Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 10:18 PM EDT

PDB ID	:	3LW5 / pdb_00003lw5
Title	:	Improved model of plant photosystem I
Authors	:	Nelson, N.; Toporik, H.
Deposited on	:	2010-02-23
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

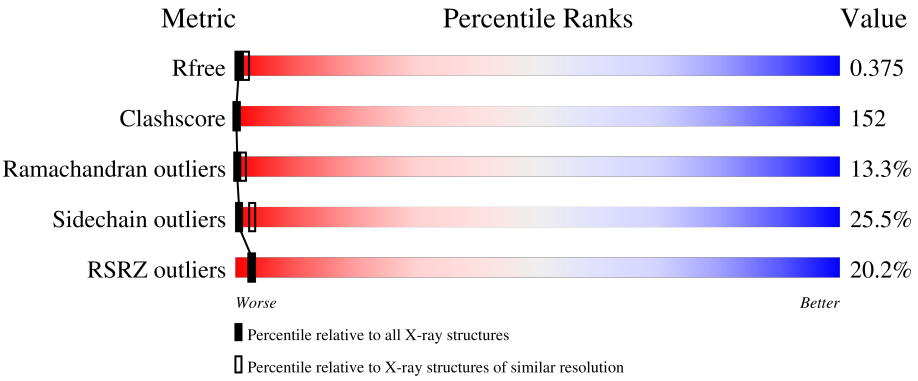
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	738	21% 7% 45% 35% 12%
2	B	733	20% 9% 44% 33% 14%
3	C	81	40% 5% 46% 33% 16%
4	D	138	17% 31% 41% 25%
5	E	64	16% 6% 34% 39% 20%

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Mol	Chain	Length	Quality of chain
6	F	154	17% 8% 36% 42% 13%
7	G	95	7% 5% 35% 36% 24%
8	H	69	7% 6% 33% 30% 30%
9	I	30	17% 67% 30%
10	J	42	14% 14% 50% 21% 14%
11	K	84	7% 11% 32% 31% 26%
12	L	161	16% 8% 36% 45% 11%
13	N	85	6% 7% 24% 35% 34%
14	R	53	28% 42% 30%
15	1	170	35% 8% 29% 35% 25%
16	2	176	23% 7% 24% 41% 27%
17	3	172	11% 9% 25% 37% 19% 9%
18	4	166	32% 6% 39% 36% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	1007	X	-	-	-
19	CLA	1	1008	X	-	-	-
19	CLA	1	1013	X	-	-	-
19	CLA	1	1014	X	-	-	-
19	CLA	1	1303	X	-	-	-
19	CLA	2	2002	X	-	-	-
19	CLA	2	2006	X	-	-	-
19	CLA	2	2007	X	-	-	-
19	CLA	2	2014	X	-	X	-
19	CLA	2	4009	X	-	-	-
19	CLA	3	2009	X	-	X	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3013	X	-	-	-
19	CLA	3	3016	X	-	-	-
19	CLA	4	1004	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	1304	X	-	X	-
19	CLA	4	1306	X	-	-	-
19	CLA	4	4002	X	-	X	-
19	CLA	4	4003	X	-	-	-
19	CLA	4	4006	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	-	-	X	-
19	CLA	A	1106	X	-	X	-
19	CLA	A	1107	X	-	X	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1112	-	-	X	-
19	CLA	A	1115	X	-	X	-
19	CLA	A	1117	X	-	X	-
19	CLA	A	1119	X	-	X	-
19	CLA	A	1122	X	-	X	-
19	CLA	A	1123	X	-	X	-
19	CLA	A	1124	X	-	X	-
19	CLA	A	1125	X	-	X	-
19	CLA	A	1126	X	-	X	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	-	-
19	CLA	A	1131	X	-	X	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	-	-	X	-
19	CLA	A	1134	-	-	X	-
19	CLA	A	1135	-	-	X	-
19	CLA	A	1136	X	-	X	-
19	CLA	A	1138	X	-	X	-
19	CLA	A	1139	-	-	X	-
19	CLA	A	1140	X	-	X	-
19	CLA	A	1141	X	-	X	-
19	CLA	A	1149	X	-	-	-
19	CLA	A	1237	X	-	X	-
19	CLA	A	9011	X	-	-	-
19	CLA	A	9012	X	-	X	-
19	CLA	A	9013	X	-	X	-
19	CLA	A	9022	X	-	X	-
19	CLA	A	9023	X	-	X	-
19	CLA	B	1202	X	-	X	-
19	CLA	B	1203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1205	X	-	X	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	X	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1214	X	-	X	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	-	-	X	-
19	CLA	B	1221	-	-	X	-
19	CLA	B	1222	X	-	X	-
19	CLA	B	1223	X	-	X	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	X	-
19	CLA	B	1226	X	-	X	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	X	-
19	CLA	B	1236	-	-	X	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1239	X	-	X	-
19	CLA	B	9010	X	-	-	-
19	CLA	F	1305	X	-	-	-
19	CLA	H	1145	X	-	X	-
19	CLA	H	1207	X	-	X	-
19	CLA	H	1241	X	-	-	-
19	CLA	H	1505	X	-	-	-
19	CLA	I	1204	X	-	-	-
19	CLA	J	1308	X	-	X	-
19	CLA	J	1311	X	-	-	-
19	CLA	K	1143	-	-	X	-
19	CLA	K	3009	X	-	-	-
19	CLA	L	1130	X	-	X	-
19	CLA	L	1148	X	-	X	-
19	CLA	L	1502	-	-	X	-
19	CLA	L	1503	X	-	-	-
19	CLA	L	1504	X	-	-	-
19	CLA	R	1144	X	-	-	-
19	CLA	R	1150	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	PQN	A	5001	X	-	-	-
20	PQN	B	5002	X	-	X	-
21	BCR	A	6002	-	-	X	-
21	BCR	A	6007	-	-	X	-
21	BCR	A	6008	-	-	X	-
21	BCR	A	6011	-	-	X	-
21	BCR	B	6010	-	-	X	-
21	BCR	B	6017	-	-	X	-
21	BCR	B	6020	-	-	X	-
21	BCR	F	6014	-	-	X	-
21	BCR	F	6016	-	-	X	-
21	BCR	I	6021	-	-	X	-
21	BCR	J	6012	-	-	X	-
21	BCR	L	6019	-	-	X	-
22	LMU	3	7005	-	-	X	-
22	LMU	4	7034	-	-	X	-
22	LMU	4	7052	-	-	X	-
22	LMU	D	7050	-	-	X	-
23	SF4	A	8001	-	-	X	-
23	SF4	C	8002	-	-	X	-
23	SF4	C	8003	-	-	X	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 36370 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5739	3762	974	985	18			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5844	3841	997	993	13			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 4 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1097	704	191	199	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	64	Total	C	N	O	0	0	0
			513	327	90	96			

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			738	481	120	137			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	69	Total	C	N	O	0	0	0
			517	334	80	103			

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			334	228	51	54	1			

- Molecule 11 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	84	Total	C	N	O	S	0	0	0
			592	377	102	110	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	161	Total	C	N	O	S	0	0	0
			1209	797	192	219	1			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called CHAIN R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 15 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	165	Total	C	N	O	S	0	0	0
			1257	816	208	229	4			

- Molecule 16 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	2	176	Total	C	N	O	S	0	0	0
			1367	895	223	245	4			

- Molecule 17 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	3	156	Total	C	N	O	S	0	0	0
			1197	784	199	209	5			

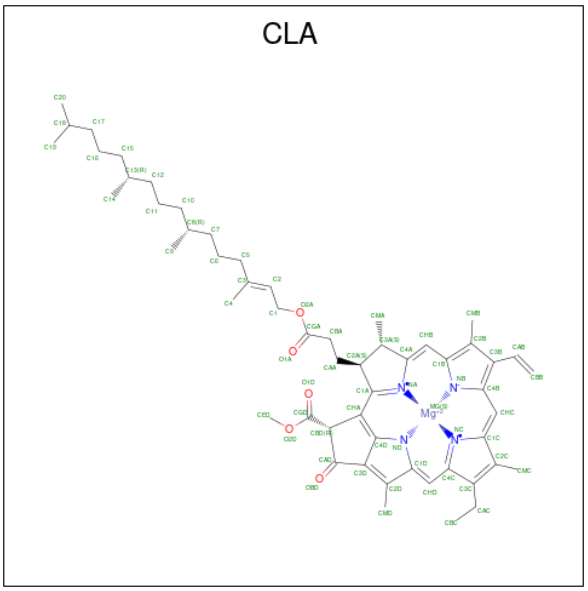
- Molecule 18 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	4	166	Total	C	N	O	S	0	0	0
			1309	856	216	234	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	SEE REMARK 999	UNP Q9SQL2

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C Mg N O 51 41 1 4 5	0	0
19	A	1	Total C Mg N O 65 55 1 4 5	0	0
19	A	1	Total C Mg N O 65 55 1 4 5	0	0
19	A	1	Total C Mg N O 46 36 1 4 5	0	0
19	A	1	Total C Mg N O 50 40 1 4 5	0	0
19	A	1	Total C Mg N O 65 55 1 4 5	0	0
19	A	1	Total C Mg N 25 20 1 4	0	0
19	A	1	Total C Mg N O 65 55 1 4 5	0	0
19	A	1	Total C Mg N O 65 55 1 4 5	0	0
19	A	1	Total C Mg N O 65 55 1 4 5	0	0
19	A	1	Total C Mg N O 65 55 1 4 5	0	0
19	A	1	Total C Mg N O 65 55 1 4 5	0	0
19	B	1	Total C Mg N O 45 35 1 4 5	0	0
19	B	1	Total C Mg N O 65 55 1 4 5	0	0
19	B	1	Total C Mg N O 65 55 1 4 5	0	0
19	B	1	Total C Mg N O 65 55 1 4 5	0	0
19	B	1	Total C Mg N O 65 55 1 4 5	0	0
19	B	1	Total C Mg N O 54 44 1 4 5	0	0
19	B	1	Total C Mg N O 55 45 1 4 5	0	0
19	B	1	Total C Mg N O 65 55 1 4 5	0	0
19	B	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	1	1	Total C Mg N O 61 51 1 4 5	0	0
19	1	1	Total C Mg N 25 20 1 4	0	0
19	1	1	Total C Mg N O 51 41 1 4 5	0	0
19	1	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N O 51 41 1 4 5	0	0
19	2	1	Total C Mg N O 56 46 1 4 5	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N O 50 40 1 4 5	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N O 65 55 1 4 5	0	0
19	2	1	Total C Mg N O 65 55 1 4 5	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N O 50 40 1 4 5	0	0
19	2	1	Total C Mg N O 50 40 1 4 5	0	0
19	2	1	Total C Mg N O 61 51 1 4 5	0	0
19	2	1	Total C Mg N O 65 55 1 4 5	0	0
19	3	1	Total C Mg N O 36 30 1 4 1	0	0
19	3	1	Total C Mg N O 46 36 1 4 5	0	0

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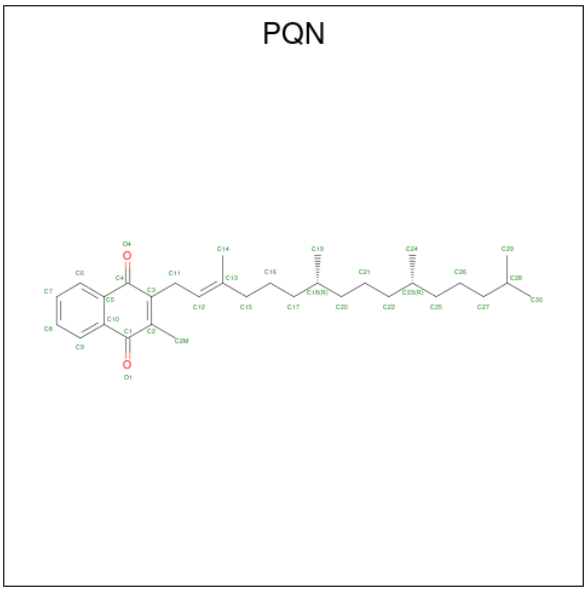
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	3	1	Total C Mg N O 56 46 1 4 5	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 36 30 1 4 1	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 42 34 1 4 3	0	0
19	3	1	Total C Mg N O 50 40 1 4 5	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 65 55 1 4 5	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 65 55 1 4 5	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 65 55 1 4 5	0	0
19	3	1	Total C Mg N O 50 40 1 4 5	0	0
19	4	1	Total C Mg N O 55 45 1 4 5	0	0
19	4	1	Total C Mg N O 36 30 1 4 1	0	0
19	4	1	Total C Mg N O 65 55 1 4 5	0	0
19	4	1	Total C Mg N O 55 45 1 4 5	0	0

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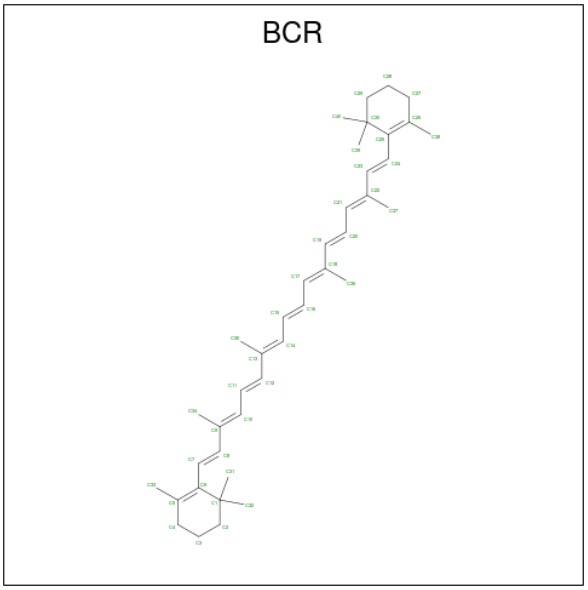
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	4	1	Total C Mg N O 50 40 1 4 5	0	0
19	4	1	Total C Mg N O 52 42 1 4 5	0	0
19	4	1	Total C Mg N O 55 45 1 4 5	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N O 55 45 1 4 5	0	0
19	4	1	Total C Mg N O 52 42 1 4 5	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N O 36 30 1 4 1	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N O 47 37 1 4 5	0	0
19	4	1	Total C Mg N O 46 36 1 4 5	0	0

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 33 31 2	0	0
20	B	1	Total C O 33 31 2	0	0

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



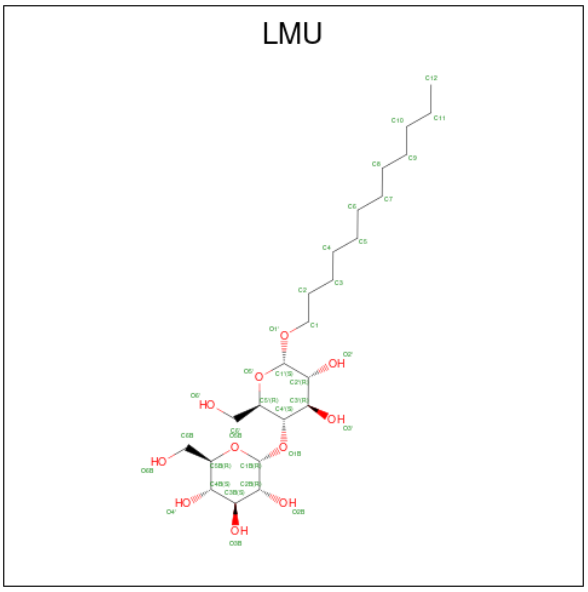
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	1	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	B	1	Total	C	O	0	0
			25	14	11		
22	B	1	Total	C	O	0	0
			35	24	11		
22	B	1	Total	C	O	0	0
			35	24	11		
22	C	1	Total	C	O	0	0
			35	24	11		
22	D	1	Total	C	O	0	0
			35	24	11		
22	E	1	Total	C	O	0	0
			35	24	11		
22	E	1	Total	C	O	0	0
			35	24	11		
22	F	1	Total	C	O	0	0
			34	23	11		

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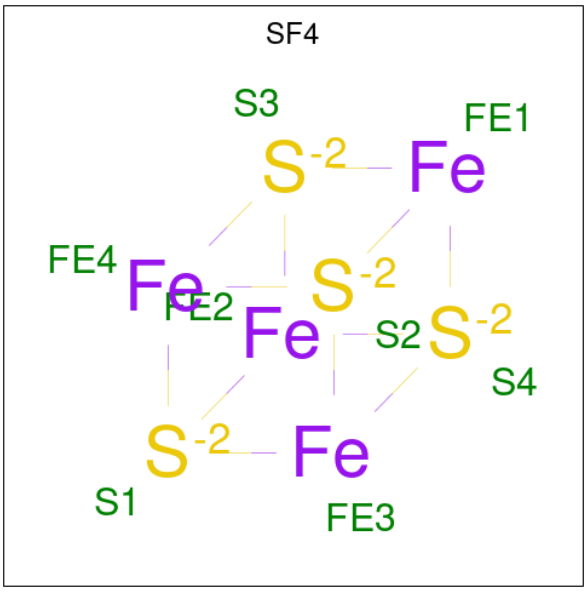
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	G	1	Total C O 35 24 11	0	0
22	G	1	Total C O 35 24 11	0	0
22	G	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	K	1	Total C O 35 24 11	0	0
22	K	1	Total C O 35 24 11	0	0
22	K	1	Total C O 35 24 11	0	0
22	K	1	Total C O 35 24 11	0	0
22	L	1	Total C O 35 24 11	0	0
22	N	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0

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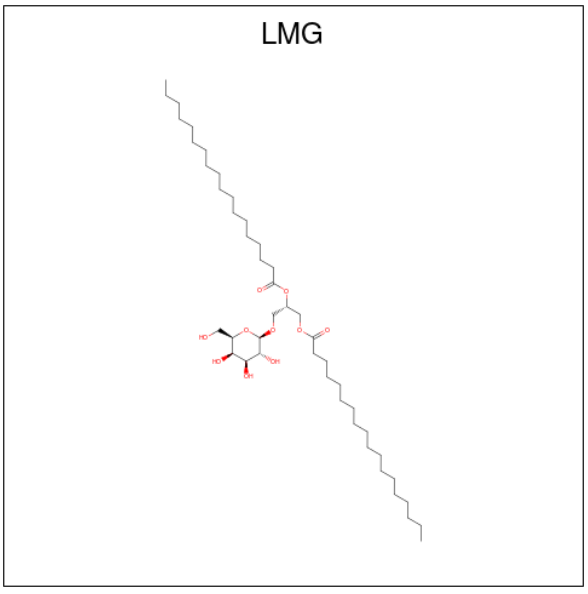
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	1	1	Total C O 35 24 11	0	0
22	1	1	Total C O 35 24 11	0	0
22	2	1	Total C O 35 24 11	0	0
22	2	1	Total C O 35 24 11	0	0
22	2	1	Total C O 35 24 11	0	0
22	2	1	Total C O 35 24 11	0	0
22	3	1	Total C O 35 24 11	0	0
22	3	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 34 23 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total Fe S 8 4 4	0	0
23	C	1	Total Fe S 8 4 4	0	0
23	C	1	Total Fe S 8 4 4	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			49	39	10		

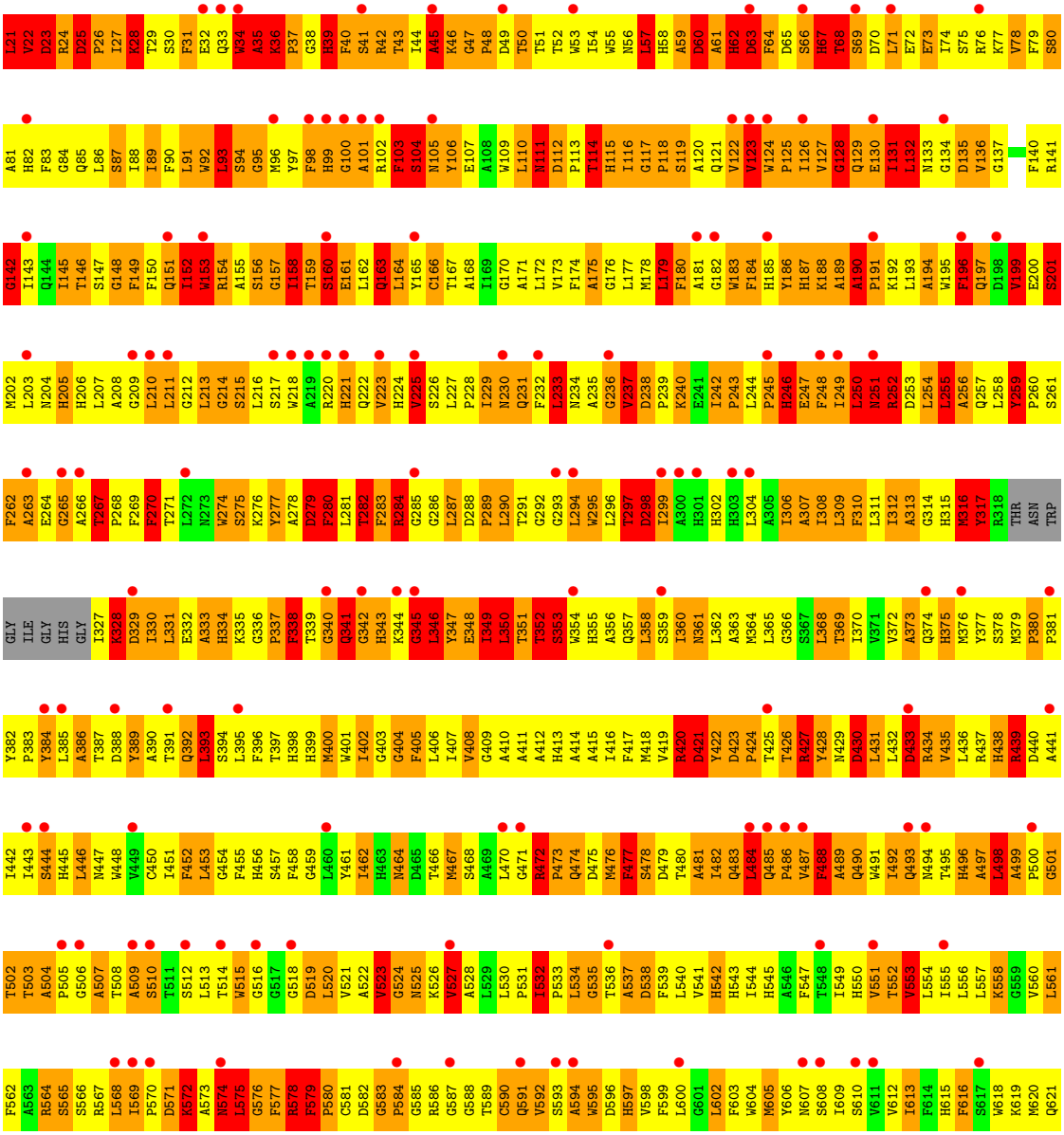
3 Residue-property plots (i)

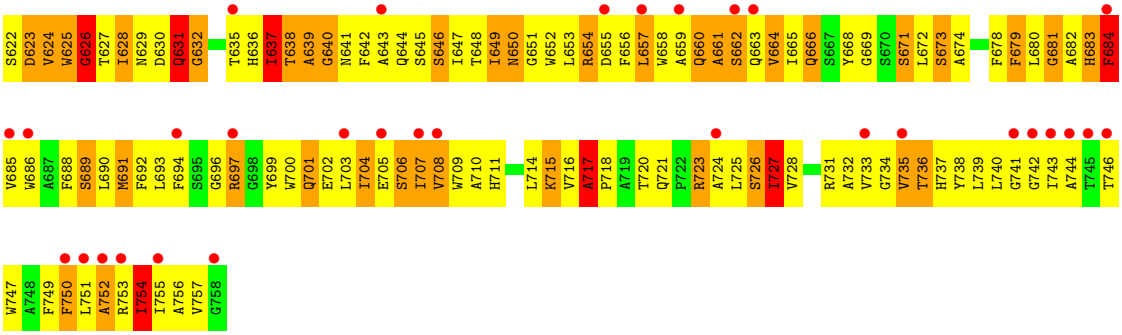
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



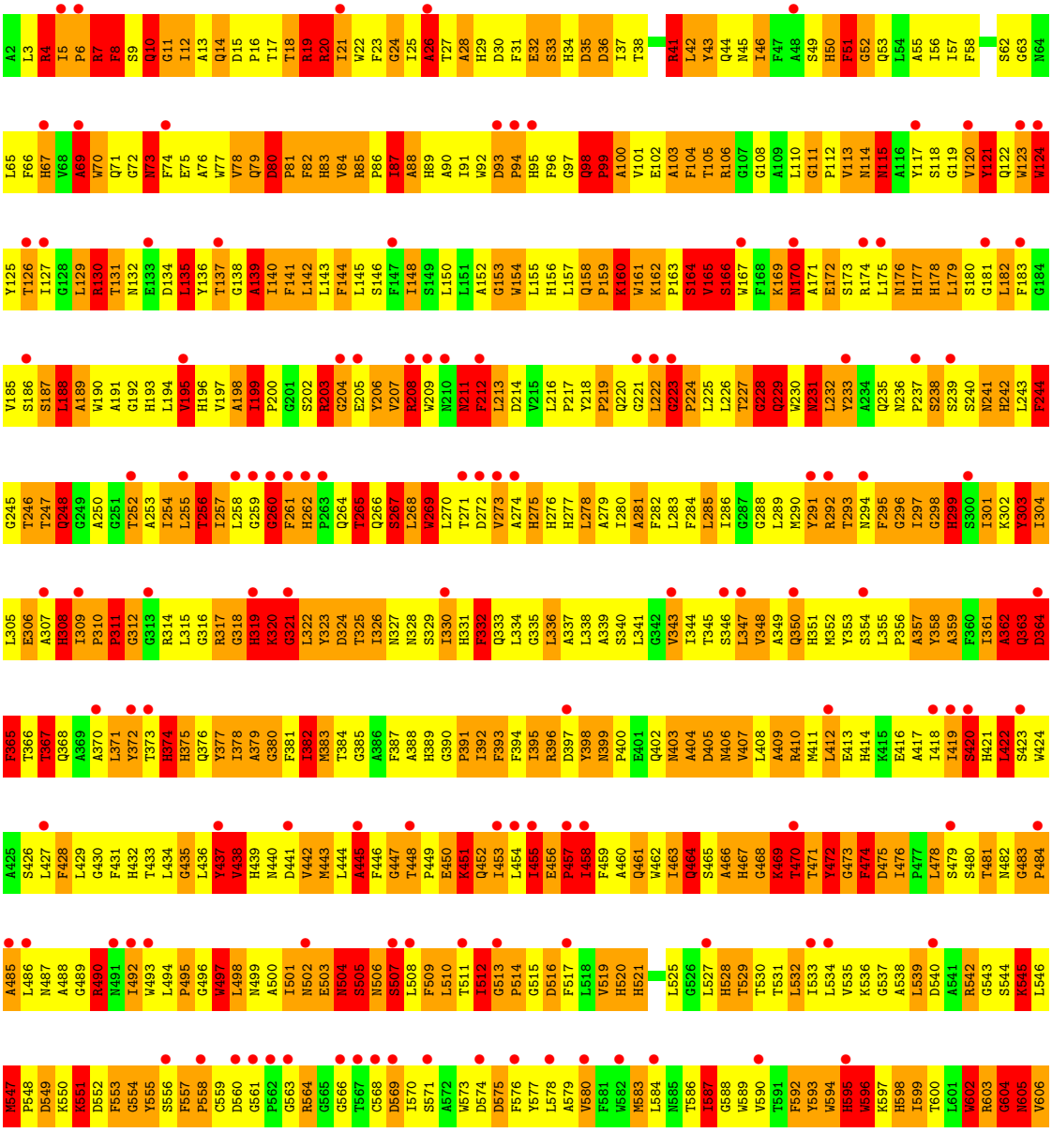


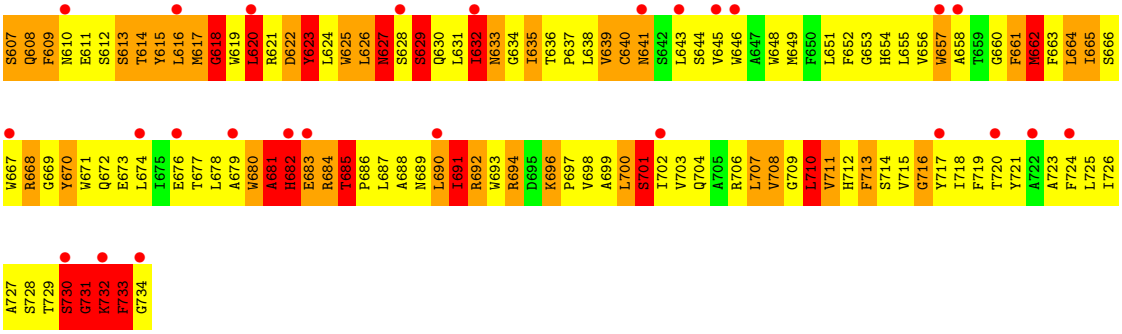


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



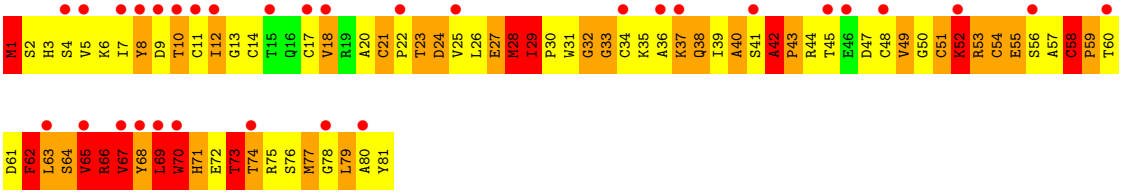




• Molecule 3: Photosystem I iron-sulfur center

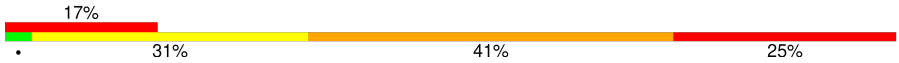
Chain C:

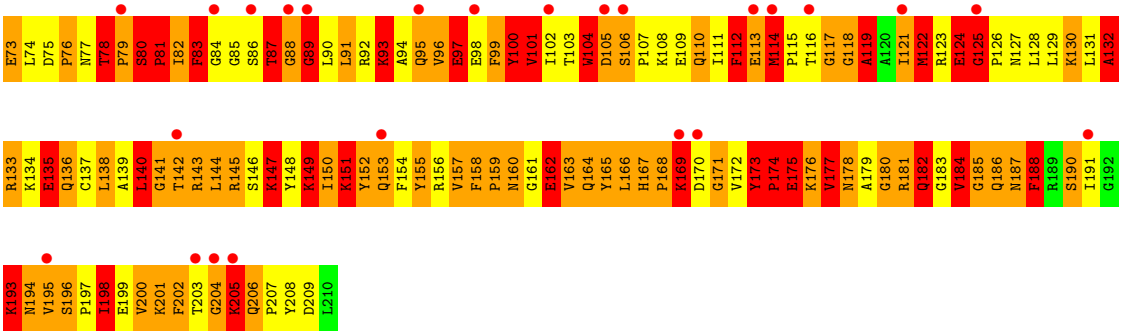




• Molecule 4: Putative uncharacterized protein

Chain D:

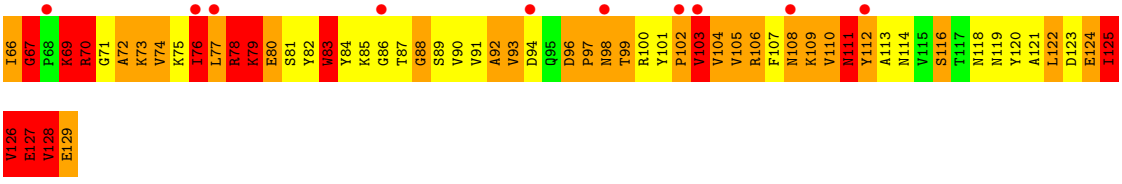




• Molecule 5: Putative uncharacterized protein

Chain E:

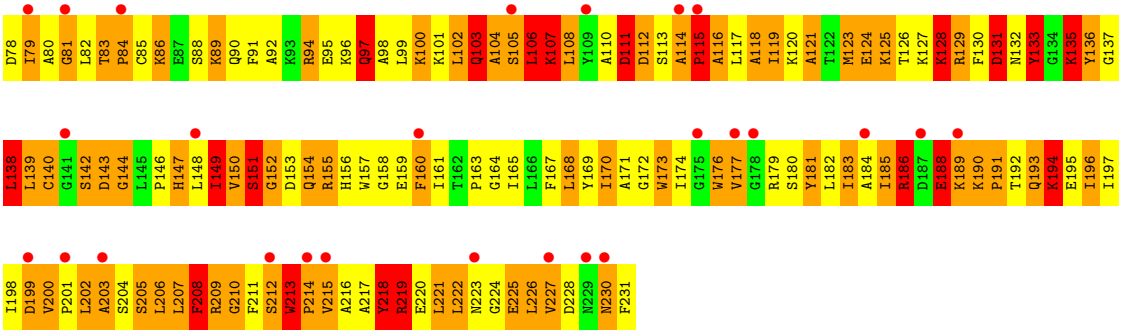




• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

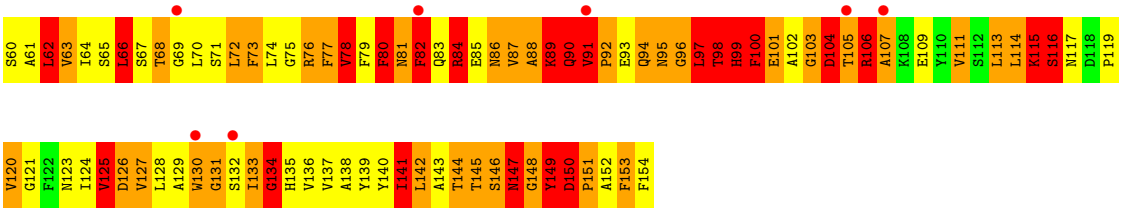
Chain F:





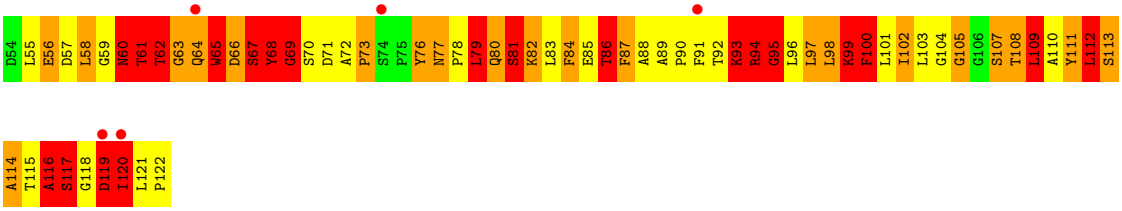
• Molecule 7: Putative uncharacterized protein





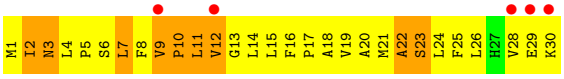
• Molecule 8: Putative uncharacterized protein



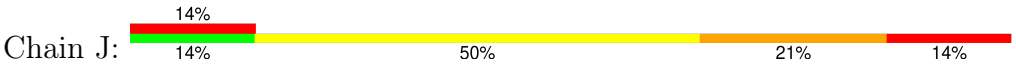


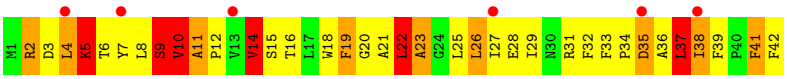
• Molecule 9: Photosystem I reaction center subunit VIII





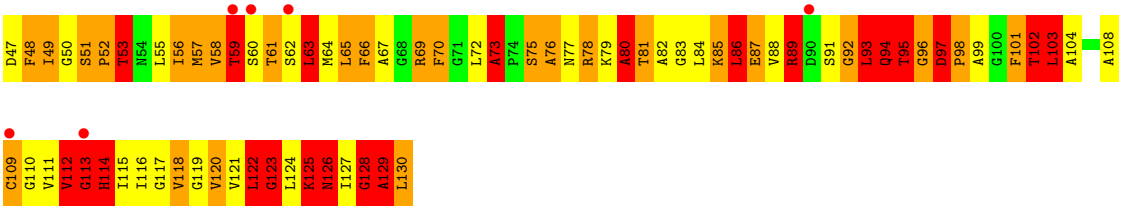
• Molecule 10: Photosystem I reaction center subunit IX





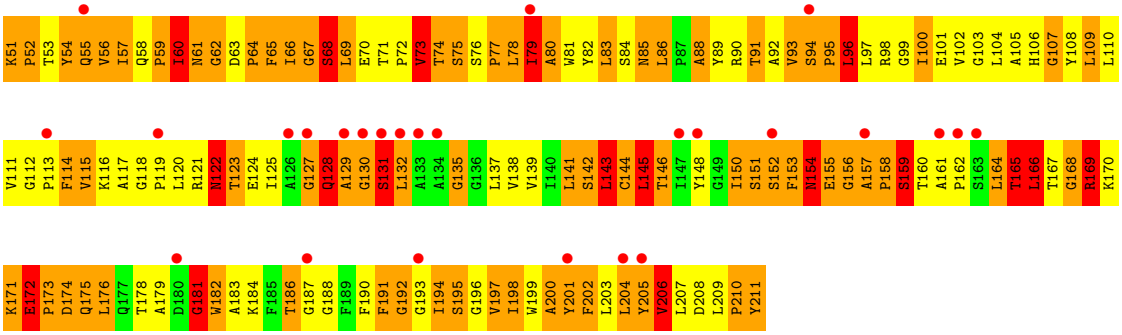
• Molecule 11: Photosystem I reaction center subunit X psaK





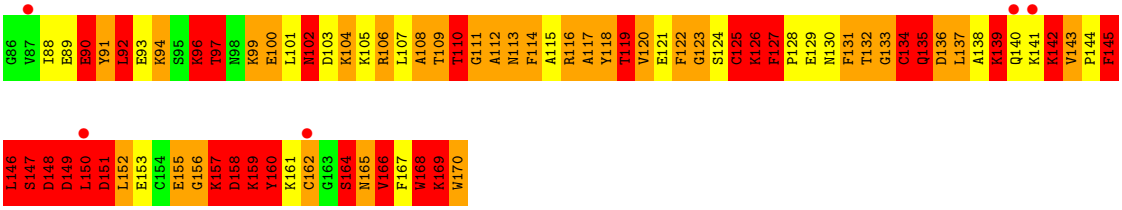
• Molecule 12: Putative uncharacterized protein





• Molecule 13: Photosystem I-N subunit





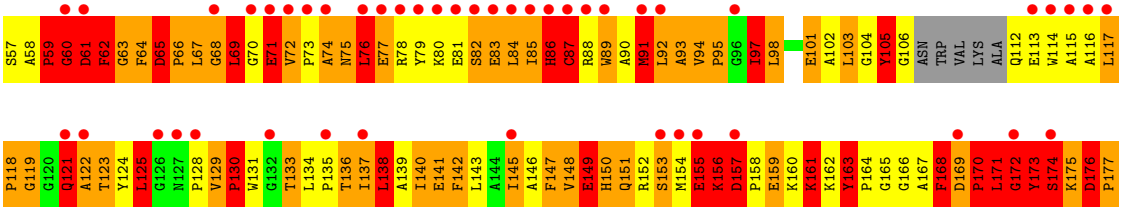
• Molecule 14: CHAIN R

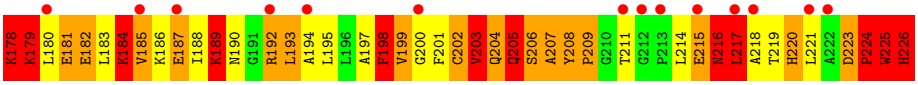




• Molecule 15: AT3g54890

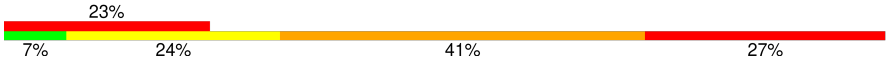


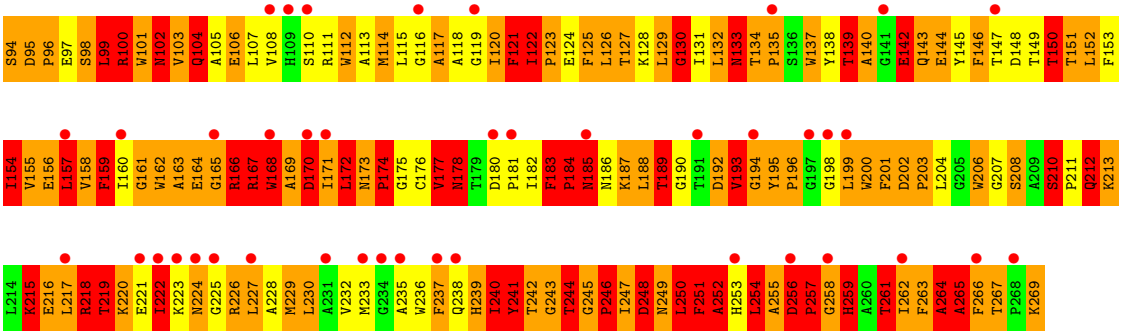




• Molecule 16: Type II chlorophyll a/b binding protein from photosystem I

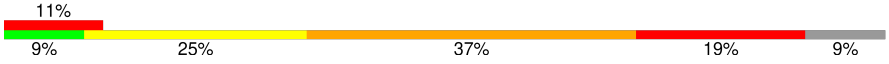
Chain 2:

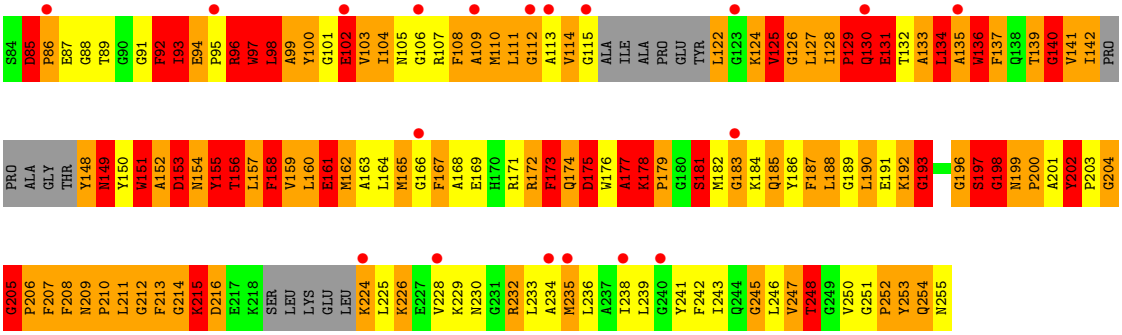




• Molecule 17: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:

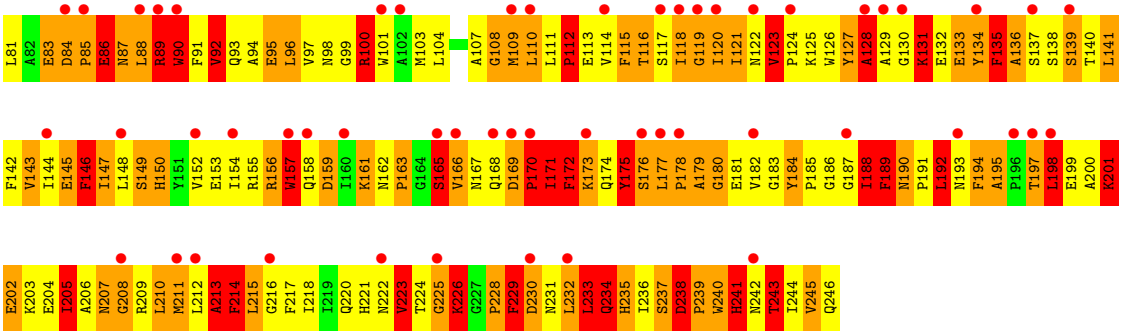




• Molecule 18: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.6 (30.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.349 , 0.383 0.353 , 0.375	Depositor DCC
R_{free} test set	4705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.12 , 75.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	36370	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, LMU, BCR, CLA, PQN, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.18	19/5932 (0.3%)	1.88	231/8096 (2.9%)
2	B	1.26	25/6054 (0.4%)	1.81	216/8273 (2.6%)
3	C	1.35	2/632 (0.3%)	2.04	24/856 (2.8%)
4	D	1.45	9/1124 (0.8%)	2.27	65/1516 (4.3%)
5	E	1.49	2/523 (0.4%)	2.15	27/710 (3.8%)
6	F	1.29	3/1250 (0.2%)	1.91	53/1687 (3.1%)
7	G	1.34	11/757 (1.5%)	2.20	52/1031 (5.0%)
8	H	1.60	7/530 (1.3%)	2.27	40/722 (5.5%)
9	I	1.05	0/235	1.16	0/320
10	J	1.05	1/344 (0.3%)	1.43	5/469 (1.1%)
11	K	1.60	11/599 (1.8%)	2.38	36/811 (4.4%)
12	L	1.39	5/1244 (0.4%)	2.08	61/1703 (3.6%)
13	N	1.54	8/699 (1.1%)	2.19	42/936 (4.5%)
15	1	1.98	26/1295 (2.0%)	2.35	89/1763 (5.0%)
16	2	1.63	23/1413 (1.6%)	2.44	98/1934 (5.1%)
17	3	1.43	12/1231 (1.0%)	2.27	76/1658 (4.6%)
18	4	1.57	19/1349 (1.4%)	2.29	88/1839 (4.8%)
All	All	1.38	183/25211 (0.7%)	2.04	1203/34324 (3.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	81
2	B	0	83
3	C	0	14
4	D	0	37
5	E	0	10
6	F	0	27

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	1	24
8	H	2	22
11	K	0	21
12	L	0	23
13	N	0	40
14	R	0	17
15	1	0	37
16	2	0	45
17	3	0	35
18	4	0	28
All	All	3	544

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	172	GLY	C-O	22.39	1.44	1.23
15	1	225	TRP	C-N	17.72	1.58	1.33
16	2	122	ILE	CA-CB	15.02	1.62	1.54
15	1	119	GLY	N-CA	14.78	1.66	1.45
15	1	63	GLY	C-O	14.09	1.42	1.23
17	3	198	GLY	N-CA	13.30	1.57	1.45
11	K	123	GLY	C-N	13.15	1.52	1.33
15	1	225	TRP	C-O	12.75	1.40	1.24
15	1	171	LEU	C-O	12.56	1.39	1.23
17	3	125	VAL	C-N	12.12	1.41	1.33
16	2	133	ASN	C-O	12.03	1.39	1.24
13	N	157	LYS	C-N	11.88	1.50	1.33
17	3	158	PHE	C-N	11.56	1.47	1.33
16	2	184	PRO	C-N	11.44	1.49	1.33
1	A	267	THR	C-O	-11.40	1.18	1.23
15	1	60	GLY	CA-C	-11.09	1.36	1.51
18	4	129	ALA	N-CA	10.85	1.58	1.45
17	3	158	PHE	C-O	10.36	1.37	1.23
15	1	172	GLY	N-CA	10.36	1.56	1.45
2	B	94	PRO	N-CD	-10.27	1.33	1.47
1	A	137	GLY	N-CA	10.14	1.54	1.45
16	2	194	GLY	N-CA	9.73	1.59	1.45
8	H	65	TRP	C-N	9.40	1.46	1.33
13	N	146	LEU	N-CA	9.37	1.58	1.46
7	G	107	ALA	N-CA	9.36	1.57	1.46
18	4	234	GLN	N-CA	9.15	1.57	1.45
12	L	132	LEU	CA-C	9.10	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	133	ASN	C-N	9.08	1.45	1.32
15	1	166	GLY	N-CA	9.07	1.58	1.45
13	N	157	LYS	C-O	9.05	1.35	1.24
18	4	235	HIS	CE1-NE2	9.01	1.41	1.32
1	A	337	PRO	N-CD	-8.87	1.35	1.47
15	1	60	GLY	N-CA	8.69	1.57	1.45
8	H	116	ALA	C-N	8.50	1.45	1.33
15	1	172	GLY	CA-C	8.48	1.63	1.52
15	1	63	GLY	CA-C	8.40	1.65	1.51
16	2	165	GLY	C-O	8.39	1.33	1.23
1	A	626	GLY	N-CA	8.36	1.53	1.45
1	A	21	LEU	C-N	8.32	1.45	1.33
15	1	60	GLY	C-N	8.27	1.44	1.33
2	B	99	PRO	N-CD	-8.23	1.36	1.47
12	L	64	PRO	N-CD	-8.22	1.36	1.47
2	B	229	GLN	C-O	8.12	1.34	1.24
18	4	229	PHE	C-N	8.07	1.45	1.33
15	1	61	ASP	N-CA	-7.96	1.34	1.46
2	B	219	PRO	N-CD	-7.81	1.36	1.47
13	N	158	ASP	N-CA	7.81	1.55	1.46
11	K	125	LYS	C-N	7.80	1.44	1.33
1	A	317	TYR	N-CA	7.68	1.56	1.46
16	2	252	ALA	CA-C	-7.62	1.43	1.52
2	B	604	GLY	CA-C	-7.58	1.47	1.52
2	B	319	HIS	N-CA	7.53	1.56	1.46
15	1	224	PRO	C-N	7.51	1.44	1.33
16	2	130	GLY	C-N	7.48	1.43	1.33
13	N	135	GLN	C-N	7.45	1.44	1.33
13	N	145	PHE	C-N	7.45	1.44	1.33
18	4	223	VAL	C-N	7.36	1.42	1.33
11	K	94	GLN	N-CA	7.34	1.55	1.46
16	2	130	GLY	C-O	-7.31	1.14	1.23
18	4	235	HIS	CG-ND1	7.25	1.46	1.38
18	4	239	PRO	N-CD	-7.23	1.37	1.47
18	4	223	VAL	C-O	7.22	1.32	1.24
18	4	229	PHE	C-O	7.16	1.33	1.24
16	2	185	ASN	N-CA	7.15	1.55	1.46
18	4	238	ASP	CA-C	-7.14	1.49	1.53
16	2	251	PHE	CA-C	-7.14	1.44	1.52
2	B	457	PRO	N-CD	-7.12	1.37	1.47
17	3	196	GLY	C-O	6.93	1.33	1.23
2	B	469	LYS	C-O	6.92	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	ALA	CA-CB	-6.86	1.42	1.53
7	G	149	TYR	C-N	6.79	1.47	1.33
4	D	205	LYS	N-CA	6.74	1.54	1.46
3	C	73	THR	CA-CB	-6.73	1.43	1.53
17	3	109	ALA	N-CA	6.72	1.54	1.46
11	K	128	GLY	C-O	6.69	1.31	1.24
15	1	173	TYR	C-O	-6.69	1.13	1.23
16	2	178	ASN	CG-OD1	6.65	1.36	1.23
15	1	69	LEU	C-O	-6.65	1.14	1.23
1	A	569	ILE	CA-CB	-6.63	1.45	1.54
2	B	470	THR	N-CA	6.59	1.54	1.46
3	C	1	MET	C-N	6.59	1.43	1.33
15	1	226	HIS	CA-C	6.59	1.66	1.52
4	D	175	GLU	N-CA	6.58	1.54	1.46
16	2	167	ARG	CZ-NH1	6.48	1.41	1.32
8	H	95	GLY	N-CA	6.46	1.54	1.45
2	B	732	LYS	C-O	6.41	1.32	1.24
8	H	95	GLY	C-N	6.41	1.42	1.33
12	L	143	LEU	CA-C	-6.33	1.44	1.52
2	B	553	PHE	CA-C	-6.32	1.46	1.52
17	3	129	PRO	N-CD	-6.31	1.39	1.47
2	B	469	LYS	C-N	6.31	1.42	1.33
16	2	175	GLY	N-CA	6.28	1.54	1.45
2	B	407	VAL	CA-CB	-6.26	1.45	1.54
11	K	92	GLY	N-CA	6.21	1.54	1.45
11	K	96	GLY	CA-C	6.17	1.60	1.51
1	A	238	ASP	CA-C	-6.14	1.47	1.52
4	D	122	MET	CA-C	6.09	1.60	1.52
12	L	62	GLY	N-CA	6.08	1.54	1.45
17	3	126	GLY	N-CA	6.07	1.53	1.45
4	D	198	ILE	CA-CB	-6.04	1.47	1.54
4	D	185	GLY	N-CA	6.01	1.54	1.45
18	4	213	ALA	CA-CB	-6.01	1.47	1.54
5	E	126	VAL	C-O	-6.00	1.17	1.24
18	4	238	ASP	C-O	-6.00	1.20	1.23
7	G	99	HIS	C-N	6.00	1.42	1.33
13	N	151	ASP	CA-C	-5.99	1.48	1.53
1	A	225	VAL	CA-CB	5.98	1.62	1.54
2	B	7	ARG	C-N	5.94	1.41	1.33
15	1	75	ASN	CA-C	-5.90	1.45	1.52
15	1	74	ALA	CA-C	-5.89	1.45	1.52
16	2	102	ASN	C-O	5.86	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	97	ILE	CA-C	5.83	1.60	1.52
16	2	250	LEU	CA-C	-5.83	1.48	1.53
8	H	117	SER	N-CA	5.79	1.53	1.46
1	A	145	ILE	CA-CB	-5.79	1.47	1.54
7	G	104	ASP	N-CA	5.78	1.53	1.45
4	D	99	PHE	C-O	5.76	1.30	1.24
15	1	226	HIS	N-CA	5.76	1.57	1.46
2	B	268	LEU	CA-C	-5.75	1.45	1.52
1	A	21	LEU	C-O	5.74	1.35	1.23
2	B	733	PHE	N-CA	5.73	1.53	1.46
4	D	152	TYR	C-O	5.73	1.30	1.23
1	A	94	SER	CA-C	-5.71	1.45	1.52
17	3	109	ALA	CA-C	5.71	1.60	1.52
16	2	171	ILE	N-CA	-5.70	1.40	1.46
12	L	150	ILE	CA-CB	-5.65	1.48	1.54
11	K	126	ASN	N-CA	5.65	1.53	1.46
6	F	186	ARG	N-CA	5.64	1.53	1.46
7	G	78	VAL	CA-C	5.61	1.59	1.52
18	4	189	PHE	CA-C	5.59	1.59	1.52
17	3	140	GLY	C-N	5.59	1.41	1.33
1	A	316	MET	C-O	5.57	1.30	1.24
2	B	696	LYS	CA-C	-5.57	1.47	1.53
18	4	230	ASP	C-O	5.56	1.30	1.24
15	1	172	GLY	C-N	5.54	1.41	1.33
8	H	108	THR	CA-C	-5.53	1.45	1.52
7	G	151	PRO	N-CD	-5.53	1.40	1.47
2	B	547	MET	C-O	-5.52	1.20	1.25
11	K	126	ASN	C-N	5.50	1.41	1.33
15	1	84	LEU	CG-CD1	-5.49	1.34	1.52
11	K	126	ASN	C-O	5.47	1.30	1.24
2	B	497	TRP	CA-C	-5.47	1.45	1.52
1	A	553	VAL	CA-CB	5.46	1.61	1.54
1	A	297	THR	CA-C	-5.45	1.45	1.52
11	K	112	VAL	C-O	5.41	1.30	1.24
18	4	88	LEU	N-CA	5.41	1.53	1.46
2	B	293	THR	CA-CB	-5.39	1.46	1.53
18	4	186	GLY	C-O	5.38	1.31	1.24
16	2	264	ALA	N-CA	5.37	1.53	1.46
16	2	166	ARG	CA-C	5.37	1.59	1.52
2	B	199	ILE	CA-CB	5.32	1.57	1.54
6	F	150	VAL	CA-CB	-5.32	1.47	1.54
1	A	22	VAL	N-CA	5.30	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	134	THR	CB-OG1	5.30	1.52	1.43
16	2	127	THR	CA-C	-5.28	1.45	1.52
7	G	100	PHE	N-CA	5.26	1.52	1.46
18	4	198	LEU	CA-C	-5.26	1.48	1.53
8	H	69	GLY	N-CA	5.25	1.52	1.45
11	K	128	GLY	C-N	5.23	1.40	1.33
16	2	125	PHE	C-O	5.23	1.30	1.24
15	1	71	GLU	CA-C	-5.21	1.46	1.52
17	3	215	LYS	CA-C	5.20	1.58	1.52
6	F	147	HIS	CA-C	-5.17	1.46	1.52
4	D	178	ASN	N-CA	5.17	1.52	1.46
18	4	128	ALA	C-N	5.17	1.40	1.33
1	A	142	GLY	CA-C	5.15	1.57	1.51
2	B	8	PHE	N-CA	5.14	1.52	1.46
18	4	90	TRP	CA-C	-5.14	1.48	1.53
17	3	135	ALA	CA-C	5.12	1.60	1.53
1	A	537	ALA	CA-CB	-5.10	1.46	1.53
15	1	209	PRO	N-CD	5.09	1.54	1.47
10	J	14	VAL	CA-CB	-5.08	1.48	1.54
2	B	458	ILE	CA-CB	-5.08	1.48	1.54
2	B	357	ALA	CA-CB	-5.07	1.45	1.53
16	2	162	TRP	N-CA	-5.06	1.40	1.46
7	G	150	ASP	N-CA	5.05	1.53	1.46
7	G	120	VAL	CA-CB	-5.04	1.47	1.54
5	E	128	VAL	C-O	-5.03	1.18	1.24
4	D	169	LYS	CA-C	5.03	1.59	1.52
13	N	164	SER	C-N	5.01	1.40	1.33
2	B	362	ALA	CA-CB	-5.00	1.45	1.53
7	G	90	GLN	C-N	5.00	1.39	1.33
7	G	125	VAL	CA-CB	-5.00	1.48	1.54

All (1203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	2	258	GLY	N-CA-C	22.18	139.35	112.73
11	K	113	GLY	N-CA-C	-18.74	90.24	112.73
18	4	84	ASP	C-N-CD	-18.22	50.30	125.00
17	3	131	GLU	N-CA-C	-18.13	90.86	111.71
4	D	122	MET	N-CA-C	17.10	130.01	111.03
4	D	169	LYS	N-CA-C	17.06	131.84	111.02
5	E	98	ASN	N-CA-C	16.92	129.17	111.07
16	2	126	LEU	N-CA-C	-16.81	90.99	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	ARG	N-CA-C	16.73	133.98	113.23
1	A	348	GLU	N-CA-C	-16.70	93.20	111.07
16	2	102	ASN	N-CA-C	-16.62	92.28	112.89
2	B	602	TRP	N-CA-C	16.52	132.00	111.69
12	L	84	SER	N-CA-C	16.43	136.11	112.94
17	3	154	ASN	N-CA-C	16.10	130.22	111.71
1	A	116	ILE	N-CA-C	15.73	128.15	111.00
5	E	70	ARG	N-CA-C	15.40	128.12	111.03
2	B	19	ARG	N-CA-C	-15.28	94.62	111.28
18	4	175	TYR	N-CA-C	-14.99	93.06	112.24
4	D	99	PHE	N-CA-C	14.55	129.15	111.40
16	2	216	GLU	N-CA-C	-14.38	95.69	111.36
1	A	524	GLY	N-CA-C	14.00	134.87	113.86
1	A	259	TYR	CA-C-N	13.87	134.76	119.92
1	A	259	TYR	C-N-CA	13.87	134.76	119.92
1	A	117	GLY	CA-C-N	13.86	133.62	119.76
1	A	117	GLY	C-N-CA	13.86	133.62	119.76
1	A	131	ILE	N-CA-C	-13.80	96.55	110.62
15	1	82	SER	N-CA-C	-13.73	95.63	112.38
1	A	353	SER	N-CA-C	13.63	128.03	111.40
18	4	215	LEU	N-CA-C	-13.61	94.78	111.11
18	4	121	ILE	N-CA-C	-13.55	97.41	110.42
2	B	625	TRP	N-CA-C	13.53	128.33	111.69
16	2	184	PRO	O-C-N	13.51	140.88	122.64
4	D	87	THR	N-CA-C	13.46	126.03	111.36
11	K	57	MET	N-CA-C	-13.42	96.66	111.28
1	A	503	THR	N-CA-C	-13.41	94.59	111.75
12	L	164	LEU	N-CA-C	13.38	125.58	111.14
17	3	205	GLY	N-CA-C	-13.36	98.79	115.09
2	B	683	GLU	N-CA-C	-13.25	96.84	111.28
18	4	194	PHE	N-CA-C	13.01	128.45	108.42
18	4	234	GLN	N-CA-C	13.01	130.62	113.97
1	A	94	SER	N-CA-C	-12.81	97.40	111.36
16	2	171	ILE	N-CA-C	-12.66	96.18	110.62
18	4	180	GLY	N-CA-C	-12.60	97.61	112.73
4	D	100	TYR	N-CA-C	12.59	128.79	111.92
16	2	169	ALA	N-CA-C	-12.58	96.01	111.11
4	D	205	LYS	N-CA-C	12.54	128.72	113.41
16	2	185	ASN	N-CA-C	12.46	129.21	113.88
17	3	125	VAL	CA-C-N	-12.44	109.68	121.62
17	3	125	VAL	C-N-CA	-12.44	109.68	121.62
1	A	298	ASP	N-CA-C	-12.40	98.15	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	177	ALA	N-CA-C	-12.39	96.34	111.33
2	B	632	ILE	CA-C-N	-12.39	104.81	123.14
2	B	632	ILE	C-N-CA	-12.39	104.81	123.14
5	E	127	GLU	N-CA-C	12.37	128.99	108.08
1	A	111	ASN	N-CA-C	-12.36	97.80	111.28
4	D	142	THR	N-CA-C	-12.33	96.31	111.11
8	H	76	TYR	N-CA-C	12.30	124.68	111.03
16	2	129	LEU	N-CA-C	-12.21	94.69	111.30
13	N	126	LYS	N-CA-C	12.09	127.86	108.76
1	A	534	LEU	N-CA-C	12.09	129.44	112.04
18	4	149	SER	N-CA-C	-12.08	98.11	111.28
16	2	184	PRO	CA-C-O	-12.01	98.75	120.60
15	1	168	PHE	N-CA-C	12.00	128.11	113.23
18	4	186	GLY	N-CA-C	11.97	138.11	114.16
11	K	52	PRO	N-CA-C	-11.95	97.51	113.65
1	A	345	GLY	N-CA-C	-11.87	96.92	114.61
2	B	498	LEU	N-CA-C	-11.80	97.14	112.24
18	4	84	ASP	N-CA-C	11.78	118.83	108.22
16	2	161	GLY	N-CA-C	-11.78	98.39	112.64
16	2	193	VAL	N-CA-C	11.73	121.45	110.42
17	3	166	GLY	N-CA-C	-11.72	98.67	112.73
1	A	123	VAL	N-CA-C	11.68	121.51	110.53
2	B	165	VAL	N-CA-C	11.54	122.19	111.45
1	A	528	ALA	N-CA-C	11.54	125.48	111.40
11	K	94	GLN	N-CA-C	11.51	127.45	113.41
15	1	76	LEU	N-CA-C	-11.49	97.32	111.11
2	B	603	ARG	CA-C-N	-11.49	112.04	122.73
2	B	603	ARG	C-N-CA	-11.49	112.04	122.73
2	B	212	PHE	N-CA-C	11.49	123.54	111.14
16	2	249	ASN	N-CA-C	11.47	123.79	111.28
17	3	98	LEU	N-CA-C	-11.45	98.82	111.07
18	4	226	LYS	N-CA-C	11.45	123.50	111.14
11	K	114	HIS	N-CA-C	-11.42	86.47	110.80
2	B	507	SER	N-CA-C	11.34	124.98	111.82
1	A	343	HIS	N-CA-C	-11.33	97.52	111.11
5	E	127	GLU	CB-CA-C	-11.33	103.49	116.63
2	B	553	PHE	N-CA-C	-11.31	94.84	113.50
2	B	203	ARG	N-CA-C	-11.29	98.73	111.71
1	A	152	ILE	N-CA-C	-11.25	99.14	110.62
2	B	303	TYR	CB-CA-C	-11.23	98.71	109.83
1	A	42	ARG	N-CA-C	11.22	124.61	111.71
3	C	42	ALA	CA-C-N	11.21	131.62	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	42	ALA	C-N-CA	11.21	131.62	120.52
8	H	68	TYR	N-CA-C	11.17	126.92	108.49
1	A	190	ALA	CA-C-N	11.16	131.57	120.52
1	A	190	ALA	C-N-CA	11.16	131.57	120.52
15	1	225	TRP	CA-C-N	-11.10	101.72	121.70
15	1	225	TRP	C-N-CA	-11.10	101.72	121.70
3	C	69	LEU	N-CA-C	11.05	125.29	111.69
13	N	157	LYS	CA-C-N	-11.05	107.47	122.72
13	N	157	LYS	C-N-CA	-11.05	107.47	122.72
16	2	177	VAL	N-CA-C	10.94	122.07	108.06
7	G	77	PHE	N-CA-C	10.93	125.14	111.69
15	1	87	CYS	N-CA-C	-10.91	99.47	111.36
16	2	201	PHE	N-CA-C	-10.85	99.46	111.28
15	1	91	MET	N-CA-C	-10.82	99.49	111.28
3	C	42	ALA	N-CA-C	10.79	120.77	108.25
7	G	133	ILE	N-CA-C	-10.77	102.33	111.91
16	2	159	PHE	N-CA-C	-10.73	99.58	111.28
15	1	216	ASN	N-CA-C	10.72	122.71	111.14
6	F	209	ARG	N-CA-C	-10.69	99.63	111.28
12	L	89	TYR	N-CA-C	10.64	125.25	110.35
12	L	198	ILE	N-CA-C	10.63	122.58	111.00
1	A	472	ARG	CA-C-N	10.61	133.10	119.84
1	A	472	ARG	C-N-CA	10.61	133.10	119.84
15	1	95	PRO	N-CA-C	-10.51	99.47	113.65
18	4	169	ASP	N-CA-C	10.50	133.01	109.81
1	A	246	HIS	N-CA-C	10.46	127.81	114.31
7	G	147	ASN	N-CA-C	10.46	122.68	111.28
4	D	83	PHE	N-CA-C	10.37	124.06	111.40
2	B	242	HIS	N-CA-C	10.36	124.44	111.69
2	B	14	GLN	N-CA-C	10.36	126.95	112.04
15	1	72	VAL	CA-C-N	-10.35	106.91	119.84
15	1	72	VAL	C-N-CA	-10.35	106.91	119.84
1	A	282	THR	N-CA-C	-10.33	97.14	111.39
15	1	129	VAL	N-CA-C	10.28	124.68	112.35
18	4	210	LEU	N-CA-C	-10.28	100.08	111.28
13	N	116	ARG	N-CA-C	-10.26	98.80	111.11
16	2	252	ALA	N-CA-C	-10.26	92.18	108.90
16	2	169	ALA	CA-C-N	-10.23	109.31	123.03
16	2	169	ALA	C-N-CA	-10.23	109.31	123.03
2	B	260	GLY	N-CA-C	10.23	126.36	110.71
1	A	47	GLY	N-CA-C	-10.22	91.49	112.34
15	1	161	LYS	N-CA-C	10.18	123.81	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ARG	N-CA-C	-10.16	99.03	111.33
6	F	219	ARG	N-CA-C	10.15	126.56	112.45
18	4	83	GLU	N-CA-C	10.10	122.05	111.14
17	3	158	PHE	N-CA-C	-10.08	90.89	108.23
15	1	174	SER	N-CA-C	10.04	122.86	108.00
2	B	121	TYR	N-CA-C	-10.04	99.18	111.33
1	A	95	GLY	N-CA-C	-10.03	100.87	112.50
15	1	207	ALA	N-CA-C	10.03	121.97	111.14
10	J	35	ASP	N-CA-C	10.01	124.35	109.24
1	A	481	ALA	N-CA-C	9.98	123.57	111.40
6	F	226	LEU	N-CA-C	-9.98	95.09	109.96
17	3	197	SER	CA-C-N	-9.97	113.30	122.17
17	3	197	SER	C-N-CA	-9.97	113.30	122.17
1	A	242	ILE	N-CA-C	9.96	130.39	108.88
8	H	79	LEU	N-CA-C	-9.92	100.46	111.28
3	C	51	CYS	N-CA-C	9.91	123.50	111.40
11	K	97	ASP	N-CA-C	9.88	131.64	109.81
1	A	342	GLY	N-CA-C	-9.88	100.30	113.24
8	H	84	PHE	N-CA-C	9.83	125.47	113.38
1	A	480	THR	N-CA-C	9.83	122.07	111.36
2	B	605	ASN	N-CA-C	-9.82	96.66	110.50
2	B	607	SER	N-CA-C	-9.82	99.33	111.11
16	2	170	ASP	N-CA-C	9.80	124.66	108.49
17	3	104	ILE	CB-CA-C	-9.79	99.44	111.97
3	C	74	THR	N-CA-C	9.78	122.02	111.36
2	B	51	PHE	N-CA-C	-9.76	101.51	113.41
13	N	159	LYS	N-CA-C	9.73	131.53	110.80
3	C	58	CYS	CA-C-N	9.72	132.00	119.84
3	C	58	CYS	C-N-CA	9.72	132.00	119.84
1	A	30	SER	N-CA-C	-9.71	100.77	111.36
2	B	502	ASN	N-CA-C	9.71	121.47	111.07
1	A	101	ALA	CA-C-N	-9.71	107.46	122.60
1	A	101	ALA	C-N-CA	-9.71	107.46	122.60
17	3	190	LEU	N-CA-C	9.69	121.60	111.14
2	B	367	THR	N-CA-C	-9.66	101.17	113.72
16	2	218	ARG	N-CA-C	-9.65	100.45	110.97
16	2	221	GLU	N-CA-C	9.63	121.54	111.14
2	B	24	GLY	N-CA-C	-9.61	101.11	112.83
15	1	184	LYS	N-CA-C	-9.60	98.48	111.54
13	N	134	CYS	N-CA-C	-9.58	90.40	110.80
1	A	637	ILE	N-CA-C	-9.57	99.70	110.62
15	1	187	GLU	N-CA-C	-9.57	99.75	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	684	ARG	N-CA-C	9.55	124.73	112.89
17	3	85	ASP	CA-C-N	9.54	129.61	119.78
17	3	85	ASP	C-N-CA	9.54	129.61	119.78
15	1	121	GLN	N-CA-C	9.54	121.44	111.14
4	D	125	GLY	N-CA-C	9.52	131.76	112.34
2	B	28	ALA	N-CA-C	-9.52	99.69	111.11
2	B	456	GLU	N-CA-C	-9.50	95.84	109.62
12	L	74	THR	N-CA-C	9.48	121.56	111.03
11	K	123	GLY	CA-C-N	-9.47	107.95	121.50
11	K	123	GLY	C-N-CA	-9.47	107.95	121.50
6	F	103	GLN	O-C-N	-9.44	110.03	122.59
4	D	166	LEU	N-CA-C	9.39	123.36	111.24
4	D	118	GLY	N-CA-C	9.39	125.08	110.71
13	N	102	ASN	N-CA-C	9.39	125.20	112.90
1	A	504	ALA	CA-C-N	9.38	131.57	119.84
1	A	504	ALA	C-N-CA	9.38	131.57	119.84
7	G	76	ARG	N-CA-C	-9.38	100.14	112.34
6	F	190	LYS	N-CA-C	9.38	121.10	109.57
15	1	171	LEU	CA-C-O	-9.35	110.50	121.44
1	A	341	GLN	N-CA-C	-9.35	100.02	111.33
6	F	196	ILE	N-CA-C	9.31	120.13	110.72
16	2	227	LEU	N-CA-C	-9.30	101.12	111.07
1	A	118	PRO	N-CA-C	9.28	125.76	111.19
7	G	116	SER	N-CA-C	9.28	123.70	112.38
17	3	102	GLU	N-CA-C	-9.24	99.92	111.75
1	A	23	ASP	N-CA-C	-9.20	96.87	110.48
7	G	143	ALA	N-CA-C	9.18	121.65	110.91
18	4	112	PRO	N-CA-C	-9.14	101.59	113.57
2	B	166	SER	CA-C-N	9.14	133.44	120.28
2	B	166	SER	C-N-CA	9.14	133.44	120.28
16	2	171	ILE	CB-CA-C	-9.14	100.06	112.04
17	3	172	ARG	N-CA-C	-9.14	101.32	111.28
2	B	227	THR	N-CA-C	-9.08	97.06	110.23
1	A	63	ASP	N-CA-C	9.08	124.79	112.90
11	K	61	THR	N-CA-C	-9.07	101.39	111.28
2	B	364	ASP	N-CA-C	9.06	122.84	111.69
13	N	151	ASP	CB-CA-C	-9.06	106.12	116.63
7	G	91	VAL	N-CA-C	-9.04	100.61	109.02
1	A	568	LEU	N-CA-C	9.03	121.20	111.36
1	A	115	HIS	N-CA-C	9.03	123.60	112.23
2	B	323	TYR	N-CA-C	9.01	121.09	111.28
11	K	63	LEU	N-CA-C	-8.98	101.49	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	SER	N-CA-C	8.98	120.76	110.97
2	B	404	ALA	N-CA-C	8.97	123.15	110.50
18	4	176	SER	N-CA-C	8.95	121.91	108.31
12	L	202	PHE	N-CA-C	-8.94	100.38	111.11
16	2	240	ILE	N-CA-C	8.94	119.74	110.62
17	3	159	VAL	CB-CA-C	-8.94	100.21	111.92
16	2	114	MET	N-CA-C	8.90	122.64	111.69
12	L	144	CYS	N-CA-C	-8.90	100.43	111.11
6	F	188	GLU	CB-CA-C	-8.87	106.34	116.63
13	N	88	ILE	N-CA-C	8.85	120.50	108.11
17	3	86	PRO	N-CA-C	8.85	125.28	111.21
18	4	176	SER	CB-CA-C	-8.82	106.40	116.54
1	A	28	LYS	CA-C-N	-8.82	110.34	122.77
1	A	28	LYS	C-N-CA	-8.82	110.34	122.77
17	3	114	VAL	N-CA-C	-8.79	101.65	110.62
5	E	67	GLY	CA-C-N	8.78	130.82	119.84
5	E	67	GLY	C-N-CA	8.78	130.82	119.84
1	A	350	LEU	N-CA-C	-8.77	100.72	111.33
2	B	469	LYS	N-CA-C	8.77	122.82	108.26
15	1	83	GLU	N-CA-C	8.77	120.91	111.36
2	B	319	HIS	N-CA-C	8.74	124.13	113.38
2	B	448	THR	CA-C-N	8.73	128.37	118.85
2	B	448	THR	C-N-CA	8.73	128.37	118.85
2	B	123	TRP	N-CA-C	8.72	122.42	111.69
16	2	254	LEU	CB-CA-C	-8.72	106.51	116.63
12	L	69	LEU	N-CA-C	-8.72	99.36	111.39
8	H	60	ASN	N-CA-C	8.72	129.37	110.80
11	K	95	THR	N-CA-C	8.69	123.07	108.90
1	A	95	GLY	CA-C-N	-8.69	109.15	120.44
1	A	95	GLY	C-N-CA	-8.69	109.15	120.44
5	E	128	VAL	N-CA-C	-8.68	91.29	109.34
3	C	53	ARG	N-CA-C	-8.65	102.49	112.87
4	D	104	TRP	N-CA-C	8.63	121.99	108.79
2	B	52	GLY	N-CA-C	-8.61	103.74	114.16
18	4	171	ILE	N-CA-C	-8.61	102.15	110.42
2	B	575	ASP	N-CA-C	-8.61	102.58	113.43
1	A	114	THR	CB-CA-C	-8.60	101.32	109.83
18	4	132	GLU	N-CA-C	8.59	124.40	112.45
2	B	468	GLY	N-CA-C	8.59	122.02	111.45
1	A	287	LEU	N-CA-C	8.58	123.17	110.48
6	F	133	TYR	N-CA-C	8.55	123.92	112.30
4	D	196	SER	CA-C-N	8.52	130.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	196	SER	C-N-CA	8.52	130.49	119.84
2	B	503	GLU	N-CA-C	8.52	123.14	111.39
18	4	241	HIS	N-CA-C	8.52	122.36	109.41
1	A	43	THR	N-CA-C	-8.51	95.86	109.39
1	A	251	ASN	CA-C-N	-8.51	111.11	122.42
1	A	251	ASN	C-N-CA	-8.51	111.11	122.42
11	K	81	THR	N-CA-C	8.50	119.12	107.73
12	L	74	THR	CB-CA-C	-8.49	97.79	110.95
13	N	149	ASP	N-CA-C	-8.48	92.73	110.80
2	B	551	LYS	N-CA-C	8.47	121.58	108.96
1	A	183	TRP	N-CA-C	-8.47	102.00	111.14
16	2	163	ALA	N-CA-C	8.46	120.12	111.07
17	3	157	LEU	N-CA-C	-8.46	101.98	111.71
10	J	27	ILE	N-CA-C	-8.45	102.00	110.62
17	3	97	TRP	N-CA-C	-8.44	102.04	111.07
15	1	202	CYS	N-CA-C	-8.43	102.09	111.28
11	K	109	CYS	N-CA-C	-8.41	101.15	111.33
7	G	121	GLY	N-CA-C	-8.41	102.10	113.37
1	A	47	GLY	CA-C-N	8.41	130.35	119.84
1	A	47	GLY	C-N-CA	8.41	130.35	119.84
1	A	28	LYS	N-CA-C	8.39	128.68	110.80
1	A	87	SER	N-CA-C	-8.39	100.09	110.41
18	4	114	VAL	N-CA-C	8.38	119.19	110.72
1	A	238	ASP	N-CA-C	-8.38	90.73	107.91
1	A	255	LEU	N-CA-C	-8.38	101.20	111.33
2	B	98	GLN	CA-C-N	8.37	130.30	119.84
2	B	98	GLN	C-N-CA	8.37	130.30	119.84
1	A	484	LEU	N-CA-C	8.36	122.77	112.23
15	1	149	GLU	N-CA-C	-8.36	102.10	111.71
1	A	295	TRP	O-C-N	8.34	133.18	122.93
2	B	120	VAL	CB-CA-C	-8.33	101.13	112.04
17	3	99	ALA	N-CA-C	-8.33	101.12	111.11
16	2	254	LEU	N-CA-C	8.31	122.12	108.08
12	L	77	PRO	N-CA-C	-8.29	101.40	113.75
4	D	141	GLY	N-CA-C	-8.29	93.53	113.18
15	1	174	SER	CB-CA-C	-8.28	104.75	116.34
5	E	104	VAL	N-CA-C	-8.28	100.85	110.21
1	A	575	LEU	N-CA-C	8.26	121.85	111.69
8	H	99	LYS	CA-C-O	-8.26	108.70	120.51
18	4	208	GLY	N-CA-C	8.25	123.33	112.77
1	A	330	ILE	CB-CA-C	-8.23	101.03	112.14
12	L	145	LEU	CA-C-N	-8.22	109.75	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	145	LEU	C-N-CA	-8.22	109.75	120.44
16	2	261	THR	N-CA-C	8.21	121.96	109.23
4	D	140	LEU	N-CA-C	-8.20	98.94	110.50
16	2	127	THR	CB-CA-C	-8.19	94.12	110.42
10	J	4	LEU	N-CA-C	8.18	120.89	107.23
2	B	93	ASP	CA-C-N	8.18	130.06	119.84
2	B	93	ASP	C-N-CA	8.18	130.06	119.84
6	F	83	THR	CA-C-N	8.17	130.05	119.84
6	F	83	THR	C-N-CA	8.17	130.05	119.84
2	B	685	THR	CA-C-N	8.15	128.18	119.78
2	B	685	THR	C-N-CA	8.15	128.18	119.78
12	L	94	SER	N-CA-C	-8.15	100.22	109.60
1	A	572	LYS	CA-C-N	-8.14	111.94	122.77
1	A	572	LYS	C-N-CA	-8.14	111.94	122.77
6	F	149	ILE	N-CA-C	8.13	118.18	110.53
1	A	156	SER	N-CA-C	-8.13	98.29	110.24
13	N	145	PHE	CA-C-N	-8.13	106.02	121.54
13	N	145	PHE	C-N-CA	-8.13	106.02	121.54
17	3	135	ALA	N-CA-C	8.11	121.50	110.55
2	B	139	ALA	N-CA-C	-8.11	102.39	111.07
1	A	523	VAL	CA-C-N	8.10	130.55	120.34
1	A	523	VAL	C-N-CA	8.10	130.55	120.34
1	A	62	HIS	N-CA-C	-8.10	95.21	108.41
1	A	569	ILE	CA-C-N	8.09	129.96	119.84
1	A	569	ILE	C-N-CA	8.09	129.96	119.84
7	G	131	GLY	N-CA-C	8.09	125.99	113.86
4	D	174	PRO	CA-C-O	-8.07	112.14	121.34
16	2	183	PHE	N-CA-C	8.06	127.64	109.81
11	K	56	ILE	N-CA-C	8.05	121.16	111.09
15	1	172	GLY	CA-C-O	8.05	130.34	122.28
8	H	67	SER	N-CA-C	-8.05	100.59	111.54
3	C	67	VAL	CB-CA-C	-8.04	99.23	112.26
2	B	261	PHE	N-CA-C	-8.03	98.39	110.28
17	3	202	TYR	CA-C-N	8.01	128.76	119.47
17	3	202	TYR	C-N-CA	8.01	128.76	119.47
6	F	151	SER	N-CA-C	8.00	123.15	113.23
2	B	140	ILE	N-CA-C	-7.99	101.97	110.36
17	3	161	GLU	CA-C-N	-7.99	110.06	120.44
17	3	161	GLU	C-N-CA	-7.99	110.06	120.44
15	1	69	LEU	N-CA-C	-7.97	100.30	110.19
6	F	106	LEU	N-CA-C	-7.95	101.32	111.02
2	B	18	THR	CA-C-N	7.94	130.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	18	THR	C-N-CA	7.94	130.92	120.28
17	3	128	ILE	N-CA-C	7.93	126.00	108.88
4	D	160	ASN	N-CA-C	7.93	122.54	111.92
16	2	151	THR	N-CA-C	-7.92	102.61	111.71
2	B	461	GLN	N-CA-C	-7.91	101.75	111.33
11	K	97	ASP	CA-C-N	-7.89	111.03	119.24
11	K	97	ASP	C-N-CA	-7.89	111.03	119.24
6	F	208	PHE	N-CA-C	-7.89	103.65	113.20
13	N	90	GLU	CA-C-N	-7.89	111.29	122.41
13	N	90	GLU	C-N-CA	-7.89	111.29	122.41
1	A	632	GLY	CA-C-N	-7.88	112.82	122.90
1	A	632	GLY	C-N-CA	-7.88	112.82	122.90
4	D	177	VAL	CB-CA-C	-7.87	99.48	110.96
6	F	131	ASP	N-CA-C	-7.87	101.68	111.75
1	A	256	ALA	N-CA-C	-7.86	101.82	111.33
1	A	101	ALA	N-CA-C	7.86	119.63	111.14
8	H	108	THR	CB-CA-C	-7.86	98.48	110.90
1	A	579	PHE	CA-C-N	7.86	129.66	119.84
1	A	579	PHE	C-N-CA	7.86	129.66	119.84
3	C	1	MET	CA-C-N	-7.85	109.78	122.26
3	C	1	MET	C-N-CA	-7.85	109.78	122.26
1	A	149	PHE	N-CA-C	-7.85	100.21	110.33
15	1	66	PRO	N-CA-C	-7.82	101.11	113.78
1	A	496	HIS	N-CA-C	7.80	119.87	111.36
1	A	22	VAL	N-CA-C	7.79	125.55	109.34
6	F	155	ARG	N-CA-C	7.79	123.11	112.90
2	B	336	LEU	N-CA-C	-7.78	103.93	113.50
15	1	91	MET	CA-C-N	7.75	130.67	120.28
15	1	91	MET	C-N-CA	7.75	130.67	120.28
1	A	194	ALA	N-CA-C	-7.74	101.97	111.33
1	A	595	TRP	N-CA-C	-7.72	102.86	111.28
2	B	710	LEU	N-CA-C	-7.68	94.44	110.80
4	D	155	TYR	N-CA-C	-7.67	97.72	109.85
8	H	72	ALA	N-CA-C	7.67	119.81	108.76
2	B	176	ASN	N-CA-C	-7.66	103.73	113.23
5	E	126	VAL	CB-CA-C	-7.66	99.78	110.96
2	B	108	GLY	N-CA-C	7.65	121.37	112.50
12	L	93	VAL	N-CA-C	-7.64	96.43	108.81
13	N	127	PHE	N-CA-C	7.64	123.18	113.25
11	K	59	THR	N-CA-C	7.64	119.24	111.07
18	4	190	ASN	N-CA-C	7.62	118.36	109.60
12	L	204	LEU	N-CA-C	-7.61	100.34	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	N	101	LEU	N-CA-C	-7.61	96.11	108.52
2	B	609	PHE	N-CA-C	-7.61	102.93	111.07
16	2	222	ILE	CA-C-N	-7.61	110.55	120.44
16	2	222	ILE	C-N-CA	-7.61	110.55	120.44
12	L	159	SER	CA-C-N	-7.60	111.89	123.14
12	L	159	SER	C-N-CA	-7.60	111.89	123.14
1	A	597	HIS	N-CA-C	-7.60	102.66	112.23
2	B	469	LYS	CA-C-N	-7.59	107.05	121.54
2	B	469	LYS	C-N-CA	-7.59	107.05	121.54
16	2	239	HIS	N-CA-C	-7.58	103.01	111.28
1	A	23	ASP	CA-C-N	-7.58	112.07	122.30
1	A	23	ASP	C-N-CA	-7.58	112.07	122.30
1	A	91	LEU	N-CA-C	-7.58	102.96	111.07
2	B	238	SER	CA-C-N	-7.57	112.09	122.77
2	B	238	SER	C-N-CA	-7.57	112.09	122.77
11	K	49	ILE	N-CA-C	-7.55	101.46	112.04
18	4	237	SER	CA-C-N	-7.54	115.86	123.10
18	4	237	SER	C-N-CA	-7.54	115.86	123.10
2	B	463	ILE	N-CA-C	-7.54	98.78	109.63
2	B	297	ILE	N-CA-C	7.53	118.26	110.05
2	B	455	ILE	N-CA-C	-7.52	97.51	108.71
6	F	114	ALA	N-CA-C	7.51	126.41	109.81
15	1	171	LEU	O-C-N	7.49	132.89	123.15
4	D	141	GLY	CA-C-N	-7.49	110.44	120.54
4	D	141	GLY	C-N-CA	-7.49	110.44	120.54
7	G	96	GLY	N-CA-C	-7.49	99.11	112.58
7	G	105	THR	CA-C-N	7.49	131.50	120.87
7	G	105	THR	C-N-CA	7.49	131.50	120.87
6	F	139	LEU	N-CA-C	7.45	119.48	111.36
2	B	72	GLY	N-CA-C	-7.45	95.53	113.18
1	A	211	LEU	N-CA-C	-7.45	102.18	111.11
4	D	96	VAL	N-CA-C	7.43	122.44	112.04
13	N	141	LYS	N-CA-C	7.43	121.59	112.23
6	F	190	LYS	CA-C-N	7.42	129.12	119.84
6	F	190	LYS	C-N-CA	7.42	129.12	119.84
7	G	150	ASP	N-CA-C	7.42	126.21	109.81
12	L	80	ALA	N-CA-C	-7.41	103.19	111.71
16	2	112	TRP	N-CA-C	-7.41	103.14	111.07
18	4	156	ARG	N-CA-C	7.40	119.42	111.36
16	2	253	HIS	CB-CA-C	7.39	123.32	110.01
18	4	230	ASP	N-CA-C	7.39	126.55	110.80
18	4	207	ASN	N-CA-C	-7.39	102.29	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	178	ASN	N-CA-C	7.39	122.68	112.04
1	A	650	ASN	N-CA-C	-7.38	103.89	113.12
1	A	571	ASP	N-CA-C	-7.38	104.66	112.93
2	B	403	ASN	N-CA-C	7.37	122.03	112.89
2	B	466	ALA	N-CA-C	-7.35	102.29	111.11
15	1	63	GLY	CA-C-O	7.34	131.59	122.78
5	E	109	LYS	N-CA-C	-7.34	99.16	110.10
16	2	208	SER	N-CA-C	7.34	120.22	109.07
4	D	114	MET	CA-C-N	7.33	127.91	120.14
4	D	114	MET	C-N-CA	7.33	127.91	120.14
6	F	111	ASP	N-CA-C	7.33	119.27	111.28
15	1	65	ASP	CA-C-N	7.32	126.85	119.24
15	1	65	ASP	C-N-CA	7.32	126.85	119.24
2	B	359	ALA	N-CA-C	-7.31	99.63	110.23
4	D	190	SER	N-CA-C	7.31	120.42	110.55
15	1	153	SER	N-CA-C	7.30	123.35	111.37
13	N	166	VAL	N-CA-C	-7.30	94.16	109.34
18	4	202	GLU	N-CA-C	-7.30	104.63	113.97
1	A	40	PHE	N-CA-C	7.29	119.66	108.07
8	H	87	PHE	N-CA-C	-7.29	99.42	111.37
13	N	127	PHE	CA-C-N	-7.28	110.74	119.84
13	N	127	PHE	C-N-CA	-7.28	110.74	119.84
15	1	69	LEU	O-C-N	-7.28	112.61	122.36
2	B	115	ASN	CA-C-N	-7.28	113.09	122.77
2	B	115	ASN	C-N-CA	-7.28	113.09	122.77
1	A	683	HIS	N-CA-C	-7.27	103.98	112.92
15	1	176	ASP	N-CA-C	7.27	121.11	110.14
5	E	112	TYR	N-CA-C	7.26	121.40	112.54
2	B	169	LYS	N-CA-C	7.21	122.17	113.23
15	1	157	ASP	N-CA-C	7.21	125.74	109.81
16	2	257	PRO	CA-C-N	7.21	127.98	119.98
16	2	257	PRO	C-N-CA	7.21	127.98	119.98
2	B	114	ASN	N-CA-C	7.18	121.80	112.89
7	G	145	THR	CB-CA-C	-7.18	98.72	110.79
12	L	94	SER	CA-C-N	7.18	127.51	119.32
12	L	94	SER	C-N-CA	7.18	127.51	119.32
15	1	189	LYS	N-CA-C	-7.18	102.49	111.11
18	4	150	HIS	N-CA-C	7.18	119.97	111.71
4	D	182	GLN	N-CA-C	7.18	119.65	108.96
4	D	143	ARG	N-CA-C	-7.17	102.50	111.11
18	4	238	ASP	CA-C-N	7.17	128.80	119.84
18	4	238	ASP	C-N-CA	7.17	128.80	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	109	LEU	N-CA-C	-7.16	102.51	111.11
16	2	99	LEU	N-CA-C	7.16	120.92	111.75
16	2	164	GLU	N-CA-C	-7.16	103.47	111.71
16	2	162	TRP	N-CA-C	-7.13	103.44	111.07
7	G	105	THR	N-CA-C	7.13	121.84	108.65
12	L	146	THR	N-CA-CB	7.13	120.35	110.01
15	1	138	LEU	N-CA-C	7.10	118.71	110.97
17	3	151	TRP	N-CA-C	-7.10	95.67	110.80
1	A	349	ILE	CB-CA-C	-7.09	102.75	112.04
4	D	144	LEU	N-CA-C	7.08	121.50	113.01
2	B	451	LYS	N-CA-C	-7.07	103.73	113.56
18	4	84	ASP	CA-C-N	7.07	128.68	119.84
18	4	84	ASP	C-N-CA	7.07	128.68	119.84
1	A	158	ILE	N-CA-C	-7.07	94.64	109.34
12	L	123	THR	N-CA-C	7.07	120.63	110.24
13	N	165	ASN	N-CA-C	-7.06	99.09	110.32
7	G	81	ASN	N-CA-C	-7.05	102.79	111.33
18	4	235	HIS	N-CA-C	7.05	119.05	111.36
12	L	78	LEU	N-CA-C	7.05	118.96	111.28
3	C	63	LEU	N-CA-C	7.03	120.89	110.48
6	F	223	ASN	N-CA-C	7.03	119.87	108.34
2	B	399	ASN	CA-C-N	7.03	127.33	119.32
2	B	399	ASN	C-N-CA	7.03	127.33	119.32
1	A	100	GLY	N-CA-C	7.02	121.15	112.73
4	D	206	GLN	N-CA-C	7.02	122.04	108.85
8	H	86	THR	N-CA-C	-7.02	103.68	111.82
1	A	338	PHE	N-CA-C	-7.00	103.65	111.28
12	L	154	ASN	N-CA-C	7.00	121.06	111.39
16	2	241	TYR	N-CA-C	7.00	122.17	112.45
1	A	523	VAL	N-CA-C	7.00	123.89	109.34
17	3	155	TYR	N-CA-C	6.99	127.27	113.29
12	L	132	LEU	CB-CA-C	-6.98	108.53	116.63
2	B	223	GLY	CA-C-N	-6.97	111.12	119.84
2	B	223	GLY	C-N-CA	-6.97	111.12	119.84
2	B	471	THR	CA-C-N	-6.97	112.46	122.36
2	B	471	THR	C-N-CA	-6.97	112.46	122.36
8	H	81	SER	N-CA-C	-6.97	97.37	108.73
16	2	142	GLU	N-CA-C	6.96	118.76	111.03
12	L	66	ILE	N-CA-C	6.96	117.72	110.62
18	4	230	ASP	CA-C-N	-6.96	112.28	122.65
18	4	230	ASP	C-N-CA	-6.96	112.28	122.65
4	D	113	GLU	N-CA-C	6.96	118.94	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	194	LYS	N-CA-C	-6.95	102.92	111.33
12	L	139	VAL	N-CA-C	6.95	117.06	110.53
1	A	492	ILE	N-CA-C	6.95	118.57	111.00
1	A	527	VAL	N-CA-C	-6.95	98.58	108.58
1	A	489	ALA	N-CA-C	6.93	118.48	111.07
16	2	246	PRO	CA-C-N	-6.93	112.17	122.01
16	2	246	PRO	C-N-CA	-6.93	112.17	122.01
1	A	423	ASP	CA-C-N	6.92	128.49	119.84
1	A	423	ASP	C-N-CA	6.92	128.49	119.84
8	H	117	SER	N-CA-C	6.92	125.53	110.80
2	B	483	GLY	N-CA-C	-6.90	98.26	112.34
2	B	620	LEU	CA-C-N	-6.90	111.47	120.44
2	B	620	LEU	C-N-CA	-6.90	111.47	120.44
6	F	202	LEU	N-CA-C	-6.89	103.98	113.56
1	A	191	PRO	N-CA-C	6.89	121.39	111.13
2	B	203	ARG	CA-C-N	6.88	126.88	120.34
2	B	203	ARG	C-N-CA	6.88	126.88	120.34
4	D	138	LEU	N-CA-C	-6.88	103.80	111.71
2	B	623	TYR	N-CA-C	-6.87	96.16	110.80
1	A	126	ILE	N-CA-C	6.87	117.79	108.17
2	B	99	PRO	CA-N-CD	-6.87	102.38	112.00
15	1	63	GLY	N-CA-C	6.86	124.49	112.83
15	1	192	ARG	N-CA-C	-6.86	103.80	111.28
4	D	101	VAL	N-CA-C	6.86	118.53	109.21
16	2	248	ASP	CA-C-N	6.84	129.45	120.28
16	2	248	ASP	C-N-CA	6.84	129.45	120.28
8	H	95	GLY	CA-C-N	-6.83	111.73	121.50
8	H	95	GLY	C-N-CA	-6.83	111.73	121.50
12	L	159	SER	N-CA-C	6.83	125.35	110.80
17	3	183	GLY	N-CA-C	-6.82	97.01	113.18
3	C	64	SER	N-CA-C	6.82	118.79	111.36
12	L	96	LEU	N-CA-C	-6.81	103.09	111.33
11	K	101	PHE	N-CA-C	6.80	120.79	112.23
15	1	163	TYR	N-CA-C	-6.79	94.80	109.81
15	1	71	GLU	N-CA-C	-6.77	102.99	111.11
17	3	153	ASP	CA-C-N	6.77	130.03	120.28
17	3	153	ASP	C-N-CA	6.77	130.03	120.28
18	4	116	THR	N-CA-C	-6.76	103.15	111.33
17	3	106	GLY	N-CA-C	-6.75	104.63	112.73
12	L	166	LEU	CA-C-N	-6.74	111.76	120.65
12	L	166	LEU	C-N-CA	-6.74	111.76	120.65
11	K	128	GLY	O-C-N	6.74	128.70	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	322	LEU	N-CA-C	-6.74	103.18	111.33
8	H	82	LYS	N-CA-C	-6.73	102.38	111.54
6	F	213	TRP	CB-CA-C	6.73	117.89	110.15
12	L	100	ILE	N-CA-C	6.73	118.33	111.00
7	G	73	PHE	N-CA-C	6.72	119.96	111.69
1	A	631	GLN	N-CA-C	-6.71	102.42	111.54
16	2	172	LEU	N-CA-C	6.71	125.08	110.80
2	B	256	THR	N-CA-C	6.70	118.38	108.60
1	A	538	ASP	N-CA-C	-6.70	105.67	114.31
1	A	68	THR	N-CA-C	6.69	119.39	108.55
15	1	170	PRO	CA-C-N	6.69	133.10	122.59
15	1	170	PRO	C-N-CA	6.69	133.10	122.59
17	3	175	ASP	N-CA-C	-6.69	103.23	111.33
18	4	214	PHE	CA-C-N	-6.69	111.50	120.54
18	4	214	PHE	C-N-CA	-6.69	111.50	120.54
2	B	69	ALA	N-CA-C	6.69	125.05	110.80
1	A	80	SER	N-CA-C	6.68	118.36	111.14
17	3	181	SER	N-CA-C	-6.67	104.08	111.82
1	A	353	SER	CB-CA-C	-6.66	99.59	110.79
1	A	340	GLY	CA-C-N	6.65	129.49	120.38
1	A	340	GLY	C-N-CA	6.65	129.49	120.38
6	F	213	TRP	N-CA-C	-6.64	98.06	109.15
6	F	147	HIS	CA-C-N	-6.64	113.68	123.11
6	F	147	HIS	C-N-CA	-6.64	113.68	123.11
1	A	60	ASP	N-CA-C	-6.63	102.53	111.54
8	H	65	TRP	CA-C-N	-6.62	111.95	121.42
8	H	65	TRP	C-N-CA	-6.62	111.95	121.42
12	L	139	VAL	CB-CA-C	-6.62	103.35	112.02
12	L	127	GLY	N-CA-C	6.62	120.17	112.50
1	A	280	PHE	N-CA-C	6.61	124.88	110.80
2	B	166	SER	N-CA-C	-6.61	104.07	111.28
16	2	130	GLY	O-C-N	6.61	131.29	122.70
5	E	72	ALA	N-CA-C	6.61	118.56	111.36
4	D	180	GLY	N-CA-C	6.60	128.82	113.18
11	K	65	LEU	N-CA-C	6.59	118.55	111.36
2	B	206	TYR	N-CA-C	6.59	119.23	110.53
1	A	201	SER	N-CA-C	6.59	120.53	112.23
18	4	205	ILE	CB-CA-C	-6.57	103.48	111.88
16	2	259	HIS	N-CA-C	6.56	118.52	108.42
1	A	245	PRO	N-CA-C	6.55	122.15	113.57
11	K	73	ALA	N-CA-C	6.55	121.66	112.75
16	2	137	TRP	N-CA-C	6.55	120.48	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	GLY	N-CA-C	-6.55	104.87	112.73
2	B	435	GLY	N-CA-C	-6.55	104.57	112.49
1	A	295	TRP	CA-C-N	6.54	134.03	121.54
1	A	295	TRP	C-N-CA	6.54	134.03	121.54
7	G	89	LYS	N-CA-C	-6.54	102.22	111.24
15	1	167	ALA	N-CA-C	6.54	120.90	107.37
16	2	117	ALA	N-CA-C	-6.53	104.41	112.38
1	A	330	ILE	N-CA-C	6.53	117.28	110.62
4	D	159	PRO	CA-C-O	-6.53	113.65	121.48
17	3	197	SER	N-CA-C	6.53	122.14	111.37
3	C	70	TRP	N-CA-C	-6.52	96.91	110.80
1	A	428	TYR	N-CA-C	6.52	118.97	110.43
15	1	71	GLU	CA-C-N	-6.52	110.07	122.13
15	1	71	GLU	C-N-CA	-6.52	110.07	122.13
2	B	618	GLY	N-CA-C	-6.51	106.34	115.32
13	N	143	VAL	CA-C-N	6.51	126.44	119.28
13	N	143	VAL	C-N-CA	6.51	126.44	119.28
4	D	94	ALA	N-CA-C	6.51	121.42	112.90
15	1	171	LEU	CA-C-N	-6.51	115.83	122.27
15	1	171	LEU	C-N-CA	-6.51	115.83	122.27
2	B	374	HIS	N-CA-C	-6.50	104.36	113.20
15	1	129	VAL	CB-CA-C	-6.48	105.51	114.00
16	2	121	PHE	CA-C-N	-6.47	115.15	120.33
16	2	121	PHE	C-N-CA	-6.47	115.15	120.33
18	4	90	TRP	CA-C-N	-6.47	112.32	122.49
18	4	90	TRP	C-N-CA	-6.47	112.32	122.49
18	4	182	VAL	N-CA-C	6.47	117.25	110.72
1	A	681	GLY	N-CA-C	-6.47	105.22	112.33
18	4	240	TRP	N-CA-C	6.47	120.14	108.69
2	B	640	CYS	N-CA-C	6.46	119.06	108.52
1	A	337	PRO	N-CA-C	6.46	122.71	113.47
12	L	64	PRO	CA-N-CD	-6.45	102.97	112.00
12	L	91	THR	CA-C-N	-6.44	111.83	120.79
12	L	91	THR	C-N-CA	-6.44	111.83	120.79
5	E	80	GLU	N-CA-C	6.44	121.34	112.90
1	A	50	THR	N-CA-C	6.44	118.85	109.07
1	A	646	SER	N-CA-C	-6.44	105.58	113.50
5	E	78	ARG	N-CA-C	6.44	121.33	112.90
17	3	247	VAL	N-CA-C	-6.43	107.22	113.53
18	4	118	ILE	N-CA-C	6.43	118.42	109.55
15	1	89	TRP	N-CA-C	-6.43	104.19	111.07
1	A	639	ALA	N-CA-C	-6.42	100.80	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	275	SER	N-CA-C	6.42	120.32	112.23
7	G	150	ASP	CA-C-N	6.42	126.33	119.85
7	G	150	ASP	C-N-CA	6.42	126.33	119.85
2	B	268	LEU	N-CA-C	-6.41	98.07	108.52
2	B	332	PHE	N-CA-C	-6.41	103.41	111.11
2	B	450	GLU	N-CA-C	-6.41	102.04	110.43
13	N	169	LYS	CA-C-N	-6.40	110.18	121.70
13	N	169	LYS	C-N-CA	-6.40	110.18	121.70
17	3	162	MET	CA-C-N	-6.40	111.90	120.54
17	3	162	MET	C-N-CA	-6.40	111.90	120.54
18	4	198	LEU	CB-CA-C	-6.40	109.18	116.54
1	A	55	TRP	N-CA-C	6.40	118.33	111.36
2	B	681	ALA	N-CA-C	-6.39	97.19	110.80
3	C	62	PHE	N-CA-C	-6.39	97.18	110.80
17	3	134	LEU	N-CA-C	6.39	119.32	108.90
6	F	115	PRO	N-CA-C	6.39	125.64	112.47
6	F	149	ILE	CB-CA-C	-6.39	103.65	112.02
2	B	17	THR	CA-C-N	6.39	130.82	120.60
2	B	17	THR	C-N-CA	6.39	130.82	120.60
15	1	93	ALA	N-CA-C	-6.38	104.33	111.28
16	2	100	ARG	CA-C-N	-6.38	112.70	122.08
16	2	100	ARG	C-N-CA	-6.38	112.70	122.08
2	B	321	GLY	N-CA-C	6.37	128.28	113.18
12	L	75	SER	N-CA-C	6.36	120.97	108.18
2	B	513	GLY	CA-C-N	6.36	127.79	119.84
2	B	513	GLY	C-N-CA	6.36	127.79	119.84
18	4	215	LEU	CA-C-N	-6.36	108.95	121.41
18	4	215	LEU	C-N-CA	-6.36	108.95	121.41
15	1	157	ASP	CA-C-N	-6.35	112.36	118.97
15	1	157	ASP	C-N-CA	-6.35	112.36	118.97
2	B	99	PRO	CA-C-N	6.35	129.43	120.28
2	B	99	PRO	C-N-CA	6.35	129.43	120.28
2	B	543	GLY	N-CA-C	6.35	120.01	112.33
2	B	222	LEU	N-CA-C	-6.35	103.65	111.33
6	F	210	GLY	N-CA-C	6.34	120.57	112.83
17	3	204	GLY	CA-C-N	-6.34	116.50	121.13
17	3	204	GLY	C-N-CA	-6.34	116.50	121.13
7	G	143	ALA	CA-C-N	-6.34	114.53	123.03
7	G	143	ALA	C-N-CA	-6.34	114.53	123.03
8	H	108	THR	N-CA-CB	6.34	119.27	110.07
6	F	97	GLN	N-CA-C	-6.33	97.31	110.80
7	G	91	VAL	CB-CA-C	-6.33	104.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	265	GLY	N-CA-C	6.33	128.17	113.18
13	N	135	GLN	CA-C-N	-6.32	109.47	121.54
13	N	135	GLN	C-N-CA	-6.32	109.47	121.54
18	4	92	VAL	CB-CA-C	-6.31	103.62	112.14
17	3	141	VAL	N-CA-C	6.31	122.46	109.34
16	2	116	GLY	N-CA-C	-6.30	104.70	112.77
1	A	628	ILE	N-CA-C	6.30	117.78	109.21
17	3	216	ASP	N-CA-C	-6.30	96.99	108.02
1	A	71	LEU	N-CA-C	-6.30	103.55	111.11
1	A	337	PRO	CA-N-CD	-6.29	103.19	112.00
4	D	206	GLN	CA-C-N	6.29	127.70	119.84
4	D	206	GLN	C-N-CA	6.29	127.70	119.84
2	B	100	ALA	N-CA-C	-6.29	104.48	111.71
8	H	87	PHE	CA-C-N	-6.29	113.81	122.30
8	H	87	PHE	C-N-CA	-6.29	113.81	122.30
2	B	124	TRP	N-CA-C	-6.28	104.35	111.07
12	L	132	LEU	N-CA-C	6.27	118.68	108.08
4	D	175	GLU	N-CA-C	6.27	124.15	110.80
5	E	99	THR	N-CA-C	6.26	118.12	109.29
8	H	108	THR	CA-C-N	-6.26	112.08	120.54
8	H	108	THR	C-N-CA	-6.26	112.08	120.54
1	A	25	ASP	CA-C-N	6.26	125.75	119.24
1	A	25	ASP	C-N-CA	6.26	125.75	119.24
1	A	121	GLN	N-CA-C	6.26	119.11	108.90
7	G	80	PHE	N-CA-C	6.26	121.06	113.17
6	F	225	GLU	CA-C-N	-6.26	111.76	121.02
6	F	225	GLU	C-N-CA	-6.26	111.76	121.02
15	1	198	PHE	N-CA-C	-6.25	104.38	111.07
2	B	358	TYR	N-CA-C	6.25	119.59	109.40
2	B	228	GLY	N-CA-C	-6.25	98.37	113.18
17	3	130	GLN	N-CA-C	-6.25	100.33	110.20
15	1	203	VAL	CA-C-N	6.25	128.65	120.28
15	1	203	VAL	C-N-CA	6.25	128.65	120.28
18	4	233	LEU	N-CA-C	6.25	121.13	112.45
1	A	161	GLU	N-CA-C	6.24	118.16	111.36
2	B	504	ASN	N-CA-C	-6.24	100.67	109.96
2	B	438	VAL	N-CA-C	-6.23	105.07	110.74
2	B	88	ALA	N-CA-C	6.23	117.95	111.03
4	D	195	VAL	N-CA-C	-6.22	103.31	111.09
7	G	99	HIS	N-CA-C	-6.22	97.55	110.80
6	F	142	SER	N-CA-C	6.22	119.68	110.48
15	1	142	PHE	CA-C-N	-6.22	111.46	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	142	PHE	C-N-CA	-6.22	111.46	120.29
1	A	231	GLN	N-CA-C	-6.21	104.05	111.69
6	F	206	LEU	N-CA-C	-6.20	104.62	111.82
12	L	135	GLY	N-CA-C	-6.20	105.12	113.24
15	1	215	GLU	CA-C-N	6.19	128.86	120.44
15	1	215	GLU	C-N-CA	6.19	128.86	120.44
2	B	104	PHE	N-CA-C	-6.19	97.61	110.80
15	1	165	GLY	CA-C-N	-6.19	109.28	121.41
15	1	165	GLY	C-N-CA	-6.19	109.28	121.41
12	L	109	LEU	N-CA-C	-6.19	100.13	109.60
12	L	173	PRO	N-CA-C	-6.17	101.29	111.11
15	1	86	HIS	N-CA-CB	-6.17	100.71	110.28
16	2	130	GLY	N-CA-C	-6.17	98.56	113.18
7	G	120	VAL	CA-C-N	6.16	128.04	120.22
7	G	120	VAL	C-N-CA	6.16	128.04	120.22
4	D	136	GLN	N-CA-C	6.16	118.07	111.36
2	B	306	GLU	CB-CA-C	-6.16	109.46	116.54
2	B	310	PRO	CA-C-N	6.16	127.53	119.84
2	B	310	PRO	C-N-CA	6.16	127.53	119.84
16	2	240	ILE	CB-CA-C	-6.15	103.83	112.14
16	2	210	SER	CA-C-N	6.15	125.55	118.85
16	2	210	SER	C-N-CA	6.15	125.55	118.85
1	A	489	ALA	CA-C-N	-6.14	114.61	122.77
1	A	489	ALA	C-N-CA	-6.14	114.61	122.77
17	3	196	GLY	N-CA-C	6.13	127.71	113.18
2	B	445	ALA	N-CA-C	-6.13	103.66	113.28
17	3	205	GLY	CA-C-N	6.12	127.05	120.13
17	3	205	GLY	C-N-CA	6.12	127.05	120.13
2	B	264	GLN	CA-C-N	6.12	133.23	121.54
2	B	264	GLN	C-N-CA	6.12	133.23	121.54
1	A	522	ALA	CA-C-N	6.12	132.98	121.97
1	A	522	ALA	C-N-CA	6.12	132.98	121.97
17	3	133	ALA	N-CA-C	6.12	119.21	111.69
2	B	21	ILE	CB-CA-C	-6.12	104.01	112.02
4	D	193	LYS	N-CA-C	6.12	123.83	110.80
6	F	114	ALA	CA-C-N	6.11	127.48	119.84
6	F	114	ALA	C-N-CA	6.11	127.48	119.84
1	A	117	GLY	N-CA-C	6.11	124.80	112.34
1	A	125	PRO	CA-C-N	-6.11	115.61	123.19
1	A	125	PRO	C-N-CA	-6.11	115.61	123.19
6	F	107	LYS	N-CA-C	-6.11	100.13	109.41
1	A	349	ILE	N-CA-C	-6.10	103.66	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	149	ASN	CA-C-N	-6.10	111.97	122.10
17	3	149	ASN	C-N-CA	-6.10	111.97	122.10
15	1	172	GLY	CA-C-N	-6.10	112.94	123.25
15	1	172	GLY	C-N-CA	-6.10	112.94	123.25
17	3	158	PHE	CA-C-N	-6.10	112.62	121.65
17	3	158	PHE	C-N-CA	-6.10	112.62	121.65
15	1	84	LEU	N-CA-C	6.10	118.01	111.36
8	H	102	ILE	CB-CA-C	-6.10	103.91	112.14
13	N	164	SER	CA-C-N	-6.09	111.65	122.07
13	N	164	SER	C-N-CA	-6.09	111.65	122.07
11	K	69	ARG	CA-C-N	-6.09	112.32	120.54
11	K	69	ARG	C-N-CA	-6.09	112.32	120.54
12	L	152	SER	N-CA-C	-6.09	98.98	108.90
18	4	137	SER	N-CA-C	6.08	117.71	111.14
12	L	65	PHE	N-CA-C	6.08	118.87	111.82
2	B	10	GLN	N-CA-C	6.07	119.16	111.69
7	G	88	ALA	N-CA-C	-6.07	104.48	113.40
1	A	233	LEU	N-CA-C	-6.07	106.01	113.41
7	G	113	LEU	N-CA-C	6.07	120.41	112.89
17	3	103	VAL	N-CA-C	6.06	116.80	110.62
5	E	125	ILE	CB-CA-C	-6.06	102.11	110.96
1	A	515	TRP	CA-C-N	6.06	126.84	119.99
1	A	515	TRP	C-N-CA	6.06	126.84	119.99
2	B	93	ASP	N-CA-C	6.05	120.23	108.85
7	G	126	ASP	N-CA-C	6.05	117.55	111.07
4	D	167	HIS	CA-C-N	-6.05	112.68	118.97
4	D	167	HIS	C-N-CA	-6.05	112.68	118.97
18	4	213	ALA	CA-C-N	6.05	128.66	120.44
18	4	213	ALA	C-N-CA	6.05	128.66	120.44
1	A	163	GLN	CA-C-N	-6.04	110.00	121.54
1	A	163	GLN	C-N-CA	-6.04	110.00	121.54
2	B	87	ILE	CB-CA-C	-6.04	102.63	110.84
11	K	63	LEU	CA-C-N	-6.03	112.60	120.44
11	K	63	LEU	C-N-CA	-6.03	112.60	120.44
18	4	211	MET	CB-CA-C	6.03	121.10	110.85
2	B	120	VAL	N-CA-C	6.03	117.49	110.62
8	H	105	GLY	N-CA-C	-6.01	105.53	112.50
10	J	11	ALA	CA-C-N	6.00	127.35	119.84
10	J	11	ALA	C-N-CA	6.00	127.35	119.84
1	A	328	LYS	N-CA-C	-6.00	103.91	111.11
1	A	507	ALA	N-CA-C	6.00	123.59	110.80
13	N	147	SER	N-CA-C	-5.99	98.04	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	68	THR	CA-C-N	5.99	126.76	119.99
7	G	68	THR	C-N-CA	5.99	126.76	119.99
7	G	68	THR	N-CA-C	-5.99	103.71	111.02
18	4	184	TYR	CA-C-N	5.98	127.32	119.84
18	4	184	TYR	C-N-CA	5.98	127.32	119.84
13	N	92	LEU	N-CA-C	-5.98	98.06	110.80
16	2	123	PRO	CA-C-N	-5.98	112.67	120.44
16	2	123	PRO	C-N-CA	-5.98	112.67	120.44
2	B	265	THR	N-CA-C	-5.97	98.07	110.80
16	2	125	PHE	N-CA-C	5.97	117.87	111.36
2	B	252	THR	N-CA-C	5.97	120.27	107.67
4	D	106	SER	N-CA-C	5.97	117.90	108.23
15	1	66	PRO	CA-C-N	-5.96	112.69	120.44
15	1	66	PRO	C-N-CA	-5.96	112.69	120.44
2	B	219	PRO	CA-N-CD	-5.95	103.67	112.00
2	B	213	LEU	N-CA-C	5.95	117.84	111.36
3	C	77	MET	N-CA-C	5.95	117.84	111.36
2	B	620	LEU	CB-CA-C	-5.94	101.55	110.88
13	N	106	ARG	N-CA-C	-5.94	103.19	111.39
4	D	112	PHE	N-CA-C	5.94	119.23	109.85
8	H	61	THR	N-CA-C	-5.94	98.15	110.80
1	A	89	ILE	N-CA-C	-5.93	104.57	110.62
8	H	111	TYR	CA-C-N	-5.92	111.24	121.66
8	H	111	TYR	C-N-CA	-5.92	111.24	121.66
2	B	324	ASP	N-CA-C	5.92	120.23	112.89
7	G	62	LEU	CA-C-N	5.92	127.94	120.72
7	G	62	LEU	C-N-CA	5.92	127.94	120.72
1	A	245	PRO	CA-C-N	-5.91	112.96	122.24
1	A	245	PRO	C-N-CA	-5.91	112.96	122.24
8	H	99	LYS	N-CA-C	-5.91	98.22	110.80
16	2	121	PHE	N-CA-C	5.91	117.39	111.07
17	3	226	LYS	N-CA-C	-5.90	106.41	113.97
13	N	88	ILE	CB-CA-C	-5.90	101.89	110.63
6	F	128	LYS	N-CA-C	-5.90	98.24	110.80
2	B	318	GLY	N-CA-C	5.90	118.71	111.93
12	L	157	ALA	CA-C-N	5.90	127.21	119.84
12	L	157	ALA	C-N-CA	5.90	127.21	119.84
16	2	194	GLY	N-CA-C	5.89	127.14	113.18
5	E	128	VAL	O-C-N	-5.89	115.21	122.57
2	B	372	TYR	N-CA-C	-5.88	105.93	113.23
11	K	102	THR	N-CA-C	5.88	120.52	113.23
15	1	65	ASP	O-C-N	5.88	128.08	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	458	ILE	N-CA-C	-5.88	104.78	110.42
3	C	37	LYS	N-CA-C	5.88	119.68	111.74
15	1	67	LEU	N-CA-C	5.88	117.36	111.07
18	4	100	ARG	N-CA-C	5.87	117.68	111.28
16	2	139	THR	CA-C-N	-5.87	113.91	122.19
16	2	139	THR	C-N-CA	-5.87	113.91	122.19
1	A	104	SER	CB-CA-C	-5.87	101.93	110.96
2	B	409	ALA	N-CA-C	-5.87	102.79	110.53
1	A	92	TRP	CA-C-N	-5.86	116.08	126.45
1	A	92	TRP	C-N-CA	-5.86	116.08	126.45
1	A	501	GLY	N-CA-C	-5.86	99.30	113.18
2	B	94	PRO	CA-N-CD	-5.86	103.80	112.00
2	B	209	TRP	N-CA-C	-5.85	104.98	111.71
2	B	596	TRP	N-CA-C	-5.85	98.34	110.80
1	A	59	ALA	N-CA-C	-5.85	102.40	110.35
16	2	127	THR	N-CA-CB	5.85	120.37	110.49
16	2	225	GLY	N-CA-C	-5.84	107.09	114.16
1	A	157	GLY	N-CA-C	-5.84	99.34	113.18
5	E	69	LYS	CA-C-N	5.84	128.57	120.63
5	E	69	LYS	C-N-CA	5.84	128.57	120.63
11	K	128	GLY	CA-C-N	-5.83	113.16	121.50
11	K	128	GLY	C-N-CA	-5.83	113.16	121.50
2	B	130	ARG	N-CA-C	5.83	117.44	111.14
2	B	244	PHE	N-CA-C	5.82	118.78	110.10
1	A	440	ASP	N-CA-C	-5.82	104.81	112.72
2	B	512	ILE	N-CA-C	5.80	121.41	109.34
4	D	162	GLU	N-CA-C	5.79	118.40	109.07
1	A	236	GLY	N-CA-C	-5.79	102.75	110.97
8	H	71	ASP	N-CA-C	5.79	118.36	111.71
12	L	79	ILE	CB-CA-C	-5.79	104.44	112.02
17	3	215	LYS	N-CA-C	5.79	118.20	109.23
17	3	211	LEU	N-CA-C	-5.77	101.87	110.23
7	G	72	LEU	N-CA-C	-5.76	98.52	110.80
12	L	131	SER	O-C-N	-5.76	114.93	122.59
2	B	627	ASN	CB-CA-C	-5.76	102.42	111.51
16	2	257	PRO	CA-C-O	-5.76	110.12	120.60
17	3	175	ASP	CA-C-N	-5.75	110.43	121.94
17	3	175	ASP	C-N-CA	-5.75	110.43	121.94
2	B	32	GLU	N-CA-C	-5.75	101.89	110.23
1	A	106	TYR	CA-C-N	-5.75	112.78	120.54
1	A	106	TYR	C-N-CA	-5.75	112.78	120.54
2	B	474	PHE	N-CA-C	-5.75	98.56	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	121	ILE	N-CA-C	5.75	116.40	108.12
7	G	106	ARG	N-CA-C	5.75	118.79	110.28
15	1	105	TYR	CB-CA-C	-5.75	109.41	117.23
18	4	145	GLU	N-CA-C	-5.74	104.38	111.33
18	4	188	ILE	N-CA-C	5.73	121.26	109.34
2	B	453	ILE	N-CA-C	5.73	116.05	107.51
15	1	170	PRO	N-CA-C	-5.73	100.67	112.47
18	4	108	GLY	CA-C-N	-5.71	110.64	121.54
18	4	108	GLY	C-N-CA	-5.71	110.64	121.54
16	2	96	PRO	CA-C-N	-5.70	115.01	123.11
16	2	96	PRO	C-N-CA	-5.70	115.01	123.11
2	B	11	GLY	N-CA-C	-5.70	105.74	112.64
15	1	148	VAL	N-CA-C	5.70	116.47	110.72
18	4	184	TYR	N-CA-C	-5.69	101.28	109.48
2	B	626	LEU	CA-C-N	-5.69	114.15	122.40
2	B	626	LEU	C-N-CA	-5.69	114.15	122.40
17	3	129	PRO	CA-N-CD	-5.69	104.04	112.00
17	3	173	PHE	N-CA-C	5.68	117.47	111.28
4	D	135	GLU	N-CA-C	-5.68	105.18	111.71
2	B	539	LEU	CA-C-N	-5.67	115.19	122.79
2	B	539	LEU	C-N-CA	-5.67	115.19	122.79
2	B	275	HIS	N-CA-C	-5.67	104.31	111.11
12	L	130	GLY	N-CA-C	5.67	121.11	111.19
4	D	153	GLN	CA-C-O	-5.66	114.71	120.71
16	2	150	THR	N-CA-C	5.66	120.31	112.90
2	B	303	TYR	N-CA-CB	-5.66	108.44	114.10
15	1	182	GLU	N-CA-C	-5.66	105.70	113.56
2	B	731	GLY	N-CA-C	-5.65	99.79	113.18
1	A	252	ARG	N-CA-C	5.65	117.50	108.41
15	1	202	CYS	CA-CB-SG	-5.64	101.43	114.40
1	A	638	THR	N-CA-C	5.64	117.60	108.41
15	1	85	ILE	CB-CA-C	-5.64	104.44	112.22
1	A	478	SER	N-CA-C	-5.63	103.05	110.43
17	3	100	TYR	N-CA-C	-5.63	105.51	112.38
18	4	123	VAL	CA-C-N	5.63	125.74	119.32
18	4	123	VAL	C-N-CA	5.63	125.74	119.32
5	E	74	VAL	N-CA-C	5.62	116.22	108.12
12	L	143	LEU	CA-C-N	-5.62	112.95	120.54
12	L	143	LEU	C-N-CA	-5.62	112.95	120.54
2	B	467	HIS	N-CA-C	5.61	117.20	111.14
2	B	312	GLY	N-CA-C	5.61	126.46	113.18
1	A	135	ASP	CA-C-N	5.60	129.93	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	ASP	C-N-CA	5.60	129.93	120.29
15	1	156	LYS	O-C-N	-5.60	115.15	122.59
1	A	706	SER	N-CA-C	-5.59	104.40	111.11
16	2	235	ALA	N-CA-C	-5.59	105.33	111.82
8	H	107	SER	CA-C-N	-5.59	112.84	120.44
8	H	107	SER	C-N-CA	-5.59	112.84	120.44
1	A	259	TYR	N-CA-C	5.58	122.15	109.81
7	G	115	LYS	N-CA-C	-5.58	99.73	108.00
1	A	341	GLN	CA-C-N	5.58	127.11	120.14
1	A	341	GLN	C-N-CA	5.58	127.11	120.14
2	B	475	ASP	N-CA-C	5.58	118.55	111.69
13	N	97	THR	CB-CA-C	-5.58	99.33	110.42
4	D	80	SER	N-CA-C	5.57	122.12	109.81
1	A	45	ALA	N-CA-C	-5.57	102.29	110.42
15	1	176	ASP	CB-CA-C	5.56	117.22	108.88
17	3	206	PRO	CB-CA-C	-5.56	104.60	111.11
2	B	199	ILE	N-CA-CB	5.56	114.78	110.45
2	B	698	VAL	N-CA-C	5.56	116.18	108.23
2	B	296	GLY	N-CA-C	5.55	123.75	115.64
16	2	251	PHE	CA-C-N	-5.55	115.16	122.99
16	2	251	PHE	C-N-CA	-5.55	115.16	122.99
12	L	194	ILE	CB-CA-C	-5.55	102.54	111.59
1	A	578	ARG	N-CA-C	5.54	118.51	111.69
1	A	380	PRO	CA-C-N	5.54	126.76	119.84
1	A	380	PRO	C-N-CA	5.54	126.76	119.84
2	B	732	LYS	N-CA-C	-5.54	99.01	110.80
1	A	684	PHE	N-CA-C	-5.53	105.64	112.72
8	H	73	PRO	N-CA-C	5.53	120.81	113.57
12	L	181	GLY	N-CA-C	-5.53	100.08	113.18
4	D	132	ALA	N-CA-C	5.52	122.56	110.80
4	D	185	GLY	N-CA-C	-5.52	100.10	113.18
1	A	69	SER	N-CA-C	-5.51	104.69	111.75
1	A	192	LYS	CA-C-N	5.51	127.60	120.44
1	A	192	LYS	C-N-CA	5.51	127.60	120.44
2	B	505	SER	N-CA-C	-5.51	99.06	110.80
15	1	146	ALA	N-CA-C	-5.51	105.38	111.71
15	1	61	ASP	CA-C-N	-5.50	114.82	123.13
15	1	61	ASP	C-N-CA	-5.50	114.82	123.13
7	G	134	GLY	N-CA-C	5.50	119.81	112.77
6	F	81	GLY	N-CA-C	-5.50	100.15	113.18
2	B	301	ILE	N-CA-C	5.49	116.22	110.62
2	B	211	ASN	CA-C-N	5.49	127.91	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	211	ASN	C-N-CA	5.49	127.91	120.44
5	E	103	VAL	N-CA-C	5.49	120.76	109.34
2	B	195	VAL	N-CA-C	5.49	116.14	110.82
2	B	159	PRO	N-CA-C	5.48	121.31	113.47
1	A	360	ILE	N-CA-C	-5.47	102.46	109.30
1	A	453	LEU	N-CA-C	-5.47	103.27	110.33
2	B	238	SER	N-CA-C	-5.47	101.09	109.41
2	B	325	THR	N-CA-C	5.47	119.13	112.23
1	A	196	PHE	N-CA-C	5.47	118.07	111.40
2	B	701	SER	N-CA-C	-5.47	103.41	110.19
4	D	173	TYR	CA-C-N	5.47	125.39	119.76
4	D	173	TYR	C-N-CA	5.47	125.39	119.76
4	D	188	PHE	CA-CB-CG	-5.46	108.34	113.80
12	L	85	ASN	CA-C-N	5.46	129.77	121.03
12	L	85	ASN	C-N-CA	5.46	129.77	121.03
11	K	85	LYS	N-CA-C	5.45	117.40	108.52
1	A	152	ILE	CA-C-N	5.45	128.59	120.31
1	A	152	ILE	C-N-CA	5.45	128.59	120.31
1	A	22	VAL	CA-C-N	-5.44	112.36	121.39
1	A	22	VAL	C-N-CA	-5.44	112.36	121.39
15	1	63	GLY	O-C-N	-5.44	115.99	122.68
1	A	452	PHE	N-CA-C	-5.44	105.00	111.03
2	B	140	ILE	CB-CA-C	-5.44	104.92	111.88
1	A	106	TYR	N-CA-C	5.43	116.89	111.07
16	2	219	THR	CA-C-N	-5.43	113.05	120.44
16	2	219	THR	C-N-CA	-5.43	113.05	120.44
1	A	717	ALA	N-CA-C	5.43	121.80	109.81
18	4	157	TRP	N-CA-C	-5.42	105.37	111.28
6	F	144	GLY	N-CA-C	-5.41	108.16	115.36
2	B	148	ILE	N-CA-C	-5.40	105.11	110.62
17	3	153	ASP	N-CA-CB	-5.40	102.24	110.07
2	B	732	LYS	CA-C-N	-5.40	111.23	121.54
2	B	732	LYS	C-N-CA	-5.40	111.23	121.54
17	3	193	GLY	N-CA-C	-5.40	106.24	112.83
18	4	241	HIS	CA-C-N	5.39	127.95	120.29
18	4	241	HIS	C-N-CA	5.39	127.95	120.29
11	K	98	PRO	CA-N-CD	-5.39	104.45	112.00
1	A	571	ASP	CA-C-N	5.39	127.94	120.29
1	A	571	ASP	C-N-CA	5.39	127.94	120.29
12	L	210	PRO	N-CA-C	-5.39	101.37	112.47
8	H	96	LEU	N-CA-C	5.39	118.33	109.76
11	K	129	ALA	N-CA-C	5.38	118.32	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	VAL	N-CA-C	-5.38	98.15	109.34
2	B	419	ILE	CB-CA-C	-5.38	106.10	111.80
17	3	96	ARG	CA-C-N	-5.38	113.45	120.44
17	3	96	ARG	C-N-CA	-5.38	113.45	120.44
16	2	103	VAL	N-CA-C	5.38	116.00	110.36
2	B	79	GLN	N-CA-C	-5.37	104.83	111.33
1	A	552	THR	N-CA-C	-5.36	102.45	110.23
2	B	680	TRP	N-CA-C	-5.36	106.75	113.72
2	B	713	PHE	N-CA-C	-5.36	105.43	111.28
16	2	132	LEU	CA-CB-CG	5.36	135.06	116.30
1	A	538	ASP	CA-C-N	5.36	127.41	120.44
1	A	538	ASP	C-N-CA	5.36	127.41	120.44
6	F	152	GLY	N-CA-C	5.35	124.15	114.46
3	C	48	CYS	N-CA-C	5.35	117.54	109.41
4	D	165	TYR	CB-CA-C	-5.35	101.99	110.81
2	B	553	PHE	CA-C-N	-5.34	110.94	121.41
2	B	553	PHE	C-N-CA	-5.34	110.94	121.41
2	B	304	ILE	CA-C-N	-5.34	111.34	121.54
2	B	304	ILE	C-N-CA	-5.34	111.34	121.54
3	C	69	LEU	N-CA-CB	-5.34	102.24	110.20
6	F	176	TRP	N-CA-C	-5.34	105.57	111.71
15	1	197	ALA	N-CA-C	5.32	117.16	111.36
2	B	422	LEU	N-CA-C	-5.31	105.61	112.68
18	4	165	SER	N-CA-C	5.31	117.05	108.34
18	4	119	GLY	N-CA-C	5.31	120.44	111.04
1	A	583	GLY	CA-C-N	5.31	126.48	119.84
1	A	583	GLY	C-N-CA	5.31	126.48	119.84
2	B	616	LEU	N-CA-C	5.31	116.87	111.14
3	C	43	PRO	CA-C-O	-5.31	115.14	122.15
1	A	214	GLY	N-CA-C	-5.30	100.61	113.18
8	H	77	ASN	N-CA-C	5.30	117.78	108.82
6	F	194	LYS	CA-C-N	5.29	127.90	120.28
6	F	194	LYS	C-N-CA	5.29	127.90	120.28
5	E	108	ASN	N-CA-C	5.29	117.96	111.82
18	4	171	ILE	CA-C-N	5.29	129.63	120.58
18	4	171	ILE	C-N-CA	5.29	129.63	120.58
13	N	119	THR	N-CA-C	-5.29	99.54	110.80
1	A	486	PRO	N-CA-C	5.29	119.62	112.48
4	D	188	PHE	N-CA-C	5.28	118.19	111.69
3	C	73	THR	CB-CA-C	-5.28	98.69	110.19
1	A	166	CYS	N-CA-C	-5.27	105.97	112.72
4	D	85	GLY	N-CA-C	5.27	120.09	112.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	103	GLN	CA-C-O	-5.27	112.98	120.51
15	1	225	TRP	N-CA-C	-5.27	99.58	110.80
18	4	182	VAL	CB-CA-C	-5.27	104.95	112.22
16	2	120	ILE	CA-C-N	-5.26	113.60	120.44
16	2	120	ILE	C-N-CA	-5.26	113.60	120.44
17	3	210	PRO	N-CA-C	-5.26	106.21	113.53
7	G	66	LEU	N-CA-C	5.26	119.97	113.50
2	B	485	ALA	N-CA-C	-5.26	101.59	109.79
18	4	129	ALA	N-CA-C	5.26	118.29	110.14
2	B	392	ILE	N-CA-C	-5.25	107.71	112.96
6	F	103	GLN	N-CA-C	-5.25	99.61	110.80
7	G	97	LEU	N-CA-C	5.25	117.73	108.75
17	3	190	LEU	CA-C-N	-5.25	115.79	122.77
17	3	190	LEU	C-N-CA	-5.25	115.79	122.77
6	F	186	ARG	N-CA-C	5.25	121.97	110.80
7	G	152	ALA	CA-C-N	5.24	128.28	120.31
7	G	152	ALA	C-N-CA	5.24	128.28	120.31
2	B	532	LEU	N-CA-C	-5.24	105.74	111.82
15	1	64	PHE	N-CA-C	5.24	121.95	110.80
1	A	338	PHE	CA-C-N	5.24	129.72	120.87
1	A	338	PHE	C-N-CA	5.24	129.72	120.87
2	B	453	ILE	CB-CA-C	-5.23	103.98	111.31
16	2	224	ASN	N-CA-C	5.23	117.89	111.82
7	G	82	PHE	CB-CA-C	-5.23	102.67	110.88
8	H	94	ARG	N-CA-C	5.23	120.00	111.37
4	D	94	ALA	CA-C-N	-5.23	113.33	120.44
4	D	94	ALA	C-N-CA	-5.23	113.33	120.44
1	A	430	ASP	N-CA-C	5.22	117.33	109.23
1	A	34	TRP	N-CA-C	-5.22	99.90	108.41
13	N	119	THR	CB-CA-C	-5.22	100.04	110.42
2	B	326	ILE	N-CA-C	5.21	117.61	111.09
5	E	70	ARG	CB-CA-C	-5.21	102.88	110.95
2	B	682	HIS	N-CA-C	-5.20	104.87	111.11
15	1	62	PHE	N-CA-C	5.20	118.14	107.69
17	3	106	GLY	CA-C-N	5.19	127.50	120.44
17	3	106	GLY	C-N-CA	5.19	127.50	120.44
2	B	82	PHE	N-CA-C	-5.19	101.23	109.59
2	B	111	GLY	N-CA-C	-5.19	101.76	112.34
5	E	76	ILE	CB-CA-C	-5.19	102.89	110.62
1	A	502	THR	CB-CA-C	5.18	121.13	110.40
2	B	607	SER	CA-C-N	5.18	127.23	120.28
2	B	607	SER	C-N-CA	5.18	127.23	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	225	GLY	CA-C-N	5.18	127.49	120.44
18	4	225	GLY	C-N-CA	5.18	127.49	120.44
11	K	72	LEU	N-CA-C	5.18	119.65	113.23
11	K	103	LEU	N-CA-C	-5.18	105.76	111.71
1	A	616	PHE	N-CA-C	5.17	117.32	111.11
8	H	112	LEU	N-CA-C	-5.17	106.82	113.23
17	3	214	GLY	N-CA-C	-5.17	106.50	112.50
12	L	206	VAL	N-CA-C	5.17	115.94	110.72
16	2	106	GLU	N-CA-C	-5.16	105.65	111.28
1	A	147	SER	CA-C-N	-5.16	111.29	121.41
1	A	147	SER	C-N-CA	-5.16	111.29	121.41
4	D	179	ALA	N-CA-C	5.16	116.83	109.14
18	4	87	ASN	N-CA-C	5.16	117.30	111.11
2	B	412	LEU	N-CA-C	-5.16	105.57	111.14
2	B	269	TRP	N-CA-C	-5.16	102.97	110.24
16	2	154	ILE	CB-CA-C	-5.16	105.27	112.02
17	3	85	ASP	N-CA-C	-5.16	103.09	109.64
18	4	147	ILE	CB-CA-C	-5.16	105.11	112.22
2	B	691	ILE	N-CA-C	-5.15	100.47	107.99
13	N	100	GLU	N-CA-C	5.14	118.70	112.23
16	2	250	LEU	N-CA-C	-5.14	99.40	108.08
18	4	188	ILE	CB-CA-C	-5.13	102.87	111.29
1	A	499	ALA	N-CA-C	5.13	120.45	113.16
7	G	99	HIS	CA-C-N	-5.13	111.74	121.54
7	G	99	HIS	C-N-CA	-5.13	111.74	121.54
13	N	139	LYS	N-CA-C	5.13	117.77	111.82
2	B	137	THR	CB-CA-C	5.13	118.42	109.65
13	N	134	CYS	CA-C-N	-5.13	113.66	121.66
13	N	134	CYS	C-N-CA	-5.13	113.66	121.66
2	B	208	ARG	N-CA-C	5.13	121.73	110.80
2	B	529	THR	N-CA-C	-5.13	105.60	111.14
4	D	83	PHE	CB-CA-C	-5.13	102.17	110.79
15	1	163	TYR	CB-CA-C	5.12	120.26	110.17
6	F	143	ASP	N-CA-C	-5.12	103.05	113.29
5	E	97	PRO	CA-C-N	5.12	127.09	120.44
5	E	97	PRO	C-N-CA	5.12	127.09	120.44
1	A	353	SER	N-CA-CB	-5.12	102.56	110.13
2	B	98	GLN	O-C-N	5.12	124.42	120.38
16	2	157	LEU	N-CA-C	5.12	116.94	111.36
7	G	145	THR	N-CA-C	5.11	117.64	111.40
16	2	225	GLY	O-C-N	5.11	128.45	122.68
12	L	172	GLU	CA-C-N	-5.11	114.68	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	172	GLU	C-N-CA	-5.11	114.68	119.89
7	G	132	SER	N-CA-C	5.11	117.83	111.24
8	H	95	GLY	N-CA-C	-5.10	101.09	113.18
16	2	250	LEU	CB-CA-C	-5.10	110.71	116.63
1	A	153	TRP	N-CA-C	5.09	117.73	111.82
2	B	20	ARG	CB-CA-C	-5.09	102.66	110.81
8	H	61	THR	CA-C-O	5.09	127.79	120.51
11	K	75	SER	N-CA-C	5.08	117.09	110.53
7	G	82	PHE	CA-C-N	-5.08	115.66	123.07
7	G	82	PHE	C-N-CA	-5.08	115.66	123.07
1	A	115	HIS	N-CA-CB	-5.07	102.49	110.30
2	B	17	THR	N-CA-C	-5.07	103.45	110.35
1	A	48	PRO	CA-C-N	5.07	127.91	120.71
1	A	48	PRO	C-N-CA	5.07	127.91	120.71
2	B	130	ARG	CA-C-N	-5.07	115.72	122.72
2	B	130	ARG	C-N-CA	-5.07	115.72	122.72
18	4	133	GLU	N-CA-C	5.07	117.51	109.50
1	A	199	VAL	CB-CA-C	-5.06	104.06	112.26
6	F	97	GLN	CA-C-O	-5.06	113.27	120.51
12	L	62	GLY	N-CA-C	5.06	125.17	113.18
1	A	352	THR	N-CA-C	5.06	116.47	109.54
2	B	87	ILE	N-CA-C	5.05	115.59	108.36
2	B	380	GLY	N-CA-C	-5.05	101.20	113.18
1	A	35	ALA	N-CA-C	5.05	121.56	110.80
1	A	565	SER	N-CA-C	5.05	117.64	109.06
7	G	120	VAL	N-CA-C	5.05	116.40	111.91
1	A	602	LEU	N-CA-C	-5.05	105.47	110.97
1	A	225	VAL	N-CA-C	5.04	119.83	109.34
13	N	142	LYS	N-CA-C	5.04	121.54	110.80
16	2	246	PRO	N-CD-CG	-5.04	95.64	103.20
2	B	299	HIS	N-CA-C	5.04	117.61	109.40
6	F	83	THR	CB-CA-C	-5.04	100.24	110.17
3	C	29	ILE	CA-C-N	5.04	125.48	120.14
3	C	29	ILE	C-N-CA	5.04	125.48	120.14
4	D	110	GLN	N-CA-C	5.04	117.32	109.52
2	B	399	ASN	N-CA-C	5.03	118.87	108.71
16	2	265	ALA	N-CA-C	5.03	121.52	110.80
1	A	493	GLN	N-CA-C	-5.03	105.08	111.11
1	A	129	GLN	N-CA-C	-5.03	103.52	110.35
1	A	122	VAL	N-CA-C	5.02	115.94	108.46
18	4	146	PHE	N-CA-C	5.02	118.67	112.54
16	2	167	ARG	N-CA-C	5.02	121.49	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	88	LEU	N-CA-C	5.02	121.50	110.80
5	E	83	TRP	CA-CB-CG	5.02	123.14	113.60
18	4	159	ASP	N-CA-C	-5.02	105.81	111.28
18	4	170	PRO	CA-C-N	-5.02	114.24	120.56
18	4	170	PRO	C-N-CA	-5.02	114.24	120.56
15	1	179	LYS	N-CA-C	5.01	116.58	108.41
7	G	149	TYR	CA-C-O	-5.01	113.34	120.51
13	N	117	ALA	N-CA-C	5.01	117.63	111.82
18	4	135	PHE	CA-C-N	-5.01	115.12	122.19
18	4	135	PHE	C-N-CA	-5.01	115.12	122.19
1	A	494	ASN	N-CA-C	5.00	117.47	111.71
18	4	189	PHE	N-CA-C	5.00	120.38	113.97
6	F	213	TRP	CA-CB-CG	5.00	123.11	113.60
11	K	53	THR	CB-CA-C	-5.00	102.48	110.79
12	L	89	TYR	CB-CA-C	-5.00	101.71	109.61
1	A	61	ALA	N-CA-C	5.00	116.81	111.36
2	B	363	GLN	N-CA-C	-5.00	105.91	113.51
16	2	99	LEU	CA-C-N	-5.00	119.01	126.86
16	2	99	LEU	C-N-CA	-5.00	119.01	126.86

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	77	PHE	CA
8	H	60	ASN	CA
8	H	68	TYR	CA

All (544) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	1	105	TYR	Peptide
15	1	118	PRO	Peptide
15	1	121	GLN	Peptide
15	1	122	ALA	Peptide
15	1	125	LEU	Peptide
15	1	130	PRO	Peptide
15	1	155	GLU	Peptide
15	1	156	LYS	Peptide
15	1	157	ASP	Peptide
15	1	170	PRO	Peptide
15	1	171	LEU	Peptide
15	1	172	GLY	Peptide

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Mol	Chain	Res	Type	Group
15	1	174	SER	Peptide
15	1	176	ASP	Peptide
15	1	178	LYS	Peptide
15	1	179	LYS	Peptide
15	1	184	LYS	Peptide
15	1	185	VAL	Peptide
15	1	204	GLN	Peptide
15	1	205	GLN	Peptide
15	1	206	SER	Peptide
15	1	208	TYR	Peptide
15	1	216	ASN	Peptide
15	1	217	LEU	Peptide
15	1	224	PRO	Peptide,Mainchain
15	1	225	TRP	Peptide
15	1	59	PRO	Peptide
15	1	60	GLY	Peptide
15	1	61	ASP	Peptide
15	1	62	PHE	Peptide
15	1	63	GLY	Peptide,Mainchain
15	1	65	ASP	Peptide
15	1	68	GLY	Mainchain
15	1	69	LEU	Mainchain
15	1	97	ILE	Peptide
16	2	100	ARG	Peptide
16	2	101	TRP	Peptide
16	2	102	ASN	Peptide
16	2	130	GLY	Peptide
16	2	133	ASN	Peptide
16	2	138	TYR	Peptide
16	2	139	THR	Peptide
16	2	140	ALA	Peptide
16	2	142	GLU	Peptide
16	2	166	ARG	Peptide
16	2	170	ASP	Peptide
16	2	172	LEU	Peptide
16	2	174	PRO	Peptide
16	2	177	VAL	Peptide
16	2	178	ASN	Peptide
16	2	181	PRO	Peptide
16	2	184	PRO	Peptide
16	2	189	THR	Peptide
16	2	193	VAL	Peptide

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Mol	Chain	Res	Type	Group
16	2	199	LEU	Peptide
16	2	210	SER	Peptide
16	2	212	GLN	Peptide
16	2	213	LYS	Peptide
16	2	215	LYS	Peptide
16	2	216	GLU	Peptide
16	2	218	ARG	Peptide
16	2	243	GLY	Peptide
16	2	244	THR	Peptide
16	2	245	GLY	Peptide
16	2	246	PRO	Peptide
16	2	247	ILE	Peptide
16	2	248	ASP	Peptide
16	2	250	LEU	Peptide
16	2	252	ALA	Peptide
16	2	255	ALA	Peptide
16	2	256	ASP	Peptide
16	2	257	PRO	Peptide
16	2	261	THR	Peptide
16	2	262	ILE	Peptide
16	2	263	PHE	Peptide
16	2	264	ALA	Peptide
16	2	266	PHE	Peptide
16	2	267	THR	Peptide
16	2	98	SER	Peptide
16	2	99	LEU	Peptide
17	3	110	MET	Peptide
17	3	122	LEU	Peptide
17	3	125	VAL	Peptide
17	3	127	LEU	Peptide
17	3	128	ILE	Peptide
17	3	129	PRO	Peptide
17	3	130	GLN	Peptide
17	3	131	GLU	Peptide
17	3	136	TRP	Peptide
17	3	139	THR	Peptide
17	3	140	GLY	Peptide
17	3	148	TYR	Peptide
17	3	149	ASN	Peptide
17	3	153	ASP	Peptide
17	3	158	PHE	Peptide
17	3	177	ALA	Peptide

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Mol	Chain	Res	Type	Group
17	3	178	LYS	Peptide
17	3	179	PRO	Peptide
17	3	181	SER	Peptide
17	3	188	LEU	Peptide
17	3	189	GLY	Peptide
17	3	193	GLY	Peptide
17	3	196	GLY	Peptide
17	3	197	SER	Peptide
17	3	198	GLY	Peptide
17	3	199	ASN	Peptide
17	3	200	PRO	Peptide
17	3	205	GLY	Peptide
17	3	212	GLY	Peptide
17	3	213	PHE	Peptide
17	3	215	LYS	Peptide
17	3	85	ASP	Peptide
17	3	93	ILE	Peptide
17	3	96	ARG	Peptide
17	3	98	LEU	Peptide
18	4	110	LEU	Peptide
18	4	112	PRO	Peptide
18	4	119	GLY	Peptide
18	4	123	VAL	Peptide
18	4	127	TYR	Peptide
18	4	128	ALA	Peptide
18	4	130	GLY	Peptide
18	4	131	LYS	Peptide
18	4	135	PHE	Peptide
18	4	136	ALA	Peptide
18	4	170	PRO	Peptide
18	4	171	ILE	Peptide
18	4	172	PHE	Peptide
18	4	175	TYR	Peptide,Mainchain
18	4	178	PRO	Peptide
18	4	189	PHE	Peptide
18	4	197	THR	Peptide
18	4	198	LEU	Peptide
18	4	213	ALA	Peptide
18	4	223	VAL	Peptide
18	4	226	LYS	Peptide
18	4	229	PHE	Peptide
18	4	232	LEU	Peptide

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Mol	Chain	Res	Type	Group
18	4	233	LEU	Peptide
18	4	243	THR	Peptide
18	4	86	GLU	Peptide
18	4	89	ARG	Peptide
1	A	103	PHE	Peptide
1	A	114	THR	Peptide
1	A	117	GLY	Peptide
1	A	119	SER	Peptide
1	A	123	VAL	Peptide
1	A	128	GLY	Peptide
1	A	132	LEU	Peptide
1	A	134	GLY	Peptide
1	A	136	VAL	Peptide
1	A	142	GLY	Peptide
1	A	146	THR	Peptide
1	A	148	GLY	Peptide
1	A	189	ALA	Peptide
1	A	197	GLN	Peptide
1	A	199	VAL	Peptide
1	A	201	SER	Peptide
1	A	21	LEU	Peptide
1	A	22	VAL	Peptide
1	A	23	ASP	Peptide
1	A	240	LYS	Peptide
1	A	246	HIS	Peptide
1	A	25	ASP	Peptide
1	A	250	LEU	Peptide
1	A	251	ASN	Peptide
1	A	257	GLN	Peptide
1	A	26	PRO	Peptide
1	A	262	PHE	Peptide
1	A	263	ALA	Peptide
1	A	27	ILE	Peptide
1	A	270	PHE	Peptide
1	A	274	TRP	Peptide
1	A	275	SER	Peptide
1	A	276	LYS	Peptide
1	A	279	ASP	Peptide
1	A	28	LYS	Peptide
1	A	280	PHE	Peptide
1	A	282	THR	Peptide
1	A	290	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	316	MET	Peptide
1	A	345	GLY	Peptide
1	A	346	LEU	Peptide
1	A	349	ILE	Peptide
1	A	352	THR	Peptide
1	A	36	LYS	Peptide
1	A	37	PRO	Peptide
1	A	38	GLY	Peptide
1	A	39	HIS	Peptide
1	A	393	LEU	Peptide
1	A	420	ARG	Peptide
1	A	427	ARG	Peptide
1	A	430	ASP	Peptide
1	A	45	ALA	Peptide
1	A	46	LYS	Peptide
1	A	47	GLY	Peptide
1	A	482	ILE	Peptide
1	A	483	GLN	Peptide
1	A	486	PRO	Peptide
1	A	488	PHE	Peptide
1	A	497	ALA	Peptide
1	A	501	GLY	Peptide
1	A	505	PRO	Peptide
1	A	506	GLY	Peptide
1	A	510	SER	Peptide
1	A	518	GLY	Peptide
1	A	519	ASP	Peptide
1	A	520	LEU	Peptide
1	A	525	ASN	Peptide
1	A	527	VAL	Peptide
1	A	535	GLY	Peptide
1	A	574	ASN	Peptide
1	A	575	LEU	Peptide
1	A	576	GLY	Peptide
1	A	62	HIS	Peptide
1	A	625	TRP	Peptide
1	A	626	GLY	Peptide
1	A	631	GLN	Peptide
1	A	64	PHE	Peptide
1	A	66	SER	Peptide
1	A	67	HIS	Peptide
1	A	73	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	93	LEU	Peptide
2	B	103	ALA	Peptide
2	B	126	THR	Peptide
2	B	130	ARG	Peptide
2	B	135	LEU	Peptide
2	B	139	ALA	Peptide
2	B	162	LYS	Peptide
2	B	166	SER	Peptide
2	B	170	ASN	Peptide
2	B	203	ARG	Peptide
2	B	204	GLY	Peptide
2	B	211	ASN	Peptide
2	B	223	GLY	Peptide
2	B	224	PRO	Peptide
2	B	228	GLY	Peptide
2	B	229	GLN	Peptide
2	B	231	ASN	Peptide
2	B	232	LEU	Peptide
2	B	238	SER	Peptide
2	B	246	THR	Peptide
2	B	248	GLN	Peptide
2	B	256	THR	Peptide
2	B	257	ILE	Peptide
2	B	259	GLY	Peptide
2	B	26	ALA	Peptide
2	B	260	GLY	Peptide
2	B	265	THR	Peptide
2	B	267	SER	Peptide
2	B	292	ARG	Peptide
2	B	298	GLY	Peptide
2	B	303	TYR	Peptide
2	B	308	HIS	Peptide
2	B	311	PRO	Peptide
2	B	320	LYS	Peptide
2	B	33	SER	Peptide
2	B	36	ASP	Peptide
2	B	363	GLN	Peptide
2	B	364	ASP	Peptide
2	B	365	PHE	Peptide
2	B	377	TYR	Peptide
2	B	4	ARG	Peptide
2	B	405	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	B	406	ASN	Peptide
2	B	445	ALA	Peptide
2	B	447	GLY	Peptide
2	B	458	ILE	Peptide
2	B	464	GLN	Peptide
2	B	468	GLY	Peptide
2	B	469	LYS	Peptide
2	B	472	TYR	Peptide
2	B	473	GLY	Peptide
2	B	474	PHE	Peptide
2	B	478	LEU	Peptide
2	B	481	THR	Peptide
2	B	483	GLY	Peptide
2	B	484	PRO	Peptide
2	B	5	ILE	Peptide
2	B	504	ASN	Peptide
2	B	507	SER	Peptide
2	B	510	LEU	Peptide
2	B	540	ASP	Peptide
2	B	549	ASP	Peptide
2	B	563	GLY	Peptide
2	B	595	HIS	Peptide
2	B	602	TRP	Peptide
2	B	603	ARG	Peptide
2	B	604	GLY	Peptide
2	B	605	ASN	Peptide
2	B	606	VAL	Peptide
2	B	618	GLY	Peptide
2	B	627	ASN	Peptide
2	B	632	ILE	Peptide
2	B	633	ASN	Peptide
2	B	635	ILE	Peptide
2	B	641	ASN	Peptide
2	B	69	ALA	Peptide
2	B	690	LEU	Peptide
2	B	7	ARG	Peptide
2	B	73	ASN	Peptide
2	B	730	SER	Peptide
2	B	732	LYS	Peptide
2	B	80	ASP	Peptide
2	B	84	VAL	Peptide
2	B	9	SER	Peptide

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Mol	Chain	Res	Type	Group
3	C	1	MET	Peptide
3	C	27	GLU	Peptide
3	C	28	MET	Peptide
3	C	29	ILE	Peptide
3	C	33	GLY	Peptide
3	C	42	ALA	Peptide
3	C	54	CYS	Peptide
3	C	65	VAL	Peptide
3	C	67	VAL	Peptide
3	C	68	TYR	Peptide
3	C	69	LEU	Peptide
3	C	70	TRP	Peptide
3	C	73	THR	Peptide
3	C	79	LEU	Peptide
4	D	108	LYS	Peptide
4	D	114	MET	Peptide
4	D	117	GLY	Peptide
4	D	118	GLY	Peptide
4	D	119	ALA	Peptide
4	D	124	GLU	Peptide
4	D	125	GLY	Peptide
4	D	145	ARG	Peptide
4	D	147	LYS	Peptide
4	D	150	ILE	Peptide
4	D	151	LYS	Peptide
4	D	158	PHE	Peptide
4	D	161	GLY	Peptide
4	D	162	GLU	Peptide
4	D	163	VAL	Peptide
4	D	168	PRO	Peptide
4	D	171	GLY	Peptide
4	D	174	PRO	Peptide
4	D	177	VAL	Peptide
4	D	181	ARG	Peptide
4	D	182	GLN	Peptide
4	D	184	VAL	Peptide
4	D	190	SER	Peptide
4	D	193	LYS	Peptide
4	D	194	ASN	Peptide
4	D	204	GLY	Peptide
4	D	209	ASP	Peptide
4	D	73	GLU	Peptide

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Mol	Chain	Res	Type	Group
4	D	78	THR	Peptide
4	D	79	PRO	Peptide
4	D	81	PRO	Peptide
4	D	83	PHE	Peptide
4	D	87	THR	Peptide
4	D	89	GLY	Peptide
4	D	91	LEU	Peptide
4	D	93	LYS	Peptide
4	D	97	GLU	Peptide
5	E	116	SER	Peptide
5	E	124	GLU	Peptide
5	E	125	ILE	Peptide
5	E	126	VAL	Mainchain
5	E	127	GLU	Peptide
5	E	67	GLY	Peptide
5	E	79	LYS	Peptide
5	E	88	GLY	Peptide
5	E	96	ASP	Peptide
5	E	97	PRO	Peptide
6	F	103	GLN	Mainchain
6	F	104	ALA	Peptide
6	F	105	SER	Peptide
6	F	107	LYS	Peptide
6	F	108	LEU	Peptide
6	F	111	ASP	Peptide
6	F	112	ASP	Peptide
6	F	115	PRO	Peptide
6	F	116	ALA	Peptide
6	F	118	ALA	Peptide
6	F	129	ARG	Peptide
6	F	133	TYR	Peptide
6	F	135	LYS	Peptide
6	F	137	GLY	Peptide
6	F	138	LEU	Peptide
6	F	151	SER	Peptide
6	F	185	ILE	Peptide
6	F	189	LYS	Peptide
6	F	196	ILE	Peptide
6	F	199	ASP	Peptide
6	F	203	ALA	Peptide
6	F	212	SER	Peptide
6	F	213	TRP	Peptide

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Mol	Chain	Res	Type	Group
6	F	218	TYR	Peptide
6	F	230	ASN	Peptide
6	F	79	ILE	Peptide
6	F	97	GLN	Mainchain
7	G	100	PHE	Peptide
7	G	103	GLY	Peptide
7	G	104	ASP	Peptide
7	G	106	ARG	Peptide
7	G	111	VAL	Peptide
7	G	114	LEU	Peptide
7	G	115	LYS	Peptide
7	G	134	GLY	Peptide
7	G	141	ILE	Peptide
7	G	146	SER	Peptide
7	G	147	ASN	Peptide
7	G	148	GLY	Peptide
7	G	149	TYR	Peptide
7	G	153	PHE	Peptide
7	G	71	SER	Peptide
7	G	78	VAL	Peptide
7	G	82	PHE	Peptide
7	G	84	ARG	Peptide
7	G	86	ASN	Peptide
7	G	90	GLN	Peptide
7	G	91	VAL	Peptide
7	G	95	ASN	Peptide
7	G	98	THR	Peptide
7	G	99	HIS	Peptide
8	H	114	ALA	Peptide
8	H	116	ALA	Peptide
8	H	118	GLY	Peptide
8	H	119	ASP	Peptide
8	H	120	ILE	Peptide
8	H	56	GLU	Peptide
8	H	58	LEU	Peptide
8	H	60	ASN	Peptide
8	H	61	THR	Peptide
8	H	62	THR	Peptide
8	H	63	GLY	Peptide
8	H	65	TRP	Peptide
8	H	67	SER	Peptide
8	H	68	TYR	Peptide

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Mol	Chain	Res	Type	Group
8	H	69	GLY	Peptide
8	H	79	LEU	Peptide
8	H	81	SER	Peptide
8	H	84	PHE	Peptide
8	H	86	THR	Peptide
8	H	93	LYS	Peptide
8	H	95	GLY	Peptide
8	H	97	LEU	Peptide
11	K	113	GLY	Peptide
11	K	118	VAL	Peptide
11	K	119	GLY	Peptide
11	K	120	VAL	Peptide
11	K	122	LEU	Peptide
11	K	123	GLY	Peptide
11	K	125	LYS	Peptide
11	K	126	ASN	Peptide
11	K	128	GLY	Peptide
11	K	129	ALA	Peptide
11	K	73	ALA	Peptide
11	K	76	ALA	Peptide
11	K	80	ALA	Peptide
11	K	86	LEU	Peptide
11	K	88	VAL	Peptide
11	K	89	ARG	Peptide
11	K	91	SER	Peptide
11	K	93	LEU	Peptide
11	K	94	GLN	Peptide
11	K	96	GLY	Peptide
11	K	97	ASP	Peptide
12	L	128	GLN	Peptide
12	L	129	ALA	Peptide
12	L	143	LEU	Peptide
12	L	152	SER	Peptide
12	L	154	ASN	Peptide
12	L	156	GLY	Peptide
12	L	157	ALA	Peptide
12	L	160	THR	Peptide
12	L	165	THR	Peptide
12	L	166	LEU	Peptide
12	L	168	GLY	Peptide
12	L	169	ARG	Peptide
12	L	174	ASP	Peptide

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Mol	Chain	Res	Type	Group
12	L	176	LEU	Peptide
12	L	206	VAL	Peptide
12	L	52	PRO	Peptide
12	L	61	ASN	Peptide
12	L	67	GLY	Peptide
12	L	68	SER	Peptide
12	L	73	VAL	Peptide
12	L	79	ILE	Peptide
12	L	88	ALA	Peptide
12	L	95	PRO	Peptide
13	N	100	GLU	Peptide
13	N	102	ASN	Peptide
13	N	108	ALA	Peptide
13	N	111	GLY	Peptide
13	N	112	ALA	Peptide
13	N	113	ASN	Peptide
13	N	118	TYR	Peptide
13	N	119	THR	Peptide
13	N	120	VAL	Peptide
13	N	123	GLY	Peptide
13	N	125	CYS	Peptide
13	N	126	LYS	Peptide
13	N	127	PHE	Peptide
13	N	129	GLU	Peptide
13	N	131	PHE	Peptide
13	N	133	GLY	Peptide
13	N	135	GLN	Peptide
13	N	136	ASP	Peptide
13	N	137	LEU	Peptide
13	N	142	LYS	Peptide
13	N	145	PHE	Peptide
13	N	147	SER	Peptide
13	N	148	ASP	Peptide
13	N	150	LEU	Peptide
13	N	151	ASP	Peptide
13	N	152	LEU	Peptide
13	N	155	GLU	Peptide
13	N	156	GLY	Peptide
13	N	157	LYS	Peptide
13	N	158	ASP	Peptide
13	N	160	TYR	Peptide
13	N	162	CYS	Peptide

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Mol	Chain	Res	Type	Group
13	N	164	SER	Peptide
13	N	166	VAL	Peptide
13	N	168	TRP	Peptide
13	N	169	LYS	Peptide
13	N	90	GLU	Peptide
13	N	92	LEU	Peptide
13	N	96	LYS	Peptide
13	N	97	THR	Peptide
14	R	28	UNK	Peptide
14	R	30	UNK	Peptide
14	R	31	UNK	Peptide
14	R	32	UNK	Peptide
14	R	33	UNK	Peptide
14	R	34	UNK	Peptide
14	R	36	UNK	Peptide
14	R	37	UNK	Peptide
14	R	40	UNK	Peptide
14	R	42	UNK	Peptide
14	R	46	UNK	Peptide
14	R	47	UNK	Peptide
14	R	48	UNK	Peptide
14	R	50	UNK	Peptide
14	R	51	UNK	Peptide
14	R	52	UNK	Peptide
14	R	7	UNK	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5574	1954	6
2	B	5844	0	5648	1960	12
3	C	619	0	605	334	0
4	D	1097	0	1101	440	4
5	E	513	0	514	254	0
6	F	1221	0	1247	385	28
7	G	738	0	709	342	6
8	H	517	0	503	210	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	229	0	252	55	1
10	J	334	0	344	85	0
11	K	592	0	618	269	5
12	L	1209	0	1220	448	64
13	N	685	0	667	354	0
14	R	265	0	67	79	0
15	1	1257	0	1220	611	36
16	2	1367	0	1312	655	34
17	3	1197	0	1137	532	2
18	4	1309	0	1264	540	45
19	1	665	0	453	118	1
19	2	663	0	494	135	0
19	3	736	0	453	157	0
19	4	729	0	496	151	0
19	A	2676	0	2544	1012	0
19	B	2177	0	2072	648	0
19	F	130	0	85	20	0
19	G	51	0	40	10	0
19	H	240	0	237	62	0
19	I	60	0	58	6	0
19	J	116	0	107	51	0
19	K	210	0	179	39	6
19	L	322	0	275	110	0
19	R	122	0	123	13	0
20	A	33	0	45	6	0
20	B	33	0	46	22	0
21	1	40	0	54	6	0
21	3	40	0	54	6	0
21	A	200	0	271	161	0
21	B	240	0	323	112	0
21	F	80	0	107	61	0
21	I	80	0	111	46	0
21	J	40	0	52	32	0
21	L	40	0	53	34	0
22	1	70	0	92	10	0
22	2	140	0	184	14	0
22	3	70	0	90	38	0
22	4	278	0	357	69	0
22	A	210	0	275	27	0
22	B	95	0	115	11	0
22	C	35	0	46	0	0
22	D	35	0	45	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	E	70	0	92	24	0
22	F	34	0	41	12	0
22	G	105	0	138	14	0
22	H	245	0	322	40	0
22	K	140	0	184	37	2
22	L	35	0	46	12	0
22	N	35	0	46	9	0
22	R	245	0	322	34	0
23	A	8	0	0	2	0
23	C	16	0	0	9	0
24	B	49	0	71	19	0
All	All	36370	0	35200	10903	127

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 152.

All (10903) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:7034:LMU:C9	22:4:7052:LMU:H1'	1.24	1.64
2:B:459:PHE:CE2	19:B:1235:CLA:C2D	1.76	1.63
19:A:1125:CLA:HBB2	19:A:1133:CLA:CMA	1.18	1.60
1:A:244:LEU:CB	1:A:247:GLU:HG3	1.25	1.60
16:2:130:GLY:CA	16:2:131:ILE:HG13	1.29	1.60
2:B:459:PHE:CD2	19:B:1235:CLA:C3D	1.79	1.59
1:A:21:LEU:CA	1:A:22:VAL:HG12	1.16	1.59
15:1:177:PRO:HD2	15:1:180:LEU:CG	1.13	1.58
1:A:281:LEU:HD13	19:A:1115:CLA:CED	1.24	1.57
1:A:281:LEU:CD2	19:A:1115:CLA:HMA3	1.33	1.57
19:2:2007:CLA:CBC	19:3:2009:CLA:HED2	1.11	1.57
5:E:89:SER:HB2	5:E:106:ARG:CZ	1.28	1.56
16:2:130:GLY:HA2	16:2:131:ILE:CG1	1.29	1.56
22:4:7034:LMU:C8	22:4:7052:LMU:H2'	1.09	1.56
18:4:158:GLN:HB3	19:4:1004:CLA:CMA	1.12	1.56
2:B:459:PHE:HD2	19:B:1235:CLA:C3D	0.91	1.56
22:4:7034:LMU:H81	22:4:7052:LMU:C2'	1.23	1.56
8:H:61:THR:CA	8:H:62:THR:HG23	1.36	1.55
13:N:130:ASN:CB	13:N:139:LYS:HG2	1.36	1.55
15:1:177:PRO:CD	15:1:180:LEU:HG	1.08	1.55
15:1:93:ALA:HB1	19:1:1006:CLA:CHC	1.34	1.54
18:4:120:ILE:CD1	18:4:226:LYS:HG3	1.12	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ARG:NH2	4:D:181:ARG:CD	1.68	1.54
18:4:120:ILE:HD11	18:4:226:LYS:CG	1.24	1.54
18:4:103:MET:HE3	18:4:208:GLY:CA	1.08	1.53
13:N:103:ASP:HB2	13:N:107:LEU:CD1	1.35	1.52
18:4:103:MET:CE	18:4:208:GLY:N	1.71	1.52
3:C:62:PHE:CZ	5:E:80:GLU:CD	1.88	1.51
17:3:103:VAL:HG13	17:3:107:ARG:CD	1.36	1.51
2:B:459:PHE:CD2	19:B:1235:CLA:C2D	1.82	1.51
8:H:58:LEU:CD1	8:H:62:THR:HG21	1.38	1.51
14:R:32:UNK:CB	14:R:33:UNK:CB	1.85	1.51
15:1:97:ILE:HD13	15:1:98:LEU:CA	1.10	1.51
17:3:113:ALA:CB	17:3:239:LEU:HD11	1.34	1.51
2:B:314:ARG:NH1	15:1:67:LEU:HD21	1.22	1.50
18:4:103:MET:CE	18:4:208:GLY:CA	1.88	1.50
18:4:172:PHE:CB	18:4:194:PHE:HE2	0.89	1.50
8:H:61:THR:HA	8:H:62:THR:CG2	1.37	1.50
1:A:244:LEU:HB2	1:A:247:GLU:CG	1.40	1.49
18:4:172:PHE:HB2	18:4:194:PHE:CE2	1.00	1.49
6:F:190:LYS:NZ	6:F:192:THR:HG21	1.18	1.49
1:A:250:LEU:HB2	17:3:136:TRP:CH2	1.47	1.49
15:1:97:ILE:CD1	15:1:98:LEU:N	1.69	1.49
2:B:89:HIS:C	2:B:113:VAL:HG11	1.10	1.49
15:1:97:ILE:CD1	15:1:98:LEU:CA	1.85	1.49
19:A:1125:CLA:CBB	19:A:1133:CLA:CMA	1.89	1.48
19:1:1013:CLA:C6	19:1:1014:CLA:HED3	1.41	1.48
1:A:281:LEU:CD1	19:A:1115:CLA:HED1	1.41	1.47
18:4:103:MET:HE2	18:4:207:ASN:C	1.35	1.47
19:L:1148:CLA:HED1	19:L:1148:CLA:C2	1.38	1.47
13:N:103:ASP:CB	13:N:107:LEU:HD12	1.43	1.47
1:A:443:ILE:HD11	1:A:557:LEU:CD2	1.41	1.46
13:N:155:GLU:HB3	13:N:157:LYS:N	1.21	1.46
17:3:135:ALA:HB1	17:3:139:THR:CB	1.44	1.46
17:3:127:LEU:CB	19:3:1147:CLA:HED3	1.45	1.45
4:D:156:ARG:NH1	4:D:158:PHE:HE1	0.97	1.45
1:A:249:ILE:CG2	17:3:136:TRP:HZ3	1.25	1.45
22:4:7034:LMU:H92	22:4:7052:LMU:C1'	1.42	1.45
2:B:123:TRP:HA	2:B:126:THR:CG2	1.44	1.44
2:B:596:TRP:CH2	2:B:612:SER:O	1.68	1.44
2:B:294:ASN:ND2	7:G:94:GLN:HG3	1.25	1.44
8:H:58:LEU:CD1	8:H:62:THR:CG2	1.91	1.44
17:3:122:LEU:CD2	19:3:3006:CLA:CHA	1.94	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:87:ASN:HB2	18:4:90:TRP:CE3	1.51	1.44
19:4:4006:CLA:C10	22:4:7034:LMU:H121	1.47	1.44
1:A:308:ILE:CD1	19:A:1115:CLA:HHC	1.47	1.43
15:1:176:ASP:HB3	15:1:180:LEU:CD1	1.46	1.43
16:2:160:ILE:CG2	19:2:2012:CLA:CBB	1.95	1.43
2:B:633:ASN:CB	2:B:636:THR:HB	1.48	1.43
21:B:6020:BCR:C33	19:L:1502:CLA:C4B	1.95	1.43
13:N:146:LEU:CD1	17:3:142:ILE:O	1.66	1.43
16:2:133:ASN:ND2	16:2:134:THR:HB	1.28	1.43
17:3:103:VAL:CG1	17:3:107:ARG:HD3	1.47	1.42
18:4:175:TYR:O	18:4:194:PHE:CE1	1.69	1.42
22:3:7003:LMU:H3B	22:3:7005:LMU:C5B	1.46	1.42
3:C:14:CYS:HA	3:C:17:CYS:SG	1.58	1.41
4:D:167:HIS:NE2	4:D:172:VAL:HG11	1.12	1.41
6:F:190:LYS:NZ	6:F:192:THR:CG2	1.82	1.41
16:2:133:ASN:HD22	16:2:134:THR:CB	1.33	1.41
13:N:155:GLU:C	13:N:157:LYS:CE	1.90	1.41
19:2:2007:CLA:CBC	19:3:2009:CLA:CED	1.95	1.40
4:D:167:HIS:NE2	4:D:172:VAL:CG1	1.84	1.40
16:2:168:TRP:HD1	16:2:171:ILE:CG2	1.35	1.40
1:A:154:ARG:NE	1:A:384:TYR:HE1	1.19	1.40
19:A:1115:CLA:CED	19:A:1115:CLA:H2A	1.49	1.39
7:G:98:THR:CB	7:G:101:GLU:CD	1.95	1.39
11:K:92:GLY:O	11:K:93:LEU:HG	1.22	1.39
13:N:139:LYS:CB	13:N:142:LYS:HD3	1.50	1.39
17:3:150:TYR:CG	17:3:151:TRP:CD1	2.10	1.39
1:A:338:PHE:CE1	19:A:1151:CLA:CBB	2.06	1.39
1:A:478:SER:CB	1:A:644:GLN:HE22	1.35	1.39
16:2:122:ILE:HD11	19:2:2002:CLA:CAB	1.51	1.39
16:2:166:ARG:N	16:2:167:ARG:HB2	1.21	1.39
1:A:342:GLY:CA	1:A:430:ASP:HB2	1.48	1.39
2:B:257:ILE:O	2:B:497:TRP:CE3	1.75	1.39
2:B:247:THR:HA	2:B:250:ALA:CB	1.52	1.39
1:A:21:LEU:N	1:A:22:VAL:CG1	1.83	1.38
22:4:7034:LMU:H111	22:4:7052:LMU:C4'	1.38	1.38
16:2:160:ILE:HG22	19:2:2012:CLA:CBB	1.52	1.38
17:3:127:LEU:CB	19:3:1147:CLA:CED	2.01	1.38
1:A:534:LEU:HD12	1:A:535:GLY:N	1.31	1.38
13:N:155:GLU:CB	13:N:157:LYS:H	1.37	1.38
1:A:21:LEU:CA	1:A:22:VAL:CG1	1.98	1.37
15:1:176:ASP:CB	15:1:180:LEU:HD12	1.54	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HA	1:A:22:VAL:CG1	1.54	1.37
1:A:249:ILE:HG23	17:3:136:TRP:CZ3	1.60	1.37
13:N:130:ASN:HB2	13:N:139:LYS:CG	1.51	1.37
16:2:168:TRP:CD1	16:2:171:ILE:HG21	1.59	1.37
18:4:158:GLN:NE2	19:4:1004:CLA:C1A	1.87	1.37
16:2:118:ALA:HA	16:2:121:PHE:CE2	1.60	1.36
1:A:279:ASP:O	1:A:281:LEU:HG	1.24	1.36
2:B:459:PHE:HE2	19:B:1235:CLA:C1D	1.39	1.36
2:B:732:LYS:HG2	2:B:734:GLY:N	1.34	1.36
12:L:205:TYR:CD1	12:L:207:LEU:HD12	1.61	1.36
13:N:132:THR:CG2	13:N:139:LYS:HD3	1.55	1.36
22:3:7003:LMU:H3B	22:3:7005:LMU:C4B	1.52	1.35
19:A:1125:CLA:CBB	19:A:1133:CLA:HMA1	1.44	1.35
2:B:120:VAL:HA	2:B:123:TRP:CD1	1.61	1.35
17:3:150:TYR:N	17:3:152:ALA:HB2	1.40	1.35
19:3:2009:CLA:HBD	19:3:2009:CLA:CGA	1.56	1.35
16:2:165:GLY:C	16:2:167:ARG:HB2	1.50	1.34
19:3:2009:CLA:H92	19:3:2009:CLA:C5	1.45	1.34
3:C:44:ARG:NH2	4:D:181:ARG:HD3	1.04	1.34
13:N:155:GLU:C	13:N:157:LYS:HE2	1.49	1.34
1:A:308:ILE:HD11	19:A:1115:CLA:CAB	1.56	1.34
2:B:732:LYS:HG2	2:B:733:PHE:C	1.52	1.34
4:D:114:MET:CG	4:D:115:PRO:O	1.76	1.34
15:1:67:LEU:HD12	15:1:68:GLY:N	1.41	1.34
18:4:103:MET:CE	18:4:208:GLY:HA2	1.49	1.34
18:4:158:GLN:CB	19:4:1004:CLA:CMA	2.03	1.33
7:G:89:LYS:HA	7:G:89:LYS:CE	1.55	1.33
18:4:158:GLN:CB	19:4:1004:CLA:HMA1	1.56	1.33
20:B:5002:PQN:H162	21:B:6017:BCR:C33	1.54	1.33
13:N:114:PHE:CD1	13:N:117:ALA:HB2	1.62	1.33
16:2:118:ALA:CA	16:2:121:PHE:HE2	1.40	1.33
16:2:134:THR:OG1	16:2:135:PRO:HD2	1.22	1.33
1:A:744:ALA:CB	21:A:6011:BCR:H391	1.59	1.32
3:C:64:SER:O	3:C:65:VAL:HG12	1.16	1.32
18:4:145:GLU:HG3	18:4:146:PHE:CD1	1.62	1.32
19:A:1119:CLA:H92	21:A:6007:BCR:C37	1.57	1.32
2:B:229:GLN:C	7:G:63:VAL:HG21	1.55	1.32
4:D:140:LEU:CD1	4:D:141:GLY:N	1.92	1.32
5:E:89:SER:OG	5:E:106:ARG:CD	1.78	1.32
19:L:1148:CLA:CED	19:L:1148:CLA:H2	1.57	1.32
2:B:304:ILE:CD1	19:B:1216:CLA:HED2	1.59	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:150:TYR:CD2	17:3:151:TRP:CD1	2.18	1.31
17:3:109:ALA:C	17:3:111:LEU:HB3	1.55	1.31
5:E:89:SER:OG	5:E:106:ARG:HD3	1.28	1.31
19:A:1125:CLA:CAB	19:A:1133:CLA:HMA3	1.59	1.31
7:G:98:THR:HG21	7:G:101:GLU:OE2	1.18	1.31
19:L:1148:CLA:HAA1	19:L:1148:CLA:CGD	1.60	1.31
15:1:91:MET:O	15:1:95:PRO:HD3	1.20	1.31
16:2:186:ASN:OD1	16:2:188:LEU:HD11	1.27	1.31
2:B:36:ASP:O	2:B:41:ARG:NH1	1.63	1.31
3:C:62:PHE:CE2	5:E:80:GLU:HG3	1.65	1.31
7:G:98:THR:HB	7:G:101:GLU:CD	1.54	1.31
16:2:117:ALA:CB	16:2:230:LEU:HG	1.58	1.31
1:A:120:ALA:H	1:A:145:ILE:CD1	1.41	1.30
19:A:1115:CLA:HED3	19:A:1115:CLA:C2A	1.61	1.30
2:B:257:ILE:O	2:B:497:TRP:CZ3	1.84	1.30
8:H:78:PRO:HD3	19:L:1501:CLA:CMD	1.61	1.30
17:3:113:ALA:HB2	17:3:239:LEU:CD1	1.62	1.30
11:K:127:ILE:C	11:K:129:ALA:HA	1.56	1.30
17:3:111:LEU:O	17:3:114:VAL:N	1.65	1.30
1:A:338:PHE:CE1	19:A:1151:CLA:HBB1	1.65	1.29
21:B:6020:BCR:H333	19:L:1502:CLA:C4B	1.56	1.29
15:1:88:ARG:O	15:1:92:LEU:HB2	1.28	1.29
1:A:281:LEU:CD2	19:A:1115:CLA:CMA	2.07	1.29
19:K:1143:CLA:CAC	22:K:7001:LMU:O3B	1.79	1.29
17:3:150:TYR:CD2	17:3:151:TRP:NE1	2.01	1.29
16:2:96:PRO:HD2	17:3:85:ASP:OD2	1.30	1.29
1:A:21:LEU:N	1:A:22:VAL:HG12	0.99	1.28
7:G:98:THR:CG2	7:G:101:GLU:OE2	1.77	1.28
8:H:119:ASP:O	8:H:120:ILE:HG22	1.24	1.28
12:L:154:ASN:O	12:L:178:THR:HG23	1.18	1.28
13:N:132:THR:HG21	13:N:139:LYS:CD	1.62	1.28
1:A:246:HIS:HA	1:A:248:PHE:CE2	1.67	1.28
19:3:2009:CLA:H52	19:3:2009:CLA:C9	1.54	1.28
1:A:157:GLY:HA3	1:A:229:ILE:CG2	1.60	1.28
1:A:668:TYR:CD1	2:B:445:ALA:HB2	1.68	1.28
2:B:122:GLN:O	2:B:126:THR:CB	1.80	1.28
16:2:134:THR:OG1	16:2:135:PRO:CD	1.80	1.28
19:2:2007:CLA:HAC2	19:3:2009:CLA:CED	1.62	1.28
4:D:140:LEU:HD12	4:D:141:GLY:N	0.95	1.27
18:4:167:ASN:OD1	19:4:4014:CLA:C2	1.80	1.27
11:K:49:ILE:C	11:K:52:PRO:CG	2.05	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:ILE:O	11:K:52:PRO:CG	1.80	1.27
11:K:49:ILE:O	11:K:52:PRO:HG2	1.14	1.27
22:4:7034:LMU:C11	22:4:7052:LMU:C4'	2.12	1.27
1:A:157:GLY:O	1:A:158:ILE:CG2	1.79	1.27
1:A:162:LEU:O	1:A:165:TYR:HB3	1.34	1.27
1:A:368:LEU:HD21	19:A:1117:CLA:C9	1.63	1.27
4:D:123:ARG:NH2	22:D:7050:LMU:C4B	1.98	1.27
4:D:156:ARG:NH1	4:D:158:PHE:CE1	1.74	1.27
5:E:89:SER:CB	5:E:106:ARG:CZ	2.11	1.27
15:1:95:PRO:O	15:1:98:LEU:HB3	1.30	1.27
19:2:2007:CLA:CAC	19:3:2009:CLA:CED	2.11	1.27
2:B:317:ARG:NH1	2:B:405:ASP:O	1.68	1.27
7:G:72:LEU:HD23	7:G:124:ILE:CD1	1.65	1.27
12:L:129:ALA:O	12:L:201:TYR:HB3	1.35	1.27
15:1:77:GLU:HA	15:1:80:LYS:CG	1.65	1.27
15:1:97:ILE:HD13	15:1:98:LEU:N	0.94	1.27
1:A:744:ALA:HB2	21:A:6011:BCR:C39	1.64	1.26
5:E:107:PHE:CE2	5:E:109:LYS:HG3	1.69	1.26
12:L:209:LEU:CD1	12:L:210:PRO:HD2	1.64	1.26
12:L:60:ILE:CG2	12:L:61:ASN:H	1.43	1.26
1:A:242:ILE:HG13	1:A:243:PRO:CD	1.65	1.26
4:D:123:ARG:NH2	22:D:7050:LMU:O4'	1.67	1.26
15:1:95:PRO:O	15:1:98:LEU:CB	1.83	1.26
16:2:130:GLY:CA	16:2:131:ILE:CG1	1.97	1.26
4:D:167:HIS:CD2	4:D:172:VAL:HG21	1.68	1.26
6:F:200:VAL:CG1	10:J:7:TYR:HB2	1.65	1.26
2:B:232:LEU:CD1	2:B:235:GLN:HG3	1.66	1.26
2:B:317:ARG:NH2	2:B:410:ARG:HG2	1.49	1.26
2:B:459:PHE:CE2	19:B:1235:CLA:CMD	2.18	1.26
4:D:200:VAL:HG21	4:D:206:GLN:NE2	1.48	1.26
13:N:155:GLU:O	13:N:157:LYS:HE3	1.22	1.26
16:2:165:GLY:C	16:2:167:ARG:CB	2.09	1.26
1:A:242:ILE:CG1	1:A:243:PRO:HD3	1.64	1.25
2:B:160:LYS:HD3	2:B:161:TRP:CE2	1.70	1.25
16:2:226:ARG:HD2	16:2:230:LEU:CD2	1.67	1.25
17:3:103:VAL:HG13	17:3:107:ARG:NE	1.49	1.25
2:B:403:ASN:O	2:B:406:ASN:HB3	1.34	1.25
3:C:5:VAL:CG2	3:C:65:VAL:HG23	1.66	1.25
19:B:1209:CLA:HAC2	19:B:1210:CLA:CBB	1.65	1.25
19:B:1209:CLA:CAC	19:B:1210:CLA:HBB2	1.65	1.25
8:H:76:TYR:OH	12:L:90:ARG:NE	1.68	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:139:LYS:CG	13:N:142:LYS:HD3	1.66	1.24
1:A:281:LEU:CD1	19:A:1115:CLA:CED	2.00	1.24
4:D:156:ARG:CZ	4:D:158:PHE:HE1	1.48	1.24
2:B:5:ILE:HG22	2:B:6:PRO:CD	1.67	1.24
16:2:254:LEU:HD22	16:2:255:ALA:N	1.49	1.24
18:4:146:PHE:HZ	19:4:4013:CLA:C4C	1.50	1.24
19:A:9012:CLA:H11	2:B:616:LEU:CD1	1.66	1.24
2:B:294:ASN:HB2	7:G:94:GLN:CD	1.62	1.24
7:G:98:THR:HB	7:G:101:GLU:OE1	1.15	1.23
1:A:284:ARG:HA	1:A:284:ARG:NH1	1.50	1.23
2:B:36:ASP:O	2:B:41:ARG:CZ	1.86	1.23
2:B:225:LEU:HD13	2:B:233:TYR:OH	1.33	1.23
7:G:72:LEU:CD2	7:G:124:ILE:CD1	2.15	1.23
8:H:76:TYR:OH	12:L:90:ARG:CD	1.84	1.23
19:A:1119:CLA:C9	21:A:6007:BCR:H373	1.67	1.23
16:2:148:ASP:CB	16:2:152:LEU:HB3	1.64	1.23
22:4:7034:LMU:C11	22:4:7052:LMU:H4'	1.67	1.23
4:D:114:MET:HG3	4:D:115:PRO:O	1.30	1.22
17:3:96:ARG:HA	17:3:99:ALA:CB	1.67	1.22
1:A:154:ARG:NE	1:A:384:TYR:CE1	2.08	1.22
4:D:80:SER:OG	4:D:126:PRO:HD2	1.06	1.22
5:E:106:ARG:NH2	5:E:107:PHE:HA	1.51	1.22
15:1:157:ASP:HB2	15:1:178:LYS:CA	1.69	1.22
6:F:190:LYS:HZ2	6:F:192:THR:CG2	1.42	1.22
7:G:149:TYR:HA	7:G:150:ASP:OD1	1.36	1.22
16:2:122:ILE:CD1	19:2:2002:CLA:C3B	2.16	1.22
22:3:7003:LMU:C3B	22:3:7005:LMU:H4B	1.68	1.22
11:K:49:ILE:C	11:K:52:PRO:CD	2.12	1.22
19:A:1237:CLA:H141	12:L:141:LEU:CD2	1.68	1.22
6:F:107:LYS:O	6:F:108:LEU:HD12	1.05	1.22
6:F:127:LYS:C	6:F:129:ARG:H	1.39	1.22
8:H:78:PRO:CD	19:L:1501:CLA:HMD2	1.68	1.22
15:1:78:ARG:HH21	15:1:179:LYS:CD	1.52	1.22
17:3:122:LEU:HD22	19:3:3006:CLA:CHA	1.60	1.22
17:3:151:TRP:CD1	17:3:152:ALA:H	1.58	1.22
2:B:469:LYS:CD	2:B:470:THR:HA	1.70	1.21
2:B:558:PRO:CB	2:B:703:VAL:HG22	1.69	1.21
12:L:72:PRO:O	12:L:73:VAL:HG22	1.36	1.21
16:2:133:ASN:ND2	16:2:134:THR:CB	1.94	1.21
19:A:1122:CLA:CHD	21:A:6007:BCR:H19C	1.68	1.21
6:F:100:LYS:O	6:F:103:GLN:HB3	1.38	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1006:CLA:CAB	19:1:1013:CLA:HBC2	1.70	1.21
18:4:169:ASP:O	18:4:173:LYS:HG2	1.36	1.21
2:B:73:ASN:O	2:B:121:TYR:OH	1.55	1.21
2:B:294:ASN:ND2	7:G:94:GLN:CG	2.02	1.21
4:D:162:GLU:O	4:D:163:VAL:HG23	1.37	1.21
19:A:1140:CLA:H141	21:A:6011:BCR:C2	1.71	1.21
2:B:398:TYR:O	4:D:197:PRO:HG2	1.37	1.21
15:1:95:PRO:HA	15:1:98:LEU:HG	1.22	1.21
1:A:250:LEU:HB2	17:3:136:TRP:CZ2	1.73	1.21
2:B:315:LEU:CD1	2:B:317:ARG:HG2	1.71	1.21
2:B:429:LEU:O	2:B:525:LEU:HD12	1.36	1.21
21:I:6021:BCR:H313	21:I:6021:BCR:C8	1.51	1.21
22:4:7034:LMU:C9	22:4:7052:LMU:C1'	2.07	1.21
2:B:123:TRP:CA	2:B:126:THR:HG22	1.68	1.20
2:B:293:THR:HG22	7:G:94:GLN:CD	1.64	1.20
16:2:240:ILE:CG2	16:2:263:PHE:HB3	1.70	1.20
17:3:111:LEU:CG	17:3:112:GLY:H	1.38	1.20
17:3:130:GLN:HB3	17:3:132:THR:N	1.56	1.20
17:3:130:GLN:CB	17:3:132:THR:H	1.55	1.20
17:3:197:SER:CB	17:3:206:PRO:HD3	1.70	1.20
19:A:1105:CLA:C3B	21:J:6012:BCR:H331	1.71	1.20
11:K:115:ILE:HG12	11:K:122:LEU:N	1.55	1.20
17:3:113:ALA:CB	17:3:239:LEU:CD1	2.15	1.20
17:3:150:TYR:CB	17:3:151:TRP:CD1	2.22	1.20
18:4:159:ASP:OD1	18:4:171:ILE:HD11	1.04	1.20
22:4:7034:LMU:H111	22:4:7052:LMU:C3'	1.70	1.20
1:A:702:GLU:OE2	2:B:550:LYS:NZ	1.74	1.20
6:F:99:LEU:O	6:F:102:LEU:HG	1.35	1.20
15:1:190:ASN:HD21	19:1:1002:CLA:C1A	1.53	1.20
18:4:169:ASP:C	18:4:173:LYS:HA	1.67	1.20
2:B:596:TRP:HH2	2:B:612:SER:O	0.94	1.20
4:D:114:MET:HG3	4:D:115:PRO:C	1.67	1.20
11:K:84:LEU:HG	11:K:85:LYS:HG2	1.24	1.20
16:2:96:PRO:CD	17:3:85:ASP:OD2	1.90	1.20
18:4:172:PHE:CB	18:4:194:PHE:CE2	1.76	1.20
1:A:223:VAL:HG23	1:A:227:LEU:CD1	1.70	1.20
11:K:113:GLY:O	11:K:116:ILE:HG22	1.41	1.20
18:4:89:ARG:HD3	18:4:90:TRP:N	1.54	1.20
18:4:158:GLN:OE1	19:4:1004:CLA:O1D	1.55	1.20
18:4:165:SER:O	18:4:168:GLN:HG3	1.06	1.20
4:D:123:ARG:NH2	22:D:7050:LMU:C6B	2.00	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:78:ARG:HD3	19:1:1011:CLA:HMC2	1.20	1.19
19:B:1235:CLA:H93	19:B:1235:CLA:CBB	1.72	1.19
5:E:89:SER:CB	5:E:106:ARG:NE	2.06	1.19
11:K:127:ILE:CA	11:K:130:LEU:HG	1.71	1.19
16:2:118:ALA:O	16:2:121:PHE:CE2	1.96	1.19
1:A:575:LEU:HD12	1:A:576:GLY:N	1.56	1.19
3:C:17:CYS:HB2	3:C:58:CYS:SG	1.83	1.19
11:K:115:ILE:HA	11:K:118:VAL:CG2	1.72	1.19
14:R:41:UNK:CB	14:R:42:UNK:HA	1.70	1.19
19:3:1147:CLA:HMC1	19:3:1147:CLA:CBC	1.73	1.19
18:4:177:LEU:CD1	18:4:178:PRO:HD3	1.69	1.19
2:B:459:PHE:CE2	19:B:1235:CLA:C1D	2.17	1.19
15:1:157:ASP:HB2	15:1:178:LYS:CB	1.73	1.19
17:3:135:ALA:HB1	17:3:139:THR:OG1	1.40	1.19
12:L:92:ALA:H	12:L:98:ARG:NH1	1.39	1.18
15:1:150:HIS:CD2	15:1:151:GLN:HE22	1.61	1.18
17:3:95:PRO:O	17:3:96:ARG:HG2	1.36	1.18
17:3:192:LYS:CE	17:3:192:LYS:HA	1.66	1.18
1:A:86:LEU:HD13	1:A:178:MET:HE2	1.19	1.18
1:A:668:TYR:CG	2:B:445:ALA:HB2	1.77	1.18
7:G:149:TYR:HA	7:G:150:ASP:CG	1.66	1.18
8:H:58:LEU:HD12	8:H:61:THR:CB	1.73	1.18
14:R:52:UNK:HA	14:R:53:UNK:CB	1.68	1.18
15:1:149:GLU:HG2	15:1:152:ARG:NH1	1.55	1.18
17:3:150:TYR:H	17:3:152:ALA:CB	1.56	1.18
1:A:425:THR:CB	1:A:428:TYR:HE1	1.55	1.18
1:A:715:LYS:HD2	6:F:230:ASN:ND2	1.58	1.18
3:C:69:LEU:HD13	3:C:70:TRP:O	1.44	1.18
6:F:185:ILE:O	6:F:186:ARG:HG2	1.44	1.18
1:A:113:PRO:O	1:A:114:THR:HG22	1.43	1.18
21:B:6020:BCR:C33	19:L:1502:CLA:CHC	2.22	1.18
15:1:177:PRO:HD2	15:1:180:LEU:CB	1.73	1.18
1:A:21:LEU:HD12	1:A:21:LEU:O	1.39	1.18
1:A:545:HIS:CG	19:A:1135:CLA:HBB2	1.79	1.18
2:B:440:ASN:OD1	2:B:614:THR:CG2	1.91	1.18
4:D:86:SER:O	12:L:67:GLY:HA3	1.42	1.18
12:L:205:TYR:CD1	12:L:207:LEU:CD1	2.25	1.18
13:N:142:LYS:HA	13:N:142:LYS:HE3	1.18	1.18
1:A:281:LEU:HD13	19:A:1115:CLA:HED2	1.22	1.17
2:B:123:TRP:CA	2:B:126:THR:CG2	2.21	1.17
19:B:1220:CLA:H151	19:B:1220:CLA:H102	1.24	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:81:THR:HG23	11:K:83:GLY:H	1.02	1.17
19:L:1503:CLA:HBC3	19:L:1503:CLA:HHD	1.18	1.17
13:N:99:LYS:HA	13:N:102:ASN:OD1	1.44	1.17
13:N:103:ASP:CB	13:N:107:LEU:CD1	2.07	1.17
15:1:92:LEU:C	15:1:95:PRO:HD2	1.68	1.17
16:2:184:PRO:HD3	16:2:187:LYS:CB	1.74	1.17
1:A:223:VAL:CG2	1:A:227:LEU:HD12	1.71	1.17
1:A:351:THR:O	19:A:1123:CLA:H191	1.43	1.17
2:B:247:THR:CG2	2:B:248:GLN:H	1.56	1.17
8:H:58:LEU:CD1	8:H:61:THR:HB	1.74	1.17
12:L:153:PHE:HA	12:L:179:ALA:HB2	1.24	1.17
16:2:182:ILE:HB	16:2:187:LYS:CB	1.72	1.17
17:3:98:LEU:HD11	19:3:3012:CLA:C2D	1.75	1.17
22:A:7016:LMU:H21	22:A:7016:LMU:H81	1.24	1.17
2:B:553:PHE:O	2:B:554:GLY:C	1.85	1.17
1:A:342:GLY:HA3	1:A:430:ASP:CB	1.75	1.17
4:D:140:LEU:HD21	4:D:144:LEU:HD12	1.26	1.17
19:K:1143:CLA:HAC2	22:K:7001:LMU:O3B	1.39	1.17
16:2:229:MET:SD	16:2:230:LEU:HD22	1.85	1.17
19:3:3008:CLA:HBA2	19:3:3008:CLA:CBD	1.75	1.17
18:4:103:MET:CE	18:4:207:ASN:C	2.09	1.17
18:4:159:ASP:OD1	18:4:171:ILE:CD1	1.92	1.17
1:A:24:ARG:HD2	1:A:24:ARG:N	1.60	1.16
19:B:1218:CLA:HBC2	19:B:1218:CLA:HHD	1.27	1.16
11:K:49:ILE:CA	11:K:52:PRO:HG3	1.73	1.16
15:1:92:LEU:O	15:1:95:PRO:HD2	1.41	1.16
19:A:1122:CLA:C4C	21:A:6007:BCR:H19C	1.75	1.16
19:A:1124:CLA:H72	19:A:1125:CLA:CED	1.76	1.16
3:C:44:ARG:NH2	4:D:181:ARG:CG	2.08	1.16
6:F:127:LYS:O	6:F:129:ARG:N	1.77	1.16
9:I:7:LEU:HD12	21:I:6021:BCR:H333	1.17	1.16
15:1:93:ALA:CB	19:1:1006:CLA:CHC	2.22	1.16
16:2:226:ARG:HD2	16:2:230:LEU:HD21	1.19	1.16
1:A:126:ILE:HD11	19:A:1107:CLA:HMA1	1.25	1.16
1:A:423:ASP:HB3	1:A:424:PRO:HG3	1.20	1.16
2:B:633:ASN:HB2	2:B:636:THR:CB	1.76	1.16
4:D:111:ILE:HG12	4:D:121:ILE:HG22	1.22	1.16
22:E:7048:LMU:C4B	22:F:7036:LMU:H6E	1.74	1.16
6:F:200:VAL:HG12	10:J:7:TYR:HB2	1.17	1.16
12:L:92:ALA:H	12:L:98:ARG:CZ	1.58	1.16
16:2:195:TYR:CD1	16:2:196:PRO:HD2	1.81	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:197:SER:OG	17:3:205:GLY:HA3	1.46	1.16
18:4:158:GLN:HE22	19:4:1004:CLA:C1A	1.51	1.16
18:4:228:PRO:HB2	18:4:229:PHE:CD1	1.80	1.16
1:A:217:SER:OG	21:A:6002:BCR:H15C	1.42	1.16
2:B:89:HIS:C	2:B:113:VAL:CG1	1.81	1.16
2:B:216:LEU:HD23	2:B:218:TYR:O	1.44	1.16
6:F:99:LEU:HA	6:F:102:LEU:HD23	1.28	1.16
19:J:1308:CLA:HHD	19:J:1308:CLA:CBC	1.74	1.16
13:N:114:PHE:CG	13:N:117:ALA:HB2	1.80	1.16
16:2:186:ASN:CG	16:2:188:LEU:HD11	1.54	1.16
15:1:171:LEU:HA	15:1:173:TYR:CE2	1.80	1.15
15:1:189:LYS:CG	19:1:1007:CLA:HMC1	1.75	1.15
16:2:125:PHE:CA	16:2:127:THR:HG23	1.76	1.15
16:2:177:VAL:HG12	16:2:178:ASN:HB2	1.18	1.15
16:2:269:LYS:HA	16:2:269:LYS:NZ	1.59	1.15
21:I:6021:BCR:HC8	21:I:6021:BCR:C31	1.74	1.15
11:K:127:ILE:HA	11:K:130:LEU:HG	1.22	1.15
19:K:1143:CLA:CBC	22:K:7001:LMU:O3B	1.95	1.15
13:N:139:LYS:HA	13:N:142:LYS:NZ	1.62	1.15
17:3:122:LEU:HD21	19:3:3006:CLA:CHA	1.65	1.15
18:4:177:LEU:CG	18:4:178:PRO:HD3	1.75	1.15
1:A:249:ILE:CG2	17:3:136:TRP:CZ3	2.18	1.15
1:A:342:GLY:CA	1:A:430:ASP:CB	2.23	1.15
2:B:470:THR:N	2:B:501:ILE:HB	1.32	1.15
3:C:10:THR:HG23	5:E:101:TYR:CD2	1.82	1.15
6:F:124:GLU:HG3	6:F:128:LYS:HD3	1.21	1.15
8:H:58:LEU:HD12	8:H:62:THR:CG2	1.66	1.15
8:H:116:ALA:HB1	8:H:117:SER:HA	1.26	1.15
16:2:156:GLU:CG	16:2:157:LEU:HD13	1.75	1.15
1:A:451:ILE:HD12	19:A:1131:CLA:HED3	1.28	1.15
4:D:132:ALA:O	4:D:133:ARG:HD3	1.44	1.15
4:D:140:LEU:HD11	4:D:144:LEU:HB2	1.22	1.15
5:E:82:TYR:HB3	5:E:83:TRP:CZ3	1.81	1.15
15:1:77:GLU:HA	15:1:80:LYS:HG2	1.23	1.15
2:B:620:LEU:HD12	2:B:624:LEU:HD23	1.23	1.15
2:B:628:SER:O	2:B:631:LEU:HD23	1.45	1.15
4:D:201:LYS:H	4:D:201:LYS:HD2	1.02	1.15
7:G:98:THR:CB	7:G:101:GLU:OE1	1.86	1.15
13:N:139:LYS:HA	13:N:142:LYS:HZ3	0.98	1.15
13:N:139:LYS:HE3	13:N:142:LYS:CE	1.76	1.15
16:2:184:PRO:HD3	16:2:187:LYS:CG	1.74	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:174:GLN:O	18:4:194:PHE:CG	1.99	1.15
1:A:281:LEU:HD22	19:A:1115:CLA:HMA3	1.24	1.14
1:A:336:GLY:CA	1:A:339:THR:OG1	1.94	1.14
19:A:1119:CLA:CMD	19:A:1121:CLA:HBB2	1.75	1.14
2:B:255:LEU:HA	2:B:271:THR:HB	1.16	1.14
2:B:429:LEU:C	2:B:525:LEU:HD12	1.70	1.14
6:F:224:GLY:C	6:F:227:VAL:HG12	1.72	1.14
8:H:58:LEU:HB3	8:H:61:THR:CG2	1.76	1.14
8:H:97:LEU:HG	8:H:98:LEU:HA	1.29	1.14
19:L:1148:CLA:HBC3	19:L:1148:CLA:HHD	1.26	1.14
16:2:182:ILE:CG2	16:2:187:LYS:HG3	1.76	1.14
18:4:168:GLN:HB3	18:4:172:PHE:HE1	1.06	1.14
1:A:150:PHE:O	1:A:151:GLN:HG3	1.46	1.14
4:D:140:LEU:HD12	4:D:140:LEU:C	1.60	1.14
16:2:112:TRP:CZ2	16:2:167:ARG:NH2	2.04	1.14
16:2:182:ILE:HG22	16:2:187:LYS:HG3	1.26	1.14
17:3:150:TYR:HB3	17:3:151:TRP:CD1	1.81	1.14
11:K:118:VAL:HG23	11:K:121:VAL:HG22	1.25	1.14
14:R:26:UNK:O	14:R:28:UNK:CB	1.96	1.14
16:2:184:PRO:HD2	16:2:185:ASN:C	1.72	1.14
18:4:158:GLN:CA	19:4:1004:CLA:HMA1	1.76	1.14
1:A:281:LEU:HD23	19:A:1115:CLA:HMA3	1.29	1.14
2:B:75:GLU:CB	2:B:132:ASN:ND2	2.09	1.14
5:E:79:LYS:HG3	5:E:84:TYR:CZ	1.82	1.14
1:A:443:ILE:CD1	1:A:557:LEU:HD22	1.77	1.14
1:A:575:LEU:HD12	1:A:576:GLY:CA	1.78	1.14
19:A:1115:CLA:H193	11:K:64:MET:HE1	1.17	1.14
17:3:141:VAL:HG23	17:3:142:ILE:HG12	1.30	1.14
18:4:175:TYR:HD2	18:4:195:ALA:O	1.26	1.14
1:A:267:THR:HG22	1:A:269:PHE:CE2	1.83	1.13
1:A:499:ALA:HB1	19:A:1133:CLA:HED1	1.24	1.13
2:B:329:SER:O	2:B:330:ILE:HG22	1.48	1.13
2:B:569:ASP:OD1	2:B:706:ARG:CZ	1.95	1.13
16:2:171:ILE:HG13	16:2:172:LEU:N	1.60	1.13
16:2:187:LYS:HA	16:2:187:LYS:HE3	1.28	1.13
1:A:397:THR:CG2	1:A:613:ILE:HG13	1.78	1.13
12:L:171:LYS:C	12:L:173:PRO:CD	2.21	1.13
22:R:7020:LMU:H5B	22:R:7020:LMU:H6E	1.30	1.13
1:A:492:ILE:HD11	19:A:1133:CLA:HMC2	1.25	1.13
2:B:469:LYS:HD2	2:B:470:THR:CA	1.77	1.13
11:K:111:VAL:O	11:K:114:HIS:HB2	1.46	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:155:GLU:C	13:N:157:LYS:HE3	1.60	1.13
15:1:177:PRO:CD	15:1:180:LEU:CG	1.86	1.13
16:2:246:PRO:HB3	16:2:247:ILE:HD13	1.13	1.13
17:3:103:VAL:HG12	17:3:107:ARG:HD3	1.30	1.13
18:4:87:ASN:HB2	18:4:90:TRP:CZ3	1.82	1.13
18:4:173:LYS:NZ	18:4:201:LYS:HG3	1.64	1.13
1:A:152:ILE:HD11	19:A:1127:CLA:O1D	1.45	1.13
2:B:22:TRP:HE1	19:B:1238:CLA:CBB	1.62	1.13
2:B:310:PRO:CB	2:B:311:PRO:HD3	1.71	1.13
22:D:7050:LMU:H6E	22:D:7050:LMU:C2B	1.78	1.13
17:3:109:ALA:CA	17:3:111:LEU:HB3	1.78	1.13
17:3:159:VAL:O	17:3:161:GLU:N	1.81	1.13
22:3:7003:LMU:C3B	22:3:7005:LMU:C4B	2.25	1.13
19:A:1124:CLA:HBC2	19:A:1124:CLA:HHD	1.29	1.12
19:A:9022:CLA:H93	19:A:9023:CLA:H91	1.28	1.12
2:B:247:THR:HA	2:B:250:ALA:HB2	1.25	1.12
2:B:294:ASN:HD22	7:G:94:GLN:CA	1.60	1.12
3:C:66:ARG:HG2	3:C:66:ARG:HH21	1.12	1.12
7:G:89:LYS:HA	7:G:89:LYS:NZ	1.63	1.12
7:G:100:PHE:N	7:G:101:GLU:HB2	1.64	1.13
11:K:78:ARG:NE	11:K:78:ARG:HA	1.60	1.12
12:L:60:ILE:HG22	12:L:61:ASN:N	1.52	1.12
12:L:141:LEU:HD11	21:L:6019:BCR:H312	1.24	1.12
22:L:7029:LMU:H1'	22:L:7029:LMU:H31	1.31	1.12
13:N:139:LYS:HB3	13:N:142:LYS:HD3	1.18	1.12
19:1:1014:CLA:HBC3	19:1:1014:CLA:HHD	1.25	1.13
16:2:148:ASP:HB3	16:2:152:LEU:CB	1.79	1.12
17:3:201:ALA:HB1	17:3:202:TYR:CE2	1.83	1.12
7:G:72:LEU:CD2	7:G:124:ILE:HD11	1.78	1.12
22:N:7049:LMU:H61	22:N:7049:LMU:H12	1.19	1.12
19:1:1010:CLA:HBC3	19:1:1010:CLA:HHD	1.26	1.12
18:4:175:TYR:CD2	18:4:195:ALA:O	2.00	1.12
1:A:217:SER:OG	21:A:6002:BCR:C15	1.98	1.12
2:B:304:ILE:HD11	19:B:1216:CLA:CED	1.79	1.12
2:B:382:ILE:HG22	2:B:383:MET:H	1.09	1.12
19:J:1308:CLA:HBA2	19:J:1308:CLA:HBD	1.28	1.12
18:4:193:ASN:O	18:4:194:PHE:CG	2.03	1.12
1:A:281:LEU:HD22	19:A:1115:CLA:CED	1.80	1.12
1:A:502:THR:HG22	1:A:504:ALA:H	1.09	1.12
2:B:310:PRO:HB2	2:B:311:PRO:HD3	1.21	1.12
2:B:314:ARG:HH12	15:1:67:LEU:CD2	1.61	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1235:CLA:H152	21:F:6016:BCR:C31	1.78	1.12
11:K:125:LYS:HB2	11:K:128:GLY:CA	1.80	1.12
22:L:7029:LMU:H4'	22:L:7029:LMU:H5B	1.27	1.12
15:1:189:LYS:CB	19:1:1007:CLA:HMC3	1.78	1.12
19:1:1014:CLA:H71	19:1:1014:CLA:H41	1.31	1.12
1:A:158:ILE:CG1	1:A:159:THR:H	1.62	1.12
1:A:669:GLY:N	2:B:445:ALA:HA	1.63	1.12
4:D:167:HIS:CE1	4:D:172:VAL:HG11	1.85	1.12
13:N:103:ASP:HB3	13:N:107:LEU:HD12	1.15	1.12
15:1:97:ILE:HD13	15:1:98:LEU:CB	1.80	1.12
17:3:98:LEU:O	17:3:101:GLY:N	1.81	1.12
17:3:103:VAL:CG1	17:3:107:ARG:CD	2.14	1.12
1:A:244:LEU:CB	1:A:247:GLU:CG	2.11	1.11
1:A:487:VAL:HG13	1:A:489:ALA:N	1.63	1.11
19:A:1115:CLA:H141	19:A:1115:CLA:H172	1.26	1.11
3:C:62:PHE:CE2	5:E:80:GLU:CG	2.33	1.11
11:K:125:LYS:CA	11:K:126:ASN:HB3	1.79	1.11
12:L:96:LEU:HD23	12:L:96:LEU:H	1.13	1.11
19:1:1014:CLA:H52	19:1:1014:CLA:H102	1.28	1.11
16:2:125:PHE:HA	16:2:127:THR:HG23	1.14	1.11
1:A:227:LEU:HD21	1:A:296:LEU:O	1.48	1.11
2:B:230:TRP:N	7:G:63:VAL:HG21	1.62	1.11
2:B:315:LEU:HD12	2:B:317:ARG:HG2	1.13	1.11
6:F:173:TRP:CZ3	6:F:211:PHE:HB2	1.84	1.11
13:N:103:ASP:HB2	13:N:107:LEU:HD11	1.22	1.11
13:N:139:LYS:CE	13:N:142:LYS:HE2	1.78	1.11
15:1:97:ILE:CD1	15:1:98:LEU:HA	1.66	1.11
17:3:243:ILE:HD11	19:3:3005:CLA:C2C	1.80	1.11
18:4:96:LEU:C	18:4:96:LEU:HD12	1.73	1.11
1:A:167:THR:HG22	19:A:1112:CLA:HAA2	1.32	1.11
1:A:472:ARG:NH1	12:L:120:LEU:HD22	1.64	1.11
19:A:1124:CLA:HED1	19:A:1125:CLA:C2D	1.80	1.11
2:B:89:HIS:O	2:B:113:VAL:HG13	1.45	1.11
2:B:90:ALA:HA	2:B:113:VAL:HG13	1.33	1.11
2:B:123:TRP:HA	2:B:126:THR:CB	1.79	1.11
3:C:44:ARG:HB3	4:D:182:GLN:NE2	1.65	1.11
13:N:132:THR:HB	13:N:139:LYS:NZ	1.65	1.11
13:N:135:GLN:HA	13:N:136:ASP:O	1.47	1.11
16:2:176:CYS:O	16:2:177:VAL:HG23	1.50	1.11
19:3:1147:CLA:HBC3	19:3:1147:CLA:CMC	1.77	1.11
2:B:53:GLN:NE2	19:B:1201:CLA:HBB1	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ARG:HB2	19:B:1210:CLA:HBC2	1.32	1.11
19:B:1202:CLA:O1A	19:B:1202:CLA:H2	1.30	1.11
19:B:1235:CLA:H152	21:F:6016:BCR:H312	1.18	1.11
5:E:96:ASP:HB3	5:E:98:ASN:H	1.03	1.11
12:L:128:GLN:HA	12:L:130:GLY:HA3	1.27	1.11
15:1:157:ASP:CB	15:1:178:LYS:HA	1.79	1.11
16:2:166:ARG:N	16:2:167:ARG:CB	2.14	1.11
17:3:135:ALA:CB	17:3:139:THR:HB	1.80	1.11
17:3:201:ALA:C	17:3:202:TYR:HD2	1.59	1.11
5:E:125:ILE:O	5:E:125:ILE:HG13	1.40	1.11
13:N:146:LEU:HD11	17:3:142:ILE:O	1.22	1.11
19:4:1304:CLA:HAA2	19:4:1304:CLA:CED	1.79	1.11
1:A:308:ILE:HD12	19:A:1115:CLA:HHC	1.20	1.10
1:A:478:SER:HB2	1:A:644:GLN:NE2	1.65	1.10
2:B:314:ARG:NH1	15:1:67:LEU:CD2	2.14	1.10
13:N:130:ASN:C	13:N:132:THR:HG22	1.75	1.10
1:A:73:GLU:O	1:A:76:ARG:N	1.85	1.10
1:A:478:SER:HB2	1:A:644:GLN:HE22	1.06	1.10
19:A:1134:CLA:CGA	19:A:1141:CLA:HBB1	1.80	1.10
21:A:6002:BCR:H311	21:A:6002:BCR:HC8	1.15	1.10
2:B:120:VAL:HG22	2:B:123:TRP:HE1	0.93	1.10
6:F:207:LEU:HD13	6:F:208:PHE:H	1.03	1.10
8:H:58:LEU:HD12	8:H:61:THR:HB	1.17	1.10
13:N:155:GLU:CA	13:N:157:LYS:HE2	1.81	1.10
15:1:157:ASP:HB2	15:1:178:LYS:HA	1.24	1.10
15:1:162:LYS:C	15:1:164:PRO:HD3	1.75	1.10
2:B:25:ILE:HG13	2:B:25:ILE:O	1.50	1.10
2:B:620:LEU:HD12	2:B:624:LEU:CD2	1.81	1.10
4:D:140:LEU:HD13	4:D:144:LEU:HG	1.19	1.10
6:F:107:LYS:O	6:F:108:LEU:CD1	1.99	1.10
6:F:130:PHE:N	6:F:133:TYR:HE1	1.50	1.10
6:F:173:TRP:HZ3	6:F:211:PHE:HB2	1.07	1.10
7:G:113:LEU:O	7:G:117:ASN:ND2	1.85	1.10
15:1:177:PRO:HD3	15:1:180:LEU:HG	1.32	1.10
16:2:184:PRO:CB	16:2:187:LYS:HD2	1.81	1.10
22:3:7003:LMU:C4B	22:3:7005:LMU:H4B	1.81	1.10
1:A:157:GLY:HA3	1:A:229:ILE:HG21	1.22	1.10
1:A:158:ILE:HG13	1:A:159:THR:N	1.56	1.10
4:D:84:GLY:O	12:L:64:PRO:HB3	1.50	1.10
5:E:111:ASN:ND2	5:E:113:ALA:H	1.50	1.10
8:H:58:LEU:HD11	8:H:62:THR:HG21	1.13	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:85:ILE:HG12	15:1:88:ARG:CZ	1.82	1.10
15:1:168:PHE:O	15:1:169:ASP:HB2	1.52	1.10
17:3:108:PHE:HB3	19:3:3013:CLA:C4	1.82	1.10
18:4:141:LEU:H	18:4:141:LEU:CD2	1.64	1.10
1:A:86:LEU:CD1	1:A:178:MET:HE2	1.81	1.10
1:A:316:MET:HB3	1:A:317:TYR:HB2	1.34	1.10
1:A:423:ASP:HB3	1:A:424:PRO:CG	1.82	1.10
2:B:20:ARG:HG3	2:B:20:ARG:HH11	1.02	1.10
2:B:140:ILE:HG13	2:B:141:PHE:N	1.59	1.10
2:B:317:ARG:NH2	2:B:410:ARG:CG	2.14	1.10
2:B:459:PHE:HD2	19:B:1235:CLA:CAD	1.63	1.10
4:D:158:PHE:HB3	4:D:159:PRO:HD2	1.34	1.10
7:G:96:GLY:C	7:G:97:LEU:HG	1.76	1.10
8:H:58:LEU:HB3	8:H:61:THR:CB	1.81	1.10
14:R:38:UNK:O	14:R:42:UNK:HA	1.48	1.10
19:A:1124:CLA:HED1	19:A:1125:CLA:C3D	1.81	1.09
2:B:131:THR:HG22	2:B:134:ASP:H	1.01	1.09
6:F:82:LEU:HG	6:F:83:THR:H	1.12	1.09
6:F:119:ILE:HG13	6:F:120:LYS:H	1.07	1.09
21:F:6016:BCR:C8	21:F:6016:BCR:H321	1.62	1.09
7:G:89:LYS:HA	7:G:89:LYS:HE3	1.32	1.09
16:2:122:ILE:HD13	19:2:2002:CLA:C3B	1.78	1.09
17:3:135:ALA:CB	17:3:139:THR:CB	2.28	1.09
22:4:7034:LMU:H112	22:4:7052:LMU:H4'	1.29	1.09
1:A:435:VAL:O	1:A:438:HIS:O	1.70	1.09
2:B:98:GLN:O	2:B:100:ALA:N	1.86	1.09
19:B:1235:CLA:H161	21:F:6016:BCR:H313	1.30	1.09
5:E:82:TYR:HB3	5:E:83:TRP:CE3	1.86	1.09
5:E:106:ARG:HH21	5:E:107:PHE:CA	1.63	1.09
5:E:127:GLU:HB3	5:E:129:GLU:O	1.49	1.09
8:H:56:GLU:HG3	8:H:57:ASP:N	1.65	1.09
12:L:131:SER:HB3	12:L:201:TYR:CE2	1.67	1.09
16:2:168:TRP:CD1	16:2:171:ILE:CG2	2.26	1.09
1:A:56:ASN:O	1:A:57:LEU:HB3	1.37	1.09
4:D:80:SER:OG	4:D:126:PRO:CD	1.99	1.09
14:R:46:UNK:CB	14:R:47:UNK:CB	2.30	1.09
19:2:2007:CLA:HBC2	19:3:2009:CLA:HED2	1.13	1.09
17:3:150:TYR:C	17:3:152:ALA:N	1.99	1.09
17:3:210:PRO:HG2	17:3:211:LEU:HD12	1.30	1.09
19:3:3008:CLA:HBA2	19:3:3008:CLA:HBD	1.15	1.09
1:A:331:LEU:HD11	1:A:346:LEU:HB3	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:GLY:H	2:B:445:ALA:HA	1.15	1.09
2:B:89:HIS:O	2:B:113:VAL:CB	2.00	1.09
2:B:545:LYS:HD3	2:B:546:LEU:H	1.01	1.09
3:C:44:ARG:CZ	4:D:181:ARG:HD3	1.83	1.09
10:J:11:ALA:HB1	10:J:12:PRO:HD2	1.29	1.09
12:L:73:VAL:O	19:L:1130:CLA:O2A	1.71	1.09
14:R:34:UNK:CB	14:R:35:UNK:CB	2.30	1.09
15:1:78:ARG:NH2	15:1:179:LYS:HB3	1.67	1.09
16:2:122:ILE:HD11	19:2:2002:CLA:C3B	1.81	1.09
16:2:182:ILE:CB	16:2:187:LYS:HG3	1.81	1.09
21:3:6022:BCR:H23C	21:3:6022:BCR:C39	1.82	1.09
18:4:158:GLN:NE2	19:4:1004:CLA:NA	2.00	1.09
1:A:24:ARG:HD2	1:A:24:ARG:H	0.92	1.09
1:A:145:ILE:HG23	19:A:1106:CLA:OBD	1.50	1.09
1:A:158:ILE:HG13	1:A:159:THR:H	1.03	1.09
1:A:331:LEU:HD21	1:A:343:HIS:O	1.53	1.09
1:A:338:PHE:HE1	19:A:1151:CLA:HBB1	0.93	1.09
2:B:315:LEU:C	2:B:315:LEU:HD13	1.78	1.09
21:B:6020:BCR:H331	19:L:1502:CLA:CHC	1.83	1.09
12:L:141:LEU:HD11	21:L:6019:BCR:C31	1.81	1.09
14:R:41:UNK:CB	14:R:42:UNK:CA	2.30	1.09
17:3:185:GLN:CG	17:3:186:TYR:H	1.65	1.09
19:A:1101:CLA:H42	19:A:1140:CLA:H61	1.12	1.08
19:A:1102:CLA:H12	19:A:1109:CLA:H61	1.28	1.08
21:A:6011:BCR:H23C	21:A:6011:BCR:H393	1.27	1.08
2:B:475:ASP:HB3	2:B:480:SER:HA	1.33	1.08
4:D:87:THR:HG23	12:L:69:LEU:HD12	1.11	1.08
22:E:7048:LMU:H4B	22:F:7036:LMU:H6E	1.15	1.08
19:J:1308:CLA:HHD	19:J:1308:CLA:HBC2	1.33	1.08
16:2:130:GLY:HA2	16:2:131:ILE:HG12	1.21	1.08
16:2:152:LEU:HD13	16:2:153:PHE:H	0.99	1.08
17:3:150:TYR:CD2	17:3:151:TRP:CE2	2.41	1.08
19:A:1119:CLA:HMD2	19:A:1121:CLA:HBB2	1.31	1.08
2:B:225:LEU:CD1	2:B:233:TYR:OH	2.00	1.08
2:B:247:THR:HG23	2:B:248:GLN:H	1.16	1.08
2:B:268:LEU:HD21	19:B:1214:CLA:HMA1	1.27	1.08
19:B:1222:CLA:HHD	19:B:1222:CLA:HBC2	1.31	1.08
3:C:14:CYS:CA	3:C:17:CYS:SG	2.41	1.08
7:G:62:LEU:HB3	7:G:65:SER:HB3	1.24	1.08
12:L:115:VAL:HG11	12:L:130:GLY:H	1.14	1.08
13:N:143:VAL:HB	13:N:144:PRO:HD2	1.15	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:147:SER:HB3	13:N:151:ASP:HA	1.19	1.08
16:2:125:PHE:HA	16:2:127:THR:CG2	1.80	1.08
17:3:96:ARG:HA	17:3:99:ALA:HB3	1.30	1.08
17:3:111:LEU:HG	17:3:112:GLY:N	1.48	1.08
18:4:103:MET:HE2	18:4:207:ASN:O	1.52	1.08
1:A:425:THR:HB	1:A:428:TYR:HE1	1.04	1.08
2:B:255:LEU:HA	2:B:271:THR:CB	1.82	1.08
2:B:527:LEU:CD1	19:B:1236:CLA:HMA3	1.84	1.08
2:B:558:PRO:HB2	2:B:703:VAL:HG22	1.16	1.08
3:C:24:ASP:HB2	23:C:8002:SF4:S2	1.92	1.08
6:F:179:ARG:HG2	6:F:183:ILE:HD11	1.25	1.08
8:H:121:LEU:HB3	8:H:122:PRO:HD2	1.13	1.08
22:H:7030:LMU:H91	22:H:7030:LMU:H52	1.32	1.08
22:R:7022:LMU:H21	22:R:7022:LMU:H2'	1.27	1.08
15:1:70:GLY:O	15:1:73:PRO:HD2	1.51	1.08
15:1:177:PRO:CD	15:1:180:LEU:CD2	2.30	1.08
17:3:150:TYR:O	17:3:151:TRP:C	1.95	1.08
18:4:89:ARG:HD3	18:4:90:TRP:H	1.08	1.08
1:A:361:ASN:ND2	19:A:1103:CLA:OBD	1.84	1.08
19:A:1115:CLA:C19	11:K:64:MET:HE1	1.84	1.08
19:A:1140:CLA:H141	21:A:6011:BCR:HC22	1.20	1.08
6:F:221:LEU:HD23	6:F:222:LEU:CD2	1.82	1.08
21:I:6021:BCR:C8	21:I:6021:BCR:C31	2.28	1.08
16:2:117:ALA:HB3	16:2:230:LEU:HG	1.28	1.08
19:2:2001:CLA:H42	19:2:2001:CLA:O1A	1.53	1.08
1:A:71:LEU:HG	1:A:72:GLU:H	1.14	1.08
1:A:492:ILE:HD11	19:A:1133:CLA:CMC	1.83	1.08
1:A:567:ARG:NH1	4:D:89:GLY:HA2	1.68	1.08
2:B:247:THR:HA	2:B:250:ALA:HB3	1.27	1.08
2:B:302:LYS:O	2:B:303:TYR:HB2	1.52	1.08
11:K:97:ASP:HB2	11:K:101:PHE:HE2	1.12	1.08
12:L:154:ASN:C	12:L:178:THR:HG23	1.79	1.08
14:R:39:UNK:C	14:R:41:UNK:CB	2.30	1.08
17:3:96:ARG:HH11	17:3:96:ARG:CG	1.67	1.08
18:4:146:PHE:CZ	19:4:4013:CLA:C1C	2.36	1.08
1:A:443:ILE:HD11	1:A:557:LEU:HD22	1.14	1.07
1:A:479:ASP:HA	1:A:536:THR:HG21	1.32	1.07
1:A:567:ARG:NH2	4:D:136:GLN:OE1	1.85	1.07
19:A:1124:CLA:HED1	19:A:1125:CLA:CMD	1.84	1.07
19:A:1141:CLA:H71	19:A:1141:CLA:H121	1.33	1.07
2:B:25:ILE:HG21	21:L:6019:BCR:H292	1.28	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:LYS:O	2:B:552:ASP:OD1	1.72	1.07
4:D:140:LEU:HD13	4:D:144:LEU:CG	1.84	1.07
12:L:171:LYS:C	12:L:173:PRO:HD2	1.79	1.07
16:2:118:ALA:O	16:2:121:PHE:CD2	2.06	1.07
16:2:227:LEU:HD21	19:2:2004:CLA:C1C	1.84	1.07
18:4:146:PHE:CZ	19:4:4013:CLA:C2C	2.37	1.07
1:A:163:GLN:HA	1:A:166:CYS:SG	1.93	1.07
2:B:119:GLY:HA3	19:B:1225:CLA:HED1	1.22	1.07
2:B:131:THR:HG22	2:B:134:ASP:N	1.70	1.07
2:B:294:ASN:ND2	7:G:94:GLN:CA	2.17	1.07
3:C:62:PHE:CZ	5:E:80:GLU:CG	2.37	1.07
4:D:87:THR:HG23	12:L:69:LEU:CD1	1.83	1.07
6:F:213:TRP:HB2	6:F:216:ALA:HB2	1.36	1.07
11:K:52:PRO:HD2	11:K:53:THR:H	1.19	1.07
12:L:131:SER:CB	12:L:201:TYR:CE2	2.31	1.07
13:N:148:ASP:N	13:N:149:ASP:HB2	1.68	1.07
15:1:77:GLU:O	15:1:80:LYS:HG3	1.55	1.07
16:2:195:TYR:HD1	16:2:196:PRO:HD2	1.04	1.07
19:A:1122:CLA:HBB2	21:A:6007:BCR:C35	1.85	1.07
2:B:89:HIS:O	2:B:113:VAL:HG12	1.34	1.07
2:B:500:ALA:O	2:B:501:ILE:HG12	1.55	1.07
2:B:551:LYS:HG2	2:B:552:ASP:H	1.17	1.07
15:1:80:LYS:O	15:1:83:GLU:HB3	1.52	1.07
1:A:51:THR:HG21	19:A:1139:CLA:HBB2	1.37	1.07
1:A:328:LYS:HD2	1:A:332:GLU:HB2	1.33	1.07
2:B:11:GLY:HA3	3:C:71:HIS:HD2	1.03	1.07
5:E:107:PHE:CE2	5:E:109:LYS:HE3	1.88	1.07
11:K:81:THR:HG23	11:K:83:GLY:N	1.68	1.07
16:2:148:ASP:HB3	16:2:152:LEU:HB3	1.15	1.07
17:3:139:THR:HG22	17:3:140:GLY:H	0.90	1.07
17:3:139:THR:HG22	17:3:140:GLY:N	1.65	1.07
2:B:122:GLN:C	2:B:126:THR:HB	1.79	1.07
12:L:164:LEU:HB2	12:L:165:THR:HG23	1.36	1.07
12:L:209:LEU:HD12	12:L:210:PRO:CD	1.83	1.07
13:N:139:LYS:HG3	13:N:142:LYS:CD	1.85	1.07
13:N:152:LEU:C	13:N:153:GLU:HG3	1.78	1.07
16:2:152:LEU:HD13	16:2:153:PHE:N	1.70	1.07
16:2:184:PRO:HB3	16:2:187:LYS:HD2	1.33	1.07
18:4:146:PHE:CZ	19:4:4013:CLA:C3C	2.38	1.07
18:4:165:SER:O	18:4:168:GLN:CG	2.02	1.07
1:A:249:ILE:C	1:A:251:ASN:H	1.60	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:SER:HB2	19:A:1126:CLA:HMA3	1.35	1.06
1:A:555:ILE:HD13	19:A:9023:CLA:HMD2	1.37	1.06
2:B:110:LEU:HD12	2:B:111:GLY:N	1.71	1.06
6:F:207:LEU:HD22	6:F:208:PHE:CA	1.85	1.06
7:G:84:ARG:HG3	7:G:85:GLU:CB	1.83	1.06
11:K:49:ILE:CA	11:K:52:PRO:CG	2.31	1.06
11:K:49:ILE:HA	11:K:52:PRO:HG3	1.11	1.06
11:K:127:ILE:HA	11:K:130:LEU:CG	1.85	1.06
16:2:168:TRP:HA	16:2:171:ILE:HG23	1.28	1.06
17:3:192:LYS:HA	17:3:192:LYS:HE2	1.27	1.06
1:A:157:GLY:O	1:A:158:ILE:HG23	0.89	1.06
1:A:478:SER:HB3	1:A:644:GLN:HE22	1.16	1.06
1:A:499:ALA:HB1	19:A:1133:CLA:CED	1.85	1.06
19:A:1105:CLA:C3B	21:J:6012:BCR:C33	2.33	1.06
2:B:123:TRP:HA	2:B:126:THR:HG22	1.13	1.06
3:C:65:VAL:HG22	3:C:66:ARG:H	1.17	1.06
7:G:84:ARG:HG3	7:G:85:GLU:N	1.65	1.06
15:1:134:LEU:HA	15:1:137:ILE:HD11	1.10	1.06
16:2:246:PRO:HB3	16:2:247:ILE:CD1	1.84	1.06
17:3:109:ALA:CA	17:3:111:LEU:CB	2.33	1.06
17:3:113:ALA:HB1	17:3:239:LEU:HD11	1.12	1.06
18:4:242:ASN:O	18:4:243:THR:HG22	1.55	1.06
1:A:316:MET:HG2	1:A:317:TYR:CD1	1.89	1.06
1:A:478:SER:CB	1:A:644:GLN:NE2	2.18	1.06
19:A:1122:CLA:HBB2	21:A:6007:BCR:H351	1.35	1.06
19:A:1134:CLA:H3A	19:A:1141:CLA:HBB2	1.31	1.06
2:B:475:ASP:CB	2:B:480:SER:HA	1.84	1.06
2:B:696:LYS:HG2	3:C:80:ALA:HA	1.38	1.06
19:J:1308:CLA:CAD	19:J:1308:CLA:HED3	1.86	1.06
11:K:125:LYS:HA	11:K:126:ASN:CB	1.84	1.06
16:2:118:ALA:CA	16:2:121:PHE:CE2	2.25	1.06
17:3:93:ILE:HG13	17:3:95:PRO:O	1.55	1.06
17:3:197:SER:OG	17:3:206:PRO:HD3	1.55	1.06
18:4:146:PHE:CZ	19:4:4013:CLA:C4C	2.37	1.06
18:4:209:ARG:O	18:4:212:LEU:O	1.72	1.06
19:4:4002:CLA:HMA2	19:4:4002:CLA:HBA1	1.35	1.06
19:A:9012:CLA:H11	2:B:616:LEU:HD13	1.35	1.06
19:A:9012:CLA:C1	2:B:616:LEU:HD13	1.85	1.06
2:B:475:ASP:O	2:B:476:ILE:HG22	1.54	1.06
4:D:163:VAL:O	4:D:164:GLN:HG3	1.53	1.06
5:E:78:ARG:HH22	5:E:125:ILE:HG21	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:143:LEU:HD22	12:L:146:THR:HG22	1.31	1.06
17:3:110:MET:O	17:3:113:ALA:HB3	1.54	1.06
1:A:21:LEU:HA	1:A:22:VAL:HG13	1.33	1.06
1:A:365:LEU:HD23	19:A:1103:CLA:HED3	1.31	1.06
1:A:578:ARG:HB2	1:A:578:ARG:CZ	1.81	1.06
1:A:707:ILE:HG22	1:A:711:HIS:NE2	1.71	1.06
2:B:122:GLN:O	2:B:126:THR:HB	0.89	1.06
2:B:294:ASN:CG	7:G:94:GLN:HG3	1.81	1.06
2:B:317:ARG:CZ	2:B:410:ARG:HG2	1.85	1.06
19:B:1235:CLA:HBB2	19:B:1235:CLA:C9	1.85	1.06
7:G:64:ILE:O	7:G:68:THR:HG23	1.53	1.06
9:I:11:LEU:HD12	21:I:6021:BCR:H10C	1.34	1.06
13:N:139:LYS:HG3	13:N:142:LYS:HD3	1.37	1.06
19:1:1014:CLA:H52	19:1:1014:CLA:C10	1.86	1.06
16:2:117:ALA:HB1	16:2:230:LEU:HG	1.37	1.06
16:2:119:GLY:O	16:2:123:PRO:CG	2.02	1.06
19:4:1004:CLA:HBC2	19:4:1004:CLA:HHD	1.30	1.06
1:A:163:GLN:HG3	1:A:164:LEU:H	1.18	1.05
1:A:188:LYS:O	1:A:190:ALA:HB2	1.56	1.05
1:A:397:THR:HG22	1:A:613:ILE:HG13	1.11	1.05
2:B:89:HIS:O	2:B:113:VAL:CG1	0.76	1.05
2:B:732:LYS:CG	2:B:733:PHE:C	2.29	1.05
5:E:78:ARG:NH2	5:E:125:ILE:HG21	1.68	1.05
8:H:76:TYR:OH	12:L:90:ARG:HD2	1.53	1.05
15:1:102:ALA:C	15:1:103:LEU:HD23	1.81	1.05
18:4:172:PHE:HB3	18:4:194:PHE:CE2	1.88	1.05
1:A:439:ARG:NH1	1:A:565:SER:O	1.90	1.05
1:A:483:GLN:HB3	1:A:485:GLN:NE2	1.71	1.05
2:B:70:TRP:HB3	2:B:136:TYR:OH	1.56	1.05
6:F:132:ASN:O	6:F:133:TYR:HD1	1.38	1.05
6:F:219:ARG:HG2	6:F:219:ARG:HH11	0.93	1.05
7:G:98:THR:OG1	7:G:101:GLU:CD	1.98	1.05
8:H:98:LEU:CD2	12:L:146:THR:HG21	1.86	1.05
12:L:60:ILE:HG22	12:L:61:ASN:H	1.02	1.05
16:2:125:PHE:C	16:2:127:THR:HG23	1.82	1.05
19:2:2007:CLA:HAC2	19:3:2009:CLA:HED3	1.38	1.05
19:2:2014:CLA:C10	19:2:2014:CLA:H152	1.75	1.05
17:3:185:GLN:HG2	17:3:186:TYR:N	1.45	1.05
1:A:281:LEU:CD2	19:A:1115:CLA:CED	2.33	1.05
1:A:425:THR:HB	1:A:428:TYR:CE1	1.90	1.05
4:D:102:ILE:HD12	4:D:137:CYS:HB3	1.39	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:SER:O	7:G:68:THR:OG1	1.74	1.05
8:H:58:LEU:HB3	8:H:61:THR:HG21	1.36	1.05
10:J:31:ARG:HH22	19:J:1311:CLA:C4B	1.69	1.05
15:1:189:LYS:CB	19:1:1007:CLA:CMC	2.33	1.05
15:1:189:LYS:HB2	19:1:1007:CLA:HMC3	1.35	1.05
16:2:182:ILE:HB	16:2:187:LYS:HB3	1.05	1.05
22:3:7003:LMU:H3B	22:3:7005:LMU:O5B	1.55	1.05
18:4:103:MET:HE3	18:4:208:GLY:HA3	1.37	1.05
1:A:259:TYR:HB3	1:A:260:PRO:HD2	1.37	1.05
1:A:279:ASP:O	1:A:281:LEU:CG	2.03	1.05
2:B:11:GLY:CA	3:C:71:HIS:HD2	1.68	1.05
2:B:87:ILE:HA	2:B:115:ASN:HA	1.38	1.05
10:J:37:LEU:O	10:J:38:ILE:HG13	1.56	1.05
15:1:78:ARG:HG3	15:1:81:GLU:OE1	1.55	1.05
19:1:1013:CLA:O1D	19:1:1013:CLA:HAA2	1.53	1.05
19:2:2014:CLA:H41	19:2:2014:CLA:H72	1.39	1.05
19:3:1147:CLA:CBC	19:3:1147:CLA:CMC	2.30	1.05
1:A:51:THR:CG2	19:A:1139:CLA:HBB2	1.85	1.05
1:A:250:LEU:CB	17:3:136:TRP:CH2	2.39	1.05
1:A:581:CYS:HB2	1:A:590:CYS:HA	1.38	1.05
1:A:715:LYS:CD	6:F:230:ASN:HD21	1.69	1.05
2:B:11:GLY:HA3	3:C:71:HIS:CD2	1.91	1.05
2:B:517:PHE:CD2	2:B:517:PHE:O	2.09	1.05
3:C:44:ARG:HB3	4:D:182:GLN:CD	1.80	1.05
4:D:114:MET:SD	4:D:115:PRO:O	2.15	1.05
5:E:127:GLU:O	5:E:128:VAL:HG23	1.55	1.05
6:F:190:LYS:HZ3	6:F:192:THR:HG22	1.17	1.05
7:G:131:GLY:HA2	7:G:136:VAL:HG23	1.35	1.05
16:2:103:VAL:HG13	16:2:104:GLN:OE1	1.56	1.05
16:2:160:ILE:HG21	19:2:2012:CLA:CBB	1.81	1.05
1:A:451:ILE:CD1	19:A:1131:CLA:CED	2.35	1.04
1:A:588:GLY:CA	2:B:668:ARG:HD3	1.86	1.04
3:C:54:CYS:SG	23:C:8002:SF4:S1	2.54	1.04
8:H:85:GLU:HG3	8:H:86:THR:H	1.10	1.04
15:1:97:ILE:CD1	15:1:98:LEU:CB	2.34	1.04
16:2:174:PRO:HB2	16:2:194:GLY:HA3	1.37	1.04
19:3:2009:CLA:HBD	19:3:2009:CLA:O1A	1.52	1.04
22:4:7034:LMU:C9	22:4:7052:LMU:H2'	1.86	1.04
1:A:120:ALA:H	1:A:145:ILE:HD11	1.15	1.04
1:A:443:ILE:CD1	1:A:557:LEU:CD2	2.33	1.04
2:B:319:HIS:CE1	2:B:322:LEU:HD12	1.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:VAL:CB	3:C:65:VAL:HG23	1.88	1.04
22:D:7050:LMU:H6E	22:D:7050:LMU:H2B	1.05	1.04
6:F:190:LYS:HZ3	6:F:192:THR:CG2	1.57	1.04
12:L:153:PHE:HB2	12:L:155:GLU:OE1	1.55	1.04
15:1:78:ARG:HH21	15:1:179:LYS:HD2	1.14	1.04
15:1:83:GLU:C	15:1:86:HIS:HD2	1.64	1.04
18:4:90:TRP:CG	18:4:91:PHE:H	1.74	1.04
22:4:7034:LMU:C8	22:4:7052:LMU:C2'	2.01	1.04
2:B:213:LEU:HD12	2:B:214:ASP:N	1.72	1.04
2:B:694:ARG:HG2	2:B:694:ARG:HH21	0.90	1.04
21:B:6020:BCR:H333	19:L:1502:CLA:CHC	1.87	1.04
15:1:162:LYS:H	15:1:164:PRO:HG3	1.18	1.04
17:3:201:ALA:HB1	17:3:202:TYR:CD2	1.92	1.04
18:4:88:LEU:C	18:4:90:TRP:HB3	1.82	1.04
18:4:158:GLN:CB	19:4:1004:CLA:HMA2	1.78	1.04
1:A:308:ILE:CD1	19:A:1115:CLA:CHC	2.34	1.04
12:L:131:SER:N	12:L:201:TYR:CE2	2.25	1.04
16:2:226:ARG:CD	16:2:230:LEU:CD2	2.35	1.04
17:3:113:ALA:HB2	17:3:239:LEU:HD11	1.11	1.04
18:4:169:ASP:HA	18:4:173:LYS:HA	1.35	1.04
19:A:9022:CLA:H151	21:B:6017:BCR:H20C	1.36	1.04
2:B:202:SER:OG	2:B:270:LEU:HD22	1.57	1.04
19:B:1220:CLA:NA	19:B:1220:CLA:C4	2.21	1.04
3:C:64:SER:O	3:C:65:VAL:CG1	2.06	1.04
22:R:7014:LMU:H62	22:R:7014:LMU:H11	1.34	1.04
16:2:165:GLY:O	16:2:167:ARG:HB3	1.55	1.04
19:3:3011:CLA:HAC2	19:3:3012:CLA:C2A	1.88	1.04
1:A:86:LEU:HD13	1:A:178:MET:CE	1.87	1.03
1:A:126:ILE:O	1:A:127:VAL:HG22	1.54	1.03
1:A:575:LEU:HD12	1:A:576:GLY:HA3	1.40	1.03
2:B:294:ASN:HD22	7:G:94:GLN:CB	1.71	1.03
2:B:469:LYS:HG3	2:B:470:THR:HG23	1.35	1.03
6:F:170:ILE:HG21	21:F:6014:BCR:C37	1.88	1.03
12:L:145:LEU:HD11	21:L:6019:BCR:H313	1.39	1.03
13:N:139:LYS:HD2	13:N:142:LYS:HZ3	1.17	1.03
16:2:186:ASN:CG	16:2:188:LEU:CD1	2.25	1.03
17:3:150:TYR:O	17:3:152:ALA:N	1.91	1.03
22:3:7003:LMU:C3B	22:3:7005:LMU:C5B	2.35	1.03
1:A:343:HIS:O	1:A:346:LEU:HB2	1.56	1.03
2:B:120:VAL:CA	2:B:123:TRP:CD1	2.39	1.03
2:B:459:PHE:CD2	19:B:1235:CLA:CMD	2.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:6016:BCR:H321	21:F:6016:BCR:HC8	1.05	1.03
7:G:102:ALA:HA	7:G:104:ASP:CG	1.82	1.03
8:H:77:ASN:CG	8:H:78:PRO:HD2	1.81	1.03
11:K:97:ASP:CB	11:K:101:PHE:HE2	1.72	1.03
16:2:156:GLU:HG2	16:2:157:LEU:HD13	1.08	1.03
17:3:122:LEU:HD21	19:3:3006:CLA:C4D	1.87	1.03
18:4:158:GLN:HE22	19:4:1004:CLA:CHA	1.72	1.03
1:A:98:PHE:O	1:A:100:GLY:N	1.90	1.03
1:A:525:ASN:HB3	1:A:526:LYS:HG3	1.40	1.03
2:B:486:LEU:HB2	19:B:1232:CLA:HMD2	1.39	1.03
13:N:130:ASN:O	13:N:132:THR:CG2	2.06	1.03
16:2:120:ILE:HG13	16:2:121:PHE:N	1.69	1.03
16:2:124:GLU:O	16:2:127:THR:HA	1.59	1.03
16:2:195:TYR:HD1	16:2:196:PRO:CD	1.70	1.03
21:3:6022:BCR:H23C	21:3:6022:BCR:H393	1.04	1.03
1:A:484:LEU:H	1:A:484:LEU:CD2	1.71	1.03
2:B:199:ILE:HG23	2:B:270:LEU:HD13	1.05	1.03
6:F:200:VAL:HG12	10:J:7:TYR:CB	1.89	1.03
7:G:72:LEU:HD22	7:G:124:ILE:HD12	1.37	1.03
8:H:58:LEU:HD12	8:H:62:THR:HG23	1.06	1.03
13:N:146:LEU:CD1	17:3:142:ILE:C	2.31	1.03
15:1:206:SER:O	15:1:209:PRO:HG3	1.59	1.03
16:2:229:MET:SD	16:2:230:LEU:HD13	1.98	1.03
18:4:111:LEU:HD12	18:4:112:PRO:CD	1.88	1.03
18:4:141:LEU:H	18:4:141:LEU:HD22	1.19	1.03
19:4:4002:CLA:CGD	19:4:4002:CLA:HAA2	1.86	1.03
19:A:1112:CLA:C3B	21:A:6002:BCR:H19C	1.89	1.03
2:B:224:PRO:HB2	2:B:227:THR:HB	1.36	1.03
2:B:490:ARG:HG3	2:B:490:ARG:NH1	1.61	1.03
3:C:5:VAL:CG2	3:C:65:VAL:CG2	2.36	1.03
5:E:99:THR:CG2	5:E:100:ARG:H	1.69	1.03
6:F:97:GLN:CD	6:F:98:ALA:H	1.67	1.03
8:H:58:LEU:CG	8:H:61:THR:HB	1.88	1.03
8:H:58:LEU:HD13	8:H:62:THR:HG21	1.41	1.03
10:J:2:ARG:HH12	10:J:8:LEU:HD13	1.21	1.03
15:1:85:ILE:HA	15:1:88:ARG:CG	1.89	1.03
19:1:1013:CLA:C6	19:1:1014:CLA:CED	2.35	1.03
19:3:3016:CLA:H142	19:3:3016:CLA:C10	1.89	1.03
18:4:210:LEU:O	18:4:214:PHE:HB2	1.59	1.03
1:A:370:ILE:HG23	1:A:403:GLY:HA3	1.36	1.02
1:A:555:ILE:HD11	19:A:9023:CLA:OBD	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:558:PRO:CG	2:B:703:VAL:HG22	1.88	1.02
7:G:64:ILE:O	7:G:68:THR:CG2	2.06	1.02
7:G:90:GLN:HB3	7:G:91:VAL:O	1.58	1.02
19:K:1143:CLA:O1A	19:K:1143:CLA:H3A	1.59	1.02
19:R:1150:CLA:HBA2	19:R:1150:CLA:HBD	1.35	1.02
15:1:170:PRO:HD2	15:1:173:TYR:CE2	1.93	1.02
19:1:1303:CLA:HMC1	19:1:1303:CLA:HBC2	1.37	1.02
18:4:103:MET:HE1	18:4:208:GLY:N	1.70	1.02
18:4:193:ASN:O	18:4:194:PHE:CD1	2.12	1.02
1:A:64:PHE:CE2	1:A:74:ILE:CG2	2.42	1.02
2:B:199:ILE:HG23	2:B:270:LEU:CD1	1.88	1.02
2:B:459:PHE:CD2	19:B:1235:CLA:CAD	2.40	1.02
2:B:504:ASN:OD1	2:B:504:ASN:O	1.77	1.02
19:B:1235:CLA:HBC1	6:F:160:PHE:CZ	1.93	1.02
7:G:98:THR:CB	7:G:101:GLU:OE2	2.01	1.02
8:H:97:LEU:CD1	8:H:100:PHE:HB2	1.88	1.02
11:K:125:LYS:HB2	11:K:128:GLY:HA2	1.38	1.02
15:1:97:ILE:HD11	15:1:98:LEU:HA	1.34	1.02
15:1:162:LYS:N	15:1:164:PRO:HG3	1.73	1.02
16:2:130:GLY:HA3	16:2:131:ILE:HG13	1.03	1.02
19:3:3011:CLA:HMA1	19:3:3011:CLA:H12	1.36	1.02
18:4:158:GLN:HB3	19:4:1004:CLA:HMA1	1.05	1.02
18:4:175:TYR:O	18:4:194:PHE:CZ	2.12	1.02
1:A:541:VAL:HG11	1:A:615:HIS:CD2	1.93	1.02
4:D:140:LEU:HA	4:D:143:ARG:HB2	1.03	1.02
7:G:124:ILE:HG12	7:G:128:LEU:CD1	1.89	1.02
8:H:58:LEU:HD12	8:H:61:THR:CA	1.89	1.02
16:2:133:ASN:HD22	16:2:134:THR:CA	1.71	1.02
16:2:246:PRO:CB	16:2:247:ILE:HD13	1.89	1.02
1:A:255:LEU:HD13	1:A:280:PHE:HZ	1.20	1.02
2:B:5:ILE:HG22	2:B:6:PRO:HD3	1.05	1.02
2:B:90:ALA:CA	2:B:113:VAL:HG13	1.88	1.02
2:B:160:LYS:HD3	2:B:161:TRP:CD2	1.94	1.02
20:B:5002:PQN:C16	21:B:6017:BCR:C33	2.37	1.02
4:D:111:ILE:HG12	4:D:121:ILE:CG2	1.88	1.02
7:G:99:HIS:C	7:G:101:GLU:HB2	1.84	1.02
19:H:1241:CLA:CAC	21:I:6021:BCR:HC31	1.88	1.02
22:R:7020:LMU:H6E	22:R:7020:LMU:C5B	1.89	1.02
15:1:189:LYS:HG3	19:1:1007:CLA:HMC1	1.06	1.02
16:2:122:ILE:O	16:2:126:LEU:HG	1.60	1.02
17:3:150:TYR:HD2	17:3:151:TRP:NE1	1.45	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:OE2	1:A:161:GLU:HG3	1.58	1.02
1:A:249:ILE:O	1:A:251:ASN:N	1.93	1.02
1:A:281:LEU:HD21	19:A:1115:CLA:CMA	1.85	1.02
19:A:1104:CLA:H43	19:A:1128:CLA:H11	1.38	1.02
2:B:310:PRO:O	19:B:1301:CLA:CHD	2.07	1.02
2:B:438:VAL:HG22	19:B:1230:CLA:HMC2	1.40	1.02
22:E:7048:LMU:C6B	22:E:7048:LMU:H3'	1.89	1.02
12:L:96:LEU:H	12:L:96:LEU:CD2	1.67	1.02
12:L:112:GLY:HA3	19:L:1503:CLA:CHC	1.90	1.02
12:L:171:LYS:O	12:L:173:PRO:HD2	1.59	1.02
16:2:122:ILE:CD1	19:2:2002:CLA:CAB	2.36	1.02
17:3:135:ALA:HB1	17:3:139:THR:HB	1.34	1.02
1:A:149:PHE:O	1:A:150:PHE:HB2	1.54	1.01
1:A:351:THR:O	19:A:1123:CLA:C19	2.07	1.01
1:A:370:ILE:HG22	1:A:400:MET:HA	1.41	1.01
2:B:542:ARG:HH11	2:B:542:ARG:CG	1.71	1.01
6:F:88:SER:OG	6:F:91:PHE:HB3	1.58	1.01
19:L:1148:CLA:HED1	19:L:1148:CLA:C1	1.90	1.01
16:2:117:ALA:O	16:2:120:ILE:HG12	1.58	1.01
1:A:21:LEU:O	1:A:21:LEU:CD1	2.08	1.01
1:A:157:GLY:HA3	1:A:229:ILE:HG22	1.40	1.01
1:A:340:GLY:O	1:A:343:HIS:HB2	1.58	1.01
2:B:120:VAL:CG2	2:B:123:TRP:HE1	1.74	1.01
4:D:95:GLN:NE2	4:D:96:VAL:HA	1.76	1.01
6:F:200:VAL:HG13	10:J:7:TYR:H	1.25	1.01
7:G:123:ASN:HA	7:G:126:ASP:OD2	1.58	1.01
19:H:1241:CLA:HAC2	21:I:6021:BCR:HC31	1.42	1.01
12:L:92:ALA:N	12:L:98:ARG:NH1	2.06	1.01
13:N:157:LYS:HB3	13:N:159:LYS:N	1.73	1.01
18:4:120:ILE:HD12	18:4:226:LYS:HG3	1.40	1.01
18:4:158:GLN:C	19:4:1004:CLA:HMA1	1.86	1.01
18:4:170:PRO:HG3	19:4:4011:CLA:C2D	1.90	1.01
19:4:1304:CLA:HAA2	19:4:1304:CLA:HED3	1.03	1.01
1:A:157:GLY:CA	1:A:229:ILE:HG21	1.89	1.01
19:A:1124:CLA:HED2	19:A:1125:CLA:CAD	1.91	1.01
19:A:1134:CLA:CBC	21:A:6008:BCR:HC31	1.90	1.01
2:B:98:GLN:C	2:B:100:ALA:H	1.63	1.01
2:B:120:VAL:HA	2:B:123:TRP:HD1	1.23	1.01
3:C:44:ARG:CA	4:D:182:GLN:OE1	2.08	1.01
5:E:99:THR:HG22	5:E:100:ARG:N	1.65	1.01
15:1:64:PHE:O	15:1:69:LEU:HD13	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:84:LEU:O	15:1:88:ARG:HG3	1.60	1.01
15:1:112:GLN:HG2	15:1:113:GLU:H	1.20	1.01
17:3:243:ILE:HG12	19:3:3005:CLA:C4C	1.88	1.01
22:3:7005:LMU:C1	22:3:7005:LMU:H51	1.88	1.01
1:A:132:LEU:HD11	1:A:674:ALA:HB2	1.41	1.01
1:A:328:LYS:CD	1:A:332:GLU:HB2	1.88	1.01
1:A:368:LEU:HD21	19:A:1117:CLA:H93	1.42	1.01
4:D:140:LEU:CD1	4:D:144:LEU:HB2	1.89	1.01
11:K:49:ILE:C	11:K:52:PRO:HG2	1.77	1.01
11:K:81:THR:CG2	11:K:83:GLY:H	1.71	1.01
15:1:97:ILE:CG1	15:1:98:LEU:N	2.22	1.01
19:1:1010:CLA:HBC3	19:1:1010:CLA:CHD	1.89	1.01
16:2:118:ALA:C	16:2:121:PHE:CE2	2.37	1.01
16:2:184:PRO:HG3	16:2:187:LYS:H	1.24	1.01
17:3:150:TYR:CB	17:3:151:TRP:HD1	1.71	1.01
1:A:227:LEU:CD2	1:A:296:LEU:O	2.09	1.01
1:A:249:ILE:HG23	17:3:136:TRP:HZ3	0.85	1.01
1:A:426:THR:HG22	1:A:428:TYR:CE2	1.96	1.01
1:A:575:LEU:CD1	1:A:576:GLY:HA3	1.90	1.01
19:A:9012:CLA:C1	2:B:616:LEU:CD1	2.39	1.01
19:B:1223:CLA:HED1	19:B:1231:CLA:HBB2	1.41	1.01
15:1:78:ARG:HD3	19:1:1011:CLA:CMC	1.91	1.01
15:1:136:THR:O	15:1:140:ILE:HG12	1.61	1.01
15:1:170:PRO:HD2	15:1:173:TYR:CD2	1.96	1.01
18:4:159:ASP:CG	18:4:171:ILE:HD11	1.85	1.01
1:A:487:VAL:HG13	1:A:489:ALA:H	0.89	1.00
19:A:1124:CLA:HBA2	19:A:1137:CLA:HED1	1.38	1.00
2:B:457:PRO:HB3	2:B:517:PHE:HB2	1.44	1.00
2:B:545:LYS:CD	2:B:546:LEU:H	1.74	1.00
19:B:1205:CLA:HBB2	19:B:1205:CLA:H92	1.44	1.00
20:B:5002:PQN:H162	21:B:6017:BCR:H333	1.05	1.00
8:H:111:TYR:C	8:H:112:LEU:HD23	1.86	1.00
11:K:49:ILE:O	11:K:52:PRO:CD	2.08	1.00
12:L:92:ALA:HB2	12:L:98:ARG:NH2	1.75	1.00
13:N:146:LEU:HD13	17:3:142:ILE:C	1.85	1.00
15:1:77:GLU:HG3	15:1:80:LYS:HD2	1.42	1.00
15:1:189:LYS:HE2	15:1:189:LYS:CA	1.86	1.00
16:2:118:ALA:C	16:2:121:PHE:HE2	1.68	1.00
17:3:95:PRO:O	17:3:96:ARG:CG	2.09	1.00
17:3:122:LEU:HD22	19:3:3006:CLA:C1A	1.90	1.00
2:B:409:ALA:O	2:B:410:ARG:HB2	1.56	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:GLY:O	7:G:97:LEU:HG	1.62	1.00
13:N:147:SER:HB3	13:N:151:ASP:CA	1.91	1.00
15:1:162:LYS:H	15:1:164:PRO:CG	1.73	1.00
22:1:7004:LMU:H12	22:1:7004:LMU:H3'	1.43	1.00
18:4:96:LEU:HD11	18:4:100:ARG:CZ	1.90	1.00
1:A:342:GLY:HA2	1:A:430:ASP:CB	1.91	1.00
2:B:120:VAL:HG22	2:B:123:TRP:NE1	1.77	1.00
19:B:1222:CLA:HBB1	19:B:1236:CLA:HHB	1.40	1.00
19:B:1228:CLA:HHD	19:B:1228:CLA:CBC	1.91	1.00
3:C:62:PHE:CE2	5:E:80:GLU:CD	2.40	1.00
3:C:69:LEU:CD1	3:C:70:TRP:O	2.09	1.00
6:F:200:VAL:CG1	10:J:7:TYR:CB	2.39	1.00
7:G:84:ARG:CG	7:G:85:GLU:N	2.24	1.00
8:H:56:GLU:HG3	8:H:57:ASP:CA	1.92	1.00
12:L:79:ILE:HD11	19:L:1130:CLA:C4	1.90	1.00
13:N:133:GLY:C	13:N:134:CYS:SG	2.44	1.00
15:1:77:GLU:HA	15:1:80:LYS:CD	1.91	1.00
15:1:134:LEU:CA	15:1:137:ILE:HD11	1.91	1.00
16:2:147:THR:HG22	16:2:148:ASP:OD2	1.61	1.00
1:A:267:THR:CG2	1:A:269:PHE:HE2	1.74	1.00
2:B:638:LEU:O	2:B:639:VAL:HG12	1.60	1.00
2:B:732:LYS:CG	2:B:734:GLY:N	2.23	1.00
4:D:140:LEU:HD21	4:D:144:LEU:CD1	1.90	1.00
4:D:187:ASN:HD22	4:D:187:ASN:N	1.60	1.00
11:K:99:ALA:O	11:K:103:LEU:HD11	1.60	1.00
15:1:93:ALA:HB1	19:1:1006:CLA:HHC	1.42	1.00
15:1:157:ASP:HB2	15:1:178:LYS:HB2	1.40	1.00
16:2:160:ILE:CG2	19:2:2012:CLA:HBB1	1.91	1.00
2:B:50:HIS:HD2	19:B:1202:CLA:HAA2	1.24	1.00
2:B:247:THR:CA	2:B:250:ALA:HB2	1.92	1.00
5:E:107:PHE:CD2	5:E:109:LYS:HG3	1.97	1.00
12:L:164:LEU:HD12	12:L:165:THR:N	1.75	1.00
15:1:95:PRO:HA	15:1:98:LEU:CG	1.92	1.00
16:2:165:GLY:O	16:2:167:ARG:CB	2.07	1.00
17:3:176:TRP:O	17:3:178:LYS:HB2	1.62	1.00
1:A:116:ILE:O	1:A:136:VAL:O	1.77	1.00
2:B:353:TYR:CG	2:B:594:TRP:HZ3	1.79	1.00
2:B:560:ASP:HB2	3:C:66:ARG:HE	1.27	1.00
4:D:140:LEU:CA	4:D:143:ARG:HB2	1.90	1.00
22:E:7048:LMU:H3'	22:E:7048:LMU:H6'2	1.44	1.00
12:L:52:PRO:HB2	12:L:55:GLN:O	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HG	19:A:1115:CLA:CBB	1.91	1.00
4:D:167:HIS:CD2	4:D:172:VAL:CG2	2.44	1.00
8:H:78:PRO:HD3	19:L:1501:CLA:HMD2	1.02	1.00
3:C:27:GLU:OE1	3:C:39:ILE:O	1.78	0.99
3:C:72:GLU:HG2	3:C:77:MET:HE2	1.44	0.99
4:D:200:VAL:CG2	4:D:206:GLN:HE21	1.74	0.99
5:E:79:LYS:HA	5:E:84:TYR:CE1	1.97	0.99
22:N:7049:LMU:H61	22:N:7049:LMU:C1	1.91	0.99
22:R:7020:LMU:H5B	22:R:7020:LMU:C6'	1.90	0.99
15:1:68:GLY:O	15:1:72:VAL:HB	1.61	0.99
16:2:218:ARG:HB2	16:2:219:THR:CG2	1.91	0.99
18:4:177:LEU:HD13	18:4:178:PRO:HD3	1.42	0.99
1:A:328:LYS:CG	1:A:332:GLU:HB2	1.92	0.99
1:A:531:PRO:O	1:A:532:ILE:HG22	1.63	0.99
19:A:1124:CLA:CED	19:A:1125:CLA:CAD	2.40	0.99
22:A:7016:LMU:H22	22:A:7016:LMU:H61	1.42	0.99
19:A:9022:CLA:HBB2	19:A:9023:CLA:C1B	1.92	0.99
2:B:58:PHE:CD2	2:B:145:LEU:HD22	1.97	0.99
2:B:160:LYS:HZ2	2:B:161:TRP:CG	1.80	0.99
2:B:430:GLY:HA2	2:B:525:LEU:HD11	1.41	0.99
13:N:114:PHE:HB3	13:N:117:ALA:HB3	1.41	0.99
16:2:104:GLN:O	16:2:107:LEU:HG	1.62	0.99
16:2:171:ILE:CG1	16:2:172:LEU:N	2.25	0.99
16:2:172:LEU:HB3	16:2:173:ASN:ND2	1.77	0.99
1:A:246:HIS:CA	1:A:248:PHE:HE2	1.75	0.99
1:A:336:GLY:HA3	1:A:339:THR:OG1	1.62	0.99
2:B:131:THR:HG22	2:B:134:ASP:HB2	1.44	0.99
19:B:1213:CLA:HHD	19:B:1213:CLA:HBC2	1.44	0.99
4:D:201:LYS:H	4:D:201:LYS:CD	1.66	0.99
1:A:208:ALA:HA	1:A:310:PHE:O	1.62	0.99
1:A:451:ILE:CD1	19:A:1131:CLA:HED3	1.92	0.99
19:A:1138:CLA:H191	6:F:181:TYR:HB3	1.41	0.99
2:B:7:ARG:HH11	2:B:7:ARG:CG	1.75	0.99
2:B:58:PHE:CE2	2:B:145:LEU:CD2	2.44	0.99
2:B:58:PHE:HB2	2:B:146:SER:HB3	1.41	0.99
2:B:73:ASN:O	2:B:121:TYR:CZ	2.16	0.99
16:2:254:LEU:C	16:2:254:LEU:CD2	2.30	0.99
17:3:127:LEU:CB	19:3:1147:CLA:HED1	1.88	0.99
18:4:232:LEU:HB2	18:4:236:ILE:HD12	1.41	0.99
1:A:22:VAL:HG22	1:A:22:VAL:O	1.59	0.99
1:A:51:THR:HG21	19:A:1139:CLA:CBB	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:TYR:N	1:A:422:TYR:HD1	1.58	0.99
3:C:72:GLU:CG	3:C:77:MET:HE2	1.92	0.99
13:N:130:ASN:HB3	13:N:139:LYS:HG2	1.40	0.99
15:1:66:PRO:HD2	15:1:67:LEU:H	1.23	0.99
17:3:173:PHE:HD1	17:3:174:GLN:N	1.59	0.99
19:4:4006:CLA:C10	22:4:7034:LMU:C12	2.40	0.99
1:A:102:ARG:C	1:A:103:PHE:HD2	1.70	0.99
2:B:294:ASN:ND2	7:G:94:GLN:N	2.11	0.99
3:C:80:ALA:O	3:C:81:TYR:HB3	1.62	0.99
15:1:137:ILE:O	15:1:141:GLU:HG2	1.63	0.99
16:2:139:THR:HG23	16:2:140:ALA:H	1.21	0.99
17:3:109:ALA:HA	17:3:111:LEU:CB	1.91	0.99
1:A:249:ILE:O	1:A:252:ARG:HG3	1.62	0.99
1:A:534:LEU:CD1	1:A:535:GLY:N	2.25	0.99
2:B:694:ARG:HG2	2:B:694:ARG:NH2	1.62	0.99
3:C:52:LYS:HZ1	3:C:64:SER:CB	1.76	0.99
4:D:103:THR:HG22	4:D:128:LEU:HG	1.42	0.99
14:R:52:UNK:CA	14:R:53:UNK:CB	2.36	0.99
19:2:2002:CLA:HBC2	19:2:2002:CLA:HHD	1.43	0.99
22:4:7052:LMU:H61	22:4:7052:LMU:O1'	1.61	0.99
2:B:199:ILE:CG2	2:B:270:LEU:HD13	1.92	0.99
19:B:1205:CLA:H92	19:B:1205:CLA:CBB	1.93	0.99
4:D:200:VAL:HG21	4:D:206:GLN:HE21	0.84	0.99
17:3:96:ARG:NH1	17:3:96:ARG:HB2	1.77	0.99
19:A:1141:CLA:H121	19:A:1141:CLA:C7	1.91	0.99
2:B:85:ARG:HG2	2:B:85:ARG:HH11	1.24	0.99
2:B:268:LEU:HD21	19:B:1214:CLA:CMA	1.91	0.99
19:B:1202:CLA:O1A	19:B:1202:CLA:H62	1.63	0.99
8:H:97:LEU:CD1	8:H:100:PHE:CB	2.41	0.99
15:1:178:LYS:HG3	15:1:179:LYS:H	1.23	0.99
16:2:237:PHE:HA	16:2:240:ILE:CD1	1.92	0.99
1:A:368:LEU:CD2	19:A:1117:CLA:C9	2.41	0.99
1:A:699:TYR:OH	2:B:533:ILE:HG22	1.61	0.99
2:B:490:ARG:HH11	2:B:490:ARG:CG	1.75	0.99
21:F:6016:BCR:HC8	21:F:6016:BCR:C32	1.89	0.99
12:L:79:ILE:CD1	19:L:1130:CLA:H42	1.92	0.99
1:A:163:GLN:CG	1:A:164:LEU:H	1.74	0.98
1:A:365:LEU:CD2	19:A:1103:CLA:HED3	1.92	0.98
1:A:715:LYS:NZ	6:F:230:ASN:OD1	1.95	0.98
2:B:58:PHE:CB	2:B:146:SER:HB3	1.93	0.98
7:G:90:GLN:HB2	7:G:92:PRO:HD3	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:70:PHE:C	11:K:70:PHE:HD1	1.71	0.98
12:L:60:ILE:CG2	12:L:61:ASN:N	2.12	0.98
12:L:96:LEU:HD23	12:L:96:LEU:N	1.77	0.98
15:1:129:VAL:HG12	15:1:130:PRO:HD3	1.41	0.98
15:1:161:LYS:HE2	15:1:162:LYS:HB2	1.45	0.98
15:1:190:ASN:HD21	19:1:1002:CLA:CHA	1.76	0.98
16:2:177:VAL:HG12	16:2:178:ASN:CB	1.93	0.98
18:4:223:VAL:O	18:4:223:VAL:HG12	1.63	0.98
1:A:567:ARG:HH12	4:D:89:GLY:HA2	1.21	0.98
11:K:63:LEU:HD13	11:K:63:LEU:N	1.75	0.98
17:3:159:VAL:HG13	17:3:160:LEU:N	1.72	0.98
1:A:106:TYR:O	1:A:110:LEU:HD23	1.61	0.98
1:A:120:ALA:N	1:A:145:ILE:CD1	2.26	0.98
1:A:397:THR:HG22	1:A:613:ILE:CG1	1.92	0.98
15:1:198:PHE:O	15:1:202:CYS:HB3	1.63	0.98
1:A:90:PHE:CE1	19:A:1103:CLA:H91	1.99	0.98
2:B:476:ILE:CG2	2:B:479:SER:OG	2.11	0.98
4:D:158:PHE:HB3	4:D:159:PRO:O	1.60	0.98
8:H:63:GLY:O	8:H:66:ASP:OD1	1.81	0.98
19:J:1308:CLA:C9	19:2:2014:CLA:O1D	2.11	0.98
17:3:150:TYR:HD2	17:3:151:TRP:CE2	1.80	0.98
1:A:605:MET:HA	1:A:608:SER:OG	1.63	0.98
1:A:711:HIS:CD2	19:A:1139:CLA:HBC1	1.98	0.98
2:B:622:ASP:HB2	2:B:626:LEU:HD12	1.42	0.98
3:C:1:MET:HG2	3:C:4:SER:OG	1.62	0.98
19:4:1304:CLA:C20	19:4:1304:CLA:H151	1.93	0.98
1:A:132:LEU:O	1:A:671:SER:O	1.80	0.98
2:B:189:ALA:HB2	19:B:1225:CLA:H203	1.46	0.98
2:B:429:LEU:O	2:B:525:LEU:CD1	2.11	0.98
13:N:146:LEU:CD2	17:3:142:ILE:O	2.10	0.98
17:3:173:PHE:HD1	17:3:173:PHE:C	1.70	0.98
1:A:249:ILE:HG21	17:3:136:TRP:HZ3	1.24	0.98
2:B:303:TYR:HA	2:B:306:GLU:HB2	1.45	0.98
22:E:7048:LMU:H72	22:E:7048:LMU:H111	1.45	0.98
8:H:58:LEU:HD13	8:H:62:THR:CG2	1.92	0.98
8:H:89:ALA:HA	8:H:92:THR:HB	1.45	0.98
19:L:1148:CLA:HHD	19:L:1148:CLA:CBC	1.93	0.98
16:2:237:PHE:CA	16:2:240:ILE:HD12	1.92	0.98
16:2:269:LYS:HA	16:2:269:LYS:HZ2	1.22	0.98
1:A:64:PHE:HZ	1:A:77:LYS:HE2	1.29	0.98
1:A:267:THR:HG22	1:A:269:PHE:HE2	1.18	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:ILE:CD1	19:B:1216:CLA:CED	2.39	0.98
13:N:132:THR:OG1	13:N:137:LEU:O	1.82	0.98
1:A:68:THR:CG2	1:A:70:ASP:H	1.76	0.98
1:A:193:LEU:HA	1:A:196:PHE:HE2	1.27	0.98
2:B:294:ASN:CB	7:G:94:GLN:CD	2.37	0.98
3:C:52:LYS:HZ1	3:C:64:SER:HB2	1.25	0.98
13:N:139:LYS:CB	13:N:142:LYS:CD	2.41	0.98
19:A:9022:CLA:C15	21:B:6017:BCR:H20C	1.93	0.98
6:F:219:ARG:HH11	6:F:219:ARG:CG	1.75	0.98
21:J:6012:BCR:H23C	21:J:6012:BCR:H393	1.46	0.98
18:4:96:LEU:HD11	18:4:100:ARG:NH1	1.77	0.98
1:A:51:THR:OG1	19:A:1139:CLA:HBB2	1.62	0.97
1:A:89:ILE:O	1:A:92:TRP:O	1.82	0.97
1:A:217:SER:HG	21:A:6002:BCR:H15C	1.24	0.97
8:H:97:LEU:HD11	8:H:100:PHE:CB	1.94	0.97
12:L:154:ASN:O	12:L:178:THR:CG2	2.11	0.97
1:A:454:GLY:H	1:A:457:SER:HB3	1.23	0.97
12:L:155:GLU:HA	12:L:178:THR:CG2	1.93	0.97
16:2:119:GLY:O	16:2:123:PRO:HG2	1.63	0.97
18:4:87:ASN:CB	18:4:90:TRP:CE3	2.46	0.97
18:4:172:PHE:HB2	18:4:194:PHE:CD2	1.97	0.97
2:B:732:LYS:HB3	2:B:733:PHE:HA	1.45	0.97
7:G:99:HIS:HA	7:G:100:PHE:HB3	1.46	0.97
19:H:1145:CLA:HMC3	19:H:1145:CLA:HBC2	1.45	0.97
22:H:7032:LMU:H31	22:H:7032:LMU:C1B	1.92	0.97
12:L:79:ILE:HD11	19:L:1130:CLA:H42	1.00	0.97
15:1:91:MET:C	15:1:95:PRO:HD3	1.87	0.97
16:2:103:VAL:CG1	16:2:104:GLN:OE1	2.12	0.97
19:2:2007:CLA:HBC1	19:3:2009:CLA:HED2	1.00	0.97
19:4:1304:CLA:H151	19:4:1304:CLA:H203	1.45	0.97
1:A:129:GLN:O	1:A:130:GLU:HB3	1.62	0.97
2:B:353:TYR:CD2	2:B:594:TRP:CZ3	2.51	0.97
11:K:127:ILE:HB	11:K:129:ALA:HB1	1.45	0.97
12:L:73:VAL:HA	19:L:1504:CLA:CMA	1.92	0.97
15:1:149:GLU:HG2	15:1:152:ARG:HH12	1.16	0.97
17:3:156:THR:O	17:3:158:PHE:C	2.08	0.97
11:K:92:GLY:O	11:K:93:LEU:CG	2.11	0.97
1:A:491:TRP:HE1	19:A:1135:CLA:H12	1.27	0.97
1:A:564:ARG:HB3	1:A:564:ARG:HH21	1.29	0.97
15:1:158:PRO:HA	15:1:175:LYS:HG3	1.46	0.97
1:A:57:LEU:HD23	1:A:57:LEU:C	1.88	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:GLU:O	2:B:176:ASN:HB2	1.64	0.97
2:B:708:VAL:O	2:B:712:HIS:HB2	1.62	0.97
16:2:113:ALA:C	16:2:114:MET:HE3	1.90	0.97
17:3:201:ALA:C	17:3:202:TYR:CD2	2.42	0.97
8:H:99:LYS:O	8:H:101:LEU:N	1.97	0.97
11:K:125:LYS:HA	11:K:126:ASN:HB3	0.97	0.97
13:N:139:LYS:HE3	13:N:142:LYS:HE2	0.98	0.97
15:1:171:LEU:HA	15:1:173:TYR:CZ	2.00	0.97
1:A:296:LEU:HD12	1:A:297:THR:HG22	1.47	0.97
19:A:1122:CLA:C1D	21:A:6007:BCR:H19C	1.93	0.97
2:B:213:LEU:HD12	2:B:214:ASP:H	1.29	0.97
2:B:527:LEU:HD13	19:B:1236:CLA:CMA	1.94	0.97
4:D:140:LEU:HA	4:D:143:ARG:CB	1.93	0.97
6:F:139:LEU:HD13	6:F:149:ILE:CD1	1.93	0.97
8:H:109:LEU:O	8:H:113:SER:HB2	1.63	0.97
18:4:169:ASP:CA	18:4:173:LYS:HA	1.94	0.97
1:A:64:PHE:CE2	1:A:74:ILE:HG21	2.00	0.97
5:E:126:VAL:C	5:E:127:GLU:HG3	1.88	0.97
6:F:221:LEU:HD23	6:F:222:LEU:HD23	1.46	0.97
22:H:7030:LMU:H91	22:H:7030:LMU:C5	1.93	0.97
11:K:49:ILE:HA	11:K:52:PRO:CG	1.92	0.97
13:N:122:PHE:N	13:N:122:PHE:HD2	1.60	0.97
15:1:67:LEU:CD1	15:1:68:GLY:N	2.27	0.97
15:1:78:ARG:NH2	15:1:179:LYS:HD2	1.80	0.97
16:2:126:LEU:HB3	19:2:2006:CLA:H192	1.45	0.97
16:2:237:PHE:HA	16:2:240:ILE:HD12	0.98	0.97
2:B:666:SER:HB3	2:B:671:TRP:HE1	1.27	0.96
5:E:99:THR:HG22	5:E:100:ARG:H	0.81	0.96
8:H:113:SER:OG	19:H:1207:CLA:H61	1.65	0.96
11:K:98:PRO:HD2	11:K:99:ALA:H	1.28	0.96
13:N:136:ASP:O	13:N:137:LEU:HD22	1.64	0.96
2:B:594:TRP:O	2:B:595:HIS:HB3	1.61	0.96
8:H:86:THR:HG22	8:H:87:PHE:O	1.65	0.96
8:H:121:LEU:HB3	8:H:122:PRO:CD	1.95	0.96
22:R:7021:LMU:H1'	22:R:7021:LMU:H31	1.45	0.96
16:2:160:ILE:HG21	19:2:2012:CLA:HBB1	1.44	0.96
1:A:426:THR:HA	1:A:428:TYR:CZ	2.00	0.96
2:B:256:THR:O	2:B:272:ASP:OD1	1.83	0.96
21:F:6016:BCR:C8	21:F:6016:BCR:C32	2.38	0.96
15:1:85:ILE:HA	15:1:88:ARG:HG3	1.47	0.96
17:3:254:GLN:HG3	17:3:255:ASN:H	1.27	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:145:GLU:HG3	18:4:146:PHE:HD1	1.20	0.96
2:B:189:ALA:CB	19:B:1225:CLA:H203	1.96	0.96
3:C:44:ARG:H	4:D:182:GLN:HG3	1.27	0.96
17:3:176:TRP:CH2	17:3:199:ASN:OD1	2.15	0.96
2:B:621:ARG:O	2:B:625:TRP:HB3	1.66	0.96
16:2:172:LEU:O	16:2:174:PRO:HD3	1.63	0.96
17:3:176:TRP:O	17:3:178:LYS:CB	2.13	0.96
18:4:173:LYS:NZ	18:4:201:LYS:CG	2.27	0.96
3:C:44:ARG:H	4:D:182:GLN:CG	1.77	0.96
5:E:127:GLU:HB3	5:E:128:VAL:O	1.65	0.96
6:F:130:PHE:H	6:F:133:TYR:HE1	1.01	0.96
13:N:157:LYS:N	13:N:157:LYS:HE2	1.80	0.96
1:A:281:LEU:HD22	19:A:1115:CLA:HED3	1.45	0.96
1:A:491:TRP:NE1	19:A:1135:CLA:H12	1.79	0.96
2:B:314:ARG:CZ	15:1:67:LEU:HD21	1.94	0.96
5:E:93:VAL:HG23	5:E:103:VAL:HB	1.46	0.96
16:2:167:ARG:HA	16:2:167:ARG:NE	1.77	0.96
18:4:111:LEU:HD12	18:4:112:PRO:N	1.80	0.96
1:A:308:ILE:HD13	19:A:1115:CLA:H102	1.48	0.96
1:A:430:ASP:O	1:A:432:LEU:N	1.98	0.96
1:A:483:GLN:C	1:A:485:GLN:HE22	1.73	0.96
2:B:480:SER:O	2:B:481:THR:HG22	1.63	0.96
2:B:527:LEU:HD22	19:B:1222:CLA:ND	1.80	0.96
1:A:24:ARG:H	1:A:24:ARG:CD	1.75	0.96
1:A:308:ILE:HD13	19:A:1115:CLA:HHC	1.46	0.96
2:B:422:LEU:HD13	2:B:535:VAL:HG11	1.47	0.96
12:L:138:VAL:O	12:L:142:SER:OG	1.84	0.96
17:3:96:ARG:HH11	17:3:96:ARG:HG3	1.25	0.96
17:3:197:SER:HB3	17:3:206:PRO:HD3	1.46	0.96
1:A:252:ARG:H	1:A:252:ARG:HD3	1.30	0.96
19:B:1219:CLA:HBB2	19:B:1219:CLA:H72	1.47	0.96
21:B:6020:BCR:H333	19:L:1502:CLA:NB	1.81	0.96
4:D:87:THR:CG2	12:L:69:LEU:HD12	1.95	0.96
19:F:1305:CLA:H42	19:4:1306:CLA:HAA1	1.45	0.96
18:4:168:GLN:HB3	18:4:172:PHE:CE1	1.99	0.96
2:B:131:THR:CG2	2:B:134:ASP:HB2	1.94	0.95
2:B:569:ASP:OD1	2:B:706:ARG:NH1	1.99	0.95
4:D:124:GLU:OE1	4:D:125:GLY:HA3	1.66	0.95
4:D:140:LEU:CD1	4:D:144:LEU:CB	2.44	0.95
6:F:207:LEU:HD21	6:F:208:PHE:CD1	2.00	0.95
12:L:141:LEU:CD1	12:L:145:LEU:CD1	2.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:143:VAL:CB	13:N:144:PRO:HD2	1.95	0.95
15:1:177:PRO:HD2	15:1:180:LEU:CD2	1.92	0.95
16:2:103:VAL:O	16:2:106:GLU:N	1.99	0.95
17:3:130:GLN:HB3	17:3:132:THR:H	0.79	0.95
18:4:175:TYR:HB3	18:4:194:PHE:CD1	2.00	0.95
1:A:412:ALA:HB2	1:A:598:VAL:HG11	1.47	0.95
2:B:282:PHE:HZ	19:B:1213:CLA:C1	1.79	0.95
2:B:292:ARG:NH1	2:B:296:GLY:H	1.63	0.95
5:E:111:ASN:HD21	5:E:113:ALA:H	0.96	0.95
6:F:148:LEU:HD12	6:F:148:LEU:O	1.65	0.95
11:K:62:SER:OG	11:K:63:LEU:HD13	1.64	0.95
12:L:137:LEU:HD23	12:L:137:LEU:C	1.91	0.95
15:1:157:ASP:CG	15:1:178:LYS:HA	1.89	0.95
15:1:200:GLY:O	15:1:203:VAL:HG12	1.66	0.95
18:4:228:PRO:HB2	18:4:229:PHE:CE1	2.00	0.95
1:A:425:THR:O	1:A:427:ARG:HD3	1.66	0.95
2:B:459:PHE:HD2	19:B:1235:CLA:C4D	1.77	0.95
5:E:107:PHE:CE2	5:E:109:LYS:CG	2.48	0.95
18:4:145:GLU:HG3	18:4:146:PHE:CE1	2.00	0.95
3:C:44:ARG:N	4:D:182:GLN:OE1	2.00	0.95
4:D:186:GLN:C	4:D:187:ASN:HD22	1.74	0.95
8:H:119:ASP:O	8:H:120:ILE:CG2	2.13	0.95
15:1:76:LEU:HB3	15:1:77:GLU:OE1	1.66	0.95
16:2:183:PHE:N	16:2:187:LYS:HG2	1.81	0.95
19:3:3008:CLA:HBA2	19:3:3008:CLA:CGD	1.95	0.95
21:A:6007:BCR:H382	21:A:6007:BCR:H23C	1.44	0.95
2:B:180:SER:HB3	2:B:288:GLY:HA3	1.47	0.95
2:B:382:ILE:CG2	2:B:383:MET:H	1.80	0.95
5:E:89:SER:HB2	5:E:106:ARG:NH1	1.81	0.95
19:J:1311:CLA:HED3	19:J:1311:CLA:C1A	1.97	0.95
15:1:94:VAL:O	15:1:97:ILE:HG23	1.64	0.95
16:2:240:ILE:HG23	16:2:263:PHE:HB3	1.46	0.95
17:3:181:SER:CB	19:3:2009:CLA:C11	2.40	0.95
1:A:188:LYS:HD2	1:A:188:LYS:C	1.92	0.95
2:B:103:ALA:HB1	2:B:106:ARG:HD2	1.49	0.95
2:B:478:LEU:O	2:B:478:LEU:HD23	1.65	0.95
6:F:204:SER:O	6:F:207:LEU:HD12	1.65	0.95
7:G:89:LYS:NZ	7:G:89:LYS:CA	2.29	0.95
8:H:76:TYR:HH	12:L:90:ARG:CD	1.67	0.95
22:R:7022:LMU:H21	22:R:7022:LMU:C2'	1.95	0.95
16:2:218:ARG:HB2	16:2:219:THR:HG22	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:187:GLY:O	18:4:188:ILE:HB	1.64	0.95
15:1:91:MET:O	15:1:95:PRO:CD	2.13	0.95
1:A:302:HIS:O	1:A:306:ILE:HG12	1.67	0.95
1:A:714:LEU:HD13	21:F:6016:BCR:H393	1.48	0.95
17:3:139:THR:CG2	17:3:140:GLY:H	1.79	0.95
18:4:172:PHE:CB	18:4:194:PHE:CZ	2.49	0.95
1:A:281:LEU:HD11	19:A:1115:CLA:HED1	1.46	0.95
19:A:9022:CLA:C9	19:A:9023:CLA:H91	1.97	0.95
22:H:7011:LMU:H2B	22:H:7011:LMU:H6E	1.46	0.95
19:L:1503:CLA:HHD	19:L:1503:CLA:CBC	1.96	0.95
13:N:165:ASN:C	13:N:167:PHE:H	1.75	0.95
15:1:128:PRO:HG2	15:1:131:TRP:CH2	2.00	0.95
17:3:173:PHE:C	17:3:173:PHE:CD1	2.40	0.95
18:4:124:PRO:HB2	18:4:126:TRP:H	1.31	0.95
2:B:294:ASN:HD22	7:G:94:GLN:N	1.64	0.95
3:C:5:VAL:HB	3:C:65:VAL:HG23	1.47	0.95
3:C:5:VAL:HG21	3:C:65:VAL:CG2	1.97	0.95
3:C:34:CYS:H	3:C:37:LYS:HB3	1.30	0.95
4:D:156:ARG:NH2	4:D:158:PHE:CE1	2.35	0.95
6:F:204:SER:O	6:F:207:LEU:N	2.00	0.95
6:F:207:LEU:CD1	6:F:208:PHE:H	1.78	0.95
7:G:72:LEU:CD2	7:G:124:ILE:HD12	1.90	0.95
19:K:1143:CLA:HBC1	22:K:7001:LMU:O3B	1.63	0.95
14:R:40:UNK:N	14:R:41:UNK:CB	2.30	0.95
15:1:189:LYS:HB2	19:1:1007:CLA:CMC	1.93	0.95
1:A:190:ALA:HB1	1:A:191:PRO:CD	1.97	0.94
1:A:586:ARG:HG3	3:C:49:VAL:HG21	1.48	0.94
19:A:1141:CLA:H12	19:A:1141:CLA:HMA2	1.47	0.94
2:B:622:ASP:CB	2:B:626:LEU:CD1	2.44	0.94
12:L:128:GLN:HA	12:L:130:GLY:CA	1.96	0.94
12:L:131:SER:CA	12:L:201:TYR:CE2	2.50	0.94
14:R:34:UNK:N	14:R:36:UNK:CB	2.30	0.94
1:A:26:PRO:HB2	1:A:27:ILE:HG13	1.49	0.94
1:A:345:GLY:C	1:A:347:TYR:H	1.73	0.94
6:F:150:VAL:HG21	6:F:160:PHE:HB2	1.48	0.94
7:G:99:HIS:CA	7:G:100:PHE:HB3	1.97	0.94
17:3:150:TYR:HB3	17:3:151:TRP:NE1	1.82	0.94
17:3:207:PHE:HD1	17:3:207:PHE:O	1.50	0.94
2:B:20:ARG:HH11	2:B:20:ARG:CG	1.78	0.94
2:B:315:LEU:HD13	2:B:315:LEU:O	1.68	0.94
2:B:490:ARG:HG3	2:B:490:ARG:HH11	0.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1220:CLA:HAA1	19:B:1220:CLA:H43	1.48	0.94
5:E:76:ILE:HB	5:E:84:TYR:O	1.67	0.94
6:F:119:ILE:HG13	6:F:120:LYS:N	1.77	0.94
17:3:103:VAL:O	17:3:107:ARG:HD2	1.67	0.94
1:A:23:ASP:CG	1:A:33:GLN:HG2	1.92	0.94
19:A:1126:CLA:H203	21:J:6012:BCR:H17C	1.46	0.94
2:B:294:ASN:HD22	7:G:94:GLN:CG	1.74	0.94
22:D:7050:LMU:H2B	22:D:7050:LMU:C6'	1.97	0.94
2:B:247:THR:CA	2:B:250:ALA:CB	2.45	0.94
2:B:542:ARG:HH11	2:B:542:ARG:HG3	1.29	0.94
6:F:213:TRP:HB2	6:F:216:ALA:CB	1.97	0.94
7:G:102:ALA:HA	7:G:104:ASP:OD1	1.63	0.94
11:K:97:ASP:HB2	11:K:101:PHE:CE2	2.02	0.94
15:1:69:LEU:C	15:1:73:PRO:HD3	1.93	0.94
16:2:168:TRP:HD1	16:2:171:ILE:HG23	1.32	0.94
1:A:248:PHE:H	1:A:248:PHE:HD2	1.11	0.94
1:A:502:THR:HB	1:A:504:ALA:HB3	1.46	0.94
1:A:588:GLY:HA3	2:B:668:ARG:HD3	1.46	0.94
19:A:1124:CLA:C7	19:A:1125:CLA:HED1	1.97	0.94
2:B:7:ARG:HH11	2:B:7:ARG:HG3	1.30	0.94
19:B:1220:CLA:HMC1	19:B:1220:CLA:HBC3	1.47	0.94
5:E:75:LYS:HA	5:E:87:THR:HG22	1.50	0.94
15:1:85:ILE:O	15:1:88:ARG:HB2	1.67	0.94
16:2:160:ILE:HG22	19:2:2012:CLA:HBB2	1.47	0.94
16:2:189:THR:O	16:2:192:ASP:O	1.86	0.94
17:3:96:ARG:CA	17:3:99:ALA:H	1.79	0.94
1:A:338:PHE:HE1	19:A:1151:CLA:CBB	1.61	0.94
19:A:1124:CLA:CED	19:A:1125:CLA:CMD	2.45	0.94
19:A:1125:CLA:CBB	19:A:1133:CLA:HMA3	1.75	0.94
2:B:317:ARG:HH22	2:B:410:ARG:CG	1.76	0.94
8:H:112:LEU:HD23	8:H:112:LEU:N	1.78	0.94
11:K:127:ILE:HG12	11:K:130:LEU:HD12	1.46	0.94
13:N:133:GLY:C	13:N:134:CYS:HG	1.74	0.94
15:1:80:LYS:O	15:1:83:GLU:CB	2.15	0.94
1:A:331:LEU:CD1	1:A:346:LEU:HB3	1.97	0.94
1:A:523:VAL:HG13	1:A:524:GLY:N	1.80	0.94
19:A:1237:CLA:H141	12:L:141:LEU:HD23	1.47	0.94
2:B:73:ASN:O	2:B:121:TYR:CE1	2.21	0.94
2:B:244:PHE:C	2:B:244:PHE:CD2	2.46	0.94
2:B:454:LEU:HD11	6:F:147:HIS:HA	1.47	0.94
4:D:141:GLY:H	4:D:144:LEU:H	1.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:GLU:C	5:E:129:GLU:CD	2.30	0.94
11:K:63:LEU:HD22	11:K:63:LEU:H	1.31	0.94
15:1:95:PRO:O	15:1:98:LEU:HB2	1.66	0.94
16:2:182:ILE:CB	16:2:187:LYS:HB3	1.97	0.94
16:2:187:LYS:HE3	16:2:187:LYS:CA	1.97	0.94
19:2:2014:CLA:H41	19:2:2014:CLA:C7	1.98	0.94
17:3:96:ARG:HH11	17:3:96:ARG:CB	1.79	0.94
17:3:150:TYR:O	17:3:152:ALA:CB	2.15	0.94
18:4:89:ARG:CD	18:4:90:TRP:H	1.79	0.94
18:4:120:ILE:HD11	18:4:226:LYS:CB	1.96	0.94
18:4:226:LYS:CE	18:4:226:LYS:H	1.80	0.94
19:A:1122:CLA:CBB	21:A:6007:BCR:H351	1.98	0.94
2:B:394:PHE:O	2:B:542:ARG:NE	2.01	0.94
4:D:123:ARG:HH21	22:D:7050:LMU:C4B	1.71	0.94
4:D:140:LEU:CD2	4:D:144:LEU:CD1	2.45	0.94
11:K:76:ALA:H	11:K:78:ARG:HH12	1.02	0.94
11:K:115:ILE:HA	11:K:118:VAL:HG22	1.46	0.94
15:1:78:ARG:NH2	15:1:179:LYS:CB	2.30	0.94
15:1:130:PRO:O	15:1:131:TRP:HE3	1.49	0.94
16:2:229:MET:SD	16:2:230:LEU:HA	2.06	0.94
18:4:87:ASN:HB2	18:4:90:TRP:CD2	2.02	0.94
1:A:157:GLY:CA	1:A:229:ILE:CG2	2.45	0.94
1:A:248:PHE:CD2	1:A:248:PHE:N	2.36	0.94
2:B:58:PHE:HB2	2:B:146:SER:CB	1.97	0.94
2:B:493:TRP:CH2	19:B:1214:CLA:H122	2.02	0.94
2:B:622:ASP:HB2	2:B:626:LEU:CD1	1.96	0.94
13:N:96:LYS:HG3	13:N:97:THR:OG1	1.67	0.94
16:2:254:LEU:CD2	16:2:255:ALA:N	2.30	0.94
18:4:169:ASP:O	18:4:173:LYS:CG	2.15	0.94
2:B:493:TRP:HE1	19:B:1213:CLA:HAC2	1.30	0.93
2:B:685:THR:OG1	19:L:1130:CLA:H3A	1.68	0.93
4:D:100:TYR:CE1	4:D:134:LYS:HG3	2.02	0.93
5:E:78:ARG:NH2	5:E:125:ILE:CG2	2.29	0.93
7:G:84:ARG:NE	7:G:85:GLU:HB3	1.83	0.93
11:K:60:SER:HA	11:K:63:LEU:HD21	1.49	0.93
16:2:237:PHE:HE1	16:2:241:TYR:CZ	1.86	0.93
1:A:244:LEU:HD12	1:A:247:GLU:CD	1.93	0.93
1:A:249:ILE:HG12	1:A:250:LEU:N	1.81	0.93
19:A:9012:CLA:H11	2:B:616:LEU:HD12	1.45	0.93
2:B:130:ARG:HH11	2:B:130:ARG:HG3	1.32	0.93
2:B:244:PHE:C	2:B:244:PHE:HD2	1.76	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:N	3:C:4:SER:OG	2.01	0.93
11:K:115:ILE:HG12	11:K:122:LEU:H	1.24	0.93
11:K:118:VAL:O	11:K:121:VAL:HG23	1.69	0.93
1:A:382:TYR:OH	19:A:1127:CLA:H42	1.67	0.93
2:B:340:SER:HA	19:B:1223:CLA:H51	1.49	0.93
2:B:560:ASP:HB2	3:C:66:ARG:NE	1.82	0.93
11:K:99:ALA:O	11:K:103:LEU:CD1	2.15	0.93
15:1:97:ILE:HD13	15:1:97:ILE:C	1.94	0.93
16:2:148:ASP:CG	16:2:152:LEU:HB3	1.92	0.93
1:A:462:ILE:HD11	19:A:9022:CLA:H51	1.50	0.93
2:B:131:THR:CG2	2:B:134:ASP:H	1.81	0.93
3:C:66:ARG:HH21	3:C:66:ARG:CG	1.81	0.93
7:G:124:ILE:HG12	7:G:128:LEU:HD12	1.48	0.93
8:H:85:GLU:HG3	8:H:86:THR:N	1.73	0.93
1:A:127:VAL:HG23	1:A:128:GLY:N	1.83	0.93
1:A:259:TYR:CB	1:A:260:PRO:HD2	1.87	0.93
1:A:426:THR:HA	1:A:428:TYR:CE2	2.04	0.93
1:A:514:THR:O	1:A:531:PRO:HA	1.69	0.93
2:B:620:LEU:HA	2:B:624:LEU:HD23	1.47	0.93
19:A:1138:CLA:HED3	19:A:1138:CLA:H2A	1.48	0.93
2:B:3:LEU:HD13	9:I:29:GLU:OE1	1.66	0.93
9:I:26:LEU:HA	9:I:29:GLU:O	1.67	0.93
16:2:101:TRP:H	16:2:103:VAL:HB	1.32	0.93
1:A:127:VAL:HG21	19:A:1107:CLA:CBB	1.99	0.93
1:A:606:TYR:O	1:A:610:SER:HB2	1.68	0.93
2:B:25:ILE:HG22	21:L:6019:BCR:H282	1.51	0.93
2:B:633:ASN:HB2	2:B:636:THR:HB	0.94	0.93
19:B:1235:CLA:C15	21:F:6016:BCR:C31	2.46	0.93
21:B:6017:BCR:H382	21:B:6017:BCR:H23C	1.49	0.93
8:H:58:LEU:CD1	8:H:62:THR:HG23	1.76	0.93
13:N:139:LYS:CG	13:N:142:LYS:CD	2.42	0.93
18:4:177:LEU:HD22	18:4:178:PRO:N	1.84	0.93
19:4:1306:CLA:HMC1	19:4:1306:CLA:HBC3	1.50	0.93
21:A:6011:BCR:C31	19:A:9013:CLA:H143	1.98	0.93
3:C:44:ARG:N	4:D:182:GLN:CD	2.27	0.93
4:D:115:PRO:O	4:D:116:THR:OG1	1.87	0.93
12:L:171:LYS:C	12:L:173:PRO:HD3	1.92	0.93
4:D:201:LYS:HD2	4:D:201:LYS:N	1.78	0.93
16:2:212:GLN:HG2	16:2:213:LYS:H	1.31	0.93
16:2:254:LEU:HD22	16:2:254:LEU:C	1.89	0.93
18:4:153:GLU:OE2	19:4:4012:CLA:C3B	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:4015:CLA:HBD	19:4:4015:CLA:HBA1	1.50	0.93
2:B:361:ILE:HG23	2:B:368:GLN:OE1	1.69	0.93
19:B:1220:CLA:H43	19:B:1220:CLA:C1A	1.99	0.93
4:D:140:LEU:CD1	4:D:144:LEU:CG	2.47	0.93
4:D:140:LEU:HD11	4:D:144:LEU:CB	1.99	0.93
6:F:207:LEU:HD22	6:F:208:PHE:N	1.84	0.93
1:A:250:LEU:CB	17:3:136:TRP:CZ2	2.50	0.92
19:A:1237:CLA:C14	12:L:141:LEU:CD2	2.46	0.92
21:A:6002:BCR:H341	21:A:6002:BCR:H12C	1.50	0.92
7:G:125:VAL:HG13	7:G:129:ALA:HB3	1.49	0.92
12:L:205:TYR:HD1	12:L:207:LEU:HD12	1.18	0.92
16:2:187:LYS:HA	16:2:187:LYS:CE	1.83	0.92
17:3:109:ALA:HA	17:3:111:LEU:HD22	1.49	0.92
17:3:207:PHE:C	17:3:207:PHE:CD1	2.45	0.92
1:A:648:THR:HG23	1:A:651:GLY:H	1.32	0.92
2:B:8:PHE:N	2:B:8:PHE:CD1	2.37	0.92
2:B:558:PRO:HB2	2:B:703:VAL:CG2	1.99	0.92
15:1:65:ASP:CG	15:1:66:PRO:N	2.24	0.92
15:1:133:THR:O	15:1:137:ILE:HD13	1.68	0.92
16:2:156:GLU:HG2	16:2:157:LEU:CD1	1.97	0.92
19:3:3016:CLA:C14	19:3:3016:CLA:H102	1.97	0.92
18:4:158:GLN:OE1	19:4:1004:CLA:CGD	2.15	0.92
1:A:668:TYR:CD1	2:B:445:ALA:CB	2.51	0.92
2:B:419:ILE:O	2:B:420:SER:OG	1.87	0.92
2:B:696:LYS:HE3	3:C:80:ALA:HB1	1.48	0.92
4:D:140:LEU:CD2	4:D:144:LEU:HD12	1.99	0.92
5:E:79:LYS:HG3	5:E:84:TYR:CE1	2.02	0.92
6:F:139:LEU:HD13	6:F:149:ILE:HD13	1.49	0.92
15:1:89:TRP:O	15:1:92:LEU:HB3	1.69	0.92
1:A:267:THR:O	1:A:269:PHE:CD2	2.22	0.92
1:A:388:ASP:OD1	1:A:391:THR:OG1	1.87	0.92
2:B:188:LEU:HD11	19:B:1212:CLA:HBB2	1.51	0.92
2:B:293:THR:HG21	19:B:1209:CLA:HMA3	1.52	0.92
19:B:1220:CLA:O2D	19:B:1220:CLA:H2A	1.70	0.92
6:F:219:ARG:HG2	6:F:219:ARG:NH1	1.62	0.92
16:2:114:MET:HG2	16:2:227:LEU:HA	1.51	0.92
1:A:120:ALA:H	1:A:145:ILE:HD12	1.34	0.92
1:A:351:THR:O	19:A:1123:CLA:C18	2.17	0.92
3:C:54:CYS:HB2	23:C:8002:SF4:S1	2.08	0.92
4:D:123:ARG:NH2	22:D:7050:LMU:C5B	2.32	0.92
5:E:78:ARG:N	5:E:78:ARG:HD2	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:1241:CLA:C4C	21:I:6021:BCR:HC22	2.00	0.92
19:R:1144:CLA:HED3	19:R:1144:CLA:CHA	2.00	0.92
16:2:173:ASN:HD22	16:2:173:ASN:N	1.65	0.92
19:2:2007:CLA:HAC2	19:3:2009:CLA:HED1	1.48	0.92
21:A:6011:BCR:C31	19:A:9013:CLA:C14	2.47	0.92
19:B:1222:CLA:HED1	19:B:1223:CLA:HMD2	1.50	0.92
19:L:1148:CLA:HAA1	19:L:1148:CLA:O2D	1.69	0.92
13:N:132:THR:HB	13:N:139:LYS:HZ3	1.31	0.92
17:3:185:GLN:HG2	17:3:186:TYR:H	0.79	0.92
1:A:358:LEU:HD11	1:A:413:HIS:CG	2.05	0.92
1:A:451:ILE:CD1	19:A:1131:CLA:HED1	2.00	0.92
1:A:672:LEU:O	1:A:674:ALA:N	2.02	0.92
2:B:694:ARG:HH21	2:B:694:ARG:CG	1.81	0.92
11:K:115:ILE:CG1	11:K:122:LEU:N	2.32	0.92
1:A:246:HIS:HA	1:A:248:PHE:HE2	0.79	0.92
1:A:379:MET:HE2	19:A:1125:CLA:HMC2	1.52	0.92
19:A:1124:CLA:H72	19:A:1125:CLA:HED2	1.51	0.92
2:B:453:ILE:HG23	2:B:453:ILE:O	1.68	0.92
5:E:126:VAL:O	5:E:127:GLU:HG3	1.69	0.92
18:4:120:ILE:HG22	18:4:121:ILE:H	1.33	0.92
1:A:51:THR:CB	19:A:1139:CLA:HBB2	1.99	0.92
1:A:390:ALA:HB2	1:A:754:ILE:HB	1.52	0.92
1:A:691:MET:HE3	20:A:5001:PQN:H2M2	1.49	0.92
19:B:1234:CLA:HMC3	19:B:1234:CLA:HBC3	1.49	0.92
5:E:96:ASP:OD2	5:E:98:ASN:CG	2.11	0.92
7:G:72:LEU:HD23	7:G:124:ILE:CG1	2.00	0.92
17:3:197:SER:OG	17:3:205:GLY:CA	2.17	0.92
19:3:3016:CLA:H142	19:3:3016:CLA:H102	1.50	0.92
18:4:146:PHE:CE2	19:4:4013:CLA:C3C	2.52	0.92
1:A:236:GLY:O	1:A:237:VAL:HG13	1.71	0.92
19:A:9023:CLA:HHB	19:A:9023:CLA:H43	1.52	0.92
2:B:317:ARG:HH22	2:B:410:ARG:HG2	1.18	0.92
3:C:39:ILE:HG23	3:C:40:ALA:N	1.85	0.92
4:D:167:HIS:HD2	4:D:172:VAL:HG21	1.20	0.92
6:F:127:LYS:C	6:F:129:ARG:N	2.07	0.92
7:G:84:ARG:HE	7:G:89:LYS:HE2	1.34	0.92
7:G:99:HIS:HA	7:G:100:PHE:CB	1.99	0.92
11:K:125:LYS:HB2	11:K:128:GLY:N	1.84	0.92
21:1:6023:BCR:C8	21:1:6023:BCR:H313	1.74	0.92
16:2:226:ARG:CB	16:2:226:ARG:HH11	1.82	0.92
17:3:109:ALA:HA	17:3:111:LEU:CG	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:222:ASN:O	18:4:223:VAL:HB	1.66	0.92
19:B:1235:CLA:C16	21:F:6016:BCR:H313	2.00	0.91
6:F:173:TRP:HZ3	6:F:211:PHE:CB	1.83	0.91
8:H:97:LEU:HD11	8:H:100:PHE:HB3	1.50	0.91
9:I:12:VAL:O	9:I:17:PRO:HD3	1.69	0.91
19:L:1148:CLA:HED1	19:L:1148:CLA:H2	0.92	0.91
18:4:174:GLN:O	18:4:194:PHE:CB	2.18	0.91
1:A:628:ILE:HD12	1:A:629:ASN:H	1.34	0.91
19:B:1220:CLA:C2	19:B:1220:CLA:H71	1.99	0.91
6:F:82:LEU:HG	6:F:83:THR:N	1.72	0.91
15:1:77:GLU:CG	15:1:80:LYS:HD2	1.99	0.91
15:1:190:ASN:ND2	19:1:1002:CLA:C1A	2.33	0.91
15:1:193:LEU:HD23	15:1:193:LEU:C	1.96	0.91
17:3:133:ALA:HB3	17:3:134:LEU:CD1	1.99	0.91
18:4:134:TYR:HB3	18:4:136:ALA:HB2	1.51	0.91
19:A:1105:CLA:HMB2	21:J:6012:BCR:HC7	1.53	0.91
19:A:1107:CLA:HBB2	19:B:1230:CLA:CMD	2.00	0.91
2:B:5:ILE:CG2	2:B:6:PRO:HD3	1.98	0.91
2:B:457:PRO:HB3	2:B:517:PHE:CD1	2.04	0.91
3:C:14:CYS:HA	3:C:17:CYS:HG	1.13	0.91
6:F:207:LEU:HD13	6:F:208:PHE:N	1.85	0.91
21:I:6021:BCR:H391	21:L:6019:BCR:H401	1.47	0.91
15:1:129:VAL:HG12	15:1:130:PRO:CD	1.99	0.91
15:1:129:VAL:CG1	15:1:130:PRO:HD3	2.00	0.91
16:2:182:ILE:HD13	16:2:190:GLY:HA3	1.51	0.91
16:2:184:PRO:CD	16:2:187:LYS:HD2	2.00	0.91
1:A:336:GLY:N	1:A:339:THR:OG1	2.02	0.91
1:A:368:LEU:HD11	19:A:1125:CLA:H61	1.52	0.91
1:A:425:THR:CB	1:A:428:TYR:CE1	2.48	0.91
2:B:443:MET:O	2:B:446:PHE:HB2	1.69	0.91
7:G:116:SER:HA	7:G:119:PRO:HG2	1.52	0.91
11:K:51:SER:N	11:K:52:PRO:CD	2.34	0.91
12:L:102:VAL:HA	19:L:1502:CLA:HED2	1.50	0.91
18:4:226:LYS:H	18:4:226:LYS:CD	1.81	0.91
1:A:328:LYS:NZ	1:A:345:GLY:CA	2.33	0.91
1:A:411:ALA:HB2	21:A:6008:BCR:H392	1.53	0.91
1:A:564:ARG:HB3	1:A:564:ARG:NH2	1.85	0.91
19:A:1149:CLA:O1D	19:A:1149:CLA:HAA1	1.71	0.91
3:C:6:LYS:HE2	4:D:191:ILE:HG13	1.49	0.91
4:D:80:SER:HG	4:D:126:PRO:HD2	1.12	0.91
5:E:96:ASP:OD2	5:E:98:ASN:OD1	1.87	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:131:GLY:O	7:G:136:VAL:HB	1.68	0.91
12:L:110:LEU:HB3	12:L:114:PHE:HE1	1.32	0.91
12:L:142:SER:O	12:L:143:LEU:HG	1.70	0.91
15:1:142:PHE:HA	15:1:145:ILE:CD1	2.00	0.91
16:2:101:TRP:CA	16:2:103:VAL:H	1.82	0.91
19:3:2009:CLA:HBA2	19:3:2009:CLA:CHA	2.00	0.91
1:A:365:LEU:HD23	19:A:1103:CLA:CED	1.99	0.91
1:A:484:LEU:H	1:A:484:LEU:HD22	1.36	0.91
11:K:118:VAL:CG2	11:K:121:VAL:HG22	2.00	0.91
19:A:1112:CLA:HHC	21:A:6002:BCR:H17C	1.50	0.91
19:A:1125:CLA:O1D	19:A:1125:CLA:HBA1	1.69	0.91
2:B:103:ALA:HA	2:B:105:THR:N	1.85	0.91
2:B:310:PRO:CG	2:B:311:PRO:HD3	2.00	0.91
4:D:95:GLN:HE21	4:D:96:VAL:HA	1.30	0.91
5:E:89:SER:O	5:E:106:ARG:N	2.03	0.91
7:G:124:ILE:O	7:G:128:LEU:HB2	1.71	0.91
16:2:182:ILE:C	16:2:187:LYS:CG	2.44	0.91
17:3:133:ALA:HB3	17:3:134:LEU:HD11	1.53	0.91
1:A:338:PHE:CE1	19:A:1151:CLA:HBB2	2.03	0.91
19:A:1113:CLA:CBB	21:A:6002:BCR:H352	2.01	0.91
4:D:83:PHE:HB3	4:D:84:GLY:O	1.71	0.91
4:D:100:TYR:CD1	4:D:134:LYS:HG3	2.06	0.91
6:F:132:ASN:O	6:F:133:TYR:CD1	2.23	0.91
7:G:63:VAL:CG2	7:G:64:ILE:H	1.84	0.91
7:G:94:GLN:O	7:G:97:LEU:HD23	1.70	0.91
7:G:125:VAL:HG13	7:G:129:ALA:CB	2.01	0.91
15:1:177:PRO:HD3	15:1:180:LEU:CD2	2.00	0.91
18:4:169:ASP:CG	18:4:174:GLN:HB2	1.95	0.91
22:4:7034:LMU:H71	22:4:7052:LMU:H11	1.53	0.91
1:A:105:ASN:OD1	1:A:118:PRO:HA	1.70	0.91
2:B:270:LEU:HD12	2:B:271:THR:N	1.86	0.91
2:B:574:ASP:HA	2:B:577:TYR:HB3	1.50	0.91
8:H:99:LYS:O	8:H:100:PHE:C	2.14	0.91
8:H:120:ILE:HG13	8:H:120:ILE:O	1.68	0.91
12:L:150:ILE:C	12:L:150:ILE:HD12	1.95	0.91
12:L:174:ASP:OD2	12:L:175:GLN:HG3	1.70	0.91
1:A:23:ASP:HB3	1:A:33:GLN:CD	1.95	0.91
19:A:1126:CLA:H203	21:J:6012:BCR:C17	2.01	0.91
19:A:1141:CLA:C7	19:A:1141:CLA:C12	2.48	0.91
2:B:110:LEU:HD12	2:B:111:GLY:CA	2.01	0.91
2:B:403:ASN:O	2:B:406:ASN:CB	2.19	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:672:GLN:HE22	3:C:79:LEU:HD12	1.35	0.91
4:D:133:ARG:H	4:D:136:GLN:NE2	1.66	0.91
15:1:177:PRO:HG2	15:1:179:LYS:O	1.70	0.91
1:A:73:GLU:HG3	1:A:74:ILE:N	1.82	0.90
2:B:257:ILE:O	2:B:497:TRP:HE3	1.38	0.90
2:B:306:GLU:HG3	2:B:307:ALA:H	1.31	0.90
3:C:52:LYS:O	3:C:52:LYS:HG3	1.71	0.90
3:C:62:PHE:CD2	5:E:80:GLU:HG3	2.07	0.90
8:H:56:GLU:CG	8:H:57:ASP:N	2.34	0.90
16:2:117:ALA:HB1	16:2:230:LEU:CG	2.02	0.90
17:3:150:TYR:H	17:3:152:ALA:HB2	0.75	0.90
18:4:177:LEU:CD2	18:4:178:PRO:HD3	2.01	0.90
1:A:195:TRP:CZ2	19:A:1108:CLA:HMA2	2.06	0.90
21:A:6002:BCR:HC8	21:A:6002:BCR:C31	2.01	0.90
2:B:560:ASP:OD1	2:B:561:GLY:N	2.04	0.90
3:C:62:PHE:HZ	5:E:80:GLU:CD	1.60	0.90
8:H:58:LEU:HB3	8:H:61:THR:HB	1.48	0.90
19:J:1308:CLA:CAD	19:J:1308:CLA:CED	2.50	0.90
14:R:33:UNK:C	14:R:36:UNK:CB	2.50	0.90
19:1:1014:CLA:HBC3	19:1:1014:CLA:CHD	2.01	0.90
24:B:7101:LMG:O3	3:C:70:TRP:CZ2	2.23	0.90
4:D:137:CYS:O	4:D:140:LEU:O	1.89	0.90
5:E:111:ASN:HB3	5:E:116:SER:OG	1.71	0.90
19:K:1146:CLA:HMA1	19:K:1146:CLA:O1A	1.71	0.90
13:N:155:GLU:HB3	13:N:157:LYS:CA	2.01	0.90
16:2:156:GLU:OE2	19:2:2013:CLA:CHD	2.18	0.90
19:3:1147:CLA:HMC1	19:3:1147:CLA:HBC3	0.92	0.90
1:A:129:GLN:NE2	19:A:1107:CLA:NA	2.19	0.90
2:B:558:PRO:HG2	2:B:703:VAL:CG2	2.02	0.90
3:C:5:VAL:HG21	3:C:65:VAL:HG23	1.52	0.90
5:E:79:LYS:HA	5:E:84:TYR:CD1	2.06	0.90
5:E:103:VAL:HG13	5:E:120:TYR:O	1.72	0.90
11:K:128:GLY:N	11:K:129:ALA:HA	1.80	0.90
17:3:154:ASN:C	17:3:155:TYR:CD2	2.49	0.90
19:3:3011:CLA:H122	19:3:3011:CLA:H172	1.52	0.90
1:A:733:VAL:O	1:A:733:VAL:HG12	1.72	0.90
2:B:75:GLU:HB2	2:B:132:ASN:ND2	1.83	0.90
21:B:6006:BCR:H331	21:B:6006:BCR:C8	2.00	0.90
6:F:130:PHE:N	6:F:133:TYR:CE1	2.37	0.90
12:L:74:THR:HG22	12:L:75:SER:OG	1.71	0.90
16:2:137:TRP:O	16:2:139:THR:HG22	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:206:PRO:HG2	17:3:208:PHE:CE2	2.06	0.90
19:4:4006:CLA:HMA3	22:4:7034:LMU:H62	1.51	0.90
19:4:4014:CLA:HHD	19:4:4014:CLA:HBC2	1.51	0.90
1:A:62:HIS:O	19:A:1128:CLA:HAA2	1.71	0.90
1:A:64:PHE:CD2	1:A:74:ILE:HG21	2.05	0.90
2:B:459:PHE:HB2	19:B:1235:CLA:CAD	2.01	0.90
8:H:58:LEU:HD12	8:H:61:THR:HA	1.52	0.90
8:H:58:LEU:CB	8:H:61:THR:HB	2.00	0.90
13:N:120:VAL:O	13:N:120:VAL:HG12	1.69	0.90
15:1:221:LEU:HD13	19:1:1003:CLA:HAC1	1.51	0.90
18:4:167:ASN:CG	19:4:4014:CLA:C2	2.45	0.90
2:B:457:PRO:HB3	2:B:517:PHE:HD1	1.37	0.90
2:B:459:PHE:HE2	19:B:1235:CLA:C2D	1.42	0.90
19:B:1226:CLA:HMC3	19:B:1226:CLA:HBC2	1.54	0.90
21:3:6022:BCR:H393	21:3:6022:BCR:C23	1.95	0.90
19:4:4002:CLA:HBA1	19:4:4002:CLA:CMA	1.94	0.90
1:A:126:ILE:HD11	19:A:1107:CLA:CMA	2.02	0.90
1:A:281:LEU:HD21	19:A:1115:CLA:HMA2	1.52	0.90
1:A:342:GLY:HA2	1:A:430:ASP:HB3	1.52	0.90
19:A:1141:CLA:H12	19:A:1141:CLA:CMA	2.01	0.90
2:B:224:PRO:HB2	2:B:227:THR:CB	2.01	0.90
2:B:229:GLN:O	7:G:63:VAL:HG21	1.70	0.90
2:B:352:MET:CE	19:B:1225:CLA:OBD	2.20	0.90
3:C:44:ARG:H	4:D:182:GLN:CD	1.79	0.90
19:J:1308:CLA:CBC	19:J:1308:CLA:CHD	2.48	0.90
11:K:70:PHE:HB3	11:K:98:PRO:HB3	1.52	0.90
12:L:131:SER:HB3	12:L:201:TYR:HE2	1.34	0.90
13:N:130:ASN:C	13:N:132:THR:CG2	2.43	0.90
16:2:131:ILE:O	16:2:131:ILE:HG22	1.71	0.90
17:3:159:VAL:CG1	17:3:160:LEU:N	2.31	0.90
17:3:205:GLY:N	17:3:206:PRO:HD2	1.85	0.90
21:B:6020:BCR:H332	19:L:1502:CLA:C4B	2.00	0.90
4:D:140:LEU:CD1	4:D:144:LEU:HG	2.00	0.90
15:1:64:PHE:CD1	15:1:65:ASP:N	2.40	0.90
17:3:109:ALA:HA	17:3:111:LEU:CD2	2.02	0.90
18:4:169:ASP:OD2	18:4:174:GLN:HB2	1.70	0.90
18:4:173:LYS:HZ2	18:4:201:LYS:CG	1.84	0.90
2:B:44:GLN:CD	2:B:163:PRO:HB2	1.97	0.90
7:G:69:GLY:O	7:G:72:LEU:HG	1.71	0.90
7:G:77:PHE:O	7:G:79:PHE:CB	2.19	0.90
1:A:71:LEU:CG	1:A:72:GLU:H	1.84	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLY:C	1:A:158:ILE:HG23	1.96	0.89
2:B:120:VAL:CA	2:B:123:TRP:HD1	1.79	0.89
2:B:269:TRP:HB2	2:B:497:TRP:HH2	1.38	0.89
2:B:312:GLY:HA3	2:B:315:LEU:CB	2.03	0.89
2:B:545:LYS:HD3	2:B:546:LEU:N	1.87	0.89
2:B:558:PRO:HG2	2:B:703:VAL:HG22	1.53	0.89
2:B:655:LEU:HD21	19:B:1239:CLA:HBB1	1.53	0.89
19:B:1222:CLA:CAD	19:B:1234:CLA:HBB1	2.03	0.89
6:F:170:ILE:HG21	21:F:6014:BCR:H371	1.52	0.89
6:F:185:ILE:C	6:F:186:ARG:HG2	1.97	0.89
13:N:143:VAL:HB	13:N:144:PRO:CD	1.99	0.89
16:2:184:PRO:HD3	16:2:187:LYS:CA	2.02	0.89
18:4:146:PHE:CZ	19:4:4013:CLA:NC	2.39	0.89
2:B:232:LEU:HD13	2:B:235:GLN:HG3	1.50	0.89
17:3:197:SER:HG	17:3:205:GLY:HA3	1.36	0.89
18:4:146:PHE:CE2	19:4:4013:CLA:C2C	2.53	0.89
22:4:7034:LMU:C11	22:4:7052:LMU:C3'	2.47	0.89
1:A:331:LEU:CD2	1:A:343:HIS:O	2.21	0.89
1:A:499:ALA:CB	19:A:1133:CLA:HED1	2.02	0.89
1:A:740:LEU:HD21	19:A:1140:CLA:CMA	2.01	0.89
21:A:6011:BCR:C39	21:A:6011:BCR:H23C	2.01	0.89
19:A:9022:CLA:H112	21:B:6017:BCR:H19C	1.53	0.89
4:D:82:ILE:O	4:D:82:ILE:HG13	1.69	0.89
11:K:48:PHE:O	11:K:52:PRO:HD3	1.72	0.89
11:K:70:PHE:C	11:K:70:PHE:CD1	2.46	0.89
15:1:170:PRO:HG2	15:1:171:LEU:CA	2.02	0.89
16:2:119:GLY:O	16:2:123:PRO:CD	2.20	0.89
18:4:96:LEU:CD1	18:4:100:ARG:CZ	2.50	0.89
18:4:110:LEU:O	18:4:113:GLU:HG3	1.71	0.89
18:4:158:GLN:HB3	19:4:1004:CLA:HMA2	0.90	0.89
18:4:173:LYS:HZ3	18:4:201:LYS:HG3	1.28	0.89
18:4:175:TYR:O	18:4:194:PHE:CD1	2.25	0.89
19:A:1237:CLA:H201	12:L:110:LEU:HD21	1.52	0.89
4:D:140:LEU:HD12	4:D:141:GLY:CA	2.02	0.89
6:F:221:LEU:HD23	6:F:222:LEU:HD21	1.52	0.89
12:L:143:LEU:HA	12:L:146:THR:H	1.36	0.89
13:N:169:LYS:HB3	13:N:170:TRP:CD1	2.06	0.89
15:1:134:LEU:HA	15:1:137:ILE:CD1	2.01	0.89
1:A:78:VAL:O	1:A:82:HIS:CD2	2.26	0.89
1:A:83:PHE:CE1	19:A:1111:CLA:HED1	2.08	0.89
1:A:244:LEU:CD1	1:A:247:GLU:CD	2.46	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HB2	17:3:136:TRP:HH2	1.36	0.89
1:A:381:PRO:HB2	19:A:1117:CLA:HAA2	1.54	0.89
5:E:79:LYS:CA	5:E:84:TYR:CE1	2.54	0.89
19:H:1145:CLA:H101	19:H:1145:CLA:H142	1.50	0.89
13:N:130:ASN:HB2	13:N:139:LYS:CD	2.02	0.89
16:2:237:PHE:HE1	16:2:241:TYR:CE1	1.90	0.89
1:A:163:GLN:HG3	1:A:164:LEU:N	1.86	0.89
1:A:547:PHE:O	1:A:551:VAL:HG13	1.73	0.89
19:A:1134:CLA:C3A	19:A:1141:CLA:HBB2	2.01	0.89
2:B:140:ILE:CG1	2:B:141:PHE:N	2.34	0.89
7:G:90:GLN:HB3	7:G:91:VAL:C	1.97	0.89
7:G:145:THR:HG23	7:G:146:SER:N	1.87	0.89
11:K:118:VAL:O	11:K:121:VAL:CG2	2.20	0.89
11:K:127:ILE:HG23	11:K:130:LEU:CG	1.95	0.89
13:N:139:LYS:HB3	13:N:142:LYS:CD	1.99	0.89
16:2:112:TRP:HZ2	16:2:167:ARG:NH2	1.30	0.89
16:2:117:ALA:CB	16:2:230:LEU:CG	2.49	0.89
18:4:173:LYS:HD2	18:4:201:LYS:HE3	1.52	0.89
1:A:24:ARG:N	1:A:24:ARG:CD	2.33	0.89
1:A:426:THR:CG2	1:A:428:TYR:CE2	2.55	0.89
1:A:715:LYS:HD2	6:F:230:ASN:HD21	0.76	0.89
5:E:78:ARG:HH22	5:E:125:ILE:CG2	1.86	0.89
13:N:130:ASN:O	13:N:132:THR:HG23	1.72	0.89
13:N:142:LYS:O	13:N:145:PHE:N	2.06	0.89
15:1:170:PRO:C	15:1:173:TYR:HE2	1.80	0.89
15:1:177:PRO:HD3	15:1:180:LEU:CG	1.92	0.89
15:1:189:LYS:HG3	19:1:1007:CLA:CMC	1.99	0.89
1:A:316:MET:HB3	1:A:317:TYR:CB	2.02	0.89
1:A:423:ASP:HB3	1:A:424:PRO:CD	2.02	0.89
2:B:391:PRO:HB3	2:B:538:ALA:HA	1.51	0.89
8:H:57:ASP:O	8:H:59:GLY:N	2.06	0.89
15:1:171:LEU:CA	15:1:173:TYR:CE2	2.55	0.89
17:3:96:ARG:HA	17:3:99:ALA:N	1.87	0.89
1:A:103:PHE:HE1	19:A:1105:CLA:O1D	1.55	0.89
3:C:44:ARG:CB	4:D:182:GLN:CD	2.45	0.89
4:D:123:ARG:HH22	22:D:7050:LMU:C4B	1.85	0.89
5:E:70:ARG:HG2	5:E:71:GLY:N	1.88	0.89
5:E:83:TRP:N	5:E:83:TRP:HE3	1.71	0.89
11:K:49:ILE:O	11:K:52:PRO:HD2	1.73	0.89
15:1:133:THR:O	15:1:136:THR:HG23	1.73	0.89
1:A:204:ASN:O	1:A:205:HIS:HB2	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:PHE:CD2	19:B:1235:CLA:C4D	2.54	0.89
2:B:535:VAL:O	2:B:539:LEU:HD23	1.72	0.89
19:B:1235:CLA:C15	21:F:6016:BCR:H312	2.03	0.89
4:D:73:GLU:O	4:D:76:PRO:HD2	1.73	0.89
4:D:203:THR:HG22	4:D:205:LYS:H	1.37	0.89
12:L:92:ALA:N	12:L:98:ARG:HH12	1.71	0.89
13:N:139:LYS:O	13:N:142:LYS:HD2	1.72	0.89
18:4:202:GLU:O	18:4:205:ILE:HG12	1.72	0.89
18:4:220:GLN:CG	19:4:1306:CLA:HAC2	2.03	0.89
1:A:71:LEU:CG	1:A:72:GLU:N	2.36	0.88
1:A:127:VAL:HG23	1:A:128:GLY:H	1.34	0.88
1:A:207:LEU:CD2	19:A:1119:CLA:HBB2	2.03	0.88
1:A:502:THR:CG2	1:A:504:ALA:H	1.86	0.88
1:A:599:PHE:CE2	1:A:731:ARG:HB3	2.06	0.88
2:B:232:LEU:CD1	2:B:235:GLN:CG	2.50	0.88
2:B:521:HIS:HE1	19:B:1235:CLA:NA	1.69	0.88
19:B:1202:CLA:O1A	19:B:1202:CLA:C2	2.20	0.88
4:D:83:PHE:CZ	4:D:114:MET:HE3	2.07	0.88
7:G:98:THR:OG1	7:G:101:GLU:HB2	1.71	0.88
8:H:78:PRO:CD	19:L:1501:CLA:CMD	2.40	0.88
11:K:52:PRO:CD	11:K:53:THR:H	1.81	0.88
12:L:79:ILE:HD12	19:L:1504:CLA:HMA2	1.55	0.88
13:N:146:LEU:CG	17:3:142:ILE:O	2.21	0.88
15:1:183:LEU:C	15:1:184:LYS:HG2	1.96	0.88
17:3:96:ARG:CA	17:3:99:ALA:CB	2.50	0.88
17:3:157:LEU:O	17:3:160:LEU:N	2.06	0.88
18:4:90:TRP:CG	18:4:91:PHE:N	2.36	0.88
1:A:316:MET:CB	1:A:317:TYR:CD1	2.57	0.88
19:A:1123:CLA:H92	19:A:1123:CLA:OBD	1.72	0.88
2:B:319:HIS:HE1	2:B:322:LEU:CD1	1.85	0.88
13:N:114:PHE:HB3	13:N:117:ALA:CB	2.02	0.88
15:1:142:PHE:HA	15:1:145:ILE:HD11	1.54	0.88
16:2:211:PRO:HD2	16:2:212:GLN:H	1.36	0.88
1:A:453:LEU:HB3	1:A:547:PHE:HB2	1.55	0.88
19:A:1122:CLA:CBB	21:A:6007:BCR:C35	2.51	0.88
2:B:382:ILE:HG22	2:B:383:MET:N	1.89	0.88
19:B:1235:CLA:H93	19:B:1235:CLA:HBB2	0.92	0.88
4:D:146:SER:O	4:D:147:LYS:HG3	1.72	0.88
5:E:96:ASP:HB3	5:E:98:ASN:N	1.88	0.88
7:G:72:LEU:HD23	7:G:124:ILE:HD11	1.34	0.88
7:G:141:ILE:O	7:G:142:LEU:HB2	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:96:ARG:CA	17:3:99:ALA:HB3	2.04	0.88
17:3:108:PHE:HB3	19:3:3013:CLA:H42	1.54	0.88
19:A:1131:CLA:H161	21:L:6019:BCR:H361	1.53	0.88
19:A:1138:CLA:H61	21:F:6014:BCR:H12C	1.52	0.88
11:K:84:LEU:CG	11:K:85:LYS:HG2	2.03	0.88
14:R:39:UNK:HA	14:R:42:UNK:CB	2.04	0.88
15:1:88:ARG:O	15:1:92:LEU:CB	2.20	0.88
16:2:184:PRO:HG3	16:2:187:LYS:N	1.89	0.88
18:4:198:LEU:HG	18:4:199:GLU:N	1.88	0.88
1:A:289:PRO:O	1:A:290:LEU:HB3	1.73	0.88
1:A:426:THR:HG22	1:A:428:TYR:HE2	1.32	0.88
16:2:182:ILE:HB	16:2:187:LYS:CG	2.02	0.88
17:3:93:ILE:CG1	17:3:95:PRO:O	2.20	0.88
17:3:159:VAL:O	17:3:162:MET:N	2.05	0.88
2:B:222:LEU:HD12	2:B:223:GLY:O	1.74	0.88
2:B:268:LEU:HD22	2:B:273:VAL:HG12	1.54	0.88
2:B:398:TYR:O	4:D:197:PRO:CG	2.20	0.88
21:B:6010:BCR:H382	21:B:6010:BCR:H23C	1.53	0.88
3:C:65:VAL:O	3:C:66:ARG:HB3	1.71	0.88
4:D:95:GLN:HE21	4:D:96:VAL:CA	1.86	0.88
11:K:56:ILE:HA	11:K:59:THR:CG2	2.02	0.88
13:N:164:SER:HA	13:N:165:ASN:C	1.98	0.88
17:3:135:ALA:CB	17:3:139:THR:OG1	2.20	0.88
2:B:87:ILE:HA	2:B:115:ASN:CA	2.04	0.88
2:B:293:THR:HG21	19:B:1209:CLA:CMA	2.04	0.88
2:B:693:TRP:CD1	19:B:1238:CLA:C2D	2.56	0.88
19:B:1214:CLA:CBD	19:B:1223:CLA:HBB2	2.04	0.88
20:B:5002:PQN:C16	21:B:6017:BCR:H333	2.00	0.88
3:C:62:PHE:CZ	5:E:80:GLU:OE2	2.24	0.88
6:F:200:VAL:HG11	10:J:7:TYR:HB2	1.54	0.88
7:G:149:TYR:CA	7:G:150:ASP:OD1	2.20	0.88
12:L:51:LYS:HE2	12:L:51:LYS:HA	1.54	0.88
12:L:102:VAL:HA	19:L:1502:CLA:CED	2.04	0.88
18:4:143:VAL:O	18:4:147:ILE:HD12	1.73	0.88
21:A:6011:BCR:C8	21:A:6011:BCR:H311	2.04	0.88
2:B:527:LEU:HD12	19:B:1236:CLA:HMA3	1.56	0.88
3:C:31:TRP:HD1	3:C:32:GLY:N	1.72	0.88
19:2:4009:CLA:H152	19:2:4009:CLA:H192	1.54	0.88
17:3:122:LEU:HD21	19:3:3006:CLA:C3D	2.02	0.88
19:3:2009:CLA:CGA	19:3:2009:CLA:CBD	2.49	0.88
19:A:9022:CLA:HBB2	19:A:9023:CLA:CHB	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:VAL:HG21	19:B:1230:CLA:HAC2	1.55	0.88
3:C:65:VAL:HG22	3:C:66:ARG:N	1.84	0.88
3:C:72:GLU:CD	3:C:77:MET:CE	2.46	0.88
5:E:107:PHE:HE2	5:E:109:LYS:HG3	1.19	0.88
7:G:72:LEU:HD12	7:G:73:PHE:CE2	2.09	0.88
8:H:119:ASP:OD2	8:H:121:LEU:HG	1.72	0.88
16:2:195:TYR:CD2	16:2:198:GLY:HA3	2.08	0.88
16:2:261:THR:HG22	16:2:262:ILE:H	1.38	0.88
19:2:2001:CLA:HMC1	19:2:2001:CLA:HBC3	1.56	0.88
1:A:252:ARG:H	1:A:252:ARG:CD	1.82	0.88
2:B:123:TRP:C	2:B:126:THR:HG22	1.99	0.88
2:B:469:LYS:HG3	2:B:470:THR:CG2	2.03	0.88
2:B:470:THR:H	2:B:501:ILE:HB	1.29	0.88
2:B:493:TRP:HH2	19:B:1214:CLA:H122	1.36	0.88
21:B:6020:BCR:H331	21:B:6020:BCR:HC8	1.55	0.88
5:E:81:SER:OG	5:E:120:TYR:OH	1.64	0.88
19:H:1145:CLA:H143	19:H:1145:CLA:H193	1.55	0.88
1:A:71:LEU:HD12	1:A:72:GLU:N	1.87	0.87
1:A:73:GLU:HA	1:A:76:ARG:HD2	1.54	0.87
1:A:154:ARG:HE	1:A:384:TYR:HE1	0.92	0.87
19:A:1115:CLA:HMC1	19:A:1115:CLA:HBC3	1.56	0.87
2:B:294:ASN:ND2	7:G:94:GLN:HA	1.88	0.87
2:B:693:TRP:HD1	19:B:1238:CLA:C2D	1.87	0.87
19:B:1228:CLA:HHD	19:B:1228:CLA:HBC2	1.56	0.87
16:2:184:PRO:CD	16:2:187:LYS:CG	2.52	0.87
18:4:173:LYS:C	18:4:194:PHE:CD2	2.52	0.87
1:A:566:SER:OG	2:B:673:GLU:OE2	1.90	0.87
19:A:1136:CLA:H192	19:L:1130:CLA:HBB1	1.54	0.87
4:D:100:TYR:CE1	4:D:134:LYS:CG	2.57	0.87
12:L:141:LEU:HD13	12:L:145:LEU:HD12	1.57	0.87
12:L:142:SER:O	12:L:143:LEU:CG	2.23	0.87
12:L:209:LEU:HD12	12:L:210:PRO:HD2	0.89	0.87
16:2:120:ILE:O	16:2:123:PRO:HD2	1.73	0.87
1:A:207:LEU:HA	1:A:211:LEU:HG	1.55	0.87
1:A:368:LEU:CD2	19:A:1117:CLA:H92	2.03	0.87
1:A:668:TYR:CG	2:B:445:ALA:CB	2.58	0.87
21:A:6002:BCR:H311	21:A:6002:BCR:C8	2.01	0.87
2:B:475:ASP:OD1	2:B:480:SER:O	1.92	0.87
3:C:43:PRO:HA	4:D:182:GLN:HB3	1.56	0.87
11:K:49:ILE:C	11:K:52:PRO:HD2	1.98	0.87
19:L:1148:CLA:C2	19:L:1148:CLA:CED	2.31	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:189:LYS:CG	19:1:1007:CLA:CMC	2.53	0.87
17:3:197:SER:CB	17:3:206:PRO:CD	2.52	0.87
18:4:172:PHE:HB3	18:4:194:PHE:CZ	2.09	0.87
1:A:150:PHE:H	1:A:153:TRP:HB2	1.39	0.87
2:B:319:HIS:HE1	2:B:322:LEU:HD12	1.32	0.87
4:D:100:TYR:CE1	4:D:134:LYS:HE3	2.09	0.87
15:1:85:ILE:HA	15:1:88:ARG:CD	2.03	0.87
16:2:103:VAL:O	16:2:105:ALA:N	2.08	0.87
1:A:71:LEU:HG	1:A:72:GLU:N	1.86	0.87
1:A:85:GLN:O	1:A:87:SER:O	1.91	0.87
1:A:92:TRP:O	1:A:93:LEU:CD2	2.23	0.87
1:A:160:SER:O	1:A:163:GLN:HG2	1.74	0.87
19:A:1124:CLA:C7	19:A:1125:CLA:CED	2.51	0.87
19:A:1140:CLA:H141	21:A:6011:BCR:HC21	1.55	0.87
2:B:303:TYR:CA	2:B:306:GLU:HB2	2.03	0.87
2:B:312:GLY:HA3	2:B:315:LEU:HB2	1.55	0.87
2:B:697:PRO:O	3:C:79:LEU:HD13	1.73	0.87
4:D:150:ILE:O	4:D:151:LYS:HG2	1.73	0.87
19:L:1503:CLA:HBC3	19:L:1503:CLA:CHD	2.05	0.87
13:N:155:GLU:CA	13:N:157:LYS:CE	2.31	0.87
15:1:141:GLU:O	15:1:145:ILE:HG13	1.74	0.87
17:3:96:ARG:HH11	17:3:96:ARG:HB2	1.36	0.87
1:A:261:SER:O	1:A:262:PHE:CD1	2.28	0.87
1:A:281:LEU:CG	19:A:1115:CLA:CED	2.53	0.87
1:A:316:MET:CG	1:A:317:TYR:CD1	2.58	0.87
1:A:470:LEU:CD1	2:B:95:HIS:HB3	2.03	0.87
21:B:6020:BCR:H331	21:B:6020:BCR:C8	2.03	0.87
15:1:92:LEU:C	15:1:95:PRO:CD	2.47	0.87
19:1:1001:CLA:CMC	19:1:1001:CLA:HBC3	2.03	0.87
17:3:201:ALA:CB	17:3:202:TYR:CD2	2.58	0.87
22:4:7053:LMU:H11	22:4:7053:LMU:H5'	1.56	0.87
1:A:89:ILE:O	1:A:92:TRP:HB3	1.75	0.87
1:A:723:ARG:H	19:A:1139:CLA:HBB1	1.37	0.87
19:A:1237:CLA:H141	12:L:141:LEU:HD21	1.56	0.87
22:H:7043:LMU:H102	22:H:7043:LMU:H62	1.55	0.87
10:J:5:LYS:HG3	16:2:178:ASN:OD1	1.75	0.87
11:K:127:ILE:CG2	11:K:130:LEU:HG	2.04	0.87
12:L:143:LEU:HD22	12:L:146:THR:CG2	2.04	0.87
15:1:189:LYS:HE2	15:1:189:LYS:HA	1.56	0.87
19:A:1119:CLA:HMD1	19:A:1121:CLA:HBB2	1.55	0.87
2:B:482:ASN:OD1	2:B:485:ALA:HB2	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:622:ASP:CB	2:B:626:LEU:HD12	2.03	0.87
6:F:132:ASN:C	6:F:133:TYR:HD1	1.82	0.87
6:F:200:VAL:CG1	10:J:7:TYR:H	1.86	0.87
9:I:24:LEU:C	9:I:26:LEU:H	1.80	0.87
12:L:70:GLU:HG2	12:L:74:THR:HG21	1.57	0.87
12:L:153:PHE:O	12:L:179:ALA:N	2.08	0.87
17:3:159:VAL:O	17:3:160:LEU:C	2.14	0.87
17:3:205:GLY:N	17:3:206:PRO:CD	2.34	0.87
1:A:246:HIS:O	1:A:248:PHE:HD2	1.57	0.87
1:A:308:ILE:HD12	19:A:1115:CLA:CHC	2.03	0.87
1:A:491:TRP:HE1	19:A:1135:CLA:C1	1.87	0.87
1:A:659:ALA:O	1:A:662:SER:OG	1.93	0.87
19:A:1134:CLA:HBC1	21:A:6008:BCR:HC31	1.54	0.87
2:B:50:HIS:CD2	19:B:1202:CLA:HAA2	2.09	0.87
8:H:109:LEU:CD2	19:H:1207:CLA:H52	2.05	0.87
13:N:114:PHE:CD1	13:N:117:ALA:CB	2.53	0.87
22:4:7053:LMU:H6E	22:4:7053:LMU:H1B	1.54	0.87
1:A:40:PHE:O	1:A:41:SER:O	1.93	0.86
1:A:387:THR:HG22	1:A:523:VAL:HG11	1.54	0.86
19:B:1214:CLA:CAD	19:B:1223:CLA:HBB2	2.05	0.86
22:H:7032:LMU:H31	22:H:7032:LMU:H1B	1.56	0.86
22:H:7032:LMU:H3'	22:H:7032:LMU:O5B	1.75	0.86
1:A:316:MET:HB3	1:A:317:TYR:CD1	2.10	0.86
1:A:502:THR:HG22	1:A:504:ALA:N	1.90	0.86
19:A:1107:CLA:HBB2	19:B:1230:CLA:HMD3	1.57	0.86
2:B:393:PHE:HD2	2:B:397:ASP:OD1	1.59	0.86
2:B:459:PHE:CE2	19:B:1235:CLA:HMD1	2.08	0.86
2:B:469:LYS:HE3	2:B:470:THR:HG23	1.56	0.86
3:C:62:PHE:CZ	5:E:80:GLU:OE1	2.28	0.86
4:D:100:TYR:CE1	4:D:134:LYS:CE	2.57	0.86
4:D:103:THR:HG22	4:D:128:LEU:CG	2.05	0.86
22:D:7050:LMU:H4'	22:D:7050:LMU:O2B	1.73	0.86
5:E:89:SER:HB2	5:E:106:ARG:NH2	1.90	0.86
16:2:184:PRO:CG	16:2:187:LYS:HD2	2.04	0.86
19:4:1304:CLA:HED3	19:4:1304:CLA:CAA	1.98	0.86
1:A:443:ILE:HD11	1:A:557:LEU:HD23	1.57	0.86
1:A:691:MET:HE3	20:A:5001:PQN:C2M	2.05	0.86
15:1:177:PRO:N	15:1:180:LEU:HG	1.89	0.86
15:1:190:ASN:ND2	19:1:1002:CLA:NA	2.23	0.86
17:3:187:PHE:C	17:3:187:PHE:CD1	2.54	0.86
17:3:202:TYR:HB3	17:3:203:PRO:CD	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:CB	1:A:317:TYR:HB2	2.03	0.86
1:A:331:LEU:HD11	1:A:346:LEU:CB	2.03	0.86
19:A:1111:CLA:HBA1	19:A:1123:CLA:H41	1.55	0.86
2:B:353:TYR:CG	2:B:594:TRP:CZ3	2.63	0.86
3:C:14:CYS:SG	3:C:18:VAL:O	2.32	0.86
4:D:82:ILE:HG23	4:D:121:ILE:O	1.74	0.86
15:1:64:PHE:CG	15:1:65:ASP:N	2.44	0.86
19:2:2001:CLA:H42	19:2:2001:CLA:CGA	2.04	0.86
17:3:151:TRP:CD1	17:3:152:ALA:N	2.41	0.86
22:4:7034:LMU:C9	22:4:7052:LMU:C2'	2.42	0.86
2:B:247:THR:CG2	2:B:248:GLN:N	2.33	0.86
2:B:254:ILE:HB	2:B:255:LEU:HD23	1.56	0.86
3:C:7:ILE:O	3:C:8:TYR:O	1.92	0.86
2:B:58:PHE:CD2	2:B:145:LEU:CD2	2.57	0.86
2:B:140:ILE:HG13	2:B:141:PHE:H	1.36	0.86
2:B:382:ILE:O	2:B:384:THR:N	2.08	0.86
2:B:556:SER:C	2:B:558:PRO:HD2	2.00	0.86
6:F:96:LYS:O	6:F:100:LYS:HB2	1.74	0.86
8:H:61:THR:CB	8:H:62:THR:HG23	2.05	0.86
19:H:1145:CLA:C2	19:H:1145:CLA:HMA1	2.05	0.86
17:3:103:VAL:O	17:3:107:ARG:HB2	1.74	0.86
17:3:150:TYR:O	17:3:152:ALA:HB3	1.73	0.86
1:A:402:ILE:HG13	19:A:1127:CLA:HBB2	1.56	0.86
2:B:310:PRO:CB	2:B:311:PRO:CD	2.54	0.86
2:B:527:LEU:HD13	19:B:1236:CLA:HMA3	1.51	0.86
2:B:561:GLY:HA3	3:C:52:LYS:HG2	1.56	0.86
6:F:97:GLN:CD	6:F:98:ALA:N	2.33	0.86
7:G:84:ARG:HG3	7:G:85:GLU:CA	2.05	0.86
11:K:97:ASP:CB	11:K:101:PHE:CE2	2.50	0.86
13:N:114:PHE:CG	13:N:117:ALA:CB	2.59	0.86
16:2:237:PHE:CE1	16:2:241:TYR:CZ	2.64	0.86
18:4:243:THR:HG23	18:4:244:ILE:O	1.74	0.86
1:A:64:PHE:CE2	1:A:74:ILE:HG23	2.09	0.86
1:A:103:PHE:HD2	1:A:103:PHE:N	1.71	0.86
1:A:240:LYS:N	1:A:243:PRO:HD2	1.89	0.86
1:A:248:PHE:HD2	1:A:248:PHE:N	1.73	0.86
1:A:267:THR:O	1:A:269:PHE:HD2	1.56	0.86
1:A:308:ILE:HD11	19:A:1115:CLA:CBB	2.04	0.86
1:A:401:TRP:CD1	19:A:1126:CLA:HHC	2.11	0.86
19:A:1105:CLA:C2B	21:J:6012:BCR:H331	2.05	0.86
2:B:444:LEU:CD2	2:B:452:GLN:HE22	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1223:CLA:H122	21:B:6010:BCR:C14	2.05	0.86
6:F:89:LYS:HG2	6:F:90:GLN:N	1.90	0.86
7:G:131:GLY:HA2	7:G:136:VAL:CG2	2.06	0.86
10:J:31:ARG:NH2	19:J:1311:CLA:C4B	2.39	0.86
16:2:148:ASP:HB3	16:2:152:LEU:CG	2.04	0.86
18:4:96:LEU:C	18:4:96:LEU:CD1	2.48	0.86
18:4:207:ASN:ND2	19:4:4002:CLA:NA	2.23	0.86
1:A:207:LEU:HD11	1:A:314:GLY:CA	2.05	0.86
2:B:123:TRP:CB	2:B:126:THR:HG21	2.06	0.86
2:B:304:ILE:O	2:B:308:HIS:HB2	1.76	0.86
2:B:421:HIS:NE2	19:B:1228:CLA:ND	2.23	0.86
19:B:1232:CLA:HMB1	21:B:6010:BCR:H292	1.56	0.86
21:B:6020:BCR:C33	19:L:1502:CLA:C3B	2.54	0.86
15:1:137:ILE:HG22	19:1:1013:CLA:HBB2	1.58	0.86
17:3:151:TRP:HD1	17:3:152:ALA:H	1.21	0.86
1:A:331:LEU:HD23	1:A:331:LEU:O	1.75	0.86
2:B:131:THR:CB	2:B:134:ASP:HB2	2.06	0.86
18:4:177:LEU:HD13	18:4:178:PRO:CD	2.05	0.86
1:A:120:ALA:N	1:A:145:ILE:HD11	1.89	0.85
1:A:472:ARG:HH12	12:L:120:LEU:HD22	1.37	0.85
1:A:483:GLN:HB3	1:A:485:GLN:CD	2.01	0.85
19:A:1124:CLA:CED	19:A:1125:CLA:HMD2	2.05	0.85
2:B:229:GLN:C	7:G:63:VAL:CG2	2.46	0.85
5:E:78:ARG:CZ	5:E:125:ILE:HG21	2.05	0.85
12:L:85:ASN:O	12:L:92:ALA:HB2	1.76	0.85
12:L:104:LEU:HD21	12:L:199:TRP:HZ2	1.41	0.85
15:1:158:PRO:HG2	15:1:159:GLU:H	1.38	0.85
19:3:3016:CLA:HMC1	19:3:3016:CLA:HBC3	1.59	0.85
1:A:190:ALA:HB1	1:A:191:PRO:HD3	1.57	0.85
19:A:1131:CLA:H52	21:B:6017:BCR:H343	1.58	0.85
4:D:140:LEU:HD12	4:D:141:GLY:H	1.06	0.85
4:D:159:PRO:HD2	4:D:159:PRO:O	1.75	0.85
12:L:78:LEU:HD12	12:L:79:ILE:N	1.91	0.85
22:R:7021:LMU:H22	22:R:7021:LMU:H62	1.57	0.85
15:1:150:HIS:CD2	15:1:151:GLN:NE2	2.43	0.85
16:2:129:LEU:O	16:2:130:GLY:C	2.19	0.85
16:2:139:THR:HG23	16:2:140:ALA:N	1.85	0.85
16:2:182:ILE:CB	16:2:187:LYS:CG	2.54	0.85
18:4:122:ASN:O	18:4:123:VAL:HG12	1.76	0.85
11:K:115:ILE:CA	11:K:118:VAL:HG22	2.05	0.85
12:L:210:PRO:C	12:L:211:TYR:CG	2.53	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:2007:CLA:HBC1	19:3:2009:CLA:CED	1.81	0.85
18:4:172:PHE:HD1	18:4:173:LYS:O	1.57	0.85
1:A:207:LEU:HD11	1:A:314:GLY:N	1.91	0.85
2:B:329:SER:O	2:B:330:ILE:CG2	2.23	0.85
2:B:596:TRP:CZ3	2:B:612:SER:O	2.30	0.85
4:D:139:ALA:O	4:D:142:THR:HG22	1.76	0.85
22:E:7048:LMU:H111	22:E:7048:LMU:C7	2.04	0.85
6:F:124:GLU:HG3	6:F:128:LYS:CD	2.06	0.85
11:K:115:ILE:CG1	11:K:121:VAL:C	2.47	0.85
13:N:155:GLU:CB	13:N:157:LYS:HE2	2.06	0.85
15:1:67:LEU:HD12	15:1:68:GLY:CA	2.06	0.85
15:1:170:PRO:C	15:1:173:TYR:CE2	2.54	0.85
21:1:6023:BCR:C8	21:1:6023:BCR:C31	2.54	0.85
1:A:64:PHE:CZ	1:A:77:LYS:HE2	2.11	0.85
2:B:551:LYS:HG2	2:B:552:ASP:N	1.91	0.85
19:B:1203:CLA:HHB	19:B:1226:CLA:HBB2	1.57	0.85
10:J:5:LYS:HD2	16:2:178:ASN:HA	1.56	0.85
12:L:174:ASP:CG	12:L:175:GLN:H	1.84	0.85
19:L:1503:CLA:HAA1	19:L:1503:CLA:CGD	2.05	0.85
13:N:142:LYS:HA	13:N:142:LYS:CE	2.00	0.85
15:1:83:GLU:C	15:1:86:HIS:CD2	2.53	0.85
15:1:116:ALA:C	15:1:117:LEU:HD22	2.00	0.85
16:2:168:TRP:HD1	16:2:171:ILE:HG21	0.91	0.85
16:2:251:PHE:O	16:2:251:PHE:CD1	2.29	0.85
17:3:101:GLY:HA2	17:3:104:ILE:HD12	1.57	0.85
2:B:388:ALA:C	2:B:391:PRO:HD2	2.00	0.85
2:B:471:THR:O	2:B:472:TYR:CD1	2.29	0.85
2:B:625:TRP:CE3	2:B:625:TRP:C	2.55	0.85
2:B:672:GLN:NE2	3:C:79:LEU:HD12	1.91	0.85
4:D:156:ARG:CZ	4:D:158:PHE:CE1	2.35	0.85
4:D:157:VAL:HG12	4:D:158:PHE:O	1.77	0.85
19:I:1204:CLA:H142	21:I:6018:BCR:H392	1.59	0.85
12:L:79:ILE:CG2	12:L:80:ALA:N	2.39	0.85
15:1:206:SER:O	15:1:209:PRO:CG	2.25	0.85
16:2:184:PRO:HB3	16:2:187:LYS:CD	2.06	0.85
18:4:215:LEU:O	18:4:216:GLY:C	2.17	0.85
1:A:308:ILE:CD1	19:A:1115:CLA:CAB	2.51	0.85
1:A:308:ILE:HD11	19:A:1115:CLA:C3B	2.06	0.85
1:A:723:ARG:CG	1:A:723:ARG:HH11	1.89	0.85
22:A:7023:LMU:H91	22:A:7023:LMU:H21	1.59	0.85
2:B:25:ILE:HG21	21:L:6019:BCR:C29	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:PRO:O	2:B:204:GLY:HA3	1.77	0.85
2:B:600:THR:O	2:B:604:GLY:CA	2.25	0.85
6:F:150:VAL:O	6:F:150:VAL:HG13	1.75	0.85
11:K:56:ILE:HG23	11:K:59:THR:HG23	1.58	0.85
12:L:125:ILE:HG21	12:L:128:GLN:OE1	1.77	0.85
13:N:139:LYS:CD	13:N:142:LYS:HZ3	1.89	0.85
1:A:71:LEU:CD1	1:A:72:GLU:N	2.39	0.85
1:A:167:THR:CG2	19:A:1112:CLA:HAA2	2.04	0.85
1:A:259:TYR:HB3	1:A:260:PRO:CD	2.07	0.85
1:A:558:LYS:NZ	2:B:674:LEU:HB2	1.92	0.85
22:A:7016:LMU:H81	22:A:7016:LMU:C2	2.04	0.85
2:B:58:PHE:HE2	2:B:145:LEU:HD21	1.42	0.85
2:B:351:HIS:HB3	19:B:1214:CLA:HED1	1.58	0.85
19:B:1220:CLA:C4	19:B:1220:CLA:C4A	2.55	0.85
7:G:77:PHE:O	7:G:79:PHE:HB2	1.76	0.85
7:G:84:ARG:HE	7:G:89:LYS:CE	1.87	0.85
19:J:1308:CLA:HHD	19:J:1308:CLA:HBC3	1.56	0.85
11:K:63:LEU:N	11:K:63:LEU:HD22	1.89	0.85
1:A:249:ILE:H	17:3:137:PHE:HZ	1.24	0.85
1:A:600:LEU:HD21	2:B:665:ILE:O	1.76	0.85
19:A:1134:CLA:HBC2	21:A:6008:BCR:HC31	1.58	0.85
4:D:171:GLY:O	4:D:172:VAL:HG23	1.77	0.85
13:N:133:GLY:HA3	13:N:134:CYS:O	1.77	0.85
15:1:92:LEU:HA	15:1:95:PRO:HG2	1.59	0.85
16:2:237:PHE:C	16:2:237:PHE:CD1	2.54	0.85
18:4:87:ASN:CG	18:4:90:TRP:CE2	2.54	0.85
18:4:173:LYS:HB2	18:4:194:PHE:HD2	1.40	0.85
1:A:661:ALA:O	1:A:664:VAL:HG22	1.77	0.85
2:B:98:GLN:O	2:B:101:VAL:N	2.08	0.85
4:D:103:THR:HG21	4:D:128:LEU:HD12	1.55	0.85
12:L:71:THR:O	12:L:74:THR:HB	1.76	0.85
12:L:92:ALA:H	12:L:98:ARG:NH2	1.72	0.85
12:L:94:SER:O	12:L:96:LEU:HD23	1.76	0.85
19:2:2014:CLA:H152	19:2:2014:CLA:H102	1.58	0.85
1:A:78:VAL:HG11	19:A:1103:CLA:HBC3	1.59	0.84
2:B:98:GLN:C	2:B:100:ALA:N	2.26	0.84
2:B:469:LYS:CG	2:B:470:THR:HG23	2.07	0.84
4:D:191:ILE:H	4:D:191:ILE:HD12	1.40	0.84
6:F:170:ILE:O	6:F:173:TRP:HD1	1.60	0.84
12:L:79:ILE:HG23	12:L:80:ALA:CA	2.07	0.84
22:L:7029:LMU:H6D	22:L:7029:LMU:H51	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:164:LEU:HD12	17:3:165:MET:N	1.90	0.84
19:3:3008:CLA:HMC3	19:3:3008:CLA:HBC2	1.59	0.84
1:A:51:THR:OG1	19:A:1139:CLA:CBB	2.24	0.84
2:B:542:ARG:HH11	2:B:542:ARG:CB	1.90	0.84
5:E:78:ARG:NH1	5:E:125:ILE:CG2	2.41	0.84
5:E:82:TYR:HB3	5:E:83:TRP:HZ3	1.40	0.84
9:I:11:LEU:CD1	21:I:6021:BCR:H10C	2.08	0.84
19:J:1308:CLA:HBD	19:J:1308:CLA:CBA	2.06	0.84
12:L:92:ALA:N	12:L:98:ARG:CZ	2.40	0.84
15:1:125:LEU:HD22	15:1:125:LEU:H	1.40	0.84
17:3:108:PHE:HB3	19:3:3013:CLA:H43	1.58	0.84
17:3:131:GLU:CB	17:3:148:TYR:CD2	2.60	0.84
19:A:1115:CLA:H172	19:A:1115:CLA:C14	2.04	0.84
21:A:6011:BCR:H311	21:A:6011:BCR:HC8	1.58	0.84
19:A:9023:CLA:CMC	2:B:661:PHE:HB2	2.06	0.84
2:B:20:ARG:HG3	2:B:20:ARG:NH1	1.86	0.84
2:B:119:GLY:CA	19:B:1225:CLA:HED1	2.04	0.84
2:B:275:HIS:O	2:B:279:ALA:N	2.09	0.84
2:B:552:ASP:OD1	2:B:553:PHE:CD2	2.30	0.84
4:D:99:PHE:N	4:D:157:VAL:O	2.10	0.84
8:H:63:GLY:C	8:H:66:ASP:OD1	2.08	0.84
19:H:1241:CLA:CAC	21:I:6021:BCR:C3	2.55	0.84
1:A:397:THR:CG2	1:A:613:ILE:CG1	2.50	0.84
1:A:423:ASP:N	1:A:424:PRO:HD3	1.92	0.84
8:H:65:TRP:N	8:H:66:ASP:HA	1.92	0.84
19:J:1308:CLA:CMA	19:2:2014:CLA:HED2	2.06	0.84
11:K:78:ARG:NE	11:K:78:ARG:CA	2.39	0.84
19:L:1148:CLA:CGD	19:L:1148:CLA:CAA	2.51	0.84
15:1:85:ILE:CA	15:1:88:ARG:HG3	2.07	0.84
17:3:171:ARG:HG2	17:3:175:ASP:OD1	1.77	0.84
18:4:146:PHE:HZ	19:4:4013:CLA:NC	1.73	0.84
1:A:596:ASP:HA	1:A:599:PHE:HB3	1.60	0.84
19:A:1112:CLA:C4B	21:A:6002:BCR:C19	2.55	0.84
19:A:1126:CLA:HBA1	19:A:1126:CLA:H43	1.60	0.84
2:B:460:ALA:O	2:B:463:ILE:O	1.95	0.84
19:B:1202:CLA:H43	21:B:6005:BCR:H313	1.58	0.84
5:E:106:ARG:HH21	5:E:107:PHE:HA	0.72	0.84
16:2:246:PRO:CB	16:2:247:ILE:CD1	2.52	0.84
21:I:6021:BCR:C4	21:I:6021:BCR:H322	2.06	0.84
11:K:124:LEU:HD12	11:K:124:LEU:O	1.77	0.84
12:L:172:GLU:N	12:L:173:PRO:HD3	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:157:LYS:HB3	13:N:159:LYS:H	1.39	0.84
16:2:229:MET:SD	16:2:230:LEU:CD2	2.66	0.84
1:A:740:LEU:HD21	19:A:1140:CLA:HMA2	1.59	0.84
19:B:1220:CLA:HBC3	19:B:1220:CLA:CMC	2.04	0.84
3:C:44:ARG:HE	4:D:182:GLN:HE21	1.21	0.84
6:F:170:ILE:CG2	21:F:6014:BCR:C37	2.56	0.84
8:H:70:SER:O	8:H:73:PRO:HD3	1.78	0.84
19:H:1241:CLA:C3C	21:I:6021:BCR:HC22	2.07	0.84
11:K:51:SER:N	11:K:52:PRO:HD3	1.92	0.84
15:1:77:GLU:CA	15:1:80:LYS:HG2	2.06	0.84
15:1:92:LEU:CA	15:1:95:PRO:CD	2.55	0.84
18:4:88:LEU:O	18:4:90:TRP:HB3	1.77	0.84
1:A:162:LEU:C	1:A:165:TYR:HB3	2.03	0.84
6:F:99:LEU:HA	6:F:102:LEU:CD2	2.07	0.84
12:L:153:PHE:N	12:L:153:PHE:CD2	2.45	0.84
18:4:205:ILE:CG1	18:4:206:ALA:N	2.40	0.84
1:A:527:VAL:HB	1:A:626:GLY:HA3	1.58	0.84
2:B:352:MET:HE1	19:B:1225:CLA:OBD	1.78	0.84
8:H:119:ASP:CG	8:H:121:LEU:HG	2.03	0.84
11:K:127:ILE:C	11:K:130:LEU:HG	2.02	0.84
12:L:60:ILE:HG23	12:L:61:ASN:H	1.39	0.84
15:1:64:PHE:O	15:1:69:LEU:CD1	2.25	0.84
1:A:284:ARG:HA	1:A:284:ARG:HH11	1.20	0.84
1:A:388:ASP:CG	1:A:391:THR:OG1	2.21	0.84
1:A:684:PHE:C	1:A:684:PHE:CD2	2.56	0.84
2:B:257:ILE:C	2:B:497:TRP:HZ3	1.86	0.84
2:B:319:HIS:CE1	2:B:322:LEU:CD1	2.60	0.84
2:B:454:LEU:CD1	6:F:147:HIS:HA	2.07	0.84
2:B:542:ARG:HG3	2:B:542:ARG:NH1	1.86	0.84
19:B:1209:CLA:HMC2	21:B:6005:BCR:H373	1.58	0.84
19:B:1235:CLA:C20	21:F:6016:BCR:HC41	2.08	0.84
5:E:93:VAL:CG2	5:E:103:VAL:HB	2.08	0.84
7:G:124:ILE:CG1	7:G:128:LEU:HD12	2.06	0.84
15:1:90:ALA:O	15:1:94:VAL:HG23	1.77	0.84
15:1:93:ALA:HB1	19:1:1006:CLA:C1C	2.07	0.84
16:2:134:THR:HG1	16:2:135:PRO:HD2	0.99	0.84
2:B:75:GLU:CB	2:B:132:ASN:HD22	1.86	0.83
3:C:44:ARG:N	4:D:182:GLN:HG3	1.93	0.83
7:G:90:GLN:CB	7:G:91:VAL:C	2.51	0.83
22:K:7042:LMU:H5'	22:K:7042:LMU:O2B	1.78	0.83
19:R:1144:CLA:HED3	19:R:1144:CLA:C1A	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:122:LEU:CD2	19:3:3006:CLA:C4D	2.52	0.83
1:A:733:VAL:HG21	19:A:1140:CLA:C2D	2.08	0.83
2:B:633:ASN:HB3	2:B:636:THR:HB	1.60	0.83
3:C:54:CYS:CB	23:C:8002:SF4:S1	2.66	0.83
16:2:101:TRP:H	16:2:103:VAL:CB	1.90	0.83
18:4:169:ASP:O	18:4:173:LYS:HA	1.77	0.83
1:A:356:ALA:O	1:A:360:ILE:HG22	1.77	0.83
19:A:9022:CLA:H151	21:B:6017:BCR:C20	2.09	0.83
2:B:308:HIS:CG	2:B:309:ILE:H	1.93	0.83
3:C:67:VAL:HG13	3:C:68:TYR:CA	2.08	0.83
17:3:96:ARG:HA	17:3:99:ALA:CA	2.08	0.83
22:A:7016:LMU:H1'	22:A:7016:LMU:H31	1.58	0.83
2:B:230:TRP:HB3	19:B:1213:CLA:HED3	1.57	0.83
2:B:302:LYS:HD3	7:G:105:THR:HA	1.60	0.83
2:B:374:HIS:HB2	19:B:1224:CLA:C1B	2.08	0.83
5:E:78:ARG:NH2	5:E:123:ASP:O	2.10	0.83
13:N:104:LYS:O	13:N:107:LEU:HB2	1.77	0.83
17:3:158:PHE:N	17:3:158:PHE:CD1	2.37	0.83
19:4:1004:CLA:HHD	19:4:1004:CLA:CBC	2.07	0.83
1:A:525:ASN:CB	1:A:526:LYS:HG3	2.08	0.83
19:B:1220:CLA:H151	19:B:1220:CLA:C10	1.97	0.83
4:D:111:ILE:CG1	4:D:121:ILE:HG22	2.07	0.83
5:E:83:TRP:HH2	5:E:116:SER:HB2	1.43	0.83
7:G:128:LEU:HD23	7:G:128:LEU:C	2.03	0.83
7:G:130:TRP:O	7:G:134:GLY:HA3	1.76	0.83
22:3:7003:LMU:C4B	22:3:7005:LMU:C4B	2.54	0.83
22:3:7003:LMU:H4B	22:3:7005:LMU:H4B	1.59	0.83
18:4:120:ILE:CD1	18:4:226:LYS:CG	2.07	0.83
1:A:203:LEU:HD22	19:A:1123:CLA:CED	2.07	0.83
1:A:249:ILE:HG21	17:3:136:TRP:CZ3	2.01	0.83
1:A:328:LYS:HG3	1:A:332:GLU:HB2	1.57	0.83
1:A:443:ILE:HD11	1:A:557:LEU:HD21	1.55	0.83
19:A:1133:CLA:OBD	19:A:1134:CLA:HAC1	1.79	0.83
2:B:586:THR:O	2:B:588:GLY:N	2.11	0.83
4:D:157:VAL:CG1	4:D:158:PHE:O	2.26	0.83
1:A:274:TRP:NE1	1:A:277:TYR:CE2	2.47	0.83
1:A:545:HIS:CB	19:A:1135:CLA:HBB2	2.08	0.83
1:A:628:ILE:CD1	1:A:632:GLY:HA2	2.08	0.83
2:B:269:TRP:HB2	2:B:497:TRP:CH2	2.14	0.83
5:E:107:PHE:HE2	5:E:109:LYS:CG	1.85	0.83
8:H:56:GLU:HG3	8:H:57:ASP:HA	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:113:SER:OG	19:H:1207:CLA:C6	2.26	0.83
12:L:100:ILE:HG22	12:L:191:PHE:O	1.79	0.83
17:3:181:SER:HB2	19:3:2009:CLA:C11	2.07	0.83
17:3:187:PHE:C	17:3:187:PHE:HD1	1.86	0.83
18:4:122:ASN:HB3	18:4:124:PRO:HD3	1.59	0.83
22:4:7053:LMU:H11	22:4:7053:LMU:C5'	2.08	0.83
1:A:555:ILE:CD1	19:A:9023:CLA:HMD2	2.08	0.83
19:A:1125:CLA:HMC1	19:A:1125:CLA:HBC2	1.61	0.83
2:B:261:PHE:HE2	2:B:499:ASN:C	1.87	0.83
2:B:470:THR:N	2:B:501:ILE:CB	2.27	0.83
12:L:145:LEU:HD11	21:L:6019:BCR:C31	2.08	0.83
12:L:168:GLY:C	12:L:170:LYS:H	1.87	0.83
17:3:243:ILE:CD1	19:3:3005:CLA:C2C	2.57	0.83
1:A:92:TRP:O	1:A:93:LEU:HD23	1.76	0.83
1:A:244:LEU:HB3	1:A:247:GLU:CG	2.07	0.83
1:A:316:MET:CB	1:A:317:TYR:HD1	1.92	0.83
19:B:1223:CLA:H8	21:B:6010:BCR:H12C	1.60	0.83
21:B:6020:BCR:H332	19:L:1502:CLA:C3B	2.08	0.83
6:F:179:ARG:CG	6:F:183:ILE:HD11	2.09	0.83
11:K:125:LYS:CA	11:K:126:ASN:CB	2.51	0.83
12:L:79:ILE:HG23	12:L:80:ALA:N	1.92	0.83
16:2:158:VAL:HG22	16:2:159:PHE:N	1.92	0.83
17:3:156:THR:O	17:3:159:VAL:N	2.11	0.83
17:3:210:PRO:CG	17:3:211:LEU:HD12	2.07	0.83
2:B:7:ARG:HG3	2:B:7:ARG:NH1	1.89	0.83
2:B:131:THR:HG22	2:B:134:ASP:CB	2.09	0.83
2:B:174:ARG:HB2	19:B:1210:CLA:CBC	2.08	0.83
6:F:228:ASP:O	6:F:231:PHE:HB3	1.79	0.83
15:1:189:LYS:HB3	19:1:1007:CLA:HMC3	1.61	0.83
16:2:236:TRP:O	16:2:240:ILE:HG13	1.79	0.83
16:2:266:PHE:CD1	16:2:267:THR:N	2.47	0.83
17:3:108:PHE:CB	19:3:3013:CLA:C4	2.57	0.83
1:A:207:LEU:O	1:A:310:PHE:HB3	1.77	0.82
1:A:249:ILE:HG12	1:A:250:LEU:H	1.41	0.82
2:B:7:ARG:HH11	2:B:7:ARG:CB	1.91	0.82
2:B:588:GLY:O	2:B:592:PHE:HB2	1.77	0.82
6:F:103:GLN:CD	6:F:104:ALA:H	1.87	0.82
13:N:99:LYS:HB3	13:N:102:ASN:HD21	1.41	0.82
14:R:41:UNK:CB	14:R:42:UNK:CB	2.56	0.82
15:1:97:ILE:CD1	15:1:98:LEU:HD23	2.09	0.82
16:2:124:GLU:O	16:2:127:THR:CA	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:4003:CLA:HMC3	19:4:4003:CLA:HBC2	1.60	0.82
1:A:236:GLY:O	1:A:237:VAL:HG22	1.78	0.82
1:A:249:ILE:C	1:A:251:ASN:N	2.31	0.82
1:A:488:PHE:CE2	1:A:533:PRO:HB2	2.14	0.82
2:B:715:VAL:HG13	2:B:719:PHE:CD2	2.13	0.82
2:B:732:LYS:HB3	2:B:733:PHE:CA	2.08	0.82
3:C:20:ALA:O	3:C:21:CYS:HB2	1.76	0.82
8:H:64:GLN:HB2	8:H:67:SER:H	1.44	0.82
19:J:1311:CLA:H141	19:2:2014:CLA:HMB2	1.61	0.82
11:K:57:MET:SD	11:K:61:THR:OG1	2.36	0.82
19:K:1143:CLA:H3A	19:K:1143:CLA:CGA	2.09	0.82
12:L:83:LEU:O	12:L:83:LEU:HD12	1.78	0.82
12:L:92:ALA:CB	12:L:98:ARG:NH2	2.41	0.82
15:1:77:GLU:CA	15:1:80:LYS:CG	2.53	0.82
1:A:668:TYR:OH	2:B:441:ASP:OD1	1.96	0.82
23:A:8001:SF4:S4	2:B:560:ASP:O	2.37	0.82
2:B:515:GLY:HA3	2:B:613:SER:HB2	1.60	0.82
8:H:109:LEU:O	8:H:113:SER:CB	2.27	0.82
19:J:1308:CLA:H92	19:2:2014:CLA:CGD	2.10	0.82
12:L:51:LYS:HE2	12:L:51:LYS:CA	2.07	0.82
12:L:210:PRO:C	12:L:211:TYR:CD2	2.57	0.82
19:2:2014:CLA:H152	19:2:2014:CLA:C8	2.10	0.82
1:A:103:PHE:N	1:A:103:PHE:CD2	2.44	0.82
2:B:7:ARG:O	2:B:7:ARG:HG2	1.79	0.82
2:B:493:TRP:NE1	19:B:1213:CLA:HAC2	1.93	0.82
2:B:618:GLY:HA2	2:B:621:ARG:HB3	1.61	0.82
24:B:7101:LMG:O3	3:C:70:TRP:CE2	2.31	0.82
6:F:103:GLN:CG	6:F:104:ALA:H	1.91	0.82
6:F:200:VAL:CG1	10:J:7:TYR:N	2.42	0.82
13:N:132:THR:OG1	13:N:138:ALA:C	2.22	0.82
13:N:157:LYS:H	13:N:157:LYS:HE2	1.42	0.82
16:2:177:VAL:CG1	16:2:178:ASN:HB2	2.05	0.82
16:2:184:PRO:CD	16:2:185:ASN:C	2.53	0.82
1:A:207:LEU:HD22	19:A:1119:CLA:HBB2	1.59	0.82
19:A:1138:CLA:HBC2	19:A:1139:CLA:C1C	2.10	0.82
19:B:1210:CLA:H141	19:B:1215:CLA:H2	1.61	0.82
4:D:86:SER:O	12:L:67:GLY:CA	2.27	0.82
4:D:163:VAL:O	4:D:164:GLN:CG	2.27	0.82
4:D:185:GLY:O	4:D:186:GLN:HG3	1.79	0.82
15:1:207:ALA:C	15:1:209:PRO:HD3	2.05	0.82
15:1:208:TYR:N	15:1:209:PRO:HD3	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:195:ALA:HB3	18:4:197:THR:O	1.79	0.82
1:A:93:LEU:CA	1:A:96:MET:H	1.91	0.82
2:B:268:LEU:HD22	2:B:273:VAL:CG1	2.10	0.82
2:B:429:LEU:HD11	19:B:1235:CLA:HMB2	1.59	0.82
19:B:1218:CLA:HBC2	19:B:1218:CLA:CHD	2.07	0.82
4:D:132:ALA:HB3	4:D:136:GLN:HE22	1.43	0.82
12:L:72:PRO:O	12:L:73:VAL:CG2	2.26	0.82
13:N:114:PHE:CB	13:N:117:ALA:HB3	2.09	0.82
15:1:177:PRO:HG2	15:1:179:LYS:C	2.04	0.82
16:2:229:MET:SD	16:2:230:LEU:CA	2.67	0.82
19:A:1134:CLA:CGA	19:A:1141:CLA:CBB	2.56	0.82
19:A:9023:CLA:HMC1	2:B:661:PHE:CB	2.09	0.82
2:B:664:LEU:C	2:B:667:TRP:HZ3	1.87	0.82
11:K:63:LEU:HD13	11:K:63:LEU:H	1.42	0.82
19:L:1130:CLA:H52	19:L:1504:CLA:HHB	1.61	0.82
13:N:148:ASP:H	13:N:149:ASP:C	1.87	0.82
18:4:96:LEU:HD12	18:4:97:VAL:N	1.95	0.82
2:B:315:LEU:HD12	2:B:317:ARG:CG	2.04	0.82
6:F:177:VAL:HA	6:F:180:SER:OG	1.78	0.82
16:2:128:LYS:HB3	16:2:131:ILE:HG12	1.59	0.82
16:2:243:GLY:C	16:2:244:THR:HG23	2.05	0.82
19:2:2014:CLA:C15	19:2:2014:CLA:H91	2.09	0.82
17:3:150:TYR:CD2	17:3:151:TRP:CG	2.67	0.82
19:4:1306:CLA:HED1	19:4:1306:CLA:H2	1.60	0.82
1:A:85:GLN:C	1:A:87:SER:O	2.22	0.82
2:B:493:TRP:CH2	19:B:1232:CLA:HMA2	2.15	0.82
7:G:99:HIS:C	7:G:101:GLU:N	2.37	0.82
7:G:124:ILE:HG12	7:G:128:LEU:HD13	1.62	0.82
15:1:114:TRP:CH2	15:1:121:GLN:HG3	2.15	0.82
19:1:1007:CLA:CBC	19:1:1007:CLA:HHD	2.09	0.82
16:2:165:GLY:CA	16:2:167:ARG:HG2	2.08	0.82
17:3:156:THR:O	17:3:156:THR:CG2	2.26	0.82
1:A:246:HIS:CD2	19:3:1147:CLA:O1D	2.33	0.82
2:B:123:TRP:CB	2:B:126:THR:CG2	2.57	0.82
2:B:440:ASN:OD1	2:B:614:THR:HG22	1.76	0.82
2:B:440:ASN:OD1	2:B:614:THR:HG21	1.77	0.82
19:B:1235:CLA:H161	21:F:6016:BCR:C31	2.08	0.82
3:C:63:LEU:CD2	3:C:65:VAL:H	1.92	0.82
11:K:78:ARG:HA	11:K:78:ARG:CZ	2.09	0.82
17:3:131:GLU:CB	17:3:148:TYR:CE2	2.62	0.82
1:A:162:LEU:O	1:A:165:TYR:CB	2.25	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:CG	19:A:1115:CLA:HED1	2.09	0.81
2:B:31:PHE:O	2:B:37:ILE:HG21	1.80	0.81
5:E:78:ARG:CZ	5:E:125:ILE:CG2	2.57	0.81
17:3:98:LEU:CD1	19:3:3012:CLA:C2D	2.57	0.81
18:4:111:LEU:HD12	18:4:112:PRO:CG	2.10	0.81
18:4:220:GLN:HG3	19:4:1306:CLA:HAC2	1.61	0.81
1:A:79:PHE:CD1	19:A:1111:CLA:HED3	2.16	0.81
19:A:1122:CLA:C4C	21:A:6007:BCR:C19	2.59	0.81
2:B:224:PRO:CB	2:B:227:THR:HB	2.10	0.81
2:B:679:ALA:O	2:B:683:GLU:OE1	1.97	0.81
7:G:100:PHE:N	7:G:101:GLU:CB	2.43	0.81
8:H:97:LEU:HG	8:H:98:LEU:CA	2.10	0.81
21:I:6021:BCR:C39	21:L:6019:BCR:H401	2.09	0.81
12:L:73:VAL:CG2	19:L:1130:CLA:OBD	2.28	0.81
12:L:115:VAL:CG1	12:L:130:GLY:H	1.91	0.81
19:2:2014:CLA:OBD	19:2:2014:CLA:HED3	1.79	0.81
18:4:173:LYS:HZ2	18:4:201:LYS:HG2	1.46	0.81
1:A:129:GLN:NE2	19:A:1107:CLA:MG	1.36	0.81
1:A:195:TRP:CZ2	19:A:1108:CLA:CMA	2.63	0.81
1:A:284:ARG:NH2	1:A:507:ALA:O	2.11	0.81
1:A:400:MET:HE3	1:A:612:VAL:HG11	1.61	0.81
1:A:426:THR:HG23	1:A:428:TYR:OH	1.79	0.81
19:A:9023:CLA:HMC1	2:B:661:PHE:HB2	1.62	0.81
2:B:79:GLN:O	2:B:80:ASP:HB3	1.79	0.81
2:B:293:THR:HG22	7:G:94:GLN:CG	2.10	0.81
2:B:586:THR:C	2:B:588:GLY:H	1.87	0.81
2:B:600:THR:O	2:B:604:GLY:HA3	1.81	0.81
2:B:633:ASN:CB	2:B:636:THR:CB	2.44	0.81
4:D:185:GLY:O	4:D:186:GLN:CG	2.28	0.81
5:E:107:PHE:CD2	5:E:109:LYS:CG	2.63	0.81
8:H:78:PRO:HB3	19:L:1501:CLA:HMD3	1.63	0.81
8:H:98:LEU:HD23	12:L:146:THR:HG21	1.61	0.81
13:N:118:TYR:O	13:N:119:THR:HG23	1.80	0.81
15:1:149:GLU:CG	15:1:152:ARG:HH12	1.93	0.81
15:1:224:PRO:CA	15:1:225:TRP:HB2	2.10	0.81
17:3:161:GLU:HA	17:3:164:LEU:HG	1.61	0.81
17:3:204:GLY:HA3	17:3:206:PRO:O	1.80	0.81
17:3:207:PHE:HD1	17:3:207:PHE:C	1.84	0.81
22:3:7005:LMU:H51	22:3:7005:LMU:H11	1.61	0.81
18:4:90:TRP:C	18:4:91:PHE:HD1	1.87	0.81
18:4:169:ASP:HA	18:4:173:LYS:CA	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:VAL:HG12	4:D:130:LYS:HB2	1.62	0.81
9:I:8:PHE:HB2	19:I:1204:CLA:OBD	1.80	0.81
11:K:56:ILE:HA	11:K:59:THR:HG22	1.62	0.81
11:K:76:ALA:H	11:K:78:ARG:NH1	1.78	0.81
12:L:141:LEU:HD13	12:L:145:LEU:CD1	2.09	0.81
12:L:168:GLY:C	12:L:170:LYS:N	2.35	0.81
15:1:77:GLU:CB	15:1:80:LYS:HD2	2.11	0.81
15:1:114:TRP:CH2	15:1:121:GLN:HA	2.14	0.81
15:1:172:GLY:HA2	15:1:173:TYR:CD2	2.14	0.81
17:3:96:ARG:NH1	17:3:96:ARG:CB	2.41	0.81
17:3:136:TRP:N	17:3:139:THR:OG1	2.13	0.81
18:4:131:LYS:H	18:4:131:LYS:HD2	1.45	0.81
1:A:158:ILE:HD13	19:A:1112:CLA:HED3	1.62	0.81
19:A:1112:CLA:C4B	21:A:6002:BCR:H19C	2.10	0.81
4:D:138:LEU:O	4:D:140:LEU:O	1.98	0.81
7:G:124:ILE:HG23	7:G:125:VAL:N	1.96	0.81
1:A:129:GLN:NE2	19:A:1107:CLA:ND	2.29	0.81
23:A:8001:SF4:S2	2:B:702:ILE:HD11	2.21	0.81
2:B:172:GLU:O	2:B:176:ASN:CB	2.28	0.81
2:B:315:LEU:CD1	2:B:317:ARG:CG	2.57	0.81
2:B:353:TYR:CD2	2:B:594:TRP:HZ3	1.96	0.81
3:C:69:LEU:HD12	3:C:70:TRP:N	1.95	0.81
19:J:1308:CLA:HBC2	19:J:1308:CLA:CHD	2.10	0.81
11:K:50:GLY:C	11:K:52:PRO:HD2	2.06	0.81
12:L:141:LEU:CD1	12:L:145:LEU:HD11	2.08	0.81
15:1:117:LEU:HD13	15:1:117:LEU:N	1.96	0.81
16:2:184:PRO:CD	16:2:187:LYS:N	2.44	0.81
17:3:94:GLU:C	17:3:94:GLU:CD	2.47	0.81
1:A:23:ASP:OD1	1:A:24:ARG:HD2	1.80	0.81
1:A:351:THR:C	19:A:1123:CLA:H191	2.05	0.81
19:A:1115:CLA:C19	11:K:64:MET:CE	2.59	0.81
2:B:140:ILE:CG1	2:B:141:PHE:H	1.92	0.81
2:B:232:LEU:HD11	2:B:235:GLN:HG3	1.59	0.81
4:D:93:LYS:HG3	4:D:96:VAL:CG1	2.10	0.81
5:E:127:GLU:CA	5:E:128:VAL:O	2.29	0.81
12:L:164:LEU:HD12	12:L:165:THR:H	1.42	0.81
17:3:201:ALA:HB1	17:3:202:TYR:HE2	1.39	0.81
1:A:23:ASP:CG	1:A:33:GLN:CG	2.54	0.81
2:B:294:ASN:CB	7:G:94:GLN:OE1	2.25	0.81
5:E:127:GLU:CB	5:E:128:VAL:O	2.28	0.81
5:E:127:GLU:CB	5:E:129:GLU:O	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:116:ALA:HB1	8:H:117:SER:CA	2.06	0.81
15:1:97:ILE:HD12	15:1:98:LEU:HD23	1.63	0.81
15:1:158:PRO:CG	15:1:159:GLU:H	1.92	0.81
16:2:128:LYS:HB3	16:2:131:ILE:HG23	1.62	0.81
16:2:182:ILE:C	16:2:187:LYS:HG3	2.05	0.81
1:A:279:ASP:C	1:A:281:LEU:HG	2.06	0.81
1:A:415:ALA:O	1:A:419:VAL:HG23	1.80	0.81
2:B:233:TYR:HD1	2:B:254:ILE:HG13	1.44	0.81
4:D:198:ILE:O	4:D:198:ILE:HG13	1.75	0.81
5:E:107:PHE:CD2	5:E:109:LYS:CD	2.64	0.81
22:E:7048:LMU:H4B	22:F:7036:LMU:C6'	2.07	0.81
6:F:103:GLN:CG	6:F:104:ALA:N	2.44	0.81
6:F:224:GLY:C	6:F:227:VAL:CG1	2.54	0.81
7:G:69:GLY:O	7:G:72:LEU:CG	2.29	0.81
13:N:114:PHE:O	13:N:117:ALA:HB3	1.80	0.81
19:1:1007:CLA:HHD	19:1:1007:CLA:HBC2	1.63	0.81
16:2:124:GLU:O	16:2:127:THR:HG22	1.81	0.81
1:A:227:LEU:HD22	1:A:296:LEU:HD13	1.61	0.81
2:B:571:SER:OG	2:B:574:ASP:OD1	1.99	0.81
4:D:123:ARG:HH22	22:D:7050:LMU:H4B	1.45	0.81
5:E:78:ARG:NH1	5:E:125:ILE:HG21	1.95	0.81
6:F:200:VAL:HG23	6:F:204:SER:H	1.46	0.81
19:2:2014:CLA:C10	19:2:2014:CLA:C15	2.59	0.81
1:A:68:THR:HG22	1:A:70:ASP:H	1.42	0.80
2:B:314:ARG:HH12	15:1:67:LEU:HD21	0.98	0.80
2:B:542:ARG:NH2	4:D:195:VAL:O	2.14	0.80
19:B:1203:CLA:H2A	19:B:1203:CLA:O1D	1.81	0.80
4:D:147:LYS:C	4:D:148:TYR:CG	2.57	0.80
5:E:90:VAL:HG12	5:E:91:VAL:N	1.95	0.80
7:G:73:PHE:O	7:G:76:ARG:HB2	1.80	0.80
16:2:182:ILE:HG22	16:2:187:LYS:CG	2.09	0.80
17:3:125:VAL:HB	17:3:126:GLY:HA2	1.61	0.80
1:A:98:PHE:O	1:A:99:HIS:C	2.24	0.80
19:A:1126:CLA:H172	21:J:6012:BCR:H17C	1.62	0.80
2:B:58:PHE:CE2	2:B:145:LEU:HD21	2.14	0.80
2:B:224:PRO:CB	2:B:227:THR:CB	2.60	0.80
2:B:304:ILE:HD11	19:B:1216:CLA:HED2	0.83	0.80
19:B:1235:CLA:C16	21:F:6016:BCR:C31	2.59	0.80
14:R:33:UNK:O	14:R:36:UNK:CB	2.30	0.80
15:1:137:ILE:HG12	15:1:138:LEU:H	1.46	0.80
18:4:174:GLN:O	18:4:194:PHE:HB3	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:THR:HA	19:A:1123:CLA:H201	1.61	0.80
2:B:131:THR:O	2:B:135:LEU:HD23	1.82	0.80
2:B:378:ILE:O	2:B:380:GLY:N	2.14	0.80
19:B:1235:CLA:HBC1	6:F:160:PHE:HZ	1.41	0.80
3:C:29:ILE:HG12	4:D:180:GLY:HA2	1.63	0.80
9:I:1:MET:O	9:I:2:ILE:HG22	1.80	0.80
15:1:85:ILE:HG12	15:1:88:ARG:NH2	1.97	0.80
17:3:113:ALA:HB1	17:3:239:LEU:CD1	1.98	0.80
19:4:1306:CLA:HBC3	19:4:1306:CLA:CMC	2.12	0.80
1:A:279:ASP:O	1:A:281:LEU:CD1	2.29	0.80
1:A:370:ILE:CG2	1:A:400:MET:HA	2.11	0.80
1:A:445:HIS:O	1:A:446:LEU:HB3	1.80	0.80
2:B:58:PHE:CE2	2:B:145:LEU:HD22	2.09	0.80
2:B:315:LEU:CD1	2:B:315:LEU:C	2.54	0.80
4:D:138:LEU:C	4:D:140:LEU:O	2.25	0.80
6:F:103:GLN:HG3	6:F:104:ALA:H	1.47	0.80
7:G:62:LEU:CB	7:G:65:SER:HB3	2.09	0.80
11:K:47:ASP:HA	11:K:51:SER:HB2	1.64	0.80
11:K:115:ILE:CG1	11:K:122:LEU:H	1.92	0.80
15:1:92:LEU:HA	15:1:95:PRO:CD	2.11	0.80
15:1:171:LEU:CA	15:1:173:TYR:CZ	2.63	0.80
16:2:177:VAL:CG1	16:2:178:ASN:CB	2.58	0.80
18:4:211:MET:HG3	19:4:4002:CLA:CBB	2.12	0.80
1:A:255:LEU:CD1	1:A:280:PHE:HZ	1.93	0.80
1:A:281:LEU:CD2	19:A:1115:CLA:HED1	2.03	0.80
1:A:328:LYS:HZ3	1:A:345:GLY:HA2	1.44	0.80
1:A:356:ALA:HB2	1:A:417:PHE:CD2	2.17	0.80
1:A:423:ASP:CB	1:A:424:PRO:HD3	2.11	0.80
2:B:257:ILE:C	2:B:497:TRP:CZ3	2.57	0.80
2:B:432:HIS:HE1	19:B:1229:CLA:NB	1.80	0.80
2:B:459:PHE:HE2	19:B:1235:CLA:CHD	1.95	0.80
2:B:628:SER:O	2:B:631:LEU:CD2	2.29	0.80
22:D:7050:LMU:C2B	22:D:7050:LMU:C6'	2.57	0.80
16:2:160:ILE:HG22	19:2:2012:CLA:CAB	2.12	0.80
1:A:76:ARG:NH1	1:A:193:LEU:HD22	1.96	0.80
1:A:123:VAL:O	19:A:1107:CLA:O1D	1.97	0.80
1:A:353:SER:O	1:A:354:TRP:HB2	1.82	0.80
1:A:425:THR:C	1:A:428:TYR:CE1	2.60	0.80
2:B:119:GLY:HA3	19:B:1225:CLA:CED	2.09	0.80
2:B:457:PRO:CB	2:B:517:PHE:HB2	2.12	0.80
19:B:1213:CLA:HHD	19:B:1213:CLA:CBC	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:115:ILE:HG12	11:K:121:VAL:C	2.06	0.80
12:L:55:GLN:C	12:L:57:ILE:H	1.90	0.80
19:L:1148:CLA:HBC3	19:L:1148:CLA:CHD	2.09	0.80
13:N:110:THR:HG22	13:N:111:GLY:H	1.46	0.80
16:2:184:PRO:HD3	16:2:187:LYS:CD	2.12	0.80
18:4:131:LYS:H	18:4:131:LYS:CD	1.95	0.80
1:A:50:THR:CG2	1:A:51:THR:N	2.44	0.80
19:A:1131:CLA:H161	21:L:6019:BCR:C36	2.12	0.80
19:A:1138:CLA:C19	6:F:181:TYR:HB3	2.10	0.80
21:A:6011:BCR:H312	19:A:9013:CLA:H143	1.62	0.80
2:B:679:ALA:O	2:B:683:GLU:CD	2.25	0.80
15:1:137:ILE:HG12	15:1:138:LEU:N	1.96	0.80
22:1:7004:LMU:O6B	22:1:7004:LMU:H1B	1.80	0.80
1:A:355:HIS:ND1	1:A:416:ILE:HG21	1.97	0.80
1:A:446:LEU:HD21	1:A:554:LEU:HA	1.62	0.80
2:B:53:GLN:C	2:B:55:ALA:H	1.90	0.80
2:B:282:PHE:CZ	19:B:1213:CLA:C1	2.64	0.80
2:B:462:TRP:CZ3	19:B:1231:CLA:CBC	2.65	0.80
2:B:628:SER:O	2:B:629:SER:C	2.24	0.80
19:B:1205:CLA:HMC2	21:B:6017:BCR:H281	1.64	0.80
4:D:102:ILE:HG13	4:D:154:PHE:HB3	1.64	0.80
5:E:126:VAL:O	5:E:127:GLU:CB	2.30	0.80
14:R:34:UNK:O	14:R:38:UNK:CB	2.30	0.80
18:4:112:PRO:HD2	18:4:113:GLU:HG3	1.62	0.80
1:A:485:GLN:CD	1:A:485:GLN:N	2.40	0.80
19:A:1149:CLA:HAA1	19:A:1149:CLA:CGD	2.12	0.80
2:B:469:LYS:HD2	2:B:470:THR:HA	0.86	0.80
19:B:1220:CLA:C4A	19:B:1220:CLA:H42	2.11	0.80
4:D:174:PRO:O	4:D:175:GLU:HG2	1.82	0.80
5:E:107:PHE:CE2	5:E:109:LYS:CE	2.65	0.80
22:H:7011:LMU:C10	22:H:7011:LMU:H61	2.12	0.80
19:J:1311:CLA:HED3	19:J:1311:CLA:CHA	2.10	0.80
13:N:132:THR:OG1	13:N:138:ALA:O	1.98	0.80
14:R:35:UNK:O	14:R:38:UNK:CB	2.29	0.80
16:2:120:ILE:HG13	16:2:121:PHE:H	1.47	0.80
16:2:134:THR:HG1	16:2:135:PRO:CD	1.74	0.80
16:2:156:GLU:CG	16:2:157:LEU:CD1	2.57	0.80
16:2:204:LEU:HD12	16:2:210:SER:O	1.82	0.80
17:3:104:ILE:HG21	19:3:3004:CLA:C1D	2.11	0.80
1:A:284:ARG:HG3	1:A:295:TRP:CD1	2.17	0.80
2:B:199:ILE:CG2	2:B:270:LEU:CD1	2.55	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:456:GLU:HA	2:B:514:PRO:HD3	1.62	0.80
19:B:1219:CLA:HBC2	19:B:1220:CLA:HBA1	1.62	0.80
5:E:126:VAL:O	5:E:127:GLU:CG	2.29	0.80
11:K:122:LEU:O	11:K:122:LEU:HD22	1.82	0.80
15:1:151:GLN:N	15:1:151:GLN:HE21	1.79	0.80
16:2:182:ILE:C	16:2:187:LYS:HG2	2.07	0.80
19:2:2007:CLA:CAC	19:3:2009:CLA:HED3	2.00	0.80
22:4:7034:LMU:H111	22:4:7052:LMU:C2'	1.99	0.80
1:A:342:GLY:HA3	1:A:430:ASP:HB2	0.81	0.79
1:A:389:TYR:CE1	1:A:625:TRP:CD1	2.70	0.79
2:B:102:GLU:O	2:B:104:PHE:HB2	1.82	0.79
2:B:293:THR:CG2	7:G:94:GLN:HG2	2.12	0.79
2:B:462:TRP:HZ3	19:B:1231:CLA:HBC2	1.47	0.79
6:F:214:PRO:O	6:F:215:VAL:HB	1.78	0.79
22:H:7011:LMU:H61	22:H:7011:LMU:H101	1.61	0.79
21:I:6021:BCR:H313	21:I:6021:BCR:HC8	0.81	0.79
11:K:89:ARG:NH1	11:K:89:ARG:HG3	1.97	0.79
13:N:169:LYS:CB	13:N:170:TRP:HD1	1.95	0.79
14:R:36:UNK:O	14:R:38:UNK:CB	2.30	0.79
16:2:166:ARG:CA	16:2:167:ARG:HB2	2.11	0.79
22:2:7006:LMU:H5'	22:2:7006:LMU:O5B	1.79	0.79
17:3:141:VAL:HG23	17:3:142:ILE:CG1	2.10	0.79
17:3:153:ASP:HB2	17:3:154:ASN:OD1	1.81	0.79
18:4:177:LEU:HD22	18:4:178:PRO:CD	2.12	0.79
1:A:152:ILE:CD1	19:A:1127:CLA:O1D	2.29	0.79
1:A:244:LEU:HD12	1:A:247:GLU:OE1	1.81	0.79
1:A:316:MET:HG2	1:A:317:TYR:HD1	1.44	0.79
19:A:1105:CLA:CBA	19:A:1107:CLA:H12	2.12	0.79
19:A:1124:CLA:HBC2	19:A:1124:CLA:CHD	2.10	0.79
2:B:306:GLU:HG3	2:B:307:ALA:N	1.97	0.79
19:B:1220:CLA:NA	19:B:1220:CLA:H41	1.95	0.79
3:C:44:ARG:N	4:D:182:GLN:CG	2.46	0.79
11:K:125:LYS:CB	11:K:128:GLY:HA2	2.13	0.79
12:L:78:LEU:HD22	19:L:1504:CLA:HED1	1.62	0.79
13:N:130:ASN:CB	13:N:139:LYS:CG	2.29	0.79
13:N:142:LYS:N	13:N:145:PHE:O	2.14	0.79
14:R:38:UNK:O	14:R:42:UNK:CA	2.29	0.79
15:1:190:ASN:ND2	19:1:1002:CLA:C4D	2.44	0.79
16:2:101:TRP:N	16:2:103:VAL:H	1.81	0.79
16:2:201:PHE:CD1	16:2:202:ASP:N	2.50	0.79
17:3:238:ILE:CD1	19:3:3003:CLA:HMC1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:142:PHE:HA	18:4:145:GLU:OE1	1.82	0.79
2:B:626:LEU:O	2:B:627:ASN:HB2	1.82	0.79
6:F:100:LYS:O	6:F:100:LYS:HD2	1.81	0.79
19:K:1142:CLA:HED2	19:K:1143:CLA:HMB3	1.64	0.79
12:L:145:LEU:HG	21:L:6019:BCR:HC7	1.62	0.79
13:N:130:ASN:HB2	13:N:139:LYS:HG2	0.80	0.79
13:N:148:ASP:HA	13:N:149:ASP:O	1.83	0.79
15:1:112:GLN:CG	15:1:113:GLU:H	1.92	0.79
16:2:186:ASN:OD1	16:2:188:LEU:CD1	2.19	0.79
17:3:111:LEU:O	17:3:114:VAL:CA	2.30	0.79
17:3:156:THR:C	17:3:158:PHE:O	2.25	0.79
17:3:252:PRO:HB3	17:3:254:GLN:HE21	1.47	0.79
18:4:87:ASN:CG	18:4:90:TRP:CD2	2.59	0.79
1:A:50:THR:HG22	1:A:51:THR:N	1.98	0.79
1:A:64:PHE:HZ	1:A:77:LYS:CE	1.95	0.79
1:A:267:THR:HG22	1:A:267:THR:O	1.81	0.79
22:E:7048:LMU:C4B	22:F:7036:LMU:C6'	2.60	0.79
18:4:205:ILE:HG12	18:4:206:ALA:N	1.98	0.79
1:A:534:LEU:HD12	1:A:535:GLY:H	0.98	0.79
1:A:579:PHE:N	1:A:579:PHE:HD1	1.81	0.79
2:B:160:LYS:NZ	2:B:161:TRP:CE3	2.49	0.79
2:B:594:TRP:O	2:B:595:HIS:CB	2.31	0.79
3:C:12:ILE:HG13	23:C:8003:SF4:S1	2.23	0.79
6:F:180:SER:C	6:F:182:LEU:H	1.91	0.79
6:F:200:VAL:HG23	6:F:204:SER:N	1.98	0.79
11:K:59:THR:O	11:K:63:LEU:HD21	1.83	0.79
12:L:172:GLU:O	12:L:173:PRO:C	2.24	0.79
13:N:114:PHE:CB	13:N:117:ALA:CB	2.60	0.79
16:2:101:TRP:N	16:2:103:VAL:HB	1.96	0.79
16:2:113:ALA:HB1	16:2:114:MET:HE1	1.64	0.79
16:2:131:ILE:O	16:2:132:LEU:HB2	1.82	0.79
16:2:227:LEU:HD21	19:2:2004:CLA:CHC	2.13	0.79
17:3:243:ILE:CD1	19:3:3005:CLA:C1C	2.59	0.79
1:A:22:VAL:O	1:A:22:VAL:CG2	2.28	0.79
1:A:284:ARG:C	1:A:284:ARG:CZ	2.56	0.79
2:B:469:LYS:NZ	2:B:471:THR:H	1.80	0.79
2:B:527:LEU:HD12	2:B:527:LEU:O	1.82	0.79
5:E:79:LYS:HE3	5:E:84:TYR:OH	1.81	0.79
5:E:127:GLU:O	5:E:128:VAL:CG2	2.29	0.79
9:I:7:LEU:CD1	21:I:6021:BCR:H333	2.08	0.79
22:L:7029:LMU:H5B	22:L:7029:LMU:C4'	2.09	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:7029:LMU:O2B	22:L:7029:LMU:H6E	1.82	0.79
13:N:138:ALA:HB3	13:N:140:GLN:HG3	1.65	0.79
15:1:178:LYS:HD2	15:1:178:LYS:C	2.08	0.79
18:4:94:ALA:O	18:4:98:ASN:OD1	2.01	0.79
21:A:6011:BCR:H313	19:A:9013:CLA:C14	2.11	0.79
2:B:93:ASP:OD1	2:B:96:PHE:CD1	2.35	0.79
2:B:475:ASP:O	2:B:476:ILE:CG2	2.30	0.79
7:G:76:ARG:NH2	7:G:117:ASN:O	2.14	0.79
7:G:131:GLY:CA	7:G:136:VAL:HG23	2.13	0.79
22:G:7026:LMU:H2B	22:G:7026:LMU:O3'	1.83	0.79
19:J:1308:CLA:H2A	19:J:1308:CLA:O2A	1.80	0.79
12:L:91:THR:HA	12:L:98:ARG:HH12	1.47	0.79
15:1:77:GLU:HG3	15:1:80:LYS:CD	2.13	0.79
15:1:147:PHE:CD1	15:1:147:PHE:C	2.60	0.79
15:1:170:PRO:CD	15:1:173:TYR:CE2	2.66	0.79
15:1:182:GLU:OE1	19:1:1001:CLA:C1D	2.31	0.79
16:2:224:ASN:OD1	16:2:227:LEU:HD22	1.82	0.79
17:3:201:ALA:CB	17:3:202:TYR:HD2	1.94	0.79
18:4:120:ILE:HG22	18:4:121:ILE:N	1.96	0.79
1:A:77:LYS:O	1:A:80:SER:OG	2.00	0.79
1:A:484:LEU:HD22	1:A:484:LEU:N	1.96	0.79
1:A:567:ARG:NH1	4:D:89:GLY:CA	2.45	0.79
2:B:363:GLN:H	2:B:365:PHE:HB3	1.46	0.79
19:B:1223:CLA:CED	19:B:1231:CLA:HBB2	2.11	0.79
3:C:1:MET:H1	3:C:4:SER:N	1.79	0.79
4:D:167:HIS:N	4:D:168:PRO:CD	2.45	0.79
15:1:78:ARG:NH2	15:1:179:LYS:CD	2.37	0.79
15:1:78:ARG:CD	19:1:1011:CLA:HMC2	2.08	0.79
15:1:162:LYS:O	15:1:164:PRO:HD3	1.83	0.79
15:1:172:GLY:HA2	15:1:173:TYR:CG	2.17	0.79
19:1:1014:CLA:H41	19:1:1014:CLA:C7	2.04	0.79
16:2:229:MET:SD	16:2:230:LEU:N	2.55	0.79
17:3:148:TYR:N	17:3:149:ASN:ND2	2.30	0.79
22:3:7003:LMU:C3B	22:3:7005:LMU:O5B	2.30	0.79
1:A:255:LEU:HD13	1:A:280:PHE:CZ	2.12	0.79
1:A:452:PHE:CE1	19:A:1136:CLA:CBB	2.66	0.79
2:B:25:ILE:O	2:B:25:ILE:CG1	2.27	0.79
2:B:53:GLN:HG3	19:B:1202:CLA:HHB	1.65	0.79
2:B:310:PRO:CG	2:B:311:PRO:CD	2.61	0.79
2:B:454:LEU:HD12	2:B:454:LEU:O	1.82	0.79
4:D:156:ARG:NE	4:D:164:GLN:HB2	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:69:GLY:HA2	7:G:72:LEU:HG	1.65	0.79
7:G:134:GLY:O	7:G:135:HIS:CG	2.36	0.79
11:K:115:ILE:C	11:K:118:VAL:HG22	2.08	0.79
13:N:148:ASP:N	13:N:149:ASP:CB	2.45	0.79
15:1:92:LEU:HA	15:1:95:PRO:CG	2.12	0.79
15:1:97:ILE:CD1	15:1:98:LEU:HB2	2.12	0.79
1:A:68:THR:HG23	1:A:70:ASP:H	1.47	0.79
1:A:316:MET:HB3	1:A:317:TYR:CG	2.18	0.79
2:B:557:PHE:N	2:B:558:PRO:CD	2.46	0.79
24:B:7101:LMG:O3	3:C:70:TRP:NE1	2.16	0.79
4:D:99:PHE:CB	4:D:157:VAL:HG12	2.13	0.79
8:H:61:THR:HA	8:H:62:THR:HG22	1.64	0.79
8:H:77:ASN:CG	8:H:78:PRO:CD	2.55	0.79
16:2:115:LEU:O	16:2:118:ALA:HB3	1.82	0.79
16:2:269:LYS:HA	16:2:269:LYS:CE	2.12	0.79
18:4:123:VAL:N	18:4:124:PRO:HD3	1.98	0.79
18:4:232:LEU:CB	18:4:236:ILE:HD12	2.12	0.79
1:A:158:ILE:CG1	1:A:159:THR:N	2.28	0.78
1:A:207:LEU:CB	19:A:1119:CLA:HBB2	2.13	0.78
1:A:296:LEU:HD12	1:A:296:LEU:C	2.08	0.78
19:A:1124:CLA:H72	19:A:1125:CLA:HED1	1.54	0.78
2:B:87:ILE:CA	2:B:115:ASN:HA	2.12	0.78
2:B:504:ASN:O	2:B:504:ASN:CG	2.25	0.78
11:K:115:ILE:HA	11:K:118:VAL:HG21	1.63	0.78
15:1:97:ILE:CD1	15:1:98:LEU:CD2	2.61	0.78
17:3:96:ARG:NH1	17:3:96:ARG:HG3	1.98	0.78
17:3:254:GLN:HG3	17:3:255:ASN:N	1.98	0.78
22:A:7016:LMU:H22	22:A:7016:LMU:C6	2.02	0.78
2:B:232:LEU:HD11	2:B:235:GLN:CG	2.14	0.78
19:B:1218:CLA:HHD	19:B:1218:CLA:CBC	2.13	0.78
3:C:72:GLU:CD	3:C:77:MET:HE1	2.07	0.78
15:1:190:ASN:HD21	19:1:1002:CLA:C4D	1.97	0.78
1:A:545:HIS:O	1:A:549:ILE:HG13	1.82	0.78
1:A:628:ILE:HD12	1:A:632:GLY:HA2	1.64	0.78
19:A:1124:CLA:H2	19:A:1124:CLA:O1A	1.80	0.78
2:B:317:ARG:NH1	2:B:410:ARG:HG2	1.98	0.78
2:B:462:TRP:CZ3	19:B:1231:CLA:HBC2	2.19	0.78
7:G:84:ARG:HA	19:G:1242:CLA:HMA2	1.64	0.78
15:1:190:ASN:ND2	19:1:1002:CLA:CHA	2.46	0.78
22:1:7013:LMU:O6B	22:1:7013:LMU:H1B	1.82	0.78
16:2:148:ASP:O	16:2:149:THR:OG1	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:173:LYS:O	18:4:194:PHE:CD2	2.36	0.78
1:A:148:GLY:O	1:A:152:ILE:HD12	1.84	0.78
1:A:578:ARG:CZ	1:A:578:ARG:CB	2.61	0.78
19:A:1112:CLA:CHC	21:A:6002:BCR:C19	2.61	0.78
19:A:1237:CLA:HMC2	19:B:1238:CLA:H11	1.66	0.78
19:B:1211:CLA:HMA1	21:B:6006:BCR:H313	1.66	0.78
3:C:62:PHE:CE1	5:E:80:GLU:HB3	2.17	0.78
4:D:99:PHE:HB2	4:D:157:VAL:HG12	1.64	0.78
5:E:89:SER:OG	5:E:106:ARG:CG	2.30	0.78
19:H:1241:CLA:HAC1	21:I:6021:BCR:C3	2.13	0.78
12:L:79:ILE:HG23	12:L:80:ALA:HA	1.65	0.78
12:L:95:PRO:O	12:L:98:ARG:N	2.16	0.78
17:3:111:LEU:C	17:3:114:VAL:H	1.91	0.78
22:4:7034:LMU:H101	22:4:7052:LMU:O3'	1.83	0.78
1:A:555:ILE:CD1	19:A:9023:CLA:OBD	2.31	0.78
19:A:1121:CLA:HAA1	11:K:78:ARG:CZ	2.12	0.78
2:B:645:VAL:HG11	19:B:1205:CLA:HAC1	1.65	0.78
3:C:44:ARG:HB3	4:D:182:GLN:HE22	1.47	0.78
19:K:1142:CLA:CED	19:K:1143:CLA:CMB	2.62	0.78
17:3:111:LEU:HG	17:3:112:GLY:H	0.63	0.78
18:4:110:LEU:O	18:4:113:GLU:CG	2.30	0.78
1:A:201:SER:O	1:A:204:ASN:HB2	1.84	0.78
1:A:203:LEU:HD22	19:A:1123:CLA:HED1	1.63	0.78
19:A:1124:CLA:O1A	19:A:1125:CLA:HED3	1.84	0.78
2:B:334:LEU:HG	2:B:334:LEU:O	1.81	0.78
6:F:220:GLU:OE1	6:F:225:GLU:HB2	1.83	0.78
19:2:2014:CLA:H72	19:2:2014:CLA:C4	2.12	0.78
19:3:3008:CLA:HBD	19:3:3008:CLA:CBA	2.06	0.78
18:4:173:LYS:O	18:4:194:PHE:CE2	2.36	0.78
19:A:1149:CLA:O1D	19:A:1149:CLA:CAA	2.31	0.78
3:C:52:LYS:NZ	3:C:64:SER:CB	2.47	0.78
4:D:174:PRO:C	4:D:175:GLU:HG2	2.08	0.78
5:E:111:ASN:HD21	5:E:113:ALA:N	1.80	0.78
6:F:190:LYS:HG3	6:F:192:THR:HG23	1.66	0.78
15:1:128:PRO:HG2	15:1:131:TRP:CZ3	2.18	0.78
16:2:171:ILE:HG13	16:2:172:LEU:CB	2.14	0.78
16:2:261:THR:CG2	16:2:262:ILE:H	1.96	0.78
17:3:103:VAL:O	17:3:107:ARG:CD	2.31	0.78
1:A:27:ILE:O	1:A:27:ILE:HG22	1.83	0.78
1:A:421:ASP:OD1	1:A:422:TYR:CE1	2.36	0.78
1:A:492:ILE:HD11	19:A:1133:CLA:C2C	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:LEU:HG	2:B:218:TYR:H	1.48	0.78
2:B:469:LYS:HZ3	2:B:471:THR:H	1.30	0.78
7:G:90:GLN:HB2	7:G:92:PRO:CD	2.13	0.78
9:I:7:LEU:HD12	21:I:6021:BCR:C33	2.09	0.78
22:L:7029:LMU:H4'	22:L:7029:LMU:C5B	2.11	0.78
15:1:66:PRO:HD2	15:1:67:LEU:N	1.91	0.78
15:1:176:ASP:HB3	15:1:180:LEU:HD12	0.79	0.78
19:1:1303:CLA:HMC1	19:1:1303:CLA:CBC	2.14	0.78
16:2:172:LEU:CA	16:2:173:ASN:HD22	1.96	0.78
16:2:254:LEU:C	16:2:254:LEU:HD23	2.05	0.78
1:A:603:PHE:HZ	1:A:693:LEU:HD21	1.49	0.78
19:A:1115:CLA:HBC3	19:A:1115:CLA:CMC	2.14	0.78
7:G:88:ALA:C	7:G:90:GLN:O	2.27	0.78
22:H:7011:LMU:H122	22:H:7011:LMU:H82	1.66	0.78
17:3:125:VAL:HG21	19:3:3010:CLA:C2C	2.13	0.78
17:3:151:TRP:CD1	17:3:151:TRP:N	2.48	0.78
1:A:425:THR:O	1:A:427:ARG:CD	2.31	0.78
1:A:502:THR:HB	1:A:504:ALA:CB	2.13	0.78
2:B:36:ASP:O	2:B:41:ARG:NE	2.17	0.78
2:B:256:THR:O	2:B:272:ASP:CG	2.27	0.78
3:C:1:MET:N	3:C:3:HIS:C	2.42	0.78
8:H:119:ASP:C	8:H:120:ILE:HG22	2.07	0.78
13:N:165:ASN:OD1	13:N:167:PHE:HA	1.84	0.78
15:1:150:HIS:CG	15:1:151:GLN:HE22	2.00	0.78
16:2:254:LEU:HD22	16:2:255:ALA:H	1.49	0.78
19:2:2002:CLA:H93	19:2:2002:CLA:H51	1.65	0.78
18:4:87:ASN:CB	18:4:90:TRP:CD2	2.67	0.78
18:4:205:ILE:HG12	18:4:206:ALA:H	1.47	0.78
1:A:190:ALA:CB	1:A:191:PRO:HD3	2.11	0.77
1:A:328:LYS:HZ3	1:A:345:GLY:CA	1.94	0.77
1:A:484:LEU:CD2	1:A:484:LEU:N	2.47	0.77
2:B:242:HIS:ND1	2:B:244:PHE:HA	1.99	0.77
2:B:257:ILE:O	2:B:497:TRP:HZ3	1.55	0.77
2:B:303:TYR:HA	2:B:306:GLU:CB	2.13	0.77
2:B:648:TRP:CZ3	21:B:6017:BCR:H392	2.19	0.77
20:B:5002:PQN:C16	21:B:6017:BCR:H331	2.10	0.77
4:D:167:HIS:N	4:D:168:PRO:HD2	2.00	0.77
7:G:123:ASN:CA	7:G:126:ASP:OD2	2.33	0.77
22:R:7021:LMU:H31	22:R:7021:LMU:C1'	2.13	0.77
15:1:78:ARG:CG	15:1:81:GLU:OE1	2.32	0.77
15:1:206:SER:O	15:1:209:PRO:CD	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PHE:H	1:A:44:ILE:CG2	1.97	0.77
1:A:291:THR:O	1:A:291:THR:HG22	1.83	0.77
15:1:162:LYS:C	15:1:164:PRO:CD	2.56	0.77
16:2:112:TRP:CZ3	16:2:164:GLU:HG3	2.19	0.77
16:2:177:VAL:CG1	16:2:178:ASN:CG	2.56	0.77
18:4:211:MET:SD	19:4:4002:CLA:CBB	2.73	0.77
2:B:255:LEU:CA	2:B:271:THR:HB	2.06	0.77
2:B:429:LEU:C	2:B:525:LEU:CD1	2.53	0.77
2:B:459:PHE:CD2	19:B:1235:CLA:HMD3	2.18	0.77
19:B:1226:CLA:H72	24:B:7101:LMG:H311	1.66	0.77
3:C:1:MET:H1	3:C:3:HIS:C	1.93	0.77
5:E:83:TRP:CE3	5:E:83:TRP:N	2.51	0.77
8:H:77:ASN:ND2	8:H:78:PRO:HG2	1.98	0.77
19:K:1142:CLA:CMD	19:K:1143:CLA:NA	2.47	0.77
13:N:132:THR:HB	13:N:139:LYS:HZ2	1.46	0.77
14:R:27:UNK:O	14:R:29:UNK:O	2.03	0.77
15:1:87:CYS:SG	15:1:88:ARG:N	2.58	0.77
16:2:184:PRO:HD3	16:2:187:LYS:HG2	1.66	0.77
16:2:222:ILE:O	16:2:226:ARG:HB2	1.83	0.77
18:4:226:LYS:CD	18:4:226:LYS:N	2.47	0.77
1:A:360:ILE:HD13	21:A:6007:BCR:H371	1.67	0.77
1:A:624:VAL:O	1:A:636:HIS:CD2	2.37	0.77
19:A:1122:CLA:CHD	21:A:6007:BCR:C19	2.58	0.77
2:B:123:TRP:O	2:B:126:THR:HG22	1.84	0.77
2:B:154:TRP:O	2:B:157:LEU:HB3	1.84	0.77
2:B:455:ILE:HG23	6:F:148:LEU:HD11	1.67	0.77
19:B:1239:CLA:H102	9:I:21:MET:SD	2.25	0.77
6:F:83:THR:HB	6:F:84:PRO:HD2	1.67	0.77
7:G:84:ARG:HG3	7:G:85:GLU:HB3	1.63	0.77
19:H:1241:CLA:C3C	21:I:6021:BCR:C2	2.62	0.77
11:K:118:VAL:HG23	11:K:121:VAL:CG2	2.11	0.77
13:N:150:LEU:HB2	13:N:152:LEU:HD23	1.67	0.77
15:1:73:PRO:O	15:1:77:GLU:HB2	1.84	0.77
15:1:177:PRO:HD2	15:1:180:LEU:CA	2.15	0.77
16:2:125:PHE:O	16:2:127:THR:HG23	1.83	0.77
17:3:150:TYR:C	17:3:151:TRP:HD1	1.90	0.77
1:A:726:SER:O	1:A:728:VAL:N	2.18	0.77
22:A:7010:LMU:H3'	22:A:7010:LMU:O2B	1.85	0.77
19:A:9022:CLA:C11	21:B:6017:BCR:H19C	2.14	0.77
2:B:103:ALA:HB1	2:B:106:ARG:CD	2.14	0.77
2:B:247:THR:HG22	2:B:248:GLN:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:HIS:CG	2:B:374:HIS:O	2.38	0.77
19:B:1228:CLA:HHD	19:B:1228:CLA:HBC3	1.66	0.77
4:D:93:LYS:CG	4:D:96:VAL:HG13	2.14	0.77
7:G:72:LEU:HD23	7:G:124:ILE:HG13	1.67	0.77
7:G:99:HIS:O	7:G:101:GLU:HB2	1.83	0.77
10:J:5:LYS:CD	16:2:178:ASN:OD1	2.32	0.77
12:L:153:PHE:CD1	12:L:155:GLU:OE1	2.38	0.77
14:R:3:UNK:O	14:R:4:UNK:CB	2.33	0.77
17:3:111:LEU:O	17:3:115:GLY:N	2.17	0.77
22:3:7003:LMU:C3B	22:3:7005:LMU:C6B	2.62	0.77
18:4:123:VAL:O	18:4:123:VAL:HG13	1.82	0.77
1:A:51:THR:CB	19:A:1139:CLA:CBB	2.63	0.77
1:A:202:MET:HG3	19:A:1111:CLA:HBC2	1.65	0.77
1:A:508:THR:O	1:A:509:ALA:CB	2.30	0.77
2:B:732:LYS:CB	2:B:733:PHE:CA	2.62	0.77
19:B:1226:CLA:HMC3	19:B:1226:CLA:CBC	2.15	0.77
7:G:75:GLY:C	7:G:77:PHE:N	2.35	0.77
8:H:58:LEU:CB	8:H:61:THR:CG2	2.51	0.77
10:J:9:SER:O	10:J:10:VAL:HB	1.85	0.77
19:J:1311:CLA:HBC3	19:J:1311:CLA:HHD	1.65	0.77
17:3:243:ILE:HG12	19:3:3005:CLA:C3C	2.14	0.77
18:4:177:LEU:CG	18:4:178:PRO:CD	2.59	0.77
1:A:581:CYS:CB	1:A:590:CYS:HA	2.14	0.77
1:A:669:GLY:H	2:B:445:ALA:CA	1.95	0.77
19:A:1103:CLA:H151	21:A:6002:BCR:H393	1.66	0.77
2:B:174:ARG:CB	19:B:1210:CLA:HBC2	2.11	0.77
2:B:293:THR:CG2	7:G:94:GLN:CD	2.54	0.77
2:B:615:TYR:HD1	2:B:615:TYR:H	1.32	0.77
19:K:3009:CLA:HBA1	19:K:3009:CLA:O2D	1.84	0.77
15:1:170:PRO:O	15:1:173:TYR:CE2	2.38	0.77
17:3:98:LEU:O	17:3:101:GLY:CA	2.33	0.77
18:4:87:ASN:CB	18:4:90:TRP:CZ3	2.66	0.77
19:4:4014:CLA:HHD	19:4:4014:CLA:CBC	2.14	0.77
1:A:472:ARG:HE	1:A:474:GLN:HG3	1.49	0.77
3:C:42:ALA:HB1	3:C:43:PRO:HD2	1.65	0.77
4:D:162:GLU:C	4:D:163:VAL:HG23	2.10	0.77
6:F:119:ILE:CG1	6:F:120:LYS:H	1.94	0.77
13:N:122:PHE:HD2	13:N:122:PHE:H	1.32	0.77
13:N:156:GLY:HA2	13:N:157:LYS:HD2	1.64	0.77
15:1:114:TRP:CZ3	15:1:121:GLN:HA	2.19	0.77
17:3:135:ALA:HB1	17:3:139:THR:CG2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1119:CLA:C3C	19:A:1125:CLA:H172	2.15	0.77
19:B:1209:CLA:HAC2	19:B:1210:CLA:HBB2	0.81	0.77
5:E:83:TRP:HE3	5:E:83:TRP:H	1.29	0.77
8:H:94:ARG:O	8:H:95:GLY:C	2.28	0.77
15:1:70:GLY:C	15:1:73:PRO:HD2	2.08	0.77
16:2:165:GLY:C	16:2:167:ARG:CG	2.58	0.77
16:2:224:ASN:O	16:2:227:LEU:HB3	1.85	0.77
1:A:57:LEU:C	1:A:57:LEU:CD2	2.57	0.77
1:A:346:LEU:C	1:A:346:LEU:CD2	2.58	0.77
2:B:75:GLU:HB2	2:B:132:ASN:CG	2.09	0.77
2:B:130:ARG:HG3	2:B:130:ARG:NH1	1.99	0.77
2:B:160:LYS:HD3	2:B:161:TRP:CZ2	2.20	0.77
2:B:374:HIS:HB2	19:B:1224:CLA:NB	2.00	0.77
3:C:8:TYR:O	3:C:60:THR:HA	1.85	0.77
3:C:33:GLY:HA2	3:C:37:LYS:HE2	1.67	0.77
4:D:95:GLN:CD	4:D:95:GLN:C	2.52	0.77
11:K:89:ARG:CG	11:K:89:ARG:HH11	1.98	0.77
17:3:134:LEU:HD12	17:3:134:LEU:N	2.00	0.77
19:A:1119:CLA:HMD3	19:A:1120:CLA:HHD	1.67	0.76
19:A:1124:CLA:CED	19:A:1125:CLA:C3D	2.58	0.76
19:A:9022:CLA:H101	21:B:6017:BCR:H17C	1.68	0.76
2:B:267:SER:HB2	2:B:356:PRO:O	1.84	0.76
2:B:314:ARG:HH12	15:1:67:LEU:CG	1.98	0.76
2:B:732:LYS:CB	2:B:733:PHE:HA	2.14	0.76
3:C:27:GLU:OE1	3:C:39:ILE:C	2.28	0.76
4:D:156:ARG:NH2	4:D:163:VAL:O	2.18	0.76
4:D:158:PHE:HB3	4:D:159:PRO:CD	2.08	0.76
5:E:79:LYS:CA	5:E:84:TYR:HE1	1.99	0.76
7:G:120:VAL:O	7:G:120:VAL:HG12	1.84	0.76
11:K:47:ASP:CA	11:K:51:SER:HB2	2.15	0.76
1:A:284:ARG:HA	1:A:284:ARG:CZ	2.14	0.76
1:A:295:TRP:O	1:A:298:ASP:OD2	2.03	0.76
1:A:714:LEU:HD13	21:F:6016:BCR:C39	2.15	0.76
2:B:87:ILE:HA	2:B:115:ASN:HB2	1.66	0.76
2:B:293:THR:O	2:B:295:PHE:CD2	2.38	0.76
4:D:103:THR:CG2	4:D:128:LEU:HG	2.15	0.76
21:J:6012:BCR:H393	21:J:6012:BCR:C23	2.14	0.76
13:N:143:VAL:CB	13:N:144:PRO:CD	2.62	0.76
16:2:107:LEU:HD12	16:2:108:VAL:N	1.99	0.76
16:2:195:TYR:CE2	16:2:198:GLY:HA3	2.20	0.76
19:2:2001:CLA:HMC1	19:2:2001:CLA:CBC	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3016:CLA:H142	19:3:3016:CLA:H101	1.64	0.76
1:A:56:ASN:O	1:A:57:LEU:CB	2.24	0.76
1:A:426:THR:CA	1:A:428:TYR:CZ	2.69	0.76
1:A:525:ASN:HD22	1:A:526:LYS:HE3	1.50	0.76
1:A:534:LEU:CD1	1:A:535:GLY:H	1.90	0.76
19:A:1117:CLA:HBB2	19:A:1117:CLA:H8	1.65	0.76
19:A:1134:CLA:O1A	19:A:1141:CLA:HBB1	1.84	0.76
22:A:7023:LMU:H2B	22:A:7023:LMU:H6'2	1.68	0.76
2:B:174:ARG:O	2:B:175:LEU:HB3	1.85	0.76
19:B:1205:CLA:HMC2	21:B:6017:BCR:C28	2.15	0.76
6:F:200:VAL:HG11	10:J:7:TYR:CB	2.11	0.76
7:G:64:ILE:O	7:G:64:ILE:HG13	1.83	0.76
7:G:124:ILE:CG1	7:G:128:LEU:CD1	2.62	0.76
12:L:115:VAL:HG11	12:L:130:GLY:N	1.95	0.76
19:L:1148:CLA:CBC	19:L:1148:CLA:CHD	2.62	0.76
16:2:172:LEU:CB	16:2:173:ASN:ND2	2.48	0.76
1:A:127:VAL:CG2	19:A:1107:CLA:CBB	2.63	0.76
1:A:150:PHE:N	1:A:153:TRP:HB2	2.01	0.76
1:A:343:HIS:O	1:A:346:LEU:CB	2.33	0.76
1:A:368:LEU:CD1	19:A:1125:CLA:H61	2.15	0.76
1:A:411:ALA:HB2	21:A:6008:BCR:C39	2.16	0.76
1:A:746:THR:HA	1:A:749:PHE:HB3	1.66	0.76
4:D:100:TYR:CD1	4:D:134:LYS:CG	2.66	0.76
12:L:54:TYR:CE1	12:L:57:ILE:HG23	2.19	0.76
15:1:177:PRO:CD	15:1:180:LEU:HD23	2.15	0.76
17:3:161:GLU:OE1	17:3:162:MET:HA	1.84	0.76
21:A:6002:BCR:H341	21:A:6002:BCR:C12	2.15	0.76
2:B:655:LEU:CD2	19:B:1239:CLA:HBB1	2.15	0.76
4:D:101:VAL:HG12	4:D:130:LYS:CB	2.16	0.76
6:F:139:LEU:CD1	6:F:149:ILE:HD13	2.15	0.76
10:J:23:ALA:O	10:J:26:LEU:HB3	1.85	0.76
22:K:7001:LMU:H42	22:K:7001:LMU:H81	1.67	0.76
12:L:153:PHE:CA	12:L:179:ALA:HB2	2.10	0.76
13:N:110:THR:CG2	13:N:111:GLY:N	2.47	0.76
14:R:34:UNK:H	14:R:36:UNK:CB	1.99	0.76
17:3:109:ALA:O	17:3:111:LEU:HB3	1.86	0.76
19:3:3011:CLA:CBC	19:3:3012:CLA:CHA	2.63	0.76
1:A:193:LEU:HA	1:A:196:PHE:CE2	2.18	0.76
2:B:292:ARG:NH2	2:B:297:ILE:N	2.33	0.76
2:B:353:TYR:O	2:B:354:SER:HB2	1.84	0.76
2:B:517:PHE:O	2:B:517:PHE:HD2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:732:LYS:HG2	2:B:733:PHE:CA	2.15	0.76
4:D:140:LEU:HD13	4:D:144:LEU:CB	2.11	0.76
7:G:88:ALA:HB3	7:G:90:GLN:O	1.86	0.76
13:N:165:ASN:C	13:N:167:PHE:N	2.39	0.76
14:R:37:UNK:O	14:R:42:UNK:C	2.34	0.76
16:2:261:THR:HG22	16:2:262:ILE:N	1.98	0.76
17:3:125:VAL:HG11	19:3:3010:CLA:CHC	2.16	0.76
17:3:177:ALA:O	17:3:178:LYS:HB2	1.84	0.76
1:A:270:PHE:CE1	19:A:1141:CLA:H2	2.21	0.76
1:A:334:HIS:HB3	19:A:1120:CLA:HMA1	1.65	0.76
1:A:389:TYR:HE1	1:A:625:TRP:CD1	2.03	0.76
1:A:697:ARG:NH2	2:B:566:GLY:O	2.17	0.76
2:B:69:ALA:HB1	2:B:135:LEU:HD12	1.65	0.76
2:B:203:ARG:HH22	2:B:254:ILE:HG22	1.50	0.76
5:E:89:SER:O	5:E:105:VAL:HB	1.86	0.76
11:K:76:ALA:N	11:K:78:ARG:HH12	1.81	0.76
12:L:129:ALA:O	12:L:201:TYR:CB	2.25	0.76
19:1:1010:CLA:CHD	19:1:1010:CLA:CBC	2.63	0.76
16:2:128:LYS:CB	16:2:131:ILE:HG12	2.16	0.76
18:4:246:GLN:O	18:4:246:GLN:HG2	1.84	0.76
1:A:23:ASP:HB3	1:A:33:GLN:OE1	1.84	0.76
1:A:431:LEU:O	1:A:435:VAL:HG12	1.85	0.76
1:A:457:SER:O	1:A:544:ILE:HD13	1.85	0.76
1:A:478:SER:HB2	1:A:644:GLN:CD	2.10	0.76
2:B:160:LYS:NZ	2:B:161:TRP:CD2	2.54	0.76
2:B:233:TYR:CD1	2:B:254:ILE:HG13	2.20	0.76
2:B:387:PHE:O	2:B:391:PRO:HD3	1.86	0.76
2:B:493:TRP:HE1	19:B:1213:CLA:CAC	1.99	0.76
4:D:156:ARG:HB2	4:D:166:LEU:CD1	2.15	0.76
5:E:90:VAL:O	5:E:91:VAL:CG2	2.34	0.76
6:F:200:VAL:HG12	10:J:7:TYR:CA	2.15	0.76
8:H:109:LEU:HD23	19:H:1207:CLA:C7	2.14	0.76
15:1:157:ASP:OD1	15:1:175:LYS:HE3	1.86	0.76
16:2:184:PRO:CG	16:2:187:LYS:N	2.49	0.76
1:A:92:TRP:CD1	19:A:1105:CLA:HBB2	2.20	0.76
19:A:1105:CLA:CMB	21:J:6012:BCR:HC7	2.15	0.76
2:B:69:ALA:CB	2:B:135:LEU:HD12	2.15	0.76
2:B:229:GLN:O	7:G:63:VAL:CG2	2.34	0.76
4:D:128:LEU:O	4:D:128:LEU:HD23	1.85	0.76
5:E:89:SER:OG	5:E:106:ARG:NE	2.15	0.76
5:E:111:ASN:ND2	5:E:113:ALA:N	2.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:11:LEU:HD12	21:I:6021:BCR:C10	2.15	0.76
15:1:183:LEU:O	15:1:184:LYS:HG2	1.85	0.76
18:4:173:LYS:CB	18:4:194:PHE:HD2	1.97	0.76
1:A:170:GLY:O	1:A:173:VAL:HG22	1.86	0.76
1:A:217:SER:OG	21:A:6002:BCR:C17	2.34	0.76
1:A:603:PHE:CZ	1:A:735:VAL:HG22	2.21	0.76
1:A:661:ALA:HA	1:A:664:VAL:HG13	1.65	0.76
2:B:469:LYS:HB3	2:B:470:THR:OG1	1.86	0.76
2:B:500:ALA:O	2:B:501:ILE:CG1	2.31	0.76
2:B:510:LEU:HD11	2:B:597:LYS:NZ	2.00	0.76
21:B:6006:BCR:H331	21:B:6006:BCR:HC8	1.66	0.76
4:D:99:PHE:HB3	4:D:157:VAL:HB	1.67	0.76
5:E:89:SER:CB	5:E:106:ARG:CD	2.61	0.76
6:F:207:LEU:HD21	6:F:208:PHE:HD1	1.48	0.76
10:J:5:LYS:HD2	16:2:178:ASN:CA	2.15	0.76
13:N:122:PHE:N	13:N:122:PHE:CD2	2.36	0.76
22:1:7004:LMU:O2'	22:1:7004:LMU:H11	1.84	0.76
16:2:160:ILE:CB	19:2:2012:CLA:CBB	2.64	0.76
1:A:187:HIS:HE1	19:A:1109:CLA:C4D	1.86	0.75
1:A:475:ASP:OD2	12:L:120:LEU:HA	1.85	0.75
2:B:200:PRO:O	2:B:204:GLY:CA	2.33	0.75
2:B:545:LYS:CG	2:B:546:LEU:N	2.48	0.75
6:F:129:ARG:HB3	6:F:133:TYR:CZ	2.21	0.75
6:F:225:GLU:N	6:F:227:VAL:HG12	2.01	0.75
11:K:127:ILE:O	11:K:130:LEU:HD23	1.86	0.75
15:1:69:LEU:CA	15:1:73:PRO:HD3	2.16	0.75
15:1:84:LEU:O	15:1:87:CYS:SG	2.44	0.75
1:A:127:VAL:HG21	19:A:1107:CLA:HBB2	1.69	0.75
19:A:1105:CLA:HBA2	19:A:1107:CLA:H12	1.68	0.75
19:A:9022:CLA:H93	19:A:9023:CLA:C9	2.11	0.75
2:B:459:PHE:CB	19:B:1235:CLA:CAD	2.64	0.75
6:F:160:PHE:O	6:F:164:GLY:HA3	1.86	0.75
6:F:173:TRP:CE3	6:F:211:PHE:N	2.54	0.75
12:L:175:GLN:O	12:L:176:LEU:HB2	1.86	0.75
19:2:2014:CLA:H102	19:2:2014:CLA:C15	2.15	0.75
1:A:422:TYR:HD1	1:A:422:TYR:H	0.82	0.75
1:A:523:VAL:HG13	1:A:524:GLY:H	1.49	0.75
1:A:624:VAL:O	1:A:636:HIS:HD2	1.69	0.75
1:A:701:GLN:OE1	5:E:112:TYR:OH	2.01	0.75
19:A:1136:CLA:H171	19:L:1504:CLA:HBB2	1.67	0.75
2:B:709:GLY:O	2:B:710:LEU:HB2	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:98:LEU:HD22	12:L:146:THR:HG21	1.69	0.75
19:J:1311:CLA:O1A	19:J:1311:CLA:H143	1.86	0.75
13:N:146:LEU:HD21	17:3:142:ILE:O	1.84	0.75
13:N:157:LYS:CB	13:N:159:LYS:H	1.98	0.75
16:2:184:PRO:CD	16:2:187:LYS:CD	2.63	0.75
19:2:2007:CLA:HBC2	19:3:2009:CLA:CED	1.89	0.75
5:E:74:VAL:HG22	5:E:90:VAL:HG22	1.67	0.75
6:F:207:LEU:CD2	6:F:208:PHE:CD1	2.69	0.75
7:G:84:ARG:HA	19:G:1242:CLA:CMA	2.16	0.75
7:G:102:ALA:HA	7:G:104:ASP:OD2	1.85	0.75
8:H:97:LEU:CD1	8:H:100:PHE:HB3	2.13	0.75
11:K:63:LEU:H	11:K:63:LEU:CD2	1.90	0.75
11:K:84:LEU:HG	11:K:85:LYS:CG	2.10	0.75
19:3:3008:CLA:CGD	19:3:3008:CLA:CBA	2.64	0.75
18:4:103:MET:HE3	18:4:208:GLY:HA2	0.75	0.75
18:4:177:LEU:CD2	18:4:178:PRO:CD	2.64	0.75
19:4:4015:CLA:HBC3	19:4:4015:CLA:HHD	1.68	0.75
22:4:7034:LMU:C8	22:4:7052:LMU:C1'	2.58	0.75
1:A:128:GLY:HA3	2:B:446:PHE:CD2	2.21	0.75
1:A:154:ARG:CZ	1:A:384:TYR:CE1	2.68	0.75
1:A:196:PHE:H	1:A:196:PHE:HD2	1.33	0.75
1:A:349:ILE:HG22	1:A:350:LEU:CA	2.16	0.75
19:A:1105:CLA:HMB3	19:A:1106:CLA:HHB	1.69	0.75
19:A:1124:CLA:HBA2	19:A:1137:CLA:CED	2.16	0.75
19:A:1124:CLA:C6	19:A:1125:CLA:HED1	2.15	0.75
2:B:88:ALA:H	2:B:115:ASN:HA	1.50	0.75
2:B:323:TYR:O	2:B:327:ASN:HB2	1.86	0.75
2:B:469:LYS:HZ2	2:B:471:THR:C	1.94	0.75
2:B:694:ARG:HD3	9:I:28:VAL:HG13	1.67	0.75
20:B:5002:PQN:H162	21:B:6017:BCR:H331	1.62	0.75
4:D:103:THR:HG21	4:D:128:LEU:CD1	2.16	0.75
5:E:91:VAL:HG12	5:E:92:ALA:H	1.51	0.75
11:K:127:ILE:HB	11:K:129:ALA:CB	2.16	0.75
12:L:153:PHE:HD1	12:L:155:GLU:OE1	1.70	0.75
15:1:134:LEU:N	15:1:135:PRO:HD3	2.00	0.75
1:A:163:GLN:O	1:A:166:CYS:N	2.07	0.75
19:A:9023:CLA:H41	19:A:9023:CLA:HMB3	1.67	0.75
2:B:91:ILE:HG21	19:B:1206:CLA:HMD1	1.69	0.75
2:B:510:LEU:HD11	2:B:597:LYS:HZ3	1.50	0.75
2:B:547:MET:HE2	2:B:550:LYS:HA	1.66	0.75
2:B:694:ARG:HD3	9:I:28:VAL:CG1	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:PHE:CB	19:I:1204:CLA:OBD	2.34	0.75
1:A:240:LYS:H	1:A:243:PRO:HD2	1.48	0.75
1:A:308:ILE:O	1:A:312:ILE:N	2.16	0.75
1:A:349:ILE:HG22	1:A:350:LEU:HA	1.67	0.75
1:A:470:LEU:HD11	2:B:95:HIS:HB3	1.68	0.75
19:A:1124:CLA:H43	19:A:1136:CLA:HBA1	1.67	0.75
19:A:9012:CLA:HED2	19:A:9012:CLA:CAD	2.16	0.75
3:C:25:VAL:HA	3:C:43:PRO:CG	2.17	0.75
5:E:129:GLU:C	5:E:129:GLU:OE1	2.30	0.75
11:K:115:ILE:CA	11:K:118:VAL:CG2	2.59	0.75
13:N:104:LYS:N	13:N:107:LEU:HD13	2.02	0.75
13:N:131:PHE:C	13:N:132:THR:HG22	2.11	0.75
13:N:156:GLY:N	13:N:157:LYS:HE2	2.02	0.75
15:1:77:GLU:HA	15:1:80:LYS:HD2	1.69	0.75
18:4:172:PHE:CD1	18:4:173:LYS:O	2.40	0.75
1:A:555:ILE:HD13	19:A:9023:CLA:CMD	2.17	0.75
1:A:700:TRP:O	1:A:704:ILE:HB	1.87	0.75
2:B:625:TRP:HE3	2:B:626:LEU:N	1.85	0.75
19:B:1222:CLA:HBC2	19:B:1222:CLA:CHD	2.12	0.75
19:B:1222:CLA:H52	19:B:1236:CLA:CAD	2.17	0.75
4:D:93:LYS:HG2	4:D:96:VAL:HG13	1.67	0.75
22:G:7026:LMU:H41	22:G:7026:LMU:H82	1.69	0.75
12:L:211:TYR:CD2	12:L:211:TYR:N	2.49	0.75
16:2:184:PRO:CD	16:2:187:LYS:HG2	2.16	0.75
16:2:229:MET:SD	16:2:230:LEU:CD1	2.75	0.75
1:A:93:LEU:HA	1:A:96:MET:HB2	1.69	0.75
1:A:430:ASP:H	1:A:433:ASP:CG	1.95	0.75
19:A:1117:CLA:HBB2	19:A:1117:CLA:H121	1.68	0.75
19:A:1133:CLA:HMC3	19:A:1133:CLA:HBC2	1.67	0.75
2:B:131:THR:C	2:B:135:LEU:HD23	2.12	0.75
19:B:1205:CLA:HBA1	19:B:1224:CLA:OBD	1.87	0.75
6:F:88:SER:OG	6:F:91:PHE:CB	2.35	0.75
7:G:63:VAL:HG23	7:G:64:ILE:N	2.01	0.75
15:1:178:LYS:HG3	15:1:179:LYS:N	1.87	0.75
16:2:229:MET:SD	16:2:229:MET:C	2.70	0.75
17:3:148:TYR:N	17:3:149:ASN:CG	2.45	0.75
1:A:168:ALA:O	1:A:171:ALA:HB3	1.86	0.74
1:A:236:GLY:C	1:A:237:VAL:HG22	2.12	0.74
1:A:284:ARG:HB3	1:A:295:TRP:CD1	2.22	0.74
1:A:514:THR:O	1:A:531:PRO:O	2.05	0.74
1:A:711:HIS:HB3	1:A:717:ALA:HB2	1.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1126:CLA:C20	21:J:6012:BCR:H17C	2.17	0.74
21:A:6011:BCR:C31	19:A:9013:CLA:H142	2.17	0.74
2:B:87:ILE:HA	2:B:115:ASN:CB	2.15	0.74
2:B:308:HIS:ND1	2:B:309:ILE:N	2.32	0.74
2:B:461:GLN:O	2:B:464:GLN:HG2	1.86	0.74
19:B:1222:CLA:HED1	19:B:1223:CLA:CMD	2.15	0.74
3:C:73:THR:OG1	3:C:76:SER:N	2.20	0.74
12:L:67:GLY:O	12:L:68:SER:HB3	1.86	0.74
12:L:128:GLN:CA	12:L:130:GLY:HA3	2.14	0.74
13:N:132:THR:HA	13:N:136:ASP:OD1	1.86	0.74
19:R:1150:CLA:HBA2	19:R:1150:CLA:CBD	2.16	0.74
1:A:209:GLY:HA2	1:A:213:LEU:HD13	1.68	0.74
1:A:346:LEU:C	1:A:346:LEU:HD23	2.11	0.74
19:A:1124:CLA:C4B	21:A:6008:BCR:H373	2.17	0.74
2:B:247:THR:HG23	2:B:248:GLN:N	1.94	0.74
19:B:1203:CLA:HBB2	19:B:1225:CLA:HHC	1.68	0.74
22:B:7040:LMU:O3'	22:B:7040:LMU:H1B	1.87	0.74
3:C:52:LYS:HE3	3:C:64:SER:HB3	1.69	0.74
15:1:78:ARG:CD	19:1:1011:CLA:CMC	2.64	0.74
22:3:7003:LMU:C3B	22:3:7005:LMU:H6'1	2.09	0.74
1:A:63:ASP:HB2	19:A:1128:CLA:HED3	1.69	0.74
1:A:129:GLN:O	1:A:130:GLU:CB	2.35	0.74
2:B:551:LYS:O	2:B:552:ASP:CG	2.30	0.74
4:D:159:PRO:O	4:D:159:PRO:CD	2.34	0.74
6:F:207:LEU:CD2	6:F:208:PHE:N	2.50	0.74
7:G:102:ALA:CA	7:G:104:ASP:CG	2.60	0.74
7:G:145:THR:HG23	7:G:146:SER:H	1.50	0.74
14:R:44:UNK:O	14:R:45:UNK:C	2.35	0.74
19:R:1144:CLA:CHA	19:R:1144:CLA:CED	2.65	0.74
16:2:117:ALA:HB1	16:2:230:LEU:CD1	2.17	0.74
17:3:191:GLU:O	17:3:191:GLU:HG2	1.85	0.74
18:4:90:TRP:CD1	18:4:92:VAL:H	2.05	0.74
1:A:25:ASP:OD1	1:A:26:PRO:HG3	1.87	0.74
21:A:6008:BCR:HC8	21:A:6008:BCR:C33	2.15	0.74
2:B:551:LYS:HZ1	4:D:194:ASN:C	1.95	0.74
3:C:62:PHE:CD1	4:D:191:ILE:HG22	2.21	0.74
4:D:156:ARG:NH1	4:D:158:PHE:CD1	2.37	0.74
13:N:155:GLU:HB3	13:N:157:LYS:HE2	1.67	0.74
14:R:24:UNK:O	14:R:27:UNK:CB	2.35	0.74
15:1:97:ILE:HD12	15:1:98:LEU:CB	2.17	0.74
16:2:153:PHE:CE2	16:2:157:LEU:CD2	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:2013:CLA:HBC3	19:2:2013:CLA:HMC1	1.67	0.74
17:3:150:TYR:CD1	17:3:151:TRP:N	2.54	0.74
18:4:159:ASP:OD2	18:4:163:PRO:HA	1.86	0.74
1:A:479:ASP:HA	1:A:536:THR:CG2	2.15	0.74
1:A:513:LEU:HD12	1:A:513:LEU:O	1.86	0.74
21:A:6011:BCR:H393	21:A:6011:BCR:C23	2.15	0.74
2:B:314:ARG:HH22	15:1:67:LEU:HG	1.51	0.74
2:B:500:ALA:HB1	2:B:503:GLU:OE2	1.87	0.74
3:C:24:ASP:CB	23:C:8002:SF4:S2	2.73	0.74
10:J:5:LYS:HD2	16:2:178:ASN:CG	2.12	0.74
22:K:7042:LMU:C6'	22:K:7042:LMU:H32	2.18	0.74
13:N:147:SER:HB2	13:N:151:ASP:OD1	1.88	0.74
1:A:423:ASP:CB	1:A:424:PRO:CD	2.63	0.74
1:A:452:PHE:HE1	19:A:1136:CLA:CBB	1.99	0.74
1:A:523:VAL:CG1	1:A:524:GLY:N	2.51	0.74
19:A:1102:CLA:C1	19:A:1109:CLA:H61	2.12	0.74
2:B:295:PHE:N	2:B:295:PHE:HD2	1.85	0.74
2:B:310:PRO:O	19:B:1301:CLA:HHD	1.86	0.74
2:B:390:GLY:O	21:B:6010:BCR:HC42	1.86	0.74
6:F:89:LYS:HG2	6:F:90:GLN:H	1.51	0.74
6:F:103:GLN:HG3	6:F:104:ALA:N	1.99	0.74
7:G:89:LYS:N	7:G:89:LYS:HZ2	1.84	0.74
14:R:7:UNK:O	14:R:11:UNK:N	2.20	0.74
15:1:123:THR:HG22	15:1:124:TYR:O	1.86	0.74
16:2:218:ARG:HB2	16:2:219:THR:HG23	1.68	0.74
17:3:96:ARG:NH1	17:3:100:TYR:CZ	2.47	0.74
18:4:201:LYS:HG2	18:4:201:LYS:O	1.86	0.74
1:A:283:PHE:O	1:A:284:ARG:NH1	2.19	0.74
1:A:328:LYS:HZ2	1:A:345:GLY:CA	1.99	0.74
1:A:693:LEU:HD21	1:A:735:VAL:H	1.51	0.74
2:B:160:LYS:CE	2:B:161:TRP:CE3	2.71	0.74
2:B:216:LEU:CD2	2:B:218:TYR:O	2.31	0.74
2:B:230:TRP:CH2	7:G:67:SER:HB2	2.21	0.74
2:B:295:PHE:HE2	7:G:94:GLN:HE22	1.35	0.74
2:B:317:ARG:NE	2:B:317:ARG:HA	2.02	0.74
5:E:74:VAL:HG22	5:E:90:VAL:CG2	2.17	0.74
8:H:112:LEU:N	8:H:112:LEU:CD2	2.51	0.74
15:1:67:LEU:HD12	15:1:67:LEU:C	2.12	0.74
22:2:7006:LMU:H22	22:2:7006:LMU:C2'	2.18	0.74
1:A:41:SER:O	1:A:44:ILE:HA	1.88	0.74
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLY:HA2	19:A:1151:CLA:CMC	2.18	0.74
1:A:349:ILE:O	1:A:352:THR:N	2.21	0.74
1:A:470:LEU:HD13	2:B:95:HIS:HB3	1.68	0.74
1:A:542:HIS:HA	1:A:545:HIS:HD2	1.53	0.74
1:A:733:VAL:HG21	19:A:1140:CLA:CMD	2.18	0.74
2:B:10:GLN:O	2:B:14:GLN:NE2	2.20	0.74
2:B:25:ILE:CG2	21:L:6019:BCR:H282	2.18	0.74
3:C:14:CYS:C	3:C:17:CYS:SG	2.69	0.74
22:F:7036:LMU:H4'	22:F:7036:LMU:O2B	1.87	0.74
8:H:67:SER:O	8:H:68:TYR:CG	2.41	0.74
8:H:77:ASN:HD21	8:H:78:PRO:HG2	1.51	0.74
11:K:114:HIS:O	11:K:115:ILE:C	2.31	0.74
12:L:164:LEU:CB	12:L:165:THR:HG23	2.16	0.74
15:1:83:GLU:OE2	15:1:83:GLU:HA	1.87	0.74
16:2:246:PRO:HB2	16:2:247:ILE:HG12	1.70	0.74
1:A:281:LEU:CD1	19:A:1115:CLA:HED2	1.94	0.74
1:A:281:LEU:HD23	19:A:1115:CLA:CMA	1.98	0.74
19:A:1101:CLA:H42	19:A:1140:CLA:C6	2.07	0.74
2:B:53:GLN:HE21	19:B:1201:CLA:HBB1	1.50	0.74
2:B:70:TRP:CD1	2:B:71:GLN:OE1	2.40	0.74
2:B:330:ILE:HD11	19:B:1202:CLA:C19	2.18	0.74
2:B:527:LEU:CD2	19:B:1222:CLA:ND	2.50	0.74
4:D:167:HIS:NE2	4:D:172:VAL:CG2	2.50	0.74
7:G:79:PHE:CG	7:G:80:PHE:N	2.50	0.74
22:H:7030:LMU:H52	22:H:7030:LMU:C9	2.16	0.74
12:L:141:LEU:CD1	21:L:6019:BCR:C31	2.65	0.74
12:L:190:PHE:CZ	12:L:194:ILE:HD12	2.21	0.74
15:1:73:PRO:HG2	15:1:74:ALA:N	2.03	0.74
16:2:220:LYS:NZ	19:2:2004:CLA:OBD	2.15	0.74
17:3:101:GLY:HA2	17:3:104:ILE:CD1	2.18	0.74
19:3:3016:CLA:C10	19:3:3016:CLA:C14	2.57	0.74
18:4:141:LEU:CD2	18:4:141:LEU:N	2.48	0.74
1:A:316:MET:HG2	1:A:317:TYR:CE1	2.21	0.74
1:A:692:PHE:CE2	19:A:1140:CLA:HBC3	2.23	0.74
19:A:1140:CLA:C14	21:A:6011:BCR:C2	2.62	0.74
2:B:32:GLU:HG2	2:B:42:LEU:CD2	2.18	0.74
19:B:1220:CLA:H102	19:B:1220:CLA:C15	2.12	0.74
19:B:1222:CLA:CBB	19:B:1236:CLA:HMB1	2.17	0.74
6:F:173:TRP:HE3	6:F:211:PHE:N	1.86	0.74
15:1:225:TRP:HD1	15:1:226:HIS:CE1	2.06	0.74
17:3:197:SER:OG	17:3:206:PRO:CD	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:123:VAL:N	18:4:124:PRO:CD	2.51	0.74
1:A:684:PHE:C	1:A:684:PHE:HD2	1.95	0.73
2:B:90:ALA:HA	2:B:113:VAL:CG1	2.02	0.73
3:C:26:LEU:H	3:C:43:PRO:HG3	1.53	0.73
3:C:73:THR:HG23	3:C:76:SER:OG	1.87	0.73
4:D:100:TYR:HE1	4:D:134:LYS:CG	2.01	0.73
4:D:140:LEU:CD1	4:D:140:LEU:C	2.32	0.73
22:E:7037:LMU:H12	22:E:7037:LMU:H51	1.69	0.73
7:G:136:VAL:O	7:G:137:VAL:C	2.28	0.73
13:N:139:LYS:CE	13:N:142:LYS:CE	2.51	0.73
1:A:591:GLN:HA	1:A:591:GLN:HE21	1.53	0.73
19:A:1136:CLA:H192	19:L:1130:CLA:CBB	2.18	0.73
19:A:1141:CLA:HMA2	19:A:1141:CLA:C1	2.18	0.73
21:A:6002:BCR:H12C	21:A:6002:BCR:C34	2.17	0.73
2:B:349:ALA:HB2	2:B:375:HIS:HB3	1.69	0.73
2:B:370:ALA:O	19:B:1224:CLA:HMA1	1.88	0.73
2:B:516:ASP:O	2:B:520:HIS:HB2	1.88	0.73
2:B:711:VAL:O	2:B:711:VAL:HG12	1.85	0.73
4:D:148:TYR:O	4:D:149:LYS:HG2	1.89	0.73
7:G:98:THR:OG1	7:G:101:GLU:CB	2.35	0.73
8:H:70:SER:O	8:H:73:PRO:CD	2.37	0.73
12:L:155:GLU:HA	12:L:178:THR:HG21	1.68	0.73
14:R:35:UNK:O	14:R:36:UNK:C	2.35	0.73
1:A:218:TRP:O	1:A:222:GLN:HB2	1.87	0.73
19:A:1124:CLA:HHD	19:A:1124:CLA:CBC	2.15	0.73
2:B:550:LYS:O	2:B:550:LYS:HG2	1.87	0.73
3:C:42:ALA:O	4:D:183:GLY:HA3	1.88	0.73
3:C:44:ARG:CB	4:D:182:GLN:OE1	2.37	0.73
3:C:67:VAL:HG13	3:C:68:TYR:HA	1.70	0.73
4:D:167:HIS:NE2	4:D:172:VAL:HG21	2.02	0.73
5:E:78:ARG:HH12	5:E:125:ILE:HG21	1.51	0.73
22:G:7026:LMU:C5	22:G:7026:LMU:H12	2.17	0.73
13:N:157:LYS:HB3	13:N:158:ASP:CA	2.18	0.73
16:2:139:THR:CG2	16:2:140:ALA:N	2.51	0.73
16:2:172:LEU:C	16:2:173:ASN:HD22	1.95	0.73
16:2:212:GLN:HG2	16:2:213:LYS:HG2	1.71	0.73
17:3:96:ARG:HA	17:3:99:ALA:H	1.41	0.73
19:3:3013:CLA:H2A	19:3:3013:CLA:O1D	1.88	0.73
18:4:100:ARG:O	18:4:104:LEU:HD12	1.89	0.73
18:4:232:LEU:HD12	18:4:234:GLN:HA	1.69	0.73
1:A:150:PHE:N	1:A:153:TRP:HE3	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:CZ	1:A:284:ARG:O	2.35	0.73
2:B:75:GLU:HB2	2:B:132:ASN:CB	2.19	0.73
4:D:167:HIS:CE1	4:D:172:VAL:CG1	2.58	0.73
14:R:38:UNK:O	14:R:41:UNK:CB	2.36	0.73
15:1:84:LEU:C	15:1:88:ARG:HG3	2.14	0.73
15:1:170:PRO:HD2	15:1:173:TYR:HE2	1.49	0.73
17:3:201:ALA:CA	17:3:202:TYR:HD2	2.02	0.73
17:3:210:PRO:CD	17:3:211:LEU:H	2.02	0.73
18:4:211:MET:CG	19:4:4002:CLA:CBB	2.65	0.73
19:4:4002:CLA:CMA	19:4:4002:CLA:CBA	2.67	0.73
1:A:29:THR:HG23	1:A:29:THR:O	1.89	0.73
1:A:73:GLU:OE1	1:A:186:TYR:OH	2.07	0.73
1:A:89:ILE:O	1:A:93:LEU:HD22	1.89	0.73
1:A:217:SER:HA	21:A:6002:BCR:H351	1.68	0.73
1:A:258:LEU:O	1:A:259:TYR:HB2	1.87	0.73
19:A:9023:CLA:H3A	19:A:9023:CLA:O2A	1.87	0.73
3:C:55:GLU:C	3:C:57:ALA:H	1.96	0.73
19:J:1308:CLA:H91	19:2:2014:CLA:O1D	1.87	0.73
18:4:173:LYS:HB2	18:4:194:PHE:CD2	2.22	0.73
18:4:201:LYS:HD3	18:4:201:LYS:N	2.03	0.73
1:A:293:GLY:O	1:A:294:LEU:CB	2.37	0.73
1:A:328:LYS:NZ	1:A:345:GLY:HA3	2.01	0.73
1:A:521:VAL:O	1:A:521:VAL:HG12	1.86	0.73
19:A:1119:CLA:CBA	19:A:1123:CLA:HBB2	2.18	0.73
19:A:1125:CLA:HBB2	19:A:1133:CLA:C3A	2.14	0.73
21:A:6002:BCR:H373	19:3:1147:CLA:HBC1	1.68	0.73
19:A:9012:CLA:C3B	2:B:589:TRP:HH2	2.02	0.73
2:B:11:GLY:CA	3:C:71:HIS:CD2	2.61	0.73
2:B:486:LEU:CD1	2:B:489:GLY:N	2.49	0.73
2:B:545:LYS:HG2	2:B:546:LEU:N	2.01	0.73
19:B:1205:CLA:H102	19:B:1205:CLA:H142	1.71	0.73
3:C:52:LYS:O	3:C:52:LYS:CG	2.37	0.73
3:C:73:THR:HG21	3:C:76:SER:HB3	1.70	0.73
6:F:105:SER:O	6:F:106:LEU:C	2.31	0.73
7:G:99:HIS:O	7:G:101:GLU:CB	2.36	0.73
8:H:80:GLN:HA	8:H:83:LEU:HD23	1.70	0.73
12:L:110:LEU:HA	12:L:113:PRO:HG2	1.71	0.73
12:L:164:LEU:C	12:L:165:THR:CG2	2.61	0.73
12:L:210:PRO:O	12:L:211:TYR:CG	2.42	0.73
15:1:95:PRO:C	15:1:98:LEU:CB	2.60	0.73
16:2:269:LYS:NZ	16:2:269:LYS:CA	2.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:202:TYR:HB3	17:3:203:PRO:HD2	1.69	0.73
19:A:1237:CLA:C20	12:L:110:LEU:HD21	2.18	0.73
19:A:9022:CLA:H13	19:B:1206:CLA:HBB2	1.70	0.73
2:B:515:GLY:CA	2:B:613:SER:HB2	2.18	0.73
7:G:89:LYS:CA	7:G:89:LYS:HZ2	2.02	0.73
17:3:92:PHE:N	17:3:92:PHE:CD1	2.57	0.73
1:A:635:THR:O	1:A:635:THR:HG22	1.88	0.73
19:A:1122:CLA:C1D	21:A:6007:BCR:C19	2.67	0.73
2:B:352:MET:HE2	19:B:1225:CLA:OBD	1.88	0.73
2:B:527:LEU:HD13	19:B:1236:CLA:HMA2	1.68	0.73
6:F:228:ASP:OD2	6:F:231:PHE:CD1	2.41	0.73
7:G:137:VAL:O	7:G:137:VAL:HG23	1.87	0.73
19:H:1145:CLA:CED	19:H:1145:CLA:HAA1	2.19	0.73
19:J:1308:CLA:HMA2	19:2:2014:CLA:HED2	1.70	0.73
19:K:1146:CLA:O1A	19:K:1146:CLA:CMA	2.37	0.73
15:1:155:GLU:O	15:1:156:LYS:HB2	1.88	0.73
21:1:6023:BCR:HC8	21:1:6023:BCR:HC21	1.70	0.73
16:2:192:ASP:OD2	16:2:194:GLY:HA2	1.87	0.73
17:3:238:ILE:HG23	17:3:241:TYR:OH	1.88	0.73
1:A:328:LYS:HG3	1:A:332:GLU:CB	2.19	0.73
1:A:575:LEU:HD11	1:A:579:PHE:HB3	1.71	0.73
19:A:1124:CLA:HED1	19:A:1125:CLA:CAD	2.12	0.73
2:B:261:PHE:CE2	2:B:500:ALA:N	2.57	0.73
2:B:493:TRP:O	2:B:495:PRO:HD3	1.88	0.73
2:B:531:THR:O	2:B:535:VAL:HG12	1.89	0.73
19:B:1228:CLA:CBC	19:B:1228:CLA:CHD	2.66	0.73
3:C:65:VAL:CG2	3:C:66:ARG:H	1.97	0.73
4:D:141:GLY:N	4:D:144:LEU:H	1.84	0.73
5:E:96:ASP:CB	5:E:98:ASN:H	1.94	0.73
12:L:54:TYR:CD1	12:L:54:TYR:N	2.53	0.73
15:1:170:PRO:C	15:1:171:LEU:HD23	2.14	0.73
16:2:153:PHE:CE2	16:2:157:LEU:HD21	2.24	0.73
19:3:3008:CLA:CGD	19:3:3008:CLA:CGA	2.66	0.73
1:A:309:LEU:HD21	19:A:1119:CLA:CMC	2.19	0.73
1:A:349:ILE:HG22	1:A:350:LEU:N	2.01	0.73
2:B:247:THR:C	2:B:250:ALA:H	1.96	0.73
2:B:454:LEU:HD12	2:B:454:LEU:C	2.13	0.73
2:B:622:ASP:HB3	2:B:626:LEU:CD1	2.18	0.73
4:D:100:TYR:HE1	4:D:134:LYS:CE	2.00	0.73
6:F:222:LEU:HD23	6:F:222:LEU:N	2.03	0.73
19:H:1145:CLA:O2D	19:H:1145:CLA:HAA2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:1311:CLA:H2	19:J:1311:CLA:C16	2.18	0.73
12:L:128:GLN:HG2	12:L:132:LEU:HD22	1.69	0.73
16:2:167:ARG:NE	16:2:167:ARG:CA	2.51	0.73
1:A:93:LEU:HA	1:A:96:MET:H	1.53	0.72
1:A:150:PHE:O	1:A:151:GLN:CG	2.34	0.72
1:A:464:ASN:HD22	1:A:464:ASN:N	1.85	0.72
2:B:87:ILE:HD12	2:B:87:ILE:N	2.03	0.72
2:B:190:TRP:HA	19:B:1211:CLA:HBB2	1.69	0.72
4:D:147:LYS:HA	4:D:148:TYR:CD1	2.23	0.72
5:E:129:GLU:OE1	5:E:129:GLU:CA	2.35	0.72
10:J:5:LYS:CG	16:2:178:ASN:OD1	2.36	0.72
15:1:170:PRO:CD	15:1:173:TYR:CD2	2.71	0.72
19:3:3008:CLA:HBC2	19:3:3008:CLA:CMC	2.19	0.72
19:4:1304:CLA:C20	19:4:1304:CLA:C15	2.63	0.72
2:B:124:TRP:CD1	2:B:129:LEU:HB3	2.24	0.72
2:B:125:TYR:CE1	2:B:130:ARG:NH1	2.56	0.72
2:B:294:ASN:HB2	7:G:94:GLN:NE2	2.03	0.72
2:B:486:LEU:CD1	2:B:489:GLY:H	2.02	0.72
2:B:542:ARG:HH11	2:B:542:ARG:HB3	1.52	0.72
2:B:553:PHE:O	2:B:555:TYR:N	2.22	0.72
19:B:1205:CLA:H141	19:B:1224:CLA:H91	1.71	0.72
24:B:7101:LMG:HC61	3:C:70:TRP:CH2	2.25	0.72
8:H:109:LEU:CD2	19:H:1207:CLA:C5	2.67	0.72
12:L:68:SER:O	12:L:69:LEU:C	2.30	0.72
17:3:173:PHE:CD1	17:3:174:GLN:N	2.51	0.72
1:A:267:THR:HG22	1:A:269:PHE:CD2	2.23	0.72
1:A:336:GLY:C	1:A:339:THR:HG1	1.96	0.72
1:A:478:SER:HB3	1:A:644:GLN:NE2	1.94	0.72
1:A:588:GLY:N	2:B:668:ARG:HD3	2.03	0.72
2:B:131:THR:HB	2:B:134:ASP:HB2	1.71	0.72
2:B:216:LEU:HD21	2:B:221:GLY:HA2	1.71	0.72
2:B:457:PRO:HB3	2:B:517:PHE:CB	2.19	0.72
3:C:5:VAL:HG23	3:C:65:VAL:CG2	2.19	0.72
5:E:111:ASN:ND2	5:E:111:ASN:C	2.46	0.72
7:G:63:VAL:HG22	7:G:64:ILE:H	1.51	0.72
7:G:129:ALA:O	7:G:131:GLY:N	2.23	0.72
8:H:111:TYR:CD1	8:H:112:LEU:CD2	2.72	0.72
19:J:1308:CLA:C9	19:2:2014:CLA:CGD	2.67	0.72
11:K:127:ILE:O	11:K:130:LEU:HG	1.90	0.72
12:L:51:LYS:N	12:L:52:PRO:HD3	2.04	0.72
13:N:157:LYS:N	13:N:157:LYS:CE	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1303:CLA:HBC2	19:1:1303:CLA:CMC	2.18	0.72
16:2:183:PHE:C	16:2:185:ASN:HA	2.14	0.72
16:2:188:LEU:HD22	16:2:188:LEU:H	1.53	0.72
17:3:238:ILE:HD11	19:3:3003:CLA:HMC1	1.71	0.72
19:3:3016:CLA:H2A	19:3:3016:CLA:O2D	1.88	0.72
18:4:98:ASN:CB	18:4:212:LEU:HD21	2.20	0.72
1:A:558:LYS:HZ2	2:B:674:LEU:HB2	1.52	0.72
21:A:6011:BCR:C32	21:J:6012:BCR:H391	2.19	0.72
2:B:256:THR:OG1	2:B:258:LEU:N	2.23	0.72
2:B:430:GLY:CA	2:B:525:LEU:HD11	2.17	0.72
3:C:12:ILE:O	3:C:38:GLN:HG3	1.89	0.72
5:E:79:LYS:CG	5:E:84:TYR:CE1	2.73	0.72
6:F:100:LYS:O	6:F:103:GLN:CB	2.31	0.72
6:F:207:LEU:HD22	6:F:208:PHE:HA	1.70	0.72
22:F:7036:LMU:O2B	22:F:7036:LMU:H6D	1.89	0.72
7:G:96:GLY:O	7:G:97:LEU:CG	2.37	0.72
8:H:113:SER:OG	19:H:1207:CLA:C5	2.37	0.72
15:1:224:PRO:HA	15:1:225:TRP:HB2	1.69	0.72
1:A:188:LYS:HE2	1:A:190:ALA:HA	1.72	0.72
1:A:475:ASP:HB3	19:A:1132:CLA:HED3	1.69	0.72
1:A:579:PHE:N	1:A:579:PHE:CD1	2.53	0.72
19:A:1105:CLA:C3B	21:J:6012:BCR:H333	2.19	0.72
2:B:160:LYS:CD	2:B:161:TRP:CD2	2.72	0.72
2:B:521:HIS:CE1	19:B:1235:CLA:NA	2.56	0.72
4:D:176:LYS:HG3	4:D:177:VAL:N	2.02	0.72
22:G:7026:LMU:H41	22:G:7026:LMU:C8	2.19	0.72
15:1:64:PHE:CE1	15:1:66:PRO:HD3	2.24	0.72
17:3:156:THR:CA	17:3:158:PHE:O	2.36	0.72
18:4:214:PHE:O	18:4:215:LEU:C	2.29	0.72
19:4:1304:CLA:O1D	19:4:1304:CLA:H2A	1.90	0.72
1:A:34:TRP:O	1:A:35:ALA:HB3	1.89	0.72
1:A:351:THR:O	19:A:1123:CLA:H201	1.89	0.72
19:A:1141:CLA:HBC3	19:A:1141:CLA:HHD	1.70	0.72
2:B:293:THR:HG23	7:G:94:GLN:HG2	1.69	0.72
2:B:362:ALA:O	2:B:363:GLN:HB3	1.88	0.72
2:B:459:PHE:H	19:B:1235:CLA:CAD	2.02	0.72
2:B:576:PHE:HE2	19:B:1226:CLA:HAC1	1.53	0.72
4:D:201:LYS:O	4:D:202:PHE:HB3	1.87	0.72
11:K:97:ASP:CA	11:K:101:PHE:CE2	2.73	0.72
13:N:139:LYS:HD2	13:N:142:LYS:NZ	2.01	0.72
15:1:134:LEU:N	15:1:135:PRO:CD	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:249:ASN:ND2	16:2:254:LEU:HG	2.04	0.72
1:A:93:LEU:HA	1:A:96:MET:CB	2.19	0.72
1:A:289:PRO:O	1:A:290:LEU:CB	2.37	0.72
1:A:355:HIS:CE1	1:A:416:ILE:HG21	2.24	0.72
2:B:77:TRP:O	2:B:81:PRO:HG3	1.89	0.72
2:B:135:LEU:HD12	2:B:135:LEU:O	1.90	0.72
2:B:639:VAL:HG22	2:B:640:CYS:H	1.55	0.72
19:B:1214:CLA:HBD	19:B:1223:CLA:HBB2	1.70	0.72
19:B:1222:CLA:HBB1	19:B:1236:CLA:CHB	2.19	0.72
7:G:89:LYS:HZ2	7:G:89:LYS:H	1.38	0.72
19:K:1142:CLA:HMD2	19:K:1143:CLA:NA	2.05	0.72
15:1:161:LYS:HE2	15:1:162:LYS:CB	2.17	0.72
17:3:103:VAL:HG13	17:3:107:ARG:CZ	2.19	0.72
19:4:1306:CLA:O2A	19:4:1306:CLA:H2A	1.89	0.72
1:A:284:ARG:CG	1:A:295:TRP:CG	2.73	0.72
1:A:355:HIS:ND1	1:A:416:ILE:CG2	2.52	0.72
1:A:422:TYR:N	1:A:422:TYR:CD1	2.31	0.72
1:A:499:ALA:CB	19:A:1133:CLA:CED	2.64	0.72
19:A:1140:CLA:C4	19:A:1140:CLA:NC	2.53	0.72
21:A:6002:BCR:H402	21:A:6002:BCR:C23	2.20	0.72
2:B:430:GLY:HA2	2:B:525:LEU:CD1	2.19	0.72
3:C:73:THR:CG2	3:C:76:SER:OG	2.38	0.72
5:E:93:VAL:HG23	5:E:103:VAL:CB	2.19	0.72
6:F:138:LEU:HD23	6:F:146:PRO:HB3	1.71	0.72
7:G:128:LEU:HD23	7:G:128:LEU:O	1.88	0.72
15:1:170:PRO:O	15:1:173:TYR:OH	2.08	0.72
16:2:206:TRP:O	16:2:208:SER:HB2	1.90	0.72
22:4:7009:LMU:H3'	22:4:7009:LMU:O5B	1.89	0.72
1:A:27:ILE:O	1:A:28:LYS:CG	2.38	0.72
2:B:70:TRP:CD1	2:B:70:TRP:H	2.07	0.72
2:B:120:VAL:HA	2:B:123:TRP:NE1	2.05	0.72
2:B:230:TRP:N	7:G:63:VAL:CG2	2.49	0.72
2:B:531:THR:HG22	19:B:1222:CLA:HMC2	1.70	0.72
19:B:1203:CLA:H91	19:B:1203:CLA:H193	1.71	0.72
3:C:52:LYS:NZ	3:C:64:SER:HB2	2.03	0.72
3:C:62:PHE:CE2	5:E:80:GLU:OE2	2.42	0.72
6:F:103:GLN:CD	6:F:104:ALA:N	2.47	0.72
19:H:1145:CLA:CED	19:H:1145:CLA:CAA	2.68	0.72
12:L:112:GLY:HA3	19:L:1503:CLA:HHC	1.69	0.72
19:L:1130:CLA:H52	19:L:1504:CLA:CHB	2.19	0.72
13:N:152:LEU:C	13:N:153:GLU:CG	2.57	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:179:LYS:HG2	15:1:180:LEU:O	1.89	0.72
18:4:232:LEU:HB2	18:4:236:ILE:CD1	2.18	0.72
1:A:316:MET:CG	1:A:317:TYR:HD1	1.97	0.72
2:B:639:VAL:HG22	2:B:640:CYS:N	2.05	0.72
19:B:1216:CLA:OBD	19:B:1219:CLA:HBC3	1.90	0.72
3:C:5:VAL:HG23	3:C:65:VAL:HG23	1.71	0.72
3:C:80:ALA:O	3:C:81:TYR:CB	2.35	0.72
5:E:78:ARG:HH12	5:E:125:ILE:CG2	2.00	0.72
22:E:7037:LMU:H12	22:E:7037:LMU:C5	2.20	0.72
22:E:7048:LMU:H22	22:E:7048:LMU:O5'	1.90	0.72
7:G:64:ILE:O	7:G:68:THR:HG21	1.88	0.72
7:G:144:THR:HG23	7:G:147:ASN:O	1.90	0.72
22:N:7049:LMU:O1'	22:N:7049:LMU:H41	1.88	0.72
15:1:92:LEU:CA	15:1:95:PRO:HD2	2.19	0.72
16:2:167:ARG:HE	16:2:168:TRP:H	1.37	0.72
1:A:293:GLY:O	1:A:294:LEU:HB3	1.89	0.71
2:B:74:PHE:O	2:B:76:ALA:N	2.23	0.71
2:B:231:ASN:HD21	7:G:61:ALA:HB3	1.53	0.71
2:B:317:ARG:NH2	2:B:410:ARG:HG3	2.05	0.71
2:B:594:TRP:CD1	2:B:594:TRP:C	2.68	0.71
2:B:729:THR:O	2:B:729:THR:HG22	1.90	0.71
6:F:96:LYS:O	6:F:100:LYS:CB	2.37	0.71
11:K:63:LEU:H	11:K:63:LEU:CD1	1.99	0.71
11:K:118:VAL:CG2	11:K:121:VAL:CG2	2.68	0.71
12:L:51:LYS:N	12:L:52:PRO:CD	2.52	0.71
17:3:252:PRO:HB3	17:3:254:GLN:NE2	2.04	0.71
18:4:226:LYS:H	18:4:226:LYS:NZ	1.87	0.71
1:A:246:HIS:CA	1:A:248:PHE:CE2	2.60	0.71
1:A:283:PHE:C	1:A:284:ARG:HH11	1.98	0.71
1:A:472:ARG:HH22	12:L:120:LEU:HD11	1.54	0.71
19:A:1141:CLA:C12	19:A:1141:CLA:H72	2.18	0.71
2:B:606:VAL:O	2:B:607:SER:C	2.33	0.71
3:C:26:LEU:N	3:C:43:PRO:HG3	2.05	0.71
4:D:146:SER:C	4:D:147:LYS:HG3	2.12	0.71
4:D:188:PHE:N	4:D:188:PHE:CD1	2.52	0.71
11:K:56:ILE:HG23	11:K:59:THR:CG2	2.19	0.71
11:K:116:ILE:HG23	11:K:117:GLY:N	2.05	0.71
11:K:127:ILE:CB	11:K:130:LEU:HG	2.20	0.71
12:L:110:LEU:HB3	12:L:114:PHE:CE1	2.22	0.71
15:1:150:HIS:CE1	15:1:151:GLN:HE22	2.07	0.71
16:2:184:PRO:HD3	16:2:187:LYS:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:104:ILE:HG21	19:3:3004:CLA:C4D	2.20	0.71
18:4:122:ASN:C	18:4:124:PRO:HD3	2.15	0.71
18:4:225:GLY:HA2	18:4:226:LYS:HZ2	1.55	0.71
1:A:92:TRP:O	1:A:93:LEU:CB	2.38	0.71
1:A:387:THR:CG2	1:A:523:VAL:HG11	2.20	0.71
1:A:472:ARG:NH1	12:L:120:LEU:CD2	2.50	0.71
19:A:1117:CLA:H202	19:A:1125:CLA:H3A	1.71	0.71
22:A:7016:LMU:H61	22:A:7016:LMU:C2	2.16	0.71
2:B:315:LEU:HD11	2:B:317:ARG:HD2	1.73	0.71
2:B:395:ILE:HD12	2:B:396:ARG:HG2	1.73	0.71
2:B:693:TRP:CD1	19:B:1238:CLA:C1D	2.74	0.71
19:B:1235:CLA:H121	21:F:6016:BCR:H312	1.70	0.71
22:B:7038:LMU:H4'	22:B:7038:LMU:O2B	1.88	0.71
3:C:72:GLU:HG2	3:C:77:MET:CE	2.19	0.71
5:E:83:TRP:CZ3	5:E:111:ASN:HB2	2.25	0.71
5:E:127:GLU:C	5:E:128:VAL:HG23	2.15	0.71
11:K:49:ILE:C	11:K:52:PRO:HD3	2.15	0.71
11:K:89:ARG:HG3	11:K:89:ARG:HH11	1.55	0.71
12:L:67:GLY:O	12:L:68:SER:CB	2.38	0.71
21:L:6019:BCR:H403	21:L:6019:BCR:C27	2.19	0.71
16:2:124:GLU:O	16:2:127:THR:CG2	2.37	0.71
16:2:227:LEU:HD21	19:2:2004:CLA:NC	2.05	0.71
17:3:98:LEU:HD21	19:3:3012:CLA:C3D	2.20	0.71
1:A:462:ILE:HG21	19:A:1132:CLA:HMC1	1.73	0.71
19:A:1124:CLA:H172	21:A:6007:BCR:H332	1.71	0.71
2:B:270:LEU:HD12	2:B:270:LEU:C	2.15	0.71
8:H:108:THR:O	8:H:109:LEU:C	2.29	0.71
11:K:59:THR:O	11:K:63:LEU:CD2	2.38	0.71
11:K:98:PRO:CD	11:K:99:ALA:H	2.01	0.71
13:N:139:LYS:CD	13:N:142:LYS:CE	2.68	0.71
15:1:67:LEU:HD12	15:1:68:GLY:H	1.51	0.71
16:2:96:PRO:HD3	17:3:85:ASP:OD2	1.87	0.71
16:2:121:PHE:H	16:2:121:PHE:HD2	1.36	0.71
16:2:148:ASP:CG	16:2:152:LEU:CB	2.63	0.71
16:2:226:ARG:HH11	16:2:226:ARG:HB2	1.56	0.71
18:4:220:GLN:CD	19:4:1306:CLA:HAC2	2.14	0.71
19:A:1102:CLA:H12	19:A:1109:CLA:H92	1.72	0.71
2:B:331:HIS:CE1	2:B:392:ILE:HG21	2.25	0.71
19:B:1223:CLA:C8	21:B:6010:BCR:H14C	2.21	0.71
6:F:170:ILE:CG2	21:F:6014:BCR:H372	2.21	0.71
11:K:112:VAL:O	11:K:113:GLY:C	2.34	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:94:SER:O	12:L:96:LEU:CD2	2.38	0.71
13:N:99:LYS:CB	13:N:102:ASN:HD21	2.03	0.71
16:2:154:ILE:HG12	16:2:155:VAL:N	2.04	0.71
16:2:223:LYS:O	16:2:226:ARG:HB3	1.90	0.71
17:3:150:TYR:CD2	17:3:151:TRP:CD2	2.78	0.71
18:4:109:MET:C	18:4:111:LEU:H	1.97	0.71
1:A:187:HIS:CE1	19:A:1109:CLA:C4D	2.67	0.71
1:A:258:LEU:HG	1:A:280:PHE:CE1	2.26	0.71
1:A:370:ILE:HG23	1:A:403:GLY:CA	2.16	0.71
1:A:379:MET:HE2	19:A:1125:CLA:CMC	2.20	0.71
1:A:479:ASP:OD1	1:A:536:THR:HG22	1.91	0.71
21:B:6004:BCR:H343	7:G:77:PHE:CD1	2.25	0.71
3:C:63:LEU:HD21	3:C:65:VAL:H	1.53	0.71
4:D:106:SER:OG	4:D:124:GLU:HG2	1.91	0.71
4:D:133:ARG:H	4:D:136:GLN:HE22	1.36	0.71
8:H:77:ASN:OD1	8:H:78:PRO:HD2	1.91	0.71
22:L:7029:LMU:H31	22:L:7029:LMU:C1'	2.16	0.71
15:1:73:PRO:CG	15:1:74:ALA:N	2.49	0.71
17:3:204:GLY:H	17:3:207:PHE:HA	1.56	0.71
18:4:226:LYS:N	18:4:226:LYS:HD3	2.04	0.71
1:A:246:HIS:C	1:A:248:PHE:CD2	2.68	0.71
1:A:615:HIS:CE1	19:A:1135:CLA:HBC3	2.26	0.71
19:A:1102:CLA:O2D	19:A:1102:CLA:H2A	1.90	0.71
19:A:1125:CLA:HMC1	19:A:1125:CLA:CBC	2.19	0.71
2:B:600:THR:O	2:B:604:GLY:HA2	1.89	0.71
19:B:1225:CLA:OBD	19:B:1225:CLA:O1D	1.97	0.71
3:C:44:ARG:HA	4:D:182:GLN:OE1	1.90	0.71
5:E:89:SER:HB3	5:E:106:ARG:NE	2.06	0.71
8:H:98:LEU:HD21	12:L:143:LEU:HD22	1.73	0.71
11:K:70:PHE:HD1	11:K:70:PHE:O	1.74	0.71
15:1:83:GLU:CA	15:1:86:HIS:CD2	2.74	0.71
16:2:107:LEU:HD12	16:2:107:LEU:C	2.15	0.71
17:3:150:TYR:CA	17:3:152:ALA:HB2	2.21	0.71
22:3:7003:LMU:O2B	22:3:7005:LMU:O5B	2.09	0.71
18:4:96:LEU:HD12	18:4:96:LEU:O	1.91	0.71
18:4:167:ASN:ND2	19:4:4014:CLA:C2	2.53	0.71
1:A:252:ARG:NH1	1:A:261:SER:OG	2.23	0.71
1:A:328:LYS:CG	1:A:332:GLU:CB	2.68	0.71
1:A:723:ARG:HH11	1:A:723:ARG:HG2	1.56	0.71
2:B:88:ALA:N	2:B:115:ASN:HA	2.05	0.71
2:B:268:LEU:CD2	19:B:1214:CLA:HMA1	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:LEU:O	2:B:326:ILE:HG22	1.90	0.71
2:B:622:ASP:HB3	2:B:626:LEU:HG	1.72	0.71
3:C:62:PHE:CG	4:D:191:ILE:HG21	2.26	0.71
5:E:90:VAL:HG12	5:E:91:VAL:H	1.56	0.71
19:H:1241:CLA:HAC1	21:I:6021:BCR:HC31	1.69	0.71
12:L:143:LEU:H	12:L:145:LEU:H	1.35	0.71
13:N:120:VAL:O	13:N:121:GLU:C	2.34	0.71
18:4:159:ASP:CG	18:4:171:ILE:CD1	2.55	0.71
18:4:242:ASN:O	18:4:243:THR:CG2	2.35	0.71
2:B:125:TYR:CD1	2:B:130:ARG:NH1	2.58	0.71
3:C:52:LYS:NZ	3:C:65:VAL:O	2.24	0.71
5:E:94:ASP:HB2	5:E:102:PRO:HB3	1.72	0.71
7:G:63:VAL:CG2	7:G:64:ILE:N	2.45	0.71
10:J:2:ARG:NH1	10:J:8:LEU:HD13	2.01	0.71
12:L:209:LEU:CG	12:L:210:PRO:HD2	2.21	0.71
19:1:1303:CLA:CMA	19:1:1303:CLA:HBA2	2.19	0.71
18:4:122:ASN:CB	18:4:124:PRO:HD3	2.19	0.71
1:A:62:HIS:ND1	1:A:62:HIS:N	2.39	0.71
5:E:81:SER:OG	5:E:120:TYR:CZ	2.37	0.71
8:H:66:ASP:O	8:H:67:SER:C	2.34	0.71
8:H:78:PRO:CG	19:L:1501:CLA:CMD	2.69	0.71
19:K:1143:CLA:HBC1	22:K:7001:LMU:C3B	2.21	0.71
16:2:171:ILE:HG13	16:2:172:LEU:CA	2.19	0.71
17:3:150:TYR:CA	17:3:151:TRP:HD1	2.04	0.71
18:4:174:GLN:O	18:4:194:PHE:CD1	2.44	0.71
1:A:66:SER:O	1:A:67:HIS:HB2	1.89	0.70
1:A:295:TRP:C	1:A:297:THR:H	1.96	0.70
1:A:362:LEU:HB3	1:A:410:ALA:HB2	1.73	0.70
1:A:545:HIS:HB3	19:A:1135:CLA:HBB2	1.71	0.70
1:A:680:LEU:HB3	19:A:9012:CLA:O2A	1.91	0.70
19:A:1140:CLA:H161	21:A:6011:BCR:HC22	1.72	0.70
19:A:9022:CLA:C9	19:A:9023:CLA:C9	2.69	0.70
3:C:44:ARG:HB3	4:D:182:GLN:OE1	1.89	0.70
3:C:49:VAL:HG22	3:C:50:GLY:H	1.55	0.70
5:E:82:TYR:HB3	5:E:83:TRP:HE3	1.54	0.70
7:G:84:ARG:NE	7:G:89:LYS:CE	2.51	0.70
12:L:82:TYR:O	12:L:83:LEU:HB3	1.91	0.70
12:L:174:ASP:CG	12:L:175:GLN:N	2.48	0.70
15:1:151:GLN:HE21	15:1:151:GLN:CA	2.02	0.70
16:2:120:ILE:CG1	16:2:121:PHE:N	2.51	0.70
16:2:134:THR:OG1	16:2:135:PRO:HD3	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:148:ASP:C	16:2:149:THR:HG1	2.00	0.70
16:2:160:ILE:CG2	19:2:2012:CLA:CAB	2.68	0.70
18:4:169:ASP:OD1	18:4:174:GLN:HB2	1.90	0.70
18:4:172:PHE:CA	18:4:194:PHE:HE2	1.94	0.70
18:4:211:MET:HG3	19:4:4002:CLA:HBB2	1.73	0.70
1:A:132:LEU:HD11	1:A:674:ALA:CB	2.20	0.70
1:A:188:LYS:HD2	1:A:189:ALA:N	2.06	0.70
1:A:389:TYR:HE2	1:A:526:LYS:HD3	1.56	0.70
2:B:400:PRO:HD2	4:D:197:PRO:HD3	1.72	0.70
2:B:663:PHE:O	2:B:664:LEU:CB	2.39	0.70
3:C:65:VAL:CG2	3:C:66:ARG:N	2.55	0.70
5:E:128:VAL:O	5:E:129:GLU:C	2.30	0.70
6:F:139:LEU:HD13	6:F:149:ILE:HD12	1.72	0.70
6:F:213:TRP:CB	6:F:216:ALA:HB2	2.17	0.70
6:F:225:GLU:O	6:F:227:VAL:HG13	1.92	0.70
19:F:1302:CLA:CMA	21:F:6016:BCR:HC32	2.21	0.70
10:J:11:ALA:HB1	10:J:12:PRO:CD	2.12	0.70
11:K:87:GLU:O	11:K:87:GLU:CD	2.34	0.70
12:L:73:VAL:HA	19:L:1504:CLA:HMA1	1.73	0.70
16:2:131:ILE:O	16:2:132:LEU:CB	2.39	0.70
16:2:173:ASN:ND2	16:2:173:ASN:N	2.36	0.70
17:3:156:THR:HA	17:3:158:PHE:O	1.89	0.70
17:3:225:LEU:HD13	17:3:228:VAL:HG21	1.72	0.70
18:4:169:ASP:C	18:4:173:LYS:CA	2.57	0.70
1:A:532:ILE:HG23	1:A:532:ILE:O	1.90	0.70
19:A:1119:CLA:HMD2	19:A:1121:CLA:CBB	2.18	0.70
19:A:1237:CLA:C14	12:L:141:LEU:HD23	2.17	0.70
21:A:6007:BCR:H382	21:A:6007:BCR:C23	2.21	0.70
2:B:110:LEU:CD1	2:B:111:GLY:N	2.53	0.70
2:B:127:ILE:O	2:B:127:ILE:CG1	2.38	0.70
2:B:160:LYS:HZ2	2:B:161:TRP:CB	2.03	0.70
2:B:680:TRP:O	2:B:681:ALA:O	2.08	0.70
3:C:31:TRP:CD1	3:C:32:GLY:N	2.58	0.70
4:D:123:ARG:O	4:D:124:GLU:HB2	1.91	0.70
6:F:159:GLU:HG2	10:J:38:ILE:HG12	1.72	0.70
21:I:6021:BCR:H322	21:I:6021:BCR:HC42	1.72	0.70
11:K:115:ILE:O	11:K:118:VAL:HG22	1.91	0.70
19:K:3009:CLA:H91	19:3:3007:CLA:HAC2	1.74	0.70
14:R:37:UNK:O	14:R:43:UNK:N	2.24	0.70
16:2:176:CYS:O	16:2:177:VAL:CG2	2.36	0.70
19:2:2014:CLA:OBD	19:2:2014:CLA:CED	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:103:VAL:CG1	17:3:107:ARG:NE	2.42	0.70
19:3:1147:CLA:CMC	19:3:1147:CLA:HBC2	2.20	0.70
22:3:7003:LMU:C2B	22:3:7005:LMU:O5B	2.39	0.70
1:A:284:ARG:CG	1:A:295:TRP:CD1	2.73	0.70
19:A:1119:CLA:CMD	19:A:1121:CLA:CBB	2.64	0.70
2:B:25:ILE:CG2	21:L:6019:BCR:H292	2.15	0.70
2:B:438:VAL:CG2	19:B:1230:CLA:HMC2	2.18	0.70
19:B:1223:CLA:HED1	19:B:1231:CLA:CBB	2.19	0.70
3:C:43:PRO:HA	4:D:182:GLN:CB	2.20	0.70
3:C:72:GLU:CG	3:C:77:MET:CE	2.66	0.70
6:F:190:LYS:CG	6:F:192:THR:HG23	2.22	0.70
6:F:204:SER:O	6:F:207:LEU:CD1	2.38	0.70
8:H:78:PRO:CG	19:L:1501:CLA:HMD2	2.21	0.70
10:J:2:ARG:HH12	10:J:8:LEU:CD1	2.00	0.70
13:N:99:LYS:CB	13:N:102:ASN:ND2	2.55	0.70
13:N:165:ASN:O	13:N:167:PHE:N	2.24	0.70
17:3:150:TYR:O	17:3:152:ALA:CA	2.38	0.70
17:3:156:THR:O	17:3:156:THR:HG23	1.90	0.70
18:4:111:LEU:HD12	18:4:112:PRO:HG3	1.74	0.70
1:A:27:ILE:O	1:A:28:LYS:HG3	1.92	0.70
1:A:578:ARG:O	1:A:579:PHE:C	2.33	0.70
2:B:244:PHE:HD2	2:B:244:PHE:O	1.75	0.70
2:B:615:TYR:HD1	2:B:615:TYR:N	1.89	0.70
19:B:1209:CLA:H61	19:B:1209:CLA:H11	1.73	0.70
4:D:100:TYR:HE1	4:D:134:LYS:CD	2.04	0.70
7:G:124:ILE:O	7:G:128:LEU:CB	2.39	0.70
15:1:101:GLU:O	15:1:101:GLU:HG2	1.89	0.70
22:4:7053:LMU:H6E	22:4:7053:LMU:C1B	2.20	0.70
1:A:246:HIS:O	1:A:248:PHE:CD2	2.43	0.70
1:A:388:ASP:CG	1:A:391:THR:HG1	1.96	0.70
2:B:58:PHE:HB3	2:B:146:SER:HB3	1.73	0.70
2:B:469:LYS:CE	2:B:470:THR:HG23	2.21	0.70
19:B:1228:CLA:HMA1	19:B:1228:CLA:H12	1.72	0.70
19:B:1235:CLA:H121	21:F:6016:BCR:C31	2.21	0.70
4:D:113:GLU:O	4:D:114:MET:HB3	1.91	0.70
5:E:111:ASN:C	5:E:111:ASN:HD22	1.99	0.70
22:R:7021:LMU:H1'	22:R:7021:LMU:C3	2.20	0.70
15:1:201:PHE:CD1	15:1:204:GLN:CD	2.70	0.70
16:2:154:ILE:CG1	16:2:155:VAL:N	2.53	0.70
19:A:1124:CLA:H2	19:A:1125:CLA:HED3	1.73	0.70
21:A:6008:BCR:H331	21:A:6008:BCR:C8	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:LEU:CD1	19:B:1212:CLA:HBB2	2.20	0.70
2:B:232:LEU:HD11	2:B:235:GLN:HB2	1.72	0.70
2:B:256:THR:O	2:B:257:ILE:HD13	1.92	0.70
2:B:314:ARG:HH12	15:1:67:LEU:CD1	2.05	0.70
2:B:329:SER:OG	2:B:332:PHE:HB2	1.91	0.70
2:B:457:PRO:CB	2:B:517:PHE:HD1	2.04	0.70
2:B:596:TRP:CH2	2:B:612:SER:C	2.67	0.70
5:E:79:LYS:HG3	5:E:84:TYR:OH	1.90	0.70
6:F:207:LEU:CG	6:F:208:PHE:N	2.54	0.70
7:G:124:ILE:CG2	7:G:125:VAL:N	2.54	0.70
19:K:1142:CLA:HED2	19:K:1143:CLA:CMB	2.21	0.70
12:L:73:VAL:HG21	19:L:1130:CLA:OBD	1.90	0.70
12:L:91:THR:CA	12:L:98:ARG:HH12	2.05	0.70
13:N:120:VAL:O	13:N:120:VAL:CG1	2.40	0.70
13:N:139:LYS:HG3	13:N:142:LYS:CE	2.22	0.70
15:1:150:HIS:CG	15:1:151:GLN:NE2	2.60	0.70
18:4:211:MET:CG	19:4:4002:CLA:HBB1	2.21	0.70
1:A:207:LEU:HB3	19:A:1119:CLA:CBB	2.22	0.70
1:A:581:CYS:HB2	1:A:590:CYS:CA	2.18	0.70
2:B:5:ILE:HG22	2:B:6:PRO:N	2.05	0.70
19:B:1222:CLA:HHD	19:B:1222:CLA:CBC	2.16	0.70
21:B:6020:BCR:C33	19:L:1502:CLA:NB	2.48	0.70
4:D:95:GLN:HG3	4:D:96:VAL:N	2.06	0.70
5:E:83:TRP:CH2	5:E:116:SER:HB2	2.27	0.70
7:G:82:PHE:HB2	7:G:83:GLN:CG	2.21	0.70
10:J:4:LEU:O	10:J:5:LYS:HB2	1.89	0.70
11:K:78:ARG:HA	11:K:78:ARG:HE	1.52	0.70
12:L:73:VAL:HA	19:L:1504:CLA:HMA3	1.73	0.70
19:R:1144:CLA:H2A	19:R:1144:CLA:O1A	1.92	0.70
18:4:126:TRP:CG	18:4:127:TYR:H	2.09	0.70
18:4:200:ALA:O	18:4:202:GLU:N	2.25	0.70
19:4:1004:CLA:HBC2	19:4:1004:CLA:CHD	2.16	0.70
1:A:244:LEU:HD13	1:A:247:GLU:OE2	1.92	0.70
1:A:564:ARG:NH2	1:A:564:ARG:CB	2.54	0.70
19:A:1112:CLA:HHC	21:A:6002:BCR:C17	2.22	0.70
19:B:1239:CLA:H192	9:I:21:MET:HB3	1.73	0.70
3:C:44:ARG:NH2	4:D:181:ARG:HG2	2.06	0.70
5:E:126:VAL:O	5:E:127:GLU:HB2	1.92	0.70
12:L:172:GLU:N	12:L:173:PRO:CD	2.40	0.70
13:N:157:LYS:HB3	13:N:158:ASP:HA	1.73	0.70
15:1:103:LEU:HD23	15:1:103:LEU:N	2.02	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:148:ASP:HB3	16:2:152:LEU:HG	1.71	0.70
19:3:2009:CLA:CHA	19:3:2009:CLA:CBA	2.70	0.70
1:A:50:THR:HG22	1:A:52:THR:H	1.57	0.70
2:B:212:PHE:CZ	19:B:1211:CLA:HHD	2.26	0.70
5:E:78:ARG:NH1	5:E:125:ILE:HB	2.07	0.70
6:F:138:LEU:CD2	6:F:146:PRO:HB3	2.22	0.70
11:K:115:ILE:HD13	11:K:122:LEU:HD12	1.73	0.70
16:2:126:LEU:C	16:2:128:LYS:H	1.97	0.70
16:2:182:ILE:HB	16:2:187:LYS:HG3	1.64	0.70
17:3:91:GLY:C	17:3:92:PHE:CD1	2.69	0.70
18:4:109:MET:O	18:4:111:LEU:N	2.25	0.70
18:4:153:GLU:OE2	19:4:4012:CLA:C4B	2.39	0.70
1:A:83:PHE:CE1	19:A:1111:CLA:CED	2.75	0.69
1:A:531:PRO:O	1:A:532:ILE:CG2	2.39	0.69
19:A:1108:CLA:HBB2	19:A:1111:CLA:HMA2	1.74	0.69
19:A:1237:CLA:C6	19:A:1237:CLA:H112	2.20	0.69
19:B:1206:CLA:H41	21:I:6018:BCR:C23	2.21	0.69
4:D:145:ARG:HH12	4:D:173:TYR:HE1	1.38	0.69
5:E:82:TYR:CE1	5:E:111:ASN:HA	2.27	0.69
22:H:7011:LMU:O6'	22:H:7011:LMU:H4B	1.92	0.69
12:L:51:LYS:HB3	12:L:51:LYS:NZ	2.06	0.69
12:L:143:LEU:CD2	12:L:146:THR:HG22	2.15	0.69
19:L:1148:CLA:H2	19:L:1148:CLA:HED3	1.70	0.69
13:N:155:GLU:CB	13:N:157:LYS:N	2.17	0.69
15:1:112:GLN:HG2	15:1:113:GLU:N	2.03	0.69
17:3:187:PHE:CD1	17:3:188:LEU:N	2.60	0.69
18:4:142:PHE:CD1	19:4:4010:CLA:C3C	2.75	0.69
22:4:7034:LMU:C8	22:4:7052:LMU:H1'	2.14	0.69
1:A:105:ASN:HB2	1:A:119:SER:O	1.93	0.69
1:A:370:ILE:HG22	1:A:400:MET:CA	2.21	0.69
19:A:1101:CLA:C4	19:A:1140:CLA:H61	2.07	0.69
2:B:229:GLN:OE1	2:B:229:GLN:HA	1.92	0.69
3:C:67:VAL:HG22	3:C:67:VAL:O	1.90	0.69
19:K:3009:CLA:C9	19:3:3007:CLA:HAC2	2.23	0.69
12:L:154:ASN:C	12:L:178:THR:CG2	2.62	0.69
15:1:98:LEU:O	15:1:98:LEU:HD13	1.92	0.69
19:1:1014:CLA:HHD	19:1:1014:CLA:CBC	2.12	0.69
17:3:150:TYR:HB3	17:3:151:TRP:HE1	1.56	0.69
19:3:3008:CLA:CBD	19:3:3008:CLA:CBA	2.65	0.69
18:4:120:ILE:HG22	18:4:121:ILE:HG23	1.74	0.69
18:4:188:ILE:HG22	18:4:189:PHE:N	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:HD21	1:A:343:HIS:C	2.16	0.69
19:A:1105:CLA:HAA2	19:A:1107:CLA:CED	2.22	0.69
19:A:1106:CLA:HBB2	19:A:1107:CLA:C4D	2.23	0.69
19:A:1119:CLA:HBA1	19:A:1123:CLA:HBB2	1.74	0.69
19:A:1122:CLA:CAB	21:A:6007:BCR:H351	2.22	0.69
2:B:187:SER:O	2:B:189:ALA:N	2.25	0.69
3:C:17:CYS:C	3:C:58:CYS:HB2	2.17	0.69
6:F:207:LEU:HD22	6:F:208:PHE:CB	2.22	0.69
7:G:64:ILE:HG13	7:G:68:THR:CG2	2.22	0.69
12:L:131:SER:N	12:L:201:TYR:CD2	2.59	0.69
13:N:124:SER:O	13:N:125:CYS:HB2	1.91	0.69
13:N:156:GLY:CA	13:N:157:LYS:HD2	2.22	0.69
15:1:201:PHE:CD1	15:1:204:GLN:NE2	2.59	0.69
19:1:1014:CLA:C10	19:1:1014:CLA:C5	2.58	0.69
16:2:243:GLY:CA	16:2:244:THR:HG23	2.22	0.69
1:A:102:ARG:C	1:A:103:PHE:CD2	2.62	0.69
1:A:472:ARG:HH22	12:L:120:LEU:CD1	2.04	0.69
2:B:118:SER:HB2	19:B:1205:CLA:OBD	1.92	0.69
2:B:292:ARG:HH21	2:B:297:ILE:C	1.99	0.69
2:B:373:THR:HA	2:B:376:GLN:HB2	1.73	0.69
6:F:193:GLN:HA	6:F:195:GLU:OE1	1.92	0.69
6:F:205:SER:C	6:F:207:LEU:HD12	2.17	0.69
7:G:116:SER:CA	7:G:119:PRO:HG2	2.21	0.69
8:H:67:SER:C	8:H:68:TYR:CG	2.69	0.69
12:L:72:PRO:C	12:L:73:VAL:HG22	2.15	0.69
12:L:137:LEU:HD23	12:L:137:LEU:O	1.91	0.69
13:N:89:GLU:OE1	13:N:89:GLU:O	2.11	0.69
13:N:146:LEU:HD11	17:3:142:ILE:C	2.03	0.69
15:1:157:ASP:CB	15:1:178:LYS:CA	2.50	0.69
17:3:93:ILE:O	17:3:93:ILE:HG23	1.92	0.69
17:3:98:LEU:HD21	19:3:3012:CLA:C2D	2.22	0.69
17:3:233:LEU:HA	17:3:236:LEU:HB3	1.73	0.69
22:3:7005:LMU:H3'	22:3:7005:LMU:O2B	1.91	0.69
18:4:193:ASN:C	18:4:194:PHE:CD1	2.69	0.69
1:A:74:ILE:O	1:A:77:LYS:N	2.22	0.69
1:A:351:THR:O	19:A:1123:CLA:C20	2.41	0.69
1:A:690:LEU:HD23	1:A:693:LEU:HD12	1.74	0.69
1:A:725:LEU:HD21	19:A:1140:CLA:HMD3	1.74	0.69
2:B:44:GLN:OE1	2:B:163:PRO:HB2	1.91	0.69
2:B:224:PRO:O	2:B:226:LEU:N	2.25	0.69
2:B:508:LEU:HB3	2:B:509:PHE:CD2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ARG:NH2	7:G:117:ASN:HA	2.07	0.69
7:G:77:PHE:O	7:G:79:PHE:HB3	1.92	0.69
19:K:1142:CLA:CED	19:K:1143:CLA:HMB3	2.22	0.69
12:L:168:GLY:O	12:L:170:LYS:N	2.25	0.69
12:L:172:GLU:O	12:L:174:ASP:O	2.10	0.69
12:L:205:TYR:CE1	12:L:207:LEU:CD1	2.75	0.69
14:R:51:UNK:O	14:R:52:UNK:CB	2.41	0.69
15:1:65:ASP:OD2	15:1:66:PRO:CA	2.40	0.69
15:1:97:ILE:HD12	15:1:98:LEU:HB2	1.73	0.69
15:1:147:PHE:O	15:1:150:HIS:HB3	1.92	0.69
17:3:192:LYS:HA	17:3:192:LYS:NZ	2.06	0.69
1:A:73:GLU:CG	1:A:74:ILE:N	2.55	0.69
1:A:281:LEU:HD13	19:A:1115:CLA:O2D	1.89	0.69
1:A:345:GLY:C	1:A:347:TYR:N	2.35	0.69
19:A:1134:CLA:CMA	19:A:1141:CLA:HBB2	2.22	0.69
19:A:9012:CLA:H12	2:B:616:LEU:HD13	1.73	0.69
2:B:438:VAL:HG22	19:B:1230:CLA:CMC	2.21	0.69
6:F:170:ILE:O	6:F:173:TRP:CD1	2.44	0.69
7:G:90:GLN:CB	7:G:91:VAL:O	2.38	0.69
8:H:114:ALA:O	8:H:115:THR:CG2	2.40	0.69
10:J:42:PHE:HD1	18:4:244:ILE:HG21	1.58	0.69
19:J:1308:CLA:HBA2	19:J:1308:CLA:CBD	2.14	0.69
11:K:125:LYS:HB2	11:K:128:GLY:H	1.57	0.69
12:L:54:TYR:HE1	12:L:57:ILE:HG23	1.58	0.69
12:L:155:GLU:HA	12:L:178:THR:HG22	1.74	0.69
13:N:130:ASN:O	13:N:132:THR:HG22	1.78	0.69
15:1:170:PRO:CD	15:1:173:TYR:HE2	2.05	0.69
16:2:94:SER:O	16:2:95:ASP:HB2	1.90	0.69
16:2:125:PHE:O	16:2:126:LEU:C	2.36	0.69
1:A:173:VAL:HG23	1:A:174:PHE:HD1	1.57	0.69
1:A:217:SER:OG	21:A:6002:BCR:H17C	1.92	0.69
19:A:1112:CLA:HED2	19:A:1112:CLA:H2A	1.74	0.69
19:A:1123:CLA:OBD	19:A:1123:CLA:H112	1.93	0.69
19:A:9023:CLA:H3A	19:A:9023:CLA:CGA	2.22	0.69
2:B:87:ILE:N	2:B:87:ILE:CD1	2.55	0.69
2:B:152:ALA:O	2:B:153:GLY:C	2.35	0.69
2:B:308:HIS:CG	2:B:309:ILE:N	2.61	0.69
6:F:138:LEU:O	6:F:140:CYS:SG	2.48	0.69
22:G:7039:LMU:H6'2	22:G:7039:LMU:H3'	1.74	0.69
12:L:204:LEU:HD13	12:L:205:TYR:N	2.08	0.69
13:N:99:LYS:CA	13:N:102:ASN:OD1	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:81:GLU:C	15:1:83:GLU:N	2.40	0.69
19:1:1013:CLA:CAD	19:1:1013:CLA:HED2	2.22	0.69
17:3:91:GLY:O	17:3:93:ILE:N	2.25	0.69
17:3:243:ILE:HD11	19:3:3005:CLA:C1C	2.20	0.69
18:4:145:GLU:CG	18:4:146:PHE:CD1	2.58	0.69
18:4:207:ASN:HD21	19:4:4002:CLA:C1A	2.06	0.69
1:A:49:ASP:HB2	1:A:720:THR:HA	1.75	0.69
1:A:491:TRP:NE1	19:A:1135:CLA:C1	2.50	0.69
19:A:1124:CLA:HED1	19:A:1125:CLA:HMD2	1.65	0.69
21:A:6011:BCR:C31	21:A:6011:BCR:C8	2.70	0.69
2:B:53:GLN:HE22	19:B:1201:CLA:HBB1	1.53	0.69
2:B:141:PHE:HA	2:B:144:PHE:CD1	2.28	0.69
2:B:625:TRP:CE3	2:B:626:LEU:N	2.60	0.69
4:D:82:ILE:CG2	4:D:121:ILE:O	2.40	0.69
6:F:97:GLN:O	6:F:98:ALA:C	2.32	0.69
19:F:1302:CLA:HBC2	19:F:1302:CLA:HHD	1.75	0.69
7:G:87:VAL:O	7:G:88:ALA:HB3	1.92	0.69
8:H:115:THR:O	8:H:116:ALA:HB3	1.90	0.69
22:H:7011:LMU:H2B	22:H:7011:LMU:C6'	2.22	0.69
19:K:1142:CLA:CED	19:K:1143:CLA:HMB1	2.22	0.69
13:N:135:GLN:HA	13:N:136:ASP:C	2.12	0.69
15:1:206:SER:O	15:1:209:PRO:HD3	1.92	0.69
15:1:217:LEU:HD23	15:1:218:ALA:HA	1.74	0.69
16:2:158:VAL:CG2	16:2:159:PHE:N	2.54	0.69
17:3:159:VAL:CG1	17:3:160:LEU:H	2.05	0.69
17:3:191:GLU:O	17:3:192:LYS:HE2	1.91	0.69
1:A:44:ILE:O	1:A:45:ALA:C	2.36	0.69
1:A:575:LEU:CD1	1:A:576:GLY:CA	2.57	0.69
19:A:9022:CLA:H151	21:B:6017:BCR:C19	2.22	0.69
2:B:127:ILE:O	2:B:127:ILE:HG13	1.93	0.69
19:B:1223:CLA:H41	19:B:1223:CLA:H72	1.74	0.69
3:C:10:THR:CG2	5:E:101:TYR:CD2	2.71	0.69
4:D:80:SER:CB	4:D:127:ASN:H	2.06	0.69
7:G:89:LYS:NZ	7:G:89:LYS:N	2.41	0.69
14:R:34:UNK:C	14:R:38:UNK:CB	2.71	0.69
15:1:170:PRO:O	15:1:173:TYR:HE2	1.73	0.69
19:1:1013:CLA:HAA2	19:1:1013:CLA:CGD	2.22	0.69
16:2:215:LYS:O	16:2:215:LYS:HG2	1.92	0.69
22:3:7005:LMU:H32	22:3:7005:LMU:H1'	1.73	0.69
18:4:103:MET:HG2	18:4:211:MET:HE3	1.75	0.69
1:A:209:GLY:CA	1:A:213:LEU:HD13	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLY:CA	19:A:1151:CLA:CMC	2.71	0.69
1:A:443:ILE:HG21	1:A:558:LYS:HB2	1.75	0.69
1:A:453:LEU:HD13	1:A:547:PHE:HA	1.73	0.69
19:A:1115:CLA:H2A	19:A:1115:CLA:HED3	0.74	0.69
3:C:44:ARG:HE	4:D:182:GLN:NE2	1.90	0.69
6:F:173:TRP:HE3	6:F:210:GLY:C	2.01	0.69
10:J:31:ARG:HA	10:J:34:PRO:HA	1.75	0.69
12:L:82:TYR:O	12:L:82:TYR:CG	2.46	0.69
13:N:157:LYS:HB3	13:N:158:ASP:C	2.17	0.69
15:1:84:LEU:O	15:1:88:ARG:CG	2.38	0.69
15:1:133:THR:C	15:1:135:PRO:CD	2.66	0.69
15:1:178:LYS:CG	15:1:179:LYS:N	2.55	0.69
16:2:131:ILE:O	16:2:131:ILE:CG2	2.41	0.69
19:2:2014:CLA:H152	19:2:2014:CLA:H91	1.75	0.69
19:3:3011:CLA:HBC1	19:3:3012:CLA:CHA	2.22	0.69
18:4:90:TRP:CD1	18:4:91:PHE:H	2.11	0.69
18:4:153:GLU:OE2	19:4:4012:CLA:CHC	2.41	0.69
20:A:5001:PQN:H241	20:A:5001:PQN:H272	1.76	0.68
2:B:262:HIS:ND1	2:B:265:THR:OG1	2.26	0.68
2:B:530:THR:HG21	19:B:1222:CLA:HAC1	1.74	0.68
2:B:535:VAL:O	2:B:539:LEU:CD2	2.41	0.68
2:B:545:LYS:CD	2:B:546:LEU:N	2.50	0.68
2:B:654:HIS:CE1	19:B:9010:CLA:NB	2.60	0.68
5:E:127:GLU:HB3	5:E:128:VAL:C	2.18	0.68
8:H:119:ASP:CB	8:H:121:LEU:HG	2.22	0.68
15:1:66:PRO:CD	15:1:67:LEU:N	2.56	0.68
17:3:93:ILE:CD1	17:3:95:PRO:O	2.41	0.68
17:3:104:ILE:HG21	19:3:3004:CLA:ND	2.08	0.68
1:A:103:PHE:CE1	19:A:1105:CLA:O1D	2.43	0.68
1:A:120:ALA:N	1:A:145:ILE:HD12	1.97	0.68
1:A:220:ARG:O	1:A:221:HIS:HB2	1.92	0.68
1:A:453:LEU:CD2	19:A:1136:CLA:CBB	2.71	0.68
19:A:9023:CLA:HMC1	19:A:9023:CLA:HBC3	1.74	0.68
2:B:90:ALA:N	2:B:113:VAL:CG1	2.55	0.68
7:G:114:LEU:C	7:G:114:LEU:HD12	2.18	0.68
11:K:127:ILE:HA	11:K:130:LEU:CD1	2.23	0.68
12:L:51:LYS:HB3	12:L:51:LYS:HZ3	1.59	0.68
12:L:112:GLY:N	12:L:113:PRO:HD2	2.08	0.68
12:L:198:ILE:O	12:L:202:PHE:N	2.21	0.68
13:N:157:LYS:CG	13:N:159:LYS:H	2.07	0.68
15:1:158:PRO:HA	15:1:175:LYS:CG	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:162:LYS:HG2	15:1:163:TYR:H	1.59	0.68
16:2:182:ILE:O	16:2:183:PHE:CD1	2.46	0.68
22:4:7033:LMU:H3'	22:4:7033:LMU:C6B	2.23	0.68
1:A:59:ALA:O	1:A:60:ASP:C	2.36	0.68
1:A:258:LEU:O	1:A:259:TYR:CB	2.42	0.68
1:A:508:THR:O	1:A:509:ALA:HB2	1.90	0.68
2:B:620:LEU:HD12	2:B:624:LEU:HD21	1.74	0.68
4:D:163:VAL:C	4:D:164:GLN:HG3	2.18	0.68
6:F:160:PHE:O	6:F:164:GLY:CA	2.40	0.68
8:H:98:LEU:HD21	12:L:143:LEU:CD2	2.24	0.68
12:L:190:PHE:CZ	12:L:194:ILE:CD1	2.77	0.68
19:L:1130:CLA:H2	19:L:1504:CLA:HMB3	1.75	0.68
15:1:135:PRO:HD2	15:1:136:THR:H	1.59	0.68
15:1:171:LEU:HA	15:1:173:TYR:CD2	2.26	0.68
16:2:177:VAL:HG13	16:2:178:ASN:CG	2.17	0.68
16:2:226:ARG:HD3	16:2:230:LEU:CD2	2.23	0.68
17:3:109:ALA:CA	17:3:111:LEU:HD22	2.23	0.68
22:3:7005:LMU:H32	22:3:7005:LMU:C1'	2.22	0.68
18:4:146:PHE:CE1	19:4:4013:CLA:C1C	2.77	0.68
1:A:217:SER:OG	21:A:6002:BCR:C16	2.40	0.68
1:A:249:ILE:N	17:3:137:PHE:HZ	1.91	0.68
1:A:668:TYR:CB	2:B:445:ALA:HB2	2.23	0.68
19:A:1133:CLA:C3D	19:A:1134:CLA:HAC1	2.22	0.68
21:A:6011:BCR:H313	19:A:9013:CLA:H143	1.74	0.68
2:B:120:VAL:C	2:B:123:TRP:HD1	2.00	0.68
2:B:314:ARG:HH12	15:1:67:LEU:HD11	1.59	0.68
2:B:469:LYS:NZ	2:B:471:THR:O	2.27	0.68
4:D:186:GLN:C	4:D:187:ASN:ND2	2.50	0.68
5:E:103:VAL:CG1	5:E:120:TYR:O	2.42	0.68
7:G:64:ILE:HG13	7:G:68:THR:HG23	1.74	0.68
11:K:55:LEU:O	11:K:58:VAL:HG12	1.94	0.68
13:N:139:LYS:CA	13:N:142:LYS:NZ	2.51	0.68
13:N:147:SER:CA	13:N:149:ASP:HB2	2.23	0.68
15:1:95:PRO:C	15:1:98:LEU:HB2	2.17	0.68
17:3:206:PRO:HG2	17:3:208:PHE:CZ	2.28	0.68
1:A:57:LEU:HD23	1:A:58:HIS:N	2.08	0.68
2:B:475:ASP:CA	2:B:480:SER:HA	2.23	0.68
19:B:1209:CLA:CMC	21:B:6005:BCR:H373	2.24	0.68
19:B:1215:CLA:CGA	19:B:1215:CLA:H3A	2.23	0.68
4:D:124:GLU:OE1	4:D:125:GLY:CA	2.41	0.68
8:H:114:ALA:O	8:H:115:THR:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:11:LEU:HG	21:I:6021:BCR:C7	2.23	0.68
11:K:47:ASP:OD2	11:K:48:PHE:N	2.27	0.68
12:L:161:ALA:N	12:L:162:PRO:HD2	2.07	0.68
13:N:139:LYS:CG	13:N:142:LYS:CE	2.71	0.68
16:2:131:ILE:O	16:2:132:LEU:CD1	2.41	0.68
16:2:171:ILE:HD11	16:2:173:ASN:HD21	1.59	0.68
16:2:184:PRO:HD2	16:2:185:ASN:O	1.93	0.68
16:2:240:ILE:HG22	16:2:263:PHE:HB3	1.72	0.68
18:4:154:ILE:O	18:4:158:GLN:HG2	1.93	0.68
19:4:4006:CLA:CMA	22:4:7034:LMU:H62	2.23	0.68
1:A:193:LEU:CA	1:A:196:PHE:HE2	2.03	0.68
2:B:22:TRP:NE1	19:B:1238:CLA:CBB	2.47	0.68
2:B:633:ASN:OD1	2:B:633:ASN:O	2.11	0.68
3:C:17:CYS:CB	3:C:58:CYS:SG	2.74	0.68
3:C:66:ARG:CG	3:C:66:ARG:NH2	2.49	0.68
16:2:167:ARG:HE	16:2:168:TRP:N	1.90	0.68
16:2:182:ILE:O	16:2:183:PHE:CG	2.47	0.68
17:3:154:ASN:O	17:3:155:TYR:CG	2.46	0.68
18:4:145:GLU:CG	18:4:146:PHE:HD1	2.03	0.68
1:A:110:LEU:O	1:A:113:PRO:HD3	1.94	0.68
1:A:532:ILE:HD13	19:A:1135:CLA:HMD1	1.76	0.68
22:A:7016:LMU:O6'	22:A:7016:LMU:H51	1.94	0.68
2:B:266:GLN:O	2:B:267:SER:CB	2.41	0.68
2:B:666:SER:HB3	2:B:671:TRP:NE1	2.05	0.68
19:B:1226:CLA:H62	24:B:7101:LMG:H182	1.75	0.68
3:C:52:LYS:NZ	3:C:64:SER:HB3	2.08	0.68
6:F:200:VAL:CG1	10:J:7:TYR:CA	2.71	0.68
22:H:7011:LMU:O6'	22:H:7011:LMU:H1B	1.93	0.68
11:K:79:LYS:O	11:K:80:ALA:HB3	1.91	0.68
12:L:150:ILE:C	12:L:150:ILE:CD1	2.63	0.68
16:2:165:GLY:C	16:2:167:ARG:HG2	2.19	0.68
18:4:202:GLU:O	18:4:205:ILE:CG1	2.40	0.68
1:A:281:LEU:CD1	1:A:282:THR:H	2.07	0.68
1:A:464:ASN:HD22	1:A:464:ASN:H	1.41	0.68
19:A:1125:CLA:H143	19:A:1125:CLA:H101	1.74	0.68
22:A:7023:LMU:H91	22:A:7023:LMU:C2	2.24	0.68
2:B:82:PHE:O	2:B:84:VAL:N	2.22	0.68
2:B:98:GLN:O	2:B:100:ALA:CA	2.42	0.68
2:B:444:LEU:CD2	2:B:452:GLN:NE2	2.56	0.68
3:C:12:ILE:HG22	3:C:38:GLN:O	1.93	0.68
3:C:44:ARG:NH2	4:D:181:ARG:CB	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:92:ALA:O	6:F:95:GLU:HB2	1.94	0.68
7:G:86:ASN:O	7:G:89:LYS:NZ	2.26	0.68
8:H:89:ALA:O	8:H:92:THR:N	2.27	0.68
19:H:1145:CLA:HBC2	19:H:1145:CLA:CMC	2.21	0.68
12:L:69:LEU:O	12:L:71:THR:HG23	1.94	0.68
16:2:160:ILE:O	16:2:161:GLY:C	2.34	0.68
17:3:111:LEU:CG	17:3:112:GLY:N	2.19	0.68
18:4:194:PHE:O	18:4:195:ALA:HB3	1.91	0.68
1:A:63:ASP:HA	19:A:1128:CLA:HED2	1.76	0.68
1:A:71:LEU:HD12	1:A:71:LEU:C	2.18	0.68
1:A:490:GLN:HG3	1:A:490:GLN:O	1.93	0.68
1:A:728:VAL:HG22	1:A:731:ARG:NH1	2.09	0.68
2:B:57:ILE:HD13	21:B:6005:BCR:H321	1.76	0.68
2:B:190:TRP:HE3	19:B:1211:CLA:CBB	2.06	0.68
2:B:225:LEU:C	2:B:227:THR:O	2.37	0.68
2:B:279:ALA:O	19:B:1213:CLA:HMB2	1.94	0.68
3:C:43:PRO:HD2	3:C:43:PRO:O	1.94	0.68
8:H:86:THR:O	8:H:88:ALA:C	2.37	0.68
12:L:150:ILE:HD12	12:L:151:SER:N	2.08	0.68
15:1:142:PHE:HA	15:1:145:ILE:HD12	1.74	0.68
15:1:177:PRO:HG2	15:1:180:LEU:N	2.09	0.68
16:2:184:PRO:N	16:2:187:LYS:HG2	2.09	0.68
16:2:263:PHE:CG	16:2:263:PHE:O	2.47	0.68
19:2:2014:CLA:H152	19:2:2014:CLA:C9	2.24	0.68
17:3:215:LYS:HB2	17:3:216:ASP:HA	1.75	0.68
1:A:545:HIS:CG	19:A:1135:CLA:CBB	2.69	0.68
1:A:628:ILE:HD12	1:A:629:ASN:N	2.09	0.68
19:A:1126:CLA:H102	21:A:6011:BCR:H372	1.76	0.68
2:B:476:ILE:HG23	2:B:476:ILE:O	1.93	0.68
5:E:78:ARG:HH12	5:E:125:ILE:CB	2.07	0.68
6:F:204:SER:C	6:F:207:LEU:HD12	2.19	0.68
7:G:76:ARG:NH1	7:G:120:VAL:HB	2.08	0.68
19:H:1145:CLA:C2	19:H:1145:CLA:CMA	2.71	0.68
15:1:73:PRO:CD	15:1:74:ALA:H	2.07	0.68
15:1:140:ILE:HD13	15:1:140:ILE:N	2.09	0.68
18:4:86:GLU:CD	18:4:86:GLU:H	1.98	0.68
18:4:141:LEU:HD22	18:4:141:LEU:N	2.01	0.68
1:A:75:SER:HB3	1:A:354:TRP:CZ2	2.29	0.67
1:A:445:HIS:O	1:A:446:LEU:CB	2.42	0.67
1:A:553:VAL:H	1:A:556:LEU:HD12	1.59	0.67
1:A:555:ILE:CD1	19:A:9023:CLA:CMD	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1124:CLA:HED3	19:A:1125:CLA:HMD2	1.75	0.67
2:B:104:PHE:O	2:B:105:THR:OG1	2.09	0.67
2:B:334:LEU:HB2	19:B:1202:CLA:HMD3	1.75	0.67
2:B:353:TYR:C	2:B:355:LEU:H	2.02	0.67
19:B:1203:CLA:H71	24:B:7101:LMG:H381	1.76	0.67
22:D:7050:LMU:O2B	22:D:7050:LMU:H5B	1.92	0.67
15:1:137:ILE:CG2	19:1:1013:CLA:HBB2	2.22	0.67
16:2:122:ILE:O	16:2:126:LEU:CG	2.40	0.67
16:2:166:ARG:CA	16:2:167:ARG:CB	2.70	0.67
16:2:167:ARG:HA	16:2:167:ARG:HE	1.55	0.67
16:2:174:PRO:HD2	16:2:189:THR:OG1	1.94	0.67
16:2:184:PRO:HD3	16:2:187:LYS:HD2	1.75	0.67
17:3:161:GLU:CD	17:3:161:GLU:C	2.61	0.67
18:4:100:ARG:O	18:4:104:LEU:CD1	2.42	0.67
18:4:172:PHE:O	18:4:173:LYS:HB2	1.94	0.67
18:4:198:LEU:HG	18:4:199:GLU:H	1.58	0.67
1:A:21:LEU:N	1:A:22:VAL:CB	2.57	0.67
1:A:249:ILE:CG1	1:A:250:LEU:N	2.52	0.67
1:A:304:LEU:HG	19:A:1115:CLA:CAB	2.24	0.67
1:A:684:PHE:HD2	1:A:685:VAL:N	1.93	0.67
2:B:69:ALA:CB	2:B:135:LEU:CD1	2.71	0.67
2:B:310:PRO:HG2	2:B:311:PRO:HD3	1.75	0.67
19:B:1202:CLA:H151	19:B:1202:CLA:OBD	1.94	0.67
3:C:7:ILE:O	3:C:8:TYR:C	2.36	0.67
5:E:101:TYR:HA	5:E:121:ALA:HB2	1.76	0.67
13:N:99:LYS:HB3	13:N:102:ASN:ND2	2.09	0.67
14:R:26:UNK:O	14:R:27:UNK:C	2.42	0.67
15:1:75:ASN:O	15:1:76:LEU:C	2.34	0.67
15:1:145:ILE:HA	15:1:148:VAL:HG12	1.76	0.67
15:1:189:LYS:CB	19:1:1007:CLA:HMC1	2.12	0.67
16:2:164:GLU:OE2	19:2:2012:CLA:NB	2.26	0.67
18:4:124:PRO:HB2	18:4:126:TRP:N	2.07	0.67
18:4:173:LYS:CA	18:4:194:PHE:HD2	2.08	0.67
1:A:720:THR:O	1:A:720:THR:HG22	1.95	0.67
19:A:1126:CLA:H111	21:J:6012:BCR:H353	1.74	0.67
2:B:176:ASN:ND2	2:B:291:TYR:O	2.27	0.67
2:B:294:ASN:HD21	7:G:94:GLN:HA	1.57	0.67
2:B:424:TRP:CZ2	19:B:1228:CLA:HAC1	2.29	0.67
21:B:6020:BCR:H23C	21:B:6020:BCR:H383	1.75	0.67
4:D:114:MET:HG3	4:D:115:PRO:CA	2.23	0.67
5:E:122:LEU:O	5:E:125:ILE:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:7011:LMU:C7	22:H:7011:LMU:H111	2.23	0.67
9:I:12:VAL:O	9:I:17:PRO:CD	2.41	0.67
19:J:1308:CLA:H92	19:2:2014:CLA:O2D	1.93	0.67
12:L:92:ALA:H	12:L:98:ARG:HH12	1.22	0.67
13:N:139:LYS:CE	13:N:142:LYS:NZ	2.57	0.67
22:N:7049:LMU:C1	22:N:7049:LMU:C6	2.71	0.67
15:1:129:VAL:CB	15:1:130:PRO:HD3	2.24	0.67
15:1:225:TRP:HB3	15:1:226:HIS:HA	1.73	0.67
17:3:238:ILE:HA	17:3:241:TYR:CE1	2.30	0.67
19:3:3016:CLA:HBC3	19:3:3016:CLA:CMC	2.25	0.67
18:4:173:LYS:HZ3	18:4:201:LYS:CG	1.98	0.67
1:A:408:VAL:HG21	1:A:602:LEU:HG	1.76	0.67
1:A:455:PHE:HD1	19:A:1131:CLA:HMA3	1.60	0.67
1:A:536:THR:HA	1:A:539:PHE:HB2	1.76	0.67
2:B:85:ARG:HH11	2:B:85:ARG:CG	2.05	0.67
2:B:233:TYR:O	2:B:253:ALA:HB1	1.94	0.67
2:B:625:TRP:C	2:B:625:TRP:CD2	2.71	0.67
5:E:85:LYS:O	5:E:86:GLY:C	2.37	0.67
5:E:107:PHE:CD2	5:E:109:LYS:HE3	2.28	0.67
15:1:68:GLY:O	15:1:72:VAL:CB	2.40	0.67
15:1:151:GLN:NE2	15:1:151:GLN:CA	2.57	0.67
15:1:201:PHE:O	15:1:204:GLN:HB2	1.95	0.67
16:2:100:ARG:O	16:2:102:ASN:N	2.26	0.67
16:2:226:ARG:HH11	16:2:226:ARG:CG	2.08	0.67
18:4:121:ILE:CG1	18:4:122:ASN:N	2.57	0.67
22:4:7053:LMU:H1B	22:4:7053:LMU:C6'	2.17	0.67
1:A:207:LEU:HA	1:A:211:LEU:CG	2.25	0.67
1:A:251:ASN:OD1	17:3:137:PHE:HD1	1.55	0.67
1:A:304:LEU:CG	19:A:1115:CLA:CBB	2.72	0.67
1:A:373:ALA:O	1:A:396:PHE:CD1	2.48	0.67
1:A:534:LEU:HD12	1:A:534:LEU:C	2.17	0.67
19:A:1112:CLA:HMC2	21:A:6002:BCR:C16	2.24	0.67
2:B:175:LEU:HD21	19:B:1216:CLA:HMA1	1.74	0.67
2:B:411:MET:CE	19:B:1220:CLA:CMC	2.72	0.67
2:B:538:ALA:O	2:B:539:LEU:C	2.38	0.67
6:F:103:GLN:OE1	6:F:103:GLN:CA	2.42	0.67
6:F:170:ILE:HG22	21:F:6014:BCR:H372	1.76	0.67
7:G:62:LEU:O	7:G:65:SER:HB3	1.94	0.67
11:K:56:ILE:HA	11:K:59:THR:HG23	1.76	0.67
14:R:26:UNK:O	14:R:28:UNK:N	2.27	0.67
15:1:73:PRO:CG	15:1:74:ALA:H	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:93:ALA:CB	19:1:1006:CLA:HHC	2.09	0.67
21:1:6023:BCR:C8	21:1:6023:BCR:HC21	2.23	0.67
16:2:211:PRO:O	16:2:212:GLN:CB	2.41	0.67
22:2:7027:LMU:O2'	22:2:7027:LMU:H12	1.95	0.67
17:3:135:ALA:C	17:3:139:THR:OG1	2.38	0.67
19:3:2009:CLA:HBD	19:3:2009:CLA:CBA	2.22	0.67
1:A:336:GLY:C	1:A:339:THR:OG1	2.36	0.67
19:A:1124:CLA:HMA1	19:A:1125:CLA:O1A	1.95	0.67
2:B:292:ARG:NH2	2:B:297:ILE:HG13	2.10	0.67
2:B:324:ASP:O	2:B:328:ASN:HB2	1.94	0.67
2:B:542:ARG:HH21	4:D:197:PRO:HG3	1.59	0.67
19:B:1223:CLA:H71	21:B:6010:BCR:H14C	1.76	0.67
7:G:114:LEU:HD12	7:G:115:LYS:N	2.09	0.67
8:H:113:SER:OG	19:H:1207:CLA:H52	1.92	0.67
10:J:26:LEU:C	10:J:26:LEU:HD23	2.20	0.67
19:J:1308:CLA:HMA1	19:J:1308:CLA:C2	2.25	0.67
15:1:85:ILE:CG1	15:1:88:ARG:CZ	2.69	0.67
16:2:103:VAL:HG12	16:2:104:GLN:OE1	1.94	0.67
18:4:121:ILE:HG13	18:4:122:ASN:N	2.07	0.67
18:4:175:TYR:HB2	18:4:195:ALA:N	2.09	0.67
19:4:4015:CLA:HBA1	19:4:4015:CLA:CBD	2.25	0.67
1:A:87:SER:O	1:A:88:ILE:HB	1.94	0.67
1:A:193:LEU:O	1:A:196:PHE:CD2	2.48	0.67
1:A:207:LEU:HB3	19:A:1119:CLA:HBB2	1.76	0.67
22:A:7016:LMU:C2	22:A:7016:LMU:C6	2.72	0.67
2:B:29:HIS:CD2	19:B:1202:CLA:CBB	2.77	0.67
2:B:73:ASN:H	2:B:73:ASN:ND2	1.90	0.67
4:D:103:THR:CG2	4:D:128:LEU:HD12	2.23	0.67
5:E:83:TRP:HH2	5:E:116:SER:CB	2.07	0.67
7:G:68:THR:HB	7:G:128:LEU:HG	1.77	0.67
8:H:86:THR:HG22	8:H:87:PHE:C	2.19	0.67
15:1:199:VAL:CG1	15:1:200:GLY:N	2.56	0.67
17:3:96:ARG:N	17:3:99:ALA:H	1.93	0.67
17:3:150:TYR:C	17:3:152:ALA:H	2.01	0.67
18:4:83:GLU:HB3	18:4:84:ASP:OD1	1.94	0.67
18:4:205:ILE:HD12	19:4:4004:CLA:CHA	2.25	0.67
1:A:224:HIS:O	1:A:225:VAL:HG22	1.95	0.67
1:A:331:LEU:HD23	1:A:331:LEU:C	2.17	0.67
1:A:334:HIS:ND1	1:A:334:HIS:N	2.41	0.67
1:A:503:THR:HB	19:A:1134:CLA:HBA1	1.75	0.67
2:B:292:ARG:NH1	2:B:296:GLY:N	2.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:GLY:O	2:B:407:VAL:HG13	1.95	0.67
19:1:1008:CLA:CGD	19:1:1008:CLA:HAA2	2.25	0.67
17:3:162:MET:HE1	19:3:3010:CLA:C3D	2.24	0.67
1:A:40:PHE:N	1:A:44:ILE:HG23	2.10	0.67
1:A:104:SER:C	1:A:106:TYR:H	2.02	0.67
1:A:127:VAL:CG2	1:A:128:GLY:H	2.03	0.67
1:A:150:PHE:C	1:A:151:GLN:HG3	2.19	0.67
19:A:9012:CLA:HMB3	19:B:9010:CLA:H18	1.77	0.67
2:B:273:VAL:O	2:B:277:HIS:HD2	1.78	0.67
19:B:1235:CLA:CBC	6:F:160:PHE:CZ	2.77	0.67
3:C:52:LYS:C	3:C:54:CYS:H	2.03	0.67
5:E:125:ILE:O	5:E:125:ILE:CG1	2.30	0.67
6:F:101:LYS:C	6:F:103:GLN:N	2.46	0.67
12:L:110:LEU:HA	12:L:113:PRO:CG	2.25	0.67
13:N:91:TYR:C	13:N:93:GLU:N	2.50	0.67
13:N:139:LYS:CD	13:N:142:LYS:NZ	2.55	0.67
15:1:182:GLU:O	15:1:183:LEU:HB2	1.93	0.67
15:1:193:LEU:C	15:1:193:LEU:CD2	2.68	0.67
19:1:1001:CLA:HBC3	19:1:1001:CLA:HMC1	1.76	0.67
19:1:1007:CLA:H122	19:1:1007:CLA:H61	1.77	0.67
16:2:126:LEU:O	16:2:128:LYS:N	2.27	0.67
17:3:191:GLU:O	17:3:192:LYS:HD2	1.95	0.67
18:4:167:ASN:HD21	19:4:4014:CLA:C2	2.08	0.67
1:A:21:LEU:HD12	1:A:21:LEU:C	2.20	0.67
1:A:79:PHE:CE1	19:A:1111:CLA:CED	2.78	0.67
2:B:92:TRP:O	2:B:92:TRP:CD1	2.48	0.67
2:B:353:TYR:HB2	2:B:594:TRP:HH2	1.60	0.67
2:B:501:ILE:HG13	2:B:502:ASN:N	2.09	0.67
19:B:1211:CLA:HMB1	21:B:6006:BCR:C8	2.25	0.67
19:B:1222:CLA:CBB	19:B:1236:CLA:CMB	2.73	0.67
3:C:52:LYS:CE	3:C:64:SER:HB3	2.24	0.67
4:D:102:ILE:O	4:D:102:ILE:CG2	2.43	0.67
7:G:139:TYR:CG	7:G:139:TYR:O	2.45	0.67
19:H:1207:CLA:CHD	21:I:6018:BCR:H342	2.25	0.67
13:N:139:LYS:O	13:N:142:LYS:CD	2.43	0.67
13:N:143:VAL:HG12	13:N:144:PRO:HD3	1.77	0.67
16:2:212:GLN:HG2	16:2:213:LYS:N	2.07	0.67
16:2:226:ARG:CD	16:2:230:LEU:HD22	2.25	0.67
17:3:154:ASN:HA	17:3:155:TYR:CE2	2.29	0.67
17:3:204:GLY:HA3	17:3:207:PHE:C	2.20	0.67
1:A:64:PHE:CD2	1:A:74:ILE:HD13	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:PHE:O	1:A:593:SER:OG	2.13	0.66
1:A:711:HIS:NE2	19:A:1139:CLA:HAC1	2.10	0.66
2:B:75:GLU:HB2	2:B:132:ASN:HB3	1.76	0.66
2:B:638:LEU:O	2:B:639:VAL:CG1	2.40	0.66
3:C:52:LYS:HZ1	3:C:64:SER:HB3	1.59	0.66
8:H:58:LEU:CB	8:H:61:THR:HG21	2.08	0.66
8:H:61:THR:CA	8:H:62:THR:CG2	2.24	0.66
15:1:128:PRO:CG	15:1:131:TRP:CH2	2.75	0.66
15:1:170:PRO:HG2	15:1:171:LEU:N	2.09	0.66
16:2:128:LYS:O	16:2:129:LEU:C	2.37	0.66
16:2:182:ILE:CG2	16:2:187:LYS:CG	2.65	0.66
17:3:108:PHE:CB	19:3:3013:CLA:H42	2.24	0.66
17:3:197:SER:HB3	17:3:206:PRO:CD	2.21	0.66
18:4:98:ASN:HB3	18:4:212:LEU:HD21	1.77	0.66
18:4:232:LEU:CB	18:4:236:ILE:CD1	2.72	0.66
1:A:149:PHE:HB3	1:A:153:TRP:CE3	2.31	0.66
1:A:451:ILE:HD11	19:A:1131:CLA:HED1	1.78	0.66
19:A:1102:CLA:H2A	19:A:1102:CLA:CED	2.25	0.66
21:A:6003:BCR:C40	21:A:6003:BCR:C23	2.73	0.66
2:B:310:PRO:HB2	2:B:311:PRO:CD	2.12	0.66
2:B:315:LEU:HD11	2:B:317:ARG:HG2	1.72	0.66
2:B:576:PHE:CE2	19:B:1226:CLA:HAC1	2.29	0.66
19:B:1239:CLA:HED1	24:B:7101:LMG:C21	2.25	0.66
3:C:61:ASP:OD2	5:E:118:ASN:ND2	2.26	0.66
4:D:102:ILE:O	4:D:102:ILE:HG23	1.93	0.66
5:E:122:LEU:O	5:E:122:LEU:HD12	1.95	0.66
6:F:188:GLU:OE2	16:2:180:ASP:OD1	2.13	0.66
7:G:84:ARG:CG	7:G:85:GLU:HB3	2.26	0.66
8:H:109:LEU:HD23	19:H:1207:CLA:H72	1.77	0.66
11:K:56:ILE:O	11:K:59:THR:HG23	1.95	0.66
11:K:99:ALA:O	11:K:103:LEU:HD12	1.95	0.66
15:1:58:ALA:HB3	15:1:59:PRO:CD	2.25	0.66
16:2:182:ILE:CA	16:2:187:LYS:HG3	2.25	0.66
16:2:237:PHE:O	16:2:237:PHE:HD1	1.77	0.66
19:2:2014:CLA:H41	19:2:2014:CLA:H93	1.75	0.66
2:B:139:ALA:O	2:B:140:ILE:C	2.36	0.66
2:B:455:ILE:HD13	6:F:148:LEU:HD21	1.77	0.66
2:B:691:ILE:O	2:B:691:ILE:CG2	2.43	0.66
4:D:86:SER:HA	12:L:69:LEU:HD21	1.78	0.66
4:D:142:THR:O	4:D:143:ARG:C	2.38	0.66
8:H:121:LEU:CB	8:H:122:PRO:HD2	2.05	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ASP:HA	11:K:51:SER:CB	2.25	0.66
13:N:168:TRP:HE3	13:N:168:TRP:O	1.78	0.66
16:2:104:GLN:H	16:2:104:GLN:CD	2.02	0.66
19:4:4006:CLA:C10	19:4:4006:CLA:H41	2.25	0.66
1:A:308:ILE:HG23	19:A:1115:CLA:H111	1.77	0.66
19:A:1138:CLA:H191	6:F:181:TYR:CB	2.19	0.66
19:A:1140:CLA:NC	19:A:1140:CLA:H43	2.11	0.66
2:B:80:ASP:OD1	2:B:80:ASP:O	2.14	0.66
2:B:202:SER:C	2:B:204:GLY:H	2.03	0.66
2:B:231:ASN:O	2:B:233:TYR:N	2.28	0.66
2:B:459:PHE:HB2	19:B:1235:CLA:CBD	2.26	0.66
19:B:1227:CLA:HMA2	19:B:1228:CLA:O2A	1.95	0.66
3:C:73:THR:CG2	3:C:76:SER:CB	2.74	0.66
4:D:167:HIS:NE2	4:D:172:VAL:CB	2.57	0.66
5:E:82:TYR:CZ	5:E:111:ASN:HA	2.30	0.66
5:E:82:TYR:CB	5:E:83:TRP:CE3	2.74	0.66
5:E:90:VAL:O	5:E:91:VAL:HG23	1.94	0.66
6:F:103:GLN:O	6:F:104:ALA:C	2.30	0.66
6:F:130:PHE:HB3	6:F:132:ASN:ND2	2.09	0.66
11:K:52:PRO:CD	11:K:53:THR:N	2.51	0.66
12:L:70:GLU:CG	12:L:74:THR:HG21	2.24	0.66
16:2:97:GLU:HG2	16:2:97:GLU:O	1.96	0.66
16:2:166:ARG:NH2	19:2:4009:CLA:O1D	2.29	0.66
17:3:96:ARG:NH1	17:3:100:TYR:CE2	2.63	0.66
17:3:130:GLN:CA	17:3:132:THR:H	2.08	0.66
1:A:296:LEU:C	1:A:296:LEU:CD1	2.69	0.66
22:A:7010:LMU:C6'	22:K:7047:LMU:H111	2.25	0.66
2:B:67:HIS:O	2:B:88:ALA:O	2.14	0.66
2:B:120:VAL:O	2:B:123:TRP:N	2.28	0.66
2:B:317:ARG:NE	2:B:317:ARG:CA	2.55	0.66
2:B:469:LYS:CB	2:B:470:THR:OG1	2.43	0.66
19:B:1217:CLA:H2	19:B:1217:CLA:NB	2.09	0.66
11:K:47:ASP:CA	11:K:51:SER:CB	2.73	0.66
13:N:151:ASP:O	13:N:152:LEU:HG	1.96	0.66
1:A:207:LEU:HD11	1:A:314:GLY:HA2	1.78	0.66
1:A:214:GLY:O	1:A:215:SER:HB3	1.94	0.66
19:A:1124:CLA:C5	19:A:1125:CLA:HED1	2.25	0.66
19:A:1138:CLA:CBC	21:F:6014:BCR:H332	2.25	0.66
2:B:123:TRP:CA	2:B:126:THR:HG21	2.18	0.66
2:B:175:LEU:O	2:B:179:LEU:HG	1.96	0.66
5:E:79:LYS:CE	5:E:84:TYR:OH	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:202:LEU:O	6:F:203:ALA:HB3	1.94	0.66
7:G:145:THR:CG2	7:G:146:SER:N	2.57	0.66
19:J:1311:CLA:CHA	19:J:1311:CLA:CED	2.74	0.66
11:K:63:LEU:HB3	11:K:102:THR:OG1	1.95	0.66
12:L:201:TYR:O	12:L:202:PHE:C	2.37	0.66
13:N:147:SER:C	13:N:149:ASP:HB2	2.21	0.66
17:3:100:TYR:CB	17:3:229:LYS:HE2	2.24	0.66
17:3:110:MET:O	17:3:114:VAL:N	2.29	0.66
18:4:169:ASP:OD1	18:4:174:GLN:CB	2.43	0.66
18:4:243:THR:HG23	18:4:244:ILE:C	2.20	0.66
1:A:109:TRP:HA	1:A:116:ILE:HG13	1.77	0.66
1:A:377:TYR:CD1	1:A:616:PHE:HE1	2.14	0.66
19:A:1129:CLA:HMB2	19:L:1130:CLA:C1D	2.26	0.66
2:B:117:TYR:HE2	2:B:366:THR:HG21	1.60	0.66
2:B:131:THR:HG22	2:B:134:ASP:CA	2.26	0.66
2:B:211:ASN:HB2	2:B:214:ASP:HB3	1.75	0.66
2:B:310:PRO:O	19:B:1301:CLA:C1D	2.44	0.66
2:B:508:LEU:CB	2:B:509:PHE:HD2	2.08	0.66
4:D:140:LEU:HD22	4:D:144:LEU:CD1	2.26	0.66
6:F:101:LYS:O	6:F:102:LEU:C	2.38	0.66
7:G:76:ARG:NH2	7:G:117:ASN:C	2.54	0.66
8:H:78:PRO:CB	19:L:1501:CLA:HMD3	2.26	0.66
9:I:14:LEU:C	9:I:17:PRO:HD2	2.20	0.66
11:K:111:VAL:HA	11:K:114:HIS:CG	2.30	0.66
12:L:142:SER:O	12:L:143:LEU:CD2	2.43	0.66
12:L:204:LEU:HD13	12:L:205:TYR:C	2.19	0.66
15:1:77:GLU:CA	15:1:80:LYS:HD2	2.25	0.66
15:1:219:THR:O	15:1:220:HIS:HB3	1.95	0.66
18:4:126:TRP:CG	18:4:127:TYR:N	2.63	0.66
18:4:143:VAL:HG12	18:4:144:ILE:N	2.11	0.66
18:4:209:ARG:HB2	19:4:4004:CLA:C3A	2.26	0.66
1:A:150:PHE:N	1:A:153:TRP:CE3	2.62	0.66
1:A:203:LEU:HD21	19:A:1123:CLA:C3D	2.26	0.66
1:A:488:PHE:CD2	1:A:533:PRO:HB2	2.31	0.66
1:A:710:ALA:CB	19:A:1138:CLA:HED2	2.26	0.66
2:B:638:LEU:C	2:B:639:VAL:HG12	2.21	0.66
4:D:148:TYR:O	4:D:149:LYS:CG	2.44	0.66
6:F:110:ALA:HA	6:F:113:SER:HB2	1.78	0.66
7:G:131:GLY:O	7:G:136:VAL:CB	2.42	0.66
8:H:67:SER:C	8:H:68:TYR:CD2	2.74	0.66
9:I:9:VAL:HG12	9:I:10:PRO:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:153:PHE:CB	12:L:155:GLU:OE1	2.38	0.66
13:N:91:TYR:O	13:N:93:GLU:N	2.27	0.66
15:1:162:LYS:CA	15:1:164:PRO:HG3	2.26	0.66
16:2:269:LYS:CE	16:2:269:LYS:CA	2.73	0.66
17:3:98:LEU:O	17:3:99:ALA:C	2.39	0.66
19:3:3017:CLA:HMA1	19:3:3017:CLA:O1A	1.95	0.66
18:4:115:PHE:O	18:4:116:THR:C	2.38	0.66
18:4:175:TYR:HB3	18:4:194:PHE:HD1	1.54	0.66
18:4:223:VAL:O	18:4:223:VAL:CG1	2.38	0.66
1:A:358:LEU:HD11	1:A:413:HIS:CB	2.26	0.66
1:A:396:PHE:CE2	1:A:616:PHE:CG	2.84	0.66
1:A:483:GLN:CB	1:A:485:GLN:NE2	2.56	0.66
1:A:532:ILE:O	1:A:533:PRO:C	2.34	0.66
1:A:606:TYR:O	1:A:610:SER:CB	2.44	0.66
1:A:678:PHE:O	1:A:680:LEU:N	2.28	0.66
1:A:715:LYS:CE	6:F:230:ASN:OD1	2.44	0.66
19:A:1125:CLA:CBB	19:A:1133:CLA:C3A	2.70	0.66
19:A:1139:CLA:CGA	19:A:1139:CLA:H42	2.25	0.66
19:A:1140:CLA:C14	21:A:6011:BCR:HC21	2.25	0.66
22:A:7023:LMU:H2B	22:A:7023:LMU:C6B	2.24	0.66
2:B:123:TRP:HA	2:B:126:THR:HB	1.58	0.66
2:B:212:PHE:HE1	19:B:1211:CLA:HMD3	1.61	0.66
2:B:633:ASN:CG	2:B:636:THR:HB	2.19	0.66
3:C:31:TRP:O	3:C:33:GLY:N	2.29	0.66
4:D:185:GLY:O	4:D:186:GLN:CB	2.43	0.66
6:F:149:ILE:O	6:F:150:VAL:HG12	1.96	0.66
11:K:69:ARG:HG3	11:K:73:ALA:HB2	1.77	0.66
11:K:127:ILE:O	11:K:130:LEU:CG	2.44	0.66
13:N:148:ASP:N	13:N:149:ASP:C	2.53	0.66
1:A:112:ASP:O	1:A:115:HIS:CD2	2.49	0.66
1:A:733:VAL:O	1:A:733:VAL:CG1	2.44	0.66
2:B:305:LEU:CD2	19:B:1220:CLA:O1D	2.45	0.66
3:C:12:ILE:HG21	3:C:27:GLU:OE1	1.96	0.66
4:D:80:SER:HG	4:D:126:PRO:CD	1.98	0.66
7:G:102:ALA:CA	7:G:104:ASP:OD1	2.39	0.66
22:H:7017:LMU:O3'	22:H:7017:LMU:H1B	1.96	0.66
12:L:92:ALA:N	12:L:98:ARG:NH2	2.41	0.66
16:2:237:PHE:CE1	16:2:241:TYR:CE1	2.79	0.66
19:2:4009:CLA:H151	19:2:4009:CLA:H8	1.75	0.66
1:A:328:LYS:HZ2	1:A:345:GLY:HA3	1.60	0.65
1:A:342:GLY:O	1:A:343:HIS:C	2.39	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:CG1	19:A:1127:CLA:HBB2	2.26	0.65
1:A:492:ILE:CD1	19:A:1133:CLA:HMC2	2.15	0.65
19:A:1106:CLA:HBB2	19:A:1107:CLA:C3D	2.26	0.65
2:B:79:GLN:O	2:B:80:ASP:CB	2.43	0.65
19:B:1205:CLA:CBB	19:B:1205:CLA:C9	2.73	0.65
4:D:140:LEU:CD1	4:D:141:GLY:H	1.82	0.65
6:F:181:TYR:HB2	6:F:203:ALA:HB2	1.78	0.65
22:F:7036:LMU:C6'	22:F:7036:LMU:O2B	2.45	0.65
7:G:125:VAL:O	7:G:129:ALA:N	2.29	0.65
19:H:1145:CLA:HMC3	19:H:1145:CLA:CBC	2.25	0.65
12:L:205:TYR:H	12:L:205:TYR:HD2	1.40	0.65
12:L:209:LEU:O	12:L:210:PRO:C	2.38	0.65
13:N:148:ASP:H	13:N:149:ASP:CB	2.08	0.65
15:1:66:PRO:O	15:1:69:LEU:O	2.14	0.65
19:1:1006:CLA:CAC	19:1:1010:CLA:CMB	2.73	0.65
19:4:1304:CLA:H151	19:4:1304:CLA:H202	1.77	0.65
19:A:1131:CLA:O1A	19:A:1237:CLA:H11	1.96	0.65
19:A:9022:CLA:H13	19:B:1206:CLA:CBB	2.26	0.65
2:B:58:PHE:HB2	2:B:146:SER:HB2	1.78	0.65
2:B:120:VAL:O	2:B:123:TRP:HD1	1.79	0.65
2:B:476:ILE:HG23	2:B:479:SER:OG	1.94	0.65
3:C:73:THR:CB	3:C:76:SER:OG	2.43	0.65
4:D:99:PHE:HB3	4:D:157:VAL:CB	2.25	0.65
8:H:64:GLN:CB	8:H:67:SER:H	2.09	0.65
8:H:85:GLU:CG	8:H:86:THR:H	1.98	0.65
11:K:127:ILE:O	11:K:129:ALA:HA	1.94	0.65
15:1:86:HIS:CD2	15:1:86:HIS:H	2.01	0.65
16:2:115:LEU:HD21	19:2:2011:CLA:NB	2.12	0.65
16:2:183:PHE:N	16:2:187:LYS:CG	2.53	0.65
18:4:142:PHE:HA	18:4:145:GLU:CD	2.20	0.65
18:4:158:GLN:CD	19:4:1004:CLA:O1D	2.37	0.65
6:F:172:GLY:O	6:F:176:TRP:HB2	1.96	0.65
8:H:58:LEU:CD1	8:H:61:THR:HA	2.26	0.65
11:K:89:ARG:NH1	11:K:89:ARG:CG	2.58	0.65
12:L:141:LEU:HD12	12:L:145:LEU:CD1	2.24	0.65
15:1:79:TYR:CB	19:1:1012:CLA:OBD	2.44	0.65
15:1:183:LEU:C	15:1:184:LYS:CG	2.69	0.65
18:4:211:MET:SD	19:4:4002:CLA:HBB1	2.36	0.65
22:4:7034:LMU:C11	22:4:7052:LMU:C2'	2.72	0.65
1:A:94:SER:OG	19:A:1105:CLA:HMC1	1.97	0.65
1:A:107:GLU:CD	1:A:161:GLU:HG3	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:O	1:A:386:ALA:CB	2.43	0.65
1:A:711:HIS:CE1	19:A:1139:CLA:HAC1	2.31	0.65
19:A:1126:CLA:H43	19:A:1126:CLA:CBA	2.25	0.65
19:A:9012:CLA:C1	2:B:616:LEU:HD12	2.14	0.65
2:B:27:THR:O	2:B:28:ALA:C	2.39	0.65
2:B:230:TRP:O	2:B:231:ASN:C	2.39	0.65
2:B:292:ARG:NH2	2:B:297:ILE:CG1	2.60	0.65
2:B:320:LYS:O	2:B:406:ASN:ND2	2.18	0.65
19:B:1214:CLA:H52	19:B:1223:CLA:HMB1	1.79	0.65
7:G:89:LYS:O	7:G:90:GLN:HG2	1.95	0.65
8:H:81:SER:O	8:H:82:LYS:C	2.37	0.65
8:H:119:ASP:HB3	8:H:121:LEU:HG	1.78	0.65
19:1:1303:CLA:HMC2	19:4:1304:CLA:HMB2	1.79	0.65
18:4:245:VAL:HG22	18:4:246:GLN:N	2.10	0.65
1:A:90:PHE:CD1	19:A:1103:CLA:H91	2.31	0.65
1:A:250:LEU:HD12	17:3:136:TRP:HZ2	1.61	0.65
1:A:660:GLN:O	1:A:661:ALA:CB	2.43	0.65
2:B:69:ALA:HB2	2:B:135:LEU:CD1	2.27	0.65
2:B:615:TYR:N	2:B:615:TYR:CD1	2.62	0.65
2:B:645:VAL:HG22	19:B:1206:CLA:HHD	1.77	0.65
19:B:1219:CLA:H72	19:B:1219:CLA:CBB	2.24	0.65
3:C:55:GLU:O	3:C:57:ALA:N	2.20	0.65
4:D:95:GLN:NE2	4:D:96:VAL:CA	2.52	0.65
7:G:128:LEU:C	7:G:128:LEU:CD2	2.70	0.65
13:N:110:THR:CG2	13:N:111:GLY:H	2.10	0.65
15:1:91:MET:O	15:1:91:MET:SD	2.55	0.65
17:3:254:GLN:CG	17:3:255:ASN:H	2.06	0.65
1:A:40:PHE:N	1:A:44:ILE:CG2	2.59	0.65
1:A:101:ALA:HB2	1:A:164:LEU:HB2	1.77	0.65
1:A:525:ASN:ND2	1:A:526:LYS:HE3	2.12	0.65
1:A:747:TRP:CE3	21:A:6011:BCR:H401	2.31	0.65
1:A:755:ILE:O	1:A:756:ALA:HB3	1.95	0.65
2:B:5:ILE:CG2	2:B:6:PRO:CD	2.62	0.65
2:B:98:GLN:N	2:B:99:PRO:HD2	2.11	0.65
2:B:444:LEU:HD21	2:B:452:GLN:HE22	1.61	0.65
2:B:469:LYS:NZ	2:B:471:THR:C	2.55	0.65
2:B:479:SER:O	2:B:480:SER:HB3	1.96	0.65
3:C:73:THR:CG2	3:C:76:SER:HB3	2.26	0.65
11:K:87:GLU:O	11:K:87:GLU:OE1	2.15	0.65
13:N:152:LEU:CB	13:N:153:GLU:HG3	2.27	0.65
13:N:169:LYS:CB	13:N:170:TRP:CD1	2.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:150:HIS:CE1	15:1:151:GLN:NE2	2.65	0.65
16:2:152:LEU:HD22	16:2:152:LEU:C	2.21	0.65
17:3:204:GLY:C	17:3:206:PRO:C	2.65	0.65
19:3:3017:CLA:HBC3	19:3:3017:CLA:CMC	2.24	0.65
18:4:90:TRP:C	18:4:91:PHE:CD1	2.74	0.65
18:4:169:ASP:O	18:4:173:LYS:CA	2.45	0.65
1:A:327:ILE:O	1:A:328:LYS:C	2.37	0.65
1:A:356:ALA:HB2	1:A:417:PHE:HD2	1.61	0.65
1:A:425:THR:OG1	1:A:428:TYR:CE1	2.49	0.65
1:A:586:ARG:CG	3:C:49:VAL:HG21	2.24	0.65
1:A:588:GLY:H	2:B:668:ARG:NH1	1.95	0.65
1:A:740:LEU:CD2	19:A:1140:CLA:CMA	2.75	0.65
2:B:65:LEU:HD22	2:B:124:TRP:CE3	2.31	0.65
2:B:171:ALA:O	2:B:172:GLU:HB2	1.97	0.65
3:C:26:LEU:H	3:C:43:PRO:CG	2.08	0.65
3:C:55:GLU:C	3:C:57:ALA:N	2.50	0.65
4:D:140:LEU:CD1	4:D:144:LEU:H	2.10	0.65
5:E:127:GLU:CD	5:E:129:GLU:O	2.40	0.65
7:G:69:GLY:CA	7:G:72:LEU:HG	2.26	0.65
7:G:89:LYS:NZ	7:G:89:LYS:H	1.95	0.65
14:R:36:UNK:O	14:R:38:UNK:N	2.30	0.65
15:1:170:PRO:HG2	15:1:171:LEU:C	2.22	0.65
15:1:208:TYR:N	15:1:209:PRO:CD	2.59	0.65
16:2:156:GLU:O	16:2:160:ILE:HD13	1.96	0.65
17:3:96:ARG:CA	17:3:99:ALA:N	2.51	0.65
18:4:158:GLN:HA	19:4:1004:CLA:H2A	1.78	0.65
1:A:105:ASN:OD1	1:A:119:SER:N	2.28	0.65
1:A:331:LEU:CD2	1:A:331:LEU:C	2.69	0.65
1:A:692:PHE:CZ	19:A:1140:CLA:HBC3	2.32	0.65
19:A:1115:CLA:H191	11:K:64:MET:CE	2.26	0.65
21:A:6011:BCR:H313	19:A:9013:CLA:H142	1.79	0.65
2:B:127:ILE:O	2:B:127:ILE:HD12	1.97	0.65
2:B:159:PRO:O	2:B:160:LYS:C	2.38	0.65
2:B:280:ILE:HD13	19:B:1215:CLA:HBB2	1.79	0.65
2:B:394:PHE:O	2:B:542:ARG:CD	2.45	0.65
2:B:583:MET:HE2	2:B:583:MET:O	1.96	0.65
19:B:1210:CLA:H151	19:B:1225:CLA:HMD1	1.78	0.65
19:B:1220:CLA:C4	19:B:1220:CLA:C1A	2.65	0.65
6:F:139:LEU:CD1	6:F:149:ILE:CD1	2.71	0.65
22:F:7036:LMU:H72	22:F:7036:LMU:C11	2.27	0.65
8:H:98:LEU:CD2	12:L:146:THR:CG2	2.71	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:1502:CLA:HAC1	21:L:6019:BCR:H322	1.78	0.65
15:1:176:ASP:HB3	15:1:180:LEU:CG	2.24	0.65
17:3:112:GLY:HA2	17:3:115:GLY:O	1.97	0.65
17:3:136:TRP:O	17:3:139:THR:N	2.29	0.65
22:3:7005:LMU:H51	22:3:7005:LMU:O1'	1.97	0.65
18:4:149:SER:HB2	18:4:153:GLU:OE1	1.95	0.65
18:4:174:GLN:C	18:4:176:SER:N	2.49	0.65
1:A:246:HIS:O	1:A:248:PHE:N	2.25	0.65
1:A:479:ASP:CG	1:A:536:THR:CG2	2.70	0.65
1:A:707:ILE:C	1:A:711:HIS:HD2	2.05	0.65
19:A:1131:CLA:C16	21:L:6019:BCR:C36	2.75	0.65
19:A:1139:CLA:H43	6:F:198:ILE:HD13	1.78	0.65
2:B:196:HIS:CE1	19:B:1212:CLA:HED2	2.32	0.65
2:B:299:HIS:CE1	19:B:1219:CLA:HMD1	2.31	0.65
2:B:312:GLY:CA	2:B:315:LEU:HB2	2.24	0.65
21:B:6020:BCR:H333	19:L:1502:CLA:C1C	2.26	0.65
5:E:111:ASN:ND2	5:E:112:TYR:N	2.45	0.65
11:K:128:GLY:N	11:K:129:ALA:CA	2.55	0.65
22:N:7049:LMU:H12	22:N:7049:LMU:C6	2.12	0.65
15:1:64:PHE:C	15:1:69:LEU:CD1	2.70	0.65
15:1:65:ASP:OD2	15:1:66:PRO:N	2.29	0.65
16:2:152:LEU:CD1	16:2:153:PHE:N	2.55	0.65
16:2:258:GLY:O	16:2:259:HIS:ND1	2.29	0.65
17:3:210:PRO:HD2	17:3:211:LEU:H	1.62	0.65
17:3:245:GLY:C	17:3:246:LEU:HD22	2.22	0.65
19:3:3011:CLA:HBC2	19:3:3012:CLA:CHA	2.26	0.65
18:4:174:GLN:C	18:4:176:SER:H	2.03	0.65
22:4:7009:LMU:H3'	22:4:7009:LMU:C5B	2.27	0.65
1:A:281:LEU:O	1:A:282:THR:C	2.38	0.65
2:B:123:TRP:HB2	2:B:126:THR:CG2	2.26	0.65
2:B:361:ILE:CG2	2:B:368:GLN:OE1	2.44	0.65
2:B:456:GLU:HA	2:B:514:PRO:CD	2.27	0.65
19:B:1235:CLA:H152	21:F:6016:BCR:H313	1.76	0.65
5:E:121:ALA:O	5:E:125:ILE:HG21	1.97	0.65
7:G:62:LEU:O	7:G:65:SER:CB	2.44	0.65
9:I:24:LEU:C	9:I:26:LEU:N	2.51	0.65
11:K:75:SER:O	11:K:76:ALA:HB3	1.97	0.65
15:1:150:HIS:C	15:1:150:HIS:ND1	2.53	0.65
16:2:152:LEU:HD22	16:2:153:PHE:N	2.12	0.65
17:3:177:ALA:O	17:3:178:LYS:CB	2.45	0.65
18:4:112:PRO:HA	18:4:117:SER:OG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LYS:HD2	1:A:332:GLU:CB	2.19	0.64
1:A:467:MET:HA	1:A:470:LEU:HB2	1.79	0.64
19:A:1102:CLA:HBA2	19:A:1109:CLA:H62	1.79	0.64
19:A:1120:CLA:H2A	19:A:1120:CLA:O1D	1.97	0.64
19:A:1133:CLA:O1A	19:A:1134:CLA:HBC3	1.97	0.64
19:A:9011:CLA:HMB2	19:A:9012:CLA:CAD	2.27	0.64
2:B:4:ARG:C	2:B:4:ARG:NE	2.55	0.64
2:B:292:ARG:NH2	2:B:297:ILE:O	2.30	0.64
2:B:444:LEU:O	2:B:445:ALA:HB3	1.97	0.64
7:G:99:HIS:C	7:G:101:GLU:CB	2.68	0.64
10:J:18:TRP:CH2	10:J:22:LEU:HD22	2.32	0.64
19:K:1143:CLA:HAC2	22:K:7001:LMU:H3O1	1.60	0.64
12:L:71:THR:HB	12:L:72:PRO:HD2	1.78	0.64
12:L:174:ASP:OD2	12:L:175:GLN:N	2.29	0.64
15:1:58:ALA:HB1	19:1:1015:CLA:C3B	2.27	0.64
15:1:170:PRO:HG2	15:1:173:TYR:CE2	2.32	0.64
19:1:1014:CLA:CHD	19:1:1014:CLA:CBC	2.72	0.64
16:2:133:ASN:HD22	16:2:134:THR:HB	0.92	0.64
1:A:43:THR:HG22	1:A:46:LYS:NZ	2.11	0.64
1:A:96:MET:HE1	19:A:1106:CLA:CED	2.26	0.64
1:A:96:MET:HE1	19:A:1106:CLA:HED2	1.78	0.64
1:A:207:LEU:CD1	1:A:314:GLY:CA	2.75	0.64
1:A:223:VAL:HG23	1:A:227:LEU:HD12	0.79	0.64
1:A:274:TRP:CG	1:A:277:TYR:O	2.49	0.64
1:A:370:ILE:CD1	19:A:1124:CLA:CAD	2.74	0.64
19:A:1133:CLA:CAD	19:A:1134:CLA:HAC1	2.27	0.64
21:A:6011:BCR:H323	21:J:6012:BCR:H391	1.77	0.64
2:B:188:LEU:O	2:B:191:ALA:N	2.30	0.64
2:B:298:GLY:HA2	19:B:1218:CLA:HMD2	1.78	0.64
2:B:558:PRO:CG	2:B:703:VAL:CG2	2.62	0.64
2:B:607:SER:O	2:B:610:ASN:HB2	1.96	0.64
19:B:1227:CLA:HAA1	19:B:1227:CLA:HED2	1.80	0.64
4:D:102:ILE:HG13	4:D:153:GLN:O	1.97	0.64
6:F:117:LEU:HA	6:F:119:ILE:HG12	1.78	0.64
19:R:1150:CLA:H92	22:R:7007:LMU:O4'	1.97	0.64
15:1:78:ARG:HH21	15:1:179:LYS:HD3	1.55	0.64
19:2:2014:CLA:H41	19:2:2014:CLA:C8	2.26	0.64
18:4:161:LYS:HD2	18:4:161:LYS:C	2.22	0.64
1:A:204:ASN:O	1:A:205:HIS:CB	2.45	0.64
1:A:266:ALA:O	1:A:267:THR:C	2.37	0.64
1:A:281:LEU:HD12	1:A:282:THR:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLN:O	1:A:377:TYR:HD2	1.81	0.64
1:A:382:TYR:CE2	19:A:1127:CLA:HED3	2.33	0.64
1:A:555:ILE:CG1	19:A:9023:CLA:OBD	2.45	0.64
1:A:618:TRP:O	1:A:622:SER:HB3	1.98	0.64
1:A:705:GLU:HA	1:A:708:VAL:HB	1.80	0.64
1:A:705:GLU:CB	2:B:545:LYS:HZ2	2.10	0.64
19:A:1132:CLA:C4	12:L:110:LEU:HD23	2.27	0.64
2:B:362:ALA:O	2:B:363:GLN:CB	2.46	0.64
2:B:561:GLY:HA3	3:C:52:LYS:CG	2.25	0.64
19:B:1220:CLA:CMC	19:B:1220:CLA:CBC	2.74	0.64
19:B:1235:CLA:CBC	6:F:160:PHE:HZ	2.10	0.64
8:H:58:LEU:CD1	8:H:61:THR:CB	2.52	0.64
11:K:115:ILE:HG12	11:K:122:LEU:CD1	2.27	0.64
13:N:114:PHE:CE2	13:N:116:ARG:HD2	2.33	0.64
14:R:38:UNK:C	14:R:39:UNK:O	2.45	0.64
16:2:184:PRO:HD3	16:2:187:LYS:HB2	1.71	0.64
22:3:7003:LMU:H3B	22:3:7005:LMU:C6B	2.19	0.64
1:A:52:THR:OG1	1:A:53:TRP:CE3	2.50	0.64
1:A:113:PRO:O	1:A:114:THR:CG2	2.35	0.64
1:A:296:LEU:CD1	1:A:297:THR:HG22	2.22	0.64
1:A:336:GLY:CA	19:A:1151:CLA:HMC1	2.27	0.64
1:A:392:GLN:HA	1:A:395:LEU:HD23	1.78	0.64
1:A:393:LEU:HG	1:A:394:SER:H	1.62	0.64
19:A:1107:CLA:HBB2	19:B:1230:CLA:HMD1	1.79	0.64
3:C:63:LEU:CD2	3:C:65:VAL:N	2.59	0.64
6:F:97:GLN:NE2	6:F:98:ALA:N	2.45	0.64
7:G:61:ALA:O	7:G:63:VAL:HG13	1.97	0.64
19:K:1142:CLA:HED1	19:K:1143:CLA:HMB1	1.77	0.64
12:L:104:LEU:HD21	12:L:199:TRP:CZ2	2.29	0.64
13:N:139:LYS:CD	13:N:142:LYS:HE2	2.28	0.64
13:N:150:LEU:H	13:N:150:LEU:HD22	1.63	0.64
19:2:2001:CLA:CGA	19:2:2001:CLA:C4	2.74	0.64
17:3:150:TYR:CB	17:3:151:TRP:NE1	2.48	0.64
1:A:40:PHE:H	1:A:44:ILE:HG23	1.62	0.64
1:A:174:PHE:CE2	19:A:1103:CLA:H152	2.31	0.64
1:A:302:HIS:HB2	19:A:1116:CLA:CHB	2.27	0.64
2:B:622:ASP:HB3	2:B:626:LEU:CG	2.27	0.64
19:B:1212:CLA:O2D	19:B:1212:CLA:OBD	2.11	0.64
4:D:77:ASN:HB3	4:D:79:PRO:CD	2.27	0.64
12:L:209:LEU:CD1	12:L:210:PRO:CD	2.59	0.64
15:1:81:GLU:C	15:1:83:GLU:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:93:ALA:HA	19:1:1006:CLA:C4B	2.28	0.64
15:1:223:ASP:OD1	18:4:140:THR:CG2	2.46	0.64
17:3:111:LEU:O	17:3:114:VAL:CB	2.45	0.64
18:4:111:LEU:CD1	18:4:112:PRO:HG3	2.26	0.64
1:A:60:ASP:CG	1:A:60:ASP:O	2.40	0.64
1:A:360:ILE:HD11	19:A:1123:CLA:HMB2	1.79	0.64
1:A:554:LEU:CD2	19:A:9023:CLA:O2D	2.46	0.64
2:B:294:ASN:CG	7:G:94:GLN:CG	2.57	0.64
2:B:310:PRO:HG2	2:B:311:PRO:CD	2.27	0.64
2:B:549:ASP:CG	3:C:63:LEU:HB2	2.22	0.64
21:B:6020:BCR:H23C	21:B:6020:BCR:C38	2.28	0.64
3:C:26:LEU:CD2	4:D:181:ARG:NH1	2.61	0.64
3:C:52:LYS:C	3:C:54:CYS:N	2.54	0.64
3:C:67:VAL:HG13	3:C:68:TYR:N	2.09	0.64
4:D:112:PHE:C	4:D:112:PHE:CD2	2.75	0.64
19:F:1302:CLA:HHB	21:F:6016:BCR:H333	1.79	0.64
8:H:79:LEU:O	8:H:80:GLN:C	2.40	0.64
11:K:62:SER:OG	11:K:63:LEU:CD1	2.42	0.64
11:K:63:LEU:N	11:K:63:LEU:CD1	2.45	0.64
13:N:110:THR:HG22	13:N:111:GLY:N	2.12	0.64
1:A:76:ARG:HH12	1:A:193:LEU:HD22	1.62	0.64
2:B:469:LYS:NZ	2:B:471:THR:N	2.46	0.64
3:C:63:LEU:HD23	3:C:65:VAL:N	2.13	0.64
4:D:93:LYS:NZ	4:D:97:GLU:OE2	2.30	0.64
4:D:98:GLU:CB	4:D:100:TYR:HE2	2.11	0.64
6:F:214:PRO:O	6:F:215:VAL:CB	2.45	0.64
11:K:59:THR:O	11:K:63:LEU:CD1	2.46	0.64
12:L:83:LEU:O	12:L:83:LEU:CD1	2.46	0.64
12:L:210:PRO:HB2	12:L:211:TYR:CD2	2.33	0.64
16:2:184:PRO:HG2	16:2:185:ASN:N	2.12	0.64
16:2:211:PRO:HD2	16:2:212:GLN:N	2.12	0.64
16:2:256:ASP:N	16:2:256:ASP:OD1	2.29	0.64
17:3:135:ALA:HB3	17:3:139:THR:HB	1.77	0.64
17:3:154:ASN:C	17:3:155:TYR:CG	2.75	0.64
18:4:158:GLN:NE2	19:4:1004:CLA:CHA	2.44	0.64
1:A:57:LEU:HD23	1:A:57:LEU:O	1.98	0.64
1:A:62:HIS:ND1	19:A:1128:CLA:HBA1	2.12	0.64
1:A:92:TRP:O	1:A:93:LEU:HB3	1.97	0.64
1:A:338:PHE:CD1	19:A:1151:CLA:HBB2	2.33	0.64
1:A:349:ILE:O	1:A:350:LEU:C	2.39	0.64
1:A:378:SER:O	1:A:379:MET:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ALA:CB	1:A:510:SER:OG	2.45	0.64
19:A:1112:CLA:HMB2	21:A:6002:BCR:C38	2.28	0.64
22:A:7045:LMU:O5B	22:A:7045:LMU:H5'	1.97	0.64
19:A:9013:CLA:H93	2:B:431:PHE:CD1	2.33	0.64
19:A:9023:CLA:HHB	19:A:9023:CLA:C4	2.27	0.64
2:B:3:LEU:CD1	9:I:29:GLU:OE1	2.44	0.64
2:B:73:ASN:O	2:B:121:TYR:HE1	1.79	0.64
2:B:202:SER:O	2:B:245:GLY:HA2	1.98	0.64
2:B:280:ILE:HA	2:B:283:LEU:HD12	1.79	0.64
2:B:293:THR:CG2	7:G:94:GLN:CG	2.72	0.64
2:B:295:PHE:CD2	2:B:295:PHE:N	2.59	0.64
2:B:683:GLU:OE2	2:B:693:TRP:HH2	1.80	0.64
2:B:692:ARG:HH22	2:B:694:ARG:HH22	1.44	0.64
4:D:103:THR:CG2	4:D:128:LEU:CG	2.75	0.64
4:D:141:GLY:O	4:D:142:THR:C	2.39	0.64
15:1:143:LEU:N	15:1:143:LEU:HD12	2.13	0.64
18:4:202:GLU:O	18:4:205:ILE:CD1	2.45	0.64
1:A:261:SER:O	1:A:262:PHE:CG	2.51	0.64
1:A:345:GLY:O	1:A:347:TYR:N	2.23	0.64
1:A:401:TRP:CD1	19:A:1126:CLA:CHC	2.80	0.64
1:A:636:HIS:O	1:A:637:ILE:C	2.41	0.64
22:A:7016:LMU:C7	22:A:7016:LMU:H112	2.28	0.64
2:B:232:LEU:HD11	2:B:235:GLN:CB	2.27	0.64
2:B:418:ILE:O	2:B:422:LEU:HD12	1.97	0.64
2:B:510:LEU:HD22	2:B:597:LYS:HD2	1.79	0.64
8:H:97:LEU:HD13	8:H:100:PHE:CB	2.28	0.64
13:N:133:GLY:HA3	13:N:134:CYS:C	2.21	0.64
14:R:27:UNK:O	14:R:29:UNK:N	2.31	0.64
15:1:77:GLU:CD	15:1:80:LYS:HZ1	2.05	0.64
15:1:224:PRO:HA	15:1:225:TRP:CB	2.26	0.64
19:2:2007:CLA:CAC	19:3:2009:CLA:HED1	2.09	0.64
17:3:176:TRP:O	17:3:178:LYS:CG	2.45	0.64
18:4:112:PRO:HB3	18:4:116:THR:O	1.98	0.64
19:4:1304:CLA:CGD	19:4:1304:CLA:C2A	2.75	0.64
1:A:40:PHE:C	1:A:41:SER:O	2.41	0.64
1:A:130:GLU:OE1	1:A:130:GLU:CA	2.45	0.64
1:A:430:ASP:OD1	1:A:433:ASP:OD2	2.15	0.64
19:A:1117:CLA:H203	19:A:1125:CLA:HAA1	1.80	0.64
2:B:388:ALA:C	2:B:391:PRO:CD	2.69	0.64
2:B:453:ILE:O	2:B:453:ILE:CG2	2.41	0.64
2:B:476:ILE:HG22	2:B:479:SER:OG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:69:GLY:C	7:G:72:LEU:HG	2.23	0.64
8:H:120:ILE:O	8:H:120:ILE:CG1	2.40	0.64
12:L:71:THR:HB	12:L:72:PRO:CD	2.27	0.64
12:L:146:THR:O	12:L:148:TYR:N	2.30	0.64
13:N:139:LYS:CA	13:N:142:LYS:HD3	2.27	0.64
16:2:206:TRP:O	16:2:208:SER:N	2.31	0.64
19:3:3011:CLA:H12	19:3:3011:CLA:CMA	2.20	0.64
18:4:87:ASN:O	18:4:90:TRP:HB2	1.98	0.64
19:4:1304:CLA:H203	19:4:1304:CLA:C15	2.23	0.64
1:A:58:HIS:HE1	19:A:1101:CLA:ND	1.97	0.63
1:A:188:LYS:CE	1:A:190:ALA:HA	2.27	0.63
1:A:245:PRO:O	1:A:248:PHE:CE2	2.51	0.63
1:A:451:ILE:HD11	19:A:1131:CLA:CED	2.29	0.63
2:B:178:HIS:C	2:B:180:SER:H	2.04	0.63
2:B:212:PHE:CZ	19:B:1211:CLA:HAC1	2.33	0.63
2:B:622:ASP:CB	2:B:626:LEU:HD11	2.28	0.63
2:B:711:VAL:HG22	24:B:7101:LMG:H391	1.80	0.63
3:C:72:GLU:CD	3:C:77:MET:HE2	2.19	0.63
3:C:73:THR:CB	3:C:76:SER:HG	2.06	0.63
4:D:100:TYR:CZ	4:D:134:LYS:HE3	2.32	0.63
4:D:103:THR:CG2	4:D:128:LEU:CD1	2.76	0.63
4:D:129:LEU:HD13	12:L:65:PHE:CE1	2.33	0.63
4:D:148:TYR:C	4:D:149:LYS:HG2	2.22	0.63
6:F:129:ARG:C	6:F:133:TYR:CE1	2.76	0.63
21:F:6016:BCR:HC8	21:F:6016:BCR:H311	1.79	0.63
13:N:142:LYS:HE3	13:N:142:LYS:CA	2.11	0.63
16:2:131:ILE:O	16:2:132:LEU:HD12	1.98	0.63
16:2:145:TYR:O	16:2:146:PHE:CG	2.51	0.63
16:2:211:PRO:CD	16:2:212:GLN:H	2.09	0.63
17:3:141:VAL:CG2	17:3:142:ILE:HG12	2.16	0.63
18:4:177:LEU:HD22	18:4:177:LEU:C	2.22	0.63
1:A:218:TRP:N	19:A:1112:CLA:HBB2	2.13	0.63
2:B:256:THR:HG1	2:B:258:LEU:H	1.44	0.63
2:B:292:ARG:NH2	2:B:297:ILE:H	1.95	0.63
2:B:454:LEU:HB2	2:B:514:PRO:HB3	1.79	0.63
3:C:73:THR:O	3:C:77:MET:HG2	1.97	0.63
19:F:1305:CLA:C4	19:4:1306:CLA:HAA1	2.23	0.63
12:L:76:SER:O	12:L:77:PRO:C	2.41	0.63
13:N:169:LYS:HB3	13:N:170:TRP:HD1	1.48	0.63
15:1:176:ASP:HB2	15:1:180:LEU:HD12	1.72	0.63
16:2:103:VAL:C	16:2:105:ALA:N	2.53	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:217:LEU:O	16:2:218:ARG:C	2.42	0.63
18:4:158:GLN:NE2	19:4:1004:CLA:C2A	2.61	0.63
18:4:158:GLN:HE22	19:4:1004:CLA:C4D	2.12	0.63
22:4:7053:LMU:H6E	22:4:7053:LMU:H2B	1.79	0.63
1:A:197:GLN:NE2	1:A:351:THR:C	2.57	0.63
2:B:117:TYR:CE2	2:B:366:THR:HG21	2.33	0.63
2:B:224:PRO:C	2:B:227:THR:HB	2.23	0.63
3:C:73:THR:OG1	3:C:76:SER:CB	2.46	0.63
4:D:140:LEU:HD13	4:D:144:LEU:N	2.13	0.63
5:E:74:VAL:CG2	5:E:90:VAL:HG22	2.27	0.63
6:F:180:SER:C	6:F:182:LEU:N	2.56	0.63
6:F:185:ILE:C	6:F:186:ARG:CG	2.71	0.63
22:H:7032:LMU:H31	22:H:7032:LMU:C2B	2.28	0.63
11:K:115:ILE:HG12	11:K:122:LEU:HD13	1.78	0.63
22:K:7042:LMU:H32	22:K:7042:LMU:H6D	1.80	0.63
12:L:153:PHE:N	12:L:153:PHE:HD2	1.92	0.63
22:R:7020:LMU:C5B	22:R:7020:LMU:C6'	2.64	0.63
16:2:163:ALA:O	16:2:167:ARG:HD2	1.98	0.63
16:2:182:ILE:HD13	16:2:187:LYS:O	1.98	0.63
16:2:189:THR:HG23	16:2:193:VAL:O	1.97	0.63
17:3:156:THR:C	17:3:158:PHE:C	2.65	0.63
22:3:7005:LMU:O3'	22:3:7005:LMU:H1B	1.99	0.63
1:A:432:LEU:HA	1:A:435:VAL:HG13	1.81	0.63
1:A:434:ARG:O	1:A:437:ARG:HB2	1.98	0.63
1:A:536:THR:O	1:A:537:ALA:HB3	1.98	0.63
1:A:569:ILE:HB	1:A:572:LYS:HB2	1.80	0.63
1:A:585:GLY:O	1:A:589:THR:OG1	2.17	0.63
1:A:699:TYR:OH	2:B:533:ILE:CG2	2.43	0.63
19:A:1237:CLA:H92	21:L:6019:BCR:H321	1.81	0.63
2:B:616:LEU:O	2:B:619:TRP:HB2	1.98	0.63
4:D:83:PHE:CZ	4:D:114:MET:CE	2.81	0.63
5:E:91:VAL:O	5:E:93:VAL:N	2.31	0.63
7:G:72:LEU:HD22	7:G:124:ILE:CD1	2.02	0.63
7:G:82:PHE:HB2	7:G:83:GLN:HG3	1.79	0.63
9:I:22:ALA:O	9:I:23:SER:C	2.40	0.63
11:K:50:GLY:C	11:K:52:PRO:CD	2.71	0.63
11:K:81:THR:OG1	11:K:82:ALA:N	2.32	0.63
22:K:7042:LMU:O3'	22:K:7042:LMU:H1B	1.96	0.63
12:L:146:THR:C	12:L:148:TYR:H	2.05	0.63
15:1:77:GLU:OE1	15:1:77:GLU:N	2.31	0.63
16:2:183:PHE:C	16:2:183:PHE:CD1	2.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:252:ALA:HB1	16:2:254:LEU:HB2	1.80	0.63
17:3:243:ILE:HD13	19:3:3005:CLA:C1C	2.29	0.63
19:4:4003:CLA:HBC2	19:4:4003:CLA:CMC	2.28	0.63
1:A:42:ARG:NH1	1:A:42:ARG:O	2.32	0.63
1:A:54:ILE:O	1:A:58:HIS:HD2	1.80	0.63
1:A:126:ILE:CD1	19:A:1107:CLA:HMA1	2.16	0.63
1:A:397:THR:OG1	19:A:1126:CLA:HMB1	1.98	0.63
1:A:711:HIS:NE2	19:A:1139:CLA:CAC	2.62	0.63
21:A:6003:BCR:H403	21:A:6003:BCR:H23C	1.80	0.63
2:B:298:GLY:HA2	19:B:1218:CLA:CMD	2.28	0.63
2:B:556:SER:C	2:B:558:PRO:CD	2.71	0.63
4:D:112:PHE:O	4:D:119:ALA:HB1	1.98	0.63
6:F:139:LEU:HD12	6:F:147:HIS:O	1.99	0.63
21:F:6016:BCR:H271	21:F:6016:BCR:H403	1.80	0.63
14:R:7:UNK:O	14:R:10:UNK:CB	2.47	0.63
15:1:201:PHE:HA	15:1:204:GLN:HB2	1.80	0.63
17:3:159:VAL:C	17:3:161:GLU:N	2.56	0.63
1:A:58:HIS:HB3	19:A:1102:CLA:HBC1	1.81	0.63
1:A:159:THR:C	1:A:163:GLN:NE2	2.57	0.63
1:A:197:GLN:NE2	1:A:351:THR:O	2.32	0.63
1:A:281:LEU:HD12	1:A:282:THR:N	2.14	0.63
1:A:368:LEU:HD22	19:A:1117:CLA:H92	1.77	0.63
1:A:582:ASP:HB3	1:A:589:THR:HG22	1.80	0.63
19:A:9023:CLA:HMC1	2:B:661:PHE:HB3	1.80	0.63
2:B:568:CYS:O	2:B:570:ILE:N	2.31	0.63
6:F:191:PRO:HG2	6:F:191:PRO:O	1.99	0.63
7:G:84:ARG:HE	7:G:85:GLU:HB3	1.60	0.63
8:H:94:ARG:O	8:H:95:GLY:O	2.16	0.63
9:I:10:PRO:HA	9:I:14:LEU:HB2	1.80	0.63
11:K:59:THR:O	11:K:63:LEU:HD11	1.98	0.63
11:K:112:VAL:C	11:K:114:HIS:H	2.06	0.63
19:K:1146:CLA:HMD3	22:K:7001:LMU:H52	1.81	0.63
16:2:114:MET:HE3	16:2:114:MET:N	2.14	0.63
19:2:2002:CLA:HBC2	19:2:2002:CLA:CHD	2.23	0.63
17:3:96:ARG:CB	17:3:99:ALA:HB3	2.27	0.63
18:4:161:LYS:C	18:4:161:LYS:CD	2.72	0.63
18:4:175:TYR:HB2	18:4:195:ALA:H	1.63	0.63
1:A:43:THR:HG22	1:A:46:LYS:HZ3	1.63	0.63
1:A:401:TRP:O	1:A:405:PHE:HB2	1.98	0.63
1:A:568:LEU:HG	2:B:676:GLU:OE2	1.98	0.63
1:A:691:MET:HB2	19:A:9013:CLA:C1C	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1140:CLA:H62	19:A:9013:CLA:H193	1.79	0.63
2:B:460:ALA:O	2:B:461:GLN:C	2.42	0.63
2:B:544:SER:O	2:B:547:MET:N	2.32	0.63
6:F:206:LEU:O	6:F:209:ARG:HB2	1.99	0.63
13:N:127:PHE:O	13:N:128:PRO:C	2.42	0.63
19:R:1144:CLA:HED3	19:R:1144:CLA:C4D	2.28	0.63
17:3:131:GLU:O	17:3:134:LEU:N	2.17	0.63
18:4:145:GLU:CG	18:4:146:PHE:CE1	2.78	0.63
1:A:98:PHE:HD1	1:A:99:HIS:H	1.43	0.63
1:A:448:TRP:CD1	19:A:1131:CLA:HED2	2.32	0.63
2:B:21:ILE:O	2:B:24:GLY:N	2.31	0.63
2:B:292:ARG:NE	2:B:297:ILE:O	2.31	0.63
2:B:348:VAL:HA	19:B:1215:CLA:H42	1.79	0.63
2:B:732:LYS:C	2:B:733:PHE:O	2.41	0.63
19:B:1226:CLA:CBC	19:B:1226:CLA:CMC	2.75	0.63
3:C:12:ILE:HD13	3:C:39:ILE:HG13	1.81	0.63
4:D:100:TYR:CD2	4:D:100:TYR:N	2.65	0.63
6:F:129:ARG:C	6:F:133:TYR:HE1	2.07	0.63
22:K:7041:LMU:H6'2	22:K:7042:LMU:H21	1.79	0.63
12:L:210:PRO:O	12:L:211:TYR:CB	2.46	0.63
15:1:225:TRP:CD1	15:1:226:HIS:CE1	2.86	0.63
16:2:233:MET:HA	16:2:236:TRP:HB2	1.80	0.63
18:4:121:ILE:C	18:4:123:VAL:H	2.07	0.63
1:A:370:ILE:HD11	19:A:1124:CLA:C3D	2.29	0.63
19:A:1113:CLA:CED	19:A:1113:CLA:HAA1	2.29	0.63
19:A:1119:CLA:H92	21:A:6007:BCR:H373	0.74	0.63
19:A:1124:CLA:HED2	19:A:1124:CLA:CAA	2.29	0.63
2:B:103:ALA:CA	2:B:105:THR:N	2.61	0.63
2:B:115:ASN:C	2:B:115:ASN:OD1	2.41	0.63
2:B:422:LEU:CD1	2:B:535:VAL:HG11	2.26	0.63
3:C:44:ARG:CB	4:D:182:GLN:NE2	2.51	0.63
4:D:112:PHE:O	4:D:119:ALA:CB	2.47	0.63
5:E:78:ARG:CD	5:E:78:ARG:H	2.11	0.63
7:G:93:GLU:OE2	7:G:98:THR:N	2.31	0.63
8:H:58:LEU:HD11	8:H:62:THR:CG2	1.92	0.63
11:K:70:PHE:CD1	11:K:70:PHE:O	2.51	0.63
12:L:131:SER:N	12:L:201:TYR:CZ	2.58	0.63
21:L:6019:BCR:H403	21:L:6019:BCR:H271	1.79	0.63
14:R:31:UNK:C	14:R:32:UNK:O	2.47	0.63
17:3:202:TYR:HB3	17:3:203:PRO:HD3	1.79	0.63
18:4:133:GLU:O	18:4:134:TYR:CD1	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:157:TRP:HB2	19:4:4012:CLA:CMA	2.29	0.63
18:4:172:PHE:CA	18:4:194:PHE:CE2	2.77	0.63
1:A:364:MET:O	1:A:368:LEU:HB2	1.99	0.62
19:A:1111:CLA:HBA1	19:A:1123:CLA:C4	2.27	0.62
19:A:1134:CLA:H3A	19:A:1141:CLA:CBB	2.19	0.62
2:B:356:PRO:O	2:B:356:PRO:HD2	1.99	0.62
2:B:470:THR:H	2:B:502:ASN:H	1.45	0.62
2:B:598:HIS:HB3	2:B:602:TRP:CZ3	2.34	0.62
2:B:663:PHE:O	2:B:664:LEU:HG	1.99	0.62
19:B:1222:CLA:HBB1	19:B:1236:CLA:CMB	2.29	0.62
19:B:1235:CLA:HHB	19:B:1236:CLA:OBD	1.98	0.62
4:D:158:PHE:CB	4:D:159:PRO:HD2	2.17	0.62
7:G:72:LEU:HD12	7:G:73:PHE:CZ	2.33	0.62
7:G:111:VAL:HG23	7:G:111:VAL:O	1.97	0.62
19:G:1242:CLA:H11	22:G:7026:LMU:H61	1.81	0.62
8:H:94:ARG:HH11	8:H:94:ARG:HB2	1.64	0.62
8:H:111:TYR:C	8:H:112:LEU:CD2	2.70	0.62
12:L:73:VAL:HG12	19:L:1504:CLA:HMA3	1.81	0.62
19:1:1008:CLA:HMA3	19:1:1008:CLA:HBA2	1.80	0.62
19:1:1010:CLA:HHD	19:1:1010:CLA:CBC	2.09	0.62
16:2:128:LYS:CB	16:2:131:ILE:HG23	2.29	0.62
16:2:171:ILE:CG1	16:2:173:ASN:HD21	2.12	0.62
16:2:247:ILE:O	16:2:248:ASP:HB2	1.98	0.62
18:4:90:TRP:O	18:4:91:PHE:CD1	2.52	0.62
1:A:105:ASN:OD1	1:A:118:PRO:CA	2.44	0.62
1:A:381:PRO:CB	19:A:1117:CLA:HAA2	2.29	0.62
1:A:442:ILE:HG23	19:A:1129:CLA:HMC3	1.80	0.62
1:A:681:GLY:HA2	1:A:684:PHE:HB3	1.79	0.62
1:A:723:ARG:HG2	1:A:723:ARG:NH1	2.13	0.62
22:A:7016:LMU:H31	22:A:7016:LMU:C1'	2.29	0.62
2:B:32:GLU:HG2	2:B:42:LEU:HD21	1.81	0.62
2:B:230:TRP:HH2	7:G:67:SER:HB2	1.64	0.62
2:B:459:PHE:HB2	19:B:1235:CLA:HBD	1.80	0.62
2:B:552:ASP:OD1	2:B:553:PHE:CE2	2.52	0.62
2:B:656:VAL:HG22	19:B:1239:CLA:HMB3	1.81	0.62
19:B:1220:CLA:O2D	19:B:1220:CLA:C2A	2.47	0.62
3:C:25:VAL:HA	3:C:43:PRO:HG3	1.80	0.62
6:F:89:LYS:O	6:F:92:ALA:N	2.32	0.62
22:H:7011:LMU:C6'	22:H:7011:LMU:H1B	2.28	0.62
11:K:56:ILE:CA	11:K:59:THR:HG23	2.29	0.62
11:K:127:ILE:O	11:K:130:LEU:CD2	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:86:LEU:HD12	12:L:86:LEU:H	1.64	0.62
13:N:156:GLY:C	13:N:157:LYS:HD2	2.24	0.62
15:1:78:ARG:O	15:1:81:GLU:HG2	1.98	0.62
15:1:138:LEU:HA	15:1:141:GLU:CG	2.29	0.62
16:2:201:PHE:CE1	16:2:202:ASP:HB3	2.34	0.62
1:A:284:ARG:NH1	1:A:284:ARG:C	2.57	0.62
1:A:364:MET:O	1:A:368:LEU:N	2.32	0.62
1:A:389:TYR:CD1	1:A:625:TRP:CG	2.87	0.62
1:A:426:THR:CG2	1:A:428:TYR:HE2	2.04	0.62
19:A:1124:CLA:C6	19:A:1125:CLA:CED	2.77	0.62
2:B:187:SER:O	2:B:188:LEU:C	2.40	0.62
2:B:269:TRP:HA	2:B:269:TRP:CE3	2.34	0.62
2:B:353:TYR:HB2	2:B:594:TRP:CH2	2.33	0.62
2:B:411:MET:CE	19:B:1220:CLA:HMC2	2.30	0.62
2:B:664:LEU:O	2:B:667:TRP:CZ3	2.52	0.62
2:B:691:ILE:O	2:B:691:ILE:HG22	1.98	0.62
3:C:11:CYS:SG	3:C:12:ILE:N	2.72	0.62
5:E:79:LYS:CB	5:E:84:TYR:CE1	2.82	0.62
5:E:103:VAL:CG2	5:E:104:VAL:O	2.47	0.62
6:F:101:LYS:O	6:F:103:GLN:N	2.32	0.62
22:H:7011:LMU:H111	22:H:7011:LMU:H72	1.81	0.62
19:J:1311:CLA:HBC3	19:J:1311:CLA:CHD	2.28	0.62
11:K:47:ASP:O	11:K:48:PHE:HB2	1.99	0.62
13:N:142:LYS:O	13:N:145:PHE:O	2.16	0.62
18:4:87:ASN:ND2	18:4:90:TRP:CE2	2.67	0.62
18:4:146:PHE:HD1	18:4:146:PHE:N	1.97	0.62
18:4:223:VAL:O	18:4:224:THR:HG23	1.99	0.62
1:A:344:LYS:C	1:A:346:LEU:H	2.08	0.62
1:A:443:ILE:HG22	2:B:674:LEU:HD11	1.80	0.62
2:B:488:ALA:HB1	19:B:1233:CLA:C1C	2.29	0.62
6:F:200:VAL:HG11	10:J:7:TYR:CG	2.34	0.62
7:G:84:ARG:CD	7:G:85:GLU:HB3	2.30	0.62
7:G:139:TYR:O	7:G:139:TYR:CD1	2.52	0.62
9:I:9:VAL:CG1	9:I:10:PRO:HD3	2.29	0.62
11:K:98:PRO:HD2	11:K:99:ALA:N	2.06	0.62
13:N:142:LYS:CA	13:N:145:PHE:O	2.47	0.62
15:1:85:ILE:CG1	15:1:88:ARG:NH2	2.62	0.62
16:2:118:ALA:CB	16:2:121:PHE:HE2	2.11	0.62
16:2:137:TRP:O	16:2:139:THR:CG2	2.47	0.62
16:2:174:PRO:HB2	16:2:194:GLY:CA	2.22	0.62
17:3:113:ALA:HB2	17:3:239:LEU:HD12	1.70	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:148:TYR:CG	17:3:148:TYR:O	2.51	0.62
18:4:172:PHE:C	18:4:194:PHE:CE2	2.77	0.62
19:4:1304:CLA:CED	19:4:1304:CLA:CAA	2.66	0.62
1:A:284:ARG:HB2	1:A:295:TRP:HB2	1.80	0.62
1:A:747:TRP:CD2	21:A:6011:BCR:H401	2.34	0.62
2:B:144:PHE:CD2	2:B:144:PHE:O	2.52	0.62
2:B:207:VAL:HG13	2:B:207:VAL:O	1.99	0.62
2:B:550:LYS:O	2:B:550:LYS:CG	2.46	0.62
19:B:1222:CLA:CBB	19:B:1236:CLA:HHB	2.24	0.62
5:E:107:PHE:CE2	5:E:109:LYS:CD	2.82	0.62
6:F:94:ARG:HA	6:F:94:ARG:HE	1.62	0.62
7:G:89:LYS:O	7:G:90:GLN:CB	2.48	0.62
16:2:98:SER:O	16:2:100:ARG:CB	2.47	0.62
17:3:130:GLN:C	17:3:132:THR:N	2.49	0.62
1:A:57:LEU:O	1:A:61:ALA:HB2	1.99	0.62
19:A:1125:CLA:HBA2	21:A:6008:BCR:H12C	1.81	0.62
19:A:1151:CLA:O2D	19:A:1151:CLA:HBA2	2.00	0.62
21:A:6011:BCR:HC31	21:F:6014:BCR:H17C	1.81	0.62
2:B:98:GLN:HA	2:B:98:GLN:NE2	2.14	0.62
2:B:247:THR:N	2:B:250:ALA:HB2	2.15	0.62
2:B:255:LEU:H	2:B:271:THR:CG2	2.13	0.62
2:B:337:ALA:HA	19:B:1221:CLA:HAA1	1.82	0.62
2:B:379:ALA:O	2:B:383:MET:HG2	1.98	0.62
5:E:89:SER:C	5:E:106:ARG:H	2.07	0.62
5:E:107:PHE:CD2	5:E:109:LYS:HD2	2.34	0.62
7:G:84:ARG:HG3	7:G:85:GLU:HB2	1.76	0.62
7:G:100:PHE:CD2	7:G:100:PHE:O	2.53	0.62
8:H:113:SER:CB	19:H:1207:CLA:H2	2.29	0.62
15:1:133:THR:C	15:1:135:PRO:HD2	2.24	0.62
15:1:225:TRP:CB	15:1:226:HIS:HA	2.29	0.62
17:3:130:GLN:CA	17:3:132:THR:N	2.63	0.62
18:4:120:ILE:O	18:4:121:ILE:C	2.43	0.62
18:4:120:ILE:CG1	18:4:226:LYS:HG3	2.17	0.62
1:A:63:ASP:HB2	19:A:1128:CLA:CED	2.28	0.62
1:A:123:VAL:O	1:A:124:TRP:HB2	1.99	0.62
1:A:159:THR:HG22	1:A:160:SER:H	1.64	0.62
1:A:707:ILE:C	1:A:711:HIS:CD2	2.77	0.62
1:A:733:VAL:CG2	19:A:1140:CLA:C3D	2.78	0.62
2:B:295:PHE:HE2	7:G:94:GLN:NE2	1.97	0.62
3:C:74:THR:HG23	3:C:75:ARG:N	2.13	0.62
4:D:140:LEU:CD2	4:D:144:LEU:HD11	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:GLN:OE1	6:F:103:GLN:HA	2.00	0.62
8:H:98:LEU:HG	8:H:98:LEU:O	1.99	0.62
10:J:5:LYS:HD2	16:2:178:ASN:CB	2.30	0.62
11:K:115:ILE:CD1	11:K:122:LEU:HD12	2.29	0.62
19:K:1142:CLA:HED1	19:K:1143:CLA:CMB	2.30	0.62
16:2:186:ASN:O	16:2:187:LYS:HB2	1.99	0.62
17:3:155:TYR:O	17:3:157:LEU:N	2.32	0.62
18:4:209:ARG:O	18:4:212:LEU:C	2.42	0.62
1:A:207:LEU:CD1	1:A:314:GLY:N	2.62	0.62
1:A:246:HIS:C	1:A:248:PHE:HD2	2.05	0.62
1:A:250:LEU:CG	17:3:136:TRP:CZ2	2.83	0.62
1:A:360:ILE:O	1:A:361:ASN:CB	2.47	0.62
1:A:452:PHE:CE1	19:A:1136:CLA:HBB2	2.34	0.62
1:A:485:GLN:N	1:A:485:GLN:OE1	2.32	0.62
19:A:1101:CLA:HBB2	19:A:1102:CLA:NC	2.15	0.62
2:B:686:PRO:HG2	19:L:1130:CLA:H12	1.82	0.62
3:C:14:CYS:SG	3:C:14:CYS:O	2.58	0.62
3:C:20:ALA:O	3:C:21:CYS:CB	2.47	0.62
3:C:31:TRP:CD1	3:C:31:TRP:C	2.78	0.62
3:C:58:CYS:HB3	23:C:8003:SF4:S2	2.40	0.62
4:D:167:HIS:NE2	4:D:172:VAL:HG13	2.02	0.62
4:D:172:VAL:O	4:D:173:TYR:CB	2.48	0.62
15:1:65:ASP:HA	15:1:69:LEU:HD13	1.80	0.62
15:1:77:GLU:C	15:1:80:LYS:HG3	2.23	0.62
16:2:249:ASN:C	16:2:249:ASN:OD1	2.42	0.62
19:2:2004:CLA:O1A	19:3:2009:CLA:CBC	2.48	0.62
17:3:204:GLY:CA	17:3:206:PRO:O	2.48	0.62
1:A:211:LEU:O	1:A:214:GLY:O	2.18	0.62
1:A:224:HIS:CE1	19:A:1113:CLA:C4C	2.83	0.62
1:A:229:ILE:CG2	1:A:229:ILE:O	2.46	0.62
1:A:298:ASP:OD2	1:A:298:ASP:N	2.32	0.62
1:A:351:THR:O	19:A:1123:CLA:H18	1.98	0.62
1:A:497:ALA:HB1	1:A:510:SER:OG	1.99	0.62
1:A:603:PHE:HZ	1:A:693:LEU:CD2	2.13	0.62
1:A:682:ALA:H	1:A:685:VAL:HG23	1.65	0.62
2:B:141:PHE:O	2:B:143:LEU:N	2.33	0.62
2:B:233:TYR:N	2:B:233:TYR:CD2	2.68	0.62
2:B:400:PRO:HD2	4:D:197:PRO:CD	2.29	0.62
2:B:438:VAL:HG23	19:B:1230:CLA:HAC1	1.82	0.62
2:B:710:LEU:C	2:B:712:HIS:N	2.56	0.62
19:B:1203:CLA:H191	19:B:1224:CLA:H141	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:CG	3:C:4:SER:OG	2.42	0.62
3:C:25:VAL:HA	3:C:43:PRO:HG2	1.79	0.62
3:C:39:ILE:HG12	3:C:40:ALA:H	1.65	0.62
19:H:1145:CLA:CMC	19:H:1145:CLA:CBC	2.77	0.62
13:N:110:THR:H	13:N:113:ASN:ND2	1.98	0.62
15:1:190:ASN:ND2	19:1:1002:CLA:ND	2.48	0.62
16:2:156:GLU:HG3	16:2:157:LEU:HD13	1.74	0.62
16:2:266:PHE:CZ	16:2:267:THR:O	2.53	0.62
17:3:110:MET:O	17:3:113:ALA:CB	2.41	0.62
18:4:90:TRP:CD1	18:4:91:PHE:N	2.67	0.62
18:4:201:LYS:H	18:4:201:LYS:CD	2.12	0.62
1:A:93:LEU:N	1:A:96:MET:H	1.98	0.62
1:A:98:PHE:O	1:A:101:ALA:N	2.33	0.62
1:A:373:ALA:HB1	1:A:396:PHE:CD1	2.35	0.62
1:A:399:HIS:O	1:A:400:MET:HB2	2.00	0.62
19:A:1104:CLA:H51	19:A:1128:CLA:C4C	2.30	0.62
19:A:1115:CLA:CED	19:A:1115:CLA:C2A	2.44	0.62
19:A:1117:CLA:C20	19:A:1125:CLA:H3A	2.30	0.62
19:A:9023:CLA:H92	19:B:1239:CLA:HBB2	1.82	0.62
2:B:120:VAL:O	2:B:121:TYR:C	2.41	0.62
2:B:178:HIS:HE1	19:B:1210:CLA:NC	1.97	0.62
2:B:262:HIS:O	2:B:265:THR:O	2.18	0.62
4:D:93:LYS:CG	4:D:96:VAL:CG1	2.74	0.62
22:H:7043:LMU:H62	22:H:7043:LMU:C10	2.28	0.62
19:L:1503:CLA:CBC	19:L:1503:CLA:CHD	2.65	0.62
16:2:95:ASP:OD2	17:3:85:ASP:O	2.13	0.62
17:3:134:LEU:HD12	17:3:134:LEU:H	1.64	0.62
1:A:54:ILE:O	1:A:58:HIS:CD2	2.53	0.61
1:A:96:MET:CE	19:A:1106:CLA:HED2	2.29	0.61
1:A:126:ILE:O	1:A:127:VAL:CG2	2.41	0.61
1:A:227:LEU:HD22	1:A:296:LEU:O	1.99	0.61
1:A:295:TRP:CD1	1:A:295:TRP:H	2.17	0.61
1:A:578:ARG:CB	1:A:578:ARG:NH1	2.63	0.61
2:B:449:PRO:O	2:B:452:GLN:HB2	2.00	0.61
2:B:557:PHE:CD1	2:B:571:SER:HB3	2.34	0.61
2:B:663:PHE:O	2:B:664:LEU:HB2	1.99	0.61
2:B:685:THR:OG1	19:L:1130:CLA:C3A	2.47	0.61
19:B:1235:CLA:H202	21:F:6016:BCR:HC41	1.82	0.61
3:C:44:ARG:NE	4:D:182:GLN:HE21	1.97	0.61
6:F:203:ALA:HB1	6:F:206:LEU:HD12	1.80	0.61
19:L:1503:CLA:HAA1	19:L:1503:CLA:O1D	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:170:PRO:HD2	15:1:173:TYR:HD2	1.56	0.61
16:2:168:TRP:O	16:2:169:ALA:C	2.43	0.61
17:3:151:TRP:HD1	17:3:151:TRP:N	1.93	0.61
22:4:7033:LMU:H3'	22:4:7033:LMU:H6'2	1.82	0.61
1:A:188:LYS:O	1:A:190:ALA:CB	2.43	0.61
1:A:193:LEU:O	1:A:196:PHE:CE2	2.52	0.61
1:A:261:SER:C	1:A:263:ALA:H	2.08	0.61
1:A:389:TYR:CE1	1:A:625:TRP:CG	2.87	0.61
1:A:459:GLY:O	1:A:462:ILE:HG22	2.00	0.61
1:A:701:GLN:O	1:A:704:ILE:N	2.33	0.61
19:A:1117:CLA:OBD	19:A:1127:CLA:H43	2.01	0.61
19:A:1131:CLA:C16	21:L:6019:BCR:H361	2.29	0.61
4:D:141:GLY:H	4:D:144:LEU:N	1.86	0.61
5:E:107:PHE:HD2	5:E:109:LYS:HD2	1.65	0.61
6:F:171:ALA:HA	6:F:174:ILE:HG12	1.80	0.61
11:K:110:GLY:O	11:K:114:HIS:CD2	2.53	0.61
13:N:147:SER:O	13:N:148:ASP:CB	2.48	0.61
15:1:93:ALA:CB	19:1:1006:CLA:C4B	2.78	0.61
16:2:168:TRP:HA	16:2:171:ILE:CG2	2.19	0.61
17:3:202:TYR:CD2	17:3:202:TYR:N	2.67	0.61
17:3:243:ILE:CG1	19:3:3005:CLA:C3C	2.78	0.61
18:4:96:LEU:HD13	18:4:100:ARG:CZ	2.30	0.61
22:4:7052:LMU:H61	22:4:7052:LMU:C1	2.29	0.61
1:A:236:GLY:O	1:A:237:VAL:CG1	2.48	0.61
1:A:263:ALA:O	1:A:264:GLU:CG	2.47	0.61
1:A:302:HIS:HB2	19:A:1116:CLA:C1B	2.30	0.61
1:A:309:LEU:O	1:A:310:PHE:HB2	2.00	0.61
1:A:575:LEU:CD1	1:A:579:PHE:HB3	2.30	0.61
19:A:1124:CLA:CHC	21:A:6008:BCR:H373	2.30	0.61
2:B:175:LEU:HD21	19:B:1216:CLA:CMA	2.30	0.61
2:B:310:PRO:HG3	19:B:1220:CLA:HMA1	1.82	0.61
2:B:493:TRP:O	2:B:495:PRO:CD	2.47	0.61
2:B:525:LEU:HD23	2:B:525:LEU:O	1.99	0.61
3:C:42:ALA:HB1	3:C:43:PRO:CD	2.30	0.61
3:C:74:THR:OG1	3:C:80:ALA:HB2	2.00	0.61
3:C:74:THR:OG1	3:C:80:ALA:CB	2.48	0.61
5:E:111:ASN:CG	5:E:116:SER:HB3	2.25	0.61
8:H:78:PRO:O	8:H:79:LEU:C	2.39	0.61
22:H:7032:LMU:H3'	22:H:7032:LMU:C5B	2.29	0.61
12:L:164:LEU:C	12:L:165:THR:HG23	2.24	0.61
13:N:139:LYS:C	13:N:142:LYS:HZ2	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:184:LYS:HE3	19:1:1001:CLA:OBD	2.00	0.61
16:2:104:GLN:OE1	16:2:104:GLN:N	2.33	0.61
16:2:160:ILE:O	16:2:163:ALA:N	2.34	0.61
16:2:172:LEU:CA	16:2:173:ASN:ND2	2.62	0.61
19:2:2007:CLA:H2A	19:2:2007:CLA:O1D	2.01	0.61
19:2:4009:CLA:H18	19:2:4009:CLA:ND	2.14	0.61
18:4:87:ASN:ND2	18:4:90:TRP:CZ2	2.68	0.61
18:4:169:ASP:HB3	19:4:4001:CLA:HMB3	1.82	0.61
1:A:73:GLU:O	1:A:74:ILE:C	2.43	0.61
1:A:93:LEU:HA	1:A:96:MET:N	2.15	0.61
1:A:206:HIS:C	1:A:211:LEU:HD23	2.26	0.61
1:A:483:GLN:HB3	1:A:485:GLN:HE22	1.61	0.61
1:A:638:THR:O	1:A:639:ALA:C	2.44	0.61
19:A:1112:CLA:C3B	21:A:6002:BCR:C19	2.72	0.61
19:A:1124:CLA:H52	19:A:1125:CLA:HED1	1.81	0.61
19:A:1237:CLA:H152	21:B:6020:BCR:H352	1.80	0.61
2:B:120:VAL:HG13	2:B:123:TRP:CD1	2.35	0.61
2:B:266:GLN:O	2:B:267:SER:HB3	1.98	0.61
2:B:544:SER:N	2:B:547:MET:O	2.34	0.61
2:B:714:SER:O	2:B:718:ILE:HG22	2.01	0.61
19:B:1215:CLA:CGA	19:B:1215:CLA:C3A	2.77	0.61
19:B:1227:CLA:HED2	19:B:1227:CLA:CAA	2.30	0.61
4:D:80:SER:N	4:D:81:PRO:HD3	2.16	0.61
21:F:6016:BCR:H403	21:F:6016:BCR:C27	2.30	0.61
11:K:60:SER:CA	11:K:63:LEU:HD21	2.28	0.61
13:N:112:ALA:N	13:N:118:TYR:CD1	2.69	0.61
13:N:132:THR:OG1	13:N:137:LEU:C	2.43	0.61
15:1:112:GLN:O	15:1:113:GLU:HB2	2.00	0.61
15:1:184:LYS:CE	19:1:1001:CLA:OBD	2.47	0.61
17:3:192:LYS:HZ3	17:3:192:LYS:CA	2.12	0.61
22:4:7034:LMU:C10	22:4:7052:LMU:O3'	2.48	0.61
1:A:258:LEU:O	1:A:259:TYR:CD2	2.54	0.61
1:A:304:LEU:HG	19:A:1115:CLA:HBB2	1.82	0.61
1:A:438:HIS:CE1	1:A:442:ILE:HD11	2.35	0.61
1:A:554:LEU:HD21	19:A:9023:CLA:O2D	1.99	0.61
1:A:604:TRP:HE1	19:A:9023:CLA:C1D	2.14	0.61
2:B:293:THR:O	2:B:295:PHE:HD2	1.82	0.61
2:B:421:HIS:NE2	19:B:1228:CLA:C4D	2.63	0.61
19:B:1214:CLA:H52	19:B:1223:CLA:CMB	2.30	0.61
5:E:106:ARG:C	5:E:106:ARG:HE	2.09	0.61
6:F:228:ASP:O	6:F:231:PHE:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:69:LEU:O	15:1:70:GLY:C	2.39	0.61
19:1:1303:CLA:CMC	19:4:1304:CLA:HMB2	2.30	0.61
19:2:2001:CLA:CBC	19:2:2001:CLA:CMC	2.76	0.61
17:3:238:ILE:HG13	19:3:3003:CLA:HMC3	1.82	0.61
21:3:6022:BCR:C8	21:3:6022:BCR:H311	2.29	0.61
18:4:177:LEU:N	18:4:178:PRO:HD2	2.16	0.61
18:4:201:LYS:N	18:4:201:LYS:CD	2.63	0.61
19:4:1306:CLA:CMC	19:4:1306:CLA:CBC	2.79	0.61
1:A:195:TRP:CE2	19:A:1108:CLA:HMA2	2.34	0.61
1:A:618:TRP:CZ2	1:A:655:ASP:HB2	2.35	0.61
1:A:700:TRP:CZ3	19:A:9013:CLA:O1D	2.53	0.61
19:A:1103:CLA:H42	21:A:6003:BCR:H313	1.82	0.61
19:A:1131:CLA:HAA1	21:B:6020:BCR:C13	2.30	0.61
22:A:7010:LMU:O6'	22:K:7047:LMU:H111	2.00	0.61
2:B:552:ASP:OD1	2:B:553:PHE:HD2	1.82	0.61
3:C:62:PHE:CG	4:D:191:ILE:CG2	2.84	0.61
4:D:173:TYR:O	4:D:173:TYR:CD2	2.52	0.61
6:F:195:GLU:H	6:F:195:GLU:CD	2.07	0.61
6:F:204:SER:O	6:F:206:LEU:N	2.33	0.61
16:2:133:ASN:HD21	16:2:134:THR:CB	2.10	0.61
16:2:154:ILE:O	16:2:158:VAL:HG12	2.01	0.61
16:2:160:ILE:CG2	19:2:2012:CLA:HBB2	2.11	0.61
1:A:375:HIS:CE1	19:A:1125:CLA:NC	2.69	0.61
1:A:631:GLN:O	1:A:632:GLY:C	2.41	0.61
1:A:648:THR:CG2	1:A:651:GLY:H	2.09	0.61
1:A:707:ILE:O	1:A:711:HIS:CD2	2.53	0.61
19:A:1106:CLA:H142	21:J:6012:BCR:C14	2.31	0.61
2:B:8:PHE:O	2:B:35:ASP:OD2	2.18	0.61
2:B:98:GLN:O	2:B:100:ALA:HB3	2.01	0.61
2:B:143:LEU:C	2:B:145:LEU:H	2.08	0.61
2:B:315:LEU:HD12	2:B:317:ARG:N	2.15	0.61
2:B:378:ILE:HA	2:B:381:PHE:HB2	1.82	0.61
2:B:440:ASN:CG	2:B:614:THR:CG2	2.71	0.61
2:B:457:PRO:O	2:B:458:ILE:C	2.44	0.61
2:B:480:SER:O	2:B:481:THR:CG2	2.45	0.61
2:B:607:SER:O	2:B:610:ASN:CB	2.49	0.61
2:B:623:TYR:H	2:B:626:LEU:HB2	1.66	0.61
19:B:1220:CLA:HAA2	19:B:1220:CLA:HBD	1.81	0.61
19:F:1302:CLA:C3B	19:F:1305:CLA:CAC	2.68	0.61
12:L:51:LYS:CA	12:L:51:LYS:CE	2.75	0.61
15:1:158:PRO:CA	15:1:175:LYS:HG3	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ASP:C	1:A:432:LEU:H	2.08	0.61
1:A:690:LEU:HD21	1:A:738:TYR:HE1	1.66	0.61
19:A:1112:CLA:HMC1	19:A:1113:CLA:HMB2	1.82	0.61
2:B:123:TRP:CB	2:B:126:THR:HG22	2.26	0.61
2:B:312:GLY:C	2:B:314:ARG:N	2.59	0.61
2:B:390:GLY:N	2:B:391:PRO:CD	2.64	0.61
2:B:558:PRO:HG2	2:B:703:VAL:CG1	2.31	0.61
2:B:692:ARG:HH22	2:B:694:ARG:NH2	1.98	0.61
2:B:696:LYS:HG2	3:C:80:ALA:CA	2.24	0.61
3:C:51:CYS:N	23:C:8002:SF4:S4	2.63	0.61
3:C:78:GLY:O	3:C:81:TYR:HE1	1.84	0.61
4:D:82:ILE:O	4:D:82:ILE:CG1	2.46	0.61
4:D:156:ARG:HB2	4:D:166:LEU:HD12	1.81	0.61
19:K:1142:CLA:HMD3	19:K:1143:CLA:NA	2.15	0.61
13:N:130:ASN:HB2	13:N:139:LYS:HD3	1.80	0.61
22:R:7020:LMU:H5B	22:R:7020:LMU:O6'	1.99	0.61
15:1:177:PRO:CG	15:1:180:LEU:HD23	2.31	0.61
19:1:1001:CLA:HBC3	19:1:1001:CLA:HMC2	1.82	0.61
17:3:156:THR:O	17:3:158:PHE:O	2.18	0.61
17:3:204:GLY:O	17:3:205:GLY:C	2.42	0.61
18:4:154:ILE:HG21	19:4:1009:CLA:HMD1	1.81	0.61
1:A:284:ARG:CB	1:A:295:TRP:CD1	2.84	0.61
1:A:393:LEU:CD1	1:A:750:PHE:CE1	2.83	0.61
19:A:1122:CLA:HBC1	21:A:6007:BCR:H393	1.83	0.61
19:A:1134:CLA:O1A	19:A:1141:CLA:CBB	2.49	0.61
2:B:426:SER:O	2:B:430:GLY:N	2.33	0.61
2:B:560:ASP:CG	3:C:66:ARG:NH1	2.59	0.61
2:B:668:ARG:HG3	2:B:699:ALA:O	2.01	0.61
19:K:1146:CLA:O1A	19:K:1146:CLA:C2A	2.48	0.61
12:L:106:HIS:HD2	19:L:1502:CLA:HED1	1.64	0.61
15:1:67:LEU:CD1	15:1:68:GLY:H	2.10	0.61
15:1:85:ILE:C	15:1:88:ARG:HB2	2.26	0.61
2:B:75:GLU:HB3	2:B:132:ASN:HD22	1.64	0.61
2:B:122:GLN:O	2:B:126:THR:CA	2.49	0.61
2:B:178:HIS:O	2:B:180:SER:N	2.34	0.61
2:B:463:ILE:O	2:B:464:GLN:CB	2.49	0.61
2:B:469:LYS:CD	2:B:470:THR:HG23	2.30	0.61
2:B:730:SER:C	2:B:731:GLY:O	2.42	0.61
19:B:1222:CLA:HBB1	19:B:1236:CLA:HMB1	1.82	0.61
11:K:76:ALA:HA	11:K:78:ARG:HH11	1.65	0.61
12:L:82:TYR:CE1	19:L:1130:CLA:H93	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:143:VAL:HG12	13:N:144:PRO:CD	2.31	0.61
22:R:7007:LMU:H1'	22:R:7007:LMU:O6'	2.00	0.61
15:1:77:GLU:O	15:1:80:LYS:CG	2.41	0.61
19:1:1014:CLA:C5	19:1:1014:CLA:H101	2.29	0.61
16:2:101:TRP:N	16:2:103:VAL:N	2.49	0.61
18:4:158:GLN:CD	19:4:1004:CLA:C1A	2.70	0.61
19:4:4002:CLA:HAA2	19:4:4002:CLA:O1D	2.01	0.61
1:A:76:ARG:O	1:A:186:TYR:HD2	1.84	0.60
1:A:101:ALA:HB1	1:A:161:GLU:O	2.01	0.60
1:A:545:HIS:HB3	19:A:1135:CLA:CBB	2.30	0.60
2:B:681:ALA:O	2:B:684:ARG:N	2.33	0.60
3:C:12:ILE:CG2	3:C:38:GLN:O	2.49	0.60
3:C:24:ASP:O	3:C:43:PRO:HG2	2.01	0.60
6:F:152:GLY:O	19:F:1302:CLA:HAC2	2.00	0.60
8:H:121:LEU:C	8:H:122:PRO:O	2.44	0.60
10:J:5:LYS:CD	16:2:178:ASN:HA	2.28	0.60
19:J:1308:CLA:CHD	19:J:1308:CLA:HBC3	2.25	0.60
14:R:41:UNK:CA	14:R:42:UNK:CB	2.77	0.60
16:2:155:VAL:O	16:2:158:VAL:HG13	2.01	0.60
16:2:172:LEU:CB	16:2:173:ASN:HD22	2.13	0.60
16:2:185:ASN:C	16:2:185:ASN:OD1	2.43	0.60
1:A:177:LEU:C	1:A:179:LEU:H	2.09	0.60
1:A:207:LEU:O	1:A:310:PHE:CB	2.49	0.60
1:A:346:LEU:O	1:A:346:LEU:HD22	2.01	0.60
1:A:425:THR:O	1:A:427:ARG:NE	2.33	0.60
1:A:484:LEU:C	1:A:485:GLN:NE2	2.59	0.60
1:A:534:LEU:HD12	1:A:535:GLY:CA	2.26	0.60
1:A:570:PRO:C	1:A:572:LYS:H	2.07	0.60
1:A:723:ARG:HH11	1:A:723:ARG:HG3	1.65	0.60
2:B:440:ASN:OD1	2:B:614:THR:HG23	1.96	0.60
2:B:553:PHE:CD1	2:B:557:PHE:HB3	2.36	0.60
2:B:664:LEU:O	2:B:667:TRP:HZ3	1.84	0.60
3:C:9:ASP:OD1	3:C:61:ASP:OD2	2.19	0.60
4:D:208:TYR:CG	4:D:208:TYR:O	2.53	0.60
7:G:100:PHE:H	7:G:101:GLU:HB2	1.62	0.60
12:L:67:GLY:C	12:L:68:SER:OG	2.45	0.60
12:L:93:VAL:O	12:L:94:SER:C	2.41	0.60
12:L:137:LEU:C	12:L:137:LEU:CD2	2.64	0.60
14:R:35:UNK:C	14:R:38:UNK:CB	2.79	0.60
15:1:169:ASP:OD2	15:1:170:PRO:HD2	2.00	0.60
15:1:189:LYS:HE2	15:1:189:LYS:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:167:ARG:CA	16:2:167:ARG:HE	2.13	0.60
17:3:131:GLU:O	17:3:134:LEU:HD12	2.02	0.60
18:4:89:ARG:NH1	18:4:90:TRP:HA	2.16	0.60
1:A:68:THR:HG22	1:A:70:ASP:N	2.14	0.60
1:A:174:PHE:O	1:A:175:ALA:HB2	2.01	0.60
1:A:246:HIS:ND1	1:A:246:HIS:N	2.50	0.60
1:A:362:LEU:HD11	19:A:1128:CLA:HBB2	1.84	0.60
1:A:679:PHE:HE1	1:A:749:PHE:HB2	1.66	0.60
19:A:1105:CLA:HMB2	21:J:6012:BCR:C7	2.27	0.60
19:A:1132:CLA:H41	12:L:110:LEU:HD23	1.82	0.60
19:A:1141:CLA:HBC3	19:A:1141:CLA:CHD	2.32	0.60
2:B:25:ILE:CG2	21:L:6019:BCR:C29	2.77	0.60
2:B:154:TRP:CD1	2:B:154:TRP:C	2.78	0.60
2:B:302:LYS:O	2:B:303:TYR:CB	2.37	0.60
2:B:553:PHE:O	2:B:554:GLY:O	2.19	0.60
2:B:704:GLN:O	2:B:708:VAL:HG23	2.02	0.60
2:B:715:VAL:HG13	2:B:719:PHE:HD2	1.64	0.60
19:B:1216:CLA:HBB2	19:B:1221:CLA:H41	1.83	0.60
6:F:228:ASP:C	6:F:231:PHE:HB3	2.25	0.60
7:G:76:ARG:NH2	7:G:117:ASN:CA	2.64	0.60
7:G:102:ALA:C	7:G:104:ASP:OD1	2.44	0.60
11:K:56:ILE:CG2	11:K:59:THR:HG23	2.28	0.60
11:K:97:ASP:O	11:K:98:PRO:C	2.44	0.60
12:L:142:SER:O	12:L:143:LEU:HD23	2.01	0.60
13:N:145:PHE:CA	13:N:146:LEU:O	2.49	0.60
16:2:101:TRP:HA	16:2:103:VAL:H	1.64	0.60
18:4:172:PHE:C	18:4:194:PHE:CD2	2.79	0.60
22:4:7034:LMU:C10	22:4:7052:LMU:C2'	2.78	0.60
1:A:23:ASP:CB	1:A:33:GLN:OE1	2.50	0.60
1:A:50:THR:CG2	1:A:51:THR:H	2.15	0.60
1:A:193:LEU:O	1:A:194:ALA:C	2.44	0.60
1:A:250:LEU:CG	17:3:136:TRP:HZ2	2.15	0.60
1:A:445:HIS:CE1	19:A:1129:CLA:HMB1	2.37	0.60
19:A:1115:CLA:H141	19:A:1115:CLA:C17	2.13	0.60
21:A:6008:BCR:C33	21:A:6008:BCR:C8	2.75	0.60
19:A:9012:CLA:H11	2:B:616:LEU:CB	2.30	0.60
2:B:86:PRO:C	2:B:87:ILE:HD12	2.26	0.60
2:B:478:LEU:O	2:B:478:LEU:CD2	2.44	0.60
19:B:1212:CLA:H2A	19:B:1212:CLA:O1D	2.02	0.60
4:D:156:ARG:CZ	4:D:164:GLN:HB2	2.32	0.60
5:E:78:ARG:CZ	5:E:125:ILE:HG22	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:TYR:CB	5:E:83:TRP:CZ3	2.72	0.60
5:E:103:VAL:HG13	5:E:120:TYR:C	2.26	0.60
6:F:207:LEU:N	6:F:207:LEU:CD1	2.64	0.60
7:G:144:THR:OG1	7:G:148:GLY:N	2.34	0.60
11:K:47:ASP:N	11:K:51:SER:HB2	2.17	0.60
15:1:85:ILE:HA	15:1:88:ARG:NE	2.14	0.60
15:1:150:HIS:NE2	15:1:151:GLN:NE2	2.47	0.60
16:2:122:ILE:N	16:2:123:PRO:CD	2.64	0.60
18:4:149:SER:CB	18:4:153:GLU:OE1	2.50	0.60
1:A:34:TRP:O	1:A:35:ALA:CB	2.49	0.60
1:A:206:HIS:O	1:A:211:LEU:HD23	2.00	0.60
1:A:287:LEU:HD22	1:A:292:GLY:O	2.00	0.60
1:A:567:ARG:HH11	4:D:88:GLY:C	2.09	0.60
1:A:630:ASP:O	1:A:631:GLN:C	2.45	0.60
1:A:704:ILE:HA	1:A:707:ILE:HG13	1.83	0.60
1:A:735:VAL:O	1:A:739:LEU:HG	2.00	0.60
2:B:652:PHE:O	2:B:656:VAL:HG23	2.00	0.60
21:B:6010:BCR:H23C	21:B:6010:BCR:C38	2.27	0.60
5:E:107:PHE:CD2	5:E:109:LYS:CE	2.84	0.60
7:G:83:GLN:O	7:G:84:ARG:HB3	2.01	0.60
19:H:1145:CLA:H143	19:H:1145:CLA:C19	2.29	0.60
9:I:8:PHE:CE1	19:I:1204:CLA:H43	2.36	0.60
19:K:1142:CLA:HMD3	19:K:1143:CLA:C1A	2.32	0.60
15:1:143:LEU:N	15:1:143:LEU:CD1	2.63	0.60
16:2:130:GLY:CA	16:2:131:ILE:HG12	1.99	0.60
16:2:183:PHE:C	16:2:183:PHE:HD1	2.09	0.60
16:2:184:PRO:CB	16:2:187:LYS:CD	2.68	0.60
16:2:184:PRO:N	16:2:185:ASN:HA	2.16	0.60
22:2:7031:LMU:H4'	22:2:7031:LMU:O2B	2.01	0.60
18:4:127:TYR:CD1	18:4:127:TYR:O	2.54	0.60
18:4:205:ILE:HG13	18:4:206:ALA:N	2.14	0.60
1:A:109:TRP:O	1:A:113:PRO:N	2.35	0.60
1:A:242:ILE:HG13	1:A:243:PRO:HD3	0.74	0.60
2:B:131:THR:CG2	2:B:134:ASP:CB	2.74	0.60
2:B:131:THR:O	2:B:134:ASP:N	2.34	0.60
19:B:1239:CLA:H151	12:L:144:CYS:SG	2.42	0.60
5:E:107:PHE:HD2	5:E:109:LYS:CD	2.12	0.60
7:G:144:THR:HG23	7:G:144:THR:O	2.01	0.60
9:I:28:VAL:O	9:I:29:GLU:CD	2.45	0.60
12:L:172:GLU:C	12:L:173:PRO:O	2.41	0.60
13:N:127:PHE:CD2	13:N:127:PHE:N	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:97:ILE:HD11	15:1:98:LEU:CD2	2.27	0.60
16:2:154:ILE:O	16:2:158:VAL:CG1	2.49	0.60
16:2:192:ASP:OD1	16:2:194:GLY:C	2.43	0.60
22:2:7006:LMU:H22	22:2:7006:LMU:O2'	2.01	0.60
17:3:104:ILE:HG21	19:3:3004:CLA:C2D	2.30	0.60
17:3:150:TYR:CG	17:3:151:TRP:NE1	2.47	0.60
18:4:173:LYS:C	18:4:194:PHE:HD2	2.10	0.60
1:A:245:PRO:C	1:A:248:PHE:HE2	2.09	0.60
19:A:1141:CLA:H121	19:A:1141:CLA:H72	1.79	0.60
19:A:9012:CLA:H122	19:A:9012:CLA:H92	1.83	0.60
19:A:9013:CLA:HMD2	2:B:533:ILE:HD13	1.84	0.60
2:B:31:PHE:HB2	2:B:42:LEU:CD1	2.32	0.60
2:B:141:PHE:HD2	2:B:144:PHE:CE1	2.20	0.60
2:B:315:LEU:HD11	2:B:317:ARG:CD	2.30	0.60
2:B:493:TRP:CZ2	19:B:1214:CLA:H122	2.36	0.60
2:B:686:PRO:HD2	19:L:1130:CLA:O1A	2.01	0.60
3:C:11:CYS:C	3:C:13:GLY:H	2.10	0.60
4:D:87:THR:H	12:L:69:LEU:HD11	1.67	0.60
5:E:110:VAL:O	5:E:111:ASN:HB3	2.00	0.60
7:G:94:GLN:O	7:G:97:LEU:CD2	2.46	0.60
7:G:131:GLY:CA	7:G:136:VAL:CG2	2.75	0.60
7:G:145:THR:CG2	7:G:146:SER:H	2.13	0.60
13:N:99:LYS:HA	13:N:102:ASN:CG	2.23	0.60
14:R:35:UNK:N	14:R:38:UNK:CB	2.65	0.60
15:1:112:GLN:C	15:1:113:GLU:OE2	2.44	0.60
16:2:269:LYS:HE3	16:2:269:LYS:C	2.26	0.60
17:3:207:PHE:O	17:3:207:PHE:CD1	2.39	0.60
19:3:3008:CLA:O1A	19:3:3008:CLA:HED3	2.01	0.60
18:4:211:MET:HE2	19:4:4002:CLA:CBB	2.32	0.60
1:A:74:ILE:O	1:A:75:SER:C	2.44	0.60
1:A:92:TRP:CD1	19:A:1105:CLA:CBB	2.83	0.60
1:A:281:LEU:CG	19:A:1115:CLA:HED2	2.23	0.60
1:A:484:LEU:C	1:A:485:GLN:CD	2.70	0.60
2:B:349:ALA:CB	2:B:375:HIS:HB3	2.31	0.60
2:B:443:MET:O	2:B:446:PHE:CB	2.48	0.60
2:B:664:LEU:C	2:B:667:TRP:CZ3	2.76	0.60
19:B:1206:CLA:H143	19:B:1224:CLA:H18	1.83	0.60
4:D:95:GLN:CG	4:D:96:VAL:N	2.63	0.60
4:D:115:PRO:C	4:D:116:THR:HG1	2.03	0.60
5:E:129:GLU:OE1	5:E:129:GLU:HA	2.00	0.60
6:F:129:ARG:HB3	6:F:133:TYR:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:153:PHE:O	12:L:178:THR:HG22	2.01	0.60
22:L:7029:LMU:O2B	22:L:7029:LMU:C6'	2.50	0.60
15:1:60:GLY:O	15:1:61:ASP:C	2.45	0.60
15:1:179:LYS:CG	15:1:180:LEU:O	2.49	0.60
16:2:229:MET:HE1	16:2:230:LEU:HD11	1.82	0.60
17:3:201:ALA:O	17:3:202:TYR:HB2	2.00	0.60
1:A:29:THR:OG1	1:A:31:PHE:HB2	2.02	0.60
1:A:343:HIS:HA	1:A:431:LEU:HD22	1.83	0.60
1:A:430:ASP:C	1:A:432:LEU:N	2.60	0.60
21:A:6008:BCR:HC8	21:A:6008:BCR:H331	1.82	0.60
19:A:9022:CLA:C13	19:B:1206:CLA:HBB2	2.32	0.60
2:B:670:TYR:C	2:B:670:TYR:CD1	2.80	0.60
3:C:43:PRO:CA	4:D:182:GLN:HG3	2.32	0.60
4:D:114:MET:HG3	4:D:115:PRO:N	2.17	0.60
5:E:72:ALA:O	5:E:73:LYS:HB3	2.02	0.60
19:F:1305:CLA:H42	19:4:1306:CLA:CAA	2.25	0.60
7:G:74:LEU:C	7:G:77:PHE:H	2.10	0.60
11:K:62:SER:HG	11:K:63:LEU:HD13	1.62	0.60
12:L:169:ARG:HG2	12:L:172:GLU:HA	1.84	0.60
13:N:132:THR:CG2	13:N:139:LYS:CD	2.46	0.60
13:N:165:ASN:OD1	13:N:167:PHE:CA	2.49	0.60
22:R:7014:LMU:H11	22:R:7014:LMU:C6	2.22	0.60
15:1:68:GLY:C	15:1:72:VAL:HB	2.25	0.60
15:1:137:ILE:C	15:1:141:GLU:OE2	2.45	0.60
16:2:112:TRP:HZ3	16:2:164:GLU:HG3	1.66	0.60
17:3:191:GLU:O	17:3:191:GLU:CG	2.49	0.60
1:A:296:LEU:HD12	1:A:297:THR:N	2.16	0.60
1:A:507:ALA:O	1:A:508:THR:C	2.44	0.60
2:B:312:GLY:C	2:B:314:ARG:H	2.07	0.60
2:B:508:LEU:CB	2:B:509:PHE:CD2	2.85	0.60
3:C:62:PHE:HZ	5:E:80:GLU:OE2	1.74	0.60
4:D:96:VAL:O	4:D:96:VAL:HG22	2.00	0.60
6:F:207:LEU:CD2	6:F:208:PHE:CB	2.80	0.60
6:F:228:ASP:HA	6:F:231:PHE:HB3	1.84	0.60
7:G:105:THR:OG1	7:G:106:ARG:N	2.34	0.60
8:H:60:ASN:O	8:H:62:THR:HA	2.01	0.60
8:H:62:THR:H	8:H:63:GLY:HA2	1.67	0.60
8:H:89:ALA:O	8:H:93:LYS:N	2.32	0.60
11:K:112:VAL:C	11:K:114:HIS:N	2.53	0.60
12:L:155:GLU:CA	12:L:178:THR:CG2	2.75	0.60
14:R:4:UNK:O	14:R:5:UNK:CB	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:114:TRP:HH2	15:1:121:GLN:HA	1.65	0.60
16:2:144:GLU:HA	16:2:144:GLU:OE2	1.97	0.60
16:2:223:LYS:O	16:2:226:ARG:CB	2.50	0.60
1:A:84:GLY:O	1:A:87:SER:O	2.19	0.59
1:A:107:GLU:HA	1:A:110:LEU:HD21	1.83	0.59
1:A:158:ILE:HG13	1:A:163:GLN:HE22	1.65	0.59
1:A:165:TYR:CD2	1:A:165:TYR:O	2.55	0.59
1:A:253:ASP:HB3	1:A:254:LEU:HD22	1.83	0.59
1:A:479:ASP:CA	1:A:536:THR:HG21	2.21	0.59
2:B:246:THR:O	2:B:246:THR:HG23	2.00	0.59
2:B:438:VAL:O	2:B:441:ASP:N	2.35	0.59
2:B:607:SER:O	2:B:610:ASN:N	2.35	0.59
22:B:7038:LMU:C6	22:B:7038:LMU:H101	2.31	0.59
22:B:7040:LMU:O3'	22:B:7040:LMU:C1B	2.50	0.59
5:E:106:ARG:NE	5:E:106:ARG:C	2.60	0.59
6:F:159:GLU:CG	10:J:38:ILE:HG12	2.31	0.59
6:F:167:PHE:HA	21:F:6014:BCR:H392	1.84	0.59
19:L:1148:CLA:C2	19:L:1148:CLA:O1A	2.50	0.59
13:N:105:LYS:O	13:N:106:ARG:C	2.44	0.59
15:1:69:LEU:C	15:1:73:PRO:CD	2.72	0.59
15:1:95:PRO:HA	15:1:98:LEU:CB	2.31	0.59
15:1:157:ASP:CB	15:1:178:LYS:HB2	2.23	0.59
15:1:170:PRO:O	15:1:171:LEU:HD23	2.02	0.59
16:2:183:PHE:CA	16:2:187:LYS:HG2	2.31	0.59
18:4:221:HIS:O	18:4:224:THR:N	2.33	0.59
1:A:361:ASN:O	1:A:365:LEU:N	2.34	0.59
1:A:580:PRO:HB3	1:A:727:ILE:HG21	1.84	0.59
21:A:6002:BCR:H402	21:A:6002:BCR:H23C	1.83	0.59
2:B:222:LEU:HD13	2:B:225:LEU:HD23	1.84	0.59
22:D:7050:LMU:O2B	22:D:7050:LMU:C4'	2.46	0.59
5:E:78:ARG:HD2	5:E:78:ARG:H	1.66	0.59
5:E:121:ALA:O	5:E:125:ILE:CG2	2.50	0.59
19:F:1302:CLA:H2A	19:F:1302:CLA:O1D	2.02	0.59
8:H:94:ARG:NH2	8:H:97:LEU:O	2.35	0.59
15:1:158:PRO:CG	15:1:159:GLU:N	2.61	0.59
19:2:2001:CLA:C4	19:2:2001:CLA:O2A	2.50	0.59
17:3:124:LYS:HZ1	17:3:148:TYR:N	2.00	0.59
18:4:90:TRP:O	18:4:91:PHE:HD1	1.84	0.59
18:4:165:SER:O	18:4:168:GLN:N	2.34	0.59
1:A:90:PHE:CE1	19:A:1103:CLA:C9	2.82	0.59
1:A:447:ASN:ND2	2:B:678:LEU:HD21	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1126:CLA:H171	21:J:6012:BCR:H15C	1.83	0.59
20:A:5001:PQN:H142	21:F:6014:BCR:HC22	1.83	0.59
2:B:126:THR:OG1	2:B:358:TYR:CD1	2.49	0.59
2:B:189:ALA:HB2	19:B:1225:CLA:C20	2.26	0.59
2:B:378:ILE:HG22	2:B:379:ALA:H	1.66	0.59
21:B:6020:BCR:C33	21:B:6020:BCR:C8	2.77	0.59
3:C:79:LEU:CD2	3:C:81:TYR:C	2.76	0.59
5:E:78:ARG:HB2	5:E:80:GLU:OE2	2.02	0.59
6:F:105:SER:HB2	6:F:108:LEU:HD13	1.83	0.59
7:G:82:PHE:HB2	7:G:83:GLN:HG2	1.84	0.59
12:L:74:THR:HG22	12:L:75:SER:CB	2.31	0.59
13:N:145:PHE:C	13:N:146:LEU:O	2.45	0.59
13:N:169:LYS:HA	13:N:170:TRP:CD1	2.37	0.59
16:2:240:ILE:HG23	16:2:263:PHE:CB	2.27	0.59
19:2:2002:CLA:H2A	19:2:2002:CLA:O1D	2.02	0.59
1:A:70:ASP:O	1:A:71:LEU:C	2.44	0.59
1:A:112:ASP:HB3	1:A:116:ILE:HD11	1.84	0.59
1:A:130:GLU:OE1	1:A:130:GLU:HA	2.02	0.59
1:A:308:ILE:CD1	19:A:1115:CLA:CBB	2.77	0.59
1:A:472:ARG:HH12	12:L:120:LEU:CD2	2.10	0.59
1:A:679:PHE:O	1:A:683:HIS:HB2	2.03	0.59
19:A:1106:CLA:HBB1	19:A:1126:CLA:H151	1.84	0.59
2:B:32:GLU:HG2	2:B:42:LEU:HD22	1.85	0.59
2:B:46:ILE:HD11	19:B:1202:CLA:H192	1.83	0.59
2:B:256:THR:C	2:B:257:ILE:HD13	2.27	0.59
2:B:463:ILE:O	2:B:464:GLN:HG2	2.01	0.59
2:B:618:GLY:HA2	2:B:621:ARG:H	1.67	0.59
6:F:225:GLU:N	6:F:227:VAL:CG1	2.64	0.59
11:K:118:VAL:O	11:K:121:VAL:HG22	1.99	0.59
16:2:266:PHE:CG	16:2:267:THR:N	2.70	0.59
18:4:87:ASN:OD1	18:4:88:LEU:N	2.35	0.59
22:4:7052:LMU:O1'	22:4:7052:LMU:C6	2.45	0.59
1:A:73:GLU:HB2	1:A:186:TYR:HE2	1.67	0.59
1:A:368:LEU:HD21	19:A:1117:CLA:H91	1.75	0.59
1:A:451:ILE:HD12	19:A:1131:CLA:CED	2.03	0.59
1:A:472:ARG:O	1:A:474:GLN:N	2.36	0.59
19:A:1151:CLA:HBA2	19:A:1151:CLA:CED	2.32	0.59
20:B:5002:PQN:H291	24:B:7101:LMG:H201	1.83	0.59
4:D:162:GLU:O	4:D:163:VAL:CG2	2.30	0.59
4:D:201:LYS:CD	4:D:201:LYS:N	2.47	0.59
22:D:7050:LMU:C6'	22:D:7050:LMU:O2B	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:136:VAL:HG22	7:G:137:VAL:HG13	1.83	0.59
7:G:144:THR:OG1	7:G:148:GLY:CA	2.50	0.59
11:K:58:VAL:O	11:K:62:SER:HB3	2.02	0.59
15:1:76:LEU:CB	15:1:77:GLU:OE1	2.48	0.59
16:2:240:ILE:HG21	16:2:263:PHE:HB3	1.79	0.59
17:3:98:LEU:CD2	19:3:3012:CLA:C3D	2.81	0.59
1:A:23:ASP:OD1	1:A:33:GLN:CG	2.51	0.59
1:A:274:TRP:CD2	1:A:277:TYR:O	2.55	0.59
1:A:454:GLY:H	1:A:457:SER:CB	2.05	0.59
1:A:575:LEU:CD1	1:A:576:GLY:N	2.48	0.59
1:A:747:TRP:CD2	21:A:6011:BCR:C40	2.85	0.59
2:B:195:VAL:HA	2:B:199:ILE:HG13	1.84	0.59
2:B:438:VAL:CG2	19:B:1230:CLA:CMC	2.80	0.59
2:B:455:ILE:HG23	6:F:148:LEU:CD1	2.32	0.59
2:B:493:TRP:CH2	19:B:1232:CLA:CMA	2.85	0.59
2:B:594:TRP:C	2:B:594:TRP:HD1	2.10	0.59
19:B:1201:CLA:C4C	21:I:6021:BCR:H401	2.33	0.59
4:D:96:VAL:O	4:D:96:VAL:CG2	2.49	0.59
4:D:112:PHE:C	4:D:112:PHE:HD2	2.09	0.59
4:D:173:TYR:O	4:D:175:GLU:CG	2.51	0.59
7:G:125:VAL:O	7:G:129:ALA:HB3	2.03	0.59
13:N:126:LYS:NZ	13:N:126:LYS:CB	2.65	0.59
14:R:26:UNK:C	14:R:28:UNK:N	2.66	0.59
15:1:102:ALA:CA	15:1:103:LEU:HD23	2.33	0.59
15:1:145:ILE:O	15:1:148:VAL:CG1	2.51	0.59
16:2:263:PHE:O	16:2:263:PHE:CD2	2.56	0.59
17:3:174:GLN:O	17:3:175:ASP:C	2.46	0.59
18:4:142:PHE:CG	19:4:4010:CLA:C3C	2.85	0.59
18:4:155:ARG:O	18:4:158:GLN:HB2	2.02	0.59
18:4:158:GLN:NE2	19:4:1004:CLA:C4A	2.65	0.59
22:4:7034:LMU:H81	22:4:7052:LMU:O2'	1.97	0.59
1:A:261:SER:C	1:A:262:PHE:CD1	2.79	0.59
1:A:330:ILE:O	1:A:334:HIS:HE1	1.86	0.59
1:A:393:LEU:HG	1:A:394:SER:N	2.17	0.59
1:A:426:THR:HA	1:A:428:TYR:CE1	2.36	0.59
1:A:455:PHE:HD1	19:A:1131:CLA:CMA	2.15	0.59
19:A:1139:CLA:H42	19:A:1139:CLA:O1A	2.02	0.59
19:A:1149:CLA:CMC	19:A:1149:CLA:HBC2	2.33	0.59
2:B:90:ALA:N	2:B:113:VAL:HG13	2.18	0.59
19:B:1213:CLA:HBA2	19:B:1213:CLA:HED2	1.85	0.59
3:C:44:ARG:NH2	4:D:181:ARG:HB3	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:88:ALA:O	7:G:89:LYS:C	2.41	0.59
11:K:78:ARG:CA	11:K:78:ARG:CZ	2.80	0.59
13:N:147:SER:HA	13:N:149:ASP:CB	2.32	0.59
14:R:39:UNK:CB	14:R:40:UNK:HA	2.33	0.59
15:1:171:LEU:CD2	15:1:173:TYR:OH	2.51	0.59
16:2:150:THR:C	16:2:152:LEU:CD1	2.76	0.59
16:2:217:LEU:HD12	16:2:218:ARG:HG3	1.85	0.59
17:3:184:LYS:O	17:3:185:GLN:HB3	2.02	0.59
1:A:46:LYS:HB2	1:A:48:PRO:O	2.03	0.59
1:A:71:LEU:HD12	1:A:72:GLU:O	2.03	0.59
1:A:86:LEU:HD12	1:A:178:MET:HE2	1.78	0.59
1:A:129:GLN:HE21	19:A:1107:CLA:MG	1.09	0.59
1:A:426:THR:HG23	1:A:428:TYR:CZ	2.38	0.59
1:A:492:ILE:HA	1:A:495:THR:HG22	1.83	0.59
19:A:1125:CLA:HBC2	19:A:1125:CLA:CMC	2.33	0.59
2:B:90:ALA:CA	2:B:113:VAL:CG1	2.63	0.59
2:B:241:ASN:CG	2:B:241:ASN:O	2.45	0.59
2:B:255:LEU:CA	2:B:271:THR:CB	2.70	0.59
2:B:289:LEU:HD21	19:B:1217:CLA:NA	2.17	0.59
2:B:290:MET:HA	19:B:1218:CLA:CAC	2.32	0.59
2:B:489:GLY:HA3	19:B:1232:CLA:OBD	2.01	0.59
2:B:493:TRP:HH2	19:B:1232:CLA:HMA2	1.66	0.59
19:B:1223:CLA:C7	21:B:6010:BCR:H14C	2.33	0.59
4:D:181:ARG:HB3	4:D:182:GLN:HG2	1.83	0.59
7:G:99:HIS:CB	7:G:100:PHE:HB3	2.33	0.59
19:H:1145:CLA:CED	19:H:1145:CLA:HAA2	2.33	0.59
11:K:55:LEU:O	11:K:58:VAL:CG1	2.51	0.59
12:L:91:THR:C	12:L:98:ARG:HH12	2.11	0.59
12:L:158:PRO:O	12:L:159:SER:CB	2.51	0.59
12:L:164:LEU:CD1	12:L:165:THR:N	2.61	0.59
19:L:1148:CLA:CED	19:L:1148:CLA:CGA	2.80	0.59
13:N:147:SER:HA	13:N:149:ASP:HB2	1.83	0.59
15:1:70:GLY:O	15:1:71:GLU:C	2.42	0.59
19:1:1007:CLA:O1D	22:4:7008:LMU:O2'	2.19	0.59
16:2:184:PRO:HG2	16:2:186:ASN:N	2.17	0.59
16:2:226:ARG:CD	16:2:230:LEU:HD23	2.30	0.59
16:2:246:PRO:HB2	16:2:247:ILE:CG1	2.32	0.59
18:4:225:GLY:CA	18:4:226:LYS:NZ	2.66	0.59
1:A:136:VAL:CG2	1:A:140:PHE:O	2.51	0.59
1:A:267:THR:CG2	1:A:267:THR:O	2.50	0.59
1:A:360:ILE:O	1:A:361:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:TYR:CE1	1:A:540:LEU:CD1	2.85	0.59
19:A:9011:CLA:HAA1	19:B:9010:CLA:HBB2	1.85	0.59
2:B:102:GLU:OE1	2:B:640:CYS:O	2.20	0.59
2:B:124:TRP:CD1	2:B:124:TRP:C	2.80	0.59
2:B:207:VAL:O	2:B:207:VAL:CG1	2.50	0.59
3:C:39:ILE:O	3:C:40:ALA:HB3	2.03	0.59
5:E:76:ILE:HG23	5:E:78:ARG:HD3	1.85	0.59
7:G:76:ARG:HH12	7:G:120:VAL:CA	2.16	0.59
7:G:88:ALA:CB	7:G:90:GLN:O	2.49	0.59
11:K:115:ILE:HD12	11:K:118:VAL:HG23	1.85	0.59
16:2:129:LEU:O	16:2:130:GLY:O	2.20	0.59
16:2:229:MET:HE1	16:2:230:LEU:CD1	2.33	0.59
18:4:103:MET:CG	18:4:211:MET:HE3	2.33	0.59
18:4:146:PHE:CD1	18:4:146:PHE:N	2.70	0.59
18:4:168:GLN:O	18:4:173:LYS:C	2.46	0.59
18:4:232:LEU:HD12	18:4:234:GLN:CA	2.32	0.59
1:A:63:ASP:OD2	1:A:65:ASP:N	2.30	0.59
1:A:628:ILE:CD1	1:A:629:ASN:H	2.13	0.59
19:A:9012:CLA:CAD	19:A:9012:CLA:CED	2.81	0.59
2:B:310:PRO:HG3	19:B:1220:CLA:CMA	2.33	0.59
2:B:315:LEU:HD11	2:B:317:ARG:CG	2.30	0.59
19:B:1222:CLA:CED	19:B:1223:CLA:OBD	2.50	0.59
5:E:90:VAL:C	5:E:91:VAL:HG23	2.28	0.59
19:J:1308:CLA:O1D	19:J:1308:CLA:CGA	2.51	0.59
13:N:104:LYS:O	13:N:107:LEU:CB	2.49	0.59
15:1:64:PHE:CE1	15:1:65:ASP:HB3	2.38	0.59
19:1:1013:CLA:CAD	19:1:1013:CLA:CED	2.79	0.59
16:2:145:TYR:O	16:2:146:PHE:CB	2.51	0.59
17:3:96:ARG:HA	17:3:99:ALA:HB2	1.78	0.59
1:A:105:ASN:CB	1:A:119:SER:O	2.51	0.58
1:A:154:ARG:CD	1:A:384:TYR:HE1	2.11	0.58
1:A:253:ASP:O	1:A:256:ALA:HB3	2.02	0.58
1:A:604:TRP:O	1:A:607:ASN:N	2.31	0.58
1:A:699:TYR:HD1	1:A:700:TRP:CD1	2.21	0.58
2:B:127:ILE:O	2:B:127:ILE:CD1	2.51	0.58
2:B:277:HIS:HE1	19:B:1215:CLA:NC	2.01	0.58
2:B:433:THR:O	2:B:436:LEU:O	2.20	0.58
2:B:535:VAL:HG13	2:B:536:LYS:N	2.17	0.58
2:B:544:SER:O	2:B:545:LYS:C	2.45	0.58
2:B:551:LYS:O	2:B:553:PHE:CE2	2.56	0.58
19:B:1222:CLA:H72	19:B:1236:CLA:C2D	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:THR:OG1	3:C:76:SER:CA	2.51	0.58
5:E:79:LYS:N	5:E:84:TYR:HE1	2.00	0.58
7:G:88:ALA:O	7:G:90:GLN:O	2.20	0.58
12:L:102:VAL:HG13	19:L:1502:CLA:CED	2.33	0.58
15:1:179:LYS:HE3	15:1:181:GLU:HA	1.85	0.58
16:2:130:GLY:HA3	16:2:131:ILE:CG1	1.92	0.58
16:2:160:ILE:HB	19:2:2012:CLA:CBB	2.33	0.58
17:3:238:ILE:HG13	19:3:3003:CLA:CMC	2.33	0.58
18:4:133:GLU:O	18:4:134:TYR:HB2	2.01	0.58
1:A:93:LEU:O	1:A:97:TYR:HD2	1.85	0.58
1:A:281:LEU:CD2	19:A:1115:CLA:HMA2	2.13	0.58
1:A:432:LEU:C	1:A:434:ARG:N	2.60	0.58
19:A:1101:CLA:HBB2	19:A:1102:CLA:C1C	2.32	0.58
19:A:1117:CLA:H121	19:A:1117:CLA:CBB	2.34	0.58
2:B:455:ILE:O	2:B:514:PRO:HG3	2.02	0.58
19:B:1214:CLA:HBD	19:B:1223:CLA:CBB	2.31	0.58
19:B:1239:CLA:C19	9:I:21:MET:HB3	2.32	0.58
20:B:5002:PQN:C19	21:B:6017:BCR:C10	2.80	0.58
3:C:34:CYS:H	3:C:37:LYS:CB	2.09	0.58
6:F:128:LYS:O	6:F:129:ARG:HD3	2.03	0.58
22:R:7022:LMU:C2'	22:R:7022:LMU:C2	2.76	0.58
18:4:87:ASN:OD1	18:4:90:TRP:CG	2.55	0.58
18:4:109:MET:C	18:4:111:LEU:N	2.61	0.58
18:4:148:LEU:O	18:4:149:SER:C	2.45	0.58
22:4:7034:LMU:H81	22:4:7052:LMU:C3'	2.23	0.58
1:A:42:ARG:C	1:A:44:ILE:N	2.60	0.58
1:A:278:ALA:O	1:A:281:LEU:HD11	2.03	0.58
1:A:581:CYS:CB	1:A:590:CYS:O	2.50	0.58
19:A:1136:CLA:C19	19:L:1130:CLA:HBB1	2.29	0.58
2:B:175:LEU:HD12	19:B:1221:CLA:HED1	1.84	0.58
2:B:555:TYR:O	2:B:571:SER:HB2	2.03	0.58
2:B:631:LEU:HD23	2:B:631:LEU:H	1.68	0.58
19:B:1223:CLA:H122	21:B:6010:BCR:C13	2.32	0.58
19:B:1229:CLA:H51	21:F:6016:BCR:C40	2.33	0.58
5:E:84:TYR:CD2	5:E:85:LYS:HG3	2.38	0.58
5:E:90:VAL:O	5:E:91:VAL:HG22	2.03	0.58
6:F:173:TRP:CZ3	6:F:211:PHE:CB	2.68	0.58
7:G:80:PHE:O	7:G:81:ASN:C	2.44	0.58
8:H:109:LEU:HD22	19:H:1207:CLA:H52	1.85	0.58
13:N:132:THR:CB	13:N:139:LYS:HD3	2.29	0.58
22:R:7020:LMU:O6'	22:R:7020:LMU:H3B	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1014:CLA:H71	19:1:1014:CLA:C4	2.19	0.58
16:2:266:PHE:CE1	16:2:267:THR:O	2.55	0.58
17:3:162:MET:CE	19:3:3010:CLA:C3D	2.81	0.58
18:4:88:LEU:O	18:4:90:TRP:CD1	2.55	0.58
18:4:228:PRO:CB	18:4:229:PHE:CD1	2.72	0.58
18:4:232:LEU:CD1	18:4:234:GLN:HA	2.33	0.58
1:A:50:THR:HG23	1:A:51:THR:H	1.69	0.58
1:A:90:PHE:HA	1:A:93:LEU:CD2	2.34	0.58
1:A:155:ALA:O	1:A:156:SER:C	2.40	0.58
1:A:255:LEU:CD1	1:A:280:PHE:CZ	2.82	0.58
1:A:746:THR:HG1	19:A:9011:CLA:CGD	2.13	0.58
2:B:89:HIS:C	2:B:113:VAL:HG13	1.98	0.58
2:B:378:ILE:CA	2:B:381:PHE:HB2	2.34	0.58
2:B:409:ALA:O	2:B:410:ARG:CB	2.34	0.58
2:B:654:HIS:HE1	19:B:9010:CLA:NB	2.01	0.58
2:B:732:LYS:CG	2:B:733:PHE:CA	2.78	0.58
19:B:1222:CLA:CHD	19:B:1222:CLA:CBC	2.79	0.58
5:E:78:ARG:HH12	5:E:125:ILE:HB	1.65	0.58
6:F:215:VAL:O	6:F:216:ALA:C	2.45	0.58
9:I:23:SER:O	9:I:26:LEU:HG	2.04	0.58
11:K:69:ARG:O	11:K:70:PHE:C	2.42	0.58
19:K:1142:CLA:CMD	19:K:1143:CLA:C1A	2.82	0.58
19:L:1501:CLA:HED2	19:L:1501:CLA:HAA2	1.85	0.58
13:N:130:ASN:O	13:N:130:ASN:OD1	2.20	0.58
14:R:35:UNK:C	14:R:36:UNK:O	2.51	0.58
15:1:188:ILE:O	15:1:189:LYS:C	2.44	0.58
15:1:223:ASP:OD1	18:4:140:THR:HG21	2.03	0.58
16:2:203:PRO:O	16:2:204:LEU:HB2	2.03	0.58
16:2:226:ARG:HH11	16:2:226:ARG:CA	2.16	0.58
16:2:244:THR:O	16:2:246:PRO:C	2.46	0.58
18:4:220:GLN:NE2	19:4:1306:CLA:HAC2	2.18	0.58
1:A:216:LEU:HD12	21:A:6002:BCR:H353	1.85	0.58
1:A:230:ASN:HA	1:A:233:LEU:HB2	1.85	0.58
1:A:332:GLU:HA	1:A:344:LYS:HG2	1.85	0.58
1:A:338:PHE:CZ	19:A:1151:CLA:CBB	2.81	0.58
1:A:368:LEU:CD2	19:A:1117:CLA:H93	2.24	0.58
2:B:29:HIS:CG	19:B:1202:CLA:HBB2	2.38	0.58
2:B:194:LEU:O	2:B:199:ILE:HG13	2.04	0.58
2:B:213:LEU:CD1	2:B:214:ASP:N	2.60	0.58
19:B:1213:CLA:CBC	19:B:1213:CLA:CHD	2.81	0.58
19:B:1223:CLA:H8	21:B:6010:BCR:H14C	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:CYS:O	3:C:35:LYS:HB2	2.04	0.58
4:D:150:ILE:O	4:D:151:LYS:CG	2.47	0.58
4:D:156:ARG:HE	4:D:164:GLN:HB2	1.64	0.58
5:E:96:ASP:OD2	5:E:98:ASN:ND2	2.36	0.58
5:E:103:VAL:HG22	5:E:104:VAL:O	2.03	0.58
6:F:99:LEU:HB3	6:F:127:LYS:HE2	1.85	0.58
8:H:64:GLN:C	8:H:66:ASP:HA	2.29	0.58
8:H:77:ASN:ND2	8:H:78:PRO:CG	2.66	0.58
22:K:7042:LMU:H2B	22:K:7042:LMU:H3'	1.85	0.58
12:L:143:LEU:N	12:L:145:LEU:H	2.01	0.58
13:N:139:LYS:CA	13:N:142:LYS:CD	2.81	0.58
15:1:116:ALA:O	15:1:117:LEU:HD22	2.02	0.58
16:2:172:LEU:C	16:2:174:PRO:HD3	2.26	0.58
16:2:195:TYR:CE2	16:2:198:GLY:CA	2.87	0.58
16:2:243:GLY:C	16:2:244:THR:CG2	2.76	0.58
19:A:1123:CLA:HMD2	19:A:1123:CLA:H121	1.85	0.58
2:B:70:TRP:CD1	2:B:70:TRP:N	2.71	0.58
2:B:290:MET:HA	19:B:1218:CLA:HAC2	1.85	0.58
2:B:469:LYS:CG	2:B:470:THR:HA	2.31	0.58
2:B:558:PRO:HB3	2:B:706:ARG:HH21	1.68	0.58
3:C:66:ARG:HB3	3:C:66:ARG:NH2	2.18	0.58
6:F:227:VAL:O	6:F:230:ASN:N	2.37	0.58
12:L:70:GLU:HG2	12:L:74:THR:CG2	2.31	0.58
14:R:52:UNK:CB	14:R:53:UNK:CB	2.82	0.58
15:1:77:GLU:CD	15:1:80:LYS:HE3	2.28	0.58
19:1:1013:CLA:HED2	19:1:1013:CLA:OBD	2.03	0.58
16:2:122:ILE:HG13	16:2:126:LEU:HD21	1.84	0.58
17:3:192:LYS:CE	17:3:192:LYS:CA	2.59	0.58
18:4:198:LEU:O	18:4:199:GLU:C	2.46	0.58
1:A:210:LEU:HD13	19:A:1111:CLA:HHB	1.85	0.58
1:A:453:LEU:HD23	19:A:1136:CLA:HBB1	1.86	0.58
1:A:603:PHE:CZ	1:A:735:VAL:CG2	2.86	0.58
19:A:1117:CLA:O1A	19:A:1127:CLA:H71	2.04	0.58
19:A:1124:CLA:O2A	19:A:1137:CLA:O2D	2.21	0.58
19:A:1237:CLA:HMD2	21:B:6017:BCR:HC31	1.85	0.58
19:A:9022:CLA:C14	19:B:1206:CLA:HBB2	2.34	0.58
2:B:145:LEU:HA	2:B:148:ILE:HD12	1.85	0.58
2:B:190:TRP:CA	19:B:1211:CLA:HBB2	2.34	0.58
2:B:294:ASN:HB2	7:G:94:GLN:OE1	1.89	0.58
2:B:394:PHE:O	2:B:542:ARG:HD3	2.04	0.58
2:B:696:LYS:CG	3:C:80:ALA:HA	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:697:PRO:O	3:C:79:LEU:CD1	2.49	0.58
4:D:77:ASN:HB3	4:D:79:PRO:HD2	1.85	0.58
5:E:90:VAL:CG1	5:E:91:VAL:N	2.65	0.58
15:1:162:LYS:CB	15:1:164:PRO:HG3	2.34	0.58
19:1:1007:CLA:CBC	19:1:1007:CLA:CHD	2.82	0.58
18:4:165:SER:O	18:4:166:VAL:C	2.45	0.58
18:4:172:PHE:O	18:4:173:LYS:CB	2.51	0.58
1:A:29:THR:OG1	1:A:31:PHE:CB	2.51	0.58
1:A:281:LEU:HB2	19:A:1115:CLA:HED2	1.85	0.58
1:A:284:ARG:HG2	1:A:295:TRP:CG	2.37	0.58
1:A:396:PHE:HE2	1:A:616:PHE:CB	2.17	0.58
1:A:397:THR:HG21	1:A:613:ILE:HG13	1.82	0.58
1:A:443:ILE:CG1	1:A:557:LEU:HD22	2.32	0.58
2:B:154:TRP:O	2:B:157:LEU:N	2.36	0.58
2:B:353:TYR:C	2:B:355:LEU:N	2.61	0.58
2:B:388:ALA:O	2:B:391:PRO:HD2	2.02	0.58
2:B:475:ASP:O	2:B:480:SER:N	2.26	0.58
2:B:692:ARG:NH2	2:B:694:ARG:NH2	2.52	0.58
19:B:1239:CLA:HMC3	19:B:1239:CLA:HBC2	1.85	0.58
3:C:34:CYS:N	3:C:37:LYS:HB3	2.10	0.58
10:J:5:LYS:HD2	16:2:178:ASN:OD1	2.02	0.58
11:K:108:ALA:O	11:K:109:CYS:C	2.45	0.58
14:R:37:UNK:C	14:R:42:UNK:O	2.52	0.58
17:3:156:THR:O	17:3:157:LEU:C	2.46	0.58
17:3:171:ARG:CG	17:3:175:ASP:OD1	2.50	0.58
22:3:7005:LMU:C1'	22:3:7005:LMU:C3	2.80	0.58
18:4:210:LEU:HD23	19:4:4002:CLA:CBB	2.34	0.58
1:A:104:SER:O	1:A:106:TYR:N	2.28	0.58
1:A:328:LYS:O	1:A:329:ASP:C	2.46	0.58
1:A:711:HIS:HB3	1:A:717:ALA:CB	2.34	0.58
19:A:9013:CLA:H11	2:B:431:PHE:CE1	2.39	0.58
2:B:25:ILE:O	2:B:26:ALA:CB	2.51	0.58
2:B:29:HIS:CD2	19:B:1202:CLA:HBB1	2.39	0.58
2:B:34:HIS:O	2:B:36:ASP:N	2.37	0.58
2:B:212:PHE:CE1	19:B:1211:CLA:HHD	2.38	0.58
2:B:375:HIS:HE1	19:B:1225:CLA:NC	2.01	0.58
6:F:102:LEU:C	6:F:103:GLN:O	2.42	0.58
7:G:99:HIS:O	7:G:101:GLU:N	2.37	0.58
10:J:11:ALA:CB	10:J:12:PRO:HD2	2.10	0.58
11:K:60:SER:HA	11:K:63:LEU:CD2	2.28	0.58
12:L:73:VAL:CA	19:L:1504:CLA:CMA	2.78	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:91:THR:O	12:L:92:ALA:C	2.41	0.58
12:L:108:TYR:HB2	12:L:200:ALA:HB2	1.85	0.58
13:N:120:VAL:O	13:N:122:PHE:CD2	2.57	0.58
15:1:65:ASP:O	15:1:68:GLY:N	2.37	0.58
15:1:157:ASP:OD2	15:1:175:LYS:HD2	2.04	0.58
15:1:199:VAL:O	15:1:200:GLY:C	2.47	0.58
16:2:201:PHE:HD1	16:2:202:ASP:CA	2.16	0.58
17:3:103:VAL:HG11	17:3:229:LYS:HG2	1.84	0.58
19:4:4006:CLA:H43	22:4:7034:LMU:H91	1.86	0.58
1:A:253:ASP:O	1:A:256:ALA:CB	2.52	0.58
1:A:329:ASP:O	1:A:332:GLU:O	2.22	0.58
19:B:1220:CLA:H93	19:B:1227:CLA:HBC1	1.86	0.58
19:B:1229:CLA:CBB	21:F:6014:BCR:H23C	2.34	0.58
5:E:107:PHE:HD2	5:E:109:LYS:CG	2.17	0.58
8:H:77:ASN:ND2	8:H:78:PRO:CD	2.67	0.58
8:H:97:LEU:HD12	8:H:100:PHE:HB2	1.83	0.58
12:L:109:LEU:O	12:L:110:LEU:C	2.47	0.58
12:L:128:GLN:HG2	12:L:132:LEU:CD2	2.02	0.58
15:1:155:GLU:OE2	15:1:155:GLU:N	2.30	0.58
15:1:171:LEU:HB3	15:1:173:TYR:CZ	2.39	0.58
15:1:176:ASP:C	15:1:180:LEU:HG	2.29	0.58
16:2:95:ASP:HB3	17:3:85:ASP:OD2	1.82	0.58
16:2:113:ALA:CB	16:2:114:MET:HE1	2.33	0.58
16:2:171:ILE:HG13	16:2:172:LEU:HB2	1.84	0.58
17:3:88:GLY:O	17:3:89:THR:C	2.47	0.58
1:A:111:ASN:O	1:A:113:PRO:HD2	2.03	0.57
1:A:217:SER:CA	21:A:6002:BCR:H351	2.34	0.57
1:A:270:PHE:CZ	19:A:1141:CLA:H2	2.39	0.57
1:A:307:ALA:O	1:A:308:ILE:C	2.48	0.57
2:B:37:ILE:HD12	2:B:37:ILE:O	2.04	0.57
2:B:74:PHE:O	2:B:77:TRP:N	2.36	0.57
2:B:411:MET:HE3	19:B:1220:CLA:HMC2	1.86	0.57
2:B:724:PHE:CD2	19:B:9010:CLA:HMD2	2.39	0.57
10:J:5:LYS:CD	16:2:178:ASN:CG	2.76	0.57
11:K:79:LYS:O	11:K:79:LYS:HG3	2.04	0.57
13:N:143:VAL:CG1	13:N:144:PRO:CD	2.82	0.57
19:1:1006:CLA:CAB	19:1:1013:CLA:CHD	2.82	0.57
16:2:118:ALA:C	16:2:121:PHE:CD2	2.75	0.57
16:2:121:PHE:CD2	16:2:121:PHE:N	2.72	0.57
19:2:2014:CLA:H41	19:2:2014:CLA:C9	2.33	0.57
1:A:40:PHE:H	1:A:44:ILE:HG22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HG22	1:A:723:ARG:HB2	1.84	0.57
1:A:187:HIS:HE1	19:A:1109:CLA:CHA	2.17	0.57
1:A:346:LEU:O	1:A:347:TYR:HB2	2.04	0.57
1:A:423:ASP:N	1:A:424:PRO:CD	2.65	0.57
1:A:705:GLU:HB3	2:B:545:LYS:NZ	2.19	0.57
21:A:6002:BCR:C31	21:A:6002:BCR:C8	2.69	0.57
2:B:317:ARG:HA	2:B:317:ARG:HE	1.68	0.57
2:B:560:ASP:CB	3:C:66:ARG:NE	2.65	0.57
3:C:12:ILE:O	3:C:12:ILE:HG22	2.03	0.57
3:C:12:ILE:HB	3:C:39:ILE:HA	1.86	0.57
5:E:91:VAL:HG12	5:E:92:ALA:N	2.18	0.57
6:F:152:GLY:O	6:F:157:TRP:CH2	2.57	0.57
7:G:103:GLY:N	7:G:104:ASP:HA	2.19	0.57
19:J:1308:CLA:H2A	19:J:1308:CLA:H2	1.86	0.57
13:N:127:PHE:H	13:N:127:PHE:HD2	1.50	0.57
14:R:38:UNK:C	14:R:42:UNK:O	2.52	0.57
15:1:66:PRO:O	15:1:69:LEU:C	2.46	0.57
15:1:73:PRO:HG2	15:1:74:ALA:H	1.65	0.57
15:1:170:PRO:HG2	15:1:171:LEU:HA	1.85	0.57
16:2:251:PHE:O	16:2:251:PHE:CG	2.57	0.57
22:2:7006:LMU:H22	22:2:7006:LMU:H2'	1.86	0.57
17:3:155:TYR:C	17:3:157:LEU:H	2.12	0.57
1:A:157:GLY:C	1:A:229:ILE:HG21	2.28	0.57
2:B:154:TRP:O	2:B:157:LEU:CB	2.52	0.57
2:B:282:PHE:O	2:B:286:ILE:HG13	2.03	0.57
2:B:393:PHE:CD2	2:B:397:ASP:OD1	2.49	0.57
2:B:414:HIS:O	2:B:414:HIS:CG	2.57	0.57
2:B:440:ASN:CG	2:B:614:THR:HG23	2.29	0.57
2:B:469:LYS:C	2:B:470:THR:OG1	2.47	0.57
19:B:1203:CLA:C4	24:B:7101:LMG:H321	2.34	0.57
19:B:1235:CLA:CGA	19:B:1235:CLA:C1A	2.82	0.57
3:C:33:GLY:HA2	3:C:37:LYS:CE	2.33	0.57
5:E:78:ARG:HB2	5:E:80:GLU:CD	2.29	0.57
13:N:114:PHE:HE2	13:N:116:ARG:HD2	1.69	0.57
15:1:81:GLU:O	15:1:82:SER:C	2.46	0.57
15:1:134:LEU:CA	15:1:137:ILE:CD1	2.71	0.57
17:3:226:LYS:HG3	17:3:229:LYS:HE3	1.86	0.57
18:4:93:GLN:OE1	18:4:170:PRO:HB2	2.04	0.57
1:A:106:TYR:O	1:A:107:GLU:C	2.43	0.57
1:A:111:ASN:OD1	1:A:238:ASP:HA	2.04	0.57
1:A:282:THR:O	1:A:283:PHE:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LYS:HZ1	2:B:674:LEU:HB2	1.67	0.57
19:A:1102:CLA:HBB2	19:A:1104:CLA:C4D	2.34	0.57
2:B:51:PHE:CD1	19:B:1210:CLA:HED1	2.40	0.57
2:B:155:LEU:O	2:B:161:TRP:NE1	2.38	0.57
2:B:486:LEU:HD13	2:B:489:GLY:N	2.19	0.57
2:B:711:VAL:O	2:B:711:VAL:CG1	2.52	0.57
4:D:98:GLU:HB2	4:D:100:TYR:HE2	1.68	0.57
11:K:116:ILE:CG2	11:K:117:GLY:N	2.68	0.57
12:L:55:GLN:O	12:L:57:ILE:N	2.38	0.57
12:L:82:TYR:O	12:L:82:TYR:CD1	2.57	0.57
13:N:147:SER:CB	13:N:151:ASP:OD1	2.52	0.57
15:1:77:GLU:C	15:1:80:LYS:CG	2.77	0.57
15:1:129:VAL:HB	15:1:130:PRO:HD3	1.85	0.57
16:2:154:ILE:HG12	16:2:155:VAL:H	1.70	0.57
16:2:182:ILE:CB	16:2:187:LYS:CB	2.61	0.57
18:4:222:ASN:O	18:4:223:VAL:CB	2.39	0.57
19:4:1004:CLA:CBC	19:4:1004:CLA:CHD	2.75	0.57
1:A:174:PHE:O	1:A:175:ALA:CB	2.51	0.57
1:A:225:VAL:O	1:A:229:ILE:HB	2.04	0.57
1:A:338:PHE:CD1	1:A:338:PHE:N	2.72	0.57
1:A:412:ALA:HA	1:A:598:VAL:HG21	1.86	0.57
19:A:1133:CLA:H2A	19:A:1133:CLA:O1D	2.04	0.57
21:A:6011:BCR:H19C	19:A:9012:CLA:H172	1.86	0.57
2:B:155:LEU:O	2:B:161:TRP:CD1	2.57	0.57
2:B:486:LEU:HD12	2:B:489:GLY:H	1.68	0.57
2:B:503:GLU:CG	2:B:503:GLU:O	2.49	0.57
20:B:5002:PQN:H161	21:B:6017:BCR:H331	1.87	0.57
21:B:6020:BCR:H331	19:L:1502:CLA:C4B	2.06	0.57
8:H:91:PHE:HB3	12:L:187:GLY:HA3	1.86	0.57
9:I:2:ILE:HG12	9:I:3:ASN:ND2	2.20	0.57
11:K:118:VAL:O	11:K:120:VAL:HA	2.03	0.57
15:1:78:ARG:HH22	15:1:179:LYS:CB	2.16	0.57
15:1:171:LEU:HD22	15:1:173:TYR:OH	2.05	0.57
19:1:1005:CLA:CBC	19:1:1005:CLA:HMC3	2.35	0.57
16:2:115:LEU:O	16:2:118:ALA:CB	2.52	0.57
17:3:103:VAL:O	17:3:107:ARG:CB	2.49	0.57
19:3:3013:CLA:O1D	19:3:3013:CLA:C2A	2.52	0.57
18:4:193:ASN:C	18:4:201:LYS:NZ	2.62	0.57
18:4:194:PHE:O	18:4:195:ALA:CB	2.51	0.57
18:4:225:GLY:CA	18:4:226:LYS:HZ2	2.17	0.57
1:A:278:ALA:O	1:A:279:ASP:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLY:O	1:A:343:HIS:CB	2.45	0.57
1:A:665:ILE:O	2:B:621:ARG:HD3	2.04	0.57
1:A:723:ARG:N	19:A:1139:CLA:HBB1	2.16	0.57
19:A:1122:CLA:NC	21:A:6007:BCR:H19C	2.20	0.57
2:B:70:TRP:H	2:B:70:TRP:HD1	1.50	0.57
2:B:93:ASP:OD1	2:B:96:PHE:HD1	1.87	0.57
2:B:347:LEU:HD13	2:B:351:HIS:HD1	1.70	0.57
20:B:5002:PQN:H191	21:B:6017:BCR:C10	2.34	0.57
3:C:1:MET:N	3:C:4:SER:CB	2.67	0.57
5:E:83:TRP:CH2	5:E:116:SER:CB	2.86	0.57
11:K:62:SER:O	11:K:63:LEU:C	2.46	0.57
11:K:125:LYS:HE3	11:K:125:LYS:O	2.04	0.57
12:L:95:PRO:O	12:L:97:LEU:N	2.38	0.57
12:L:100:ILE:CG2	12:L:191:PHE:O	2.50	0.57
15:1:182:GLU:O	15:1:183:LEU:CB	2.53	0.57
19:1:1001:CLA:CMC	19:1:1001:CLA:CBC	2.80	0.57
16:2:171:ILE:CD1	16:2:173:ASN:HD21	2.17	0.57
17:3:155:TYR:CD2	17:3:155:TYR:N	2.72	0.57
17:3:210:PRO:CD	17:3:211:LEU:N	2.67	0.57
18:4:93:GLN:CD	18:4:170:PRO:HB2	2.30	0.57
18:4:133:GLU:O	18:4:134:TYR:CB	2.51	0.57
1:A:51:THR:CG2	19:A:1139:CLA:CBB	2.61	0.57
1:A:240:LYS:CA	1:A:243:PRO:HD2	2.33	0.57
19:A:1119:CLA:C2C	19:A:1125:CLA:C17	2.82	0.57
19:A:1134:CLA:O2A	19:A:1141:CLA:HBB1	2.04	0.57
19:A:1137:CLA:HBC3	19:A:1137:CLA:CMC	2.34	0.57
19:A:9013:CLA:H93	2:B:431:PHE:HD1	1.69	0.57
2:B:457:PRO:HG3	2:B:517:PHE:HB2	1.87	0.57
2:B:531:THR:HG22	19:B:1222:CLA:CMC	2.35	0.57
4:D:100:TYR:N	4:D:100:TYR:HD2	2.01	0.57
22:D:7050:LMU:H42	22:D:7050:LMU:H82	1.85	0.57
6:F:214:PRO:C	6:F:215:VAL:HG23	2.30	0.57
10:J:37:LEU:C	10:J:38:ILE:HG13	2.25	0.57
11:K:76:ALA:HA	11:K:78:ARG:NH1	2.18	0.57
11:K:114:HIS:O	11:K:116:ILE:N	2.38	0.57
13:N:146:LEU:O	13:N:147:SER:HB2	2.04	0.57
15:1:93:ALA:HB1	19:1:1006:CLA:C4B	2.24	0.57
15:1:97:ILE:HG12	15:1:98:LEU:N	2.18	0.57
17:3:104:ILE:CG2	19:3:3004:CLA:C1D	2.83	0.57
18:4:159:ASP:O	18:4:163:PRO:HA	2.04	0.57
1:A:213:LEU:O	1:A:217:SER:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:PRO:C	1:A:248:PHE:CE2	2.82	0.57
1:A:259:TYR:CE2	1:A:280:PHE:HA	2.40	0.57
2:B:42:LEU:O	2:B:43:TYR:C	2.47	0.57
2:B:91:ILE:HG12	2:B:112:PRO:O	2.04	0.57
2:B:221:GLY:O	2:B:222:LEU:C	2.46	0.57
2:B:254:ILE:HB	2:B:255:LEU:CD2	2.32	0.57
2:B:649:MET:O	2:B:653:GLY:N	2.37	0.57
2:B:715:VAL:O	2:B:716:GLY:C	2.48	0.57
3:C:1:MET:H2	3:C:3:HIS:N	2.02	0.57
4:D:181:ARG:CB	4:D:182:GLN:HG2	2.35	0.57
6:F:200:VAL:HG13	10:J:7:TYR:N	2.02	0.57
7:G:144:THR:OG1	7:G:148:GLY:HA3	2.05	0.57
13:N:139:LYS:HA	13:N:142:LYS:CE	2.34	0.57
13:N:144:PRO:HG2	13:N:158:ASP:O	2.05	0.57
15:1:92:LEU:CA	15:1:95:PRO:HD3	2.35	0.57
19:1:1303:CLA:HMC2	19:4:1304:CLA:CMB	2.34	0.57
17:3:204:GLY:N	17:3:207:PHE:HA	2.18	0.57
1:A:110:LEU:HD11	1:A:239:PRO:HG2	1.86	0.57
1:A:250:LEU:CB	17:3:136:TRP:HH2	2.02	0.57
1:A:308:ILE:CG2	19:A:1115:CLA:H111	2.35	0.57
1:A:389:TYR:CD1	1:A:625:TRP:CD1	2.92	0.57
1:A:603:PHE:CE2	1:A:735:VAL:HG22	2.40	0.57
2:B:276:HIS:HB2	19:B:1214:CLA:C1B	2.35	0.57
2:B:293:THR:HG21	19:B:1209:CLA:HMA2	1.86	0.57
2:B:302:LYS:NZ	7:G:103:GLY:HA3	2.19	0.57
2:B:303:TYR:N	2:B:306:GLU:HB2	2.19	0.57
2:B:444:LEU:C	2:B:446:PHE:H	2.11	0.57
2:B:454:LEU:HD13	2:B:514:PRO:HG2	1.86	0.57
2:B:465:SER:O	2:B:466:ALA:C	2.44	0.57
2:B:469:LYS:HG3	2:B:470:THR:CB	2.35	0.57
2:B:471:THR:CG2	2:B:502:ASN:HD22	2.18	0.57
2:B:486:LEU:HD13	2:B:489:GLY:H	1.70	0.57
19:B:1205:CLA:C4C	19:B:1205:CLA:H42	2.35	0.57
3:C:2:SER:O	3:C:69:LEU:HB3	2.05	0.57
3:C:64:SER:C	3:C:65:VAL:HG12	2.17	0.57
4:D:172:VAL:O	4:D:173:TYR:HB3	2.05	0.57
5:E:89:SER:OG	5:E:106:ARG:HG3	2.05	0.57
22:E:7048:LMU:H3'	22:E:7048:LMU:C5B	2.34	0.57
6:F:150:VAL:HG21	6:F:160:PHE:CB	2.31	0.57
6:F:157:TRP:HB3	19:F:1305:CLA:HHC	1.85	0.57
7:G:63:VAL:HG23	7:G:64:ILE:H	1.59	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:69:GLY:O	7:G:72:LEU:CB	2.53	0.57
12:L:54:TYR:O	12:L:55:GLN:HB3	2.05	0.57
13:N:148:ASP:CA	13:N:149:ASP:C	2.77	0.57
15:1:71:GLU:HG2	15:1:72:VAL:HG23	1.85	0.57
15:1:78:ARG:HH21	15:1:179:LYS:CB	2.07	0.57
15:1:97:ILE:HD11	15:1:98:LEU:HD23	1.85	0.57
16:2:128:LYS:CG	16:2:131:ILE:HG23	2.35	0.57
17:3:130:GLN:CB	17:3:132:THR:N	2.37	0.57
19:4:4014:CLA:CBC	19:4:4014:CLA:CHD	2.83	0.57
1:A:63:ASP:CG	1:A:65:ASP:H	2.13	0.57
1:A:284:ARG:CA	1:A:298:ASP:OD1	2.53	0.57
1:A:484:LEU:H	1:A:484:LEU:HD23	1.66	0.57
1:A:567:ARG:HH11	4:D:89:GLY:CA	2.16	0.57
1:A:697:ARG:HD3	2:B:566:GLY:O	2.05	0.57
19:A:1132:CLA:O1D	12:L:119:PRO:HA	2.05	0.57
19:A:1136:CLA:CGA	19:A:1136:CLA:C1A	2.83	0.57
2:B:223:GLY:O	2:B:224:PRO:C	2.45	0.57
2:B:232:LEU:CD1	2:B:235:GLN:HB2	2.35	0.57
2:B:233:TYR:HB3	2:B:254:ILE:O	2.04	0.57
2:B:272:ASP:C	2:B:274:ALA:H	2.13	0.57
2:B:643:LEU:HD22	2:B:646:TRP:CD1	2.40	0.57
2:B:668:ARG:NE	2:B:699:ALA:O	2.38	0.57
13:N:146:LEU:CG	13:N:148:ASP:O	2.52	0.57
16:2:195:TYR:CD1	16:2:196:PRO:CD	2.60	0.57
16:2:201:PHE:HD1	16:2:202:ASP:N	2.00	0.57
19:2:2002:CLA:HHD	19:2:2002:CLA:CBC	2.28	0.57
18:4:87:ASN:OD1	18:4:90:TRP:CD1	2.58	0.57
1:A:390:ALA:HB1	1:A:754:ILE:HD13	1.86	0.56
19:A:1131:CLA:H101	19:A:1131:CLA:C14	2.35	0.56
19:A:1135:CLA:HBD	19:A:1135:CLA:HBA2	1.85	0.56
2:B:88:ALA:H	2:B:115:ASN:CA	2.17	0.56
2:B:186:SER:C	2:B:187:SER:O	2.48	0.56
2:B:457:PRO:CG	2:B:517:PHE:HB2	2.34	0.56
2:B:570:ILE:O	2:B:570:ILE:HG13	2.04	0.56
2:B:725:LEU:HD12	2:B:726:ILE:N	2.20	0.56
21:B:6020:BCR:C38	21:B:6020:BCR:C23	2.82	0.56
4:D:100:TYR:HE1	4:D:134:LYS:HG3	1.58	0.56
4:D:102:ILE:CG1	4:D:154:PHE:HB3	2.35	0.56
4:D:177:VAL:HG22	4:D:178:ASN:HA	1.87	0.56
6:F:114:ALA:N	6:F:115:PRO:HD3	2.20	0.56
7:G:96:GLY:O	7:G:97:LEU:CD2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:HIS:HA	7:G:100:PHE:HB2	1.85	0.56
19:H:1145:CLA:H101	19:H:1145:CLA:C14	2.22	0.56
11:K:58:VAL:HG12	11:K:59:THR:N	2.19	0.56
11:K:76:ALA:N	11:K:78:ARG:NH1	2.46	0.56
11:K:115:ILE:HD12	11:K:118:VAL:CG2	2.34	0.56
12:L:164:LEU:HD12	12:L:165:THR:CA	2.34	0.56
13:N:148:ASP:CA	13:N:149:ASP:O	2.53	0.56
15:1:95:PRO:CA	15:1:98:LEU:CB	2.83	0.56
16:2:103:VAL:C	16:2:105:ALA:H	2.13	0.56
16:2:195:TYR:CE1	16:2:196:PRO:HD2	2.37	0.56
19:2:2004:CLA:O1A	19:3:2009:CLA:HBC2	2.05	0.56
17:3:159:VAL:O	17:3:161:GLU:CA	2.53	0.56
18:4:146:PHE:HE2	19:4:4013:CLA:C3C	2.17	0.56
1:A:97:TYR:O	1:A:98:PHE:O	2.23	0.56
1:A:236:GLY:O	1:A:237:VAL:CG2	2.53	0.56
1:A:370:ILE:CD1	19:A:1124:CLA:O1D	2.53	0.56
1:A:438:HIS:HB2	1:A:441:ALA:HB3	1.85	0.56
1:A:502:THR:C	1:A:504:ALA:N	2.51	0.56
1:A:558:LYS:NZ	2:B:674:LEU:HD22	2.20	0.56
19:A:1124:CLA:CHD	19:A:1124:CLA:CBC	2.77	0.56
19:A:1124:CLA:O1A	19:A:1124:CLA:C2	2.51	0.56
2:B:172:GLU:C	2:B:176:ASN:HB2	2.29	0.56
2:B:371:LEU:HD21	19:B:1225:CLA:HED3	1.87	0.56
2:B:510:LEU:C	2:B:510:LEU:HD12	2.29	0.56
19:B:1213:CLA:HED2	19:B:1213:CLA:CBA	2.36	0.56
3:C:26:LEU:HD21	4:D:181:ARG:NH1	2.20	0.56
4:D:138:LEU:O	4:D:138:LEU:HD23	2.05	0.56
4:D:167:HIS:CD2	4:D:167:HIS:O	2.59	0.56
4:D:187:ASN:N	4:D:187:ASN:ND2	2.37	0.56
6:F:82:LEU:CG	6:F:83:THR:N	2.58	0.56
6:F:207:LEU:CD2	6:F:208:PHE:CG	2.88	0.56
7:G:133:ILE:HG23	7:G:133:ILE:O	2.03	0.56
22:H:7002:LMU:H1B	22:H:7002:LMU:O6B	2.05	0.56
16:2:117:ALA:HB3	16:2:230:LEU:CG	2.20	0.56
16:2:195:TYR:HB3	16:2:201:PHE:CE2	2.39	0.56
17:3:148:TYR:CD2	17:3:148:TYR:C	2.78	0.56
17:3:214:GLY:HA3	17:3:215:LYS:HE2	1.85	0.56
19:4:4015:CLA:HBC3	19:4:4015:CLA:CHD	2.34	0.56
1:A:111:ASN:HB3	1:A:112:ASP:OD1	2.04	0.56
1:A:203:LEU:CD2	19:A:1123:CLA:CED	2.83	0.56
1:A:224:HIS:HE1	19:A:1113:CLA:C4C	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:HIS:C	1:A:248:PHE:CE2	2.83	0.56
1:A:263:ALA:O	1:A:264:GLU:HG2	2.06	0.56
1:A:462:ILE:HD11	19:A:9022:CLA:C5	2.32	0.56
1:A:733:VAL:HG22	19:A:1140:CLA:C3D	2.35	0.56
19:A:1112:CLA:CAB	21:A:6002:BCR:H19C	2.36	0.56
19:A:1119:CLA:C4C	19:A:1125:CLA:H172	2.35	0.56
19:A:9022:CLA:CBB	19:A:9023:CLA:CHB	2.79	0.56
19:A:9023:CLA:H142	21:I:6018:BCR:C4	2.36	0.56
2:B:293:THR:H	19:B:1217:CLA:CED	2.18	0.56
2:B:495:PRO:O	2:B:499:ASN:ND2	2.39	0.56
19:B:1206:CLA:H203	21:I:6018:BCR:H372	1.85	0.56
19:B:1206:CLA:H122	21:I:6018:BCR:H373	1.87	0.56
21:B:6010:BCR:H321	21:B:6010:BCR:HC8	1.88	0.56
4:D:104:TRP:N	4:D:104:TRP:CD1	2.73	0.56
6:F:215:VAL:O	6:F:218:TYR:N	2.38	0.56
7:G:90:GLN:N	7:G:90:GLN:OE1	2.39	0.56
8:H:104:GLY:O	8:H:105:GLY:C	2.47	0.56
11:K:57:MET:O	11:K:61:THR:OG1	2.22	0.56
11:K:60:SER:O	11:K:61:THR:C	2.44	0.56
11:K:70:PHE:CB	11:K:98:PRO:HB3	2.32	0.56
11:K:122:LEU:HD22	11:K:122:LEU:C	2.30	0.56
12:L:141:LEU:CD1	21:L:6019:BCR:H312	2.17	0.56
15:1:64:PHE:CD1	15:1:65:ASP:HB3	2.40	0.56
15:1:77:GLU:CD	15:1:80:LYS:CE	2.78	0.56
15:1:90:ALA:O	15:1:91:MET:C	2.45	0.56
15:1:91:MET:SD	15:1:94:VAL:HB	2.45	0.56
16:2:103:VAL:O	16:2:104:GLN:C	2.48	0.56
16:2:150:THR:O	16:2:152:LEU:HD13	2.05	0.56
16:2:172:LEU:O	16:2:174:PRO:CD	2.46	0.56
19:2:2001:CLA:O1A	19:2:2001:CLA:C1A	2.53	0.56
17:3:184:LYS:O	17:3:185:GLN:CB	2.53	0.56
18:4:111:LEU:HD12	18:4:112:PRO:HD3	1.78	0.56
18:4:156:ARG:HD2	19:4:4011:CLA:C2D	2.35	0.56
18:4:177:LEU:N	18:4:178:PRO:CD	2.68	0.56
18:4:226:LYS:N	18:4:226:LYS:HZ3	2.04	0.56
18:4:246:GLN:O	18:4:246:GLN:CG	2.52	0.56
19:4:1306:CLA:H2	19:4:1306:CLA:CED	2.31	0.56
1:A:68:THR:HG23	1:A:69:SER:N	2.20	0.56
1:A:187:HIS:CE1	19:A:1109:CLA:C1A	2.74	0.56
19:A:1138:CLA:CBB	19:A:1138:CLA:H101	2.35	0.56
2:B:25:ILE:CG2	21:L:6019:BCR:C28	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:LEU:CD1	19:B:1221:CLA:HED1	2.35	0.56
2:B:315:LEU:O	2:B:315:LEU:HD22	2.06	0.56
2:B:558:PRO:HG3	2:B:574:ASP:OD1	2.06	0.56
2:B:623:TYR:O	2:B:624:LEU:HB3	2.03	0.56
19:B:1220:CLA:H43	19:B:1220:CLA:CAA	2.31	0.56
3:C:7:ILE:HD13	3:C:54:CYS:SG	2.45	0.56
3:C:23:THR:HG21	3:C:47:ASP:OD2	2.06	0.56
19:J:1308:CLA:HMA2	19:2:2014:CLA:CED	2.34	0.56
15:1:157:ASP:O	15:1:158:PRO:C	2.48	0.56
15:1:170:PRO:O	15:1:173:TYR:CZ	2.58	0.56
15:1:189:LYS:CA	15:1:189:LYS:CE	2.74	0.56
16:2:112:TRP:CG	19:2:2012:CLA:O1D	2.58	0.56
16:2:165:GLY:HA2	16:2:167:ARG:HG2	1.86	0.56
18:4:95:GLU:HA	18:4:98:ASN:OD1	2.05	0.56
18:4:121:ILE:CG1	18:4:122:ASN:H	2.18	0.56
18:4:144:ILE:O	18:4:145:GLU:C	2.46	0.56
1:A:130:GLU:O	1:A:130:GLU:CD	2.48	0.56
1:A:242:ILE:CB	1:A:243:PRO:HD3	2.34	0.56
1:A:267:THR:CG2	1:A:269:PHE:CE2	2.59	0.56
1:A:281:LEU:HD22	19:A:1115:CLA:HED2	1.83	0.56
1:A:402:ILE:C	1:A:404:GLY:H	2.13	0.56
1:A:438:HIS:HA	4:D:87:THR:OG1	2.05	0.56
1:A:564:ARG:CB	1:A:564:ARG:CZ	2.83	0.56
1:A:578:ARG:HB2	1:A:578:ARG:NH1	2.19	0.56
1:A:645:SER:OG	1:A:655:ASP:OD1	2.15	0.56
19:A:1102:CLA:CBA	19:A:1109:CLA:H62	2.35	0.56
19:A:1115:CLA:CMC	19:A:1115:CLA:CBC	2.82	0.56
19:A:9023:CLA:HBA2	19:A:9023:CLA:HED3	1.87	0.56
2:B:131:THR:HG22	2:B:131:THR:O	2.04	0.56
2:B:230:TRP:H	7:G:63:VAL:HG21	1.63	0.56
2:B:586:THR:C	2:B:588:GLY:N	2.56	0.56
20:B:5002:PQN:H302	21:L:6019:BCR:H24C	1.86	0.56
3:C:1:MET:H3	3:C:4:SER:CB	2.16	0.56
5:E:78:ARG:NH1	5:E:125:ILE:CB	2.65	0.56
6:F:221:LEU:CD2	6:F:222:LEU:HD21	2.31	0.56
8:H:121:LEU:O	8:H:122:PRO:C	2.47	0.56
11:K:127:ILE:HG12	11:K:130:LEU:CD1	2.28	0.56
11:K:127:ILE:HG23	11:K:130:LEU:HG	1.64	0.56
13:N:133:GLY:O	13:N:134:CYS:SG	2.60	0.56
13:N:146:LEU:HG	13:N:148:ASP:O	2.06	0.56
15:1:123:THR:O	15:1:124:TYR:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:221:LEU:CD1	19:1:1003:CLA:HAC1	2.29	0.56
17:3:164:LEU:CD1	17:3:165:MET:SD	2.93	0.56
18:4:145:GLU:OE2	18:4:146:PHE:HE1	1.88	0.56
18:4:207:ASN:OD1	19:4:4002:CLA:NB	2.39	0.56
1:A:331:LEU:CD2	1:A:331:LEU:O	2.52	0.56
1:A:685:VAL:HG22	19:A:1140:CLA:HBB2	1.86	0.56
1:A:700:TRP:HZ3	19:A:9013:CLA:O1D	1.89	0.56
19:A:9023:CLA:HMC1	19:A:9023:CLA:CBC	2.35	0.56
2:B:193:HIS:HB2	19:B:1211:CLA:CHC	2.36	0.56
2:B:351:HIS:O	2:B:355:LEU:HB2	2.05	0.56
2:B:355:LEU:HD21	2:B:508:LEU:HD21	1.87	0.56
19:B:1205:CLA:H142	19:B:1205:CLA:C10	2.34	0.56
3:C:72:GLU:OE2	3:C:77:MET:HE1	2.05	0.56
4:D:140:LEU:CD1	4:D:144:LEU:N	2.69	0.56
5:E:90:VAL:CG1	5:E:91:VAL:H	2.19	0.56
6:F:199:ASP:HA	10:J:9:SER:HA	1.87	0.56
8:H:82:LYS:HG2	8:H:85:GLU:CB	2.36	0.56
8:H:82:LYS:HG2	8:H:85:GLU:HB3	1.87	0.56
19:H:1145:CLA:HMA1	19:H:1145:CLA:O2A	2.04	0.56
13:N:113:ASN:OD1	13:N:113:ASN:O	2.24	0.56
22:R:7021:LMU:H41	22:R:7021:LMU:H6D	1.87	0.56
15:1:151:GLN:NE2	15:1:151:GLN:HA	2.19	0.56
15:1:170:PRO:CG	15:1:173:TYR:CE2	2.88	0.56
16:2:157:LEU:HD13	16:2:157:LEU:N	2.19	0.56
18:4:212:LEU:O	18:4:213:ALA:HB3	2.04	0.56
1:A:57:LEU:CD2	1:A:58:HIS:N	2.68	0.56
1:A:426:THR:CG2	1:A:428:TYR:CZ	2.88	0.56
1:A:451:ILE:HD13	19:A:1131:CLA:HED1	1.84	0.56
19:A:1112:CLA:CHC	21:A:6002:BCR:C17	2.82	0.56
19:A:1127:CLA:H51	21:A:6003:BCR:H331	1.87	0.56
2:B:436:LEU:O	2:B:437:TYR:HB2	2.06	0.56
2:B:614:THR:CG2	2:B:614:THR:O	2.50	0.56
4:D:147:LYS:O	4:D:148:TYR:CG	2.58	0.56
4:D:177:VAL:O	4:D:177:VAL:HG13	2.05	0.56
5:E:75:LYS:HA	5:E:87:THR:CG2	2.31	0.56
6:F:88:SER:O	6:F:91:PHE:N	2.39	0.56
6:F:148:LEU:O	6:F:148:LEU:CD1	2.48	0.56
6:F:221:LEU:C	6:F:222:LEU:HD23	2.31	0.56
7:G:151:PRO:O	7:G:151:PRO:HD2	2.05	0.56
10:J:31:ARG:NH2	19:J:1311:CLA:C3B	2.69	0.56
13:N:164:SER:CA	13:N:165:ASN:C	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:7021:LMU:H22	22:R:7021:LMU:C6	2.33	0.56
15:1:81:GLU:CG	15:1:82:SER:N	2.68	0.56
15:1:117:LEU:N	15:1:117:LEU:CD1	2.67	0.56
15:1:170:PRO:CG	15:1:171:LEU:N	2.58	0.56
17:3:125:VAL:HG21	19:3:3010:CLA:C1C	2.35	0.56
1:A:58:HIS:CE1	19:A:1101:CLA:ND	2.74	0.56
1:A:190:ALA:HB1	1:A:191:PRO:HD2	1.85	0.56
1:A:336:GLY:HA2	19:A:1151:CLA:HMC1	1.84	0.56
1:A:479:ASP:CG	1:A:536:THR:HG22	2.29	0.56
1:A:544:ILE:HD11	19:A:9011:CLA:H193	1.88	0.56
1:A:665:ILE:C	1:A:665:ILE:HD12	2.30	0.56
1:A:716:VAL:O	19:A:1139:CLA:HMD2	2.06	0.56
19:A:1116:CLA:H52	19:A:1133:CLA:HBA1	1.87	0.56
19:A:1119:CLA:H18	21:A:6007:BCR:H383	1.87	0.56
19:A:1127:CLA:CHD	21:A:6003:BCR:H333	2.36	0.56
2:B:317:ARG:CZ	2:B:410:ARG:CG	2.68	0.56
2:B:404:ALA:O	2:B:405:ASP:CG	2.48	0.56
24:B:7101:LMG:O3	3:C:70:TRP:HZ2	1.84	0.56
3:C:43:PRO:O	3:C:43:PRO:CD	2.54	0.56
3:C:66:ARG:HG2	3:C:66:ARG:NH2	1.95	0.56
5:E:73:LYS:O	5:E:73:LYS:HG3	2.06	0.56
6:F:184:ALA:C	6:F:185:ILE:HG23	2.29	0.56
6:F:215:VAL:O	6:F:218:TYR:HB2	2.06	0.56
10:J:2:ARG:HB3	10:J:7:TYR:CZ	2.41	0.56
15:1:78:ARG:HH21	15:1:179:LYS:CG	2.15	0.56
15:1:161:LYS:O	15:1:161:LYS:HD2	2.06	0.56
16:2:146:PHE:N	16:2:146:PHE:CD1	2.73	0.56
16:2:226:ARG:HA	16:2:229:MET:HB3	1.87	0.56
22:3:7003:LMU:C2B	22:3:7005:LMU:H6'1	2.36	0.56
1:A:252:ARG:NH2	1:A:261:SER:OG	2.39	0.56
1:A:426:THR:CA	1:A:428:TYR:CE2	2.84	0.56
1:A:580:PRO:HA	1:A:728:VAL:CG2	2.36	0.56
1:A:586:ARG:HG3	3:C:49:VAL:CG2	2.31	0.56
1:A:639:ALA:O	1:A:641:ASN:N	2.39	0.56
19:A:1124:CLA:CHB	21:A:6008:BCR:H363	2.35	0.56
19:A:9023:CLA:H142	21:I:6018:BCR:HC42	1.87	0.56
2:B:12:ILE:HG22	2:B:13:ALA:N	2.20	0.56
2:B:197:VAL:O	2:B:198:ALA:HB2	2.06	0.56
2:B:324:ASP:O	2:B:328:ASN:CG	2.48	0.56
2:B:419:ILE:HG12	2:B:536:LYS:HB2	1.88	0.56
2:B:457:PRO:HB3	2:B:517:PHE:CG	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:SER:OG	2:B:506:ASN:OD1	2.23	0.56
5:E:79:LYS:N	5:E:84:TYR:CE1	2.74	0.56
7:G:89:LYS:HA	7:G:89:LYS:HZ1	1.63	0.56
8:H:109:LEU:HD23	19:H:1207:CLA:H52	1.86	0.56
13:N:131:PHE:CA	13:N:132:THR:HG22	2.35	0.56
14:R:36:UNK:C	14:R:38:UNK:N	2.66	0.56
19:3:3013:CLA:H91	19:3:3013:CLA:H121	1.87	0.56
1:A:98:PHE:CZ	19:A:1105:CLA:HMD3	2.41	0.56
1:A:159:THR:HG22	1:A:160:SER:N	2.20	0.56
1:A:358:LEU:HD21	1:A:413:HIS:ND1	2.21	0.56
1:A:545:HIS:CE1	1:A:612:VAL:HG22	2.41	0.56
19:A:1112:CLA:CMB	21:A:6002:BCR:H382	2.36	0.56
2:B:471:THR:HG22	2:B:502:ASN:HD22	1.71	0.56
2:B:493:TRP:O	2:B:495:PRO:HG3	2.06	0.56
2:B:655:LEU:CD2	19:B:1239:CLA:CBB	2.84	0.56
2:B:707:LEU:O	2:B:710:LEU:HB3	2.06	0.56
2:B:732:LYS:HG2	2:B:733:PHE:HA	1.88	0.56
19:B:1203:CLA:C19	19:B:1224:CLA:H141	2.36	0.56
4:D:184:VAL:HG12	4:D:185:GLY:N	2.21	0.56
5:E:96:ASP:CG	5:E:98:ASN:OD1	2.49	0.56
6:F:168:LEU:O	6:F:171:ALA:O	2.23	0.56
9:I:10:PRO:O	9:I:15:LEU:N	2.32	0.56
10:J:32:PHE:HE2	10:J:33:PHE:CZ	2.23	0.56
11:K:56:ILE:O	11:K:56:ILE:HG22	2.05	0.56
19:K:1146:CLA:O1A	19:K:1146:CLA:H2A	2.05	0.56
12:L:51:LYS:N	12:L:51:LYS:CD	2.66	0.56
12:L:164:LEU:O	12:L:165:THR:HG22	2.05	0.56
13:N:146:LEU:C	13:N:147:SER:O	2.48	0.56
15:1:170:PRO:HG2	15:1:173:TYR:CD2	2.41	0.56
15:1:178:LYS:C	15:1:178:LYS:CD	2.71	0.56
16:2:122:ILE:N	16:2:123:PRO:HD3	2.20	0.56
19:A:9012:CLA:C3B	2:B:589:TRP:CH2	2.85	0.55
2:B:382:ILE:CG2	2:B:383:MET:N	2.48	0.55
2:B:438:VAL:CG2	19:B:1230:CLA:HAC1	2.35	0.55
19:B:1220:CLA:H93	19:B:1227:CLA:CBC	2.37	0.55
6:F:149:ILE:HG22	6:F:151:SER:N	2.21	0.55
6:F:200:VAL:CG2	6:F:204:SER:N	2.70	0.55
11:K:124:LEU:O	11:K:126:ASN:CB	2.54	0.55
12:L:82:TYR:O	12:L:83:LEU:CB	2.54	0.55
12:L:104:LEU:HD11	12:L:199:TRP:CZ2	2.41	0.55
19:L:1148:CLA:CED	19:L:1148:CLA:C1	2.77	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:125:LEU:O	15:1:125:LEU:HD23	2.06	0.55
16:2:150:THR:O	16:2:153:PHE:N	2.39	0.55
16:2:254:LEU:HD22	16:2:256:ASP:H	1.69	0.55
18:4:108:GLY:C	18:4:109:MET:O	2.49	0.55
1:A:362:LEU:CB	1:A:410:ALA:HB2	2.36	0.55
19:A:1124:CLA:HED2	19:A:1124:CLA:HAA1	1.87	0.55
19:A:1131:CLA:H52	21:B:6017:BCR:C34	2.34	0.55
19:A:1141:CLA:H71	19:A:1141:CLA:C12	2.09	0.55
2:B:290:MET:O	2:B:290:MET:HG2	2.06	0.55
2:B:347:LEU:HD22	2:B:351:HIS:CE1	2.42	0.55
2:B:356:PRO:O	2:B:356:PRO:CD	2.55	0.55
2:B:560:ASP:OD1	3:C:52:LYS:NZ	2.35	0.55
4:D:123:ARG:NH2	22:D:7050:LMU:H6'1	1.59	0.55
6:F:90:GLN:HG2	6:F:143:ASP:H	1.70	0.55
8:H:111:TYR:CD1	8:H:112:LEU:HD21	2.41	0.55
9:I:14:LEU:O	9:I:17:PRO:HD2	2.06	0.55
12:L:169:ARG:HG2	12:L:172:GLU:CA	2.37	0.55
13:N:155:GLU:CB	13:N:157:LYS:CA	2.79	0.55
22:N:7049:LMU:O1'	22:N:7049:LMU:C6	2.55	0.55
1:A:316:MET:CA	1:A:317:TYR:HB2	2.31	0.55
1:A:393:LEU:HD11	1:A:750:PHE:CE1	2.41	0.55
19:A:1124:CLA:H2	19:A:1125:CLA:CED	2.35	0.55
19:A:1126:CLA:C20	21:J:6012:BCR:C17	2.79	0.55
19:A:1138:CLA:CMD	21:F:6014:BCR:HC41	2.36	0.55
2:B:98:GLN:O	2:B:100:ALA:CB	2.55	0.55
2:B:292:ARG:HH21	2:B:297:ILE:HG13	1.70	0.55
2:B:459:PHE:CD2	19:B:1235:CLA:C1D	2.66	0.55
3:C:44:ARG:CA	4:D:182:GLN:CD	2.69	0.55
6:F:88:SER:O	6:F:89:LYS:C	2.48	0.55
7:G:106:ARG:HB2	7:G:107:ALA:HA	1.88	0.55
8:H:61:THR:HA	8:H:62:THR:HG23	0.63	0.55
19:H:1145:CLA:HMA1	19:H:1145:CLA:C1	2.35	0.55
11:K:78:ARG:CZ	11:K:78:ARG:H	2.20	0.55
11:K:81:THR:HG23	11:K:82:ALA:N	2.22	0.55
11:K:97:ASP:HA	11:K:101:PHE:CE2	2.41	0.55
12:L:141:LEU:O	12:L:145:LEU:HD12	2.07	0.55
13:N:139:LYS:HG3	13:N:142:LYS:CG	2.37	0.55
15:1:115:ALA:O	15:1:116:ALA:HB3	2.05	0.55
18:4:191:PRO:O	18:4:192:LEU:HB2	2.06	0.55
22:4:7053:LMU:H6E	22:4:7053:LMU:C2B	2.36	0.55
1:A:29:THR:O	1:A:29:THR:CG2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:C	1:A:235:ALA:H	2.14	0.55
1:A:458:PHE:CD2	19:A:9022:CLA:HMB3	2.41	0.55
1:A:541:VAL:HG12	1:A:545:HIS:NE2	2.22	0.55
1:A:629:ASN:O	1:A:632:GLY:N	2.39	0.55
19:A:1124:CLA:HED3	19:A:1125:CLA:CMD	2.30	0.55
19:A:9023:CLA:HBC1	2:B:665:ILE:HD12	1.89	0.55
2:B:459:PHE:CG	19:B:1235:CLA:CAD	2.89	0.55
2:B:544:SER:O	2:B:547:MET:C	2.49	0.55
2:B:617:MET:HG3	2:B:618:GLY:N	2.21	0.55
2:B:622:ASP:CB	2:B:626:LEU:CG	2.85	0.55
19:B:1222:CLA:CED	19:B:1223:CLA:CMD	2.85	0.55
19:B:1224:CLA:O1D	19:B:1225:CLA:CMA	2.54	0.55
3:C:12:ILE:HB	3:C:38:GLN:O	2.07	0.55
4:D:91:LEU:C	4:D:91:LEU:HD12	2.32	0.55
5:E:96:ASP:CB	5:E:98:ASN:OD1	2.54	0.55
5:E:102:PRO:O	5:E:120:TYR:O	2.24	0.55
6:F:94:ARG:HA	6:F:94:ARG:NE	2.21	0.55
7:G:68:THR:OG1	7:G:69:GLY:N	2.39	0.55
8:H:60:ASN:C	8:H:60:ASN:OD1	2.47	0.55
10:J:10:VAL:CG1	10:J:11:ALA:N	2.68	0.55
12:L:92:ALA:CB	12:L:98:ARG:CZ	2.84	0.55
19:L:1130:CLA:HAC2	19:L:1504:CLA:HMC3	1.87	0.55
19:L:1148:CLA:HAA1	19:L:1148:CLA:O1D	2.03	0.55
15:1:141:GLU:O	15:1:145:ILE:CG1	2.53	0.55
17:3:94:GLU:HB3	17:3:95:PRO:HD3	1.88	0.55
17:3:97:TRP:O	17:3:98:LEU:C	2.48	0.55
22:3:7003:LMU:O2B	22:3:7005:LMU:C6B	2.55	0.55
18:4:126:TRP:HA	19:4:4006:CLA:HMD1	1.87	0.55
1:A:107:GLU:OE2	1:A:161:GLU:CG	2.45	0.55
1:A:158:ILE:HD13	19:A:1112:CLA:CED	2.36	0.55
1:A:201:SER:O	1:A:204:ASN:N	2.40	0.55
1:A:338:PHE:HB3	19:A:1129:CLA:HBD	1.89	0.55
1:A:492:ILE:O	1:A:493:GLN:C	2.47	0.55
19:A:1106:CLA:CMB	19:A:1107:CLA:H11	2.36	0.55
19:A:1141:CLA:CMA	19:A:1141:CLA:C1	2.80	0.55
2:B:261:PHE:CE2	2:B:499:ASN:C	2.76	0.55
2:B:542:ARG:NH1	2:B:542:ARG:HB3	2.18	0.55
2:B:686:PRO:C	2:B:688:ALA:H	2.14	0.55
4:D:80:SER:H	4:D:81:PRO:HD3	1.70	0.55
6:F:100:LYS:O	6:F:100:LYS:CD	2.53	0.55
12:L:102:VAL:CA	19:L:1502:CLA:HED2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:144:PRO:HA	13:N:151:ASP:CG	2.31	0.55
15:1:147:PHE:CD1	15:1:147:PHE:O	2.59	0.55
16:2:120:ILE:C	16:2:123:PRO:HD2	2.31	0.55
16:2:187:LYS:HE3	16:2:187:LYS:C	2.31	0.55
17:3:161:GLU:HA	17:3:164:LEU:CG	2.32	0.55
22:3:7003:LMU:H3B	22:3:7005:LMU:C3B	2.31	0.55
19:4:4002:CLA:CGD	19:4:4002:CLA:CAA	2.75	0.55
1:A:64:PHE:N	1:A:64:PHE:CD1	2.73	0.55
19:A:1106:CLA:H111	21:J:6012:BCR:C11	2.36	0.55
2:B:49:SER:O	2:B:52:GLY:N	2.40	0.55
2:B:175:LEU:HA	2:B:178:HIS:HB2	1.88	0.55
2:B:710:LEU:C	2:B:712:HIS:H	2.13	0.55
21:B:6010:BCR:H382	21:B:6010:BCR:C23	2.34	0.55
21:B:6017:BCR:H23C	21:B:6017:BCR:C38	2.26	0.55
4:D:95:GLN:NE2	4:D:95:GLN:C	2.64	0.55
4:D:173:TYR:O	4:D:175:GLU:HG3	2.07	0.55
5:E:82:TYR:CB	5:E:83:TRP:HZ3	2.14	0.55
6:F:123:MET:O	6:F:126:THR:N	2.39	0.55
6:F:209:ARG:O	6:F:212:SER:C	2.50	0.55
8:H:89:ALA:N	8:H:90:PRO:HD2	2.22	0.55
11:K:50:GLY:N	11:K:52:PRO:CD	2.68	0.55
13:N:104:LYS:O	13:N:107:LEU:CA	2.55	0.55
13:N:139:LYS:HG3	13:N:142:LYS:HE2	1.87	0.55
15:1:137:ILE:HB	15:1:141:GLU:OE2	2.07	0.55
19:1:1005:CLA:HMC3	19:1:1005:CLA:HBC2	1.89	0.55
16:2:165:GLY:O	16:2:167:ARG:CG	2.54	0.55
17:3:176:TRP:O	17:3:177:ALA:C	2.49	0.55
17:3:210:PRO:CG	17:3:211:LEU:N	2.69	0.55
18:4:173:LYS:CA	18:4:194:PHE:CD2	2.89	0.55
18:4:174:GLN:CA	18:4:176:SER:H	2.19	0.55
1:A:23:ASP:CB	1:A:33:GLN:CD	2.74	0.55
1:A:230:ASN:OD1	1:A:296:LEU:HD22	2.07	0.55
1:A:373:ALA:O	1:A:396:PHE:HD1	1.88	0.55
1:A:420:ARG:HB3	1:A:420:ARG:CZ	2.32	0.55
1:A:710:ALA:HB1	19:A:1138:CLA:HED2	1.88	0.55
19:A:9012:CLA:CED	19:B:9010:CLA:H2	2.36	0.55
2:B:18:THR:O	2:B:21:ILE:N	2.40	0.55
2:B:596:TRP:O	2:B:597:LYS:HB3	2.06	0.55
2:B:682:HIS:O	2:B:683:GLU:C	2.50	0.55
2:B:707:LEU:CD1	2:B:711:VAL:HG21	2.37	0.55
2:B:732:LYS:CG	2:B:733:PHE:HA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1205:CLA:CGA	19:B:1205:CLA:C1A	2.85	0.55
19:B:1225:CLA:H101	21:B:6006:BCR:H343	1.89	0.55
4:D:129:LEU:HD12	4:D:130:LYS:H	1.71	0.55
5:E:69:LYS:HE3	5:E:69:LYS:H	1.71	0.55
19:G:1242:CLA:O1A	22:G:7026:LMU:H101	2.07	0.55
13:N:146:LEU:HD13	17:3:142:ILE:HB	1.89	0.55
13:N:147:SER:O	13:N:148:ASP:CG	2.50	0.55
13:N:155:GLU:CB	13:N:157:LYS:CE	2.78	0.55
13:N:169:LYS:CA	13:N:170:TRP:HD1	2.20	0.55
15:1:122:ALA:HB3	15:1:124:TYR:H	1.72	0.55
16:2:228:ALA:O	16:2:229:MET:C	2.44	0.55
17:3:110:MET:CE	17:3:238:ILE:H	2.20	0.55
17:3:154:ASN:HA	17:3:155:TYR:CD2	2.41	0.55
22:3:7005:LMU:C2B	22:3:7005:LMU:C3'	2.85	0.55
18:4:232:LEU:HD12	18:4:233:LEU:C	2.31	0.55
1:A:109:TRP:CH2	1:A:154:ARG:HD3	2.42	0.55
19:A:1113:CLA:HBA2	19:A:1113:CLA:H42	1.88	0.55
19:A:1131:CLA:HAA1	21:B:6020:BCR:C14	2.37	0.55
19:A:1237:CLA:H112	19:A:1237:CLA:H61	1.87	0.55
21:A:6011:BCR:C19	19:A:9012:CLA:H172	2.37	0.55
22:A:7010:LMU:H22	22:K:7047:LMU:H101	1.89	0.55
2:B:160:LYS:CE	2:B:161:TRP:CD2	2.90	0.55
2:B:334:LEU:O	2:B:334:LEU:CG	2.51	0.55
2:B:419:ILE:C	2:B:420:SER:OG	2.50	0.55
2:B:473:GLY:O	2:B:474:PHE:HB2	2.06	0.55
2:B:502:ASN:ND2	2:B:511:THR:HG21	2.22	0.55
2:B:507:SER:O	2:B:508:LEU:HB2	2.05	0.55
2:B:607:SER:OG	2:B:608:GLN:N	2.39	0.55
4:D:98:GLU:HB2	4:D:100:TYR:CE2	2.42	0.55
4:D:146:SER:O	4:D:147:LYS:CG	2.51	0.55
5:E:93:VAL:O	5:E:93:VAL:CG1	2.54	0.55
6:F:194:LYS:O	6:F:197:ILE:O	2.25	0.55
19:F:1305:CLA:HED2	19:F:1305:CLA:CAD	2.36	0.55
7:G:134:GLY:O	7:G:135:HIS:ND1	2.40	0.55
8:H:61:THR:C	8:H:62:THR:HG23	2.25	0.55
22:H:7032:LMU:H31	22:H:7032:LMU:O5B	2.07	0.55
12:L:166:LEU:O	12:L:167:THR:C	2.45	0.55
15:1:133:THR:C	15:1:137:ILE:HD13	2.31	0.55
16:2:101:TRP:CA	16:2:103:VAL:N	2.62	0.55
16:2:145:TYR:C	16:2:146:PHE:CG	2.85	0.55
17:3:96:ARG:CA	17:3:99:ALA:HB2	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:124:PRO:O	18:4:125:LYS:CB	2.55	0.55
18:4:158:GLN:HE21	19:4:1004:CLA:C4A	2.18	0.55
18:4:169:ASP:O	18:4:173:LYS:CB	2.54	0.55
19:4:4002:CLA:O1A	19:4:4002:CLA:C2	2.52	0.55
22:4:7033:LMU:H3'	22:4:7033:LMU:O5B	2.05	0.55
1:A:229:ILE:HG22	1:A:229:ILE:O	2.06	0.55
1:A:281:LEU:HD22	19:A:1115:CLA:H2A	1.87	0.55
1:A:466:THR:HG22	2:B:648:TRP:NE1	2.21	0.55
1:A:472:ARG:N	1:A:473:PRO:CD	2.68	0.55
2:B:31:PHE:O	2:B:32:GLU:C	2.50	0.55
2:B:224:PRO:HB2	2:B:227:THR:CG2	2.36	0.55
2:B:348:VAL:HG12	2:B:349:ALA:N	2.22	0.55
19:B:1210:CLA:H41	19:B:1215:CLA:CBC	2.36	0.55
3:C:62:PHE:CE1	5:E:80:GLU:CB	2.87	0.55
4:D:167:HIS:HD2	4:D:167:HIS:O	1.90	0.55
22:E:7048:LMU:C7	22:E:7048:LMU:C11	2.83	0.55
7:G:134:GLY:O	7:G:135:HIS:CD2	2.60	0.55
19:G:1242:CLA:H3A	19:G:1242:CLA:O2A	2.06	0.55
8:H:107:SER:O	8:H:111:TYR:HB2	2.07	0.55
19:H:1145:CLA:O2D	19:H:1145:CLA:CAA	2.55	0.55
11:K:115:ILE:O	11:K:116:ILE:C	2.47	0.55
12:L:205:TYR:CD1	12:L:207:LEU:HD13	2.33	0.55
13:N:139:LYS:C	13:N:142:LYS:NZ	2.64	0.55
15:1:170:PRO:HB2	15:1:171:LEU:O	2.06	0.55
15:1:171:LEU:HD23	15:1:171:LEU:N	2.22	0.55
22:1:7004:LMU:H3'	22:1:7004:LMU:C1	2.25	0.55
19:2:2014:CLA:C4A	19:2:2014:CLA:HBA2	2.35	0.55
17:3:206:PRO:HD2	17:3:206:PRO:O	2.07	0.55
17:3:238:ILE:CD1	19:3:3003:CLA:CMC	2.84	0.55
18:4:83:GLU:C	18:4:84:ASP:CG	2.74	0.55
18:4:125:LYS:NZ	18:4:136:ALA:O	2.34	0.55
18:4:172:PHE:HB2	18:4:173:LYS:O	2.06	0.55
1:A:250:LEU:CD1	17:3:136:TRP:HZ2	2.20	0.55
1:A:336:GLY:HA3	19:A:1151:CLA:CMC	2.37	0.55
1:A:461:TYR:CE1	1:A:540:LEU:HD11	2.42	0.55
1:A:607:ASN:HD21	19:A:9022:CLA:C2C	2.19	0.55
19:A:1140:CLA:H192	10:J:19:PHE:CD2	2.42	0.55
19:A:9013:CLA:H3A	19:A:9013:CLA:CGA	2.37	0.55
2:B:104:PHE:O	2:B:105:THR:CB	2.54	0.55
2:B:163:PRO:C	2:B:164:SER:OG	2.48	0.55
2:B:560:ASP:OD1	3:C:65:VAL:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1213:CLA:HBC2	19:B:1213:CLA:CHD	2.29	0.55
19:B:1235:CLA:C15	21:F:6016:BCR:H313	2.25	0.55
3:C:26:LEU:HD22	4:D:181:ARG:HH11	1.71	0.55
4:D:101:VAL:HA	4:D:130:LYS:HA	1.87	0.55
4:D:203:THR:HG22	4:D:205:LYS:N	2.16	0.55
6:F:158:GLY:O	10:J:38:ILE:HG23	2.06	0.55
6:F:225:GLU:O	6:F:227:VAL:CG1	2.54	0.55
19:G:1242:CLA:HAA2	19:G:1242:CLA:HBD	1.88	0.55
8:H:55:LEU:O	8:H:56:GLU:C	2.50	0.55
22:K:7042:LMU:H32	22:K:7042:LMU:O5'	2.06	0.55
12:L:125:ILE:HG12	12:L:127:GLY:H	1.72	0.55
13:N:118:TYR:O	13:N:119:THR:CG2	2.53	0.55
13:N:169:LYS:HA	13:N:170:TRP:HD1	1.71	0.55
15:1:170:PRO:CD	15:1:173:TYR:HD2	2.16	0.55
15:1:193:LEU:HD23	15:1:193:LEU:O	2.07	0.55
16:2:149:THR:O	16:2:152:LEU:HD11	2.07	0.55
16:2:184:PRO:N	16:2:187:LYS:CD	2.70	0.55
17:3:98:LEU:HD21	17:3:102:GLU:HG3	1.88	0.55
17:3:185:GLN:CG	17:3:186:TYR:N	2.33	0.55
17:3:233:LEU:C	17:3:235:MET:N	2.65	0.55
18:4:202:GLU:HA	18:4:205:ILE:HG23	1.89	0.55
22:4:7053:LMU:H72	22:4:7053:LMU:C11	2.37	0.55
1:A:75:SER:HB3	1:A:354:TRP:HZ2	1.71	0.54
1:A:255:LEU:O	1:A:256:ALA:C	2.49	0.54
1:A:448:TRP:CD1	19:A:1131:CLA:CED	2.90	0.54
1:A:622:SER:OG	1:A:642:PHE:HB2	2.07	0.54
1:A:728:VAL:HG22	1:A:731:ARG:HH12	1.72	0.54
22:A:7023:LMU:C6B	22:A:7023:LMU:C2B	2.82	0.54
2:B:314:ARG:NH1	15:1:67:LEU:HD11	2.23	0.54
2:B:330:ILE:HD11	19:B:1202:CLA:H193	1.87	0.54
19:B:1201:CLA:HBC3	19:B:1226:CLA:H51	1.88	0.54
6:F:89:LYS:O	6:F:90:GLN:C	2.47	0.54
21:I:6021:BCR:C39	21:L:6019:BCR:C40	2.81	0.54
10:J:10:VAL:HG13	10:J:11:ALA:N	2.21	0.54
11:K:56:ILE:O	11:K:56:ILE:CG2	2.55	0.54
15:1:130:PRO:O	15:1:131:TRP:CE3	2.42	0.54
15:1:145:ILE:O	15:1:148:VAL:HG12	2.07	0.54
16:2:161:GLY:O	16:2:162:TRP:C	2.50	0.54
16:2:224:ASN:C	16:2:227:LEU:H	2.15	0.54
16:2:269:LYS:HA	16:2:269:LYS:HZ1	1.65	0.54
19:3:3011:CLA:H3A	19:3:3011:CLA:CGA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:OG1	19:A:1139:CLA:CAB	2.54	0.54
1:A:286:GLY:O	1:A:295:TRP:CD1	2.59	0.54
1:A:295:TRP:CD1	1:A:295:TRP:N	2.75	0.54
1:A:396:PHE:HE2	1:A:616:PHE:CG	2.26	0.54
1:A:426:THR:HA	1:A:428:TYR:CD2	2.43	0.54
19:A:1101:CLA:O1D	19:A:1101:CLA:HBA2	2.07	0.54
19:A:1120:CLA:HBC3	19:A:1122:CLA:HED1	1.90	0.54
21:A:6007:BCR:H23C	21:A:6007:BCR:C38	2.21	0.54
2:B:20:ARG:CG	2:B:20:ARG:NH1	2.49	0.54
2:B:23:PHE:O	2:B:24:GLY:C	2.49	0.54
2:B:124:TRP:NE1	2:B:129:LEU:O	2.36	0.54
2:B:174:ARG:NH1	19:B:1221:CLA:CMD	2.70	0.54
2:B:229:GLN:OE1	2:B:229:GLN:CA	2.53	0.54
2:B:317:ARG:NH1	2:B:405:ASP:C	2.58	0.54
2:B:376:GLN:OE1	2:B:376:GLN:HA	2.06	0.54
2:B:462:TRP:CZ3	19:B:1231:CLA:HBC1	2.42	0.54
19:B:1221:CLA:C8	19:B:1223:CLA:H43	2.38	0.54
19:B:1224:CLA:O1D	19:B:1225:CLA:HMA1	2.08	0.54
4:D:125:GLY:HA2	4:D:127:ASN:N	2.22	0.54
6:F:169:TYR:C	6:F:169:TYR:CD2	2.85	0.54
12:L:76:SER:OG	12:L:78:LEU:CD1	2.55	0.54
1:A:203:LEU:HD21	19:A:1123:CLA:C4D	2.37	0.54
1:A:285:GLY:O	1:A:294:LEU:CD1	2.56	0.54
1:A:462:ILE:CG2	19:A:1132:CLA:HMC1	2.37	0.54
19:A:1126:CLA:C10	21:A:6011:BCR:H372	2.38	0.54
19:A:1135:CLA:HBD	19:A:1135:CLA:CBA	2.37	0.54
2:B:70:TRP:NE1	2:B:71:GLN:OE1	2.40	0.54
2:B:160:LYS:NZ	2:B:161:TRP:CB	2.69	0.54
2:B:303:TYR:HA	2:B:306:GLU:CG	2.36	0.54
2:B:326:ILE:O	2:B:326:ILE:HG12	2.07	0.54
19:B:1220:CLA:HMD1	19:B:1221:CLA:CBB	2.37	0.54
3:C:67:VAL:CG1	3:C:68:TYR:N	2.68	0.54
5:E:127:GLU:C	5:E:128:VAL:CG2	2.77	0.54
7:G:84:ARG:HG2	7:G:85:GLU:H	1.72	0.54
12:L:79:ILE:HD12	19:L:1504:CLA:CMA	2.34	0.54
12:L:129:ALA:C	12:L:201:TYR:HB3	2.26	0.54
16:2:133:ASN:ND2	16:2:134:THR:CA	2.52	0.54
19:2:2006:CLA:H102	19:2:2006:CLA:H161	1.89	0.54
17:3:239:LEU:HA	17:3:242:PHE:HB2	1.89	0.54
18:4:127:TYR:O	18:4:128:ALA:CB	2.55	0.54
1:A:73:GLU:HB2	1:A:186:TYR:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HD3	1:A:191:PRO:O	2.07	0.54
1:A:244:LEU:HD13	1:A:247:GLU:CD	2.28	0.54
1:A:302:HIS:HD2	19:A:1116:CLA:NB	2.03	0.54
1:A:471:GLY:O	1:A:472:ARG:HG2	2.07	0.54
1:A:672:LEU:HD23	1:A:672:LEU:H	1.72	0.54
1:A:693:LEU:HD11	1:A:738:TYR:CD1	2.43	0.54
19:A:1105:CLA:HAA2	19:A:1107:CLA:HED1	1.90	0.54
19:A:1106:CLA:CHC	19:A:1107:CLA:HMD1	2.38	0.54
19:A:1124:CLA:CED	19:A:1125:CLA:HMD1	2.37	0.54
2:B:233:TYR:H	2:B:233:TYR:HD2	1.55	0.54
2:B:292:ARG:HH22	2:B:297:ILE:HG12	1.73	0.54
2:B:297:ILE:HG21	7:G:77:PHE:CZ	2.43	0.54
2:B:450:GLU:O	2:B:451:LYS:CB	2.52	0.54
2:B:454:LEU:HD11	6:F:147:HIS:CA	2.29	0.54
3:C:7:ILE:C	3:C:8:TYR:O	2.50	0.54
3:C:44:ARG:NE	4:D:182:GLN:NE2	2.55	0.54
4:D:100:TYR:HE1	4:D:134:LYS:HE3	1.61	0.54
7:G:89:LYS:C	7:G:90:GLN:CG	2.78	0.54
10:J:22:LEU:O	10:J:25:LEU:N	2.41	0.54
22:K:7041:LMU:H1B	22:K:7041:LMU:O6'	2.08	0.54
13:N:104:LYS:H	13:N:107:LEU:HD13	1.73	0.54
16:2:184:PRO:CG	16:2:186:ASN:N	2.71	0.54
16:2:249:ASN:HD22	16:2:254:LEU:HG	1.71	0.54
17:3:107:ARG:NH1	17:3:233:LEU:H	2.06	0.54
17:3:197:SER:OG	17:3:205:GLY:C	2.50	0.54
22:3:7005:LMU:O2B	22:3:7005:LMU:C3'	2.55	0.54
1:A:73:GLU:O	1:A:76:ARG:CA	2.55	0.54
1:A:129:GLN:HE22	19:A:1107:CLA:C1A	2.13	0.54
1:A:159:THR:C	1:A:160:SER:OG	2.50	0.54
1:A:163:GLN:CG	1:A:164:LEU:N	2.37	0.54
1:A:370:ILE:HD12	19:A:1124:CLA:O1D	2.07	0.54
1:A:656:PHE:HD2	1:A:657:LEU:HD12	1.72	0.54
19:A:1237:CLA:C14	12:L:141:LEU:HD22	2.36	0.54
2:B:33:SER:H	2:B:37:ILE:HD13	1.73	0.54
2:B:160:LYS:HE3	2:B:161:TRP:CE3	2.41	0.54
2:B:646:TRP:CH2	2:B:726:ILE:HG21	2.43	0.54
2:B:668:ARG:NH2	2:B:672:GLN:OE1	2.41	0.54
2:B:720:THR:O	2:B:724:PHE:N	2.41	0.54
4:D:83:PHE:CE1	4:D:114:MET:CE	2.91	0.54
4:D:163:VAL:O	4:D:164:GLN:CB	2.56	0.54
7:G:84:ARG:CG	7:G:85:GLU:CB	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:139:LYS:O	13:N:142:LYS:NZ	2.40	0.54
13:N:169:LYS:CA	13:N:170:TRP:CD1	2.91	0.54
15:1:201:PHE:CE1	15:1:204:GLN:NE2	2.75	0.54
15:1:207:ALA:C	15:1:209:PRO:CD	2.79	0.54
17:3:139:THR:CG2	17:3:140:GLY:N	2.38	0.54
17:3:164:LEU:HD12	17:3:164:LEU:C	2.33	0.54
18:4:174:GLN:C	18:4:195:ALA:H	2.15	0.54
18:4:178:PRO:O	18:4:194:PHE:HZ	1.89	0.54
18:4:201:LYS:CG	18:4:201:LYS:O	2.52	0.54
1:A:436:LEU:O	1:A:439:ARG:HB3	2.07	0.54
1:A:491:TRP:CE2	19:A:1135:CLA:H12	2.42	0.54
1:A:706:SER:HB3	2:B:419:ILE:O	2.07	0.54
19:A:1133:CLA:C1B	21:A:6008:BCR:H333	2.37	0.54
19:A:1138:CLA:C6	21:F:6014:BCR:H12C	2.33	0.54
19:A:9022:CLA:H152	21:B:6017:BCR:H20C	1.85	0.54
19:A:9023:CLA:HBC3	2:B:661:PHE:HB3	1.89	0.54
2:B:228:GLY:O	2:B:229:GLN:OE1	2.26	0.54
2:B:310:PRO:CG	19:B:1220:CLA:HMA1	2.38	0.54
2:B:631:LEU:HB3	2:B:727:ALA:HB1	1.90	0.54
2:B:663:PHE:O	2:B:664:LEU:CG	2.55	0.54
19:B:1218:CLA:CHD	19:B:1218:CLA:CBC	2.76	0.54
19:B:1220:CLA:HAA2	19:B:1220:CLA:CBD	2.37	0.54
19:B:1232:CLA:HBB2	21:B:6010:BCR:H281	1.89	0.54
4:D:170:ASP:HB2	4:D:181:ARG:HH21	1.71	0.54
6:F:92:ALA:O	6:F:96:LYS:HG3	2.06	0.54
7:G:98:THR:OG1	7:G:101:GLU:CG	2.54	0.54
22:G:7051:LMU:H5'	22:G:7051:LMU:O2'	2.04	0.54
19:H:1241:CLA:O1D	19:H:1241:CLA:H2A	2.07	0.54
11:K:47:ASP:O	11:K:48:PHE:CB	2.55	0.54
12:L:60:ILE:HG12	12:L:68:SER:OG	2.08	0.54
13:N:110:THR:HG23	13:N:111:GLY:N	2.22	0.54
13:N:123:GLY:CA	13:N:131:PHE:CD1	2.90	0.54
15:1:69:LEU:O	15:1:73:PRO:HD3	2.07	0.54
16:2:128:LYS:HB3	16:2:131:ILE:CG2	2.33	0.54
17:3:96:ARG:O	17:3:100:TYR:CD2	2.61	0.54
17:3:103:VAL:CG1	17:3:107:ARG:CZ	2.85	0.54
17:3:176:TRP:CZ2	17:3:199:ASN:OD1	2.61	0.54
17:3:204:GLY:C	17:3:206:PRO:HD2	2.33	0.54
1:A:207:LEU:HA	1:A:211:LEU:HB2	1.89	0.54
1:A:284:ARG:CB	1:A:295:TRP:HB2	2.37	0.54
1:A:344:LYS:C	1:A:346:LEU:N	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1140:CLA:C19	10:J:19:PHE:CD2	2.90	0.54
2:B:137:THR:OG1	2:B:140:ILE:HG12	2.08	0.54
2:B:233:TYR:N	2:B:233:TYR:HD2	2.04	0.54
2:B:236:ASN:N	2:B:237:PRO:HD3	2.23	0.54
2:B:361:ILE:O	2:B:362:ALA:HB3	2.08	0.54
19:B:1222:CLA:HED2	19:B:1223:CLA:OBD	2.07	0.54
6:F:204:SER:O	6:F:207:LEU:CB	2.55	0.54
7:G:72:LEU:HD21	7:G:124:ILE:HD11	1.84	0.54
8:H:81:SER:O	8:H:83:LEU:N	2.41	0.54
8:H:109:LEU:HD23	19:H:1207:CLA:C5	2.36	0.54
22:H:7011:LMU:C6'	22:H:7011:LMU:C1B	2.86	0.54
19:J:1308:CLA:O1D	19:J:1308:CLA:C1	2.56	0.54
11:K:76:ALA:CA	11:K:78:ARG:NH1	2.71	0.54
13:N:89:GLU:O	13:N:89:GLU:CD	2.51	0.54
13:N:132:THR:HG1	13:N:137:LEU:C	2.16	0.54
13:N:156:GLY:CA	13:N:157:LYS:HE2	2.36	0.54
15:1:170:PRO:CG	15:1:173:TYR:CD2	2.91	0.54
15:1:225:TRP:HB3	15:1:226:HIS:ND1	2.22	0.54
16:2:211:PRO:CD	16:2:212:GLN:N	2.70	0.54
16:2:249:ASN:O	16:2:250:LEU:HB3	2.06	0.54
17:3:150:TYR:CE2	17:3:151:TRP:CD2	2.96	0.54
19:4:4006:CLA:HBA2	19:4:4006:CLA:HBD	1.89	0.54
1:A:25:ASP:OD1	1:A:26:PRO:CG	2.56	0.54
1:A:425:THR:OG1	1:A:428:TYR:HE1	1.82	0.54
1:A:618:TRP:CZ2	1:A:655:ASP:CB	2.91	0.54
19:A:9023:CLA:HMC3	2:B:661:PHE:HB2	1.88	0.54
2:B:224:PRO:C	2:B:227:THR:CB	2.81	0.54
2:B:225:LEU:O	2:B:230:TRP:NE1	2.40	0.54
2:B:393:PHE:CZ	2:B:398:TYR:HD2	2.24	0.54
2:B:486:LEU:HD12	2:B:489:GLY:N	2.21	0.54
2:B:625:TRP:CE3	2:B:625:TRP:O	2.59	0.54
19:B:1221:CLA:HMA1	19:B:1221:CLA:H61	1.90	0.54
22:G:7026:LMU:H12	22:G:7026:LMU:H51	1.89	0.54
8:H:78:PRO:CG	19:L:1501:CLA:HMD3	2.37	0.54
8:H:108:THR:OG1	8:H:109:LEU:N	2.38	0.54
11:K:111:VAL:C	11:K:114:HIS:HB2	2.27	0.54
19:K:1142:CLA:OBD	19:K:1143:CLA:CHB	2.56	0.54
19:K:1146:CLA:O1A	19:K:1146:CLA:C3A	2.56	0.54
12:L:81:TRP:O	12:L:83:LEU:N	2.37	0.54
12:L:172:GLU:O	12:L:173:PRO:O	2.25	0.54
13:N:144:PRO:CG	13:N:158:ASP:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:67:LEU:O	15:1:69:LEU:O	2.26	0.54
15:1:68:GLY:O	15:1:73:PRO:HD3	2.07	0.54
15:1:104:GLY:O	15:1:105:TYR:HB2	2.08	0.54
15:1:177:PRO:O	15:1:179:LYS:N	2.41	0.54
15:1:183:LEU:O	15:1:184:LYS:CG	2.55	0.54
17:3:233:LEU:C	17:3:235:MET:H	2.14	0.54
19:4:4006:CLA:HMA3	22:4:7034:LMU:C6	2.30	0.54
1:A:398:HIS:CD2	19:A:1126:CLA:ND	2.76	0.54
1:A:402:ILE:HG13	19:A:1127:CLA:CBB	2.33	0.54
1:A:453:LEU:HD21	19:A:1136:CLA:CBB	2.38	0.54
19:A:1125:CLA:HBA1	19:A:1125:CLA:CGD	2.37	0.54
2:B:8:PHE:O	2:B:35:ASP:CG	2.50	0.54
2:B:321:GLY:O	2:B:322:LEU:C	2.49	0.54
2:B:324:ASP:O	2:B:328:ASN:CB	2.54	0.54
2:B:440:ASN:O	2:B:444:LEU:HD23	2.07	0.54
3:C:79:LEU:CD2	3:C:81:TYR:O	2.56	0.54
4:D:99:PHE:CB	4:D:157:VAL:CG1	2.84	0.54
4:D:99:PHE:HB3	4:D:157:VAL:CG1	2.38	0.54
4:D:100:TYR:HD1	4:D:134:LYS:CG	2.18	0.54
4:D:157:VAL:HG13	4:D:158:PHE:O	2.06	0.54
5:E:118:ASN:OD1	5:E:119:ASN:N	2.41	0.54
6:F:149:ILE:HG22	6:F:150:VAL:N	2.21	0.54
6:F:204:SER:O	6:F:205:SER:C	2.51	0.54
6:F:228:ASP:CA	6:F:231:PHE:HB3	2.38	0.54
7:G:89:LYS:HE3	7:G:89:LYS:CA	2.22	0.54
8:H:97:LEU:HD11	8:H:100:PHE:HB2	1.66	0.54
12:L:52:PRO:O	12:L:53:THR:C	2.50	0.54
13:N:150:LEU:O	13:N:151:ASP:HB2	2.07	0.54
15:1:171:LEU:N	15:1:173:TYR:CE2	2.76	0.54
17:3:99:ALA:C	17:3:101:GLY:N	2.64	0.54
18:4:193:ASN:O	18:4:194:PHE:CB	2.52	0.54
1:A:29:THR:OG1	1:A:31:PHE:N	2.40	0.54
1:A:79:PHE:CE1	19:A:1111:CLA:HED3	2.39	0.54
1:A:119:SER:HA	1:A:145:ILE:HD12	1.90	0.54
1:A:158:ILE:HG12	1:A:159:THR:H	1.68	0.54
1:A:479:ASP:OD1	1:A:536:THR:CG2	2.55	0.54
19:A:1104:CLA:H51	19:A:1128:CLA:NC	2.23	0.54
2:B:55:ALA:HB1	2:B:150:LEU:CD1	2.38	0.54
2:B:255:LEU:H	2:B:271:THR:HG21	1.73	0.54
2:B:269:TRP:HE3	2:B:270:LEU:H	1.55	0.54
2:B:343:VAL:CG1	19:B:1223:CLA:H2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:VAL:HG21	19:B:1230:CLA:CAC	2.33	0.54
2:B:506:ASN:CG	2:B:506:ASN:O	2.51	0.54
2:B:545:LYS:O	2:B:548:PRO:HD3	2.09	0.54
19:B:1205:CLA:CMC	21:B:6017:BCR:H281	2.37	0.54
12:L:111:VAL:C	12:L:113:PRO:HD2	2.32	0.54
13:N:93:GLU:HG2	13:N:94:LYS:N	2.23	0.54
22:R:7007:LMU:H71	22:R:7007:LMU:H11	1.90	0.54
15:1:114:TRP:CH2	15:1:121:GLN:CA	2.89	0.54
16:2:254:LEU:HD22	16:2:256:ASP:N	2.23	0.54
19:3:3008:CLA:CMC	19:3:3008:CLA:CBC	2.86	0.54
18:4:98:ASN:HB2	18:4:212:LEU:HD21	1.90	0.54
18:4:197:THR:OG1	19:4:4001:CLA:HBA2	2.07	0.54
1:A:110:LEU:C	1:A:113:PRO:HD3	2.32	0.53
1:A:249:ILE:CG2	17:3:137:PHE:CE2	2.92	0.53
1:A:252:ARG:CD	1:A:252:ARG:N	2.52	0.53
1:A:274:TRP:HB3	1:A:277:TYR:H	1.73	0.53
2:B:135:LEU:O	2:B:135:LEU:HG	2.07	0.53
2:B:143:LEU:C	2:B:145:LEU:N	2.66	0.53
2:B:212:PHE:HZ	19:B:1211:CLA:HHD	1.73	0.53
2:B:462:TRP:CH2	19:B:1231:CLA:HBC1	2.43	0.53
2:B:509:PHE:CD2	2:B:509:PHE:N	2.76	0.53
19:B:1202:CLA:HMC2	19:B:1226:CLA:H3A	1.89	0.53
19:B:1216:CLA:C3	19:B:1221:CLA:H92	2.38	0.53
5:E:79:LYS:CB	5:E:84:TYR:HE1	2.19	0.53
12:L:51:LYS:N	12:L:51:LYS:HD2	2.23	0.53
13:N:132:THR:CA	13:N:137:LEU:O	2.56	0.53
13:N:150:LEU:CB	13:N:152:LEU:HD23	2.38	0.53
15:1:112:GLN:CG	15:1:113:GLU:N	2.62	0.53
15:1:123:THR:O	15:1:124:TYR:HB2	2.08	0.53
16:2:215:LYS:HA	16:2:217:LEU:HD23	1.89	0.53
16:2:218:ARG:CB	16:2:219:THR:HG22	2.28	0.53
16:2:254:LEU:CD2	16:2:256:ASP:H	2.20	0.53
17:3:155:TYR:C	17:3:157:LEU:N	2.62	0.53
17:3:171:ARG:O	17:3:172:ARG:C	2.49	0.53
17:3:232:ARG:HA	17:3:235:MET:HB2	1.90	0.53
18:4:124:PRO:O	18:4:125:LYS:HG3	2.08	0.53
18:4:170:PRO:O	18:4:171:ILE:C	2.50	0.53
18:4:217:PHE:CD1	18:4:221:HIS:ND1	2.76	0.53
18:4:226:LYS:H	18:4:226:LYS:HD3	1.57	0.53
1:A:23:ASP:OD2	1:A:24:ARG:CZ	2.56	0.53
1:A:62:HIS:CE1	19:A:1128:CLA:CGA	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:HE2	1:A:74:ILE:CG2	2.12	0.53
1:A:261:SER:C	1:A:263:ALA:N	2.66	0.53
1:A:453:LEU:HD23	19:A:1136:CLA:CBB	2.37	0.53
2:B:247:THR:HG22	2:B:248:GLN:N	2.15	0.53
2:B:278:LEU:HG	19:B:1213:CLA:CMA	2.38	0.53
2:B:304:ILE:O	2:B:308:HIS:CB	2.52	0.53
2:B:391:PRO:HB3	2:B:538:ALA:CA	2.30	0.53
2:B:469:LYS:HE3	2:B:470:THR:CG2	2.34	0.53
2:B:560:ASP:CG	3:C:66:ARG:CZ	2.81	0.53
4:D:87:THR:N	12:L:69:LEU:HD11	2.22	0.53
4:D:158:PHE:CB	4:D:159:PRO:O	2.46	0.53
5:E:84:TYR:HD2	5:E:85:LYS:HG3	1.72	0.53
8:H:98:LEU:O	8:H:102:ILE:HG13	2.08	0.53
11:K:63:LEU:O	11:K:64:MET:C	2.50	0.53
12:L:81:TRP:C	12:L:83:LEU:H	2.17	0.53
16:2:164:GLU:HA	16:2:167:ARG:NH1	2.22	0.53
17:3:167:PHE:O	17:3:168:ALA:C	2.50	0.53
19:3:2009:CLA:CBD	19:3:2009:CLA:CBA	2.85	0.53
18:4:131:LYS:O	18:4:131:LYS:HG2	2.08	0.53
18:4:209:ARG:O	18:4:212:LEU:N	2.41	0.53
18:4:209:ARG:HG2	18:4:210:LEU:N	2.15	0.53
1:A:462:ILE:CD1	19:A:9022:CLA:H72	2.38	0.53
2:B:196:HIS:CE1	19:B:1212:CLA:ND	2.75	0.53
2:B:222:LEU:HA	19:B:1212:CLA:HMD1	1.91	0.53
2:B:293:THR:HG22	7:G:94:GLN:NE2	2.18	0.53
2:B:298:GLY:CA	19:B:1218:CLA:HMD2	2.37	0.53
2:B:625:TRP:CD2	2:B:625:TRP:O	2.61	0.53
3:C:62:PHE:CD1	5:E:80:GLU:HB3	2.43	0.53
6:F:227:VAL:HG23	6:F:228:ASP:N	2.23	0.53
11:K:113:GLY:O	11:K:116:ILE:CG2	2.34	0.53
13:N:90:GLU:OE1	13:N:91:TYR:CZ	2.61	0.53
16:2:266:PHE:CE2	16:2:267:THR:O	2.62	0.53
17:3:109:ALA:C	17:3:111:LEU:CB	2.51	0.53
17:3:162:MET:O	17:3:163:ALA:C	2.46	0.53
22:3:7005:LMU:O2B	22:3:7005:LMU:H5'	2.09	0.53
18:4:142:PHE:HA	18:4:145:GLU:CG	2.38	0.53
1:A:431:LEU:H	1:A:434:ARG:NE	2.06	0.53
1:A:534:LEU:HB2	1:A:538:ASP:CB	2.39	0.53
1:A:696:GLY:HA3	2:B:569:ASP:HB2	1.89	0.53
19:A:1107:CLA:CBB	19:B:1230:CLA:HMD1	2.38	0.53
2:B:65:LEU:HD22	2:B:124:TRP:HE3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:PHE:O	2:B:66:PHE:CG	2.60	0.53
2:B:294:ASN:ND2	7:G:93:GLU:C	2.66	0.53
2:B:367:THR:O	2:B:367:THR:CG2	2.56	0.53
2:B:482:ASN:O	2:B:484:PRO:HD2	2.08	0.53
3:C:65:VAL:H	3:C:66:ARG:HH22	1.57	0.53
3:C:65:VAL:N	3:C:66:ARG:HH22	2.06	0.53
4:D:80:SER:HB2	4:D:127:ASN:HA	1.90	0.53
4:D:156:ARG:HB2	4:D:166:LEU:HD11	1.89	0.53
13:N:99:LYS:HB2	13:N:102:ASN:ND2	2.24	0.53
22:R:7021:LMU:H41	22:R:7021:LMU:C6'	2.38	0.53
15:1:81:GLU:HG2	15:1:82:SER:N	2.22	0.53
16:2:125:PHE:O	16:2:127:THR:CG2	2.56	0.53
16:2:150:THR:C	16:2:152:LEU:HD13	2.33	0.53
16:2:189:THR:O	16:2:190:GLY:C	2.50	0.53
22:2:7006:LMU:O6B	22:2:7006:LMU:H3'	2.08	0.53
17:3:111:LEU:C	17:3:113:ALA:N	2.62	0.53
17:3:192:LYS:HZ3	17:3:192:LYS:C	2.16	0.53
17:3:236:LEU:C	17:3:238:ILE:H	2.17	0.53
18:4:179:ALA:O	18:4:180:GLY:C	2.49	0.53
18:4:215:LEU:O	18:4:217:PHE:N	2.41	0.53
19:4:4002:CLA:HMA3	19:4:4002:CLA:O2A	2.07	0.53
1:A:79:PHE:CE2	1:A:185:HIS:NE2	2.76	0.53
1:A:466:THR:O	1:A:470:LEU:HG	2.08	0.53
1:A:482:ILE:CG2	1:A:482:ILE:O	2.55	0.53
1:A:624:VAL:HG12	1:A:625:TRP:N	2.22	0.53
1:A:628:ILE:CD1	1:A:629:ASN:N	2.71	0.53
1:A:673:SER:OG	2:B:445:ALA:O	2.16	0.53
1:A:703:LEU:O	1:A:707:ILE:HG12	2.08	0.53
2:B:165:VAL:O	2:B:166:SER:C	2.50	0.53
2:B:316:GLY:O	2:B:317:ARG:NE	2.41	0.53
2:B:459:PHE:N	19:B:1235:CLA:CAD	2.71	0.53
2:B:508:LEU:HB3	2:B:509:PHE:CE2	2.42	0.53
2:B:509:PHE:HD2	2:B:509:PHE:N	2.06	0.53
3:C:2:SER:O	3:C:3:HIS:ND1	2.42	0.53
6:F:176:TRP:CZ3	6:F:217:ALA:HB2	2.43	0.53
6:F:203:ALA:O	6:F:205:SER:N	2.42	0.53
8:H:58:LEU:CB	8:H:61:THR:CB	2.60	0.53
10:J:21:ALA:O	10:J:22:LEU:C	2.51	0.53
12:L:73:VAL:HG12	19:L:1504:CLA:CMA	2.39	0.53
12:L:190:PHE:CE2	12:L:194:ILE:HD12	2.44	0.53
13:N:126:LYS:HD2	13:N:127:PHE:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:143:VAL:O	13:N:151:ASP:OD1	2.26	0.53
15:1:199:VAL:HG13	15:1:200:GLY:N	2.23	0.53
16:2:168:TRP:CD1	16:2:171:ILE:HD13	2.43	0.53
17:3:132:THR:HG23	17:3:133:ALA:N	2.23	0.53
17:3:150:TYR:C	17:3:151:TRP:CD1	2.77	0.53
1:A:91:LEU:O	19:A:1105:CLA:HMC3	2.09	0.53
1:A:281:LEU:HD12	1:A:282:THR:HG23	1.91	0.53
1:A:362:LEU:HB3	1:A:406:LEU:O	2.08	0.53
1:A:466:THR:HG22	2:B:648:TRP:HE1	1.72	0.53
1:A:707:ILE:HG22	1:A:711:HIS:CD2	2.41	0.53
19:A:1119:CLA:C2C	19:A:1125:CLA:H172	2.38	0.53
19:A:1126:CLA:C17	21:J:6012:BCR:H17C	2.36	0.53
19:A:9012:CLA:NB	19:A:9013:CLA:HBB2	2.24	0.53
2:B:464:GLN:HG3	2:B:464:GLN:O	2.01	0.53
2:B:574:ASP:O	2:B:578:LEU:HG	2.08	0.53
19:B:1216:CLA:HBD	19:B:1216:CLA:HBA1	1.90	0.53
19:B:1222:CLA:CMB	21:B:6010:BCR:H352	2.39	0.53
6:F:192:THR:O	6:F:193:GLN:CG	2.56	0.53
6:F:228:ASP:O	6:F:231:PHE:HD1	1.90	0.53
6:F:230:ASN:C	6:F:231:PHE:O	2.51	0.53
7:G:123:ASN:O	7:G:126:ASP:OD2	2.27	0.53
8:H:77:ASN:ND2	8:H:78:PRO:O	2.42	0.53
8:H:119:ASP:OD2	8:H:121:LEU:CG	2.50	0.53
22:H:7028:LMU:O6'	22:H:7028:LMU:H1'	2.09	0.53
12:L:141:LEU:HD11	12:L:145:LEU:HD11	1.90	0.53
12:L:205:TYR:CD2	12:L:205:TYR:O	2.62	0.53
13:N:147:SER:O	13:N:151:ASP:CG	2.52	0.53
15:1:199:VAL:O	15:1:201:PHE:N	2.41	0.53
18:4:217:PHE:CE1	18:4:221:HIS:ND1	2.77	0.53
1:A:472:ARG:N	1:A:473:PRO:HD2	2.22	0.53
19:A:1106:CLA:H93	21:J:6012:BCR:H311	1.89	0.53
19:A:1131:CLA:H152	21:L:6019:BCR:C36	2.39	0.53
21:A:6002:BCR:C23	21:A:6002:BCR:C40	2.87	0.53
2:B:278:LEU:O	2:B:281:ALA:N	2.42	0.53
2:B:292:ARG:NH2	2:B:297:ILE:CA	2.71	0.53
2:B:560:ASP:CG	2:B:561:GLY:N	2.66	0.53
19:B:1235:CLA:H61	21:F:6016:BCR:H323	1.91	0.53
19:B:1239:CLA:H51	20:B:5002:PQN:H251	1.90	0.53
22:B:7038:LMU:H101	22:B:7038:LMU:H61	1.91	0.53
3:C:12:ILE:CB	3:C:38:GLN:O	2.56	0.53
3:C:61:ASP:CG	5:E:118:ASN:HD21	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:TYR:CD1	4:D:134:LYS:HG2	2.42	0.53
12:L:63:ASP:OD1	12:L:63:ASP:O	2.26	0.53
13:N:139:LYS:O	13:N:140:GLN:C	2.51	0.53
14:R:26:UNK:O	14:R:28:UNK:CA	2.57	0.53
15:1:177:PRO:HD3	15:1:180:LEU:HD21	1.85	0.53
16:2:156:GLU:HG3	16:2:157:LEU:CD1	2.36	0.53
17:3:150:TYR:N	17:3:152:ALA:CB	2.32	0.53
18:4:169:ASP:HA	18:4:173:LYS:C	2.33	0.53
1:A:182:GLY:C	19:A:1109:CLA:HAC1	2.33	0.53
1:A:209:GLY:HA2	1:A:213:LEU:CD1	2.38	0.53
1:A:224:HIS:CE1	19:A:1113:CLA:NC	2.77	0.53
1:A:282:THR:O	1:A:283:PHE:C	2.52	0.53
1:A:492:ILE:CD1	19:A:1133:CLA:C2C	2.85	0.53
1:A:750:PHE:O	1:A:752:ALA:N	2.41	0.53
19:A:1122:CLA:CBB	21:A:6007:BCR:H353	2.36	0.53
2:B:138:GLY:O	2:B:139:ALA:C	2.50	0.53
2:B:212:PHE:CE1	19:B:1211:CLA:HMD3	2.44	0.53
2:B:364:ASP:OD2	2:B:367:THR:HB	2.08	0.53
2:B:367:THR:O	2:B:367:THR:HG22	2.08	0.53
19:B:1220:CLA:C9	19:B:1227:CLA:HBC2	2.39	0.53
4:D:140:LEU:HD12	4:D:144:LEU:H	1.74	0.53
4:D:148:TYR:C	4:D:148:TYR:CD2	2.86	0.53
5:E:100:ARG:O	5:E:121:ALA:CB	2.57	0.53
6:F:160:PHE:O	6:F:164:GLY:N	2.42	0.53
7:G:89:LYS:C	7:G:90:GLN:HG2	2.34	0.53
7:G:98:THR:HB	7:G:101:GLU:OE2	1.81	0.53
12:L:98:ARG:O	12:L:102:VAL:HG23	2.07	0.53
12:L:148:TYR:C	12:L:150:ILE:H	2.16	0.53
13:N:118:TYR:C	13:N:119:THR:OG1	2.52	0.53
13:N:130:ASN:HB2	13:N:132:THR:HG21	1.91	0.53
13:N:144:PRO:C	13:N:151:ASP:OD1	2.52	0.53
15:1:101:GLU:O	15:1:101:GLU:CG	2.54	0.53
15:1:176:ASP:CB	15:1:180:LEU:CD1	2.39	0.53
19:1:1014:CLA:H52	19:1:1014:CLA:H101	1.79	0.53
16:2:126:LEU:O	16:2:129:LEU:N	2.41	0.53
16:2:137:TRP:O	16:2:137:TRP:CD1	2.62	0.53
16:2:200:TRP:CD1	16:2:200:TRP:H	2.26	0.53
16:2:240:ILE:CG2	16:2:263:PHE:CB	2.65	0.53
19:3:1147:CLA:HBC2	19:3:1147:CLA:HMC2	1.91	0.53
22:4:7053:LMU:H5B	22:4:7053:LMU:O2B	2.08	0.53
1:A:32:GLU:OE1	1:A:33:GLN:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:O	1:A:284:ARG:NE	2.42	0.53
1:A:369:THR:CG2	19:A:1127:CLA:HMC2	2.39	0.53
1:A:612:VAL:O	1:A:615:HIS:HB3	2.09	0.53
19:A:1126:CLA:C17	21:J:6012:BCR:H15C	2.39	0.53
19:A:1131:CLA:H11	19:A:1237:CLA:H43	1.90	0.53
2:B:232:LEU:CD1	2:B:235:GLN:CB	2.86	0.53
2:B:282:PHE:HE2	19:B:1213:CLA:H3A	1.74	0.53
2:B:311:PRO:HG3	19:B:1301:CLA:NC	2.24	0.53
2:B:312:GLY:HA3	2:B:315:LEU:HB3	1.87	0.53
2:B:595:HIS:CE1	2:B:599:ILE:HD11	2.43	0.53
2:B:622:ASP:HB3	2:B:626:LEU:HD11	1.91	0.53
6:F:181:TYR:O	6:F:181:TYR:CD2	2.61	0.53
19:L:1148:CLA:O2D	19:L:1148:CLA:CAA	2.52	0.53
15:1:74:ALA:HB3	15:1:75:ASN:CG	2.34	0.53
16:2:128:LYS:O	16:2:131:ILE:HA	2.08	0.53
16:2:246:PRO:HB2	16:2:247:ILE:CD1	2.36	0.53
19:2:2007:CLA:C1B	19:2:2007:CLA:H2	2.38	0.53
17:3:104:ILE:HG21	19:3:3004:CLA:C3D	2.39	0.53
18:4:150:HIS:CE1	18:4:154:ILE:HD11	2.43	0.53
19:4:1004:CLA:O1D	19:4:1004:CLA:H2A	2.08	0.53
1:A:104:SER:C	1:A:106:TYR:N	2.66	0.53
1:A:302:HIS:HE1	19:A:1117:CLA:CHB	2.22	0.53
1:A:346:LEU:CD2	1:A:346:LEU:O	2.56	0.53
1:A:415:ALA:HB2	1:A:560:VAL:HG12	1.91	0.53
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.44	0.53
1:A:443:ILE:HG22	2:B:674:LEU:CD1	2.39	0.53
1:A:464:ASN:H	1:A:464:ASN:ND2	2.07	0.53
1:A:628:ILE:CG1	1:A:629:ASN:N	2.70	0.53
19:A:9023:CLA:H111	21:B:6017:BCR:C35	2.39	0.53
2:B:66:PHE:O	2:B:66:PHE:CD2	2.61	0.53
2:B:120:VAL:CB	2:B:123:TRP:HE1	2.21	0.53
2:B:310:PRO:CD	2:B:311:PRO:CD	2.87	0.53
2:B:325:THR:HG21	2:B:403:ASN:HD21	1.74	0.53
2:B:330:ILE:CD1	19:B:1202:CLA:C19	2.86	0.53
2:B:577:TYR:CE2	2:B:578:LEU:HD23	2.45	0.53
2:B:580:VAL:CG1	2:B:710:LEU:HD21	2.39	0.53
2:B:609:PHE:O	2:B:613:SER:N	2.36	0.53
3:C:36:ALA:C	3:C:37:LYS:HG2	2.34	0.53
4:D:129:LEU:CD1	12:L:65:PHE:CD1	2.92	0.53
5:E:75:LYS:CA	5:E:87:THR:HG22	2.31	0.53
5:E:89:SER:O	5:E:105:VAL:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:E:7048:LMU:O5'	22:E:7048:LMU:C2	2.57	0.53
6:F:228:ASP:O	6:F:231:PHE:CD1	2.62	0.53
9:I:20:ALA:O	9:I:24:LEU:HB3	2.08	0.53
15:1:134:LEU:O	15:1:137:ILE:HG12	2.09	0.53
16:2:184:PRO:HD2	16:2:186:ASN:N	2.22	0.53
17:3:150:TYR:CG	17:3:151:TRP:N	2.77	0.53
18:4:220:GLN:NE2	19:4:1306:CLA:CAC	2.72	0.53
1:A:582:ASP:HB3	1:A:589:THR:CG2	2.38	0.52
19:A:1119:CLA:HMD1	19:A:1121:CLA:CBB	2.32	0.52
2:B:127:ILE:HD13	2:B:193:HIS:HE1	1.74	0.52
2:B:244:PHE:CD2	2:B:245:GLY:N	2.77	0.52
2:B:294:ASN:ND2	7:G:94:GLN:CB	2.46	0.52
2:B:347:LEU:CD2	2:B:351:HIS:CE1	2.92	0.52
2:B:353:TYR:O	2:B:355:LEU:N	2.41	0.52
2:B:469:LYS:C	2:B:501:ILE:CA	2.68	0.52
2:B:687:LEU:HD12	21:B:6020:BCR:HC31	1.91	0.52
2:B:708:VAL:O	2:B:710:LEU:O	2.27	0.52
19:B:1203:CLA:H91	19:B:1203:CLA:H161	1.91	0.52
19:B:1216:CLA:OBD	19:B:1219:CLA:CBC	2.57	0.52
4:D:133:ARG:H	4:D:136:GLN:HE21	1.53	0.52
4:D:167:HIS:H	4:D:168:PRO:CD	2.21	0.52
4:D:205:LYS:N	4:D:205:LYS:HE2	2.24	0.52
6:F:142:SER:C	6:F:144:GLY:H	2.17	0.52
6:F:228:ASP:OD2	6:F:231:PHE:CG	2.63	0.52
12:L:143:LEU:H	12:L:145:LEU:N	2.05	0.52
14:R:32:UNK:CB	14:R:33:UNK:CA	2.76	0.52
22:1:7004:LMU:O6B	22:1:7004:LMU:C1B	2.55	0.52
22:1:7004:LMU:O2'	22:1:7004:LMU:C1	2.50	0.52
16:2:101:TRP:H	16:2:103:VAL:CG1	2.21	0.52
1:A:348:GLU:O	1:A:349:ILE:C	2.52	0.52
1:A:458:PHE:CD2	19:A:9022:CLA:CMB	2.92	0.52
1:A:746:THR:O	1:A:750:PHE:N	2.36	0.52
19:A:9012:CLA:HED1	19:B:9010:CLA:H61	1.90	0.52
2:B:222:LEU:HA	19:B:1212:CLA:CMD	2.40	0.52
2:B:569:ASP:OD1	2:B:706:ARG:NE	2.42	0.52
2:B:608:GLN:O	2:B:612:SER:HB2	2.08	0.52
19:B:1231:CLA:ND	19:B:1232:CLA:HBB1	2.24	0.52
4:D:129:LEU:HD13	12:L:65:PHE:CZ	2.44	0.52
7:G:84:ARG:CG	7:G:85:GLU:H	2.13	0.52
7:G:136:VAL:O	7:G:137:VAL:HG22	2.09	0.52
19:J:1308:CLA:H2A	19:J:1308:CLA:C2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:62:SER:HG	11:K:63:LEU:CD1	2.21	0.52
12:L:55:GLN:O	12:L:57:ILE:HG13	2.08	0.52
12:L:205:TYR:HD1	12:L:207:LEU:CD1	1.90	0.52
13:N:131:PHE:N	13:N:132:THR:HG22	2.19	0.52
13:N:133:GLY:CA	13:N:134:CYS:O	2.54	0.52
13:N:143:VAL:CG1	13:N:144:PRO:HD2	2.39	0.52
13:N:150:LEU:HD13	13:N:150:LEU:N	2.25	0.52
15:1:65:ASP:OD2	15:1:66:PRO:HA	2.08	0.52
16:2:176:CYS:H	16:2:188:LEU:HB2	1.73	0.52
17:3:225:LEU:HD13	17:3:228:VAL:CG2	2.38	0.52
22:3:7005:LMU:O3'	22:3:7005:LMU:C1B	2.57	0.52
18:4:174:GLN:HB3	18:4:195:ALA:HA	1.92	0.52
18:4:195:ALA:CB	18:4:197:THR:O	2.55	0.52
1:A:309:LEU:O	1:A:310:PHE:CB	2.56	0.52
1:A:690:LEU:CD2	2:B:661:PHE:HE1	2.21	0.52
19:A:1105:CLA:C4B	21:J:6012:BCR:C33	2.86	0.52
19:A:1117:CLA:H93	19:A:1117:CLA:H193	1.91	0.52
19:A:1126:CLA:H43	19:A:1126:CLA:CGA	2.39	0.52
2:B:131:THR:C	2:B:135:LEU:CD2	2.80	0.52
2:B:297:ILE:HG21	7:G:77:PHE:HZ	1.73	0.52
2:B:376:GLN:HB3	2:B:587:ILE:HD12	1.92	0.52
2:B:416:GLU:CD	2:B:416:GLU:H	2.16	0.52
2:B:556:SER:HG	2:B:573:TRP:CG	2.27	0.52
3:C:26:LEU:HD22	4:D:181:ARG:NH1	2.23	0.52
4:D:148:TYR:O	4:D:149:LYS:CB	2.56	0.52
7:G:60:SER:OG	7:G:61:ALA:N	2.42	0.52
7:G:72:LEU:CD1	7:G:73:PHE:CZ	2.93	0.52
7:G:125:VAL:HG13	7:G:129:ALA:HB2	1.88	0.52
19:J:1308:CLA:CBA	19:J:1308:CLA:CBD	2.83	0.52
19:K:1143:CLA:CGA	19:K:1143:CLA:C3A	2.85	0.52
12:L:102:VAL:HA	19:L:1502:CLA:HED1	1.89	0.52
13:N:114:PHE:O	13:N:118:TYR:N	2.42	0.52
13:N:136:ASP:OD1	13:N:137:LEU:O	2.28	0.52
16:2:133:ASN:HD21	16:2:134:THR:HB	1.57	0.52
17:3:233:LEU:O	17:3:236:LEU:N	2.43	0.52
18:4:142:PHE:O	18:4:143:VAL:C	2.51	0.52
19:4:1304:CLA:CAA	19:4:1304:CLA:CGD	2.87	0.52
1:A:70:ASP:C	1:A:72:GLU:HG2	2.34	0.52
1:A:252:ARG:NH2	1:A:252:ARG:O	2.42	0.52
1:A:592:VAL:HG23	1:A:593:SER:N	2.25	0.52
19:A:1106:CLA:HMB2	19:A:1107:CLA:H11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1135:CLA:HBA2	19:A:1135:CLA:O1D	2.09	0.52
2:B:53:GLN:C	2:B:55:ALA:N	2.58	0.52
2:B:203:ARG:O	2:B:245:GLY:C	2.53	0.52
2:B:497:TRP:C	2:B:499:ASN:N	2.62	0.52
2:B:574:ASP:OD2	2:B:706:ARG:NE	2.43	0.52
2:B:624:LEU:CD2	19:B:9010:CLA:H93	2.40	0.52
2:B:668:ARG:HH12	2:B:672:GLN:HG2	1.73	0.52
2:B:673:GLU:O	2:B:676:GLU:HB2	2.09	0.52
6:F:190:LYS:CG	6:F:192:THR:CG2	2.88	0.52
7:G:85:GLU:HG3	7:G:86:ASN:N	2.24	0.52
8:H:116:ALA:CB	8:H:117:SER:CA	2.85	0.52
19:H:1505:CLA:HAA1	19:H:1505:CLA:H42	1.92	0.52
12:L:52:PRO:HB2	12:L:55:GLN:C	2.32	0.52
17:3:213:PHE:HB2	17:3:215:LYS:N	2.24	0.52
1:A:240:LYS:O	1:A:240:LYS:HD2	2.10	0.52
1:A:365:LEU:HD22	19:A:1103:CLA:HED3	1.87	0.52
1:A:599:PHE:CE2	1:A:735:VAL:HG21	2.45	0.52
1:A:607:ASN:ND2	19:A:9022:CLA:C2C	2.73	0.52
1:A:697:ARG:C	1:A:699:TYR:H	2.17	0.52
19:A:1119:CLA:HMB2	19:A:1123:CLA:CED	2.39	0.52
19:A:9012:CLA:HBB2	19:A:9013:CLA:C1B	2.39	0.52
2:B:135:LEU:O	2:B:135:LEU:CD1	2.57	0.52
2:B:183:PHE:HB3	2:B:284:PHE:HD2	1.74	0.52
2:B:350:GLN:O	2:B:353:TYR:CD1	2.62	0.52
2:B:353:TYR:O	2:B:354:SER:CB	2.47	0.52
2:B:444:LEU:C	2:B:446:PHE:N	2.68	0.52
3:C:31:TRP:HD1	3:C:31:TRP:C	2.16	0.52
3:C:36:ALA:O	3:C:37:LYS:HG2	2.09	0.52
4:D:100:TYR:HD1	4:D:134:LYS:HG3	1.64	0.52
5:E:91:VAL:HB	5:E:104:VAL:CG1	2.40	0.52
7:G:69:GLY:HA2	7:G:72:LEU:CG	2.38	0.52
8:H:67:SER:O	8:H:68:TYR:CD1	2.62	0.52
19:I:1204:CLA:C14	21:I:6018:BCR:H392	2.37	0.52
12:L:194:ILE:O	12:L:195:SER:CB	2.58	0.52
12:L:205:TYR:CG	12:L:207:LEU:HD12	2.36	0.52
19:L:1148:CLA:O2D	19:L:1148:CLA:CGA	2.57	0.52
13:N:123:GLY:CA	13:N:131:PHE:HD1	2.22	0.52
13:N:147:SER:O	13:N:148:ASP:HB2	2.10	0.52
15:1:163:TYR:N	15:1:164:PRO:HD3	2.23	0.52
16:2:113:ALA:CB	16:2:114:MET:CE	2.87	0.52
16:2:145:TYR:C	16:2:146:PHE:CD1	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:261:THR:C	16:2:262:ILE:HG23	2.35	0.52
19:3:3008:CLA:H2A	19:3:3008:CLA:O2A	2.09	0.52
18:4:174:GLN:HA	18:4:176:SER:H	1.74	0.52
18:4:177:LEU:HD22	18:4:178:PRO:CA	2.40	0.52
18:4:241:HIS:CE1	18:4:242:ASN:OD1	2.62	0.52
1:A:39:HIS:ND1	1:A:39:HIS:O	2.43	0.52
1:A:49:ASP:OD2	1:A:49:ASP:N	2.41	0.52
1:A:629:ASN:OD1	1:A:630:ASP:N	2.43	0.52
19:A:9012:CLA:H12	2:B:616:LEU:CD1	2.32	0.52
2:B:443:MET:HG2	2:B:451:LYS:O	2.10	0.52
2:B:469:LYS:C	2:B:501:ILE:HA	2.34	0.52
2:B:475:ASP:CG	2:B:480:SER:HA	2.35	0.52
2:B:694:ARG:CD	9:I:28:VAL:CG1	2.87	0.52
3:C:12:ILE:CB	3:C:39:ILE:HA	2.39	0.52
5:E:127:GLU:CG	5:E:129:GLU:O	2.57	0.52
22:F:7036:LMU:O2B	22:F:7036:LMU:C4'	2.58	0.52
19:H:1241:CLA:HAC1	21:I:6021:BCR:HC32	1.90	0.52
12:L:76:SER:O	12:L:79:ILE:N	2.42	0.52
16:2:155:VAL:HA	16:2:158:VAL:CG1	2.40	0.52
19:2:2004:CLA:O1A	19:3:2009:CLA:HBC3	2.10	0.52
17:3:103:VAL:HG11	17:3:229:LYS:CG	2.39	0.52
17:3:109:ALA:HA	17:3:111:LEU:CD1	2.39	0.52
17:3:159:VAL:O	17:3:161:GLU:C	2.53	0.52
19:3:2009:CLA:C5	19:3:2009:CLA:C9	2.26	0.52
18:4:174:GLN:O	18:4:175:TYR:CB	2.58	0.52
1:A:396:PHE:CG	1:A:396:PHE:O	2.62	0.52
1:A:587:GLY:HA3	2:B:668:ARG:CZ	2.40	0.52
19:A:9022:CLA:H151	21:B:6017:BCR:H19C	1.92	0.52
2:B:224:PRO:HG3	7:G:153:PHE:CB	2.40	0.52
2:B:323:TYR:CE1	19:B:1221:CLA:HBC1	2.45	0.52
6:F:132:ASN:C	6:F:133:TYR:CD1	2.74	0.52
10:J:26:LEU:H	10:J:28:GLU:H	1.56	0.52
12:L:93:VAL:HG12	12:L:94:SER:O	2.10	0.52
13:N:157:LYS:HG2	13:N:159:LYS:HG3	1.92	0.52
14:R:39:UNK:CA	14:R:41:UNK:CB	2.88	0.52
15:1:149:GLU:HG2	15:1:152:ARG:HH11	1.61	0.52
15:1:171:LEU:CB	15:1:173:TYR:CZ	2.93	0.52
16:2:123:PRO:O	16:2:124:GLU:C	2.50	0.52
19:3:3008:CLA:O1A	19:3:3008:CLA:CED	2.58	0.52
18:4:112:PRO:CB	18:4:116:THR:O	2.57	0.52
18:4:131:LYS:O	18:4:131:LYS:CG	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:HG3	1:A:74:ILE:CA	2.40	0.52
1:A:100:GLY:HA3	1:A:153:TRP:HH2	1.75	0.52
1:A:246:HIS:C	1:A:248:PHE:H	2.15	0.52
1:A:435:VAL:HA	1:A:438:HIS:HE1	1.75	0.52
1:A:681:GLY:C	1:A:683:HIS:H	2.16	0.52
1:A:692:PHE:CD2	1:A:733:VAL:HG12	2.45	0.52
1:A:711:HIS:CD2	19:A:1139:CLA:CBC	2.84	0.52
19:A:9011:CLA:H192	19:A:9022:CLA:C2B	2.39	0.52
19:A:9012:CLA:H11	2:B:616:LEU:HB2	1.92	0.52
2:B:25:ILE:O	2:B:26:ALA:HB3	2.08	0.52
2:B:135:LEU:O	2:B:135:LEU:CG	2.58	0.52
2:B:180:SER:OG	2:B:181:GLY:N	2.35	0.52
2:B:278:LEU:HD21	19:B:1213:CLA:CGA	2.40	0.52
2:B:393:PHE:CE2	2:B:398:TYR:HD2	2.27	0.52
2:B:609:PHE:O	2:B:613:SER:OG	2.27	0.52
19:B:1221:CLA:H61	19:B:1221:CLA:CMA	2.40	0.52
19:B:1226:CLA:HMD1	24:B:7101:LMG:H341	1.91	0.52
3:C:5:VAL:HG23	3:C:65:VAL:HG21	1.91	0.52
3:C:28:MET:SD	4:D:176:LYS:C	2.93	0.52
3:C:43:PRO:HA	4:D:182:GLN:HG3	1.92	0.52
3:C:44:ARG:NH2	4:D:181:ARG:NE	2.49	0.52
6:F:193:GLN:CA	6:F:195:GLU:OE1	2.57	0.52
10:J:9:SER:O	10:J:10:VAL:CB	2.57	0.52
12:L:73:VAL:CA	19:L:1504:CLA:HMA1	2.38	0.52
12:L:104:LEU:HD12	12:L:196:GLY:CA	2.38	0.52
13:N:165:ASN:OD1	13:N:167:PHE:N	2.42	0.52
16:2:182:ILE:CA	16:2:187:LYS:CG	2.87	0.52
16:2:211:PRO:HB2	16:2:215:LYS:HZ1	1.75	0.52
1:A:176:GLY:O	1:A:180:PHE:HB2	2.10	0.52
1:A:181:ALA:HB2	19:A:1108:CLA:HBC2	1.92	0.52
1:A:309:LEU:HD23	1:A:309:LEU:C	2.35	0.52
1:A:373:ALA:HB1	1:A:396:PHE:HD1	1.75	0.52
1:A:553:VAL:HG22	21:A:6008:BCR:H401	1.91	0.52
1:A:574:ASN:OD1	1:A:574:ASN:N	2.42	0.52
1:A:595:TRP:HE3	1:A:596:ASP:OD2	1.92	0.52
19:A:1137:CLA:HBA2	19:A:1137:CLA:CHA	2.39	0.52
19:A:1237:CLA:H152	21:B:6020:BCR:C35	2.40	0.52
2:B:44:GLN:OE1	2:B:163:PRO:CB	2.57	0.52
2:B:110:LEU:HD12	2:B:111:GLY:HA2	1.88	0.52
2:B:123:TRP:HB2	2:B:126:THR:HG21	1.82	0.52
2:B:211:ASN:CB	2:B:214:ASP:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:GLN:O	2:B:363:GLN:HG3	2.09	0.52
2:B:387:PHE:HE2	19:B:1222:CLA:HHC	1.75	0.52
2:B:463:ILE:O	2:B:464:GLN:HB3	2.08	0.52
2:B:636:THR:O	2:B:636:THR:HG23	2.08	0.52
2:B:694:ARG:NH2	2:B:694:ARG:CG	2.47	0.52
19:B:1234:CLA:HMC3	19:B:1234:CLA:CBC	2.31	0.52
19:F:1305:CLA:HED2	19:F:1305:CLA:OBD	2.09	0.52
22:K:7042:LMU:H71	22:K:7042:LMU:H22	1.92	0.52
12:L:161:ALA:H	12:L:162:PRO:HD2	1.72	0.52
13:N:136:ASP:OD1	13:N:136:ASP:N	2.43	0.52
19:R:1144:CLA:C1A	19:R:1144:CLA:CED	2.83	0.52
15:1:186:LYS:O	15:1:187:GLU:C	2.49	0.52
19:1:1008:CLA:HAA2	19:1:1008:CLA:CBD	2.40	0.52
16:2:237:PHE:CD1	16:2:237:PHE:O	2.57	0.52
19:3:3016:CLA:CMC	19:3:3016:CLA:CBC	2.87	0.52
22:3:7003:LMU:O4'	22:3:7005:LMU:C4B	2.56	0.52
18:4:93:GLN:HE22	18:4:171:ILE:HG12	1.75	0.52
18:4:139:SER:O	18:4:141:LEU:HD22	2.09	0.52
1:A:44:ILE:O	1:A:45:ALA:O	2.28	0.52
1:A:51:THR:HG23	1:A:52:THR:N	2.25	0.52
1:A:157:GLY:CA	1:A:229:ILE:HG22	2.25	0.52
1:A:478:SER:HB2	1:A:644:GLN:OE1	2.08	0.52
1:A:483:GLN:CB	1:A:485:GLN:HE22	2.21	0.52
1:A:664:VAL:CG2	1:A:665:ILE:HG23	2.40	0.52
1:A:733:VAL:HG21	19:A:1140:CLA:C3D	2.40	0.52
19:A:1149:CLA:O1D	19:A:1149:CLA:CBA	2.58	0.52
19:A:9022:CLA:O2A	2:B:651:LEU:HB3	2.10	0.52
2:B:172:GLU:CD	2:B:301:ILE:HG13	2.35	0.52
2:B:200:PRO:O	2:B:204:GLY:HA2	2.10	0.52
2:B:455:ILE:HA	6:F:148:LEU:HG	1.91	0.52
2:B:628:SER:O	2:B:630:GLN:N	2.43	0.52
3:C:62:PHE:CE1	5:E:80:GLU:CD	2.75	0.52
4:D:155:TYR:CE1	4:D:168:PRO:HG3	2.45	0.52
4:D:173:TYR:O	4:D:175:GLU:HG2	2.10	0.52
5:E:78:ARG:NH2	5:E:125:ILE:HG22	2.19	0.52
6:F:207:LEU:CD1	6:F:208:PHE:N	2.51	0.52
12:L:169:ARG:NE	12:L:169:ARG:O	2.43	0.52
13:N:132:THR:CA	13:N:136:ASP:OD1	2.54	0.52
16:2:118:ALA:HA	16:2:121:PHE:CD2	2.34	0.52
16:2:152:LEU:CD1	16:2:152:LEU:N	2.73	0.52
16:2:247:ILE:O	16:2:248:ASP:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:101:GLY:O	17:3:102:GLU:C	2.53	0.52
18:4:83:GLU:O	18:4:84:ASP:CG	2.53	0.52
18:4:95:GLU:CG	18:4:96:LEU:N	2.69	0.52
1:A:154:ARG:HG3	1:A:383:PRO:HB2	1.92	0.51
1:A:291:THR:O	1:A:293:GLY:N	2.36	0.51
1:A:545:HIS:ND1	19:A:1135:CLA:HBB2	2.22	0.51
1:A:555:ILE:HG23	2:B:670:TYR:HE2	1.75	0.51
19:A:1132:CLA:HBC2	19:H:1207:CLA:HBC1	1.92	0.51
19:A:9022:CLA:H122	19:A:9022:CLA:H71	1.92	0.51
19:A:9023:CLA:CAD	2:B:670:TYR:OH	2.58	0.51
2:B:30:ASP:CG	2:B:30:ASP:O	2.53	0.51
2:B:222:LEU:HB2	19:B:1212:CLA:HMD2	1.92	0.51
2:B:527:LEU:CD2	19:B:1222:CLA:C1D	2.87	0.51
2:B:597:LYS:O	2:B:598:HIS:HB2	2.10	0.51
3:C:28:MET:HG3	4:D:175:GLU:HA	1.92	0.51
4:D:99:PHE:C	4:D:100:TYR:HD2	2.18	0.51
4:D:129:LEU:HD11	12:L:65:PHE:CD1	2.44	0.51
6:F:85:CYS:O	6:F:86:LYS:C	2.52	0.51
21:I:6021:BCR:H392	21:L:6019:BCR:C40	2.39	0.51
11:K:56:ILE:HG12	11:K:59:THR:HG21	1.92	0.51
12:L:178:THR:HG22	12:L:179:ALA:H	1.74	0.51
13:N:90:GLU:OE1	13:N:91:TYR:CE1	2.62	0.51
13:N:109:THR:O	13:N:111:GLY:N	2.42	0.51
16:2:113:ALA:HB1	16:2:114:MET:CE	2.38	0.51
18:4:121:ILE:O	18:4:123:VAL:N	2.41	0.51
1:A:374:GLN:O	1:A:377:TYR:CD2	2.63	0.51
1:A:421:ASP:OD1	1:A:421:ASP:N	2.43	0.51
1:A:603:PHE:CZ	1:A:693:LEU:CD2	2.93	0.51
1:A:694:PHE:HZ	2:B:661:PHE:CD1	2.28	0.51
19:A:1103:CLA:H201	21:A:6003:BCR:C18	2.40	0.51
19:A:9022:CLA:H62	2:B:648:TRP:CZ2	2.45	0.51
19:A:9023:CLA:HED3	19:A:9023:CLA:CBA	2.40	0.51
19:B:1203:CLA:CBB	19:B:1225:CLA:HHC	2.39	0.51
19:B:1239:CLA:C19	9:I:21:MET:CB	2.88	0.51
22:B:7038:LMU:C6	22:B:7038:LMU:C10	2.88	0.51
3:C:67:VAL:O	3:C:67:VAL:CG2	2.57	0.51
4:D:171:GLY:O	4:D:172:VAL:CG2	2.53	0.51
7:G:89:LYS:O	7:G:90:GLN:CG	2.57	0.51
12:L:110:LEU:CA	12:L:113:PRO:HG2	2.40	0.51
14:R:39:UNK:CA	14:R:42:UNK:CB	2.85	0.51
15:1:150:HIS:ND1	15:1:150:HIS:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:157:ASP:OD2	15:1:178:LYS:HA	2.08	0.51
17:3:150:TYR:C	17:3:152:ALA:CB	2.83	0.51
17:3:159:VAL:HG12	17:3:160:LEU:H	1.75	0.51
17:3:176:TRP:O	17:3:178:LYS:CA	2.57	0.51
17:3:210:PRO:CG	17:3:211:LEU:H	2.23	0.51
18:4:173:LYS:HD2	18:4:201:LYS:CE	2.33	0.51
1:A:411:ALA:CB	21:A:6008:BCR:H392	2.34	0.51
1:A:461:TYR:CZ	1:A:540:LEU:CD1	2.93	0.51
1:A:629:ASN:CG	1:A:630:ASP:N	2.68	0.51
1:A:733:VAL:HG21	19:A:1140:CLA:HMD1	1.91	0.51
19:A:1126:CLA:CGA	19:A:1126:CLA:C1A	2.89	0.51
2:B:102:GLU:OE2	2:B:641:ASN:HA	2.09	0.51
2:B:124:TRP:C	2:B:124:TRP:HD1	2.17	0.51
2:B:154:TRP:O	2:B:155:LEU:C	2.52	0.51
2:B:235:GLN:O	2:B:236:ASN:C	2.53	0.51
2:B:405:ASP:C	2:B:405:ASP:OD1	2.52	0.51
2:B:620:LEU:O	2:B:621:ARG:C	2.50	0.51
2:B:620:LEU:CD1	19:B:9010:CLA:H93	2.39	0.51
2:B:662:MET:HE3	2:B:671:TRP:CH2	2.45	0.51
22:B:7038:LMU:H1B	22:B:7038:LMU:O6'	2.10	0.51
6:F:83:THR:HB	6:F:84:PRO:CD	2.36	0.51
6:F:150:VAL:O	6:F:150:VAL:CG1	2.49	0.51
8:H:80:GLN:CA	8:H:83:LEU:HD23	2.40	0.51
22:H:7011:LMU:H6E	22:H:7011:LMU:C2B	2.32	0.51
12:L:205:TYR:CE1	12:L:207:LEU:HD13	2.45	0.51
12:L:211:TYR:N	12:L:211:TYR:HD2	2.07	0.51
13:N:120:VAL:HG12	13:N:122:PHE:CE2	2.45	0.51
14:R:38:UNK:O	14:R:42:UNK:C	2.59	0.51
15:1:77:GLU:HG3	15:1:80:LYS:NZ	2.25	0.51
15:1:93:ALA:HA	19:1:1006:CLA:C3B	2.41	0.51
16:2:177:VAL:CG1	16:2:178:ASN:N	2.73	0.51
16:2:249:ASN:OD1	16:2:249:ASN:O	2.28	0.51
17:3:192:LYS:NZ	17:3:192:LYS:CA	2.71	0.51
1:A:207:LEU:CD2	19:A:1119:CLA:CBB	2.83	0.51
1:A:358:LEU:C	1:A:358:LEU:HD12	2.35	0.51
1:A:368:LEU:CD1	19:A:1125:CLA:C6	2.88	0.51
19:A:1126:CLA:H18	19:A:9012:CLA:H18	1.92	0.51
19:A:1132:CLA:H111	21:B:6020:BCR:H10C	1.91	0.51
19:A:1135:CLA:HBA2	19:A:1135:CLA:CGD	2.39	0.51
2:B:75:GLU:CG	2:B:132:ASN:CG	2.70	0.51
2:B:98:GLN:NE2	2:B:98:GLN:CA	2.71	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:LEU:CD1	2:B:317:ARG:HD2	2.40	0.51
2:B:317:ARG:CZ	2:B:317:ARG:HB3	2.39	0.51
2:B:487:ASN:OD1	2:B:487:ASN:C	2.53	0.51
2:B:494:LEU:O	2:B:494:LEU:HD12	2.11	0.51
2:B:561:GLY:HA3	3:C:52:LYS:CB	2.41	0.51
2:B:561:GLY:CA	3:C:52:LYS:HG2	2.36	0.51
2:B:662:MET:HG2	20:B:5002:PQN:O1	2.11	0.51
4:D:177:VAL:HG23	4:D:178:ASN:C	2.35	0.51
5:E:73:LYS:HG3	5:E:128:VAL:HG11	1.93	0.51
6:F:100:LYS:HZ2	6:F:103:GLN:HB2	1.75	0.51
6:F:121:ALA:C	6:F:123:MET:N	2.69	0.51
6:F:202:LEU:O	6:F:203:ALA:CB	2.59	0.51
19:J:1308:CLA:C2	19:J:1308:CLA:O1D	2.58	0.51
11:K:64:MET:O	11:K:67:ALA:HB3	2.11	0.51
13:N:157:LYS:N	13:N:157:LYS:CD	2.74	0.51
15:1:65:ASP:CG	15:1:66:PRO:CA	2.83	0.51
15:1:182:GLU:OE1	19:1:1001:CLA:C2D	2.58	0.51
16:2:122:ILE:HD11	19:2:2002:CLA:CBB	2.26	0.51
17:3:113:ALA:CB	17:3:239:LEU:HD12	2.28	0.51
17:3:134:LEU:CD1	17:3:134:LEU:N	2.65	0.51
18:4:95:GLU:O	18:4:98:ASN:N	2.43	0.51
18:4:96:LEU:CD1	18:4:96:LEU:O	2.57	0.51
18:4:176:SER:C	18:4:178:PRO:HD2	2.35	0.51
1:A:185:HIS:O	1:A:186:TYR:C	2.54	0.51
1:A:295:TRP:HB3	1:A:297:THR:HG23	1.92	0.51
1:A:374:GLN:O	1:A:376:MET:N	2.43	0.51
1:A:571:ASP:HB3	3:C:53:ARG:HH12	1.74	0.51
1:A:678:PHE:O	1:A:681:GLY:O	2.29	0.51
1:A:680:LEU:HD21	2:B:617:MET:HE3	1.92	0.51
19:A:1125:CLA:HBA2	21:A:6008:BCR:C12	2.41	0.51
19:A:1132:CLA:HBC3	19:A:1132:CLA:CMC	2.41	0.51
19:A:1237:CLA:CMD	21:B:6017:BCR:HC31	2.39	0.51
2:B:340:SER:O	2:B:344:ILE:HG13	2.11	0.51
2:B:558:PRO:HG2	2:B:703:VAL:HG13	1.92	0.51
2:B:639:VAL:CG2	2:B:640:CYS:N	2.74	0.51
6:F:208:PHE:O	6:F:209:ARG:C	2.48	0.51
19:F:1302:CLA:HBC2	19:F:1302:CLA:CHD	2.38	0.51
7:G:123:ASN:O	7:G:124:ILE:C	2.52	0.51
11:K:48:PHE:C	11:K:52:PRO:HD3	2.34	0.51
13:N:126:LYS:HZ3	13:N:126:LYS:HB3	1.74	0.51
15:1:67:LEU:CG	15:1:68:GLY:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:84:LEU:N	15:1:86:HIS:HD2	2.07	0.51
15:1:168:PHE:O	15:1:169:ASP:CB	2.39	0.51
15:1:179:LYS:HG2	15:1:180:LEU:C	2.35	0.51
16:2:184:PRO:CA	16:2:187:LYS:HD2	2.40	0.51
16:2:200:TRP:CD1	16:2:200:TRP:N	2.79	0.51
19:2:4009:CLA:H152	19:2:4009:CLA:C19	2.33	0.51
1:A:52:THR:HG1	1:A:53:TRP:HE3	1.57	0.51
1:A:214:GLY:O	1:A:215:SER:CB	2.58	0.51
1:A:274:TRP:NE1	1:A:277:TYR:CD2	2.78	0.51
1:A:483:GLN:CA	1:A:485:GLN:HE22	2.23	0.51
1:A:488:PHE:HB3	1:A:535:GLY:H	1.76	0.51
1:A:575:LEU:HD11	1:A:579:PHE:CG	2.45	0.51
19:A:1101:CLA:HBB1	19:A:1109:CLA:H151	1.91	0.51
19:A:1105:CLA:HBA2	19:A:1107:CLA:C1	2.40	0.51
19:A:1107:CLA:HBA2	19:A:1107:CLA:CHA	2.40	0.51
19:A:1124:CLA:CHC	21:A:6008:BCR:C37	2.89	0.51
19:A:1124:CLA:HAA2	19:A:1125:CLA:CAD	2.41	0.51
19:A:9012:CLA:C4B	19:A:9013:CLA:HBB2	2.41	0.51
2:B:98:GLN:HE21	2:B:101:VAL:HG23	1.76	0.51
2:B:225:LEU:N	2:B:227:THR:O	2.44	0.51
2:B:257:ILE:HD13	2:B:257:ILE:N	2.25	0.51
2:B:365:PHE:HD1	2:B:602:TRP:CE2	2.29	0.51
2:B:411:MET:HE2	19:B:1220:CLA:CMC	2.40	0.51
2:B:450:GLU:C	2:B:452:GLN:H	2.18	0.51
2:B:471:THR:O	2:B:472:TYR:C	2.48	0.51
2:B:555:TYR:CD2	2:B:573:TRP:HB2	2.44	0.51
2:B:558:PRO:CB	2:B:703:VAL:CG2	2.64	0.51
2:B:564:ARG:NH2	3:C:66:ARG:HH12	2.09	0.51
19:B:1220:CLA:HAA1	19:B:1220:CLA:H12	1.93	0.51
4:D:74:LEU:HD11	12:L:58:GLN:OE1	2.10	0.51
4:D:147:LYS:C	4:D:148:TYR:CD1	2.88	0.51
6:F:161:ILE:O	6:F:164:GLY:N	2.36	0.51
6:F:184:ALA:C	6:F:185:ILE:CG2	2.84	0.51
11:K:60:SER:O	11:K:63:LEU:HD22	2.11	0.51
13:N:115:ALA:O	13:N:116:ARG:C	2.49	0.51
13:N:152:LEU:O	13:N:153:GLU:HG3	2.08	0.51
13:N:168:TRP:O	13:N:168:TRP:CE3	2.63	0.51
14:R:37:UNK:O	14:R:42:UNK:O	2.29	0.51
15:1:71:GLU:CG	15:1:72:VAL:N	2.71	0.51
16:2:201:PHE:CD1	16:2:202:ASP:CA	2.93	0.51
18:4:201:LYS:HD3	18:4:201:LYS:H	1.71	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:CD1	19:A:1111:CLA:CED	2.90	0.51
1:A:244:LEU:CB	1:A:247:GLU:CD	2.81	0.51
1:A:468:SER:HB2	1:A:476:MET:SD	2.51	0.51
1:A:660:GLN:HE21	1:A:660:GLN:H	1.58	0.51
19:A:1115:CLA:HED3	19:A:1115:CLA:C1A	2.36	0.51
19:A:1126:CLA:H71	21:A:6011:BCR:H372	1.93	0.51
19:A:1131:CLA:C16	21:L:6019:BCR:H362	2.40	0.51
2:B:10:GLN:O	2:B:11:GLY:C	2.49	0.51
2:B:230:TRP:O	2:B:232:LEU:N	2.43	0.51
2:B:292:ARG:HH22	2:B:297:ILE:CG1	2.24	0.51
2:B:378:ILE:H	2:B:381:PHE:HD1	1.59	0.51
2:B:493:TRP:CB	19:B:1232:CLA:HED2	2.41	0.51
2:B:621:ARG:O	2:B:625:TRP:CB	2.52	0.51
19:B:1205:CLA:H102	19:B:1205:CLA:C14	2.40	0.51
19:B:1228:CLA:HBC2	19:B:1228:CLA:CHD	2.35	0.51
3:C:1:MET:N	3:C:3:HIS:N	2.59	0.51
3:C:5:VAL:HG23	3:C:5:VAL:O	2.11	0.51
4:D:172:VAL:HG12	4:D:173:TYR:N	2.26	0.51
5:E:111:ASN:CG	5:E:112:TYR:N	2.68	0.51
6:F:131:ASP:OD2	6:F:131:ASP:N	2.43	0.51
19:J:1311:CLA:C1A	19:J:1311:CLA:CED	2.83	0.51
13:N:159:LYS:O	13:N:160:TYR:C	2.54	0.51
15:1:157:ASP:OD1	15:1:157:ASP:C	2.53	0.51
17:3:96:ARG:CG	17:3:96:ARG:NH1	2.39	0.51
18:4:94:ALA:HA	19:4:4012:CLA:OBD	2.11	0.51
1:A:240:LYS:O	1:A:240:LYS:CG	2.58	0.51
1:A:313:ALA:C	1:A:315:HIS:H	2.19	0.51
1:A:332:GLU:HA	1:A:344:LYS:CG	2.41	0.51
1:A:435:VAL:O	1:A:438:HIS:ND1	2.43	0.51
1:A:755:ILE:O	1:A:756:ALA:CB	2.59	0.51
2:B:160:LYS:NZ	2:B:161:TRP:CG	2.65	0.51
2:B:288:GLY:O	2:B:289:LEU:HB2	2.10	0.51
2:B:341:LEU:O	2:B:345:THR:OG1	2.14	0.51
2:B:596:TRP:O	2:B:597:LYS:CB	2.58	0.51
19:B:1222:CLA:CHB	19:B:1236:CLA:HAA2	2.41	0.51
4:D:123:ARG:HG2	4:D:124:GLU:N	2.24	0.51
5:E:103:VAL:HG23	5:E:104:VAL:O	2.11	0.51
8:H:58:LEU:N	8:H:61:THR:HG21	2.23	0.51
8:H:94:ARG:HB2	8:H:94:ARG:NH1	2.25	0.51
12:L:107:GLY:O	12:L:109:LEU:N	2.44	0.51
14:R:27:UNK:C	14:R:29:UNK:N	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:30:UNK:O	14:R:32:UNK:N	2.43	0.51
15:1:162:LYS:N	15:1:164:PRO:CG	2.49	0.51
19:2:2004:CLA:H43	19:3:2009:CLA:HBC3	1.93	0.51
22:2:7006:LMU:H122	22:3:7005:LMU:O3'	2.10	0.51
17:3:96:ARG:H	17:3:99:ALA:H	1.58	0.51
17:3:125:VAL:CB	17:3:126:GLY:HA2	2.31	0.51
18:4:237:SER:O	18:4:238:ASP:C	2.50	0.51
19:4:1304:CLA:H2A	19:4:1304:CLA:CGD	2.41	0.51
1:A:431:LEU:CA	1:A:434:ARG:HB2	2.41	0.51
1:A:497:ALA:HB1	1:A:510:SER:HG	1.76	0.51
19:A:1106:CLA:H112	19:A:1126:CLA:H91	1.93	0.51
19:A:1117:CLA:ND	19:A:1127:CLA:H72	2.26	0.51
19:A:1125:CLA:CAB	19:A:1133:CLA:CMA	2.32	0.51
19:A:1126:CLA:C7	21:A:6011:BCR:C37	2.88	0.51
2:B:189:ALA:HB1	19:B:1225:CLA:H203	1.91	0.51
2:B:194:LEU:O	2:B:198:ALA:HB3	2.11	0.51
2:B:256:THR:O	2:B:272:ASP:OD2	2.29	0.51
2:B:290:MET:SD	2:B:291:TYR:CE1	3.04	0.51
2:B:297:ILE:HD11	19:B:1217:CLA:O2D	2.10	0.51
2:B:304:ILE:HD13	19:B:1216:CLA:CED	2.38	0.51
2:B:458:ILE:O	2:B:461:GLN:N	2.43	0.51
19:B:1217:CLA:HMA2	7:G:77:PHE:CD2	2.45	0.51
3:C:63:LEU:HD21	3:C:65:VAL:N	2.24	0.51
4:D:162:GLU:C	4:D:163:VAL:CG2	2.81	0.51
6:F:82:LEU:O	6:F:140:CYS:O	2.29	0.51
6:F:107:LYS:C	6:F:108:LEU:HD12	2.13	0.51
7:G:100:PHE:CD2	7:G:100:PHE:C	2.87	0.51
10:J:42:PHE:CD1	18:4:244:ILE:HG21	2.43	0.51
13:N:123:GLY:HA3	13:N:131:PHE:CD1	2.45	0.51
15:1:138:LEU:O	15:1:139:ALA:C	2.53	0.51
15:1:189:LYS:HB3	19:1:1007:CLA:CMC	2.27	0.51
16:2:157:LEU:CD1	16:2:157:LEU:N	2.73	0.51
16:2:183:PHE:O	16:2:185:ASN:HA	2.11	0.51
17:3:191:GLU:O	17:3:192:LYS:CE	2.57	0.51
17:3:201:ALA:O	17:3:202:TYR:CB	2.58	0.51
18:4:133:GLU:O	18:4:134:TYR:HD1	1.93	0.51
18:4:226:LYS:N	18:4:226:LYS:NZ	2.56	0.51
1:A:270:PHE:CD2	1:A:270:PHE:N	2.79	0.51
1:A:583:GLY:O	1:A:585:GLY:N	2.44	0.51
19:A:1113:CLA:HAA1	19:A:1113:CLA:HED2	1.91	0.51
19:A:1122:CLA:CAB	21:A:6007:BCR:C35	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ILE:O	2:B:22:TRP:C	2.54	0.51
2:B:536:LYS:O	2:B:537:GLY:C	2.54	0.51
2:B:560:ASP:OD2	3:C:66:ARG:NH1	2.44	0.51
3:C:42:ALA:CB	3:C:43:PRO:CD	2.88	0.51
6:F:132:ASN:O	6:F:132:ASN:CG	2.54	0.51
7:G:131:GLY:C	7:G:136:VAL:HB	2.35	0.51
11:K:115:ILE:CG1	11:K:122:LEU:CD1	2.89	0.51
11:K:124:LEU:HD12	11:K:124:LEU:C	2.36	0.51
15:1:69:LEU:HA	15:1:73:PRO:HD3	1.91	0.51
15:1:177:PRO:HG3	15:1:180:LEU:HD23	1.93	0.51
19:1:1010:CLA:O1D	19:1:1010:CLA:C4D	2.50	0.51
16:2:153:PHE:CD2	16:2:157:LEU:HD22	2.45	0.51
16:2:201:PHE:CD1	16:2:202:ASP:HB3	2.46	0.51
17:3:226:LYS:O	17:3:229:LYS:HB3	2.11	0.51
1:A:39:HIS:HA	1:A:44:ILE:HG21	1.92	0.50
1:A:333:ALA:HB3	1:A:334:HIS:ND1	2.27	0.50
19:A:1106:CLA:H43	21:A:6011:BCR:H383	1.92	0.50
2:B:122:GLN:HG2	2:B:361:ILE:HG13	1.94	0.50
2:B:229:GLN:O	7:G:63:VAL:HG11	2.12	0.50
2:B:469:LYS:HZ3	2:B:471:THR:N	2.03	0.50
7:G:75:GLY:O	7:G:78:VAL:N	2.45	0.50
19:H:1207:CLA:HMA2	19:H:1207:CLA:O2A	2.10	0.50
9:I:29:GLU:HA	9:I:29:GLU:OE2	2.11	0.50
12:L:96:LEU:HG	12:L:97:LEU:CD2	2.41	0.50
12:L:106:HIS:HD2	19:L:1502:CLA:CED	2.23	0.50
13:N:123:GLY:HA3	13:N:131:PHE:HD1	1.76	0.50
13:N:142:LYS:O	13:N:145:PHE:CD1	2.64	0.50
14:R:38:UNK:C	14:R:42:UNK:C	2.89	0.50
16:2:161:GLY:N	19:2:2012:CLA:HBB2	2.26	0.50
17:3:100:TYR:HB3	17:3:229:LYS:HE2	1.92	0.50
19:3:3011:CLA:HMA1	19:3:3011:CLA:C1	2.25	0.50
18:4:127:TYR:O	18:4:128:ALA:HB3	2.10	0.50
18:4:206:ALA:O	18:4:207:ASN:C	2.54	0.50
1:A:71:LEU:HD12	1:A:72:GLU:C	2.36	0.50
1:A:135:ASP:OD2	1:A:141:ARG:N	2.44	0.50
1:A:285:GLY:O	1:A:294:LEU:HD11	2.11	0.50
1:A:340:GLY:O	1:A:343:HIS:N	2.33	0.50
1:A:377:TYR:HD1	1:A:616:PHE:HE1	1.56	0.50
1:A:405:PHE:CD1	1:A:605:MET:HE1	2.47	0.50
1:A:473:PRO:O	1:A:474:GLN:C	2.54	0.50
19:A:1119:CLA:HMB2	19:A:1123:CLA:HED2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:9012:CLA:HED2	19:A:9012:CLA:C3D	2.41	0.50
19:A:9012:CLA:H91	19:A:9012:CLA:H152	1.92	0.50
2:B:120:VAL:HG13	2:B:123:TRP:NE1	2.27	0.50
2:B:303:TYR:H	2:B:306:GLU:HB2	1.76	0.50
2:B:556:SER:O	24:B:7101:LMG:HC2	2.11	0.50
2:B:583:MET:HA	19:B:1222:CLA:HBC1	1.93	0.50
2:B:598:HIS:HB3	2:B:602:TRP:CH2	2.46	0.50
19:B:1238:CLA:H91	21:I:6018:BCR:H333	1.93	0.50
4:D:126:PRO:HB2	4:D:128:LEU:HB2	1.93	0.50
5:E:128:VAL:O	5:E:129:GLU:O	2.28	0.50
7:G:98:THR:OG1	7:G:99:HIS:C	2.55	0.50
19:H:1145:CLA:CMA	19:H:1145:CLA:C1	2.89	0.50
10:J:14:VAL:O	10:J:14:VAL:HG13	2.11	0.50
14:R:35:UNK:O	14:R:42:UNK:O	2.30	0.50
15:1:224:PRO:HA	15:1:225:TRP:C	2.36	0.50
16:2:126:LEU:HB3	19:2:2006:CLA:C19	2.29	0.50
16:2:126:LEU:HD13	19:2:2006:CLA:H172	1.93	0.50
16:2:236:TRP:CZ2	19:2:2003:CLA:CHB	2.94	0.50
17:3:95:PRO:O	17:3:96:ARG:CD	2.58	0.50
18:4:147:ILE:O	18:4:150:HIS:HB3	2.10	0.50
18:4:154:ILE:O	18:4:155:ARG:C	2.54	0.50
1:A:281:LEU:HD22	19:A:1115:CLA:CMA	2.11	0.50
1:A:472:ARG:O	1:A:474:GLN:HG3	2.12	0.50
1:A:483:GLN:CB	1:A:485:GLN:CD	2.79	0.50
1:A:626:GLY:O	1:A:627:THR:HG22	2.11	0.50
19:A:1102:CLA:HBC3	19:A:1102:CLA:HHD	1.92	0.50
19:A:1103:CLA:C4	21:A:6003:BCR:H313	2.41	0.50
19:A:1123:CLA:HMD2	19:A:1123:CLA:H142	1.92	0.50
19:A:1128:CLA:C10	19:A:1128:CLA:H152	2.41	0.50
19:A:1135:CLA:HBA2	19:A:1135:CLA:CBD	2.41	0.50
2:B:407:VAL:C	2:B:409:ALA:O	2.55	0.50
2:B:429:LEU:HD21	19:B:1235:CLA:C3B	2.42	0.50
2:B:573:TRP:O	2:B:577:TYR:N	2.37	0.50
2:B:605:ASN:C	2:B:605:ASN:OD1	2.53	0.50
4:D:180:GLY:O	4:D:182:GLN:N	2.44	0.50
6:F:100:LYS:C	6:F:103:GLN:HB3	2.29	0.50
11:K:94:GLN:CD	11:K:94:GLN:N	2.69	0.50
11:K:115:ILE:O	11:K:118:VAL:N	2.44	0.50
13:N:142:LYS:CE	13:N:142:LYS:CA	2.80	0.50
13:N:148:ASP:H	13:N:150:LEU:N	2.09	0.50
13:N:152:LEU:CA	13:N:153:GLU:HG3	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:44:UNK:O	14:R:45:UNK:O	2.30	0.50
16:2:114:MET:HG3	16:2:230:LEU:HB2	1.92	0.50
16:2:241:TYR:HD2	16:2:242:THR:N	2.10	0.50
18:4:161:LYS:NZ	18:4:162:ASN:ND2	2.60	0.50
18:4:223:VAL:C	18:4:224:THR:HG23	2.36	0.50
1:A:109:TRP:O	1:A:112:ASP:N	2.44	0.50
1:A:284:ARG:HG3	1:A:295:TRP:NE1	2.26	0.50
1:A:502:THR:O	1:A:504:ALA:O	2.30	0.50
1:A:536:THR:O	1:A:536:THR:HG23	2.11	0.50
1:A:550:HIS:O	1:A:552:THR:O	2.29	0.50
1:A:734:GLY:O	1:A:736:THR:N	2.44	0.50
2:B:351:HIS:NE2	19:B:1223:CLA:NC	2.59	0.50
2:B:394:PHE:C	2:B:542:ARG:HD3	2.36	0.50
2:B:447:GLY:C	2:B:449:PRO:HD3	2.37	0.50
2:B:594:TRP:HD1	2:B:595:HIS:HB2	1.76	0.50
2:B:622:ASP:HB2	2:B:626:LEU:HD11	1.84	0.50
19:B:1203:CLA:H43	24:B:7101:LMG:H321	1.92	0.50
3:C:10:THR:HG23	5:E:101:TYR:CG	2.41	0.50
6:F:88:SER:HG	6:F:91:PHE:HB3	1.73	0.50
19:K:1143:CLA:CAC	22:K:7001:LMU:C3B	2.86	0.50
19:L:1130:CLA:H92	19:L:1504:CLA:H2	1.92	0.50
13:N:104:LYS:O	13:N:107:LEU:N	2.44	0.50
13:N:120:VAL:CG1	13:N:122:PHE:CE2	2.94	0.50
22:R:7025:LMU:H21	22:R:7025:LMU:O2'	2.11	0.50
15:1:77:GLU:CD	15:1:80:LYS:NZ	2.69	0.50
15:1:225:TRP:HB3	15:1:226:HIS:CA	2.41	0.50
16:2:227:LEU:CD2	19:2:2004:CLA:NC	2.72	0.50
16:2:261:THR:CG2	16:2:262:ILE:N	2.59	0.50
17:3:201:ALA:CB	17:3:202:TYR:CE2	2.74	0.50
1:A:245:PRO:O	1:A:248:PHE:CZ	2.64	0.50
1:A:747:TRP:CE3	21:A:6011:BCR:C40	2.94	0.50
19:A:9022:CLA:C10	21:B:6017:BCR:H19C	2.40	0.50
2:B:6:PRO:O	2:B:6:PRO:HG2	2.12	0.50
2:B:196:HIS:NE2	19:B:1212:CLA:ND	2.59	0.50
2:B:247:THR:CA	2:B:250:ALA:HB3	2.20	0.50
2:B:451:LYS:HD3	19:B:1230:CLA:O2D	2.10	0.50
2:B:593:TYR:O	2:B:596:TRP:O	2.29	0.50
2:B:649:MET:HE1	19:B:1205:CLA:HBC3	1.93	0.50
2:B:726:ILE:C	2:B:728:SER:H	2.19	0.50
19:B:1224:CLA:CGA	19:B:1224:CLA:H3A	2.34	0.50
5:E:127:GLU:OE1	5:E:129:GLU:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:173:TRP:CZ3	6:F:211:PHE:N	2.80	0.50
6:F:226:LEU:HA	6:F:230:ASN:HD22	1.77	0.50
7:G:81:ASN:OD1	7:G:82:PHE:N	2.43	0.50
7:G:87:VAL:O	7:G:88:ALA:CB	2.57	0.50
8:H:78:PRO:HG3	19:L:1501:CLA:CMD	2.40	0.50
12:L:208:ASP:OD2	12:L:209:LEU:O	2.29	0.50
14:R:38:UNK:O	14:R:39:UNK:O	2.30	0.50
19:1:1008:CLA:HBA2	19:1:1008:CLA:CMA	2.42	0.50
17:3:192:LYS:O	17:3:193:GLY:C	2.54	0.50
22:4:7033:LMU:H6'2	22:4:7033:LMU:O2'	2.12	0.50
1:A:23:ASP:OD1	1:A:33:GLN:HG3	2.12	0.50
1:A:95:GLY:O	1:A:96:MET:C	2.52	0.50
1:A:203:LEU:CD2	19:A:1123:CLA:O2D	2.59	0.50
1:A:205:HIS:CE1	19:A:1111:CLA:HMC2	2.47	0.50
1:A:656:PHE:O	1:A:659:ALA:N	2.45	0.50
19:A:1104:CLA:HBA2	19:A:1104:CLA:HED2	1.93	0.50
19:A:1112:CLA:CHC	21:A:6002:BCR:H17C	2.31	0.50
19:A:1137:CLA:HBC3	19:A:1137:CLA:HMC1	1.92	0.50
19:A:9012:CLA:HED1	19:B:9010:CLA:H2	1.94	0.50
2:B:92:TRP:CZ2	9:I:6:SER:HB2	2.47	0.50
2:B:175:LEU:HD12	2:B:179:LEU:HD23	1.93	0.50
2:B:278:LEU:HG	19:B:1213:CLA:HMA1	1.93	0.50
2:B:292:ARG:HH21	2:B:297:ILE:CA	2.25	0.50
2:B:354:SER:O	2:B:508:LEU:HD23	2.12	0.50
2:B:456:GLU:CB	6:F:147:HIS:ND1	2.75	0.50
2:B:667:TRP:O	2:B:669:GLY:N	2.44	0.50
19:B:1208:CLA:HBD	19:B:1208:CLA:O2A	2.11	0.50
19:B:1209:CLA:H61	19:B:1209:CLA:C1	2.42	0.50
19:B:1222:CLA:O1A	19:B:1236:CLA:HAA1	2.12	0.50
3:C:29:ILE:HG22	3:C:30:PRO:O	2.12	0.50
4:D:103:THR:C	4:D:104:TRP:HD1	2.19	0.50
22:H:7032:LMU:H22	22:H:7032:LMU:H6'2	1.93	0.50
13:N:155:GLU:O	13:N:157:LYS:CE	2.08	0.50
22:R:7020:LMU:H6E	22:R:7020:LMU:O6B	2.11	0.50
16:2:113:ALA:C	16:2:114:MET:CE	2.75	0.50
16:2:219:THR:O	16:2:223:LYS:HB2	2.12	0.50
19:3:3017:CLA:HBC3	19:3:3017:CLA:HMC2	1.94	0.50
18:4:158:GLN:C	19:4:1004:CLA:CMA	2.74	0.50
19:4:4003:CLA:CMC	19:4:4003:CLA:CBC	2.89	0.50
1:A:148:GLY:O	1:A:152:ILE:CD1	2.57	0.50
1:A:370:ILE:HD13	19:A:1124:CLA:CAD	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ASP:O	1:A:660:GLN:NE2	2.45	0.50
1:A:662:SER:O	1:A:666:GLN:HB2	2.12	0.50
1:A:705:GLU:CB	2:B:545:LYS:NZ	2.75	0.50
19:A:1141:CLA:H72	19:A:1141:CLA:H122	1.90	0.50
2:B:224:PRO:HG3	7:G:153:PHE:HB3	1.94	0.50
2:B:330:ILE:HD12	2:B:333:GLN:HE21	1.77	0.50
2:B:519:VAL:HG11	2:B:593:TYR:HB2	1.94	0.50
2:B:626:LEU:O	2:B:627:ASN:CB	2.47	0.50
4:D:140:LEU:HD22	4:D:144:LEU:HD11	1.92	0.50
4:D:147:LYS:CA	4:D:148:TYR:CD1	2.93	0.50
4:D:184:VAL:HG12	4:D:185:GLY:H	1.76	0.50
6:F:88:SER:HG	6:F:91:PHE:CB	2.25	0.50
11:K:51:SER:H	11:K:52:PRO:HD3	1.75	0.50
15:1:168:PHE:O	15:1:168:PHE:HD1	1.95	0.50
19:1:1005:CLA:CHA	19:1:1005:CLA:HBA1	2.42	0.50
17:3:109:ALA:O	17:3:111:LEU:CD2	2.60	0.50
17:3:246:LEU:HB3	17:3:248:THR:HG23	1.92	0.50
18:4:188:ILE:HG22	18:4:189:PHE:HD2	1.77	0.50
1:A:409:GLY:C	1:A:411:ALA:H	2.19	0.50
1:A:431:LEU:N	1:A:434:ARG:HE	2.10	0.50
2:B:348:VAL:HG21	19:B:1225:CLA:HHD	1.94	0.50
2:B:420:SER:O	2:B:424:TRP:N	2.36	0.50
2:B:431:PHE:HE2	19:B:1229:CLA:CED	2.25	0.50
2:B:508:LEU:HB2	2:B:509:PHE:HD2	1.76	0.50
2:B:693:TRP:CD1	19:B:1238:CLA:CMD	2.94	0.50
4:D:103:THR:OG1	4:D:153:GLN:HB2	2.11	0.50
22:H:7002:LMU:O6B	22:H:7002:LMU:C1B	2.58	0.50
12:L:70:GLU:OE2	12:L:75:SER:OG	2.19	0.50
13:N:90:GLU:OE1	13:N:91:TYR:CD1	2.65	0.50
13:N:168:TRP:CZ3	13:N:170:TRP:HB3	2.47	0.50
14:R:8:UNK:CB	19:R:1144:CLA:CED	2.90	0.50
14:R:34:UNK:O	14:R:36:UNK:O	2.30	0.50
15:1:150:HIS:O	15:1:153:SER:HB3	2.12	0.50
16:2:158:VAL:O	16:2:159:PHE:C	2.52	0.50
16:2:249:ASN:OD1	16:2:250:LEU:O	2.30	0.50
17:3:104:ILE:CG2	19:3:3004:CLA:C2D	2.90	0.50
18:4:120:ILE:HD11	18:4:226:LYS:HG3	0.51	0.50
18:4:122:ASN:HB3	18:4:124:PRO:CD	2.36	0.50
22:4:7034:LMU:C10	22:4:7052:LMU:C3'	2.90	0.50
1:A:167:THR:HG22	19:A:1112:CLA:CAA	2.23	0.50
1:A:240:LYS:O	1:A:240:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:HIS:CD2	19:A:1116:CLA:NB	2.78	0.50
1:A:348:GLU:O	1:A:351:THR:HG22	2.12	0.50
1:A:348:GLU:O	1:A:351:THR:CG2	2.60	0.50
19:A:1237:CLA:HMB1	19:L:1502:CLA:HBC1	1.92	0.50
2:B:190:TRP:CZ2	19:B:1215:CLA:HMD1	2.47	0.50
2:B:338:LEU:O	2:B:339:ALA:HB3	2.11	0.50
2:B:472:TYR:O	2:B:472:TYR:HD1	1.95	0.50
2:B:620:LEU:CA	2:B:624:LEU:HD23	2.32	0.50
2:B:707:LEU:HD11	2:B:711:VAL:HG21	1.93	0.50
2:B:732:LYS:CG	2:B:734:GLY:CA	2.88	0.50
19:B:1202:CLA:H162	19:B:1210:CLA:OBD	2.12	0.50
3:C:63:LEU:HD23	3:C:63:LEU:C	2.37	0.50
6:F:105:SER:O	6:F:107:LYS:N	2.45	0.50
6:F:129:ARG:NH1	6:F:132:ASN:OD1	2.45	0.50
6:F:200:VAL:HG12	10:J:7:TYR:C	2.36	0.50
19:J:1308:CLA:HBD	19:J:1308:CLA:CGA	2.42	0.50
11:K:53:THR:HA	11:K:56:ILE:HB	1.94	0.50
11:K:116:ILE:HG23	11:K:117:GLY:H	1.74	0.50
12:L:112:GLY:N	12:L:113:PRO:CD	2.75	0.50
12:L:138:VAL:HG21	12:L:194:ILE:HG13	1.94	0.50
13:N:132:THR:HG21	13:N:139:LYS:HD3	0.66	0.50
14:R:35:UNK:O	14:R:36:UNK:O	2.30	0.50
15:1:137:ILE:O	15:1:141:GLU:CG	2.49	0.50
17:3:108:PHE:HD2	19:3:3013:CLA:H43	1.77	0.50
17:3:109:ALA:HA	17:3:111:LEU:HB3	1.60	0.50
17:3:161:GLU:O	17:3:162:MET:C	2.50	0.50
17:3:176:TRP:C	17:3:178:LYS:N	2.67	0.50
18:4:167:ASN:O	18:4:168:GLN:HB2	2.12	0.50
18:4:170:PRO:C	18:4:173:LYS:N	2.70	0.50
1:A:378:SER:OG	19:A:1125:CLA:HBC2	2.12	0.49
1:A:499:ALA:HB3	1:A:500:PRO:CD	2.42	0.49
1:A:744:ALA:HB2	21:A:6011:BCR:H391	0.69	0.49
19:A:1126:CLA:H72	21:A:6011:BCR:H371	1.94	0.49
2:B:46:ILE:HG21	19:B:1202:CLA:HBC3	1.94	0.49
2:B:69:ALA:HB1	2:B:135:LEU:CD1	2.37	0.49
2:B:275:HIS:O	2:B:278:LEU:HB3	2.11	0.49
2:B:306:GLU:CG	2:B:307:ALA:H	2.00	0.49
2:B:315:LEU:CD1	2:B:316:GLY:C	2.85	0.49
2:B:330:ILE:HG13	2:B:330:ILE:O	2.10	0.49
2:B:434:LEU:O	2:B:438:VAL:HG13	2.12	0.49
2:B:592:PHE:HA	2:B:721:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:685:THR:HG1	19:L:1130:CLA:H3A	1.74	0.49
19:B:1225:CLA:H142	21:B:6006:BCR:C10	2.42	0.49
4:D:132:ALA:CB	4:D:136:GLN:HE22	2.21	0.49
5:E:76:ILE:O	5:E:84:TYR:O	2.30	0.49
5:E:111:ASN:CG	5:E:116:SER:CB	2.85	0.49
7:G:102:ALA:CA	7:G:104:ASP:OD2	2.59	0.49
7:G:144:THR:CG2	7:G:147:ASN:O	2.58	0.49
22:H:7032:LMU:H31	22:H:7032:LMU:H2B	1.93	0.49
10:J:22:LEU:O	10:J:23:ALA:C	2.55	0.49
14:R:38:UNK:O	14:R:42:UNK:O	2.30	0.49
22:R:7007:LMU:O6B	22:R:7007:LMU:H1B	2.12	0.49
15:1:77:GLU:HG3	15:1:80:LYS:CE	2.42	0.49
16:2:171:ILE:CG1	16:2:172:LEU:H	2.23	0.49
17:3:94:GLU:CD	17:3:94:GLU:O	2.54	0.49
17:3:161:GLU:CA	17:3:164:LEU:HG	2.39	0.49
18:4:170:PRO:HG2	18:4:171:ILE:HG13	1.94	0.49
19:4:1004:CLA:OBD	19:4:1004:CLA:O2D	2.29	0.49
1:A:90:PHE:O	1:A:91:LEU:C	2.52	0.49
1:A:150:PHE:H	1:A:153:TRP:CB	2.19	0.49
1:A:170:GLY:C	1:A:173:VAL:HG22	2.37	0.49
1:A:210:LEU:HB2	19:A:1111:CLA:HMB2	1.95	0.49
1:A:217:SER:HG	21:A:6002:BCR:H17C	1.76	0.49
1:A:233:LEU:O	1:A:235:ALA:N	2.30	0.49
1:A:262:PHE:O	1:A:265:GLY:N	2.44	0.49
1:A:382:TYR:HE2	19:A:1127:CLA:HED3	1.75	0.49
1:A:400:MET:HE3	1:A:612:VAL:CG1	2.35	0.49
1:A:639:ALA:O	1:A:640:GLY:C	2.53	0.49
1:A:686:TRP:O	1:A:689:SER:OG	2.19	0.49
1:A:692:PHE:CE2	1:A:733:VAL:HG11	2.46	0.49
19:A:1112:CLA:HMC2	21:A:6002:BCR:C15	2.41	0.49
19:A:1112:CLA:HBA2	19:3:1147:CLA:HMC3	1.94	0.49
19:A:1141:CLA:O2D	19:A:1141:CLA:O1A	2.29	0.49
21:A:6011:BCR:H353	19:A:9012:CLA:H41	1.94	0.49
2:B:21:ILE:HD11	19:B:1238:CLA:HMA1	1.93	0.49
2:B:244:PHE:CD2	2:B:244:PHE:O	2.58	0.49
2:B:393:PHE:CZ	2:B:398:TYR:CD2	3.01	0.49
2:B:396:ARG:NH1	19:B:1226:CLA:HED2	2.27	0.49
2:B:503:GLU:O	2:B:504:ASN:C	2.55	0.49
19:B:1205:CLA:H42	19:B:1205:CLA:CHD	2.42	0.49
19:B:1222:CLA:H72	19:B:1236:CLA:C3D	2.41	0.49
19:B:1225:CLA:H62	21:B:6006:BCR:HC7	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1235:CLA:C12	21:F:6016:BCR:C31	2.90	0.49
3:C:5:VAL:CG2	3:C:65:VAL:HG21	2.35	0.49
4:D:105:ASP:HB2	4:D:151:LYS:HB2	1.94	0.49
19:H:1207:CLA:HBB2	9:I:13:GLY:O	2.11	0.49
10:J:5:LYS:CE	16:2:178:ASN:CG	2.85	0.49
22:K:7042:LMU:H5'	22:K:7042:LMU:C2B	2.41	0.49
12:L:124:GLU:O	12:L:124:GLU:HG3	2.13	0.49
13:N:90:GLU:OE1	13:N:91:TYR:CE2	2.65	0.49
22:R:7020:LMU:O2'	22:R:7020:LMU:H5'	2.12	0.49
15:1:183:LEU:O	15:1:184:LYS:C	2.54	0.49
19:2:2002:CLA:C4C	19:2:2002:CLA:H42	2.42	0.49
17:3:101:GLY:C	17:3:103:VAL:N	2.65	0.49
1:A:130:GLU:OE1	1:A:130:GLU:O	2.29	0.49
1:A:267:THR:HG21	1:A:269:PHE:HE2	1.67	0.49
1:A:284:ARG:CZ	1:A:284:ARG:CA	2.88	0.49
1:A:539:PHE:HD2	1:A:539:PHE:O	1.95	0.49
2:B:222:LEU:HB3	19:B:1212:CLA:CAD	2.43	0.49
3:C:17:CYS:SG	3:C:18:VAL:N	2.86	0.49
4:D:95:GLN:NE2	4:D:96:VAL:N	2.60	0.49
22:E:7048:LMU:O4'	22:F:7036:LMU:C6'	2.60	0.49
6:F:123:MET:C	6:F:127:LYS:HB2	2.37	0.49
6:F:181:TYR:CD2	6:F:181:TYR:C	2.90	0.49
7:G:116:SER:OG	7:G:119:PRO:HG2	2.12	0.49
12:L:207:LEU:HD23	12:L:208:ASP:C	2.37	0.49
15:1:125:LEU:HD22	15:1:125:LEU:N	2.13	0.49
15:1:158:PRO:CD	15:1:159:GLU:H	2.24	0.49
16:2:244:THR:O	16:2:245:GLY:C	2.55	0.49
1:A:251:ASN:OD1	17:3:137:PHE:CD1	2.45	0.49
1:A:312:ILE:O	1:A:313:ALA:HB2	2.11	0.49
1:A:369:THR:HG21	1:A:402:ILE:CG2	2.42	0.49
1:A:372:VAL:HG22	19:A:1117:CLA:C4	2.42	0.49
1:A:432:LEU:O	1:A:435:VAL:N	2.45	0.49
19:A:1119:CLA:C9	21:A:6007:BCR:C37	2.53	0.49
2:B:123:TRP:CA	2:B:126:THR:HB	2.37	0.49
2:B:312:GLY:O	2:B:314:ARG:N	2.36	0.49
2:B:330:ILE:CD1	19:B:1202:CLA:H193	2.43	0.49
2:B:462:TRP:HZ3	19:B:1231:CLA:CBC	2.10	0.49
2:B:500:ALA:HB3	2:B:507:SER:O	2.13	0.49
19:B:1217:CLA:HBB2	7:G:74:LEU:HD22	1.94	0.49
19:B:1223:CLA:H41	19:B:1223:CLA:C7	2.32	0.49
4:D:105:ASP:HB2	4:D:151:LYS:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:80:ALA:O	6:F:81:GLY:C	2.55	0.49
7:G:89:LYS:O	7:G:90:GLN:HB2	2.11	0.49
7:G:144:THR:OG1	7:G:147:ASN:C	2.56	0.49
10:J:10:VAL:HG13	10:J:11:ALA:H	1.76	0.49
12:L:76:SER:O	12:L:78:LEU:N	2.45	0.49
13:N:150:LEU:O	13:N:151:ASP:CB	2.60	0.49
15:1:161:LYS:C	15:1:161:LYS:CD	2.85	0.49
19:1:1008:CLA:H43	19:1:1008:CLA:CGA	2.42	0.49
16:2:211:PRO:O	16:2:212:GLN:HB3	2.11	0.49
16:2:249:ASN:O	16:2:250:LEU:C	2.47	0.49
22:4:7052:LMU:H12	22:4:7052:LMU:H52	1.93	0.49
1:A:107:GLU:CD	1:A:161:GLU:CG	2.85	0.49
1:A:130:GLU:C	1:A:132:LEU:N	2.65	0.49
1:A:598:VAL:O	1:A:598:VAL:HG12	2.13	0.49
1:A:629:ASN:CG	1:A:630:ASP:H	2.21	0.49
19:A:1102:CLA:HBA2	19:A:1109:CLA:C6	2.41	0.49
2:B:396:ARG:HH11	19:B:1226:CLA:HED2	1.78	0.49
2:B:646:TRP:CZ2	2:B:726:ILE:HG21	2.48	0.49
19:B:1205:CLA:H71	19:B:1205:CLA:H2	1.95	0.49
19:B:1214:CLA:H12	19:B:1214:CLA:C1A	2.42	0.49
19:B:1229:CLA:HBB2	21:F:6014:BCR:H23C	1.94	0.49
4:D:206:GLN:O	4:D:208:TYR:N	2.45	0.49
7:G:62:LEU:HB3	7:G:65:SER:CB	2.16	0.49
7:G:89:LYS:CA	7:G:89:LYS:HZ1	2.19	0.49
8:H:99:LYS:O	8:H:102:ILE:N	2.42	0.49
22:H:7011:LMU:C6'	22:H:7011:LMU:C2B	2.90	0.49
12:L:164:LEU:HD13	12:L:165:THR:OG1	2.12	0.49
13:N:133:GLY:CA	13:N:134:CYS:CB	2.89	0.49
15:1:157:ASP:OD1	15:1:157:ASP:O	2.29	0.49
16:2:182:ILE:HD13	16:2:190:GLY:CA	2.34	0.49
16:2:200:TRP:HB3	16:2:202:ASP:OD1	2.12	0.49
18:4:232:LEU:HB3	18:4:236:ILE:CD1	2.42	0.49
18:4:239:PRO:HD2	18:4:240:TRP:H	1.78	0.49
1:A:126:ILE:O	1:A:126:ILE:HG13	2.11	0.49
1:A:209:GLY:C	1:A:213:LEU:HB2	2.37	0.49
1:A:385:LEU:O	1:A:386:ALA:HB3	2.12	0.49
1:A:503:THR:HB	19:A:1134:CLA:CBA	2.43	0.49
1:A:571:ASP:O	1:A:574:ASN:ND2	2.46	0.49
1:A:623:ASP:O	1:A:624:VAL:HB	2.12	0.49
19:A:1104:CLA:HMA1	19:A:1104:CLA:H2	1.95	0.49
19:A:1119:CLA:HMC3	19:A:1119:CLA:HBC2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:6002:BCR:C12	21:A:6002:BCR:C34	2.84	0.49
2:B:131:THR:CG2	2:B:134:ASP:N	2.55	0.49
2:B:160:LYS:HG3	2:B:161:TRP:H	1.75	0.49
2:B:639:VAL:CG2	2:B:640:CYS:H	2.23	0.49
19:B:1222:CLA:C1B	19:B:1236:CLA:HMA2	2.42	0.49
3:C:62:PHE:CE1	5:E:80:GLU:CG	2.93	0.49
6:F:154:GLN:C	6:F:154:GLN:OE1	2.55	0.49
7:G:76:ARG:HH11	7:G:120:VAL:HB	1.78	0.49
15:1:73:PRO:O	15:1:74:ALA:C	2.54	0.49
15:1:186:LYS:O	15:1:189:LYS:HG2	2.12	0.49
16:2:131:ILE:C	16:2:133:ASN:H	2.20	0.49
16:2:200:TRP:H	16:2:200:TRP:HD1	1.61	0.49
17:3:107:ARG:CZ	17:3:233:LEU:N	2.75	0.49
17:3:200:PRO:O	17:3:201:ALA:C	2.54	0.49
18:4:203:LYS:NZ	19:4:4002:CLA:CAD	2.71	0.49
18:4:220:GLN:CD	19:4:1306:CLA:CAC	2.85	0.49
1:A:88:ILE:O	1:A:92:TRP:HB2	2.13	0.49
1:A:216:LEU:HD12	21:A:6002:BCR:C35	2.43	0.49
1:A:377:TYR:CD1	1:A:616:PHE:CE1	2.99	0.49
1:A:397:THR:HG21	1:A:613:ILE:CG1	2.41	0.49
1:A:446:LEU:CD2	1:A:554:LEU:HA	2.38	0.49
1:A:462:ILE:HD13	19:A:9022:CLA:H93	1.95	0.49
1:A:618:TRP:O	1:A:618:TRP:CD1	2.66	0.49
1:A:618:TRP:CH2	1:A:655:ASP:HB2	2.48	0.49
1:A:656:PHE:O	1:A:658:TRP:N	2.46	0.49
2:B:197:VAL:O	2:B:198:ALA:CB	2.60	0.49
2:B:270:LEU:HD12	2:B:271:THR:CA	2.43	0.49
2:B:311:PRO:HG3	19:B:1301:CLA:C4C	2.42	0.49
2:B:399:ASN:O	2:B:402:GLN:N	2.45	0.49
2:B:618:GLY:CA	2:B:621:ARG:H	2.26	0.49
19:B:1205:CLA:HMC2	21:B:6017:BCR:H282	1.93	0.49
3:C:29:ILE:HD11	4:D:180:GLY:O	2.12	0.49
3:C:39:ILE:O	3:C:40:ALA:CB	2.61	0.49
3:C:66:ARG:NH2	3:C:66:ARG:CB	2.75	0.49
4:D:77:ASN:C	4:D:79:PRO:CD	2.86	0.49
22:E:7037:LMU:H5B	22:E:7037:LMU:O2B	2.12	0.49
6:F:200:VAL:CG2	6:F:203:ALA:C	2.85	0.49
6:F:224:GLY:O	6:F:226:LEU:O	2.30	0.49
9:I:11:LEU:CD1	21:I:6021:BCR:C10	2.81	0.49
13:N:156:GLY:HA2	13:N:157:LYS:CD	2.38	0.49
13:N:156:GLY:CA	13:N:157:LYS:CE	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:97:ILE:HD12	15:1:98:LEU:CD2	2.32	0.49
16:2:218:ARG:HH12	19:2:2001:CLA:HBB2	1.78	0.49
17:3:206:PRO:HG2	17:3:208:PHE:CD2	2.47	0.49
19:3:2009:CLA:H92	19:3:2009:CLA:H52	0.60	0.49
1:A:23:ASP:OD1	1:A:24:ARG:CD	2.56	0.49
1:A:75:SER:CB	1:A:354:TRP:HZ2	2.24	0.49
1:A:89:ILE:O	1:A:93:LEU:CD2	2.61	0.49
1:A:184:PHE:CE2	19:A:1108:CLA:C2D	2.96	0.49
1:A:578:ARG:O	1:A:579:PHE:O	2.30	0.49
19:A:1126:CLA:H2A	19:A:1126:CLA:O1D	2.12	0.49
19:A:1138:CLA:HBC3	21:F:6014:BCR:H332	1.93	0.49
2:B:87:ILE:O	2:B:121:TYR:HE2	1.96	0.49
2:B:103:ALA:HB2	2:B:105:THR:O	2.13	0.49
2:B:216:LEU:HD21	2:B:221:GLY:CA	2.42	0.49
2:B:247:THR:C	2:B:250:ALA:N	2.70	0.49
2:B:257:ILE:HG22	2:B:495:PRO:HG2	1.95	0.49
2:B:394:PHE:CE2	2:B:412:LEU:HD21	2.48	0.49
2:B:476:ILE:CG2	2:B:476:ILE:O	2.58	0.49
2:B:492:ILE:O	2:B:493:TRP:HB2	2.13	0.49
2:B:527:LEU:HD23	19:B:1222:CLA:C1D	2.43	0.49
2:B:614:THR:HG23	2:B:614:THR:O	2.12	0.49
2:B:644:SER:O	2:B:645:VAL:C	2.54	0.49
2:B:707:LEU:HD11	19:B:1226:CLA:C9	2.42	0.49
3:C:28:MET:HB3	4:D:176:LYS:O	2.13	0.49
3:C:73:THR:OG1	3:C:76:SER:OG	1.76	0.49
4:D:199:GLU:O	4:D:200:VAL:C	2.56	0.49
7:G:75:GLY:C	7:G:77:PHE:H	2.20	0.49
19:H:1145:CLA:H193	19:H:1145:CLA:C14	2.37	0.49
10:J:20:GLY:O	10:J:21:ALA:HB3	2.11	0.49
11:K:78:ARG:HB3	11:K:79:LYS:H	1.49	0.49
15:1:73:PRO:CD	15:1:74:ALA:N	2.72	0.49
15:1:78:ARG:HG2	19:1:1011:CLA:HMC1	1.93	0.49
15:1:85:ILE:N	15:1:88:ARG:HG3	2.27	0.49
15:1:158:PRO:HA	15:1:175:LYS:CB	2.42	0.49
15:1:177:PRO:CD	15:1:180:LEU:CA	2.89	0.49
16:2:95:ASP:CB	17:3:85:ASP:OD2	2.50	0.49
16:2:149:THR:O	16:2:152:LEU:CD1	2.61	0.49
16:2:183:PHE:O	16:2:184:PRO:C	2.55	0.49
18:4:121:ILE:C	18:4:123:VAL:N	2.71	0.49
1:A:23:ASP:CG	1:A:24:ARG:HD2	2.37	0.49
1:A:223:VAL:O	1:A:228:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:O	1:A:313:ALA:CB	2.60	0.49
1:A:355:HIS:O	1:A:358:LEU:HG	2.12	0.49
1:A:370:ILE:CD1	19:A:1124:CLA:C3D	2.90	0.49
1:A:487:VAL:CG1	1:A:489:ALA:N	2.55	0.49
1:A:701:GLN:HA	1:A:701:GLN:NE2	2.26	0.49
19:A:1107:CLA:HBA2	19:A:1107:CLA:HBD	1.93	0.49
2:B:223:GLY:O	2:B:225:LEU:HB3	2.13	0.49
2:B:232:LEU:HD12	2:B:235:GLN:HG3	1.78	0.49
2:B:469:LYS:HG3	2:B:470:THR:OG1	2.12	0.49
2:B:622:ASP:CB	2:B:626:LEU:HG	2.40	0.49
6:F:149:ILE:HG22	6:F:151:SER:H	1.78	0.49
7:G:61:ALA:O	7:G:63:VAL:CG1	2.61	0.49
7:G:119:PRO:HB2	7:G:120:VAL:HG23	1.95	0.49
12:L:101:GLU:HG3	19:L:1501:CLA:C1A	2.43	0.49
12:L:146:THR:C	12:L:148:TYR:N	2.69	0.49
13:N:113:ASN:OD1	13:N:113:ASN:C	2.56	0.49
13:N:127:PHE:HD1	13:N:128:PRO:HA	1.78	0.49
19:R:1144:CLA:HBA2	19:R:1144:CLA:HBD	1.95	0.49
15:1:84:LEU:N	15:1:84:LEU:HD12	2.28	0.49
15:1:204:GLN:HE21	19:1:1003:CLA:CBB	2.26	0.49
15:1:223:ASP:CB	15:1:224:PRO:HD2	2.43	0.49
16:2:149:THR:OG1	16:2:150:THR:N	2.46	0.49
16:2:182:ILE:HG21	16:2:187:LYS:HE2	1.95	0.49
19:2:2002:CLA:CHD	19:2:2002:CLA:CBC	2.90	0.49
17:3:206:PRO:CD	17:3:206:PRO:O	2.61	0.49
18:4:177:LEU:HD22	18:4:178:PRO:CB	2.43	0.49
18:4:177:LEU:CD2	18:4:178:PRO:N	2.68	0.49
18:4:202:GLU:HA	18:4:205:ILE:CG2	2.42	0.49
1:A:224:HIS:HE1	19:A:1113:CLA:CHD	2.26	0.49
1:A:226:SER:O	1:A:230:ASN:ND2	2.46	0.49
1:A:302:HIS:HE1	19:A:1117:CLA:C1B	2.25	0.49
1:A:532:ILE:O	1:A:532:ILE:HG12	2.13	0.49
1:A:575:LEU:HD11	1:A:579:PHE:CB	2.40	0.49
1:A:628:ILE:CD1	1:A:629:ASN:O	2.61	0.49
1:A:723:ARG:H	19:A:1139:CLA:CBB	2.17	0.49
19:A:1138:CLA:H52	19:A:1138:CLA:NC	2.27	0.49
19:A:9022:CLA:H71	19:A:9022:CLA:C12	2.41	0.49
19:A:9022:CLA:H142	19:B:1206:CLA:HBB2	1.94	0.49
2:B:120:VAL:O	2:B:123:TRP:CD1	2.64	0.49
2:B:549:ASP:HB2	3:C:63:LEU:HD12	1.95	0.49
2:B:590:VAL:O	2:B:593:TYR:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:649:MET:SD	2:B:723:ALA:HB2	2.53	0.49
19:B:1221:CLA:CMB	19:B:1223:CLA:H92	2.43	0.49
5:E:122:LEU:O	5:E:124:GLU:C	2.56	0.49
5:E:128:VAL:C	5:E:129:GLU:O	2.56	0.49
6:F:199:ASP:CA	10:J:9:SER:HA	2.42	0.49
7:G:83:GLN:OE1	19:G:1242:CLA:C2D	2.60	0.49
8:H:98:LEU:O	8:H:99:LYS:O	2.30	0.49
12:L:54:TYR:CD1	12:L:57:ILE:HG23	2.47	0.49
12:L:208:ASP:OD2	12:L:208:ASP:C	2.55	0.49
13:N:148:ASP:H	13:N:149:ASP:CA	2.26	0.49
15:1:158:PRO:CD	15:1:159:GLU:N	2.76	0.49
16:2:125:PHE:CA	16:2:127:THR:CG2	2.60	0.49
17:3:110:MET:C	17:3:113:ALA:HB3	2.35	0.49
17:3:157:LEU:O	17:3:160:LEU:HB3	2.12	0.49
18:4:112:PRO:CA	18:4:117:SER:OG	2.61	0.49
1:A:39:HIS:HA	1:A:44:ILE:CG2	2.43	0.48
1:A:130:GLU:O	1:A:131:ILE:C	2.51	0.48
1:A:132:LEU:O	1:A:671:SER:C	2.52	0.48
1:A:246:HIS:NE2	19:3:1147:CLA:O1D	2.46	0.48
1:A:366:GLY:O	1:A:403:GLY:HA2	2.13	0.48
1:A:378:SER:OG	1:A:512:SER:OG	2.29	0.48
1:A:412:ALA:O	1:A:415:ALA:HB3	2.13	0.48
1:A:423:ASP:H	1:A:424:PRO:HD3	1.76	0.48
1:A:488:PHE:CD1	1:A:535:GLY:N	2.81	0.48
1:A:648:THR:C	1:A:650:ASN:H	2.21	0.48
19:A:1113:CLA:HMC1	19:A:1113:CLA:HBC3	1.95	0.48
19:A:1131:CLA:H101	19:A:1131:CLA:H143	1.94	0.48
19:A:1132:CLA:O1D	12:L:119:PRO:O	2.31	0.48
2:B:85:ARG:HG2	2:B:85:ARG:NH1	2.04	0.48
2:B:427:LEU:HB3	19:B:1229:CLA:HED1	1.95	0.48
2:B:438:VAL:O	2:B:442:VAL:N	2.44	0.48
2:B:454:LEU:HD13	2:B:514:PRO:CG	2.43	0.48
2:B:507:SER:O	2:B:508:LEU:CB	2.60	0.48
2:B:657:TRP:O	2:B:660:GLY:N	2.34	0.48
19:B:1225:CLA:H62	21:B:6006:BCR:C32	2.42	0.48
6:F:96:LYS:C	6:F:97:GLN:O	2.53	0.48
6:F:207:LEU:C	6:F:209:ARG:H	2.21	0.48
19:F:1302:CLA:C3B	19:F:1305:CLA:HAC2	2.41	0.48
7:G:99:HIS:O	7:G:101:GLU:CA	2.61	0.48
7:G:116:SER:OG	7:G:119:PRO:HB2	2.13	0.48
22:G:7026:LMU:H3'	22:G:7026:LMU:H11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:1311:CLA:O1A	19:J:1311:CLA:C14	2.59	0.48
13:N:146:LEU:HD21	13:N:148:ASP:O	2.12	0.48
15:1:85:ILE:CA	15:1:88:ARG:CG	2.72	0.48
15:1:138:LEU:HA	15:1:141:GLU:CD	2.38	0.48
21:1:6023:BCR:HC8	21:1:6023:BCR:C2	2.42	0.48
16:2:153:PHE:CD2	16:2:157:LEU:CD2	2.96	0.48
16:2:226:ARG:CG	16:2:226:ARG:NH1	2.67	0.48
17:3:100:TYR:HA	17:3:229:LYS:HE2	1.94	0.48
17:3:182:MET:HG2	17:3:183:GLY:N	2.28	0.48
18:4:83:GLU:C	18:4:84:ASP:OD1	2.56	0.48
18:4:107:ALA:O	18:4:110:LEU:HB3	2.13	0.48
18:4:170:PRO:C	18:4:173:LYS:H	2.21	0.48
1:A:89:ILE:O	1:A:92:TRP:C	2.54	0.48
1:A:159:THR:O	1:A:163:GLN:CD	2.56	0.48
1:A:258:LEU:HG	1:A:280:PHE:CD1	2.47	0.48
1:A:439:ARG:HG2	1:A:562:PHE:CE2	2.47	0.48
1:A:464:ASN:O	1:A:468:SER:N	2.42	0.48
1:A:552:THR:O	1:A:553:VAL:HB	2.13	0.48
1:A:618:TRP:HB2	1:A:656:PHE:CE1	2.48	0.48
1:A:679:PHE:O	1:A:683:HIS:CB	2.61	0.48
19:A:1151:CLA:CED	19:A:1151:CLA:CBA	2.91	0.48
2:B:4:ARG:CZ	2:B:4:ARG:O	2.60	0.48
2:B:317:ARG:HH12	2:B:410:ARG:HG2	1.75	0.48
3:C:72:GLU:CB	3:C:77:MET:HE2	2.41	0.48
5:E:83:TRP:CH2	5:E:116:SER:OG	2.63	0.48
7:G:100:PHE:O	7:G:100:PHE:HD2	1.96	0.48
7:G:120:VAL:O	7:G:120:VAL:CG1	2.57	0.48
10:J:14:VAL:O	10:J:14:VAL:CG1	2.59	0.48
12:L:108:TYR:C	12:L:109:LEU:O	2.52	0.48
16:2:241:TYR:O	16:2:242:THR:C	2.52	0.48
19:2:2013:CLA:HMC1	19:2:2013:CLA:CBC	2.39	0.48
17:3:108:PHE:CD2	19:3:3013:CLA:H43	2.48	0.48
18:4:123:VAL:O	18:4:123:VAL:HG22	2.13	0.48
18:4:239:PRO:HD2	18:4:240:TRP:N	2.28	0.48
1:A:39:HIS:O	1:A:40:PHE:HB3	2.12	0.48
1:A:210:LEU:CD1	19:A:1111:CLA:CMB	2.90	0.48
1:A:309:LEU:HA	1:A:312:ILE:O	2.13	0.48
1:A:350:LEU:HA	1:A:350:LEU:HD23	1.37	0.48
1:A:382:TYR:HB2	1:A:385:LEU:HD11	1.95	0.48
1:A:441:ALA:HA	1:A:444:SER:HB3	1.95	0.48
1:A:665:ILE:HD13	2:B:621:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1139:CLA:O1A	19:A:1139:CLA:C3	2.62	0.48
21:A:6007:BCR:C23	21:A:6007:BCR:C38	2.85	0.48
2:B:361:ILE:O	2:B:362:ALA:O	2.31	0.48
2:B:373:THR:O	2:B:377:TYR:N	2.36	0.48
2:B:404:ALA:O	2:B:405:ASP:OD1	2.30	0.48
3:C:43:PRO:HA	4:D:182:GLN:CG	2.43	0.48
4:D:140:LEU:CB	4:D:143:ARG:HB2	2.40	0.48
6:F:78:ASP:OD1	6:F:154:GLN:NE2	2.39	0.48
6:F:128:LYS:C	6:F:129:ARG:HD3	2.37	0.48
6:F:220:GLU:HG3	6:F:220:GLU:O	2.13	0.48
10:J:21:ALA:O	10:J:23:ALA:N	2.46	0.48
11:K:115:ILE:CG1	11:K:122:LEU:HD12	2.43	0.48
12:L:205:TYR:O	12:L:205:TYR:CG	2.65	0.48
13:N:136:ASP:CG	13:N:137:LEU:N	2.71	0.48
15:1:199:VAL:HG12	15:1:200:GLY:N	2.28	0.48
17:3:205:GLY:H	17:3:206:PRO:HD2	1.76	0.48
1:A:23:ASP:CG	1:A:24:ARG:CD	2.87	0.48
1:A:109:TRP:O	1:A:112:ASP:C	2.56	0.48
1:A:148:GLY:C	1:A:149:PHE:O	2.51	0.48
1:A:249:ILE:HG23	17:3:137:PHE:CE2	2.49	0.48
1:A:250:LEU:H	17:3:136:TRP:HH2	1.60	0.48
1:A:370:ILE:HD11	19:A:1124:CLA:CAD	2.41	0.48
1:A:420:ARG:CZ	1:A:420:ARG:CB	2.91	0.48
1:A:619:LYS:O	1:A:621:GLN:N	2.46	0.48
19:A:1103:CLA:H141	19:A:1103:CLA:H161	1.68	0.48
19:A:1122:CLA:ND	21:A:6007:BCR:H19C	2.27	0.48
19:A:1128:CLA:H192	21:A:6011:BCR:H20C	1.95	0.48
19:A:1141:CLA:H12	19:A:1141:CLA:HMA3	1.87	0.48
2:B:98:GLN:HB2	2:B:99:PRO:HD2	1.96	0.48
2:B:314:ARG:CZ	15:1:67:LEU:CD2	2.77	0.48
2:B:666:SER:CB	2:B:671:TRP:HE1	2.13	0.48
2:B:707:LEU:HD13	24:B:7101:LMG:H301	1.96	0.48
19:B:1239:CLA:HBC2	19:B:1239:CLA:CMC	2.43	0.48
4:D:173:TYR:O	4:D:173:TYR:CG	2.62	0.48
9:I:19:VAL:O	9:I:23:SER:N	2.46	0.48
11:K:125:LYS:CG	11:K:128:GLY:HA2	2.43	0.48
12:L:164:LEU:C	12:L:165:THR:HG22	2.37	0.48
13:N:110:THR:O	13:N:112:ALA:O	2.31	0.48
15:1:223:ASP:O	15:1:225:TRP:HB2	2.13	0.48
16:2:160:ILE:CB	19:2:2012:CLA:HBB1	2.37	0.48
16:2:169:ALA:O	16:2:170:ASP:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:184:PRO:N	16:2:187:LYS:HD2	2.28	0.48
17:3:156:THR:O	17:3:156:THR:HG22	2.06	0.48
18:4:204:GLU:O	18:4:205:ILE:C	2.54	0.48
1:A:130:GLU:OE1	1:A:133:ASN:HB3	2.13	0.48
1:A:244:LEU:CD1	1:A:247:GLU:OE2	2.56	0.48
1:A:502:THR:CB	1:A:504:ALA:H	2.25	0.48
19:A:1112:CLA:HMB2	21:A:6002:BCR:H382	1.93	0.48
19:A:1119:CLA:H162	21:A:6008:BCR:H271	1.96	0.48
19:A:1128:CLA:HBD	19:A:1128:CLA:HAA1	1.96	0.48
19:A:1138:CLA:HBC3	19:A:1138:CLA:HHD	1.96	0.48
2:B:230:TRP:CE3	19:B:1213:CLA:HAA2	2.49	0.48
2:B:374:HIS:HB2	19:B:1224:CLA:C4B	2.42	0.48
2:B:697:PRO:CG	19:B:1238:CLA:HBC3	2.44	0.48
3:C:7:ILE:HG21	3:C:54:CYS:SG	2.54	0.48
6:F:83:THR:CB	6:F:84:PRO:CD	2.91	0.48
7:G:84:ARG:NH1	7:G:89:LYS:H	2.11	0.48
8:H:113:SER:OG	19:H:1207:CLA:H2	2.12	0.48
22:K:7042:LMU:H71	22:K:7042:LMU:C2	2.43	0.48
13:N:143:VAL:HG11	13:N:155:GLU:OE1	2.14	0.48
15:1:68:GLY:HA2	15:1:72:VAL:HB	1.93	0.48
15:1:83:GLU:OE2	15:1:83:GLU:CA	2.55	0.48
15:1:163:TYR:N	15:1:164:PRO:CD	2.76	0.48
16:2:100:ARG:O	16:2:101:TRP:C	2.55	0.48
16:2:147:THR:HG22	16:2:148:ASP:CG	2.35	0.48
18:4:207:ASN:ND2	19:4:4002:CLA:C1A	2.72	0.48
1:A:73:GLU:O	1:A:76:ARG:HB2	2.14	0.48
1:A:262:PHE:C	1:A:262:PHE:CD2	2.91	0.48
1:A:390:ALA:HA	1:A:393:LEU:CD2	2.44	0.48
1:A:680:LEU:HD21	2:B:617:MET:CE	2.43	0.48
19:A:1119:CLA:HAA2	19:A:1123:CLA:HBB2	1.95	0.48
19:A:1140:CLA:H102	19:A:9013:CLA:H152	1.95	0.48
19:A:1149:CLA:HBC2	19:A:1149:CLA:HMC3	1.96	0.48
2:B:22:TRP:HE1	19:B:1238:CLA:CAB	2.17	0.48
2:B:621:ARG:C	2:B:625:TRP:HB3	2.35	0.48
2:B:709:GLY:O	2:B:710:LEU:CB	2.59	0.48
19:B:1214:CLA:H112	19:B:1232:CLA:H3A	1.96	0.48
3:C:73:THR:HG23	3:C:76:SER:CB	2.42	0.48
4:D:123:ARG:NH2	22:D:7050:LMU:H4B	1.98	0.48
7:G:73:PHE:O	7:G:76:ARG:CB	2.56	0.48
7:G:98:THR:OG1	7:G:100:PHE:N	2.47	0.48
8:H:111:TYR:CD1	8:H:112:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:LYS:HE3	16:2:178:ASN:CG	2.38	0.48
12:L:79:ILE:O	12:L:80:ALA:C	2.56	0.48
19:L:1502:CLA:CMC	19:L:1502:CLA:HBC3	2.44	0.48
22:R:7020:LMU:H6E	22:R:7020:LMU:C6B	2.42	0.48
15:1:58:ALA:CB	19:1:1015:CLA:C2B	2.91	0.48
19:1:1007:CLA:HAA1	22:4:7008:LMU:O3'	2.13	0.48
22:1:7013:LMU:O6B	22:1:7013:LMU:C1B	2.58	0.48
18:4:177:LEU:CD2	18:4:177:LEU:C	2.84	0.48
1:A:87:SER:HB3	1:A:178:MET:O	2.14	0.48
1:A:98:PHE:O	1:A:100:GLY:CA	2.62	0.48
1:A:402:ILE:HD11	19:A:1127:CLA:CBB	2.44	0.48
1:A:411:ALA:O	1:A:412:ALA:C	2.57	0.48
19:A:1105:CLA:CGA	19:A:1107:CLA:H12	2.43	0.48
19:A:1112:CLA:CMB	21:A:6002:BCR:C38	2.90	0.48
19:A:1133:CLA:C2B	21:A:6008:BCR:H333	2.44	0.48
19:A:9011:CLA:CBB	19:A:9012:CLA:HED1	2.43	0.48
19:A:9013:CLA:CMD	2:B:533:ILE:HG21	2.44	0.48
2:B:98:GLN:CB	2:B:99:PRO:HD2	2.44	0.48
2:B:103:ALA:HA	2:B:105:THR:CA	2.43	0.48
2:B:103:ALA:CB	2:B:105:THR:O	2.61	0.48
2:B:183:PHE:HE1	19:B:1210:CLA:H71	1.79	0.48
2:B:305:LEU:HD23	19:B:1220:CLA:O1D	2.14	0.48
2:B:326:ILE:HG13	2:B:332:PHE:HB3	1.96	0.48
2:B:389:HIS:HE1	19:B:1226:CLA:NC	2.11	0.48
2:B:436:LEU:O	2:B:437:TYR:CB	2.61	0.48
2:B:559:CYS:SG	2:B:560:ASP:N	2.86	0.48
2:B:649:MET:CE	21:B:6017:BCR:H272	2.44	0.48
19:B:1202:CLA:H43	21:B:6005:BCR:C31	2.38	0.48
4:D:86:SER:CA	12:L:69:LEU:HD21	2.43	0.48
8:H:86:THR:HG23	8:H:89:ALA:HB2	1.94	0.48
11:K:116:ILE:CG2	11:K:117:GLY:H	2.26	0.48
12:L:97:LEU:O	12:L:98:ARG:C	2.55	0.48
12:L:165:THR:O	12:L:166:LEU:C	2.57	0.48
13:N:139:LYS:CG	13:N:142:LYS:HE2	2.41	0.48
13:N:155:GLU:OE2	13:N:157:LYS:O	2.32	0.48
16:2:128:LYS:C	16:2:130:GLY:N	2.66	0.48
16:2:157:LEU:HD12	16:2:157:LEU:HA	1.59	0.48
16:2:233:MET:SD	16:2:236:TRP:CD1	3.07	0.48
17:3:103:VAL:C	17:3:107:ARG:HD2	2.38	0.48
17:3:191:GLU:O	17:3:192:LYS:CD	2.62	0.48
18:4:87:ASN:OD1	18:4:90:TRP:CD2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:168:GLN:O	18:4:172:PHE:CD1	2.66	0.48
18:4:169:ASP:HB3	19:4:4001:CLA:CMB	2.43	0.48
18:4:209:ARG:O	18:4:212:LEU:CA	2.61	0.48
1:A:71:LEU:O	1:A:72:GLU:C	2.53	0.48
1:A:93:LEU:H	1:A:96:MET:H	1.60	0.48
1:A:188:LYS:O	1:A:188:LYS:HD2	2.14	0.48
1:A:281:LEU:CB	19:A:1115:CLA:HED2	2.44	0.48
1:A:316:MET:CA	1:A:317:TYR:HD1	2.27	0.48
1:A:316:MET:HA	1:A:317:TYR:HD1	1.79	0.48
1:A:547:PHE:HE2	19:A:9023:CLA:O1A	1.97	0.48
1:A:690:LEU:HD21	2:B:661:PHE:HE1	1.78	0.48
19:A:1102:CLA:HMC3	19:A:1104:CLA:O2D	2.13	0.48
2:B:7:ARG:NH1	2:B:7:ARG:CB	2.69	0.48
2:B:110:LEU:HD12	2:B:110:LEU:C	2.34	0.48
2:B:294:ASN:CG	7:G:94:GLN:CD	2.80	0.48
2:B:382:ILE:HD11	19:B:1203:CLA:H142	1.95	0.48
2:B:493:TRP:HB2	19:B:1232:CLA:HED2	1.96	0.48
3:C:1:MET:SD	3:C:4:SER:CB	3.02	0.48
3:C:66:ARG:HB3	3:C:66:ARG:CZ	2.44	0.48
6:F:82:LEU:HG	6:F:83:THR:OG1	2.14	0.48
6:F:157:TRP:HZ3	19:F:1302:CLA:HMC1	1.79	0.48
11:K:48:PHE:HB2	11:K:50:GLY:H	1.79	0.48
19:K:1142:CLA:HBD	19:K:1142:CLA:HAA2	1.94	0.48
13:N:133:GLY:CA	13:N:134:CYS:HB2	2.44	0.48
13:N:148:ASP:N	13:N:149:ASP:CA	2.76	0.48
13:N:157:LYS:CB	13:N:159:LYS:N	2.57	0.48
22:N:7049:LMU:O1'	22:N:7049:LMU:C4	2.61	0.48
15:1:189:LYS:N	15:1:189:LYS:CE	2.77	0.48
19:1:1010:CLA:HBA2	19:1:1010:CLA:CMA	2.44	0.48
16:2:229:MET:CE	16:2:230:LEU:HD13	2.43	0.48
16:2:269:LYS:CE	16:2:269:LYS:C	2.87	0.48
17:3:95:PRO:C	17:3:96:ARG:HG2	2.27	0.48
19:3:3017:CLA:O1A	19:3:3017:CLA:CMA	2.60	0.48
18:4:243:THR:CG2	18:4:244:ILE:O	2.53	0.48
19:4:4002:CLA:HMA2	19:4:4002:CLA:CBA	2.22	0.48
1:A:249:ILE:HG22	17:3:137:PHE:CE2	2.49	0.48
1:A:390:ALA:CB	1:A:754:ILE:HD13	2.43	0.48
1:A:575:LEU:HD12	1:A:575:LEU:C	2.32	0.48
1:A:607:ASN:O	1:A:608:SER:C	2.57	0.48
19:A:1119:CLA:H43	19:A:1122:CLA:H2	1.96	0.48
19:A:1136:CLA:H71	19:A:1136:CLA:H112	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1140:CLA:H62	19:A:9013:CLA:H171	1.96	0.48
19:A:9011:CLA:C1A	19:B:9010:CLA:HBB2	2.44	0.48
2:B:62:SER:OG	2:B:63:GLY:N	2.47	0.48
2:B:500:ALA:CB	2:B:503:GLU:OE2	2.60	0.48
2:B:594:TRP:CD2	2:B:598:HIS:CE1	3.02	0.48
2:B:685:THR:O	2:B:685:THR:HG22	2.14	0.48
19:B:1231:CLA:HMD1	19:B:1232:CLA:C2C	2.44	0.48
22:B:7038:LMU:O6'	22:B:7038:LMU:C1B	2.62	0.48
4:D:165:TYR:CD2	4:D:168:PRO:HG2	2.49	0.48
6:F:194:LYS:N	6:F:195:GLU:OE2	2.47	0.48
6:F:204:SER:O	6:F:207:LEU:HB3	2.14	0.48
11:K:56:ILE:C	11:K:59:THR:HG23	2.39	0.48
11:K:125:LYS:CD	11:K:128:GLY:HA2	2.44	0.48
19:L:1148:CLA:HED3	19:L:1148:CLA:H72	1.96	0.48
13:N:132:THR:CB	13:N:137:LEU:O	2.62	0.48
14:R:38:UNK:O	14:R:39:UNK:C	2.62	0.48
15:1:77:GLU:CG	15:1:80:LYS:CD	2.78	0.48
15:1:92:LEU:N	15:1:95:PRO:HD3	2.26	0.48
15:1:162:LYS:CG	15:1:163:TYR:H	2.24	0.48
16:2:128:LYS:HB3	16:2:131:ILE:CG1	2.35	0.48
16:2:184:PRO:CG	16:2:185:ASN:N	2.77	0.48
18:4:131:LYS:CD	18:4:131:LYS:N	2.69	0.48
18:4:177:LEU:CD1	18:4:178:PRO:CD	2.59	0.48
22:4:7019:LMU:H32	22:4:7019:LMU:O2'	2.13	0.48
1:A:113:PRO:C	1:A:114:THR:HG22	2.29	0.48
1:A:316:MET:CA	1:A:317:TYR:CB	2.91	0.48
1:A:358:LEU:O	1:A:361:ASN:HB3	2.14	0.48
1:A:426:THR:HG23	1:A:428:TYR:CE2	2.45	0.48
1:A:493:GLN:HG2	1:A:516:GLY:H	1.79	0.48
1:A:588:GLY:N	2:B:668:ARG:NH1	2.60	0.48
1:A:664:VAL:HG23	1:A:665:ILE:HG23	1.95	0.48
1:A:701:GLN:NE2	1:A:724:ALA:H	2.12	0.48
1:A:733:VAL:HG22	19:A:1140:CLA:CAD	2.43	0.48
19:A:1119:CLA:HMC3	19:A:1119:CLA:CBC	2.44	0.48
2:B:172:GLU:OE1	2:B:301:ILE:HG13	2.14	0.48
2:B:618:GLY:HA2	2:B:621:ARG:CB	2.40	0.48
6:F:207:LEU:HD13	6:F:207:LEU:N	2.28	0.48
6:F:207:LEU:C	6:F:209:ARG:N	2.69	0.48
7:G:80:PHE:CE1	7:G:83:GLN:O	2.67	0.48
12:L:85:ASN:O	12:L:92:ALA:CB	2.55	0.48
13:N:133:GLY:HA2	13:N:134:CYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:94:VAL:O	15:1:98:LEU:HB2	2.14	0.48
15:1:136:THR:O	15:1:137:ILE:C	2.56	0.48
19:2:2001:CLA:HBA2	19:2:2001:CLA:H3A	1.67	0.48
17:3:96:ARG:NH1	17:3:100:TYR:OH	2.43	0.48
1:A:63:ASP:CA	19:A:1128:CLA:HED2	2.43	0.47
1:A:93:LEU:CA	1:A:96:MET:N	2.69	0.47
1:A:211:LEU:HB3	1:A:310:PHE:CD2	2.49	0.47
1:A:545:HIS:ND1	19:A:1135:CLA:CBB	2.76	0.47
19:A:1124:CLA:H43	19:A:1136:CLA:CBA	2.39	0.47
19:A:1126:CLA:C7	21:A:6011:BCR:H371	2.44	0.47
19:A:1128:CLA:H152	19:A:1128:CLA:H101	1.96	0.47
2:B:161:TRP:O	2:B:162:LYS:C	2.57	0.47
2:B:377:TYR:O	2:B:378:ILE:HB	2.14	0.47
2:B:497:TRP:C	2:B:499:ASN:H	2.21	0.47
2:B:542:ARG:CG	2:B:542:ARG:NH1	2.41	0.47
2:B:599:ILE:O	2:B:734:GLY:C	2.57	0.47
2:B:658:ALA:O	2:B:661:PHE:HD2	1.96	0.47
3:C:61:ASP:CG	5:E:118:ASN:ND2	2.72	0.47
4:D:97:GLU:HB2	4:D:98:GLU:HG2	1.96	0.47
4:D:149:LYS:HE3	4:D:149:LYS:HB3	1.28	0.47
6:F:121:ALA:HB1	6:F:125:LYS:HB3	1.95	0.47
6:F:205:SER:C	6:F:207:LEU:CD1	2.86	0.47
8:H:81:SER:O	8:H:83:LEU:HD22	2.14	0.47
19:H:1145:CLA:HAA1	19:H:1145:CLA:HED2	1.93	0.47
12:L:204:LEU:CD1	12:L:205:TYR:C	2.85	0.47
13:N:132:THR:CB	13:N:139:LYS:CD	2.90	0.47
15:1:93:ALA:CA	19:1:1006:CLA:C4B	2.91	0.47
15:1:114:TRP:HH2	15:1:121:GLN:CA	2.27	0.47
16:2:128:LYS:HD2	16:2:128:LYS:HA	1.61	0.47
18:4:169:ASP:OD1	18:4:174:GLN:CA	2.62	0.47
18:4:177:LEU:HD13	18:4:178:PRO:HD2	1.95	0.47
18:4:209:ARG:HA	18:4:212:LEU:HD12	1.95	0.47
22:4:7034:LMU:C11	22:4:7052:LMU:O3'	2.61	0.47
1:A:122:VAL:O	19:A:1105:CLA:HED2	2.14	0.47
1:A:252:ARG:O	1:A:252:ARG:CZ	2.62	0.47
1:A:258:LEU:O	1:A:259:TYR:HD2	1.96	0.47
1:A:595:TRP:CZ3	1:A:728:VAL:HG13	2.50	0.47
19:A:1106:CLA:ND	19:A:1126:CLA:H42	2.29	0.47
19:A:1117:CLA:HBC1	21:A:6003:BCR:H12C	1.96	0.47
2:B:167:TRP:CZ2	19:B:1210:CLA:CAC	2.97	0.47
2:B:174:ARG:HH12	19:B:1221:CLA:HMD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:PRO:HD2	2:B:497:TRP:HB2	1.95	0.47
2:B:607:SER:HA	2:B:610:ASN:ND2	2.29	0.47
2:B:662:MET:O	2:B:663:PHE:C	2.57	0.47
2:B:668:ARG:CG	2:B:699:ALA:O	2.62	0.47
19:B:1227:CLA:H3A	19:B:1227:CLA:HBA2	1.50	0.47
3:C:9:ASP:OD1	3:C:61:ASP:CG	2.57	0.47
3:C:11:CYS:SG	23:C:8003:SF4:S3	3.12	0.47
12:L:161:ALA:N	12:L:162:PRO:CD	2.77	0.47
15:1:58:ALA:HB3	15:1:59:PRO:HD3	1.96	0.47
15:1:145:ILE:O	15:1:148:VAL:HG13	2.14	0.47
16:2:184:PRO:CD	16:2:185:ASN:HA	2.44	0.47
18:4:138:SER:O	18:4:139:SER:CB	2.61	0.47
18:4:225:GLY:HA2	18:4:226:LYS:NZ	2.24	0.47
1:A:50:THR:HG22	1:A:52:THR:N	2.27	0.47
1:A:64:PHE:CG	1:A:74:ILE:HD13	2.49	0.47
1:A:107:GLU:CD	1:A:161:GLU:CD	2.82	0.47
1:A:220:ARG:O	1:A:221:HIS:CB	2.62	0.47
1:A:350:LEU:O	1:A:350:LEU:HD22	2.14	0.47
1:A:362:LEU:HG	1:A:406:LEU:HG	1.96	0.47
1:A:438:HIS:HB2	1:A:441:ALA:CB	2.44	0.47
1:A:651:GLY:O	1:A:655:ASP:N	2.41	0.47
1:A:653:LEU:HD13	19:B:9010:CLA:HBC2	1.96	0.47
2:B:19:ARG:O	2:B:23:PHE:HB2	2.15	0.47
2:B:55:ALA:HB1	2:B:150:LEU:HD12	1.97	0.47
2:B:183:PHE:HB3	2:B:284:PHE:CD2	2.48	0.47
2:B:198:ALA:H	2:B:200:PRO:HG2	1.80	0.47
2:B:292:ARG:HH12	2:B:295:PHE:N	2.13	0.47
2:B:587:ILE:HA	2:B:587:ILE:HD13	1.72	0.47
19:B:1206:CLA:HAA1	19:B:1206:CLA:H12	1.97	0.47
21:B:6006:BCR:HC8	21:B:6006:BCR:C33	2.39	0.47
6:F:99:LEU:O	6:F:102:LEU:CG	2.30	0.47
6:F:103:GLN:OE1	6:F:103:GLN:C	2.57	0.47
6:F:127:LYS:O	6:F:129:ARG:CA	2.60	0.47
11:K:47:ASP:N	11:K:51:SER:CB	2.77	0.47
11:K:75:SER:O	11:K:76:ALA:CB	2.61	0.47
12:L:83:LEU:HD13	12:L:88:ALA:CB	2.44	0.47
12:L:209:LEU:CG	12:L:210:PRO:CD	2.92	0.47
13:N:120:VAL:HG12	13:N:122:PHE:CD2	2.49	0.47
16:2:168:TRP:NE1	16:2:171:ILE:HG21	2.21	0.47
18:4:214:PHE:O	18:4:215:LEU:O	2.32	0.47
1:A:27:ILE:O	1:A:28:LYS:CD	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HG22	1:A:45:ALA:H	1.79	0.47
1:A:119:SER:OG	1:A:143:ILE:C	2.57	0.47
1:A:126:ILE:CD1	19:A:1107:CLA:CMA	2.86	0.47
1:A:349:ILE:O	1:A:351:THR:N	2.47	0.47
1:A:619:LYS:HG2	1:A:642:PHE:CE1	2.50	0.47
19:A:1113:CLA:HBC3	19:A:1113:CLA:CMC	2.45	0.47
19:A:1126:CLA:HBD	19:A:1126:CLA:HAA1	1.95	0.47
2:B:98:GLN:CB	2:B:99:PRO:CD	2.92	0.47
2:B:130:ARG:NH1	2:B:130:ARG:CG	2.71	0.47
2:B:375:HIS:CE1	19:B:1225:CLA:NC	2.82	0.47
2:B:693:TRP:HD1	19:B:1238:CLA:C3D	2.27	0.47
19:B:1210:CLA:H151	19:B:1225:CLA:CMD	2.45	0.47
4:D:132:ALA:HB3	4:D:136:GLN:NE2	2.21	0.47
5:E:81:SER:O	5:E:82:TYR:C	2.53	0.47
6:F:192:THR:O	6:F:193:GLN:HG3	2.14	0.47
19:H:1145:CLA:HAA1	19:H:1145:CLA:HED1	1.96	0.47
19:H:1145:CLA:CMA	19:H:1145:CLA:O2A	2.63	0.47
12:L:91:THR:HA	12:L:98:ARG:NH1	2.22	0.47
12:L:143:LEU:N	12:L:145:LEU:N	2.60	0.47
12:L:181:GLY:O	12:L:184:LYS:HG2	2.14	0.47
13:N:157:LYS:HG2	13:N:159:LYS:CG	2.44	0.47
17:3:124:LYS:CG	17:3:124:LYS:O	2.62	0.47
18:4:161:LYS:HZ1	18:4:162:ASN:HD21	1.60	0.47
18:4:176:SER:OG	18:4:177:LEU:HD13	2.14	0.47
1:A:73:GLU:O	1:A:76:ARG:CB	2.62	0.47
1:A:143:ILE:HG23	1:A:143:ILE:HD12	1.64	0.47
1:A:304:LEU:CD1	19:A:1115:CLA:CBB	2.93	0.47
1:A:330:ILE:O	1:A:330:ILE:HG22	2.13	0.47
1:A:409:GLY:C	1:A:411:ALA:N	2.72	0.47
1:A:454:GLY:N	1:A:457:SER:HB3	2.07	0.47
19:A:1102:CLA:H12	19:A:1109:CLA:C6	2.20	0.47
19:A:1106:CLA:ND	19:A:1126:CLA:C4	2.77	0.47
19:A:1138:CLA:HBB1	19:A:1138:CLA:H122	1.97	0.47
19:A:9012:CLA:H152	19:A:9012:CLA:H101	1.94	0.47
2:B:73:ASN:ND2	2:B:73:ASN:N	2.61	0.47
2:B:78:VAL:O	2:B:79:GLN:C	2.56	0.47
2:B:157:LEU:HB3	2:B:158:GLN:HG2	1.96	0.47
2:B:224:PRO:CB	2:B:227:THR:OG1	2.62	0.47
2:B:326:ILE:O	2:B:326:ILE:CG1	2.60	0.47
2:B:365:PHE:HD1	2:B:602:TRP:NE1	2.12	0.47
2:B:544:SER:O	2:B:546:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1218:CLA:HMA2	19:B:1219:CLA:C3D	2.44	0.47
6:F:97:GLN:O	6:F:99:LEU:N	2.47	0.47
6:F:185:ILE:O	6:F:186:ARG:CG	2.37	0.47
8:H:120:ILE:O	8:H:121:LEU:O	2.31	0.47
9:I:4:LEU:HG	9:I:4:LEU:O	2.15	0.47
12:L:59:PRO:O	12:L:60:ILE:HB	2.14	0.47
13:N:114:PHE:C	13:N:117:ALA:HB3	2.39	0.47
22:R:7014:LMU:H1B	22:R:7014:LMU:H3'	1.27	0.47
17:3:233:LEU:C	17:3:236:LEU:H	2.22	0.47
18:4:159:ASP:OD2	18:4:163:PRO:CA	2.60	0.47
18:4:161:LYS:NZ	18:4:162:ASN:HD21	2.12	0.47
18:4:214:PHE:O	18:4:218:ILE:HG13	2.15	0.47
1:A:159:THR:CA	1:A:163:GLN:HE22	2.27	0.47
1:A:279:ASP:O	1:A:281:LEU:HD11	2.12	0.47
1:A:308:ILE:O	1:A:311:LEU:HB2	2.14	0.47
1:A:310:PHE:H	1:A:313:ALA:HB3	1.79	0.47
1:A:452:PHE:O	1:A:456:HIS:ND1	2.35	0.47
1:A:709:TRP:CH2	2:B:417:ALA:HB2	2.50	0.47
19:A:1133:CLA:H3A	19:A:1133:CLA:HBA2	1.58	0.47
2:B:124:TRP:HD1	2:B:124:TRP:O	1.98	0.47
2:B:260:GLY:O	2:B:262:HIS:NE2	2.47	0.47
2:B:493:TRP:O	2:B:495:PRO:CG	2.62	0.47
2:B:527:LEU:CD2	19:B:1222:CLA:C4D	2.92	0.47
19:B:1216:CLA:HMD3	19:B:1219:CLA:HAC1	1.97	0.47
19:B:1231:CLA:HMD3	19:B:1232:CLA:C1C	2.45	0.47
6:F:207:LEU:HD22	6:F:208:PHE:CG	2.49	0.47
7:G:130:TRP:O	7:G:134:GLY:CA	2.55	0.47
10:J:31:ARG:NH2	19:J:1311:CLA:CHC	2.77	0.47
12:L:114:PHE:HD1	12:L:114:PHE:H	1.61	0.47
14:R:46:UNK:CB	14:R:47:UNK:CA	2.92	0.47
15:1:65:ASP:OD1	15:1:66:PRO:HG3	2.14	0.47
15:1:129:VAL:HG12	15:1:130:PRO:CG	2.45	0.47
15:1:155:GLU:OE1	15:1:156:LYS:N	2.45	0.47
15:1:198:PHE:C	15:1:199:VAL:O	2.57	0.47
16:2:168:TRP:CD1	16:2:171:ILE:HG23	2.19	0.47
1:A:25:ASP:OD1	1:A:26:PRO:CD	2.62	0.47
1:A:51:THR:HG21	1:A:723:ARG:H	1.80	0.47
1:A:89:ILE:O	1:A:92:TRP:CB	2.55	0.47
1:A:167:THR:CG2	19:A:1112:CLA:CAA	2.87	0.47
1:A:201:SER:O	1:A:204:ASN:CB	2.58	0.47
1:A:223:VAL:CG1	1:A:224:HIS:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PHE:CZ	19:A:1141:CLA:C2	2.97	0.47
1:A:281:LEU:CD2	19:A:1115:CLA:HED2	2.37	0.47
1:A:296:LEU:HD12	1:A:297:THR:CG2	2.31	0.47
1:A:331:LEU:CD2	1:A:343:HIS:C	2.83	0.47
1:A:346:LEU:CD2	1:A:347:TYR:HB2	2.45	0.47
1:A:346:LEU:HD11	19:A:1122:CLA:HBC3	1.97	0.47
1:A:390:ALA:HA	1:A:393:LEU:HD23	1.96	0.47
1:A:466:THR:CG2	2:B:648:TRP:HE1	2.28	0.47
1:A:473:PRO:C	1:A:475:ASP:N	2.71	0.47
1:A:581:CYS:HB3	1:A:590:CYS:O	2.14	0.47
1:A:584:PRO:HB2	3:C:67:VAL:HA	1.96	0.47
1:A:599:PHE:CD2	1:A:735:VAL:HG21	2.49	0.47
1:A:661:ALA:O	1:A:665:ILE:HG13	2.15	0.47
19:A:1102:CLA:O1A	19:A:1109:CLA:HBA2	2.15	0.47
19:A:1104:CLA:HBA2	19:A:1104:CLA:CED	2.45	0.47
19:A:1106:CLA:H111	21:J:6012:BCR:C10	2.45	0.47
19:A:1120:CLA:O2D	19:A:1120:CLA:OBD	2.33	0.47
19:A:1121:CLA:HAA1	11:K:78:ARG:NH1	2.29	0.47
19:A:1122:CLA:C1B	21:A:6007:BCR:C15	2.93	0.47
19:A:1138:CLA:H52	19:A:1138:CLA:C4C	2.45	0.47
2:B:34:HIS:O	2:B:37:ILE:HG23	2.15	0.47
2:B:154:TRP:O	2:B:158:GLN:HG2	2.14	0.47
2:B:197:VAL:O	2:B:197:VAL:HG12	2.15	0.47
2:B:224:PRO:O	2:B:227:THR:N	2.43	0.47
2:B:503:GLU:O	2:B:503:GLU:HG2	2.13	0.47
2:B:564:ARG:NH2	3:C:66:ARG:NH1	2.63	0.47
2:B:655:LEU:HD21	19:B:1239:CLA:CBB	2.37	0.47
2:B:710:LEU:HA	2:B:713:PHE:HB3	1.97	0.47
2:B:732:LYS:HG2	2:B:734:GLY:H	1.58	0.47
19:B:1201:CLA:HBB2	19:B:1203:CLA:C4D	2.45	0.47
19:B:1206:CLA:H43	21:I:6018:BCR:H21C	1.96	0.47
19:B:1221:CLA:HMB1	19:B:1223:CLA:H92	1.96	0.47
3:C:11:CYS:C	3:C:13:GLY:N	2.71	0.47
3:C:62:PHE:CE1	5:E:80:GLU:OE1	2.68	0.47
4:D:100:TYR:CE2	4:D:156:ARG:HG3	2.50	0.47
4:D:100:TYR:OH	4:D:134:LYS:HE3	2.14	0.47
4:D:114:MET:CG	4:D:115:PRO:N	2.78	0.47
4:D:137:CYS:O	4:D:138:LEU:C	2.55	0.47
5:E:90:VAL:C	5:E:91:VAL:CG2	2.85	0.47
5:E:127:GLU:HB3	5:E:129:GLU:C	2.32	0.47
6:F:123:MET:O	6:F:125:LYS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:130:PHE:O	6:F:131:ASP:C	2.56	0.47
6:F:168:LEU:HD13	6:F:168:LEU:HA	1.75	0.47
6:F:181:TYR:C	6:F:181:TYR:HD2	2.22	0.47
7:G:90:GLN:HB2	7:G:91:VAL:C	2.36	0.47
8:H:66:ASP:C	8:H:68:TYR:N	2.71	0.47
19:H:1207:CLA:HHD	21:I:6018:BCR:H342	1.96	0.47
10:J:19:PHE:O	10:J:23:ALA:HB3	2.14	0.47
10:J:25:LEU:HA	10:J:28:GLU:HB2	1.97	0.47
21:J:6012:BCR:C23	21:J:6012:BCR:C39	2.83	0.47
11:K:101:PHE:O	11:K:104:ALA:HB3	2.15	0.47
12:L:104:LEU:HD12	12:L:196:GLY:HA2	1.97	0.47
13:N:104:LYS:O	13:N:105:LYS:C	2.58	0.47
13:N:108:ALA:C	13:N:109:THR:HG1	2.23	0.47
13:N:112:ALA:O	13:N:113:ASN:C	2.58	0.47
13:N:146:LEU:O	13:N:147:SER:O	2.33	0.47
13:N:147:SER:C	13:N:151:ASP:N	2.71	0.47
15:1:68:GLY:C	15:1:69:LEU:O	2.56	0.47
15:1:133:THR:O	15:1:135:PRO:HD2	2.15	0.47
15:1:155:GLU:CD	15:1:156:LYS:N	2.73	0.47
15:1:216:ASN:O	15:1:217:LEU:HB2	2.12	0.47
22:1:7013:LMU:H41	22:1:7013:LMU:H1'	1.97	0.47
16:2:150:THR:CG2	16:2:151:THR:N	2.76	0.47
16:2:167:ARG:HE	16:2:167:ARG:C	2.22	0.47
16:2:269:LYS:HE3	16:2:269:LYS:O	2.15	0.47
17:3:99:ALA:O	17:3:100:TYR:C	2.58	0.47
19:3:3017:CLA:H3A	19:3:3017:CLA:HBA1	1.29	0.47
18:4:81:LEU:O	18:4:83:GLU:OE2	2.33	0.47
18:4:99:GLY:O	18:4:103:MET:HG3	2.14	0.47
18:4:172:PHE:CD1	18:4:176:SER:O	2.68	0.47
18:4:211:MET:CE	19:4:4002:CLA:CBB	2.92	0.47
18:4:217:PHE:HE1	18:4:221:HIS:CG	2.31	0.47
22:4:7052:LMU:H111	22:4:7052:LMU:H82	1.67	0.47
1:A:207:LEU:HA	1:A:211:LEU:CB	2.44	0.47
1:A:252:ARG:O	1:A:252:ARG:NE	2.48	0.47
1:A:369:THR:HG21	1:A:402:ILE:HG22	1.96	0.47
1:A:374:GLN:C	1:A:376:MET:N	2.71	0.47
1:A:644:GLN:HG3	1:A:644:GLN:O	2.15	0.47
19:A:1105:CLA:HBA2	19:A:1105:CLA:H3A	1.49	0.47
19:A:1136:CLA:ND	19:A:1136:CLA:H11	2.29	0.47
19:A:9011:CLA:CMC	2:B:624:LEU:HG	2.44	0.47
19:A:9013:CLA:H2	19:A:9013:CLA:CMA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ARG:NH1	19:B:1221:CLA:HMD2	2.30	0.47
2:B:312:GLY:O	19:B:1301:CLA:CAD	2.62	0.47
2:B:611:GLU:OE1	6:F:143:ASP:OD2	2.33	0.47
2:B:666:SER:O	2:B:667:TRP:HB2	2.14	0.47
19:B:1218:CLA:HMA2	19:B:1219:CLA:C4D	2.44	0.47
19:B:1219:CLA:H3A	19:B:1219:CLA:HBA2	1.51	0.47
3:C:10:THR:CG2	5:E:101:TYR:CG	2.98	0.47
3:C:69:LEU:HD12	3:C:70:TRP:H	1.78	0.47
4:D:135:GLU:O	4:D:139:ALA:HB2	2.13	0.47
4:D:204:GLY:C	4:D:205:LYS:HE2	2.40	0.47
6:F:100:LYS:HA	6:F:100:LYS:HD3	1.30	0.47
6:F:172:GLY:O	6:F:176:TRP:CB	2.61	0.47
10:J:5:LYS:CE	16:2:178:ASN:OD1	2.63	0.47
11:K:81:THR:CG2	11:K:83:GLY:N	2.49	0.47
11:K:86:LEU:O	11:K:87:GLU:CB	2.62	0.47
13:N:157:LYS:CB	13:N:158:ASP:HA	2.42	0.47
22:1:7013:LMU:H42	22:1:7013:LMU:H11	1.81	0.47
16:2:100:ARG:N	16:2:101:TRP:HB2	2.29	0.47
16:2:122:ILE:O	16:2:126:LEU:CD2	2.62	0.47
16:2:142:GLU:O	16:2:143:GLN:HG2	2.15	0.47
16:2:172:LEU:O	16:2:172:LEU:HD12	2.15	0.47
16:2:238:GLN:O	16:2:239:HIS:C	2.57	0.47
19:2:2002:CLA:O2D	19:2:2002:CLA:OBD	2.33	0.47
19:2:2014:CLA:OBD	19:2:2014:CLA:O2D	2.32	0.47
17:3:95:PRO:C	17:3:96:ARG:CG	2.85	0.47
22:4:7008:LMU:C6'	22:4:7008:LMU:H1B	2.45	0.47
1:A:188:LYS:C	1:A:188:LYS:CD	2.65	0.47
1:A:281:LEU:HD21	19:A:1115:CLA:HED1	1.94	0.47
1:A:370:ILE:CG2	1:A:403:GLY:HA3	2.26	0.47
1:A:594:ALA:O	1:A:598:VAL:HG23	2.14	0.47
1:A:736:THR:HG21	19:A:1128:CLA:H91	1.96	0.47
19:A:1119:CLA:H61	21:A:6008:BCR:H19C	1.96	0.47
19:A:1124:CLA:HAA1	19:A:1124:CLA:HBD	1.97	0.47
19:A:1126:CLA:H193	19:A:1126:CLA:H162	1.77	0.47
19:A:1140:CLA:HBA2	19:A:1140:CLA:H3A	1.47	0.47
21:A:6011:BCR:H333	19:B:1230:CLA:HBB2	1.95	0.47
2:B:4:ARG:HE	2:B:4:ARG:HB2	1.46	0.47
2:B:225:LEU:HD11	2:B:233:TYR:OH	2.06	0.47
2:B:443:MET:HA	2:B:443:MET:HE3	1.96	0.47
2:B:560:ASP:OD1	3:C:66:ARG:HB3	2.15	0.47
2:B:679:ALA:HB1	2:B:683:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:136:VAL:O	7:G:137:VAL:CG2	2.63	0.47
10:J:15:SER:HA	10:J:18:TRP:HB3	1.96	0.47
12:L:206:VAL:O	12:L:207:LEU:O	2.33	0.47
13:N:132:THR:O	13:N:133:GLY:C	2.55	0.47
13:N:142:LYS:HB3	13:N:143:VAL:H	1.61	0.47
14:R:34:UNK:CB	14:R:35:UNK:CA	2.80	0.47
16:2:155:VAL:HA	16:2:158:VAL:HG13	1.97	0.47
16:2:215:LYS:O	16:2:215:LYS:CG	2.60	0.47
17:3:94:GLU:CB	17:3:95:PRO:HD3	2.45	0.47
18:4:140:THR:O	18:4:144:ILE:HD12	2.15	0.47
1:A:261:SER:C	1:A:262:PHE:CG	2.93	0.47
1:A:603:PHE:CE2	2:B:665:ILE:HG21	2.50	0.47
19:A:1115:CLA:C14	19:A:1115:CLA:C17	2.75	0.47
19:A:1133:CLA:C3D	19:A:1134:CLA:CAC	2.92	0.47
21:A:6003:BCR:C8	21:A:6003:BCR:H311	2.44	0.47
2:B:224:PRO:CB	2:B:227:THR:HG21	2.45	0.47
2:B:290:MET:HG3	19:B:1218:CLA:C2C	2.45	0.47
2:B:343:VAL:HG11	19:B:1223:CLA:H2	1.96	0.47
2:B:555:TYR:CE2	2:B:573:TRP:HA	2.50	0.47
19:B:1205:CLA:HBB2	19:B:1205:CLA:C9	2.29	0.47
19:B:1205:CLA:CMC	21:B:6017:BCR:C28	2.91	0.47
19:B:1210:CLA:H192	19:B:1215:CLA:OBD	2.15	0.47
19:B:1213:CLA:HMC3	19:B:1214:CLA:H143	1.97	0.47
21:B:6017:BCR:C33	21:B:6017:BCR:HC8	2.45	0.47
3:C:11:CYS:O	3:C:13:GLY:N	2.48	0.47
3:C:12:ILE:O	3:C:38:GLN:CG	2.62	0.47
4:D:99:PHE:HB3	4:D:157:VAL:HG12	1.95	0.47
5:E:110:VAL:O	5:E:111:ASN:CB	2.61	0.47
6:F:207:LEU:HD21	6:F:208:PHE:CG	2.48	0.47
7:G:124:ILE:CG2	7:G:125:VAL:H	2.26	0.47
8:H:108:THR:O	8:H:109:LEU:O	2.33	0.47
22:H:7032:LMU:O2'	22:H:7032:LMU:H12	2.15	0.47
10:J:2:ARG:NH1	10:J:8:LEU:HB2	2.30	0.47
11:K:55:LEU:O	11:K:58:VAL:HB	2.15	0.47
11:K:78:ARG:CZ	11:K:78:ARG:N	2.78	0.47
22:R:7021:LMU:O3'	22:R:7021:LMU:H1B	2.13	0.47
15:1:142:PHE:C	15:1:143:LEU:HD12	2.40	0.47
19:1:1001:CLA:CMA	19:1:1001:CLA:HBA1	2.44	0.47
16:2:145:TYR:O	16:2:146:PHE:HB2	2.15	0.47
16:2:264:ALA:O	16:2:265:ALA:CB	2.63	0.47
17:3:107:ARG:NH1	17:3:229:LYS:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:109:ALA:O	17:3:111:LEU:HD23	2.14	0.47
18:4:144:ILE:HA	18:4:147:ILE:HD13	1.97	0.47
18:4:206:ALA:C	18:4:208:GLY:N	2.66	0.47
18:4:209:ARG:O	18:4:212:LEU:HB2	2.15	0.47
1:A:84:GLY:O	1:A:88:ILE:HD12	2.15	0.46
1:A:263:ALA:O	1:A:264:GLU:HG3	2.13	0.46
1:A:581:CYS:HB2	1:A:590:CYS:O	2.14	0.46
1:A:592:VAL:HG23	1:A:593:SER:H	1.80	0.46
1:A:739:LEU:O	1:A:743:ILE:HG13	2.15	0.46
19:A:1107:CLA:CBB	19:B:1230:CLA:CMD	2.84	0.46
19:A:1119:CLA:CAA	19:A:1123:CLA:HBB2	2.45	0.46
19:A:1124:CLA:H162	19:A:1124:CLA:H111	1.96	0.46
19:A:1138:CLA:HBD	19:A:1138:CLA:HAA1	1.95	0.46
2:B:15:ASP:O	2:B:20:ARG:HG3	2.15	0.46
2:B:74:PHE:C	2:B:76:ALA:N	2.73	0.46
2:B:693:TRP:NE1	19:B:1238:CLA:HMD3	2.29	0.46
3:C:62:PHE:CD1	4:D:191:ILE:CG2	2.92	0.46
4:D:123:ARG:HH21	22:D:7050:LMU:C6B	2.17	0.46
6:F:192:THR:O	6:F:193:GLN:CB	2.63	0.46
7:G:123:ASN:C	7:G:126:ASP:OD2	2.58	0.46
8:H:98:LEU:O	8:H:98:LEU:CG	2.63	0.46
19:H:1505:CLA:HAA2	19:H:1505:CLA:HBD	1.96	0.46
22:H:7030:LMU:H61	22:H:7030:LMU:H32	1.62	0.46
11:K:56:ILE:CA	11:K:59:THR:CG2	2.81	0.46
11:K:115:ILE:O	11:K:118:VAL:CG2	2.60	0.46
12:L:82:TYR:OH	19:L:1502:CLA:HBA2	2.15	0.46
12:L:178:THR:HG22	12:L:179:ALA:N	2.30	0.46
13:N:160:TYR:O	13:N:164:SER:O	2.33	0.46
15:1:133:THR:O	15:1:136:THR:CG2	2.53	0.46
16:2:174:PRO:CD	16:2:189:THR:OG1	2.61	0.46
16:2:184:PRO:CD	16:2:186:ASN:C	2.87	0.46
16:2:229:MET:CE	16:2:230:LEU:CD1	2.94	0.46
18:4:173:LYS:CE	18:4:201:LYS:HG3	2.43	0.46
18:4:178:PRO:O	18:4:194:PHE:CZ	2.67	0.46
1:A:124:TRP:HA	1:A:124:TRP:CE3	2.50	0.46
1:A:129:GLN:NE2	19:A:1107:CLA:NB	2.64	0.46
1:A:187:HIS:HE1	19:A:1109:CLA:C1A	2.06	0.46
1:A:245:PRO:O	1:A:248:PHE:HE2	1.93	0.46
1:A:308:ILE:CG2	19:A:1115:CLA:C11	2.94	0.46
1:A:473:PRO:O	1:A:475:ASP:N	2.48	0.46
1:A:536:THR:O	1:A:537:ALA:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ARG:HA	1:A:573:ALA:HB2	1.97	0.46
19:A:1101:CLA:H42	19:A:1140:CLA:H8	1.97	0.46
19:A:1105:CLA:C4B	21:J:6012:BCR:H333	2.45	0.46
19:A:1125:CLA:HBB2	19:A:1133:CLA:HMA1	0.48	0.46
2:B:80:ASP:HA	2:B:81:PRO:HD3	1.75	0.46
2:B:320:LYS:HG3	2:B:321:GLY:H	1.80	0.46
2:B:353:TYR:CB	2:B:594:TRP:CZ3	2.98	0.46
2:B:471:THR:O	2:B:472:TYR:HD1	1.92	0.46
2:B:488:ALA:HB2	19:B:1233:CLA:C3C	2.45	0.46
2:B:564:ARG:CZ	3:C:64:SER:H	2.28	0.46
2:B:668:ARG:NH1	2:B:672:GLN:HG2	2.30	0.46
19:B:1222:CLA:H11	19:B:1236:CLA:CBD	2.46	0.46
19:B:1233:CLA:HBA2	19:B:1233:CLA:H3A	1.71	0.46
3:C:79:LEU:HD22	3:C:81:TYR:O	2.15	0.46
4:D:172:VAL:CG1	4:D:173:TYR:N	2.78	0.46
6:F:169:TYR:OH	6:F:211:PHE:HA	2.15	0.46
22:H:7032:LMU:H1B	22:H:7032:LMU:O1'	2.15	0.46
10:J:26:LEU:HA	10:J:29:ILE:HG22	1.97	0.46
14:R:6:UNK:CB	14:R:10:UNK:CB	2.92	0.46
22:R:7021:LMU:H41	22:R:7021:LMU:O6'	2.16	0.46
19:1:1001:CLA:H3A	19:1:1001:CLA:HBA2	1.30	0.46
16:2:128:LYS:HB2	16:2:131:ILE:HG12	1.96	0.46
17:3:154:ASN:O	17:3:155:TYR:CD2	2.62	0.46
17:3:187:PHE:CE1	17:3:188:LEU:HB2	2.51	0.46
18:4:193:ASN:C	18:4:194:PHE:CG	2.87	0.46
1:A:393:LEU:HD11	1:A:750:PHE:CD1	2.51	0.46
1:A:707:ILE:HD12	19:A:1138:CLA:HMD2	1.98	0.46
19:A:1149:CLA:O1D	19:A:1149:CLA:HBA2	2.14	0.46
19:A:9013:CLA:HMD2	2:B:533:ILE:CD1	2.43	0.46
2:B:38:THR:HG23	2:B:41:ARG:NH1	2.30	0.46
2:B:595:HIS:HD2	2:B:623:TYR:OH	1.99	0.46
2:B:596:TRP:CD1	2:B:623:TYR:HB2	2.50	0.46
2:B:693:TRP:HD1	19:B:1238:CLA:C1D	2.18	0.46
3:C:18:VAL:HB	3:C:58:CYS:HB2	1.97	0.46
4:D:140:LEU:HD22	4:D:144:LEU:HG	1.96	0.46
5:E:73:LYS:HG3	5:E:128:VAL:CG1	2.46	0.46
9:I:8:PHE:CE1	21:I:6021:BCR:HC7	2.50	0.46
10:J:2:ARG:HB3	10:J:7:TYR:CE1	2.50	0.46
22:K:7047:LMU:O2B	22:K:7047:LMU:H6E	2.16	0.46
12:L:92:ALA:N	12:L:98:ARG:HH22	2.12	0.46
22:N:7049:LMU:H4'	22:N:7049:LMU:O6B	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:66:PRO:CD	15:1:67:LEU:H	2.06	0.46
15:1:103:LEU:N	15:1:103:LEU:CD2	2.71	0.46
19:1:1010:CLA:O1D	19:1:1010:CLA:C3D	2.54	0.46
16:2:184:PRO:CD	16:2:185:ASN:CA	2.93	0.46
16:2:218:ARG:NH1	19:2:2001:CLA:HBB2	2.30	0.46
16:2:267:THR:O	16:2:267:THR:HG23	2.14	0.46
17:3:158:PHE:HA	17:3:159:VAL:C	2.40	0.46
21:3:6022:BCR:C39	21:3:6022:BCR:C23	2.63	0.46
1:A:96:MET:HE1	19:A:1106:CLA:O2D	2.14	0.46
1:A:389:TYR:HD1	1:A:625:TRP:CG	2.32	0.46
19:A:1102:CLA:HBB2	19:A:1104:CLA:C3D	2.46	0.46
19:A:1138:CLA:H191	6:F:181:TYR:CG	2.51	0.46
19:A:1140:CLA:H43	19:A:1140:CLA:ND	2.30	0.46
2:B:37:ILE:HD12	2:B:37:ILE:C	2.41	0.46
2:B:141:PHE:O	2:B:142:LEU:C	2.58	0.46
2:B:247:THR:O	2:B:250:ALA:N	2.49	0.46
2:B:310:PRO:HD2	2:B:311:PRO:HD2	1.97	0.46
2:B:655:LEU:HD22	19:B:1239:CLA:CBB	2.45	0.46
19:B:1220:CLA:C9	19:B:1227:CLA:CBC	2.94	0.46
19:B:1225:CLA:H62	21:B:6006:BCR:H321	1.97	0.46
3:C:12:ILE:HG21	3:C:39:ILE:C	2.40	0.46
4:D:114:MET:SD	4:D:115:PRO:HD2	2.55	0.46
4:D:147:LYS:O	4:D:148:TYR:CD2	2.68	0.46
6:F:133:TYR:CD1	6:F:133:TYR:N	2.83	0.46
19:J:1311:CLA:O1A	19:J:1311:CLA:C15	2.64	0.46
11:K:97:ASP:O	11:K:97:ASP:OD1	2.32	0.46
15:1:75:ASN:O	15:1:76:LEU:O	2.34	0.46
16:2:125:PHE:C	16:2:127:THR:N	2.60	0.46
19:2:2013:CLA:CBC	19:2:2013:CLA:CMC	2.93	0.46
17:3:182:MET:CG	17:3:183:GLY:N	2.78	0.46
18:4:112:PRO:O	18:4:115:PHE:O	2.34	0.46
19:4:4014:CLA:HBC2	19:4:4014:CLA:CHD	2.34	0.46
1:A:42:ARG:O	1:A:44:ILE:HG13	2.15	0.46
1:A:163:GLN:HG2	1:A:164:LEU:H	1.74	0.46
1:A:392:GLN:CG	1:A:392:GLN:O	2.64	0.46
1:A:532:ILE:HD13	19:A:1135:CLA:CMD	2.45	0.46
1:A:539:PHE:HE2	1:A:543:HIS:CE1	2.34	0.46
1:A:586:ARG:HA	3:C:77:MET:O	2.15	0.46
1:A:626:GLY:O	1:A:627:THR:CG2	2.64	0.46
1:A:692:PHE:CD2	1:A:733:VAL:CG1	2.97	0.46
19:A:1237:CLA:H201	12:L:110:LEU:CD2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:5001:PQN:H243	20:A:5001:PQN:H212	1.76	0.46
2:B:15:ASP:O	2:B:20:ARG:CG	2.63	0.46
2:B:87:ILE:C	2:B:115:ASN:HA	2.40	0.46
2:B:377:TYR:CD1	2:B:718:ILE:HD12	2.51	0.46
2:B:594:TRP:CD1	2:B:595:HIS:N	2.84	0.46
22:E:7048:LMU:H3'	22:E:7048:LMU:O5B	2.15	0.46
8:H:98:LEU:C	8:H:99:LYS:O	2.56	0.46
9:I:9:VAL:H	9:I:10:PRO:CD	2.28	0.46
9:I:12:VAL:HG12	9:I:13:GLY:N	2.31	0.46
10:J:2:ARG:HH22	10:J:8:LEU:HD22	1.80	0.46
19:J:1308:CLA:H93	19:J:1308:CLA:H61	1.70	0.46
12:L:96:LEU:HG	12:L:97:LEU:HD23	1.97	0.46
12:L:109:LEU:HG	12:L:110:LEU:H	1.81	0.46
12:L:113:PRO:O	12:L:117:ALA:HB3	2.16	0.46
16:2:189:THR:CG2	16:2:193:VAL:O	2.61	0.46
17:3:94:GLU:CA	17:3:94:GLU:OE2	2.63	0.46
18:4:93:GLN:O	18:4:97:VAL:HG23	2.15	0.46
18:4:107:ALA:O	18:4:109:MET:O	2.33	0.46
18:4:110:LEU:HA	18:4:113:GLU:CD	2.40	0.46
1:A:336:GLY:HA3	19:A:1151:CLA:HMC1	1.96	0.46
1:A:426:THR:N	1:A:428:TYR:CZ	2.84	0.46
1:A:430:ASP:HA	1:A:434:ARG:HH21	1.80	0.46
1:A:476:MET:HE3	1:A:644:GLN:HE21	1.80	0.46
1:A:497:ALA:HB2	1:A:510:SER:OG	2.14	0.46
19:A:1104:CLA:HED2	19:A:1104:CLA:H12	1.97	0.46
2:B:139:ALA:O	2:B:141:PHE:N	2.49	0.46
2:B:321:GLY:O	2:B:325:THR:HG22	2.15	0.46
2:B:502:ASN:OD1	2:B:502:ASN:C	2.59	0.46
19:B:1220:CLA:H42	19:B:1220:CLA:CHB	2.43	0.46
21:B:6004:BCR:H343	7:G:77:PHE:CE1	2.50	0.46
3:C:51:CYS:SG	3:C:53:ARG:N	2.89	0.46
6:F:95:GLU:OE1	6:F:129:ARG:O	2.33	0.46
6:F:152:GLY:HA2	6:F:157:TRP:CE3	2.51	0.46
7:G:127:VAL:O	7:G:128:LEU:C	2.57	0.46
12:L:175:GLN:O	12:L:176:LEU:CB	2.55	0.46
13:N:132:THR:CB	13:N:139:LYS:NZ	2.57	0.46
14:R:1:UNK:O	14:R:2:UNK:O	2.34	0.46
15:1:72:VAL:O	15:1:73:PRO:C	2.54	0.46
15:1:84:LEU:HA	15:1:87:CYS:HB3	1.97	0.46
16:2:172:LEU:HB3	16:2:173:ASN:HD21	1.73	0.46
16:2:177:VAL:HG13	16:2:178:ASN:OD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:184:PRO:HG2	16:2:185:ASN:CA	2.45	0.46
19:2:2001:CLA:O1A	19:2:2001:CLA:NA	2.49	0.46
17:3:150:TYR:CE2	17:3:151:TRP:CE2	2.99	0.46
19:3:3013:CLA:O2D	19:3:3013:CLA:OBD	2.33	0.46
1:A:284:ARG:HH12	1:A:507:ALA:HB2	1.10	0.46
1:A:584:PRO:HB2	3:C:67:VAL:CA	2.45	0.46
1:A:656:PHE:O	1:A:657:LEU:C	2.58	0.46
1:A:697:ARG:NH1	1:A:724:ALA:HB3	2.30	0.46
19:A:1117:CLA:HBC1	21:A:6003:BCR:C12	2.46	0.46
19:A:1135:CLA:H2	19:A:1135:CLA:O1A	2.16	0.46
21:A:6003:BCR:C23	21:A:6003:BCR:H402	2.44	0.46
19:A:9023:CLA:CMC	19:A:9023:CLA:CBC	2.93	0.46
2:B:268:LEU:O	2:B:269:TRP:C	2.58	0.46
2:B:435:GLY:HA3	19:B:1230:CLA:HBB1	1.97	0.46
2:B:587:ILE:O	2:B:587:ILE:CG2	2.62	0.46
2:B:605:ASN:OD1	2:B:605:ASN:O	2.34	0.46
2:B:623:TYR:O	2:B:624:LEU:CB	2.64	0.46
19:B:1235:CLA:CBB	19:B:1235:CLA:C9	2.66	0.46
3:C:69:LEU:H	3:C:69:LEU:HG	1.20	0.46
5:E:124:GLU:HB2	5:E:126:VAL:HG13	1.97	0.46
6:F:167:PHE:CD1	21:F:6014:BCR:H23C	2.51	0.46
6:F:180:SER:O	6:F:182:LEU:N	2.38	0.46
6:F:190:LYS:HA	6:F:191:PRO:HD3	1.54	0.46
7:G:134:GLY:O	7:G:135:HIS:CE1	2.69	0.46
8:H:86:THR:HA	8:H:92:THR:HG21	1.98	0.46
19:J:1308:CLA:HMA1	19:2:2014:CLA:HED2	1.93	0.46
19:L:1130:CLA:H72	19:L:1504:CLA:HBA1	1.98	0.46
14:R:8:UNK:CB	19:R:1144:CLA:HED1	2.46	0.46
16:2:114:MET:O	16:2:117:ALA:HB3	2.16	0.46
16:2:122:ILE:HG13	16:2:126:LEU:CD2	2.46	0.46
19:3:3016:CLA:H102	19:3:3016:CLA:H143	1.90	0.46
22:3:7005:LMU:H3'	22:3:7005:LMU:C2B	2.46	0.46
1:A:119:SER:C	1:A:145:ILE:HD12	2.41	0.46
1:A:199:VAL:O	1:A:199:VAL:CG1	2.58	0.46
1:A:284:ARG:CB	1:A:295:TRP:CG	2.99	0.46
1:A:341:GLN:HE21	1:A:341:GLN:HB2	1.56	0.46
1:A:402:ILE:CD1	19:A:1127:CLA:CBB	2.94	0.46
1:A:487:VAL:HG13	1:A:488:PHE:C	2.36	0.46
1:A:655:ASP:O	1:A:659:ALA:HB3	2.16	0.46
1:A:708:VAL:HA	1:A:711:HIS:HD2	1.80	0.46
19:A:1109:CLA:C4A	19:A:1109:CLA:CBA	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:GLN:O	2:B:55:ALA:N	2.41	0.46
2:B:196:HIS:CE1	19:B:1212:CLA:C4D	2.98	0.46
2:B:217:PRO:HD2	19:B:1212:CLA:HED1	1.98	0.46
2:B:310:PRO:C	19:B:1301:CLA:CHD	2.86	0.46
19:B:1235:CLA:C6	21:F:6016:BCR:H323	2.46	0.46
3:C:7:ILE:O	3:C:60:THR:HA	2.16	0.46
4:D:90:LEU:O	12:L:66:ILE:HG23	2.16	0.46
11:K:95:THR:O	11:K:95:THR:HG22	2.16	0.46
12:L:63:ASP:OD1	12:L:63:ASP:C	2.59	0.46
12:L:131:SER:HA	12:L:197:VAL:CG1	2.45	0.46
12:L:155:GLU:H	12:L:155:GLU:HG2	1.15	0.46
19:L:1504:CLA:H62	19:L:1504:CLA:H41	1.62	0.46
22:L:7029:LMU:H1'	22:L:7029:LMU:C3	2.23	0.46
15:1:83:GLU:HA	15:1:86:HIS:CD2	2.51	0.46
15:1:97:ILE:HD11	15:1:98:LEU:HD22	1.97	0.46
15:1:201:PHE:CE1	15:1:204:GLN:OE1	2.69	0.46
19:2:4009:CLA:H71	19:2:4009:CLA:H111	1.68	0.46
17:3:184:LYS:HD3	19:3:2009:CLA:H61	1.60	0.46
19:3:2009:CLA:O1A	19:3:2009:CLA:CBD	2.44	0.46
18:4:98:ASN:HB3	18:4:212:LEU:CD2	2.45	0.46
18:4:158:GLN:CD	19:4:1004:CLA:C2A	2.89	0.46
1:A:110:LEU:O	1:A:111:ASN:C	2.57	0.46
1:A:112:ASP:N	1:A:113:PRO:CD	2.78	0.46
1:A:196:PHE:CD2	1:A:196:PHE:N	2.76	0.46
1:A:417:PHE:CD1	1:A:417:PHE:C	2.94	0.46
1:A:431:LEU:H	1:A:434:ARG:HE	1.62	0.46
1:A:555:ILE:HD11	19:A:9023:CLA:CAD	2.41	0.46
1:A:715:LYS:CD	6:F:230:ASN:ND2	2.48	0.46
19:A:1117:CLA:H71	19:A:1117:CLA:CAB	2.46	0.46
19:A:1126:CLA:H71	21:A:6011:BCR:C37	2.45	0.46
19:A:1237:CLA:CGA	19:A:1237:CLA:C1A	2.94	0.46
19:A:1237:CLA:HMD1	21:B:6017:BCR:H313	1.98	0.46
2:B:29:HIS:NE2	19:B:1202:CLA:HBB1	2.31	0.46
2:B:100:ALA:O	2:B:102:GLU:O	2.33	0.46
2:B:255:LEU:N	2:B:271:THR:HG21	2.31	0.46
2:B:330:ILE:HD12	2:B:333:GLN:NE2	2.30	0.46
19:B:1222:CLA:H52	19:B:1236:CLA:CBD	2.45	0.46
20:B:5002:PQN:H142	20:B:5002:PQN:C2M	2.46	0.46
5:E:73:LYS:O	5:E:73:LYS:CG	2.64	0.46
5:E:73:LYS:CG	5:E:128:VAL:HG11	2.44	0.46
5:E:77:LEU:C	5:E:78:ARG:HD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:VAL:O	5:E:93:VAL:HG12	2.15	0.46
6:F:153:ASP:N	6:F:153:ASP:OD1	2.47	0.46
6:F:177:VAL:CA	6:F:180:SER:OG	2.57	0.46
7:G:82:PHE:CB	7:G:83:GLN:HG2	2.46	0.46
9:I:12:VAL:HG13	21:I:6018:BCR:H271	1.97	0.46
10:J:19:PHE:CD2	10:J:19:PHE:C	2.94	0.46
19:L:1130:CLA:H142	19:L:1504:CLA:H43	1.97	0.46
16:2:157:LEU:O	16:2:161:GLY:N	2.39	0.46
16:2:206:TRP:O	16:2:208:SER:CB	2.62	0.46
18:4:103:MET:HG2	18:4:211:MET:HB2	1.96	0.46
1:A:105:ASN:HA	1:A:140:PHE:HE2	1.81	0.46
1:A:308:ILE:HD11	19:A:1115:CLA:C4B	2.46	0.46
1:A:308:ILE:HG21	19:A:1115:CLA:C11	2.46	0.46
1:A:520:LEU:HB3	22:A:7044:LMU:H2'	1.62	0.46
1:A:531:PRO:C	1:A:532:ILE:HG22	2.39	0.46
1:A:654:ARG:HG3	1:A:655:ASP:N	2.30	0.46
1:A:701:GLN:OE1	5:E:112:TYR:CE1	2.69	0.46
19:A:9022:CLA:H91	19:A:9023:CLA:C9	2.43	0.46
2:B:25:ILE:HG21	21:L:6019:BCR:C28	2.45	0.46
2:B:278:LEU:O	2:B:279:ALA:C	2.58	0.46
2:B:317:ARG:HH22	2:B:410:ARG:CB	2.28	0.46
2:B:431:PHE:CD2	19:B:1229:CLA:HMA1	2.50	0.46
2:B:646:TRP:CH2	2:B:726:ILE:HD13	2.50	0.46
2:B:662:MET:HE2	20:B:5002:PQN:H2M3	1.98	0.46
19:B:1208:CLA:HAA2	19:B:1208:CLA:H12	1.98	0.46
19:B:1227:CLA:HMB1	19:B:1228:CLA:C4A	2.46	0.46
19:B:1234:CLA:O2D	19:B:1234:CLA:OBD	2.34	0.46
4:D:80:SER:HB2	4:D:127:ASN:H	1.80	0.46
4:D:95:GLN:HE21	4:D:96:VAL:CB	2.29	0.46
5:E:108:ASN:OD1	5:E:109:LYS:N	2.49	0.46
22:E:7037:LMU:C5	22:E:7037:LMU:C1	2.92	0.46
6:F:139:LEU:O	6:F:140:CYS:O	2.32	0.46
8:H:91:PHE:HB3	12:L:187:GLY:CA	2.46	0.46
22:H:7011:LMU:H111	22:H:7011:LMU:C6	2.46	0.46
13:N:156:GLY:CA	13:N:157:LYS:CD	2.94	0.46
15:1:91:MET:O	15:1:94:VAL:HB	2.16	0.46
15:1:201:PHE:CD1	15:1:204:GLN:OE1	2.69	0.46
1:A:70:ASP:CB	1:A:72:GLU:HG2	2.46	0.45
1:A:120:ALA:HB3	19:A:1106:CLA:HED3	1.98	0.45
1:A:183:TRP:O	1:A:185:HIS:N	2.49	0.45
1:A:240:LYS:H	1:A:243:PRO:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ILE:HD13	19:A:1131:CLA:CED	2.35	0.45
1:A:502:THR:HG22	1:A:503:THR:N	2.32	0.45
1:A:592:VAL:O	1:A:597:HIS:CD2	2.69	0.45
1:A:604:TRP:O	1:A:605:MET:C	2.59	0.45
1:A:660:GLN:O	1:A:661:ALA:HB3	2.16	0.45
2:B:4:ARG:C	2:B:5:ILE:HG12	2.41	0.45
2:B:5:ILE:CG2	2:B:6:PRO:N	2.75	0.45
2:B:65:LEU:HD11	21:B:6006:BCR:HC42	1.97	0.45
2:B:199:ILE:CG2	2:B:270:LEU:HD11	2.43	0.45
2:B:229:GLN:NE2	7:G:154:PHE:CE1	2.79	0.45
2:B:377:TYR:OH	2:B:717:TYR:HE1	1.99	0.45
2:B:551:LYS:HE3	2:B:551:LYS:HB3	1.55	0.45
19:B:1229:CLA:HBB2	21:F:6014:BCR:C26	2.46	0.45
6:F:214:PRO:C	6:F:215:VAL:CG2	2.86	0.45
21:F:6016:BCR:H24C	21:F:6016:BCR:H371	1.75	0.45
11:K:98:PRO:CD	11:K:99:ALA:N	2.64	0.45
22:R:7020:LMU:H92	22:R:7020:LMU:H62	1.54	0.45
15:1:156:LYS:HB3	15:1:158:PRO:CD	2.46	0.45
17:3:109:ALA:HA	17:3:111:LEU:HD13	1.97	0.45
17:3:209:ASN:HD22	17:3:209:ASN:HA	1.55	0.45
17:3:238:ILE:HA	17:3:241:TYR:CZ	2.50	0.45
18:4:89:ARG:CD	18:4:89:ARG:N	2.79	0.45
18:4:121:ILE:HG12	18:4:122:ASN:H	1.81	0.45
1:A:23:ASP:HA	1:A:24:ARG:HE	1.81	0.45
1:A:252:ARG:CZ	1:A:261:SER:OG	2.64	0.45
1:A:462:ILE:HG21	19:A:1132:CLA:CMC	2.43	0.45
19:A:1101:CLA:C1	19:A:1140:CLA:H2	2.47	0.45
19:A:1122:CLA:HBC1	21:A:6007:BCR:C39	2.46	0.45
19:A:1237:CLA:CMD	21:B:6017:BCR:H313	2.46	0.45
2:B:50:HIS:HB2	2:B:53:GLN:HB2	1.98	0.45
2:B:73:ASN:C	2:B:121:TYR:OH	2.48	0.45
2:B:240:SER:O	2:B:242:HIS:N	2.49	0.45
2:B:463:ILE:O	2:B:464:GLN:CG	2.64	0.45
2:B:636:THR:O	2:B:636:THR:CG2	2.64	0.45
2:B:683:GLU:OE1	4:D:91:LEU:HD13	2.16	0.45
4:D:78:THR:N	4:D:79:PRO:CD	2.79	0.45
22:E:7037:LMU:H4B	22:E:7037:LMU:H1B	1.54	0.45
22:G:7039:LMU:H4B	22:G:7039:LMU:H1B	1.64	0.45
8:H:86:THR:O	8:H:88:ALA:N	2.49	0.45
8:H:94:ARG:CZ	8:H:97:LEU:O	2.65	0.45
11:K:50:GLY:CA	11:K:52:PRO:HD2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:90:GLU:OE2	13:N:91:TYR:CG	2.69	0.45
13:N:127:PHE:CD1	13:N:128:PRO:HA	2.51	0.45
15:1:155:GLU:O	15:1:156:LYS:CB	2.61	0.45
15:1:181:GLU:O	15:1:182:GLU:HB3	2.16	0.45
16:2:266:PHE:CD1	16:2:267:THR:O	2.68	0.45
22:2:7006:LMU:O5B	22:2:7006:LMU:C5'	2.50	0.45
18:4:103:MET:SD	18:4:211:MET:HE3	2.56	0.45
18:4:238:ASP:OD2	18:4:238:ASP:N	2.47	0.45
22:4:7053:LMU:O2B	22:4:7053:LMU:C5B	2.60	0.45
1:A:23:ASP:OD1	1:A:24:ARG:N	2.50	0.45
1:A:71:LEU:CD1	1:A:71:LEU:C	2.82	0.45
1:A:164:LEU:HA	1:A:167:THR:OG1	2.17	0.45
1:A:462:ILE:CG2	19:A:1132:CLA:CMC	2.94	0.45
1:A:566:SER:HG	2:B:673:GLU:CD	2.06	0.45
1:A:596:ASP:HA	1:A:599:PHE:CB	2.38	0.45
1:A:628:ILE:HG13	1:A:629:ASN:N	2.25	0.45
1:A:672:LEU:C	1:A:674:ALA:N	2.74	0.45
19:A:1132:CLA:H172	19:A:1136:CLA:C20	2.46	0.45
19:A:1138:CLA:HMD2	21:F:6014:BCR:HC41	1.96	0.45
19:A:9011:CLA:HBB2	19:A:9012:CLA:HED1	1.98	0.45
19:A:9012:CLA:HBB2	19:A:9013:CLA:C2B	2.47	0.45
19:A:9023:CLA:H141	19:A:9023:CLA:H161	1.72	0.45
2:B:224:PRO:CA	2:B:227:THR:OG1	2.64	0.45
2:B:451:LYS:CD	19:B:1230:CLA:O2D	2.65	0.45
19:B:1223:CLA:C7	19:B:1223:CLA:C4	2.94	0.45
3:C:28:MET:HA	3:C:29:ILE:O	2.17	0.45
3:C:69:LEU:HD12	3:C:70:TRP:O	2.11	0.45
4:D:121:ILE:O	4:D:121:ILE:HG13	2.17	0.45
22:D:7050:LMU:H82	22:D:7050:LMU:C4	2.46	0.45
5:E:85:LYS:O	5:E:87:THR:CG2	2.64	0.45
6:F:99:LEU:CA	6:F:102:LEU:CD2	2.89	0.45
7:G:70:LEU:O	7:G:70:LEU:HG	2.16	0.45
7:G:76:ARG:NH1	7:G:120:VAL:CA	2.80	0.45
7:G:136:VAL:C	7:G:137:VAL:HG22	2.41	0.45
11:K:66:PHE:HE2	11:K:102:THR:HG22	1.82	0.45
11:K:126:ASN:OD1	11:K:126:ASN:O	2.34	0.45
15:1:64:PHE:CD1	15:1:65:ASP:CB	2.99	0.45
16:2:127:THR:OG1	16:2:129:LEU:N	2.49	0.45
17:3:204:GLY:O	17:3:206:PRO:C	2.59	0.45
18:4:135:PHE:H	18:4:136:ALA:HB2	1.81	0.45
1:A:23:ASP:OD1	1:A:23:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:HG22	1:A:43:THR:O	2.17	0.45
1:A:70:ASP:O	1:A:72:GLU:HB2	2.16	0.45
1:A:107:GLU:HA	1:A:110:LEU:CD2	2.46	0.45
1:A:149:PHE:O	1:A:150:PHE:CB	2.36	0.45
1:A:165:TYR:O	1:A:165:TYR:HD2	1.97	0.45
1:A:208:ALA:HA	1:A:310:PHE:C	2.37	0.45
1:A:212:GLY:C	1:A:214:GLY:H	2.23	0.45
1:A:421:ASP:OD1	1:A:422:TYR:HE1	1.92	0.45
1:A:492:ILE:O	1:A:495:THR:HG22	2.17	0.45
1:A:539:PHE:C	1:A:539:PHE:CD2	2.94	0.45
1:A:553:VAL:O	1:A:557:LEU:HB2	2.16	0.45
19:A:1138:CLA:HMD1	21:F:6014:BCR:HC41	1.98	0.45
2:B:97:GLY:O	2:B:100:ALA:HB2	2.17	0.45
2:B:339:ALA:O	2:B:340:SER:CB	2.64	0.45
2:B:373:THR:C	2:B:375:HIS:H	2.24	0.45
2:B:564:ARG:CZ	3:C:64:SER:N	2.80	0.45
2:B:564:ARG:HH21	3:C:66:ARG:NH1	2.14	0.45
19:B:1223:CLA:H72	19:B:1223:CLA:C4	2.45	0.45
19:B:1234:CLA:HBC3	19:B:1234:CLA:CMC	2.35	0.45
3:C:70:TRP:O	3:C:71:HIS:C	2.59	0.45
4:D:116:THR:O	4:D:117:GLY:O	2.34	0.45
4:D:123:ARG:O	4:D:124:GLU:CB	2.63	0.45
5:E:99:THR:CG2	5:E:100:ARG:N	2.42	0.45
6:F:113:SER:C	6:F:115:PRO:HD3	2.42	0.45
6:F:224:GLY:CA	6:F:227:VAL:CG1	2.94	0.45
7:G:84:ARG:HA	19:G:1242:CLA:HMA1	1.97	0.45
12:L:131:SER:O	12:L:132:LEU:HB3	2.15	0.45
19:L:1502:CLA:HBA1	19:L:1502:CLA:CHA	2.47	0.45
15:1:145:ILE:HG13	15:1:145:ILE:H	1.52	0.45
19:1:1007:CLA:HHD	19:1:1007:CLA:HBC3	1.96	0.45
17:3:186:TYR:HD2	17:3:188:LEU:O	1.99	0.45
17:3:233:LEU:HA	17:3:236:LEU:CB	2.44	0.45
18:4:124:PRO:O	18:4:125:LYS:HB2	2.17	0.45
18:4:124:PRO:O	18:4:125:LYS:CG	2.63	0.45
18:4:217:PHE:CE1	18:4:221:HIS:CG	3.04	0.45
22:4:7033:LMU:H5'	22:4:7033:LMU:H1B	1.73	0.45
1:A:284:ARG:O	1:A:285:GLY:C	2.56	0.45
21:A:6003:BCR:C8	21:A:6003:BCR:C31	2.95	0.45
2:B:70:TRP:CB	2:B:136:TYR:OH	2.46	0.45
2:B:73:ASN:H	2:B:73:ASN:HD22	1.59	0.45
2:B:75:GLU:CB	2:B:132:ASN:CG	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:LEU:HD13	19:B:1221:CLA:CBB	2.46	0.45
2:B:395:ILE:HD13	2:B:555:TYR:H	1.81	0.45
2:B:450:GLU:C	2:B:452:GLN:N	2.73	0.45
2:B:498:LEU:O	2:B:498:LEU:HD23	2.16	0.45
2:B:505:SER:OG	2:B:506:ASN:N	2.49	0.45
2:B:533:ILE:CD1	2:B:579:ALA:HA	2.46	0.45
2:B:646:TRP:O	2:B:649:MET:HB3	2.17	0.45
19:B:1230:CLA:HED2	19:B:1230:CLA:H2A	1.98	0.45
19:B:1231:CLA:HBA2	19:B:1231:CLA:H3A	1.53	0.45
19:B:9010:CLA:H161	19:B:9010:CLA:H193	1.74	0.45
5:E:108:ASN:O	5:E:109:LYS:C	2.57	0.45
5:E:123:ASP:HA	5:E:124:GLU:HA	1.57	0.45
6:F:103:GLN:OE1	6:F:104:ALA:N	2.50	0.45
12:L:158:PRO:O	12:L:159:SER:HB3	2.16	0.45
12:L:167:THR:OG1	12:L:168:GLY:N	2.47	0.45
13:N:90:GLU:OE1	13:N:91:TYR:CD2	2.69	0.45
22:R:7007:LMU:H6D	22:R:7007:LMU:O5B	2.17	0.45
22:R:7014:LMU:H62	22:R:7014:LMU:C1	2.25	0.45
17:3:176:TRP:O	17:3:178:LYS:HG3	2.16	0.45
19:4:1304:CLA:HAA2	19:4:1304:CLA:O2D	2.13	0.45
1:A:39:HIS:ND1	1:A:39:HIS:C	2.75	0.45
1:A:94:SER:O	1:A:95:GLY:C	2.58	0.45
1:A:98:PHE:C	1:A:100:GLY:N	2.68	0.45
1:A:109:TRP:O	1:A:112:ASP:CA	2.65	0.45
1:A:136:VAL:HG23	1:A:140:PHE:O	2.15	0.45
1:A:177:LEU:C	1:A:179:LEU:N	2.75	0.45
1:A:210:LEU:N	1:A:213:LEU:H	2.15	0.45
1:A:252:ARG:HE	1:A:252:ARG:HB2	1.34	0.45
1:A:362:LEU:HD11	19:A:1128:CLA:CBB	2.45	0.45
1:A:401:TRP:HD1	19:A:1126:CLA:CHC	2.30	0.45
1:A:496:HIS:O	1:A:499:ALA:HB2	2.17	0.45
1:A:569:ILE:HG22	1:A:571:ASP:N	2.32	0.45
1:A:708:VAL:O	1:A:711:HIS:HB2	2.17	0.45
19:A:9013:CLA:H2	19:A:9013:CLA:HMA2	1.97	0.45
2:B:7:ARG:HD2	2:B:7:ARG:N	2.31	0.45
2:B:141:PHE:O	2:B:144:PHE:N	2.50	0.45
2:B:305:LEU:O	2:B:308:HIS:CB	2.65	0.45
2:B:469:LYS:CG	2:B:470:THR:OG1	2.65	0.45
2:B:515:GLY:HA3	2:B:613:SER:CB	2.39	0.45
19:B:1203:CLA:H193	19:B:1203:CLA:H161	1.78	0.45
19:B:1230:CLA:H3A	19:B:1230:CLA:HBA1	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:TRP:NE1	4:D:127:ASN:OD1	2.48	0.45
5:E:89:SER:CB	5:E:106:ARG:NH1	2.57	0.45
6:F:124:GLU:N	6:F:127:LYS:HB2	2.32	0.45
6:F:128:LYS:O	6:F:129:ARG:CD	2.64	0.45
8:H:115:THR:O	8:H:116:ALA:CB	2.58	0.45
11:K:125:LYS:CB	11:K:128:GLY:H	2.26	0.45
22:K:7042:LMU:H6D	22:K:7042:LMU:C3	2.44	0.45
12:L:143:LEU:HA	12:L:146:THR:N	2.18	0.45
12:L:206:VAL:O	12:L:206:VAL:HG22	2.17	0.45
13:N:96:LYS:HG3	13:N:97:THR:HG1	1.77	0.45
13:N:136:ASP:O	13:N:137:LEU:CD2	2.51	0.45
15:1:114:TRP:CZ3	15:1:121:GLN:CA	2.96	0.45
16:2:215:LYS:HB2	16:2:217:LEU:HG	1.98	0.45
16:2:241:TYR:CD2	16:2:242:THR:N	2.84	0.45
22:2:7031:LMU:H21	22:2:7031:LMU:H52	1.56	0.45
17:3:98:LEU:O	17:3:101:GLY:HA3	2.16	0.45
17:3:108:PHE:CD2	19:3:3013:CLA:C4	2.99	0.45
19:3:3006:CLA:C3B	19:3:3013:CLA:H11	2.46	0.45
18:4:172:PHE:CD2	18:4:172:PHE:N	2.82	0.45
18:4:215:LEU:O	18:4:218:ILE:N	2.49	0.45
19:4:4001:CLA:HAA2	19:4:4001:CLA:HBD	1.99	0.45
1:A:105:ASN:HA	1:A:105:ASN:HD22	1.55	0.45
1:A:185:HIS:O	1:A:188:LYS:N	2.49	0.45
1:A:421:ASP:OD1	1:A:422:TYR:CD1	2.70	0.45
1:A:443:ILE:CG2	2:B:674:LEU:CD1	2.95	0.45
1:A:525:ASN:HD22	1:A:526:LYS:CE	2.24	0.45
1:A:555:ILE:HG23	2:B:670:TYR:CE2	2.51	0.45
1:A:685:VAL:O	1:A:688:PHE:HB3	2.17	0.45
1:A:691:MET:O	20:A:5001:PQN:O1	2.35	0.45
19:A:1110:CLA:HBD	19:A:1110:CLA:HAA1	1.98	0.45
19:A:1115:CLA:H93	19:A:1115:CLA:H61	1.81	0.45
19:A:1116:CLA:C4C	19:A:1116:CLA:H62	2.47	0.45
19:A:1138:CLA:HBC2	19:A:1139:CLA:NC	2.32	0.45
19:A:9012:CLA:H41	19:A:9012:CLA:H62	1.80	0.45
2:B:14:GLN:O	2:B:15:ASP:C	2.56	0.45
2:B:364:ASP:C	2:B:365:PHE:HD2	2.25	0.45
2:B:440:ASN:OD1	2:B:452:GLN:CD	2.60	0.45
2:B:608:GLN:O	2:B:608:GLN:HG3	2.16	0.45
3:C:12:ILE:CG2	3:C:39:ILE:HA	2.47	0.45
4:D:74:LEU:CD1	12:L:58:GLN:OE1	2.64	0.45
4:D:101:VAL:O	4:D:101:VAL:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:1145:CLA:H3A	19:H:1145:CLA:HBA1	1.35	0.45
11:K:47:ASP:C	11:K:51:SER:H	2.24	0.45
12:L:195:SER:C	12:L:197:VAL:H	2.25	0.45
22:N:7049:LMU:H41	22:N:7049:LMU:H5'	1.98	0.45
15:1:155:GLU:CD	15:1:155:GLU:H	2.19	0.45
15:1:205:GLN:HE21	15:1:205:GLN:HB2	1.62	0.45
16:2:167:ARG:NE	16:2:168:TRP:H	2.10	0.45
16:2:212:GLN:CG	16:2:213:LYS:N	2.74	0.45
17:3:154:ASN:O	17:3:158:PHE:CZ	2.70	0.45
17:3:156:THR:C	17:3:158:PHE:N	2.69	0.45
19:3:3006:CLA:HHC	19:3:3013:CLA:H11	1.98	0.45
19:4:1304:CLA:C2	19:4:1304:CLA:O1A	2.64	0.45
1:A:75:SER:HB3	1:A:354:TRP:CE2	2.52	0.45
1:A:210:LEU:HD13	19:A:1111:CLA:CMB	2.47	0.45
1:A:210:LEU:CD1	19:A:1111:CLA:HMB2	2.46	0.45
1:A:213:LEU:HD12	1:A:311:LEU:HD21	1.97	0.45
1:A:254:LEU:HA	1:A:254:LEU:HD13	1.41	0.45
1:A:413:HIS:ND1	1:A:416:ILE:HD12	2.32	0.45
1:A:569:ILE:CG1	1:A:586:ARG:NH1	2.80	0.45
1:A:668:TYR:HA	2:B:445:ALA:HB1	1.98	0.45
1:A:672:LEU:C	1:A:674:ALA:H	2.16	0.45
1:A:708:VAL:HA	1:A:711:HIS:CD2	2.52	0.45
19:A:1106:CLA:HBA2	19:A:1106:CLA:H3A	1.35	0.45
2:B:29:HIS:CG	19:B:1202:CLA:CBB	2.99	0.45
2:B:175:LEU:HD13	19:B:1221:CLA:O2D	2.16	0.45
2:B:182:LEU:O	2:B:186:SER:HB2	2.17	0.45
2:B:606:VAL:O	2:B:608:GLN:N	2.49	0.45
2:B:668:ARG:HG3	2:B:699:ALA:C	2.42	0.45
19:B:1203:CLA:H41	24:B:7101:LMG:H321	1.98	0.45
3:C:44:ARG:CD	4:D:182:GLN:NE2	2.80	0.45
5:E:111:ASN:HB3	5:E:116:SER:HG	1.78	0.45
6:F:129:ARG:HD2	6:F:129:ARG:HA	1.61	0.45
7:G:109:GLU:HG3	7:G:109:GLU:O	2.17	0.45
19:G:1242:CLA:HBC3	19:G:1242:CLA:HHD	1.97	0.45
12:L:54:TYR:HE1	12:L:57:ILE:CG2	2.28	0.45
21:L:6019:BCR:C8	21:L:6019:BCR:H331	2.46	0.45
15:1:68:GLY:O	15:1:73:PRO:CD	2.65	0.45
15:1:151:GLN:NE2	15:1:151:GLN:N	2.56	0.45
16:2:170:ASP:C	16:2:172:LEU:N	2.67	0.45
19:2:2007:CLA:CGA	19:2:2007:CLA:C1A	2.95	0.45
17:3:204:GLY:C	17:3:206:PRO:O	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3008:CLA:CGA	19:3:3008:CLA:O1D	2.64	0.45
19:4:1304:CLA:H161	19:4:1304:CLA:H122	1.38	0.45
1:A:42:ARG:O	1:A:44:ILE:N	2.49	0.45
1:A:74:ILE:O	1:A:76:ARG:N	2.50	0.45
1:A:119:SER:CA	1:A:145:ILE:HD12	2.47	0.45
1:A:249:ILE:HG22	17:3:137:PHE:HE2	1.82	0.45
1:A:284:ARG:N	1:A:298:ASP:OD1	2.49	0.45
1:A:418:MET:O	1:A:564:ARG:HD2	2.16	0.45
1:A:421:ASP:H	1:A:422:TYR:HD1	1.64	0.45
1:A:482:ILE:O	1:A:482:ILE:HG23	2.13	0.45
1:A:536:THR:HA	1:A:539:PHE:CB	2.46	0.45
1:A:697:ARG:C	1:A:699:TYR:N	2.74	0.45
19:A:1117:CLA:HAC2	21:A:6003:BCR:H352	1.98	0.45
19:A:1126:CLA:H171	21:J:6012:BCR:H351	1.98	0.45
22:A:7010:LMU:O5'	22:K:7047:LMU:H122	2.17	0.45
2:B:156:HIS:O	2:B:163:PRO:HB3	2.17	0.45
2:B:167:TRP:CZ2	19:B:1210:CLA:HAC2	2.52	0.45
2:B:255:LEU:HA	2:B:271:THR:OG1	2.16	0.45
2:B:284:PHE:CE1	19:B:1216:CLA:HHC	2.52	0.45
2:B:370:ALA:HB2	2:B:725:LEU:HD11	1.99	0.45
2:B:493:TRP:CZ3	19:B:1232:CLA:HMA3	2.52	0.45
2:B:535:VAL:C	2:B:539:LEU:HD23	2.39	0.45
2:B:637:PRO:O	2:B:639:VAL:N	2.44	0.45
19:B:1223:CLA:H202	19:B:1223:CLA:H162	1.80	0.45
3:C:36:ALA:O	3:C:37:LYS:CG	2.65	0.45
3:C:44:ARG:HG3	3:C:44:ARG:O	2.17	0.45
4:D:103:THR:C	4:D:104:TRP:CD1	2.95	0.45
4:D:113:GLU:O	4:D:114:MET:CB	2.59	0.45
7:G:101:GLU:HA	7:G:105:THR:HG21	1.12	0.45
7:G:137:VAL:O	7:G:137:VAL:CG2	2.60	0.45
7:G:149:TYR:CG	7:G:150:ASP:OD1	2.70	0.45
19:J:1311:CLA:O1A	19:J:1311:CLA:H152	2.16	0.45
11:K:58:VAL:CG1	11:K:59:THR:N	2.76	0.45
12:L:54:TYR:O	12:L:55:GLN:CB	2.65	0.45
12:L:148:TYR:O	12:L:151:SER:HB3	2.17	0.45
12:L:156:GLY:N	12:L:178:THR:HG21	2.32	0.45
12:L:195:SER:C	12:L:197:VAL:N	2.75	0.45
13:N:90:GLU:OE1	13:N:91:TYR:CG	2.70	0.45
13:N:114:PHE:HE2	13:N:116:ARG:CD	2.29	0.45
13:N:155:GLU:CA	13:N:157:LYS:H	2.19	0.45
15:1:57:SER:O	15:1:58:ALA:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:120:ILE:CG1	16:2:121:PHE:H	2.24	0.45
16:2:152:LEU:HD13	16:2:152:LEU:N	2.32	0.45
16:2:164:GLU:HG2	16:2:167:ARG:HD3	1.98	0.45
18:4:201:LYS:O	18:4:205:ILE:HG23	2.17	0.45
1:A:76:ARG:C	1:A:186:TYR:HD2	2.25	0.45
1:A:159:THR:O	1:A:163:GLN:OE1	2.35	0.45
1:A:196:PHE:HD2	1:A:196:PHE:N	2.07	0.45
1:A:217:SER:CB	21:A:6002:BCR:H351	2.46	0.45
1:A:531:PRO:O	1:A:532:ILE:CB	2.65	0.45
19:A:1106:CLA:C4	21:A:6011:BCR:H383	2.46	0.45
19:A:1138:CLA:HBC1	21:F:6014:BCR:C33	2.47	0.45
2:B:4:ARG:C	2:B:4:ARG:CZ	2.90	0.45
2:B:129:LEU:HA	19:B:1211:CLA:HED3	1.99	0.45
2:B:172:GLU:HG3	2:B:301:ILE:CG1	2.47	0.45
2:B:193:HIS:HD2	19:B:1211:CLA:NC	2.15	0.45
2:B:289:LEU:O	19:B:1218:CLA:HAC1	2.16	0.45
2:B:454:LEU:CD1	2:B:454:LEU:C	2.86	0.45
2:B:568:CYS:C	2:B:570:ILE:HG23	2.42	0.45
19:B:1202:CLA:H2	19:B:1202:CLA:H62	1.37	0.45
6:F:199:ASP:HB2	10:J:7:TYR:O	2.17	0.45
7:G:99:HIS:CA	7:G:100:PHE:CB	2.62	0.45
11:K:55:LEU:O	11:K:58:VAL:CB	2.65	0.45
22:K:7041:LMU:H1B	22:K:7041:LMU:H4B	1.67	0.45
12:L:92:ALA:H	12:L:98:ARG:HH22	1.59	0.45
12:L:131:SER:CB	12:L:201:TYR:HE2	2.05	0.45
12:L:154:ASN:O	12:L:154:ASN:CG	2.58	0.45
12:L:168:GLY:O	12:L:170:LYS:O	2.34	0.45
12:L:169:ARG:CZ	12:L:169:ARG:HA	2.47	0.45
19:L:1148:CLA:CED	19:L:1148:CLA:HAA1	2.46	0.45
15:1:80:LYS:C	15:1:83:GLU:H	2.24	0.45
16:2:211:PRO:O	16:2:212:GLN:HB2	2.17	0.45
16:2:227:LEU:HD21	19:2:2004:CLA:C4B	2.46	0.45
16:2:250:LEU:HD23	16:2:251:PHE:CD1	2.52	0.45
18:4:89:ARG:CD	18:4:90:TRP:N	2.45	0.45
1:A:23:ASP:C	1:A:33:GLN:OE1	2.60	0.44
1:A:239:PRO:O	1:A:240:LYS:HB3	2.17	0.44
1:A:434:ARG:O	1:A:435:VAL:C	2.60	0.44
19:A:1116:CLA:H12	19:A:1116:CLA:C4A	2.47	0.44
19:A:1132:CLA:H172	19:A:1136:CLA:H202	1.99	0.44
19:A:1132:CLA:H3A	19:A:1132:CLA:HBA1	1.78	0.44
21:A:6011:BCR:H322	21:J:6012:BCR:H391	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:9011:CLA:HMC2	2:B:624:LEU:HG	1.98	0.44
2:B:38:THR:OG1	2:B:41:ARG:HB2	2.17	0.44
2:B:255:LEU:HD13	2:B:275:HIS:HB2	1.99	0.44
2:B:292:ARG:NH1	2:B:295:PHE:N	2.65	0.44
2:B:382:ILE:O	2:B:385:GLY:N	2.48	0.44
2:B:412:LEU:O	2:B:413:GLU:C	2.58	0.44
2:B:420:SER:H	2:B:422:LEU:H	1.65	0.44
2:B:535:VAL:CG1	2:B:536:LYS:N	2.79	0.44
2:B:580:VAL:HG11	2:B:710:LEU:HD11	1.98	0.44
2:B:593:TYR:CZ	19:B:1234:CLA:HBC2	2.52	0.44
2:B:697:PRO:CB	19:B:1238:CLA:HBC3	2.48	0.44
4:D:95:GLN:HE21	4:D:96:VAL:N	2.16	0.44
4:D:131:LEU:HD13	4:D:136:GLN:HB3	1.99	0.44
4:D:140:LEU:CD2	4:D:144:LEU:CG	2.96	0.44
4:D:169:LYS:HZ3	4:D:169:LYS:HB2	1.81	0.44
5:E:82:TYR:CB	5:E:83:TRP:HE3	2.20	0.44
5:E:89:SER:O	5:E:105:VAL:CA	2.65	0.44
6:F:206:LEU:O	6:F:207:LEU:C	2.60	0.44
7:G:151:PRO:O	7:G:151:PRO:CD	2.65	0.44
22:H:7028:LMU:O6'	22:H:7028:LMU:C1'	2.65	0.44
12:L:69:LEU:HD23	12:L:69:LEU:HA	1.80	0.44
12:L:112:GLY:HA2	12:L:115:VAL:HG22	1.99	0.44
15:1:58:ALA:HB3	15:1:59:PRO:HD2	1.99	0.44
15:1:70:GLY:N	15:1:73:PRO:CD	2.80	0.44
15:1:138:LEU:HA	15:1:141:GLU:HG3	1.99	0.44
17:3:157:LEU:O	17:3:159:VAL:C	2.59	0.44
22:3:7005:LMU:C2	22:3:7005:LMU:O5'	2.64	0.44
18:4:168:GLN:O	18:4:172:PHE:HD1	2.00	0.44
22:4:7033:LMU:H61	22:4:7033:LMU:H31	1.83	0.44
1:A:59:ALA:O	1:A:61:ALA:N	2.50	0.44
1:A:331:LEU:HD22	1:A:343:HIS:O	2.15	0.44
1:A:369:THR:HG21	19:A:1127:CLA:HMC2	1.99	0.44
1:A:431:LEU:N	1:A:434:ARG:HB2	2.32	0.44
1:A:499:ALA:HB1	19:A:1133:CLA:O2D	2.14	0.44
1:A:555:ILE:HD11	19:A:9023:CLA:CMD	2.48	0.44
1:A:567:ARG:HH11	4:D:89:GLY:N	2.15	0.44
2:B:120:VAL:CA	2:B:123:TRP:NE1	2.71	0.44
2:B:131:THR:O	2:B:135:LEU:N	2.49	0.44
2:B:256:THR:OG1	2:B:257:ILE:N	2.50	0.44
2:B:261:PHE:HE2	2:B:499:ASN:O	2.00	0.44
2:B:378:ILE:HG22	2:B:379:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:482:ASN:C	2:B:484:PRO:HD2	2.42	0.44
2:B:493:TRP:HB3	2:B:494:LEU:H	1.54	0.44
2:B:584:LEU:HD11	2:B:714:SER:OG	2.18	0.44
2:B:597:LYS:HG2	19:B:1234:CLA:HBC1	1.99	0.44
2:B:718:ILE:HD11	19:B:1224:CLA:HHC	1.97	0.44
19:B:1226:CLA:C20	19:B:1239:CLA:HBA1	2.47	0.44
4:D:141:GLY:O	4:D:142:THR:O	2.34	0.44
4:D:145:ARG:NH1	4:D:173:TYR:HE1	2.12	0.44
5:E:85:LYS:HE3	5:E:85:LYS:HB3	1.67	0.44
5:E:127:GLU:HA	5:E:128:VAL:O	2.13	0.44
6:F:157:TRP:HB3	19:F:1305:CLA:HMC3	1.99	0.44
6:F:190:LYS:HZ2	6:F:192:THR:HG21	0.48	0.44
7:G:64:ILE:CG1	7:G:68:THR:HG23	2.45	0.44
7:G:76:ARG:HH12	7:G:120:VAL:N	2.16	0.44
7:G:119:PRO:HB3	19:G:1242:CLA:CBC	2.47	0.44
11:K:86:LEU:O	11:K:87:GLU:HB2	2.16	0.44
11:K:111:VAL:HA	11:K:114:HIS:ND1	2.30	0.44
12:L:182:TRP:O	12:L:186:THR:HG23	2.17	0.44
19:L:1501:CLA:H3A	19:L:1501:CLA:HBA2	1.57	0.44
13:N:132:THR:HA	13:N:137:LEU:O	2.18	0.44
15:1:68:GLY:CA	15:1:72:VAL:HB	2.47	0.44
15:1:177:PRO:O	15:1:178:LYS:HG3	2.17	0.44
15:1:202:CYS:O	15:1:202:CYS:SG	2.71	0.44
16:2:155:VAL:C	16:2:158:VAL:HG13	2.42	0.44
17:3:124:LYS:NZ	17:3:148:TYR:N	2.65	0.44
18:4:173:LYS:CD	18:4:201:LYS:HG3	2.46	0.44
22:4:7053:LMU:H51	22:4:7053:LMU:H21	1.57	0.44
1:A:85:GLN:O	1:A:89:ILE:HG13	2.18	0.44
1:A:106:TYR:O	1:A:110:LEU:CD2	2.50	0.44
1:A:359:SER:OG	1:A:414:ALA:HB2	2.16	0.44
1:A:467:MET:HE1	1:A:475:ASP:O	2.16	0.44
1:A:488:PHE:CD1	1:A:488:PHE:N	2.83	0.44
1:A:493:GLN:HE21	1:A:515:TRP:HA	1.82	0.44
1:A:499:ALA:HB3	1:A:500:PRO:HD2	1.99	0.44
1:A:502:THR:CG2	1:A:503:THR:N	2.81	0.44
19:A:1103:CLA:H161	19:A:1103:CLA:H202	1.62	0.44
19:A:1112:CLA:C4B	21:A:6002:BCR:C20	2.94	0.44
19:A:1140:CLA:H43	19:A:1140:CLA:C4C	2.46	0.44
2:B:114:ASN:O	2:B:115:ASN:CG	2.61	0.44
2:B:174:ARG:HH11	19:B:1221:CLA:HMD1	1.81	0.44
2:B:244:PHE:HD2	2:B:245:GLY:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:LEU:HD21	19:B:1214:CLA:HMA3	1.89	0.44
2:B:292:ARG:CZ	2:B:297:ILE:O	2.65	0.44
19:B:1220:CLA:H141	19:B:1220:CLA:H161	1.67	0.44
3:C:44:ARG:O	3:C:44:ARG:CG	2.65	0.44
4:D:80:SER:HB2	4:D:127:ASN:CA	2.47	0.44
7:G:84:ARG:NE	7:G:89:LYS:CD	2.80	0.44
10:J:26:LEU:HD23	10:J:26:LEU:O	2.17	0.44
12:L:55:GLN:C	12:L:57:ILE:N	2.57	0.44
12:L:105:ALA:HB2	19:L:1501:CLA:HMA2	2.00	0.44
14:R:5:UNK:O	14:R:6:UNK:CB	2.65	0.44
15:1:177:PRO:HG2	15:1:180:LEU:CA	2.47	0.44
16:2:113:ALA:O	16:2:114:MET:HE3	2.15	0.44
16:2:171:ILE:HG12	16:2:172:LEU:N	2.26	0.44
19:2:2006:CLA:H112	19:2:2006:CLA:H71	1.72	0.44
17:3:151:TRP:CG	17:3:152:ALA:N	2.84	0.44
17:3:224:LYS:O	17:3:226:LYS:N	2.50	0.44
19:4:1304:CLA:CAA	19:4:1304:CLA:O2D	2.65	0.44
22:4:7052:LMU:H12	22:4:7052:LMU:C5	2.47	0.44
1:A:308:ILE:CG1	19:A:1115:CLA:CBB	2.96	0.44
1:A:432:LEU:HB3	1:A:433:ASP:H	1.71	0.44
1:A:539:PHE:HE2	1:A:543:HIS:HE1	1.65	0.44
1:A:549:ILE:O	1:A:552:THR:O	2.34	0.44
1:A:615:HIS:ND1	19:A:1135:CLA:HBC3	2.32	0.44
1:A:669:GLY:CA	2:B:445:ALA:HA	2.44	0.44
1:A:709:TRP:O	1:A:710:ALA:C	2.59	0.44
2:B:120:VAL:CB	2:B:123:TRP:NE1	2.80	0.44
2:B:316:GLY:O	2:B:317:ARG:CD	2.64	0.44
2:B:495:PRO:HB2	2:B:496:GLY:H	1.40	0.44
19:B:1217:CLA:NA	19:B:1217:CLA:O2A	2.51	0.44
19:B:1229:CLA:H143	19:B:1229:CLA:H162	1.84	0.44
4:D:173:TYR:CZ	4:D:175:GLU:OE2	2.70	0.44
6:F:149:ILE:O	6:F:150:VAL:CG1	2.64	0.44
6:F:227:VAL:O	6:F:228:ASP:C	2.60	0.44
12:L:205:TYR:N	12:L:205:TYR:CD2	2.84	0.44
13:N:104:LYS:HB3	13:N:105:LYS:H	1.53	0.44
15:1:68:GLY:O	15:1:72:VAL:CA	2.64	0.44
15:1:183:LEU:C	15:1:185:VAL:N	2.64	0.44
16:2:150:THR:O	16:2:151:THR:C	2.58	0.44
17:3:93:ILE:HA	17:3:95:PRO:HD2	1.99	0.44
17:3:164:LEU:HD12	17:3:165:MET:SD	2.58	0.44
17:3:190:LEU:HD23	17:3:190:LEU:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3011:CLA:CAC	19:3:3012:CLA:C2A	2.78	0.44
18:4:158:GLN:CD	19:4:1004:CLA:H2A	2.41	0.44
1:A:98:PHE:CD1	1:A:99:HIS:N	2.77	0.44
1:A:122:VAL:HG13	1:A:133:ASN:HD21	1.83	0.44
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.77	0.44
1:A:218:TRP:CA	19:A:1112:CLA:HBB2	2.48	0.44
1:A:227:LEU:O	1:A:231:GLN:HB2	2.18	0.44
1:A:389:TYR:HD1	1:A:625:TRP:CD2	2.36	0.44
1:A:680:LEU:HB3	19:A:9012:CLA:C2	2.48	0.44
19:A:1107:CLA:HBA2	19:A:1107:CLA:CBD	2.47	0.44
19:A:1125:CLA:CBA	21:A:6008:BCR:H12C	2.45	0.44
19:A:1133:CLA:CMC	19:A:1133:CLA:CBC	2.95	0.44
19:A:1140:CLA:H71	19:A:9013:CLA:H171	1.98	0.44
2:B:33:SER:H	2:B:37:ILE:CD1	2.30	0.44
2:B:75:GLU:O	2:B:79:GLN:HG2	2.17	0.44
2:B:167:TRP:CZ2	19:B:1210:CLA:HAC1	2.53	0.44
2:B:469:LYS:CD	2:B:470:THR:CA	2.60	0.44
2:B:697:PRO:HB3	19:B:1238:CLA:HBC3	1.99	0.44
19:B:1229:CLA:CBB	21:F:6014:BCR:C23	2.96	0.44
3:C:10:THR:HG23	5:E:101:TYR:HD2	1.67	0.44
4:D:99:PHE:CD1	4:D:99:PHE:O	2.71	0.44
4:D:141:GLY:N	4:D:143:ARG:N	2.66	0.44
4:D:158:PHE:HB3	4:D:159:PRO:C	2.36	0.44
7:G:116:SER:O	7:G:119:PRO:N	2.50	0.44
8:H:97:LEU:HG	8:H:98:LEU:N	2.32	0.44
11:K:49:ILE:CA	11:K:52:PRO:HG2	2.23	0.44
12:L:114:PHE:N	12:L:114:PHE:CD1	2.85	0.44
12:L:138:VAL:CG2	12:L:194:ILE:HG13	2.47	0.44
13:N:147:SER:C	13:N:151:ASP:H	2.25	0.44
15:1:94:VAL:O	15:1:95:PRO:C	2.56	0.44
16:2:97:GLU:OE1	16:2:97:GLU:N	2.51	0.44
16:2:156:GLU:OE2	19:2:2013:CLA:HHD	2.11	0.44
16:2:184:PRO:N	16:2:187:LYS:CG	2.74	0.44
16:2:195:TYR:HD1	16:2:196:PRO:N	2.14	0.44
16:2:226:ARG:NH1	16:2:226:ARG:HG2	2.33	0.44
17:3:151:TRP:HD1	17:3:152:ALA:N	1.97	0.44
17:3:226:LYS:O	17:3:226:LYS:HG2	2.18	0.44
1:A:51:THR:CG2	1:A:723:ARG:HB2	2.47	0.44
1:A:450:CYS:O	1:A:453:LEU:O	2.35	0.44
1:A:527:VAL:CB	1:A:626:GLY:HA3	2.41	0.44
1:A:723:ARG:CG	1:A:723:ARG:NH1	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1119:CLA:HBA1	19:A:1123:CLA:CBB	2.46	0.44
19:A:1139:CLA:C4	6:F:198:ILE:HD13	2.45	0.44
19:A:1140:CLA:C6	19:A:9013:CLA:H193	2.45	0.44
22:A:7023:LMU:H41	22:A:7023:LMU:H92	1.99	0.44
2:B:55:ALA:HB1	2:B:150:LEU:HD11	2.00	0.44
2:B:182:LEU:HD13	19:B:1210:CLA:HHB	1.99	0.44
2:B:387:PHE:HB2	2:B:534:LEU:HD13	1.98	0.44
2:B:493:TRP:CZ3	19:B:1232:CLA:CMA	3.01	0.44
2:B:708:VAL:C	2:B:710:LEU:O	2.61	0.44
3:C:9:ASP:OD1	3:C:61:ASP:HB2	2.17	0.44
3:C:62:PHE:CD1	5:E:80:GLU:CB	3.00	0.44
4:D:148:TYR:O	4:D:149:LYS:NZ	2.44	0.44
4:D:151:LYS:HB3	4:D:151:LYS:HE2	1.72	0.44
7:G:79:PHE:CE2	7:G:80:PHE:HB2	2.53	0.44
8:H:89:ALA:HB3	8:H:90:PRO:HD3	1.99	0.44
8:H:112:LEU:HD22	8:H:112:LEU:HA	1.74	0.44
9:I:12:VAL:CG1	21:I:6018:BCR:H271	2.48	0.44
11:K:127:ILE:CA	11:K:129:ALA:HA	2.40	0.44
22:K:7042:LMU:O2B	22:K:7042:LMU:C5'	2.59	0.44
12:L:83:LEU:HD13	12:L:88:ALA:HB3	1.98	0.44
13:N:90:GLU:OE2	13:N:91:TYR:N	2.51	0.44
22:R:7022:LMU:H81	22:R:7022:LMU:H111	1.72	0.44
15:1:73:PRO:HD2	15:1:74:ALA:H	1.82	0.44
15:1:134:LEU:C	15:1:137:ILE:HD11	2.40	0.44
19:1:1010:CLA:HBA2	19:1:1010:CLA:HMA2	1.99	0.44
16:2:128:LYS:HG3	16:2:131:ILE:HG23	1.98	0.44
16:2:164:GLU:HB3	19:2:2012:CLA:CHB	2.47	0.44
17:3:96:ARG:NH2	17:3:100:TYR:OH	2.51	0.44
17:3:164:LEU:O	17:3:167:PHE:HB2	2.18	0.44
22:3:7005:LMU:O1'	22:3:7005:LMU:C5	2.63	0.44
18:4:157:TRP:O	18:4:158:GLN:C	2.61	0.44
18:4:232:LEU:HB3	18:4:236:ILE:HD13	1.99	0.44
1:A:49:ASP:HA	6:F:193:GLN:OE1	2.18	0.44
1:A:93:LEU:HA	1:A:96:MET:CG	2.48	0.44
1:A:357:GLN:OE1	1:A:357:GLN:O	2.36	0.44
1:A:358:LEU:HD11	1:A:413:HIS:CD2	2.48	0.44
1:A:370:ILE:HD11	19:A:1124:CLA:O1D	2.17	0.44
1:A:538:ASP:O	1:A:542:HIS:CD2	2.71	0.44
1:A:588:GLY:HA3	2:B:668:ARG:HB3	1.99	0.44
2:B:10:GLN:HE21	2:B:10:GLN:HB2	1.53	0.44
2:B:160:LYS:NZ	2:B:161:TRP:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:HIS:O	2:B:194:LEU:C	2.59	0.44
2:B:488:ALA:HB2	19:B:1233:CLA:C2C	2.48	0.44
2:B:510:LEU:CD2	2:B:597:LYS:HD2	2.47	0.44
2:B:707:LEU:HD13	24:B:7101:LMG:H331	1.98	0.44
2:B:732:LYS:CB	2:B:733:PHE:C	2.86	0.44
19:B:1202:CLA:NC	19:B:1226:CLA:HMB1	2.33	0.44
19:B:1229:CLA:HBD	19:B:1229:CLA:HBA1	1.98	0.44
3:C:43:PRO:C	4:D:182:GLN:HG3	2.43	0.44
4:D:110:GLN:O	4:D:122:MET:HG3	2.18	0.44
5:E:81:SER:OG	5:E:120:TYR:CE1	2.68	0.44
6:F:94:ARG:O	6:F:95:GLU:C	2.61	0.44
7:G:144:THR:O	7:G:144:THR:CG2	2.66	0.44
11:K:110:GLY:O	11:K:114:HIS:CG	2.70	0.44
12:L:56:VAL:O	12:L:56:VAL:HG23	2.17	0.44
12:L:76:SER:C	12:L:78:LEU:N	2.72	0.44
12:L:76:SER:H	12:L:79:ILE:HG22	1.83	0.44
12:L:81:TRP:C	12:L:83:LEU:N	2.74	0.44
12:L:153:PHE:CG	12:L:155:GLU:OE1	2.71	0.44
12:L:155:GLU:CA	12:L:178:THR:HG21	2.43	0.44
13:N:126:LYS:NZ	13:N:126:LYS:HB3	2.32	0.44
16:2:137:TRP:CD1	16:2:139:THR:HG22	2.53	0.44
16:2:149:THR:C	16:2:152:LEU:HD12	2.43	0.44
18:4:242:ASN:O	18:4:243:THR:CB	2.66	0.44
1:A:183:TRP:C	1:A:185:HIS:H	2.26	0.44
1:A:620:MET:HG3	1:A:625:TRP:CE2	2.52	0.44
19:A:1126:CLA:H171	19:A:1126:CLA:H122	2.00	0.44
19:A:1131:CLA:HBB2	19:A:1132:CLA:H2	2.00	0.44
19:A:1141:CLA:H41	19:A:1141:CLA:H62	1.48	0.44
19:A:1237:CLA:CMB	19:L:1502:CLA:HBC1	2.47	0.44
2:B:37:ILE:HG13	4:D:202:PHE:HD2	1.83	0.44
2:B:163:PRO:O	2:B:164:SER:CB	2.66	0.44
2:B:293:THR:CG2	19:B:1209:CLA:HMA2	2.47	0.44
2:B:444:LEU:O	2:B:445:ALA:CB	2.62	0.44
2:B:535:VAL:HG13	2:B:536:LYS:H	1.83	0.44
19:B:1206:CLA:C4	21:I:6018:BCR:H21C	2.48	0.44
19:B:1218:CLA:HBA2	19:B:1219:CLA:O1A	2.18	0.44
19:B:1220:CLA:C4	19:B:1220:CLA:HAA1	2.33	0.44
22:B:7012:LMU:H1B	22:B:7012:LMU:H3'	1.36	0.44
3:C:59:PRO:HB3	3:C:61:ASP:OD2	2.18	0.44
4:D:148:TYR:C	4:D:149:LYS:CG	2.88	0.44
6:F:84:PRO:HA	6:F:138:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:1505:CLA:H41	19:H:1505:CLA:C10	2.47	0.44
19:J:1311:CLA:H152	19:2:2014:CLA:CMB	2.48	0.44
19:K:1143:CLA:H43	19:K:1143:CLA:O2A	2.18	0.44
19:K:1146:CLA:CMC	19:K:1146:CLA:HBC2	2.48	0.44
12:L:68:SER:O	12:L:70:GLU:N	2.50	0.44
12:L:100:ILE:HG22	12:L:188:GLY:O	2.18	0.44
13:N:106:ARG:C	13:N:108:ALA:N	2.76	0.44
13:N:131:PHE:HA	13:N:133:GLY:H	1.83	0.44
14:R:34:UNK:C	14:R:36:UNK:O	2.66	0.44
15:1:161:LYS:HG3	15:1:162:LYS:N	2.33	0.44
15:1:223:ASP:HB3	15:1:224:PRO:HD2	1.99	0.44
16:2:122:ILE:CD1	19:2:2002:CLA:C2B	2.89	0.44
17:3:155:TYR:HB2	17:3:157:LEU:HG	1.99	0.44
17:3:176:TRP:C	17:3:178:LYS:CA	2.91	0.44
17:3:204:GLY:HA3	17:3:207:PHE:O	2.17	0.44
1:A:119:SER:OG	1:A:136:VAL:HG11	2.18	0.44
1:A:629:ASN:O	1:A:630:ASP:C	2.60	0.44
1:A:701:GLN:OE1	5:E:112:TYR:CZ	2.71	0.44
19:A:1124:CLA:HAA2	19:A:1125:CLA:OBD	2.18	0.44
2:B:214:ASP:OD1	2:B:214:ASP:O	2.36	0.44
2:B:586:THR:O	2:B:590:VAL:HG12	2.17	0.44
2:B:649:MET:HE3	21:B:6017:BCR:H272	2.00	0.44
3:C:61:ASP:O	3:C:62:PHE:CD2	2.71	0.44
3:C:65:VAL:C	3:C:66:ARG:NH2	2.76	0.44
6:F:83:THR:CB	6:F:84:PRO:HD2	2.41	0.44
6:F:102:LEU:HD12	6:F:103:GLN:N	2.33	0.44
7:G:138:ALA:O	7:G:140:TYR:N	2.50	0.44
19:H:1145:CLA:CAA	19:H:1145:CLA:HED1	2.44	0.44
11:K:84:LEU:HG	11:K:85:LYS:N	2.33	0.44
11:K:127:ILE:HA	11:K:130:LEU:CD2	2.42	0.44
12:L:173:PRO:CD	12:L:173:PRO:O	2.65	0.44
15:1:114:TRP:CH2	15:1:121:GLN:CG	2.95	0.44
15:1:114:TRP:HZ3	15:1:121:GLN:HA	1.76	0.44
16:2:112:TRP:CZ3	16:2:164:GLU:CG	2.97	0.44
16:2:184:PRO:CG	16:2:185:ASN:C	2.90	0.44
19:3:3011:CLA:H92	19:3:3011:CLA:H142	1.99	0.44
18:4:172:PHE:O	18:4:194:PHE:CD2	2.71	0.44
1:A:23:ASP:CG	1:A:24:ARG:NE	2.76	0.43
1:A:133:ASN:HA	1:A:142:GLY:O	2.18	0.43
1:A:181:ALA:HA	1:A:184:PHE:HB3	1.99	0.43
1:A:398:HIS:HD2	19:A:1126:CLA:ND	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:PHE:C	1:A:680:LEU:H	2.26	0.43
1:A:711:HIS:O	1:A:716:VAL:HG22	2.18	0.43
19:A:1115:CLA:H61	19:A:1115:CLA:H41	1.68	0.43
19:A:1138:CLA:OBD	2:B:427:LEU:HD22	2.18	0.43
19:A:1139:CLA:OBD	6:F:182:LEU:HD11	2.18	0.43
2:B:170:ASN:O	2:B:171:ALA:HB3	2.18	0.43
2:B:304:ILE:O	2:B:308:HIS:CD2	2.71	0.43
2:B:309:ILE:HG22	2:B:319:HIS:HD2	1.82	0.43
2:B:310:PRO:HD2	2:B:311:PRO:CD	2.48	0.43
2:B:337:ALA:O	2:B:339:ALA:O	2.35	0.43
2:B:388:ALA:HA	2:B:391:PRO:CG	2.48	0.43
2:B:454:LEU:HD11	6:F:146:PRO:O	2.18	0.43
2:B:513:GLY:O	2:B:516:ASP:OD1	2.36	0.43
2:B:527:LEU:CD1	19:B:1236:CLA:CMA	2.60	0.43
2:B:529:THR:O	2:B:532:LEU:HG	2.17	0.43
2:B:549:ASP:HB2	3:C:63:LEU:HB2	2.00	0.43
2:B:635:ILE:O	2:B:636:THR:C	2.60	0.43
19:B:1206:CLA:H93	19:B:1206:CLA:H61	1.83	0.43
19:B:1209:CLA:HMC2	21:B:6005:BCR:C37	2.40	0.43
19:B:1223:CLA:C10	21:B:6010:BCR:H14C	2.48	0.43
3:C:12:ILE:HG21	3:C:39:ILE:CA	2.47	0.43
8:H:57:ASP:C	8:H:59:GLY:N	2.76	0.43
8:H:65:TRP:N	8:H:66:ASP:CA	2.74	0.43
8:H:76:TYR:HH	12:L:90:ARG:HD3	1.70	0.43
8:H:109:LEU:HD23	19:H:1207:CLA:C6	2.47	0.43
19:H:1145:CLA:CGA	19:H:1145:CLA:C3A	2.95	0.43
11:K:125:LYS:HD2	11:K:128:GLY:CA	2.48	0.43
12:L:76:SER:OG	12:L:78:LEU:HD11	2.17	0.43
12:L:125:ILE:HG23	12:L:128:GLN:H	1.82	0.43
14:R:27:UNK:O	14:R:29:UNK:C	2.65	0.43
14:R:50:UNK:HA	14:R:51:UNK:HA	1.70	0.43
16:2:101:TRP:N	16:2:103:VAL:CB	2.66	0.43
16:2:182:ILE:HG22	16:2:187:LYS:CD	2.48	0.43
16:2:182:ILE:CD1	16:2:187:LYS:O	2.64	0.43
17:3:204:GLY:CA	17:3:207:PHE:HA	2.48	0.43
22:4:7034:LMU:H92	22:4:7052:LMU:C1	2.47	0.43
1:A:36:LYS:HA	1:A:37:PRO:HD3	1.60	0.43
1:A:207:LEU:C	1:A:207:LEU:HD12	2.44	0.43
1:A:662:SER:HA	1:A:665:ILE:HD11	2.00	0.43
19:A:1131:CLA:CBC	19:A:1136:CLA:HBC2	2.48	0.43
2:B:98:GLN:O	2:B:100:ALA:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLN:H	2:B:99:PRO:HD2	1.82	0.43
2:B:216:LEU:HD11	2:B:221:GLY:HA2	2.00	0.43
2:B:224:PRO:HB3	2:B:227:THR:HG21	2.00	0.43
2:B:317:ARG:CZ	2:B:317:ARG:CB	2.94	0.43
2:B:358:TYR:O	2:B:359:ALA:C	2.60	0.43
2:B:618:GLY:HA2	2:B:621:ARG:N	2.31	0.43
2:B:724:PHE:CE2	19:B:9010:CLA:HMD2	2.53	0.43
19:B:1205:CLA:C14	19:B:1224:CLA:H91	2.44	0.43
19:B:1205:CLA:H193	19:B:1224:CLA:H192	1.99	0.43
19:B:1208:CLA:HBD	19:B:1208:CLA:C1	2.48	0.43
21:B:6010:BCR:C8	21:B:6010:BCR:H311	2.47	0.43
4:D:129:LEU:HD13	12:L:65:PHE:CD1	2.53	0.43
4:D:133:ARG:N	4:D:136:GLN:HE22	2.09	0.43
11:K:57:MET:O	11:K:58:VAL:C	2.57	0.43
11:K:84:LEU:HD11	11:K:85:LYS:HE3	2.01	0.43
11:K:113:GLY:O	11:K:114:HIS:O	2.36	0.43
12:L:104:LEU:HD23	19:L:1501:CLA:HMA1	2.00	0.43
13:N:90:GLU:HA	13:N:91:TYR:CD2	2.53	0.43
13:N:146:LEU:HD22	17:3:142:ILE:O	2.11	0.43
16:2:226:ARG:HD3	16:2:226:ARG:HA	1.60	0.43
22:2:7006:LMU:H3'	22:2:7006:LMU:C5B	2.48	0.43
1:A:86:LEU:HD13	1:A:178:MET:HE1	1.91	0.43
1:A:207:LEU:CG	19:A:1119:CLA:HBB2	2.49	0.43
1:A:244:LEU:HB3	1:A:247:GLU:HG2	1.92	0.43
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.39	0.43
1:A:270:PHE:HE1	19:A:1141:CLA:H2	1.78	0.43
1:A:458:PHE:CD1	1:A:458:PHE:C	2.97	0.43
19:A:1124:CLA:H61	19:A:1125:CLA:CED	2.49	0.43
19:A:1136:CLA:H18	19:A:1136:CLA:H151	1.84	0.43
22:A:7016:LMU:H112	22:A:7016:LMU:H71	1.97	0.43
2:B:293:THR:O	2:B:295:PHE:CE2	2.72	0.43
2:B:420:SER:HA	2:B:423:SER:OG	2.19	0.43
2:B:439:HIS:C	2:B:439:HIS:CD2	2.96	0.43
2:B:532:LEU:HA	2:B:535:VAL:HG12	2.00	0.43
19:B:1201:CLA:CHD	21:I:6021:BCR:H401	2.48	0.43
19:B:1201:CLA:HBA2	19:B:1201:CLA:H3A	1.57	0.43
19:B:1215:CLA:CGA	19:B:1215:CLA:C4A	2.96	0.43
19:B:1235:CLA:H41	21:F:6016:BCR:H323	2.00	0.43
6:F:136:TYR:HD1	6:F:138:LEU:CD1	2.30	0.43
11:K:124:LEU:O	11:K:126:ASN:HB3	2.17	0.43
12:L:95:PRO:O	12:L:96:LEU:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:110:LEU:HA	12:L:113:PRO:HG3	2.00	0.43
12:L:170:LYS:HE2	12:L:170:LYS:HB2	1.65	0.43
22:L:7029:LMU:C4'	22:L:7029:LMU:C5B	2.82	0.43
13:N:138:ALA:O	13:N:139:LYS:HD2	2.17	0.43
15:1:116:ALA:HA	15:1:117:LEU:HD22	1.99	0.43
15:1:176:ASP:HB3	15:1:180:LEU:HD11	1.74	0.43
16:2:182:ILE:CG2	16:2:187:LYS:HE2	2.48	0.43
19:2:2014:CLA:H91	19:2:2014:CLA:H151	1.96	0.43
18:4:111:LEU:O	18:4:112:PRO:C	2.61	0.43
18:4:198:LEU:HG	18:4:199:GLU:CA	2.48	0.43
18:4:220:GLN:HG3	19:4:1306:CLA:CAC	2.42	0.43
18:4:228:PRO:O	18:4:228:PRO:CG	2.66	0.43
1:A:22:VAL:H	1:A:25:ASP:HB2	1.83	0.43
1:A:27:ILE:O	1:A:28:LYS:CB	2.65	0.43
1:A:295:TRP:C	1:A:297:THR:N	2.66	0.43
1:A:400:MET:HG3	1:A:609:ILE:HG23	2.00	0.43
1:A:401:TRP:CZ3	1:A:609:ILE:HB	2.52	0.43
1:A:478:SER:OG	1:A:481:ALA:N	2.45	0.43
1:A:599:PHE:CE2	1:A:735:VAL:CG2	3.00	0.43
1:A:684:PHE:CD2	1:A:685:VAL:N	2.78	0.43
1:A:707:ILE:HG12	1:A:707:ILE:H	1.49	0.43
19:A:1125:CLA:H101	19:A:1125:CLA:C14	2.44	0.43
19:A:1136:CLA:O1D	19:A:1136:CLA:H2A	2.18	0.43
22:A:7010:LMU:H3'	22:A:7010:LMU:H2O1	1.81	0.43
2:B:90:ALA:C	2:B:113:VAL:HG13	2.43	0.43
2:B:285:LEU:HD11	19:B:1217:CLA:HBC2	2.00	0.43
2:B:304:ILE:O	2:B:308:HIS:CG	2.72	0.43
2:B:469:LYS:CG	2:B:470:THR:CB	2.97	0.43
2:B:493:TRP:CZ2	19:B:1214:CLA:C12	3.01	0.43
2:B:598:HIS:O	2:B:599:ILE:C	2.61	0.43
2:B:620:LEU:O	2:B:625:TRP:HB3	2.18	0.43
19:B:1216:CLA:C2	19:B:1221:CLA:H92	2.49	0.43
20:B:5002:PQN:H2M1	20:B:5002:PQN:H111	1.87	0.43
4:D:100:TYR:CE1	4:D:134:LYS:CD	2.88	0.43
4:D:100:TYR:CE1	4:D:134:LYS:HE2	2.50	0.43
6:F:90:GLN:CG	6:F:143:ASP:HA	2.48	0.43
7:G:76:ARG:HH22	7:G:117:ASN:C	2.21	0.43
19:H:1241:CLA:H92	19:H:1241:CLA:H62	1.88	0.43
22:K:7042:LMU:H32	22:K:7042:LMU:C5'	2.49	0.43
15:1:64:PHE:C	15:1:69:LEU:HD13	2.32	0.43
15:1:155:GLU:N	15:1:155:GLU:CD	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:243:GLY:N	16:2:244:THR:HG23	2.33	0.43
22:2:7027:LMU:O2'	22:2:7027:LMU:C1	2.66	0.43
18:4:134:TYR:C	18:4:136:ALA:N	2.74	0.43
18:4:190:ASN:HA	18:4:191:PRO:HD3	1.74	0.43
1:A:207:LEU:CB	19:A:1119:CLA:CBB	2.83	0.43
1:A:233:LEU:C	1:A:235:ALA:N	2.76	0.43
1:A:382:TYR:CD2	19:A:1127:CLA:HED3	2.53	0.43
1:A:457:SER:OG	1:A:544:ILE:HA	2.19	0.43
1:A:479:ASP:CA	1:A:536:THR:CG2	2.90	0.43
1:A:678:PHE:C	1:A:680:LEU:N	2.77	0.43
1:A:701:GLN:O	1:A:702:GLU:C	2.61	0.43
19:A:1102:CLA:HBB2	19:A:1104:CLA:CHA	2.49	0.43
19:A:1131:CLA:H93	19:A:1131:CLA:H61	1.86	0.43
19:A:9023:CLA:H202	19:A:9023:CLA:H162	1.85	0.43
2:B:303:TYR:CA	2:B:306:GLU:CB	2.85	0.43
2:B:471:THR:HG23	2:B:502:ASN:HB2	1.99	0.43
2:B:514:PRO:HG2	6:F:147:HIS:CE1	2.54	0.43
2:B:551:LYS:C	2:B:552:ASP:OD1	2.56	0.43
19:B:1222:CLA:C2B	21:B:6010:BCR:C35	2.97	0.43
3:C:1:MET:N	3:C:4:SER:N	2.57	0.43
3:C:69:LEU:O	3:C:70:TRP:C	2.60	0.43
4:D:87:THR:HG23	12:L:69:LEU:CG	2.45	0.43
4:D:95:GLN:O	4:D:159:PRO:HG3	2.17	0.43
21:F:6016:BCR:C31	21:F:6016:BCR:HC8	2.40	0.43
7:G:69:GLY:O	7:G:72:LEU:CD1	2.67	0.43
8:H:76:TYR:HH	12:L:90:ARG:HD2	1.48	0.43
8:H:114:ALA:O	8:H:115:THR:HG22	2.15	0.43
8:H:119:ASP:HB3	8:H:121:LEU:CG	2.47	0.43
10:J:41:PHE:CD1	10:J:41:PHE:N	2.87	0.43
22:K:7042:LMU:H81	22:K:7042:LMU:H52	1.52	0.43
13:N:156:GLY:C	13:N:157:LYS:CD	2.90	0.43
15:1:98:LEU:HA	15:1:98:LEU:HD22	1.45	0.43
17:3:149:ASN:HA	17:3:150:TYR:HA	1.40	0.43
17:3:211:LEU:HD12	17:3:211:LEU:H	1.84	0.43
18:4:100:ARG:O	18:4:104:LEU:HD13	2.19	0.43
18:4:111:LEU:CD1	18:4:112:PRO:HD3	2.48	0.43
18:4:120:ILE:HD11	18:4:226:LYS:CA	2.48	0.43
1:A:372:VAL:O	1:A:374:GLN:N	2.51	0.43
19:A:9023:CLA:H41	19:A:9023:CLA:CMB	2.45	0.43
2:B:172:GLU:HG3	2:B:301:ILE:HG12	2.00	0.43
2:B:212:PHE:HZ	19:B:1211:CLA:HAC1	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:ALA:CB	2:B:507:SER:O	2.66	0.43
2:B:568:CYS:HB3	2:B:569:ASP:H	1.65	0.43
19:B:1201:CLA:HBC3	19:B:1226:CLA:H41	2.00	0.43
19:B:1220:CLA:O1D	19:B:1220:CLA:OBD	2.35	0.43
19:B:1222:CLA:H11	19:B:1236:CLA:HBD	2.00	0.43
19:B:1225:CLA:H141	19:B:1225:CLA:H162	1.91	0.43
3:C:47:ASP:OD1	4:D:134:LYS:NZ	2.51	0.43
6:F:167:PHE:HA	21:F:6014:BCR:C39	2.47	0.43
7:G:89:LYS:CE	7:G:89:LYS:CA	2.47	0.43
22:H:7043:LMU:H71	22:H:7043:LMU:H112	2.00	0.43
15:1:71:GLU:OE1	15:1:76:LEU:HD11	2.17	0.43
15:1:97:ILE:HD13	15:1:98:LEU:HB2	1.78	0.43
15:1:117:LEU:HD13	15:1:117:LEU:H	1.78	0.43
15:1:155:GLU:HB2	15:1:160:LYS:HD2	1.99	0.43
15:1:161:LYS:HD2	15:1:161:LYS:C	2.43	0.43
15:1:177:PRO:CD	15:1:180:LEU:N	2.82	0.43
19:1:1008:CLA:HBC3	19:1:1008:CLA:CMC	2.48	0.43
16:2:112:TRP:O	16:2:113:ALA:C	2.61	0.43
17:3:210:PRO:CD	17:3:211:LEU:HD12	2.48	0.43
17:3:238:ILE:HD12	19:3:3003:CLA:HMC1	1.96	0.43
19:3:3016:CLA:CMA	19:3:3016:CLA:O1A	2.67	0.43
1:A:23:ASP:OD2	1:A:33:GLN:HG2	2.16	0.43
1:A:40:PHE:O	1:A:44:ILE:HA	2.18	0.43
1:A:63:ASP:OD2	1:A:64:PHE:N	2.52	0.43
1:A:183:TRP:CZ3	1:A:188:LYS:HB3	2.54	0.43
1:A:295:TRP:HB3	1:A:297:THR:CG2	2.48	0.43
1:A:338:PHE:CZ	19:A:1151:CLA:HBB1	2.38	0.43
1:A:561:LEU:HA	1:A:561:LEU:HD23	1.77	0.43
19:A:9011:CLA:H111	19:A:9011:CLA:H71	1.87	0.43
2:B:188:LEU:HG	2:B:189:ALA:N	2.34	0.43
2:B:689:ASN:OD1	2:B:689:ASN:N	2.52	0.43
19:B:1209:CLA:C3C	19:B:1210:CLA:HBB2	2.40	0.43
20:B:5002:PQN:H192	21:B:6017:BCR:C8	2.48	0.43
22:B:7038:LMU:H1B	22:B:7038:LMU:C6'	2.48	0.43
4:D:140:LEU:HD13	4:D:144:LEU:CA	2.49	0.43
4:D:167:HIS:HD2	4:D:172:VAL:CG2	2.03	0.43
6:F:117:LEU:CA	6:F:119:ILE:HG12	2.46	0.43
6:F:121:ALA:O	6:F:123:MET:N	2.50	0.43
7:G:75:GLY:N	7:G:77:PHE:H	2.17	0.43
12:L:135:GLY:O	12:L:138:VAL:HG22	2.19	0.43
12:L:137:LEU:HD23	12:L:138:VAL:N	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:171:LYS:O	12:L:173:PRO:CD	2.38	0.43
13:N:139:LYS:HA	13:N:139:LYS:HD2	1.14	0.43
13:N:145:PHE:N	13:N:145:PHE:CD1	2.80	0.43
15:1:58:ALA:HB1	19:1:1015:CLA:C2B	2.48	0.43
15:1:77:GLU:CG	15:1:80:LYS:CE	2.96	0.43
15:1:114:TRP:HH2	15:1:121:GLN:HG3	1.75	0.43
15:1:182:GLU:C	15:1:183:LEU:HG	2.44	0.43
16:2:119:GLY:O	16:2:123:PRO:HD3	2.14	0.43
17:3:238:ILE:HD13	17:3:238:ILE:N	2.34	0.43
18:4:193:ASN:O	18:4:201:LYS:NZ	2.52	0.43
19:4:1304:CLA:H3A	19:4:1304:CLA:HBA2	1.19	0.43
22:4:7053:LMU:C11	22:4:7053:LMU:C7	2.97	0.43
1:A:374:GLN:C	1:A:376:MET:H	2.25	0.43
1:A:446:LEU:HD13	19:A:1137:CLA:HMB1	1.99	0.43
1:A:740:LEU:CD2	19:A:1140:CLA:HMA3	2.47	0.43
19:A:1120:CLA:HBA2	19:A:1120:CLA:H3A	1.84	0.43
19:A:1138:CLA:HBB2	19:B:1229:CLA:H43	2.00	0.43
2:B:29:HIS:CB	19:B:1226:CLA:HBA1	2.49	0.43
2:B:50:HIS:CA	2:B:53:GLN:HB2	2.49	0.43
2:B:172:GLU:O	2:B:173:SER:C	2.61	0.43
2:B:224:PRO:CB	2:B:227:THR:CG2	2.96	0.43
2:B:323:TYR:HD2	7:G:104:ASP:H	1.65	0.43
2:B:431:PHE:CE2	19:B:1229:CLA:CED	3.02	0.43
2:B:517:PHE:O	2:B:517:PHE:CG	2.64	0.43
2:B:557:PHE:N	2:B:558:PRO:HD3	2.30	0.43
2:B:596:TRP:NE1	2:B:623:TYR:HB2	2.34	0.43
4:D:84:GLY:C	12:L:64:PRO:HB3	2.32	0.43
4:D:103:THR:HG22	4:D:128:LEU:CB	2.48	0.43
6:F:96:LYS:O	6:F:97:GLN:O	2.36	0.43
8:H:94:ARG:HD2	12:L:183:ALA:HB1	2.00	0.43
9:I:24:LEU:HD23	21:L:6019:BCR:H23C	2.01	0.43
12:L:102:VAL:HG22	19:L:1502:CLA:HED2	2.01	0.43
12:L:111:VAL:O	12:L:115:VAL:N	2.52	0.43
12:L:174:ASP:O	12:L:175:GLN:O	2.36	0.43
15:1:149:GLU:CD	19:1:1012:CLA:C1B	2.87	0.43
16:2:148:ASP:O	16:2:151:THR:N	2.52	0.43
18:4:173:LYS:NZ	18:4:201:LYS:HG2	2.14	0.43
18:4:198:LEU:CG	18:4:199:GLU:N	2.59	0.43
18:4:245:VAL:HG22	18:4:246:GLN:H	1.82	0.43
1:A:210:LEU:HD12	19:A:1111:CLA:CMB	2.48	0.43
1:A:282:THR:C	1:A:283:PHE:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:O	1:A:372:VAL:HB	2.19	0.43
1:A:408:VAL:HG11	1:A:602:LEU:HD23	2.00	0.43
1:A:711:HIS:CB	1:A:717:ALA:HB2	2.43	0.43
19:A:1237:CLA:CAB	19:B:1238:CLA:HMD2	2.49	0.43
2:B:89:HIS:CA	2:B:113:VAL:HG11	2.22	0.43
2:B:242:HIS:O	2:B:243:LEU:HB2	2.19	0.43
2:B:290:MET:O	2:B:299:HIS:HB2	2.19	0.43
2:B:432:HIS:CE1	19:B:1229:CLA:NB	2.72	0.43
19:B:1203:CLA:H3A	19:B:1203:CLA:HBA1	1.74	0.43
19:B:1214:CLA:HBA2	19:B:1214:CLA:H3A	1.33	0.43
19:B:1220:CLA:C2A	19:B:1220:CLA:CGD	2.96	0.43
19:B:1231:CLA:CMD	19:B:1232:CLA:C1C	2.97	0.43
4:D:122:MET:O	4:D:123:ARG:HB3	2.19	0.43
5:E:86:GLY:HA3	5:E:109:LYS:NZ	2.33	0.43
6:F:205:SER:O	6:F:207:LEU:CD1	2.67	0.43
9:I:8:PHE:CZ	21:I:6021:BCR:C7	3.02	0.43
11:K:60:SER:O	11:K:63:LEU:CD2	2.67	0.43
11:K:127:ILE:HG23	11:K:130:LEU:CD1	2.46	0.43
12:L:207:LEU:HD23	12:L:208:ASP:N	2.33	0.43
13:N:99:LYS:CB	13:N:102:ASN:CG	2.92	0.43
13:N:133:GLY:CA	13:N:134:CYS:C	2.86	0.43
16:2:148:ASP:CA	16:2:152:LEU:HB3	2.41	0.43
16:2:186:ASN:O	16:2:187:LYS:CB	2.65	0.43
22:2:7046:LMU:H41	22:2:7046:LMU:H6D	2.01	0.43
17:3:197:SER:CB	17:3:206:PRO:CG	2.97	0.43
19:3:3016:CLA:H41	19:3:3016:CLA:H61	1.58	0.43
21:3:6022:BCR:H14C	21:3:6022:BCR:H11C	1.56	0.43
18:4:85:PRO:HB3	18:4:188:ILE:HA	2.00	0.43
19:4:1306:CLA:H92	19:4:1306:CLA:H61	1.87	0.43
1:A:284:ARG:H	1:A:298:ASP:CG	2.26	0.43
1:A:615:HIS:CE1	19:A:1135:CLA:CBC	3.00	0.43
1:A:732:ALA:HB1	19:A:1140:CLA:HED2	2.01	0.43
19:A:1134:CLA:HBD	19:A:1134:CLA:HAA1	2.01	0.43
19:A:1134:CLA:HMA3	19:A:1141:CLA:HBB2	1.98	0.43
19:A:9013:CLA:HHD	19:A:9013:CLA:HAC1	1.88	0.43
2:B:98:GLN:CA	2:B:98:GLN:HE21	2.30	0.43
2:B:119:GLY:O	2:B:122:GLN:OE1	2.37	0.43
2:B:294:ASN:CG	7:G:93:GLU:HB2	2.44	0.43
2:B:444:LEU:HD23	2:B:452:GLN:HE22	1.80	0.43
2:B:456:GLU:HA	2:B:514:PRO:HG3	2.01	0.43
2:B:496:GLY:O	2:B:499:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:TYR:C	5:E:82:TYR:CD2	2.96	0.43
22:H:7011:LMU:C7	22:H:7011:LMU:C11	2.94	0.43
19:K:1143:CLA:O2A	19:K:1143:CLA:C4	2.67	0.43
22:R:7022:LMU:O2'	22:R:7022:LMU:H1B	2.19	0.43
15:1:171:LEU:N	15:1:171:LEU:CD2	2.81	0.43
16:2:156:GLU:OE2	19:2:2013:CLA:C1D	2.67	0.43
18:4:110:LEU:HA	18:4:113:GLU:OE2	2.19	0.43
22:4:7053:LMU:C1B	22:4:7053:LMU:C6'	2.89	0.43
1:A:255:LEU:O	1:A:259:TYR:O	2.37	0.42
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.83	0.42
1:A:538:ASP:O	1:A:542:HIS:HD2	2.02	0.42
1:A:682:ALA:HA	1:A:685:VAL:HB	2.01	0.42
1:A:744:ALA:HA	1:A:747:TRP:HB3	2.00	0.42
2:B:229:GLN:O	7:G:63:VAL:CG1	2.67	0.42
2:B:390:GLY:HA3	21:B:6010:BCR:HC22	2.01	0.42
2:B:395:ILE:HG21	2:B:554:GLY:HA3	2.00	0.42
2:B:498:LEU:O	2:B:499:ASN:OD1	2.36	0.42
2:B:551:LYS:NZ	4:D:194:ASN:O	2.34	0.42
2:B:721:TYR:HA	2:B:724:PHE:HB3	2.00	0.42
20:B:5002:PQN:H192	21:B:6017:BCR:C10	2.49	0.42
3:C:74:THR:CG2	3:C:75:ARG:N	2.81	0.42
4:D:124:GLU:OE1	4:D:125:GLY:N	2.52	0.42
7:G:76:ARG:NH1	7:G:120:VAL:CB	2.78	0.42
7:G:96:GLY:O	7:G:97:LEU:HD23	2.18	0.42
8:H:70:SER:O	8:H:73:PRO:HD2	2.19	0.42
8:H:110:ALA:HA	8:H:113:SER:HB2	2.01	0.42
10:J:5:LYS:HE3	16:2:178:ASN:ND2	2.34	0.42
13:N:132:THR:CG2	13:N:139:LYS:CE	2.97	0.42
13:N:138:ALA:C	13:N:139:LYS:HD2	2.44	0.42
15:1:83:GLU:O	15:1:83:GLU:CD	2.62	0.42
21:1:6023:BCR:C33	21:1:6023:BCR:H322	2.31	0.42
22:2:7027:LMU:H62	22:2:7027:LMU:H31	1.51	0.42
1:A:77:LYS:HG3	19:A:1109:CLA:HMD3	2.01	0.42
1:A:96:MET:O	1:A:99:HIS:HB2	2.18	0.42
1:A:130:GLU:C	1:A:132:LEU:H	2.27	0.42
1:A:154:ARG:HA	1:A:154:ARG:HD2	1.48	0.42
1:A:396:PHE:CE2	1:A:616:PHE:CB	2.99	0.42
19:A:1237:CLA:H61	19:A:1237:CLA:C11	2.49	0.42
19:A:9022:CLA:CAD	19:B:9010:CLA:HMB1	2.49	0.42
2:B:75:GLU:HB3	2:B:132:ASN:ND2	2.17	0.42
2:B:161:TRP:CD1	2:B:161:TRP:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ARG:C	2:B:176:ASN:H	2.27	0.42
2:B:177:HIS:CE1	19:B:1209:CLA:NC	2.86	0.42
2:B:377:TYR:O	2:B:378:ILE:CB	2.66	0.42
2:B:414:HIS:O	2:B:414:HIS:CD2	2.72	0.42
2:B:429:LEU:HD11	19:B:1235:CLA:CMB	2.39	0.42
2:B:476:ILE:HG21	2:B:479:SER:OG	2.12	0.42
2:B:575:ASP:O	2:B:579:ALA:N	2.49	0.42
2:B:710:LEU:H	2:B:713:PHE:H	1.66	0.42
24:B:7101:LMG:HO3	24:B:7101:LMG:HO4	1.59	0.42
4:D:80:SER:HB2	4:D:127:ASN:N	2.34	0.42
5:E:88:GLY:HA3	5:E:107:PHE:HB2	2.01	0.42
6:F:207:LEU:CD1	6:F:207:LEU:H	2.32	0.42
8:H:64:GLN:HB2	8:H:67:SER:N	2.23	0.42
12:L:209:LEU:HG	12:L:210:PRO:CD	2.49	0.42
14:R:8:UNK:CB	19:R:1144:CLA:O2D	2.67	0.42
16:2:150:THR:CA	16:2:152:LEU:CD1	2.97	0.42
16:2:184:PRO:HG2	16:2:185:ASN:C	2.43	0.42
16:2:189:THR:OG1	16:2:193:VAL:O	2.36	0.42
19:2:2002:CLA:HBA2	19:2:2002:CLA:H3A	1.76	0.42
19:2:2004:CLA:O1D	19:3:2009:CLA:HBB2	2.19	0.42
17:3:111:LEU:O	17:3:114:VAL:C	2.62	0.42
17:3:133:ALA:HB3	17:3:134:LEU:CG	2.49	0.42
17:3:210:PRO:HG2	17:3:211:LEU:N	2.33	0.42
1:A:159:THR:O	1:A:160:SER:OG	2.34	0.42
1:A:249:ILE:HG23	17:3:137:PHE:CZ	2.54	0.42
1:A:337:PRO:HB2	19:A:1151:CLA:HBB2	2.00	0.42
1:A:427:ARG:HG2	1:A:428:TYR:HA	2.02	0.42
1:A:452:PHE:CD1	19:A:1136:CLA:HBB2	2.54	0.42
1:A:476:MET:O	1:A:477:PHE:HB2	2.19	0.42
1:A:551:VAL:HG21	1:A:604:TRP:CZ2	2.53	0.42
1:A:569:ILE:HG22	1:A:572:LYS:N	2.34	0.42
1:A:628:ILE:HD11	1:A:629:ASN:O	2.20	0.42
1:A:690:LEU:HB2	19:A:9013:CLA:HMC2	2.02	0.42
19:A:1119:CLA:C1C	19:A:1125:CLA:H171	2.49	0.42
19:A:1126:CLA:C7	21:A:6011:BCR:H372	2.49	0.42
19:A:1135:CLA:H11	19:A:1136:CLA:O1A	2.19	0.42
19:A:1139:CLA:O1A	19:A:1139:CLA:C4	2.67	0.42
19:A:1141:CLA:O1A	19:A:1141:CLA:H2A	2.08	0.42
2:B:120:VAL:CG1	2:B:123:TRP:CD1	3.01	0.42
2:B:267:SER:OG	2:B:268:LEU:N	2.49	0.42
2:B:289:LEU:HA	19:B:1217:CLA:O1D	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:THR:HA	2:B:729:THR:HG21	2.00	0.42
2:B:449:PRO:O	2:B:452:GLN:CB	2.67	0.42
2:B:463:ILE:CG2	2:B:467:HIS:HE1	2.32	0.42
2:B:490:ARG:NH1	2:B:490:ARG:CG	2.47	0.42
2:B:633:ASN:HB2	2:B:636:THR:H	1.84	0.42
2:B:684:ARG:HD3	2:B:684:ARG:HA	1.76	0.42
19:B:1238:CLA:H172	19:B:1239:CLA:H13	2.02	0.42
4:D:101:VAL:HG12	4:D:130:LYS:HB3	1.98	0.42
7:G:77:PHE:CE2	7:G:79:PHE:CD2	3.07	0.42
7:G:150:ASP:N	7:G:151:PRO:HD3	2.33	0.42
9:I:10:PRO:O	9:I:11:LEU:C	2.62	0.42
19:K:1142:CLA:OBD	19:K:1143:CLA:C1B	2.68	0.42
12:L:111:VAL:H	12:L:113:PRO:HD2	1.84	0.42
15:1:116:ALA:C	15:1:117:LEU:CD2	2.84	0.42
15:1:116:ALA:CA	15:1:117:LEU:HD22	2.49	0.42
15:1:201:PHE:C	15:1:204:GLN:HB2	2.43	0.42
16:2:204:LEU:CD1	16:2:210:SER:O	2.62	0.42
16:2:224:ASN:HD21	16:2:227:LEU:HD23	1.84	0.42
18:4:122:ASN:OD1	18:4:124:PRO:HA	2.19	0.42
18:4:144:ILE:HA	18:4:147:ILE:CD1	2.49	0.42
18:4:231:ASN:O	18:4:235:HIS:HB3	2.18	0.42
22:4:7034:LMU:C10	22:4:7052:LMU:H2'	2.45	0.42
1:A:350:LEU:O	1:A:350:LEU:CD2	2.67	0.42
1:A:427:ARG:HE	1:A:428:TYR:HD1	1.66	0.42
1:A:645:SER:O	1:A:651:GLY:HA3	2.19	0.42
1:A:733:VAL:HG13	1:A:737:HIS:CE1	2.54	0.42
19:A:1131:CLA:O1A	19:A:1237:CLA:C1	2.65	0.42
19:A:1132:CLA:H41	19:A:1132:CLA:H61	1.60	0.42
2:B:50:HIS:HA	2:B:53:GLN:H	1.85	0.42
2:B:169:LYS:O	2:B:170:ASN:C	2.58	0.42
2:B:230:TRP:H	7:G:63:VAL:CG2	2.23	0.42
2:B:299:HIS:CE1	19:B:1219:CLA:OBD	2.73	0.42
2:B:302:LYS:HZ2	7:G:103:GLY:HA3	1.84	0.42
2:B:316:GLY:O	2:B:317:ARG:HD2	2.19	0.42
2:B:424:TRP:CH2	19:B:1228:CLA:HAC1	2.55	0.42
2:B:486:LEU:O	2:B:487:ASN:HB3	2.20	0.42
2:B:674:LEU:O	2:B:678:LEU:HB2	2.19	0.42
19:B:1222:CLA:CBB	19:B:1236:CLA:HMB2	2.50	0.42
4:D:123:ARG:HH21	22:D:7050:LMU:C5B	2.13	0.42
6:F:88:SER:O	6:F:91:PHE:HB3	2.19	0.42
6:F:112:ASP:O	6:F:113:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:1207:CLA:O2A	19:H:1207:CLA:CMA	2.68	0.42
21:I:6018:BCR:H272	21:I:6021:BCR:H352	2.01	0.42
10:J:36:ALA:O	10:J:37:LEU:HB2	2.18	0.42
19:J:1308:CLA:CBD	19:J:1308:CLA:CGA	2.97	0.42
12:L:111:VAL:C	12:L:115:VAL:HG22	2.44	0.42
19:1:1001:CLA:HBA1	19:1:1001:CLA:HMA1	2.01	0.42
16:2:192:ASP:CG	16:2:194:GLY:C	2.87	0.42
17:3:132:THR:CG2	17:3:133:ALA:N	2.82	0.42
19:3:3016:CLA:O1A	19:3:3016:CLA:C3A	2.68	0.42
22:3:7005:LMU:O2B	22:3:7005:LMU:C5'	2.67	0.42
18:4:110:LEU:O	18:4:113:GLU:CD	2.62	0.42
1:A:94:SER:OG	1:A:95:GLY:N	2.53	0.42
1:A:249:ILE:CG2	17:3:137:PHE:CZ	3.03	0.42
1:A:334:HIS:CB	19:A:1120:CLA:HMA1	2.43	0.42
1:A:442:ILE:HG23	19:A:1129:CLA:CMC	2.48	0.42
1:A:613:ILE:HG23	1:A:750:PHE:HE2	1.83	0.42
1:A:620:MET:C	1:A:623:ASP:O	2.62	0.42
19:A:1131:CLA:C15	21:L:6019:BCR:C36	2.97	0.42
2:B:91:ILE:CG2	19:B:1206:CLA:HMD1	2.45	0.42
2:B:180:SER:O	2:B:181:GLY:C	2.62	0.42
2:B:252:THR:HG22	2:B:252:THR:O	2.19	0.42
2:B:256:THR:N	2:B:271:THR:OG1	2.52	0.42
2:B:292:ARG:NE	2:B:292:ARG:HA	2.34	0.42
2:B:408:LEU:O	2:B:411:MET:HB2	2.20	0.42
2:B:596:TRP:CH2	2:B:612:SER:HB3	2.55	0.42
2:B:615:TYR:O	2:B:619:TRP:HD1	2.03	0.42
4:D:77:ASN:HB3	4:D:79:PRO:HD3	2.01	0.42
4:D:139:ALA:O	4:D:142:THR:CG2	2.59	0.42
6:F:138:LEU:HD22	6:F:146:PRO:HB3	2.01	0.42
6:F:200:VAL:HG23	6:F:203:ALA:C	2.43	0.42
12:L:78:LEU:HD12	12:L:79:ILE:H	1.79	0.42
12:L:95:PRO:O	12:L:98:ARG:HG3	2.19	0.42
13:N:134:CYS:O	13:N:136:ASP:O	2.37	0.42
13:N:155:GLU:CB	13:N:157:LYS:HA	2.50	0.42
16:2:100:ARG:C	16:2:102:ASN:N	2.76	0.42
17:3:253:TYR:O	17:3:254:GLN:C	2.62	0.42
18:4:96:LEU:CD1	18:4:100:ARG:NE	2.83	0.42
18:4:217:PHE:CE1	18:4:221:HIS:CE1	3.08	0.42
18:4:233:LEU:H	18:4:233:LEU:HG	1.79	0.42
1:A:68:THR:HG22	1:A:70:ASP:O	2.20	0.42
1:A:149:PHE:HB3	1:A:153:TRP:CZ3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:C	1:A:228:PRO:HD2	2.44	0.42
1:A:652:TRP:O	1:A:656:PHE:HB3	2.19	0.42
1:A:741:GLY:O	1:A:743:ILE:N	2.53	0.42
19:A:1101:CLA:C4	19:A:1140:CLA:H8	2.50	0.42
19:A:1124:CLA:HBB2	19:A:1137:CLA:CMA	2.49	0.42
2:B:319:HIS:CE1	2:B:322:LEU:HD11	2.50	0.42
2:B:346:SER:O	2:B:350:GLN:N	2.50	0.42
2:B:450:GLU:O	2:B:451:LYS:HB2	2.19	0.42
2:B:455:ILE:C	2:B:514:PRO:HG3	2.44	0.42
2:B:488:ALA:CB	19:B:1233:CLA:C1C	2.96	0.42
2:B:596:TRP:C	2:B:597:LYS:O	2.62	0.42
19:B:1202:CLA:CAB	19:B:1203:CLA:HBA2	2.49	0.42
3:C:38:GLN:HE21	3:C:38:GLN:HB3	1.65	0.42
4:D:74:LEU:O	4:D:75:ASP:C	2.62	0.42
5:E:91:VAL:CG1	5:E:92:ALA:H	2.26	0.42
6:F:97:GLN:HE21	6:F:97:GLN:HB3	1.52	0.42
12:L:104:LEU:HA	12:L:192:GLY:O	2.19	0.42
12:L:107:GLY:C	12:L:109:LEU:H	2.27	0.42
22:L:7029:LMU:O2'	22:L:7029:LMU:H11	2.20	0.42
14:R:38:UNK:C	14:R:42:UNK:CA	2.97	0.42
15:1:177:PRO:O	15:1:178:LYS:CB	2.68	0.42
15:1:177:PRO:C	15:1:179:LYS:N	2.78	0.42
16:2:107:LEU:CD1	16:2:108:VAL:HG23	2.49	0.42
16:2:195:TYR:CD2	16:2:198:GLY:CA	2.93	0.42
17:3:174:GLN:HE21	17:3:174:GLN:HB2	1.47	0.42
18:4:89:ARG:HD3	18:4:89:ARG:N	2.33	0.42
18:4:120:ILE:CG2	18:4:121:ILE:N	2.65	0.42
18:4:189:PHE:N	18:4:189:PHE:CD2	2.88	0.42
1:A:119:SER:HA	1:A:145:ILE:CD1	2.50	0.42
1:A:299:ILE:HA	1:A:299:ILE:HD12	1.78	0.42
19:A:1103:CLA:HBA1	19:A:1103:CLA:H3A	1.71	0.42
19:A:1136:CLA:H203	19:L:1130:CLA:HBB2	2.02	0.42
2:B:160:LYS:HB2	2:B:160:LYS:HE2	1.43	0.42
2:B:225:LEU:CA	2:B:227:THR:O	2.67	0.42
2:B:262:HIS:HB2	2:B:265:THR:O	2.20	0.42
2:B:556:SER:CA	2:B:558:PRO:HD2	2.50	0.42
2:B:681:ALA:O	2:B:682:HIS:C	2.62	0.42
6:F:211:PHE:C	6:F:213:TRP:H	2.27	0.42
7:G:83:GLN:O	7:G:84:ARG:CB	2.67	0.42
11:K:102:THR:O	11:K:103:LEU:C	2.60	0.42
11:K:115:ILE:HG12	11:K:122:LEU:HD12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:82:TYR:HE1	19:L:1130:CLA:H93	1.80	0.42
12:L:94:SER:C	12:L:96:LEU:HD23	2.43	0.42
12:L:150:ILE:HD12	12:L:150:ILE:O	2.18	0.42
15:1:168:PHE:O	15:1:168:PHE:CD1	2.72	0.42
16:2:114:MET:HG2	16:2:227:LEU:CA	2.36	0.42
16:2:167:ARG:HB3	16:2:169:ALA:H	1.84	0.42
17:3:150:TYR:C	17:3:152:ALA:CA	2.88	0.42
17:3:212:GLY:O	17:3:213:PHE:C	2.62	0.42
18:4:121:ILE:O	18:4:122:ASN:HB3	2.20	0.42
1:A:21:LEU:CD1	1:A:21:LEU:C	2.86	0.42
1:A:53:TRP:O	1:A:56:ASN:O	2.38	0.42
1:A:93:LEU:O	1:A:97:TYR:CD2	2.70	0.42
1:A:271:THR:O	1:A:271:THR:HG22	2.20	0.42
1:A:335:LYS:HG2	1:A:336:GLY:N	2.35	0.42
1:A:534:LEU:HB2	1:A:538:ASP:HB3	2.02	0.42
1:A:660:GLN:O	1:A:661:ALA:HB2	2.17	0.42
1:A:705:GLU:HB3	2:B:545:LYS:HZ1	1.84	0.42
1:A:733:VAL:CG2	19:A:1140:CLA:C2D	2.87	0.42
2:B:74:PHE:O	2:B:75:GLU:C	2.61	0.42
2:B:126:THR:HG21	2:B:358:TYR:CE1	2.54	0.42
2:B:350:GLN:HG3	2:B:372:TYR:HE1	1.85	0.42
2:B:431:PHE:CE2	19:B:1229:CLA:HED3	2.55	0.42
2:B:445:ALA:N	2:B:447:GLY:H	2.17	0.42
2:B:700:LEU:C	2:B:701:SER:O	2.59	0.42
2:B:715:VAL:O	2:B:719:PHE:N	2.42	0.42
3:C:8:TYR:HB2	3:C:41:SER:OG	2.18	0.42
4:D:130:LYS:O	4:D:130:LYS:HG3	2.19	0.42
5:E:111:ASN:CB	5:E:116:SER:OG	2.54	0.42
6:F:205:SER:CA	6:F:207:LEU:HD12	2.49	0.42
7:G:76:ARG:HH12	7:G:120:VAL:H	1.66	0.42
22:H:7002:LMU:O2'	22:H:7002:LMU:H5'	2.19	0.42
10:J:9:SER:HB2	10:J:10:VAL:H	1.67	0.42
12:L:78:LEU:HD22	19:L:1504:CLA:CED	2.42	0.42
12:L:145:LEU:O	12:L:182:TRP:HZ3	2.02	0.42
12:L:209:LEU:HG	12:L:210:PRO:N	2.33	0.42
13:N:90:GLU:CD	13:N:91:TYR:CG	2.98	0.42
13:N:112:ALA:O	13:N:113:ASN:O	2.37	0.42
13:N:139:LYS:C	13:N:142:LYS:CD	2.93	0.42
15:1:92:LEU:HA	15:1:95:PRO:HD2	1.92	0.42
15:1:148:VAL:O	15:1:148:VAL:CG2	2.65	0.42
15:1:178:LYS:HD2	15:1:178:LYS:O	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:183:LEU:C	15:1:185:VAL:H	2.27	0.42
16:2:111:ARG:O	16:2:112:TRP:C	2.62	0.42
16:2:118:ALA:CB	16:2:121:PHE:CE2	2.96	0.42
16:2:238:GLN:HA	16:2:241:TYR:CE2	2.54	0.42
17:3:107:ARG:HG2	17:3:232:ARG:HB2	2.01	0.42
17:3:213:PHE:HB2	17:3:215:LYS:C	2.45	0.42
18:4:162:ASN:HA	18:4:163:PRO:HD3	1.68	0.42
18:4:171:ILE:N	18:4:173:LYS:H	2.17	0.42
19:4:4006:CLA:HED2	19:4:4006:CLA:H2A	2.01	0.42
1:A:68:THR:CG2	1:A:69:SER:N	2.79	0.42
1:A:210:LEU:HD12	19:A:1111:CLA:HMB3	2.02	0.42
1:A:250:LEU:HD12	17:3:136:TRP:CZ2	2.49	0.42
1:A:389:TYR:CE2	1:A:526:LYS:HD3	2.45	0.42
1:A:457:SER:O	1:A:544:ILE:CD1	2.64	0.42
1:A:488:PHE:HD1	1:A:535:GLY:CA	2.33	0.42
1:A:554:LEU:HD11	2:B:674:LEU:HD21	2.01	0.42
1:A:555:ILE:HD11	19:A:9023:CLA:C3D	2.49	0.42
19:A:1138:CLA:H2A	19:A:1138:CLA:CED	2.35	0.42
22:A:7045:LMU:H21	22:A:7045:LMU:H1'	1.69	0.42
2:B:123:TRP:HB3	2:B:126:THR:HG21	1.99	0.42
2:B:144:PHE:O	2:B:144:PHE:HD2	2.02	0.42
2:B:182:LEU:HG	2:B:183:PHE:N	2.34	0.42
2:B:293:THR:CG2	19:B:1209:CLA:CMA	2.89	0.42
2:B:310:PRO:HG2	2:B:311:PRO:HD2	1.99	0.42
2:B:331:HIS:CE1	2:B:392:ILE:CG2	2.97	0.42
2:B:387:PHE:CB	2:B:534:LEU:HD13	2.50	0.42
2:B:399:ASN:OD1	2:B:402:GLN:HB2	2.20	0.42
2:B:430:GLY:CA	2:B:525:LEU:CD1	2.88	0.42
2:B:459:PHE:CZ	19:B:1235:CLA:HMD1	2.54	0.42
2:B:648:TRP:HZ3	21:B:6017:BCR:H383	1.84	0.42
2:B:655:LEU:HD22	19:B:1239:CLA:CAB	2.50	0.42
2:B:692:ARG:NH2	2:B:694:ARG:HH22	2.10	0.42
2:B:694:ARG:HE	12:L:151:SER:HA	1.85	0.42
19:B:1201:CLA:H2A	19:B:1201:CLA:O1D	2.19	0.42
19:B:1208:CLA:H8	19:B:1208:CLA:H51	1.75	0.42
19:B:1220:CLA:H203	19:B:1220:CLA:H11	2.02	0.42
3:C:1:MET:H2	3:C:3:HIS:C	2.26	0.42
6:F:100:LYS:NZ	6:F:103:GLN:HB2	2.35	0.42
7:G:102:ALA:N	7:G:104:ASP:OD2	2.53	0.42
7:G:125:VAL:O	7:G:129:ALA:CB	2.67	0.42
9:I:20:ALA:O	9:I:24:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:18:TRP:CZ2	10:J:22:LEU:HD22	2.55	0.42
19:J:1308:CLA:O2A	19:J:1308:CLA:C2A	2.53	0.42
11:K:48:PHE:O	11:K:52:PRO:CD	2.57	0.42
11:K:125:LYS:HD2	11:K:128:GLY:HA3	2.01	0.42
11:K:127:ILE:C	11:K:130:LEU:CD2	2.93	0.42
13:N:92:LEU:HD12	13:N:92:LEU:HA	1.68	0.42
13:N:146:LEU:HD12	13:N:146:LEU:HA	1.72	0.42
16:2:133:ASN:ND2	16:2:134:THR:OG1	2.50	0.42
16:2:226:ARG:HD3	16:2:229:MET:HB3	2.01	0.42
16:2:237:PHE:O	16:2:238:GLN:C	2.62	0.42
19:2:2006:CLA:HMA1	19:2:2006:CLA:H61	2.01	0.42
17:3:94:GLU:N	17:3:95:PRO:CD	2.83	0.42
17:3:98:LEU:CD2	19:3:3012:CLA:C2D	2.94	0.42
18:4:142:PHE:CA	18:4:145:GLU:OE1	2.63	0.42
18:4:192:LEU:CD1	18:4:193:ASN:H	2.33	0.42
1:A:92:TRP:O	1:A:93:LEU:CG	2.68	0.42
1:A:105:ASN:CG	1:A:119:SER:H	2.27	0.42
1:A:132:LEU:O	1:A:143:ILE:HD11	2.20	0.42
1:A:159:THR:C	1:A:163:GLN:HE22	2.28	0.42
1:A:288:ASP:HB2	1:A:291:THR:O	2.19	0.42
1:A:378:SER:O	1:A:512:SER:OG	2.29	0.42
1:A:580:PRO:HA	1:A:728:VAL:HG23	2.01	0.42
1:A:584:PRO:HG3	2:B:559:CYS:SG	2.59	0.42
1:A:651:GLY:O	1:A:655:ASP:HB2	2.20	0.42
19:A:1115:CLA:H51	19:A:1115:CLA:H11	1.74	0.42
19:A:1122:CLA:ND	21:A:6007:BCR:C19	2.83	0.42
19:A:1129:CLA:HHB	19:L:1130:CLA:CAD	2.50	0.42
19:A:1139:CLA:H3A	19:A:1139:CLA:HBA1	1.69	0.42
2:B:202:SER:CB	2:B:270:LEU:HD22	2.46	0.42
2:B:273:VAL:O	2:B:277:HIS:CD2	2.65	0.42
2:B:292:ARG:HH12	2:B:295:PHE:H	1.66	0.42
2:B:343:VAL:HG12	19:B:1223:CLA:H2	2.02	0.42
2:B:398:TYR:CD1	2:B:400:PRO:HD3	2.55	0.42
2:B:623:TYR:HH	2:B:721:TYR:HH	1.68	0.42
19:B:1222:CLA:CED	19:B:1223:CLA:HMD1	2.49	0.42
19:B:1229:CLA:H51	21:F:6016:BCR:H403	2.01	0.42
3:C:1:MET:H2	3:C:3:HIS:H	1.66	0.42
5:E:79:LYS:CA	5:E:84:TYR:CD1	2.90	0.42
6:F:117:LEU:CD1	6:F:120:LYS:HB2	2.49	0.42
8:H:98:LEU:HD23	12:L:146:THR:CG2	2.41	0.42
19:H:1207:CLA:H102	19:H:1207:CLA:H152	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:79:ILE:HG22	12:L:80:ALA:N	2.30	0.42
13:N:146:LEU:HD11	13:N:148:ASP:O	2.20	0.42
13:N:156:GLY:C	13:N:157:LYS:HE2	2.41	0.42
15:1:105:TYR:C	15:1:106:GLY:O	2.62	0.42
15:1:173:TYR:O	15:1:174:SER:OG	2.29	0.42
16:2:149:THR:HG1	16:2:150:THR:N	2.18	0.42
16:2:226:ARG:CA	16:2:226:ARG:NH1	2.83	0.42
17:3:136:TRP:N	17:3:139:THR:HG1	2.17	0.42
19:4:1304:CLA:C15	19:4:1304:CLA:H202	2.40	0.42
1:A:64:PHE:CZ	1:A:74:ILE:HG23	2.52	0.41
1:A:75:SER:CB	1:A:354:TRP:CZ2	2.98	0.41
1:A:93:LEU:HA	1:A:96:MET:HG2	2.02	0.41
1:A:153:TRP:O	1:A:154:ARG:C	2.59	0.41
1:A:252:ARG:NE	1:A:252:ARG:CA	2.77	0.41
1:A:363:ALA:N	1:A:410:ALA:CB	2.83	0.41
1:A:448:TRP:HD1	19:A:1131:CLA:CED	2.32	0.41
1:A:485:GLN:OE1	1:A:485:GLN:CA	2.67	0.41
1:A:525:ASN:CB	1:A:526:LYS:CG	2.90	0.41
1:A:701:GLN:HE21	1:A:724:ALA:HB2	1.85	0.41
19:A:1101:CLA:H12	19:A:1140:CLA:C6	2.49	0.41
2:B:42:LEU:O	2:B:45:ASN:N	2.53	0.41
2:B:103:ALA:HA	2:B:104:PHE:C	2.42	0.41
2:B:120:VAL:CG2	2:B:123:TRP:NE1	2.57	0.41
2:B:344:ILE:HD13	19:B:1215:CLA:H71	2.02	0.41
2:B:471:THR:C	2:B:472:TYR:CD1	2.96	0.41
2:B:475:ASP:OD1	2:B:480:SER:C	2.60	0.41
2:B:645:VAL:HG13	21:B:6017:BCR:H282	2.02	0.41
2:B:661:PHE:HA	2:B:664:LEU:HB2	2.02	0.41
19:B:1211:CLA:C2B	21:B:6006:BCR:H11C	2.50	0.41
4:D:196:SER:HA	4:D:197:PRO:HD3	1.33	0.41
4:D:203:THR:CG2	4:D:205:LYS:HG2	2.50	0.41
5:E:122:LEU:HD12	5:E:122:LEU:HA	1.57	0.41
6:F:140:CYS:H	6:F:146:PRO:HA	1.85	0.41
6:F:184:ALA:O	6:F:185:ILE:CG2	2.68	0.41
7:G:124:ILE:CD1	7:G:128:LEU:CD1	2.98	0.41
8:H:58:LEU:HG	8:H:61:THR:HB	1.93	0.41
10:J:26:LEU:C	10:J:26:LEU:CD2	2.93	0.41
12:L:92:ALA:HB3	12:L:98:ARG:CZ	2.50	0.41
15:1:130:PRO:HB2	15:1:131:TRP:H	1.63	0.41
15:1:177:PRO:CG	15:1:180:LEU:N	2.79	0.41
15:1:201:PHE:CA	15:1:204:GLN:HB2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:161:GLU:CD	17:3:161:GLU:O	2.62	0.41
17:3:204:GLY:HA3	17:3:207:PHE:CA	2.49	0.41
19:3:3013:CLA:H51	19:3:3013:CLA:H12	1.83	0.41
18:4:122:ASN:O	18:4:123:VAL:CG1	2.59	0.41
18:4:158:GLN:O	18:4:159:ASP:C	2.62	0.41
18:4:173:LYS:CB	18:4:194:PHE:CD2	2.87	0.41
22:4:7033:LMU:H3'	22:4:7033:LMU:H1B	1.73	0.41
1:A:240:LYS:HA	1:A:243:PRO:HD2	2.01	0.41
1:A:260:PRO:C	1:A:262:PHE:H	2.28	0.41
1:A:293:GLY:O	1:A:380:PRO:O	2.37	0.41
1:A:349:ILE:CG2	1:A:350:LEU:HA	2.45	0.41
1:A:488:PHE:CD1	1:A:535:GLY:CA	3.03	0.41
1:A:564:ARG:CZ	1:A:564:ARG:HB2	2.49	0.41
19:A:1131:CLA:H191	20:B:5002:PQN:H303	2.02	0.41
2:B:4:ARG:HH21	2:B:5:ILE:N	2.19	0.41
2:B:18:THR:C	2:B:20:ARG:N	2.74	0.41
2:B:110:LEU:CG	2:B:111:GLY:N	2.83	0.41
2:B:314:ARG:HH22	15:1:67:LEU:CG	2.28	0.41
2:B:365:PHE:CD1	2:B:602:TRP:CD1	3.08	0.41
2:B:431:PHE:HE2	19:B:1229:CLA:HED3	1.85	0.41
19:B:1229:CLA:C5	21:F:6016:BCR:H403	2.49	0.41
4:D:187:ASN:HB2	4:D:188:PHE:H	1.60	0.41
5:E:82:TYR:CD2	5:E:83:TRP:CE3	3.08	0.41
6:F:173:TRP:CZ3	6:F:211:PHE:CA	3.03	0.41
6:F:224:GLY:O	6:F:227:VAL:HG12	2.14	0.41
19:F:1305:CLA:HAA2	19:F:1305:CLA:HBD	2.02	0.41
7:G:90:GLN:CB	7:G:92:PRO:N	2.83	0.41
9:I:17:PRO:O	9:I:18:ALA:C	2.62	0.41
22:K:7041:LMU:O2'	22:K:7041:LMU:H5'	2.20	0.41
12:L:114:PHE:HD1	12:L:114:PHE:N	2.17	0.41
13:N:114:PHE:CD2	13:N:116:ARG:HD2	2.55	0.41
13:N:155:GLU:CD	13:N:157:LYS:O	2.63	0.41
15:1:157:ASP:CG	15:1:175:LYS:HE3	2.45	0.41
15:1:158:PRO:HD2	15:1:159:GLU:O	2.20	0.41
16:2:103:VAL:HG13	16:2:104:GLN:N	2.35	0.41
17:3:241:TYR:OH	19:3:3003:CLA:CHC	2.68	0.41
17:3:243:ILE:CG1	19:3:3005:CLA:C4C	2.79	0.41
22:3:7003:LMU:C2B	22:3:7005:LMU:C6B	2.96	0.41
18:4:120:ILE:HD11	18:4:226:LYS:CD	2.29	0.41
18:4:202:GLU:O	18:4:205:ILE:HD13	2.19	0.41
1:A:105:ASN:HB2	1:A:140:PHE:HZ	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:O	1:A:159:THR:CB	2.68	0.41
1:A:388:ASP:O	1:A:389:TYR:C	2.63	0.41
1:A:443:ILE:HD12	1:A:443:ILE:N	2.35	0.41
1:A:553:VAL:CG2	21:A:6008:BCR:H401	2.50	0.41
1:A:661:ALA:HB2	19:A:9011:CLA:HMD1	2.01	0.41
19:A:1117:CLA:HBA2	19:A:1117:CLA:H3A	1.62	0.41
19:A:1119:CLA:C2C	19:A:1125:CLA:H171	2.50	0.41
19:A:1131:CLA:HED1	19:A:1237:CLA:O1A	2.20	0.41
19:A:9011:CLA:H162	19:A:9011:CLA:H122	1.68	0.41
19:A:9023:CLA:C9	19:B:1239:CLA:HBB2	2.48	0.41
2:B:75:GLU:HB2	2:B:132:ASN:HD22	1.63	0.41
2:B:188:LEU:O	2:B:189:ALA:C	2.63	0.41
2:B:323:TYR:CD1	19:B:1221:CLA:HBC1	2.54	0.41
2:B:428:PHE:C	2:B:428:PHE:CD2	2.99	0.41
2:B:583:MET:O	2:B:587:ILE:HB	2.20	0.41
2:B:661:PHE:O	2:B:665:ILE:N	2.52	0.41
21:B:6017:BCR:C38	21:B:6017:BCR:C23	2.97	0.41
6:F:170:ILE:CG2	21:F:6014:BCR:H371	2.32	0.41
8:H:86:THR:O	8:H:87:PHE:C	2.57	0.41
8:H:97:LEU:HD11	8:H:101:LEU:H	1.85	0.41
11:K:115:ILE:CD1	11:K:122:LEU:H	2.32	0.41
12:L:164:LEU:H	12:L:164:LEU:HG	1.53	0.41
12:L:171:LYS:CA	12:L:173:PRO:HD3	2.48	0.41
19:L:1501:CLA:H11	19:L:1501:CLA:C4D	2.50	0.41
16:2:192:ASP:OD2	16:2:194:GLY:CA	2.65	0.41
19:2:2001:CLA:O2A	19:2:2001:CLA:H43	2.20	0.41
19:2:2004:CLA:HED2	19:3:2009:CLA:CAB	2.50	0.41
17:3:104:ILE:O	17:3:105:ASN:C	2.62	0.41
17:3:208:PHE:HD1	17:3:208:PHE:HA	1.76	0.41
17:3:238:ILE:CG1	19:3:3003:CLA:CMC	2.99	0.41
1:A:123:VAL:HG23	1:A:124:TRP:O	2.19	0.41
1:A:218:TRP:NE1	1:A:222:GLN:OE1	2.54	0.41
1:A:365:LEU:O	1:A:369:THR:HG23	2.21	0.41
1:A:443:ILE:CG2	2:B:674:LEU:HD11	2.47	0.41
1:A:572:LYS:HZ3	1:A:572:LYS:HG3	1.51	0.41
1:A:578:ARG:NH1	1:A:578:ARG:HB3	2.32	0.41
2:B:77:TRP:O	2:B:81:PRO:HB3	2.20	0.41
2:B:292:ARG:NH2	2:B:297:ILE:C	2.75	0.41
2:B:497:TRP:O	2:B:498:LEU:HB3	2.21	0.41
19:B:1229:CLA:CBB	21:F:6014:BCR:C26	2.99	0.41
19:F:1305:CLA:CAD	19:F:1305:CLA:CED	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:70:SER:C	8:H:73:PRO:HD3	2.42	0.41
22:H:7032:LMU:H1B	22:H:7032:LMU:H5'	1.84	0.41
11:K:112:VAL:O	11:K:114:HIS:N	2.53	0.41
16:2:123:PRO:HA	16:2:126:LEU:HG	2.00	0.41
17:3:135:ALA:HB1	17:3:139:THR:HG21	1.98	0.41
17:3:137:PHE:CD2	17:3:137:PHE:N	2.88	0.41
18:4:145:GLU:CD	18:4:146:PHE:CE1	2.98	0.41
22:4:7034:LMU:H81	22:4:7052:LMU:H2'	0.42	0.41
1:A:158:ILE:CD1	19:A:1112:CLA:HED3	2.40	0.41
1:A:214:GLY:HA3	21:A:6003:BCR:C15	2.51	0.41
1:A:258:LEU:HG	1:A:280:PHE:HE1	1.82	0.41
1:A:476:MET:HE3	1:A:644:GLN:NE2	2.35	0.41
19:A:1138:CLA:HBC3	19:A:1138:CLA:CHD	2.50	0.41
19:A:1139:CLA:H42	19:A:1139:CLA:O2A	2.19	0.41
2:B:104:PHE:HZ	2:B:645:VAL:HG23	1.84	0.41
2:B:193:HIS:CD2	19:B:1211:CLA:NB	2.88	0.41
2:B:430:GLY:N	2:B:525:LEU:CD1	2.83	0.41
2:B:580:VAL:HG11	2:B:710:LEU:HD21	2.02	0.41
2:B:594:TRP:HD1	2:B:595:HIS:N	2.17	0.41
2:B:631:LEU:HG	2:B:632:ILE:N	2.34	0.41
2:B:645:VAL:HA	19:B:1206:CLA:HAC1	2.03	0.41
2:B:715:VAL:O	2:B:719:PHE:HB2	2.20	0.41
19:B:1211:CLA:H111	19:B:1211:CLA:H71	1.47	0.41
19:B:1222:CLA:CMB	21:B:6010:BCR:C35	2.99	0.41
19:B:1222:CLA:NB	19:B:1236:CLA:HMA2	2.35	0.41
19:B:1225:CLA:H3A	19:B:1225:CLA:HBA2	1.62	0.41
19:B:1228:CLA:HBC3	19:B:1228:CLA:CHD	2.41	0.41
4:D:140:LEU:CD1	4:D:141:GLY:CA	2.80	0.41
6:F:118:ALA:O	6:F:121:ALA:O	2.38	0.41
6:F:157:TRP:HZ3	19:F:1302:CLA:CMC	2.34	0.41
6:F:188:GLU:HB3	6:F:189:LYS:H	1.23	0.41
13:N:132:THR:C	13:N:136:ASP:OD1	2.64	0.41
19:1:1006:CLA:HHC	19:1:1013:CLA:HBC1	2.02	0.41
16:2:117:ALA:HB1	16:2:230:LEU:HD12	2.01	0.41
16:2:122:ILE:C	16:2:126:LEU:HG	2.37	0.41
16:2:160:ILE:C	16:2:162:TRP:N	2.72	0.41
16:2:264:ALA:O	16:2:265:ALA:HB3	2.20	0.41
19:2:2004:CLA:C3	19:3:2009:CLA:HBC3	2.50	0.41
17:3:151:TRP:CG	17:3:152:ALA:H	2.24	0.41
1:A:79:PHE:CE1	19:A:1111:CLA:HED1	2.55	0.41
1:A:109:TRP:HH2	1:A:154:ARG:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HB	1:A:124:TRP:O	2.21	0.41
1:A:328:LYS:HZ2	1:A:345:GLY:N	2.17	0.41
1:A:355:HIS:ND1	1:A:416:ILE:HG22	2.31	0.41
1:A:425:THR:O	1:A:428:TYR:CE1	2.73	0.41
1:A:431:LEU:O	1:A:435:VAL:CG1	2.61	0.41
1:A:685:VAL:HG22	19:A:1140:CLA:CBB	2.48	0.41
1:A:705:GLU:O	1:A:706:SER:C	2.61	0.41
19:A:1106:CLA:O2D	19:A:1106:CLA:H2A	2.21	0.41
19:A:1107:CLA:CHA	19:A:1107:CLA:CBA	2.98	0.41
19:A:1116:CLA:HHD	19:A:1116:CLA:HAC2	1.96	0.41
2:B:67:HIS:CD2	2:B:89:HIS:HB2	2.55	0.41
2:B:93:ASP:HA	2:B:94:PRO:HD2	1.48	0.41
2:B:152:ALA:HB2	19:B:1208:CLA:C2C	2.50	0.41
2:B:192:GLY:HA2	19:B:1212:CLA:CHC	2.51	0.41
2:B:217:PRO:HB2	2:B:218:TYR:HD1	1.85	0.41
2:B:397:ASP:O	2:B:398:TYR:HB3	2.20	0.41
2:B:443:MET:CG	2:B:451:LYS:O	2.68	0.41
2:B:680:TRP:O	2:B:684:ARG:HB2	2.20	0.41
19:B:1203:CLA:O1D	19:B:1203:CLA:C2A	2.60	0.41
4:D:167:HIS:O	4:D:168:PRO:C	2.60	0.41
7:G:97:LEU:O	7:G:98:THR:O	2.39	0.41
7:G:116:SER:O	7:G:119:PRO:CD	2.68	0.41
8:H:109:LEU:HD21	19:H:1207:CLA:C5	2.50	0.41
12:L:210:PRO:O	12:L:211:TYR:HB3	2.18	0.41
13:N:146:LEU:HD22	17:3:142:ILE:CA	2.50	0.41
14:R:27:UNK:C	14:R:29:UNK:C	2.98	0.41
15:1:77:GLU:OE1	15:1:80:LYS:HE3	2.20	0.41
15:1:115:ALA:O	15:1:116:ALA:CB	2.69	0.41
19:1:1014:CLA:H102	19:1:1014:CLA:C5	2.18	0.41
16:2:187:LYS:O	16:2:188:LEU:C	2.61	0.41
17:3:107:ARG:NH1	17:3:233:LEU:N	2.69	0.41
17:3:251:GLY:O	17:3:252:PRO:C	2.62	0.41
19:3:3013:CLA:H3A	19:3:3013:CLA:HBA2	1.87	0.41
18:4:194:PHE:N	18:4:201:LYS:HZ2	2.19	0.41
1:A:249:ILE:HG12	17:3:136:TRP:HH2	1.85	0.41
1:A:389:TYR:HE2	1:A:526:LYS:CD	2.29	0.41
1:A:537:ALA:O	1:A:642:PHE:HE2	2.04	0.41
1:A:550:HIS:C	1:A:552:THR:O	2.63	0.41
1:A:624:VAL:O	1:A:625:TRP:C	2.63	0.41
1:A:708:VAL:N	1:A:711:HIS:HD2	2.19	0.41
19:A:1106:CLA:HMC2	19:A:1107:CLA:HHD	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1122:CLA:CBC	21:A:6007:BCR:H393	2.51	0.41
19:A:1126:CLA:C11	21:J:6012:BCR:H353	2.48	0.41
19:A:1133:CLA:CMC	19:A:1133:CLA:HBC2	2.44	0.41
2:B:91:ILE:HG21	2:B:91:ILE:HD13	1.78	0.41
2:B:98:GLN:N	2:B:99:PRO:CD	2.81	0.41
2:B:98:GLN:NE2	2:B:101:VAL:HG23	2.36	0.41
2:B:160:LYS:NZ	2:B:161:TRP:N	2.69	0.41
2:B:289:LEU:HD22	21:B:6004:BCR:H352	2.02	0.41
2:B:294:ASN:HB2	7:G:94:GLN:CG	2.45	0.41
2:B:458:ILE:HD11	6:F:149:ILE:HG13	2.02	0.41
2:B:549:ASP:CB	3:C:63:LEU:HB2	2.51	0.41
2:B:573:TRP:CZ3	2:B:703:VAL:HG13	2.55	0.41
19:B:1239:CLA:H2	20:B:5002:PQN:H251	2.02	0.41
3:C:58:CYS:HA	3:C:59:PRO:HD2	1.57	0.41
4:D:101:VAL:O	4:D:101:VAL:CG2	2.67	0.41
5:E:76:ILE:CB	5:E:84:TYR:O	2.53	0.41
22:E:7048:LMU:O4'	22:F:7036:LMU:H6E	2.15	0.41
19:F:1305:CLA:H12	19:4:1306:CLA:HAA1	2.02	0.41
22:K:7041:LMU:H82	22:K:7041:LMU:H111	1.95	0.41
12:L:83:LEU:HA	12:L:86:LEU:HD13	2.02	0.41
12:L:145:LEU:O	12:L:146:THR:C	2.61	0.41
15:1:67:LEU:CD1	15:1:67:LEU:C	2.81	0.41
15:1:101:GLU:OE2	15:1:101:GLU:C	2.64	0.41
15:1:138:LEU:O	15:1:141:GLU:HG3	2.21	0.41
19:1:1014:CLA:C12	19:1:1014:CLA:H91	2.50	0.41
16:2:155:VAL:CA	16:2:158:VAL:HG13	2.50	0.41
16:2:202:ASP:OD2	16:2:202:ASP:C	2.58	0.41
19:2:2006:CLA:H72	19:2:2006:CLA:H41	2.02	0.41
19:2:2014:CLA:C15	19:2:2014:CLA:C9	2.84	0.41
18:4:210:LEU:HD23	19:4:4002:CLA:CAB	2.51	0.41
1:A:57:LEU:HD22	1:A:58:HIS:CD2	2.54	0.41
1:A:109:TRP:HD1	1:A:116:ILE:HB	1.84	0.41
1:A:349:ILE:CG2	1:A:350:LEU:CA	2.95	0.41
1:A:473:PRO:C	1:A:475:ASP:H	2.29	0.41
1:A:479:ASP:CB	1:A:536:THR:CG2	2.99	0.41
1:A:514:THR:HA	1:A:530:LEU:O	2.21	0.41
1:A:547:PHE:CE2	19:A:9023:CLA:O1A	2.73	0.41
1:A:709:TRP:CZ3	2:B:417:ALA:HA	2.55	0.41
19:A:1124:CLA:HMA3	21:A:6008:BCR:H16C	2.03	0.41
22:A:7016:LMU:H1'	22:A:7016:LMU:H6D	1.76	0.41
2:B:52:GLY:O	2:B:56:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ARG:HA	2:B:208:ARG:HD2	1.98	0.41
2:B:353:TYR:CB	2:B:594:TRP:CH2	3.01	0.41
2:B:410:ARG:HA	2:B:410:ARG:HD2	1.49	0.41
2:B:576:PHE:CD1	2:B:576:PHE:C	2.99	0.41
2:B:622:ASP:CA	2:B:626:LEU:HD12	2.48	0.41
3:C:33:GLY:HA2	3:C:37:LYS:HB3	2.02	0.41
4:D:114:MET:HG2	4:D:115:PRO:O	1.98	0.41
9:I:8:PHE:CD1	19:I:1204:CLA:H12	2.56	0.41
19:J:1308:CLA:H93	19:2:2014:CLA:O1D	2.13	0.41
19:J:1311:CLA:HBA2	19:J:1311:CLA:H3A	1.27	0.41
11:K:127:ILE:O	11:K:130:LEU:CA	2.69	0.41
22:K:7001:LMU:H42	22:K:7001:LMU:H102	2.01	0.41
12:L:94:SER:C	12:L:96:LEU:CD2	2.94	0.41
12:L:107:GLY:C	12:L:109:LEU:N	2.78	0.41
12:L:148:TYR:C	12:L:150:ILE:N	2.78	0.41
12:L:210:PRO:HB2	12:L:211:TYR:CE2	2.55	0.41
13:N:127:PHE:CG	13:N:128:PRO:HD3	2.55	0.41
13:N:142:LYS:O	13:N:143:VAL:C	2.63	0.41
13:N:164:SER:HA	13:N:165:ASN:O	2.18	0.41
15:1:85:ILE:HG12	15:1:88:ARG:NE	2.26	0.41
15:1:90:ALA:C	15:1:92:LEU:N	2.75	0.41
15:1:200:GLY:HA3	19:1:1003:CLA:HBB2	2.02	0.41
15:1:201:PHE:HA	15:1:204:GLN:CB	2.49	0.41
16:2:110:SER:HB3	16:2:227:LEU:HD13	2.02	0.41
19:2:2014:CLA:H91	19:2:2014:CLA:C16	2.51	0.41
19:3:3011:CLA:H11	19:3:3011:CLA:HBA2	1.88	0.41
18:4:169:ASP:OD1	18:4:174:GLN:N	2.54	0.41
18:4:175:TYR:CB	18:4:194:PHE:CD1	2.90	0.41
1:A:173:VAL:O	1:A:175:ALA:O	2.39	0.41
1:A:288:ASP:O	1:A:292:GLY:HA2	2.20	0.41
1:A:288:ASP:OD1	1:A:295:TRP:CD2	2.74	0.41
1:A:378:SER:O	1:A:378:SER:OG	2.35	0.41
1:A:466:THR:HG22	2:B:648:TRP:CE2	2.56	0.41
1:A:580:PRO:HB3	1:A:727:ILE:CG2	2.51	0.41
1:A:663:GLN:HB3	1:A:752:ALA:O	2.21	0.41
19:A:1102:CLA:HBC3	19:A:1102:CLA:CHD	2.50	0.41
19:A:1126:CLA:C17	19:A:1126:CLA:H122	2.50	0.41
2:B:4:ARG:NH2	2:B:5:ILE:N	2.69	0.41
2:B:7:ARG:CD	2:B:7:ARG:H	2.32	0.41
2:B:88:ALA:HB1	19:B:1205:CLA:O2D	2.20	0.41
2:B:112:PRO:C	2:B:113:VAL:HG22	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:O	2:B:145:LEU:HB3	2.21	0.41
2:B:175:LEU:HD13	19:B:1221:CLA:CED	2.51	0.41
2:B:182:LEU:HA	19:B:1210:CLA:HMB3	2.03	0.41
2:B:253:ALA:O	2:B:254:ILE:C	2.64	0.41
2:B:305:LEU:HD22	19:B:1220:CLA:O1D	2.18	0.41
2:B:355:LEU:HD21	2:B:508:LEU:CD2	2.51	0.41
2:B:395:ILE:H	2:B:395:ILE:HG13	1.75	0.41
2:B:439:HIS:HB2	19:B:1230:CLA:C1C	2.50	0.41
2:B:478:LEU:O	2:B:478:LEU:CG	2.68	0.41
2:B:517:PHE:CD2	2:B:517:PHE:C	2.92	0.41
2:B:729:THR:O	2:B:729:THR:CG2	2.61	0.41
19:B:1214:CLA:H12	19:B:1214:CLA:NA	2.36	0.41
19:B:1220:CLA:CMD	19:B:1221:CLA:CBB	2.99	0.41
19:B:1226:CLA:CMC	19:B:1226:CLA:HBC3	2.49	0.41
3:C:39:ILE:CG1	3:C:40:ALA:H	2.32	0.41
4:D:110:GLN:O	4:D:122:MET:CG	2.69	0.41
5:E:106:ARG:CZ	5:E:106:ARG:O	2.67	0.41
22:E:7048:LMU:H4'	22:E:7048:LMU:H1'	1.79	0.41
6:F:101:LYS:O	6:F:104:ALA:HB3	2.21	0.41
6:F:116:ALA:O	6:F:119:ILE:HD13	2.21	0.41
6:F:127:LYS:O	6:F:129:ARG:C	2.63	0.41
6:F:225:GLU:C	6:F:227:VAL:HG12	2.46	0.41
8:H:100:PHE:O	8:H:101:LEU:C	2.63	0.41
8:H:107:SER:O	8:H:111:TYR:CB	2.68	0.41
8:H:111:TYR:CB	8:H:112:LEU:HD23	2.51	0.41
8:H:111:TYR:CG	8:H:112:LEU:HD23	2.56	0.41
22:H:7017:LMU:H1B	22:H:7017:LMU:H6'2	1.72	0.41
9:I:11:LEU:O	9:I:16:PHE:N	2.51	0.41
11:K:126:ASN:O	11:K:126:ASN:CG	2.63	0.41
22:K:7042:LMU:H121	22:K:7042:LMU:H91	1.75	0.41
12:L:103:GLY:HA3	12:L:192:GLY:HA3	2.02	0.41
12:L:111:VAL:HG23	12:L:112:GLY:H	1.86	0.41
13:N:142:LYS:C	13:N:145:PHE:O	2.63	0.41
15:1:135:PRO:HD2	15:1:136:THR:N	2.32	0.41
16:2:106:GLU:HG2	19:2:2004:CLA:HBC2	2.02	0.41
16:2:167:ARG:C	16:2:169:ALA:N	2.79	0.41
16:2:266:PHE:CD2	16:2:267:THR:O	2.74	0.41
19:2:2001:CLA:CMC	19:2:2001:CLA:HBC2	2.50	0.41
17:3:111:LEU:CD2	17:3:112:GLY:H	2.21	0.41
17:3:178:LYS:HB3	17:3:179:PRO:HD3	2.03	0.41
17:3:178:LYS:HB3	17:3:179:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:7005:LMU:H71	22:3:7005:LMU:H42	1.79	0.41
18:4:95:GLU:HG3	18:4:96:LEU:N	2.35	0.41
18:4:154:ILE:CG2	19:4:1009:CLA:HMD1	2.49	0.41
19:4:1004:CLA:H11	19:4:1004:CLA:H52	1.83	0.41
1:A:82:HIS:O	1:A:83:PHE:C	2.61	0.41
1:A:236:GLY:O	1:A:237:VAL:CB	2.69	0.41
1:A:281:LEU:CD2	19:A:1115:CLA:HED3	2.22	0.41
1:A:484:LEU:CA	1:A:485:GLN:NE2	2.84	0.41
1:A:684:PHE:HB2	19:A:9012:CLA:HAA1	2.02	0.41
1:A:720:THR:O	1:A:720:THR:CG2	2.65	0.41
19:A:1104:CLA:H11	19:A:1128:CLA:O2A	2.21	0.41
19:A:1106:CLA:H142	21:J:6012:BCR:C13	2.50	0.41
19:A:1106:CLA:CBB	19:A:1107:CLA:C3D	2.95	0.41
19:A:1112:CLA:CMC	21:A:6002:BCR:C15	2.99	0.41
19:A:1119:CLA:H112	19:A:1119:CLA:H91	1.83	0.41
2:B:131:THR:O	2:B:135:LEU:CD2	2.62	0.41
2:B:334:LEU:HD22	19:B:1202:CLA:CHD	2.51	0.41
3:C:28:MET:HE2	3:C:38:GLN:HE21	1.86	0.41
4:D:93:LYS:HG3	4:D:96:VAL:HG11	1.99	0.41
4:D:185:GLY:O	4:D:186:GLN:HB2	2.19	0.41
5:E:66:ILE:HG13	5:E:67:GLY:N	2.36	0.41
22:E:7037:LMU:O2B	22:E:7037:LMU:C5B	2.66	0.41
22:E:7048:LMU:H6'2	22:E:7048:LMU:O2'	2.21	0.41
6:F:201:PRO:O	6:F:202:LEU:HB2	2.21	0.41
7:G:87:VAL:O	7:G:90:GLN:O	2.38	0.41
7:G:149:TYR:CA	7:G:150:ASP:CG	2.61	0.41
22:G:7039:LMU:H82	22:G:7039:LMU:H112	1.61	0.41
11:K:92:GLY:O	11:K:93:LEU:CB	2.66	0.41
22:K:7041:LMU:H2B	22:K:7041:LMU:H4'	1.79	0.41
12:L:93:VAL:C	12:L:94:SER:O	2.56	0.41
12:L:172:GLU:CG	12:L:173:PRO:N	2.73	0.41
15:1:68:GLY:O	15:1:73:PRO:N	2.55	0.41
19:1:1014:CLA:H121	19:1:1014:CLA:C9	2.51	0.41
16:2:107:LEU:HD11	16:2:108:VAL:HG23	2.03	0.41
16:2:184:PRO:CD	16:2:186:ASN:N	2.83	0.41
19:2:2004:CLA:C4	19:3:2009:CLA:HBC3	2.51	0.41
17:3:157:LEU:O	17:3:160:LEU:CA	2.69	0.41
1:A:60:ASP:O	1:A:60:ASP:OD1	2.38	0.40
1:A:86:LEU:C	1:A:87:SER:O	2.59	0.40
1:A:127:VAL:CG2	19:A:1107:CLA:HBB2	2.39	0.40
1:A:201:SER:O	1:A:204:ASN:CA	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD21	19:A:1119:CLA:HMC2	2.02	0.40
1:A:375:HIS:ND1	1:A:375:HIS:N	2.69	0.40
1:A:648:THR:O	1:A:649:ILE:HG22	2.21	0.40
19:A:1125:CLA:CMC	19:A:1125:CLA:CBC	2.91	0.40
2:B:15:ASP:HA	2:B:16:PRO:HD3	1.89	0.40
2:B:29:HIS:HB3	19:B:1226:CLA:HBA1	2.03	0.40
2:B:169:LYS:O	2:B:170:ASN:O	2.39	0.40
2:B:174:ARG:NH1	19:B:1221:CLA:HMD1	2.36	0.40
2:B:334:LEU:HB2	19:B:1202:CLA:CMD	2.49	0.40
2:B:472:TYR:O	2:B:473:GLY:C	2.64	0.40
2:B:535:VAL:CG1	2:B:536:LYS:H	2.34	0.40
2:B:583:MET:HE2	2:B:583:MET:C	2.46	0.40
19:B:1235:CLA:HBC1	6:F:160:PHE:CE1	2.48	0.40
20:B:5002:PQN:H161	20:B:5002:PQN:H141	1.60	0.40
4:D:125:GLY:HA2	4:D:127:ASN:H	1.85	0.40
4:D:134:LYS:HE2	4:D:166:LEU:HD11	2.03	0.40
6:F:102:LEU:O	6:F:103:GLN:O	2.39	0.40
22:F:7036:LMU:H1'	22:F:7036:LMU:O6'	2.21	0.40
8:H:56:GLU:O	8:H:57:ASP:C	2.63	0.40
11:K:50:GLY:N	11:K:52:PRO:HD3	2.36	0.40
12:L:145:LEU:CG	21:L:6019:BCR:HC7	2.41	0.40
12:L:202:PHE:O	12:L:203:LEU:C	2.63	0.40
13:N:155:GLU:CB	13:N:157:LYS:NZ	2.82	0.40
19:1:1013:CLA:OBD	19:1:1013:CLA:HMD1	2.21	0.40
17:3:85:ASP:HA	17:3:86:PRO:HD3	1.40	0.40
17:3:168:ALA:O	17:3:169:GLU:C	2.63	0.40
19:3:3013:CLA:HHD	19:3:3013:CLA:HBC2	2.02	0.40
18:4:179:ALA:C	18:4:181:GLU:N	2.73	0.40
18:4:180:GLY:O	18:4:183:GLY:N	2.54	0.40
19:4:4006:CLA:HBA2	19:4:4006:CLA:CBD	2.51	0.40
1:A:210:LEU:CD1	19:A:1111:CLA:HMB3	2.50	0.40
1:A:363:ALA:N	1:A:410:ALA:HB2	2.36	0.40
1:A:434:ARG:HA	1:A:437:ARG:HD2	2.03	0.40
1:A:586:ARG:HB2	1:A:589:THR:OG1	2.22	0.40
1:A:630:ASP:C	1:A:632:GLY:N	2.74	0.40
21:A:6011:BCR:H323	21:J:6012:BCR:C39	2.49	0.40
19:A:9023:CLA:O2A	19:A:9023:CLA:C3A	2.65	0.40
2:B:279:ALA:HA	19:B:1213:CLA:HMA2	2.03	0.40
2:B:285:LEU:HD12	21:B:6004:BCR:C17	2.50	0.40
2:B:310:PRO:CG	2:B:311:PRO:HD2	2.50	0.40
2:B:320:LYS:HG3	2:B:321:GLY:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:631:LEU:O	2:B:634:GLY:N	2.53	0.40
19:B:1232:CLA:CBB	21:B:6010:BCR:C28	2.99	0.40
4:D:155:TYR:CD1	4:D:168:PRO:HG3	2.57	0.40
4:D:169:LYS:HB2	4:D:169:LYS:NZ	2.36	0.40
6:F:116:ALA:O	6:F:119:ILE:HG12	2.20	0.40
6:F:160:PHE:C	6:F:163:PRO:HD2	2.47	0.40
7:G:90:GLN:HB2	7:G:92:PRO:N	2.37	0.40
7:G:131:GLY:HA2	7:G:136:VAL:CB	2.50	0.40
22:G:7039:LMU:H3'	22:G:7039:LMU:C6B	2.49	0.40
11:K:56:ILE:HG12	11:K:59:THR:CG2	2.50	0.40
22:K:7042:LMU:H22	22:K:7042:LMU:C7	2.50	0.40
12:L:182:TRP:CZ3	12:L:186:THR:HG21	2.56	0.40
12:L:194:ILE:O	12:L:195:SER:HB3	2.21	0.40
15:1:140:ILE:N	15:1:140:ILE:CD1	2.72	0.40
19:1:1002:CLA:HMC1	19:1:1002:CLA:HBC3	2.03	0.40
19:1:1005:CLA:CBC	19:1:1005:CLA:CMC	2.99	0.40
16:2:95:ASP:HA	16:2:96:PRO:HD3	1.93	0.40
17:3:108:PHE:HD2	19:3:3013:CLA:C4	2.34	0.40
18:4:88:LEU:O	18:4:90:TRP:CB	2.59	0.40
18:4:108:GLY:O	18:4:109:MET:O	2.39	0.40
18:4:149:SER:OG	18:4:150:HIS:N	2.54	0.40
18:4:153:GLU:OE2	19:4:4012:CLA:HHC	2.17	0.40
18:4:232:LEU:HD12	18:4:234:GLN:N	2.36	0.40
18:4:243:THR:HG23	18:4:244:ILE:N	2.36	0.40
1:A:157:GLY:C	1:A:158:ILE:CG2	2.66	0.40
1:A:170:GLY:O	1:A:173:VAL:CG2	2.64	0.40
1:A:352:THR:HG22	19:A:1123:CLA:H201	2.03	0.40
1:A:409:GLY:O	1:A:411:ALA:N	2.55	0.40
1:A:472:ARG:HH22	12:L:120:LEU:HD13	1.85	0.40
1:A:492:ILE:HD13	19:A:1133:CLA:CHC	2.50	0.40
1:A:569:ILE:HG12	1:A:586:ARG:NH1	2.36	0.40
1:A:631:GLN:O	1:A:631:GLN:HG2	2.21	0.40
1:A:755:ILE:H	1:A:755:ILE:HG13	1.62	0.40
19:A:1119:CLA:CGA	19:A:1123:CLA:HBB2	2.51	0.40
19:A:1120:CLA:CGA	19:A:1120:CLA:C1A	2.99	0.40
19:A:9013:CLA:H91	19:A:9013:CLA:H112	1.78	0.40
2:B:262:HIS:HB2	2:B:265:THR:OG1	2.21	0.40
2:B:357:ALA:C	2:B:358:TYR:CD1	2.99	0.40
2:B:486:LEU:HB2	19:B:1232:CLA:CMD	2.28	0.40
2:B:653:GLY:HA3	2:B:720:THR:OG1	2.20	0.40
2:B:655:LEU:O	2:B:656:VAL:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:700:LEU:HD23	2:B:700:LEU:N	2.36	0.40
19:B:1205:CLA:H162	19:B:1224:CLA:H192	2.03	0.40
19:B:1227:CLA:HMB1	19:B:1228:CLA:CHB	2.51	0.40
20:B:5002:PQN:H141	21:B:6017:BCR:H331	2.04	0.40
21:B:6004:BCR:H15C	21:B:6004:BCR:H351	1.88	0.40
22:B:7040:LMU:C1B	22:B:7040:LMU:H3O2	2.34	0.40
4:D:140:LEU:HD22	4:D:144:LEU:CG	2.49	0.40
21:F:6014:BCR:C33	21:F:6014:BCR:HC8	2.52	0.40
7:G:66:LEU:HD23	7:G:69:GLY:HA3	2.03	0.40
8:H:103:LEU:O	8:H:107:SER:HB3	2.22	0.40
10:J:5:LYS:CG	16:2:178:ASN:HA	2.52	0.40
19:K:1143:CLA:CBC	22:K:7001:LMU:C3B	2.91	0.40
13:N:123:GLY:O	13:N:124:SER:O	2.39	0.40
15:1:148:VAL:O	15:1:148:VAL:HG22	2.19	0.40
15:1:177:PRO:HG2	15:1:180:LEU:HA	2.03	0.40
16:2:107:LEU:C	16:2:107:LEU:CD1	2.86	0.40
16:2:160:ILE:HG21	19:2:2012:CLA:CAB	2.41	0.40
16:2:172:LEU:HD12	16:2:172:LEU:HA	1.75	0.40
17:3:197:SER:HB3	17:3:206:PRO:CG	2.51	0.40
19:3:3011:CLA:H41	19:3:3011:CLA:H62	1.80	0.40
18:4:217:PHE:O	18:4:220:GLN:HB2	2.21	0.40
18:4:228:PRO:C	18:4:229:PHE:CG	2.99	0.40
22:4:7009:LMU:C3'	22:4:7009:LMU:H5B	2.52	0.40
1:A:261:SER:O	1:A:262:PHE:CE1	2.73	0.40
1:A:295:TRP:CB	1:A:297:THR:HG23	2.51	0.40
1:A:368:LEU:HD12	19:A:1125:CLA:C6	2.52	0.40
19:A:1107:CLA:HBC3	19:A:1107:CLA:CMC	2.52	0.40
19:A:1119:CLA:H101	19:A:1122:CLA:H93	2.02	0.40
19:A:1119:CLA:H8	21:A:6008:BCR:H19C	2.03	0.40
19:A:1124:CLA:H172	21:A:6007:BCR:C33	2.46	0.40
19:A:1138:CLA:H202	19:A:1139:CLA:H41	2.03	0.40
2:B:222:LEU:HD12	2:B:222:LEU:C	2.46	0.40
2:B:427:LEU:C	19:B:1229:CLA:HED2	2.47	0.40
2:B:547:MET:HE2	2:B:550:LYS:CA	2.44	0.40
2:B:569:ASP:HB3	2:B:574:ASP:HB3	2.04	0.40
2:B:586:THR:O	2:B:589:TRP:N	2.54	0.40
2:B:596:TRP:CZ2	2:B:612:SER:HB3	2.56	0.40
2:B:635:ILE:O	2:B:636:THR:O	2.38	0.40
19:B:1217:CLA:HMA2	7:G:77:PHE:CE2	2.56	0.40
19:B:1235:CLA:H121	21:F:6016:BCR:H311	1.98	0.40
19:B:1235:CLA:C12	21:F:6016:BCR:H311	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:E:7037:LMU:C7	22:E:7037:LMU:H32	2.51	0.40
6:F:130:PHE:O	6:F:132:ASN:O	2.39	0.40
6:F:154:GLN:OE1	6:F:155:ARG:N	2.55	0.40
6:F:230:ASN:O	6:F:231:PHE:O	2.40	0.40
7:G:99:HIS:C	7:G:101:GLU:H	2.27	0.40
9:I:15:LEU:HD12	9:I:18:ALA:HB3	2.03	0.40
11:K:123:GLY:HA3	11:K:124:LEU:HA	1.82	0.40
11:K:127:ILE:CB	11:K:129:ALA:HB1	2.33	0.40
12:L:210:PRO:CB	12:L:211:TYR:CD2	3.03	0.40
22:L:7029:LMU:H6E	22:L:7029:LMU:H2O1	1.85	0.40
15:1:194:ALA:O	15:1:195:LEU:C	2.64	0.40
19:1:1006:CLA:CAB	19:1:1013:CLA:HHD	2.51	0.40
19:1:1007:CLA:H11	19:1:1007:CLA:H51	1.92	0.40
16:2:222:ILE:O	16:2:226:ARG:N	2.51	0.40
19:2:2004:CLA:HED2	19:3:2009:CLA:CBB	2.51	0.40
19:2:2006:CLA:HED2	19:2:2006:CLA:OBD	2.22	0.40
17:3:111:LEU:CD2	17:3:112:GLY:N	2.83	0.40
17:3:124:LYS:CG	17:3:149:ASN:HB3	2.49	0.40
17:3:131:GLU:C	17:3:133:ALA:N	2.79	0.40
19:3:1147:CLA:HBA2	19:3:1147:CLA:H3A	1.72	0.40
18:4:212:LEU:O	18:4:213:ALA:CB	2.70	0.40
1:A:146:THR:HA	1:A:391:THR:HG22	2.03	0.40
1:A:217:SER:C	19:A:1112:CLA:HBB2	2.46	0.40
1:A:222:GLN:O	1:A:227:LEU:HG	2.21	0.40
1:A:286:GLY:O	1:A:295:TRP:NE1	2.55	0.40
1:A:447:ASN:ND2	2:B:678:LEU:CD2	2.82	0.40
1:A:452:PHE:C	1:A:453:LEU:O	2.59	0.40
19:A:1101:CLA:H12	19:A:1140:CLA:H61	2.02	0.40
19:A:1104:CLA:HBA2	19:A:1104:CLA:H12	1.79	0.40
19:A:9022:CLA:C14	19:H:1207:CLA:HBC3	2.52	0.40
2:B:102:GLU:O	2:B:103:ALA:C	2.64	0.40
2:B:120:VAL:CB	2:B:123:TRP:CD1	3.03	0.40
2:B:185:VAL:HA	2:B:188:LEU:HB3	2.04	0.40
2:B:272:ASP:C	2:B:274:ALA:N	2.76	0.40
2:B:421:HIS:CE1	19:B:1228:CLA:C4D	3.04	0.40
2:B:463:ILE:HD12	19:B:1234:CLA:CGA	2.51	0.40
2:B:488:ALA:CB	19:B:1233:CLA:C2C	3.00	0.40
2:B:557:PHE:O	2:B:557:PHE:CD2	2.74	0.40
19:B:1218:CLA:CBA	19:B:1219:CLA:O1A	2.70	0.40
21:B:6005:BCR:H321	21:B:6005:BCR:HC7	1.87	0.40
6:F:103:GLN:O	6:F:105:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:121:ALA:HA	6:F:124:GLU:HB3	2.04	0.40
6:F:123:MET:O	6:F:127:LYS:N	2.54	0.40
22:G:7026:LMU:C8	22:G:7026:LMU:C4	2.96	0.40
8:H:89:ALA:O	8:H:90:PRO:C	2.64	0.40
8:H:91:PHE:CZ	8:H:98:LEU:HD13	2.56	0.40
19:K:1143:CLA:CMC	19:K:1143:CLA:HBC2	2.52	0.40
12:L:52:PRO:O	12:L:54:TYR:N	2.55	0.40
13:N:91:TYR:HD2	13:N:91:TYR:HA	1.68	0.40
15:1:65:ASP:HA	15:1:69:LEU:CD1	2.49	0.40
15:1:173:TYR:HD2	15:1:173:TYR:HA	1.49	0.40
15:1:192:ARG:CG	15:1:193:LEU:N	2.82	0.40
19:2:2002:CLA:H72	19:2:2002:CLA:H41	2.04	0.40
19:2:2014:CLA:HED3	19:2:2014:CLA:CAD	2.50	0.40
17:3:197:SER:CB	17:3:206:PRO:HG3	2.52	0.40
17:3:197:SER:OG	17:3:198:GLY:N	2.53	0.40
22:4:7034:LMU:H71	22:4:7052:LMU:C1	2.38	0.40

All (127) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:173:TYR:OH	16:2:132:LEU:C[2_646]	0.71	1.49
6:F:130:PHE:CG	12:L:170:LYS:NZ[2_556]	0.72	1.48
2:B:205:GLU:OE2	11:K:69:ARG:NH1[1_554]	0.79	1.41
12:L:123:THR:O	18:4:180:GLY:CA[1_455]	0.88	1.32
15:1:171:LEU:N	16:2:132:LEU:N[2_646]	0.98	1.22
15:1:173:TYR:OH	16:2:132:LEU:CA[2_646]	1.01	1.19
12:L:203:LEU:C	18:4:184:TYR:OH[1_455]	1.02	1.18
12:L:205:TYR:OH	18:4:181:GLU:O[1_455]	1.02	1.18
12:L:124:GLU:OE1	18:4:172:PHE:CE2[1_455]	1.06	1.14
15:1:171:LEU:CD2	16:2:131:ILE:C[2_646]	1.07	1.13
15:1:171:LEU:CD2	16:2:131:ILE:O[2_646]	1.08	1.12
12:L:124:GLU:OE1	18:4:172:PHE:CZ[1_455]	1.09	1.11
2:B:248:GLN:NE2	19:K:3009:CLA:C2C[1_554]	1.11	1.09
12:L:124:GLU:CD	18:4:172:PHE:CE2[1_455]	1.11	1.09
15:1:173:TYR:CE1	16:2:132:LEU:O[2_646]	1.13	1.07
12:L:124:GLU:CD	18:4:172:PHE:CZ[1_455]	1.15	1.05
15:1:118:PRO:O	17:3:89:THR:CG2[1_554]	1.17	1.03
6:F:130:PHE:CD2	12:L:170:LYS:NZ[2_556]	1.18	1.02
6:F:130:PHE:CE1	12:L:170:LYS:CE[2_556]	1.18	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:GLU:OE2	11:K:69:ARG:CZ[1_554]	1.19	1.01
15:1:170:PRO:O	16:2:132:LEU:CB[2_646]	1.20	1.00
12:L:203:LEU:O	18:4:184:TYR:CE2[1_455]	1.27	0.93
15:1:170:PRO:O	16:2:132:LEU:CA[2_646]	1.30	0.90
6:F:130:PHE:CD1	12:L:170:LYS:NZ[2_556]	1.32	0.88
6:F:131:ASP:OD2	12:L:170:LYS:CD[2_556]	1.32	0.88
1:A:348:GLU:OE2	7:G:147:ASN:OD1[1_556]	1.33	0.87
15:1:173:TYR:CZ	16:2:132:LEU:O[2_646]	1.37	0.83
6:F:131:ASP:OD1	12:L:170:LYS:CG[2_556]	1.38	0.82
2:B:205:GLU:CD	11:K:69:ARG:NH1[1_554]	1.39	0.81
4:D:160:ASN:CG	6:F:101:LYS:NZ[2_546]	1.39	0.81
12:L:203:LEU:O	18:4:184:TYR:CZ[1_455]	1.40	0.80
12:L:122:ASN:ND2	18:4:181:GLU:OE1[1_455]	1.46	0.74
15:1:173:TYR:CZ	16:2:132:LEU:C[2_646]	1.47	0.73
6:F:131:ASP:CG	12:L:170:LYS:CD[2_556]	1.49	0.71
12:L:123:THR:O	18:4:180:GLY:N[1_455]	1.50	0.70
12:L:124:GLU:OE2	18:4:172:PHE:CZ[1_455]	1.50	0.70
8:H:81:SER:OG	18:4:240:TRP:CZ3[2_546]	1.51	0.69
12:L:124:GLU:OE2	18:4:172:PHE:CE1[1_455]	1.52	0.68
6:F:130:PHE:CZ	12:L:170:LYS:CE[2_556]	1.53	0.67
12:L:124:GLU:N	18:4:177:LEU:O[1_455]	1.54	0.66
12:L:205:TYR:OH	18:4:181:GLU:C[1_455]	1.55	0.65
15:1:171:LEU:CG	16:2:131:ILE:CA[2_646]	1.55	0.65
6:F:130:PHE:CD1	12:L:170:LYS:CE[2_556]	1.56	0.64
12:L:203:LEU:O	18:4:184:TYR:OH[1_455]	1.58	0.62
15:1:173:TYR:CZ	16:2:132:LEU:CA[2_646]	1.59	0.61
12:L:122:ASN:CG	18:4:181:GLU:OE1[1_455]	1.60	0.60
12:L:202:PHE:O	18:4:184:TYR:OH[1_455]	1.61	0.59
6:F:131:ASP:OD1	12:L:170:LYS:CD[2_556]	1.62	0.58
15:1:171:LEU:CG	16:2:131:ILE:C[2_646]	1.62	0.58
12:L:122:ASN:OD1	18:4:181:GLU:OE1[1_455]	1.64	0.56
12:L:124:GLU:OE2	18:4:176:SER:O[1_455]	1.65	0.55
15:1:173:TYR:OH	16:2:132:LEU:O[2_646]	1.66	0.54
15:1:118:PRO:C	17:3:89:THR:CG2[1_554]	1.67	0.53
12:L:203:LEU:CA	18:4:184:TYR:OH[1_455]	1.68	0.52
15:1:171:LEU:CG	16:2:131:ILE:N[2_646]	1.68	0.52
2:B:205:GLU:OE2	11:K:69:ARG:NH2[1_554]	1.70	0.50
19:K:1142:CLA:O2A	19:1:1008:CLA:O2D[1_456]	1.70	0.50
15:1:173:TYR:OH	16:2:133:ASN:N[2_646]	1.71	0.49
4:D:160:ASN:ND2	6:F:101:LYS:NZ[2_546]	1.72	0.48
15:1:171:LEU:CD1	16:2:131:ILE:CB[2_646]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:173:TYR:OH	16:2:132:LEU:CB[2_646]	1.72	0.48
6:F:120:LYS:NZ	12:L:155:GLU:CG[2_556]	1.73	0.47
15:1:171:LEU:CA	16:2:132:LEU:N[2_646]	1.73	0.47
12:L:124:GLU:OE2	18:4:172:PHE:CE2[1_455]	1.74	0.46
12:L:204:LEU:N	18:4:184:TYR:OH[1_455]	1.75	0.45
12:L:124:GLU:OE2	18:4:172:PHE:CD1[1_455]	1.76	0.44
12:L:203:LEU:C	18:4:184:TYR:CZ[1_455]	1.76	0.44
15:1:170:PRO:C	16:2:132:LEU:CA[2_646]	1.81	0.39
12:L:205:TYR:CZ	18:4:181:GLU:O[1_455]	1.83	0.37
15:1:170:PRO:O	16:2:132:LEU:CG[2_646]	1.83	0.37
1:A:348:GLU:OE2	7:G:147:ASN:CG[1_556]	1.84	0.36
6:F:120:LYS:NZ	12:L:155:GLU:CD[2_556]	1.85	0.35
6:F:130:PHE:CE2	12:L:170:LYS:NZ[2_556]	1.85	0.35
1:A:200:GLU:OE1	2:B:220:GLN:NE2[1_556]	1.86	0.34
8:H:81:SER:OG	18:4:240:TRP:CH2[2_546]	1.86	0.34
6:F:130:PHE:CE1	12:L:170:LYS:CD[2_556]	1.88	0.32
15:1:171:LEU:CD2	16:2:132:LEU:N[2_646]	1.88	0.32
6:F:130:PHE:CD1	12:L:170:LYS:CD[2_556]	1.89	0.31
12:L:122:ASN:OD1	18:4:181:GLU:CD[1_455]	1.91	0.29
2:B:248:GLN:NE2	19:K:3009:CLA:CHC[1_554]	1.92	0.28
6:F:120:LYS:CE	12:L:155:GLU:CG[2_556]	1.92	0.28
12:L:204:LEU:CD2	18:4:185:PRO:O[1_455]	1.92	0.28
15:1:171:LEU:CG	16:2:132:LEU:N[2_646]	1.93	0.27
12:L:124:GLU:OE2	18:4:172:PHE:CD2[1_455]	1.95	0.25
7:G:85:GLU:OE2	22:K:7047:LMU:C7[2_546]	1.96	0.24
15:1:171:LEU:CD2	16:2:133:ASN:N[2_646]	1.96	0.24
2:B:205:GLU:OE1	11:K:69:ARG:NH1[1_554]	1.97	0.23
12:L:124:GLU:OE2	18:4:172:PHE:CG[1_455]	1.97	0.23
15:1:171:LEU:CB	16:2:132:LEU:N[2_646]	1.97	0.23
15:1:173:TYR:CE2	16:2:132:LEU:CA[2_646]	1.97	0.23
6:F:130:PHE:CE1	12:L:170:LYS:NZ[2_556]	1.98	0.22
2:B:248:GLN:CD	19:K:3009:CLA:CMC[1_554]	1.99	0.21
2:B:248:GLN:CD	19:K:3009:CLA:C2C[1_554]	1.99	0.21
2:B:5:ILE:CD1	6:F:111:ASP:OD1[2_546]	2.00	0.20
6:F:131:ASP:CG	12:L:170:LYS:CG[2_556]	2.01	0.19
15:1:170:PRO:O	16:2:132:LEU:N[2_646]	2.01	0.19
12:L:122:ASN:O	18:4:179:ALA:N[1_455]	2.02	0.18
12:L:203:LEU:N	18:4:184:TYR:OH[1_455]	2.02	0.18
4:D:160:ASN:OD1	6:F:101:LYS:NZ[2_546]	2.03	0.17
12:L:202:PHE:C	18:4:184:TYR:OH[1_455]	2.03	0.17
15:1:171:LEU:N	16:2:132:LEU:CA[2_646]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLU:OE2	7:G:147:ASN:ND2[1_556]	2.04	0.16
2:B:239:SER:OG	19:K:3009:CLA:CAA[1_554]	2.04	0.16
4:D:160:ASN:CB	6:F:101:LYS:NZ[2_546]	2.04	0.16
6:F:120:LYS:NZ	12:L:155:GLU:OE2[2_556]	2.05	0.15
15:1:171:LEU:N	16:2:131:ILE:C[2_646]	2.06	0.14
7:G:85:GLU:OE2	22:K:7047:LMU:C9[2_546]	2.07	0.13
1:A:348:GLU:CD	7:G:147:ASN:OD1[1_556]	2.10	0.10
15:1:171:LEU:CD2	16:2:131:ILE:CA[2_646]	2.10	0.10
6:F:130:PHE:CE2	12:L:170:LYS:CE[2_556]	2.11	0.09
12:L:123:THR:C	18:4:180:GLY:CA[1_455]	2.11	0.09
1:A:474:GLN:O	18:4:175:TYR:OH[1_455]	2.12	0.08
12:L:124:GLU:CD	18:4:172:PHE:CD2[1_455]	2.12	0.08
12:L:209:LEU:CD2	18:4:189:PHE:CE1[1_455]	2.13	0.07
15:1:173:TYR:CE1	16:2:132:LEU:C[2_646]	2.13	0.07
6:F:130:PHE:CG	12:L:170:LYS:CE[2_556]	2.14	0.06
12:L:204:LEU:CD2	18:4:185:PRO:C[1_455]	2.14	0.06
15:1:171:LEU:CD1	16:2:131:ILE:N[2_646]	2.14	0.06
6:F:130:PHE:CZ	12:L:170:LYS:NZ[2_556]	2.15	0.05
12:L:204:LEU:N	18:4:184:TYR:CZ[1_455]	2.15	0.05
15:1:171:LEU:CG	16:2:131:ILE:CB[2_646]	2.15	0.05
12:L:203:LEU:C	18:4:184:TYR:CE2[1_455]	2.16	0.04
12:L:123:THR:C	18:4:180:GLY:N[1_455]	2.17	0.03
6:F:112:ASP:OD2	9:I:30:LYS:NZ[2_556]	2.18	0.02
12:L:124:GLU:CD	18:4:172:PHE:CE1[1_455]	2.18	0.02
12:L:202:PHE:O	18:4:184:TYR:CZ[1_455]	2.19	0.01
15:1:171:LEU:CD1	16:2:131:ILE:CA[2_646]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	726/738 (98%)	483 (66%)	139 (19%)	104 (14%)	0 1
2	B	731/733 (100%)	527 (72%)	111 (15%)	93 (13%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	79/81 (98%)	42 (53%)	18 (23%)	19 (24%)	0 0
4	D	136/138 (99%)	94 (69%)	24 (18%)	18 (13%)	0 1
5	E	62/64 (97%)	44 (71%)	11 (18%)	7 (11%)	0 2
6	F	152/154 (99%)	105 (69%)	27 (18%)	20 (13%)	0 1
7	G	93/95 (98%)	60 (64%)	22 (24%)	11 (12%)	0 1
8	H	67/69 (97%)	49 (73%)	9 (13%)	9 (13%)	0 1
9	I	28/30 (93%)	11 (39%)	9 (32%)	8 (29%)	0 0
10	J	40/42 (95%)	19 (48%)	11 (28%)	10 (25%)	0 0
11	K	82/84 (98%)	66 (80%)	9 (11%)	7 (8%)	0 4
12	L	159/161 (99%)	110 (69%)	23 (14%)	26 (16%)	0 1
13	N	83/85 (98%)	50 (60%)	19 (23%)	14 (17%)	0 1
15	1	161/170 (95%)	119 (74%)	28 (17%)	14 (9%)	0 4
16	2	174/176 (99%)	129 (74%)	26 (15%)	19 (11%)	0 2
17	3	148/172 (86%)	111 (75%)	20 (14%)	17 (12%)	0 2
18	4	164/166 (99%)	129 (79%)	21 (13%)	14 (8%)	0 4
All	All	3085/3158 (98%)	2148 (70%)	527 (17%)	410 (13%)	0 1

All (410) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	41	SER
1	A	98	PHE
1	A	99	HIS
1	A	158	ILE
1	A	164	LEU
1	A	175	ALA
1	A	205	HIS
1	A	221	HIS
1	A	237	VAL
1	A	268	PRO
1	A	279	ASP
1	A	283	PHE
1	A	307	ALA
1	A	310	PHE
1	A	317	TYR
1	A	329	ASP

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Mol	Chain	Res	Type
1	A	333	ALA
1	A	346	LEU
1	A	361	ASN
1	A	386	ALA
1	A	389	TYR
1	A	424	PRO
1	A	431	LEU
1	A	433	ASP
1	A	473	PRO
1	A	474	GLN
1	A	477	PHE
1	A	509	ALA
1	A	523	VAL
1	A	532	ILE
1	A	553	VAL
1	A	594	ALA
1	A	643	ALA
1	A	657	LEU
1	A	673	SER
1	A	679	PHE
1	A	727	ILE
1	A	735	VAL
1	A	750	PHE
1	A	751	LEU
1	A	752	ALA
1	A	757	VAL
2	B	35	ASP
2	B	80	ASP
2	B	83	HIS
2	B	99	PRO
2	B	105	THR
2	B	142	LEU
2	B	160	LYS
2	B	170	ASN
2	B	182	LEU
2	B	187	SER
2	B	198	ALA
2	B	208	ARG
2	B	231	ASN
2	B	267	SER
2	B	308	HIS
2	B	321	GLY

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Mol	Chain	Res	Type
2	B	378	ILE
2	B	382	ILE
2	B	383	MET
2	B	420	SER
2	B	490	ARG
2	B	495	PRO
2	B	506	ASN
2	B	512	ILE
2	B	545	LYS
2	B	554	GLY
2	B	555	TYR
2	B	569	ASP
2	B	587	ILE
2	B	599	ILE
2	B	629	SER
2	B	639	VAL
2	B	661	PHE
2	B	662	MET
2	B	668	ARG
2	B	681	ALA
2	B	710	LEU
2	B	733	PHE
3	C	8	TYR
3	C	21	CYS
3	C	32	GLY
3	C	49	VAL
3	C	56	SER
3	C	59	PRO
3	C	62	PHE
3	C	65	VAL
4	D	107	PRO
4	D	124	GLU
4	D	132	ALA
4	D	151	LYS
4	D	173	TYR
4	D	186	GLN
4	D	193	LYS
4	D	207	PRO
5	E	73	LYS
5	E	92	ALA
5	E	102	PRO
5	E	103	VAL

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Mol	Chain	Res	Type
5	E	128	VAL
6	F	84	PRO
6	F	119	ILE
6	F	124	GLU
6	F	191	PRO
6	F	193	GLN
7	G	84	ARG
7	G	92	PRO
7	G	98	THR
7	G	130	TRP
7	G	142	LEU
7	G	150	ASP
8	H	62	THR
8	H	99	LYS
9	I	22	ALA
9	I	23	SER
10	J	5	LYS
10	J	6	THR
10	J	10	VAL
10	J	22	LEU
10	J	26	LEU
10	J	38	ILE
11	K	87	GLU
11	K	93	LEU
12	L	60	ILE
12	L	73	VAL
12	L	83	LEU
12	L	121	ARG
12	L	122	ASN
12	L	143	LEU
12	L	169	ARG
12	L	195	SER
13	N	97	THR
13	N	125	CYS
13	N	134	CYS
13	N	146	LEU
13	N	148	ASP
13	N	149	ASP
15	1	65	ASP
15	1	97	ILE
15	1	130	PRO
15	1	156	LYS

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Mol	Chain	Res	Type
15	1	169	ASP
15	1	170	PRO
15	1	177	PRO
15	1	217	LEU
15	1	225	TRP
16	2	139	THR
16	2	174	PRO
16	2	183	PHE
16	2	207	GLY
16	2	212	GLN
16	2	246	PRO
16	2	257	PRO
16	2	265	ALA
17	3	92	PHE
17	3	129	PRO
17	3	151	TRP
17	3	160	LEU
17	3	178	LYS
17	3	254	GLN
18	4	85	PRO
18	4	109	MET
18	4	120	ILE
18	4	134	TYR
1	A	22	VAL
1	A	35	ALA
1	A	57	LEU
1	A	160	SER
1	A	163	GLN
1	A	210	LEU
1	A	215	SER
1	A	247	GLU
1	A	249	ILE
1	A	250	LEU
1	A	294	LEU
1	A	308	ILE
1	A	313	ALA
1	A	347	TYR
1	A	373	ALA
1	A	400	MET
1	A	439	ARG
1	A	446	LEU
1	A	476	MET

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Mol	Chain	Res	Type
1	A	592	VAL
1	A	624	VAL
1	A	640	GLY
1	A	649	ILE
1	A	661	ALA
1	A	671	SER
1	A	717	ALA
2	B	26	ALA
2	B	153	GLY
2	B	178	HIS
2	B	179	LEU
2	B	188	LEU
2	B	330	ILE
2	B	371	LEU
2	B	375	HIS
2	B	379	ALA
2	B	437	TYR
2	B	501	ILE
2	B	505	SER
2	B	528	HIS
2	B	657	TRP
2	B	664	LEU
2	B	707	LEU
2	B	731	GLY
2	B	732	LYS
3	C	10	THR
3	C	12	ILE
3	C	28	MET
3	C	40	ALA
3	C	66	ARG
4	D	76	PRO
4	D	81	PRO
4	D	119	ALA
4	D	149	LYS
4	D	164	GLN
5	E	110	VAL
5	E	111	ASN
6	F	128	LYS
6	F	135	LYS
6	F	138	LEU
6	F	140	CYS
6	F	205	SER

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Mol	Chain	Res	Type
7	G	62	LEU
7	G	141	ILE
8	H	64	GLN
8	H	100	PHE
8	H	116	ALA
9	I	25	PHE
10	J	37	LEU
11	K	86	LEU
11	K	114	HIS
11	K	126	ASN
12	L	68	SER
12	L	200	ALA
13	N	109	THR
13	N	119	THR
13	N	147	SER
15	1	59	PRO
16	2	104	GLN
16	2	133	ASN
16	2	146	PHE
16	2	248	ASP
17	3	152	ALA
17	3	250	VAL
17	3	252	PRO
18	4	192	LEU
1	A	127	VAL
1	A	184	PHE
1	A	213	LEU
1	A	243	PRO
1	A	421	ASP
1	A	498	LEU
1	A	742	GLY
2	B	42	LEU
2	B	81	PRO
2	B	141	PHE
2	B	189	ALA
2	B	273	VAL
2	B	335	GLY
2	B	362	ALA
2	B	470	THR
2	B	558	PRO
2	B	592	PHE
3	C	23	THR

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Mol	Chain	Res	Type
3	C	52	LYS
4	D	88	GLY
4	D	175	GLU
4	D	184	VAL
6	F	102	LEU
6	F	103	GLN
6	F	121	ALA
6	F	186	ARG
8	H	98	LEU
10	J	9	SER
10	J	23	ALA
10	J	39	PHE
12	L	193	GLY
13	N	110	THR
13	N	132	THR
13	N	142	LYS
13	N	159	LYS
15	1	224	PRO
16	2	168	TRP
17	3	112	GLY
18	4	173	LYS
18	4	201	LYS
18	4	228	PRO
18	4	230	ASP
1	A	67	HIS
1	A	186	TYR
1	A	234	ASN
1	A	259	TYR
1	A	306	ILE
1	A	404	GLY
1	A	574	ASN
1	A	701	GLN
2	B	41	ARG
2	B	43	TYR
2	B	69	ALA
2	B	164	SER
2	B	281	ALA
2	B	309	ILE
2	B	474	PHE
2	B	476	ILE
2	B	593	TYR
2	B	595	HIS

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Mol	Chain	Res	Type
6	F	97	GLN
6	F	115	PRO
6	F	123	MET
6	F	160	PHE
8	H	69	GLY
8	H	117	SER
9	I	2	ILE
9	I	5	PRO
9	I	9	VAL
12	L	56	VAL
12	L	57	ILE
12	L	59	PRO
12	L	131	SER
12	L	159	SER
12	L	181	GLY
15	1	220	HIS
16	2	203	PRO
17	3	140	GLY
17	3	156	THR
17	3	248	THR
1	A	151	GLN
1	A	179	LEU
1	A	230	ASN
1	A	472	ARG
1	A	580	PRO
1	A	718	PRO
2	B	172	GLU
2	B	265	THR
2	B	278	LEU
2	B	311	PRO
2	B	391	PRO
2	B	398	TYR
2	B	457	PRO
2	B	514	PRO
2	B	596	TRP
2	B	623	TYR
2	B	730	SER
3	C	55	GLU
3	C	58	CYS
4	D	202	PHE
7	G	90	GLN
7	G	149	TYR

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Mol	Chain	Res	Type
8	H	120	ILE
11	K	48	PHE
11	K	80	ALA
12	L	55	GLN
12	L	175	GLN
15	1	119	GLY
16	2	95	ASP
16	2	206	TRP
17	3	202	TYR
17	3	230	ASN
17	3	234	ALA
18	4	179	ALA
18	4	223	VAL
18	4	243	THR
1	A	36	LYS
1	A	130	GLU
1	A	225	VAL
1	A	289	PRO
1	A	542	HIS
1	A	721	GLN
2	B	598	HIS
3	C	71	HIS
6	F	214	PRO
16	2	135	PRO
18	4	195	ALA
1	A	223	VAL
1	A	584	PRO
2	B	557	PHE
2	B	711	VAL
2	B	716	GLY
3	C	22	PRO
4	D	89	GLY
15	1	223	ASP
1	A	112	ASP
1	A	125	PRO
1	A	229	ILE
1	A	754	ILE
2	B	708	VAL
12	L	192	GLY
16	2	196	PRO
17	3	245	GLY
2	B	219	PRO

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Mol	Chain	Res	Type
12	L	107	GLY
12	L	118	GLY
12	L	158	PRO
1	A	124	TRP
1	A	190	ALA
6	F	215	VAL
7	G	78	VAL
9	I	12	VAL
12	L	99	GLY
13	N	166	VAL
16	2	130	GLY
18	4	163	PRO
9	I	10	PRO
12	L	62	GLY
12	L	115	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	590/599 (98%)	461 (78%)	129 (22%)	1 5
2	B	597/599 (100%)	464 (78%)	133 (22%)	1 5
3	C	70/70 (100%)	60 (86%)	10 (14%)	3 14
4	D	117/117 (100%)	83 (71%)	34 (29%)	0 2
5	E	56/56 (100%)	39 (70%)	17 (30%)	0 1
6	F	127/127 (100%)	91 (72%)	36 (28%)	0 2
7	G	78/79 (99%)	59 (76%)	19 (24%)	1 3
8	H	55/55 (100%)	43 (78%)	12 (22%)	1 5
9	I	26/26 (100%)	23 (88%)	3 (12%)	5 21
10	J	35/36 (97%)	23 (66%)	12 (34%)	0 1
11	K	62/62 (100%)	43 (69%)	19 (31%)	0 1
12	L	127/127 (100%)	102 (80%)	25 (20%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	N	74/74 (100%)	53 (72%)	21 (28%)	0 2
15	1	126/134 (94%)	75 (60%)	51 (40%)	0 0
16	2	139/142 (98%)	89 (64%)	50 (36%)	0 1
17	3	113/129 (88%)	73 (65%)	40 (35%)	0 1
18	4	136/140 (97%)	103 (76%)	33 (24%)	1 3
All	All	2528/2572 (98%)	1884 (74%)	644 (26%)	0 3

All (644) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	24	ARG
1	A	31	PHE
1	A	34	TRP
1	A	39	HIS
1	A	57	LEU
1	A	60	ASP
1	A	62	HIS
1	A	63	ASP
1	A	68	THR
1	A	78	VAL
1	A	93	LEU
1	A	103	PHE
1	A	104	SER
1	A	105	ASN
1	A	110	LEU
1	A	111	ASN
1	A	131	ILE
1	A	132	LEU
1	A	152	ILE
1	A	153	TRP
1	A	159	THR
1	A	160	SER
1	A	172	LEU
1	A	179	LEU
1	A	180	PHE
1	A	187	HIS
1	A	188	LYS
1	A	196	PHE
1	A	225	VAL

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Mol	Chain	Res	Type
1	A	232	PHE
1	A	233	LEU
1	A	246	HIS
1	A	248	PHE
1	A	250	LEU
1	A	252	ARG
1	A	254	LEU
1	A	255	LEU
1	A	267	THR
1	A	270	PHE
1	A	277	TYR
1	A	284	ARG
1	A	297	THR
1	A	298	ASP
1	A	299	ILE
1	A	309	LEU
1	A	312	ILE
1	A	328	LYS
1	A	331	LEU
1	A	334	HIS
1	A	338	PHE
1	A	341	GLN
1	A	349	ILE
1	A	350	LEU
1	A	351	THR
1	A	353	SER
1	A	358	LEU
1	A	368	LEU
1	A	369	THR
1	A	375	HIS
1	A	384	TYR
1	A	392	GLN
1	A	393	LEU
1	A	402	ILE
1	A	405	PHE
1	A	407	ILE
1	A	408	VAL
1	A	420	ARG
1	A	421	ASP
1	A	422	TYR
1	A	426	THR
1	A	427	ARG

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Mol	Chain	Res	Type
1	A	429	ASN
1	A	433	ASP
1	A	434	ARG
1	A	435	VAL
1	A	438	HIS
1	A	439	ARG
1	A	444	SER
1	A	462	ILE
1	A	464	ASN
1	A	467	MET
1	A	477	PHE
1	A	484	LEU
1	A	485	GLN
1	A	487	VAL
1	A	488	PHE
1	A	490	GLN
1	A	498	LEU
1	A	519	ASP
1	A	523	VAL
1	A	527	VAL
1	A	532	ILE
1	A	551	VAL
1	A	553	VAL
1	A	558	LYS
1	A	561	LEU
1	A	564	ARG
1	A	572	LYS
1	A	577	PHE
1	A	578	ARG
1	A	579	PHE
1	A	590	CYS
1	A	591	GLN
1	A	605	MET
1	A	613	ILE
1	A	623	ASP
1	A	637	ILE
1	A	646	SER
1	A	647	ILE
1	A	654	ARG
1	A	660	GLN
1	A	662	SER
1	A	664	VAL

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Mol	Chain	Res	Type
1	A	666	GLN
1	A	684	PHE
1	A	689	SER
1	A	691	MET
1	A	697	ARG
1	A	704	ILE
1	A	707	ILE
1	A	708	VAL
1	A	715	LYS
1	A	723	ARG
1	A	726	SER
1	A	727	ILE
1	A	736	THR
1	A	753	ARG
1	A	754	ILE
2	B	4	ARG
2	B	6	PRO
2	B	7	ARG
2	B	8	PHE
2	B	10	GLN
2	B	12	ILE
2	B	19	ARG
2	B	20	ARG
2	B	41	ARG
2	B	46	ILE
2	B	50	HIS
2	B	51	PHE
2	B	67	HIS
2	B	70	TRP
2	B	73	ASN
2	B	78	VAL
2	B	83	HIS
2	B	85	ARG
2	B	87	ILE
2	B	98	GLN
2	B	106	ARG
2	B	113	VAL
2	B	115	ASN
2	B	121	TYR
2	B	124	TRP
2	B	129	LEU
2	B	130	ARG

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Mol	Chain	Res	Type
2	B	131	THR
2	B	135	LEU
2	B	144	PHE
2	B	154	TRP
2	B	158	GLN
2	B	160	LYS
2	B	161	TRP
2	B	164	SER
2	B	165	VAL
2	B	177	HIS
2	B	188	LEU
2	B	195	VAL
2	B	199	ILE
2	B	206	TYR
2	B	207	VAL
2	B	212	PHE
2	B	229	GLN
2	B	233	TYR
2	B	241	ASN
2	B	244	PHE
2	B	247	THR
2	B	248	GLN
2	B	254	ILE
2	B	255	LEU
2	B	262	HIS
2	B	267	SER
2	B	269	TRP
2	B	285	LEU
2	B	291	TYR
2	B	295	PHE
2	B	299	HIS
2	B	317	ARG
2	B	319	HIS
2	B	320	LYS
2	B	332	PHE
2	B	343	VAL
2	B	347	LEU
2	B	348	VAL
2	B	350	GLN
2	B	361	ILE
2	B	365	PHE
2	B	367	THR

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Mol	Chain	Res	Type
2	B	374	HIS
2	B	382	ILE
2	B	393	PHE
2	B	395	ILE
2	B	396	ARG
2	B	410	ARG
2	B	420	SER
2	B	422	LEU
2	B	428	PHE
2	B	437	TYR
2	B	438	VAL
2	B	442	VAL
2	B	443	MET
2	B	448	THR
2	B	451	LYS
2	B	452	GLN
2	B	455	ILE
2	B	464	GLN
2	B	469	LYS
2	B	472	TYR
2	B	474	PHE
2	B	490	ARG
2	B	492	ILE
2	B	497	TRP
2	B	509	PHE
2	B	512	ILE
2	B	516	ASP
2	B	519	VAL
2	B	520	HIS
2	B	521	HIS
2	B	528	HIS
2	B	542	ARG
2	B	545	LYS
2	B	547	MET
2	B	551	LYS
2	B	564	ARG
2	B	580	VAL
2	B	583	MET
2	B	587	ILE
2	B	594	TRP
2	B	596	TRP
2	B	608	GLN

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Mol	Chain	Res	Type
2	B	613	SER
2	B	614	THR
2	B	615	TYR
2	B	617	MET
2	B	620	LEU
2	B	622	ASP
2	B	629	SER
2	B	662	MET
2	B	665	ILE
2	B	670	TYR
2	B	677	THR
2	B	682	HIS
2	B	685	THR
2	B	690	LEU
2	B	691	ILE
2	B	692	ARG
2	B	694	ARG
2	B	700	LEU
2	B	701	SER
2	B	710	LEU
2	B	732	LYS
2	B	733	PHE
3	C	1	MET
3	C	18	VAL
3	C	24	ASP
3	C	28	MET
3	C	38	GLN
3	C	45	THR
3	C	52	LYS
3	C	66	ARG
3	C	69	LEU
3	C	70	TRP
4	D	78	THR
4	D	80	SER
4	D	82	ILE
4	D	83	PHE
4	D	92	ARG
4	D	93	LYS
4	D	95	GLN
4	D	97	GLU
4	D	100	TYR
4	D	101	VAL

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Mol	Chain	Res	Type
4	D	104	TRP
4	D	105	ASP
4	D	109	GLU
4	D	112	PHE
4	D	122	MET
4	D	124	GLU
4	D	130	LYS
4	D	133	ARG
4	D	135	GLU
4	D	140	LEU
4	D	147	LYS
4	D	149	LYS
4	D	152	TYR
4	D	157	VAL
4	D	162	GLU
4	D	169	LYS
4	D	176	LYS
4	D	177	VAL
4	D	187	ASN
4	D	188	PHE
4	D	198	ILE
4	D	200	VAL
4	D	201	LYS
4	D	205	LYS
5	E	66	ILE
5	E	69	LYS
5	E	70	ARG
5	E	76	ILE
5	E	77	LEU
5	E	78	ARG
5	E	79	LYS
5	E	83	TRP
5	E	93	VAL
5	E	105	VAL
5	E	106	ARG
5	E	111	ASN
5	E	114	ASN
5	E	122	LEU
5	E	126	VAL
5	E	128	VAL
5	E	129	GLU
6	F	79	ILE

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Mol	Chain	Res	Type
6	F	86	LYS
6	F	89	LYS
6	F	94	ARG
6	F	100	LYS
6	F	103	GLN
6	F	106	LEU
6	F	107	LYS
6	F	125	LYS
6	F	128	LYS
6	F	131	ASP
6	F	135	LYS
6	F	136	TYR
6	F	138	LEU
6	F	149	ILE
6	F	151	SER
6	F	154	GLN
6	F	156	HIS
6	F	165	ILE
6	F	168	LEU
6	F	170	ILE
6	F	173	TRP
6	F	177	VAL
6	F	181	TYR
6	F	183	ILE
6	F	188	GLU
6	F	194	LYS
6	F	200	VAL
6	F	207	LEU
6	F	208	PHE
6	F	213	TRP
6	F	218	TYR
6	F	219	ARG
6	F	221	LEU
6	F	222	LEU
6	F	227	VAL
7	G	63	VAL
7	G	66	LEU
7	G	80	PHE
7	G	87	VAL
7	G	89	LYS
7	G	90	GLN
7	G	91	VAL

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Mol	Chain	Res	Type
7	G	94	GLN
7	G	95	ASN
7	G	97	LEU
7	G	98	THR
7	G	99	HIS
7	G	101	GLU
7	G	104	ASP
7	G	116	SER
7	G	125	VAL
7	G	127	VAL
7	G	144	THR
7	G	147	ASN
8	H	66	ASP
8	H	79	LEU
8	H	80	GLN
8	H	86	THR
8	H	93	LYS
8	H	94	ARG
8	H	99	LYS
8	H	100	PHE
8	H	109	LEU
8	H	112	LEU
8	H	113	SER
8	H	119	ASP
9	I	3	ASN
9	I	7	LEU
9	I	11	LEU
10	J	2	ARG
10	J	3	ASP
10	J	5	LYS
10	J	9	SER
10	J	10	VAL
10	J	14	VAL
10	J	16	THR
10	J	19	PHE
10	J	22	LEU
10	J	35	ASP
10	J	37	LEU
10	J	41	PHE
11	K	51	SER
11	K	53	THR
11	K	58	VAL

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Mol	Chain	Res	Type
11	K	59	THR
11	K	63	LEU
11	K	65	LEU
11	K	66	PHE
11	K	70	PHE
11	K	77	ASN
11	K	78	ARG
11	K	89	ARG
11	K	95	THR
11	K	102	THR
11	K	103	LEU
11	K	112	VAL
11	K	114	HIS
11	K	122	LEU
11	K	125	LYS
11	K	130	LEU
12	L	51	LYS
12	L	54	TYR
12	L	60	ILE
12	L	86	LEU
12	L	96	LEU
12	L	114	PHE
12	L	116	LYS
12	L	122	ASN
12	L	128	GLN
12	L	141	LEU
12	L	142	SER
12	L	145	LEU
12	L	151	SER
12	L	153	PHE
12	L	155	GLU
12	L	165	THR
12	L	171	LYS
12	L	172	GLU
12	L	182	TRP
12	L	186	THR
12	L	191	PHE
12	L	197	VAL
12	L	201	TYR
12	L	205	TYR
12	L	211	TYR
13	N	90	GLU

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Mol	Chain	Res	Type
13	N	91	TYR
13	N	94	LYS
13	N	96	LYS
13	N	99	LYS
13	N	104	LYS
13	N	110	THR
13	N	114	PHE
13	N	122	PHE
13	N	126	LYS
13	N	135	GLN
13	N	139	LYS
13	N	142	LYS
13	N	145	PHE
13	N	150	LEU
13	N	157	LYS
13	N	160	TYR
13	N	161	LYS
13	N	162	CYS
13	N	168	TRP
13	N	170	TRP
15	1	62	PHE
15	1	71	GLU
15	1	76	LEU
15	1	77	GLU
15	1	86	HIS
15	1	87	CYS
15	1	91	MET
15	1	92	LEU
15	1	94	VAL
15	1	97	ILE
15	1	98	LEU
15	1	101	GLU
15	1	103	LEU
15	1	117	LEU
15	1	123	THR
15	1	125	LEU
15	1	133	THR
15	1	136	THR
15	1	137	ILE
15	1	138	LEU
15	1	140	ILE
15	1	141	GLU

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Mol	Chain	Res	Type
15	1	145	ILE
15	1	147	PHE
15	1	149	GLU
15	1	150	HIS
15	1	151	GLN
15	1	154	MET
15	1	155	GLU
15	1	159	GLU
15	1	161	LYS
15	1	163	TYR
15	1	168	PHE
15	1	170	PRO
15	1	171	LEU
15	1	173	TYR
15	1	175	LYS
15	1	178	LYS
15	1	181	GLU
15	1	189	LYS
15	1	193	LEU
15	1	198	PHE
15	1	199	VAL
15	1	203	VAL
15	1	205	GLN
15	1	211	THR
15	1	214	LEU
15	1	215	GLU
15	1	224	PRO
15	1	225	TRP
15	1	226	HIS
16	2	94	SER
16	2	99	LEU
16	2	104	GLN
16	2	121	PHE
16	2	122	ILE
16	2	133	ASN
16	2	139	THR
16	2	143	GLN
16	2	144	GLU
16	2	150	THR
16	2	152	LEU
16	2	154	ILE
16	2	155	VAL

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Mol	Chain	Res	Type
16	2	156	GLU
16	2	157	LEU
16	2	158	VAL
16	2	159	PHE
16	2	167	ARG
16	2	168	TRP
16	2	173	ASN
16	2	183	PHE
16	2	185	ASN
16	2	187	LYS
16	2	188	LEU
16	2	189	THR
16	2	192	ASP
16	2	195	TYR
16	2	199	LEU
16	2	200	TRP
16	2	202	ASP
16	2	215	LYS
16	2	217	LEU
16	2	218	ARG
16	2	219	THR
16	2	220	LYS
16	2	222	ILE
16	2	226	ARG
16	2	229	MET
16	2	230	LEU
16	2	232	VAL
16	2	237	PHE
16	2	240	ILE
16	2	241	TYR
16	2	242	THR
16	2	244	THR
16	2	251	PHE
16	2	254	LEU
16	2	256	ASP
16	2	259	HIS
16	2	269	LYS
17	3	87	GLU
17	3	92	PHE
17	3	93	ILE
17	3	94	GLU
17	3	96	ARG

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Mol	Chain	Res	Type
17	3	97	TRP
17	3	102	GLU
17	3	108	PHE
17	3	111	LEU
17	3	124	LYS
17	3	134	LEU
17	3	136	TRP
17	3	137	PHE
17	3	142	ILE
17	3	151	TRP
17	3	153	ASP
17	3	155	TYR
17	3	156	THR
17	3	158	PHE
17	3	161	GLU
17	3	165	MET
17	3	167	PHE
17	3	173	PHE
17	3	174	GLN
17	3	175	ASP
17	3	181	SER
17	3	185	GLN
17	3	187	PHE
17	3	192	LYS
17	3	202	TYR
17	3	207	PHE
17	3	208	PHE
17	3	209	ASN
17	3	215	LYS
17	3	224	LYS
17	3	232	ARG
17	3	235	MET
17	3	247	VAL
17	3	248	THR
17	3	253	TYR
18	4	86	GLU
18	4	89	ARG
18	4	90	TRP
18	4	92	VAL
18	4	95	GLU
18	4	96	LEU
18	4	100	ARG

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Mol	Chain	Res	Type
18	4	101	TRP
18	4	115	PHE
18	4	118	ILE
18	4	131	LYS
18	4	139	SER
18	4	141	LEU
18	4	143	VAL
18	4	146	PHE
18	4	152	VAL
18	4	157	TRP
18	4	161	LYS
18	4	165	SER
18	4	166	VAL
18	4	172	PHE
18	4	175	TYR
18	4	177	LEU
18	4	188	ILE
18	4	192	LEU
18	4	201	LYS
18	4	205	ILE
18	4	214	PHE
18	4	226	LYS
18	4	234	GLN
18	4	238	ASP
18	4	241	HIS
18	4	245	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	82	HIS
1	A	115	HIS
1	A	129	GLN
1	A	163	GLN
1	A	187	HIS
1	A	224	HIS
1	A	273	ASN
1	A	302	HIS
1	A	303	HIS
1	A	315	HIS
1	A	341	GLN

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Mol	Chain	Res	Type
1	A	464	ASN
1	A	493	GLN
1	A	525	ASN
1	A	542	HIS
1	A	543	HIS
1	A	545	HIS
1	A	591	GLN
1	A	607	ASN
1	A	644	GLN
1	A	660	GLN
1	A	683	HIS
1	A	711	HIS
1	A	729	GLN
2	B	10	GLN
2	B	50	HIS
2	B	53	GLN
2	B	67	HIS
2	B	73	ASN
2	B	83	HIS
2	B	98	GLN
2	B	114	ASN
2	B	158	GLN
2	B	170	ASN
2	B	178	HIS
2	B	193	HIS
2	B	231	ASN
2	B	277	HIS
2	B	294	ASN
2	B	319	HIS
2	B	331	HIS
2	B	333	GLN
2	B	375	HIS
2	B	402	GLN
2	B	403	ASN
2	B	432	HIS
2	B	452	GLN
2	B	502	ASN
2	B	521	HIS
2	B	595	HIS
2	B	598	HIS
2	B	610	ASN
2	B	633	ASN

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Mol	Chain	Res	Type
2	B	712	HIS
3	C	71	HIS
4	D	95	GLN
4	D	110	GLN
4	D	136	GLN
4	D	182	GLN
4	D	187	ASN
5	E	111	ASN
6	F	97	GLN
6	F	193	GLN
7	G	147	ASN
8	H	77	ASN
8	H	80	GLN
9	I	27	HIS
11	K	77	ASN
11	K	114	HIS
12	L	85	ASN
12	L	106	HIS
12	L	122	ASN
13	N	98	ASN
13	N	130	ASN
13	N	135	GLN
15	1	86	HIS
15	1	112	GLN
15	1	151	GLN
15	1	190	ASN
15	1	204	GLN
15	1	205	GLN
15	1	226	HIS
16	2	133	ASN
16	2	173	ASN
16	2	238	GLN
17	3	149	ASN
17	3	174	GLN
17	3	209	ASN
17	3	254	GLN
18	4	158	GLN
18	4	190	ASN
18	4	246	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

252 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	LMU	R	7021	-	36,36,36	0.75	1 (2%)	47,47,47	1.37	6 (12%)
19	CLA	A	1104	-	61,65,73	2.28	14 (22%)	72,103,113	2.88	29 (40%)
19	CLA	L	1130	1	69,73,73	2.22	15 (21%)	82,113,113	2.56	26 (31%)
22	LMU	B	7012	-	26,26,36	0.79	1 (3%)	37,37,47	1.43	8 (21%)
19	CLA	B	1217	-	54,58,73	2.38	14 (25%)	64,95,113	2.95	26 (40%)
19	CLA	A	1116	1	56,60,73	2.46	13 (23%)	65,97,113	2.96	26 (40%)
19	CLA	L	1502	12	51,55,73	2.50	13 (25%)	60,91,113	3.18	24 (40%)
19	CLA	1	1014	-	65,69,73	2.32	17 (26%)	77,108,113	2.65	23 (29%)
19	CLA	B	1223	2	69,73,73	2.18	15 (21%)	82,113,113	2.45	25 (30%)
19	CLA	3	3005	-	24,32,73	2.35	8 (33%)	31,54,113	2.90	17 (54%)
19	CLA	3	3012	-	24,32,73	2.37	9 (37%)	31,54,113	2.98	18 (58%)
19	CLA	A	1115	-	69,73,73	2.22	17 (24%)	82,113,113	2.65	23 (28%)
19	CLA	A	1106	-	69,73,73	2.16	16 (23%)	82,113,113	2.62	28 (34%)
21	BCR	F	6016	-	41,41,41	1.58	9 (21%)	56,56,56	3.72	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LMU	4	7034	22	36,36,36	0.64	0	47,47,47	0.71	0
19	CLA	B	1209	2	59,63,73	2.30	16 (27%)	70,101,113	2.70	25 (35%)
19	CLA	B	1213	-	50,54,73	2.50	13 (26%)	59,90,113	2.89	26 (44%)
19	CLA	B	1219	2	59,63,73	2.47	16 (27%)	70,101,113	2.70	21 (30%)
19	CLA	A	1129	1	54,58,73	2.46	14 (25%)	64,95,113	2.98	25 (39%)
19	CLA	B	1238	-	69,73,73	2.16	14 (20%)	82,113,113	2.67	29 (35%)
19	CLA	3	3008	-	54,58,73	2.47	18 (33%)	64,95,113	3.09	25 (39%)
19	CLA	3	3011	-	69,73,73	2.15	16 (23%)	82,113,113	2.51	23 (28%)
22	LMU	R	7025	-	36,36,36	0.77	1 (2%)	47,47,47	1.21	4 (8%)
19	CLA	H	1241	-	59,63,73	2.40	12 (20%)	70,101,113	2.65	25 (35%)
19	CLA	B	1234	2	64,68,73	2.21	15 (23%)	76,107,113	2.89	20 (26%)
19	CLA	2	1307	-	24,32,73	2.38	8 (33%)	31,54,113	2.87	19 (61%)
19	CLA	2	2005	-	24,32,73	2.35	8 (33%)	31,54,113	2.92	18 (58%)
19	CLA	4	4001	-	54,58,73	2.51	14 (25%)	64,95,113	2.78	23 (35%)
21	BCR	B	6005	-	41,41,41	1.19	4 (9%)	56,56,56	4.84	32 (57%)
21	BCR	I	6018	-	41,41,41	1.30	4 (9%)	56,56,56	4.80	32 (57%)
19	CLA	A	1110	1	58,62,73	2.37	15 (25%)	68,99,113	2.60	24 (35%)
19	CLA	3	2009	17	60,64,73	2.44	19 (31%)	71,102,113	2.74	27 (38%)
19	CLA	F	1302	19	45,49,73	2.68	16 (35%)	54,84,113	3.09	24 (44%)
19	CLA	4	4002	18	56,60,73	2.70	23 (41%)	65,97,113	3.28	34 (52%)
19	CLA	B	1206	2	69,73,73	2.13	15 (21%)	82,113,113	2.45	22 (26%)
19	CLA	B	1233	-	55,59,73	2.49	12 (21%)	64,96,113	2.98	26 (40%)
22	LMU	D	7050	4	36,36,36	0.62	1 (2%)	47,47,47	0.83	1 (2%)
19	CLA	A	1133	1	54,58,73	2.46	15 (27%)	64,95,113	2.85	25 (39%)
19	CLA	A	1126	-	69,73,73	2.15	15 (21%)	82,113,113	2.59	28 (34%)
22	LMU	B	7040	-	36,36,36	0.75	1 (2%)	47,47,47	1.62	10 (21%)
19	CLA	B	1222	-	62,66,73	2.29	15 (24%)	73,104,113	2.74	26 (35%)
19	CLA	B	1229	2	69,73,73	2.23	16 (23%)	82,113,113	2.83	25 (30%)
19	CLA	B	1228	2	54,58,73	2.36	13 (24%)	64,95,113	2.98	29 (45%)
19	CLA	4	4013	18	24,32,73	2.33	8 (33%)	31,54,113	2.66	19 (61%)
19	CLA	K	3009	2	69,73,73	2.20	13 (18%)	82,113,113	2.55	28 (34%)
19	CLA	3	3007	-	46,50,73	2.50	12 (26%)	53,85,113	3.14	26 (49%)
19	CLA	A	9011	-	69,73,73	2.15	17 (24%)	82,113,113	2.67	27 (32%)
19	CLA	A	1121	1	46,50,73	2.55	13 (28%)	53,85,113	3.25	24 (45%)
19	CLA	A	1103	1	69,73,73	2.12	14 (20%)	82,113,113	2.67	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LMU	H	7043	-	36,36,36	0.86	2 (5%)	47,47,47	1.66	10 (21%)
19	CLA	A	1135	-	55,59,73	2.45	17 (30%)	64,96,113	2.75	23 (35%)
19	CLA	2	2002	-	60,64,73	2.36	14 (23%)	71,102,113	2.87	31 (43%)
21	BCR	3	6022	-	41,41,41	1.23	3 (7%)	56,56,56	5.03	26 (46%)
19	CLA	A	1136	1	69,73,73	2.16	16 (23%)	82,113,113	2.60	25 (30%)
22	LMU	A	7016	-	36,36,36	0.68	0	47,47,47	1.44	6 (12%)
22	LMU	H	7030	-	36,36,36	0.77	2 (5%)	47,47,47	1.20	5 (10%)
19	CLA	B	1220	-	69,73,73	2.47	22 (31%)	82,113,113	2.76	30 (36%)
19	CLA	A	1137	-	51,55,73	2.51	16 (31%)	60,91,113	2.96	25 (41%)
22	LMU	4	7009	-	35,35,36	1.36	2 (5%)	46,46,47	1.26	4 (8%)
19	CLA	A	1132	-	69,73,73	2.20	14 (20%)	82,113,113	2.82	29 (35%)
19	CLA	4	1004	18	59,63,73	2.45	18 (30%)	70,101,113	2.89	29 (41%)
19	CLA	3	1118	-	38,44,73	2.81	13 (34%)	52,78,113	3.36	23 (44%)
19	CLA	J	1308	19	59,63,73	2.40	19 (32%)	70,101,113	2.96	27 (38%)
22	LMU	3	7003	-	36,36,36	0.80	0	47,47,47	1.48	7 (14%)
21	BCR	I	6021	-	41,41,41	1.97	8 (19%)	56,56,56	4.87	32 (57%)
22	LMU	R	7020	-	36,36,36	0.67	0	47,47,47	1.40	6 (12%)
22	LMU	K	7047	-	36,36,36	0.80	1 (2%)	47,47,47	1.06	3 (6%)
21	BCR	1	6023	-	41,41,41	1.56	3 (7%)	56,56,56	6.49	30 (53%)
19	CLA	L	1503	-	54,58,73	2.60	19 (35%)	64,95,113	3.22	24 (37%)
19	CLA	1	1013	-	55,59,73	2.67	20 (36%)	64,96,113	3.54	26 (40%)
22	LMU	G	7026	-	36,36,36	0.87	2 (5%)	47,47,47	1.52	6 (12%)
19	CLA	3	3006	-	24,32,73	2.36	9 (37%)	31,54,113	2.92	17 (54%)
19	CLA	H	1505	-	59,63,73	2.36	13 (22%)	70,101,113	2.89	27 (38%)
20	PQN	A	5001	-	34,34,34	1.73	2 (5%)	43,45,45	1.44	7 (16%)
19	CLA	A	1127	1	59,63,73	2.30	16 (27%)	70,101,113	2.73	25 (35%)
19	CLA	B	1227	2	54,58,73	2.56	15 (27%)	64,95,113	2.75	25 (39%)
19	CLA	B	1221	-	58,62,73	2.41	19 (32%)	68,99,113	2.77	26 (38%)
19	CLA	B	1301	-	38,44,73	2.90	13 (34%)	52,78,113	3.36	29 (55%)
19	CLA	A	1139	-	55,59,73	2.45	16 (29%)	64,96,113	2.91	25 (39%)
23	SF4	C	8003	3	0,12,12	-	-	-		
19	CLA	1	1015	-	24,32,73	2.41	8 (33%)	31,54,113	2.82	18 (58%)
21	BCR	A	6007	-	41,41,41	1.45	4 (9%)	56,56,56	3.89	32 (57%)
21	BCR	A	6011	-	41,41,41	1.22	4 (9%)	56,56,56	4.29	31 (55%)
19	CLA	A	1119	-	69,73,73	2.19	15 (21%)	82,113,113	2.62	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A	1102	19	59,63,73	2.38	15 (25%)	70,101,113	2.80	27 (38%)
19	CLA	A	1107	-	59,63,73	2.30	14 (23%)	70,101,113	2.77	31 (44%)
19	CLA	1	1012	15	38,44,73	2.79	11 (28%)	52,78,113	3.11	21 (40%)
19	CLA	R	1150	-	69,73,73	2.26	13 (18%)	82,113,113	2.60	28 (34%)
22	LMU	A	7044	-	36,36,36	0.87	1 (2%)	47,47,47	1.59	9 (19%)
19	CLA	2	2011	-	24,32,73	2.36	8 (33%)	31,54,113	2.81	18 (58%)
19	CLA	A	1109	19,1	69,73,73	2.14	13 (18%)	82,113,113	2.81	29 (35%)
21	BCR	B	6006	-	41,41,41	1.49	8 (19%)	56,56,56	4.62	26 (46%)
19	CLA	A	9013	-	69,73,73	2.28	16 (23%)	82,113,113	2.71	28 (34%)
22	LMU	G	7051	-	36,36,36	0.87	1 (2%)	47,47,47	2.12	11 (23%)
19	CLA	3	3014	-	24,32,73	2.43	9 (37%)	31,54,113	3.01	19 (61%)
19	CLA	B	1224	-	69,73,73	2.27	15 (21%)	82,113,113	2.76	23 (28%)
22	LMU	C	7015	-	36,36,36	0.69	1 (2%)	47,47,47	1.28	6 (12%)
19	CLA	2	2010	-	24,32,73	2.36	7 (29%)	31,54,113	2.74	17 (54%)
19	CLA	2	2014	19	65,69,73	2.30	21 (32%)	77,108,113	2.78	27 (35%)
19	CLA	A	1140	1	69,73,73	2.15	16 (23%)	82,113,113	2.51	26 (31%)
19	CLA	B	1235	2	69,73,73	2.10	14 (20%)	82,113,113	2.48	23 (28%)
19	CLA	B	1226	2	69,73,73	2.15	16 (23%)	82,113,113	2.72	27 (32%)
19	CLA	K	1142	-	49,53,73	2.56	15 (30%)	58,89,113	2.91	19 (32%)
19	CLA	2	2007	-	69,73,73	2.15	12 (17%)	82,113,113	2.58	28 (34%)
19	CLA	4	4014	-	51,55,73	2.50	15 (29%)	60,91,113	3.30	26 (43%)
19	CLA	2	2004	-	54,58,73	2.45	14 (25%)	64,95,113	2.69	22 (34%)
19	CLA	A	9012	-	69,73,73	2.21	17 (24%)	82,113,113	2.58	25 (30%)
22	LMU	G	7039	-	36,36,36	0.68	0	47,47,47	1.37	4 (8%)
22	LMU	R	7022	-	36,36,36	0.73	1 (2%)	47,47,47	1.34	7 (14%)
22	LMU	F	7036	-	35,35,36	0.76	1 (2%)	46,46,47	1.44	6 (13%)
19	CLA	4	4007	-	56,60,73	2.41	14 (25%)	65,97,113	2.70	25 (38%)
19	CLA	H	1207	-	69,73,73	2.23	15 (21%)	82,113,113	2.79	26 (31%)
22	LMU	E	7048	-	36,36,36	0.83	1 (2%)	47,47,47	2.05	10 (21%)
19	CLA	H	1145	-	69,73,73	2.14	16 (23%)	82,113,113	2.86	26 (31%)
22	LMU	H	7017	-	36,36,36	0.74	1 (2%)	47,47,47	1.92	11 (23%)
19	CLA	A	1309	-	24,32,73	2.33	8 (33%)	31,54,113	2.78	18 (58%)
19	CLA	2	4009	-	69,73,73	2.19	14 (20%)	82,113,113	2.71	26 (31%)
19	CLA	4	4006	-	59,63,73	2.36	12 (20%)	70,101,113	2.72	25 (35%)
19	CLA	3	1147	17	50,54,73	2.88	25 (50%)	59,90,113	3.20	34 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	1211	-	69,73,73	2.18	13 (18%)	82,113,113	2.51	26 (31%)
19	CLA	3	3010	-	24,32,73	2.33	9 (37%)	31,54,113	2.81	18 (58%)
19	CLA	2	2003	16	24,32,73	2.36	8 (33%)	31,54,113	2.89	19 (61%)
21	BCR	B	6020	-	41,41,41	1.89	10 (24%)	56,56,56	4.54	27 (48%)
21	BCR	L	6019	-	41,41,41	1.50	11 (26%)	56,56,56	4.39	24 (42%)
22	LMU	R	7007	-	36,36,36	0.58	1 (2%)	47,47,47	0.81	2 (4%)
22	LMU	R	7024	-	36,36,36	0.76	1 (2%)	47,47,47	1.47	8 (17%)
22	LMU	2	7027	-	36,36,36	0.81	1 (2%)	47,47,47	1.69	11 (23%)
19	CLA	B	1202	-	69,73,73	2.17	15 (21%)	82,113,113	2.91	30 (36%)
22	LMU	R	7014	-	36,36,36	0.91	2 (5%)	47,47,47	2.03	8 (17%)
19	CLA	A	1124	-	69,73,73	2.14	15 (21%)	82,113,113	2.55	26 (31%)
19	CLA	3	3015	-	24,32,73	2.38	7 (29%)	31,54,113	2.77	19 (61%)
22	LMU	B	7038	-	36,36,36	0.74	0	47,47,47	1.71	11 (23%)
22	LMU	4	7018	-	36,36,36	0.75	1 (2%)	47,47,47	1.08	3 (6%)
19	CLA	F	1305	19	57,61,73	2.62	23 (40%)	67,98,113	2.80	27 (40%)
19	CLA	3	3017	-	54,58,73	2.51	17 (31%)	64,95,113	3.24	29 (45%)
19	CLA	3	3013	17	69,73,73	2.29	20 (28%)	82,113,113	2.94	25 (30%)
19	CLA	L	1504	-	59,63,73	2.38	13 (22%)	70,101,113	2.73	30 (42%)
22	LMU	H	7002	-	36,36,36	0.61	0	47,47,47	1.54	7 (14%)
19	CLA	K	1146	-	54,58,73	2.65	21 (38%)	64,95,113	3.00	27 (42%)
19	CLA	1	1001	15	50,54,73	2.73	20 (40%)	59,90,113	3.56	31 (52%)
19	CLA	1	1303	-	55,59,73	2.71	24 (43%)	64,96,113	3.15	29 (45%)
23	SF4	C	8002	3	0,12,12	-	-	-		
22	LMU	A	7023	-	36,36,36	0.60	0	47,47,47	1.19	4 (8%)
19	CLA	B	9010	2	69,73,73	2.12	16 (23%)	82,113,113	2.62	33 (40%)
24	LMG	B	7101	-	49,49,55	1.04	3 (6%)	57,57,63	1.02	3 (5%)
19	CLA	A	1120	-	55,59,73	2.48	15 (27%)	64,96,113	2.91	24 (37%)
19	CLA	2	2008	-	24,32,73	2.41	8 (33%)	31,54,113	2.95	18 (58%)
22	LMU	3	7005	-	36,36,36	0.71	0	47,47,47	2.12	13 (27%)
19	CLA	4	4011	-	24,32,73	2.49	8 (33%)	31,54,113	2.88	19 (61%)
22	LMU	4	7053	-	35,35,36	0.71	1 (2%)	46,46,47	1.27	6 (13%)
19	CLA	3	3004	-	24,32,73	2.33	10 (41%)	31,54,113	3.10	19 (61%)
21	BCR	A	6003	-	41,41,41	1.42	2 (4%)	56,56,56	4.20	29 (51%)
19	CLA	A	1237	-	69,73,73	2.12	15 (21%)	82,113,113	2.73	28 (34%)
19	CLA	2	2006	-	69,73,73	2.17	13 (18%)	82,113,113	2.69	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	B	6010	-	41,41,41	1.20	2 (4%)	56,56,56	4.37	30 (53%)
22	LMU	4	7052	22	36,36,36	1.23	4 (11%)	47,47,47	1.81	8 (17%)
19	CLA	1	1003	-	51,55,73	2.50	12 (23%)	60,91,113	3.17	26 (43%)
19	CLA	B	1218	-	50,54,73	2.48	15 (30%)	59,90,113	3.11	19 (32%)
19	CLA	B	1215	2	64,68,73	2.21	14 (21%)	76,107,113	2.69	29 (38%)
19	CLA	1	1005	-	50,54,73	2.78	14 (28%)	59,90,113	2.85	22 (37%)
21	BCR	J	6012	-	41,41,41	1.31	5 (12%)	56,56,56	5.56	27 (48%)
22	LMU	2	7046	-	36,36,36	0.71	1 (2%)	47,47,47	0.88	3 (6%)
21	BCR	A	6008	-	41,41,41	1.16	4 (9%)	56,56,56	4.18	28 (50%)
19	CLA	J	1311	-	65,69,73	2.24	15 (23%)	77,108,113	2.72	25 (32%)
19	CLA	K	1143	-	54,58,73	2.44	14 (25%)	64,95,113	2.82	27 (42%)
19	CLA	L	1148	-	59,63,73	2.64	24 (40%)	70,101,113	3.37	34 (48%)
19	CLA	4	1306	-	59,63,73	2.31	13 (22%)	70,101,113	2.83	26 (37%)
22	LMU	1	7004	-	36,36,36	0.68	1 (2%)	47,47,47	0.81	1 (2%)
19	CLA	A	1138	-	69,73,73	2.17	14 (20%)	82,113,113	2.54	25 (30%)
22	LMU	N	7049	-	36,36,36	0.58	1 (2%)	47,47,47	1.37	4 (8%)
20	PQN	B	5002	-	34,34,34	1.64	2 (5%)	43,45,45	1.52	6 (13%)
19	CLA	A	1125	1	69,73,73	2.18	16 (23%)	82,113,113	2.43	23 (28%)
19	CLA	A	1134	1	49,53,73	2.54	15 (30%)	58,89,113	3.09	22 (37%)
19	CLA	1	1002	15	51,55,73	2.54	14 (27%)	60,91,113	2.82	23 (38%)
19	CLA	4	4012	-	38,44,73	2.79	12 (31%)	52,78,113	3.45	25 (48%)
19	CLA	1	1008	-	55,59,73	2.51	14 (25%)	64,96,113	3.36	25 (39%)
19	CLA	I	1204	-	64,68,73	2.26	15 (23%)	76,107,113	2.73	22 (28%)
22	LMU	K	7001	-	36,36,36	0.82	2 (5%)	47,47,47	1.38	7 (14%)
19	CLA	2	2012	16	54,58,73	2.40	14 (25%)	64,95,113	2.89	25 (39%)
19	CLA	B	1236	-	51,55,73	2.47	15 (29%)	60,91,113	2.94	26 (43%)
19	CLA	B	1208	2	58,62,73	2.61	13 (22%)	71,100,113	2.76	28 (39%)
19	CLA	3	3003	-	38,44,73	2.80	12 (31%)	52,78,113	3.07	22 (42%)
22	LMU	H	7032	-	36,36,36	0.73	1 (2%)	47,47,47	1.45	6 (12%)
22	LMU	2	7006	-	36,36,36	0.64	1 (2%)	47,47,47	0.73	0
19	CLA	B	1201	-	49,53,73	2.61	17 (34%)	58,89,113	3.06	21 (36%)
19	CLA	1	1006	19	38,44,73	2.92	13 (34%)	52,78,113	3.24	23 (44%)
19	CLA	4	4005	-	24,32,73	2.39	9 (37%)	31,54,113	2.92	18 (58%)
19	CLA	B	1230	2	54,58,73	2.50	18 (33%)	64,95,113	2.93	24 (37%)
19	CLA	F	1240	-	38,44,73	2.79	15 (39%)	52,78,113	3.09	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LMU	A	7045	-	36,36,36	0.75	1 (2%)	47,47,47	1.50	9 (19%)
19	CLA	2	2013	-	54,58,73	2.51	12 (22%)	64,95,113	2.97	25 (39%)
19	CLA	4	4004	-	24,32,73	2.39	7 (29%)	31,54,113	2.87	17 (54%)
22	LMU	H	7011	-	36,36,36	0.77	2 (5%)	47,47,47	1.99	10 (21%)
19	CLA	A	9022	-	69,73,73	2.16	15 (21%)	82,113,113	2.63	28 (34%)
22	LMU	L	7029	-	36,36,36	0.69	1 (2%)	47,47,47	0.74	0
23	SF4	A	8001	2,1	0,12,12	-	-	-		
19	CLA	A	9023	-	69,73,73	2.22	14 (20%)	82,113,113	2.57	28 (34%)
19	CLA	B	1232	19	49,53,73	2.59	13 (26%)	58,89,113	3.04	22 (37%)
19	CLA	4	1009	-	38,44,73	3.01	14 (36%)	52,78,113	3.46	21 (40%)
19	CLA	B	1212	2	64,68,73	2.21	12 (18%)	76,107,113	2.53	25 (32%)
19	CLA	4	4010	-	24,32,73	2.33	8 (33%)	31,54,113	2.86	18 (58%)
22	LMU	A	7010	-	36,36,36	1.32	2 (5%)	47,47,47	1.21	5 (10%)
22	LMU	4	7033	-	36,36,36	0.76	1 (2%)	47,47,47	1.61	9 (19%)
19	CLA	A	1117	-	69,73,73	2.17	15 (21%)	82,113,113	2.58	27 (32%)
22	LMU	A	7035	-	36,36,36	0.61	0	47,47,47	1.59	8 (17%)
19	CLA	3	3002	-	24,32,73	2.44	8 (33%)	31,54,113	2.79	19 (61%)
19	CLA	A	1123	-	69,73,73	2.10	15 (21%)	82,113,113	2.45	24 (29%)
19	CLA	A	1141	-	69,73,73	2.17	14 (20%)	82,113,113	2.63	26 (31%)
19	CLA	B	1205	-	69,73,73	2.18	13 (18%)	82,113,113	2.70	25 (30%)
19	CLA	4	4015	-	50,54,73	2.54	20 (40%)	59,90,113	2.98	25 (42%)
22	LMU	4	7019	-	36,36,36	0.82	1 (2%)	47,47,47	1.36	9 (19%)
19	CLA	A	1122	-	59,63,73	2.38	15 (25%)	70,101,113	2.75	24 (34%)
19	CLA	A	1128	1	69,73,73	2.16	15 (21%)	82,113,113	2.55	26 (31%)
19	CLA	B	1210	-	69,73,73	2.20	16 (23%)	82,113,113	2.46	24 (29%)
19	CLA	A	1151	-	54,58,73	2.49	17 (31%)	64,95,113	2.73	23 (35%)
22	LMU	K	7041	-	36,36,36	0.57	0	47,47,47	1.07	3 (6%)
19	CLA	4	4003	-	59,63,73	2.38	16 (27%)	70,101,113	2.66	24 (34%)
19	CLA	2	2001	-	55,59,73	2.43	16 (29%)	64,96,113	2.81	25 (39%)
21	BCR	B	6017	-	41,41,41	1.33	5 (12%)	56,56,56	4.06	25 (44%)
19	CLA	B	1231	2,19	49,53,73	2.62	16 (32%)	58,89,113	2.96	21 (36%)
19	CLA	1	1310	-	24,32,73	2.37	7 (29%)	31,54,113	3.08	19 (61%)
21	BCR	A	6002	-	41,41,41	1.83	5 (12%)	56,56,56	4.74	35 (62%)
19	CLA	G	1242	-	55,59,73	2.48	14 (25%)	64,96,113	2.92	27 (42%)
19	CLA	A	1112	1	49,53,73	2.56	13 (26%)	58,89,113	2.92	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A	1108	-	49,53,73	2.64	16 (32%)	58,89,113	3.02	24 (41%)
22	LMU	H	7028	-	36,36,36	0.59	0	47,47,47	0.99	2 (4%)
22	LMU	2	7031	-	36,36,36	1.23	2 (5%)	47,47,47	1.35	6 (12%)
19	CLA	A	1149	-	50,54,73	2.78	16 (32%)	61,90,113	3.76	34 (55%)
19	CLA	B	1216	-	65,69,73	2.18	16 (24%)	77,108,113	2.73	25 (32%)
19	CLA	1	1011	-	38,44,73	3.12	19 (50%)	52,78,113	3.82	26 (50%)
19	CLA	A	1131	1	69,73,73	2.20	16 (23%)	82,113,113	2.60	23 (28%)
19	CLA	A	1105	1	50,54,73	2.49	12 (24%)	59,90,113	2.93	25 (42%)
19	CLA	A	1113	1	54,58,73	2.51	13 (24%)	64,95,113	2.76	26 (40%)
19	CLA	B	1203	-	69,73,73	2.18	16 (23%)	82,113,113	2.87	32 (39%)
19	CLA	3	3016	-	69,73,73	2.18	15 (21%)	82,113,113	2.57	24 (29%)
19	CLA	A	1111	1	58,62,73	2.29	15 (25%)	68,99,113	2.78	26 (38%)
19	CLA	A	1101	-	54,58,73	2.39	14 (25%)	64,95,113	3.06	26 (40%)
19	CLA	L	1501	12	54,58,73	2.47	15 (27%)	64,95,113	2.83	25 (39%)
19	CLA	3	3001	-	24,32,73	2.44	9 (37%)	31,54,113	2.87	20 (64%)
21	BCR	B	6004	-	41,41,41	1.11	4 (9%)	56,56,56	4.38	30 (53%)
21	BCR	F	6014	-	41,41,41	1.27	4 (9%)	56,56,56	4.95	27 (48%)
19	CLA	B	1214	-	63,67,73	2.30	14 (22%)	74,105,113	2.51	22 (29%)
22	LMU	E	7037	-	36,36,36	0.74	1 (2%)	47,47,47	1.77	11 (23%)
22	LMU	4	7008	-	36,36,36	0.58	0	47,47,47	0.88	1 (2%)
22	LMU	K	7042	-	36,36,36	0.63	0	47,47,47	1.17	5 (10%)
19	CLA	R	1144	-	61,65,73	2.33	13 (21%)	72,103,113	2.81	28 (38%)
19	CLA	B	1239	-	69,73,73	2.10	15 (21%)	82,113,113	2.69	27 (32%)
19	CLA	1	1010	19	50,54,73	2.79	22 (44%)	59,90,113	3.38	28 (47%)
22	LMU	1	7013	-	36,36,36	0.71	1 (2%)	47,47,47	1.07	1 (2%)
19	CLA	1	1007	-	65,69,73	2.25	15 (23%)	77,108,113	2.59	28 (36%)
19	CLA	B	1225	-	69,73,73	2.11	14 (20%)	82,113,113	2.73	28 (34%)
19	CLA	4	1304	-	69,73,73	2.26	21 (30%)	82,113,113	3.03	32 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMU	R	7021	-	-	14/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1104	-	1/1/13/20	7/30/106/115	-
19	CLA	L	1130	1	1/1/15/20	17/39/115/115	-
22	LMU	B	7012	-	-	5/11/51/61	0/2/2/2
19	CLA	B	1217	-	-	7/21/97/115	-
19	CLA	A	1116	1	-	11/24/100/115	-
19	CLA	L	1502	12	-	9/18/94/115	-
19	CLA	1	1014	-	1/1/14/20	15/35/111/115	-
19	CLA	B	1223	2	1/1/15/20	19/39/115/115	-
19	CLA	A	1115	-	1/1/15/20	15/39/115/115	-
19	CLA	A	1106	-	1/1/15/20	22/39/115/115	-
21	BCR	F	6016	-	-	13/29/63/63	0/2/2/2
22	LMU	4	7034	22	-	13/21/61/61	0/2/2/2
19	CLA	B	1209	2	1/1/13/20	10/27/103/115	-
19	CLA	B	1213	-	-	12/17/93/115	-
19	CLA	B	1219	2	1/1/13/20	10/27/103/115	-
19	CLA	A	1129	1	-	4/21/97/115	-
19	CLA	B	1238	-	1/1/15/20	19/39/115/115	-
19	CLA	3	3008	-	-	7/21/97/115	-
19	CLA	3	3011	-	1/1/15/20	20/39/115/115	-
22	LMU	R	7025	-	-	13/21/61/61	0/2/2/2
19	CLA	H	1241	-	1/1/13/20	7/27/103/115	-
19	CLA	B	1234	2	1/1/14/20	14/33/109/115	-
19	CLA	4	4001	-	-	5/21/97/115	-
21	BCR	B	6005	-	-	8/29/63/63	0/2/2/2
21	BCR	I	6018	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1110	1	-	13/26/102/115	-
19	CLA	3	2009	17	1/1/13/20	16/29/105/115	-
19	CLA	F	1302	19	-	7/10/86/115	-
19	CLA	4	4002	18	1/1/12/20	7/24/100/115	-
19	CLA	B	1206	2	1/1/15/20	18/39/115/115	-
19	CLA	B	1233	-	-	10/23/99/115	-
22	LMU	D	7050	4	-	11/21/61/61	0/2/2/2
19	CLA	A	1133	1	-	12/21/97/115	-
19	CLA	A	1126	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMU	B	7040	-	-	14/21/61/61	0/2/2/2
19	CLA	B	1222	-	1/1/13/20	15/31/107/115	-
19	CLA	B	1229	2	1/1/15/20	18/39/115/115	-
19	CLA	B	1228	2	-	13/21/97/115	-
19	CLA	K	3009	2	1/1/15/20	20/39/115/115	-
19	CLA	3	3007	-	-	4/12/88/115	-
19	CLA	A	9011	-	1/1/15/20	23/39/115/115	-
19	CLA	A	1121	1	-	4/12/88/115	-
19	CLA	A	1103	1	1/1/15/20	22/39/115/115	-
22	LMU	H	7043	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1135	-	-	9/23/99/115	-
19	CLA	2	2002	-	1/1/13/20	10/29/105/115	-
21	BCR	3	6022	-	-	19/29/63/63	0/2/2/2
19	CLA	A	1136	1	1/1/15/20	11/39/115/115	-
22	LMU	A	7016	-	-	11/21/61/61	0/2/2/2
22	LMU	H	7030	-	-	14/21/61/61	0/2/2/2
19	CLA	B	1220	-	-	18/39/115/115	-
19	CLA	A	1137	-	-	10/18/94/115	-
22	LMU	4	7009	-	-	13/20/60/61	0/2/2/2
19	CLA	A	1132	-	1/1/15/20	23/39/115/115	-
19	CLA	4	1004	18	1/1/13/20	11/27/103/115	-
19	CLA	J	1308	19	1/1/13/20	14/27/103/115	-
22	LMU	3	7003	-	-	14/21/61/61	0/2/2/2
21	BCR	I	6021	-	-	12/29/63/63	0/2/2/2
22	LMU	R	7020	-	-	11/21/61/61	0/2/2/2
22	LMU	K	7047	-	-	9/21/61/61	0/2/2/2
21	BCR	1	6023	-	-	15/29/63/63	0/2/2/2
19	CLA	L	1503	-	1/1/12/20	10/21/97/115	-
19	CLA	1	1013	-	1/1/12/20	8/23/99/115	-
22	LMU	G	7026	-	-	15/21/61/61	0/2/2/2
19	CLA	H	1505	-	1/1/13/20	12/27/103/115	-
20	PQN	A	5001	-	1/1/8/9	11/23/43/43	0/2/2/2
19	CLA	A	1127	1	1/1/13/20	10/27/103/115	-
19	CLA	B	1227	2	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1221	-	-	8/26/102/115	-
23	SF4	C	8003	3	-	-	0/6/5/5
19	CLA	A	1139	-	-	11/23/99/115	-
21	BCR	A	6007	-	-	14/29/63/63	0/2/2/2
21	BCR	A	6011	-	-	11/29/63/63	0/2/2/2
19	CLA	A	1119	-	1/1/15/20	17/39/115/115	-
19	CLA	A	1102	19	1/1/13/20	12/27/103/115	-
19	CLA	A	1107	-	1/1/13/20	12/27/103/115	-
19	CLA	R	1150	-	1/1/15/20	20/39/115/115	-
22	LMU	A	7044	-	-	16/21/61/61	0/2/2/2
19	CLA	A	1109	19,1	1/1/15/20	25/39/115/115	-
21	BCR	B	6006	-	-	11/29/63/63	0/2/2/2
19	CLA	A	9013	-	1/1/15/20	22/39/115/115	-
22	LMU	G	7051	-	-	13/21/61/61	0/2/2/2
19	CLA	B	1224	-	1/1/15/20	16/39/115/115	-
22	LMU	C	7015	-	-	14/21/61/61	0/2/2/2
19	CLA	2	2014	19	1/1/14/20	18/35/111/115	-
19	CLA	2	2007	-	1/1/15/20	18/39/115/115	-
19	CLA	A	1140	1	1/1/15/20	17/39/115/115	-
19	CLA	B	1226	2	1/1/15/20	27/39/115/115	-
19	CLA	B	1235	2	1/1/15/20	13/39/115/115	-
19	CLA	K	1142	-	-	3/15/91/115	-
19	CLA	4	4014	-	-	13/18/94/115	-
19	CLA	2	2004	-	-	10/21/97/115	-
19	CLA	A	9012	-	1/1/15/20	20/39/115/115	-
22	LMU	G	7039	-	-	17/21/61/61	0/2/2/2
22	LMU	R	7022	-	-	14/21/61/61	0/2/2/2
22	LMU	F	7036	-	-	11/20/60/61	0/2/2/2
19	CLA	4	4007	-	-	12/24/100/115	-
19	CLA	H	1207	-	1/1/15/20	18/39/115/115	-
22	LMU	E	7048	-	-	12/21/61/61	0/2/2/2
19	CLA	H	1145	-	2/2/15/20	20/39/115/115	-
22	LMU	H	7017	-	-	13/21/61/61	0/2/2/2
21	BCR	L	6019	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	2	4009	-	1/1/15/20	17/39/115/115	-
19	CLA	4	4006	-	1/1/13/20	12/27/103/115	-
19	CLA	3	1147	17	-	9/17/93/115	-
19	CLA	B	1211	-	1/1/15/20	23/39/115/115	-
21	BCR	B	6020	-	-	14/29/63/63	0/2/2/2
22	LMU	R	7007	-	-	16/21/61/61	0/2/2/2
22	LMU	R	7024	-	-	14/21/61/61	0/2/2/2
22	LMU	2	7027	-	-	11/21/61/61	0/2/2/2
19	CLA	B	1202	-	1/1/15/20	20/39/115/115	-
22	LMU	R	7014	-	-	12/21/61/61	0/2/2/2
19	CLA	A	1124	-	1/1/15/20	20/39/115/115	-
22	LMU	B	7038	-	-	13/21/61/61	0/2/2/2
22	LMU	4	7018	-	-	13/21/61/61	0/2/2/2
19	CLA	F	1305	19	3/3/12/20	12/25/101/115	-
19	CLA	3	3017	-	-	8/21/97/115	-
19	CLA	3	3013	17	1/1/15/20	18/39/115/115	-
19	CLA	L	1504	-	1/1/13/20	8/27/103/115	-
22	LMU	H	7002	-	-	14/21/61/61	0/2/2/2
19	CLA	K	1146	-	-	8/21/97/115	-
19	CLA	1	1001	15	-	10/17/93/115	-
19	CLA	1	1303	-	2/2/12/20	11/23/99/115	-
23	SF4	C	8002	3	-	-	0/6/5/5
22	LMU	A	7023	-	-	17/21/61/61	0/2/2/2
19	CLA	B	9010	2	1/1/15/20	18/39/115/115	-
24	LMG	B	7101	-	-	24/44/64/70	0/1/1/1
19	CLA	A	1120	-	-	10/23/99/115	-
22	LMU	3	7005	-	-	15/21/61/61	0/2/2/2
22	LMU	4	7053	-	-	13/20/60/61	0/2/2/2
21	BCR	A	6003	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1237	-	1/1/15/20	15/39/115/115	-
19	CLA	2	2006	-	1/1/15/20	18/39/115/115	-
21	BCR	B	6010	-	-	13/29/63/63	0/2/2/2
22	LMU	4	7052	22	-	18/21/61/61	0/2/2/2
19	CLA	1	1003	-	-	9/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1218	-	-	12/17/93/115	-
19	CLA	B	1215	2	1/1/14/20	13/33/109/115	-
19	CLA	1	1005	-	-	7/17/93/115	-
21	BCR	J	6012	-	-	13/29/63/63	0/2/2/2
22	LMU	2	7046	-	-	16/21/61/61	0/2/2/2
21	BCR	A	6008	-	-	15/29/63/63	0/2/2/2
19	CLA	J	1311	-	1/1/14/20	23/35/111/115	-
19	CLA	K	1143	-	-	7/21/97/115	-
19	CLA	L	1148	-	2/2/13/20	13/27/103/115	-
19	CLA	4	1306	-	1/1/13/20	14/27/103/115	-
22	LMU	1	7004	-	-	16/21/61/61	0/2/2/2
19	CLA	A	1138	-	1/1/15/20	19/39/115/115	-
22	LMU	N	7049	-	-	16/21/61/61	0/2/2/2
20	PQN	B	5002	-	1/1/8/9	9/23/43/43	0/2/2/2
19	CLA	A	1125	1	1/1/15/20	24/39/115/115	-
19	CLA	A	1134	1	-	9/15/91/115	-
19	CLA	1	1002	15	-	11/18/94/115	-
19	CLA	1	1008	-	1/1/12/20	10/23/99/115	-
19	CLA	I	1204	-	1/1/14/20	12/33/109/115	-
22	LMU	K	7001	-	-	13/21/61/61	0/2/2/2
19	CLA	2	2012	16	-	4/21/97/115	-
19	CLA	B	1236	-	-	10/18/94/115	-
19	CLA	B	1208	2	1/1/13/20	9/25/101/115	-
22	LMU	H	7032	-	-	18/21/61/61	0/2/2/2
22	LMU	2	7006	-	-	14/21/61/61	0/2/2/2
19	CLA	B	1201	-	-	6/15/91/115	-
19	CLA	B	1230	2	-	10/21/97/115	-
22	LMU	H	7011	-	-	17/21/61/61	0/2/2/2
22	LMU	A	7045	-	-	14/21/61/61	0/2/2/2
19	CLA	2	2013	-	-	8/21/97/115	-
19	CLA	A	9022	-	1/1/15/20	19/39/115/115	-
22	LMU	L	7029	-	-	16/21/61/61	0/2/2/2
23	SF4	A	8001	2,1	-	-	0/6/5/5
19	CLA	A	9023	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1232	19	-	8/15/91/115	-
22	LMU	4	7033	-	-	11/21/61/61	0/2/2/2
19	CLA	B	1212	2	1/1/14/20	12/33/109/115	-
22	LMU	A	7010	-	-	18/21/61/61	0/2/2/2
19	CLA	A	1117	-	1/1/15/20	19/39/115/115	-
19	CLA	A	1123	-	1/1/15/20	20/39/115/115	-
19	CLA	A	1141	-	1/1/15/20	20/39/115/115	-
19	CLA	B	1205	-	1/1/15/20	12/39/115/115	-
19	CLA	4	4015	-	-	12/17/93/115	-
22	LMU	4	7019	-	-	15/21/61/61	0/2/2/2
19	CLA	A	1122	-	1/1/13/20	10/27/103/115	-
19	CLA	A	1128	1	1/1/15/20	18/39/115/115	-
19	CLA	B	1210	-	1/1/15/20	23/39/115/115	-
19	CLA	A	1151	-	-	9/21/97/115	-
22	LMU	K	7041	-	-	12/21/61/61	0/2/2/2
19	CLA	4	4003	-	1/1/13/20	14/27/103/115	-
19	CLA	2	2001	-	-	10/23/99/115	-
21	BCR	B	6017	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1231	2,19	-	9/15/91/115	-
21	BCR	A	6002	-	-	16/29/63/63	0/2/2/2
19	CLA	G	1242	-	-	10/23/99/115	-
19	CLA	A	1112	1	-	11/15/91/115	-
19	CLA	A	1108	-	-	6/15/91/115	-
22	LMU	H	7028	-	-	13/21/61/61	0/2/2/2
22	LMU	2	7031	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1149	-	2/2/11/20	12/16/92/115	-
19	CLA	B	1216	-	1/1/14/20	17/35/111/115	-
19	CLA	3	3016	-	1/1/15/20	23/39/115/115	-
19	CLA	A	1131	1	1/1/15/20	19/39/115/115	-
19	CLA	B	1203	-	1/1/15/20	19/39/115/115	-
19	CLA	A	1105	1	-	8/17/93/115	-
19	CLA	A	1113	1	-	8/21/97/115	-
21	BCR	B	6004	-	-	16/29/63/63	0/2/2/2
19	CLA	A	1111	1	-	13/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1101	-	-	6/21/97/115	-
19	CLA	L	1501	12	-	8/21/97/115	-
21	BCR	F	6014	-	-	17/29/63/63	0/2/2/2
22	LMU	A	7035	-	-	13/21/61/61	0/2/2/2
22	LMU	E	7037	-	-	16/21/61/61	0/2/2/2
19	CLA	B	1214	-	1/1/13/20	12/32/108/115	-
22	LMU	4	7008	-	-	12/21/61/61	0/2/2/2
22	LMU	K	7042	-	-	18/21/61/61	0/2/2/2
19	CLA	R	1144	-	1/1/13/20	14/30/106/115	-
19	CLA	B	1239	-	1/1/15/20	19/39/115/115	-
19	CLA	1	1010	19	-	8/17/93/115	-
22	LMU	1	7013	-	-	10/21/61/61	0/2/2/2
19	CLA	1	1007	-	1/1/14/20	21/35/111/115	-
19	CLA	B	1225	-	1/1/15/20	17/39/115/115	-
19	CLA	4	1304	-	2/2/15/20	19/39/115/115	-

All (2668) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1011	CLA	CAB-C3B	-8.57	1.33	1.50
19	1	1006	CLA	CAB-C3B	-8.56	1.33	1.50
19	1	1005	CLA	OBD-CAD	8.45	1.37	1.22
19	4	1009	CLA	CAB-C3B	-8.22	1.33	1.50
19	B	1208	CLA	CAB-C3B	-7.94	1.34	1.50
19	4	4012	CLA	CAB-C3B	-7.93	1.34	1.50
19	B	1301	CLA	CAB-C3B	-7.87	1.34	1.50
20	A	5001	PQN	C3-C2	7.81	1.49	1.35
19	1	1012	CLA	CAB-C3B	-7.73	1.34	1.50
20	B	5002	PQN	C3-C2	7.66	1.48	1.35
19	A	1149	CLA	CAB-C3B	-7.65	1.35	1.50
19	3	1118	CLA	CAB-C3B	-7.46	1.35	1.50
19	A	1107	CLA	CHD-C1D	7.21	1.52	1.38
19	3	1147	CLA	C1B-NB	-7.15	1.28	1.37
19	3	3003	CLA	CAB-C3B	-7.12	1.36	1.50
21	A	6002	BCR	C11-C10	7.12	1.65	1.43
19	2	2004	CLA	CHC-C1C	7.10	1.52	1.38
19	4	4001	CLA	CHC-C1C	7.07	1.52	1.38
21	I	6021	BCR	C30-C25	-7.00	1.44	1.53
19	A	1108	CLA	CHC-C1C	6.96	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	3009	CLA	CHC-C1C	6.94	1.52	1.38
19	2	2008	CLA	CHC-C1C	6.88	1.52	1.38
19	B	1210	CLA	CHC-C1C	6.88	1.52	1.38
19	4	4011	CLA	CHC-C1C	6.85	1.52	1.38
19	B	1212	CLA	CHC-C1C	6.81	1.52	1.38
21	1	6023	BCR	C11-C10	-6.81	1.22	1.43
19	B	1233	CLA	CHC-C1C	6.79	1.52	1.38
19	1	1008	CLA	CHC-C1C	6.78	1.52	1.38
19	A	1113	CLA	CHD-C1D	6.77	1.51	1.38
19	4	4006	CLA	CHC-C1C	6.77	1.52	1.38
19	A	1151	CLA	CHD-C1D	6.75	1.51	1.38
19	L	1148	CLA	CHC-C1C	6.72	1.51	1.38
19	A	1102	CLA	CHC-C1C	6.68	1.51	1.38
19	4	4013	CLA	CHC-C1C	6.68	1.51	1.38
19	A	1119	CLA	CHC-C1C	6.67	1.51	1.38
19	L	1504	CLA	CHC-C1C	6.67	1.51	1.38
19	G	1242	CLA	CHC-C1C	6.66	1.51	1.38
19	4	1009	CLA	CHC-C1C	6.65	1.51	1.38
19	B	1224	CLA	CHC-C1C	6.65	1.51	1.38
19	B	1229	CLA	CHC-C1C	6.65	1.51	1.38
19	B	1232	CLA	CHC-C1C	6.64	1.51	1.38
19	3	3002	CLA	CHC-C1C	6.64	1.51	1.38
19	A	1131	CLA	CHD-C1D	6.64	1.51	1.38
19	1	1012	CLA	CHC-C1C	6.63	1.51	1.38
19	R	1150	CLA	CHC-C1C	6.63	1.51	1.38
19	A	1120	CLA	CHC-C1C	6.63	1.51	1.38
19	I	1204	CLA	CHC-C1C	6.62	1.51	1.38
19	F	1240	CLA	CAB-C3B	-6.62	1.37	1.50
19	B	1227	CLA	CHD-C1D	6.60	1.51	1.38
19	2	2012	CLA	CHD-C1D	6.59	1.51	1.38
19	B	1227	CLA	CHC-C1C	6.57	1.51	1.38
19	B	1236	CLA	CHC-C1C	6.56	1.51	1.38
19	A	1129	CLA	CHC-C1C	6.55	1.51	1.38
19	B	1217	CLA	CHC-C1C	6.54	1.51	1.38
19	A	1132	CLA	CHD-C1D	6.54	1.51	1.38
19	B	1214	CLA	CHC-C1C	6.53	1.51	1.38
19	3	3010	CLA	CHC-C1C	6.52	1.51	1.38
19	A	9023	CLA	CHD-C1D	6.51	1.51	1.38
19	B	1201	CLA	CHC-C1C	6.51	1.51	1.38
19	2	2007	CLA	CHD-C1D	6.48	1.51	1.38
19	A	9023	CLA	CHC-C1C	6.47	1.51	1.38
19	B	1238	CLA	CHC-C1C	6.47	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1208	CLA	CHD-C1D	6.47	1.51	1.38
19	H	1241	CLA	CHC-C1C	6.47	1.51	1.38
19	L	1501	CLA	CHC-C1C	6.47	1.51	1.38
19	3	3001	CLA	CHC-C1C	6.46	1.51	1.38
19	2	2002	CLA	CHC-C1C	6.46	1.51	1.38
19	A	1106	CLA	CHC-C1C	6.45	1.51	1.38
19	3	3015	CLA	CHC-C1C	6.45	1.51	1.38
19	2	2011	CLA	CHC-C1C	6.44	1.51	1.38
19	3	3007	CLA	CHD-C1D	6.43	1.51	1.38
19	B	1201	CLA	CHD-C1D	6.43	1.51	1.38
19	H	1505	CLA	O2D-CGD	6.43	1.49	1.33
19	1	1015	CLA	CHC-C1C	6.42	1.51	1.38
19	A	1121	CLA	CHD-C1D	6.42	1.51	1.38
19	2	2013	CLA	CHC-C1C	6.42	1.51	1.38
19	A	1112	CLA	CHC-C1C	6.42	1.51	1.38
19	B	1231	CLA	CHC-C1C	6.42	1.51	1.38
19	A	1111	CLA	CHC-C1C	6.41	1.51	1.38
19	1	1014	CLA	O2D-CGD	6.41	1.49	1.33
19	B	1222	CLA	CHC-C1C	6.40	1.51	1.38
19	L	1502	CLA	CHC-C1C	6.39	1.51	1.38
19	A	1129	CLA	CHD-C1D	6.38	1.50	1.38
19	A	1113	CLA	CHC-C1C	6.38	1.51	1.38
19	A	1133	CLA	CHC-C1C	6.38	1.51	1.38
19	A	1149	CLA	CHD-C1D	6.38	1.50	1.38
19	2	2004	CLA	CHD-C1D	6.38	1.50	1.38
19	B	1215	CLA	CHC-C1C	6.37	1.51	1.38
19	H	1241	CLA	CHD-C1D	6.37	1.50	1.38
19	A	9013	CLA	CHD-C1D	6.37	1.50	1.38
19	A	1127	CLA	CHC-C1C	6.37	1.51	1.38
19	B	1219	CLA	CHD-C1D	6.37	1.50	1.38
19	A	1108	CLA	CHD-C1D	6.36	1.50	1.38
19	1	1003	CLA	CHC-C1C	6.36	1.51	1.38
19	A	1116	CLA	CHD-C1D	6.35	1.50	1.38
19	3	3017	CLA	CHD-C1D	6.35	1.50	1.38
19	B	1208	CLA	CHC-C1C	6.34	1.51	1.38
19	A	1116	CLA	CHC-C1C	6.33	1.51	1.38
19	H	1505	CLA	CHC-C1C	6.33	1.51	1.38
19	F	1240	CLA	CHC-C1C	6.33	1.51	1.38
19	A	1108	CLA	CHD-C4C	6.32	1.53	1.39
19	A	1113	CLA	CHD-C4C	6.31	1.53	1.39
19	3	3008	CLA	CHC-C1C	6.31	1.51	1.38
19	A	1105	CLA	CHD-C1D	6.31	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	1505	CLA	CHD-C1D	6.31	1.50	1.38
19	4	1306	CLA	CHD-C1D	6.30	1.50	1.38
19	B	1220	CLA	C3D-C4D	-6.30	1.30	1.44
19	A	1128	CLA	CHC-C1C	6.30	1.51	1.38
19	R	1144	CLA	CHC-C1C	6.30	1.51	1.38
19	G	1242	CLA	CHD-C1D	6.30	1.50	1.38
19	B	9010	CLA	CHC-C1C	6.29	1.51	1.38
19	A	1117	CLA	CHC-C1C	6.29	1.51	1.38
19	A	1149	CLA	CHC-C1C	6.28	1.51	1.38
19	A	1149	CLA	O2D-CGD	6.28	1.48	1.33
19	L	1148	CLA	C3D-C4D	-6.28	1.30	1.44
19	3	3003	CLA	CHC-C1C	6.28	1.51	1.38
19	A	1126	CLA	CHC-C1C	6.27	1.51	1.38
19	H	1207	CLA	CHC-C1C	6.27	1.51	1.38
19	4	4007	CLA	CHD-C1D	6.27	1.50	1.38
19	4	4012	CLA	CHC-C1C	6.27	1.51	1.38
19	A	1117	CLA	CHD-C1D	6.26	1.50	1.38
19	2	2003	CLA	CHC-C1C	6.26	1.50	1.38
19	3	3016	CLA	CHC-C1C	6.26	1.51	1.38
19	2	2007	CLA	CHD-C4C	6.26	1.53	1.39
19	A	1151	CLA	CHD-C4C	6.25	1.53	1.39
19	A	1135	CLA	CHC-C1C	6.25	1.51	1.38
19	A	1137	CLA	CHC-C1C	6.25	1.51	1.38
19	A	1126	CLA	CHD-C4C	6.24	1.53	1.39
19	2	2012	CLA	CHD-C4C	6.24	1.53	1.39
19	A	9013	CLA	CHD-C4C	6.23	1.53	1.39
19	B	1235	CLA	CHD-C1D	6.23	1.50	1.38
19	A	1124	CLA	CHC-C1C	6.22	1.50	1.38
19	B	1223	CLA	CHC-C1C	6.22	1.50	1.38
19	4	4004	CLA	CHC-C1C	6.22	1.50	1.38
19	2	2014	CLA	CHC-C1C	6.21	1.50	1.38
19	2	2012	CLA	CHC-C1C	6.21	1.50	1.38
19	A	1109	CLA	CHD-C1D	6.21	1.50	1.38
19	A	9011	CLA	CHC-C1C	6.21	1.50	1.38
19	3	3007	CLA	CHC-C1C	6.21	1.50	1.38
19	K	1142	CLA	CHC-C1C	6.21	1.50	1.38
19	L	1130	CLA	CHD-C4C	6.20	1.53	1.39
19	1	1002	CLA	O2D-CGD	6.20	1.48	1.33
19	B	1224	CLA	CHD-C4C	6.19	1.53	1.39
19	3	3014	CLA	CHC-C1C	6.19	1.50	1.38
19	J	1311	CLA	CHC-C1C	6.19	1.50	1.38
19	4	1004	CLA	CHC-C1C	6.19	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1005	CLA	CHD-C1D	6.19	1.50	1.38
19	1	1001	CLA	O2D-CGD	6.18	1.48	1.33
19	B	1202	CLA	CHD-C4C	6.18	1.53	1.39
19	1	1010	CLA	C3D-C4D	-6.18	1.30	1.44
19	L	1130	CLA	CHD-C1D	6.17	1.50	1.38
19	B	1213	CLA	CHC-C1C	6.17	1.50	1.38
19	1	1003	CLA	CHD-C1D	6.17	1.50	1.38
19	H	1241	CLA	CHD-C4C	6.17	1.53	1.39
19	3	1118	CLA	CHD-C1D	6.17	1.50	1.38
19	2	2010	CLA	CHC-C1C	6.16	1.50	1.38
19	A	1123	CLA	CHC-C1C	6.16	1.50	1.38
19	L	1503	CLA	CHC-C1C	6.15	1.50	1.38
19	3	3013	CLA	O2D-CGD	6.15	1.48	1.33
19	H	1241	CLA	O2D-CGD	6.15	1.48	1.33
19	A	1112	CLA	CHD-C1D	6.14	1.50	1.38
19	3	3005	CLA	CHC-C1C	6.14	1.50	1.38
19	4	4003	CLA	CHD-C1D	6.14	1.50	1.38
19	A	1140	CLA	CHC-C1C	6.14	1.50	1.38
19	A	1120	CLA	CHD-C1D	6.14	1.50	1.38
19	K	1143	CLA	CHD-C1D	6.14	1.50	1.38
19	A	9012	CLA	CHC-C1C	6.14	1.50	1.38
19	A	1109	CLA	CHC-C1C	6.13	1.50	1.38
19	4	4005	CLA	CHC-C1C	6.13	1.50	1.38
19	B	1202	CLA	CHD-C1D	6.13	1.50	1.38
19	B	1238	CLA	CHD-C1D	6.12	1.50	1.38
19	A	9022	CLA	CHC-C1C	6.12	1.50	1.38
19	B	1219	CLA	CHC-C1C	6.12	1.50	1.38
19	R	1144	CLA	CHD-C1D	6.12	1.50	1.38
19	B	1219	CLA	CHD-C4C	6.12	1.53	1.39
19	1	1012	CLA	CHD-C1D	6.12	1.50	1.38
19	3	2009	CLA	CHC-C1C	6.12	1.50	1.38
19	1	1006	CLA	CHD-C1D	6.12	1.50	1.38
19	B	1205	CLA	CHC-C1C	6.12	1.50	1.38
19	4	4001	CLA	CHD-C1D	6.12	1.50	1.38
19	2	2001	CLA	CHC-C1C	6.11	1.50	1.38
19	3	3003	CLA	CHD-C1D	6.11	1.50	1.38
19	B	1301	CLA	CHC-C1C	6.11	1.50	1.38
19	B	1232	CLA	CHD-C1D	6.11	1.50	1.38
19	1	1008	CLA	CHD-C1D	6.11	1.50	1.38
19	2	2001	CLA	CHD-C1D	6.11	1.50	1.38
19	3	3017	CLA	CHD-C4C	6.11	1.53	1.39
19	G	1242	CLA	O2D-CGD	6.11	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1141	CLA	CHC-C1C	6.10	1.50	1.38
19	B	1216	CLA	CHC-C1C	6.10	1.50	1.38
19	A	1138	CLA	CHC-C1C	6.10	1.50	1.38
19	A	1115	CLA	CHC-C1C	6.09	1.50	1.38
19	B	1227	CLA	CHD-C4C	6.09	1.53	1.39
19	B	1226	CLA	CHC-C1C	6.09	1.50	1.38
19	A	1134	CLA	CHC-C1C	6.09	1.50	1.38
19	B	1219	CLA	O2D-CGD	6.09	1.48	1.33
19	3	1118	CLA	CHC-C1C	6.08	1.50	1.38
19	A	1116	CLA	O2D-CGD	6.08	1.48	1.33
19	B	1206	CLA	CHC-C1C	6.08	1.50	1.38
19	A	1121	CLA	CHD-C4C	6.08	1.53	1.39
19	L	1503	CLA	O2D-CGD	6.08	1.48	1.33
19	I	1204	CLA	CHD-C1D	6.08	1.50	1.38
19	B	1224	CLA	CHD-C1D	6.08	1.50	1.38
19	F	1302	CLA	CHC-C1C	6.08	1.50	1.38
19	A	1122	CLA	CHD-C1D	6.07	1.50	1.38
19	A	1125	CLA	CHC-C1C	6.07	1.50	1.38
19	2	4009	CLA	CHC-C1C	6.07	1.50	1.38
19	1	1310	CLA	CHC-C1C	6.07	1.50	1.38
19	4	4015	CLA	CHC-C1C	6.07	1.50	1.38
19	1	1006	CLA	CHC-C1C	6.07	1.50	1.38
19	A	1136	CLA	CHC-C1C	6.07	1.50	1.38
19	B	1205	CLA	CHD-C1D	6.06	1.50	1.38
19	A	1139	CLA	CHC-C1C	6.06	1.50	1.38
19	A	1119	CLA	CHD-C1D	6.06	1.50	1.38
19	B	1220	CLA	C4C-C3C	-6.06	1.34	1.45
19	A	1104	CLA	CHC-C1C	6.06	1.50	1.38
19	2	2006	CLA	CHC-C1C	6.06	1.50	1.38
19	B	1301	CLA	CHD-C1D	6.05	1.50	1.38
19	B	1208	CLA	CHD-C4C	6.05	1.53	1.39
21	A	6003	BCR	C24-C23	6.05	1.51	1.33
19	1	1005	CLA	CHC-C1C	6.05	1.50	1.38
19	2	2002	CLA	CHD-C1D	6.05	1.50	1.38
19	A	1106	CLA	CHD-C1D	6.05	1.50	1.38
19	B	1211	CLA	CHC-C1C	6.05	1.50	1.38
19	A	1141	CLA	CHD-C1D	6.05	1.50	1.38
19	3	3013	CLA	C3D-C4D	-6.04	1.30	1.44
19	B	1235	CLA	CHD-C4C	6.04	1.53	1.39
19	1	1007	CLA	O2D-CGD	6.04	1.48	1.33
19	R	1150	CLA	CHD-C1D	6.04	1.50	1.38
19	B	1234	CLA	CHD-C1D	6.04	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1120	CLA	CHD-C4C	6.04	1.52	1.39
19	A	1110	CLA	CHD-C1D	6.03	1.50	1.38
19	H	1145	CLA	CHC-C1C	6.03	1.50	1.38
19	L	1130	CLA	CHC-C1C	6.03	1.50	1.38
19	A	1107	CLA	CHD-C4C	6.02	1.52	1.39
19	2	2013	CLA	CHD-C1D	6.02	1.50	1.38
19	A	1126	CLA	CHD-C1D	6.02	1.50	1.38
19	B	1218	CLA	CHC-C1C	6.02	1.50	1.38
19	3	1147	CLA	CAB-C3B	-6.02	1.31	1.47
19	B	1218	CLA	O2D-CGD	6.01	1.48	1.33
19	2	2006	CLA	O2D-CGD	6.01	1.48	1.33
19	B	1211	CLA	CHD-C1D	6.01	1.50	1.38
19	A	1149	CLA	CHD-C4C	6.01	1.52	1.39
19	B	1205	CLA	CHD-C4C	6.01	1.52	1.39
19	B	1211	CLA	CHD-C4C	6.00	1.52	1.39
19	A	1111	CLA	CHD-C1D	6.00	1.50	1.38
19	1	1007	CLA	CHC-C1C	6.00	1.50	1.38
19	A	1132	CLA	CHD-C4C	6.00	1.52	1.39
19	R	1150	CLA	O2D-CGD	6.00	1.48	1.33
19	L	1502	CLA	CHD-C4C	6.00	1.52	1.39
19	2	2002	CLA	CHD-C4C	6.00	1.52	1.39
19	1	1002	CLA	CHC-C1C	5.99	1.50	1.38
19	L	1501	CLA	O2D-CGD	5.99	1.48	1.33
19	3	3006	CLA	CHC-C1C	5.99	1.50	1.38
19	1	1002	CLA	CHD-C1D	5.99	1.50	1.38
19	K	1143	CLA	CHC-C1C	5.99	1.50	1.38
19	A	1237	CLA	CHC-C1C	5.98	1.50	1.38
19	4	4002	CLA	CHC-C1C	5.98	1.50	1.38
19	F	1240	CLA	CHD-C4C	5.98	1.52	1.39
19	B	1201	CLA	CHD-C4C	5.98	1.52	1.39
19	H	1207	CLA	CHD-C1D	5.97	1.50	1.38
19	4	4014	CLA	CHC-C1C	5.97	1.50	1.38
19	A	1101	CLA	CHC-C1C	5.97	1.50	1.38
19	A	1133	CLA	CHD-C1D	5.97	1.50	1.38
19	A	1110	CLA	CHD-C4C	5.96	1.52	1.39
19	L	1148	CLA	CHD-C1D	5.96	1.50	1.38
19	A	1103	CLA	CHD-C4C	5.96	1.52	1.39
19	3	1147	CLA	C4B-NB	-5.96	1.30	1.37
19	A	1123	CLA	CHD-C1D	5.96	1.50	1.38
19	B	1226	CLA	CHD-C1D	5.95	1.50	1.38
19	A	1309	CLA	CHC-C1C	5.95	1.50	1.38
19	B	1234	CLA	CHD-C4C	5.95	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1122	CLA	CHC-C1C	5.95	1.50	1.38
19	4	1304	CLA	CHD-C4C	5.95	1.52	1.39
19	4	4003	CLA	CHC-C1C	5.94	1.50	1.38
19	A	1151	CLA	CHC-C1C	5.94	1.50	1.38
19	A	1136	CLA	CHD-C1D	5.94	1.50	1.38
19	4	4006	CLA	O2D-CGD	5.93	1.47	1.33
19	4	4007	CLA	CHC-C1C	5.93	1.50	1.38
19	3	3011	CLA	CHC-C1C	5.93	1.50	1.38
19	4	4010	CLA	CHC-C1C	5.93	1.50	1.38
19	A	1110	CLA	CHC-C1C	5.93	1.50	1.38
19	H	1145	CLA	CHD-C1D	5.92	1.50	1.38
19	4	4007	CLA	O2D-CGD	5.92	1.47	1.33
19	F	1302	CLA	CHD-C1D	5.92	1.50	1.38
19	2	2007	CLA	CHC-C1C	5.92	1.50	1.38
19	B	1209	CLA	CHC-C1C	5.92	1.50	1.38
19	A	1112	CLA	CHD-C4C	5.92	1.52	1.39
19	A	1113	CLA	O2D-CGD	5.91	1.47	1.33
19	2	2005	CLA	CHC-C1C	5.91	1.50	1.38
19	A	1104	CLA	CHD-C1D	5.91	1.50	1.38
19	B	1230	CLA	CHD-C1D	5.90	1.50	1.38
19	A	1131	CLA	CHC-C1C	5.90	1.50	1.38
19	L	1502	CLA	CHD-C1D	5.90	1.50	1.38
19	4	4001	CLA	O2D-CGD	5.90	1.47	1.33
19	F	1240	CLA	CHD-C1D	5.90	1.49	1.38
19	B	1238	CLA	CHD-C4C	5.89	1.52	1.39
19	A	1102	CLA	CHD-C4C	5.89	1.52	1.39
19	B	1233	CLA	CHD-C1D	5.89	1.49	1.38
19	A	9022	CLA	CHD-C1D	5.89	1.49	1.38
19	B	1234	CLA	CHC-C1C	5.88	1.50	1.38
19	A	1123	CLA	CHD-C4C	5.88	1.52	1.39
19	4	1306	CLA	CHC-C1C	5.88	1.50	1.38
19	B	1233	CLA	O2D-CGD	5.88	1.47	1.33
19	A	1105	CLA	CHC-C1C	5.87	1.50	1.38
19	B	1214	CLA	CHD-C4C	5.87	1.52	1.39
19	2	4009	CLA	CHD-C1D	5.86	1.49	1.38
19	K	1142	CLA	CHD-C1D	5.86	1.49	1.38
19	2	1307	CLA	CHC-C1C	5.86	1.50	1.38
19	A	1138	CLA	CHD-C1D	5.86	1.49	1.38
19	4	4002	CLA	C4C-C3C	-5.86	1.35	1.45
19	3	3011	CLA	CHD-C1D	5.86	1.49	1.38
19	A	1105	CLA	CHD-C4C	5.85	1.52	1.39
19	B	1228	CLA	O2D-CGD	5.85	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	1242	CLA	CHD-C4C	5.85	1.52	1.39
19	A	1101	CLA	CHD-C4C	5.85	1.52	1.39
19	A	1121	CLA	O2D-CGD	5.84	1.47	1.33
19	A	1102	CLA	CHD-C1D	5.84	1.49	1.38
19	A	1108	CLA	O2D-CGD	5.84	1.47	1.33
19	A	1129	CLA	CHD-C4C	5.84	1.52	1.39
19	B	1225	CLA	CHC-C1C	5.83	1.50	1.38
19	K	1146	CLA	CHD-C1D	5.83	1.49	1.38
19	4	1306	CLA	CHD-C4C	5.83	1.52	1.39
19	3	3003	CLA	CHD-C4C	5.83	1.52	1.39
19	1	1014	CLA	CHC-C1C	5.83	1.50	1.38
19	A	1133	CLA	CHD-C4C	5.82	1.52	1.39
19	2	2013	CLA	O2D-CGD	5.82	1.47	1.33
19	A	1149	CLA	O2A-CGA	5.82	1.50	1.33
19	A	1104	CLA	CHD-C4C	5.82	1.52	1.39
19	A	1133	CLA	O2D-CGD	5.81	1.47	1.33
19	1	1013	CLA	CAB-C3B	-5.81	1.31	1.47
19	3	3016	CLA	CHD-C1D	5.81	1.49	1.38
19	A	1119	CLA	CHD-C4C	5.81	1.52	1.39
19	4	1304	CLA	CHC-C1C	5.81	1.50	1.38
19	1	1303	CLA	C3D-C4D	-5.80	1.31	1.44
19	R	1144	CLA	O2D-CGD	5.80	1.47	1.33
19	A	1120	CLA	O2D-CGD	5.80	1.47	1.33
19	B	1203	CLA	CHD-C1D	5.80	1.49	1.38
19	B	1220	CLA	CAB-C3B	-5.80	1.31	1.47
19	A	1134	CLA	CHD-C1D	5.79	1.49	1.38
19	4	4003	CLA	CHD-C4C	5.79	1.52	1.39
21	A	6002	BCR	C11-C12	5.79	1.49	1.34
19	3	3008	CLA	O2D-CGD	5.79	1.47	1.33
19	A	1101	CLA	CHD-C1D	5.79	1.49	1.38
19	A	9022	CLA	CHD-C4C	5.79	1.52	1.39
19	B	1213	CLA	O2D-CGD	5.78	1.47	1.33
19	A	1139	CLA	CHD-C1D	5.78	1.49	1.38
19	R	1144	CLA	CHD-C4C	5.78	1.52	1.39
19	3	3007	CLA	O2D-CGD	5.78	1.47	1.33
19	B	1214	CLA	O2D-CGD	5.78	1.47	1.33
19	K	1146	CLA	O2D-CGD	5.78	1.47	1.33
19	3	3008	CLA	CHD-C1D	5.77	1.49	1.38
19	A	1116	CLA	CHD-C4C	5.77	1.52	1.39
19	B	1221	CLA	CHD-C4C	5.77	1.52	1.39
19	A	1137	CLA	CHD-C1D	5.77	1.49	1.38
19	B	1203	CLA	CAB-C3B	-5.77	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1005	CLA	O2D-CGD	5.77	1.47	1.33
19	J	1311	CLA	O2D-CGD	5.77	1.47	1.33
19	A	9013	CLA	CAB-C3B	-5.77	1.32	1.47
19	2	2002	CLA	O2D-CGD	5.77	1.47	1.33
19	A	1109	CLA	CHD-C4C	5.77	1.52	1.39
19	4	1004	CLA	CHD-C1D	5.77	1.49	1.38
19	A	1122	CLA	CHD-C4C	5.77	1.52	1.39
19	B	1223	CLA	CHD-C1D	5.77	1.49	1.38
19	B	1232	CLA	CHD-C4C	5.76	1.52	1.39
19	F	1305	CLA	CHC-C1C	5.76	1.50	1.38
19	J	1311	CLA	CHD-C1D	5.76	1.49	1.38
19	A	1110	CLA	O2D-CGD	5.76	1.47	1.33
19	1	1013	CLA	O2D-CGD	5.76	1.47	1.33
19	A	1103	CLA	O2D-CGD	5.75	1.47	1.33
19	A	1128	CLA	CHD-C4C	5.75	1.52	1.39
19	A	1135	CLA	CHD-C1D	5.75	1.49	1.38
19	1	1003	CLA	CHD-C4C	5.75	1.52	1.39
19	1	1006	CLA	CHD-C4C	5.75	1.52	1.39
19	1	1012	CLA	CHD-C4C	5.75	1.52	1.39
19	B	9010	CLA	CHD-C1D	5.75	1.49	1.38
19	B	1229	CLA	CHD-C1D	5.74	1.49	1.38
19	A	1124	CLA	CHD-C1D	5.74	1.49	1.38
19	A	1111	CLA	CHD-C4C	5.74	1.52	1.39
19	A	1121	CLA	CHC-C1C	5.74	1.50	1.38
19	A	1103	CLA	CHC-C1C	5.74	1.50	1.38
19	B	1235	CLA	CHC-C1C	5.73	1.50	1.38
19	K	1143	CLA	CHD-C4C	5.73	1.52	1.39
19	F	1305	CLA	CHD-C1D	5.73	1.49	1.38
19	A	9013	CLA	CHC-C1C	5.73	1.50	1.38
19	2	2004	CLA	CHD-C4C	5.73	1.52	1.39
19	4	4002	CLA	C3D-C4D	-5.72	1.31	1.44
19	A	1132	CLA	CHC-C1C	5.72	1.49	1.38
19	3	3011	CLA	CHD-C4C	5.72	1.52	1.39
19	A	1131	CLA	CHD-C4C	5.72	1.52	1.39
19	H	1505	CLA	CHD-C4C	5.72	1.52	1.39
19	A	1106	CLA	CHD-C4C	5.71	1.52	1.39
19	K	1146	CLA	C3D-C4D	-5.71	1.31	1.44
19	3	1118	CLA	CHD-C4C	5.71	1.52	1.39
19	B	1210	CLA	CHD-C1D	5.71	1.49	1.38
19	B	1213	CLA	CHD-C1D	5.71	1.49	1.38
19	A	1103	CLA	CHD-C1D	5.71	1.49	1.38
19	B	1212	CLA	CHD-C1D	5.71	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1122	CLA	O2D-CGD	5.70	1.47	1.33
19	A	1115	CLA	CHD-C1D	5.70	1.49	1.38
19	B	1215	CLA	CHD-C1D	5.70	1.49	1.38
19	A	1138	CLA	CHD-C4C	5.70	1.52	1.39
19	4	4002	CLA	C1B-NB	-5.70	1.30	1.37
19	L	1502	CLA	O2D-CGD	5.70	1.47	1.33
19	1	1013	CLA	C3D-C4D	-5.69	1.31	1.44
19	2	2007	CLA	O2D-CGD	5.69	1.47	1.33
19	B	1203	CLA	CHD-C4C	5.69	1.52	1.39
19	A	1119	CLA	O2D-CGD	5.69	1.47	1.33
19	B	1206	CLA	CHD-C4C	5.69	1.52	1.39
19	B	1202	CLA	CHC-C1C	5.68	1.49	1.38
19	B	1218	CLA	CHD-C4C	5.68	1.52	1.39
19	H	1207	CLA	O2D-CGD	5.68	1.47	1.33
19	A	1104	CLA	O2D-CGD	5.68	1.47	1.33
19	A	1112	CLA	O2D-CGD	5.68	1.47	1.33
19	B	1239	CLA	CHD-C1D	5.67	1.49	1.38
19	L	1504	CLA	CHD-C1D	5.67	1.49	1.38
19	B	1231	CLA	O2D-CGD	5.67	1.47	1.33
19	B	1209	CLA	CHD-C1D	5.67	1.49	1.38
19	B	1224	CLA	C3D-C4D	-5.67	1.31	1.44
19	2	4009	CLA	O2D-CGD	5.66	1.47	1.33
19	B	1230	CLA	O2D-CGD	5.66	1.47	1.33
19	B	1222	CLA	CHD-C1D	5.66	1.49	1.38
19	1	1005	CLA	CHD-C4C	5.66	1.52	1.39
19	B	1221	CLA	CHD-C1D	5.65	1.49	1.38
19	A	1140	CLA	CHD-C1D	5.65	1.49	1.38
19	4	4014	CLA	O2D-CGD	5.65	1.47	1.33
19	L	1503	CLA	CHD-C4C	5.65	1.52	1.39
19	B	1217	CLA	CHD-C1D	5.64	1.49	1.38
19	B	1214	CLA	CHD-C1D	5.64	1.49	1.38
19	A	1127	CLA	CHD-C1D	5.64	1.49	1.38
19	F	1305	CLA	C3D-C4D	-5.64	1.31	1.44
19	2	2001	CLA	CHD-C4C	5.64	1.52	1.39
19	B	1205	CLA	O2D-CGD	5.64	1.47	1.33
19	3	3007	CLA	CHD-C4C	5.63	1.52	1.39
19	L	1501	CLA	CHD-C1D	5.62	1.49	1.38
19	B	1228	CLA	CHC-C1C	5.62	1.49	1.38
19	1	1013	CLA	CHC-C1C	5.62	1.49	1.38
19	A	1141	CLA	CHD-C4C	5.62	1.52	1.39
19	H	1207	CLA	C3D-C4D	-5.61	1.31	1.44
19	H	1207	CLA	CHD-C4C	5.61	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1010	CLA	CHC-C1C	5.61	1.49	1.38
21	F	6016	BCR	C30-C25	-5.61	1.46	1.53
19	L	1504	CLA	CHD-C4C	5.61	1.52	1.39
19	A	1117	CLA	CHD-C4C	5.61	1.52	1.39
19	J	1308	CLA	CHC-C1C	5.60	1.49	1.38
19	3	3012	CLA	CHD-C1D	5.60	1.52	1.38
19	B	1227	CLA	O2D-CGD	5.60	1.47	1.33
19	K	3009	CLA	CHD-C1D	5.60	1.49	1.38
19	B	1206	CLA	CHD-C1D	5.59	1.49	1.38
19	4	4001	CLA	CHD-C4C	5.59	1.51	1.39
19	4	4007	CLA	CHD-C4C	5.59	1.51	1.39
19	B	1221	CLA	CHC-C1C	5.59	1.49	1.38
19	B	9010	CLA	CHD-C4C	5.59	1.51	1.39
19	A	1135	CLA	CHD-C4C	5.59	1.51	1.39
19	3	2009	CLA	CHD-C1D	5.59	1.49	1.38
19	A	1140	CLA	CHD-C4C	5.58	1.51	1.39
19	B	1232	CLA	O2D-CGD	5.58	1.47	1.33
19	B	1208	CLA	O2A-CGA	5.58	1.49	1.33
19	B	1239	CLA	CHC-C1C	5.58	1.49	1.38
19	B	1228	CLA	CHD-C4C	5.58	1.51	1.39
19	L	1504	CLA	O2D-CGD	5.57	1.46	1.33
19	B	1229	CLA	CHC-C4B	5.57	1.51	1.39
19	A	9012	CLA	CHD-C1D	5.57	1.49	1.38
19	3	3008	CLA	CHD-C4C	5.56	1.51	1.39
19	B	1233	CLA	CHD-C4C	5.56	1.51	1.39
19	B	1220	CLA	C1B-NB	-5.56	1.30	1.37
19	4	4014	CLA	O2A-CGA	5.56	1.49	1.33
19	1	1303	CLA	CHD-C4C	5.56	1.51	1.39
19	K	1146	CLA	CHC-C1C	5.56	1.49	1.38
19	B	1212	CLA	O2D-CGD	5.56	1.46	1.33
19	4	4006	CLA	CHD-C4C	5.56	1.51	1.39
19	B	1213	CLA	CHD-C4C	5.55	1.51	1.39
19	A	1134	CLA	CHD-C4C	5.55	1.51	1.39
19	B	1223	CLA	CHD-C4C	5.55	1.51	1.39
19	A	1127	CLA	CHD-C4C	5.55	1.51	1.39
19	A	1151	CLA	O2D-CGD	5.55	1.46	1.33
19	4	1009	CLA	CHD-C1D	5.55	1.49	1.38
19	1	1001	CLA	C3D-C4D	-5.55	1.31	1.44
19	A	1136	CLA	CHD-C4C	5.55	1.51	1.39
19	B	1203	CLA	CHC-C1C	5.55	1.49	1.38
19	B	1205	CLA	CAB-C3B	-5.55	1.32	1.47
19	B	1210	CLA	CHC-C4B	5.54	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3016	CLA	CHD-C4C	5.54	1.51	1.39
19	4	4006	CLA	CHD-C1D	5.54	1.49	1.38
19	B	1211	CLA	O2D-CGD	5.54	1.46	1.33
19	1	1008	CLA	O2D-CGD	5.54	1.46	1.33
19	R	1150	CLA	CHD-C4C	5.54	1.51	1.39
19	A	1237	CLA	CHD-C4C	5.53	1.51	1.39
19	A	1125	CLA	CHD-C1D	5.53	1.49	1.38
19	R	1150	CLA	OBD-CAD	5.53	1.32	1.22
19	F	1302	CLA	CHD-C4C	5.53	1.51	1.39
19	3	1147	CLA	C3D-C4D	-5.52	1.31	1.44
19	A	9011	CLA	O2D-CGD	5.52	1.46	1.33
19	1	1002	CLA	CHD-C4C	5.52	1.51	1.39
19	B	1210	CLA	CAB-C3B	-5.52	1.32	1.47
19	A	1124	CLA	CHD-C4C	5.52	1.51	1.39
19	K	3009	CLA	CHD-C4C	5.52	1.51	1.39
19	3	3008	CLA	C3D-C4D	-5.52	1.31	1.44
19	A	1237	CLA	O2D-CGD	5.52	1.46	1.33
19	L	1130	CLA	O2D-CGD	5.51	1.46	1.33
19	A	1105	CLA	O2D-CGD	5.51	1.46	1.33
19	3	2009	CLA	C3D-C4D	-5.51	1.31	1.44
19	A	1132	CLA	O2D-CGD	5.51	1.46	1.33
19	B	1217	CLA	CHD-C4C	5.51	1.51	1.39
19	2	2012	CLA	CAB-C3B	-5.50	1.32	1.47
19	B	1225	CLA	CHD-C1D	5.50	1.49	1.38
19	A	9011	CLA	CHC-C4B	5.50	1.51	1.39
19	2	2014	CLA	CHD-C1D	5.50	1.49	1.38
19	B	1230	CLA	CHD-C4C	5.49	1.51	1.39
19	1	1003	CLA	CHC-C4B	5.49	1.51	1.39
19	A	1137	CLA	CHD-C4C	5.49	1.51	1.39
19	A	1139	CLA	CHD-C4C	5.49	1.51	1.39
19	B	1223	CLA	O2D-CGD	5.49	1.46	1.33
19	A	1122	CLA	O2A-CGA	5.49	1.49	1.33
19	1	1008	CLA	CHD-C4C	5.48	1.51	1.39
19	3	3004	CLA	CHC-C1C	5.48	1.49	1.38
19	G	1242	CLA	CHC-C4B	5.48	1.51	1.39
19	A	1139	CLA	CAB-C3B	-5.48	1.32	1.47
19	2	4009	CLA	CHD-C4C	5.47	1.51	1.39
19	4	4012	CLA	CHD-C1D	5.47	1.49	1.38
19	K	1142	CLA	CHD-C4C	5.47	1.51	1.39
19	A	1120	CLA	CHC-C4B	5.47	1.51	1.39
19	4	4014	CLA	C3D-C4D	-5.47	1.31	1.44
19	B	1236	CLA	O2D-CGD	5.47	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1210	CLA	CHD-C4C	5.47	1.51	1.39
19	F	1302	CLA	O2D-CGD	5.47	1.46	1.33
19	K	3009	CLA	CHC-C4B	5.47	1.51	1.39
19	4	4003	CLA	O2D-CGD	5.46	1.46	1.33
19	B	1231	CLA	CHD-C4C	5.45	1.51	1.39
19	B	1233	CLA	CHC-C4B	5.45	1.51	1.39
19	1	1012	CLA	CHC-C4B	5.45	1.51	1.39
19	4	4002	CLA	O2D-CGD	5.45	1.46	1.33
19	B	1212	CLA	CHC-C4B	5.45	1.51	1.39
19	A	1128	CLA	O2D-CGD	5.44	1.46	1.33
19	B	1227	CLA	C3D-C4D	-5.44	1.31	1.44
19	4	4011	CLA	CHD-C1D	5.44	1.51	1.38
19	A	9012	CLA	CHD-C4C	5.44	1.51	1.39
19	4	1004	CLA	CHD-C4C	5.44	1.51	1.39
19	3	2009	CLA	O2D-CGD	5.44	1.46	1.33
19	A	1141	CLA	O2D-CGD	5.43	1.46	1.33
19	4	1004	CLA	O2D-CGD	5.43	1.46	1.33
19	R	1150	CLA	CHC-C4B	5.43	1.51	1.39
19	1	1001	CLA	CHD-C1D	5.43	1.49	1.38
19	1	1011	CLA	CHD-C1D	5.43	1.49	1.38
19	A	9023	CLA	CAB-C3B	-5.43	1.32	1.47
19	2	2004	CLA	O2D-CGD	5.42	1.46	1.33
19	3	3011	CLA	O2D-CGD	5.42	1.46	1.33
19	A	1103	CLA	O2A-CGA	5.42	1.49	1.33
19	B	1215	CLA	O2D-CGD	5.42	1.46	1.33
19	J	1311	CLA	CHD-C4C	5.41	1.51	1.39
19	1	1007	CLA	CHD-C4C	5.41	1.51	1.39
19	A	1128	CLA	CHD-C1D	5.41	1.49	1.38
19	B	1222	CLA	CHD-C4C	5.41	1.51	1.39
19	F	1302	CLA	CHC-C4B	5.40	1.51	1.39
19	B	1209	CLA	O2D-CGD	5.40	1.46	1.33
19	1	1303	CLA	O2D-CGD	5.40	1.46	1.33
19	K	1146	CLA	CHD-C4C	5.40	1.51	1.39
19	I	1204	CLA	CHC-C4B	5.40	1.51	1.39
19	4	1306	CLA	O2D-CGD	5.40	1.46	1.33
19	4	1009	CLA	C3D-C4D	-5.40	1.32	1.44
19	A	9011	CLA	CHD-C4C	5.39	1.51	1.39
19	A	9023	CLA	CHD-C4C	5.39	1.51	1.39
19	L	1148	CLA	CHD-C4C	5.39	1.51	1.39
19	4	4014	CLA	CHD-C1D	5.39	1.48	1.38
19	B	1226	CLA	C3D-C4D	-5.39	1.32	1.44
19	K	1143	CLA	O2D-CGD	5.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	2002	CLA	O2A-CGA	5.39	1.49	1.33
19	B	1216	CLA	CHD-C1D	5.38	1.48	1.38
19	1	1014	CLA	C3D-C4D	-5.38	1.32	1.44
19	4	4002	CLA	CHD-C1D	5.38	1.48	1.38
19	2	2006	CLA	CHD-C4C	5.38	1.51	1.39
19	A	9012	CLA	O2D-CGD	5.38	1.46	1.33
19	B	1216	CLA	CHD-C4C	5.37	1.51	1.39
19	B	1217	CLA	CHC-C4B	5.37	1.51	1.39
19	1	1002	CLA	O2A-CGA	5.37	1.49	1.33
21	I	6021	BCR	C24-C23	5.37	1.49	1.33
19	B	1209	CLA	CHD-C4C	5.37	1.51	1.39
19	A	1129	CLA	O2A-CGA	5.37	1.49	1.33
19	I	1204	CLA	CHD-C4C	5.36	1.51	1.39
19	B	1220	CLA	CHC-C1C	5.36	1.49	1.38
19	4	1009	CLA	CHD-C4C	5.36	1.51	1.39
19	B	1221	CLA	O2D-CGD	5.36	1.46	1.33
19	L	1503	CLA	CHD-C1D	5.36	1.48	1.38
19	A	9023	CLA	O2D-CGD	5.36	1.46	1.33
19	A	1135	CLA	C3D-C4D	-5.36	1.32	1.44
19	B	1212	CLA	CHD-C4C	5.36	1.51	1.39
19	2	2002	CLA	CHC-C4B	5.36	1.51	1.39
19	B	1230	CLA	CHC-C1C	5.36	1.49	1.38
19	2	2013	CLA	O2A-CGA	5.35	1.49	1.33
19	A	1138	CLA	CAB-C3B	-5.35	1.33	1.47
19	A	1237	CLA	CHD-C1D	5.35	1.48	1.38
19	3	3016	CLA	O2D-CGD	5.35	1.46	1.33
19	A	1115	CLA	C3D-C4D	-5.35	1.32	1.44
19	A	1126	CLA	CAB-C3B	-5.35	1.33	1.47
19	2	2006	CLA	CHD-C1D	5.35	1.48	1.38
19	4	4012	CLA	CHD-C4C	5.34	1.51	1.39
19	B	1220	CLA	CHD-C1D	5.34	1.48	1.38
19	L	1504	CLA	OBD-CAD	5.34	1.31	1.22
19	A	1102	CLA	O2A-CGA	5.34	1.48	1.33
19	A	1135	CLA	CAB-C3B	-5.34	1.33	1.47
19	B	1221	CLA	CAB-C3B	-5.33	1.33	1.47
19	B	1229	CLA	CHD-C4C	5.33	1.51	1.39
19	J	1308	CLA	C3D-C4D	-5.33	1.32	1.44
19	B	1228	CLA	CHD-C1D	5.32	1.48	1.38
19	J	1308	CLA	CHD-C1D	5.32	1.48	1.38
19	A	1110	CLA	CHC-C4B	5.31	1.51	1.39
19	B	1301	CLA	CHD-C4C	5.31	1.51	1.39
19	B	1236	CLA	C3D-C4D	-5.31	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1127	CLA	O2D-CGD	5.31	1.46	1.33
19	A	1132	CLA	C3D-C4D	-5.31	1.32	1.44
19	4	4014	CLA	CHD-C4C	5.31	1.51	1.39
19	B	1224	CLA	O2D-CGD	5.31	1.46	1.33
19	1	1014	CLA	CHD-C1D	5.30	1.48	1.38
19	4	1304	CLA	CAB-C3B	-5.30	1.33	1.47
19	B	1231	CLA	CHD-C1D	5.30	1.48	1.38
19	J	1308	CLA	O2D-CGD	5.30	1.46	1.33
19	L	1148	CLA	CHC-C4B	5.29	1.51	1.39
19	A	1125	CLA	C3D-C4D	-5.29	1.32	1.44
19	A	1115	CLA	CHD-C4C	5.29	1.51	1.39
19	3	2009	CLA	CHD-C4C	5.29	1.51	1.39
19	A	1109	CLA	O2D-CGD	5.29	1.46	1.33
19	2	2001	CLA	O2D-CGD	5.29	1.46	1.33
19	2	1307	CLA	CHD-C1D	5.28	1.51	1.38
19	B	1219	CLA	CAB-C3B	-5.28	1.33	1.47
19	A	1137	CLA	CAB-C3B	-5.28	1.33	1.47
19	A	1119	CLA	CHC-C4B	5.28	1.51	1.39
19	A	1140	CLA	O2D-CGD	5.28	1.46	1.33
19	A	1139	CLA	O2D-CGD	5.28	1.46	1.33
19	A	1102	CLA	CHC-C4B	5.28	1.51	1.39
19	A	1136	CLA	CAB-C3B	-5.27	1.33	1.47
19	B	1238	CLA	O2D-CGD	5.27	1.46	1.33
19	B	1215	CLA	CHD-C4C	5.27	1.51	1.39
19	A	9022	CLA	O2D-CGD	5.27	1.46	1.33
19	H	1505	CLA	CHC-C4B	5.27	1.51	1.39
19	J	1308	CLA	CAB-C3B	-5.26	1.33	1.47
19	B	1229	CLA	CAB-C3B	-5.26	1.33	1.47
19	B	1217	CLA	O2D-CGD	5.26	1.46	1.33
19	B	1224	CLA	CHC-C4B	5.26	1.51	1.39
19	B	1225	CLA	CHD-C4C	5.26	1.51	1.39
19	2	2014	CLA	C3D-C4D	-5.26	1.32	1.44
19	A	1129	CLA	C3D-C4D	-5.25	1.32	1.44
19	3	3013	CLA	CAB-C3B	-5.25	1.33	1.47
19	B	1208	CLA	CHC-C4B	5.25	1.51	1.39
19	A	1138	CLA	O2D-CGD	5.25	1.46	1.33
19	R	1144	CLA	O2A-CGA	5.24	1.48	1.33
19	H	1145	CLA	CHD-C4C	5.24	1.51	1.39
19	2	2014	CLA	O2D-CGD	5.24	1.46	1.33
19	1	1003	CLA	O2D-CGD	5.24	1.46	1.33
19	B	1201	CLA	O2A-CGA	5.23	1.48	1.30
19	L	1502	CLA	CHC-C4B	5.23	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1214	CLA	O2A-CGA	5.23	1.48	1.33
19	B	1235	CLA	CAB-C3B	-5.22	1.33	1.47
19	1	1015	CLA	CHD-C1D	5.22	1.51	1.38
19	B	1202	CLA	O2D-CGD	5.22	1.46	1.33
19	B	1211	CLA	O2A-CGA	5.22	1.48	1.33
19	L	1503	CLA	CHC-C4B	5.22	1.51	1.39
19	K	3009	CLA	O2D-CGD	5.21	1.46	1.33
19	A	1127	CLA	CAB-C3B	-5.21	1.33	1.47
19	1	1007	CLA	CHD-C1D	5.21	1.48	1.38
19	A	1125	CLA	CHD-C4C	5.21	1.51	1.39
19	B	1230	CLA	C3D-C4D	-5.21	1.32	1.44
19	A	1103	CLA	CAB-C3B	-5.21	1.33	1.47
19	2	2004	CLA	CHC-C4B	5.20	1.51	1.39
19	2	2013	CLA	CHD-C4C	5.20	1.51	1.39
19	B	1236	CLA	CHD-C1D	5.20	1.48	1.38
19	B	1202	CLA	O2A-CGA	5.20	1.48	1.33
19	2	2013	CLA	C3D-C4D	-5.20	1.32	1.44
19	A	1106	CLA	C3D-C4D	-5.20	1.32	1.44
19	A	1108	CLA	C3D-C4D	-5.20	1.32	1.44
19	3	3012	CLA	CHC-C1C	5.20	1.48	1.38
19	A	1116	CLA	CHC-C4B	5.20	1.51	1.39
19	4	4012	CLA	CHC-C4B	5.20	1.51	1.39
19	A	1108	CLA	CHC-C4B	5.20	1.51	1.39
20	A	5001	PQN	C10-C5	5.19	1.49	1.40
19	A	1136	CLA	C3D-C4D	-5.19	1.32	1.44
19	3	3017	CLA	CHC-C1C	5.19	1.48	1.38
19	B	1236	CLA	CHC-C4B	5.19	1.51	1.39
19	B	1236	CLA	CHD-C4C	5.19	1.51	1.39
19	K	1143	CLA	C3D-C4D	-5.19	1.32	1.44
19	1	1011	CLA	C3D-C4D	-5.19	1.32	1.44
19	A	9022	CLA	CAB-C3B	-5.19	1.33	1.47
19	A	1124	CLA	CAB-C3B	-5.19	1.33	1.47
19	B	1301	CLA	CHC-C4B	5.19	1.51	1.39
19	B	1234	CLA	CAB-C3B	-5.18	1.33	1.47
19	I	1204	CLA	C3D-C4D	-5.18	1.32	1.44
19	1	1003	CLA	C3D-C4D	-5.18	1.32	1.44
19	A	1128	CLA	C3D-C4D	-5.18	1.32	1.44
19	B	1239	CLA	O2D-CGD	5.18	1.46	1.33
19	4	1304	CLA	O2D-CGD	5.17	1.46	1.33
19	L	1501	CLA	CHC-C4B	5.17	1.51	1.39
19	B	1239	CLA	CHD-C4C	5.17	1.51	1.39
19	A	1117	CLA	O2A-CGA	5.17	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	4002	CLA	CHD-C4C	5.16	1.51	1.39
19	F	1305	CLA	CHD-C4C	5.16	1.51	1.39
19	L	1501	CLA	CHD-C4C	5.16	1.50	1.39
19	B	1227	CLA	O2A-CGA	5.16	1.48	1.33
19	B	1213	CLA	CHC-C4B	5.16	1.51	1.39
19	B	1219	CLA	C3D-C4D	-5.16	1.32	1.44
19	A	1125	CLA	CAB-C3B	-5.15	1.33	1.47
19	I	1204	CLA	O2A-CGA	5.15	1.48	1.33
19	A	1137	CLA	C3D-C4D	-5.15	1.32	1.44
19	3	3013	CLA	CHD-C1D	5.15	1.48	1.38
19	A	1134	CLA	O2D-CGD	5.15	1.45	1.33
19	1	1011	CLA	CHC-C1C	5.15	1.48	1.38
19	4	4006	CLA	CHC-C4B	5.15	1.51	1.39
19	A	1110	CLA	O2A-CGA	5.14	1.48	1.33
19	1	1010	CLA	CHD-C4C	5.14	1.50	1.39
19	3	3002	CLA	CHD-C1D	5.14	1.50	1.38
19	A	9013	CLA	O2D-CGD	5.14	1.45	1.33
19	B	1231	CLA	C3D-C4D	-5.13	1.32	1.44
19	1	1011	CLA	CHD-C4C	5.13	1.50	1.39
19	K	1142	CLA	O2D-CGD	5.13	1.45	1.33
19	A	1138	CLA	C3D-C4D	-5.13	1.32	1.44
19	A	9012	CLA	CAB-C3B	-5.13	1.33	1.47
19	4	4001	CLA	CHC-C4B	5.13	1.50	1.39
19	2	4009	CLA	C3D-C4D	-5.13	1.32	1.44
19	A	1112	CLA	CHC-C4B	5.12	1.50	1.39
19	4	4004	CLA	CHD-C1D	5.12	1.50	1.38
19	4	4015	CLA	CAB-C3B	-5.12	1.33	1.47
19	A	1127	CLA	O2A-CGA	5.12	1.48	1.33
19	B	1232	CLA	CHC-C4B	5.11	1.50	1.39
19	B	1218	CLA	CHD-C1D	5.11	1.48	1.38
19	3	3016	CLA	C3D-C4D	-5.11	1.32	1.44
19	A	1140	CLA	C3D-C4D	-5.11	1.32	1.44
19	R	1150	CLA	CAB-C3B	-5.11	1.33	1.47
19	1	1010	CLA	C4C-C3C	-5.11	1.36	1.45
19	B	1208	CLA	C3D-C4D	-5.11	1.32	1.44
19	3	3003	CLA	CHC-C4B	5.11	1.50	1.39
19	B	1238	CLA	CHC-C4B	5.10	1.50	1.39
19	B	1216	CLA	C3D-C4D	-5.10	1.32	1.44
19	A	1116	CLA	O2A-CGA	5.10	1.48	1.33
19	4	4005	CLA	CHD-C1D	5.09	1.50	1.38
19	1	1303	CLA	CHC-C1C	5.09	1.48	1.38
19	A	1101	CLA	O2D-CGD	5.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1203	CLA	O2D-CGD	5.09	1.45	1.33
19	K	1142	CLA	C3D-C4D	-5.09	1.32	1.44
19	1	1008	CLA	CHC-C4B	5.09	1.50	1.39
19	J	1311	CLA	C3D-C4D	-5.09	1.32	1.44
19	3	3013	CLA	C4C-C3C	-5.09	1.36	1.45
21	A	6007	BCR	C30-C25	-5.09	1.47	1.53
19	B	1229	CLA	O2A-CGA	5.08	1.48	1.33
19	B	1226	CLA	CHD-C4C	5.08	1.50	1.39
19	1	1001	CLA	CHD-C4C	5.08	1.50	1.39
19	A	1134	CLA	C3D-C4D	-5.08	1.32	1.44
19	4	1304	CLA	C3D-C4D	-5.07	1.32	1.44
19	B	1222	CLA	CAB-C3B	-5.07	1.33	1.47
19	B	1211	CLA	CAB-C3B	-5.07	1.33	1.47
19	B	1231	CLA	CAB-C3B	-5.07	1.33	1.47
19	B	1233	CLA	C3D-C4D	-5.07	1.32	1.44
19	B	1210	CLA	O2D-CGD	5.07	1.45	1.33
19	3	1147	CLA	CHC-C1C	5.07	1.48	1.38
19	1	1014	CLA	CAB-C3B	-5.07	1.33	1.47
19	3	3017	CLA	C3D-C4D	-5.07	1.32	1.44
19	B	1214	CLA	CHC-C4B	5.07	1.50	1.39
19	A	1135	CLA	O2D-CGD	5.07	1.45	1.33
19	F	1302	CLA	C3D-C4D	-5.06	1.32	1.44
19	1	1001	CLA	O2D-CED	5.06	1.56	1.45
19	B	1215	CLA	C3D-C4D	-5.06	1.32	1.44
19	B	1231	CLA	CHC-C4B	5.06	1.50	1.39
19	A	1141	CLA	CAB-C3B	-5.06	1.33	1.47
19	1	1010	CLA	O2D-CGD	5.06	1.45	1.33
19	A	1111	CLA	O2D-CGD	5.06	1.45	1.33
19	1	1005	CLA	C3D-C4D	-5.06	1.32	1.44
19	B	1223	CLA	C3D-C4D	-5.06	1.32	1.44
19	B	1203	CLA	C3D-C4D	-5.06	1.32	1.44
19	A	1113	CLA	CHC-C4B	5.06	1.50	1.39
19	2	2006	CLA	C3D-C4D	-5.06	1.32	1.44
19	B	1218	CLA	O2A-CGA	5.05	1.48	1.33
19	B	1222	CLA	C3D-C4D	-5.05	1.32	1.44
19	A	1122	CLA	CHC-C4B	5.05	1.50	1.39
19	K	3009	CLA	C3D-C4D	-5.05	1.32	1.44
19	A	9013	CLA	C3D-C4D	-5.05	1.32	1.44
19	A	1126	CLA	CHC-C4B	5.05	1.50	1.39
19	L	1501	CLA	O2A-CGA	5.05	1.48	1.33
19	3	3015	CLA	CHD-C1D	5.04	1.50	1.38
19	A	1139	CLA	C3D-C4D	-5.04	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	9011	CLA	CHD-C1D	5.04	1.48	1.38
19	B	1216	CLA	O2D-CGD	5.04	1.45	1.33
19	B	1201	CLA	O2D-CGD	5.04	1.45	1.33
19	I	1204	CLA	O2D-CGD	5.04	1.45	1.33
19	B	1226	CLA	O2D-CGD	5.04	1.45	1.33
19	1	1014	CLA	CHD-C4C	5.04	1.50	1.39
19	A	9022	CLA	O2A-CGA	5.04	1.48	1.33
19	A	9022	CLA	CHC-C4B	5.03	1.50	1.39
19	3	3016	CLA	CAB-C3B	-5.03	1.34	1.47
19	B	1229	CLA	C3D-C4D	-5.03	1.32	1.44
19	R	1150	CLA	O2A-CGA	5.03	1.48	1.33
19	3	2009	CLA	CAB-C3B	-5.03	1.34	1.47
19	K	1146	CLA	CAB-C3B	-5.03	1.34	1.47
19	L	1130	CLA	CAB-C3B	-5.03	1.34	1.47
19	A	1140	CLA	CHC-C4B	5.03	1.50	1.39
19	H	1145	CLA	O2D-CGD	5.02	1.45	1.33
19	A	1125	CLA	O2D-CGD	5.02	1.45	1.33
19	1	1013	CLA	CHD-C1D	5.02	1.48	1.38
19	2	2014	CLA	CHD-C4C	5.02	1.50	1.39
19	A	1135	CLA	CHC-C4B	5.02	1.50	1.39
19	A	1120	CLA	C3D-C4D	-5.02	1.32	1.44
19	A	1124	CLA	CHC-C4B	5.02	1.50	1.39
19	L	1501	CLA	C3D-C4D	-5.02	1.32	1.44
19	4	4006	CLA	C3D-C4D	-5.02	1.32	1.44
19	A	1129	CLA	O2D-CGD	5.01	1.45	1.33
19	B	1227	CLA	CHC-C4B	5.01	1.50	1.39
19	1	1303	CLA	CHD-C1D	5.01	1.48	1.38
19	1	1007	CLA	CHC-C4B	5.01	1.50	1.39
19	B	1231	CLA	OBD-CAD	5.01	1.31	1.22
19	B	1223	CLA	CAB-C3B	-5.00	1.34	1.47
19	B	1209	CLA	C3D-C4D	-5.00	1.32	1.44
19	B	1232	CLA	CAB-C3B	-5.00	1.34	1.47
19	A	1102	CLA	O2D-CGD	5.00	1.45	1.33
19	J	1308	CLA	CHD-C4C	5.00	1.50	1.39
19	A	9013	CLA	CHC-C4B	5.00	1.50	1.39
19	F	1305	CLA	CAB-C3B	-5.00	1.34	1.47
19	3	3017	CLA	O2D-CGD	5.00	1.45	1.33
19	K	3009	CLA	O2A-CGA	5.00	1.47	1.33
19	R	1144	CLA	CHC-C4B	5.00	1.50	1.39
19	G	1242	CLA	C3D-C4D	-5.00	1.32	1.44
19	B	1208	CLA	O2D-CGD	4.99	1.45	1.33
19	3	3014	CLA	CHD-C1D	4.99	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1117	CLA	O2D-CGD	4.99	1.45	1.33
19	A	1237	CLA	CAB-C3B	-4.99	1.34	1.47
19	H	1241	CLA	CHC-C4B	4.99	1.50	1.39
19	2	2006	CLA	CHC-C4B	4.99	1.50	1.39
19	3	3001	CLA	CHD-C1D	4.99	1.50	1.38
19	B	1225	CLA	C3D-C4D	-4.99	1.33	1.44
19	4	1306	CLA	O2A-CGA	4.98	1.47	1.33
19	4	4003	CLA	CAB-C3B	-4.98	1.34	1.47
19	B	1222	CLA	O2D-CGD	4.98	1.45	1.33
19	1	1303	CLA	OBD-CAD	4.98	1.31	1.22
19	B	1234	CLA	C3D-C4D	-4.98	1.33	1.44
19	K	1142	CLA	CHC-C4B	4.98	1.50	1.39
19	4	1004	CLA	C3D-C4D	-4.97	1.33	1.44
19	F	1302	CLA	CAB-C3B	-4.97	1.34	1.47
19	B	1206	CLA	CHC-C4B	4.97	1.50	1.39
19	1	1010	CLA	CHD-C1D	4.97	1.48	1.38
19	B	1223	CLA	CHC-C4B	4.97	1.50	1.39
19	A	1107	CLA	CHC-C1C	4.96	1.48	1.38
19	4	1004	CLA	CAB-C3B	-4.96	1.34	1.47
19	K	1142	CLA	O2A-CGA	4.96	1.47	1.30
19	A	1133	CLA	C3D-C4D	-4.96	1.33	1.44
19	2	2010	CLA	CHD-C1D	4.96	1.50	1.38
19	4	1304	CLA	CHD-C1D	4.95	1.48	1.38
19	A	1115	CLA	CAB-C3B	-4.95	1.34	1.47
19	A	1115	CLA	CHC-C4B	4.95	1.50	1.39
19	1	1001	CLA	OBD-CAD	4.95	1.31	1.22
19	B	1227	CLA	CAB-C3B	-4.95	1.34	1.47
19	B	1206	CLA	O2D-CGD	4.95	1.45	1.33
19	1	1011	CLA	C1B-NB	-4.95	1.31	1.37
19	A	1237	CLA	C3D-C4D	-4.94	1.33	1.44
19	4	1306	CLA	CAB-C3B	-4.94	1.34	1.47
19	4	4003	CLA	C3D-C4D	-4.94	1.33	1.44
19	A	1136	CLA	O2D-CGD	4.94	1.45	1.33
19	2	2001	CLA	CHC-C4B	4.94	1.50	1.39
19	3	3016	CLA	CHC-C4B	4.94	1.50	1.39
19	L	1504	CLA	O2A-CGA	4.94	1.47	1.33
19	A	9012	CLA	CHC-C4B	4.94	1.50	1.39
19	A	1106	CLA	CHC-C4B	4.94	1.50	1.39
19	B	1238	CLA	O2A-CGA	4.93	1.47	1.33
19	B	1211	CLA	C3D-C4D	-4.93	1.33	1.44
19	1	1006	CLA	CHC-C4B	4.93	1.50	1.39
19	B	1233	CLA	O2A-CGA	4.93	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1220	CLA	CHC-C4B	4.93	1.50	1.39
19	1	1007	CLA	CAB-C3B	-4.93	1.34	1.47
19	B	1225	CLA	CAB-C3B	-4.93	1.34	1.47
19	F	1240	CLA	C3D-C4D	-4.92	1.33	1.44
19	B	1202	CLA	CAB-C3B	-4.92	1.34	1.47
19	B	1224	CLA	CAB-C3B	-4.92	1.34	1.47
19	A	1141	CLA	CHC-C4B	4.92	1.50	1.39
19	3	3008	CLA	CAB-C3B	-4.92	1.34	1.47
19	A	1112	CLA	OBD-CAD	4.91	1.30	1.22
19	3	3013	CLA	CHD-C4C	4.91	1.50	1.39
19	A	9012	CLA	O2A-CGA	4.91	1.47	1.33
19	2	2014	CLA	CAB-C3B	-4.91	1.34	1.47
19	B	1218	CLA	CHC-C4B	4.91	1.50	1.39
19	A	1131	CLA	C3D-C4D	-4.91	1.33	1.44
19	B	1236	CLA	O2A-CGA	4.91	1.47	1.33
19	B	1235	CLA	C3D-C4D	-4.91	1.33	1.44
19	L	1504	CLA	CHC-C4B	4.90	1.50	1.39
19	F	1305	CLA	O2D-CGD	4.90	1.45	1.33
19	3	1118	CLA	CHC-C4B	4.90	1.50	1.39
19	A	1108	CLA	O2A-CGA	4.90	1.47	1.30
19	3	2009	CLA	CHC-C4B	4.90	1.50	1.39
19	A	1140	CLA	CAB-C3B	-4.90	1.34	1.47
19	A	1132	CLA	CAB-C3B	-4.90	1.34	1.47
19	A	1110	CLA	C3D-C4D	-4.90	1.33	1.44
19	4	4015	CLA	CHD-C1D	4.90	1.48	1.38
19	B	1221	CLA	C3D-C4D	-4.90	1.33	1.44
19	B	1233	CLA	CAB-C3B	-4.90	1.34	1.47
19	L	1503	CLA	CAB-C3B	-4.90	1.34	1.47
19	A	1124	CLA	C3D-C4D	-4.90	1.33	1.44
19	A	1137	CLA	O2D-CGD	4.90	1.45	1.33
19	4	1009	CLA	CHC-C4B	4.90	1.50	1.39
19	B	1216	CLA	O2A-CGA	4.89	1.47	1.33
19	B	1202	CLA	C3D-C4D	-4.89	1.33	1.44
19	1	1005	CLA	CHC-C4B	4.89	1.50	1.39
19	4	4014	CLA	CHC-C4B	4.89	1.50	1.39
19	2	2001	CLA	C3D-C4D	-4.89	1.33	1.44
19	3	3013	CLA	CHC-C1C	4.89	1.48	1.38
19	B	1234	CLA	O2A-CGA	4.89	1.47	1.33
19	A	1113	CLA	O2A-CGA	4.89	1.47	1.33
19	I	1204	CLA	CAB-C3B	-4.88	1.34	1.47
19	L	1502	CLA	CAB-C3B	-4.88	1.34	1.47
19	4	1009	CLA	OBD-CAD	4.88	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1013	CLA	C4C-C3C	-4.88	1.36	1.45
19	3	3005	CLA	CHD-C1D	4.88	1.50	1.38
19	R	1144	CLA	C3D-C4D	-4.88	1.33	1.44
19	A	1131	CLA	CAB-C3B	-4.88	1.34	1.47
19	2	4009	CLA	O2A-CGA	4.88	1.47	1.33
19	A	1137	CLA	CHC-C4B	4.88	1.50	1.39
19	3	3003	CLA	C3D-C4D	-4.88	1.33	1.44
19	J	1311	CLA	CHC-C4B	4.88	1.50	1.39
19	A	1141	CLA	C3D-C4D	-4.87	1.33	1.44
19	F	1240	CLA	CHC-C4B	4.87	1.50	1.39
19	3	3007	CLA	C3D-C4D	-4.87	1.33	1.44
19	B	1220	CLA	CHD-C4C	4.87	1.50	1.39
19	B	1222	CLA	CHC-C4B	4.87	1.50	1.39
24	B	7101	LMG	O7-C10	4.87	1.48	1.34
19	4	4015	CLA	CHD-C4C	4.86	1.50	1.39
19	B	9010	CLA	CHC-C4B	4.86	1.50	1.39
19	2	2012	CLA	O2D-CGD	4.86	1.45	1.33
19	A	1111	CLA	O2A-CGA	4.86	1.47	1.33
19	B	1231	CLA	O2A-CGA	4.86	1.46	1.30
19	4	4003	CLA	O2A-CGA	4.86	1.47	1.33
19	B	1239	CLA	O2A-CGA	4.86	1.47	1.33
19	B	1228	CLA	O2A-CGA	4.85	1.47	1.33
19	1	1014	CLA	CHC-C4B	4.85	1.50	1.39
19	A	1132	CLA	O2A-CGA	4.85	1.47	1.33
19	F	1305	CLA	CHC-C4B	4.85	1.50	1.39
19	1	1008	CLA	O2A-CGA	4.85	1.47	1.33
19	4	4015	CLA	C3D-C4D	-4.85	1.33	1.44
19	A	1115	CLA	O2D-CGD	4.85	1.45	1.33
19	2	2006	CLA	OBD-CAD	4.85	1.30	1.22
19	L	1130	CLA	CHC-C4B	4.84	1.50	1.39
19	A	1105	CLA	C3D-C4D	-4.84	1.33	1.44
19	B	1239	CLA	C3D-C4D	-4.84	1.33	1.44
19	1	1007	CLA	C3D-C4D	-4.84	1.33	1.44
19	B	9010	CLA	O2D-CGD	4.84	1.45	1.33
19	A	1106	CLA	O2D-CGD	4.83	1.45	1.33
19	A	9011	CLA	CAB-C3B	-4.83	1.34	1.47
19	B	1301	CLA	C3D-C4D	-4.83	1.33	1.44
19	A	1113	CLA	CAB-C3B	-4.83	1.34	1.47
19	H	1207	CLA	O2A-CGA	4.83	1.47	1.33
19	L	1502	CLA	O2A-CGA	4.83	1.47	1.33
19	B	1234	CLA	O2D-CGD	4.83	1.45	1.33
19	A	1125	CLA	CHC-C4B	4.83	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1013	CLA	CHD-C4C	4.83	1.50	1.39
19	A	9022	CLA	C3D-C4D	-4.83	1.33	1.44
19	3	2009	CLA	O2A-CGA	4.83	1.47	1.33
19	1	1011	CLA	C3A-C2A	-4.82	1.50	1.54
19	B	1228	CLA	C3D-C4D	-4.82	1.33	1.44
19	B	1225	CLA	CHC-C4B	4.82	1.50	1.39
19	H	1145	CLA	CAB-C3B	-4.82	1.34	1.47
19	A	1121	CLA	OBD-CAD	4.82	1.30	1.22
19	B	1239	CLA	CAB-C3B	-4.82	1.34	1.47
19	3	3008	CLA	CHC-C4B	4.82	1.50	1.39
19	4	4007	CLA	CHC-C4B	4.81	1.50	1.39
19	H	1207	CLA	CHC-C4B	4.81	1.50	1.39
19	A	1109	CLA	CHC-C4B	4.81	1.50	1.39
19	B	1232	CLA	O2A-CGA	4.81	1.46	1.30
19	A	1116	CLA	C3D-C4D	-4.81	1.33	1.44
19	A	1138	CLA	CHC-C4B	4.81	1.50	1.39
19	2	2012	CLA	CHC-C4B	4.81	1.50	1.39
19	1	1014	CLA	O2A-CGA	4.81	1.47	1.33
19	L	1503	CLA	C3D-C4D	-4.81	1.33	1.44
19	L	1130	CLA	O2A-CGA	4.81	1.47	1.33
19	A	1101	CLA	CAB-C3B	-4.81	1.34	1.47
21	A	6007	BCR	C20-C21	4.81	1.58	1.43
19	A	1107	CLA	CAB-C3B	-4.81	1.34	1.47
19	2	2005	CLA	CHD-C1D	4.81	1.50	1.38
19	K	1146	CLA	CHC-C4B	4.80	1.50	1.39
19	A	1123	CLA	C3D-C4D	-4.80	1.33	1.44
19	3	3006	CLA	CHD-C1D	4.80	1.50	1.38
19	A	1151	CLA	C3D-C4D	-4.80	1.33	1.44
19	B	1219	CLA	CHC-C4B	4.80	1.50	1.39
19	H	1241	CLA	OBD-CAD	4.80	1.30	1.22
19	A	1102	CLA	C3D-C4D	-4.80	1.33	1.44
19	A	1136	CLA	CHC-C4B	4.80	1.50	1.39
19	2	2013	CLA	CHC-C4B	4.80	1.50	1.39
19	J	1311	CLA	CAB-C3B	-4.80	1.34	1.47
19	A	1134	CLA	CHC-C4B	4.80	1.50	1.39
19	2	2001	CLA	CAB-C3B	-4.80	1.34	1.47
19	1	1005	CLA	O2A-CGA	4.79	1.47	1.33
19	2	2006	CLA	CAB-C3B	-4.79	1.34	1.47
19	A	1116	CLA	CAB-C3B	-4.79	1.34	1.47
19	A	1123	CLA	O2D-CGD	4.79	1.45	1.33
19	B	1201	CLA	C3D-C4D	-4.79	1.33	1.44
19	2	2014	CLA	CHC-C4B	4.79	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1151	CLA	CHC-C4B	4.79	1.50	1.39
19	1	1005	CLA	CAB-C3B	-4.78	1.34	1.47
19	A	1128	CLA	CHC-C4B	4.78	1.50	1.39
19	A	1105	CLA	CHC-C4B	4.78	1.50	1.39
19	A	1124	CLA	O2D-CGD	4.78	1.45	1.33
19	A	1134	CLA	CAB-C3B	-4.78	1.34	1.47
19	L	1504	CLA	C3D-C4D	-4.78	1.33	1.44
19	2	4009	CLA	CHC-C4B	4.78	1.50	1.39
19	B	1206	CLA	CAB-C3B	-4.78	1.34	1.47
19	4	1004	CLA	CHC-C4B	4.78	1.50	1.39
19	B	1217	CLA	O2A-CGA	4.78	1.47	1.33
19	A	1109	CLA	O2A-CGA	4.77	1.47	1.33
19	A	1121	CLA	CAB-C3B	-4.77	1.34	1.47
19	B	1238	CLA	C3D-C4D	-4.77	1.33	1.44
19	B	1216	CLA	CAB-C3B	-4.77	1.34	1.47
19	B	1213	CLA	OBD-CAD	4.77	1.30	1.22
19	A	9023	CLA	O2A-CGA	4.77	1.47	1.33
19	1	1010	CLA	C1B-NB	-4.77	1.31	1.37
19	B	1211	CLA	CHC-C4B	4.77	1.50	1.39
19	A	1123	CLA	CHC-C4B	4.77	1.50	1.39
19	A	1139	CLA	CHC-C4B	4.76	1.50	1.39
19	A	1107	CLA	C3D-C4D	-4.76	1.33	1.44
19	1	1310	CLA	CHD-C1D	4.76	1.50	1.38
19	1	1013	CLA	O2A-CGA	4.76	1.47	1.33
19	H	1505	CLA	C3D-C4D	-4.76	1.33	1.44
19	L	1503	CLA	O2A-CGA	4.76	1.47	1.33
19	B	1228	CLA	CHC-C4B	4.75	1.50	1.39
19	A	1119	CLA	C3D-C4D	-4.75	1.33	1.44
19	B	1201	CLA	CHC-C4B	4.75	1.50	1.39
19	B	1221	CLA	O2A-CGA	4.75	1.47	1.33
21	B	6020	BCR	C30-C25	-4.75	1.47	1.53
19	A	1127	CLA	CHC-C4B	4.75	1.50	1.39
19	B	9010	CLA	C3D-C4D	-4.75	1.33	1.44
19	A	1109	CLA	CAB-C3B	-4.75	1.34	1.47
19	A	1125	CLA	O2A-CGA	4.75	1.47	1.33
19	H	1241	CLA	O2A-CGA	4.75	1.47	1.33
19	A	1133	CLA	CHC-C4B	4.74	1.50	1.39
19	3	3011	CLA	C3D-C4D	-4.74	1.33	1.44
19	A	1309	CLA	CHD-C1D	4.74	1.50	1.38
19	3	3011	CLA	O2A-CGA	4.74	1.47	1.33
19	A	1151	CLA	OBD-CAD	4.73	1.30	1.22
19	B	1210	CLA	O2A-CGA	4.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1218	CLA	C3D-C4D	-4.73	1.33	1.44
19	A	1117	CLA	CAB-C3B	-4.73	1.34	1.47
19	1	1001	CLA	CHC-C1C	4.73	1.48	1.38
19	A	1104	CLA	CHC-C4B	4.73	1.50	1.39
19	1	1303	CLA	CAB-C3B	-4.73	1.34	1.47
19	A	1129	CLA	CHC-C4B	4.73	1.50	1.39
19	2	2007	CLA	O2A-CGA	4.72	1.47	1.33
20	B	5002	PQN	C10-C5	4.72	1.48	1.40
19	4	4003	CLA	CHC-C4B	4.72	1.50	1.39
19	A	1113	CLA	C3D-C4D	-4.72	1.33	1.44
19	A	1133	CLA	O2A-CGA	4.72	1.47	1.33
19	H	1505	CLA	O2A-CGA	4.72	1.47	1.33
19	B	1230	CLA	CHC-C4B	4.72	1.50	1.39
19	4	4007	CLA	CAB-C3B	-4.72	1.34	1.47
19	A	1104	CLA	C3D-C4D	-4.72	1.33	1.44
19	1	1006	CLA	C3D-C4D	-4.72	1.33	1.44
19	B	1209	CLA	CHC-C4B	4.72	1.50	1.39
19	K	1143	CLA	CHC-C4B	4.72	1.50	1.39
19	K	1143	CLA	CAB-C3B	-4.71	1.34	1.47
19	A	1119	CLA	O2A-CGA	4.71	1.47	1.33
19	F	1305	CLA	OBD-CAD	4.71	1.30	1.22
19	L	1148	CLA	O2A-CGA	4.71	1.47	1.33
19	1	1006	CLA	OBD-CAD	4.71	1.30	1.22
19	A	1107	CLA	O2A-CGA	4.71	1.47	1.33
19	1	1303	CLA	C1B-NB	-4.71	1.31	1.37
19	B	1205	CLA	CHC-C4B	4.71	1.50	1.39
19	B	1233	CLA	OBD-CAD	4.71	1.30	1.22
19	B	1216	CLA	CHC-C4B	4.71	1.50	1.39
19	4	4007	CLA	O2A-CGA	4.70	1.47	1.33
19	B	1221	CLA	OBD-CAD	4.70	1.30	1.22
19	A	1111	CLA	CHC-C4B	4.70	1.50	1.39
19	A	1237	CLA	CHC-C4B	4.70	1.50	1.39
19	B	1225	CLA	O2D-CGD	4.70	1.44	1.33
19	B	1215	CLA	CHC-C4B	4.70	1.50	1.39
19	3	1118	CLA	OBD-CAD	4.70	1.30	1.22
19	A	9013	CLA	OBD-CAD	4.70	1.30	1.22
19	H	1241	CLA	CAB-C3B	-4.69	1.34	1.47
19	B	1214	CLA	C3D-C4D	-4.69	1.33	1.44
19	3	3010	CLA	CHD-C1D	4.69	1.49	1.38
19	4	4006	CLA	OBD-CAD	4.69	1.30	1.22
19	B	1212	CLA	O2A-CGA	4.69	1.47	1.33
19	1	1008	CLA	C3D-C4D	-4.69	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	2007	CLA	OBD-CAD	4.69	1.30	1.22
19	3	3011	CLA	CHC-C4B	4.68	1.49	1.39
19	3	3004	CLA	CHD-C1D	4.68	1.49	1.38
19	3	1118	CLA	C3D-C4D	-4.68	1.33	1.44
19	A	1126	CLA	C3D-C4D	-4.68	1.33	1.44
19	A	1103	CLA	C3D-C4D	-4.68	1.33	1.44
19	B	1210	CLA	C3D-C4D	-4.68	1.33	1.44
19	A	1122	CLA	C3D-C4D	-4.68	1.33	1.44
19	4	4015	CLA	O2A-CGA	4.66	1.47	1.33
19	3	3016	CLA	O2A-CGA	4.66	1.46	1.33
19	J	1311	CLA	O2A-CGA	4.66	1.46	1.33
19	4	4010	CLA	CHD-C1D	4.66	1.49	1.38
19	3	3007	CLA	CHC-C4B	4.66	1.49	1.39
19	B	1221	CLA	CHC-C4B	4.65	1.49	1.39
19	A	1120	CLA	O2A-CGA	4.65	1.46	1.33
19	1	1007	CLA	O2A-CGA	4.65	1.46	1.33
19	B	1213	CLA	C3D-C4D	-4.65	1.33	1.44
19	4	4015	CLA	CHC-C4B	4.65	1.49	1.39
19	1	1010	CLA	CAB-C3B	-4.65	1.35	1.47
19	4	4001	CLA	C3D-C4D	-4.64	1.33	1.44
19	2	2002	CLA	C3D-C4D	-4.64	1.33	1.44
19	2	2004	CLA	C3D-C4D	-4.64	1.33	1.44
19	A	1131	CLA	O2D-CGD	4.64	1.44	1.33
19	B	1229	CLA	O2D-CGD	4.64	1.44	1.33
19	B	1215	CLA	CAB-C3B	-4.63	1.35	1.47
19	K	1146	CLA	C1B-NB	-4.63	1.31	1.37
19	K	3009	CLA	CAB-C3B	-4.63	1.35	1.47
19	B	1232	CLA	C3D-C4D	-4.63	1.33	1.44
19	B	1201	CLA	OBD-CAD	4.63	1.30	1.22
19	B	1212	CLA	C3D-C4D	-4.63	1.33	1.44
19	A	1131	CLA	CHC-C4B	4.62	1.49	1.39
19	B	1217	CLA	CAB-C3B	-4.62	1.35	1.47
19	3	3011	CLA	CAB-C3B	-4.62	1.35	1.47
19	A	1101	CLA	O2A-CGA	4.62	1.46	1.33
19	A	1117	CLA	CHC-C4B	4.62	1.49	1.39
19	2	2004	CLA	O2A-CGA	4.62	1.46	1.33
19	3	3017	CLA	CAB-C3B	-4.62	1.35	1.47
19	B	1301	CLA	OBD-CAD	4.62	1.30	1.22
19	J	1308	CLA	CHC-C4B	4.61	1.49	1.39
19	A	9023	CLA	CHC-C4B	4.61	1.49	1.39
19	2	2012	CLA	O2A-CGA	4.60	1.46	1.33
19	1	1303	CLA	C3A-C2A	-4.60	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	9012	CLA	C3D-C4D	-4.60	1.33	1.44
19	A	1123	CLA	CAB-C3B	-4.60	1.35	1.47
19	H	1505	CLA	CAB-C3B	-4.59	1.35	1.47
19	L	1501	CLA	CAB-C3B	-4.59	1.35	1.47
19	4	4012	CLA	C3D-C4D	-4.59	1.33	1.44
19	L	1148	CLA	C4B-NB	-4.59	1.31	1.37
19	H	1241	CLA	C3D-C4D	-4.59	1.33	1.44
19	1	1007	CLA	OBD-CAD	4.58	1.30	1.22
19	4	4001	CLA	O2A-CGA	4.58	1.46	1.33
19	B	1239	CLA	CHC-C4B	4.58	1.49	1.39
19	4	4001	CLA	OBD-CAD	4.58	1.30	1.22
19	B	1206	CLA	C3D-C4D	-4.58	1.33	1.44
19	A	1112	CLA	O2A-CGA	4.57	1.45	1.30
19	A	1134	CLA	O2A-CGA	4.57	1.45	1.30
19	A	1101	CLA	C3D-C4D	-4.57	1.33	1.44
19	G	1242	CLA	O2A-CGA	4.57	1.46	1.33
19	2	2013	CLA	CAB-C3B	-4.57	1.35	1.47
19	B	1222	CLA	O2A-CGA	4.56	1.46	1.33
19	4	4007	CLA	C3D-C4D	-4.56	1.33	1.44
19	1	1008	CLA	CAB-C3B	-4.56	1.35	1.47
19	1	1003	CLA	O2A-CGA	4.56	1.46	1.33
19	A	1101	CLA	CHC-C4B	4.56	1.49	1.39
19	A	1122	CLA	CAB-C3B	-4.56	1.35	1.47
19	H	1145	CLA	CHC-C4B	4.55	1.49	1.39
19	A	1109	CLA	C3D-C4D	-4.55	1.33	1.44
19	A	1112	CLA	C3D-C4D	-4.55	1.33	1.44
19	2	2003	CLA	CHD-C1D	4.55	1.49	1.38
19	1	1002	CLA	C1B-NB	-4.55	1.31	1.37
19	A	1149	CLA	CHC-C4B	4.55	1.49	1.39
19	A	1111	CLA	C3D-C4D	-4.55	1.34	1.44
19	K	3009	CLA	OBD-CAD	4.55	1.30	1.22
19	R	1150	CLA	C3D-C4D	-4.55	1.34	1.44
19	2	2007	CLA	CHC-C4B	4.55	1.49	1.39
19	L	1502	CLA	C3D-C4D	-4.55	1.34	1.44
19	3	1147	CLA	C1D-ND	-4.55	1.31	1.37
19	B	1235	CLA	O2D-CGD	4.55	1.44	1.33
19	A	1151	CLA	O2A-CGA	4.55	1.46	1.33
19	L	1130	CLA	C3D-C4D	-4.54	1.34	1.44
19	A	1112	CLA	CAB-C3B	-4.54	1.35	1.47
19	1	1003	CLA	CAB-C3B	-4.54	1.35	1.47
19	B	1214	CLA	CAB-C3B	-4.54	1.35	1.47
19	H	1207	CLA	CAB-C3B	-4.54	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1131	CLA	O2A-CGA	4.54	1.46	1.33
19	A	1133	CLA	CAB-C3B	-4.52	1.35	1.47
19	2	2008	CLA	CHD-C1D	4.52	1.49	1.38
19	B	1201	CLA	CAB-C3B	-4.52	1.35	1.47
19	2	4009	CLA	CAB-C3B	-4.52	1.35	1.47
19	A	1151	CLA	CAB-C3B	-4.51	1.35	1.47
19	A	1107	CLA	O2D-CGD	4.51	1.44	1.33
19	L	1504	CLA	CAB-C3B	-4.51	1.35	1.47
19	1	1012	CLA	C3D-C4D	-4.51	1.34	1.44
19	B	1219	CLA	OBD-CAD	4.51	1.30	1.22
19	2	2011	CLA	CHD-C1D	4.51	1.49	1.38
19	A	1121	CLA	CHC-C4B	4.51	1.49	1.39
19	B	1219	CLA	O2A-CGA	4.50	1.46	1.33
19	A	1102	CLA	OBD-CAD	4.50	1.30	1.22
19	K	1142	CLA	CAB-C3B	-4.49	1.35	1.47
19	A	1126	CLA	O2D-CGD	4.49	1.44	1.33
19	B	1238	CLA	CAB-C3B	-4.49	1.35	1.47
19	F	1302	CLA	C3A-C2A	-4.49	1.50	1.54
19	1	1002	CLA	CAB-C3B	-4.48	1.35	1.47
19	B	1202	CLA	CHC-C4B	4.48	1.49	1.39
19	A	1117	CLA	C3D-C4D	-4.48	1.34	1.44
19	A	1141	CLA	O2A-CGA	4.47	1.46	1.33
19	B	1228	CLA	CAB-C3B	-4.47	1.35	1.47
19	1	1002	CLA	C3D-C4D	-4.46	1.34	1.44
19	H	1145	CLA	C3D-C4D	-4.46	1.34	1.44
19	2	2012	CLA	C3D-C4D	-4.45	1.34	1.44
19	F	1305	CLA	C3A-C2A	-4.45	1.42	1.54
19	B	1209	CLA	O2A-CGA	4.45	1.46	1.33
19	B	1211	CLA	OBD-CAD	4.45	1.30	1.22
19	1	1303	CLA	O2A-CGA	4.44	1.46	1.33
19	A	1106	CLA	O2A-CGA	4.44	1.46	1.33
19	4	4013	CLA	CHD-C1D	4.44	1.49	1.38
19	1	1003	CLA	OBD-CAD	4.44	1.30	1.22
19	B	9010	CLA	CAB-C3B	-4.43	1.35	1.47
19	A	1128	CLA	O2A-CGA	4.43	1.46	1.33
19	1	1011	CLA	CHC-C4B	4.43	1.49	1.39
19	4	4006	CLA	CAB-C3B	-4.43	1.35	1.47
19	B	1223	CLA	O2A-CGA	4.42	1.46	1.33
19	A	1132	CLA	CHC-C4B	4.42	1.49	1.39
19	3	1147	CLA	C4C-C3C	-4.41	1.37	1.45
19	A	9023	CLA	C3D-C4D	-4.41	1.34	1.44
19	4	4001	CLA	CAB-C3B	-4.41	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1123	CLA	O2A-CGA	4.41	1.46	1.33
19	3	3003	CLA	OBD-CAD	4.41	1.30	1.22
19	B	1235	CLA	O2A-CGA	4.40	1.46	1.33
19	3	3007	CLA	CAB-C3B	-4.40	1.35	1.47
19	G	1242	CLA	CAB-C3B	-4.40	1.35	1.47
19	B	1230	CLA	O2A-CGA	4.40	1.46	1.33
19	A	1120	CLA	CAB-C3B	-4.40	1.35	1.47
19	A	1104	CLA	CAB-C3B	-4.40	1.35	1.47
19	A	1104	CLA	OBD-CAD	4.39	1.30	1.22
19	1	1002	CLA	CHC-C4B	4.39	1.49	1.39
19	L	1503	CLA	OBD-CAD	4.39	1.30	1.22
19	3	1147	CLA	CHD-C1D	4.39	1.47	1.38
19	4	4006	CLA	O2A-CGA	4.38	1.46	1.33
19	A	1105	CLA	CAB-C3B	-4.38	1.35	1.47
19	B	1205	CLA	O2A-CGA	4.38	1.46	1.33
19	1	1001	CLA	CAB-C3B	-4.38	1.35	1.47
19	A	1121	CLA	C3D-C4D	-4.38	1.34	1.44
19	A	1140	CLA	O2A-CGA	4.37	1.46	1.33
19	B	1226	CLA	CHC-C4B	4.37	1.49	1.39
19	4	4015	CLA	O2D-CGD	4.37	1.44	1.33
19	J	1308	CLA	C4C-C3C	-4.37	1.37	1.45
19	A	1135	CLA	O2A-CGA	4.37	1.46	1.33
19	G	1242	CLA	OBD-CAD	4.36	1.30	1.22
19	A	1119	CLA	CAB-C3B	-4.36	1.35	1.47
19	4	1306	CLA	CHC-C4B	4.35	1.49	1.39
21	3	6022	BCR	C30-C25	-4.35	1.48	1.53
19	4	1306	CLA	C3D-C4D	-4.35	1.34	1.44
19	B	1220	CLA	C1D-ND	-4.35	1.32	1.37
19	A	1139	CLA	O2A-CGA	4.35	1.46	1.33
19	2	2007	CLA	C3D-C4D	-4.35	1.34	1.44
19	4	1306	CLA	OBD-CAD	4.35	1.30	1.22
19	2	2001	CLA	O2A-CGA	4.35	1.46	1.33
19	2	2011	CLA	CHC-C4B	4.34	1.51	1.39
19	2	2007	CLA	CAB-C3B	-4.34	1.35	1.47
19	A	1103	CLA	CHC-C4B	4.33	1.49	1.39
19	1	1010	CLA	O2A-CGA	4.33	1.46	1.33
19	3	3002	CLA	CHC-C4B	4.33	1.51	1.39
19	3	1147	CLA	O2D-CGD	4.33	1.43	1.33
19	3	3007	CLA	OBD-CAD	4.32	1.29	1.22
19	A	1138	CLA	O2A-CGA	4.32	1.45	1.33
19	4	1004	CLA	O2A-CGA	4.32	1.45	1.33
19	1	1001	CLA	C1B-NB	-4.32	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1212	CLA	CAB-C3B	-4.32	1.35	1.47
19	2	2006	CLA	O2A-CGA	4.32	1.45	1.33
19	A	1106	CLA	CAB-C3B	-4.31	1.35	1.47
19	R	1150	CLA	CHB-C1B	4.31	1.49	1.39
19	A	1127	CLA	C3D-C4D	-4.30	1.34	1.44
19	A	1104	CLA	O2A-CGA	4.30	1.45	1.33
19	A	1105	CLA	O2A-CGA	4.29	1.46	1.33
19	A	1111	CLA	CAB-C3B	-4.29	1.35	1.47
19	B	1225	CLA	CHB-C1B	4.29	1.49	1.39
19	3	3013	CLA	CHC-C4B	4.29	1.49	1.39
19	L	1148	CLA	O2D-CGD	4.29	1.43	1.33
19	H	1207	CLA	OBD-CAD	4.28	1.29	1.22
19	B	1217	CLA	C3D-C4D	-4.28	1.34	1.44
19	B	1236	CLA	CAB-C3B	-4.27	1.36	1.47
19	B	1209	CLA	CAB-C3B	-4.27	1.36	1.47
19	L	1148	CLA	CAB-C3B	-4.27	1.36	1.47
19	1	1008	CLA	OBD-CAD	4.27	1.29	1.22
19	B	1234	CLA	CHC-C4B	4.26	1.49	1.39
19	4	4007	CLA	OBD-CAD	4.26	1.29	1.22
19	A	1108	CLA	OBD-CAD	4.25	1.29	1.22
19	B	1214	CLA	OBD-CAD	4.25	1.29	1.22
19	B	1213	CLA	CAB-C3B	-4.24	1.36	1.47
19	L	1504	CLA	CHB-C1B	4.23	1.48	1.39
19	3	3001	CLA	CHC-C4B	4.23	1.51	1.39
19	3	3008	CLA	O2A-CGA	4.23	1.45	1.33
19	4	1004	CLA	O2D-CED	4.22	1.54	1.45
19	B	1205	CLA	C3D-C4D	-4.22	1.34	1.44
19	3	3017	CLA	C1B-NB	-4.22	1.32	1.37
19	K	1143	CLA	O2A-CGA	4.22	1.45	1.33
19	4	4012	CLA	OBD-CAD	4.22	1.29	1.22
19	1	1013	CLA	CHC-C4B	4.21	1.48	1.39
19	L	1501	CLA	CHB-C1B	4.21	1.48	1.39
19	2	2004	CLA	CAB-C3B	-4.21	1.36	1.47
19	4	4003	CLA	OBD-CAD	4.21	1.29	1.22
19	B	1230	CLA	CAB-C3B	-4.20	1.36	1.47
19	2	4009	CLA	OBD-CAD	4.20	1.29	1.22
19	B	1215	CLA	O2A-CGA	4.20	1.45	1.33
19	A	1137	CLA	O2A-CGA	4.20	1.45	1.33
19	B	1235	CLA	CHC-C4B	4.19	1.48	1.39
19	A	1237	CLA	O2A-CGA	4.19	1.45	1.33
19	B	1218	CLA	OBD-CAD	4.19	1.29	1.22
19	A	9011	CLA	O2A-CGA	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1130	CLA	OBD-CAD	4.19	1.29	1.22
19	A	1121	CLA	CHB-C1B	4.18	1.48	1.39
19	A	1122	CLA	OBD-CAD	4.18	1.29	1.22
19	K	1146	CLA	O2A-CGA	4.18	1.45	1.33
19	4	4005	CLA	CHC-C4B	4.17	1.51	1.39
19	4	1009	CLA	C3A-C2A	-4.17	1.50	1.54
19	A	1102	CLA	CAB-C3B	-4.17	1.36	1.47
19	4	4011	CLA	CHC-C4B	4.17	1.51	1.39
19	1	1013	CLA	CHB-C1B	4.17	1.48	1.39
19	1	1001	CLA	O2A-CGA	4.17	1.45	1.33
19	A	1149	CLA	C3D-C4D	-4.17	1.34	1.44
19	A	1129	CLA	CAB-C3B	-4.17	1.36	1.47
21	B	6010	BCR	C30-C25	-4.17	1.48	1.53
19	A	9022	CLA	OBD-CAD	4.16	1.29	1.22
19	4	4002	CLA	O2A-CGA	4.16	1.45	1.33
19	A	9011	CLA	C3D-C4D	-4.16	1.34	1.44
19	B	1226	CLA	O2A-CGA	4.15	1.45	1.33
19	2	2013	CLA	OBD-CAD	4.15	1.29	1.22
19	3	3013	CLA	O2A-CGA	4.15	1.45	1.33
19	A	1105	CLA	OBD-CAD	4.15	1.29	1.22
19	4	1304	CLA	CHC-C4B	4.15	1.48	1.39
19	4	4001	CLA	CHB-C1B	4.15	1.48	1.39
19	4	1304	CLA	C1B-NB	-4.15	1.32	1.37
19	B	1203	CLA	CHC-C4B	4.14	1.48	1.39
19	J	1308	CLA	O2A-CGA	4.14	1.45	1.33
19	3	3017	CLA	O2A-CGA	4.14	1.45	1.33
19	B	1203	CLA	O2A-CGA	4.14	1.45	1.33
19	A	1113	CLA	OBD-CAD	4.14	1.29	1.22
19	B	1224	CLA	O2A-CGA	4.14	1.45	1.33
19	3	3014	CLA	CHC-C4B	4.14	1.50	1.39
19	R	1144	CLA	CAB-C3B	-4.13	1.36	1.47
19	A	1136	CLA	O2A-CGA	4.12	1.45	1.33
19	B	1216	CLA	CHB-C1B	4.12	1.48	1.39
19	4	4002	CLA	C1C-C2C	-4.11	1.36	1.44
19	1	1014	CLA	C4C-C3C	-4.11	1.38	1.45
19	A	1115	CLA	O2A-CGA	4.11	1.45	1.33
19	K	1146	CLA	C4C-C3C	-4.11	1.38	1.45
19	H	1145	CLA	O2A-CGA	4.10	1.45	1.33
19	1	1002	CLA	OBD-CAD	4.10	1.29	1.22
19	A	1237	CLA	CHB-C1B	4.10	1.48	1.39
19	1	1013	CLA	C1B-NB	-4.10	1.32	1.37
19	A	9011	CLA	C4C-C3C	-4.10	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1225	CLA	OBD-CAD	4.09	1.29	1.22
19	3	3007	CLA	CHB-C1B	4.09	1.48	1.39
19	A	1124	CLA	O2A-CGA	4.09	1.45	1.33
19	A	1120	CLA	OBD-CAD	4.09	1.29	1.22
19	B	1208	CLA	OBD-CAD	4.09	1.29	1.22
19	B	1220	CLA	O2A-CGA	4.09	1.45	1.33
19	B	1234	CLA	CHB-C1B	4.08	1.48	1.39
19	A	1131	CLA	OBD-CAD	4.07	1.29	1.22
19	B	1213	CLA	O2A-CGA	4.07	1.45	1.33
19	B	9010	CLA	OBD-CAD	4.07	1.29	1.22
19	4	4013	CLA	CHC-C4B	4.07	1.50	1.39
19	3	3015	CLA	CHC-C4B	4.07	1.50	1.39
19	A	1101	CLA	OBD-CAD	4.06	1.29	1.22
19	A	1128	CLA	CAB-C3B	-4.06	1.36	1.47
19	A	1110	CLA	OBD-CAD	4.06	1.29	1.22
19	A	1117	CLA	C4C-C3C	-4.05	1.38	1.45
19	1	1007	CLA	CHB-C1B	4.05	1.48	1.39
19	4	4002	CLA	CHC-C4B	4.05	1.48	1.39
19	1	1011	CLA	C1C-C2C	-4.05	1.36	1.44
19	4	4007	CLA	CHB-C1B	4.05	1.48	1.39
19	4	1304	CLA	C4C-C3C	-4.05	1.38	1.45
19	B	1230	CLA	OBD-CAD	4.05	1.29	1.22
19	A	1141	CLA	OBD-CAD	4.04	1.29	1.22
19	K	1146	CLA	C1C-C2C	-4.04	1.36	1.44
19	3	3017	CLA	CHC-C4B	4.04	1.48	1.39
19	3	3006	CLA	CHC-C4B	4.03	1.50	1.39
19	H	1505	CLA	OBD-CAD	4.03	1.29	1.22
19	3	3011	CLA	OBD-CAD	4.03	1.29	1.22
19	1	1010	CLA	CHC-C4B	4.03	1.48	1.39
19	3	1147	CLA	OBD-CAD	4.03	1.29	1.22
21	B	6020	BCR	C21-C22	-4.02	1.26	1.35
24	B	7101	LMG	O8-C28	4.02	1.45	1.33
19	2	2001	CLA	OBD-CAD	4.01	1.29	1.22
19	A	1128	CLA	OBD-CAD	4.01	1.29	1.22
19	4	4006	CLA	CHB-C1B	4.01	1.48	1.39
19	1	1303	CLA	CHC-C4B	4.01	1.48	1.39
19	B	1301	CLA	C3A-C2A	-4.00	1.51	1.54
19	A	1110	CLA	CAB-C3B	-4.00	1.36	1.47
19	2	2002	CLA	CAB-C3B	-4.00	1.36	1.47
19	A	1126	CLA	O2A-CGA	4.00	1.45	1.33
19	B	1225	CLA	O2A-CGA	3.99	1.45	1.33
19	2	2014	CLA	O2A-CGA	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	1240	CLA	OBD-CAD	3.99	1.29	1.22
19	K	1143	CLA	OBD-CAD	3.99	1.29	1.22
19	2	2002	CLA	OBD-CAD	3.99	1.29	1.22
19	A	1149	CLA	CHB-C1B	3.99	1.48	1.39
19	4	4010	CLA	CHC-C4B	3.99	1.50	1.39
19	A	9013	CLA	O2A-CGA	3.99	1.45	1.33
19	B	9010	CLA	O2A-CGA	3.98	1.45	1.33
19	B	1218	CLA	CAB-C3B	-3.98	1.36	1.47
19	A	1237	CLA	OBD-CAD	3.98	1.29	1.22
19	F	1305	CLA	C1B-NB	-3.97	1.32	1.37
19	B	1232	CLA	OBD-CAD	3.97	1.29	1.22
19	1	1310	CLA	MG-NA	-3.96	1.96	2.06
21	B	6005	BCR	C30-C25	-3.96	1.48	1.53
19	F	1302	CLA	OBD-CAD	3.95	1.29	1.22
19	A	1107	CLA	CHC-C4B	3.95	1.48	1.39
19	4	1304	CLA	OBD-CAD	3.94	1.29	1.22
19	A	1101	CLA	CHB-C1B	3.93	1.48	1.39
19	1	1303	CLA	C1C-C2C	-3.93	1.36	1.44
19	3	3016	CLA	OBD-CAD	3.92	1.29	1.22
19	F	1305	CLA	C4C-C3C	-3.92	1.38	1.45
19	K	3009	CLA	CHB-C1B	3.92	1.48	1.39
19	2	2010	CLA	CHC-C4B	3.92	1.50	1.39
19	3	3005	CLA	CHC-C4B	3.92	1.50	1.39
19	3	3004	CLA	MG-NA	-3.91	1.97	2.06
19	3	1118	CLA	CHB-C1B	3.91	1.48	1.39
19	3	3013	CLA	CHB-C1B	3.91	1.48	1.39
19	4	1304	CLA	O2A-CGA	3.91	1.44	1.33
19	2	2005	CLA	CHC-C4B	3.91	1.50	1.39
19	4	4015	CLA	CHB-C1B	3.90	1.48	1.39
19	1	1014	CLA	OBD-CAD	3.90	1.29	1.22
19	B	1233	CLA	CHB-C1B	3.90	1.48	1.39
19	B	1220	CLA	O2D-CGD	3.90	1.42	1.33
19	L	1502	CLA	OBD-CAD	3.90	1.29	1.22
19	2	2014	CLA	C1B-NB	-3.90	1.32	1.37
19	B	1226	CLA	C4C-C3C	-3.90	1.38	1.45
19	A	9012	CLA	OBD-CAD	3.89	1.29	1.22
19	3	3017	CLA	OBD-CAD	3.89	1.29	1.22
19	H	1505	CLA	CHB-C1B	3.89	1.48	1.39
19	1	1006	CLA	CHB-C1B	3.89	1.48	1.39
19	A	1126	CLA	OBD-CAD	3.88	1.29	1.22
19	4	4004	CLA	CHC-C4B	3.88	1.50	1.39
19	A	1105	CLA	CHB-C1B	3.88	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	6006	BCR	C24-C23	3.88	1.44	1.33
19	1	1015	CLA	CHC-C4B	3.88	1.50	1.39
19	4	4015	CLA	C4C-C3C	-3.88	1.38	1.45
19	1	1013	CLA	OBD-CAD	3.88	1.29	1.22
19	A	1125	CLA	C4C-C3C	-3.87	1.38	1.45
19	4	4006	CLA	C4C-C3C	-3.87	1.38	1.45
19	2	2003	CLA	CHC-C4B	3.87	1.50	1.39
19	4	1304	CLA	C1C-C2C	-3.86	1.36	1.44
19	2	2012	CLA	CHB-C1B	3.86	1.48	1.39
19	F	1305	CLA	O2A-CGA	3.86	1.44	1.33
19	A	1138	CLA	OBD-CAD	3.86	1.29	1.22
19	B	1229	CLA	OBD-CAD	3.86	1.29	1.22
19	A	1107	CLA	OBD-CAD	3.85	1.29	1.22
19	A	1107	CLA	CHB-C1B	3.85	1.48	1.39
19	B	1206	CLA	O2A-CGA	3.85	1.44	1.33
19	2	4009	CLA	CHB-C1B	3.84	1.48	1.39
19	A	1127	CLA	OBD-CAD	3.84	1.29	1.22
19	A	1309	CLA	CHC-C4B	3.83	1.50	1.39
19	B	1215	CLA	CHB-C1B	3.83	1.48	1.39
19	A	9023	CLA	C4C-C3C	-3.83	1.38	1.45
19	J	1311	CLA	OBD-CAD	3.82	1.29	1.22
19	3	1147	CLA	CHD-C4C	3.82	1.47	1.39
19	2	2014	CLA	OBD-CAD	3.82	1.29	1.22
19	4	4012	CLA	C3A-C2A	-3.82	1.51	1.54
19	F	1240	CLA	C3A-C2A	-3.82	1.51	1.54
19	B	1210	CLA	C4C-C3C	-3.82	1.38	1.45
19	B	1301	CLA	CHB-C1B	3.81	1.48	1.39
21	B	6020	BCR	C31-C1	-3.81	1.46	1.53
19	2	2006	CLA	CHB-C1B	3.81	1.48	1.39
19	A	1135	CLA	OBD-CAD	3.81	1.29	1.22
19	A	1119	CLA	OBD-CAD	3.81	1.29	1.22
19	4	4002	CLA	CAB-C3B	-3.80	1.37	1.47
19	1	1303	CLA	C4C-C3C	-3.80	1.38	1.45
19	1	1310	CLA	CHC-C4B	3.80	1.50	1.39
19	R	1144	CLA	CHB-C1B	3.80	1.47	1.39
19	A	1116	CLA	CHB-C1B	3.80	1.47	1.39
22	4	7052	LMU	O6'-C6'	3.79	1.58	1.42
19	2	2008	CLA	CHC-C4B	3.79	1.50	1.39
19	4	4014	CLA	OBD-CAD	3.79	1.29	1.22
19	B	1222	CLA	CHB-C1B	3.78	1.47	1.39
19	A	1107	CLA	C1C-C2C	-3.78	1.36	1.44
19	B	1235	CLA	CHB-C1B	3.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1213	CLA	CHB-C1B	3.77	1.47	1.39
19	A	1139	CLA	C4C-C3C	-3.77	1.38	1.45
19	B	1209	CLA	OBD-CAD	3.77	1.29	1.22
19	1	1012	CLA	CHB-C1B	3.76	1.47	1.39
19	B	1239	CLA	CHB-C1B	3.76	1.47	1.39
19	3	2009	CLA	C4C-C3C	-3.75	1.38	1.45
19	2	2013	CLA	C1B-NB	-3.75	1.32	1.37
19	A	1116	CLA	OBD-CAD	3.74	1.28	1.22
19	B	1219	CLA	C1B-NB	-3.74	1.32	1.37
19	3	3010	CLA	CHC-C4B	3.74	1.49	1.39
19	4	1004	CLA	OBD-CAD	3.74	1.28	1.22
19	1	1008	CLA	CHB-C1B	3.74	1.47	1.39
19	B	1236	CLA	CHB-C1B	3.74	1.47	1.39
19	A	1134	CLA	OBD-CAD	3.73	1.28	1.22
19	1	1001	CLA	C4C-C3C	-3.72	1.38	1.45
19	B	1224	CLA	OBD-CAD	3.72	1.28	1.22
19	B	1206	CLA	C1B-NB	-3.71	1.33	1.37
19	B	1225	CLA	C4C-C3C	-3.71	1.38	1.45
19	B	1215	CLA	C4C-C3C	-3.71	1.38	1.45
19	A	1115	CLA	C1B-NB	-3.71	1.33	1.37
19	A	1103	CLA	CHB-C1B	3.70	1.47	1.39
19	K	1142	CLA	OBD-CAD	3.70	1.28	1.22
19	A	1134	CLA	C4C-C3C	-3.70	1.38	1.45
19	B	1226	CLA	CHB-C1B	3.69	1.47	1.39
19	A	9013	CLA	C4C-C3C	-3.69	1.38	1.45
19	A	1139	CLA	OBD-CAD	3.69	1.28	1.22
19	B	1226	CLA	OBD-CAD	3.69	1.28	1.22
19	A	1149	CLA	OBD-CAD	3.69	1.28	1.22
19	3	3003	CLA	CHB-C1B	3.69	1.47	1.39
19	4	4002	CLA	C1B-C2B	-3.69	1.34	1.43
19	A	1125	CLA	CHB-C1B	3.69	1.47	1.39
19	B	1217	CLA	CHB-C1B	3.69	1.47	1.39
19	A	1131	CLA	C4C-C3C	-3.68	1.38	1.45
19	3	3017	CLA	C1C-C2C	-3.68	1.37	1.44
19	A	9012	CLA	C1B-NB	-3.67	1.33	1.37
19	A	1113	CLA	CHB-C1B	3.67	1.47	1.39
19	1	1003	CLA	CHB-C1B	3.67	1.47	1.39
21	B	6017	BCR	C30-C25	-3.66	1.49	1.53
19	B	1232	CLA	CHB-C1B	3.66	1.47	1.39
19	B	1205	CLA	OBD-CAD	3.66	1.28	1.22
19	2	2007	CLA	CHB-C1B	3.66	1.47	1.39
21	F	6014	BCR	C30-C25	-3.66	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1226	CLA	CAB-C3B	-3.66	1.37	1.47
19	H	1145	CLA	OBD-CAD	3.65	1.28	1.22
19	A	1129	CLA	CHB-C1B	3.65	1.47	1.39
19	L	1501	CLA	OBD-CAD	3.65	1.28	1.22
19	A	1138	CLA	CHB-C1B	3.64	1.47	1.39
19	B	1236	CLA	C4C-C3C	-3.64	1.38	1.45
19	R	1144	CLA	OBD-CAD	3.64	1.28	1.22
19	B	1230	CLA	CHB-C1B	3.64	1.47	1.39
19	1	1010	CLA	MG-NA	-3.63	1.97	2.06
19	B	1231	CLA	C4C-C3C	-3.63	1.38	1.45
19	B	1212	CLA	OBD-CAD	3.63	1.28	1.22
19	A	1133	CLA	OBD-CAD	3.63	1.28	1.22
19	L	1504	CLA	C4C-C3C	-3.62	1.38	1.45
19	B	1208	CLA	CHB-C1B	3.62	1.47	1.39
19	1	1014	CLA	CHB-C1B	3.62	1.47	1.39
21	I	6018	BCR	C20-C21	-3.61	1.32	1.43
19	3	3014	CLA	MG-NA	-3.61	1.97	2.06
19	2	1307	CLA	CHC-C4B	3.61	1.49	1.39
19	A	1133	CLA	C1B-NB	-3.61	1.33	1.37
19	J	1308	CLA	C1B-NB	-3.61	1.33	1.37
19	B	1212	CLA	CHB-C1B	3.61	1.47	1.39
19	1	1011	CLA	OBD-CAD	3.61	1.28	1.22
19	A	1136	CLA	OBD-CAD	3.61	1.28	1.22
19	A	1124	CLA	OBD-CAD	3.60	1.28	1.22
21	J	6012	BCR	C30-C25	-3.60	1.49	1.53
19	K	1146	CLA	OBD-CAD	3.60	1.28	1.22
19	A	1137	CLA	C4C-C3C	-3.60	1.38	1.45
19	2	2004	CLA	OBD-CAD	3.60	1.28	1.22
21	B	6017	BCR	C32-C1	3.60	1.60	1.53
19	A	9013	CLA	C1B-NB	-3.59	1.33	1.37
19	A	1137	CLA	OBD-CAD	3.59	1.28	1.22
19	A	1109	CLA	OBD-CAD	3.59	1.28	1.22
19	B	1238	CLA	OBD-CAD	3.59	1.28	1.22
19	2	2004	CLA	CHB-C1B	3.59	1.47	1.39
19	B	1230	CLA	C1B-NB	-3.59	1.33	1.37
19	1	1012	CLA	OBD-CAD	3.59	1.28	1.22
21	F	6016	BCR	C32-C1	-3.59	1.47	1.53
21	J	6012	BCR	C20-C21	-3.58	1.32	1.43
19	J	1308	CLA	OBD-CAD	3.58	1.28	1.22
19	B	1230	CLA	C1C-C2C	-3.58	1.37	1.44
19	B	1210	CLA	C1B-NB	-3.58	1.33	1.37
19	H	1145	CLA	C1B-NB	-3.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1128	CLA	CHB-C1B	3.58	1.47	1.39
19	B	1206	CLA	OBD-CAD	3.58	1.28	1.22
19	4	1306	CLA	CHB-C1B	3.57	1.47	1.39
19	A	1135	CLA	CHB-C1B	3.56	1.47	1.39
19	3	3012	CLA	CHC-C4B	3.56	1.49	1.39
19	A	1140	CLA	OBD-CAD	3.56	1.28	1.22
19	B	1227	CLA	OBD-CAD	3.56	1.28	1.22
19	L	1148	CLA	C1B-NB	-3.56	1.33	1.37
21	A	6011	BCR	C30-C25	-3.55	1.49	1.53
19	H	1241	CLA	CHB-C1B	3.55	1.47	1.39
21	B	6020	BCR	C20-C21	-3.55	1.32	1.43
19	B	1202	CLA	OBD-CAD	3.55	1.28	1.22
19	1	1005	CLA	CHB-C1B	3.55	1.47	1.39
19	B	1203	CLA	C4B-NB	-3.54	1.33	1.37
21	A	6002	BCR	C20-C21	-3.53	1.32	1.43
19	4	4014	CLA	CHB-C1B	3.53	1.47	1.39
19	B	1222	CLA	OBD-CAD	3.53	1.28	1.22
19	A	1137	CLA	CHB-C1B	3.52	1.47	1.39
19	B	1221	CLA	C1B-NB	-3.52	1.33	1.37
19	B	1228	CLA	CHB-C1B	3.52	1.47	1.39
19	2	2012	CLA	OBD-CAD	3.52	1.28	1.22
19	L	1148	CLA	OBD-CAD	3.51	1.28	1.22
19	A	1132	CLA	CHB-C1B	3.51	1.47	1.39
22	2	7031	LMU	O1'-C1'	3.51	1.46	1.40
19	B	1223	CLA	CHB-C1B	3.51	1.47	1.39
19	1	1011	CLA	MG-NA	-3.51	1.97	2.06
19	A	1108	CLA	CAB-C3B	-3.50	1.38	1.47
19	4	4005	CLA	CHD-C4C	3.50	1.52	1.40
19	2	2001	CLA	C4C-C3C	-3.50	1.39	1.45
19	B	1234	CLA	OBD-CAD	3.50	1.28	1.22
19	B	1231	CLA	CHB-C1B	3.49	1.47	1.39
19	2	2003	CLA	MG-NA	-3.49	1.98	2.06
19	2	2008	CLA	MG-NA	-3.48	1.98	2.06
19	B	1203	CLA	C1C-C2C	-3.48	1.37	1.44
19	3	2009	CLA	C1B-NB	-3.48	1.33	1.37
19	A	1140	CLA	CHB-C1B	3.48	1.47	1.39
21	B	6020	BCR	C20-C19	-3.47	1.25	1.34
19	A	1140	CLA	C4C-C3C	-3.47	1.39	1.45
19	B	1214	CLA	C1B-NB	-3.46	1.33	1.37
19	K	1143	CLA	CHB-C1B	3.46	1.47	1.39
19	A	1127	CLA	CHB-C1B	3.46	1.47	1.39
19	B	1223	CLA	OBD-CAD	3.46	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3016	CLA	C1B-NB	-3.46	1.33	1.37
19	2	4009	CLA	C1B-NB	-3.46	1.33	1.37
19	B	1228	CLA	OBD-CAD	3.46	1.28	1.22
19	A	9012	CLA	C4C-C3C	-3.46	1.39	1.45
19	L	1501	CLA	C4C-C3C	-3.45	1.39	1.45
19	J	1311	CLA	CHB-C1B	3.45	1.47	1.39
19	A	1115	CLA	C4C-C3C	-3.45	1.39	1.45
19	B	1235	CLA	C1B-NB	-3.45	1.33	1.37
19	A	1141	CLA	C4C-C3C	-3.45	1.39	1.45
19	A	1124	CLA	CHB-C1B	3.44	1.47	1.39
19	3	3001	CLA	CHD-C4C	3.44	1.52	1.40
21	B	6006	BCR	C20-C21	-3.44	1.32	1.43
19	L	1503	CLA	C1B-NB	-3.44	1.33	1.37
19	A	1112	CLA	CHB-C1B	3.44	1.47	1.39
19	A	9011	CLA	CHB-C1B	3.44	1.47	1.39
19	A	1122	CLA	C1B-NB	-3.43	1.33	1.37
19	I	1204	CLA	CHB-C1B	3.43	1.47	1.39
19	A	1136	CLA	C4C-C3C	-3.43	1.39	1.45
19	A	1117	CLA	OBD-CAD	3.43	1.28	1.22
19	A	1132	CLA	OBD-CAD	3.43	1.28	1.22
19	G	1242	CLA	CHB-C1B	3.43	1.47	1.39
19	A	1111	CLA	OBD-CAD	3.43	1.28	1.22
19	B	9010	CLA	CHB-C1B	3.43	1.47	1.39
19	L	1148	CLA	C1B-C2B	-3.43	1.35	1.43
19	B	1222	CLA	C4C-C3C	-3.43	1.39	1.45
19	B	1209	CLA	CHB-C1B	3.43	1.47	1.39
19	B	1223	CLA	C1B-NB	-3.42	1.33	1.37
19	A	1139	CLA	C1B-NB	-3.42	1.33	1.37
19	A	9011	CLA	OBD-CAD	3.42	1.28	1.22
19	3	3011	CLA	C1B-NB	-3.42	1.33	1.37
19	K	1146	CLA	C1B-C2B	-3.42	1.35	1.43
19	1	1310	CLA	CHD-C4C	3.42	1.52	1.40
19	A	1108	CLA	CHB-C1B	3.42	1.47	1.39
19	K	1142	CLA	C4C-C3C	-3.41	1.39	1.45
19	1	1303	CLA	C4B-NB	-3.41	1.33	1.37
19	A	1106	CLA	OBD-CAD	3.41	1.28	1.22
19	J	1311	CLA	C4C-C3C	-3.41	1.39	1.45
19	4	4002	CLA	MG-NA	-3.41	1.98	2.06
19	F	1305	CLA	CHB-C1B	3.41	1.47	1.39
19	4	4007	CLA	C4C-C3C	-3.41	1.39	1.45
19	A	1117	CLA	CHB-C1B	3.41	1.47	1.39
19	4	4003	CLA	CHB-C1B	3.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1148	CLA	C3A-C2A	-3.41	1.45	1.54
19	L	1130	CLA	CHB-C1B	3.40	1.47	1.39
21	I	6021	BCR	C26-C25	-3.40	1.28	1.34
19	3	3012	CLA	CHD-C4C	3.40	1.51	1.40
19	B	1224	CLA	CHB-C1B	3.40	1.47	1.39
19	A	1139	CLA	CHB-C1B	3.40	1.47	1.39
19	1	1001	CLA	CHC-C4B	3.40	1.47	1.39
19	A	1131	CLA	C1B-NB	-3.40	1.33	1.37
19	B	1229	CLA	C4C-C3C	-3.40	1.39	1.45
19	A	1109	CLA	CHB-C1B	3.40	1.47	1.39
19	I	1204	CLA	C4C-C3C	-3.40	1.39	1.45
19	A	1111	CLA	CHB-C1B	3.39	1.47	1.39
19	2	2003	CLA	CHD-C4C	3.39	1.51	1.40
19	A	1119	CLA	CHB-C1B	3.39	1.47	1.39
19	A	1136	CLA	CHB-C1B	3.39	1.47	1.39
19	A	1138	CLA	C4C-C3C	-3.39	1.39	1.45
19	K	1143	CLA	C4C-C3C	-3.39	1.39	1.45
19	B	1223	CLA	C4C-C3C	-3.39	1.39	1.45
19	L	1148	CLA	C4C-C3C	-3.39	1.39	1.45
19	1	1013	CLA	C1C-C2C	-3.39	1.37	1.44
19	B	1214	CLA	CHB-C1B	3.39	1.47	1.39
19	4	1009	CLA	CHB-C1B	3.38	1.47	1.39
19	A	1135	CLA	C4C-C3C	-3.38	1.39	1.45
21	3	6022	BCR	C20-C21	-3.38	1.32	1.43
19	A	9023	CLA	OBD-CAD	3.37	1.28	1.22
19	A	1115	CLA	OBD-CAD	3.37	1.28	1.22
19	B	1205	CLA	CHB-C1B	3.36	1.47	1.39
19	3	3013	CLA	C1C-C2C	-3.36	1.37	1.44
19	K	3009	CLA	C4C-C3C	-3.36	1.39	1.45
19	2	2010	CLA	CHD-C4C	3.36	1.51	1.40
19	3	3008	CLA	CHB-C1B	3.36	1.47	1.39
19	3	3015	CLA	CHB-C1B	3.36	1.48	1.39
21	A	6008	BCR	C30-C25	-3.36	1.49	1.53
19	1	1015	CLA	CHD-C4C	3.36	1.51	1.40
19	B	1235	CLA	C4C-C3C	-3.36	1.39	1.45
19	1	1010	CLA	C1D-ND	-3.36	1.33	1.37
19	1	1008	CLA	C4C-C3C	-3.35	1.39	1.45
19	A	1134	CLA	CHB-C1B	3.35	1.46	1.39
19	1	1011	CLA	C4C-C3C	-3.35	1.37	1.44
19	B	1219	CLA	CHB-C1B	3.35	1.46	1.39
19	F	1302	CLA	CHB-C1B	3.35	1.46	1.39
19	3	3013	CLA	C4B-NB	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1104	CLA	CHB-C1B	3.35	1.46	1.39
19	K	1142	CLA	CHB-C1B	3.34	1.46	1.39
19	3	3016	CLA	C4C-C3C	-3.34	1.39	1.45
19	H	1207	CLA	C4C-C3C	-3.34	1.39	1.45
19	4	1004	CLA	C1B-NB	-3.34	1.33	1.37
21	1	6023	BCR	C10-C9	-3.34	1.28	1.35
19	4	4004	CLA	CHD-C4C	3.34	1.51	1.40
19	4	4003	CLA	C1B-NB	-3.33	1.33	1.37
19	4	1004	CLA	CHB-C1B	3.33	1.46	1.39
19	H	1145	CLA	C4C-C3C	-3.33	1.39	1.45
19	L	1503	CLA	CHB-C1B	3.33	1.46	1.39
19	1	1014	CLA	C1B-NB	-3.33	1.33	1.37
19	1	1001	CLA	C1C-C2C	-3.32	1.37	1.44
19	R	1150	CLA	C1B-NB	-3.32	1.33	1.37
19	B	1218	CLA	C4C-C3C	-3.32	1.39	1.45
19	A	1131	CLA	CHB-C1B	3.32	1.46	1.39
19	B	9010	CLA	C4C-C3C	-3.32	1.39	1.45
19	3	2009	CLA	OBD-CAD	3.32	1.28	1.22
19	4	4010	CLA	CHD-C4C	3.32	1.51	1.40
19	B	1230	CLA	C4C-C3C	-3.32	1.39	1.45
19	3	3008	CLA	OBD-CAD	3.32	1.28	1.22
19	3	3013	CLA	C1B-NB	-3.31	1.33	1.37
19	B	1211	CLA	CHB-C1B	3.31	1.46	1.39
21	B	6020	BCR	C17-C18	-3.31	1.28	1.35
19	B	1229	CLA	CHB-C1B	3.31	1.46	1.39
19	3	2009	CLA	CHB-C1B	3.31	1.46	1.39
19	A	1120	CLA	CHB-C1B	3.30	1.46	1.39
19	1	1013	CLA	C3D-CAD	-3.30	1.34	1.45
19	F	1305	CLA	C4B-NB	-3.30	1.33	1.37
19	3	3005	CLA	CHD-C4C	3.30	1.51	1.40
19	A	1106	CLA	C4C-C3C	-3.30	1.39	1.45
19	2	2001	CLA	CHB-C1B	3.30	1.46	1.39
19	A	1109	CLA	C4C-C3C	-3.29	1.39	1.45
19	4	4001	CLA	C4C-C3C	-3.29	1.39	1.45
19	A	1123	CLA	OBD-CAD	3.29	1.28	1.22
19	B	1220	CLA	C1C-C2C	-3.29	1.37	1.44
19	A	1133	CLA	CHB-C1B	3.29	1.46	1.39
19	A	1101	CLA	C4C-C3C	-3.29	1.39	1.45
19	3	3008	CLA	C1B-NB	-3.29	1.33	1.37
22	4	7019	LMU	O1'-C1'	3.29	1.45	1.40
19	1	1303	CLA	C1B-C2B	-3.29	1.35	1.43
19	B	1301	CLA	C1B-NB	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1217	CLA	OBD-CAD	3.28	1.28	1.22
19	1	1010	CLA	OBD-CAD	3.28	1.28	1.22
19	3	3002	CLA	CHD-C4C	3.28	1.51	1.40
19	B	1228	CLA	C4C-C3C	-3.28	1.39	1.45
19	A	1129	CLA	OBD-CAD	3.28	1.28	1.22
19	B	1216	CLA	C4C-C3C	-3.28	1.39	1.45
19	A	1125	CLA	C1B-NB	-3.28	1.33	1.37
19	L	1503	CLA	C4C-C3C	-3.27	1.39	1.45
19	B	1209	CLA	C1B-NB	-3.27	1.33	1.37
21	A	6003	BCR	C30-C25	-3.27	1.49	1.53
19	A	9023	CLA	CHB-C1B	3.27	1.46	1.39
19	1	1005	CLA	C1B-NB	-3.27	1.33	1.37
19	A	1122	CLA	CHB-C1B	3.27	1.46	1.39
19	J	1308	CLA	C1C-C2C	-3.27	1.37	1.44
19	4	4012	CLA	CHB-C1B	3.27	1.46	1.39
19	B	1201	CLA	C1B-NB	-3.27	1.33	1.37
19	B	1227	CLA	C1B-NB	-3.27	1.33	1.37
21	I	6018	BCR	C30-C25	-3.27	1.49	1.53
22	A	7010	LMU	O1'-C1'	3.27	1.45	1.40
19	2	2014	CLA	C4C-C3C	-3.26	1.39	1.45
19	L	1148	CLA	CMA-C3A	3.26	1.60	1.53
19	A	1126	CLA	CHB-C1B	3.26	1.46	1.39
19	A	1123	CLA	CHB-C1B	3.26	1.46	1.39
19	B	1224	CLA	C4C-C3C	-3.26	1.39	1.45
19	1	1010	CLA	C4B-NB	-3.25	1.33	1.37
19	B	1202	CLA	C1C-C2C	-3.25	1.37	1.44
19	A	1124	CLA	C4C-C3C	-3.25	1.39	1.45
19	B	1202	CLA	CHB-C1B	3.24	1.46	1.39
19	2	2014	CLA	C4B-NB	-3.23	1.33	1.37
19	3	3016	CLA	CHB-C1B	3.23	1.46	1.39
19	3	3014	CLA	CHD-C4C	3.23	1.51	1.40
19	3	3004	CLA	CHD-C4C	3.23	1.51	1.40
19	3	1147	CLA	C1D-C2D	-3.23	1.38	1.45
19	3	3006	CLA	CHD-C4C	3.23	1.51	1.40
19	B	1208	CLA	C4C-C3C	-3.22	1.39	1.45
21	F	6014	BCR	C40-C30	3.22	1.59	1.53
19	A	1141	CLA	CHB-C1B	3.22	1.46	1.39
19	A	1136	CLA	C1B-NB	-3.22	1.33	1.37
19	4	4013	CLA	CHB-C1B	3.22	1.48	1.39
19	B	1220	CLA	MG-NA	-3.22	1.98	2.06
19	A	1151	CLA	C1B-NB	-3.21	1.33	1.37
19	2	1307	CLA	MG-NA	-3.21	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1217	CLA	C4C-C3C	-3.21	1.39	1.45
19	B	1220	CLA	CHB-C1B	3.21	1.46	1.39
19	4	4003	CLA	C4C-C3C	-3.21	1.39	1.45
19	F	1302	CLA	C1B-NB	-3.21	1.33	1.37
21	L	6019	BCR	C21-C22	-3.20	1.28	1.35
19	B	1239	CLA	OBD-CAD	3.20	1.28	1.22
19	A	1116	CLA	C4C-C3C	-3.20	1.39	1.45
19	A	1110	CLA	CHB-C1B	3.19	1.46	1.39
19	4	4011	CLA	MG-NA	-3.19	1.98	2.06
19	A	9023	CLA	C1C-C2C	-3.19	1.38	1.44
19	3	3015	CLA	CHD-C4C	3.19	1.51	1.40
19	B	1213	CLA	C4C-C3C	-3.19	1.39	1.45
19	K	1143	CLA	C1B-NB	-3.19	1.33	1.37
19	1	1010	CLA	C1B-C2B	-3.19	1.35	1.43
19	A	1110	CLA	C4C-C3C	-3.19	1.39	1.45
19	A	1102	CLA	CHB-C1B	3.19	1.46	1.39
21	A	6011	BCR	C8-C7	3.18	1.42	1.33
19	3	3004	CLA	CHC-C4B	3.17	1.48	1.39
19	2	2010	CLA	MG-NA	-3.17	1.98	2.06
19	A	1137	CLA	C1B-NB	-3.17	1.33	1.37
19	2	2001	CLA	C1B-NB	-3.17	1.33	1.37
19	3	3008	CLA	C4C-C3C	-3.17	1.39	1.45
22	4	7009	LMU	O1'-C1'	3.17	1.45	1.40
19	K	1146	CLA	MG-NA	-3.16	1.98	2.06
19	B	1238	CLA	C4C-C3C	-3.16	1.39	1.45
21	B	6004	BCR	C30-C25	-3.16	1.49	1.53
19	B	1210	CLA	CHB-C1B	3.16	1.46	1.39
19	2	2010	CLA	CHB-C1B	3.16	1.48	1.39
19	A	1120	CLA	C1B-NB	-3.16	1.33	1.37
19	G	1242	CLA	C4C-C3C	-3.16	1.39	1.45
19	F	1302	CLA	C4C-C3C	-3.15	1.39	1.45
19	B	1206	CLA	C4C-C3C	-3.15	1.39	1.45
19	A	1309	CLA	CHD-C4C	3.15	1.51	1.40
19	H	1207	CLA	CHB-C1B	3.14	1.46	1.39
19	A	1134	CLA	C1B-NB	-3.14	1.33	1.37
19	B	1232	CLA	C1B-NB	-3.14	1.33	1.37
19	A	9013	CLA	CHB-C1B	3.14	1.46	1.39
19	A	1132	CLA	C1C-C2C	-3.14	1.38	1.44
19	3	3017	CLA	C4B-NB	-3.14	1.33	1.37
19	1	1011	CLA	C4B-NB	-3.14	1.33	1.37
19	1	1010	CLA	C1D-C2D	-3.13	1.39	1.45
19	B	1232	CLA	C4C-C3C	-3.13	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1008	CLA	C2A-C1A	-3.13	1.45	1.52
19	4	4004	CLA	MG-NA	-3.13	1.98	2.06
19	A	9012	CLA	CHB-C1B	3.12	1.46	1.39
19	B	1205	CLA	C1C-C2C	-3.12	1.38	1.44
19	B	1206	CLA	CHB-C1B	3.12	1.46	1.39
19	3	3013	CLA	OBD-CAD	3.12	1.27	1.22
19	A	1104	CLA	C4C-C3C	-3.12	1.39	1.45
19	4	4011	CLA	CHD-C4C	3.11	1.50	1.40
21	L	6019	BCR	C31-C1	-3.11	1.47	1.53
19	3	3017	CLA	C4C-C3C	-3.11	1.39	1.45
19	2	2004	CLA	C4C-C3C	-3.11	1.39	1.45
19	3	3012	CLA	MG-NA	-3.10	1.98	2.06
19	1	1010	CLA	C1C-C2C	-3.10	1.38	1.44
19	B	1216	CLA	OBD-CAD	3.10	1.27	1.22
21	1	6023	BCR	C11-C12	-3.09	1.26	1.34
19	B	9010	CLA	C1D-ND	-3.09	1.33	1.37
19	B	1203	CLA	MG-NA	-3.09	1.98	2.06
19	L	1502	CLA	CHB-C1B	3.09	1.46	1.39
22	G	7051	LMU	O1'-C1'	3.09	1.45	1.40
19	K	1142	CLA	C1B-NB	-3.09	1.33	1.37
19	4	4002	CLA	CHB-C4A	-3.09	1.30	1.37
19	A	1309	CLA	MG-NA	-3.09	1.98	2.06
19	K	1146	CLA	C1D-ND	-3.08	1.33	1.37
21	I	6018	BCR	C10-C9	-3.08	1.28	1.35
19	2	2002	CLA	C1B-NB	-3.08	1.33	1.37
19	A	1128	CLA	C1B-NB	-3.08	1.33	1.37
19	B	1203	CLA	C4C-C3C	-3.08	1.39	1.45
19	B	1203	CLA	CHB-C1B	3.08	1.46	1.39
19	A	1237	CLA	C4C-C3C	-3.08	1.39	1.45
19	B	1202	CLA	C4C-C3C	-3.08	1.39	1.45
19	A	1134	CLA	C1C-C2C	-3.08	1.38	1.44
19	3	1147	CLA	CHB-C1B	3.07	1.46	1.39
19	A	1138	CLA	C1B-NB	-3.07	1.33	1.37
19	J	1308	CLA	CHB-C1B	3.07	1.46	1.39
19	1	1015	CLA	CHB-C1B	3.07	1.48	1.39
19	B	1210	CLA	OBD-CAD	3.07	1.27	1.22
19	A	1309	CLA	CHB-C1B	3.07	1.48	1.39
19	4	4015	CLA	C1B-NB	-3.07	1.33	1.37
19	2	1307	CLA	CHD-C4C	3.07	1.50	1.40
19	B	1236	CLA	OBD-CAD	3.07	1.27	1.22
19	H	1145	CLA	MG-NA	-3.07	1.99	2.06
19	4	1009	CLA	C1B-NB	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1109	CLA	C1C-C2C	-3.06	1.38	1.44
19	4	4015	CLA	OBD-CAD	3.06	1.27	1.22
19	J	1308	CLA	MG-NA	-3.06	1.99	2.06
19	B	1238	CLA	CHB-C1B	3.06	1.46	1.39
19	A	9022	CLA	CHB-C1B	3.05	1.46	1.39
19	2	2005	CLA	MG-NA	-3.05	1.99	2.06
19	3	3010	CLA	MG-NA	-3.05	1.99	2.06
19	4	1306	CLA	C1C-C2C	-3.05	1.38	1.44
19	2	2008	CLA	CHA-C1A	3.05	1.50	1.41
19	A	1104	CLA	C1B-NB	-3.05	1.33	1.37
19	A	1111	CLA	C1C-C2C	-3.04	1.38	1.44
19	4	4015	CLA	C4B-NB	-3.04	1.33	1.37
19	3	3010	CLA	CHD-C4C	3.04	1.50	1.40
19	4	1004	CLA	C4C-C3C	-3.04	1.39	1.45
19	2	2006	CLA	C4C-C3C	-3.04	1.39	1.45
19	4	4013	CLA	CHD-C4C	3.04	1.50	1.40
19	2	2011	CLA	CHD-C4C	3.04	1.50	1.40
19	3	3006	CLA	CHA-C1A	3.04	1.50	1.41
19	1	1001	CLA	C4B-NB	-3.03	1.33	1.37
19	2	2008	CLA	CHD-C4C	3.03	1.50	1.40
19	J	1311	CLA	C1B-NB	-3.03	1.33	1.37
21	B	6020	BCR	C11-C12	-3.03	1.26	1.34
19	B	1205	CLA	C4C-C3C	-3.03	1.39	1.45
21	I	6021	BCR	C32-C1	-3.03	1.48	1.53
19	A	9022	CLA	C4C-C3C	-3.02	1.39	1.45
19	4	4010	CLA	MG-NA	-3.02	1.99	2.06
19	A	1132	CLA	C4B-NB	-3.02	1.33	1.37
19	4	4001	CLA	C1B-NB	-3.02	1.33	1.37
19	3	3001	CLA	CHB-C1B	3.02	1.47	1.39
19	A	1125	CLA	OBD-CAD	3.02	1.27	1.22
21	I	6021	BCR	C10-C9	-3.02	1.28	1.35
19	B	1213	CLA	C1C-C2C	-3.01	1.38	1.44
19	F	1305	CLA	CAA-C2A	-3.01	1.48	1.54
19	2	2014	CLA	CHB-C4A	-3.01	1.30	1.37
19	B	1215	CLA	OBD-CAD	3.00	1.27	1.22
19	1	1001	CLA	CHB-C1B	3.00	1.46	1.39
19	B	1205	CLA	C1B-NB	-3.00	1.33	1.37
19	F	1240	CLA	CHB-C1B	3.00	1.46	1.39
19	L	1503	CLA	CBD-CAD	-3.00	1.43	1.56
21	B	6020	BCR	C2-C1	-2.99	1.47	1.54
19	4	4005	CLA	MG-NA	-2.99	1.99	2.06
19	4	4005	CLA	CHB-C1B	2.99	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3006	CLA	CHB-C1B	2.99	1.47	1.39
19	3	3005	CLA	CHB-C1B	2.99	1.47	1.39
19	2	2002	CLA	CHB-C1B	2.99	1.46	1.39
19	L	1501	CLA	C1B-NB	-2.98	1.33	1.37
19	B	1209	CLA	C4C-C3C	-2.98	1.40	1.45
19	1	1001	CLA	C1D-C2D	-2.98	1.39	1.45
19	B	1227	CLA	CHB-C1B	2.98	1.46	1.39
21	L	6019	BCR	C24-C23	2.98	1.42	1.33
19	1	1006	CLA	C3A-C2A	-2.98	1.51	1.54
19	B	1226	CLA	C1C-C2C	-2.98	1.38	1.44
19	2	2011	CLA	MG-NA	-2.97	1.99	2.06
19	B	1235	CLA	C1C-C2C	-2.97	1.38	1.44
19	3	3001	CLA	MG-NA	-2.97	1.99	2.06
19	2	4009	CLA	C1C-C2C	-2.97	1.38	1.44
19	4	4015	CLA	C1C-C2C	-2.97	1.38	1.44
19	B	1208	CLA	C1B-NB	-2.96	1.34	1.37
19	B	1217	CLA	C1B-NB	-2.96	1.34	1.37
19	B	1221	CLA	CHB-C1B	2.96	1.46	1.39
19	3	1147	CLA	CHC-C4B	2.96	1.46	1.39
19	4	1009	CLA	C4B-NB	-2.96	1.34	1.37
19	K	1143	CLA	C1C-C2C	-2.96	1.38	1.44
19	3	1147	CLA	C1C-C2C	-2.96	1.38	1.44
19	B	1220	CLA	C4B-NB	-2.96	1.34	1.37
19	B	1218	CLA	CHB-C1B	2.95	1.46	1.39
19	3	3001	CLA	CHA-C1A	2.95	1.49	1.41
19	A	1127	CLA	C1B-NB	-2.95	1.34	1.37
19	2	2013	CLA	C4C-C3C	-2.95	1.40	1.45
19	A	9011	CLA	C1B-NB	-2.95	1.34	1.37
19	B	1226	CLA	C1B-NB	-2.95	1.34	1.37
19	3	1147	CLA	C1B-C2B	-2.95	1.36	1.43
19	A	1135	CLA	C1B-NB	-2.95	1.34	1.37
19	B	1203	CLA	C1B-NB	-2.95	1.34	1.37
19	4	1004	CLA	C1C-C2C	-2.95	1.38	1.44
19	A	1108	CLA	C4C-C3C	-2.95	1.40	1.45
19	3	3006	CLA	MG-NA	-2.94	1.99	2.06
19	3	3013	CLA	C1D-ND	-2.94	1.34	1.37
19	A	1131	CLA	C1C-C2C	-2.94	1.38	1.44
19	3	1147	CLA	MG-NA	-2.94	1.99	2.06
21	B	6017	BCR	C10-C9	-2.94	1.29	1.35
19	3	3012	CLA	CHA-C1A	2.94	1.49	1.41
19	A	1120	CLA	C4C-C3C	-2.94	1.40	1.45
19	B	1233	CLA	C4C-C3C	-2.94	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1102	CLA	C4C-C3C	-2.94	1.40	1.45
19	A	1140	CLA	C1B-NB	-2.93	1.34	1.37
19	3	3005	CLA	CHA-C1A	2.93	1.49	1.41
19	4	4014	CLA	C4C-C3C	-2.93	1.40	1.45
19	2	2013	CLA	CHB-C1B	2.93	1.46	1.39
19	A	1128	CLA	C4C-C3C	-2.93	1.40	1.45
19	1	1005	CLA	C4C-C3C	-2.93	1.40	1.45
21	B	6020	BCR	C11-C10	2.92	1.52	1.43
19	2	2007	CLA	C1B-NB	-2.92	1.34	1.37
19	4	1306	CLA	C1B-NB	-2.92	1.34	1.37
19	1	1014	CLA	C1C-C2C	-2.92	1.38	1.44
19	2	4009	CLA	C4C-C3C	-2.92	1.40	1.45
19	3	3002	CLA	CHB-C1B	2.92	1.47	1.39
19	4	4002	CLA	OBD-CAD	2.91	1.27	1.22
19	L	1503	CLA	CMA-C3A	2.91	1.59	1.53
19	2	2004	CLA	C1B-NB	-2.91	1.34	1.37
19	1	1007	CLA	C4C-C3C	-2.90	1.40	1.45
19	A	1141	CLA	C1B-NB	-2.90	1.34	1.37
19	B	1203	CLA	OBD-CAD	2.90	1.27	1.22
22	4	7052	LMU	O1'-C1'	2.90	1.45	1.40
19	4	4010	CLA	CHB-C1B	2.90	1.47	1.39
22	A	7044	LMU	O1'-C1'	2.90	1.45	1.40
19	A	1103	CLA	C1C-C2C	-2.89	1.38	1.44
19	2	2005	CLA	CHB-C1B	2.89	1.47	1.39
19	1	1303	CLA	MG-ND	-2.89	2.00	2.05
19	A	1151	CLA	CHB-C1B	2.89	1.45	1.39
19	A	1115	CLA	C4B-NB	-2.89	1.34	1.37
19	B	1206	CLA	C1B-C2B	-2.88	1.36	1.43
19	2	2006	CLA	C1B-NB	-2.88	1.34	1.37
19	B	1236	CLA	C1C-C2C	-2.88	1.38	1.44
19	B	1209	CLA	C1C-C2C	-2.88	1.38	1.44
19	H	1207	CLA	C1B-NB	-2.87	1.34	1.37
19	A	9013	CLA	C1C-C2C	-2.87	1.38	1.44
19	2	2005	CLA	CHD-C4C	2.87	1.50	1.40
19	B	1206	CLA	C1C-C2C	-2.87	1.38	1.44
19	B	1212	CLA	C4C-C3C	-2.86	1.40	1.45
19	A	1126	CLA	C1C-C2C	-2.86	1.38	1.44
19	4	4004	CLA	CHB-C1B	2.86	1.47	1.39
19	B	9010	CLA	C1B-NB	-2.86	1.34	1.37
19	4	4011	CLA	CHB-C1B	2.85	1.47	1.39
19	A	1103	CLA	OBD-CAD	2.85	1.27	1.22
19	A	1119	CLA	C1C-C2C	-2.85	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	2007	CLA	C1C-C2C	-2.85	1.38	1.44
19	4	4003	CLA	C1C-C2C	-2.85	1.38	1.44
19	L	1148	CLA	MG-NA	-2.84	1.99	2.06
19	B	1221	CLA	C4B-NB	-2.84	1.34	1.37
19	A	1129	CLA	C1B-NB	-2.84	1.34	1.37
19	2	2014	CLA	C1B-C2B	-2.83	1.36	1.43
19	B	1224	CLA	C1B-NB	-2.83	1.34	1.37
19	A	1106	CLA	C1B-NB	-2.83	1.34	1.37
19	R	1144	CLA	C1B-NB	-2.83	1.34	1.37
19	4	4014	CLA	C1C-C2C	-2.83	1.38	1.44
19	3	3012	CLA	C3D-C4D	-2.82	1.37	1.44
19	B	1238	CLA	C1C-C2C	-2.82	1.38	1.44
19	A	1106	CLA	CHB-C1B	2.82	1.45	1.39
19	A	1126	CLA	C4B-NB	-2.82	1.34	1.37
19	1	1003	CLA	C1B-NB	-2.82	1.34	1.37
19	A	1135	CLA	C1C-C2C	-2.82	1.38	1.44
19	A	1126	CLA	C4C-C3C	-2.81	1.40	1.45
19	L	1130	CLA	C1B-NB	-2.81	1.34	1.37
19	1	1303	CLA	C1D-C2D	-2.81	1.39	1.45
19	2	2001	CLA	C1C-C2C	-2.80	1.38	1.44
19	A	1105	CLA	C4C-C3C	-2.80	1.40	1.45
19	4	4002	CLA	C4B-NB	-2.80	1.34	1.37
19	3	1118	CLA	C4C-C3C	-2.80	1.38	1.44
19	A	1136	CLA	C1C-C2C	-2.80	1.38	1.44
19	1	1002	CLA	CHB-C1B	2.79	1.45	1.39
22	H	7032	LMU	O1'-C1'	2.79	1.44	1.40
19	2	2011	CLA	CHB-C1B	2.79	1.47	1.39
21	F	6016	BCR	C39-C30	2.79	1.59	1.53
19	3	3013	CLA	C1C-NC	-2.79	1.33	1.37
19	A	1124	CLA	C1C-C2C	-2.79	1.38	1.44
19	A	1112	CLA	C1B-NB	-2.79	1.34	1.37
19	B	1214	CLA	C4C-C3C	-2.79	1.40	1.45
19	3	1147	CLA	MG-ND	-2.79	2.00	2.05
19	B	1226	CLA	MG-NA	-2.79	1.99	2.06
19	R	1144	CLA	C4C-C3C	-2.79	1.40	1.45
19	B	1220	CLA	C1B-C2B	-2.79	1.36	1.43
19	B	1235	CLA	OBD-CAD	2.79	1.27	1.22
19	1	1015	CLA	MG-NA	-2.78	1.99	2.06
19	A	1122	CLA	C4C-C3C	-2.78	1.40	1.45
19	4	4013	CLA	CHA-C1A	2.78	1.49	1.41
19	1	1013	CLA	C4B-NB	-2.78	1.34	1.37
19	A	1139	CLA	C1C-C2C	-2.77	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	1305	CLA	C1D-ND	-2.77	1.34	1.37
19	3	3011	CLA	CHB-C1B	2.77	1.45	1.39
19	4	4014	CLA	MG-NA	-2.77	1.99	2.06
19	3	1147	CLA	O2A-CGA	2.77	1.41	1.33
22	R	7025	LMU	O1'-C1'	2.76	1.44	1.40
19	B	1238	CLA	C1B-NB	-2.76	1.34	1.37
19	L	1130	CLA	C4C-C3C	-2.76	1.40	1.45
19	B	1216	CLA	C1B-NB	-2.76	1.34	1.37
19	3	1147	CLA	C1C-NC	-2.76	1.33	1.37
19	3	3003	CLA	C3A-C2A	-2.76	1.52	1.54
19	1	1001	CLA	MG-NA	-2.76	1.99	2.06
19	B	1201	CLA	C4C-C3C	-2.75	1.40	1.45
19	A	1110	CLA	C1C-C2C	-2.75	1.38	1.44
19	4	1304	CLA	C1B-C2B	-2.75	1.36	1.43
19	B	1222	CLA	C1B-NB	-2.75	1.34	1.37
19	H	1505	CLA	C4C-C3C	-2.75	1.40	1.45
19	4	1004	CLA	C5-C3	2.74	1.56	1.51
19	3	3017	CLA	C1B-C2B	-2.74	1.36	1.43
19	A	9011	CLA	C1D-C2D	-2.74	1.39	1.45
19	A	1107	CLA	C4B-NB	-2.74	1.34	1.37
19	3	1118	CLA	C1C-C2C	-2.73	1.39	1.44
19	A	9023	CLA	C1B-NB	-2.73	1.34	1.37
19	4	4007	CLA	C1C-C2C	-2.73	1.39	1.44
19	L	1148	CLA	CHB-C4A	-2.73	1.30	1.37
19	1	1007	CLA	C1B-NB	-2.73	1.34	1.37
19	1	1015	CLA	CHA-C1A	2.72	1.49	1.41
19	A	1137	CLA	C1C-C2C	-2.72	1.39	1.44
19	H	1145	CLA	C1C-C2C	-2.72	1.39	1.44
19	B	1222	CLA	CBC-CAC	2.72	1.63	1.51
19	B	1201	CLA	CHB-C1B	2.72	1.45	1.39
19	K	1146	CLA	CHB-C1B	2.72	1.45	1.39
19	2	1307	CLA	CHB-C1B	2.72	1.47	1.39
19	A	1115	CLA	C1B-C2B	-2.72	1.36	1.43
19	A	1125	CLA	C1C-C2C	-2.71	1.39	1.44
19	F	1305	CLA	C1C-C2C	-2.71	1.39	1.44
19	B	1220	CLA	C1C-NC	-2.71	1.33	1.37
22	2	7046	LMU	O1'-C1'	2.71	1.44	1.40
19	A	1115	CLA	C1C-C2C	-2.71	1.39	1.44
19	F	1305	CLA	C2A-C1A	-2.71	1.46	1.52
19	B	1231	CLA	C1B-NB	-2.71	1.34	1.37
19	A	1117	CLA	C1B-NB	-2.71	1.34	1.37
19	3	3015	CLA	MG-NA	-2.71	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3005	CLA	MG-NA	-2.70	1.99	2.06
19	3	3010	CLA	CHA-C1A	2.70	1.49	1.41
19	3	3015	CLA	CHA-C1A	2.70	1.49	1.41
19	2	2011	CLA	CHA-C1A	2.70	1.49	1.41
19	A	1149	CLA	C1C-C2C	-2.69	1.39	1.44
19	3	3016	CLA	C1C-C2C	-2.69	1.39	1.44
19	4	4004	CLA	CHA-C1A	2.69	1.49	1.41
19	B	1221	CLA	C4C-C3C	-2.69	1.40	1.45
19	4	1009	CLA	C4C-C3C	-2.69	1.39	1.44
21	B	6006	BCR	C23-C22	2.69	1.51	1.46
19	3	3002	CLA	MG-NA	-2.69	1.99	2.06
19	A	1124	CLA	C1B-NB	-2.69	1.34	1.37
19	2	2008	CLA	CHB-C1B	2.69	1.47	1.39
19	1	1010	CLA	CHB-C4A	-2.69	1.31	1.37
19	A	9022	CLA	C1B-NB	-2.69	1.34	1.37
19	4	1304	CLA	MG-NA	-2.69	1.99	2.06
19	1	1012	CLA	C1B-NB	-2.69	1.34	1.37
19	2	2014	CLA	C1C-C2C	-2.68	1.39	1.44
19	F	1240	CLA	C1C-C2C	-2.68	1.39	1.44
19	A	1140	CLA	C1C-C2C	-2.68	1.39	1.44
19	B	1227	CLA	C4C-C3C	-2.67	1.40	1.45
19	2	2005	CLA	C3D-C4D	-2.67	1.37	1.44
19	B	1227	CLA	C1C-C2C	-2.67	1.39	1.44
22	L	7029	LMU	O1'-C1'	2.67	1.44	1.40
19	A	1138	CLA	C1C-C2C	-2.67	1.39	1.44
19	A	1102	CLA	C1B-NB	-2.67	1.34	1.37
19	3	2009	CLA	C1C-C2C	-2.66	1.39	1.44
19	A	1110	CLA	C1B-NB	-2.66	1.34	1.37
19	A	1127	CLA	C4C-C3C	-2.66	1.40	1.45
19	B	1223	CLA	C1C-C2C	-2.66	1.39	1.44
21	B	6005	BCR	C20-C21	-2.66	1.34	1.43
19	3	3014	CLA	C3D-C4D	-2.65	1.37	1.44
19	A	1111	CLA	C4C-C3C	-2.65	1.40	1.45
19	2	2003	CLA	CHB-C1B	2.65	1.47	1.39
19	1	1006	CLA	C1C-C2C	-2.65	1.39	1.44
19	A	1151	CLA	C1C-C2C	-2.65	1.39	1.44
19	I	1204	CLA	C1B-NB	-2.65	1.34	1.37
19	A	1115	CLA	MG-NA	-2.64	2.00	2.06
19	A	1121	CLA	C4C-C3C	-2.64	1.40	1.45
19	2	1307	CLA	CHA-C1A	2.64	1.48	1.41
19	B	1215	CLA	C1C-C2C	-2.64	1.39	1.44
19	3	3002	CLA	CHA-C1A	2.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	1308	CLA	C4B-NB	-2.64	1.34	1.37
19	A	1101	CLA	C1C-C2C	-2.64	1.39	1.44
19	A	1126	CLA	C1B-NB	-2.64	1.34	1.37
19	A	1121	CLA	C1C-C2C	-2.63	1.39	1.44
19	B	1225	CLA	C1D-C2D	-2.63	1.40	1.45
19	J	1311	CLA	C1C-C2C	-2.63	1.39	1.44
19	4	4015	CLA	MG-NA	-2.63	2.00	2.06
19	2	2014	CLA	C1D-ND	-2.63	1.34	1.37
19	4	4007	CLA	C1B-NB	-2.63	1.34	1.37
21	A	6002	BCR	C30-C25	-2.63	1.50	1.53
19	A	1117	CLA	C1C-C2C	-2.63	1.39	1.44
19	3	3003	CLA	C4C-C3C	-2.62	1.39	1.44
19	H	1145	CLA	CHB-C1B	2.62	1.45	1.39
19	A	1105	CLA	C1B-NB	-2.62	1.34	1.37
21	F	6014	BCR	C20-C21	-2.62	1.35	1.43
22	H	7043	LMU	O1'-C1'	2.62	1.44	1.40
22	K	7047	LMU	O1'-C1'	2.62	1.44	1.40
19	A	1108	CLA	C1C-C2C	-2.61	1.39	1.44
19	A	1104	CLA	C1C-C2C	-2.61	1.39	1.44
19	L	1502	CLA	C1B-NB	-2.61	1.34	1.37
19	A	1113	CLA	C1B-NB	-2.61	1.34	1.37
19	B	1220	CLA	C1D-C2D	-2.61	1.40	1.45
19	B	1234	CLA	C4C-C3C	-2.61	1.40	1.45
19	1	1003	CLA	C4C-C3C	-2.61	1.40	1.45
19	B	1230	CLA	C1C-NC	-2.60	1.33	1.37
19	A	9023	CLA	MG-NA	-2.60	2.00	2.06
22	4	7052	LMU	O1'-C1	2.60	1.50	1.43
21	B	6006	BCR	C30-C25	-2.60	1.50	1.53
19	1	1005	CLA	C1C-C2C	-2.60	1.39	1.44
19	B	1208	CLA	C1C-C2C	-2.60	1.39	1.44
19	3	1118	CLA	C1B-NB	-2.60	1.34	1.37
19	3	3012	CLA	CHB-C1B	2.60	1.46	1.39
19	B	1202	CLA	MG-NA	-2.60	2.00	2.06
19	B	1202	CLA	C1B-NB	-2.60	1.34	1.37
19	B	1220	CLA	C4D-CHA	-2.60	1.29	1.38
21	I	6021	BCR	C31-C1	-2.60	1.48	1.53
19	R	1150	CLA	C4C-C3C	-2.59	1.40	1.45
19	4	4015	CLA	C1B-C2B	-2.59	1.37	1.43
19	2	2002	CLA	C1C-C2C	-2.59	1.39	1.44
19	L	1148	CLA	C1C-NC	-2.59	1.33	1.37
19	A	1123	CLA	C1B-NB	-2.59	1.34	1.37
19	B	1219	CLA	C1C-C2C	-2.59	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1141	CLA	C1C-C2C	-2.59	1.39	1.44
19	4	1304	CLA	CHB-C4A	-2.58	1.31	1.37
19	1	1006	CLA	C1B-NB	-2.58	1.34	1.37
19	3	3017	CLA	CHB-C1B	2.58	1.45	1.39
19	4	4011	CLA	C3D-C4D	-2.58	1.37	1.44
19	3	3014	CLA	CHA-C1A	2.58	1.48	1.41
19	F	1302	CLA	C1C-C2C	-2.58	1.39	1.44
19	3	3011	CLA	C1B-C2B	-2.58	1.37	1.43
19	4	4014	CLA	C4B-NB	-2.58	1.34	1.37
22	A	7010	LMU	C4-C3	2.58	1.64	1.51
21	B	6010	BCR	C21-C22	-2.58	1.29	1.35
19	4	4002	CLA	C3A-C2A	-2.57	1.47	1.54
19	2	1307	CLA	C3D-C4D	-2.57	1.37	1.44
22	4	7018	LMU	O1'-C1'	2.57	1.44	1.40
19	A	1115	CLA	CHB-C1B	2.57	1.45	1.39
19	1	1005	CLA	MG-NA	-2.56	2.00	2.06
19	A	1108	CLA	C1B-NB	-2.56	1.34	1.37
19	1	1011	CLA	CHB-C1B	2.56	1.45	1.39
19	A	1139	CLA	MG-NA	-2.56	2.00	2.06
19	1	1002	CLA	C1B-C2B	-2.55	1.37	1.43
19	B	1210	CLA	C1C-C2C	-2.55	1.39	1.44
19	A	1132	CLA	C1B-NB	-2.55	1.34	1.37
19	3	3007	CLA	C1B-NB	-2.55	1.34	1.37
19	B	1214	CLA	C1C-C2C	-2.55	1.39	1.44
21	L	6019	BCR	C30-C25	-2.55	1.50	1.53
21	F	6016	BCR	C1-C6	-2.55	1.50	1.53
22	G	7026	LMU	O1'-C1'	2.55	1.44	1.40
22	4	7009	LMU	O6'-C6'	2.55	1.53	1.42
19	A	9012	CLA	C1B-C2B	-2.55	1.37	1.43
19	4	4010	CLA	CHA-C1A	2.55	1.48	1.41
19	K	1146	CLA	MG-ND	-2.54	2.00	2.05
19	1	1007	CLA	C1C-C2C	-2.54	1.39	1.44
19	B	1225	CLA	C1D-ND	-2.54	1.34	1.37
19	B	1230	CLA	C4B-NB	-2.54	1.34	1.37
19	1	1303	CLA	C1D-ND	-2.54	1.34	1.37
19	1	1011	CLA	C1C-NC	-2.54	1.33	1.37
19	L	1503	CLA	C4B-NB	-2.54	1.34	1.37
19	B	1233	CLA	C1B-NB	-2.54	1.34	1.37
19	B	1219	CLA	C4C-C3C	-2.54	1.40	1.45
19	4	4014	CLA	C1B-NB	-2.54	1.34	1.37
19	4	1304	CLA	CHB-C1B	2.54	1.45	1.39
19	B	1239	CLA	C1B-NB	-2.54	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1222	CLA	C1C-C2C	-2.53	1.39	1.44
19	K	1142	CLA	MG-NA	-2.53	2.00	2.06
19	A	1129	CLA	C1C-C2C	-2.53	1.39	1.44
19	B	1238	CLA	MG-NA	-2.53	2.00	2.06
19	1	1014	CLA	MG-NA	-2.53	2.00	2.06
19	1	1303	CLA	CHB-C1B	2.53	1.45	1.39
19	1	1303	CLA	C1C-NC	-2.53	1.33	1.37
19	A	1133	CLA	C4C-C3C	-2.53	1.40	1.45
19	4	4002	CLA	C1D-ND	-2.53	1.34	1.37
19	A	1113	CLA	C4C-C3C	-2.53	1.40	1.45
19	B	1221	CLA	C1C-C2C	-2.53	1.39	1.44
19	A	1116	CLA	C1C-C2C	-2.52	1.39	1.44
19	L	1503	CLA	C1B-C2B	-2.52	1.37	1.43
19	B	1224	CLA	C1C-C2C	-2.52	1.39	1.44
19	A	1141	CLA	MG-NA	-2.52	2.00	2.06
19	H	1241	CLA	C1B-NB	-2.52	1.34	1.37
19	A	1106	CLA	C1B-C2B	-2.52	1.37	1.43
19	A	1122	CLA	C1C-C2C	-2.52	1.39	1.44
19	H	1505	CLA	C1B-NB	-2.51	1.34	1.37
19	4	4010	CLA	C3D-C4D	-2.51	1.37	1.44
19	1	1013	CLA	CBD-CGD	-2.51	1.44	1.52
19	3	1147	CLA	C3B-C4B	-2.51	1.35	1.42
19	A	1125	CLA	MG-NA	-2.51	2.00	2.06
19	B	9010	CLA	C1C-C2C	-2.51	1.39	1.44
19	3	3011	CLA	C4C-C3C	-2.51	1.40	1.45
19	A	9013	CLA	MG-NA	-2.51	2.00	2.06
22	A	7045	LMU	O1'-C1'	2.51	1.44	1.40
19	2	2002	CLA	C4C-C3C	-2.51	1.40	1.45
19	4	4012	CLA	C1C-C2C	-2.50	1.39	1.44
19	2	2010	CLA	CHA-C1A	2.50	1.48	1.41
19	1	1006	CLA	C4C-C3C	-2.50	1.39	1.44
21	I	6021	BCR	C11-C10	2.50	1.50	1.43
19	A	1309	CLA	CHA-C1A	2.50	1.48	1.41
19	F	1305	CLA	C1B-C2B	-2.50	1.37	1.43
19	A	9012	CLA	C1C-C2C	-2.50	1.39	1.44
19	B	1228	CLA	C1B-NB	-2.50	1.34	1.37
19	1	1012	CLA	C4C-C3C	-2.49	1.39	1.44
19	3	3017	CLA	MG-NA	-2.49	2.00	2.06
19	I	1204	CLA	OBD-CAD	2.49	1.26	1.22
21	A	6008	BCR	C10-C9	-2.49	1.30	1.35
22	B	7012	LMU	O1'-C1'	2.48	1.44	1.40
19	L	1502	CLA	C1C-C2C	-2.48	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3002	CLA	C3D-C4D	-2.47	1.38	1.44
19	B	1227	CLA	C1B-C2B	-2.47	1.37	1.43
19	4	1009	CLA	C1B-C2B	-2.47	1.37	1.43
19	A	1237	CLA	C1B-NB	-2.47	1.34	1.37
19	L	1504	CLA	C1B-NB	-2.47	1.34	1.37
21	A	6007	BCR	C10-C9	-2.46	1.30	1.35
19	A	1116	CLA	C1B-NB	-2.46	1.34	1.37
19	4	1304	CLA	C4B-NB	-2.46	1.34	1.37
19	2	2003	CLA	C3D-C4D	-2.46	1.38	1.44
21	F	6016	BCR	C20-C19	-2.46	1.28	1.34
22	H	7030	LMU	O6B-C6B	2.46	1.52	1.42
19	A	1107	CLA	C1B-NB	-2.45	1.34	1.37
19	1	1011	CLA	C1B-C2B	-2.45	1.37	1.43
19	3	3011	CLA	C4B-NB	-2.45	1.34	1.37
19	B	1201	CLA	C1B-C2B	-2.45	1.37	1.43
19	A	1309	CLA	C3D-C4D	-2.45	1.38	1.44
21	B	6005	BCR	C10-C9	-2.45	1.30	1.35
21	A	6008	BCR	C21-C22	-2.45	1.30	1.35
19	2	2005	CLA	CHA-C1A	2.45	1.48	1.41
19	2	2012	CLA	C1C-C2C	-2.44	1.39	1.44
19	L	1502	CLA	C4C-C3C	-2.44	1.40	1.45
19	3	3003	CLA	C1B-NB	-2.44	1.34	1.37
19	A	1134	CLA	MG-NA	-2.44	2.00	2.06
19	B	1229	CLA	C1B-NB	-2.44	1.34	1.37
19	A	1117	CLA	C1B-C2B	-2.44	1.37	1.43
19	A	1122	CLA	C1B-C2B	-2.44	1.37	1.43
19	B	1234	CLA	C1C-C2C	-2.44	1.39	1.44
19	2	2014	CLA	CHB-C1B	2.44	1.44	1.39
19	2	2003	CLA	CHA-C1A	2.44	1.48	1.41
19	A	1121	CLA	C1B-NB	-2.44	1.34	1.37
19	A	9012	CLA	C4B-NB	-2.44	1.34	1.37
19	L	1148	CLA	C1D-ND	-2.44	1.34	1.37
19	A	9011	CLA	C1D-ND	-2.44	1.34	1.37
19	3	3017	CLA	CHB-C4A	-2.43	1.31	1.37
19	1	1013	CLA	C1C-NC	-2.43	1.34	1.37
19	A	1128	CLA	C1C-C2C	-2.43	1.39	1.44
19	A	1149	CLA	C1B-NB	-2.43	1.34	1.37
19	A	1113	CLA	C1C-C2C	-2.43	1.39	1.44
19	A	9011	CLA	C1C-C2C	-2.43	1.39	1.44
19	3	3008	CLA	MG-NA	-2.43	2.00	2.06
21	L	6019	BCR	C20-C19	-2.43	1.28	1.34
19	B	1218	CLA	C1B-NB	-2.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1125	CLA	C4B-NB	-2.42	1.34	1.37
19	B	1229	CLA	C1B-C2B	-2.42	1.37	1.43
21	L	6019	BCR	C2-C1	-2.42	1.48	1.54
19	A	1124	CLA	MG-NA	-2.42	2.00	2.06
19	F	1240	CLA	C4C-C3C	-2.42	1.39	1.44
19	2	2006	CLA	C1C-C2C	-2.42	1.39	1.44
19	1	1014	CLA	C1D-ND	-2.41	1.34	1.37
19	3	3004	CLA	CHB-C1B	2.41	1.46	1.39
19	3	1118	CLA	C3A-C2A	-2.41	1.52	1.54
19	A	1131	CLA	MG-NA	-2.41	2.00	2.06
19	3	3008	CLA	C1C-C2C	-2.41	1.39	1.44
19	B	1211	CLA	C1C-C2C	-2.41	1.39	1.44
19	B	1211	CLA	C4C-C3C	-2.40	1.41	1.45
21	L	6019	BCR	C11-C10	2.40	1.50	1.43
19	1	1010	CLA	MG-NB	-2.40	2.01	2.05
19	4	4002	CLA	C1D-C2D	-2.40	1.40	1.45
19	A	1112	CLA	C1C-C2C	-2.40	1.39	1.44
19	1	1310	CLA	C3D-C4D	-2.40	1.38	1.44
19	A	1127	CLA	C1C-C2C	-2.40	1.39	1.44
19	B	1201	CLA	MG-NA	-2.40	2.00	2.06
19	B	1301	CLA	C1C-C2C	-2.40	1.39	1.44
19	B	1213	CLA	C1B-NB	-2.40	1.34	1.37
19	A	1107	CLA	C4C-C3C	-2.39	1.41	1.45
19	3	3014	CLA	CHB-C1B	2.39	1.46	1.39
19	K	1142	CLA	C1C-C2C	-2.39	1.39	1.44
19	1	1303	CLA	MG-NA	-2.39	2.00	2.06
19	3	3003	CLA	C1C-C2C	-2.39	1.39	1.44
19	3	1147	CLA	MG-NB	-2.38	2.01	2.05
19	1	1310	CLA	CHB-C1B	2.38	1.46	1.39
21	F	6016	BCR	C21-C22	-2.38	1.30	1.35
19	A	1151	CLA	C4C-C3C	-2.37	1.41	1.45
22	G	7026	LMU	O3B-C3B	2.37	1.48	1.43
22	R	7024	LMU	O1'-C1'	2.37	1.44	1.40
19	A	1237	CLA	C1C-C2C	-2.37	1.39	1.44
19	A	1136	CLA	MG-NA	-2.37	2.00	2.06
19	A	1133	CLA	C1C-C2C	-2.37	1.39	1.44
19	B	1210	CLA	MG-NA	-2.37	2.00	2.06
19	A	1115	CLA	CHB-C4A	-2.36	1.31	1.37
19	3	2009	CLA	C1B-C2B	-2.36	1.37	1.43
19	A	1137	CLA	MG-NA	-2.36	2.00	2.06
19	3	3004	CLA	C3D-C4D	-2.36	1.38	1.44
19	B	1231	CLA	C1C-C2C	-2.36	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	7014	LMU	O2B-C2B	2.36	1.48	1.43
19	B	1234	CLA	C1B-NB	-2.36	1.34	1.37
19	3	2009	CLA	MG-NA	-2.35	2.00	2.06
19	4	1004	CLA	MG-NA	-2.35	2.00	2.06
19	1	1001	CLA	O1D-CGD	2.35	1.27	1.21
19	4	4015	CLA	C1D-C2D	-2.35	1.40	1.45
19	L	1503	CLA	CBD-CGD	-2.35	1.45	1.52
22	2	7027	LMU	O1'-C1'	2.35	1.44	1.40
19	4	1004	CLA	C4B-NB	-2.35	1.34	1.37
19	A	1135	CLA	MG-NA	-2.35	2.00	2.06
21	J	6012	BCR	C32-C1	2.35	1.58	1.53
19	B	1229	CLA	C1C-C2C	-2.34	1.39	1.44
19	B	1239	CLA	C4C-C3C	-2.34	1.41	1.45
19	A	1106	CLA	C1D-ND	-2.34	1.34	1.37
19	1	1002	CLA	C4C-C3C	-2.34	1.41	1.45
21	J	6012	BCR	C21-C22	-2.34	1.30	1.35
19	B	1221	CLA	C1B-C2B	-2.33	1.37	1.43
19	3	3016	CLA	MG-NA	-2.33	2.00	2.06
19	B	1209	CLA	C1D-ND	-2.33	1.34	1.37
19	1	1008	CLA	C3A-C2A	-2.33	1.48	1.54
19	B	1218	CLA	C1B-C2B	-2.33	1.37	1.43
19	B	1231	CLA	C1D-C2D	-2.33	1.40	1.45
19	J	1308	CLA	C1B-C2B	-2.33	1.37	1.43
19	B	1223	CLA	MG-NA	-2.33	2.00	2.06
19	3	3004	CLA	CHA-C1A	2.32	1.47	1.41
19	4	4002	CLA	C1C-NC	-2.32	1.34	1.37
19	4	1009	CLA	C1C-C2C	-2.32	1.39	1.44
19	K	3009	CLA	C1B-NB	-2.32	1.34	1.37
19	B	1225	CLA	C1C-C2C	-2.32	1.39	1.44
19	A	9012	CLA	MG-NA	-2.32	2.00	2.06
19	1	1010	CLA	CHB-C1B	2.32	1.44	1.39
19	L	1130	CLA	C1B-C2B	-2.32	1.37	1.43
19	A	1149	CLA	CMA-C3A	2.32	1.58	1.53
21	L	6019	BCR	C20-C21	-2.32	1.36	1.43
19	A	1126	CLA	C1B-C2B	-2.32	1.37	1.43
19	3	3004	CLA	C2C-C1C	-2.31	1.37	1.43
19	K	1142	CLA	C1B-C2B	-2.31	1.37	1.43
19	3	3001	CLA	C3D-C4D	-2.31	1.38	1.44
19	B	1227	CLA	C1D-ND	-2.31	1.34	1.37
19	A	1119	CLA	C4C-C3C	-2.31	1.41	1.45
19	A	1120	CLA	C1B-C2B	-2.31	1.37	1.43
19	4	1304	CLA	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1102	CLA	C1C-C2C	-2.31	1.39	1.44
19	A	1104	CLA	MG-NA	-2.31	2.00	2.06
19	3	2009	CLA	C4-C3	2.31	1.56	1.50
19	L	1501	CLA	C1D-ND	-2.30	1.34	1.37
19	A	1123	CLA	C4C-C3C	-2.30	1.41	1.45
19	3	2009	CLA	C1D-ND	-2.30	1.34	1.37
19	4	4005	CLA	CHA-C1A	2.30	1.47	1.41
19	3	3013	CLA	MG-NA	-2.30	2.00	2.06
19	A	1138	CLA	MG-NA	-2.30	2.00	2.06
19	1	1002	CLA	C1C-C2C	-2.30	1.39	1.44
21	A	6008	BCR	C40-C30	-2.30	1.49	1.53
19	2	2014	CLA	MG-NA	-2.29	2.00	2.06
22	F	7036	LMU	O1'-C1'	2.29	1.44	1.40
19	L	1130	CLA	C1C-C2C	-2.29	1.39	1.44
19	A	1101	CLA	C1B-NB	-2.29	1.34	1.37
19	4	4014	CLA	C1D-ND	-2.29	1.34	1.37
19	A	9022	CLA	MG-NA	-2.29	2.00	2.06
19	1	1012	CLA	C1C-C2C	-2.29	1.39	1.44
19	A	1139	CLA	C1B-C2B	-2.29	1.37	1.43
19	2	2002	CLA	MG-NA	-2.29	2.00	2.06
19	A	1129	CLA	C4C-C3C	-2.29	1.41	1.45
19	J	1311	CLA	MG-NA	-2.28	2.00	2.06
19	4	4012	CLA	C1B-NB	-2.28	1.34	1.37
19	L	1148	CLA	C1C-C2C	-2.28	1.39	1.44
21	B	6017	BCR	C39-C30	-2.28	1.49	1.53
21	F	6014	BCR	C20-C19	-2.28	1.28	1.34
19	A	1119	CLA	C1B-NB	-2.28	1.34	1.37
21	A	6011	BCR	C31-C1	-2.28	1.49	1.53
19	A	1139	CLA	C4B-NB	-2.27	1.34	1.37
19	3	3011	CLA	C1C-C2C	-2.27	1.39	1.44
19	1	1303	CLA	CHB-C4A	-2.27	1.32	1.37
19	A	1133	CLA	MG-NA	-2.27	2.00	2.06
19	3	3010	CLA	C3D-C4D	-2.27	1.38	1.44
19	A	1101	CLA	C4B-NB	-2.26	1.34	1.37
19	A	9022	CLA	C1C-C2C	-2.26	1.39	1.44
21	B	6020	BCR	C39-C30	-2.26	1.49	1.53
19	4	4002	CLA	CAA-C2A	-2.26	1.50	1.54
19	A	9012	CLA	CHB-C4A	-2.26	1.32	1.37
19	1	1015	CLA	C3D-C4D	-2.26	1.38	1.44
21	L	6019	BCR	C39-C30	-2.26	1.49	1.53
21	F	6016	BCR	C11-C10	2.26	1.50	1.43
19	2	2001	CLA	MG-NA	-2.26	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	6006	BCR	C37-C22	2.26	1.55	1.50
19	B	1214	CLA	C1B-C2B	-2.25	1.37	1.43
19	A	1103	CLA	C1B-NB	-2.25	1.34	1.37
19	4	4015	CLA	C1D-ND	-2.25	1.34	1.37
19	2	2014	CLA	C1D-C2D	-2.25	1.40	1.45
19	A	1123	CLA	C1C-C2C	-2.25	1.39	1.44
22	B	7040	LMU	O1'-C1'	2.25	1.43	1.40
19	B	1224	CLA	MG-NA	-2.25	2.00	2.06
19	B	1231	CLA	C1D-ND	-2.24	1.34	1.37
19	1	1014	CLA	C4B-NB	-2.24	1.34	1.37
19	3	3010	CLA	CHB-C1B	2.24	1.45	1.39
21	B	6006	BCR	C31-C1	-2.24	1.49	1.53
19	B	1234	CLA	C4B-NB	-2.24	1.34	1.37
19	3	3012	CLA	C2C-C1C	-2.24	1.37	1.43
19	B	1230	CLA	MG-NA	-2.24	2.00	2.06
19	3	3006	CLA	C3D-C2D	2.24	1.40	1.35
19	B	1201	CLA	CHB-C4A	-2.24	1.32	1.37
19	1	1011	CLA	CHB-C4A	-2.23	1.32	1.37
19	A	1123	CLA	C1B-C2B	-2.23	1.37	1.43
19	B	1218	CLA	C1C-C2C	-2.23	1.40	1.44
19	4	4012	CLA	MG-NA	-2.23	2.01	2.06
19	1	1011	CLA	C3B-C2B	-2.23	1.35	1.44
19	A	1151	CLA	CHB-C4A	-2.22	1.32	1.37
19	4	4002	CLA	CHB-C1B	2.22	1.44	1.39
19	A	1237	CLA	C1D-C2D	-2.22	1.40	1.45
19	3	3007	CLA	C1C-C2C	-2.22	1.40	1.44
19	B	1217	CLA	C1C-C2C	-2.22	1.40	1.44
19	A	1106	CLA	MG-NA	-2.22	2.01	2.06
19	2	2014	CLA	MG-ND	-2.22	2.01	2.05
19	A	1120	CLA	C1C-C2C	-2.22	1.40	1.44
19	I	1204	CLA	C4B-NB	-2.21	1.35	1.37
19	2	2011	CLA	C3D-C4D	-2.21	1.38	1.44
19	A	1103	CLA	C4C-C3C	-2.21	1.41	1.45
19	A	1135	CLA	C1B-C2B	-2.21	1.37	1.43
21	F	6016	BCR	C31-C1	-2.21	1.49	1.53
22	4	7052	LMU	C2-C1	2.21	1.60	1.51
19	B	1201	CLA	C4B-NB	-2.21	1.35	1.37
19	L	1148	CLA	C3D-CAD	-2.21	1.37	1.45
22	H	7043	LMU	C5-C4	2.21	1.62	1.51
19	A	1140	CLA	MG-NA	-2.21	2.01	2.06
19	A	1119	CLA	C1B-C2B	-2.21	1.37	1.43
19	2	2008	CLA	C3D-C4D	-2.21	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3013	CLA	C1B-C2B	-2.20	1.38	1.43
21	L	6019	BCR	C32-C1	-2.20	1.49	1.53
19	1	1013	CLA	MG-NA	-2.20	2.01	2.06
19	3	3016	CLA	C1B-C2B	-2.20	1.38	1.43
19	B	9010	CLA	MG-NA	-2.20	2.01	2.06
19	B	1239	CLA	C1D-ND	-2.20	1.35	1.37
19	4	1004	CLA	C2-C3	2.20	1.38	1.33
19	A	9013	CLA	C4B-NB	-2.20	1.35	1.37
19	B	1232	CLA	C1C-C2C	-2.20	1.40	1.44
19	B	1226	CLA	C1D-ND	-2.20	1.35	1.37
19	A	1132	CLA	C4C-C3C	-2.20	1.41	1.45
22	E	7037	LMU	O1'-C1'	2.20	1.43	1.40
22	H	7030	LMU	O1'-C1'	2.19	1.43	1.40
19	4	4006	CLA	C1D-ND	-2.19	1.35	1.37
19	4	4005	CLA	C3D-C2D	2.19	1.40	1.35
19	4	1304	CLA	C1C-NC	-2.19	1.34	1.37
19	A	1136	CLA	C4B-NB	-2.19	1.35	1.37
19	B	1206	CLA	C1D-ND	-2.19	1.35	1.37
19	1	1001	CLA	C1D-ND	-2.19	1.35	1.37
22	1	7004	LMU	O1'-C1'	2.19	1.43	1.40
19	B	1220	CLA	CHB-C4A	-2.18	1.32	1.37
19	A	9011	CLA	C1B-C2B	-2.18	1.38	1.43
19	4	4011	CLA	CHA-C1A	2.18	1.47	1.41
19	B	1230	CLA	C1D-C2D	-2.18	1.41	1.45
19	B	1228	CLA	C1C-C2C	-2.18	1.40	1.44
19	B	1226	CLA	C3D-CAD	-2.18	1.38	1.45
19	A	1111	CLA	C1B-NB	-2.18	1.35	1.37
19	2	2014	CLA	C3A-C2A	-2.18	1.48	1.54
22	H	7011	LMU	O1'-C1'	2.18	1.43	1.40
19	L	1148	CLA	MG-ND	-2.18	2.01	2.05
19	B	1231	CLA	C4B-NB	-2.18	1.35	1.37
21	B	6004	BCR	C10-C9	-2.17	1.30	1.35
19	3	1147	CLA	O2D-CED	-2.17	1.40	1.45
19	B	1236	CLA	C1D-ND	-2.17	1.35	1.37
22	N	7049	LMU	O1'-C1'	2.17	1.43	1.40
19	A	9013	CLA	C1C-NC	-2.17	1.34	1.37
19	F	1302	CLA	MG-NA	-2.17	2.01	2.06
19	F	1240	CLA	C1B-C2B	-2.17	1.38	1.43
19	A	1124	CLA	C1B-C2B	-2.17	1.38	1.43
19	B	1219	CLA	MG-NA	-2.17	2.01	2.06
19	A	1137	CLA	C4B-NB	-2.17	1.35	1.37
19	H	1207	CLA	C1C-C2C	-2.17	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	7017	LMU	O1'-C1'	2.16	1.43	1.40
19	A	1117	CLA	MG-NA	-2.16	2.01	2.06
19	B	1216	CLA	C1D-C2D	-2.16	1.41	1.45
21	J	6012	BCR	C10-C9	-2.16	1.30	1.35
21	A	6002	BCR	C39-C30	-2.16	1.49	1.53
19	J	1308	CLA	C3D-CAD	-2.16	1.38	1.45
22	K	7001	LMU	O3B-C3B	2.16	1.48	1.43
19	1	1013	CLA	C2-C3	2.16	1.38	1.33
19	B	1223	CLA	C1B-C2B	-2.16	1.38	1.43
19	A	1102	CLA	CHB-C4A	-2.16	1.32	1.37
19	1	1014	CLA	C1D-C2D	-2.16	1.41	1.45
19	A	1112	CLA	C4C-C3C	-2.15	1.41	1.45
19	R	1144	CLA	C1C-C2C	-2.15	1.40	1.44
22	C	7015	LMU	O1'-C1'	2.15	1.43	1.40
19	3	3008	CLA	C1B-C2B	-2.15	1.38	1.43
19	1	1001	CLA	C3D-CAD	-2.15	1.38	1.45
21	A	6011	BCR	C21-C22	-2.15	1.30	1.35
19	3	2009	CLA	C4B-NB	-2.15	1.35	1.37
22	E	7048	LMU	O1'-C1'	2.15	1.43	1.40
19	4	1304	CLA	C1D-ND	-2.15	1.35	1.37
19	3	3011	CLA	MG-NA	-2.15	2.01	2.06
22	4	7053	LMU	O1'-C1'	2.15	1.43	1.40
19	L	1148	CLA	C4D-CHA	-2.15	1.31	1.38
19	B	9010	CLA	C1D-C2D	-2.15	1.41	1.45
19	3	3013	CLA	C3D-CAD	-2.15	1.38	1.45
19	B	1219	CLA	C4B-NB	-2.15	1.35	1.37
19	A	1128	CLA	C1B-C2B	-2.15	1.38	1.43
19	I	1204	CLA	C1C-C2C	-2.14	1.40	1.44
19	1	1010	CLA	C3D-CAD	-2.14	1.38	1.45
19	B	1224	CLA	C1B-C2B	-2.14	1.38	1.43
19	2	4009	CLA	C1D-ND	-2.14	1.35	1.37
19	2	2004	CLA	C1C-C2C	-2.14	1.40	1.44
19	4	4003	CLA	C1B-C2B	-2.14	1.38	1.43
19	K	1143	CLA	MG-NA	-2.14	2.01	2.06
19	A	1119	CLA	C4B-NB	-2.14	1.35	1.37
24	B	7101	LMG	O1-C1	2.14	1.43	1.40
19	K	1146	CLA	C4B-NB	-2.14	1.35	1.37
19	2	2001	CLA	C1B-C2B	-2.14	1.38	1.43
22	R	7014	LMU	O1'-C1'	2.14	1.43	1.40
19	A	1131	CLA	C4B-NB	-2.13	1.35	1.37
19	3	3013	CLA	C1D-C2D	-2.13	1.41	1.45
19	H	1241	CLA	C1C-C2C	-2.13	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1102	CLA	C1B-C2B	-2.13	1.38	1.43
19	A	1133	CLA	C4B-NB	-2.13	1.35	1.37
22	K	7001	LMU	O1'-C1'	2.13	1.43	1.40
19	B	1301	CLA	C4C-C3C	-2.13	1.40	1.44
19	A	1120	CLA	MG-NA	-2.13	2.01	2.06
19	2	2012	CLA	C4B-NB	-2.13	1.35	1.37
19	B	1220	CLA	MG-NB	-2.13	2.01	2.05
19	A	1136	CLA	C1B-C2B	-2.13	1.38	1.43
19	F	1240	CLA	CHB-C4A	-2.12	1.32	1.37
22	1	7013	LMU	O1'-C1'	2.12	1.43	1.40
19	B	1216	CLA	C1C-C2C	-2.12	1.40	1.44
21	3	6022	BCR	C21-C22	-2.12	1.30	1.35
22	R	7021	LMU	O1'-C1'	2.12	1.43	1.40
19	1	1007	CLA	MG-NA	-2.12	2.01	2.06
19	B	1301	CLA	MG-NA	-2.12	2.01	2.06
21	B	6004	BCR	C21-C22	-2.12	1.30	1.35
19	3	1147	CLA	C3A-C2A	-2.11	1.48	1.54
22	2	7006	LMU	O1'-C1'	2.11	1.43	1.40
19	3	3008	CLA	C1D-ND	-2.11	1.35	1.37
21	F	6016	BCR	C11-C12	-2.11	1.29	1.34
19	A	1110	CLA	MG-NA	-2.11	2.01	2.06
19	4	4013	CLA	C3D-C4D	-2.11	1.38	1.44
19	A	1106	CLA	C1C-C2C	-2.11	1.40	1.44
21	B	6005	BCR	C21-C22	-2.11	1.30	1.35
22	R	7022	LMU	O1'-C1'	2.11	1.43	1.40
19	B	1220	CLA	C3D-CAD	-2.11	1.38	1.45
21	I	6021	BCR	C4-C5	2.11	1.54	1.51
19	B	1217	CLA	MG-NA	-2.11	2.01	2.06
19	H	1207	CLA	MG-NA	-2.11	2.01	2.06
19	A	1151	CLA	C4B-NB	-2.11	1.35	1.37
19	A	1128	CLA	C1D-C2D	-2.11	1.41	1.45
19	B	1203	CLA	C1C-NC	-2.11	1.34	1.37
19	A	1108	CLA	MG-NA	-2.10	2.01	2.06
19	A	1122	CLA	C4B-NB	-2.10	1.35	1.37
19	B	1216	CLA	MG-NA	-2.10	2.01	2.06
19	A	1110	CLA	C4B-NB	-2.10	1.35	1.37
19	K	1146	CLA	C1D-C2D	-2.10	1.41	1.45
19	1	1013	CLA	CBD-CAD	-2.10	1.47	1.56
19	K	1146	CLA	CHB-C4A	-2.10	1.32	1.37
21	B	6006	BCR	C32-C1	-2.10	1.49	1.53
19	J	1308	CLA	C1D-ND	-2.10	1.35	1.37
19	B	1209	CLA	MG-NA	-2.10	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1239	CLA	MG-NA	-2.10	2.01	2.06
21	L	6019	BCR	C10-C9	-2.10	1.31	1.35
19	2	2012	CLA	C1B-NB	-2.10	1.35	1.37
19	1	1303	CLA	MG-NB	-2.10	2.01	2.05
19	A	1237	CLA	MG-NA	-2.09	2.01	2.06
19	A	9022	CLA	C1B-C2B	-2.09	1.38	1.43
19	B	1216	CLA	C1D-ND	-2.09	1.35	1.37
19	4	4005	CLA	C3D-C4D	-2.09	1.39	1.44
19	F	1305	CLA	CHB-C4A	-2.09	1.32	1.37
19	A	1109	CLA	C4B-NB	-2.09	1.35	1.37
19	L	1504	CLA	MG-NA	-2.09	2.01	2.06
19	4	4013	CLA	MG-NA	-2.09	2.01	2.06
19	H	1145	CLA	C3A-C2A	-2.09	1.48	1.54
19	1	1011	CLA	C1D-ND	-2.09	1.35	1.37
19	B	1212	CLA	C1C-C2C	-2.08	1.40	1.44
19	3	3004	CLA	C3C-C4C	-2.08	1.38	1.43
19	4	4015	CLA	CBD-CGD	-2.08	1.46	1.52
19	A	1134	CLA	C1B-C2B	-2.08	1.38	1.43
19	A	1123	CLA	C4B-NB	-2.08	1.35	1.37
19	B	1230	CLA	C1D-ND	-2.08	1.35	1.37
19	B	1229	CLA	CHB-C4A	-2.08	1.32	1.37
19	B	1221	CLA	C1D-C2D	-2.08	1.41	1.45
22	2	7031	LMU	C6'-C5'	2.08	1.58	1.51
19	2	2004	CLA	MG-NA	-2.08	2.01	2.06
19	1	1006	CLA	MG-NA	-2.08	2.01	2.06
19	3	3008	CLA	C3D-CAD	-2.07	1.38	1.45
19	A	1111	CLA	C1B-C2B	-2.07	1.38	1.43
19	3	3010	CLA	C3D-C2D	2.07	1.40	1.35
19	1	1008	CLA	C1C-C2C	-2.07	1.40	1.44
19	4	4015	CLA	MG-ND	-2.07	2.01	2.05
19	B	1221	CLA	CHB-C4A	-2.07	1.32	1.37
19	4	1306	CLA	MG-NA	-2.07	2.01	2.06
19	L	1501	CLA	C1D-C2D	-2.07	1.41	1.45
19	K	3009	CLA	C1D-C2D	-2.07	1.41	1.45
19	F	1305	CLA	MG-NA	-2.07	2.01	2.06
19	3	3001	CLA	C3D-C2D	2.07	1.40	1.35
19	A	1151	CLA	C1B-C2B	-2.07	1.38	1.43
19	A	1108	CLA	C3A-C2A	-2.06	1.48	1.54
19	A	1135	CLA	C4B-NB	-2.06	1.35	1.37
19	A	1127	CLA	C1B-C2B	-2.06	1.38	1.43
19	B	1222	CLA	MG-NA	-2.06	2.01	2.06
19	B	1236	CLA	MG-NA	-2.06	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1239	CLA	C3B-C4B	-2.06	1.36	1.42
19	G	1242	CLA	C4B-NB	-2.06	1.35	1.37
21	A	6007	BCR	C40-C30	-2.06	1.49	1.53
21	B	6017	BCR	C21-C22	-2.06	1.31	1.35
19	G	1242	CLA	C1B-NB	-2.06	1.35	1.37
19	B	1221	CLA	C2-C3	2.06	1.37	1.33
19	L	1148	CLA	MG-NB	-2.06	2.01	2.05
19	A	1149	CLA	C2A-C1A	-2.05	1.47	1.52
19	A	1140	CLA	C1D-ND	-2.05	1.35	1.37
19	F	1302	CLA	C4B-NB	-2.05	1.35	1.37
19	L	1130	CLA	C4B-NB	-2.05	1.35	1.37
19	3	1147	CLA	C3B-C2B	-2.05	1.34	1.41
19	B	1234	CLA	C3D-CAD	-2.05	1.38	1.45
21	I	6018	BCR	C32-C1	-2.05	1.49	1.53
19	F	1240	CLA	C4B-NB	-2.05	1.35	1.37
19	I	1204	CLA	C1B-C2B	-2.05	1.38	1.43
19	J	1311	CLA	C1B-C2B	-2.05	1.38	1.43
22	D	7050	LMU	O1'-C1'	2.05	1.43	1.40
21	B	6004	BCR	C32-C1	-2.05	1.49	1.53
19	B	1202	CLA	C3A-C2A	-2.05	1.48	1.54
19	4	4001	CLA	C1C-C2C	-2.05	1.40	1.44
19	B	1215	CLA	C1D-C2D	-2.04	1.41	1.45
19	A	9011	CLA	MG-NA	-2.04	2.01	2.06
19	A	1149	CLA	C4C-C3C	-2.04	1.41	1.45
19	4	1304	CLA	C3A-C2A	-2.04	1.48	1.54
22	R	7007	LMU	O1'-C1'	2.04	1.43	1.40
19	L	1501	CLA	C1C-C2C	-2.04	1.40	1.44
19	3	3006	CLA	C3C-C4C	-2.04	1.38	1.43
19	R	1150	CLA	C1C-C2C	-2.04	1.40	1.44
19	A	1103	CLA	MG-NA	-2.04	2.01	2.06
19	B	1211	CLA	CHB-C4A	-2.04	1.32	1.37
19	L	1503	CLA	CHB-C4A	-2.04	1.32	1.37
19	B	1235	CLA	C4B-NB	-2.04	1.35	1.37
19	2	2012	CLA	C4C-C3C	-2.04	1.41	1.45
19	B	1219	CLA	C1B-C2B	-2.04	1.38	1.43
19	A	1140	CLA	C1B-C2B	-2.04	1.38	1.43
19	B	1210	CLA	CHB-C4A	-2.03	1.32	1.37
19	B	1210	CLA	C1B-C2B	-2.03	1.38	1.43
22	H	7011	LMU	O5B-C1B	2.03	1.47	1.41
19	3	1118	CLA	MG-NA	-2.03	2.01	2.06
19	3	3005	CLA	C3D-C2D	2.03	1.39	1.35
19	H	1207	CLA	C1D-ND	-2.03	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	1308	CLA	CHB-C4A	-2.03	1.32	1.37
19	4	4002	CLA	C2A-C1A	-2.03	1.47	1.52
19	H	1145	CLA	CHB-C4A	-2.03	1.32	1.37
19	3	3008	CLA	C4B-NB	-2.03	1.35	1.37
19	B	1218	CLA	MG-NA	-2.03	2.01	2.06
19	1	1010	CLA	C3B-C4B	-2.02	1.37	1.42
19	A	1149	CLA	CBD-CAD	-2.02	1.47	1.56
21	B	6006	BCR	C19-C18	2.02	1.50	1.46
19	A	1127	CLA	MG-NA	-2.02	2.01	2.06
19	A	1131	CLA	C1B-C2B	-2.02	1.38	1.43
19	4	4003	CLA	MG-NA	-2.02	2.01	2.06
19	F	1305	CLA	C1D-C2D	-2.02	1.41	1.45
19	1	1007	CLA	C1D-ND	-2.02	1.35	1.37
19	2	2001	CLA	C4B-NB	-2.02	1.35	1.37
19	F	1305	CLA	C1C-NC	-2.02	1.34	1.37
22	4	7033	LMU	O1'-C1'	2.02	1.43	1.40
19	B	1209	CLA	C4B-NB	-2.02	1.35	1.37
19	B	1201	CLA	C1C-C2C	-2.02	1.40	1.44
19	A	1127	CLA	C4B-NB	-2.02	1.35	1.37
19	4	4007	CLA	C1B-C2B	-2.01	1.38	1.43
19	B	1229	CLA	C1A-CHA	2.01	1.51	1.43
19	B	1221	CLA	C1A-CHA	2.01	1.51	1.43
19	L	1503	CLA	C1C-C2C	-2.01	1.40	1.44
19	A	1108	CLA	C1B-C2B	-2.01	1.38	1.43
19	A	1111	CLA	MG-NA	-2.01	2.01	2.06
19	3	3007	CLA	C4C-C3C	-2.01	1.41	1.45
19	A	1135	CLA	C1D-ND	-2.01	1.35	1.37
19	A	1125	CLA	C1D-ND	-2.01	1.35	1.37
19	1	1303	CLA	CAA-CBA	2.01	1.58	1.52
19	F	1302	CLA	C1B-C2B	-2.01	1.38	1.43
19	4	4003	CLA	C4B-NB	-2.01	1.35	1.37
19	A	1151	CLA	MG-NA	-2.01	2.01	2.06
19	B	1215	CLA	MG-NA	-2.01	2.01	2.06
19	K	1146	CLA	C1C-NC	-2.01	1.34	1.37
19	H	1505	CLA	C1C-C2C	-2.01	1.40	1.44
19	4	4001	CLA	C5-C3	2.01	1.55	1.50
19	B	1236	CLA	C1D-C2D	-2.01	1.41	1.45
19	A	1129	CLA	MG-NA	-2.01	2.01	2.06
19	F	1240	CLA	C1B-NB	-2.00	1.35	1.37
19	3	2009	CLA	C3D-CAD	-2.00	1.38	1.45
19	A	1137	CLA	C1B-C2B	-2.00	1.38	1.43
19	3	3014	CLA	C2C-C1C	-2.00	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	1242	CLA	MG-NA	-2.00	2.01	2.06
19	A	1121	CLA	C4B-NB	-2.00	1.35	1.37

All (5208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	6012	BCR	C20-C21-C22	30.62	170.21	127.28
21	A	6002	BCR	C20-C21-C22	25.17	162.58	127.28
21	3	6022	BCR	C20-C21-C22	24.97	162.30	127.28
21	F	6014	BCR	C20-C21-C22	23.10	159.67	127.28
21	B	6005	BCR	C20-C21-C22	22.66	159.05	127.28
21	1	6023	BCR	C2-C1-C6	-21.73	78.87	110.44
21	L	6019	BCR	C20-C21-C22	21.55	157.50	127.28
21	B	6006	BCR	C20-C21-C22	21.12	156.90	127.28
21	1	6023	BCR	C11-C10-C9	20.99	156.72	127.28
21	B	6010	BCR	C20-C21-C22	20.54	156.09	127.28
21	B	6020	BCR	C20-C21-C22	20.33	155.79	127.28
21	B	6004	BCR	C20-C21-C22	18.99	153.91	127.28
21	I	6018	BCR	C11-C10-C9	17.90	152.38	127.28
21	A	6008	BCR	C20-C21-C22	17.17	151.36	127.28
21	B	6017	BCR	C20-C21-C22	16.99	151.11	127.28
21	B	6006	BCR	C11-C10-C9	16.12	149.89	127.28
21	J	6012	BCR	C11-C10-C9	15.89	149.57	127.28
21	I	6021	BCR	C24-C23-C22	-15.79	102.88	126.23
21	F	6014	BCR	C21-C20-C19	15.74	168.81	123.20
21	1	6023	BCR	C29-C30-C25	-15.55	87.86	110.44
21	I	6018	BCR	C20-C21-C22	15.41	148.89	127.28
21	A	6002	BCR	C21-C20-C19	15.17	167.16	123.20
21	A	6007	BCR	C11-C10-C9	15.15	148.52	127.28
21	A	6011	BCR	C20-C21-C22	14.95	148.24	127.28
21	I	6021	BCR	C20-C21-C22	14.91	148.18	127.28
21	A	6011	BCR	C11-C10-C9	14.90	148.17	127.28
21	3	6022	BCR	C21-C20-C19	14.82	166.13	123.20
21	F	6016	BCR	C20-C21-C22	14.48	147.59	127.28
21	1	6023	BCR	C32-C1-C6	-13.99	88.31	110.24
21	B	6005	BCR	C11-C10-C9	13.89	146.76	127.28
21	J	6012	BCR	C21-C20-C19	13.75	163.04	123.20
21	A	6003	BCR	C20-C21-C22	13.46	146.16	127.28
21	B	6005	BCR	C21-C20-C19	13.44	162.16	123.20
21	1	6023	BCR	C10-C11-C12	13.37	161.95	123.20
19	1	1011	CLA	CAB-C3B-C4B	-13.22	105.28	125.42
21	B	6017	BCR	C11-C10-C9	13.12	145.68	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	I	6021	BCR	C11-C10-C9	12.76	145.17	127.28
21	A	6008	BCR	C11-C10-C9	12.72	145.11	127.28
19	2	4009	CLA	OBD-CAD-C3D	-12.71	98.70	128.42
21	F	6014	BCR	C11-C10-C9	12.67	145.04	127.28
19	1	1013	CLA	OBD-CAD-C3D	-12.38	99.48	128.42
19	3	3013	CLA	OBD-CAD-C3D	-12.13	100.06	128.42
21	B	6020	BCR	C15-C16-C17	-12.03	98.91	123.52
21	1	6023	BCR	C31-C1-C6	-11.90	91.58	110.24
19	4	1009	CLA	CAB-C3B-C4B	-11.81	107.43	125.42
19	B	1301	CLA	CAB-C3B-C4B	-11.71	107.59	125.42
21	B	6004	BCR	C11-C10-C9	11.67	143.65	127.28
19	4	4012	CLA	CAB-C3B-C4B	-11.51	107.89	125.42
21	I	6018	BCR	C24-C23-C22	-11.31	109.51	126.23
19	4	4014	CLA	OBD-CAD-C3D	-11.20	102.24	128.42
19	2	2006	CLA	OBD-CAD-C3D	-11.14	102.38	128.42
19	A	1149	CLA	CAB-C3B-C4B	-10.98	108.70	125.42
21	B	6006	BCR	C21-C20-C19	10.93	154.87	123.20
19	L	1503	CLA	OBD-CAD-C3D	-10.89	102.97	128.42
21	B	6010	BCR	C11-C10-C9	10.84	142.48	127.28
19	1	1012	CLA	CAB-C3B-C4B	-10.83	108.92	125.42
19	1	1303	CLA	OBD-CAD-C3D	-10.79	103.20	128.42
19	3	1118	CLA	CAB-C3B-C4B	-10.78	109.01	125.42
21	A	6011	BCR	C21-C20-C19	10.69	154.16	123.20
21	B	6020	BCR	C7-C8-C9	-10.68	110.43	126.23
19	A	1129	CLA	OBD-CAD-C3D	-10.68	103.45	128.42
19	H	1207	CLA	OBD-CAD-C3D	-10.64	103.56	128.42
19	B	1233	CLA	OBD-CAD-C3D	-10.63	103.57	128.42
19	B	1234	CLA	OBD-CAD-C3D	-10.61	103.61	128.42
21	A	6003	BCR	C11-C10-C9	10.60	142.15	127.28
19	B	1224	CLA	OBD-CAD-C3D	-10.60	103.64	128.42
21	L	6019	BCR	C11-C10-C9	10.55	142.08	127.28
19	3	3017	CLA	OBD-CAD-C3D	-10.53	103.80	128.42
19	A	1149	CLA	OBD-CAD-C3D	-10.53	103.81	128.42
21	A	6003	BCR	C21-C20-C19	10.52	153.69	123.20
19	I	1204	CLA	OBD-CAD-C3D	-10.51	103.84	128.42
21	I	6018	BCR	C7-C8-C9	-10.49	110.72	126.23
21	B	6004	BCR	C21-C20-C19	10.47	153.54	123.20
19	A	1237	CLA	OBD-CAD-C3D	-10.47	103.95	128.42
19	3	3008	CLA	CBB-CAB-C3B	10.41	179.53	127.53
19	B	1218	CLA	OBD-CAD-C3D	-10.41	104.09	128.42
19	A	1128	CLA	OBD-CAD-C3D	-10.40	104.10	128.42
21	3	6022	BCR	C11-C10-C9	10.36	141.81	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	I	1204	CLA	CBB-CAB-C3B	10.35	179.24	127.53
19	A	1134	CLA	CBB-CAB-C3B	10.34	179.20	127.53
19	A	1119	CLA	OBD-CAD-C3D	-10.31	104.32	128.42
21	B	6010	BCR	C21-C20-C19	10.29	153.00	123.20
19	J	1308	CLA	CBB-CAB-C3B	10.29	178.91	127.53
19	A	1137	CLA	CBB-CAB-C3B	10.27	178.82	127.53
19	K	3009	CLA	CBB-CAB-C3B	10.25	178.75	127.53
19	H	1145	CLA	OBD-CAD-C3D	-10.21	104.56	128.42
19	L	1503	CLA	CBB-CAB-C3B	10.18	178.41	127.53
21	L	6019	BCR	C21-C20-C19	10.18	152.70	123.20
19	4	1004	CLA	CBB-CAB-C3B	10.16	178.31	127.53
19	1	1001	CLA	OBD-CAD-C3D	-10.15	104.69	128.42
19	A	9013	CLA	CBB-CAB-C3B	10.10	178.00	127.53
19	1	1006	CLA	OBD-CAD-C3D	-10.10	104.81	128.42
19	L	1501	CLA	CBB-CAB-C3B	10.08	177.89	127.53
19	L	1130	CLA	CBB-CAB-C3B	10.08	177.86	127.53
19	2	2013	CLA	OBD-CAD-C3D	-10.03	104.98	128.42
19	A	1141	CLA	CBB-CAB-C3B	10.02	177.61	127.53
19	4	4014	CLA	CBB-CAB-C3B	10.02	177.61	127.53
19	B	1228	CLA	CBB-CAB-C3B	10.02	177.59	127.53
19	B	1222	CLA	CBB-CAB-C3B	10.01	177.56	127.53
21	B	6020	BCR	C21-C20-C19	10.00	152.19	123.20
19	L	1148	CLA	OBD-CAD-C3D	-9.98	105.08	128.42
19	H	1145	CLA	CBB-CAB-C3B	9.97	177.33	127.53
19	4	4015	CLA	CBB-CAB-C3B	9.97	177.33	127.53
19	B	1206	CLA	OBD-CAD-C3D	-9.97	105.12	128.42
19	A	1126	CLA	OBD-CAD-C3D	-9.95	105.17	128.42
19	4	1004	CLA	OBD-CAD-C3D	-9.94	105.18	128.42
19	B	1220	CLA	OBD-CAD-C3D	-9.91	105.25	128.42
19	B	1219	CLA	CBB-CAB-C3B	9.91	177.03	127.53
19	A	1105	CLA	CBB-CAB-C3B	9.91	177.02	127.53
19	B	1220	CLA	CBB-CAB-C3B	9.88	176.87	127.53
19	J	1311	CLA	CBB-CAB-C3B	9.88	176.87	127.53
19	A	1106	CLA	OBD-CAD-C3D	-9.87	105.34	128.42
19	B	1232	CLA	CBB-CAB-C3B	9.86	176.81	127.53
19	B	1229	CLA	CBB-CAB-C3B	9.86	176.78	127.53
19	B	1230	CLA	OBD-CAD-C3D	-9.86	105.37	128.42
19	A	1136	CLA	CBB-CAB-C3B	9.83	176.63	127.53
19	3	1147	CLA	CBB-CAB-C3B	9.83	176.63	127.53
19	B	1234	CLA	CBB-CAB-C3B	9.82	176.58	127.53
19	3	3011	CLA	CBB-CAB-C3B	9.81	176.52	127.53
19	1	1003	CLA	CBB-CAB-C3B	9.80	176.50	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	F	6016	BCR	C21-C20-C19	9.76	151.49	123.20
19	F	1302	CLA	CBB-CAB-C3B	9.76	176.27	127.53
19	B	1203	CLA	CBB-CAB-C3B	9.75	176.25	127.53
21	3	6022	BCR	C10-C11-C12	9.75	151.45	123.20
21	1	6023	BCR	C24-C23-C22	-9.72	111.85	126.23
19	A	1116	CLA	CBB-CAB-C3B	9.72	176.08	127.53
19	2	2006	CLA	CBB-CAB-C3B	9.72	176.08	127.53
19	L	1502	CLA	CBB-CAB-C3B	9.72	176.08	127.53
19	3	1118	CLA	OBD-CAD-C3D	-9.69	105.76	128.42
19	B	1216	CLA	CBB-CAB-C3B	9.68	175.88	127.53
19	A	1131	CLA	CBB-CAB-C3B	9.68	175.87	127.53
21	A	6003	BCR	C10-C11-C12	9.67	151.22	123.20
19	4	4002	CLA	OBD-CAD-C3D	-9.66	105.85	128.42
19	A	1134	CLA	OBD-CAD-C3D	-9.64	105.87	128.42
19	B	1232	CLA	OBD-CAD-C3D	-9.64	105.89	128.42
19	B	1205	CLA	CBB-CAB-C3B	9.63	175.66	127.53
19	B	1221	CLA	CBB-CAB-C3B	9.62	175.59	127.53
19	A	1122	CLA	OBD-CAD-C3D	-9.58	106.03	128.42
19	1	1005	CLA	CBB-CAB-C3B	9.58	175.38	127.53
21	A	6008	BCR	C21-C20-C19	9.57	150.92	123.20
19	A	9012	CLA	CBB-CAB-C3B	9.56	175.30	127.53
19	A	1140	CLA	CBB-CAB-C3B	9.56	175.28	127.53
19	A	1122	CLA	CBB-CAB-C3B	9.56	175.27	127.53
19	3	3007	CLA	CBB-CAB-C3B	9.54	175.19	127.53
19	3	3013	CLA	CBB-CAB-C3B	9.54	175.18	127.53
19	4	4001	CLA	OBD-CAD-C3D	-9.51	106.19	128.42
19	A	1138	CLA	CBB-CAB-C3B	9.48	174.90	127.53
19	R	1150	CLA	CBB-CAB-C3B	9.48	174.88	127.53
19	K	1146	CLA	CBB-CAB-C3B	9.46	174.78	127.53
19	H	1505	CLA	CBB-CAB-C3B	9.46	174.77	127.53
19	A	9023	CLA	CBB-CAB-C3B	9.45	174.76	127.53
19	B	1209	CLA	OBD-CAD-C3D	-9.41	106.41	128.42
19	A	9013	CLA	OBD-CAD-C3D	-9.40	106.43	128.42
19	3	3016	CLA	OBD-CAD-C3D	-9.40	106.45	128.42
19	B	1231	CLA	OBD-CAD-C3D	-9.37	106.52	128.42
19	H	1207	CLA	CBB-CAB-C3B	9.36	174.27	127.53
19	A	1104	CLA	CBB-CAB-C3B	9.35	174.25	127.53
19	A	1120	CLA	OBD-CAD-C3D	-9.35	106.56	128.42
19	F	1305	CLA	OBD-CAD-C3D	-9.35	106.57	128.42
19	B	1239	CLA	CBB-CAB-C3B	9.34	174.18	127.53
21	A	6011	BCR	C10-C11-C12	9.34	150.25	123.20
19	L	1503	CLA	O2D-CGD-CBD	9.32	127.53	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1237	CLA	CBB-CAB-C3B	9.31	174.05	127.53
19	A	1133	CLA	CBB-CAB-C3B	9.31	174.03	127.53
19	2	2014	CLA	OBD-CAD-C3D	-9.31	106.67	128.42
19	A	1108	CLA	OBD-CAD-C3D	-9.30	106.68	128.42
19	4	4003	CLA	CBB-CAB-C3B	9.29	173.93	127.53
19	B	1217	CLA	CBB-CAB-C3B	9.28	173.90	127.53
19	A	1132	CLA	CBB-CAB-C3B	9.28	173.88	127.53
19	2	2014	CLA	CBB-CAB-C3B	9.27	173.84	127.53
19	1	1303	CLA	CBB-CAB-C3B	9.26	173.81	127.53
19	3	3008	CLA	OBD-CAD-C3D	-9.26	106.77	128.42
21	B	6017	BCR	C21-C20-C19	9.26	150.03	123.20
19	1	1014	CLA	OBD-CAD-C3D	-9.23	106.83	128.42
19	1	1013	CLA	CMD-C2D-C1D	9.23	140.98	124.73
19	4	1304	CLA	OBD-CAD-C3D	-9.23	106.84	128.42
19	1	1008	CLA	CBB-CAB-C3B	9.23	173.63	127.53
19	A	1139	CLA	CBB-CAB-C3B	9.21	173.55	127.53
19	A	1103	CLA	OBD-CAD-C3D	-9.20	106.90	128.42
19	A	1115	CLA	CBB-CAB-C3B	9.20	173.51	127.53
19	A	1116	CLA	OBD-CAD-C3D	-9.20	106.92	128.42
21	I	6018	BCR	C21-C20-C19	9.19	149.84	123.20
19	4	4006	CLA	CBB-CAB-C3B	9.19	173.45	127.53
19	B	1215	CLA	CBB-CAB-C3B	9.18	173.41	127.53
19	K	1142	CLA	CBB-CAB-C3B	9.16	173.32	127.53
19	3	3016	CLA	CBB-CAB-C3B	9.16	173.29	127.53
19	A	1131	CLA	OBD-CAD-C3D	-9.16	107.02	128.42
19	4	1009	CLA	OBD-CAD-C3D	-9.15	107.03	128.42
19	4	4012	CLA	OBD-CAD-C3D	-9.14	107.04	128.42
19	A	1104	CLA	OBD-CAD-C3D	-9.14	107.06	128.42
19	B	1208	CLA	CAB-C3B-C4B	-9.13	111.51	125.42
19	3	3003	CLA	CAB-C3B-C4B	-9.11	111.54	125.42
19	A	1139	CLA	OBD-CAD-C3D	-9.11	107.13	128.42
19	B	1229	CLA	CAA-C2A-C3A	-9.11	88.39	113.00
19	G	1242	CLA	CBB-CAB-C3B	9.09	172.92	127.53
19	A	1115	CLA	OBD-CAD-C3D	-9.09	107.18	128.42
19	R	1144	CLA	OBD-CAD-C3D	-9.09	107.18	128.42
19	B	1202	CLA	CBB-CAB-C3B	9.08	172.91	127.53
19	A	1124	CLA	OBD-CAD-C3D	-9.08	107.20	128.42
19	1	1001	CLA	CBB-CAB-C3B	9.07	172.85	127.53
19	A	1125	CLA	OBD-CAD-C3D	-9.07	107.22	128.42
19	A	1149	CLA	C4D-C3D-CAD	9.06	117.95	108.11
19	3	2009	CLA	CBB-CAB-C3B	9.05	172.73	127.53
19	2	4009	CLA	CBB-CAB-C3B	9.04	172.69	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1010	CLA	OBD-CAD-C3D	-9.01	107.36	128.42
19	4	1304	CLA	CBB-CAB-C3B	9.01	172.52	127.53
19	3	2009	CLA	OBD-CAD-C3D	-8.99	107.39	128.42
19	1	1011	CLA	OBD-CAD-C3D	-8.99	107.40	128.42
21	B	6020	BCR	C15-C14-C13	-8.99	114.67	127.28
19	1	1003	CLA	OBD-CAD-C3D	-8.99	107.42	128.42
19	A	1129	CLA	CBB-CAB-C3B	8.97	172.36	127.53
19	2	2001	CLA	CBB-CAB-C3B	8.96	172.31	127.53
21	F	6014	BCR	C10-C11-C12	8.96	149.16	123.20
19	F	1302	CLA	OBD-CAD-C3D	-8.96	107.48	128.42
19	A	1119	CLA	CBB-CAB-C3B	8.96	172.28	127.53
21	A	6003	BCR	C24-C23-C22	-8.96	112.99	126.23
19	R	1144	CLA	CBB-CAB-C3B	8.95	172.22	127.53
19	B	1233	CLA	CBB-CAB-C3B	8.94	172.21	127.53
19	2	2002	CLA	CBB-CAB-C3B	8.91	172.06	127.53
19	A	1120	CLA	CBB-CAB-C3B	8.89	171.94	127.53
19	4	4002	CLA	CBB-CAB-C3B	8.86	171.81	127.53
19	B	1228	CLA	OBD-CAD-C3D	-8.84	107.75	128.42
19	B	1214	CLA	CBB-CAB-C3B	8.83	171.63	127.53
19	A	1141	CLA	OBD-CAD-C3D	-8.82	107.79	128.42
19	J	1311	CLA	OBD-CAD-C3D	-8.81	107.82	128.42
21	I	6021	BCR	C16-C15-C14	-8.81	105.50	123.52
19	B	1218	CLA	CBB-CAB-C3B	8.81	171.52	127.53
19	B	9010	CLA	OBD-CAD-C3D	-8.79	107.87	128.42
19	A	1101	CLA	O2D-CGD-CBD	8.76	126.55	111.23
19	B	1216	CLA	OBD-CAD-C3D	-8.75	107.95	128.42
19	K	1142	CLA	OBD-CAD-C3D	-8.75	107.97	128.42
19	3	3007	CLA	OBD-CAD-C3D	-8.74	107.98	128.42
19	A	9022	CLA	CBB-CAB-C3B	8.74	171.17	127.53
19	K	1146	CLA	OBD-CAD-C3D	-8.74	108.00	128.42
19	B	1202	CLA	OBD-CAD-C3D	-8.72	108.04	128.42
19	A	9022	CLA	OBD-CAD-C3D	-8.71	108.06	128.42
19	K	1143	CLA	OBD-CAD-C3D	-8.70	108.08	128.42
19	B	1222	CLA	OBD-CAD-C3D	-8.68	108.12	128.42
19	1	1001	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	4	4001	CLA	CBB-CAB-C3B	8.68	170.88	127.53
19	A	1124	CLA	CBB-CAB-C3B	8.67	170.83	127.53
22	H	7011	LMU	C1B-O1B-C4'	-8.66	97.46	117.98
19	A	1101	CLA	OBD-CAD-C3D	-8.65	108.20	128.42
19	A	1113	CLA	CBB-CAB-C3B	8.64	170.69	127.53
19	A	1113	CLA	OBD-CAD-C3D	-8.63	108.25	128.42
19	A	9012	CLA	OBD-CAD-C3D	-8.62	108.27	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	2004	CLA	CBB-CAB-C3B	8.60	170.51	127.53
19	3	3003	CLA	OBD-CAD-C3D	-8.60	108.32	128.42
19	A	1151	CLA	CBB-CAB-C3B	8.60	170.48	127.53
19	2	2012	CLA	OBD-CAD-C3D	-8.59	108.34	128.42
21	I	6021	BCR	C30-C25-C26	-8.53	110.98	122.64
19	1	1010	CLA	CBB-CAB-C3B	8.53	170.14	127.53
19	A	1136	CLA	OBD-CAD-C3D	-8.52	108.50	128.42
19	B	1212	CLA	CBB-CAB-C3B	8.51	170.02	127.53
19	B	1211	CLA	CBB-CAB-C3B	8.49	169.94	127.53
19	A	1111	CLA	CBB-CAB-C3B	8.46	169.82	127.53
19	A	1137	CLA	OBD-CAD-C3D	-8.46	108.64	128.42
19	1	1013	CLA	CBB-CAB-C3B	8.44	169.71	127.53
19	H	1241	CLA	OBD-CAD-C3D	-8.44	108.69	128.42
19	B	1229	CLA	OBD-CAD-C3D	-8.44	108.69	128.42
19	B	1210	CLA	CBB-CAB-C3B	8.43	169.64	127.53
19	2	2013	CLA	CBB-CAB-C3B	8.43	169.62	127.53
21	L	6019	BCR	C10-C11-C12	8.42	147.60	123.20
21	J	6012	BCR	C10-C11-C12	8.37	147.45	123.20
21	B	6005	BCR	C10-C11-C12	8.37	147.44	123.20
19	L	1148	CLA	CBB-CAB-C3B	8.37	169.33	127.53
19	A	1105	CLA	OBD-CAD-C3D	-8.35	108.89	128.42
19	A	9011	CLA	CBB-CAB-C3B	8.35	169.23	127.53
19	A	1103	CLA	CBB-CAB-C3B	8.34	169.22	127.53
19	B	1227	CLA	CBB-CAB-C3B	8.33	169.15	127.53
19	L	1504	CLA	CBB-CAB-C3B	8.33	169.15	127.53
19	B	1227	CLA	OBD-CAD-C3D	-8.32	108.97	128.42
19	A	1121	CLA	CBB-CAB-C3B	8.31	169.03	127.53
19	B	1206	CLA	CBB-CAB-C3B	8.29	168.93	127.53
19	B	1217	CLA	OBD-CAD-C3D	-8.28	109.05	128.42
19	H	1505	CLA	OBD-CAD-C3D	-8.27	109.09	128.42
19	1	1007	CLA	CBB-CAB-C3B	8.23	168.64	127.53
19	A	1123	CLA	CBB-CAB-C3B	8.22	168.62	127.53
21	A	6007	BCR	C10-C11-C12	8.22	147.02	123.20
19	B	1203	CLA	OBD-CAD-C3D	-8.22	109.21	128.42
19	B	1231	CLA	CBB-CAB-C3B	8.21	168.56	127.53
19	B	1215	CLA	OBD-CAD-C3D	-8.21	109.22	128.42
19	A	1133	CLA	OBD-CAD-C3D	-8.20	109.24	128.42
19	K	1143	CLA	CBB-CAB-C3B	8.17	168.35	127.53
19	H	1241	CLA	CBB-CAB-C3B	8.17	168.32	127.53
19	1	1014	CLA	CBB-CAB-C3B	8.16	168.30	127.53
19	2	2001	CLA	OBD-CAD-C3D	-8.15	109.36	128.42
19	A	1127	CLA	O2D-CGD-CBD	8.15	125.48	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	J	1308	CLA	OBD-CAD-C3D	-8.15	109.38	128.42
19	A	1135	CLA	CBB-CAB-C3B	8.14	168.21	127.53
19	B	1225	CLA	CBB-CAB-C3B	8.14	168.18	127.53
19	A	1140	CLA	OBD-CAD-C3D	-8.13	109.42	128.42
19	B	1223	CLA	OBD-CAD-C3D	-8.13	109.42	128.42
19	A	1110	CLA	CBB-CAB-C3B	8.11	168.05	127.53
19	A	1109	CLA	CBB-CAB-C3B	8.11	168.04	127.53
19	1	1008	CLA	C3A-C2A-C1A	8.10	113.48	101.34
19	L	1502	CLA	OBD-CAD-C3D	-8.10	109.50	128.42
19	4	1306	CLA	CBB-CAB-C3B	8.08	167.91	127.53
19	A	1135	CLA	OBD-CAD-C3D	-8.08	109.52	128.42
19	4	4003	CLA	OBD-CAD-C3D	-8.06	109.57	128.42
19	B	1223	CLA	CBB-CAB-C3B	8.06	167.80	127.53
19	B	1224	CLA	CBB-CAB-C3B	8.06	167.80	127.53
19	A	1127	CLA	OBD-CAD-C3D	-8.06	109.58	128.42
19	B	1238	CLA	CBB-CAB-C3B	8.05	167.73	127.53
19	B	1219	CLA	OBD-CAD-C3D	-8.04	109.61	128.42
19	B	1212	CLA	OBD-CAD-C3D	-8.04	109.63	128.42
21	I	6021	BCR	C21-C20-C19	8.04	146.49	123.20
19	4	4007	CLA	OBD-CAD-C3D	-8.00	109.72	128.42
19	B	1205	CLA	O2D-CGD-CBD	7.99	125.20	111.23
19	B	1201	CLA	CBB-CAB-C3B	7.96	167.31	127.53
19	B	1225	CLA	O2D-CGD-CBD	7.94	125.12	111.23
21	A	6007	BCR	C24-C23-C22	-7.94	114.49	126.23
19	A	1138	CLA	OBD-CAD-C3D	-7.92	109.91	128.42
19	2	2007	CLA	OBD-CAD-C3D	-7.90	109.94	128.42
19	B	1213	CLA	OBD-CAD-C3D	-7.88	110.00	128.42
21	1	6023	BCR	C30-C25-C26	-7.85	111.91	122.64
19	B	1236	CLA	OBD-CAD-C3D	-7.85	110.07	128.42
19	L	1501	CLA	OBD-CAD-C3D	-7.84	110.09	128.42
21	B	6006	BCR	C10-C11-C12	7.84	145.91	123.20
19	4	1306	CLA	OBD-CAD-C3D	-7.79	110.22	128.42
21	3	6022	BCR	C16-C17-C18	-7.78	116.37	127.28
19	A	1117	CLA	CBB-CAB-C3B	7.77	166.35	127.53
21	A	6008	BCR	C10-C11-C12	7.76	145.68	123.20
19	B	1201	CLA	OBD-CAD-C3D	-7.72	110.37	128.42
19	A	1132	CLA	OBD-CAD-C3D	-7.71	110.39	128.42
21	B	6010	BCR	C10-C11-C12	7.67	145.43	123.20
21	B	6006	BCR	C24-C23-C22	-7.67	114.89	126.23
19	A	1125	CLA	CBB-CAB-C3B	7.64	165.71	127.53
19	G	1242	CLA	OBD-CAD-C3D	-7.62	110.60	128.42
21	F	6016	BCR	C11-C10-C9	7.61	137.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1213	CLA	CBB-CAB-C3B	7.60	165.48	127.53
19	2	2002	CLA	OBD-CAD-C3D	-7.59	110.67	128.42
19	1	1011	CLA	CMD-C2D-C1D	7.57	138.05	124.73
21	B	6020	BCR	C3-C4-C5	-7.54	100.61	114.06
19	2	2004	CLA	OBD-CAD-C3D	-7.54	110.79	128.42
19	B	1211	CLA	CMD-C2D-C1D	7.52	137.97	124.73
19	3	3008	CLA	CMD-C2D-C1D	7.51	137.96	124.73
19	1	1008	CLA	CMD-C2D-C1D	7.50	137.93	124.73
19	A	1102	CLA	CBB-CAB-C3B	7.49	164.97	127.53
19	A	1149	CLA	CMD-C2D-C1D	7.48	137.91	124.73
19	L	1148	CLA	CMD-C2D-C1D	7.48	137.90	124.73
19	B	1226	CLA	OBD-CAD-C3D	-7.48	110.94	128.42
21	1	6023	BCR	C21-C20-C19	7.45	144.78	123.20
19	H	1145	CLA	C4D-C3D-CAD	7.44	116.19	108.11
19	A	1121	CLA	OBD-CAD-C3D	-7.44	111.03	128.42
19	3	3017	CLA	CBB-CAB-C3B	7.44	164.69	127.53
19	1	1005	CLA	O2D-CGD-CBD	7.42	124.20	111.23
19	B	1238	CLA	CMD-C2D-C1D	7.41	137.78	124.73
19	1	1011	CLA	CAB-C3B-C2B	-7.37	103.95	123.53
19	3	3017	CLA	O2D-CGD-CBD	7.37	124.12	111.23
19	A	1110	CLA	OBD-CAD-C3D	-7.37	111.19	128.42
19	1	1006	CLA	CAB-C3B-C4B	-7.37	114.20	125.42
19	B	1226	CLA	O2D-CGD-CBD	7.36	124.10	111.23
19	B	1301	CLA	OBD-CAD-C3D	-7.36	111.21	128.42
19	B	1234	CLA	CMD-C2D-C1D	7.34	137.66	124.73
19	A	1101	CLA	CBB-CAB-C3B	7.34	164.19	127.53
19	4	1304	CLA	CGD-CBD-CAD	7.34	134.60	110.85
19	A	1126	CLA	CBB-CAB-C3B	7.34	164.18	127.53
19	1	1008	CLA	OBD-CAD-C3D	-7.32	111.31	128.42
19	R	1144	CLA	CMD-C2D-C1D	7.31	137.61	124.73
19	A	1112	CLA	OBD-CAD-C3D	-7.31	111.33	128.42
19	A	1151	CLA	OBD-CAD-C3D	-7.30	111.35	128.42
19	A	9011	CLA	C4D-C3D-CAD	7.29	116.03	108.11
19	H	1505	CLA	CMD-C2D-C1D	7.29	137.57	124.73
19	1	1013	CLA	C4D-C3D-CAD	7.27	116.00	108.11
19	1	1003	CLA	CMD-C2D-C1D	7.27	137.53	124.73
19	B	1236	CLA	CBB-CAB-C3B	7.25	163.73	127.53
19	A	1112	CLA	CBB-CAB-C3B	7.24	163.68	127.53
19	2	2007	CLA	O2D-CGD-CBD	7.22	123.86	111.23
19	A	1127	CLA	CBB-CAB-C3B	7.21	163.56	127.53
19	A	1109	CLA	CMD-C2D-C1D	7.21	137.43	124.73
19	B	1209	CLA	CBB-CAB-C3B	7.21	163.54	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1226	CLA	CMD-C2D-C1D	7.21	137.42	124.73
22	G	7051	LMU	O1B-C4'-C3'	7.19	125.51	107.23
19	2	2007	CLA	CBB-CAB-C3B	7.17	163.35	127.53
19	3	3011	CLA	OBD-CAD-C3D	-7.16	111.68	128.42
21	B	6004	BCR	C10-C11-C12	7.16	143.95	123.20
19	B	1218	CLA	CMD-C2D-C1D	7.16	137.33	124.73
19	A	1107	CLA	OBD-CAD-C3D	-7.16	111.69	128.42
19	3	3013	CLA	O2D-CGD-CBD	7.15	123.74	111.23
19	R	1150	CLA	CMD-C2D-C1D	7.14	137.30	124.73
19	2	2002	CLA	CMD-C2D-C1D	7.13	137.29	124.73
19	L	1148	CLA	O2D-CGD-CBD	7.11	123.67	111.23
19	L	1148	CLA	C1-C2-C3	-7.10	114.56	126.20
19	B	1238	CLA	OBD-CAD-C3D	-7.09	111.85	128.42
21	I	6018	BCR	C40-C30-C25	7.08	121.35	110.24
19	1	1003	CLA	C4D-C3D-CAD	7.08	115.79	108.11
19	B	1210	CLA	OBD-CAD-C3D	-7.07	111.89	128.42
19	1	1007	CLA	OBD-CAD-C3D	-7.06	111.91	128.42
19	1	1001	CLA	C4D-C3D-CAD	7.06	115.78	108.11
19	4	4007	CLA	CBB-CAB-C3B	7.06	162.79	127.53
19	2	2012	CLA	CBB-CAB-C3B	7.05	162.75	127.53
19	A	1132	CLA	CMD-C2D-C1D	7.05	137.14	124.73
19	B	1225	CLA	OBD-CAD-C3D	-7.05	111.95	128.42
19	A	9023	CLA	OBD-CAD-C3D	-7.03	111.99	128.42
19	B	1234	CLA	O2D-CGD-CBD	7.03	123.51	111.23
19	A	1120	CLA	CMD-C2D-C1D	7.03	137.10	124.73
19	B	1201	CLA	O2D-CGD-CBD	7.02	123.50	111.23
19	A	1129	CLA	O2D-CGD-CBD	7.02	123.49	111.23
21	B	6017	BCR	C10-C11-C12	7.01	143.50	123.20
21	A	6007	BCR	C20-C21-C22	6.99	137.09	127.28
19	A	9011	CLA	OBD-CAD-C3D	-6.97	112.12	128.42
21	I	6018	BCR	C3-C4-C5	-6.97	101.63	114.06
19	F	1240	CLA	C1B-C2B-C3B	-6.97	100.48	107.03
19	L	1501	CLA	O2D-CGD-CBD	6.96	123.40	111.23
19	3	1147	CLA	C4D-C3D-CAD	6.96	115.66	108.11
19	4	1304	CLA	CMD-C2D-C1D	6.96	136.98	124.73
19	B	1226	CLA	C4D-C3D-CAD	6.95	115.66	108.11
21	F	6016	BCR	C15-C14-C13	-6.95	117.53	127.28
19	4	1306	CLA	O2D-CGD-CBD	6.95	123.37	111.23
19	4	1009	CLA	C1D-CHD-C4C	-6.94	111.26	126.02
19	B	1239	CLA	OBD-CAD-C3D	-6.93	112.21	128.42
19	1	1002	CLA	CBB-CAB-C3B	6.91	162.06	127.53
19	4	4014	CLA	CMD-C2D-C1D	6.90	136.87	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	3009	CLA	OBD-CAD-C3D	-6.89	112.31	128.42
19	A	1111	CLA	OBD-CAD-C3D	-6.88	112.33	128.42
19	A	1128	CLA	O2D-CGD-CBD	6.87	123.25	111.23
19	A	1107	CLA	CBB-CAB-C3B	6.87	161.84	127.53
19	L	1148	CLA	C1D-CHD-C4C	-6.86	111.45	126.02
19	B	1235	CLA	O2D-CGD-CBD	6.84	123.18	111.23
19	B	1216	CLA	O2D-CGD-CBD	6.82	123.16	111.23
19	4	4015	CLA	O2D-CGD-CBD	6.82	123.15	111.23
19	3	3008	CLA	C4D-C3D-CAD	6.82	115.51	108.11
19	4	4006	CLA	OBD-CAD-C3D	-6.82	112.48	128.42
19	1	1008	CLA	C4D-C3D-CAD	6.82	115.51	108.11
19	B	1202	CLA	CAA-C2A-C3A	-6.82	94.58	113.00
19	A	1132	CLA	O2D-CGD-CBD	6.79	123.10	111.23
19	A	1151	CLA	CMD-C2D-C1D	6.79	136.68	124.73
19	R	1144	CLA	C4D-C3D-CAD	6.78	115.47	108.11
19	4	1304	CLA	C1D-CHD-C4C	-6.78	111.60	126.02
19	B	9010	CLA	CBB-CAB-C3B	6.78	161.42	127.53
19	A	1149	CLA	O2D-CGD-CBD	6.78	123.09	111.23
19	4	4002	CLA	C1D-CHD-C4C	-6.78	111.62	126.02
19	A	1123	CLA	OBD-CAD-C3D	-6.77	112.58	128.42
19	3	3017	CLA	C4D-C3D-CAD	6.77	115.46	108.11
19	B	1235	CLA	CBB-CAB-C3B	6.76	161.28	127.53
19	A	1121	CLA	O2D-CGD-CBD	6.76	123.04	111.23
19	B	1233	CLA	CMD-C2D-C1D	6.75	136.62	124.73
19	A	1133	CLA	CMD-C2D-C1D	6.74	136.59	124.73
19	A	1116	CLA	CMD-C2D-C1D	6.73	136.58	124.73
19	F	1240	CLA	CMD-C2D-C1D	6.73	136.57	124.73
19	1	1303	CLA	C1D-CHD-C4C	-6.73	111.72	126.02
19	J	1308	CLA	CMD-C2D-C1D	6.73	136.57	124.73
22	E	7048	LMU	C1B-C2B-C3B	-6.72	95.86	110.01
19	1	1001	CLA	CMD-C2D-C1D	6.72	136.56	124.73
19	F	1302	CLA	CMD-C2D-C1D	6.72	136.56	124.73
19	B	1208	CLA	CMD-C2D-C1D	6.70	136.53	124.73
22	3	7005	LMU	C2'-C3'-C4'	-6.70	94.48	109.68
19	A	1121	CLA	C4D-C3D-CAD	6.69	115.37	108.11
19	B	1202	CLA	CMD-C2D-C1D	6.68	136.50	124.73
19	L	1504	CLA	O2D-CGD-CBD	6.67	122.88	111.23
19	B	1235	CLA	OBD-CAD-C3D	-6.67	112.84	128.42
19	4	4002	CLA	CHD-C4C-NC	6.66	134.56	124.23
21	I	6021	BCR	C2-C1-C6	-6.63	100.81	110.44
19	1	1011	CLA	C4D-C3D-CAD	6.61	115.29	108.11
19	3	3007	CLA	CMD-C2D-C1D	6.61	136.37	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	1004	CLA	CMD-C2D-C1D	6.61	136.37	124.73
19	B	1214	CLA	OBD-CAD-C3D	-6.60	112.98	128.42
19	3	3017	CLA	CMD-C2D-C1D	6.60	136.35	124.73
19	B	1224	CLA	O2D-CGD-CBD	6.59	122.75	111.23
21	I	6021	BCR	C16-C17-C18	-6.59	118.04	127.28
19	B	1231	CLA	C4D-C3D-CAD	6.59	115.26	108.11
19	B	1218	CLA	C4D-C3D-CAD	6.59	115.26	108.11
19	A	1119	CLA	CMD-C2D-C1D	6.58	136.32	124.73
19	A	1109	CLA	C3B-C2B-C1B	-6.58	99.41	107.17
19	1	1303	CLA	O2D-CGD-CBD	6.58	122.73	111.23
19	3	1147	CLA	C1D-CHD-C4C	-6.57	112.06	126.02
19	B	1222	CLA	CMD-C2D-C1D	6.56	136.28	124.73
22	H	7002	LMU	O1B-C4'-C3'	6.56	123.90	107.23
19	F	1305	CLA	CBB-CAB-C3B	6.56	160.28	127.53
19	B	1217	CLA	CMD-C2D-C1D	6.55	136.27	124.73
19	B	1217	CLA	C4D-C3D-CAD	6.53	115.20	108.11
19	B	1224	CLA	CMD-C2D-C1D	6.53	136.23	124.73
21	A	6011	BCR	C15-C14-C13	-6.53	118.12	127.28
19	H	1145	CLA	CMD-C2D-C1D	6.53	136.22	124.73
19	H	1241	CLA	O2D-CGD-CBD	6.53	122.64	111.23
21	A	6003	BCR	C32-C1-C6	-6.53	100.01	110.24
19	4	4015	CLA	OBD-CAD-C3D	-6.52	113.18	128.42
19	B	1201	CLA	CMD-C2D-C1D	6.52	136.21	124.73
19	A	1108	CLA	O2D-CGD-CBD	6.51	122.62	111.23
19	L	1504	CLA	OBD-CAD-C3D	-6.51	113.20	128.42
22	E	7048	LMU	C3B-C4B-C5B	6.51	122.03	110.23
19	1	1005	CLA	CMD-C2D-C1D	6.50	136.18	124.73
22	R	7014	LMU	C4B-C3B-C2B	-6.50	99.42	110.83
19	H	1207	CLA	C3B-C2B-C1B	-6.50	99.51	107.17
19	B	1226	CLA	CBB-CAB-C3B	6.50	159.99	127.53
19	3	2009	CLA	C4D-C3D-CAD	6.49	115.15	108.11
19	B	1213	CLA	CMD-C2D-C1D	6.48	136.14	124.73
19	J	1311	CLA	O2D-CGD-CBD	6.47	122.53	111.23
19	L	1502	CLA	CAA-C2A-C3A	-6.46	95.54	113.00
19	A	1117	CLA	OBD-CAD-C3D	-6.45	113.33	128.42
19	B	1225	CLA	C4A-NA-C1A	6.45	109.62	106.68
19	A	1122	CLA	C4D-C3D-CAD	6.44	115.10	108.11
19	B	1234	CLA	C4D-C3D-CAD	6.43	115.08	108.11
19	A	1121	CLA	CMD-C2D-C1D	6.42	136.03	124.73
19	B	1221	CLA	O2D-CGD-CBD	6.40	122.43	111.23
19	A	1138	CLA	CMD-C2D-C1D	6.40	136.00	124.73
19	B	1203	CLA	O2D-CGD-CBD	6.40	122.42	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L	1130	CLA	OBD-CAD-C3D	-6.40	113.46	128.42
19	A	1134	CLA	CMD-C2D-C1D	6.40	135.99	124.73
19	A	1102	CLA	C3B-C2B-C1B	-6.39	99.63	107.17
19	A	1124	CLA	CMD-C2D-C1D	6.39	135.98	124.73
19	1	1010	CLA	CMD-C2D-C1D	6.38	135.97	124.73
21	B	6006	BCR	C16-C17-C18	-6.38	118.33	127.28
19	A	1141	CLA	CMD-C2D-C1D	6.37	135.95	124.73
19	K	1146	CLA	CMD-C2D-C1D	6.37	135.95	124.73
19	1	1013	CLA	C1D-CHD-C4C	-6.36	112.50	126.02
19	2	2014	CLA	C1D-CHD-C4C	-6.36	112.50	126.02
21	A	6007	BCR	C16-C17-C18	-6.36	118.36	127.28
19	4	1304	CLA	C4D-CHA-C1A	6.35	128.82	121.24
19	B	1230	CLA	C4D-C3D-CAD	6.35	115.00	108.11
19	4	1306	CLA	C4D-C3D-CAD	6.35	115.00	108.11
19	1	1003	CLA	O2D-CGD-CBD	6.34	122.32	111.23
19	B	1230	CLA	O2D-CGD-CBD	6.34	122.31	111.23
19	B	1236	CLA	O2D-CGD-CBD	6.34	122.31	111.23
19	A	1139	CLA	CMD-C2D-C1D	6.33	135.88	124.73
19	A	1109	CLA	OBD-CAD-C3D	-6.33	113.62	128.42
19	L	1503	CLA	C1D-CHD-C4C	-6.33	112.57	126.02
19	2	2012	CLA	C4D-C3D-CAD	6.32	114.97	108.11
19	4	1304	CLA	CHD-C4C-NC	6.32	134.03	124.23
19	G	1242	CLA	CMD-C2D-C1D	6.32	135.86	124.73
19	3	1118	CLA	CMD-C2D-C1D	6.32	135.85	124.73
19	4	4012	CLA	C4D-C3D-CAD	6.32	114.97	108.11
19	4	4003	CLA	CMD-C2D-C1D	6.31	135.85	124.73
19	B	1229	CLA	O2D-CGD-CBD	6.31	122.26	111.23
19	3	3013	CLA	C1D-CHD-C4C	-6.31	112.62	126.02
19	K	1143	CLA	CMD-C2D-C1D	6.30	135.83	124.73
19	A	1126	CLA	CMD-C2D-C1D	6.30	135.82	124.73
19	1	1002	CLA	CMD-C2D-C1D	6.30	135.82	124.73
19	2	2001	CLA	CMD-C2D-C1D	6.30	135.82	124.73
19	A	1116	CLA	C4D-C3D-CAD	6.30	114.95	108.11
19	B	1202	CLA	O2D-CGD-CBD	6.30	122.24	111.23
19	B	1235	CLA	CMD-C2D-C1D	6.28	135.79	124.73
19	B	1228	CLA	O2D-CGD-CBD	6.28	122.21	111.23
22	H	7017	LMU	C1B-O1B-C4'	-6.26	103.13	117.98
19	3	3013	CLA	CMD-C2D-C1D	6.26	135.75	124.73
19	J	1311	CLA	CMD-C2D-C1D	6.26	135.75	124.73
19	A	1107	CLA	CMD-C2D-C1D	6.26	135.75	124.73
19	B	1219	CLA	CMD-C2D-C1D	6.26	135.75	124.73
19	A	1102	CLA	CMD-C2D-C1D	6.25	135.74	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	2009	CLA	CMD-C2D-C1D	6.25	135.74	124.73
19	L	1502	CLA	CMD-C2D-C1D	6.25	135.73	124.73
19	4	1306	CLA	CMD-C2D-C1D	6.24	135.72	124.73
19	A	1123	CLA	CMD-C2D-C1D	6.24	135.72	124.73
19	1	1012	CLA	CAB-C3B-C2B	-6.24	106.96	123.53
19	B	1209	CLA	CMD-C2D-C1D	6.24	135.71	124.73
19	3	3004	CLA	C4A-NA-C1A	6.23	109.52	106.68
19	4	1009	CLA	C4D-C3D-CAD	6.23	114.87	108.11
19	B	1239	CLA	C4D-C3D-CAD	6.23	114.87	108.11
19	1	1010	CLA	C1D-CHD-C4C	-6.22	112.79	126.02
19	1	1006	CLA	CMD-C2D-C1D	6.22	135.68	124.73
19	4	4015	CLA	C1D-CHD-C4C	-6.22	112.81	126.02
19	4	4006	CLA	C4D-C3D-CAD	6.21	114.85	108.11
19	B	1209	CLA	C4D-C3D-CAD	6.21	114.85	108.11
19	1	1006	CLA	C4D-C3D-CAD	6.21	114.85	108.11
19	L	1130	CLA	CMD-C2D-C1D	6.20	135.64	124.73
19	K	1146	CLA	C4D-C3D-CAD	6.20	114.83	108.11
19	F	1302	CLA	C4D-C3D-CAD	6.19	114.82	108.11
19	A	1149	CLA	CAA-C2A-C3A	6.18	129.71	113.00
19	1	1014	CLA	C1D-CHD-C4C	-6.18	112.89	126.02
19	A	1135	CLA	CMD-C2D-C1D	6.18	135.60	124.73
19	2	2012	CLA	CMD-C2D-C1D	6.18	135.60	124.73
19	1	1013	CLA	CHD-C4C-NC	6.17	133.80	124.23
19	2	4009	CLA	O2D-CGD-CBD	6.17	122.01	111.23
19	B	1208	CLA	O2D-CGD-CBD	6.16	122.00	111.23
19	1	1007	CLA	C4D-C3D-CAD	6.16	114.79	108.11
19	1	1303	CLA	CAA-C2A-C1A	6.15	132.14	111.97
19	2	2006	CLA	C1D-CHD-C4C	-6.15	112.94	126.02
19	A	1106	CLA	CMD-C2D-C1D	6.15	135.56	124.73
19	L	1504	CLA	CMD-C2D-C1D	6.15	135.56	124.73
19	1	1010	CLA	C4D-C3D-CAD	6.15	114.78	108.11
19	A	1105	CLA	O2D-CGD-CBD	6.15	121.97	111.23
19	A	1108	CLA	CMD-C2D-C1D	6.14	135.53	124.73
19	B	1219	CLA	C4D-C3D-CAD	6.13	114.77	108.11
19	A	9022	CLA	O2D-CGD-CBD	6.13	121.95	111.23
19	L	1502	CLA	O2D-CGD-CBD	6.13	121.95	111.23
19	B	1201	CLA	C4D-C3D-CAD	6.13	114.76	108.11
19	A	1110	CLA	CMD-C2D-C1D	6.13	135.52	124.73
19	A	1101	CLA	CMD-C2D-C1D	6.12	135.51	124.73
22	A	7035	LMU	O1B-C4'-C3'	6.12	122.79	107.23
21	B	6010	BCR	C24-C23-C22	-6.12	117.18	126.23
19	H	1505	CLA	C4D-C3D-CAD	6.12	114.75	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1232	CLA	CMD-C2D-C1D	6.12	135.50	124.73
19	B	1211	CLA	C4D-C3D-CAD	6.11	114.74	108.11
19	A	1131	CLA	C4D-C3D-CAD	6.11	114.74	108.11
19	B	9010	CLA	C4D-C3D-CAD	6.10	114.73	108.11
19	1	1012	CLA	CMD-C2D-C1D	6.10	135.46	124.73
21	B	6005	BCR	C31-C1-C6	-6.09	100.70	110.24
19	B	1210	CLA	C1D-CHD-C4C	-6.09	113.08	126.02
19	B	1221	CLA	C1D-CHD-C4C	-6.09	113.08	126.02
19	A	1112	CLA	O2D-CGD-CBD	6.08	121.86	111.23
19	B	1230	CLA	CMD-C2D-C1D	6.08	135.44	124.73
19	1	1002	CLA	OBD-CAD-C3D	-6.08	114.22	128.42
19	B	1301	CLA	CMD-C2D-C1D	6.07	135.42	124.73
19	A	1136	CLA	CMD-C2D-C1D	6.07	135.42	124.73
19	A	1112	CLA	CMD-C2D-C1D	6.07	135.41	124.73
19	2	2006	CLA	CMD-C2D-C1D	6.06	135.40	124.73
19	1	1001	CLA	C1D-CHD-C4C	-6.06	113.14	126.02
19	A	1104	CLA	CMD-C2D-C1D	6.06	135.40	124.73
19	2	2002	CLA	O2D-CGD-CBD	6.06	121.82	111.23
21	1	6023	BCR	C28-C27-C26	-6.06	103.26	114.06
19	I	1204	CLA	C1D-CHD-C4C	-6.05	113.16	126.02
19	L	1503	CLA	CMD-C2D-C1D	6.04	135.37	124.73
21	1	6023	BCR	C40-C30-C29	-6.04	85.76	108.95
19	A	1149	CLA	CAB-C3B-C2B	-6.04	107.50	123.53
19	3	3013	CLA	CHD-C4C-NC	6.04	133.59	124.23
19	B	1218	CLA	C1D-CHD-C4C	-6.04	113.19	126.02
19	2	2004	CLA	CMD-C2D-C1D	6.03	135.35	124.73
19	K	1142	CLA	C1D-CHD-C4C	-6.03	113.20	126.02
19	1	1014	CLA	O2D-CGD-CBD	6.03	121.77	111.23
19	4	4006	CLA	CMD-C2D-C1D	6.03	135.34	124.73
19	A	1141	CLA	C4D-C3D-CAD	6.03	114.65	108.11
19	A	1137	CLA	CMD-C2D-C1D	6.03	135.34	124.73
19	B	1201	CLA	C2B-C1B-NB	6.02	116.57	110.33
19	B	1202	CLA	C4D-C3D-CAD	6.02	114.65	108.11
19	R	1150	CLA	C4D-C3D-CAD	6.02	114.64	108.11
19	1	1002	CLA	C4D-C3D-CAD	6.01	114.63	108.11
19	K	3009	CLA	O2D-CGD-CBD	6.00	121.72	111.23
19	B	1226	CLA	C1D-CHD-C4C	-6.00	113.27	126.02
19	B	1211	CLA	OBD-CAD-C3D	-6.00	114.40	128.42
19	3	3016	CLA	CMD-C2D-C1D	5.99	135.28	124.73
19	B	1225	CLA	C4D-C3D-CAD	5.99	114.62	108.11
19	4	1004	CLA	C4D-C3D-CAD	5.99	114.61	108.11
19	L	1130	CLA	O2D-CGD-CBD	5.99	121.70	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1301	CLA	CAB-C3B-C2B	-5.99	107.63	123.53
19	B	1232	CLA	C4D-C3D-CAD	5.99	114.61	108.11
19	3	3013	CLA	CHD-C4C-C3C	-5.98	116.05	124.77
19	F	1305	CLA	C1D-CHD-C4C	-5.98	113.32	126.02
19	A	1136	CLA	C4D-C3D-CAD	5.97	114.59	108.11
19	B	1231	CLA	CMD-C2D-C1D	5.97	135.25	124.73
19	A	1109	CLA	C4D-C3D-CAD	5.97	114.59	108.11
19	1	1006	CLA	C1D-CHD-C4C	-5.97	113.33	126.02
19	H	1145	CLA	C2B-C1B-NB	5.97	116.52	110.33
19	4	4007	CLA	C4D-C3D-CAD	5.97	114.59	108.11
19	2	2002	CLA	C4D-C3D-CAD	5.96	114.58	108.11
19	B	1205	CLA	C4D-C3D-CAD	5.96	114.58	108.11
19	1	1010	CLA	CHD-C4C-NC	5.96	133.47	124.23
19	A	1107	CLA	O2D-CGD-CBD	5.95	121.63	111.23
19	B	1231	CLA	C1D-CHD-C4C	-5.95	113.38	126.02
19	B	1229	CLA	CMD-C2D-C1D	5.95	135.20	124.73
19	3	3011	CLA	CMD-C2D-C1D	5.95	135.20	124.73
19	4	4006	CLA	C1D-CHD-C4C	-5.95	113.38	126.02
19	1	1013	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
19	J	1308	CLA	C1D-CHD-C4C	-5.95	113.38	126.02
19	2	2014	CLA	C4D-C3D-CAD	5.94	114.56	108.11
19	3	2009	CLA	C1D-CHD-C4C	-5.94	113.39	126.02
19	1	1010	CLA	CGD-CBD-CAD	-5.94	91.61	110.85
19	3	3007	CLA	C4D-C3D-CAD	5.94	114.56	108.11
19	A	1131	CLA	CMD-C2D-C1D	5.93	135.18	124.73
21	A	6008	BCR	C16-C17-C18	-5.93	118.96	127.28
19	J	1311	CLA	C4D-C3D-CAD	5.93	114.55	108.11
19	1	1011	CLA	C1D-CHD-C4C	-5.93	113.43	126.02
19	B	1206	CLA	C4D-C3D-CAD	5.92	114.54	108.11
19	2	2004	CLA	C4D-C3D-CAD	5.92	114.54	108.11
19	A	1125	CLA	C1D-CHD-C4C	-5.92	113.44	126.02
19	B	1239	CLA	C3B-C2B-C1B	-5.92	100.19	107.17
19	4	1009	CLA	CMD-C2D-C1D	5.91	135.14	124.73
19	A	1139	CLA	C4D-C3D-CAD	5.91	114.53	108.11
19	I	1204	CLA	CMD-C2D-C1D	5.91	135.14	124.73
19	A	9013	CLA	O2D-CGD-CBD	5.91	121.56	111.23
19	1	1008	CLA	O2D-CGD-CBD	5.91	121.56	111.23
19	B	1213	CLA	O2D-CGD-CBD	5.90	121.54	111.23
19	4	4001	CLA	CMD-C2D-C1D	5.90	135.11	124.73
19	1	1013	CLA	C4A-NA-C1A	5.90	109.37	106.68
19	B	1238	CLA	C4D-C3D-CAD	5.89	114.50	108.11
19	4	1304	CLA	CHC-C1C-NC	5.89	133.18	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1109	CLA	C1D-CHD-C4C	-5.89	113.50	126.02
19	3	3016	CLA	C1D-CHD-C4C	-5.88	113.51	126.02
19	A	1137	CLA	C1D-CHD-C4C	-5.88	113.51	126.02
19	A	1120	CLA	C4D-C3D-CAD	5.88	114.50	108.11
19	B	1203	CLA	C1D-CHD-C4C	-5.88	113.52	126.02
19	K	1142	CLA	C4D-C3D-CAD	5.88	114.49	108.11
19	1	1012	CLA	OBD-CAD-C3D	-5.88	114.68	128.42
19	B	1210	CLA	CMD-C2D-C1D	5.88	135.07	124.73
19	A	1140	CLA	CMD-C2D-C1D	5.87	135.07	124.73
19	A	1237	CLA	C4D-C3D-CAD	5.87	114.48	108.11
19	B	1223	CLA	CMD-C2D-C1D	5.87	135.07	124.73
19	B	1233	CLA	C4D-C3D-CAD	5.87	114.48	108.11
19	A	1115	CLA	CMD-C2D-C1D	5.86	135.05	124.73
19	B	1236	CLA	CMD-C2D-C1D	5.86	135.05	124.73
21	A	6007	BCR	C31-C1-C6	-5.86	101.05	110.24
19	H	1207	CLA	CMD-C2D-C1D	5.86	135.05	124.73
19	A	9013	CLA	C4D-C3D-CAD	5.86	114.47	108.11
19	4	4001	CLA	C1D-CHD-C4C	-5.86	113.58	126.02
19	J	1311	CLA	C1D-CHD-C4C	-5.85	113.58	126.02
19	A	9012	CLA	C1D-CHD-C4C	-5.85	113.58	126.02
19	B	1236	CLA	C1D-CHD-C4C	-5.85	113.58	126.02
19	B	1216	CLA	C4D-C3D-CAD	5.84	114.45	108.11
19	R	1150	CLA	OBD-CAD-C3D	-5.84	114.75	128.42
19	A	1106	CLA	CBB-CAB-C3B	5.84	156.72	127.53
19	A	1134	CLA	C4D-C3D-CAD	5.84	114.45	108.11
21	F	6014	BCR	C32-C1-C6	-5.83	101.09	110.24
19	4	4002	CLA	CAA-C2A-C1A	5.83	131.09	111.97
19	B	1223	CLA	C4D-C3D-CAD	5.83	114.44	108.11
19	A	9013	CLA	CMD-C2D-C1D	5.82	134.98	124.73
19	2	2013	CLA	C1D-CHD-C4C	-5.82	113.65	126.02
19	1	1014	CLA	CMD-C2D-C1D	5.81	134.97	124.73
19	A	1122	CLA	CMD-C2D-C1D	5.81	134.96	124.73
19	B	1208	CLA	OBD-CAD-C3D	-5.81	114.83	128.42
22	G	7051	LMU	C3'-C4'-C5'	-5.81	98.05	110.93
19	A	1115	CLA	C1D-CHD-C4C	-5.81	113.67	126.02
19	A	1128	CLA	C4D-C3D-CAD	5.81	114.42	108.11
19	A	1132	CLA	C4D-C3D-CAD	5.81	114.42	108.11
19	3	1118	CLA	C4D-C3D-CAD	5.81	114.41	108.11
19	1	1007	CLA	C1D-CHD-C4C	-5.81	113.68	126.02
19	A	1128	CLA	C1D-CHD-C4C	-5.80	113.69	126.02
19	4	4001	CLA	C4D-C3D-CAD	5.80	114.41	108.11
19	B	1222	CLA	C4D-C3D-CAD	5.80	114.41	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1213	CLA	C4D-C3D-CAD	5.79	114.40	108.11
19	K	3009	CLA	C4D-C3D-CAD	5.79	114.39	108.11
21	B	6010	BCR	C7-C8-C9	-5.78	117.68	126.23
21	A	6003	BCR	C23-C24-C25	-5.78	111.55	127.00
19	B	1230	CLA	C1D-CHD-C4C	-5.78	113.73	126.02
19	2	2001	CLA	C1D-CHD-C4C	-5.78	113.74	126.02
19	B	1220	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
19	A	9023	CLA	C4D-C3D-CAD	5.77	114.38	108.11
19	4	4007	CLA	CMD-C2D-C1D	5.77	134.89	124.73
19	A	1119	CLA	C4D-C3D-CAD	5.77	114.37	108.11
19	B	1215	CLA	C1D-CHD-C4C	-5.77	113.76	126.02
19	L	1148	CLA	C4D-C3D-CAD	5.77	114.37	108.11
19	4	4003	CLA	C4D-C3D-CAD	5.76	114.37	108.11
21	B	6004	BCR	C32-C1-C6	-5.76	101.20	110.24
19	F	1240	CLA	OBD-CAD-C3D	-5.76	114.95	128.42
20	B	5002	PQN	C11-C12-C13	-5.76	116.91	126.83
19	K	1143	CLA	C1D-CHD-C4C	-5.76	113.78	126.02
19	B	1214	CLA	CMD-C2D-C1D	5.76	134.87	124.73
19	2	4009	CLA	CMD-C2D-C1D	5.76	134.87	124.73
19	2	2001	CLA	C4D-C3D-CAD	5.75	114.36	108.11
19	3	1118	CLA	C1D-CHD-C4C	-5.75	113.80	126.02
19	1	1007	CLA	CMD-C2D-C1D	5.75	134.85	124.73
19	2	2006	CLA	C4D-C3D-CAD	5.75	114.35	108.11
19	A	1120	CLA	O2D-CGD-CBD	5.75	121.27	111.23
19	B	1221	CLA	CMD-C2D-C1D	5.74	134.84	124.73
19	2	2012	CLA	C4A-NA-C1A	5.74	109.30	106.68
19	B	1206	CLA	C1D-CHD-C4C	-5.73	113.83	126.02
19	F	1240	CLA	C1D-CHD-C4C	-5.73	113.83	126.02
19	4	4012	CLA	C1D-CHD-C4C	-5.73	113.84	126.02
19	A	1102	CLA	C2B-C1B-NB	5.73	116.27	110.33
19	B	1201	CLA	C1D-CHD-C4C	-5.73	113.84	126.02
19	4	4014	CLA	C1D-CHD-C4C	-5.73	113.84	126.02
19	F	1240	CLA	C4D-C3D-CAD	5.73	114.33	108.11
19	4	4004	CLA	C3A-C4A-CHB	-5.73	116.90	123.91
19	J	1308	CLA	O2D-CGD-CBD	5.72	121.23	111.23
19	A	9023	CLA	CMD-C2D-C1D	5.72	134.81	124.73
21	A	6008	BCR	C31-C1-C6	-5.72	101.27	110.24
19	A	1106	CLA	C4D-C3D-CAD	5.72	114.32	108.11
19	L	1502	CLA	C4D-C3D-CAD	5.72	114.32	108.11
19	A	1133	CLA	C4D-C3D-CAD	5.72	114.32	108.11
19	2	2012	CLA	O2D-CGD-CBD	5.72	121.23	111.23
22	3	7005	LMU	C1B-O5B-C5B	-5.72	102.55	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1205	CLA	O1D-CGD-CBD	-5.72	113.24	124.52
19	B	1218	CLA	CHD-C4C-NC	5.72	133.09	124.23
21	I	6021	BCR	C1-C6-C5	-5.71	114.83	122.64
19	3	3003	CLA	C1D-CHD-C4C	-5.71	113.88	126.02
19	A	1111	CLA	CMD-C2D-C1D	5.71	134.78	124.73
19	A	1139	CLA	C1D-CHD-C4C	-5.71	113.88	126.02
19	B	1223	CLA	C1D-CHD-C4C	-5.71	113.88	126.02
19	A	1111	CLA	C1D-CHD-C4C	-5.71	113.89	126.02
19	H	1207	CLA	C2B-C1B-NB	5.71	116.25	110.33
19	B	1229	CLA	C4D-C3D-CAD	5.71	114.31	108.11
19	A	1136	CLA	C1D-CHD-C4C	-5.71	113.89	126.02
19	3	3003	CLA	CMD-C2D-C1D	5.71	134.78	124.73
19	A	1117	CLA	C4D-C3D-CAD	5.70	114.30	108.11
19	B	1234	CLA	C1D-CHD-C4C	-5.70	113.89	126.02
19	A	1103	CLA	CMD-C2D-C1D	5.70	134.77	124.73
19	A	1132	CLA	C1D-CHD-C4C	-5.70	113.91	126.02
19	L	1501	CLA	C1D-CHD-C4C	-5.70	113.91	126.02
19	A	1117	CLA	C1D-CHD-C4C	-5.69	113.92	126.02
19	B	1229	CLA	C1D-CHD-C4C	-5.69	113.92	126.02
21	J	6012	BCR	C24-C23-C22	-5.69	117.82	126.23
19	3	3014	CLA	C3A-C4A-CHB	-5.69	116.94	123.91
19	A	1111	CLA	C4D-C3D-CAD	5.68	114.28	108.11
19	3	3008	CLA	C1D-CHD-C4C	-5.68	113.94	126.02
19	L	1501	CLA	C4D-C3D-CAD	5.68	114.28	108.11
19	4	1304	CLA	C4D-C3D-CAD	5.68	114.27	108.11
21	A	6011	BCR	C7-C8-C9	-5.67	117.85	126.23
22	N	7049	LMU	C1B-O1B-C4'	-5.67	104.54	117.98
19	B	1224	CLA	C1D-CHD-C4C	-5.66	113.98	126.02
19	A	1126	CLA	C4D-C3D-CAD	5.66	114.25	108.11
19	B	1225	CLA	C1D-CHD-C4C	-5.66	114.00	126.02
19	4	4003	CLA	O2D-CGD-CBD	5.65	121.12	111.23
19	2	2013	CLA	C4A-NA-C1A	5.65	109.26	106.68
21	I	6021	BCR	C34-C9-C10	-5.65	113.66	122.82
19	B	1208	CLA	C4D-C3D-CAD	5.65	114.24	108.11
19	B	1301	CLA	C4D-C3D-CAD	5.65	114.24	108.11
19	A	1140	CLA	C4D-C3D-CAD	5.65	114.24	108.11
19	H	1505	CLA	C1D-CHD-C4C	-5.64	114.03	126.02
19	A	9011	CLA	C3B-C2B-C1B	-5.64	100.52	107.17
19	4	4002	CLA	CHC-C1C-NC	5.64	132.80	124.31
19	A	1137	CLA	C4D-C3D-CAD	5.64	114.23	108.11
19	L	1503	CLA	C4D-C3D-CAD	5.63	114.22	108.11
19	A	1140	CLA	C1D-CHD-C4C	-5.63	114.05	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1010	CLA	CHD-C4C-C3C	-5.63	116.56	124.77
19	2	2013	CLA	O2D-CGD-CBD	5.63	121.07	111.23
19	4	4006	CLA	CHD-C4C-NC	5.63	132.96	124.23
19	K	1142	CLA	CMD-C2D-C1D	5.63	134.63	124.73
21	1	6023	BCR	C20-C19-C18	5.63	141.79	126.36
19	B	1205	CLA	OBD-CAD-C3D	-5.62	115.27	128.42
21	A	6007	BCR	C21-C20-C19	5.62	139.49	123.20
19	2	4009	CLA	C4D-C3D-CAD	5.61	114.20	108.11
19	B	1217	CLA	C1D-CHD-C4C	-5.61	114.09	126.02
19	A	1126	CLA	C1D-CHD-C4C	-5.61	114.10	126.02
19	H	1207	CLA	C4D-C3D-CAD	5.61	114.20	108.11
19	A	1134	CLA	C1D-CHD-C4C	-5.61	114.10	126.02
19	B	1203	CLA	CMD-C2D-C1D	5.61	134.60	124.73
19	A	1116	CLA	C1D-CHD-C4C	-5.61	114.11	126.02
19	A	1125	CLA	C4D-C3D-CAD	5.60	114.19	108.11
19	K	3009	CLA	CMD-C2D-C1D	5.60	134.59	124.73
21	F	6016	BCR	C10-C11-C12	5.60	139.42	123.20
19	1	1012	CLA	C1D-CHD-C4C	-5.60	114.13	126.02
19	B	1238	CLA	O2D-CGD-CBD	5.59	121.01	111.23
19	A	1141	CLA	C1D-CHD-C4C	-5.59	114.13	126.02
19	B	1212	CLA	C1D-CHD-C4C	-5.59	114.14	126.02
19	A	1125	CLA	CMD-C2D-C1D	5.59	134.57	124.73
19	G	1242	CLA	C1D-CHD-C4C	-5.59	114.15	126.02
19	A	9023	CLA	C1D-CHD-C4C	-5.58	114.15	126.02
19	A	1138	CLA	C4D-C3D-CAD	5.58	114.17	108.11
19	L	1504	CLA	C1D-CHD-C4C	-5.58	114.16	126.02
19	1	1014	CLA	C4D-C3D-CAD	5.58	114.16	108.11
19	B	1234	CLA	O2D-CGD-O1D	-5.57	113.00	123.85
21	1	6023	BCR	C39-C30-C25	5.57	118.98	110.24
19	F	1302	CLA	C1D-CHD-C4C	-5.57	114.18	126.02
19	1	1011	CLA	CBD-CAD-C3D	-5.57	100.81	108.25
19	A	1104	CLA	C4D-C3D-CAD	5.57	114.16	108.11
21	A	6003	BCR	C16-C17-C18	-5.57	119.47	127.28
19	A	1104	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
19	B	1227	CLA	C4D-C3D-CAD	5.56	114.14	108.11
19	A	1237	CLA	CMD-C2D-C1D	5.56	134.51	124.73
19	B	1210	CLA	CHD-C4C-NC	5.56	132.85	124.23
19	A	1103	CLA	C1D-CHD-C4C	-5.56	114.21	126.02
19	4	4006	CLA	CHD-C4C-C3C	-5.55	116.67	124.77
19	A	1135	CLA	C1D-CHD-C4C	-5.55	114.22	126.02
21	1	6023	BCR	C39-C30-C29	-5.55	87.65	108.95
19	A	1112	CLA	C3B-C2B-C1B	-5.54	100.63	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1105	CLA	C4D-C3D-CAD	5.54	114.12	108.11
19	A	1124	CLA	C1D-CHD-C4C	-5.54	114.25	126.02
19	A	1131	CLA	C1D-CHD-C4C	-5.54	114.25	126.02
19	A	9011	CLA	CMD-C2D-C1D	5.53	134.47	124.73
19	1	1012	CLA	C4D-C3D-CAD	5.53	114.11	108.11
19	B	1224	CLA	C4D-C3D-CAD	5.53	114.11	108.11
21	B	6004	BCR	C16-C17-C18	-5.53	119.53	127.28
19	B	1203	CLA	C3B-C2B-C1B	-5.52	100.66	107.17
19	H	1145	CLA	C1D-CHD-C4C	-5.52	114.29	126.02
19	A	1110	CLA	C1D-CHD-C4C	-5.52	114.30	126.02
19	A	1124	CLA	C4D-C3D-CAD	5.52	114.10	108.11
19	3	3006	CLA	C3A-C4A-CHB	-5.51	117.16	123.91
19	1	1011	CLA	CHD-C4C-NC	5.51	132.78	124.23
19	B	1216	CLA	C1D-CHD-C4C	-5.51	114.30	126.02
19	B	1210	CLA	C4D-C3D-CAD	5.51	114.09	108.11
19	A	1101	CLA	C4D-C3D-CAD	5.51	114.09	108.11
19	A	1135	CLA	O2D-CGD-CBD	5.51	120.86	111.23
19	A	1110	CLA	C4D-C3D-CAD	5.51	114.09	108.11
19	2	2014	CLA	O2D-CGD-CBD	5.51	120.86	111.23
19	4	4012	CLA	CBD-CAD-C3D	-5.50	100.91	108.25
19	B	1222	CLA	C1D-CHD-C4C	-5.50	114.33	126.02
19	F	1305	CLA	O2D-CGD-CBD	5.50	120.84	111.23
19	A	1117	CLA	CMD-C2D-C1D	5.50	134.41	124.73
19	B	1208	CLA	C1D-CHD-C4C	-5.49	114.34	126.02
19	4	1009	CLA	CHD-C4C-NC	5.49	132.75	124.23
21	I	6021	BCR	C38-C26-C25	-5.49	118.49	124.48
19	K	3009	CLA	C1D-CHD-C4C	-5.49	114.35	126.02
19	A	1124	CLA	O2D-CGD-CBD	5.49	120.83	111.23
22	3	7003	LMU	C4B-C3B-C2B	5.49	120.47	110.83
19	4	1004	CLA	C1D-CHD-C4C	-5.49	114.35	126.02
19	3	3016	CLA	C4D-C3D-CAD	5.49	114.07	108.11
19	F	1240	CLA	C2B-C1B-NB	5.49	116.02	110.33
19	3	3006	CLA	CHD-C4C-NC	5.49	132.58	124.24
19	2	2014	CLA	CAA-C2A-C3A	-5.49	98.17	113.00
19	J	1308	CLA	C4D-C3D-CAD	5.48	114.06	108.11
19	L	1503	CLA	CHD-C4C-NC	5.48	132.73	124.23
19	1	1005	CLA	C1D-CHD-C4C	-5.48	114.37	126.02
19	J	1308	CLA	CHD-C4C-NC	5.48	132.73	124.23
19	G	1242	CLA	C4-C3-C5	5.48	122.58	116.13
19	A	1123	CLA	C1D-CHD-C4C	-5.48	114.38	126.02
22	4	7052	LMU	O1'-C1'-C2'	5.47	116.58	108.27
19	B	1219	CLA	C1D-CHD-C4C	-5.47	114.40	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	F	1305	CLA	CMA-C3A-C4A	5.47	126.47	111.77
19	A	1112	CLA	C2B-C1B-NB	5.47	116.00	110.33
19	B	1217	CLA	CHD-C4C-NC	5.46	132.70	124.23
19	A	1119	CLA	C1D-CHD-C4C	-5.46	114.41	126.02
19	B	1202	CLA	C1D-CHD-C4C	-5.46	114.41	126.02
19	A	1113	CLA	C4D-C3D-CAD	5.46	114.04	108.11
19	B	1230	CLA	CBB-CAB-C3B	5.46	154.80	127.53
19	B	1228	CLA	CHD-C4C-NC	5.46	132.69	124.23
21	F	6016	BCR	C24-C23-C22	-5.46	118.16	126.23
19	A	1135	CLA	C4D-C3D-CAD	5.46	114.03	108.11
19	1	1008	CLA	C1D-CHD-C4C	-5.45	114.43	126.02
19	B	1218	CLA	CHD-C4C-C3C	-5.45	116.82	124.77
19	G	1242	CLA	O2D-CGD-CBD	5.45	120.76	111.23
19	A	9022	CLA	C1D-CHD-C4C	-5.45	114.45	126.02
19	H	1241	CLA	C1D-CHD-C4C	-5.44	114.46	126.02
19	A	1138	CLA	C1D-CHD-C4C	-5.44	114.47	126.02
19	A	1128	CLA	CMD-C2D-C1D	5.43	134.30	124.73
19	A	1106	CLA	O2D-CGD-CBD	5.43	120.73	111.23
21	F	6016	BCR	C3-C4-C5	-5.43	104.38	114.06
19	A	1117	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
19	B	1215	CLA	C4D-C3D-CAD	5.42	114.00	108.11
19	A	1105	CLA	CMD-C2D-C1D	5.42	134.28	124.73
19	A	1237	CLA	O2D-CGD-CBD	5.42	120.71	111.23
19	K	1143	CLA	C4D-C3D-CAD	5.42	113.99	108.11
19	B	1239	CLA	CMD-C2D-C1D	5.42	134.27	124.73
19	L	1504	CLA	C4D-C3D-CAD	5.41	113.99	108.11
19	B	1239	CLA	CHC-C4B-NB	5.41	132.17	124.05
19	B	1213	CLA	C1D-CHD-C4C	-5.41	114.52	126.02
19	1	1008	CLA	CBA-CAA-C2A	-5.41	97.69	113.79
19	I	1204	CLA	O2D-CGD-CBD	5.41	120.68	111.23
21	B	6017	BCR	C31-C1-C6	-5.40	101.77	110.24
19	4	1009	CLA	CBD-CAD-C3D	-5.40	101.04	108.25
19	A	1113	CLA	CMD-C2D-C1D	5.40	134.24	124.73
19	A	9011	CLA	CHD-C4C-C3C	-5.40	116.90	124.77
19	A	1137	CLA	O2D-CGD-CBD	5.40	120.67	111.23
19	A	1129	CLA	CMD-C2D-C1D	5.40	134.23	124.73
19	2	2013	CLA	C4D-C3D-CAD	5.40	113.97	108.11
19	A	1112	CLA	C4D-C3D-CAD	5.39	113.97	108.11
21	3	6022	BCR	C7-C8-C9	-5.39	118.26	126.23
19	A	1151	CLA	C1D-CHD-C4C	-5.39	114.56	126.02
19	A	1103	CLA	C4D-C3D-CAD	5.39	113.96	108.11
19	B	1220	CLA	CHD-C4C-NC	5.39	132.59	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1149	CLA	CMD-C2D-C3D	-5.39	115.33	127.69
21	B	6004	BCR	C15-C14-C13	-5.39	119.72	127.28
19	2	2001	CLA	O2D-CGD-CBD	5.39	120.65	111.23
19	H	1241	CLA	C4D-C3D-CAD	5.39	113.96	108.11
19	H	1207	CLA	C1D-CHD-C4C	-5.38	114.58	126.02
19	A	1123	CLA	C4D-C3D-CAD	5.37	113.94	108.11
19	2	2014	CLA	CMD-C2D-C1D	5.37	134.19	124.73
21	I	6021	BCR	C8-C9-C10	5.37	127.46	119.01
19	A	1122	CLA	C1D-CHD-C4C	-5.37	114.60	126.02
19	3	3003	CLA	CHD-C4C-NC	5.37	132.55	124.23
21	F	6016	BCR	C32-C1-C6	-5.37	101.83	110.24
19	A	1115	CLA	O2D-CGD-CBD	5.37	120.61	111.23
21	L	6019	BCR	C31-C1-C6	-5.37	101.83	110.24
19	B	1232	CLA	C1D-CHD-C4C	-5.36	114.63	126.02
19	B	1301	CLA	CBD-CAD-C3D	-5.36	101.09	108.25
19	2	4009	CLA	C1D-CHD-C4C	-5.36	114.64	126.02
19	A	1111	CLA	CHC-C1C-NC	5.35	132.38	124.31
19	A	1127	CLA	C1D-CHD-C4C	-5.35	114.64	126.02
19	4	4002	CLA	C4D-C3D-CAD	5.35	113.92	108.11
19	3	3017	CLA	C4B-CHC-C1C	-5.35	113.67	126.25
19	1	1003	CLA	C1D-CHD-C4C	-5.35	114.66	126.02
19	A	1107	CLA	C1D-CHD-C4C	-5.35	114.66	126.02
21	1	6023	BCR	C38-C26-C25	-5.34	118.65	124.48
19	A	1102	CLA	C1D-CHD-C4C	-5.34	114.66	126.02
19	A	1107	CLA	CHC-C1C-NC	5.34	132.35	124.31
19	4	1304	CLA	CAA-C2A-C3A	-5.33	98.59	113.00
19	A	1132	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
19	A	1129	CLA	C1D-CHD-C4C	-5.32	114.70	126.02
19	B	1232	CLA	O2D-CGD-CBD	5.32	120.54	111.23
19	A	1115	CLA	C2B-C1B-NB	5.32	115.85	110.33
19	2	2013	CLA	CMD-C2D-C1D	5.32	134.10	124.73
19	B	1217	CLA	O2D-CGD-CBD	5.32	120.53	111.23
21	1	6023	BCR	C40-C30-C25	5.32	118.58	110.24
19	B	1216	CLA	CMD-C2D-C1D	5.32	134.09	124.73
19	3	1118	CLA	CAB-C3B-C2B	-5.32	109.41	123.53
19	4	4003	CLA	C1D-CHD-C4C	-5.32	114.72	126.02
19	A	1133	CLA	C1D-CHD-C4C	-5.31	114.73	126.02
19	2	2007	CLA	C4D-C3D-CAD	5.31	113.87	108.11
19	R	1144	CLA	C1D-CHD-C4C	-5.31	114.74	126.02
19	4	4014	CLA	C4D-C3D-CAD	5.31	113.87	108.11
19	B	1205	CLA	C4A-NA-C1A	5.31	109.10	106.68
19	B	1214	CLA	O2D-CGD-CBD	5.30	120.50	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1107	CLA	C4D-C3D-CAD	5.30	113.86	108.11
19	1	1001	CLA	O2D-CGD-CBD	5.30	120.50	111.23
19	3	3007	CLA	O2D-CGD-CBD	5.30	120.50	111.23
19	B	1203	CLA	C4D-C3D-CAD	5.30	113.86	108.11
19	F	1240	CLA	CHD-C4C-NC	5.30	132.45	124.23
19	R	1150	CLA	C1D-CHD-C4C	-5.30	114.76	126.02
21	3	6022	BCR	C16-C15-C14	-5.29	112.69	123.52
19	B	1239	CLA	C1D-CHD-C4C	-5.29	114.78	126.02
19	3	3011	CLA	C1D-CHD-C4C	-5.28	114.79	126.02
19	A	1101	CLA	C1D-CHD-C4C	-5.28	114.79	126.02
19	L	1502	CLA	C1D-CHD-C4C	-5.28	114.80	126.02
19	1	1001	CLA	CHC-C4B-NB	5.28	131.97	124.05
21	I	6021	BCR	C29-C30-C25	-5.28	102.78	110.44
19	G	1242	CLA	C4D-C3D-CAD	5.27	113.83	108.11
19	1	1002	CLA	C1D-CHD-C4C	-5.27	114.81	126.02
19	1	1010	CLA	O2D-CGD-CBD	5.27	120.45	111.23
21	A	6008	BCR	C32-C1-C6	-5.27	101.98	110.24
21	A	6008	BCR	C20-C19-C18	-5.27	111.91	126.36
19	3	3001	CLA	C3A-C4A-CHB	-5.27	117.46	123.91
19	A	1237	CLA	C1D-CHD-C4C	-5.27	114.83	126.02
19	1	1310	CLA	C3A-C4A-CHB	-5.26	117.46	123.91
19	B	1228	CLA	CMD-C2D-C1D	5.26	134.00	124.73
19	1	1010	CLA	CAA-C2A-C1A	5.26	129.22	111.97
21	1	6023	BCR	C15-C14-C13	-5.26	119.90	127.28
19	G	1242	CLA	C2B-C1B-NB	5.26	115.78	110.33
19	3	3016	CLA	O2D-CGD-CBD	5.26	120.43	111.23
19	K	1146	CLA	O2D-CGD-CBD	5.25	120.40	111.23
19	A	1117	CLA	CHD-C4C-NC	5.24	132.35	124.23
19	B	1214	CLA	C1D-CHD-C4C	-5.24	114.89	126.02
19	B	1205	CLA	C1D-CHD-C4C	-5.23	114.89	126.02
19	A	1115	CLA	C4D-C3D-CAD	5.23	113.79	108.11
19	B	1210	CLA	CHD-C4C-C3C	-5.23	117.14	124.77
19	B	1224	CLA	C2B-C1B-NB	5.23	115.75	110.33
19	1	1007	CLA	O2D-CGD-CBD	5.23	120.38	111.23
22	A	7044	LMU	O1'-C1'-C2'	5.23	116.22	108.27
19	A	1139	CLA	CHD-C4C-NC	5.23	132.34	124.23
19	L	1503	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
19	J	1308	CLA	C4A-NA-C1A	5.23	109.06	106.68
19	2	2014	CLA	C2B-C1B-NB	5.23	115.75	110.33
19	B	1228	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
19	A	1134	CLA	CHD-C4C-NC	5.22	132.33	124.23
19	A	9011	CLA	CHD-C4C-NC	5.22	132.33	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1120	CLA	C1D-CHD-C4C	-5.22	114.92	126.02
19	4	4002	CLA	C3A-C2A-C1A	5.22	109.16	101.34
19	B	1228	CLA	C1D-CHD-C4C	-5.22	114.93	126.02
19	K	3009	CLA	CHD-C4C-C3C	-5.22	117.17	124.77
19	A	9012	CLA	C2B-C1B-NB	5.21	115.73	110.33
19	A	1104	CLA	C1D-CHD-C4C	-5.21	114.94	126.02
21	B	6017	BCR	C15-C14-C13	-5.21	119.97	127.28
19	1	1015	CLA	C3A-C4A-CHB	-5.21	117.53	123.91
19	B	1206	CLA	CMD-C2D-C1D	5.21	133.90	124.73
19	3	3005	CLA	C3A-C4A-CHB	-5.21	117.53	123.91
19	1	1008	CLA	CGD-CBD-CAD	-5.20	94.00	110.85
19	A	1108	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
19	4	4012	CLA	CMD-C2D-C1D	5.20	133.88	124.73
19	A	1121	CLA	C1D-CHD-C4C	-5.20	114.98	126.02
19	B	1209	CLA	C1D-CHD-C4C	-5.19	114.98	126.02
19	B	1233	CLA	C1D-CHD-C4C	-5.19	114.98	126.02
19	A	1106	CLA	C2B-C1B-NB	5.18	115.70	110.33
19	A	1151	CLA	C4D-C3D-CAD	5.18	113.73	108.11
19	1	1006	CLA	CHD-C4C-NC	5.18	132.26	124.23
21	F	6014	BCR	C7-C8-C9	-5.18	118.58	126.23
19	A	1102	CLA	CHD-C4C-NC	5.17	132.25	124.23
19	4	4014	CLA	O2D-CGD-CBD	5.17	120.27	111.23
19	A	9022	CLA	C4-C3-C5	5.17	124.20	115.23
19	2	2008	CLA	C4A-NA-C1A	5.17	109.04	106.68
19	B	1211	CLA	CMD-C2D-C3D	-5.16	115.85	127.69
19	1	1014	CLA	CHD-C4C-NC	5.16	132.23	124.23
19	B	1205	CLA	CMD-C2D-C1D	5.16	133.82	124.73
21	B	6004	BCR	C24-C23-C22	-5.16	118.60	126.23
22	G	7026	LMU	C1'-O5'-C5'	5.16	123.79	113.72
19	K	1146	CLA	C1D-CHD-C4C	-5.15	115.06	126.02
19	L	1148	CLA	CMA-C3A-C4A	5.15	125.62	111.77
19	B	1223	CLA	O2D-CGD-CBD	5.15	120.24	111.23
19	2	2007	CLA	CMD-C2D-C1D	5.15	133.80	124.73
19	A	1112	CLA	C1D-CHD-C4C	-5.15	115.07	126.02
19	A	1102	CLA	C1-O2A-CGA	5.15	129.12	116.65
19	A	1149	CLA	C1D-CHD-C4C	-5.15	115.08	126.02
19	3	3017	CLA	C1D-CHD-C4C	-5.15	115.08	126.02
21	A	6008	BCR	C15-C14-C13	-5.15	120.06	127.28
19	B	1214	CLA	C4D-C3D-CAD	5.15	113.70	108.11
19	3	2009	CLA	CHD-C4C-NC	5.14	132.21	124.23
19	1	1002	CLA	C4A-NA-C1A	5.14	109.03	106.68
19	3	3004	CLA	CHD-C4C-NC	5.14	132.06	124.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1235	CLA	C1D-CHD-C4C	-5.14	115.09	126.02
19	4	4015	CLA	CHD-C4C-C3C	-5.14	117.28	124.77
19	3	3016	CLA	CHD-C4C-NC	5.14	132.20	124.23
19	1	1013	CLA	CMD-C2D-C3D	-5.14	115.90	127.69
19	1	1010	CLA	C4B-CHC-C1C	-5.14	114.16	126.25
19	1	1310	CLA	C2A-C1A-CHA	-5.14	113.87	122.63
19	A	1101	CLA	C3B-C2B-C1B	-5.14	101.12	107.17
19	I	1204	CLA	C4D-C3D-CAD	5.13	113.68	108.11
19	2	2011	CLA	C3A-C4A-CHB	-5.13	117.63	123.91
19	K	1142	CLA	O2D-CGD-CBD	5.13	120.19	111.23
19	1	1001	CLA	C4B-CHC-C1C	-5.13	114.19	126.25
19	A	1116	CLA	O2D-CGD-CBD	5.12	120.19	111.23
19	A	1134	CLA	O2D-CGD-CBD	5.12	120.19	111.23
19	A	9013	CLA	C1D-CHD-C4C	-5.12	115.13	126.02
19	B	9010	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
19	2	2006	CLA	CHD-C4C-NC	5.12	132.16	124.23
19	2	2002	CLA	C1D-CHD-C4C	-5.12	115.15	126.02
19	B	1236	CLA	C4D-C3D-CAD	5.11	113.66	108.11
19	A	9022	CLA	CMD-C2D-C1D	5.11	133.73	124.73
19	A	1127	CLA	C4D-C3D-CAD	5.11	113.66	108.11
19	3	3013	CLA	C4D-C3D-CAD	5.11	113.66	108.11
19	A	1113	CLA	C1D-CHD-C4C	-5.11	115.16	126.02
19	2	2004	CLA	C1D-CHD-C4C	-5.11	115.16	126.02
19	L	1130	CLA	C1D-CHD-C4C	-5.11	115.16	126.02
19	1	1006	CLA	CBD-CAD-C3D	-5.11	101.43	108.25
19	A	1119	CLA	O2D-CGD-CBD	5.11	120.16	111.23
21	L	6019	BCR	C24-C23-C22	-5.11	118.68	126.23
19	3	1147	CLA	CHD-C4C-NC	5.11	132.15	124.23
19	A	1106	CLA	C1D-CHD-C4C	-5.10	115.17	126.02
22	E	7037	LMU	C1B-O5B-C5B	-5.10	103.75	113.72
19	A	1117	CLA	C2B-C1B-NB	5.10	115.62	110.33
19	A	1141	CLA	O2D-CGD-CBD	5.10	120.15	111.23
19	A	1137	CLA	CHD-C4C-NC	5.10	132.14	124.23
19	A	1138	CLA	O2D-CGD-CBD	5.10	120.15	111.23
19	B	1225	CLA	CHD-C4C-C3C	-5.10	117.34	124.77
19	A	1108	CLA	C4D-C3D-CAD	5.10	113.64	108.11
19	1	1014	CLA	CHD-C4C-C3C	-5.09	117.34	124.77
19	A	1111	CLA	O2D-CGD-CBD	5.09	120.13	111.23
19	A	9011	CLA	C1D-CHD-C4C	-5.09	115.19	126.02
19	4	1306	CLA	C4B-CHC-C1C	-5.09	114.27	126.25
19	H	1241	CLA	CMD-C2D-C1D	5.09	133.69	124.73
19	A	1136	CLA	O2D-CGD-CBD	5.08	120.11	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	3004	CLA	CHC-C1C-NC	5.08	131.80	124.33
19	1	1303	CLA	CHD-C4C-NC	5.08	132.10	124.23
21	B	6010	BCR	C29-C30-C25	-5.08	103.07	110.44
19	B	1220	CLA	CMD-C2D-C1D	5.07	133.66	124.73
21	A	6011	BCR	C32-C1-C6	-5.07	102.29	110.24
21	A	6007	BCR	C15-C14-C13	-5.07	120.17	127.28
19	A	9012	CLA	C4D-C3D-CAD	5.06	113.61	108.11
19	A	1103	CLA	C4B-CHC-C1C	-5.06	114.34	126.25
19	B	1236	CLA	CHD-C4C-NC	5.06	132.08	124.23
19	3	3008	CLA	CMD-C2D-C3D	-5.06	116.09	127.69
19	B	1227	CLA	CMD-C2D-C1D	5.06	133.63	124.73
19	G	1242	CLA	CHD-C4C-NC	5.05	132.07	124.23
19	A	1109	CLA	CMB-C2B-C1B	5.05	133.11	125.42
19	4	4007	CLA	C1D-CHD-C4C	-5.05	115.28	126.02
19	A	1125	CLA	CHD-C4C-NC	5.05	132.06	124.23
19	3	1147	CLA	CHD-C4C-C3C	-5.05	117.41	124.77
19	A	9012	CLA	CMD-C2D-C1D	5.04	133.61	124.73
19	B	1212	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
19	2	2012	CLA	C1D-CHD-C4C	-5.04	115.30	126.02
19	3	3005	CLA	CHD-C4C-NC	5.04	131.90	124.24
19	L	1148	CLA	O2D-CGD-O1D	-5.04	114.05	123.85
21	A	6002	BCR	C15-C14-C13	-5.04	120.22	127.28
19	B	1203	CLA	C4A-NA-C1A	5.03	108.98	106.68
19	B	1203	CLA	C2B-C1B-NB	5.03	115.54	110.33
19	4	4010	CLA	C3A-C4A-CHB	-5.03	117.75	123.91
19	B	1222	CLA	CHD-C4C-NC	5.03	132.02	124.23
19	B	1220	CLA	C1D-CHD-C4C	-5.03	115.34	126.02
19	L	1148	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
19	1	1310	CLA	C4A-NA-C1A	5.02	108.97	106.68
19	F	1240	CLA	CBD-CAD-C3D	-5.02	101.55	108.25
19	3	1118	CLA	CHD-C4C-NC	5.01	132.00	124.23
19	A	1106	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
21	A	6008	BCR	C7-C8-C9	-5.01	118.82	126.23
19	3	3007	CLA	C1D-CHD-C4C	-5.01	115.37	126.02
19	B	1221	CLA	C4D-C3D-CAD	5.01	113.55	108.11
19	3	3008	CLA	CHD-C4C-NC	5.01	132.00	124.23
21	1	6023	BCR	C36-C18-C19	5.01	125.74	118.09
19	2	2003	CLA	CHD-C4C-NC	5.01	131.85	124.24
19	3	3011	CLA	C2B-C1B-NB	5.01	115.52	110.33
19	4	4015	CLA	CHD-C4C-NC	5.00	131.99	124.23
19	A	1105	CLA	C1D-CHD-C4C	-5.00	115.39	126.02
19	A	1133	CLA	O2D-CGD-CBD	5.00	119.96	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	2008	CLA	CHD-C4C-NC	5.00	131.83	124.24
19	K	1143	CLA	CHD-C4C-NC	4.99	131.97	124.23
19	J	1311	CLA	CHD-C4C-NC	4.99	131.97	124.23
19	A	1136	CLA	CHD-C4C-NC	4.99	131.97	124.23
19	K	1142	CLA	CHD-C4C-NC	4.99	131.96	124.23
19	A	9022	CLA	C2B-C1B-NB	4.98	115.49	110.33
19	A	1104	CLA	O2D-CGD-CBD	4.98	119.94	111.23
19	A	1138	CLA	CHD-C4C-NC	4.98	131.95	124.23
21	A	6002	BCR	C32-C1-C6	-4.98	102.44	110.24
19	B	1223	CLA	CHD-C4C-NC	4.98	131.95	124.23
19	A	1103	CLA	CHC-C1C-NC	4.97	131.80	124.31
21	B	6010	BCR	C31-C1-C6	-4.97	102.45	110.24
21	I	6021	BCR	C38-C26-C27	4.97	124.19	113.60
22	4	7033	LMU	C3B-C4B-C5B	4.96	119.23	110.23
19	3	1147	CLA	C4A-NA-C1A	4.96	108.94	106.68
19	L	1148	CLA	CMD-C2D-C3D	-4.96	116.31	127.69
19	B	1224	CLA	CHD-C4C-NC	4.96	131.92	124.23
19	1	1008	CLA	C2A-C3A-C4A	-4.96	93.86	101.87
19	3	1147	CLA	O2D-CGD-CBD	4.96	119.90	111.23
19	A	9013	CLA	CHD-C4C-NC	4.96	131.92	124.23
21	L	6019	BCR	C7-C8-C9	-4.95	118.91	126.23
19	B	1229	CLA	CHD-C4C-NC	4.95	131.91	124.23
19	A	1149	CLA	C4A-NA-C1A	4.95	108.94	106.68
19	B	1239	CLA	C4A-NA-C1A	4.95	108.94	106.68
19	3	3017	CLA	CBC-CAC-C3C	-4.95	99.00	112.42
19	A	1104	CLA	C2B-C1B-NB	4.95	115.46	110.33
19	B	9010	CLA	C4B-CHC-C1C	-4.95	114.61	126.25
19	B	1233	CLA	O2D-CGD-CBD	4.95	119.88	111.23
19	3	3004	CLA	C2A-C1A-CHA	-4.94	114.20	122.63
19	4	4005	CLA	C2A-C1A-CHA	-4.94	114.21	122.63
19	F	1305	CLA	C1-C2-C3	-4.94	118.11	126.20
19	B	1301	CLA	C1D-CHD-C4C	-4.94	115.53	126.02
19	B	1208	CLA	CAB-C3B-C2B	-4.93	110.43	123.53
19	A	1109	CLA	CHD-C4C-NC	4.93	131.88	124.23
19	A	1139	CLA	O2D-CGD-CBD	4.93	119.85	111.23
19	A	1141	CLA	CHD-C4C-NC	4.93	131.88	124.23
19	B	1231	CLA	CHD-C4C-NC	4.93	131.88	124.23
19	B	1227	CLA	C1D-CHD-C4C	-4.93	115.54	126.02
19	A	1128	CLA	CHD-C4C-NC	4.93	131.87	124.23
19	L	1504	CLA	CHD-C4C-NC	4.93	131.87	124.23
21	3	6022	BCR	C2-C1-C6	-4.92	103.29	110.44
19	1	1303	CLA	CHC-C1C-NC	4.92	131.72	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	6007	BCR	C7-C8-C9	-4.92	118.95	126.23
19	B	1226	CLA	CHC-C4B-NB	4.92	131.43	124.05
19	4	4010	CLA	CHD-C4C-NC	4.92	131.72	124.24
19	B	1238	CLA	C1D-CHD-C4C	-4.92	115.56	126.02
22	R	7014	LMU	O1B-C1B-C2B	4.92	120.19	108.09
19	2	2001	CLA	CHD-C4C-NC	4.92	131.85	124.23
19	2	2005	CLA	C2A-C1A-CHA	-4.92	114.25	122.63
19	4	4015	CLA	C4D-C3D-CAD	4.91	113.44	108.11
19	A	9011	CLA	C3B-C4B-NB	-4.91	106.15	110.53
19	3	3003	CLA	C4D-C3D-CAD	4.91	113.43	108.11
19	B	1235	CLA	C4D-C3D-CAD	4.90	113.43	108.11
22	4	7033	LMU	C1B-O1B-C4'	-4.90	106.37	117.98
19	A	9012	CLA	CHD-C4C-NC	4.90	131.83	124.23
19	A	1111	CLA	C2B-C1B-NB	4.90	115.40	110.33
19	L	1130	CLA	CHD-C4C-NC	4.90	131.82	124.23
19	B	1201	CLA	CHD-C4C-NC	4.89	131.82	124.23
22	R	7021	LMU	O1B-C4'-C3'	4.89	119.67	107.23
19	1	1013	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
19	1	1012	CLA	CBD-CAD-C3D	-4.89	101.72	108.25
21	A	6003	BCR	C7-C8-C9	-4.89	119.00	126.23
19	A	1104	CLA	CHD-C4C-NC	4.89	131.81	124.23
19	B	1215	CLA	CHD-C4C-C3C	-4.89	117.65	124.77
19	A	1140	CLA	CHD-C4C-NC	4.89	131.81	124.23
19	K	1143	CLA	O2D-CGD-CBD	4.88	119.77	111.23
21	I	6018	BCR	C16-C15-C14	-4.88	113.53	123.52
19	A	1109	CLA	CHC-C1C-NC	4.88	131.66	124.31
19	B	1238	CLA	C4B-CHC-C1C	-4.88	114.78	126.25
19	A	1103	CLA	CHD-C4C-NC	4.88	131.79	124.23
22	F	7036	LMU	O1'-C1'-C2'	4.88	115.68	108.27
21	F	6014	BCR	C37-C22-C21	-4.88	114.92	122.82
19	4	1306	CLA	CHC-C1C-NC	4.88	131.65	124.31
19	B	9010	CLA	C1D-CHD-C4C	-4.88	115.66	126.02
19	1	1011	CLA	CMD-C2D-C3D	-4.87	116.51	127.69
19	A	1103	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
19	4	4001	CLA	O2D-CGD-CBD	4.87	119.75	111.23
19	1	1008	CLA	C4A-NA-C1A	4.87	108.90	106.68
19	1	1003	CLA	CMD-C2D-C3D	-4.87	116.52	127.69
19	3	3017	CLA	CHC-C4B-NB	4.87	131.35	124.05
19	A	1135	CLA	CHD-C4C-NC	4.87	131.78	124.23
19	3	3011	CLA	O2D-CGD-CBD	4.87	119.74	111.23
19	A	1108	CLA	C1D-CHD-C4C	-4.87	115.68	126.02
21	F	6014	BCR	C15-C14-C13	-4.87	120.45	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	9023	CLA	CHC-C1C-NC	4.87	131.64	124.31
19	1	1303	CLA	C4-C3-C5	4.86	121.85	116.13
19	B	1232	CLA	CHD-C4C-NC	4.86	131.77	124.23
19	B	1226	CLA	CMD-C2D-C3D	-4.86	116.54	127.69
21	B	6017	BCR	C7-C8-C9	-4.85	119.05	126.23
19	B	1220	CLA	C6-C5-C3	-4.85	101.65	113.47
19	B	1238	CLA	CMD-C2D-C3D	-4.85	116.57	127.69
19	A	1126	CLA	C2B-C1B-NB	4.85	115.35	110.33
19	A	1101	CLA	CHD-C4C-NC	4.85	131.75	124.23
19	K	1146	CLA	C2B-C1B-NB	4.85	115.35	110.33
19	A	1115	CLA	C1-C2-C3	-4.84	118.26	126.20
21	F	6016	BCR	C31-C1-C6	-4.84	102.65	110.24
19	A	9011	CLA	C4B-CHC-C1C	-4.84	114.86	126.25
19	B	1238	CLA	CHD-C4C-NC	4.84	131.74	124.23
19	A	1108	CLA	CBB-CAB-C3B	4.84	151.70	127.53
19	B	1238	CLA	C2B-C1B-NB	4.84	115.34	110.33
19	2	2008	CLA	C3A-C4A-CHB	-4.84	117.99	123.91
19	L	1501	CLA	CHD-C4C-C3C	-4.84	117.72	124.77
19	B	1203	CLA	CHC-C1C-NC	4.84	131.59	124.31
19	3	3006	CLA	CHC-C1C-NC	4.83	131.44	124.33
19	A	1109	CLA	C4B-C3B-C2B	4.83	113.31	107.30
19	2	2007	CLA	C1D-CHD-C4C	-4.83	115.76	126.02
19	A	1131	CLA	CHD-C4C-NC	4.82	131.71	124.23
19	K	3009	CLA	CHD-C4C-NC	4.82	131.71	124.23
19	2	2005	CLA	CHC-C1C-NC	4.82	131.41	124.33
19	A	9012	CLA	CHD-C4C-C3C	-4.82	117.75	124.77
21	B	6005	BCR	C32-C1-C6	-4.81	102.69	110.24
19	A	1125	CLA	CHD-C4C-C3C	-4.81	117.76	124.77
19	A	1109	CLA	CMD-C2D-C3D	-4.80	116.67	127.69
19	H	1207	CLA	O2D-CGD-CBD	4.80	119.62	111.23
19	A	1132	CLA	CMD-C2D-C3D	-4.80	116.68	127.69
21	A	6007	BCR	C2-C1-C6	-4.80	103.47	110.44
21	F	6016	BCR	C16-C17-C18	-4.80	120.55	127.28
19	1	1002	CLA	C2B-C1B-NB	4.80	115.30	110.33
19	B	1217	CLA	CHD-C4C-C3C	-4.80	117.78	124.77
19	3	3008	CLA	O2D-CGD-CBD	4.80	119.62	111.23
19	4	4002	CLA	C2B-C1B-NB	4.79	115.30	110.33
19	A	1129	CLA	C4D-C3D-CAD	4.79	113.31	108.11
19	1	1001	CLA	CHD-C4C-NC	4.79	131.66	124.23
19	J	1308	CLA	CHD-C4C-C3C	-4.79	117.80	124.77
19	1	1007	CLA	CHD-C4C-C3C	-4.78	117.80	124.77
19	B	1236	CLA	C3B-C2B-C1B	-4.78	101.53	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1001	CLA	CMD-C2D-C3D	-4.78	116.73	127.69
21	B	6005	BCR	C16-C17-C18	-4.78	120.58	127.28
19	B	1216	CLA	CHD-C4C-C3C	-4.78	117.81	124.77
19	L	1501	CLA	CHD-C4C-NC	4.77	131.63	124.23
21	A	6003	BCR	C3-C4-C5	-4.77	105.55	114.06
19	2	2007	CLA	CHC-C1C-NC	4.77	131.50	124.31
19	2	2002	CLA	C2B-C1B-NB	4.77	115.27	110.33
19	L	1148	CLA	C4-C3-C5	4.77	123.50	115.23
19	B	1239	CLA	C4B-CHC-C1C	-4.77	115.03	126.25
22	4	7052	LMU	C1'-O5'-C5'	-4.77	104.41	113.72
19	H	1505	CLA	CHD-C4C-NC	4.77	131.62	124.23
19	F	1305	CLA	CMD-C2D-C1D	4.77	133.12	124.73
19	I	1204	CLA	CHD-C4C-NC	4.77	131.62	124.23
19	A	1121	CLA	O1D-CGD-CBD	-4.77	115.12	124.52
19	L	1502	CLA	C2B-C1B-NB	4.76	115.27	110.33
19	B	1215	CLA	CHD-C4C-NC	4.76	131.62	124.23
19	B	1212	CLA	CMD-C2D-C1D	4.76	133.12	124.73
21	L	6019	BCR	C29-C30-C25	-4.76	103.52	110.44
19	B	1213	CLA	C4A-NA-C1A	4.76	108.85	106.68
19	3	3013	CLA	O1D-CGD-CBD	-4.76	115.13	124.52
19	4	1009	CLA	C1B-C2B-C3B	-4.76	102.56	107.03
19	4	1304	CLA	C4B-CHC-C1C	-4.76	115.06	126.25
19	3	3017	CLA	CHC-C1C-NC	4.76	131.47	124.31
19	A	1121	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
19	A	1107	CLA	C4B-CHC-C1C	-4.76	115.06	126.25
19	3	3011	CLA	C4D-C3D-CAD	4.75	113.27	108.11
19	3	3010	CLA	C3A-C4A-CHB	-4.75	118.09	123.91
19	B	9010	CLA	C2B-C1B-NB	4.75	115.25	110.33
19	B	1220	CLA	C4D-C3D-CAD	4.75	113.26	108.11
19	A	1111	CLA	CHD-C4C-NC	4.75	131.59	124.23
19	B	1216	CLA	CHD-C4C-NC	4.75	131.59	124.23
21	1	6023	BCR	C16-C15-C14	-4.75	113.81	123.52
19	A	1123	CLA	C2B-C1B-NB	4.74	115.25	110.33
19	3	3003	CLA	CHD-C4C-C3C	-4.74	117.54	125.03
19	B	1202	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
19	B	1211	CLA	C1D-CHD-C4C	-4.74	115.94	126.02
19	4	4007	CLA	CHD-C4C-NC	4.74	131.58	124.23
19	B	1202	CLA	CHC-C1C-NC	4.74	131.45	124.31
21	A	6007	BCR	C32-C1-C6	-4.74	102.81	110.24
19	B	1231	CLA	CHD-C4C-C3C	-4.74	117.87	124.77
19	4	4007	CLA	O2D-CGD-CBD	4.74	119.51	111.23
19	B	1229	CLA	CHD-C4C-C3C	-4.73	117.87	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1013	CLA	O2A-CGA-CBA	4.73	126.27	111.83
19	3	1147	CLA	CAC-C3C-C4C	4.73	130.95	124.79
19	F	1302	CLA	CHD-C4C-NC	4.73	131.57	124.23
19	2	2004	CLA	C2B-C1B-NB	4.73	115.23	110.33
19	L	1504	CLA	CHD-C4C-C3C	-4.73	117.88	124.77
19	A	1109	CLA	C2B-C1B-NB	4.73	115.23	110.33
19	B	1202	CLA	CHD-C4C-NC	4.73	131.56	124.23
21	B	6004	BCR	C7-C8-C9	-4.73	119.24	126.23
21	B	6004	BCR	C20-C19-C18	-4.72	113.41	126.36
19	A	1115	CLA	CHD-C4C-NC	4.72	131.55	124.23
19	F	1305	CLA	CHD-C4C-NC	4.72	131.55	124.23
19	K	1146	CLA	C4B-CHC-C1C	-4.72	115.15	126.25
22	E	7037	LMU	C4B-C3B-C2B	-4.72	102.55	110.83
19	L	1502	CLA	CHD-C4C-NC	4.72	131.54	124.23
19	A	9022	CLA	CHD-C4C-NC	4.71	131.54	124.23
19	B	1215	CLA	CMD-C2D-C1D	4.71	133.03	124.73
19	K	1146	CLA	CHC-C1C-NC	4.71	131.41	124.31
19	1	1303	CLA	CMD-C2D-C1D	4.71	133.03	124.73
19	2	2007	CLA	C2B-C1B-NB	4.71	115.21	110.33
19	B	1233	CLA	C4-C3-C5	4.71	121.67	116.13
19	A	1120	CLA	C2B-C1B-NB	4.71	115.21	110.33
19	A	1127	CLA	CMD-C2D-C1D	4.70	133.01	124.73
19	B	1215	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
19	2	2007	CLA	C4B-CHC-C1C	-4.70	115.19	126.25
19	4	1304	CLA	CHD-C4C-C3C	-4.70	117.92	124.77
19	B	1235	CLA	CHD-C4C-NC	4.70	131.52	124.23
19	1	1008	CLA	CAA-C2A-C3A	4.70	125.69	113.00
19	B	1226	CLA	CHD-C4C-NC	4.70	131.51	124.23
19	2	2003	CLA	C3A-C4A-CHB	-4.69	118.16	123.91
19	A	9011	CLA	CHC-C4B-NB	4.69	131.09	124.05
19	3	1118	CLA	CBD-CAD-C3D	-4.69	101.99	108.25
19	L	1130	CLA	C2B-C1B-NB	4.69	115.19	110.33
19	1	1008	CLA	CMD-C2D-C3D	-4.69	116.94	127.69
19	2	1307	CLA	C3A-C4A-CHB	-4.68	118.18	123.91
22	R	7014	LMU	O2B-C2B-C3B	4.68	121.41	110.38
19	4	1009	CLA	CHD-C4C-C3C	-4.68	117.64	125.03
19	B	1234	CLA	CHD-C4C-NC	4.67	131.48	124.23
19	B	1239	CLA	CHD-C4C-C3C	-4.67	117.96	124.77
21	J	6012	BCR	C15-C14-C13	-4.67	120.73	127.28
19	A	1102	CLA	OBD-CAD-C3D	-4.67	117.50	128.42
19	A	1140	CLA	O2D-CGD-CBD	4.67	119.39	111.23
19	B	1226	CLA	C4B-CHC-C1C	-4.67	115.28	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1126	CLA	CHD-C4C-NC	4.66	131.46	124.23
19	R	1144	CLA	O2D-CGD-CBD	4.66	119.38	111.23
19	A	1124	CLA	CHD-C4C-NC	4.66	131.46	124.23
19	A	9023	CLA	CHD-C4C-NC	4.66	131.45	124.23
21	B	6004	BCR	C31-C1-C6	-4.66	102.94	110.24
19	3	3013	CLA	C4B-CHC-C1C	-4.65	115.30	126.25
19	A	1149	CLA	CHC-C1C-NC	4.65	131.32	124.31
19	B	1234	CLA	CMD-C2D-C3D	-4.65	117.02	127.69
19	1	1002	CLA	C4B-CHC-C1C	-4.65	115.31	126.25
19	B	1213	CLA	CHD-C4C-NC	4.65	131.44	124.23
19	1	1012	CLA	CHD-C4C-NC	4.65	131.44	124.23
19	4	4002	CLA	CHD-C4C-C3C	-4.65	117.99	124.77
19	A	1110	CLA	CHD-C4C-NC	4.65	131.44	124.23
19	1	1008	CLA	CHD-C4C-NC	4.65	131.44	124.23
21	B	6020	BCR	C4-C5-C6	-4.65	116.42	122.70
19	B	1229	CLA	C2B-C1B-NB	4.64	115.14	110.33
19	3	3004	CLA	C1B-NB-C4B	-4.64	103.05	106.31
19	4	4012	CLA	CAB-C3B-C2B	-4.64	111.21	123.53
19	3	3002	CLA	C2A-C1A-CHA	-4.64	114.72	122.63
19	B	1238	CLA	CHC-C1C-NC	4.64	131.29	124.31
19	B	1209	CLA	O2D-CGD-CBD	4.63	119.33	111.23
19	R	1144	CLA	CMD-C2D-C3D	-4.63	117.06	127.69
19	A	9023	CLA	C2B-C1B-NB	4.63	115.13	110.33
19	A	1237	CLA	CHD-C4C-C3C	-4.63	118.02	124.77
19	A	1125	CLA	O2D-CGD-CBD	4.63	119.33	111.23
19	R	1150	CLA	CMD-C2D-C3D	-4.63	117.07	127.69
19	2	2008	CLA	CHC-C1C-NC	4.63	131.13	124.33
19	B	1235	CLA	C4B-CHC-C1C	-4.63	115.36	126.25
19	B	1203	CLA	CHD-C4C-NC	4.62	131.40	124.23
19	3	3004	CLA	C1C-CHC-C4B	-4.62	113.86	126.04
21	3	6022	BCR	C31-C1-C6	-4.62	103.00	110.24
22	E	7048	LMU	C1B-O1B-C4'	-4.62	107.03	117.98
22	3	7005	LMU	O1B-C1B-O5B	-4.62	98.54	110.69
21	1	6023	BCR	C19-C18-C17	-4.62	111.75	119.01
19	A	1128	CLA	C4A-NA-C1A	4.62	108.78	106.68
19	B	1212	CLA	C4D-C3D-CAD	4.62	113.12	108.11
21	I	6018	BCR	C10-C11-C12	4.61	136.57	123.20
22	H	7032	LMU	C1B-O5B-C5B	4.61	122.73	113.72
19	A	1102	CLA	O2A-CGA-CBA	4.61	125.90	111.83
19	4	1306	CLA	C4A-NA-C1A	4.61	108.78	106.68
19	B	1202	CLA	CMD-C2D-C3D	-4.61	117.12	127.69
19	B	1225	CLA	O2D-CGD-O1D	-4.61	114.88	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1212	CLA	C2B-C1B-NB	4.61	115.10	110.33
21	I	6021	BCR	C31-C1-C6	-4.61	103.02	110.24
19	H	1207	CLA	CHD-C4C-NC	4.60	131.37	124.23
19	A	1117	CLA	C4B-CHC-C1C	-4.60	115.42	126.25
21	A	6002	BCR	C11-C10-C9	-4.60	120.82	127.28
19	A	1108	CLA	C2B-C1B-NB	4.60	115.10	110.33
19	3	3014	CLA	C2A-C1A-CHA	-4.60	114.79	122.63
19	B	1225	CLA	CHD-C4C-NC	4.60	131.36	124.23
19	A	1126	CLA	C1-C2-C3	-4.60	118.67	126.20
19	A	1151	CLA	C2B-C1B-NB	4.60	115.09	110.33
19	A	1108	CLA	C4B-CHC-C1C	-4.60	115.44	126.25
19	B	1201	CLA	C3B-C2B-C1B	-4.59	101.75	107.17
19	2	1307	CLA	C2A-C1A-CHA	-4.59	114.80	122.63
19	A	9022	CLA	C4D-C3D-CAD	4.59	113.09	108.11
19	B	1202	CLA	C4B-CHC-C1C	-4.59	115.45	126.25
19	3	3012	CLA	C3A-C4A-CHB	-4.59	118.29	123.91
19	3	3005	CLA	CHC-C1C-NC	4.59	131.07	124.33
19	H	1505	CLA	CMD-C2D-C3D	-4.59	117.17	127.69
19	B	1202	CLA	C2B-C1B-NB	4.59	115.08	110.33
19	L	1503	CLA	O1D-CGD-CBD	-4.58	115.47	124.52
19	2	2010	CLA	CHD-C4C-NC	4.58	131.20	124.24
19	A	1102	CLA	C3B-C4B-NB	-4.58	106.44	110.53
19	4	4014	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
19	3	3003	CLA	CAB-C3B-C2B	-4.58	111.38	123.53
19	3	2009	CLA	CHD-C4C-C3C	-4.57	118.10	124.77
19	4	4011	CLA	C2A-C1A-CHA	-4.57	114.83	122.63
19	2	2011	CLA	CHD-C4C-NC	4.57	131.19	124.24
19	B	1232	CLA	CHD-C4C-C3C	-4.57	118.11	124.77
19	B	1231	CLA	C4A-NA-C1A	4.57	108.76	106.68
19	4	4005	CLA	CHD-C4C-NC	4.56	131.18	124.24
19	3	3012	CLA	C1C-CHC-C4B	-4.56	114.00	126.04
21	L	6019	BCR	C39-C30-C25	4.56	117.40	110.24
19	A	9013	CLA	C2B-C1B-NB	4.56	115.06	110.33
19	1	1007	CLA	CHD-C4C-NC	4.56	131.30	124.23
19	B	1208	CLA	CMD-C2D-C3D	-4.56	117.23	127.69
19	A	1102	CLA	C4B-CHC-C1C	-4.56	115.53	126.25
19	3	3017	CLA	CMD-C2D-C3D	-4.56	117.23	127.69
19	B	1206	CLA	CHD-C4C-NC	4.56	131.30	124.23
19	1	1005	CLA	CHD-C4C-C3C	-4.56	118.13	124.77
19	B	1233	CLA	CHD-C4C-NC	4.55	131.29	124.23
19	A	1106	CLA	CHD-C4C-NC	4.55	131.29	124.23
21	1	6023	BCR	C40-C30-C39	4.55	121.66	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	G	1242	CLA	CHD-C4C-C3C	-4.55	118.14	124.77
19	A	1149	CLA	O2A-CGA-CBA	4.55	125.70	111.83
19	B	1208	CLA	CHD-C4C-NC	4.54	131.28	124.23
19	A	1116	CLA	CHD-C4C-NC	4.54	131.28	124.23
19	1	1011	CLA	CHC-C1C-NC	4.54	131.15	124.31
19	4	4015	CLA	CMD-C2D-C1D	4.54	132.73	124.73
19	2	2010	CLA	C3A-C4A-CHB	-4.54	118.35	123.91
19	F	1302	CLA	O2D-CGD-CBD	4.54	119.17	111.23
19	B	1214	CLA	CHD-C4C-NC	4.54	131.27	124.23
19	2	2005	CLA	C1C-CHC-C4B	-4.54	114.07	126.04
19	B	1228	CLA	C4D-C3D-CAD	4.54	113.03	108.11
19	3	3001	CLA	CHD-C4C-NC	4.54	131.13	124.24
19	3	3006	CLA	C4C-CHD-C1D	-4.54	113.06	125.98
19	4	4002	CLA	C4A-NA-C1A	4.53	108.75	106.68
19	B	1229	CLA	O2D-CGD-O1D	-4.53	115.03	123.85
19	4	4011	CLA	C3A-C4A-CHB	-4.53	118.36	123.91
19	1	1005	CLA	O2D-CGD-O1D	-4.53	115.03	123.85
19	B	1226	CLA	C4A-NA-C1A	4.53	108.75	106.68
19	2	2006	CLA	CHD-C4C-C3C	-4.53	118.17	124.77
19	B	1220	CLA	C4B-CHC-C1C	-4.53	115.60	126.25
19	1	1001	CLA	CHB-C4A-NA	4.53	130.94	124.40
19	1	1303	CLA	C4B-CHC-C1C	-4.53	115.60	126.25
19	A	1127	CLA	CHD-C4C-NC	4.53	131.25	124.23
19	4	4002	CLA	C4B-CHC-C1C	-4.52	115.61	126.25
19	B	1222	CLA	CHD-C4C-C3C	-4.52	118.18	124.77
19	A	1121	CLA	C4B-CHC-C1C	-4.52	115.61	126.25
19	4	4007	CLA	C4B-CHC-C1C	-4.52	115.63	126.25
21	1	6023	BCR	C3-C4-C5	-4.52	106.00	114.06
19	B	1212	CLA	CHD-C4C-NC	4.51	131.23	124.23
19	4	1004	CLA	CHD-C4C-NC	4.51	131.23	124.23
19	B	1238	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
19	1	1008	CLA	CHD-C4C-C3C	-4.51	118.20	124.77
19	B	1215	CLA	C2B-C1B-NB	4.51	115.00	110.33
19	R	1150	CLA	CHD-C4C-NC	4.51	131.22	124.23
19	4	1009	CLA	CAB-C3B-C2B	-4.51	111.56	123.53
19	A	1121	CLA	C4A-NA-C1A	4.51	108.73	106.68
19	A	1151	CLA	CMD-C2D-C3D	-4.51	117.36	127.69
19	A	1309	CLA	C2A-C1A-CHA	-4.51	114.95	122.63
19	B	1236	CLA	CHD-C4C-C3C	-4.51	118.20	124.77
19	A	1119	CLA	C2B-C1B-NB	4.51	115.00	110.33
19	2	2003	CLA	CHC-C1C-NC	4.50	130.95	124.33
19	B	1218	CLA	O2D-CGD-CBD	4.50	119.10	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	1147	CLA	OBD-CAD-C3D	-4.50	117.89	128.42
21	F	6014	BCR	C24-C23-C22	-4.50	119.57	126.23
19	4	4004	CLA	CHD-C4C-NC	4.50	131.08	124.24
19	1	1011	CLA	C4B-CHC-C1C	-4.50	115.66	126.25
19	B	1227	CLA	O2D-CGD-CBD	4.50	119.10	111.23
19	2	2002	CLA	CMD-C2D-C3D	-4.50	117.36	127.69
19	A	1123	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
19	3	3002	CLA	CHD-C4C-NC	4.50	131.08	124.24
19	B	1220	CLA	O2D-CGD-CBD	4.50	119.10	111.23
19	B	1221	CLA	CHD-C4C-NC	4.50	131.21	124.23
19	B	1201	CLA	CMD-C2D-C3D	-4.50	117.37	127.69
19	A	1309	CLA	CHC-C1C-NC	4.50	130.94	124.33
19	A	1132	CLA	CHC-C1C-NC	4.50	131.08	124.31
19	A	1309	CLA	CHD-C4C-NC	4.49	131.07	124.24
19	B	1236	CLA	CHC-C1C-NC	4.49	131.07	124.31
19	B	1215	CLA	CHC-C1C-NC	4.49	131.07	124.31
19	H	1145	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
19	A	1132	CLA	C2B-C1B-NB	4.49	114.98	110.33
19	B	1201	CLA	O2D-CGD-O1D	-4.49	115.11	123.85
19	4	4002	CLA	CMD-C2D-C1D	4.48	132.62	124.73
21	A	6003	BCR	C31-C1-C6	-4.48	103.21	110.24
19	H	1505	CLA	CHD-C4C-C3C	-4.48	118.24	124.77
19	4	4012	CLA	C1B-C2B-C3B	-4.48	102.82	107.03
19	A	1102	CLA	C4D-C3D-CAD	4.48	112.97	108.11
19	A	1107	CLA	CHC-C4B-NB	4.48	130.77	124.05
19	B	1222	CLA	O2D-CGD-CBD	4.48	119.06	111.23
19	B	1212	CLA	O2D-CGD-CBD	4.48	119.06	111.23
19	L	1130	CLA	C4D-C3D-CAD	4.48	112.97	108.11
19	3	3015	CLA	CHD-C4C-NC	4.48	131.04	124.24
19	B	1230	CLA	CHD-C4C-C3C	-4.47	118.25	124.77
19	L	1148	CLA	CHD-C4C-C3C	-4.47	118.25	124.77
22	2	7031	LMU	O1B-C1B-C2B	4.47	119.10	108.09
19	1	1001	CLA	CHC-C1C-NC	4.47	131.05	124.31
19	2	2003	CLA	C2A-C1A-CHA	-4.47	115.01	122.63
19	I	1204	CLA	CHD-C4C-C3C	-4.47	118.26	124.77
19	B	1211	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
21	I	6018	BCR	C29-C30-C25	-4.46	103.96	110.44
19	B	1210	CLA	C2B-C1B-NB	4.46	114.95	110.33
19	2	2007	CLA	O2D-CGD-O1D	-4.46	115.16	123.85
19	1	1310	CLA	C3B-C2B-C1B	-4.46	101.84	106.81
19	B	1214	CLA	C2B-C1B-NB	4.46	114.95	110.33
19	B	1226	CLA	CHD-C4C-C3C	-4.46	118.27	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1134	CLA	CHC-C1C-NC	4.46	131.03	124.31
19	B	1238	CLA	CHD-C4C-C3C	-4.46	118.27	124.77
19	2	2002	CLA	CHD-C4C-NC	4.46	131.14	124.23
19	3	3016	CLA	CHD-C4C-C3C	-4.46	118.28	124.77
19	4	4010	CLA	C4C-CHD-C1D	-4.45	113.30	125.98
21	A	6011	BCR	C31-C1-C6	-4.45	103.26	110.24
19	4	1306	CLA	C2B-C1B-NB	4.45	114.94	110.33
19	K	1143	CLA	CHC-C1C-NC	4.45	131.01	124.31
19	A	1131	CLA	C4B-CHC-C1C	-4.45	115.79	126.25
19	A	1110	CLA	O2D-CGD-CBD	4.45	119.01	111.23
19	A	1108	CLA	CHD-C4C-NC	4.45	131.13	124.23
19	A	1119	CLA	CMD-C2D-C3D	-4.45	117.49	127.69
19	A	9011	CLA	C4B-C3B-C2B	4.45	112.83	107.30
19	1	1006	CLA	CHD-C4C-C3C	-4.45	118.01	125.03
19	R	1144	CLA	CHD-C4C-NC	4.45	131.13	124.23
19	4	4007	CLA	C4A-NA-C1A	4.45	108.71	106.68
19	1	1310	CLA	CHD-C4C-NC	4.44	130.99	124.24
19	B	1233	CLA	C2B-C1B-NB	4.44	114.93	110.33
19	A	1120	CLA	CHD-C4C-NC	4.44	131.12	124.23
19	4	1304	CLA	CMD-C2D-C3D	-4.44	117.50	127.69
19	L	1148	CLA	C2B-C1B-NB	4.44	114.93	110.33
19	2	2005	CLA	CHD-C4C-NC	4.44	130.99	124.24
19	K	1142	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
21	A	6003	BCR	C2-C1-C6	-4.44	104.00	110.44
19	3	3001	CLA	C2A-C1A-CHA	-4.43	115.07	122.63
19	A	1117	CLA	CHD-C4C-C3C	-4.43	118.31	124.77
19	3	3012	CLA	CHC-C1C-NC	4.43	130.84	124.33
19	1	1005	CLA	CHD-C4C-NC	4.43	131.10	124.23
19	1	1013	CLA	C4B-CHC-C1C	-4.43	115.83	126.25
19	1	1013	CLA	CHC-C1C-NC	4.43	130.98	124.31
19	A	1131	CLA	O2D-CGD-CBD	4.42	118.97	111.23
19	2	2008	CLA	C2A-C1A-CHA	-4.42	115.09	122.63
19	1	1010	CLA	CHC-C4B-NB	4.42	130.69	124.05
19	3	3003	CLA	CBD-CAD-C3D	-4.42	102.35	108.25
19	A	1104	CLA	CHD-C4C-C3C	-4.42	118.33	124.77
19	A	1137	CLA	CHD-C4C-C3C	-4.42	118.33	124.77
19	3	3005	CLA	C4A-NA-C1A	4.42	108.69	106.68
19	4	1009	CLA	C2B-C1B-NB	4.42	114.91	110.33
19	3	3015	CLA	C2A-C1A-CHA	-4.42	115.10	122.63
19	4	1004	CLA	C2B-C1B-NB	4.41	114.90	110.33
19	A	1116	CLA	CHD-C4C-C3C	-4.41	118.34	124.77
19	L	1504	CLA	O2D-CGD-O1D	-4.41	115.27	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	I	6018	BCR	C28-C27-C26	-4.41	106.20	114.06
19	4	4012	CLA	CHD-C4C-NC	4.40	131.06	124.23
19	2	1307	CLA	C1B-NB-C4B	-4.40	103.22	106.31
19	F	1305	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
19	A	1237	CLA	CHD-C4C-NC	4.40	131.06	124.23
19	4	4014	CLA	CHD-C4C-NC	4.40	131.05	124.23
19	B	1211	CLA	C4B-CHC-C1C	-4.40	115.90	126.25
21	A	6008	BCR	C3-C4-C5	-4.40	106.21	114.06
19	F	1240	CLA	CMD-C2D-C3D	-4.40	117.61	127.69
19	4	1306	CLA	CAC-C3C-C4C	4.40	130.51	124.79
19	3	3010	CLA	CHD-C4C-NC	4.40	130.92	124.24
19	3	3010	CLA	C2A-C1A-CHA	-4.40	115.14	122.63
19	4	4007	CLA	CHC-C1C-NC	4.39	130.93	124.31
19	2	2013	CLA	CHD-C4C-C3C	-4.39	118.37	124.77
19	3	3004	CLA	C3A-C4A-CHB	-4.39	118.53	123.91
19	3	3012	CLA	C2D-C3D-C4D	-4.39	102.01	107.35
19	3	1147	CLA	C4B-CHC-C1C	-4.39	115.92	126.25
19	B	1230	CLA	CHD-C4C-NC	4.39	131.04	124.23
19	4	4001	CLA	CHD-C4C-NC	4.39	131.04	124.23
19	2	2006	CLA	C2B-C1B-NB	4.39	114.88	110.33
19	B	1224	CLA	CMD-C2D-C3D	-4.39	117.62	127.69
19	A	1139	CLA	C4B-CHC-C1C	-4.38	115.94	126.25
19	1	1003	CLA	CHD-C4C-NC	4.38	131.03	124.23
19	A	1149	CLA	O2D-CGD-O1D	-4.38	115.32	123.85
19	A	1120	CLA	CMD-C2D-C3D	-4.38	117.64	127.69
19	A	1121	CLA	CHD-C4C-NC	4.38	131.02	124.23
19	A	1122	CLA	CHD-C4C-NC	4.38	131.02	124.23
19	H	1145	CLA	C4B-CHC-C1C	-4.37	115.97	126.25
19	B	1225	CLA	CMD-C2D-C1D	4.37	132.42	124.73
19	R	1150	CLA	CHD-C4C-C3C	-4.37	118.40	124.77
19	A	1149	CLA	C3A-C2A-C1A	4.37	107.88	101.34
19	1	1013	CLA	CGD-CBD-CAD	-4.37	96.71	110.85
19	B	1301	CLA	CHD-C4C-NC	4.37	131.00	124.23
19	3	3015	CLA	C3A-C4A-CHB	-4.37	118.56	123.91
19	A	1108	CLA	CMD-C2D-C3D	-4.37	117.67	127.69
19	F	1240	CLA	CHC-C1C-NC	4.37	130.89	124.31
19	K	1143	CLA	C4B-CHC-C1C	-4.37	115.98	126.25
19	A	1139	CLA	CHD-C4C-C3C	-4.37	118.41	124.77
19	B	1212	CLA	CHD-C4C-C3C	-4.37	118.41	124.77
19	B	1223	CLA	CHD-C4C-C3C	-4.36	118.41	124.77
19	3	3013	CLA	CHC-C4B-NB	4.36	130.60	124.05
19	A	1109	CLA	C4A-NA-C1A	4.36	108.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1224	CLA	CHD-C4C-C3C	-4.36	118.41	124.77
19	J	1311	CLA	CHD-C4C-C3C	-4.36	118.41	124.77
21	A	6007	BCR	C20-C19-C18	-4.36	114.40	126.36
19	A	1101	CLA	C4B-CHC-C1C	-4.36	115.99	126.25
19	B	1227	CLA	C2B-C1B-NB	4.36	114.84	110.33
19	A	1113	CLA	CHD-C4C-NC	4.36	130.99	124.23
19	3	3008	CLA	CHD-C4C-C3C	-4.35	118.42	124.77
21	A	6003	BCR	C15-C14-C13	-4.35	121.17	127.28
19	B	1201	CLA	CHC-C1C-NC	4.35	130.87	124.31
19	H	1145	CLA	CHD-C4C-NC	4.35	130.98	124.23
19	A	1133	CLA	CMD-C2D-C3D	-4.35	117.71	127.69
19	3	3015	CLA	CHC-C1C-NC	4.35	130.73	124.33
21	B	6017	BCR	C32-C1-C6	-4.35	103.42	110.24
21	A	6011	BCR	C2-C1-C6	-4.35	104.12	110.44
19	A	1119	CLA	CHD-C4C-NC	4.35	130.97	124.23
19	B	1232	CLA	C4B-CHC-C1C	-4.35	116.02	126.25
19	B	1201	CLA	CHD-C4C-C3C	-4.35	118.43	124.77
19	A	1108	CLA	C3B-C4B-NB	-4.35	106.65	110.53
19	A	1109	CLA	C4B-CHC-C1C	-4.35	116.02	126.25
19	A	1127	CLA	C4B-CHC-C1C	-4.35	116.03	126.25
19	B	1219	CLA	C4B-CHC-C1C	-4.34	116.03	126.25
19	3	3012	CLA	C3B-C2B-C1B	-4.34	101.98	106.81
21	L	6019	BCR	C23-C24-C25	-4.34	115.40	127.00
19	B	1224	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
19	K	1146	CLA	CHD-C4C-NC	4.34	130.96	124.23
19	B	1236	CLA	C2B-C1B-NB	4.34	114.83	110.33
19	B	9010	CLA	CHD-C4C-NC	4.34	130.96	124.23
19	A	1134	CLA	C4B-CHC-C1C	-4.34	116.05	126.25
19	1	1003	CLA	O2D-CGD-O1D	-4.34	115.41	123.85
19	A	1102	CLA	CMD-C2D-C3D	-4.34	117.74	127.69
19	2	2013	CLA	C4B-CHC-C1C	-4.34	116.05	126.25
19	A	1133	CLA	C2B-C1B-NB	4.34	114.82	110.33
19	A	9011	CLA	C2B-C1B-NB	4.34	114.82	110.33
19	B	1218	CLA	C2B-C1B-NB	4.34	114.82	110.33
19	4	4015	CLA	O1D-CGD-CBD	-4.33	115.97	124.52
19	B	1232	CLA	C2B-C1B-NB	4.33	114.82	110.33
19	L	1130	CLA	C4-C3-C5	4.33	122.74	115.23
19	A	9013	CLA	CHD-C4C-C3C	-4.33	118.46	124.77
19	3	3005	CLA	C4C-CHD-C1D	-4.33	113.65	125.98
19	A	1113	CLA	C2B-C1B-NB	4.33	114.81	110.33
21	F	6014	BCR	C29-C30-C25	-4.33	104.15	110.44
19	F	1305	CLA	O2D-CGD-O1D	-4.33	115.43	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1101	CLA	CHD-C4C-C3C	-4.33	118.47	124.77
19	4	4001	CLA	CHD-C4C-C3C	-4.32	118.47	124.77
19	4	4005	CLA	C3A-C4A-CHB	-4.32	118.61	123.91
19	A	9012	CLA	O2D-CGD-CBD	4.32	118.79	111.23
19	4	4005	CLA	CHA-C4D-ND	4.32	130.95	124.84
21	B	6017	BCR	C15-C16-C17	-4.32	114.68	123.52
19	B	1210	CLA	CHC-C1C-NC	4.32	130.82	124.31
21	A	6007	BCR	C33-C5-C6	-4.32	119.77	124.48
19	3	2009	CLA	C4B-CHC-C1C	-4.32	116.09	126.25
19	1	1310	CLA	CHC-C1C-NC	4.32	130.68	124.33
19	4	4003	CLA	CHD-C4C-NC	4.32	130.92	124.23
22	4	7019	LMU	C2'-C3'-C4'	4.32	119.48	109.68
19	A	1132	CLA	C4B-CHC-C1C	-4.32	116.10	126.25
19	B	9010	CLA	CHC-C1C-NC	4.31	130.81	124.31
19	A	1103	CLA	CHC-C4B-NB	4.31	130.52	124.05
19	3	1118	CLA	CHD-C4C-C3C	-4.31	118.22	125.03
19	1	1013	CLA	CMB-C2B-C1B	4.31	131.98	125.42
19	R	1150	CLA	O2A-CGA-CBA	4.31	124.98	111.83
19	A	1141	CLA	C2B-C1B-NB	4.31	114.80	110.33
19	B	1230	CLA	C4B-CHC-C1C	-4.31	116.11	126.25
19	4	4005	CLA	C4C-CHD-C1D	-4.31	113.71	125.98
19	A	1111	CLA	C1-C2-C3	-4.31	119.14	126.20
19	B	1233	CLA	CHD-C4C-C3C	-4.31	118.49	124.77
19	A	1128	CLA	CHD-C4C-C3C	-4.31	118.50	124.77
19	A	1132	CLA	CHC-C4B-NB	4.30	130.50	124.05
19	K	1146	CLA	CMD-C2D-C3D	-4.30	117.82	127.69
19	B	1215	CLA	O2D-CGD-CBD	4.30	118.75	111.23
19	3	3014	CLA	C2D-C3D-C4D	-4.30	102.13	107.35
19	B	1206	CLA	C4B-CHC-C1C	-4.30	116.14	126.25
19	3	3008	CLA	C2B-C1B-NB	4.30	114.78	110.33
19	3	3006	CLA	C4A-NA-C1A	4.30	108.64	106.68
19	A	1309	CLA	C3A-C4A-CHB	-4.29	118.65	123.91
19	4	4011	CLA	CHA-C4D-ND	4.29	130.91	124.84
19	B	1216	CLA	C4B-CHC-C1C	-4.29	116.15	126.25
19	L	1148	CLA	CHD-C4C-NC	4.29	130.89	124.23
19	A	1129	CLA	CHC-C1C-NC	4.29	130.78	124.31
19	A	1107	CLA	CMD-C2D-C3D	-4.29	117.85	127.69
19	B	1236	CLA	C4B-CHC-C1C	-4.29	116.16	126.25
19	4	1304	CLA	C2B-C1B-NB	4.29	114.78	110.33
22	1	7013	LMU	O1B-C4'-C3'	4.29	118.14	107.23
19	B	1239	CLA	C4B-C3B-C2B	4.29	112.64	107.30
19	2	2014	CLA	CHD-C4C-NC	4.29	130.88	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	4012	CLA	CBD-CHA-C1A	4.29	133.85	127.38
21	3	6022	BCR	C33-C5-C6	-4.29	119.81	124.48
19	A	1102	CLA	C4B-C3B-C2B	4.29	112.63	107.30
22	B	7040	LMU	O5B-C5B-C4B	-4.29	101.97	109.70
19	1	1011	CLA	C2B-C1B-NB	4.29	114.77	110.33
19	B	1218	CLA	CMD-C2D-C3D	-4.29	117.86	127.69
19	A	1126	CLA	O2D-CGD-CBD	4.29	118.72	111.23
19	B	1235	CLA	CHC-C1C-NC	4.29	130.76	124.31
19	H	1145	CLA	CHC-C1C-NC	4.28	130.76	124.31
22	B	7040	LMU	C1B-O1B-C4'	-4.28	107.82	117.98
19	3	3007	CLA	CMD-C2D-C3D	-4.28	117.87	127.69
19	A	1131	CLA	C2B-C1B-NB	4.28	114.77	110.33
19	A	1122	CLA	C4B-CHC-C1C	-4.28	116.18	126.25
19	2	2005	CLA	C2D-C3D-C4D	-4.28	102.15	107.35
19	3	1147	CLA	CAA-C2A-C1A	4.28	126.00	111.97
19	1	1006	CLA	CHC-C1C-NC	4.28	130.76	124.31
19	1	1003	CLA	CGD-CBD-CAD	-4.28	97.00	110.85
19	A	1151	CLA	CHD-C4C-NC	4.28	130.86	124.23
19	B	1210	CLA	O2D-CGD-CBD	4.27	118.70	111.23
19	A	1141	CLA	CHD-C4C-C3C	-4.27	118.54	124.77
19	A	1101	CLA	O2D-CGD-O1D	-4.27	115.53	123.85
19	R	1150	CLA	C4B-CHC-C1C	-4.27	116.21	126.25
19	4	4004	CLA	C3B-C2B-C1B	-4.27	102.06	106.81
19	3	3002	CLA	C3A-C4A-CHB	-4.27	118.68	123.91
21	L	6019	BCR	C3-C4-C5	-4.27	106.45	114.06
19	B	1217	CLA	C4B-CHC-C1C	-4.27	116.22	126.25
19	2	2013	CLA	CHC-C4B-NB	4.26	130.45	124.05
19	2	2001	CLA	CHD-C4C-C3C	-4.26	118.56	124.77
19	H	1145	CLA	CHB-C4A-NA	4.26	130.55	124.40
19	A	1116	CLA	CMD-C2D-C3D	-4.26	117.92	127.69
19	4	4007	CLA	CHD-C4C-C3C	-4.26	118.56	124.77
19	1	1012	CLA	CMD-C2D-C3D	-4.26	117.92	127.69
19	4	4015	CLA	C2B-C1B-NB	4.26	114.74	110.33
19	B	1226	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
19	2	2010	CLA	CHC-C1C-NC	4.26	130.59	124.33
19	3	3012	CLA	C2A-C1A-CHA	-4.26	115.37	122.63
19	A	1138	CLA	CMD-C2D-C3D	-4.26	117.93	127.69
21	A	6002	BCR	C31-C1-C6	-4.26	103.57	110.24
19	1	1014	CLA	C4B-CHC-C1C	-4.25	116.24	126.25
19	A	1102	CLA	CHD-C4C-C3C	-4.25	118.57	124.77
19	B	1211	CLA	CHD-C4C-NC	4.25	130.82	124.23
19	B	1219	CLA	CMD-C2D-C3D	-4.25	117.95	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	4014	CLA	C4A-NA-C1A	4.25	108.62	106.68
22	R	7014	LMU	O1'-C1'-C2'	4.25	114.72	108.27
19	A	1121	CLA	CHC-C4B-NB	4.24	130.42	124.05
19	3	3014	CLA	CHD-C4C-NC	4.24	130.69	124.24
19	3	3011	CLA	CHD-C4C-NC	4.24	130.81	124.23
19	F	1302	CLA	CMD-C2D-C3D	-4.24	117.96	127.69
19	A	1129	CLA	C4B-CHC-C1C	-4.24	116.27	126.25
19	F	1302	CLA	CHD-C4C-C3C	-4.24	118.59	124.77
19	2	2008	CLA	C1B-NB-C4B	-4.24	103.34	106.31
19	A	1104	CLA	C4B-CHC-C1C	-4.24	116.28	126.25
19	3	3002	CLA	C4A-NA-C1A	4.24	108.61	106.68
19	A	1108	CLA	CHC-C1C-NC	4.24	130.69	124.31
19	2	2006	CLA	C4B-CHC-C1C	-4.24	116.29	126.25
19	B	1219	CLA	CHD-C4C-NC	4.24	130.80	124.23
19	A	1136	CLA	CHC-C1C-NC	4.24	130.69	124.31
19	1	1002	CLA	CHC-C1C-NC	4.23	130.69	124.31
19	B	1227	CLA	C4B-CHC-C1C	-4.23	116.30	126.25
19	A	1112	CLA	CMB-C2B-C1B	4.23	131.86	125.42
19	B	1215	CLA	C4B-CHC-C1C	-4.23	116.30	126.25
19	4	1004	CLA	CHC-C1C-NC	4.23	130.68	124.31
19	2	2012	CLA	O2D-CGD-O1D	-4.23	115.62	123.85
19	A	1122	CLA	C2B-C1B-NB	4.23	114.71	110.33
19	G	1242	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
21	F	6016	BCR	C8-C7-C6	-4.23	115.70	127.00
19	3	3010	CLA	C4A-NA-C1A	4.23	108.61	106.68
19	A	1128	CLA	CBB-CAB-C3B	4.23	148.65	127.53
19	A	1133	CLA	CHD-C4C-NC	4.22	130.78	124.23
19	A	1140	CLA	CHD-C4C-C3C	-4.22	118.61	124.77
19	1	1012	CLA	CHD-C4C-C3C	-4.22	118.36	125.03
19	L	1502	CLA	C4B-CHC-C1C	-4.22	116.32	126.25
19	A	1111	CLA	C4A-NA-C1A	4.22	108.61	106.68
19	A	1105	CLA	C4B-CHC-C1C	-4.22	116.32	126.25
19	B	1228	CLA	C4B-CHC-C1C	-4.22	116.32	126.25
19	B	1209	CLA	C4B-CHC-C1C	-4.22	116.33	126.25
21	A	6002	BCR	C2-C1-C6	-4.22	104.31	110.44
19	4	4004	CLA	C4C-CHD-C1D	-4.22	113.96	125.98
19	L	1501	CLA	C2B-C1B-NB	4.22	114.70	110.33
19	A	1237	CLA	C4A-NA-C1A	4.22	108.60	106.68
19	A	1149	CLA	C4B-CHC-C1C	-4.21	116.34	126.25
19	H	1505	CLA	C4B-CHC-C1C	-4.21	116.34	126.25
19	3	3001	CLA	C4A-NA-C1A	4.21	108.60	106.68
19	A	1126	CLA	CMD-C2D-C3D	-4.21	118.03	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1138	CLA	C4B-CHC-C1C	-4.21	116.34	126.25
19	2	2011	CLA	C3B-C2B-C1B	-4.21	102.12	106.81
19	4	4012	CLA	C4A-NA-C1A	4.21	108.60	106.68
19	B	1205	CLA	C4B-CHC-C1C	-4.21	116.35	126.25
19	2	2003	CLA	C1B-NB-C4B	-4.21	103.36	106.31
19	A	1139	CLA	CMD-C2D-C3D	-4.21	118.05	127.69
19	A	1112	CLA	CHD-C4C-NC	4.20	130.75	124.23
22	H	7017	LMU	C1'-O5'-C5'	4.20	121.93	113.72
19	1	1015	CLA	CHC-C1C-NC	4.20	130.51	124.33
19	A	1132	CLA	C4-C3-C5	4.20	122.52	115.23
19	B	1301	CLA	C4A-NA-C1A	4.20	108.59	106.68
19	3	3012	CLA	C4A-NA-C1A	4.20	108.59	106.68
19	A	1110	CLA	C2B-C1B-NB	4.20	114.68	110.33
19	H	1241	CLA	C2B-C1B-NB	4.20	114.68	110.33
19	4	4003	CLA	C4B-CHC-C1C	-4.20	116.38	126.25
19	4	4011	CLA	C3B-C2B-C1B	-4.20	102.14	106.81
19	A	1309	CLA	C1C-CHC-C4B	-4.20	114.97	126.04
19	4	4005	CLA	CHC-C1C-NC	4.20	130.50	124.33
19	1	1310	CLA	C1B-NB-C4B	-4.19	103.37	106.31
22	R	7014	LMU	C1'-C2'-C3'	-4.19	101.19	110.01
19	B	1213	CLA	CHD-C4C-C3C	-4.19	118.66	124.77
19	A	1119	CLA	CHC-C1C-NC	4.19	130.63	124.31
19	1	1002	CLA	CAA-C2A-C1A	4.19	125.72	111.97
19	B	1208	CLA	C2B-C1B-NB	4.19	114.67	110.33
19	L	1130	CLA	C4B-CHC-C1C	-4.19	116.39	126.25
19	3	3007	CLA	C4B-CHC-C1C	-4.19	116.39	126.25
19	2	2004	CLA	CHD-C4C-NC	4.19	130.73	124.23
19	B	1239	CLA	CMB-C2B-C1B	4.19	131.80	125.42
19	1	1006	CLA	C4B-CHC-C1C	-4.19	116.39	126.25
19	A	1151	CLA	CHC-C1C-NC	4.19	130.62	124.31
19	B	1209	CLA	CHC-C1C-NC	4.19	130.62	124.31
19	A	1136	CLA	C4B-CHC-C1C	-4.19	116.39	126.25
19	2	2001	CLA	C2B-C1B-NB	4.19	114.67	110.33
19	A	1109	CLA	C1-C2-C3	-4.19	119.34	126.20
19	A	1127	CLA	CHC-C1C-NC	4.19	130.62	124.31
19	2	2010	CLA	C4C-CHD-C1D	-4.18	114.06	125.98
19	4	1004	CLA	CMD-C2D-C3D	-4.18	118.10	127.69
19	A	1123	CLA	CMD-C2D-C3D	-4.18	118.10	127.69
19	3	3017	CLA	CHD-C4C-NC	4.18	130.71	124.23
19	4	4013	CLA	CHD-C4C-NC	4.18	130.59	124.24
19	4	4010	CLA	C2A-C1A-CHA	-4.18	115.50	122.63
19	4	4010	CLA	CHC-C1C-NC	4.18	130.47	124.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	3007	CLA	CHC-C1C-NC	4.18	130.60	124.31
19	1	1006	CLA	C4A-NA-C1A	4.18	108.58	106.68
19	B	1218	CLA	C4B-CHC-C1C	-4.18	116.42	126.25
19	H	1145	CLA	CHD-C4C-C3C	-4.18	118.68	124.77
19	1	1015	CLA	C2A-C1A-CHA	-4.18	115.51	122.63
19	A	1127	CLA	C2B-C1B-NB	4.17	114.66	110.33
19	2	2001	CLA	CMD-C2D-C3D	-4.17	118.12	127.69
19	3	3014	CLA	C3B-C2B-C1B	-4.17	102.17	106.81
19	4	4014	CLA	CAC-C3C-C4C	4.17	130.22	124.79
19	1	1005	CLA	OBD-CAD-C3D	-4.17	118.66	128.42
19	4	4004	CLA	C1B-NB-C4B	-4.17	103.38	106.31
19	B	1214	CLA	CHC-C1C-NC	4.17	130.59	124.31
19	3	2009	CLA	CMD-C2D-C3D	-4.17	118.12	127.69
19	B	1226	CLA	CHC-C1C-NC	4.17	130.59	124.31
19	4	4014	CLA	C2B-C1B-NB	4.17	114.65	110.33
19	3	3002	CLA	C4C-CHD-C1D	-4.17	114.10	125.98
19	2	2008	CLA	C4C-CHD-C1D	-4.17	114.10	125.98
22	G	7039	LMU	C1B-O5B-C5B	-4.17	105.58	113.72
19	B	1223	CLA	C4B-CHC-C1C	-4.17	116.44	126.25
19	2	1307	CLA	C2D-C3D-C4D	-4.17	102.29	107.35
19	H	1505	CLA	C4-C3-C5	4.17	122.46	115.23
19	2	2001	CLA	CHC-C1C-NC	4.16	130.58	124.31
19	B	1221	CLA	OBD-CAD-C3D	-4.16	118.69	128.42
19	B	1217	CLA	C2B-C1B-NB	4.16	114.64	110.33
19	2	2005	CLA	C3A-C4A-CHB	-4.16	118.81	123.91
19	A	1138	CLA	CHC-C1C-NC	4.16	130.58	124.31
21	A	6002	BCR	C7-C8-C9	-4.16	120.08	126.23
21	I	6018	BCR	C4-C5-C6	-4.16	117.08	122.70
19	A	1141	CLA	CMD-C2D-C3D	-4.16	118.15	127.69
19	L	1504	CLA	C4A-NA-C1A	4.16	108.58	106.68
21	B	6005	BCR	C38-C26-C25	-4.16	119.94	124.48
19	L	1502	CLA	CHC-C1C-NC	4.16	130.57	124.31
19	A	9023	CLA	CHB-C4A-NA	4.16	130.40	124.40
19	2	1307	CLA	C4A-NA-C1A	4.16	108.58	106.68
19	3	3014	CLA	C4A-NA-C1A	4.16	108.58	106.68
19	2	2004	CLA	O2D-CGD-CBD	4.16	118.50	111.23
19	A	1134	CLA	CMD-C2D-C3D	-4.16	118.16	127.69
19	4	4013	CLA	C3A-C4A-CHB	-4.16	118.82	123.91
21	B	6004	BCR	C23-C24-C25	-4.15	115.90	127.00
19	A	9012	CLA	C4B-CHC-C1C	-4.15	116.48	126.25
19	B	1225	CLA	C4B-CHC-C1C	-4.15	116.48	126.25
19	A	1136	CLA	CHD-C4C-C3C	-4.15	118.72	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1103	CLA	C2B-C1B-NB	4.15	114.63	110.33
19	A	1139	CLA	C2B-C1B-NB	4.15	114.63	110.33
21	A	6002	BCR	C10-C11-C12	-4.15	111.18	123.20
19	3	3013	CLA	CED-O2D-CGD	4.15	125.33	115.92
22	4	7052	LMU	C1'-C2'-C3'	4.15	118.73	110.01
19	A	1141	CLA	C4B-CHC-C1C	-4.15	116.50	126.25
19	A	1106	CLA	C4B-CHC-C1C	-4.15	116.50	126.25
19	B	9010	CLA	C4A-NA-C1A	4.14	108.57	106.68
19	A	1237	CLA	C4B-CHC-C1C	-4.14	116.50	126.25
19	1	1002	CLA	CHD-C4C-C3C	-4.14	118.73	124.77
19	3	1147	CLA	CMD-C2D-C1D	4.14	132.02	124.73
19	A	1115	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
19	B	1224	CLA	O2A-CGA-CBA	4.14	124.46	111.83
19	3	3012	CLA	CHD-C4C-NC	4.14	130.53	124.24
19	A	1123	CLA	CHD-C4C-NC	4.14	130.65	124.23
19	A	1105	CLA	CHD-C4C-NC	4.14	130.65	124.23
19	4	1306	CLA	CMD-C2D-C3D	-4.14	118.20	127.69
19	A	1102	CLA	CHC-C1C-NC	4.14	130.54	124.31
19	3	3001	CLA	C4C-CHD-C1D	-4.14	114.19	125.98
19	A	1106	CLA	CHD-C4C-C3C	-4.14	118.74	124.77
21	A	6008	BCR	C23-C24-C25	-4.14	115.95	127.00
19	3	3016	CLA	C4B-CHC-C1C	-4.14	116.52	126.25
21	A	6011	BCR	C33-C5-C6	-4.14	119.97	124.48
19	F	1302	CLA	C2B-C1B-NB	4.13	114.61	110.33
19	2	2010	CLA	C2A-C1A-CHA	-4.13	115.58	122.63
19	1	1015	CLA	C4A-NA-C1A	4.13	108.56	106.68
19	3	3003	CLA	C2B-C1B-NB	4.13	114.61	110.33
19	A	1115	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
19	B	1203	CLA	C6-C5-C3	-4.13	103.40	113.47
19	A	1113	CLA	O2D-CGD-CBD	4.13	118.45	111.23
21	B	6020	BCR	C36-C18-C19	4.13	124.40	118.09
22	G	7051	LMU	O1'-C1'-C2'	4.13	114.55	108.27
19	A	1103	CLA	O2D-CGD-CBD	4.13	118.45	111.23
21	A	6011	BCR	C23-C24-C25	-4.13	115.96	127.00
21	I	6021	BCR	C8-C7-C6	-4.13	115.96	127.00
21	B	6006	BCR	C40-C30-C25	4.13	116.72	110.24
24	B	7101	LMG	O7-C10-C11	4.13	120.42	111.48
19	A	1138	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
19	A	9023	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
19	B	1209	CLA	CMD-C2D-C3D	-4.13	118.22	127.69
19	4	4011	CLA	C3D-C4D-CHA	-4.13	115.98	125.20
19	A	1140	CLA	C4B-CHC-C1C	-4.13	116.54	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	3002	CLA	CHC-C1C-NC	4.13	130.40	124.33
19	2	2012	CLA	C4B-CHC-C1C	-4.13	116.55	126.25
19	3	3016	CLA	C2B-C1B-NB	4.13	114.60	110.33
19	A	1135	CLA	CHD-C4C-C3C	-4.12	118.76	124.77
19	B	1221	CLA	C2B-C1B-NB	4.12	114.60	110.33
19	A	1123	CLA	C4B-CHC-C1C	-4.12	116.55	126.25
21	A	6002	BCR	C11-C12-C13	-4.12	115.06	126.36
19	H	1207	CLA	C4B-CHC-C1C	-4.12	116.56	126.25
19	2	4009	CLA	C4B-CHC-C1C	-4.12	116.56	126.25
19	B	1214	CLA	C4B-CHC-C1C	-4.12	116.56	126.25
19	2	2011	CLA	C4C-CHD-C1D	-4.12	114.24	125.98
19	H	1145	CLA	CMD-C2D-C3D	-4.12	118.24	127.69
19	A	1139	CLA	CHC-C1C-NC	4.12	130.51	124.31
19	1	1015	CLA	CHD-C4C-NC	4.12	130.50	124.24
19	I	1204	CLA	C2B-C1B-NB	4.12	114.60	110.33
21	1	6023	BCR	C32-C1-C2	4.12	124.75	108.95
19	A	1129	CLA	O2D-CGD-O1D	-4.12	115.84	123.85
19	B	1205	CLA	C1-C2-C3	-4.11	119.45	126.20
19	2	2013	CLA	CHD-C4C-NC	4.11	130.61	124.23
19	A	1116	CLA	O2A-CGA-CBA	4.11	124.37	111.83
19	B	1205	CLA	CHC-C1C-NC	4.11	130.50	124.31
22	B	7038	LMU	C3'-C4'-C5'	-4.11	101.82	110.93
19	A	1135	CLA	C4B-CHC-C1C	-4.11	116.58	126.25
19	B	1222	CLA	CMD-C2D-C3D	-4.11	118.27	127.69
19	4	4014	CLA	CHC-C4B-NB	4.11	130.21	124.05
19	1	1006	CLA	CBD-CHA-C1A	4.11	133.58	127.38
19	4	4012	CLA	C2B-C1B-NB	4.10	114.58	110.33
19	B	1235	CLA	O2D-CGD-O1D	-4.10	115.86	123.85
19	3	1118	CLA	CMD-C2D-C3D	-4.10	118.28	127.69
22	H	7043	LMU	O5B-C5B-C4B	4.10	117.09	109.70
19	1	1003	CLA	CHD-C4C-C3C	-4.10	118.79	124.77
19	A	1121	CLA	CMD-C2D-C3D	-4.10	118.28	127.69
19	H	1207	CLA	CHD-C4C-C3C	-4.10	118.79	124.77
19	3	3014	CLA	C1C-CHC-C4B	-4.10	115.22	126.04
19	3	1118	CLA	C4B-CHC-C1C	-4.10	116.61	126.25
19	K	1143	CLA	CMD-C2D-C3D	-4.10	118.29	127.69
19	B	1202	CLA	C4A-NA-C1A	4.10	108.55	106.68
19	L	1503	CLA	C2B-C1B-NB	4.10	114.58	110.33
21	F	6016	BCR	C39-C30-C25	4.10	116.67	110.24
19	2	2003	CLA	C4C-CHD-C1D	-4.09	114.31	125.98
19	R	1144	CLA	CHD-C4C-C3C	-4.09	118.80	124.77
19	B	1208	CLA	C1B-C2B-C3B	-4.09	103.18	107.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1006	CLA	C1B-C2B-C3B	-4.09	103.18	107.03
19	B	1230	CLA	CHC-C4B-NB	4.09	130.19	124.05
19	A	1237	CLA	C3B-C2B-C1B	-4.09	102.34	107.17
19	3	3016	CLA	CHC-C1C-NC	4.09	130.48	124.31
19	B	1222	CLA	C4B-CHC-C1C	-4.09	116.62	126.25
19	A	1113	CLA	CHC-C1C-NC	4.09	130.47	124.31
19	1	1007	CLA	C4B-CHC-C1C	-4.09	116.63	126.25
19	B	1209	CLA	CHD-C4C-NC	4.09	130.57	124.23
19	B	1233	CLA	CMD-C2D-C3D	-4.09	118.31	127.69
19	3	3011	CLA	C4B-CHC-C1C	-4.09	116.63	126.25
19	B	1230	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
19	L	1130	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
19	4	4011	CLA	C4C-CHD-C1D	-4.09	114.33	125.98
19	A	1117	CLA	CHC-C1C-NC	4.09	130.47	124.31
19	B	1211	CLA	O2D-CGD-CBD	4.08	118.37	111.23
19	1	1010	CLA	C4A-NA-C1A	4.08	108.54	106.68
19	2	2003	CLA	C4A-NA-C1A	4.08	108.54	106.68
19	3	3014	CLA	CHC-C1C-NC	4.08	130.33	124.33
19	A	1136	CLA	CMD-C2D-C3D	-4.08	118.33	127.69
19	4	4004	CLA	C4A-NA-C1A	4.08	108.54	106.68
19	2	2006	CLA	CHC-C1C-NC	4.08	130.46	124.31
22	2	7027	LMU	C1B-O1B-C4'	-4.08	108.31	117.98
19	B	1229	CLA	C4B-CHC-C1C	-4.08	116.65	126.25
19	J	1308	CLA	C4B-CHC-C1C	-4.08	116.65	126.25
19	3	3010	CLA	CHC-C1C-NC	4.08	130.33	124.33
19	A	1131	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
19	R	1144	CLA	C4B-CHC-C1C	-4.08	116.66	126.25
22	H	7043	LMU	C1B-O5B-C5B	4.08	121.68	113.72
19	2	2012	CLA	CMD-C2D-C3D	-4.08	118.34	127.69
19	A	1115	CLA	C4-C3-C5	4.08	122.30	115.23
19	1	1002	CLA	CHD-C4C-NC	4.08	130.55	124.23
19	B	1239	CLA	O2A-CGA-CBA	4.07	124.26	111.83
19	1	1008	CLA	C4B-CHC-C1C	-4.07	116.67	126.25
19	2	1307	CLA	CHD-C4C-NC	4.07	130.43	124.24
19	2	2010	CLA	C1B-NB-C4B	-4.07	103.45	106.31
19	1	1013	CLA	CHC-C4B-NB	4.07	130.16	124.05
19	2	2005	CLA	C3D-C4D-CHA	-4.07	116.11	125.20
19	B	1301	CLA	CAA-C2A-C3A	-4.07	106.89	116.23
19	A	1135	CLA	CMD-C2D-C3D	-4.07	118.36	127.69
19	4	1004	CLA	C4B-CHC-C1C	-4.07	116.68	126.25
19	J	1311	CLA	C4B-CHC-C1C	-4.07	116.68	126.25
19	3	3012	CLA	C1B-NB-C4B	-4.07	103.46	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1235	CLA	C2B-C1B-NB	4.07	114.55	110.33
19	4	4002	CLA	O2A-CGA-CBA	4.07	124.23	111.83
21	I	6021	BCR	C27-C26-C25	-4.07	117.21	122.70
22	3	7003	LMU	C1B-O1B-C4'	-4.07	108.34	117.98
19	3	3007	CLA	CAC-C3C-C4C	4.06	130.08	124.79
19	A	1124	CLA	C2B-C1B-NB	4.06	114.54	110.33
19	A	1131	CLA	CHD-C4C-C3C	-4.06	118.85	124.77
19	A	9022	CLA	C4A-NA-C1A	4.06	108.53	106.68
19	A	1124	CLA	CMD-C2D-C3D	-4.06	118.38	127.69
19	A	1124	CLA	CHC-C1C-NC	4.06	130.43	124.31
19	A	1111	CLA	C4B-CHC-C1C	-4.06	116.70	126.25
19	K	1142	CLA	C4B-CHC-C1C	-4.06	116.70	126.25
19	A	1101	CLA	C2B-C1B-NB	4.06	114.53	110.33
19	A	1128	CLA	C4B-CHC-C1C	-4.06	116.71	126.25
19	H	1241	CLA	C4B-CHC-C1C	-4.06	116.71	126.25
19	2	2001	CLA	C4B-CHC-C1C	-4.06	116.71	126.25
21	I	6021	BCR	C15-C16-C17	4.06	131.82	123.52
19	3	2009	CLA	CHC-C1C-NC	4.05	130.42	124.31
19	A	1151	CLA	C4B-CHC-C1C	-4.05	116.72	126.25
19	B	9010	CLA	CMD-C2D-C1D	4.05	131.87	124.73
19	B	1221	CLA	C4A-NA-C1A	4.05	108.53	106.68
19	2	2006	CLA	C4A-NA-C1A	4.05	108.53	106.68
19	B	1235	CLA	C3B-C2B-C1B	-4.05	102.39	107.17
19	A	1134	CLA	CHD-C4C-C3C	-4.05	118.87	124.77
19	2	4009	CLA	CHD-C4C-NC	4.05	130.51	124.23
19	B	1224	CLA	O1D-CGD-CBD	-4.05	116.54	124.52
19	3	3011	CLA	CHC-C1C-NC	4.05	130.41	124.31
19	4	4004	CLA	CHC-C1C-NC	4.05	130.28	124.33
19	H	1505	CLA	O2D-CGD-CBD	4.05	118.30	111.23
19	H	1241	CLA	CHC-C1C-NC	4.04	130.40	124.31
19	3	3012	CLA	CHC-C4B-NB	4.04	129.92	124.08
19	A	9013	CLA	C1-C2-C3	4.04	132.82	126.20
19	B	1217	CLA	CMD-C2D-C3D	-4.04	118.42	127.69
19	A	1135	CLA	C2B-C1B-NB	4.04	114.51	110.33
19	1	1010	CLA	CMD-C2D-C3D	-4.04	118.43	127.69
19	A	1121	CLA	CHC-C1C-NC	4.04	130.39	124.31
19	4	1009	CLA	CMD-C2D-C3D	-4.04	118.44	127.69
19	3	3013	CLA	CHC-C1C-NC	4.03	130.39	124.31
19	A	1112	CLA	CHD-C4C-C3C	-4.03	118.89	124.77
19	3	1147	CLA	C2B-C1B-NB	4.03	114.51	110.33
19	4	1004	CLA	O2D-CGD-CBD	4.03	118.28	111.23
19	4	4003	CLA	CMD-C2D-C3D	-4.03	118.44	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1011	CLA	CHD-C4C-C3C	-4.03	118.67	125.03
20	A	5001	PQN	C14-C13-C15	4.03	122.22	115.23
19	B	1227	CLA	C3B-C2B-C1B	-4.03	102.42	107.17
19	4	4010	CLA	C1C-CHC-C4B	-4.03	115.42	126.04
19	A	1237	CLA	C6-C5-C3	-4.02	103.67	113.47
19	B	1211	CLA	CHC-C1C-NC	4.02	130.37	124.31
19	B	1227	CLA	C1-O2A-CGA	4.02	126.39	116.65
19	4	1306	CLA	CHC-C4B-NB	4.02	130.09	124.05
21	B	6020	BCR	C7-C6-C5	-4.02	112.29	121.56
19	B	1231	CLA	O2D-CGD-CBD	4.02	118.26	111.23
19	2	2004	CLA	C4B-CHC-C1C	-4.02	116.79	126.25
19	A	1116	CLA	C4B-CHC-C1C	-4.02	116.79	126.25
19	B	1206	CLA	CHD-C4C-C3C	-4.02	118.91	124.77
19	A	1124	CLA	C4B-CHC-C1C	-4.02	116.80	126.25
21	B	6010	BCR	C2-C1-C6	-4.02	104.60	110.44
19	4	4013	CLA	C2A-C1A-CHA	-4.02	115.78	122.63
19	A	1137	CLA	CHC-C1C-NC	4.01	130.36	124.31
19	B	1234	CLA	C4B-CHC-C1C	-4.01	116.81	126.25
19	3	3003	CLA	C4B-CHC-C1C	-4.01	116.81	126.25
19	A	1128	CLA	CHC-C1C-NC	4.01	130.35	124.31
19	1	1303	CLA	CHD-C4C-C3C	-4.01	118.93	124.77
19	2	2006	CLA	C3B-C2B-C1B	-4.01	102.44	107.17
21	I	6018	BCR	C23-C22-C21	4.01	125.31	119.01
19	A	1109	CLA	CHC-C4B-NB	4.01	130.06	124.05
19	J	1308	CLA	CHC-C1C-NC	4.01	130.35	124.31
19	J	1311	CLA	CMD-C2D-C3D	-4.01	118.50	127.69
22	R	7024	LMU	O5B-C1B-C2B	4.01	118.61	110.37
19	B	1239	CLA	CHD-C4C-NC	4.01	130.45	124.23
21	B	6005	BCR	C15-C14-C13	-4.01	121.66	127.28
19	A	9022	CLA	O2D-CGD-O1D	-4.01	116.05	123.85
19	4	4011	CLA	C4A-NA-C1A	4.00	108.51	106.68
19	B	1222	CLA	CHC-C1C-NC	4.00	130.34	124.31
19	A	1137	CLA	C4B-CHC-C1C	-4.00	116.83	126.25
19	4	4003	CLA	CHC-C1C-NC	4.00	130.34	124.31
19	B	1205	CLA	CHD-C4C-NC	4.00	130.44	124.23
19	3	3010	CLA	C4C-CHD-C1D	-4.00	114.58	125.98
19	B	1219	CLA	CHC-C1C-NC	4.00	130.34	124.31
22	K	7001	LMU	C1B-C2B-C3B	4.00	118.43	110.01
19	4	4014	CLA	C4B-CHC-C1C	-4.00	116.84	126.25
19	3	3015	CLA	C1C-CHC-C4B	-4.00	115.49	126.04
19	1	1002	CLA	CMD-C2D-C3D	-4.00	118.51	127.69
19	A	1136	CLA	C1-C2-C3	-4.00	119.64	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	4015	CLA	C3B-C2B-C1B	-4.00	102.45	107.17
21	A	6002	BCR	C39-C30-C25	4.00	116.52	110.24
19	F	1305	CLA	C4D-C3D-CAD	4.00	112.45	108.11
19	4	4005	CLA	C3D-C4D-CHA	-4.00	116.27	125.20
19	A	1120	CLA	CHD-C4C-C3C	-4.00	118.94	124.77
19	3	3008	CLA	C4B-CHC-C1C	-4.00	116.85	126.25
19	B	1220	CLA	O2D-CGD-O1D	-4.00	116.07	123.85
19	H	1145	CLA	CMA-C3A-C4A	-4.00	101.03	111.77
19	4	4011	CLA	CHD-C4C-NC	4.00	130.31	124.24
19	1	1010	CLA	CHC-C1C-NC	3.99	130.33	124.31
19	B	1301	CLA	CBD-CHA-C1A	3.99	133.41	127.38
19	2	2007	CLA	C3B-C2B-C1B	-3.99	102.46	107.17
19	B	1221	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
19	3	3015	CLA	C4C-CHD-C1D	-3.99	114.62	125.98
22	H	7017	LMU	O5B-C5B-C4B	-3.99	102.51	109.70
19	B	1206	CLA	C2B-C1B-NB	3.98	114.46	110.33
19	A	1107	CLA	C3B-C2B-C1B	-3.98	102.47	107.17
19	B	1203	CLA	CHB-C4A-NA	3.98	130.15	124.40
19	B	1214	CLA	CHD-C4C-C3C	-3.98	118.97	124.77
19	K	3009	CLA	O2D-CGD-O1D	-3.98	116.10	123.85
19	2	2007	CLA	C6-C5-C3	-3.98	103.78	113.47
19	B	1210	CLA	C4B-CHC-C1C	-3.98	116.90	126.25
19	1	1310	CLA	C1C-CHC-C4B	-3.98	115.55	126.04
19	3	3006	CLA	C1C-CHC-C4B	-3.98	115.56	126.04
19	A	1132	CLA	O1D-CGD-CBD	-3.98	116.68	124.52
19	B	1230	CLA	O1D-CGD-CBD	-3.97	116.68	124.52
19	A	9022	CLA	CHD-C4C-C3C	-3.97	118.98	124.77
19	B	1234	CLA	CHD-C4C-C3C	-3.97	118.98	124.77
21	F	6016	BCR	C20-C19-C18	-3.97	115.47	126.36
19	F	1240	CLA	CHD-C4C-C3C	-3.97	118.76	125.03
19	B	1235	CLA	C4-C3-C5	3.97	122.12	115.23
19	2	2004	CLA	CMD-C2D-C3D	-3.97	118.58	127.69
19	B	1217	CLA	C4A-NA-C1A	3.97	108.49	106.68
21	L	6019	BCR	C27-C26-C25	-3.97	117.34	122.70
19	3	3005	CLA	C2A-C1A-CHA	-3.97	115.87	122.63
19	4	4005	CLA	C4A-NA-C1A	3.97	108.49	106.68
19	A	1137	CLA	C2B-C1B-NB	3.97	114.44	110.33
19	A	1103	CLA	C4A-NA-C1A	3.97	108.49	106.68
19	A	9013	CLA	C3B-C2B-C1B	-3.96	102.50	107.17
19	3	3017	CLA	C2B-C1B-NB	3.96	114.44	110.33
19	2	2003	CLA	C1C-CHC-C4B	-3.96	115.59	126.04
19	1	1310	CLA	C4C-CHD-C1D	-3.96	114.69	125.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1141	CLA	CHC-C1C-NC	3.96	130.28	124.31
22	E	7048	LMU	O5B-C5B-C6B	3.96	116.25	106.44
19	L	1502	CLA	CMD-C2D-C3D	-3.96	118.61	127.69
19	B	9010	CLA	CHD-C4C-C3C	-3.96	119.00	124.77
19	B	1213	CLA	CHC-C1C-NC	3.96	130.27	124.31
19	B	1231	CLA	CMD-C2D-C3D	-3.96	118.61	127.69
19	3	3008	CLA	CHC-C1C-NC	3.96	130.27	124.31
19	K	1143	CLA	C2B-C1B-NB	3.96	114.43	110.33
19	2	2002	CLA	CHC-C1C-NC	3.96	130.27	124.31
19	A	1136	CLA	C2B-C1B-NB	3.96	114.43	110.33
19	4	4014	CLA	CHD-C4C-C3C	-3.95	119.01	124.77
19	3	3011	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
19	K	1142	CLA	CMD-C2D-C3D	-3.95	118.62	127.69
19	B	1215	CLA	C4A-NA-C1A	3.95	108.48	106.68
19	A	9022	CLA	CHC-C1C-NC	3.95	130.26	124.31
19	L	1502	CLA	CHB-C4A-NA	3.95	130.10	124.40
19	B	1230	CLA	CHC-C1C-NC	3.95	130.26	124.31
19	F	1240	CLA	C4B-CHC-C1C	-3.95	116.96	126.25
19	3	3003	CLA	CHC-C1C-NC	3.95	130.26	124.31
19	B	1235	CLA	CMD-C2D-C3D	-3.95	118.63	127.69
19	A	9013	CLA	C4B-CHC-C1C	-3.95	116.97	126.25
19	A	9023	CLA	C3B-C2B-C1B	-3.95	102.52	107.17
19	A	1116	CLA	CHC-C1C-NC	3.95	130.25	124.31
19	A	1121	CLA	C2B-C1B-NB	3.94	114.42	110.33
21	B	6004	BCR	C2-C1-C6	-3.94	104.71	110.44
19	1	1011	CLA	C1B-C2B-C3B	-3.94	103.32	107.03
19	L	1130	CLA	CHD-C4C-C3C	-3.94	119.02	124.77
19	2	2012	CLA	CHC-C1C-NC	3.94	130.25	124.31
19	3	3005	CLA	C1C-CHC-C4B	-3.94	115.64	126.04
19	A	1107	CLA	CHC-C1C-C2C	-3.94	115.74	126.95
19	1	1310	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
19	3	3017	CLA	C4A-NA-C1A	3.94	108.48	106.68
19	A	1125	CLA	C4B-CHC-C1C	-3.94	116.98	126.25
21	F	6014	BCR	C2-C1-C6	-3.94	104.72	110.44
19	A	1127	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
19	B	1211	CLA	C2B-C1B-NB	3.94	114.41	110.33
19	1	1015	CLA	C4C-CHD-C1D	-3.94	114.76	125.98
21	B	6005	BCR	C24-C23-C22	-3.94	120.41	126.23
19	A	9022	CLA	C4B-CHC-C1C	-3.93	117.00	126.25
19	A	1129	CLA	CHD-C4C-NC	3.93	130.33	124.23
19	A	1131	CLA	CHC-C1C-NC	3.93	130.23	124.31
19	1	1005	CLA	CMD-C2D-C3D	-3.93	118.67	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1301	CLA	CHD-C4C-C3C	-3.93	118.82	125.03
19	A	1119	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
19	B	1230	CLA	C2B-C1B-NB	3.93	114.40	110.33
19	A	1110	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
22	2	7027	LMU	O1'-C1'-C2'	3.93	114.24	108.27
19	1	1008	CLA	C2B-C1B-NB	3.93	114.40	110.33
21	1	6023	BCR	C38-C26-C27	3.93	121.97	113.60
19	4	4013	CLA	C1C-CHC-C4B	-3.92	115.69	126.04
19	3	3010	CLA	CHA-C4D-ND	3.92	130.38	124.84
19	4	4003	CLA	C2B-C1B-NB	3.92	114.39	110.33
19	B	1220	CLA	C2A-C1A-CHA	-3.92	117.06	123.87
19	4	4015	CLA	C4A-NA-C1A	3.92	108.47	106.68
19	3	3001	CLA	C3B-C2B-C1B	-3.92	102.44	106.81
19	4	4006	CLA	O2D-CGD-CBD	3.92	118.09	111.23
21	A	6003	BCR	C38-C26-C25	-3.92	120.21	124.48
19	4	4012	CLA	C4B-CHC-C1C	-3.92	117.03	126.25
19	R	1150	CLA	CMB-C2B-C1B	3.92	131.38	125.42
22	2	7031	LMU	O1'-C1'-C2'	3.92	114.22	108.27
19	A	9012	CLA	C3B-C2B-C1B	-3.92	102.55	107.17
19	1	1002	CLA	CED-O2D-CGD	3.91	124.80	115.92
19	A	1140	CLA	CHC-C1C-NC	3.91	130.21	124.31
19	H	1207	CLA	C3B-C4B-NB	-3.91	107.04	110.53
19	3	3014	CLA	C1B-NB-C4B	-3.91	103.57	106.31
19	4	4004	CLA	C2A-C1A-CHA	-3.91	115.97	122.63
19	4	4005	CLA	C1C-CHC-C4B	-3.91	115.73	126.04
19	2	2002	CLA	C4B-CHC-C1C	-3.91	117.06	126.25
19	3	3001	CLA	C1B-NB-C4B	-3.91	103.57	106.31
19	J	1308	CLA	CMD-C2D-C3D	-3.91	118.73	127.69
19	1	1010	CLA	C3B-C2B-C1B	-3.91	102.56	107.17
21	I	6021	BCR	C15-C14-C13	3.91	132.76	127.28
19	A	1112	CLA	CHC-C1C-NC	3.91	130.20	124.31
19	A	1138	CLA	C2B-C1B-NB	3.91	114.38	110.33
19	1	1303	CLA	C2B-C1B-NB	3.91	114.38	110.33
19	1	1012	CLA	C2B-C1B-NB	3.91	114.38	110.33
19	4	4010	CLA	CHA-C4D-ND	3.90	130.36	124.84
19	A	1124	CLA	CHD-C4C-C3C	-3.90	119.08	124.77
21	A	6011	BCR	C29-C30-C25	-3.90	104.77	110.44
19	3	3010	CLA	C1C-CHC-C4B	-3.90	115.75	126.04
19	2	4009	CLA	CMD-C2D-C3D	-3.90	118.75	127.69
19	A	1109	CLA	C3B-C4B-NB	-3.90	107.05	110.53
19	A	1137	CLA	CMD-C2D-C3D	-3.90	118.75	127.69
19	J	1311	CLA	C2B-C1B-NB	3.90	114.37	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1236	CLA	CMB-C2B-C1B	3.90	131.35	125.42
19	A	1109	CLA	CHD-C4C-C3C	-3.90	119.09	124.77
19	1	1006	CLA	C2B-C1B-NB	3.90	114.37	110.33
19	A	1104	CLA	CHC-C1C-NC	3.90	130.18	124.31
19	B	1223	CLA	CHC-C1C-NC	3.90	130.18	124.31
19	B	1203	CLA	CMB-C2B-C1B	3.90	131.35	125.42
19	A	1135	CLA	CHC-C1C-NC	3.89	130.18	124.31
19	A	9012	CLA	CHC-C1C-NC	3.89	130.18	124.31
21	A	6003	BCR	C15-C16-C17	-3.89	115.56	123.52
19	B	1210	CLA	CMD-C2D-C3D	-3.89	118.76	127.69
19	A	1125	CLA	C2B-C1B-NB	3.89	114.36	110.33
19	4	4014	CLA	CMD-C2D-C3D	-3.89	118.77	127.69
19	A	1123	CLA	CHD-C4C-C3C	-3.89	119.10	124.77
19	K	1146	CLA	O2A-CGA-CBA	3.89	123.69	111.83
19	A	1132	CLA	CHD-C4C-NC	3.89	130.26	124.23
19	4	1004	CLA	CHD-C4C-C3C	-3.89	119.10	124.77
19	2	2008	CLA	C1C-CHC-C4B	-3.89	115.79	126.04
19	B	1226	CLA	CMB-C2B-C1B	3.89	131.34	125.42
19	3	3014	CLA	C3D-C4D-CHA	-3.89	116.52	125.20
19	2	2014	CLA	CHC-C1C-NC	3.88	130.16	124.31
19	3	3012	CLA	C3D-C4D-CHA	-3.88	116.53	125.20
21	J	6012	BCR	C2-C1-C6	-3.88	104.80	110.44
19	A	1131	CLA	CHC-C4B-NB	3.88	129.87	124.05
19	B	9010	CLA	CHC-C4B-NB	3.88	129.87	124.05
19	A	1113	CLA	CMD-C2D-C3D	-3.88	118.79	127.69
19	A	9023	CLA	C4B-CHC-C1C	-3.88	117.12	126.25
19	1	1310	CLA	C3D-C4D-CHA	-3.88	116.54	125.20
19	2	2011	CLA	C1C-CHC-C4B	-3.88	115.81	126.04
19	A	1131	CLA	CMD-C2D-C3D	-3.88	118.80	127.69
19	B	1221	CLA	C4B-CHC-C1C	-3.88	117.13	126.25
19	A	1134	CLA	C2B-C1B-NB	3.87	114.34	110.33
22	A	7023	LMU	C2'-C3'-C4'	3.87	118.47	109.68
19	2	2011	CLA	CHC-C1C-NC	3.87	130.02	124.33
19	R	1150	CLA	C1-C2-C3	3.87	132.54	126.20
21	B	6017	BCR	C39-C30-C25	3.87	116.32	110.24
19	B	1214	CLA	CMD-C2D-C3D	-3.87	118.81	127.69
19	L	1501	CLA	CMD-C2D-C1D	3.87	131.54	124.73
19	J	1311	CLA	CHC-C1C-NC	3.87	130.14	124.31
21	I	6021	BCR	C7-C8-C9	3.87	131.96	126.23
19	H	1241	CLA	CHD-C4C-NC	3.87	130.23	124.23
22	E	7037	LMU	C1B-O1B-C4'	-3.87	108.81	117.98
19	F	1240	CLA	C4B-C3B-C2B	3.87	110.67	107.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1219	CLA	C4-C3-C5	3.87	121.94	115.23
21	B	6010	BCR	C15-C14-C13	-3.87	121.86	127.28
19	4	4015	CLA	C4B-CHC-C1C	-3.87	117.16	126.25
19	B	1203	CLA	C4B-CHC-C1C	-3.86	117.16	126.25
22	B	7038	LMU	C1'-O5'-C5'	3.86	121.27	113.72
19	A	1123	CLA	O2D-CGD-CBD	3.86	117.98	111.23
22	A	7016	LMU	C4B-C3B-C2B	3.86	117.61	110.83
19	A	1140	CLA	C2B-C1B-NB	3.86	114.33	110.33
19	F	1240	CLA	C4A-NA-C1A	3.86	108.44	106.68
19	A	1117	CLA	C3B-C4B-NB	-3.86	107.08	110.53
21	F	6014	BCR	C31-C1-C6	-3.86	104.19	110.24
21	A	6003	BCR	C20-C19-C18	-3.86	115.78	126.36
19	A	1151	CLA	O2D-CGD-CBD	3.86	117.98	111.23
19	3	3001	CLA	CHC-C1C-NC	3.86	130.00	124.33
19	4	4014	CLA	CMB-C2B-C1B	3.86	131.30	125.42
19	B	1228	CLA	C4A-NA-C1A	3.86	108.44	106.68
21	I	6018	BCR	C12-C13-C14	-3.86	112.94	119.01
19	1	1010	CLA	C2B-C1B-NB	3.86	114.32	110.33
19	1	1007	CLA	CAC-C3C-C4C	3.86	129.81	124.79
21	3	6022	BCR	C37-C22-C21	-3.85	116.57	122.82
19	B	1219	CLA	C2B-C1B-NB	3.85	114.32	110.33
19	1	1006	CLA	CAB-C3B-C2B	-3.85	113.30	123.53
19	A	1113	CLA	C4B-CHC-C1C	-3.85	117.19	126.25
19	4	4013	CLA	C4C-CHD-C1D	-3.85	115.00	125.98
19	H	1145	CLA	CAA-C2A-C3A	-3.85	102.59	113.00
19	4	4013	CLA	CHC-C1C-NC	3.85	129.99	124.33
19	3	1147	CLA	CBA-CAA-C2A	-3.85	102.34	113.79
19	1	1001	CLA	C3B-C2B-C1B	-3.85	102.63	107.17
19	A	1106	CLA	CMD-C2D-C3D	-3.85	118.86	127.69
19	B	1223	CLA	CMD-C2D-C3D	-3.85	118.86	127.69
19	3	3016	CLA	CMD-C2D-C3D	-3.85	118.86	127.69
19	2	2011	CLA	C2A-C1A-CHA	-3.85	116.07	122.63
19	H	1505	CLA	CHC-C1C-NC	3.85	130.11	124.31
22	B	7038	LMU	C1B-O5B-C5B	3.85	121.23	113.72
19	B	1225	CLA	CHC-C4B-NB	3.84	129.81	124.05
19	B	1228	CLA	C2B-C1B-NB	3.84	114.31	110.33
19	A	9013	CLA	CMD-C2D-C3D	-3.84	118.88	127.69
19	2	2010	CLA	C1C-CHC-C4B	-3.84	115.91	126.04
19	3	1147	CLA	CHC-C1C-NC	3.84	130.10	124.31
19	L	1501	CLA	C4B-CHC-C1C	-3.84	117.22	126.25
19	4	4006	CLA	CMD-C2D-C3D	-3.84	118.88	127.69
22	H	7017	LMU	C4B-C3B-C2B	3.84	117.57	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	2014	CLA	CHD-C4C-C3C	-3.84	119.17	124.77
19	1	1006	CLA	CMD-C2D-C3D	-3.84	118.88	127.69
21	B	6020	BCR	C8-C9-C10	3.84	125.05	119.01
19	4	4013	CLA	CHA-C4D-ND	3.84	130.26	124.84
21	B	6005	BCR	C29-C30-C25	-3.84	104.87	110.44
19	2	4009	CLA	CHD-C4C-C3C	-3.84	119.18	124.77
19	2	2014	CLA	C3B-C2B-C1B	-3.83	102.65	107.17
21	B	6017	BCR	C16-C17-C18	-3.83	121.90	127.28
19	B	1230	CLA	CMD-C2D-C3D	-3.83	118.90	127.69
19	B	1225	CLA	CMB-C2B-C1B	3.83	131.25	125.42
19	3	1118	CLA	C1B-C2B-C3B	-3.83	103.43	107.03
19	A	1110	CLA	CMD-C2D-C3D	-3.83	118.90	127.69
22	G	7051	LMU	C1'-O5'-C5'	-3.83	106.24	113.72
19	A	1237	CLA	CMB-C2B-C1B	3.83	131.25	125.42
19	1	1005	CLA	C4B-CHC-C1C	-3.83	117.24	126.25
19	3	3003	CLA	C1B-C2B-C3B	-3.83	103.43	107.03
19	1	1010	CLA	C3A-C2A-C1A	3.83	107.07	101.34
19	B	1233	CLA	C4B-CHC-C1C	-3.83	117.25	126.25
19	B	1209	CLA	C4A-NA-C1A	3.83	108.42	106.68
19	B	1227	CLA	CHC-C1C-NC	3.83	130.07	124.31
19	A	1120	CLA	C4B-CHC-C1C	-3.83	117.25	126.25
19	1	1012	CLA	CHC-C1C-NC	3.83	130.07	124.31
19	2	2012	CLA	C2B-C1B-NB	3.83	114.29	110.33
19	B	1201	CLA	C4B-CHC-C1C	-3.83	117.25	126.25
19	B	1221	CLA	CMD-C2D-C3D	-3.83	118.92	127.69
19	H	1207	CLA	C4B-C3B-C2B	3.83	112.06	107.30
21	A	6007	BCR	C29-C30-C25	-3.82	104.88	110.44
21	B	6017	BCR	C29-C30-C25	-3.82	104.88	110.44
19	A	1126	CLA	C3B-C2B-C1B	-3.82	102.66	107.17
19	F	1305	CLA	CBA-CAA-C2A	-3.82	102.42	113.79
19	A	1127	CLA	CHD-C4C-C3C	-3.82	119.20	124.77
19	B	1208	CLA	C4B-CHC-C1C	-3.82	117.27	126.25
19	3	3006	CLA	C2A-C1A-CHA	-3.82	116.12	122.63
19	A	1132	CLA	CMB-C2B-C1B	3.82	131.23	125.42
19	1	1014	CLA	CHC-C4B-NB	3.82	129.78	124.05
19	A	1133	CLA	C4B-CHC-C1C	-3.82	117.27	126.25
19	A	1125	CLA	CHC-C1C-NC	3.82	130.06	124.31
19	2	2002	CLA	C1-O2A-CGA	3.82	125.89	116.65
19	L	1504	CLA	CMD-C2D-C3D	-3.82	118.94	127.69
19	A	1101	CLA	CHC-C4B-NB	3.81	129.77	124.05
21	A	6002	BCR	C28-C27-C26	-3.81	107.26	114.06
19	A	1151	CLA	C3B-C2B-C1B	-3.81	102.67	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	9010	CLA	O2D-CGD-CBD	3.81	117.89	111.23
19	4	1306	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
19	B	1213	CLA	C4B-CHC-C1C	-3.81	117.28	126.25
19	2	4009	CLA	CHC-C1C-NC	3.81	130.05	124.31
19	A	1309	CLA	C4C-CHD-C1D	-3.81	115.12	125.98
22	F	7036	LMU	O1B-C1B-C2B	3.81	117.46	108.09
19	1	1008	CLA	CHC-C1C-NC	3.81	130.04	124.31
21	J	6012	BCR	C15-C16-C17	-3.81	115.73	123.52
22	G	7039	LMU	O1B-C1B-C2B	3.81	117.45	108.09
21	I	6018	BCR	C30-C25-C24	3.81	125.97	115.65
19	2	2012	CLA	C3B-C2B-C1B	-3.81	102.68	107.17
19	A	1107	CLA	C2B-C1B-NB	3.80	114.27	110.33
22	R	7021	LMU	C1B-O5B-C5B	3.80	121.15	113.72
19	1	1003	CLA	C4B-CHC-C1C	-3.80	117.30	126.25
19	4	4013	CLA	C4A-NA-C1A	3.80	108.41	106.68
21	B	6017	BCR	C24-C23-C22	-3.80	120.61	126.23
21	F	6014	BCR	C20-C19-C18	-3.80	115.94	126.36
19	B	1203	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
19	A	1109	CLA	CAA-C2A-C3A	-3.80	102.73	113.00
19	2	1307	CLA	C3B-C2B-C1B	-3.80	102.58	106.81
19	4	4002	CLA	C2A-C3A-C4A	-3.80	95.73	101.87
19	B	1205	CLA	C2B-C1B-NB	3.80	114.27	110.33
19	1	1012	CLA	C4B-CHC-C1C	-3.80	117.31	126.25
19	1	1001	CLA	CAC-C3C-C4C	3.80	129.73	124.79
19	B	1208	CLA	CHC-C1C-NC	3.80	130.03	124.31
19	2	2004	CLA	CHC-C1C-NC	3.79	130.02	124.31
19	L	1130	CLA	CHC-C1C-NC	3.79	130.02	124.31
19	A	1112	CLA	CMD-C2D-C3D	-3.79	119.00	127.69
21	B	6006	BCR	C20-C19-C18	-3.79	115.97	126.36
21	A	6008	BCR	C24-C23-C22	-3.79	120.63	126.23
19	4	1004	CLA	C1-C2-C3	-3.79	119.99	126.20
22	R	7020	LMU	C1B-O5B-C5B	3.79	121.12	113.72
19	K	1142	CLA	C2B-C1B-NB	3.79	114.25	110.33
19	A	9023	CLA	CGD-CBD-CAD	3.79	123.11	110.85
19	B	1224	CLA	C4B-CHC-C1C	-3.79	117.34	126.25
19	4	4010	CLA	C3B-C2B-C1B	-3.79	102.60	106.81
19	A	1103	CLA	CMD-C2D-C3D	-3.79	119.01	127.69
19	A	1116	CLA	C2B-C1B-NB	3.78	114.25	110.33
19	1	1015	CLA	C1C-CHC-C4B	-3.78	116.06	126.04
19	1	1001	CLA	CHD-C4C-C3C	-3.78	119.26	124.77
19	2	2014	CLA	C4B-CHC-C1C	-3.78	117.35	126.25
19	2	2012	CLA	CAC-C3C-C4C	3.78	129.71	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	4012	CLA	CHC-C1C-NC	3.78	130.01	124.31
19	2	2004	CLA	CHD-C4C-C3C	-3.78	119.26	124.77
19	4	4011	CLA	CHC-C1C-NC	3.78	129.89	124.33
19	R	1144	CLA	C2B-C1B-NB	3.78	114.25	110.33
21	3	6022	BCR	C38-C26-C25	-3.78	120.36	124.48
21	B	6020	BCR	C37-C22-C23	3.78	123.86	118.09
19	4	4005	CLA	C1B-NB-C4B	-3.78	103.66	106.31
21	A	6002	BCR	C38-C26-C25	-3.78	120.36	124.48
21	F	6014	BCR	C33-C5-C6	-3.78	120.36	124.48
19	A	1129	CLA	O2A-CGA-CBA	3.78	123.35	111.83
19	B	1211	CLA	CHC-C4B-NB	3.78	129.71	124.05
19	A	1112	CLA	C4B-CHC-C1C	-3.77	117.37	126.25
19	A	1106	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
21	B	6006	BCR	C27-C26-C25	-3.77	117.61	122.70
19	3	3002	CLA	CHA-C4D-ND	3.77	130.17	124.84
19	B	1212	CLA	C4B-CHC-C1C	-3.77	117.38	126.25
19	2	1307	CLA	C3D-C4D-CHA	-3.77	116.78	125.20
21	F	6016	BCR	C29-C30-C25	-3.77	104.96	110.44
19	K	1142	CLA	CHC-C1C-NC	3.77	129.99	124.31
19	1	1008	CLA	C3B-C2B-C1B	-3.77	102.73	107.17
19	B	1220	CLA	C2B-C1B-NB	3.76	114.23	110.33
19	2	2002	CLA	C3B-C2B-C1B	-3.76	102.73	107.17
19	A	1101	CLA	CHC-C1C-NC	3.76	129.98	124.31
19	1	1007	CLA	C2B-C1B-NB	3.76	114.23	110.33
19	3	3008	CLA	O2A-CGA-CBA	3.76	123.30	111.83
19	A	1107	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
19	A	1105	CLA	CHD-C4C-C3C	-3.76	119.29	124.77
19	A	1122	CLA	CMD-C2D-C3D	-3.76	119.07	127.69
19	B	1206	CLA	CHC-C1C-NC	3.76	129.97	124.31
19	1	1007	CLA	CHC-C1C-NC	3.76	129.97	124.31
19	A	1140	CLA	CMD-C2D-C3D	-3.76	119.07	127.69
19	3	3007	CLA	CHD-C4C-NC	3.76	130.06	124.23
19	A	1111	CLA	CMD-C2D-C3D	-3.76	119.07	127.69
19	1	1002	CLA	O2A-CGA-CBA	3.76	123.29	111.83
19	B	1205	CLA	CHC-C4B-NB	3.76	129.68	124.05
21	B	6006	BCR	C16-C15-C14	-3.75	115.84	123.52
19	4	1306	CLA	C3B-C2B-C1B	-3.75	102.75	107.17
19	B	1213	CLA	CMD-C2D-C3D	-3.75	119.09	127.69
19	B	1231	CLA	C2B-C1B-NB	3.75	114.22	110.33
19	B	1301	CLA	C4B-CHC-C1C	-3.75	117.43	126.25
21	A	6007	BCR	C23-C24-C25	-3.75	116.98	127.00
19	3	3002	CLA	C1B-NB-C4B	-3.75	103.68	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	4001	CLA	C4B-CHC-C1C	-3.75	117.43	126.25
21	F	6016	BCR	C34-C9-C8	3.75	123.81	118.09
19	A	1127	CLA	C1-O2A-CGA	3.75	125.72	116.65
21	L	6019	BCR	C15-C16-C17	-3.75	115.85	123.52
19	3	3006	CLA	C3B-C2B-C1B	-3.74	102.64	106.81
19	B	1216	CLA	C2B-C1B-NB	3.74	114.21	110.33
22	4	7052	LMU	O5'-C5'-C4'	-3.74	101.98	109.72
19	B	1202	CLA	CMB-C2B-C1B	3.74	131.12	125.42
19	3	3002	CLA	C1C-CHC-C4B	-3.74	116.17	126.04
19	A	1123	CLA	CHC-C1C-NC	3.74	129.95	124.31
19	A	9022	CLA	C3B-C2B-C1B	-3.74	102.76	107.17
19	4	4001	CLA	CMD-C2D-C3D	-3.74	119.11	127.69
19	L	1502	CLA	CHD-C4C-C3C	-3.74	119.32	124.77
19	1	1014	CLA	CHC-C1C-NC	3.74	129.94	124.31
19	L	1148	CLA	O2A-CGA-CBA	3.74	123.23	111.83
19	4	4006	CLA	C4B-CHC-C1C	-3.74	117.46	126.25
19	1	1011	CLA	CBD-CHA-C1A	3.74	133.02	127.38
19	L	1501	CLA	CED-O2D-CGD	3.73	124.39	115.92
19	A	9013	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
22	G	7051	LMU	C1B-O1B-C4'	3.73	126.83	117.98
19	F	1302	CLA	C4B-CHC-C1C	-3.73	117.47	126.25
19	B	1203	CLA	CMD-C2D-C3D	-3.73	119.13	127.69
19	A	9012	CLA	CAA-C2A-C1A	3.73	124.20	111.97
19	B	1234	CLA	CHC-C4B-NB	3.73	129.65	124.05
21	A	6003	BCR	C16-C15-C14	-3.73	115.88	123.52
19	2	2002	CLA	CHD-C4C-C3C	-3.73	119.33	124.77
19	B	1225	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
21	F	6014	BCR	C38-C26-C25	-3.73	120.41	124.48
22	4	7009	LMU	O1'-C1'-C2'	3.73	113.94	108.27
19	L	1502	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
19	B	1232	CLA	CHC-C1C-NC	3.73	129.93	124.31
19	4	4014	CLA	CHC-C1C-NC	3.73	129.92	124.31
19	L	1504	CLA	C4B-CHC-C1C	-3.73	117.49	126.25
19	A	1110	CLA	C4A-NA-C1A	3.72	108.38	106.68
21	A	6003	BCR	C33-C5-C6	-3.72	120.42	124.48
19	K	1146	CLA	CHD-C4C-C3C	-3.72	119.35	124.77
19	H	1505	CLA	CHC-C4B-NB	3.72	129.63	124.05
19	A	1237	CLA	C1-C2-C3	-3.72	120.10	126.20
19	A	1110	CLA	C4B-CHC-C1C	-3.72	117.50	126.25
19	B	1234	CLA	CHC-C1C-NC	3.72	129.91	124.31
21	B	6010	BCR	C16-C17-C18	-3.72	122.06	127.28
19	3	3017	CLA	CAA-C2A-C3A	-3.72	102.95	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1225	CLA	CHC-C1C-NC	3.72	129.91	124.31
19	B	1218	CLA	CHC-C1C-NC	3.72	129.91	124.31
19	1	1011	CLA	CHC-C4B-NB	3.72	129.62	124.05
21	A	6008	BCR	C38-C26-C25	-3.72	120.43	124.48
19	1	1003	CLA	C2B-C1B-NB	3.72	114.18	110.33
19	B	1231	CLA	C4B-CHC-C1C	-3.71	117.51	126.25
19	A	1105	CLA	CHC-C4B-NB	3.71	129.62	124.05
19	2	2012	CLA	CHD-C4C-NC	3.71	129.99	124.23
19	A	1104	CLA	CMD-C2D-C3D	-3.71	119.18	127.69
19	3	3011	CLA	CMD-C2D-C3D	-3.71	119.19	127.69
19	H	1505	CLA	C4A-NA-C1A	3.71	108.37	106.68
19	B	1220	CLA	CAA-C2A-C1A	-3.71	99.83	111.97
19	K	1143	CLA	CHD-C4C-C3C	-3.71	119.37	124.77
19	A	1127	CLA	O2D-CGD-O1D	-3.71	116.64	123.85
19	B	1231	CLA	C3B-C2B-C1B	-3.70	102.80	107.17
19	B	1227	CLA	CMD-C2D-C3D	-3.70	119.19	127.69
21	B	6006	BCR	C29-C30-C25	-3.70	105.06	110.44
19	3	1147	CLA	CMC-C2C-C1C	3.70	130.82	125.03
19	3	3015	CLA	CHA-C4D-ND	3.70	130.07	124.84
19	4	4011	CLA	C1C-CHC-C4B	-3.70	116.28	126.04
19	B	1202	CLA	CHB-C4A-NA	3.70	129.74	124.40
19	4	4012	CLA	CHD-C4C-C3C	-3.70	119.19	125.03
21	A	6007	BCR	C3-C4-C5	-3.70	107.46	114.06
19	A	1103	CLA	CHD-C4C-C3C	-3.70	119.38	124.77
19	A	1309	CLA	CHA-C4D-ND	3.70	130.06	124.84
19	A	1107	CLA	CAC-C3C-C4C	3.70	129.60	124.79
21	B	6020	BCR	C1-C6-C7	3.69	125.67	115.65
19	L	1503	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
19	2	1307	CLA	C4C-CHD-C1D	-3.69	115.46	125.98
19	L	1502	CLA	C4A-NA-C1A	3.69	108.36	106.68
19	1	1005	CLA	CED-O2D-CGD	3.69	124.29	115.92
19	B	1233	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
19	2	2011	CLA	CHC-C4B-NB	3.69	129.41	124.08
21	F	6016	BCR	C30-C25-C26	-3.69	117.60	122.64
19	3	3017	CLA	CHB-C4A-NA	3.69	129.72	124.40
19	4	4002	CLA	CBC-CAC-C3C	-3.68	102.43	112.42
22	R	7020	LMU	O1'-C1'-C2'	3.68	113.87	108.27
19	A	1102	CLA	O2D-CGD-CBD	3.68	117.67	111.23
21	B	6010	BCR	C38-C26-C25	-3.68	120.47	124.48
19	2	2012	CLA	CHC-C4B-NB	3.68	129.57	124.05
19	A	1119	CLA	C4B-CHC-C1C	-3.68	117.60	126.25
19	4	4013	CLA	CHC-C4B-NB	3.68	129.40	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L	1148	CLA	C4D-CHA-C1A	3.68	125.63	121.24
19	1	1015	CLA	C3B-C2B-C1B	-3.68	102.72	106.81
19	A	1133	CLA	CHC-C1C-NC	3.68	129.85	124.31
19	A	1111	CLA	CHD-C4C-C3C	-3.67	119.42	124.77
22	A	7044	LMU	O2'-C2'-C1'	3.67	118.83	110.08
20	B	5002	PQN	C2M-C2-C3	-3.67	118.42	124.45
19	A	1121	CLA	CHD-C4C-C3C	-3.67	119.42	124.77
19	3	3007	CLA	C4A-NA-C1A	3.67	108.35	106.68
19	R	1144	CLA	O2A-CGA-CBA	3.67	123.02	111.83
21	B	6020	BCR	C20-C19-C18	-3.67	116.31	126.36
19	B	1209	CLA	C2B-C1B-NB	3.67	114.13	110.33
19	2	2007	CLA	CHD-C4C-NC	3.66	129.91	124.23
19	B	1235	CLA	CHC-C4B-NB	3.66	129.54	124.05
19	B	1228	CLA	C1-C2-C3	-3.66	120.84	126.76
19	A	1101	CLA	CMD-C2D-C3D	-3.66	119.29	127.69
19	B	1223	CLA	C2B-C1B-NB	3.66	114.12	110.33
21	B	6004	BCR	C28-C27-C26	-3.66	107.53	114.06
19	3	3001	CLA	C2D-C3D-C4D	-3.66	102.90	107.35
19	3	3004	CLA	C4C-CHD-C1D	-3.66	115.56	125.98
19	B	1229	CLA	CHC-C1C-NC	3.66	129.82	124.31
19	2	2005	CLA	CHA-C4D-ND	3.66	130.01	124.84
19	4	4003	CLA	CHD-C4C-C3C	-3.66	119.44	124.77
19	B	1217	CLA	CHC-C1C-NC	3.66	129.82	124.31
19	F	1240	CLA	CAB-C3B-C4B	-3.66	119.85	125.42
19	1	1007	CLA	C3B-C2B-C1B	-3.66	102.86	107.17
19	R	1144	CLA	CHC-C1C-NC	3.66	129.82	124.31
19	B	1238	CLA	O2A-CGA-CBA	3.66	122.98	111.83
19	A	1115	CLA	CMD-C2D-C3D	-3.66	119.31	127.69
19	L	1130	CLA	CMD-C2D-C3D	-3.66	119.31	127.69
19	A	1120	CLA	C4-C3-C5	3.65	120.43	116.13
19	3	3015	CLA	C1B-NB-C4B	-3.65	103.75	106.31
19	B	9010	CLA	CAA-C2A-C3A	-3.65	103.13	113.00
19	B	1220	CLA	CHC-C4B-NB	3.65	129.53	124.05
19	A	1129	CLA	C2B-C1B-NB	3.65	114.11	110.33
22	A	7035	LMU	C3'-C4'-C5'	-3.65	102.84	110.93
19	A	1149	CLA	CHD-C4C-NC	3.65	129.89	124.23
21	J	6012	BCR	C7-C8-C9	-3.65	120.84	126.23
22	A	7045	LMU	O5B-C1B-C2B	3.65	117.86	110.37
19	A	9022	CLA	CHB-C4A-NA	3.65	129.66	124.40
21	L	6019	BCR	C36-C18-C19	3.65	123.66	118.09
19	4	4001	CLA	O2A-CGA-CBA	3.65	122.95	111.83
19	2	2007	CLA	CHC-C4B-NB	3.64	129.51	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1011	CLA	C4A-NA-C1A	3.64	108.34	106.68
19	L	1501	CLA	CHC-C1C-NC	3.64	129.80	124.31
21	L	6019	BCR	C33-C5-C6	-3.64	120.51	124.48
19	2	2005	CLA	C4C-CHD-C1D	-3.64	115.61	125.98
19	3	2009	CLA	C2B-C1B-NB	3.64	114.10	110.33
19	B	1239	CLA	CHC-C1C-NC	3.64	129.79	124.31
19	B	1205	CLA	C3B-C2B-C1B	-3.64	102.88	107.17
19	4	4015	CLA	CGD-CBD-CAD	-3.64	99.07	110.85
19	B	1229	CLA	C3B-C2B-C1B	-3.64	102.88	107.17
19	L	1502	CLA	C3B-C2B-C1B	-3.64	102.88	107.17
19	A	9011	CLA	CMD-C2D-C3D	-3.64	119.35	127.69
21	B	6004	BCR	C29-C30-C25	-3.64	105.16	110.44
19	A	1110	CLA	CHC-C1C-NC	3.63	129.78	124.31
19	4	4007	CLA	CMD-C2D-C3D	-3.63	119.36	127.69
19	4	1009	CLA	CHC-C1C-NC	3.63	129.78	124.31
19	3	1118	CLA	C2B-C1B-NB	3.63	114.09	110.33
21	B	6017	BCR	C2-C1-C6	-3.63	105.16	110.44
19	B	1202	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
21	B	6004	BCR	C33-C5-C6	-3.63	120.52	124.48
19	B	1218	CLA	CHB-C4A-NA	3.63	129.64	124.40
19	A	1309	CLA	C4A-NA-C1A	3.63	108.33	106.68
19	4	4006	CLA	C4A-NA-C1A	3.63	108.33	106.68
19	3	3014	CLA	C4C-CHD-C1D	-3.63	115.64	125.98
19	1	1013	CLA	C1-C2-C3	-3.63	120.25	126.20
21	B	6020	BCR	C33-C5-C4	3.63	121.33	113.60
19	K	3009	CLA	C4B-CHC-C1C	-3.62	117.73	126.25
19	2	2010	CLA	CHA-C4D-ND	3.62	129.96	124.84
19	A	1108	CLA	C2A-C1A-CHA	-3.62	117.58	123.87
19	B	1209	CLA	CHC-C4B-NB	3.62	129.48	124.05
19	B	1239	CLA	C2B-C1B-NB	3.62	114.08	110.33
19	B	1236	CLA	CMD-C2D-C3D	-3.62	119.39	127.69
21	B	6005	BCR	C33-C5-C6	-3.62	120.53	124.48
19	B	1202	CLA	CHC-C4B-NB	3.62	129.48	124.05
19	2	2007	CLA	CHC-C1C-C2C	-3.62	116.66	126.95
19	R	1150	CLA	O2D-CGD-CBD	3.62	117.56	111.23
19	2	2006	CLA	CED-O2D-CGD	3.62	124.12	115.92
19	A	1121	CLA	CAA-C2A-C1A	3.62	120.14	112.14
19	A	9012	CLA	O2A-CGA-CBA	3.61	122.85	111.83
19	2	2013	CLA	CHC-C1C-NC	3.61	129.75	124.31
19	B	1221	CLA	CHD-C4C-C3C	-3.61	119.51	124.77
19	B	1225	CLA	O2A-CGA-CBA	3.61	122.85	111.83
19	B	1205	CLA	CMD-C2D-C3D	-3.61	119.41	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	4010	CLA	CHC-C4B-NB	3.61	129.30	124.08
19	B	1222	CLA	C2B-C1B-NB	3.61	114.07	110.33
19	R	1150	CLA	CHC-C1C-NC	3.61	129.75	124.31
19	A	1103	CLA	CMB-C2B-C1B	3.61	130.91	125.42
21	B	6010	BCR	C38-C26-C27	3.61	121.29	113.60
19	B	1226	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
19	B	1227	CLA	CHC-C4B-NB	3.60	129.45	124.05
19	H	1505	CLA	CMB-C2B-C1B	3.60	130.91	125.42
19	1	1015	CLA	C2D-C3D-C4D	-3.60	102.97	107.35
19	B	1238	CLA	CHC-C4B-NB	3.60	129.45	124.05
19	A	1113	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
19	H	1207	CLA	CMD-C2D-C3D	-3.60	119.43	127.69
19	A	1104	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
19	A	1106	CLA	CHC-C1C-NC	3.60	129.73	124.31
19	A	1107	CLA	CHD-C4C-NC	3.60	129.81	124.23
19	4	4011	CLA	C2D-C3D-C4D	-3.60	102.98	107.35
22	4	7052	LMU	C6'-C5'-C4'	3.60	123.50	113.38
21	A	6007	BCR	C38-C26-C25	-3.60	120.56	124.48
19	3	3010	CLA	CHC-C4B-NB	3.60	129.28	124.08
19	A	1126	CLA	CHD-C4C-C3C	-3.60	119.53	124.77
19	B	1224	CLA	CHC-C1C-NC	3.60	129.73	124.31
19	1	1015	CLA	C1B-NB-C4B	-3.59	103.79	106.31
19	2	2002	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
19	2	2006	CLA	CMD-C2D-C3D	-3.59	119.45	127.69
19	A	1122	CLA	CHC-C1C-NC	3.59	129.72	124.31
19	B	1229	CLA	CMD-C2D-C3D	-3.59	119.46	127.69
22	E	7048	LMU	C1B-O5B-C5B	-3.59	106.71	113.72
21	B	6004	BCR	C3-C4-C5	-3.59	107.66	114.06
19	A	1133	CLA	CHD-C4C-C3C	-3.59	119.54	124.77
19	3	3014	CLA	CHC-C4B-NB	3.59	129.26	124.08
19	3	3010	CLA	C3B-C2B-C1B	-3.59	102.82	106.81
22	B	7040	LMU	O1B-C1B-C2B	3.59	116.91	108.09
19	A	1309	CLA	C1B-NB-C4B	-3.58	103.80	106.31
19	A	1105	CLA	C2B-C1B-NB	3.58	114.04	110.33
19	H	1505	CLA	C2B-C1B-NB	3.58	114.04	110.33
19	A	9023	CLA	CMD-C2D-C3D	-3.58	119.47	127.69
19	B	1228	CLA	C3B-C2B-C1B	-3.58	102.95	107.17
19	A	9023	CLA	O2D-CGD-CBD	3.58	117.49	111.23
19	B	1206	CLA	CHC-C4B-NB	3.58	129.42	124.05
19	3	1118	CLA	CHC-C4B-NB	3.58	129.42	124.05
19	1	1014	CLA	C1-C2-C3	-3.58	120.33	126.20
19	2	2003	CLA	C3B-C2B-C1B	-3.58	102.83	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	3009	CLA	C2B-C1B-NB	3.58	114.04	110.33
19	1	1001	CLA	C2B-C1B-NB	3.58	114.03	110.33
21	J	6012	BCR	C29-C30-C25	-3.57	105.25	110.44
19	4	1306	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
19	L	1504	CLA	C4-C3-C5	3.57	121.43	115.23
19	G	1242	CLA	CMD-C2D-C3D	-3.57	119.49	127.69
19	2	2005	CLA	CHC-C4B-NB	3.57	129.24	124.08
19	B	1216	CLA	CHC-C4B-NB	3.57	129.41	124.05
19	L	1148	CLA	CHC-C4B-NB	3.57	129.41	124.05
19	B	1232	CLA	CMD-C2D-C3D	-3.57	119.51	127.69
19	3	3004	CLA	CHC-C4B-NB	3.57	129.23	124.08
19	A	1104	CLA	CHC-C4B-NB	3.57	129.40	124.05
21	J	6012	BCR	C23-C24-C25	-3.57	117.47	127.00
19	B	1208	CLA	CHD-C4C-C3C	-3.57	119.58	124.77
19	H	1145	CLA	CAA-C2A-C1A	3.56	123.66	111.97
22	R	7014	LMU	C1B-O1B-C4'	-3.56	109.53	117.98
19	J	1308	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
19	3	3002	CLA	C3D-C4D-CHA	-3.56	117.24	125.20
19	3	3010	CLA	C3D-C4D-CHA	-3.56	117.24	125.20
19	2	2013	CLA	CGD-CBD-CAD	-3.56	99.31	110.85
19	4	4011	CLA	CHC-C4B-NB	3.56	129.23	124.08
19	B	1213	CLA	C2B-C1B-NB	3.56	114.02	110.33
22	G	7051	LMU	O5'-C5'-C6'	3.56	115.26	106.44
19	A	9011	CLA	CED-O2D-CGD	3.56	123.99	115.92
19	B	1301	CLA	CMD-C2D-C3D	-3.56	119.53	127.69
22	C	7015	LMU	C1B-C2B-C3B	3.56	117.49	110.01
19	4	4001	CLA	CHC-C1C-NC	3.56	129.67	124.31
22	H	7011	LMU	C3'-C4'-C5'	3.56	118.81	110.93
19	A	1113	CLA	CHD-C4C-C3C	-3.56	119.59	124.77
19	2	2007	CLA	CMD-C2D-C3D	-3.56	119.53	127.69
19	3	3005	CLA	C1B-NB-C4B	-3.56	103.82	106.31
19	B	1228	CLA	CHC-C1C-NC	3.55	129.66	124.31
21	J	6012	BCR	C8-C7-C6	-3.55	117.50	127.00
21	B	6004	BCR	C40-C30-C25	3.55	115.81	110.24
19	F	1302	CLA	CHC-C1C-NC	3.55	129.66	124.31
19	4	4007	CLA	C2B-C1B-NB	3.55	114.01	110.33
19	2	4009	CLA	CHC-C4B-NB	3.55	129.37	124.05
21	A	6011	BCR	C15-C16-C17	-3.55	116.26	123.52
19	4	4005	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
19	B	1235	CLA	CHD-C4C-C3C	-3.54	119.61	124.77
19	B	1221	CLA	CHC-C1C-NC	3.54	129.65	124.31
19	B	1227	CLA	CHD-C4C-NC	3.54	129.72	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1117	CLA	C1-C2-C3	-3.54	120.39	126.20
19	3	3005	CLA	C3B-C2B-C1B	-3.54	102.87	106.81
19	3	3011	CLA	C1-C2-C3	-3.54	120.39	126.20
19	B	1219	CLA	CHC-C4B-NB	3.54	129.36	124.05
19	4	4006	CLA	C4-C3-C5	3.54	121.37	115.23
19	I	1204	CLA	CMD-C2D-C3D	-3.54	119.58	127.69
19	3	1118	CLA	CBD-CHA-C1A	3.54	132.72	127.38
19	A	1115	CLA	CHC-C1C-NC	3.54	129.64	124.31
19	3	3006	CLA	C1B-NB-C4B	-3.54	103.83	106.31
22	R	7025	LMU	C1'-O5'-C5'	3.53	120.62	113.72
19	A	1122	CLA	CHD-C4C-C3C	-3.53	119.62	124.77
19	3	1118	CLA	CHC-C1C-NC	3.53	129.63	124.31
21	3	6022	BCR	C11-C12-C13	-3.53	116.68	126.36
19	4	1306	CLA	CHC-C1C-C2C	-3.53	116.91	126.95
19	A	1111	CLA	C3B-C2B-C1B	-3.53	103.01	107.17
19	3	3017	CLA	CHC-C1C-C2C	-3.53	116.92	126.95
19	A	1237	CLA	CHC-C4B-NB	3.53	129.34	124.05
22	B	7038	LMU	O5B-C5B-C4B	3.53	116.06	109.70
19	1	1005	CLA	CHC-C1C-NC	3.53	129.62	124.31
19	3	3011	CLA	CHB-C4A-NA	3.53	129.49	124.40
19	4	4010	CLA	C1B-NB-C4B	-3.53	103.84	106.31
19	B	1215	CLA	C1-C2-C3	-3.53	120.42	126.20
19	2	1307	CLA	CHC-C1C-NC	3.53	129.51	124.33
19	3	3007	CLA	CHC-C4B-NB	3.52	129.34	124.05
19	L	1148	CLA	C4-C3-C2	-3.52	114.58	123.63
19	3	3005	CLA	CHC-C4B-NB	3.52	129.17	124.08
19	A	1126	CLA	CHC-C1C-NC	3.52	129.61	124.31
19	2	2011	CLA	C1B-NB-C4B	-3.52	103.84	106.31
19	A	1108	CLA	CHC-C4B-NB	3.52	129.33	124.05
19	1	1015	CLA	C3D-C4D-CHA	-3.52	117.34	125.20
22	H	7032	LMU	C1B-C2B-C3B	-3.52	102.61	110.01
19	A	1105	CLA	CMD-C2D-C3D	-3.52	119.62	127.69
19	A	1133	CLA	C1-C2-C3	-3.52	121.07	126.76
19	A	1117	CLA	CHC-C4B-NB	3.52	129.32	124.05
19	A	1132	CLA	CHC-C1C-C2C	-3.52	116.96	126.95
19	H	1207	CLA	CHC-C1C-NC	3.51	129.60	124.31
19	A	1107	CLA	C4A-NA-C1A	3.51	108.28	106.68
19	A	1125	CLA	CMD-C2D-C3D	-3.51	119.63	127.69
22	G	7026	LMU	C1B-O1B-C4'	-3.51	109.65	117.98
19	A	1237	CLA	C2B-C1B-NB	3.51	113.97	110.33
19	A	1123	CLA	CHC-C4B-NB	3.51	129.32	124.05
19	K	3009	CLA	CMD-C2D-C3D	-3.51	119.64	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	J	1308	CLA	C2B-C1B-NB	3.51	113.97	110.33
19	3	3013	CLA	C4A-NA-C1A	3.51	108.28	106.68
19	A	1129	CLA	CMD-C2D-C3D	-3.51	119.64	127.69
19	3	3017	CLA	C3B-C2B-C1B	-3.51	103.03	107.17
19	B	1215	CLA	O2A-CGA-CBA	3.51	122.53	111.83
19	I	1204	CLA	C4B-CHC-C1C	-3.51	118.00	126.25
19	I	1204	CLA	CHC-C1C-NC	3.51	129.59	124.31
19	4	4010	CLA	C3D-C4D-CHA	-3.50	117.38	125.20
19	A	1309	CLA	C3D-C4D-CHA	-3.50	117.38	125.20
19	H	1207	CLA	CHC-C4B-NB	3.50	129.30	124.05
21	A	6002	BCR	C23-C24-C25	-3.50	117.65	127.00
19	B	1205	CLA	O2A-CGA-CBA	3.50	122.50	111.83
19	A	9023	CLA	C1-O2A-CGA	3.49	125.11	116.65
19	4	4004	CLA	C2D-C3D-C4D	-3.49	103.10	107.35
22	H	7011	LMU	O1B-C1B-O5B	3.49	119.89	110.69
19	J	1308	CLA	C1-C2-C3	-3.49	120.47	126.20
19	3	3007	CLA	C2B-C1B-NB	3.49	113.95	110.33
19	A	1115	CLA	C4B-CHC-C1C	-3.49	118.04	126.25
19	A	1140	CLA	C1-C2-C3	-3.49	120.48	126.20
19	3	3003	CLA	CMD-C2D-C3D	-3.49	119.69	127.69
19	3	3011	CLA	CHD-C4C-C3C	-3.49	119.69	124.77
19	B	1221	CLA	O2A-CGA-CBA	3.49	122.46	111.83
21	F	6014	BCR	C23-C22-C21	3.48	124.49	119.01
19	3	2009	CLA	O2D-CGD-CBD	3.48	117.32	111.23
19	3	3015	CLA	C3D-C4D-CHA	-3.48	117.42	125.20
19	A	1141	CLA	C3B-C2B-C1B	-3.48	103.06	107.17
21	J	6012	BCR	C28-C27-C26	-3.48	107.85	114.06
19	A	1122	CLA	CHC-C4B-NB	3.48	129.27	124.05
22	4	7053	LMU	O1B-C1B-C2B	3.48	116.64	108.09
19	A	1128	CLA	O2D-CGD-O1D	-3.47	117.08	123.85
22	H	7043	LMU	O5B-C1B-C2B	3.47	117.51	110.37
19	A	1237	CLA	CHC-C1C-NC	3.47	129.54	124.31
21	A	6007	BCR	C28-C27-C26	-3.47	107.86	114.06
21	3	6022	BCR	C20-C19-C18	-3.47	116.86	126.36
19	3	3001	CLA	C1C-CHC-C4B	-3.47	116.90	126.04
19	A	1117	CLA	C4B-C3B-C2B	3.46	111.61	107.30
21	A	6002	BCR	C24-C23-C22	-3.46	121.11	126.23
19	1	1011	CLA	CMB-C2B-C1B	3.46	130.69	125.42
19	A	1107	CLA	O2A-CGA-CBA	3.46	122.39	111.83
19	2	2004	CLA	C3B-C2B-C1B	-3.46	103.09	107.17
19	A	1102	CLA	CHC-C4B-NB	3.46	129.24	124.05
19	B	1230	CLA	CED-O2D-CGD	3.46	123.76	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	4013	CLA	C3D-C4D-CHA	-3.46	117.48	125.20
19	4	4002	CLA	O2A-CGA-O1A	-3.46	114.98	123.63
22	H	7043	LMU	O1B-C4'-C3'	3.46	116.02	107.23
19	4	1304	CLA	O2A-CGA-O1A	-3.46	114.98	123.63
19	B	1217	CLA	CHC-C4B-NB	3.46	129.24	124.05
19	2	2008	CLA	C2D-C3D-C4D	-3.46	103.15	107.35
19	1	1007	CLA	CMD-C2D-C3D	-3.46	119.77	127.69
19	A	1309	CLA	CHC-C4B-NB	3.45	129.07	124.08
19	A	1108	CLA	C4B-C3B-C2B	3.45	111.60	107.30
21	B	6005	BCR	C33-C5-C4	3.45	120.96	113.60
19	A	1108	CLA	CMA-C3A-C2A	-3.45	100.64	113.98
19	3	3006	CLA	CHC-C4B-NB	3.45	129.07	124.08
19	A	1139	CLA	C3B-C2B-C1B	-3.45	103.10	107.17
21	A	6007	BCR	C40-C30-C25	3.45	115.65	110.24
19	4	4006	CLA	C4-C3-C2	-3.45	114.77	123.63
21	F	6016	BCR	C15-C16-C17	-3.45	116.47	123.52
19	B	1228	CLA	CHC-C4B-NB	3.45	129.22	124.05
21	J	6012	BCR	C31-C1-C6	-3.45	104.84	110.24
19	B	1225	CLA	CHB-C4A-NA	3.45	129.37	124.40
19	3	3014	CLA	CHA-C4D-ND	3.45	129.71	124.84
21	B	6010	BCR	C36-C18-C19	3.45	123.35	118.09
21	B	6004	BCR	C38-C26-C25	-3.44	120.73	124.48
19	3	3005	CLA	C2D-C3D-C4D	-3.44	103.17	107.35
19	4	1009	CLA	C4B-CHC-C1C	-3.44	118.15	126.25
22	A	7016	LMU	C2'-C3'-C4'	3.44	117.49	109.68
22	A	7044	LMU	C3'-C4'-C5'	3.44	118.56	110.93
19	1	1013	CLA	CBA-CAA-C2A	3.44	124.03	113.79
19	B	1301	CLA	C2B-C1B-NB	3.44	113.89	110.33
22	A	7045	LMU	O1'-C1'-C2'	3.44	113.50	108.27
19	A	1123	CLA	C4-C3-C5	3.44	121.19	115.23
19	1	1002	CLA	CHC-C4B-NB	3.44	129.20	124.05
19	B	1216	CLA	C1-C2-C3	-3.43	120.57	126.20
19	2	2011	CLA	C4A-NA-C1A	3.43	108.25	106.68
19	2	2013	CLA	CAA-C2A-C1A	3.43	123.22	111.97
19	A	1139	CLA	CHC-C4B-NB	3.43	129.20	124.05
19	3	3012	CLA	C3D-C4D-ND	3.43	114.19	109.50
19	B	1213	CLA	O1D-CGD-CBD	-3.43	117.75	124.52
19	4	4012	CLA	CHC-C4B-NB	3.43	129.19	124.05
19	B	1203	CLA	O2A-CGA-CBA	3.43	122.29	111.83
19	A	1126	CLA	O2A-CGA-CBA	3.43	122.29	111.83
19	R	1150	CLA	CHC-C4B-NB	3.43	129.19	124.05
19	1	1014	CLA	O1D-CGD-CBD	-3.43	117.76	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1014	CLA	CMD-C2D-C3D	-3.43	119.83	127.69
21	A	6011	BCR	C28-C27-C26	-3.43	107.95	114.06
19	K	1146	CLA	CHB-C4A-NA	3.42	129.34	124.40
22	H	7017	LMU	O4'-C4B-C5B	-3.42	100.89	109.32
19	3	3008	CLA	C4A-NA-C1A	3.42	108.24	106.68
19	J	1308	CLA	CHC-C4B-NB	3.42	129.19	124.05
19	J	1308	CLA	CHB-C4A-NA	3.42	129.34	124.40
19	F	1305	CLA	C4B-CHC-C1C	-3.42	118.20	126.25
19	4	4004	CLA	C1C-CHC-C4B	-3.42	117.02	126.04
19	4	4005	CLA	C2D-C3D-C4D	-3.42	103.19	107.35
19	2	2005	CLA	C4A-NA-C1A	3.42	108.24	106.68
19	3	3015	CLA	C4A-NA-C1A	3.42	108.24	106.68
19	B	1218	CLA	O1D-CGD-CBD	-3.42	117.77	124.52
19	2	2006	CLA	CHC-C4B-NB	3.42	129.18	124.05
21	B	6010	BCR	C33-C5-C6	-3.41	120.76	124.48
21	B	6005	BCR	C3-C4-C5	-3.41	107.97	114.06
19	A	1113	CLA	O2A-CGA-CBA	3.41	122.25	111.83
19	A	1117	CLA	CMD-C2D-C3D	-3.41	119.86	127.69
19	B	1202	CLA	O2A-CGA-CBA	3.41	122.23	111.83
19	I	1204	CLA	C3B-C2B-C1B	-3.41	103.15	107.17
19	4	4007	CLA	CHC-C4B-NB	3.41	129.16	124.05
19	A	9023	CLA	C4A-NA-C1A	3.41	108.23	106.68
19	1	1012	CLA	C4A-NA-C1A	3.41	108.23	106.68
19	A	1121	CLA	CMB-C2B-C1B	3.41	130.61	125.42
21	A	6002	BCR	C3-C4-C5	-3.41	107.98	114.06
19	A	1309	CLA	C3B-C2B-C1B	-3.41	103.02	106.81
19	2	2003	CLA	C3D-C4D-CHA	-3.41	117.59	125.20
19	A	1151	CLA	CHC-C4B-NB	3.41	129.16	124.05
19	B	1216	CLA	C3B-C2B-C1B	-3.41	103.15	107.17
19	B	1301	CLA	C1B-C2B-C3B	-3.41	103.83	107.03
19	3	2009	CLA	CHC-C4B-NB	3.40	129.16	124.05
19	A	1127	CLA	CHC-C4B-NB	3.40	129.16	124.05
19	A	1105	CLA	CHC-C1C-NC	3.40	129.44	124.31
19	2	2011	CLA	C2D-C3D-C4D	-3.40	103.22	107.35
19	B	1209	CLA	CHD-C4C-C3C	-3.40	119.81	124.77
19	2	2011	CLA	C3D-C4D-CHA	-3.40	117.61	125.20
22	C	7015	LMU	O1'-C1'-C2'	3.40	113.44	108.27
19	B	1202	CLA	CHD-C4C-C3C	-3.40	119.82	124.77
22	H	7032	LMU	C2'-C3'-C4'	3.40	117.39	109.68
19	A	1149	CLA	C2B-C1B-NB	3.40	113.85	110.33
19	A	1149	CLA	CAC-C3C-C4C	3.40	129.21	124.79
19	A	1120	CLA	CHC-C1C-NC	3.40	129.43	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	7036	LMU	C2'-C3'-C4'	-3.40	101.97	109.68
19	A	1117	CLA	O2D-CGD-CBD	3.40	117.17	111.23
19	1	1008	CLA	CAA-CBA-CGA	3.39	122.84	113.21
19	B	1221	CLA	CHC-C4B-NB	3.39	129.14	124.05
19	B	1212	CLA	CHC-C1C-NC	3.39	129.42	124.31
19	3	3001	CLA	C3D-C4D-CHA	-3.39	117.63	125.20
19	3	1118	CLA	C4A-NA-C1A	3.39	108.23	106.68
19	A	1129	CLA	CHC-C4B-NB	3.39	129.13	124.05
19	B	1220	CLA	C3B-C2B-C1B	-3.39	103.17	107.17
19	4	4015	CLA	CHC-C1C-NC	3.39	129.41	124.31
19	2	2010	CLA	C4A-NA-C1A	3.39	108.22	106.68
22	B	7040	LMU	O3'-C3'-C2'	-3.39	102.39	110.38
19	A	1137	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
22	A	7045	LMU	C3B-C4B-C5B	-3.39	104.09	110.23
19	B	1231	CLA	CHC-C4B-NB	3.39	129.13	124.05
22	R	7024	LMU	C1B-O5B-C5B	3.39	120.33	113.72
19	4	4006	CLA	C2B-C1B-NB	3.39	113.84	110.33
19	A	1122	CLA	O2D-CGD-CBD	3.39	117.15	111.23
21	I	6021	BCR	C10-C11-C12	3.38	133.01	123.20
22	A	7045	LMU	C1B-O5B-C5B	3.38	120.33	113.72
19	4	4005	CLA	CHC-C4B-NB	3.38	128.97	124.08
19	I	1204	CLA	O2A-CGA-CBA	3.38	122.15	111.83
22	R	7024	LMU	C3B-C4B-C5B	-3.38	104.10	110.23
19	1	1008	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
21	B	6005	BCR	C34-C9-C10	-3.38	117.34	122.82
21	A	6003	BCR	C39-C30-C25	3.38	115.54	110.24
19	3	3015	CLA	C3B-C2B-C1B	-3.38	103.05	106.81
19	A	1149	CLA	CHC-C1C-C2C	-3.38	117.34	126.95
19	2	1307	CLA	C1C-CHC-C4B	-3.38	117.13	126.04
19	A	1237	CLA	CMD-C2D-C3D	-3.38	119.94	127.69
19	A	1127	CLA	O1D-CGD-CBD	-3.38	117.86	124.52
19	2	2002	CLA	O2A-CGA-CBA	3.38	122.13	111.83
19	1	1003	CLA	CHC-C4B-NB	3.37	129.11	124.05
21	I	6018	BCR	C15-C14-C13	3.37	132.01	127.28
19	1	1010	CLA	C2A-C3A-C4A	-3.37	96.42	101.87
19	A	1108	CLA	CHD-C4C-C3C	-3.37	119.86	124.77
19	4	4015	CLA	CHC-C4B-NB	3.37	129.10	124.05
19	1	1001	CLA	CHC-C1C-C2C	-3.37	117.37	126.95
19	A	1120	CLA	C3B-C2B-C1B	-3.37	103.20	107.17
19	1	1007	CLA	CHC-C4B-NB	3.37	129.10	124.05
19	A	1149	CLA	CED-O2D-CGD	3.37	123.55	115.92
22	H	7030	LMU	C3B-C4B-C5B	-3.37	104.13	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	F	1305	CLA	CHC-C4B-NB	3.37	129.10	124.05
19	3	3004	CLA	C3B-C2B-C1B	-3.37	103.06	106.81
21	A	6002	BCR	C33-C5-C6	-3.37	120.81	124.48
22	G	7039	LMU	C1B-C2B-C3B	-3.36	102.93	110.01
19	K	3009	CLA	CMC-C2C-C1C	3.36	130.29	125.03
19	1	1310	CLA	CHA-C4D-ND	3.36	129.59	124.84
19	B	1233	CLA	CHC-C1C-NC	3.36	129.37	124.31
19	B	9010	CLA	CBA-CAA-C2A	-3.36	103.80	113.79
19	3	3004	CLA	CHA-C4D-ND	3.36	129.58	124.84
19	1	1310	CLA	CHC-C4B-NB	3.36	128.93	124.08
19	A	1128	CLA	C4-C3-C5	3.36	121.05	115.23
19	2	2011	CLA	CHA-C4D-ND	3.35	129.58	124.84
19	B	1227	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
19	B	1205	CLA	CHB-C4A-NA	3.35	129.24	124.40
19	B	1239	CLA	C3B-C4B-NB	-3.35	107.54	110.53
19	B	1216	CLA	CHC-C1C-NC	3.35	129.36	124.31
22	G	7051	LMU	O3'-C3'-C2'	-3.35	102.48	110.38
19	A	1101	CLA	O1D-CGD-CBD	-3.35	117.92	124.52
19	4	1304	CLA	O2A-CGA-CBA	3.35	122.04	111.83
19	H	1505	CLA	CED-O2D-CGD	3.35	123.51	115.92
19	3	1147	CLA	CHC-C4B-NB	3.35	129.07	124.05
19	4	4012	CLA	CAA-C2A-C3A	-3.34	108.57	116.23
21	B	6005	BCR	C7-C8-C9	-3.34	121.30	126.23
19	1	1303	CLA	CHC-C4B-NB	3.34	129.06	124.05
19	L	1503	CLA	C4B-CHC-C1C	-3.34	118.40	126.25
19	1	1011	CLA	CAA-C2A-C3A	-3.34	108.58	116.23
21	1	6023	BCR	C7-C8-C9	-3.34	121.30	126.23
22	B	7038	LMU	O1B-C4'-C3'	3.33	115.71	107.23
19	A	1134	CLA	C4A-NA-C1A	3.33	108.20	106.68
19	3	3010	CLA	C1B-NB-C4B	-3.33	103.97	106.31
19	A	1109	CLA	C11-C12-C13	-3.33	104.89	115.97
19	A	1119	CLA	C3B-C2B-C1B	-3.33	103.24	107.17
19	H	1241	CLA	CHB-C4A-NA	3.33	129.21	124.40
19	A	1111	CLA	CHB-C4A-NA	3.33	129.21	124.40
19	4	4014	CLA	CHB-C4A-NA	3.33	129.21	124.40
19	A	1128	CLA	CMD-C2D-C3D	-3.33	120.05	127.69
19	1	1005	CLA	C4D-C3D-CAD	3.33	111.72	108.11
21	F	6014	BCR	C16-C17-C18	-3.33	122.61	127.28
19	K	1146	CLA	C1-C2-C3	-3.33	121.38	126.76
21	L	6019	BCR	C28-C27-C26	-3.33	108.12	114.06
19	R	1150	CLA	C4A-NA-C1A	3.33	108.20	106.68
19	L	1501	CLA	O2D-CGD-O1D	-3.32	117.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1151	CLA	CAC-C3C-C4C	3.32	129.12	124.79
21	I	6018	BCR	C39-C30-C25	3.32	115.45	110.24
22	B	7038	LMU	C2'-C3'-C4'	-3.32	102.14	109.68
19	A	1125	CLA	C3B-C2B-C1B	-3.32	103.25	107.17
19	A	1106	CLA	C6-C5-C3	-3.32	105.37	113.47
19	2	2003	CLA	C2D-C3D-C4D	-3.32	103.31	107.35
19	B	1221	CLA	CGD-CBD-CAD	-3.32	100.09	110.85
19	1	1014	CLA	C2B-C1B-NB	3.32	113.77	110.33
19	1	1015	CLA	CHC-C4B-NB	3.32	128.88	124.08
19	A	1103	CLA	CHC-C1C-C2C	-3.32	117.52	126.95
19	A	9013	CLA	CHC-C4B-NB	3.32	129.03	124.05
21	A	6007	BCR	C33-C5-C4	3.32	120.67	113.60
19	K	1143	CLA	CHC-C4B-NB	3.32	129.02	124.05
19	G	1242	CLA	CHC-C1C-NC	3.31	129.30	124.31
19	H	1145	CLA	C4A-NA-C1A	3.31	108.19	106.68
19	1	1007	CLA	C4A-NA-C1A	3.31	108.19	106.68
19	A	1115	CLA	CHB-C4A-NA	3.31	129.18	124.40
19	4	4002	CLA	O2D-CGD-CBD	3.31	117.02	111.23
22	H	7028	LMU	O1'-C1'-C2'	3.31	113.30	108.27
19	4	4003	CLA	CHC-C4B-NB	3.31	129.01	124.05
19	3	3004	CLA	C3D-C4D-CHA	-3.31	117.81	125.20
21	A	6008	BCR	C33-C5-C6	-3.31	120.87	124.48
19	2	2008	CLA	C3D-C4D-CHA	-3.31	117.81	125.20
19	1	1008	CLA	CHC-C4B-NB	3.31	129.01	124.05
19	A	1135	CLA	C3B-C2B-C1B	-3.31	103.27	107.17
19	2	1307	CLA	C3D-C4D-ND	3.31	114.02	109.50
21	B	6010	BCR	C3-C4-C5	-3.30	108.16	114.06
21	A	6011	BCR	C36-C18-C19	3.30	123.14	118.09
19	K	1146	CLA	CMA-C3A-C4A	-3.30	102.89	111.77
19	A	1110	CLA	CHC-C4B-NB	3.30	129.00	124.05
19	A	1113	CLA	C3B-C2B-C1B	-3.30	103.28	107.17
21	B	6010	BCR	C27-C26-C25	-3.30	118.24	122.70
19	3	1147	CLA	CHB-C1B-NB	-3.30	119.10	124.05
19	4	1304	CLA	O2D-CGD-CBD	3.30	117.00	111.23
19	A	1126	CLA	C4B-CHC-C1C	-3.30	118.49	126.25
19	B	1219	CLA	CHD-C4C-C3C	-3.30	119.96	124.77
22	H	7043	LMU	C1B-C2B-C3B	3.30	116.95	110.01
19	3	3015	CLA	CHC-C4B-NB	3.30	128.85	124.08
19	L	1148	CLA	CBA-CAA-C2A	3.30	123.60	113.79
19	1	1303	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
19	4	1004	CLA	C3B-C2B-C1B	-3.30	103.28	107.17
19	A	1110	CLA	C3B-C2B-C1B	-3.30	103.28	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	7022	LMU	C1-O1'-C1'	3.29	119.31	113.68
19	3	3013	CLA	C4-C3-C5	3.29	120.94	115.23
19	J	1308	CLA	CED-O2D-CGD	3.29	123.38	115.92
19	1	1303	CLA	CHC-C1C-C2C	-3.29	117.59	126.95
22	A	7010	LMU	O5'-C5'-C6'	3.29	114.59	106.44
19	B	1228	CLA	CMB-C2B-C1B	3.29	130.43	125.42
19	B	1203	CLA	CHC-C1C-C2C	-3.29	117.60	126.95
19	3	3017	CLA	CAC-C3C-C4C	3.29	129.07	124.79
19	A	1133	CLA	C3B-C2B-C1B	-3.29	103.29	107.17
19	F	1240	CLA	CMB-C2B-C3B	3.29	132.26	123.53
22	A	7016	LMU	O1'-C1'-C2'	3.29	113.26	108.27
19	1	1005	CLA	C2B-C1B-NB	3.28	113.73	110.33
19	A	1112	CLA	O1D-CGD-CBD	-3.28	118.04	124.52
20	A	5001	PQN	C2M-C2-C3	-3.28	119.05	124.45
19	A	1104	CLA	C1-C2-C3	-3.28	120.82	126.20
21	F	6014	BCR	C3-C4-C5	-3.28	108.20	114.06
19	2	2014	CLA	CHB-C4A-NA	3.28	129.13	124.40
19	A	1127	CLA	C4A-NA-C1A	3.28	108.17	106.68
19	B	1230	CLA	C4A-NA-C1A	3.28	108.17	106.68
19	A	9012	CLA	CHB-C4A-NA	3.28	129.13	124.40
19	1	1015	CLA	CHA-C4D-ND	3.28	129.47	124.84
19	2	2006	CLA	O2D-CGD-CBD	3.28	116.96	111.23
19	4	4012	CLA	CMD-C2D-C3D	-3.28	120.17	127.69
19	A	9011	CLA	C4A-NA-C1A	3.27	108.17	106.68
19	H	1241	CLA	CMD-C2D-C3D	-3.27	120.18	127.69
19	B	1218	CLA	C3B-C2B-C1B	-3.27	103.31	107.17
22	4	7052	LMU	C3'-C4'-C5'	-3.27	103.68	110.93
19	3	3013	CLA	CMD-C2D-C3D	-3.27	120.19	127.69
19	B	1208	CLA	O2A-CGA-CBA	3.27	121.80	111.83
19	L	1503	CLA	CMD-C2D-C3D	-3.27	120.19	127.69
22	G	7051	LMU	O5B-C1B-C2B	-3.27	103.66	110.37
19	A	1141	CLA	C4A-NA-C1A	3.27	108.17	106.68
19	B	1301	CLA	CHC-C4B-NB	3.27	128.95	124.05
19	4	4004	CLA	C3D-C4D-CHA	-3.26	117.91	125.20
22	4	7009	LMU	C2'-C3'-C4'	3.26	117.09	109.68
21	I	6018	BCR	C38-C26-C25	-3.26	120.92	124.48
19	4	4014	CLA	O2A-CGA-CBA	3.26	121.78	111.83
19	A	1141	CLA	CHC-C4B-NB	3.26	128.94	124.05
19	B	1223	CLA	CHC-C4B-NB	3.26	128.94	124.05
21	A	6011	BCR	C24-C23-C22	-3.26	121.42	126.23
19	3	3005	CLA	C3D-C4D-CHA	-3.26	117.93	125.20
19	B	1214	CLA	O2D-CGD-O1D	-3.26	117.51	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	I	6021	BCR	C20-C19-C18	-3.26	117.44	126.36
21	A	6011	BCR	C40-C30-C39	3.25	117.95	108.63
22	3	7005	LMU	C1'-O5'-C5'	3.25	120.07	113.72
19	4	4002	CLA	CBA-CAA-C2A	-3.25	104.12	113.79
22	2	7027	LMU	C1'-O5'-C5'	3.25	120.07	113.72
19	4	4010	CLA	C4A-NA-C1A	3.25	108.16	106.68
19	L	1130	CLA	CHC-C4B-NB	3.25	128.93	124.05
19	3	3011	CLA	CHC-C4B-NB	3.25	128.92	124.05
19	F	1240	CLA	CHB-C4A-NA	3.25	129.09	124.40
21	3	6022	BCR	C15-C14-C13	-3.25	122.72	127.28
19	A	1124	CLA	C3B-C2B-C1B	-3.25	103.34	107.17
21	B	6005	BCR	C28-C27-C26	-3.25	108.27	114.06
19	L	1148	CLA	CAA-CBA-CGA	-3.24	104.00	113.21
19	A	1122	CLA	CAC-C3C-C4C	3.24	129.01	124.79
19	A	9013	CLA	CHC-C1C-NC	3.24	129.20	124.31
19	1	1303	CLA	O2A-CGA-CBA	3.24	121.72	111.83
19	H	1145	CLA	O2A-CGA-CBA	3.24	121.72	111.83
22	K	7001	LMU	O5B-C5B-C6B	3.24	114.47	106.44
19	A	1117	CLA	O2A-CGA-CBA	3.24	121.71	111.83
21	A	6011	BCR	C38-C26-C25	-3.24	120.95	124.48
19	2	2007	CLA	C4A-NA-C1A	3.24	108.16	106.68
19	B	1301	CLA	CHC-C1C-NC	3.24	129.19	124.31
19	B	1221	CLA	CHB-C4A-NA	3.24	129.07	124.40
19	4	4006	CLA	CHC-C1C-NC	3.24	129.18	124.31
19	1	1003	CLA	CMB-C2B-C1B	3.23	130.34	125.42
19	2	2013	CLA	CHB-C4A-NA	3.23	129.07	124.40
19	1	1006	CLA	CHC-C4B-NB	3.23	128.90	124.05
19	G	1242	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
19	2	2001	CLA	C4-C3-C5	3.23	119.93	116.13
19	H	1145	CLA	CHB-C1B-NB	-3.23	119.21	124.05
19	B	1236	CLA	CHC-C4B-NB	3.23	128.89	124.05
19	B	1217	CLA	C3B-C2B-C1B	-3.23	103.36	107.17
19	3	1147	CLA	C3B-C2B-C1B	-3.23	103.36	107.17
19	2	2014	CLA	CMD-C2D-C3D	-3.23	120.29	127.69
19	B	1212	CLA	C4-C3-C5	3.23	120.83	115.23
19	B	1232	CLA	C3B-C2B-C1B	-3.23	103.37	107.17
19	B	1227	CLA	CED-O2D-CGD	3.22	123.23	115.92
19	3	3005	CLA	CHA-C4D-ND	3.22	129.40	124.84
19	1	1013	CLA	CAA-C2A-C1A	-3.22	101.41	111.97
19	1	1005	CLA	CHC-C4B-NB	3.22	128.88	124.05
19	B	1301	CLA	CMA-C3A-C2A	-3.22	108.84	116.23
19	B	1212	CLA	CHC-C4B-NB	3.22	128.88	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	7033	LMU	O5'-C1'-C2'	3.22	116.98	110.37
19	4	4012	CLA	CHB-C4A-NA	3.22	129.05	124.40
19	1	1003	CLA	C4A-NA-C1A	3.22	108.15	106.68
19	A	1107	CLA	CMB-C2B-C1B	3.22	130.32	125.42
19	3	3002	CLA	C3B-C2B-C1B	-3.22	103.23	106.81
21	B	6006	BCR	C31-C1-C6	-3.22	105.20	110.24
19	B	1203	CLA	CHC-C4B-NB	3.22	128.87	124.05
19	R	1150	CLA	O2A-C1-C2	3.22	120.48	108.11
22	H	7002	LMU	O5'-C5'-C6'	3.21	114.41	106.44
19	B	1239	CLA	CMD-C2D-C3D	-3.21	120.32	127.69
19	A	1111	CLA	CHC-C1C-C2C	-3.21	117.82	126.95
19	G	1242	CLA	C4B-CHC-C1C	-3.21	118.70	126.25
22	2	7027	LMU	C2'-C3'-C4'	3.21	116.96	109.68
19	2	2005	CLA	C3D-C4D-ND	3.21	113.89	109.50
19	B	1232	CLA	CHC-C4B-NB	3.21	128.86	124.05
21	B	6020	BCR	C16-C17-C18	-3.21	122.78	127.28
22	H	7017	LMU	O5B-C5B-C6B	3.21	114.39	106.44
22	3	7005	LMU	O1B-C4'-C3'	3.21	115.38	107.23
21	I	6021	BCR	C30-C25-C24	3.21	124.35	115.65
19	B	1236	CLA	O1D-CGD-CBD	-3.21	118.19	124.52
19	2	2010	CLA	CHC-C4B-NB	3.21	128.71	124.08
19	2	2013	CLA	C2B-C1B-NB	3.21	113.65	110.33
19	4	1004	CLA	C4A-NA-C1A	3.20	108.14	106.68
19	4	4006	CLA	CMB-C2B-C1B	3.20	130.30	125.42
19	B	1220	CLA	CBC-CAC-C3C	-3.20	103.74	112.42
19	3	3013	CLA	C3B-C2B-C1B	-3.20	103.39	107.17
19	1	1310	CLA	C3D-C4D-ND	3.20	113.87	109.50
21	A	6011	BCR	C16-C17-C18	-3.20	122.79	127.28
22	B	7012	LMU	C3B-C4B-C5B	3.20	116.03	110.23
19	K	1142	CLA	CHC-C4B-NB	3.20	128.85	124.05
19	A	1123	CLA	O2A-CGA-CBA	3.20	121.58	111.83
19	B	1211	CLA	CMB-C2B-C1B	3.20	130.28	125.42
22	4	7053	LMU	C4B-C3B-C2B	-3.20	105.22	110.83
19	F	1302	CLA	C3B-C2B-C1B	-3.20	103.40	107.17
22	H	7011	LMU	O1B-C4'-C3'	3.19	115.35	107.23
19	L	1504	CLA	CHC-C1C-NC	3.19	129.12	124.31
21	B	6004	BCR	C33-C5-C4	3.19	120.41	113.60
21	I	6018	BCR	C24-C25-C26	-3.19	114.20	121.56
19	3	3017	CLA	O1D-CGD-CBD	-3.19	118.22	124.52
19	A	1131	CLA	O2A-CGA-CBA	3.19	121.56	111.83
19	2	2005	CLA	C1B-NB-C4B	-3.19	104.07	106.31
19	3	3001	CLA	CHA-C4D-ND	3.19	129.35	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1140	CLA	CHC-C4B-NB	3.19	128.83	124.05
19	A	1135	CLA	CHC-C4B-NB	3.19	128.83	124.05
19	A	1107	CLA	C4-C3-C5	3.19	120.76	115.23
19	3	3010	CLA	C2D-C3D-C4D	-3.19	103.48	107.35
19	2	2006	CLA	C4-C3-C5	3.18	120.76	115.23
19	B	1225	CLA	CHB-C1B-NB	-3.18	119.27	124.05
19	A	9022	CLA	C1-O2A-CGA	3.18	124.36	116.65
19	A	1105	CLA	C3B-C2B-C1B	-3.18	103.42	107.17
19	K	1142	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
19	1	1303	CLA	CGD-CBD-CAD	-3.18	100.54	110.85
19	2	2013	CLA	O2A-CGA-CBA	3.18	121.54	111.83
19	2	4009	CLA	C2B-C1B-NB	3.18	113.62	110.33
19	3	3017	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
19	3	3007	CLA	C3B-C2B-C1B	-3.18	103.42	107.17
19	4	4012	CLA	CAC-C3C-C4C	3.18	130.00	125.03
19	4	1306	CLA	CHB-C4A-NA	3.18	128.99	124.40
19	H	1505	CLA	O2A-CGA-CBA	3.18	121.53	111.83
19	2	2014	CLA	C4-C3-C5	3.18	120.75	115.23
22	4	7033	LMU	C4B-C3B-C2B	3.18	116.41	110.83
19	B	1234	CLA	CMB-C2B-C1B	3.18	130.26	125.42
19	F	1305	CLA	C4-C3-C5	3.18	120.74	115.23
21	B	6020	BCR	C24-C23-C22	-3.18	121.54	126.23
21	I	6018	BCR	C38-C26-C27	3.18	120.37	113.60
22	4	7018	LMU	C1B-O5B-C5B	3.18	119.92	113.72
19	B	1231	CLA	CHC-C1C-NC	3.18	129.09	124.31
19	B	1212	CLA	CED-O2D-CGD	3.18	123.12	115.92
19	H	1241	CLA	CED-O2D-CGD	3.18	123.12	115.92
22	H	7028	LMU	C1B-O1B-C4'	-3.18	110.45	117.98
19	A	1106	CLA	CHC-C4B-NB	3.17	128.81	124.05
19	B	1234	CLA	C3B-C2B-C1B	-3.17	103.43	107.17
19	B	1212	CLA	O2A-CGA-CBA	3.17	121.50	111.83
19	R	1144	CLA	C4-C3-C5	3.17	120.73	115.23
21	1	6023	BCR	C30-C25-C24	3.17	124.25	115.65
21	A	6002	BCR	C16-C17-C18	-3.17	122.83	127.28
19	B	1216	CLA	CMD-C2D-C3D	-3.17	120.42	127.69
19	A	1103	CLA	CAC-C3C-C4C	3.17	128.91	124.79
21	1	6023	BCR	C8-C7-C6	-3.17	118.53	127.00
19	A	1131	CLA	C4A-NA-C1A	3.17	108.12	106.68
22	A	7044	LMU	O5'-C5'-C4'	3.17	116.27	109.72
22	E	7037	LMU	O5B-C5B-C6B	3.17	114.29	106.44
19	B	9010	CLA	O2A-CGA-CBA	3.17	121.49	111.83
19	L	1130	CLA	O2D-CGD-O1D	-3.17	117.69	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1106	CLA	CHB-C4A-NA	3.16	128.97	124.40
22	R	7024	LMU	C2'-C3'-C4'	3.16	116.86	109.68
19	B	1218	CLA	CHC-C4B-NB	3.16	128.79	124.05
19	B	1211	CLA	CHD-C4C-C3C	-3.16	120.16	124.77
19	B	1239	CLA	CHB-C1B-NB	-3.16	119.31	124.05
19	A	1136	CLA	C4A-NA-C1A	3.16	108.12	106.68
21	F	6016	BCR	C27-C26-C25	-3.16	118.43	122.70
19	B	1205	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
19	4	4014	CLA	CHB-C1B-NB	-3.16	119.31	124.05
19	H	1241	CLA	C4-C3-C5	3.16	120.71	115.23
19	B	1226	CLA	CMA-C3A-C2A	-3.16	101.78	113.98
19	3	3016	CLA	C4-C3-C5	3.16	120.70	115.23
19	2	2014	CLA	CAC-C3C-C4C	3.15	128.89	124.79
19	1	1014	CLA	C4A-NA-C1A	3.15	108.12	106.68
19	A	9012	CLA	O2A-CGA-O1A	-3.15	115.74	123.63
19	A	1116	CLA	CHC-C4B-NB	3.15	128.78	124.05
19	A	1136	CLA	C3B-C2B-C1B	-3.15	103.45	107.17
21	A	6002	BCR	C32-C1-C31	3.15	117.66	108.63
19	B	1231	CLA	CHB-C4A-NA	3.15	128.95	124.40
19	A	1109	CLA	CAA-C2A-C1A	-3.15	101.65	111.97
19	A	1104	CLA	C4A-NA-C1A	3.15	108.12	106.68
19	2	2005	CLA	C3B-C2B-C1B	-3.15	103.30	106.81
19	A	1117	CLA	C4-C3-C5	3.15	120.69	115.23
19	4	4006	CLA	C3B-C2B-C1B	-3.15	103.46	107.17
19	A	9022	CLA	CMD-C2D-C3D	-3.15	120.47	127.69
19	2	2012	CLA	CHB-C4A-NA	3.15	128.94	124.40
21	B	6005	BCR	C38-C26-C27	3.15	120.31	113.60
19	A	1137	CLA	C3B-C2B-C1B	-3.15	103.46	107.17
19	A	1125	CLA	C4A-NA-C1A	3.15	108.11	106.68
19	A	1149	CLA	CBA-CAA-C2A	3.14	123.15	113.79
19	J	1311	CLA	CHC-C4B-NB	3.14	128.77	124.05
22	A	7045	LMU	C2'-C3'-C4'	3.14	116.81	109.68
19	B	1236	CLA	C4A-NA-C1A	3.14	108.11	106.68
19	3	3012	CLA	CHA-C4D-ND	3.14	129.28	124.84
19	L	1148	CLA	C3B-C4B-NB	-3.14	107.73	110.53
19	B	1221	CLA	CAA-CBA-CGA	-3.14	104.30	113.21
19	K	3009	CLA	C4A-NA-C1A	3.14	108.11	106.68
19	A	1109	CLA	CHC-C1C-C2C	-3.14	118.03	126.95
19	2	2013	CLA	C1-O2A-CGA	3.14	124.24	116.65
19	A	1136	CLA	CHC-C4B-NB	3.14	128.75	124.05
19	A	1151	CLA	CHD-C4C-C3C	-3.14	120.20	124.77
21	3	6022	BCR	C23-C24-C25	-3.13	118.63	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	3007	CLA	CHD-C4C-C3C	-3.13	120.21	124.77
19	B	1234	CLA	C2B-C1B-NB	3.13	113.57	110.33
19	R	1150	CLA	C2B-C1B-NB	3.13	113.57	110.33
19	A	1116	CLA	C1-O2A-CGA	3.13	124.22	116.65
19	A	9011	CLA	CHC-C1C-NC	3.13	129.02	124.31
21	B	6005	BCR	C2-C1-C6	-3.12	105.90	110.44
19	4	1304	CLA	CHC-C1C-C2C	-3.12	118.07	126.95
19	B	1221	CLA	C3B-C2B-C1B	-3.12	103.49	107.17
22	B	7012	LMU	O1'-C1'-C2'	3.12	113.02	108.27
19	3	3014	CLA	C3D-C4D-ND	3.12	113.77	109.50
19	A	1127	CLA	CMD-C2D-C3D	-3.12	120.53	127.69
19	3	1147	CLA	CMD-C2D-C3D	-3.12	120.53	127.69
21	B	6005	BCR	C4-C5-C6	-3.12	118.49	122.70
19	3	3008	CLA	C1-C2-C3	-3.12	121.71	126.76
19	A	1117	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
19	3	3012	CLA	C4C-CHD-C1D	-3.12	117.09	125.98
19	L	1504	CLA	CHC-C4B-NB	3.12	128.73	124.05
21	B	6005	BCR	C39-C30-C25	3.12	115.13	110.24
19	1	1005	CLA	C4A-NA-C1A	3.11	108.10	106.68
22	H	7011	LMU	O3'-C3'-C4'	-3.11	101.96	109.94
19	L	1503	CLA	C4D-CHA-C1A	3.11	124.95	121.24
19	3	3002	CLA	CHC-C4B-NB	3.11	128.57	124.08
19	3	2009	CLA	C4-C3-C5	3.11	120.62	115.23
21	B	6017	BCR	C36-C18-C19	3.11	122.84	118.09
19	2	2002	CLA	C4-C3-C2	-3.11	115.65	123.63
19	2	2010	CLA	C3B-C2B-C1B	-3.10	103.35	106.81
22	B	7012	LMU	O5B-C5B-C4B	3.10	115.29	109.70
19	B	1235	CLA	CBC-CAC-C3C	-3.10	104.01	112.42
19	B	1209	CLA	C3B-C2B-C1B	-3.10	103.51	107.17
22	A	7010	LMU	C2'-C3'-C4'	3.10	116.72	109.68
19	R	1144	CLA	C1-O2A-CGA	3.10	124.16	116.65
19	R	1144	CLA	CHC-C4B-NB	3.10	128.70	124.05
21	A	6007	BCR	C34-C9-C10	-3.10	117.80	122.82
21	I	6021	BCR	C32-C1-C31	3.10	117.50	108.63
19	B	1213	CLA	CHC-C4B-NB	3.10	128.69	124.05
19	B	1224	CLA	CAA-C2A-C3A	-3.09	104.64	113.00
19	3	3004	CLA	C2C-C1C-CHC	-3.09	117.74	125.84
19	A	1309	CLA	C2D-C3D-C4D	-3.09	103.59	107.35
19	3	3006	CLA	C2D-C3D-C4D	-3.09	103.59	107.35
19	B	1226	CLA	C2A-C1A-CHA	-3.09	118.50	123.87
19	B	9010	CLA	CHB-C4A-NA	3.09	128.86	124.40
19	B	1220	CLA	CBA-CAA-C2A	3.09	122.98	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	R	1144	CLA	CED-O2D-CGD	3.09	122.92	115.92
19	2	1307	CLA	CHA-C4D-ND	3.09	129.20	124.84
19	4	4006	CLA	C1D-ND-C4D	-3.09	104.15	106.31
19	B	1229	CLA	CHC-C4B-NB	3.09	128.68	124.05
22	K	7041	LMU	O1B-C1B-C2B	3.09	115.68	108.09
19	3	3008	CLA	C3B-C2B-C1B	-3.08	103.53	107.17
19	H	1505	CLA	C3B-C2B-C1B	-3.08	103.53	107.17
21	A	6011	BCR	C38-C26-C27	3.08	120.17	113.60
19	A	1132	CLA	CMA-C3A-C2A	-3.08	102.06	113.98
19	1	1002	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
19	A	1129	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
19	4	1009	CLA	CAA-C2A-C3A	-3.08	109.17	116.23
19	A	1126	CLA	CHB-C4A-NA	3.08	128.85	124.40
19	A	1106	CLA	C3B-C4B-NB	-3.08	107.78	110.53
19	B	1235	CLA	CMB-C2B-C1B	3.08	130.11	125.42
19	B	1209	CLA	C4-C3-C2	-3.08	115.72	123.63
19	1	1007	CLA	O2A-CGA-CBA	3.08	121.22	111.83
19	3	1147	CLA	O1D-CGD-CBD	-3.08	118.45	124.52
19	B	1219	CLA	CED-O2D-CGD	3.08	122.89	115.92
22	E	7048	LMU	O1B-C1B-C2B	3.08	115.66	108.09
19	B	1208	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
19	A	9013	CLA	CHB-C4A-NA	3.07	128.84	124.40
19	2	2003	CLA	CHC-C4B-NB	3.07	128.52	124.08
19	B	1213	CLA	C3B-C2B-C1B	-3.07	103.55	107.17
19	A	1101	CLA	C1-C2-C3	-3.07	121.79	126.76
19	A	1112	CLA	C4B-C3B-C2B	3.07	111.12	107.30
19	A	1129	CLA	C3B-C2B-C1B	-3.07	103.55	107.17
19	L	1130	CLA	O2A-CGA-CBA	3.07	121.19	111.83
19	2	2010	CLA	C3D-C4D-CHA	-3.07	118.35	125.20
22	H	7017	LMU	C1B-O5B-C5B	-3.07	107.73	113.72
19	A	1102	CLA	CMB-C2B-C1B	3.07	130.09	125.42
19	1	1310	CLA	CHB-C4A-NA	3.07	128.79	124.43
21	B	6004	BCR	C34-C9-C10	-3.07	117.85	122.82
19	A	9011	CLA	CHB-C4A-NA	3.07	128.82	124.40
22	R	7022	LMU	O1B-C4'-C3'	3.07	115.02	107.23
22	4	7053	LMU	O1B-C4'-C5'	3.07	117.52	109.48
19	A	9011	CLA	CMB-C2B-C1B	3.06	130.09	125.42
19	B	1222	CLA	C4A-NA-C1A	3.06	108.08	106.68
19	2	4009	CLA	O2A-CGA-CBA	3.06	121.17	111.83
19	4	4011	CLA	C1B-NB-C4B	-3.06	104.16	106.31
19	A	1115	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
19	2	2001	CLA	C3B-C2B-C1B	-3.06	103.56	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1231	CLA	CED-O2D-CGD	3.06	122.86	115.92
19	L	1148	CLA	CMA-C3A-C2A	3.06	125.81	113.98
19	A	1124	CLA	CHC-C4B-NB	3.06	128.64	124.05
19	3	3016	CLA	CHC-C4B-NB	3.06	128.64	124.05
19	A	9022	CLA	CAC-C3C-C4C	3.06	128.77	124.79
19	B	1209	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
21	L	6019	BCR	C38-C26-C27	3.06	120.12	113.60
21	B	6017	BCR	C37-C22-C21	-3.06	117.86	122.82
19	A	1138	CLA	C3B-C2B-C1B	-3.06	103.56	107.17
19	B	1215	CLA	CGD-CBD-CAD	-3.06	100.95	110.85
19	2	2002	CLA	CMB-C2B-C1B	3.06	130.07	125.42
19	K	3009	CLA	CHC-C4B-NB	3.06	128.63	124.05
19	2	2014	CLA	O2A-CGA-CBA	3.06	121.15	111.83
21	3	6022	BCR	C32-C1-C6	-3.05	105.45	110.24
22	E	7037	LMU	O4'-C4B-C5B	3.05	116.84	109.32
19	L	1502	CLA	CHC-C4B-NB	3.05	128.63	124.05
19	B	1208	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
19	A	1121	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
19	3	3004	CLA	C2D-C3D-C4D	-3.05	103.64	107.35
19	3	3005	CLA	CHB-C4A-NA	3.05	128.77	124.43
19	1	1012	CLA	CBD-CHA-C1A	3.05	131.99	127.38
19	A	1134	CLA	CHC-C4B-NB	3.05	128.62	124.05
19	B	1214	CLA	O2A-CGA-CBA	3.05	121.13	111.83
19	H	1241	CLA	O2A-CGA-CBA	3.05	121.13	111.83
21	B	6010	BCR	C40-C30-C39	3.05	117.36	108.63
22	R	7014	LMU	O5B-C5B-C6B	3.05	113.99	106.44
19	3	3001	CLA	CHC-C4B-NB	3.05	128.48	124.08
19	J	1311	CLA	C3B-C2B-C1B	-3.05	103.58	107.17
19	K	1146	CLA	O2A-CGA-O1A	-3.05	116.01	123.63
19	A	1133	CLA	O2A-CGA-CBA	3.05	121.12	111.83
19	A	1125	CLA	CHC-C4B-NB	3.05	128.62	124.05
19	B	1201	CLA	C4A-NA-C1A	3.04	108.07	106.68
19	1	1012	CLA	C1B-C2B-C3B	-3.04	104.17	107.03
22	B	7038	LMU	O5'-C1'-C2'	3.04	116.62	110.37
19	1	1014	CLA	C3B-C2B-C1B	-3.04	103.58	107.17
19	B	1235	CLA	CHC-C1C-C2C	-3.04	118.30	126.95
21	A	6003	BCR	C29-C30-C25	-3.04	106.03	110.44
19	B	1224	CLA	O2A-CGA-O1A	-3.04	116.03	123.63
19	2	2012	CLA	CHD-C4C-C3C	-3.04	120.34	124.77
19	J	1311	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
22	K	7047	LMU	O1B-C4'-C5'	3.04	117.44	109.48
19	2	2001	CLA	CHC-C4B-NB	3.04	128.60	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	7003	LMU	O4'-C4B-C3B	3.03	117.53	110.38
19	L	1503	CLA	CHC-C1C-NC	3.03	128.88	124.31
19	B	1205	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
19	B	1203	CLA	CHD-C4C-C3C	-3.03	120.35	124.77
19	K	1143	CLA	C3B-C2B-C1B	-3.03	103.59	107.17
19	F	1305	CLA	C2B-C1B-NB	3.03	113.47	110.33
19	A	1104	CLA	O2A-CGA-CBA	3.03	121.07	111.83
22	H	7032	LMU	C4B-C3B-C2B	-3.03	105.52	110.83
19	2	2003	CLA	CHA-C4D-ND	3.03	129.12	124.84
19	A	1109	CLA	O2D-CGD-CBD	3.03	116.52	111.23
22	K	7001	LMU	O1'-C1'-C2'	3.03	112.87	108.27
19	2	2013	CLA	CMD-C2D-C3D	-3.03	120.75	127.69
19	B	1210	CLA	C4A-NA-C1A	3.02	108.06	106.68
19	A	1113	CLA	C1-O2A-CGA	3.02	123.97	116.65
19	A	1104	CLA	C4B-C3B-C2B	3.02	111.06	107.30
19	4	4004	CLA	CHC-C4B-NB	3.02	128.44	124.08
21	B	6017	BCR	C16-C15-C14	-3.02	117.34	123.52
19	A	1140	CLA	C3B-C2B-C1B	-3.02	103.61	107.17
19	3	3007	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
19	3	3016	CLA	C3B-C2B-C1B	-3.02	103.61	107.17
19	H	1241	CLA	C3B-C2B-C1B	-3.01	103.62	107.17
19	A	1128	CLA	CHC-C4B-NB	3.01	128.57	124.05
21	F	6014	BCR	C39-C30-C25	3.01	114.97	110.24
19	4	1004	CLA	CAC-C3C-C4C	3.01	128.71	124.79
19	B	1235	CLA	O2A-CGA-CBA	3.01	121.02	111.83
19	A	1135	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
19	A	1104	CLA	C3B-C4B-NB	-3.01	107.84	110.53
19	B	1216	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
19	2	2008	CLA	C3B-C2B-C1B	-3.01	103.46	106.81
19	A	1110	CLA	CHB-C4A-NA	3.01	128.74	124.40
21	A	6002	BCR	C29-C30-C25	-3.01	106.07	110.44
19	1	1001	CLA	O1D-CGD-CBD	-3.01	118.58	124.52
19	A	1115	CLA	C4A-NA-C1A	3.01	108.05	106.68
19	A	1149	CLA	C1B-C2B-C3B	-3.01	104.20	107.03
19	2	2002	CLA	CHC-C4B-NB	3.01	128.56	124.05
22	2	7027	LMU	C1'-C2'-C3'	3.01	116.33	110.01
22	A	7044	LMU	C3B-C4B-C5B	3.01	115.68	110.23
19	B	1214	CLA	C4A-NA-C1A	3.01	108.05	106.68
19	L	1502	CLA	CGD-CBD-CAD	-3.00	101.12	110.85
19	A	1149	CLA	CGD-CBD-CAD	3.00	120.57	110.85
19	B	1219	CLA	O2D-CGD-CBD	3.00	116.48	111.23
21	B	6010	BCR	C28-C27-C26	-3.00	108.70	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1203	CLA	CHB-C1B-NB	-3.00	119.54	124.05
19	2	2002	CLA	C4A-NA-C1A	3.00	108.05	106.68
19	2	2012	CLA	CMB-C2B-C1B	3.00	129.99	125.42
19	H	1145	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
19	2	2002	CLA	C1D-ND-C4D	-3.00	104.21	106.31
19	J	1311	CLA	O2A-CGA-CBA	3.00	120.98	111.83
19	B	1219	CLA	C3B-C2B-C1B	-3.00	103.63	107.17
19	1	1003	CLA	C3B-C2B-C1B	-3.00	103.63	107.17
21	B	6020	BCR	C39-C30-C25	3.00	114.94	110.24
19	1	1303	CLA	CMA-C3A-C4A	3.00	119.83	111.77
19	2	4009	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
19	A	9022	CLA	C5-C3-C2	-3.00	114.44	121.17
19	B	9010	CLA	CMD-C2D-C3D	-3.00	120.82	127.69
19	B	1226	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
19	B	1213	CLA	CAC-C3C-C4C	3.00	128.69	124.79
19	1	1003	CLA	CHC-C1C-NC	3.00	128.82	124.31
21	B	6020	BCR	C19-C18-C17	-2.99	114.30	119.01
19	1	1002	CLA	C3B-C2B-C1B	-2.99	103.64	107.17
19	A	1133	CLA	CHC-C4B-NB	2.99	128.54	124.05
19	3	3011	CLA	CAC-C3C-C4C	2.99	128.68	124.79
19	4	4002	CLA	CMD-C2D-C3D	-2.99	120.83	127.69
19	B	1205	CLA	CHD-C4C-C3C	-2.99	120.41	124.77
19	A	1149	CLA	CAA-C2A-C1A	2.99	121.77	111.97
19	B	1223	CLA	C4-C3-C5	2.99	120.42	115.23
21	B	6004	BCR	C39-C30-C25	2.99	114.93	110.24
19	B	1232	CLA	O1D-CGD-CBD	-2.99	118.63	124.52
22	K	7041	LMU	C4B-C3B-C2B	-2.99	105.59	110.83
22	K	7001	LMU	C3B-C4B-C5B	-2.98	104.82	110.23
22	A	7016	LMU	C1B-C2B-C3B	2.98	116.29	110.01
19	B	1202	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
22	3	7005	LMU	O1B-C1B-C2B	2.98	115.43	108.09
19	A	1122	CLA	C3B-C2B-C1B	-2.98	103.65	107.17
19	A	1138	CLA	CHC-C4B-NB	2.98	128.52	124.05
19	B	1216	CLA	C4-C3-C5	2.98	120.40	115.23
19	A	1120	CLA	CHC-C4B-NB	2.98	128.52	124.05
19	F	1305	CLA	CBC-CAC-C3C	-2.98	104.34	112.42
19	A	1132	CLA	CAC-C3C-C4C	2.98	128.67	124.79
19	B	1222	CLA	CHC-C4B-NB	2.98	128.52	124.05
22	K	7042	LMU	C1B-O1B-C4'	-2.98	110.92	117.98
19	A	1101	CLA	C4B-C3B-C2B	2.98	111.01	107.30
21	J	6012	BCR	C38-C26-C25	-2.98	121.23	124.48
19	L	1148	CLA	CHB-C4A-NA	2.98	128.70	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	F	1240	CLA	CHC-C4B-NB	2.98	128.51	124.05
19	B	1230	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
19	B	1227	CLA	CHD-C4C-C3C	-2.98	120.43	124.77
19	3	1147	CLA	O2A-CGA-O1A	-2.98	114.32	123.20
19	A	1128	CLA	CMB-C2B-C1B	2.98	129.95	125.42
19	L	1148	CLA	C1-O2A-CGA	2.97	123.85	116.65
19	A	1129	CLA	CHD-C4C-C3C	-2.97	120.44	124.77
22	E	7037	LMU	O1B-C1B-O5B	2.97	118.52	110.69
19	1	1001	CLA	CAC-C3C-C2C	-2.97	122.10	127.56
19	3	3003	CLA	CBD-CHA-C1A	2.97	131.87	127.38
19	4	4002	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
19	A	1131	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	E	7048	LMU	O4'-C4B-C5B	-2.97	102.01	109.32
22	H	7017	LMU	C3B-C4B-C5B	2.97	115.62	110.23
19	K	3009	CLA	O2A-CGA-CBA	2.97	120.89	111.83
19	2	1307	CLA	CHC-C4B-NB	2.97	128.37	124.08
19	B	1206	CLA	CMD-C2D-C3D	-2.97	120.88	127.69
19	3	3016	CLA	C1-C2-C3	-2.97	121.34	126.20
19	4	4015	CLA	CHB-C4A-NA	2.96	128.68	124.40
19	B	1206	CLA	C4A-NA-C1A	2.96	108.03	106.68
19	B	1228	CLA	CMD-C2D-C3D	-2.96	120.89	127.69
19	2	2002	CLA	C4-C3-C5	2.96	120.37	115.23
21	B	6006	BCR	C40-C30-C39	2.96	117.11	108.63
21	B	6017	BCR	C28-C27-C26	-2.96	108.78	114.06
19	B	1218	CLA	C4A-NA-C1A	2.96	108.03	106.68
19	L	1502	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
19	A	9023	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
21	I	6018	BCR	C27-C26-C25	-2.96	118.71	122.70
19	A	1103	CLA	O2A-CGA-CBA	2.96	120.85	111.83
19	1	1007	CLA	C4-C3-C5	2.96	120.36	115.23
19	A	9023	CLA	CMA-C3A-C4A	-2.96	103.83	111.77
19	B	1226	CLA	C2B-C1B-NB	2.95	113.39	110.33
19	A	1116	CLA	C3B-C2B-C1B	-2.95	103.69	107.17
19	A	1140	CLA	O2A-CGA-CBA	2.95	120.84	111.83
19	H	1241	CLA	CHD-C4C-C3C	-2.95	120.47	124.77
19	F	1302	CLA	CHC-C4B-NB	2.95	128.47	124.05
19	2	2013	CLA	CHC-C1C-C2C	-2.95	118.56	126.95
21	A	6003	BCR	C28-C27-C26	-2.95	108.80	114.06
19	3	3011	CLA	C4A-NA-C1A	2.95	108.02	106.68
21	B	6005	BCR	C1-C6-C5	-2.95	118.61	122.64
19	2	2008	CLA	CHC-C4B-NB	2.95	128.34	124.08
19	3	3006	CLA	C3D-C4D-CHA	-2.95	118.62	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1220	CLA	C1D-ND-C4D	-2.95	104.25	106.31
19	G	1242	CLA	C4A-NA-C1A	2.95	108.02	106.68
19	A	1137	CLA	CHC-C4B-NB	2.95	128.47	124.05
19	K	1143	CLA	CHC-C1C-C2C	-2.94	118.58	126.95
19	4	4007	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
19	B	1215	CLA	CMD-C2D-C3D	-2.94	120.94	127.69
19	A	9023	CLA	O2A-CGA-CBA	2.94	120.80	111.83
19	B	1238	CLA	C4A-NA-C1A	2.94	108.02	106.68
19	F	1305	CLA	CMD-C2D-C3D	-2.94	120.95	127.69
19	4	4012	CLA	CMB-C2B-C1B	2.94	129.90	125.42
19	B	9010	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
19	L	1148	CLA	C4B-CHC-C1C	-2.94	119.33	126.25
19	L	1504	CLA	C2B-C1B-NB	2.94	113.38	110.33
19	B	1222	CLA	C3B-C2B-C1B	-2.94	103.70	107.17
19	K	1142	CLA	C3B-C2B-C1B	-2.94	103.70	107.17
21	I	6021	BCR	C23-C24-C25	-2.94	119.15	127.00
19	A	1149	CLA	CHC-C4B-NB	2.94	128.46	124.05
19	B	1212	CLA	C3B-C4B-NB	-2.94	107.91	110.53
19	4	4003	CLA	C3B-C2B-C1B	-2.94	103.71	107.17
19	3	3001	CLA	CHB-C4A-NA	2.94	128.61	124.43
19	I	1204	CLA	C4A-NA-C1A	2.93	108.02	106.68
19	4	4013	CLA	C2D-C3D-C4D	-2.93	103.78	107.35
19	A	1124	CLA	C1-C2-C3	-2.93	121.39	126.20
19	4	1306	CLA	CAC-C3C-C2C	-2.93	122.17	127.56
19	4	4007	CLA	C1-C2-C3	-2.93	121.39	126.20
19	B	1201	CLA	CHB-C4A-NA	2.93	128.63	124.40
19	R	1150	CLA	CED-O2D-CGD	2.93	122.57	115.92
19	1	1002	CLA	O2D-CGD-CBD	2.93	116.36	111.23
19	A	9012	CLA	CMD-C2D-C3D	-2.93	120.97	127.69
19	L	1504	CLA	C1D-ND-C4D	-2.93	104.26	106.31
19	A	9022	CLA	CMB-C2B-C1B	2.93	129.87	125.42
19	A	1141	CLA	C4-C3-C5	2.92	120.30	115.23
19	J	1308	CLA	C4-C3-C5	2.92	120.30	115.23
19	L	1503	CLA	C1-C2-C3	-2.92	122.03	126.76
19	A	1104	CLA	C2A-C1A-CHA	-2.92	118.80	123.87
19	4	4004	CLA	CHB-C4A-NA	2.92	128.58	124.43
19	B	1215	CLA	CHC-C4B-NB	2.92	128.43	124.05
22	3	7005	LMU	O2'-C2'-C1'	2.92	117.03	110.08
19	A	1138	CLA	C4-C3-C5	2.92	120.30	115.23
19	2	2008	CLA	CHB-C4A-NA	2.92	128.58	124.43
21	A	6011	BCR	C3-C4-C5	-2.92	108.85	114.06
19	G	1242	CLA	C1-C2-C3	-2.92	121.42	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1126	CLA	C4A-NA-C1A	2.92	108.01	106.68
19	A	1137	CLA	C4A-NA-C1A	2.92	108.01	106.68
19	K	1143	CLA	O2A-CGA-CBA	2.92	120.73	111.83
19	2	2013	CLA	O1D-CGD-CBD	-2.92	118.76	124.52
21	A	6008	BCR	C37-C22-C23	2.92	122.54	118.09
21	A	6007	BCR	C38-C26-C27	2.92	119.81	113.60
19	4	4004	CLA	CHA-C4D-ND	2.92	128.96	124.84
19	1	1011	CLA	CHC-C1C-C2C	-2.91	118.66	126.95
19	1	1013	CLA	CHC-C1C-C2C	-2.91	118.66	126.95
19	A	1104	CLA	CED-O2D-CGD	2.91	122.53	115.92
19	K	3009	CLA	C3B-C2B-C1B	-2.91	103.73	107.17
19	B	1238	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	A	9023	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
19	A	1124	CLA	C4A-NA-C1A	2.91	108.01	106.68
19	3	3007	CLA	CMB-C2B-C1B	2.91	129.85	125.42
19	3	2009	CLA	C3B-C2B-C1B	-2.91	103.74	107.17
19	B	1211	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
19	A	1120	CLA	O2A-CGA-CBA	2.91	120.71	111.83
19	H	1505	CLA	C1-O2A-CGA	2.91	123.70	116.65
19	A	1103	CLA	C1-O2A-CGA	2.91	123.70	116.65
19	A	1111	CLA	CAC-C3C-C4C	2.91	128.58	124.79
19	L	1504	CLA	O2A-CGA-CBA	2.91	120.70	111.83
19	F	1305	CLA	CMB-C2B-C1B	2.91	129.85	125.42
19	J	1311	CLA	CED-O2D-CGD	2.91	122.51	115.92
19	3	3012	CLA	C2C-C1C-CHC	-2.91	118.22	125.84
19	B	1221	CLA	CHC-C1C-C2C	-2.91	118.69	126.95
19	B	1206	CLA	O2A-CGA-O1A	-2.90	116.36	123.63
22	4	7052	LMU	O5'-C1'-O1'	-2.90	103.18	110.04
22	B	7038	LMU	O1B-C1B-C2B	2.90	115.23	108.09
19	4	1009	CLA	C4A-NA-C1A	2.90	108.00	106.68
19	4	1306	CLA	C4-C3-C5	2.90	120.27	115.23
21	B	6010	BCR	C34-C9-C10	-2.90	118.11	122.82
19	4	1004	CLA	CHC-C4B-NB	2.90	128.40	124.05
22	A	7044	LMU	O2'-C2'-C3'	-2.90	103.54	110.38
19	F	1302	CLA	CMA-C3A-C2A	-2.90	109.58	116.23
19	A	1141	CLA	CHB-C4A-NA	2.90	128.58	124.40
21	B	6010	BCR	C37-C22-C21	-2.90	118.12	122.82
19	1	1001	CLA	CBC-CAC-C3C	-2.90	104.57	112.42
19	2	2008	CLA	C4D-ND-C1D	-2.90	104.28	106.31
22	R	7024	LMU	C1'-C2'-C3'	2.90	116.10	110.01
19	4	1004	CLA	O2A-CGA-CBA	2.89	120.66	111.83
21	B	6010	BCR	C32-C1-C31	2.89	116.92	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	6010	BCR	C32-C1-C6	-2.89	105.70	110.24
19	4	4001	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
19	B	1229	CLA	CHB-C4A-NA	2.89	128.57	124.40
19	A	1133	CLA	CMB-C2B-C1B	2.89	129.82	125.42
19	L	1504	CLA	C2A-C1A-CHA	-2.89	118.85	123.87
19	A	1127	CLA	CMB-C2B-C1B	2.89	129.82	125.42
19	B	1239	CLA	CHB-C4A-NA	2.89	128.57	124.40
21	B	6017	BCR	C27-C26-C25	-2.89	118.80	122.70
19	1	1001	CLA	CED-O2D-CGD	2.89	122.46	115.92
19	F	1305	CLA	O2A-CGA-CBA	2.89	120.64	111.83
19	B	1217	CLA	C1D-ND-C4D	-2.89	104.29	106.31
19	F	1240	CLA	CBD-CHA-C1A	2.89	131.74	127.38
19	A	9013	CLA	C4A-NA-C1A	2.88	108.00	106.68
19	B	1229	CLA	C4-C3-C5	2.88	120.23	115.23
19	B	1219	CLA	CHC-C1C-C2C	-2.88	118.75	126.95
19	B	1215	CLA	CMB-C2B-C1B	2.88	129.81	125.42
19	B	1220	CLA	CHC-C1C-NC	2.88	128.65	124.31
19	I	1204	CLA	CHC-C4B-NB	2.88	128.37	124.05
19	R	1144	CLA	C4A-NA-C1A	2.88	107.99	106.68
19	B	1233	CLA	CHC-C4B-NB	2.88	128.37	124.05
19	3	3014	CLA	CHB-C4A-NA	2.88	128.53	124.43
19	B	1239	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
19	H	1145	CLA	C4-C3-C5	2.88	120.22	115.23
19	B	1205	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
19	A	9012	CLA	C1-C2-C3	-2.88	121.48	126.20
19	L	1503	CLA	C3B-C2B-C1B	-2.88	103.78	107.17
19	A	1102	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
19	A	1106	CLA	C4A-NA-C1A	2.88	107.99	106.68
19	1	1303	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
19	H	1145	CLA	CHC-C4B-NB	2.87	128.36	124.05
19	2	2012	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
19	3	3016	CLA	O2A-CGA-CBA	2.87	120.60	111.83
19	B	1216	CLA	O1D-CGD-CBD	-2.87	118.85	124.52
19	A	1124	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
19	1	1002	CLA	CHB-C4A-NA	2.87	128.54	124.40
19	B	1234	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
22	A	7010	LMU	O1'-C1'-C2'	2.87	112.63	108.27
19	B	1211	CLA	CHB-C4A-NA	2.87	128.54	124.40
19	3	3008	CLA	CED-O2D-CGD	2.87	122.43	115.92
19	3	3004	CLA	CHB-C4A-NA	2.87	128.51	124.43
19	H	1241	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
22	4	7018	LMU	O1'-C1'-C2'	2.87	112.63	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1001	CLA	CAA-C2A-C3A	-2.87	105.25	113.00
19	K	1146	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
19	3	3013	CLA	O2A-CGA-CBA	2.87	120.57	111.83
19	4	4013	CLA	C3B-C2B-C1B	-2.87	103.62	106.81
19	4	1306	CLA	O2A-CGA-CBA	2.87	120.57	111.83
19	K	1143	CLA	C4A-NA-C1A	2.86	107.99	106.68
19	B	1301	CLA	CMB-C2B-C1B	2.86	129.78	125.42
22	3	7005	LMU	O5B-C5B-C4B	-2.86	104.54	109.70
19	3	3013	CLA	C2A-C1A-CHA	-2.86	118.90	123.87
19	B	1222	CLA	O2A-CGA-CBA	2.86	120.57	111.83
19	A	1122	CLA	C4-C3-C5	2.86	120.20	115.23
22	3	7005	LMU	O3'-C3'-C4'	2.86	117.28	109.94
19	2	2008	CLA	C3D-C4D-ND	2.86	113.41	109.50
19	2	2002	CLA	CAC-C3C-C4C	2.86	128.51	124.79
22	R	7025	LMU	O5'-C5'-C4'	2.86	115.64	109.72
19	4	4010	CLA	C2D-C3D-C4D	-2.86	103.87	107.35
19	R	1144	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
19	3	1147	CLA	CAC-C3C-C2C	-2.86	122.30	127.56
19	3	1147	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
19	3	3017	CLA	CAC-C3C-C2C	-2.86	122.30	127.56
19	B	1216	CLA	CAA-C2A-C1A	2.86	121.35	111.97
19	A	1101	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
19	4	4001	CLA	C2B-C1B-NB	2.86	113.29	110.33
22	H	7043	LMU	C1'-O5'-C5'	2.86	119.30	113.72
19	R	1144	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
19	B	1225	CLA	CMA-C3A-C2A	-2.85	102.94	113.98
19	H	1241	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
19	B	1222	CLA	C4-C3-C5	2.85	120.18	115.23
19	A	9013	CLA	CMB-C2B-C1B	2.85	129.76	125.42
19	3	3006	CLA	CHB-C4A-NA	2.85	128.49	124.43
19	A	9012	CLA	O1D-CGD-CBD	-2.85	118.89	124.52
19	L	1501	CLA	C3B-C2B-C1B	-2.85	103.81	107.17
19	1	1005	CLA	CAA-C2A-C3A	-2.85	105.29	113.00
19	B	1234	CLA	C1-O2A-CGA	2.85	123.55	116.65
19	J	1308	CLA	CGD-CBD-CAD	-2.85	101.61	110.85
22	H	7030	LMU	O1'-C1'-C2'	2.85	112.60	108.27
19	A	9011	CLA	O2A-CGA-CBA	2.85	120.53	111.83
19	G	1242	CLA	CHB-C4A-NA	2.85	128.51	124.40
22	K	7001	LMU	O5B-C5B-C4B	-2.85	104.56	109.70
22	3	7005	LMU	O5B-C5B-C6B	2.85	113.50	106.44
21	J	6012	BCR	C16-C17-C18	-2.85	123.28	127.28
21	B	6020	BCR	C8-C7-C6	-2.85	119.39	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1124	CLA	O2A-CGA-CBA	2.85	120.52	111.83
19	A	1149	CLA	CHD-C4C-C3C	-2.85	120.62	124.77
22	H	7017	LMU	O5'-C1'-C2'	2.85	116.22	110.37
19	B	1225	CLA	C16-C15-C13	-2.85	106.50	115.97
19	B	1228	CLA	CED-O2D-CGD	2.85	122.37	115.92
19	2	2008	CLA	C3C-C4C-CHD	-2.85	117.84	125.23
19	L	1148	CLA	CHC-C1C-NC	2.85	128.60	124.31
19	A	1133	CLA	CHB-C4A-NA	2.85	128.51	124.40
19	A	1101	CLA	O2A-CGA-CBA	2.84	120.51	111.83
19	F	1240	CLA	CAA-C2A-C3A	-2.84	109.71	116.23
21	A	6003	BCR	C33-C5-C4	2.84	119.66	113.60
19	B	1209	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
19	4	1004	CLA	CHB-C4A-NA	2.84	128.50	124.40
22	E	7037	LMU	O5'-C5'-C6'	2.84	113.48	106.44
19	B	1236	CLA	C3B-C4B-NB	-2.84	107.99	110.53
22	R	7022	LMU	O1B-C1B-C2B	2.84	115.08	108.09
19	4	4002	CLA	CGD-CBD-CAD	2.84	120.04	110.85
19	B	1224	CLA	CHB-C4A-NA	2.84	128.50	124.40
19	1	1006	CLA	CHB-C4A-NA	2.84	128.50	124.40
19	K	1146	CLA	C3B-C2B-C1B	-2.84	103.82	107.17
19	B	1222	CLA	C1-C2-C3	-2.84	121.55	126.20
22	A	7010	LMU	C4B-C3B-C2B	2.84	115.81	110.83
19	A	1139	CLA	C4-C3-C5	2.83	119.46	116.13
21	A	6002	BCR	C20-C19-C18	-2.83	118.59	126.36
21	A	6011	BCR	C27-C26-C25	-2.83	118.88	122.70
19	B	1233	CLA	CMB-C2B-C1B	2.83	129.73	125.42
21	3	6022	BCR	C32-C1-C31	2.83	116.74	108.63
19	B	1223	CLA	C3B-C2B-C1B	-2.83	103.83	107.17
19	4	4002	CLA	CED-O2D-CGD	2.83	122.34	115.92
19	4	4011	CLA	CHD-C1D-ND	2.83	128.84	124.84
19	B	1228	CLA	O2A-CGA-CBA	2.83	120.46	111.83
19	A	1103	CLA	CED-O2D-CGD	2.83	122.33	115.92
19	A	1119	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
19	4	4003	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
19	A	1133	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
19	A	1116	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
19	A	1110	CLA	O2A-CGA-CBA	2.82	120.44	111.83
20	B	5002	PQN	C16-C15-C13	-2.82	106.59	113.47
19	A	1131	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
19	1	1003	CLA	O2A-CGA-CBA	2.82	120.44	111.83
19	B	1208	CLA	CHC-C4B-NB	2.82	128.28	124.05
19	H	1145	CLA	CGD-CBD-CAD	2.82	119.98	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1239	CLA	O2A-CGA-O1A	-2.82	116.57	123.63
19	A	1132	CLA	CED-O2D-CGD	2.82	122.31	115.92
19	A	1113	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
19	4	4005	CLA	CHB-C4A-NA	2.82	128.44	124.43
21	B	6010	BCR	C16-C15-C14	-2.82	117.75	123.52
19	2	2007	CLA	O2A-CGA-CBA	2.82	120.42	111.83
19	L	1130	CLA	C4A-NA-C1A	2.82	107.96	106.68
19	B	1227	CLA	CGD-CBD-CAD	2.82	119.96	110.85
19	4	4001	CLA	CHC-C4B-NB	2.82	128.27	124.05
19	J	1308	CLA	C3B-C2B-C1B	-2.81	103.85	107.17
19	4	1004	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
19	K	1146	CLA	CHC-C4B-NB	2.81	128.27	124.05
19	4	4006	CLA	CHC-C4B-NB	2.81	128.27	124.05
19	A	1106	CLA	C4B-C3B-C2B	2.81	110.80	107.30
22	R	7020	LMU	C3B-C4B-C5B	-2.81	105.13	110.23
21	J	6012	BCR	C40-C30-C25	2.81	114.65	110.24
19	A	1106	CLA	CAA-C2A-C1A	-2.81	102.76	111.97
19	A	1132	CLA	O2A-CGA-CBA	2.81	120.41	111.83
19	2	2005	CLA	C2C-C1C-CHC	-2.81	118.47	125.84
19	B	1211	CLA	CAC-C3C-C4C	2.81	128.45	124.79
19	3	3006	CLA	CHA-C4D-ND	2.81	128.81	124.84
19	H	1207	CLA	O2A-CGA-CBA	2.81	120.40	111.83
19	G	1242	CLA	C1D-ND-C4D	-2.81	104.34	106.31
19	A	1108	CLA	O1D-CGD-CBD	-2.81	118.98	124.52
19	4	1009	CLA	CHC-C4B-NB	2.81	128.26	124.05
19	A	1128	CLA	C1-C2-C3	-2.81	121.60	126.20
19	K	1146	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
19	4	1304	CLA	C11-C10-C8	-2.80	106.64	115.97
19	4	4003	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
19	A	1108	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
19	A	1134	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
19	1	1013	CLA	O2D-CGD-CBD	2.80	116.13	111.23
21	A	6007	BCR	C15-C16-C17	-2.80	117.78	123.52
19	B	1205	CLA	CMB-C2B-C1B	2.80	129.69	125.42
19	B	1217	CLA	O2A-CGA-CBA	2.80	120.38	111.83
19	4	4013	CLA	C1B-NB-C4B	-2.80	104.35	106.31
19	A	9011	CLA	CMC-C2C-C1C	2.80	129.41	125.03
19	A	1127	CLA	CHB-C4A-NA	2.80	128.44	124.40
19	A	1136	CLA	CHC-C1C-C2C	-2.80	118.99	126.95
19	3	3006	CLA	C2C-C1C-CHC	-2.80	118.51	125.84
21	I	6018	BCR	C31-C1-C6	-2.80	105.86	110.24
19	A	1122	CLA	CHB-C4A-NA	2.80	128.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	9013	CLA	O2A-CGA-CBA	2.80	120.36	111.83
19	A	1151	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
19	A	1103	CLA	C4B-C3B-C2B	2.80	110.78	107.30
19	A	9012	CLA	CHC-C4B-NB	2.79	128.24	124.05
19	B	1227	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
22	4	7052	LMU	O6'-C6'-C5'	-2.79	101.83	111.33
19	L	1502	CLA	O2A-CGA-CBA	2.79	120.35	111.83
21	B	6006	BCR	C38-C26-C27	2.79	119.55	113.60
19	3	3003	CLA	CHC-C4B-NB	2.79	128.24	124.05
19	A	1109	CLA	CHB-C4A-NA	2.79	128.43	124.40
19	B	1239	CLA	C4-C3-C5	2.79	120.07	115.23
19	B	1202	CLA	C1-C2-C3	2.79	130.77	126.20
22	2	7046	LMU	O1B-C4'-C3'	2.79	114.32	107.23
21	L	6019	BCR	C40-C30-C39	2.79	116.61	108.63
19	K	1146	CLA	CED-O2D-CGD	2.79	122.24	115.92
19	1	1008	CLA	O2A-CGA-CBA	2.79	120.33	111.83
19	4	1304	CLA	CED-O2D-CGD	2.78	122.23	115.92
19	B	1233	CLA	CED-O2D-CGD	2.78	122.23	115.92
19	2	2008	CLA	CHA-C4D-ND	2.78	128.77	124.84
19	2	2014	CLA	CHC-C4B-NB	2.78	128.22	124.05
19	A	1119	CLA	C1-O2A-CGA	2.78	123.38	116.65
21	A	6003	BCR	C40-C30-C25	2.78	114.61	110.24
19	L	1502	CLA	CED-O2D-CGD	2.78	122.22	115.92
19	3	3003	CLA	C4A-NA-C1A	2.78	107.95	106.68
21	J	6012	BCR	C34-C9-C10	-2.78	118.31	122.82
21	A	6003	BCR	C11-C12-C13	-2.78	118.75	126.36
21	B	6006	BCR	C28-C27-C26	-2.78	109.11	114.06
19	B	9010	CLA	C4B-C3B-C2B	2.77	110.75	107.30
19	A	1115	CLA	O2A-CGA-CBA	2.77	120.29	111.83
19	1	1006	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
19	B	9010	CLA	CMB-C2B-C1B	2.77	129.64	125.42
22	C	7015	LMU	C4B-C3B-C2B	2.77	115.70	110.83
19	A	1127	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
22	A	7044	LMU	C1B-O5B-C5B	2.77	119.13	113.72
19	2	2003	CLA	C3D-C4D-ND	2.77	113.29	109.50
19	A	1137	CLA	O2A-CGA-CBA	2.77	120.28	111.83
19	B	1221	CLA	C1-O2A-CGA	2.77	123.36	116.65
19	B	1230	CLA	O2A-CGA-CBA	2.77	120.28	111.83
19	3	3013	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
19	K	1142	CLA	C2A-C1A-CHA	-2.77	119.06	123.87
19	A	1149	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
19	B	1226	CLA	O1D-CGD-CBD	-2.77	119.06	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	7040	LMU	O2'-C2'-C3'	-2.77	103.85	110.38
22	R	7024	LMU	O1'-C1'-C2'	2.77	112.48	108.27
19	F	1305	CLA	CED-O2D-CGD	2.77	122.19	115.92
22	R	7020	LMU	O5B-C1B-C2B	2.77	116.05	110.37
19	3	3006	CLA	C3C-C4C-CHD	-2.77	118.05	125.23
19	A	1120	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	F	1302	CLA	CAA-C2A-C3A	-2.76	109.89	116.23
19	H	1241	CLA	O1D-CGD-CBD	-2.76	119.07	124.52
19	1	1303	CLA	CMD-C2D-C3D	-2.76	121.36	127.69
19	3	3011	CLA	CED-O2D-CGD	2.76	122.18	115.92
19	A	1105	CLA	O1D-CGD-CBD	-2.76	119.08	124.52
19	B	1226	CLA	CHB-C1B-NB	-2.76	119.91	124.05
19	4	4007	CLA	C3B-C2B-C1B	-2.76	103.92	107.17
22	R	7020	LMU	C3'-C4'-C5'	-2.76	104.81	110.93
19	1	1013	CLA	CHB-C4A-NA	2.76	128.38	124.40
21	B	6005	BCR	C40-C30-C39	2.76	116.53	108.63
19	B	1215	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
19	B	1227	CLA	C1-C2-C3	-2.76	122.30	126.76
22	B	7040	LMU	C1'-C2'-C3'	2.76	115.81	110.01
21	3	6022	BCR	C40-C30-C39	2.75	116.52	108.63
21	B	6005	BCR	C20-C19-C18	-2.75	118.81	126.36
19	3	3008	CLA	O2A-CGA-O1A	-2.75	116.74	123.63
19	2	4009	CLA	C3B-C2B-C1B	-2.75	103.92	107.17
19	2	2006	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
19	4	4006	CLA	CED-O2D-CGD	2.75	122.16	115.92
19	J	1311	CLA	C4-C3-C5	2.75	120.00	115.23
19	4	4012	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
22	4	7019	LMU	C1'-C2'-C3'	2.75	115.80	110.01
21	A	6007	BCR	C8-C7-C6	-2.75	119.66	127.00
19	B	1213	CLA	CHB-C4A-NA	2.75	128.37	124.40
21	3	6022	BCR	C34-C9-C10	-2.75	118.36	122.82
19	A	1134	CLA	C3B-C2B-C1B	-2.75	103.93	107.17
19	4	4002	CLA	CMB-C2B-C3B	2.75	133.01	126.55
19	H	1207	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
21	1	6023	BCR	C31-C1-C2	2.75	119.49	108.95
19	A	1116	CLA	O1D-CGD-CBD	-2.74	119.10	124.52
19	A	1132	CLA	CHB-C4A-NA	2.74	128.36	124.40
19	B	1215	CLA	CHB-C4A-NA	2.74	128.36	124.40
19	R	1150	CLA	CGD-CBD-CAD	-2.74	101.96	110.85
19	2	2001	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
19	B	1220	CLA	C3D-C4D-ND	2.74	114.45	109.99
22	H	7002	LMU	O1'-C1'-C2'	2.74	112.44	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L	1501	CLA	C1-O2A-CGA	2.74	123.29	116.65
21	A	6011	BCR	C34-C9-C10	-2.74	118.38	122.82
21	1	6023	BCR	C23-C24-C25	2.74	134.31	127.00
19	4	4002	CLA	CMA-C3A-C4A	-2.74	104.41	111.77
19	2	2014	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
21	A	6002	BCR	C37-C22-C21	-2.74	118.38	122.82
19	3	3015	CLA	C2C-C1C-CHC	-2.73	118.67	125.84
21	B	6017	BCR	C34-C9-C10	-2.73	118.39	122.82
19	B	1228	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
19	B	1225	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
19	2	2014	CLA	C3A-C2A-C1A	2.73	105.43	101.34
19	H	1241	CLA	CHC-C4B-NB	2.73	128.15	124.05
19	A	9023	CLA	CED-O2D-CGD	2.73	122.11	115.92
19	A	1122	CLA	C4A-NA-C1A	2.73	107.92	106.68
19	B	1216	CLA	C4A-NA-C1A	2.73	107.92	106.68
19	2	1307	CLA	CHB-C4A-NA	2.73	128.31	124.43
19	3	3002	CLA	C2D-C3D-C4D	-2.73	104.03	107.35
19	A	1133	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
22	H	7032	LMU	C3'-C4'-C5'	2.73	116.98	110.93
19	A	1138	CLA	C1-C2-C3	-2.73	121.73	126.20
19	4	1304	CLA	C1-C2-C3	-2.73	121.73	126.20
19	A	1128	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
19	B	1206	CLA	C4-C3-C5	2.73	119.96	115.23
21	B	6005	BCR	C16-C15-C14	-2.73	117.94	123.52
19	A	9022	CLA	CHC-C4B-NB	2.73	128.14	124.05
21	A	6008	BCR	C29-C30-C25	-2.73	106.48	110.44
19	B	1209	CLA	CAC-C3C-C4C	2.72	128.33	124.79
19	A	1237	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
19	3	3016	CLA	CHC-C1C-C2C	-2.72	119.21	126.95
19	A	1151	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
19	2	2003	CLA	C4D-ND-C1D	-2.72	104.40	106.31
19	3	3002	CLA	CHB-C4A-NA	2.72	128.30	124.43
19	A	1129	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
19	B	1210	CLA	C3B-C2B-C1B	-2.72	103.96	107.17
19	A	1101	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
19	A	1138	CLA	O2A-CGA-CBA	2.72	120.13	111.83
19	L	1503	CLA	O2A-CGA-CBA	2.72	120.13	111.83
19	B	1213	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
19	3	3011	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
21	B	6006	BCR	C23-C24-C25	-2.72	119.74	127.00
19	F	1305	CLA	C3B-C2B-C1B	-2.72	103.97	107.17
19	4	4010	CLA	C2C-C1C-CHC	-2.72	118.72	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1138	CLA	CHC-C1C-C2C	-2.72	119.23	126.95
21	3	6022	BCR	C24-C23-C22	-2.71	122.22	126.23
21	A	6007	BCR	C32-C1-C31	2.71	116.41	108.63
19	R	1150	CLA	CHC-C1C-C2C	-2.71	119.23	126.95
19	B	1211	CLA	C4A-NA-C1A	2.71	107.92	106.68
21	B	6017	BCR	C3-C4-C5	-2.71	109.22	114.06
21	A	6011	BCR	C8-C7-C6	-2.71	119.75	127.00
22	R	7024	LMU	O5'-C5'-C6'	2.71	113.16	106.44
19	4	1304	CLA	C7-C6-C5	-2.71	106.03	113.26
19	B	1206	CLA	CGD-CBD-CAD	2.71	119.62	110.85
19	A	1105	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
19	4	4014	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
21	A	6002	BCR	C33-C5-C4	2.71	119.37	113.60
19	A	1120	CLA	C1-C2-C3	-2.71	121.76	126.20
22	E	7048	LMU	C1'-C2'-C3'	-2.71	104.31	110.01
19	B	1206	CLA	O2A-CGA-CBA	2.71	120.08	111.83
19	B	1229	CLA	C4A-NA-C1A	2.70	107.91	106.68
19	B	1214	CLA	C3B-C2B-C1B	-2.70	103.98	107.17
19	A	1309	CLA	C2C-C1C-CHC	-2.70	118.75	125.84
22	2	7027	LMU	C6B-C5B-C4B	2.70	119.66	113.02
21	B	6020	BCR	C30-C25-C26	2.70	126.33	122.64
19	1	1013	CLA	C1D-ND-C4D	-2.70	104.42	106.31
19	B	1229	CLA	C1-C2-C3	-2.70	121.77	126.20
19	A	1104	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
19	A	1106	CLA	C1-C2-C3	-2.70	121.77	126.20
19	A	1128	CLA	CED-O2D-CGD	2.70	122.04	115.92
19	1	1303	CLA	C3B-C2B-C1B	-2.70	103.99	107.17
19	B	1212	CLA	CMD-C2D-C3D	-2.70	121.50	127.69
19	4	1304	CLA	CHC-C4B-NB	2.70	128.10	124.05
19	B	1203	CLA	CAC-C3C-C4C	2.70	128.30	124.79
19	A	1126	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
19	2	4009	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
21	A	6002	BCR	C1-C6-C7	2.70	122.96	115.65
19	1	1015	CLA	C3D-C4D-ND	2.70	113.19	109.50
19	1	1002	CLA	C3A-C2A-C1A	2.70	105.38	101.34
19	A	9011	CLA	CAA-C2A-C3A	-2.70	105.71	113.00
19	A	1105	CLA	CAA-C2A-C1A	-2.69	103.14	111.97
19	3	3015	CLA	C2D-C3D-C4D	-2.69	104.08	107.35
19	F	1305	CLA	CHC-C1C-NC	2.69	128.37	124.31
22	H	7002	LMU	O5B-C1B-C2B	-2.69	104.84	110.37
21	B	6005	BCR	C23-C24-C25	-2.69	119.81	127.00
19	B	1206	CLA	C3B-C2B-C1B	-2.69	104.00	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	I	6018	BCR	C35-C13-C12	2.69	122.20	118.09
19	3	3008	CLA	CHC-C4B-NB	2.69	128.09	124.05
19	L	1501	CLA	O1D-CGD-CBD	-2.69	119.21	124.52
19	B	1211	CLA	C4B-C3B-C2B	2.69	110.65	107.30
19	A	1134	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
21	B	6004	BCR	C4-C5-C6	-2.69	119.07	122.70
19	4	4012	CLA	CHB-C1B-NB	-2.69	120.02	124.05
19	A	1123	CLA	O2A-CGA-O1A	-2.69	116.91	123.63
19	A	1122	CLA	C1-C2-C3	-2.69	121.80	126.20
22	3	7005	LMU	C1'-C2'-C3'	-2.69	104.36	110.01
22	H	7043	LMU	C1'-C2'-C3'	2.69	115.66	110.01
19	A	1141	CLA	O2A-CGA-CBA	2.69	120.02	111.83
19	B	1236	CLA	CHB-C1B-NB	-2.69	120.02	124.05
22	H	7043	LMU	C6'-C5'-C4'	-2.68	105.83	113.38
22	R	7025	LMU	C1B-O1B-C4'	-2.68	111.61	117.98
20	A	5001	PQN	C21-C20-C18	-2.68	107.05	115.97
22	A	7035	LMU	O5'-C5'-C4'	-2.68	104.18	109.72
19	1	1011	CLA	CAC-C3C-C4C	2.68	129.22	125.03
19	B	1223	CLA	C1-C2-C3	-2.68	121.81	126.20
19	B	1211	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
19	1	1010	CLA	O2A-CGA-CBA	2.68	122.27	112.14
19	B	1203	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
19	B	1236	CLA	C4B-C3B-C2B	2.68	110.63	107.30
19	B	1228	CLA	O1D-CGD-CBD	-2.68	119.24	124.52
19	B	1202	CLA	C4-C3-C5	2.67	119.87	115.23
22	F	7036	LMU	O2'-C2'-C1'	2.67	116.45	110.08
21	L	6019	BCR	C32-C1-C6	-2.67	106.05	110.24
19	4	1009	CLA	CMB-C2B-C3B	2.67	130.63	123.53
19	J	1308	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
19	R	1144	CLA	C1D-ND-C4D	-2.67	104.44	106.31
19	A	1111	CLA	CAA-C2A-C1A	-2.67	103.22	111.97
19	B	1211	CLA	C3B-C4B-NB	-2.67	108.15	110.53
19	1	1013	CLA	CHB-C1B-NB	-2.67	120.04	124.05
19	A	1106	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
19	B	1229	CLA	C1-O2A-CGA	2.67	123.11	116.65
19	A	1112	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
19	B	1233	CLA	C4A-NA-C1A	2.67	107.90	106.68
19	3	3005	CLA	C3C-C4C-CHD	-2.67	118.30	125.23
21	F	6016	BCR	C31-C1-C2	2.67	119.19	108.95
21	B	6006	BCR	C15-C14-C13	-2.67	123.54	127.28
19	A	1110	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
21	J	6012	BCR	C39-C30-C25	2.66	114.42	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1134	CLA	CHB-C4A-NA	2.66	128.25	124.40
19	A	1126	CLA	C1-O2A-CGA	2.66	123.10	116.65
19	L	1502	CLA	CMA-C3A-C4A	-2.66	104.62	111.77
19	A	1137	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
19	4	4007	CLA	CHB-C4A-NA	2.66	128.24	124.40
19	3	3014	CLA	C2C-C1C-CHC	-2.66	118.87	125.84
19	4	4002	CLA	CHB-C1B-C2B	-2.66	119.70	127.43
19	A	1117	CLA	CMB-C2B-C1B	2.66	129.47	125.42
22	R	7020	LMU	C1B-C2B-C3B	2.66	115.60	110.01
19	1	1014	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
19	4	1304	CLA	CBC-CAC-C3C	-2.66	105.22	112.42
19	A	1131	CLA	CHB-C4A-NA	2.66	128.23	124.40
19	2	2001	CLA	O2A-CGA-CBA	2.66	119.93	111.83
19	4	4004	CLA	C3D-C4D-ND	2.66	113.13	109.50
19	2	2010	CLA	C2C-C1C-CHC	-2.66	118.88	125.84
19	H	1505	CLA	CGD-CBD-CAD	-2.66	102.25	110.85
19	1	1012	CLA	CHC-C4B-NB	2.66	128.03	124.05
22	4	7053	LMU	C1'-C2'-C3'	2.65	115.59	110.01
19	B	1221	CLA	CAC-C3C-C4C	2.65	128.24	124.79
19	1	1001	CLA	CMB-C2B-C1B	2.65	129.46	125.42
19	A	1136	CLA	O2A-CGA-CBA	2.65	119.92	111.83
19	B	1209	CLA	CHB-C4A-NA	2.65	128.23	124.40
22	4	7009	LMU	O1B-C1B-C2B	2.65	114.61	108.09
19	3	3011	CLA	C4-C3-C5	2.65	119.83	115.23
19	H	1241	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
19	A	1149	CLA	CMB-C2B-C1B	2.65	129.45	125.42
19	4	4002	CLA	CHB-C4A-NA	2.65	128.22	124.40
19	A	1103	CLA	C4-C3-C5	2.65	119.82	115.23
19	H	1207	CLA	CMB-C2B-C1B	2.65	129.45	125.42
19	3	1118	CLA	CHC-C1C-C2C	-2.64	119.43	126.95
19	4	4011	CLA	C3D-C4D-ND	2.64	113.11	109.50
19	1	1011	CLA	CHC-C4B-C3B	-2.64	119.76	127.43
19	B	1233	CLA	C1-C2-C3	-2.64	121.87	126.20
19	A	1120	CLA	CHB-C4A-NA	2.64	128.21	124.40
19	B	1223	CLA	O2A-CGA-CBA	2.64	119.89	111.83
19	B	1212	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
19	A	1101	CLA	C4A-NA-C1A	2.64	107.88	106.68
19	B	1238	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
19	2	2010	CLA	C3C-C4C-CHD	-2.64	118.38	125.23
21	B	6004	BCR	C38-C26-C27	2.64	119.22	113.60
19	A	1119	CLA	CED-O2D-CGD	2.64	121.90	115.92
19	K	3009	CLA	CHC-C1C-NC	2.64	128.29	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	3005	CLA	C2C-C1C-CHC	-2.64	118.93	125.84
22	R	7014	LMU	O5'-C1'-O1'	2.64	116.28	110.04
19	B	1212	CLA	C4-C3-C2	-2.64	116.86	123.63
19	A	1124	CLA	CHC-C1C-C2C	-2.64	119.46	126.95
19	A	1123	CLA	CHB-C4A-NA	2.64	128.20	124.40
19	A	1139	CLA	CHC-C1C-C2C	-2.64	119.46	126.95
19	A	1112	CLA	C3B-C4B-NB	-2.63	108.18	110.53
19	A	1115	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
19	B	1230	CLA	CAA-CBA-CGA	-2.63	105.73	113.21
19	L	1501	CLA	CMD-C2D-C3D	-2.63	121.65	127.69
19	2	2007	CLA	CHB-C1B-NB	-2.63	120.10	124.05
19	1	1015	CLA	CHB-C4A-NA	2.63	128.17	124.43
19	R	1144	CLA	C3B-C2B-C1B	-2.63	104.07	107.17
19	2	2005	CLA	C3C-C4C-CHD	-2.63	118.40	125.23
19	R	1144	CLA	CHC-C1C-C2C	-2.63	119.47	126.95
19	4	1304	CLA	C3B-C2B-C1B	-2.63	104.07	107.17
19	A	1110	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
19	2	2013	CLA	C3B-C2B-C1B	-2.63	104.07	107.17
19	A	1132	CLA	C4A-NA-C1A	2.63	107.88	106.68
19	B	1235	CLA	C4A-NA-C1A	2.63	107.88	106.68
22	3	7003	LMU	O2B-C2B-C3B	2.63	116.57	110.38
21	B	6004	BCR	C16-C15-C14	-2.63	118.14	123.52
19	2	2006	CLA	CMB-C2B-C1B	2.63	129.42	125.42
19	B	1212	CLA	C4B-C3B-C2B	2.63	110.57	107.30
19	3	1118	CLA	CHC-C4B-C3B	-2.63	119.80	127.43
21	B	6010	BCR	C15-C16-C17	-2.62	118.15	123.52
19	4	4003	CLA	CED-O2D-CGD	2.62	121.87	115.92
19	B	1232	CLA	C4A-NA-C1A	2.62	107.88	106.68
21	I	6018	BCR	C39-C30-C29	-2.62	98.88	108.95
19	4	4014	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
19	4	4005	CLA	C2C-C1C-CHC	-2.62	118.97	125.84
19	A	1136	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
19	B	1216	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
19	B	1202	CLA	CAA-C2A-C1A	-2.62	103.39	111.97
19	B	1238	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
19	A	1104	CLA	CAA-C2A-C1A	-2.62	103.39	111.97
19	A	1109	CLA	C3A-C2A-C1A	2.62	105.26	101.34
19	3	1118	CLA	CAA-C2A-C3A	-2.62	110.23	116.23
19	A	1115	CLA	CHC-C4B-NB	2.62	127.97	124.05
19	4	4003	CLA	O2A-CGA-CBA	2.62	119.81	111.83
19	A	1108	CLA	CED-O2D-CGD	2.62	121.85	115.92
19	A	1116	CLA	CED-O2D-CGD	2.62	121.85	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1236	CLA	CHC-C1C-C2C	-2.62	119.52	126.95
19	B	1236	CLA	CAA-C2A-C3A	-2.61	105.93	113.00
21	I	6018	BCR	C31-C1-C2	2.61	118.98	108.95
19	A	1112	CLA	CHC-C4B-NB	2.61	127.97	124.05
19	A	1117	CLA	CHC-C1C-C2C	-2.61	119.53	126.95
19	A	1124	CLA	CAC-C3C-C4C	2.61	128.19	124.79
19	4	1009	CLA	CHB-C4A-NA	2.61	128.17	124.40
19	A	1141	CLA	CHC-C1C-C2C	-2.61	119.53	126.95
19	B	1301	CLA	CGD-CBD-CAD	-2.61	103.60	114.30
19	A	1128	CLA	CAA-C2A-C1A	-2.61	103.42	111.97
19	A	1113	CLA	CAA-C2A-C3A	-2.61	105.95	113.00
19	A	1138	CLA	C4A-NA-C1A	2.61	107.87	106.68
19	A	1113	CLA	C1-C2-C3	-2.61	122.54	126.76
19	A	1140	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
19	B	1214	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
22	A	7035	LMU	O5'-C1'-C2'	2.61	115.72	110.37
19	3	3008	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
19	J	1311	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
21	I	6018	BCR	C8-C9-C10	2.61	123.11	119.01
19	H	1505	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
19	A	1103	CLA	CHB-C4A-NA	2.60	128.16	124.40
19	2	2007	CLA	CHD-C4C-C3C	-2.60	120.98	124.77
19	A	1101	CLA	C3B-C4B-NB	-2.60	108.20	110.53
21	1	6023	BCR	C27-C26-C25	-2.60	119.19	122.70
19	A	1124	CLA	CHB-C4A-NA	2.60	128.16	124.40
19	A	1140	CLA	C4A-NA-C1A	2.60	107.87	106.68
21	I	6021	BCR	C39-C30-C25	2.60	114.33	110.24
19	B	1206	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
19	A	1123	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
22	H	7032	LMU	O5'-C1'-C2'	-2.60	105.02	110.37
19	1	1010	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
19	K	3009	CLA	C1-O2A-CGA	2.60	122.95	116.65
22	A	7023	LMU	O1'-C1'-C2'	2.60	112.22	108.27
19	4	4014	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
22	4	7019	LMU	C1B-C2B-C3B	2.60	115.48	110.01
19	B	1219	CLA	C5-C3-C2	-2.60	115.33	121.17
19	L	1501	CLA	C4A-NA-C1A	2.60	107.87	106.68
19	2	2003	CLA	CHB-C4A-NA	2.60	128.13	124.43
19	3	1147	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
19	1	1010	CLA	CHB-C4A-NA	2.60	128.15	124.40
19	2	2004	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
19	2	4009	CLA	O1D-CGD-CBD	-2.60	119.39	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1237	CLA	C6-C7-C8	-2.60	107.33	115.97
19	B	1220	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
19	4	1306	CLA	CHD-C4C-NC	2.60	128.26	124.23
19	A	1138	CLA	CED-O2D-CGD	2.60	121.81	115.92
19	4	4015	CLA	C1D-ND-C4D	-2.60	104.49	106.31
19	A	1132	CLA	CHB-C1B-NB	-2.60	120.15	124.05
22	H	7030	LMU	C4B-C3B-C2B	-2.60	106.27	110.83
19	A	1149	CLA	CHC-C4B-C3B	-2.60	119.89	127.43
21	B	6017	BCR	C34-C9-C8	2.60	122.05	118.09
22	B	7012	LMU	C2'-C3'-C4'	2.60	115.57	109.68
21	B	6005	BCR	C37-C22-C23	2.60	122.05	118.09
19	A	1122	CLA	CAA-C2A-C3A	-2.60	105.99	113.00
19	2	2007	CLA	C1-O2A-CGA	2.59	122.93	116.65
19	A	1102	CLA	CBA-CAA-C2A	2.59	121.51	113.79
19	3	1118	CLA	CMB-C2B-C1B	2.59	129.37	125.42
19	F	1240	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
19	R	1150	CLA	CMA-C3A-C4A	2.59	118.74	111.77
22	H	7030	LMU	O5B-C5B-C6B	2.59	112.86	106.44
19	3	3016	CLA	CHB-C4A-NA	2.59	128.14	124.40
19	B	1218	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
19	B	1223	CLA	CHC-C1C-C2C	-2.59	119.59	126.95
19	A	1125	CLA	O2A-CGA-CBA	2.59	119.73	111.83
19	B	1225	CLA	C2B-C1B-NB	2.59	113.01	110.33
19	F	1302	CLA	CHC-C1C-C2C	-2.59	119.59	126.95
21	B	6005	BCR	C32-C1-C2	2.59	118.89	108.95
19	A	1113	CLA	CGD-CBD-CAD	2.59	119.22	110.85
19	B	1222	CLA	CAC-C3C-C4C	2.59	128.16	124.79
19	A	1104	CLA	CHB-C4A-NA	2.59	128.13	124.40
24	B	7101	LMG	O8-C28-C29	2.59	119.72	111.83
19	B	1221	CLA	CMB-C2B-C1B	2.59	129.36	125.42
19	A	1108	CLA	C3D-C4D-ND	2.59	114.19	109.99
19	L	1503	CLA	CHC-C4B-NB	2.59	127.93	124.05
19	A	1108	CLA	CHC-C1C-C2C	-2.59	119.60	126.95
22	4	7033	LMU	O5B-C5B-C6B	2.58	112.84	106.44
19	3	3002	CLA	C3C-C4C-CHD	-2.58	118.52	125.23
21	A	6002	BCR	C38-C26-C27	2.58	119.10	113.60
22	K	7001	LMU	O1B-C4'-C5'	2.58	116.25	109.48
19	B	1239	CLA	CAA-CBA-CGA	2.58	120.54	113.21
19	B	1214	CLA	C1-C2-C3	-2.58	121.97	126.20
19	A	1107	CLA	CHB-C1B-NB	-2.58	120.18	124.05
19	H	1207	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	A	1135	CLA	CHC-C1C-C2C	-2.58	119.62	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	R	1150	CLA	C4-C3-C2	-2.58	117.00	123.63
19	3	3001	CLA	C3D-C4D-ND	2.58	113.03	109.50
19	B	1214	CLA	CED-O2D-CGD	2.58	121.76	115.92
19	4	4013	CLA	C3C-C4C-CHD	-2.58	118.54	125.23
19	3	3013	CLA	C2B-C1B-NB	2.58	113.00	110.33
19	B	9010	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
19	L	1503	CLA	CAA-C2A-C1A	2.58	120.42	111.97
19	G	1242	CLA	CAA-CBA-CGA	-2.58	105.89	113.21
19	G	1242	CLA	CED-O2D-CGD	2.58	121.76	115.92
19	3	3016	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
19	B	1238	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
19	A	9022	CLA	O2A-CGA-CBA	2.57	119.68	111.83
21	I	6018	BCR	C33-C5-C4	2.57	119.08	113.60
19	1	1303	CLA	C4A-NA-C1A	-2.57	105.51	106.68
19	B	1233	CLA	O2A-CGA-CBA	2.57	119.67	111.83
22	N	7049	LMU	C1B-C2B-C3B	-2.57	104.60	110.01
19	1	1007	CLA	C1D-ND-C4D	-2.57	104.51	106.31
19	B	1214	CLA	CHB-C4A-NA	2.57	128.11	124.40
19	A	1111	CLA	C3D-C4D-ND	2.57	114.16	109.99
19	B	1232	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
19	A	1132	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
19	B	1203	CLA	CBC-CAC-C3C	-2.57	105.46	112.42
19	3	3015	CLA	C3C-C4C-CHD	-2.57	118.56	125.23
19	B	1301	CLA	CHB-C4A-NA	2.57	128.10	124.40
19	K	1143	CLA	CHB-C4A-NA	2.57	128.10	124.40
22	R	7021	LMU	O1'-C1'-C2'	2.56	112.17	108.27
19	B	1301	CLA	CHB-C1B-NB	-2.56	120.20	124.05
19	B	1224	CLA	CHC-C4B-NB	2.56	127.90	124.05
21	B	6006	BCR	C8-C7-C6	-2.56	120.15	127.00
19	2	2002	CLA	CHC-C1C-C2C	-2.56	119.66	126.95
19	B	1208	CLA	CHC-C1C-C2C	-2.56	119.66	126.95
19	A	9023	CLA	CMB-C2B-C1B	2.56	129.32	125.42
19	L	1148	CLA	C2D-C1D-ND	-2.56	107.59	110.13
19	B	1213	CLA	C1D-ND-C4D	-2.56	104.52	106.31
19	2	2004	CLA	CED-O2D-CGD	2.56	121.72	115.92
19	1	1007	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
19	L	1504	CLA	C3B-C2B-C1B	-2.56	104.15	107.17
21	3	6022	BCR	C38-C26-C27	2.56	119.06	113.60
19	A	1129	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
19	A	1110	CLA	CMB-C2B-C1B	2.56	129.32	125.42
19	B	1301	CLA	CHC-C4B-C3B	-2.56	120.00	127.43
22	3	7005	LMU	O5'-C5'-C6'	2.56	112.78	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	7004	LMU	O1'-C1'-C2'	2.56	112.16	108.27
19	A	1119	CLA	C4-C3-C5	2.56	119.67	115.23
19	A	1136	CLA	CHB-C4A-NA	2.56	128.09	124.40
19	A	1237	CLA	CAC-C3C-C4C	2.56	128.12	124.79
19	4	4005	CLA	CHD-C1D-ND	2.56	128.46	124.84
21	F	6014	BCR	C23-C24-C25	-2.56	120.17	127.00
19	A	9013	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
19	B	9010	CLA	CHB-C1B-NB	-2.56	120.22	124.05
19	B	1227	CLA	CAC-C3C-C4C	2.56	128.12	124.79
19	B	1201	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
19	1	1310	CLA	C2C-C1C-CHC	-2.55	119.15	125.84
19	A	1133	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
19	3	3011	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
19	4	4004	CLA	C2C-C1C-CHC	-2.55	119.16	125.84
22	B	7040	LMU	C2'-C3'-C4'	2.55	115.47	109.68
19	2	2008	CLA	C2C-C1C-CHC	-2.55	119.16	125.84
19	B	1217	CLA	C3D-C4D-ND	2.55	114.13	109.99
19	A	1121	CLA	CHB-C1B-NB	-2.55	120.22	124.05
19	B	1203	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
19	4	1304	CLA	C16-C15-C13	-2.55	107.50	115.97
19	1	1005	CLA	C2A-C1A-CHA	-2.55	119.45	123.87
19	B	1214	CLA	C1-O2A-CGA	2.55	122.81	116.65
19	L	1504	CLA	C4-C3-C2	-2.55	117.09	123.63
19	3	3013	CLA	C4-C3-C2	-2.55	117.09	123.63
22	2	7027	LMU	C3B-C4B-C5B	2.55	114.85	110.23
19	J	1311	CLA	CHB-C4A-NA	2.55	128.07	124.40
22	H	7011	LMU	O5B-C5B-C6B	2.55	112.75	106.44
21	A	6011	BCR	C39-C30-C25	2.54	114.23	110.24
21	A	6002	BCR	C15-C16-C17	-2.54	118.31	123.52
19	L	1130	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
19	2	2004	CLA	CHC-C4B-NB	2.54	127.86	124.05
22	K	7047	LMU	C1'-O5'-C5'	2.54	118.69	113.72
19	2	2004	CLA	CHB-C4A-NA	2.54	128.07	124.40
19	4	4010	CLA	C3C-C4C-CHD	-2.54	118.63	125.23
19	A	1132	CLA	CHD-C4C-C3C	-2.54	121.07	124.77
19	A	1133	CLA	C4A-NA-C1A	2.54	107.84	106.68
19	3	1118	CLA	CHB-C4A-NA	2.54	128.07	124.40
19	A	1122	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
19	B	1228	CLA	C1D-ND-C4D	-2.54	104.53	106.31
21	B	6020	BCR	C10-C11-C12	2.54	130.56	123.20
21	A	6008	BCR	C16-C15-C14	-2.54	118.33	123.52
19	A	1125	CLA	CHC-C1C-C2C	-2.54	119.74	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1210	CLA	O2A-CGA-CBA	2.54	119.57	111.83
19	3	1147	CLA	O2A-CGA-CBA	2.54	121.72	112.14
19	A	1135	CLA	O2A-CGA-CBA	2.54	119.56	111.83
19	B	1223	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
19	2	4009	CLA	C4A-NA-C1A	2.53	107.83	106.68
19	B	1206	CLA	O2D-CGD-CBD	2.53	115.66	111.23
21	A	6008	BCR	C33-C5-C4	2.53	119.00	113.60
19	1	1005	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
19	A	1105	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
19	1	1003	CLA	CHB-C4A-NA	2.53	128.05	124.40
19	3	3007	CLA	C3D-C4D-ND	2.53	114.10	109.99
19	B	1230	CLA	CAC-C3C-C4C	2.53	128.08	124.79
19	J	1311	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
19	3	3010	CLA	C2C-C1C-CHC	-2.53	119.21	125.84
19	3	3008	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
19	3	3007	CLA	CAC-C3C-C2C	-2.53	122.91	127.56
19	2	2007	CLA	CGD-CBD-CAD	2.53	119.03	110.85
19	B	1214	CLA	CHC-C4B-NB	2.53	127.84	124.05
19	B	1239	CLA	CMA-C3A-C2A	-2.53	104.22	113.98
19	A	1119	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
19	A	9012	CLA	CED-O2D-CGD	2.52	121.64	115.92
19	R	1150	CLA	CHB-C1B-NB	-2.52	120.26	124.05
19	F	1305	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
19	B	1216	CLA	O2A-CGA-CBA	2.52	119.53	111.83
19	B	1231	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
22	K	7042	LMU	O5'-C5'-C6'	2.52	112.69	106.44
19	A	1116	CLA	C4A-NA-C1A	2.52	107.83	106.68
22	A	7035	LMU	O3'-C3'-C4'	2.52	116.41	109.94
19	H	1207	CLA	CAC-C3C-C4C	2.52	128.07	124.79
21	B	6006	BCR	C30-C25-C26	-2.52	119.19	122.64
19	4	4015	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
22	2	7027	LMU	O1B-C1B-C2B	2.52	114.29	108.09
19	2	2004	CLA	C4A-NA-C1A	2.52	107.83	106.68
22	4	7019	LMU	O5B-C5B-C6B	2.52	112.68	106.44
19	2	2007	CLA	CHB-C4A-NA	2.52	128.03	124.40
19	B	9010	CLA	C3B-C4B-NB	-2.51	108.28	110.53
19	I	1204	CLA	O1D-CGD-CBD	-2.51	119.56	124.52
19	B	1217	CLA	CHC-C1C-C2C	-2.51	119.80	126.95
19	B	1222	CLA	CHC-C1C-C2C	-2.51	119.80	126.95
19	2	2011	CLA	C3C-C4C-CHD	-2.51	118.70	125.23
19	3	3003	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
19	2	2014	CLA	O2D-CGD-O1D	-2.51	118.96	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	2002	CLA	C3D-C4D-ND	2.51	114.07	109.99
19	2	2004	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
19	2	2001	CLA	CHB-C4A-NA	2.51	128.03	124.40
21	J	6012	BCR	C38-C26-C27	2.51	118.95	113.60
19	B	1203	CLA	C16-C15-C13	-2.51	107.62	115.97
21	A	6011	BCR	C37-C22-C23	2.51	121.92	118.09
19	J	1308	CLA	O2A-CGA-CBA	2.51	119.48	111.83
19	B	1234	CLA	O2A-CGA-CBA	2.51	119.48	111.83
21	A	6002	BCR	C8-C9-C10	2.51	122.95	119.01
19	A	9013	CLA	C2A-C1A-CHA	-2.51	119.52	123.87
21	J	6012	BCR	C33-C5-C6	-2.50	121.75	124.48
19	F	1240	CLA	CAA-C2A-C1A	-2.50	105.62	111.81
19	H	1145	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
22	H	7017	LMU	O1B-C1B-C2B	2.50	114.25	108.09
19	1	1008	CLA	C1D-ND-C4D	-2.50	104.56	106.31
21	I	6018	BCR	C2-C1-C6	-2.50	106.80	110.44
19	F	1302	CLA	CMB-C2B-C1B	2.50	129.23	125.42
21	F	6016	BCR	C34-C9-C10	-2.50	118.76	122.82
19	4	1004	CLA	C4-C3-C5	2.50	119.57	115.23
19	A	1119	CLA	CHB-C4A-NA	2.50	128.01	124.40
19	A	1106	CLA	CAA-C2A-C3A	-2.50	106.24	113.00
19	A	1105	CLA	CAC-C3C-C4C	2.50	128.04	124.79
19	2	2003	CLA	CHB-C1B-NB	-2.50	120.47	124.08
19	B	1229	CLA	CAA-CBA-CGA	-2.50	106.12	113.21
19	1	1015	CLA	C2C-C1C-CHC	-2.50	119.30	125.84
22	2	7031	LMU	O5B-C5B-C4B	2.50	114.19	109.70
19	B	1210	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
19	I	1204	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
19	L	1130	CLA	C1-O2A-CGA	2.49	122.69	116.65
22	A	7016	LMU	C1'-O5'-C5'	-2.49	108.85	113.72
19	A	1116	CLA	CHB-C4A-NA	2.49	128.00	124.40
22	A	7035	LMU	C2'-C3'-C4'	-2.49	104.02	109.68
19	3	3001	CLA	C2C-C1C-CHC	-2.49	119.31	125.84
22	K	7041	LMU	C1'-O5'-C5'	2.49	118.58	113.72
19	B	1215	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
19	1	1010	CLA	CAC-C3C-C4C	-2.49	121.55	124.79
19	A	1120	CLA	CED-O2D-CGD	2.49	121.56	115.92
19	1	1011	CLA	C1D-ND-C4D	-2.49	104.56	106.31
19	1	1008	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
19	A	1151	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	L	1130	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
19	2	2003	CLA	C2C-C1C-CHC	-2.49	119.32	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1151	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
22	N	7049	LMU	O1'-C1'-C2'	2.49	112.05	108.27
19	A	1137	CLA	CHB-C4A-NA	2.48	127.99	124.40
19	4	4011	CLA	CHB-C4A-NA	2.48	127.96	124.43
19	4	4006	CLA	C3D-C4D-ND	2.48	114.02	109.99
22	A	7045	LMU	C1'-C2'-C3'	2.48	115.23	110.01
19	2	2001	CLA	C4A-NA-C1A	2.48	107.81	106.68
19	3	3007	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
19	A	1107	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
19	H	1145	CLA	C1-C2-C3	-2.48	122.13	126.20
19	B	1238	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
19	3	3007	CLA	CHB-C1B-NB	-2.48	120.33	124.05
21	A	6008	BCR	C38-C26-C27	2.48	118.88	113.60
19	B	1233	CLA	CHB-C4A-NA	2.48	127.98	124.40
19	A	9011	CLA	C6-C7-C8	-2.48	107.73	115.97
19	3	3004	CLA	CHB-C1B-NB	-2.48	120.50	124.08
19	L	1504	CLA	CHB-C1B-NB	-2.48	120.33	124.05
19	B	1211	CLA	CED-O2D-CGD	2.48	121.54	115.92
19	2	1307	CLA	C2C-C1C-CHC	-2.48	119.35	125.84
21	B	6006	BCR	C34-C9-C10	-2.48	118.80	122.82
19	A	1105	CLA	C4A-NA-C1A	2.48	107.81	106.68
19	B	1301	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
19	K	1142	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
19	A	9012	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
19	3	3010	CLA	CHB-C4A-NA	2.47	127.95	124.43
19	4	4002	CLA	C3D-C4D-ND	2.47	114.01	109.99
19	1	1007	CLA	CHB-C1B-NB	-2.47	120.34	124.05
19	2	2004	CLA	O2A-CGA-CBA	2.47	119.37	111.83
19	B	1225	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
19	A	1119	CLA	CAA-C2A-C3A	-2.47	106.32	113.00
21	B	6004	BCR	C35-C13-C12	2.47	121.86	118.09
19	H	1241	CLA	C4-C3-C2	-2.47	117.28	123.63
22	2	7027	LMU	O5'-C5'-C6'	2.47	112.56	106.44
19	A	1140	CLA	CHB-C4A-NA	2.47	127.97	124.40
19	B	1239	CLA	O2D-CGD-CBD	2.47	115.55	111.23
19	A	1119	CLA	CHC-C4B-NB	2.47	127.75	124.05
19	B	1222	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	4	1304	CLA	CMA-C3A-C4A	2.47	118.41	111.77
19	3	3016	CLA	C4A-NA-C1A	2.47	107.81	106.68
21	A	6008	BCR	C32-C1-C2	2.47	118.42	108.95
19	B	1231	CLA	O2A-CGA-CBA	2.47	121.80	114.00
19	B	1222	CLA	C1D-ND-C4D	-2.47	104.58	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1106	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
19	B	1236	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	1	1005	CLA	C3B-C2B-C1B	-2.47	104.26	107.17
19	A	1102	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
19	B	1228	CLA	CHB-C4A-NA	2.46	127.96	124.40
19	L	1148	CLA	CAC-C3C-C4C	2.46	128.00	124.79
19	A	1125	CLA	CHB-C4A-NA	2.46	127.96	124.40
19	A	1112	CLA	C1D-ND-C4D	-2.46	104.58	106.31
19	2	4009	CLA	CAC-C3C-C4C	2.46	127.99	124.79
19	3	3010	CLA	C3C-C4C-CHD	-2.46	118.84	125.23
22	E	7037	LMU	O1B-C1B-C2B	2.46	114.14	108.09
19	A	1139	CLA	C4A-NA-C1A	2.46	107.80	106.68
19	B	1227	CLA	CHB-C4A-NA	2.46	127.95	124.40
19	A	1129	CLA	CGD-CBD-CAD	2.46	118.81	110.85
19	A	1101	CLA	CHB-C4A-NA	2.46	127.95	124.40
19	A	1128	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
19	B	1210	CLA	C4-C3-C5	2.46	119.49	115.23
21	3	6022	BCR	C28-C27-C26	-2.46	109.67	114.06
19	1	1011	CLA	CHB-C4A-NA	2.46	127.94	124.40
19	A	1237	CLA	CHB-C1B-NB	-2.46	120.36	124.05
22	H	7002	LMU	C3'-C4'-C5'	-2.46	105.49	110.93
19	B	1226	CLA	C7-C6-C5	-2.46	106.72	113.26
19	3	3004	CLA	C3C-C4C-CHD	-2.46	118.85	125.23
19	B	1230	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
19	J	1311	CLA	C4A-NA-C1A	2.45	107.80	106.68
19	G	1242	CLA	C3D-C4D-ND	2.45	113.98	109.99
22	H	7002	LMU	O3'-C3'-C2'	-2.45	104.59	110.38
19	A	9012	CLA	C4-C3-C5	2.45	119.48	115.23
19	K	1146	CLA	CMB-C2B-C3B	2.45	132.32	126.55
21	F	6014	BCR	C16-C15-C14	-2.45	118.50	123.52
19	B	1210	CLA	C11-C10-C8	-2.45	107.82	115.97
19	4	1004	CLA	CMB-C2B-C1B	2.45	129.15	125.42
19	A	1111	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
19	A	1107	CLA	C3D-C4D-ND	2.45	113.97	109.99
22	4	7018	LMU	O5'-C5'-C6'	2.45	112.51	106.44
19	B	1225	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
19	1	1310	CLA	C4D-ND-C1D	-2.45	104.59	106.31
19	3	3002	CLA	C2C-C1C-CHC	-2.45	119.42	125.84
19	A	1105	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
19	B	1206	CLA	CHB-C4A-NA	2.45	127.93	124.40
19	A	1122	CLA	CMC-C2C-C1C	2.45	128.86	125.03
19	4	4012	CLA	CMC-C2C-C1C	2.45	128.86	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	7051	LMU	O5'-C5'-C4'	-2.45	104.67	109.72
19	4	1306	CLA	CHB-C1B-NB	-2.45	120.38	124.05
19	A	1125	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
19	A	1110	CLA	CHB-C1B-NB	-2.45	120.38	124.05
19	A	9011	CLA	CHB-C1B-NB	-2.45	120.38	124.05
19	H	1505	CLA	CHB-C1B-NB	-2.45	120.38	124.05
19	B	1238	CLA	CHB-C4A-NA	2.45	127.93	124.40
19	H	1207	CLA	CMC-C2C-C1C	2.45	128.86	125.03
19	R	1150	CLA	CAA-CBA-CGA	2.44	120.15	113.21
19	B	1229	CLA	C3A-C2A-C1A	2.44	105.00	101.34
21	B	6017	BCR	C38-C26-C27	2.44	118.81	113.60
19	A	1123	CLA	C4A-NA-C1A	2.44	107.79	106.68
19	A	1138	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
19	3	2009	CLA	C6-C7-C8	-2.44	107.85	115.97
19	A	1126	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
19	1	1012	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
19	3	2009	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
19	1	1014	CLA	O2A-CGA-CBA	2.44	119.28	111.83
19	1	1003	CLA	CAC-C3C-C4C	2.44	127.97	124.79
21	A	6008	BCR	C40-C30-C25	2.44	114.07	110.24
19	B	1203	CLA	C1-C2-C3	-2.44	122.20	126.20
19	H	1145	CLA	CMB-C2B-C1B	2.44	129.13	125.42
22	2	7031	LMU	C1-O1'-C1'	2.44	117.84	113.68
19	A	1309	CLA	C3C-C4C-CHD	-2.44	118.90	125.23
19	L	1148	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
19	A	1138	CLA	C2A-C1A-CHA	-2.44	119.64	123.87
19	L	1504	CLA	CMB-C2B-C1B	2.44	129.13	125.42
19	B	1215	CLA	CHB-C1B-NB	-2.44	120.39	124.05
19	B	1228	CLA	C2A-C1A-CHA	-2.44	119.64	123.87
19	A	1112	CLA	C3D-C4D-ND	2.43	113.94	109.99
19	4	1304	CLA	C3D-C4D-ND	2.43	113.94	109.99
19	L	1130	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	4	7019	LMU	O5'-C5'-C4'	2.43	114.76	109.72
19	A	1128	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
21	A	6007	BCR	C23-C22-C21	-2.43	115.18	119.01
19	B	1230	CLA	C1-O2A-CGA	2.43	122.54	116.65
19	4	1304	CLA	C1D-ND-C4D	-2.43	104.61	106.31
19	4	4003	CLA	C4-C3-C5	2.43	119.45	115.23
19	2	4009	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
19	3	3017	CLA	CHD-C4C-C3C	-2.43	121.23	124.77
19	B	1228	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
19	A	1149	CLA	CAA-CBA-CGA	-2.43	106.31	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	5001	PQN	C30-C28-C29	2.43	121.37	110.53
19	A	1135	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
19	1	1010	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
19	4	1306	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
19	G	1242	CLA	O2A-CGA-CBA	2.43	119.23	111.83
19	B	1215	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
21	B	6017	BCR	C33-C5-C6	-2.42	121.84	124.48
22	H	7011	LMU	O3B-C3B-C4B	-2.42	104.66	110.38
19	2	2011	CLA	C3D-C4D-ND	2.42	112.81	109.50
19	I	1204	CLA	CMB-C2B-C1B	2.42	129.11	125.42
21	A	6003	BCR	C38-C26-C27	2.42	118.76	113.60
19	L	1501	CLA	CHC-C1C-C2C	-2.42	120.06	126.95
19	A	9011	CLA	CMA-C3A-C2A	-2.42	104.61	113.98
19	B	1238	CLA	C4-C3-C5	2.42	119.43	115.23
19	2	2014	CLA	C1-C2-C3	-2.42	122.23	126.20
19	A	1115	CLA	CHC-C1C-C2C	-2.42	120.06	126.95
20	B	5002	PQN	C2M-C2-C1	2.42	121.14	116.68
19	4	4002	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
22	G	7026	LMU	O5'-C5'-C4'	2.42	114.73	109.72
19	A	1106	CLA	O2A-CGA-CBA	2.42	119.22	111.83
19	B	1203	CLA	CMA-C3A-C2A	-2.42	104.63	113.98
21	A	6003	BCR	C34-C9-C10	-2.42	118.90	122.82
19	A	1105	CLA	CGD-CBD-CAD	-2.42	103.02	110.85
19	A	9022	CLA	CHC-C1C-C2C	-2.42	120.08	126.95
19	1	1006	CLA	CMB-C2B-C1B	2.42	129.10	125.42
19	2	2010	CLA	C1C-NC-C4C	-2.42	105.58	106.68
19	B	1225	CLA	C1-C2-C3	-2.42	122.24	126.20
19	B	1210	CLA	O1D-CGD-CBD	-2.41	119.75	124.52
22	A	7016	LMU	C3'-C4'-C5'	2.41	116.28	110.93
19	I	1204	CLA	CHB-C4A-NA	2.41	127.88	124.40
21	A	6002	BCR	C7-C6-C5	-2.41	116.00	121.56
21	A	6008	BCR	C8-C7-C6	-2.41	120.55	127.00
22	A	7023	LMU	C3'-C4'-C5'	2.41	116.28	110.93
19	A	9013	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
19	K	3009	CLA	C4-C3-C5	2.41	119.41	115.23
19	A	1111	CLA	C1D-ND-C4D	-2.41	104.62	106.31
19	A	1127	CLA	O2A-CGA-CBA	2.41	119.19	111.83
19	1	1003	CLA	CHC-C1C-C2C	-2.41	120.10	126.95
19	3	3015	CLA	CHB-C4A-NA	2.41	127.86	124.43
19	3	3007	CLA	CHB-C4A-NA	2.41	127.88	124.40
21	F	6014	BCR	C40-C30-C39	2.41	115.53	108.63
21	A	6007	BCR	C34-C9-C8	2.41	121.77	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1141	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
21	F	6014	BCR	C33-C5-C4	2.41	118.73	113.60
19	3	3017	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
19	A	1112	CLA	CED-O2D-CGD	2.40	121.37	115.92
19	B	1208	CLA	C1-O2A-CGA	2.40	122.47	116.65
22	G	7051	LMU	O3B-C3B-C4B	-2.40	104.71	110.38
19	A	9012	CLA	O2A-C1-C2	2.40	117.35	108.11
19	B	1225	CLA	C4B-C3B-C2B	2.40	110.29	107.30
19	3	2009	CLA	C3D-C4D-ND	2.40	113.89	109.99
19	B	1229	CLA	CHC-C1C-C2C	-2.40	120.13	126.95
19	4	4005	CLA	C3D-C4D-ND	2.40	112.78	109.50
19	2	2002	CLA	CHB-C4A-NA	2.40	127.86	124.40
19	B	1224	CLA	C4-C3-C5	2.40	119.39	115.23
19	B	1215	CLA	CAC-C3C-C4C	2.40	127.91	124.79
19	4	4012	CLA	CHC-C4B-C3B	-2.40	120.46	127.43
19	K	1143	CLA	CBC-CAC-C3C	-2.40	105.92	112.42
19	A	1125	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
21	A	6011	BCR	C33-C5-C4	2.40	118.71	113.60
22	G	7026	LMU	O4'-C4B-C5B	2.40	115.23	109.32
19	4	4001	CLA	CED-O2D-CGD	2.40	121.35	115.92
19	4	4007	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
19	B	9010	CLA	C16-C17-C18	-2.40	105.24	115.94
19	3	2009	CLA	C4-C3-C2	-2.40	117.47	123.63
19	B	1208	CLA	C4A-NA-C1A	2.39	107.77	106.68
19	4	4003	CLA	C4A-NA-C1A	2.39	107.77	106.68
19	B	1219	CLA	CAC-C3C-C4C	2.39	127.90	124.79
19	4	4006	CLA	O2A-CGA-CBA	2.39	119.13	111.83
19	G	1242	CLA	C2A-C1A-CHA	-2.39	119.71	123.87
19	H	1207	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
19	B	1233	CLA	C1D-ND-C4D	-2.39	104.63	106.31
19	L	1504	CLA	C1-O2A-CGA	2.39	122.44	116.65
19	A	1237	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
19	4	4007	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
19	1	1001	CLA	CHB-C1B-NB	-2.39	120.46	124.05
19	A	1141	CLA	C3D-C4D-ND	2.39	113.87	109.99
19	1	1007	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
19	A	1141	CLA	CMB-C2B-C1B	2.39	129.06	125.42
19	A	1135	CLA	C1-C2-C3	-2.39	122.28	126.20
19	B	1212	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	A	7023	LMU	O5B-C5B-C6B	2.39	112.36	106.44
19	2	2011	CLA	C2C-C1C-CHC	-2.39	119.58	125.84
19	4	4010	CLA	CHB-C4A-NA	2.39	127.83	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1134	CLA	C3D-C4D-ND	2.39	113.87	109.99
19	A	1138	CLA	C3D-C4D-ND	2.39	113.87	109.99
19	A	9023	CLA	C3D-C4D-ND	2.38	113.86	109.99
19	1	1303	CLA	CBA-CAA-C2A	-2.38	106.70	113.79
19	A	1107	CLA	C1-C2-C3	2.38	130.10	126.20
19	3	3007	CLA	C2A-C1A-CHA	-2.38	119.73	123.87
19	1	1003	CLA	CMC-C2C-C1C	2.38	128.75	125.03
19	F	1302	CLA	CHB-C4A-NA	2.38	127.84	124.40
19	3	3012	CLA	C3D-C2D-C1D	2.38	110.24	107.35
19	B	1210	CLA	CBA-CAA-C2A	-2.38	106.71	113.79
21	B	6006	BCR	C3-C4-C5	-2.38	109.81	114.06
22	K	7042	LMU	O5B-C1B-C2B	2.38	115.26	110.37
19	4	4001	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
19	B	1223	CLA	C4A-NA-C1A	2.38	107.76	106.68
19	1	1303	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
19	A	1139	CLA	CHB-C4A-NA	2.38	127.83	124.40
19	3	3012	CLA	C4D-ND-C1D	-2.38	104.64	106.31
19	L	1504	CLA	CMC-C2C-C1C	2.38	128.75	125.03
19	F	1240	CLA	C3D-C4D-ND	2.38	113.85	109.99
19	4	1306	CLA	C4D-CHA-C1A	-2.38	118.41	121.24
19	A	1112	CLA	C4A-NA-C1A	2.38	107.76	106.68
19	A	1135	CLA	CHB-C4A-NA	2.38	127.83	124.40
19	A	1126	CLA	CHC-C1C-C2C	-2.38	120.20	126.95
22	B	7038	LMU	C6B-C5B-C4B	-2.37	107.19	113.02
19	A	1136	CLA	C4-C3-C5	2.37	119.35	115.23
19	A	1136	CLA	C2A-C1A-CHA	-2.37	119.75	123.87
19	A	1141	CLA	C6-C5-C3	-2.37	107.69	113.47
22	E	7037	LMU	C3B-C4B-C5B	-2.37	105.93	110.23
22	A	7035	LMU	O1B-C4'-C5'	2.37	115.70	109.48
19	4	4013	CLA	C2C-C1C-CHC	-2.37	119.63	125.84
19	3	2009	CLA	C4A-NA-C1A	2.37	107.76	106.68
19	H	1207	CLA	C1-C2-C3	2.37	130.08	126.20
21	B	6005	BCR	C34-C9-C8	2.37	121.71	118.09
19	3	3013	CLA	C1-O2A-CGA	2.37	122.39	116.65
19	A	1139	CLA	O2A-CGA-CBA	2.37	119.06	111.83
19	1	1001	CLA	CBA-CAA-C2A	-2.37	106.74	113.79
19	A	1120	CLA	C4A-NA-C1A	2.37	107.76	106.68
19	B	1229	CLA	CMB-C2B-C1B	2.37	129.03	125.42
19	A	1105	CLA	C3D-C4D-ND	2.37	113.83	109.99
19	A	1135	CLA	C3D-C4D-ND	2.37	113.83	109.99
19	B	1217	CLA	CHB-C4A-NA	2.37	127.82	124.40
19	J	1308	CLA	CAA-C2A-C3A	-2.37	106.60	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	7026	LMU	O1B-C1B-C2B	2.37	113.91	108.09
19	R	1144	CLA	C4-C3-C2	-2.37	117.55	123.63
19	3	1147	CLA	CHD-C1D-ND	2.37	128.13	124.80
19	2	4009	CLA	CED-O2D-CGD	2.37	121.28	115.92
19	1	1005	CLA	CHB-C4A-NA	2.37	127.81	124.40
19	A	1116	CLA	C3D-C4D-ND	2.37	113.83	109.99
19	B	1236	CLA	O2A-CGA-CBA	2.37	119.05	111.83
19	3	3001	CLA	C3C-C4C-CHD	-2.36	119.09	125.23
19	B	1232	CLA	O2A-CGA-O1A	-2.36	117.25	123.33
19	A	1109	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
19	B	1224	CLA	CAA-C2A-C1A	-2.36	104.23	111.97
19	2	2005	CLA	CHB-C4A-NA	2.36	127.79	124.43
19	A	1133	CLA	CHB-C1B-NB	-2.36	120.50	124.05
19	2	2006	CLA	O2A-CGA-CBA	2.36	119.04	111.83
19	3	3008	CLA	C2A-C1A-CHA	-2.36	119.77	123.87
19	I	1204	CLA	C1-O2A-CGA	2.36	122.37	116.65
19	A	1109	CLA	C4-C3-C5	2.36	119.33	115.23
19	A	1137	CLA	CMB-C2B-C1B	2.36	129.01	125.42
19	4	4001	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
22	B	7040	LMU	O1'-C1'-C2'	2.36	111.86	108.27
19	4	1306	CLA	C1-O2A-CGA	2.36	122.36	116.65
19	4	4006	CLA	C2A-C1A-CHA	-2.36	119.78	123.87
19	A	1128	CLA	C2B-C1B-NB	2.35	112.77	110.33
19	F	1240	CLA	C3B-C4B-NB	-2.35	107.88	110.33
21	A	6002	BCR	C8-C7-C6	-2.35	120.71	127.00
19	2	2010	CLA	CHB-C1B-NB	-2.35	120.68	124.08
19	A	1122	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	F	1305	CLA	CHB-C4A-NA	2.35	127.80	124.40
19	2	2011	CLA	CHB-C4A-NA	2.35	127.78	124.43
19	3	3012	CLA	CHB-C4A-NA	2.35	127.77	124.43
19	3	3016	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
19	2	2003	CLA	C3C-C4C-CHD	-2.35	119.13	125.23
19	A	1129	CLA	CHB-C4A-NA	2.35	127.79	124.40
19	L	1504	CLA	C3D-C4D-ND	2.35	113.80	109.99
19	B	1217	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
19	2	4009	CLA	C1-O2A-CGA	2.35	122.33	116.65
19	A	1137	CLA	C3D-C4D-ND	2.35	113.80	109.99
19	K	3009	CLA	C2A-C1A-CHA	-2.35	119.80	123.87
19	2	2006	CLA	CHB-C4A-NA	2.35	127.78	124.40
19	A	1103	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
19	B	1209	CLA	C5-C3-C2	2.35	126.43	121.17
19	4	1306	CLA	CMB-C2B-C1B	2.34	128.99	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	2012	CLA	O2A-CGA-CBA	2.34	118.98	111.83
19	A	1126	CLA	CMA-C3A-C4A	-2.34	105.47	111.77
19	3	2009	CLA	O2A-CGA-CBA	2.34	118.97	111.83
19	1	1007	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
19	B	1224	CLA	CHC-C1C-C2C	-2.34	120.30	126.95
19	4	4015	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
19	B	1301	CLA	CMC-C2C-C1C	2.34	128.69	125.03
21	A	6007	BCR	C40-C30-C39	2.34	115.32	108.63
19	1	1001	CLA	CHC-C4B-C3B	-2.34	117.23	127.37
19	4	4014	CLA	CAC-C3C-C2C	-2.34	123.27	127.56
19	B	1201	CLA	C1D-ND-C4D	-2.34	104.67	106.31
22	B	7038	LMU	O5'-C5'-C6'	2.33	112.22	106.44
19	4	4002	CLA	C4B-C3B-C2B	-2.33	104.40	107.30
19	3	3008	CLA	CHB-C4A-NA	2.33	127.77	124.40
19	4	4002	CLA	C3C-C4C-NC	-2.33	107.44	110.43
19	2	2007	CLA	CMB-C2B-C1B	2.33	128.97	125.42
19	3	3017	CLA	O2A-CGA-CBA	2.33	118.94	111.83
19	B	1225	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
19	B	1222	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
19	B	1232	CLA	O2A-CGA-CBA	2.33	121.36	114.00
19	4	4010	CLA	CHD-C1D-ND	2.33	128.13	124.84
19	4	4007	CLA	CED-O2D-CGD	2.33	121.20	115.92
19	2	4009	CLA	C4-C3-C2	-2.33	117.65	123.63
19	A	9023	CLA	CHB-C1B-NB	-2.33	120.56	124.05
19	1	1015	CLA	C3C-C4C-CHD	-2.33	119.19	125.23
21	A	6007	BCR	C4-C5-C6	-2.33	119.56	122.70
19	3	3008	CLA	C1D-ND-C4D	-2.33	104.68	106.31
19	2	2007	CLA	C6-C7-C8	-2.33	108.23	115.97
19	A	1113	CLA	CHB-C4A-NA	2.33	127.76	124.40
19	4	4011	CLA	C3C-C4C-CHD	-2.33	119.19	125.23
19	A	1151	CLA	O2A-CGA-CBA	2.33	118.93	111.83
19	B	1238	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
19	2	1307	CLA	C4D-ND-C1D	-2.33	104.68	106.31
19	4	4004	CLA	C3C-C4C-CHD	-2.33	119.19	125.23
19	4	4002	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
19	3	3005	CLA	C3D-C4D-ND	2.32	112.68	109.50
19	1	1310	CLA	CHB-C1B-NB	-2.32	120.72	124.08
19	1	1005	CLA	CGD-CBD-CAD	2.32	118.37	110.85
21	B	6020	BCR	C31-C1-C6	-2.32	106.60	110.24
21	A	6002	BCR	C40-C30-C39	2.32	115.29	108.63
19	A	1112	CLA	CHB-C1B-NB	-2.32	120.56	124.05
19	A	1104	CLA	CMB-C2B-C1B	2.32	128.96	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1232	CLA	CED-O2D-CGD	2.32	121.18	115.92
19	1	1310	CLA	C3C-C4C-CHD	-2.32	119.20	125.23
19	4	4005	CLA	C3C-C4C-CHD	-2.32	119.20	125.23
19	2	1307	CLA	CHB-C1B-NB	-2.32	120.73	124.08
19	B	1210	CLA	CHC-C4B-NB	2.32	127.53	124.05
19	A	1102	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
19	A	1138	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	A	1139	CLA	C2A-C1A-CHA	-2.32	119.84	123.87
19	B	1201	CLA	C3D-C4D-ND	2.32	113.76	109.99
19	B	9010	CLA	C1D-ND-C4D	-2.32	104.69	106.31
19	4	4006	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
19	A	9022	CLA	CAA-C2A-C1A	2.32	119.57	111.97
19	3	3008	CLA	C3D-C4D-ND	2.32	113.75	109.99
22	R	7007	LMU	O1'-C1'-C2'	2.32	111.79	108.27
19	B	1236	CLA	CED-O2D-CGD	2.32	121.17	115.92
19	1	1012	CLA	CHB-C4A-NA	2.32	127.74	124.40
19	R	1144	CLA	C3D-C4D-ND	2.32	113.75	109.99
19	1	1001	CLA	C4D-CHA-C1A	-2.31	118.48	121.24
19	A	1309	CLA	CHB-C1B-NB	-2.31	120.73	124.08
19	A	1113	CLA	CHC-C4B-NB	2.31	127.52	124.05
22	H	7043	LMU	O5'-C1'-C2'	2.31	115.12	110.37
19	2	2012	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
19	B	1226	CLA	O2A-CGA-CBA	2.31	118.89	111.83
19	B	1211	CLA	O2A-CGA-CBA	2.31	118.88	111.83
19	B	1208	CLA	CHB-C4A-NA	2.31	127.73	124.40
19	B	1212	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
22	2	7031	LMU	O5'-C1'-O1'	2.31	115.50	110.04
19	1	1014	CLA	C4-C3-C5	2.31	119.23	115.23
19	A	1139	CLA	C3D-C4D-ND	2.31	113.74	109.99
19	2	2013	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
19	2	2001	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
19	3	2009	CLA	CGD-CBD-CAD	-2.30	103.39	110.85
19	A	1119	CLA	O2A-CGA-CBA	2.30	118.86	111.83
19	A	1117	CLA	CAA-CBA-CGA	-2.30	106.67	113.21
19	4	4015	CLA	CBA-CAA-C2A	-2.30	106.94	113.79
19	A	1126	CLA	CHC-C4B-NB	2.30	127.50	124.05
19	4	4003	CLA	CHB-C4A-NA	2.30	127.72	124.40
22	A	7035	LMU	O5'-C5'-C6'	2.30	112.14	106.44
19	1	1001	CLA	CGD-CBD-CAD	-2.30	103.40	110.85
21	F	6016	BCR	C38-C26-C27	2.30	118.50	113.60
21	B	6010	BCR	C40-C30-C25	-2.30	106.64	110.24
22	4	7033	LMU	O1B-C1B-C2B	2.30	113.75	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1116	CLA	CHB-C1B-NB	-2.30	120.60	124.05
19	A	1103	CLA	CHB-C1B-NB	-2.30	120.60	124.05
19	B	1212	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
21	L	6019	BCR	C8-C7-C6	-2.30	120.86	127.00
19	3	1147	CLA	C3B-C4B-NB	2.30	112.58	110.53
19	B	1238	CLA	C3D-C4D-ND	2.30	113.72	109.99
19	B	1213	CLA	CED-O2D-CGD	2.30	121.12	115.92
19	2	2001	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
21	F	6014	BCR	C34-C9-C10	-2.30	119.10	122.82
19	B	1301	CLA	C1D-ND-C4D	-2.29	104.70	106.31
19	3	2009	CLA	CAC-C3C-C4C	2.29	127.78	124.79
19	L	1148	CLA	C4B-C3B-C2B	2.29	110.15	107.30
21	3	6022	BCR	C37-C22-C23	2.29	121.59	118.09
21	I	6018	BCR	C34-C9-C10	-2.29	119.10	122.82
19	A	1129	CLA	CAC-C3C-C4C	2.29	127.77	124.79
21	F	6016	BCR	C33-C5-C6	-2.29	121.99	124.48
19	A	1140	CLA	C3D-C4D-ND	2.29	113.70	109.99
19	B	9010	CLA	C1-O2A-CGA	2.29	122.19	116.65
19	B	1235	CLA	CHB-C1B-NB	-2.29	120.62	124.05
19	A	1113	CLA	CED-O2D-CGD	2.29	121.10	115.92
19	A	1102	CLA	C1D-ND-C4D	-2.28	104.71	106.31
22	G	7026	LMU	O3'-C3'-C4'	2.28	115.79	109.94
19	B	1223	CLA	O1D-CGD-CBD	-2.28	120.01	124.52
19	B	1225	CLA	C11-C12-C13	-2.28	108.38	115.97
19	A	1107	CLA	C5-C3-C2	-2.28	116.04	121.17
22	E	7037	LMU	O2'-C2'-C1'	-2.28	104.63	110.08
19	A	1128	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
19	4	1004	CLA	CED-O2D-CGD	2.28	121.09	115.92
19	B	1202	CLA	CHB-C1B-NB	-2.28	120.62	124.05
19	A	9023	CLA	CHC-C4B-NB	2.28	127.47	124.05
19	J	1308	CLA	CMB-C2B-C1B	2.28	128.89	125.42
19	A	9013	CLA	CGD-CBD-CAD	2.28	118.23	110.85
19	K	1146	CLA	C4A-NA-C1A	2.28	107.72	106.68
22	A	7044	LMU	C2'-C3'-C4'	2.28	114.86	109.68
19	4	4002	CLA	C4-C3-C2	-2.28	117.77	123.63
22	4	7053	LMU	O2B-C2B-C3B	-2.28	105.00	110.38
19	1	1011	CLA	C3D-C4D-ND	2.28	113.69	109.99
22	H	7043	LMU	O5'-C5'-C6'	2.28	112.09	106.44
21	F	6014	BCR	C15-C16-C17	-2.28	118.86	123.52
21	A	6007	BCR	C27-C26-C25	-2.28	119.63	122.70
22	2	7027	LMU	C3'-C4'-C5'	2.28	115.98	110.93
19	R	1150	CLA	O2A-CGA-O1A	-2.28	117.93	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	3009	CLA	CHB-C4A-NA	2.28	127.68	124.40
19	B	1228	CLA	O2A-C1-C2	2.27	116.86	108.11
19	4	1009	CLA	CBD-CHA-C1A	2.27	130.81	127.38
21	B	6020	BCR	C34-C9-C10	-2.27	119.13	122.82
19	A	1309	CLA	CHB-C4A-NA	2.27	127.66	124.43
19	A	1112	CLA	CHB-C4A-NA	2.27	127.68	124.40
21	B	6010	BCR	C33-C5-C4	2.27	118.44	113.60
19	B	1233	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
19	2	2004	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
19	3	3004	CLA	C3D-C4D-ND	2.27	112.61	109.50
19	A	1136	CLA	C3D-C4D-ND	2.27	113.68	109.99
19	R	1150	CLA	CAA-C2A-C1A	2.27	119.41	111.97
19	F	1305	CLA	C4-C3-C2	-2.27	117.80	123.63
19	K	1143	CLA	CAC-C3C-C4C	2.27	127.74	124.79
19	A	1107	CLA	CHD-C4C-C3C	-2.27	121.47	124.77
19	1	1012	CLA	C3D-C4D-ND	2.27	113.67	109.99
19	B	1233	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
19	A	1140	CLA	C2A-C1A-CHA	-2.27	119.93	123.87
19	K	1143	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
22	4	7053	LMU	O1'-C1'-C2'	2.27	111.71	108.27
19	A	1116	CLA	CMB-C2B-C1B	2.27	128.87	125.42
19	B	1209	CLA	CHB-C1B-NB	-2.26	120.65	124.05
19	3	3014	CLA	C3D-C2D-C1D	2.26	110.10	107.35
19	3	3003	CLA	CMB-C2B-C3B	2.26	129.55	123.53
19	L	1148	CLA	CHB-C1B-C2B	-2.26	120.86	127.43
19	B	9010	CLA	C3D-C4D-ND	2.26	113.66	109.99
19	L	1130	CLA	C3D-C4D-ND	2.26	113.66	109.99
19	3	1147	CLA	CAA-CBA-CGA	2.26	119.63	113.21
19	A	9023	CLA	CMA-C3A-C2A	-2.26	105.24	113.98
19	4	4003	CLA	C1-O2A-CGA	2.26	122.12	116.65
19	B	1236	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
19	L	1130	CLA	CMB-C2B-C3B	2.26	131.87	126.55
19	2	2002	CLA	C3A-C2A-C1A	2.26	104.72	101.34
22	H	7002	LMU	C1B-O1B-C4'	2.26	123.33	117.98
21	B	6020	BCR	C39-C30-C29	-2.26	100.28	108.95
22	4	7033	LMU	C2'-C3'-C4'	2.26	114.81	109.68
19	3	3002	CLA	C3D-C4D-ND	2.26	112.59	109.50
22	N	7049	LMU	O5B-C5B-C4B	-2.26	105.63	109.70
19	A	9011	CLA	CHC-C1C-C2C	-2.26	120.54	126.95
19	A	1117	CLA	C4A-NA-C1A	2.26	107.71	106.68
19	J	1311	CLA	C1-O2A-CGA	2.25	122.11	116.65
19	4	4007	CLA	C1D-ND-C4D	-2.25	104.73	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	7033	LMU	C1'-C2'-C3'	2.25	114.75	110.01
19	B	1226	CLA	C3D-C4D-ND	2.25	113.65	109.99
19	B	1215	CLA	CED-O2D-CGD	2.25	121.03	115.92
19	2	2004	CLA	C1-O2A-CGA	2.25	122.10	116.65
19	A	1123	CLA	CMB-C2B-C1B	2.25	128.85	125.42
19	A	1131	CLA	C3D-C4D-ND	2.25	113.65	109.99
19	B	1232	CLA	CHB-C4A-NA	2.25	127.65	124.40
22	B	7040	LMU	O3B-C3B-C2B	-2.25	105.07	110.38
19	A	1151	CLA	C5-C3-C4	2.25	119.77	114.59
19	L	1504	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
19	A	1102	CLA	CHB-C4A-NA	2.25	127.64	124.40
19	1	1006	CLA	C1D-ND-C4D	-2.25	104.73	106.31
20	A	5001	PQN	C8-C7-C6	2.25	123.01	120.24
19	3	3006	CLA	C3D-C4D-ND	2.24	112.57	109.50
19	2	2010	CLA	CHB-C4A-NA	2.24	127.62	124.43
24	B	7101	LMG	O7-C10-O9	-2.24	118.46	123.70
19	B	1217	CLA	CMA-C3A-C2A	-2.24	105.31	113.98
19	2	1307	CLA	C3C-C4C-CHD	-2.24	119.40	125.23
19	3	2009	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
19	2	2001	CLA	C3D-C4D-ND	2.24	113.63	109.99
19	H	1207	CLA	C1-O2A-CGA	2.24	122.08	116.65
21	B	6020	BCR	C37-C22-C21	-2.24	119.18	122.82
21	A	6002	BCR	C16-C15-C14	-2.24	118.93	123.52
19	A	1117	CLA	CHB-C4A-NA	2.24	127.63	124.40
19	2	2007	CLA	CAC-C3C-C4C	2.24	127.70	124.79
19	A	1134	CLA	C1D-ND-C4D	-2.24	104.74	106.31
19	4	1004	CLA	C1D-ND-C4D	-2.24	104.74	106.31
19	2	4009	CLA	C4-C3-C5	2.24	119.11	115.23
19	4	1304	CLA	CHA-C1A-NA	-2.24	121.32	126.39
19	A	1129	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
21	A	6011	BCR	C19-C18-C17	-2.24	115.49	119.01
21	A	6008	BCR	C28-C27-C26	-2.24	110.06	114.06
19	B	1223	CLA	C3D-C4D-ND	2.24	113.62	109.99
19	A	1104	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
21	F	6014	BCR	C32-C1-C31	2.24	115.04	108.63
19	A	9022	CLA	CHB-C1B-NB	-2.24	120.69	124.05
19	1	1011	CLA	CHB-C1B-NB	-2.24	120.69	124.05
19	K	1143	CLA	C1-C2-C3	-2.24	123.14	126.76
19	B	1238	CLA	C1D-ND-C4D	-2.24	104.74	106.31
19	K	1142	CLA	C3D-C4D-ND	2.24	113.62	109.99
19	L	1501	CLA	C3D-C4D-ND	2.23	113.62	109.99
19	A	1107	CLA	CAC-C3C-C2C	-2.23	123.45	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1134	CLA	C2A-C1A-CHA	-2.23	119.99	123.87
19	A	1117	CLA	C6-C5-C3	-2.23	108.03	113.47
19	A	1309	CLA	C3D-C4D-ND	2.23	112.55	109.50
19	1	1002	CLA	C1-O2A-CGA	2.23	123.01	116.67
22	H	7017	LMU	C1'-C2'-C3'	2.23	114.71	110.01
21	F	6014	BCR	C38-C26-C27	2.23	118.35	113.60
19	A	1237	CLA	O2A-CGA-CBA	2.23	118.64	111.83
19	4	4015	CLA	CHB-C1B-NB	-2.23	120.70	124.05
19	B	1223	CLA	CHB-C4A-NA	2.23	127.62	124.40
19	K	1146	CLA	C4D-CHA-C1A	-2.23	118.58	121.24
19	A	1102	CLA	C4-C3-C5	2.23	119.10	115.23
19	2	2014	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
19	G	1242	CLA	CMB-C2B-C1B	2.23	128.81	125.42
19	A	1110	CLA	C3D-C4D-ND	2.23	113.61	109.99
21	B	6005	BCR	C36-C18-C19	2.23	121.49	118.09
19	B	1221	CLA	CBC-CAC-C3C	-2.23	106.39	112.42
21	A	6007	BCR	C16-C15-C14	-2.22	118.97	123.52
19	B	1208	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
21	B	6006	BCR	C1-C6-C7	2.22	121.68	115.65
19	B	1227	CLA	CMB-C2B-C1B	2.22	128.80	125.42
21	B	6005	BCR	C15-C16-C17	-2.22	118.97	123.52
19	2	2006	CLA	CHB-C1B-NB	-2.22	120.72	124.05
19	B	1203	CLA	C11-C12-C13	-2.22	108.58	115.97
22	3	7003	LMU	O1'-C1'-C2'	2.22	111.65	108.27
19	3	3017	CLA	C2D-C1D-ND	-2.22	107.93	110.13
19	L	1130	CLA	CBA-CAA-C2A	2.22	120.40	113.79
19	A	1132	CLA	C2D-C1D-ND	-2.22	107.93	110.13
19	B	1220	CLA	CHB-C1B-NB	-2.22	120.72	124.05
19	B	1219	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
19	B	1216	CLA	CMC-C2C-C1C	2.22	128.50	125.03
19	B	1228	CLA	CHB-C1B-NB	-2.22	120.72	124.05
19	4	4013	CLA	CHB-C4A-NA	2.22	127.58	124.43
22	R	7025	LMU	O1B-C1B-C2B	2.22	113.54	108.09
21	B	6004	BCR	C40-C30-C29	-2.22	100.44	108.95
19	B	1209	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
19	A	1121	CLA	C4B-C3B-C2B	2.22	110.06	107.30
19	A	1116	CLA	C1D-ND-C4D	-2.21	104.76	106.31
19	4	4014	CLA	CED-O2D-CGD	2.21	120.94	115.92
19	B	1202	CLA	C11-C12-C13	-2.21	108.61	115.97
19	2	2002	CLA	CAA-C2A-C1A	-2.21	104.73	111.97
19	L	1504	CLA	CED-O2D-CGD	2.21	120.93	115.92
19	3	3004	CLA	C3B-C4B-CHC	-2.21	118.93	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	2001	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
19	4	1304	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
19	B	9010	CLA	C7-C6-C5	-2.21	107.38	113.26
19	B	1210	CLA	C3D-C4D-ND	2.21	113.58	109.99
19	A	1137	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
22	A	7045	LMU	O1'-C1-C2	2.21	116.85	109.37
21	I	6021	BCR	C28-C27-C26	-2.21	110.12	114.06
22	K	7042	LMU	C4B-C3B-C2B	-2.21	106.96	110.83
19	B	1217	CLA	O2D-CGD-O1D	-2.21	119.56	123.85
19	K	1146	CLA	C5-C3-C4	2.21	119.66	114.59
19	4	4001	CLA	C4A-NA-C1A	2.21	107.69	106.68
19	4	4013	CLA	C1C-NC-C4C	-2.21	105.67	106.68
19	A	1149	CLA	C2A-C3A-C4A	-2.21	98.31	101.87
19	B	1213	CLA	O2A-CGA-CBA	2.20	120.47	112.14
21	B	6017	BCR	C32-C1-C2	2.20	117.41	108.95
19	A	1110	CLA	CED-O2D-CGD	2.20	120.92	115.92
19	A	1131	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
19	3	3017	CLA	CHC-C4B-C3B	-2.20	117.81	127.37
19	A	1139	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
19	4	1304	CLA	CMB-C2B-C1B	2.20	128.77	125.42
19	B	1208	CLA	CAC-C3C-C4C	2.20	127.66	124.79
22	4	7019	LMU	O2'-C2'-C3'	-2.20	105.19	110.38
22	C	7015	LMU	O5B-C5B-C4B	-2.20	105.73	109.70
22	H	7011	LMU	O1'-C1'-C2'	2.20	111.62	108.27
19	3	3015	CLA	C3D-C4D-ND	2.20	112.51	109.50
19	A	1107	CLA	CHC-C4B-C3B	-2.20	117.83	127.37
19	A	1102	CLA	C3D-C4D-ND	2.20	113.56	109.99
19	A	1124	CLA	C3D-C4D-ND	2.20	113.56	109.99
19	A	9013	CLA	O2A-C1-C2	2.20	116.57	108.11
19	A	1126	CLA	C4-C3-C2	-2.20	117.98	123.63
21	A	6011	BCR	C1-C6-C7	2.20	121.61	115.65
21	J	6012	BCR	C40-C30-C39	2.20	114.93	108.63
19	B	1216	CLA	CHB-C1B-NB	-2.20	120.75	124.05
22	4	7019	LMU	C3'-C4'-C5'	2.20	115.80	110.93
19	A	1120	CLA	CHC-C1C-C2C	-2.20	120.71	126.95
19	1	1010	CLA	O2A-CGA-O1A	-2.20	116.64	123.20
19	K	3009	CLA	CAA-CBA-CGA	-2.20	106.97	113.21
19	B	1231	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
19	A	1121	CLA	CHB-C4A-NA	2.20	127.57	124.40
19	4	1009	CLA	CHC-C1C-C2C	-2.19	120.71	126.95
19	4	4014	CLA	C1-O2A-CGA	2.19	122.91	116.67
19	1	1303	CLA	CHA-C4D-ND	2.19	137.08	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	2009	CLA	CHB-C4A-NA	2.19	127.57	124.40
19	L	1503	CLA	CHB-C4A-NA	2.19	127.56	124.40
19	1	1001	CLA	C2D-C1D-ND	-2.19	107.96	110.13
21	I	6018	BCR	C40-C30-C29	-2.19	100.55	108.95
21	B	6005	BCR	C27-C26-C25	-2.19	119.75	122.70
19	H	1241	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
21	L	6019	BCR	C40-C30-C29	-2.19	100.55	108.95
21	F	6016	BCR	C33-C5-C4	2.19	118.26	113.60
21	F	6016	BCR	C35-C13-C14	-2.19	119.27	122.82
19	B	9010	CLA	CBC-CAC-C3C	-2.19	106.49	112.42
19	F	1305	CLA	C3D-C4D-ND	2.19	113.54	109.99
19	1	1007	CLA	C1-O2A-CGA	2.19	121.94	116.65
19	3	3003	CLA	CHB-C4A-NA	2.19	127.56	124.40
19	B	1228	CLA	CAC-C3C-C4C	2.19	127.64	124.79
19	4	4007	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
19	B	1217	CLA	CHB-C1B-NB	-2.19	120.77	124.05
19	B	1218	CLA	O2A-CGA-CBA	2.18	120.39	112.14
20	B	5002	PQN	C11-C3-C2	-2.18	121.14	124.89
21	F	6016	BCR	C4-C5-C6	-2.18	119.75	122.70
19	A	1110	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
19	B	1212	CLA	C3D-C4D-ND	2.18	113.53	109.99
19	H	1207	CLA	CED-O2D-CGD	2.18	120.87	115.92
19	A	1141	CLA	C1-C2-C3	-2.18	122.62	126.20
22	R	7022	LMU	O5'-C5'-C4'	2.18	114.23	109.72
19	4	4001	CLA	CAC-C3C-C4C	2.18	127.63	124.79
19	A	1133	CLA	CMA-C3A-C4A	-2.18	105.91	111.77
19	1	1001	CLA	CMC-C2C-C1C	2.18	128.44	125.03
19	4	4006	CLA	CHB-C4A-NA	2.18	127.55	124.40
19	B	1230	CLA	CHB-C1B-NB	-2.18	120.78	124.05
19	2	2005	CLA	C4D-ND-C1D	-2.18	104.78	106.31
19	L	1501	CLA	O2A-CGA-CBA	2.18	118.48	111.83
19	4	4007	CLA	O2A-CGA-CBA	2.18	118.48	111.83
19	B	1213	CLA	CHB-C1B-NB	-2.18	120.78	124.05
19	B	1201	CLA	CMB-C2B-C1B	2.18	128.74	125.42
19	F	1302	CLA	C1D-ND-C4D	-2.18	104.78	106.31
19	A	9013	CLA	C3D-C4D-ND	2.18	113.53	109.99
19	L	1504	CLA	CHB-C4A-NA	2.18	127.54	124.40
19	A	1133	CLA	C1-O2A-CGA	2.18	121.92	116.65
19	B	1238	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
19	2	2014	CLA	CHB-C1B-C2B	-2.18	121.11	127.43
19	A	9013	CLA	CHB-C1B-NB	-2.17	120.79	124.05
19	B	1210	CLA	C16-C15-C13	-2.17	108.74	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1101	CLA	C5-C3-C4	2.17	119.59	114.59
19	L	1503	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
19	B	1301	CLA	C3D-C4D-ND	2.17	113.52	109.99
22	B	7012	LMU	O5'-C5'-C4'	2.17	114.22	109.72
19	B	1220	CLA	CMB-C2B-C1B	2.17	128.73	125.42
21	B	6010	BCR	C1-C6-C7	2.17	121.54	115.65
19	B	1222	CLA	C3D-C4D-ND	2.17	113.52	109.99
19	K	3009	CLA	CMB-C2B-C1B	2.17	128.73	125.42
19	B	1217	CLA	C5-C3-C4	2.17	119.59	114.59
21	A	6008	BCR	C2-C1-C6	-2.17	107.28	110.44
19	A	1124	CLA	C2A-C1A-CHA	-2.17	120.10	123.87
19	2	2012	CLA	CHB-C1B-NB	-2.17	120.79	124.05
21	L	6019	BCR	C19-C18-C17	-2.17	115.59	119.01
19	B	1234	CLA	C4A-NA-C1A	2.17	107.67	106.68
19	L	1504	CLA	CMA-C3A-C4A	2.17	117.60	111.77
19	4	4011	CLA	C2C-C1C-CHC	-2.17	120.16	125.84
19	J	1311	CLA	C3D-C4D-ND	2.17	113.51	109.99
21	A	6011	BCR	C11-C12-C13	-2.17	120.42	126.36
19	J	1308	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
22	C	7015	LMU	O2'-C2'-C3'	2.17	115.48	110.38
22	H	7011	LMU	O5B-C1B-C2B	2.17	114.82	110.37
19	4	1004	CLA	C4-C3-C2	-2.17	118.06	123.63
19	A	1237	CLA	C1D-ND-C4D	-2.17	104.79	106.31
19	3	3014	CLA	CHB-C1B-NB	-2.17	120.95	124.08
20	B	5002	PQN	C14-C13-C12	-2.17	118.07	123.63
21	I	6021	BCR	C31-C1-C2	2.17	117.26	108.95
19	A	1149	CLA	CHB-C4A-NA	2.16	127.52	124.40
19	A	1237	CLA	CHB-C4A-NA	2.16	127.52	124.40
19	A	1113	CLA	C3D-C4D-ND	2.16	113.50	109.99
22	4	7033	LMU	O5'-C5'-C6'	2.16	111.80	106.44
19	A	9012	CLA	C4A-NA-C1A	2.16	107.67	106.68
19	A	1136	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
19	B	1208	CLA	CHC-C4B-C3B	-2.16	121.15	127.43
19	A	1140	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
19	A	1123	CLA	C1-C2-C3	-2.16	122.66	126.20
19	1	1003	CLA	CAA-CBA-CGA	-2.16	107.07	113.21
19	A	1120	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
19	4	4007	CLA	C3D-C4D-ND	2.16	113.50	109.99
19	B	1208	CLA	CMB-C2B-C1B	2.16	128.71	125.42
19	A	1138	CLA	C1D-ND-C4D	-2.16	104.80	106.31
19	L	1501	CLA	CHC-C4B-NB	2.16	127.29	124.05
19	B	1211	CLA	C3D-C4D-ND	2.16	113.50	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	7003	LMU	O1B-C4'-C3'	2.16	112.72	107.23
19	B	1208	CLA	C3D-C4D-ND	2.16	113.49	109.99
19	1	1003	CLA	C2A-C1A-CHA	-2.16	120.13	123.87
21	J	6012	BCR	C34-C9-C8	2.16	121.38	118.09
21	B	6004	BCR	C8-C7-C6	-2.16	121.24	127.00
19	1	1006	CLA	CMA-C3A-C2A	-2.15	111.29	116.23
22	3	7005	LMU	O5'-C1'-C2'	2.15	114.80	110.37
19	4	1004	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
19	1	1303	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
22	B	7012	LMU	C3'-C4'-C5'	2.15	115.70	110.93
19	A	1141	CLA	C1D-ND-C4D	-2.15	104.80	106.31
19	A	1128	CLA	CHB-C4A-NA	2.15	127.50	124.40
19	F	1302	CLA	C2A-C1A-CHA	-2.15	120.13	123.86
22	G	7039	LMU	C1B-O1B-C4'	-2.15	112.88	117.98
22	E	7037	LMU	C1'-C2'-C3'	2.15	114.53	110.01
19	4	4015	CLA	O2A-CGA-CBA	2.15	120.26	112.14
22	K	7042	LMU	C1'-O5'-C5'	-2.15	109.52	113.72
19	A	1122	CLA	CAC-C3C-C2C	-2.15	123.61	127.56
19	F	1302	CLA	C3D-C4D-ND	2.15	113.48	109.99
19	B	1220	CLA	O2A-CGA-CBA	2.15	118.38	111.83
19	3	1118	CLA	CHB-C1B-NB	-2.15	120.83	124.05
19	K	3009	CLA	C1D-ND-C4D	-2.14	104.81	106.31
20	A	5001	PQN	C2M-C2-C1	2.14	120.62	116.68
19	A	1105	CLA	CMC-C2C-C1C	2.14	128.38	125.03
19	L	1501	CLA	C1D-ND-C4D	-2.14	104.81	106.31
19	B	1226	CLA	CHB-C4A-NA	2.14	127.49	124.40
21	A	6008	BCR	C35-C13-C12	2.14	121.36	118.09
19	B	1203	CLA	C3D-C4D-ND	2.14	113.47	109.99
19	B	1219	CLA	C3D-C4D-ND	2.14	113.47	109.99
19	B	1227	CLA	C2D-C1D-ND	-2.14	108.01	110.13
19	K	1142	CLA	CHB-C4A-NA	2.14	127.49	124.40
19	A	1107	CLA	C2A-C1A-CHA	-2.14	120.15	123.87
21	B	6010	BCR	C7-C6-C5	-2.14	116.62	121.56
22	E	7048	LMU	O1B-C1B-O5B	2.14	116.33	110.69
19	K	1143	CLA	C3D-C4D-ND	2.14	113.47	109.99
19	A	1137	CLA	C2A-C1A-CHA	-2.14	120.15	123.87
19	A	1139	CLA	C1-O2A-CGA	2.14	121.83	116.65
21	A	6002	BCR	C4-C5-C6	-2.14	119.81	122.70
19	H	1505	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
21	J	6012	BCR	C27-C26-C25	-2.14	119.81	122.70
19	B	1238	CLA	C1-C2-C3	-2.14	122.69	126.20
22	K	7001	LMU	C4B-C3B-C2B	2.14	114.58	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	7022	LMU	O1'-C1'-C2'	2.14	111.52	108.27
21	B	6006	BCR	C35-C13-C12	2.14	121.35	118.09
19	B	1213	CLA	CMB-C2B-C1B	2.14	128.67	125.42
19	A	1123	CLA	CED-O2D-CGD	2.14	120.76	115.92
19	3	1147	CLA	CGD-CBD-CAD	-2.13	103.94	110.85
21	A	6008	BCR	C15-C16-C17	-2.13	119.15	123.52
19	B	1213	CLA	CAA-C2A-C1A	2.13	118.97	111.97
19	2	2002	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
19	A	1107	CLA	C2D-C1D-ND	-2.13	108.02	110.13
19	J	1311	CLA	C1-C2-C3	-2.13	122.71	126.20
19	A	1111	CLA	C1-O2A-CGA	2.13	121.81	116.65
21	A	6002	BCR	C34-C9-C10	-2.13	119.36	122.82
19	A	9013	CLA	C16-C15-C13	-2.13	108.89	115.97
21	B	6006	BCR	C40-C30-C29	-2.13	100.78	108.95
19	G	1242	CLA	C4-C3-C2	-2.13	118.16	123.63
19	3	3016	CLA	C2A-C1A-CHA	-2.13	120.17	123.87
19	A	1134	CLA	CED-O2D-CGD	2.13	120.74	115.92
22	4	7019	LMU	O1'-C1'-C2'	2.13	111.50	108.27
19	A	1106	CLA	CMB-C2B-C1B	2.13	128.66	125.42
19	A	1126	CLA	C11-C10-C8	-2.13	108.90	115.97
19	B	1220	CLA	C6-C7-C8	-2.13	108.90	115.97
19	2	2007	CLA	C3D-C4D-ND	2.13	113.44	109.99
19	3	3007	CLA	C1D-ND-C4D	-2.13	104.82	106.31
22	F	7036	LMU	O5'-C5'-C6'	2.13	111.71	106.44
19	B	1221	CLA	CMC-C2C-C1C	2.12	128.35	125.03
22	K	7047	LMU	C1B-O5B-C5B	2.12	117.87	113.72
22	R	7022	LMU	O5B-C5B-C4B	2.12	113.53	109.70
19	F	1240	CLA	CGD-CBD-CAD	-2.12	105.59	114.30
19	A	1112	CLA	CAC-C3C-C4C	2.12	127.55	124.79
19	B	1226	CLA	C4B-C3B-C2B	2.12	109.94	107.30
19	A	1116	CLA	C4-C3-C5	2.12	118.91	115.23
19	B	1209	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	B	1215	CLA	C4B-C3B-C2B	2.12	109.94	107.30
19	A	1126	CLA	C6-C7-C8	-2.12	108.92	115.97
19	B	1203	CLA	C4B-C3B-C2B	2.12	109.94	107.30
19	A	1139	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
19	A	1131	CLA	C1-O2A-CGA	2.12	121.78	116.65
22	H	7011	LMU	O5'-C1'-C2'	-2.12	106.02	110.37
19	1	1007	CLA	C3D-C4D-ND	2.12	113.43	109.99
19	1	1002	CLA	CAA-CBA-CGA	2.12	119.22	113.21
19	2	2013	CLA	CMB-C2B-C1B	2.12	128.65	125.42
21	A	6008	BCR	C39-C30-C25	2.12	113.56	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	6012	BCR	C36-C18-C19	2.12	121.32	118.09
21	A	6002	BCR	C40-C30-C29	-2.12	100.83	108.95
19	3	3002	CLA	CHB-C1B-NB	-2.11	121.02	124.08
19	B	1233	CLA	CHB-C1B-NB	-2.11	120.88	124.05
19	A	1141	CLA	CED-O2D-CGD	2.11	120.71	115.92
19	3	3003	CLA	C3D-C4D-ND	2.11	113.42	109.99
19	3	3016	CLA	CED-O2D-CGD	2.11	120.71	115.92
21	I	6018	BCR	C30-C25-C26	-2.11	119.75	122.64
19	A	1123	CLA	CAC-C3C-C4C	2.11	127.54	124.79
19	B	9010	CLA	C11-C10-C8	-2.11	108.94	115.97
19	4	4011	CLA	CHB-C1B-NB	-2.11	121.03	124.08
19	3	3017	CLA	C1-C2-C3	-2.11	123.34	126.76
19	L	1148	CLA	C3D-C4D-ND	2.11	113.42	109.99
19	4	1004	CLA	C3D-C4D-ND	2.11	113.42	109.99
19	I	1204	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
19	A	1149	CLA	CHB-C1B-NB	-2.11	120.88	124.05
19	B	1206	CLA	CED-O2D-CGD	2.11	120.70	115.92
19	B	9010	CLA	CMA-C3A-C2A	-2.11	105.83	113.98
19	R	1150	CLA	C3B-C2B-C1B	-2.11	104.69	107.17
19	B	1223	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
19	1	1010	CLA	C3D-C4D-ND	2.11	113.41	109.99
19	A	1109	CLA	CHB-C1B-NB	-2.11	120.89	124.05
19	3	2009	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
19	K	1143	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
19	A	1104	CLA	C3D-C4D-ND	2.11	113.41	109.99
19	2	2012	CLA	CAC-C3C-C2C	-2.10	123.69	127.56
19	3	3003	CLA	CHC-C4B-C3B	-2.10	121.32	127.43
19	A	1101	CLA	CMB-C2B-C1B	2.10	128.62	125.42
19	A	9022	CLA	CMC-C2C-C1C	2.10	128.32	125.03
21	J	6012	BCR	C16-C15-C14	-2.10	119.22	123.52
19	F	1302	CLA	C4A-NA-C1A	2.10	107.64	106.68
19	A	1106	CLA	C1-O2A-CGA	2.10	121.74	116.65
19	A	1136	CLA	CMB-C2B-C1B	2.10	128.62	125.42
19	A	1113	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
19	1	1006	CLA	CHC-C4B-C3B	-2.10	121.33	127.43
19	2	2001	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
19	K	3009	CLA	C6-C7-C8	-2.10	108.98	115.97
19	B	1202	CLA	C3D-C4D-ND	2.10	113.40	109.99
19	A	1104	CLA	CHB-C1B-NB	-2.10	120.90	124.05
19	A	1129	CLA	C1-O2A-CGA	2.10	121.73	116.65
19	3	3010	CLA	C3D-C4D-ND	2.10	112.37	109.50
19	A	1121	CLA	C3D-C4D-ND	2.10	113.40	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1205	CLA	CHB-C1B-NB	-2.10	120.90	124.05
19	G	1242	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
19	L	1130	CLA	C1D-ND-C4D	-2.10	104.84	106.31
21	A	6003	BCR	C37-C22-C23	2.10	121.29	118.09
21	I	6021	BCR	C35-C13-C12	2.10	121.29	118.09
19	1	1014	CLA	CHB-C4A-NA	2.10	127.42	124.40
19	B	1235	CLA	C3D-C4D-ND	2.09	113.39	109.99
19	1	1012	CLA	CHC-C4B-C3B	-2.09	121.35	127.43
19	B	1222	CLA	C2A-C1A-CHA	-2.09	120.23	123.87
19	3	1147	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
19	A	1140	CLA	C4-C3-C5	2.09	118.86	115.23
21	I	6021	BCR	C7-C6-C5	2.09	126.38	121.56
19	A	1111	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
19	2	2013	CLA	CHC-C4B-C3B	-2.09	118.30	127.37
19	4	4001	CLA	CGD-CBD-CAD	-2.09	104.08	110.85
22	R	7021	LMU	C6B-C5B-C4B	-2.09	107.89	113.02
19	1	1007	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
22	A	7044	LMU	O5B-C5B-C4B	2.09	113.46	109.70
19	A	1135	CLA	C4A-NA-C1A	2.09	107.63	106.68
19	3	1147	CLA	CHB-C4A-NA	2.09	127.41	124.40
19	A	1126	CLA	C7-C6-C5	-2.09	107.70	113.26
19	B	1232	CLA	C1D-ND-C4D	-2.09	104.85	106.31
19	B	1223	CLA	C1-O2A-CGA	2.09	121.70	116.65
19	A	1117	CLA	C3A-C2A-C1A	2.09	104.46	101.34
21	I	6021	BCR	C32-C1-C6	-2.09	106.97	110.24
19	3	3010	CLA	CHD-C1D-ND	2.09	127.79	124.84
19	3	3011	CLA	C5-C3-C2	-2.09	116.49	121.17
19	A	1237	CLA	CED-O2D-CGD	2.08	120.64	115.92
19	B	1205	CLA	C3A-C2A-C1A	2.08	104.46	101.34
19	L	1502	CLA	CAC-C3C-C4C	2.08	127.50	124.79
19	3	3001	CLA	CHB-C1B-NB	-2.08	121.07	124.08
21	L	6019	BCR	C33-C5-C4	2.08	118.03	113.60
19	K	1143	CLA	CED-O2D-CGD	2.08	120.64	115.92
19	L	1501	CLA	C2A-C1A-CHA	-2.08	120.26	123.87
19	1	1010	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
19	2	2014	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
19	A	1113	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	3	1147	CLA	CHC-C4B-C3B	-2.08	118.35	127.37
21	B	6010	BCR	C39-C30-C25	2.08	113.50	110.24
19	2	2002	CLA	C2A-C1A-CHA	-2.08	120.26	123.87
19	B	1227	CLA	C3D-C4D-ND	2.08	113.36	109.99
19	1	1007	CLA	C1-C2-C3	-2.08	122.80	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	1013	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
19	A	1125	CLA	C3D-C4D-ND	2.08	113.36	109.99
19	A	1137	CLA	C1D-ND-C4D	-2.08	104.86	106.31
19	A	1128	CLA	O2A-CGA-CBA	2.08	118.16	111.83
19	2	2012	CLA	C5-C3-C4	2.08	119.36	114.59
19	A	1125	CLA	CMB-C2B-C1B	2.07	128.58	125.42
22	2	7046	LMU	O1B-C4'-C5'	2.07	114.92	109.48
19	1	1003	CLA	CHB-C1B-NB	-2.07	120.94	124.05
22	D	7050	LMU	C1'-O5'-C5'	-2.07	109.67	113.72
19	A	1135	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
19	A	1111	CLA	C4-C3-C5	2.07	118.83	115.23
19	K	3009	CLA	C3D-C4D-ND	2.07	113.36	109.99
19	B	1222	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
19	A	1139	CLA	C1-C2-C3	-2.07	122.80	126.20
19	R	1144	CLA	CAA-CBA-CGA	2.07	119.09	113.21
19	1	1014	CLA	CMB-C2B-C1B	2.07	128.57	125.42
19	B	1220	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
19	B	1201	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
19	B	1216	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
19	B	1231	CLA	CMB-C2B-C1B	2.07	128.57	125.42
21	B	6004	BCR	C15-C16-C17	-2.07	119.29	123.52
19	4	4001	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
19	2	2007	CLA	CED-O2D-CGD	2.07	120.61	115.92
19	L	1503	CLA	CAA-CBA-CGA	-2.07	107.34	113.21
19	4	4015	CLA	CMB-C2B-C1B	2.07	128.56	125.42
21	L	6019	BCR	C30-C25-C26	-2.07	119.81	122.64
19	B	1220	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
19	L	1148	CLA	CAA-C2A-C1A	2.06	118.74	111.97
21	B	6020	BCR	C23-C24-C25	-2.06	121.48	127.00
19	A	1127	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
19	B	1215	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
22	2	7031	LMU	O1B-C4'-C5'	2.06	114.89	109.48
19	A	1127	CLA	CGD-CBD-CAD	2.06	117.52	110.85
21	A	6003	BCR	C4-C5-C6	-2.06	119.92	122.70
22	4	7019	LMU	O5'-C5'-C6'	2.06	111.55	106.44
19	4	1004	CLA	CHB-C1B-NB	-2.06	120.96	124.05
22	A	7045	LMU	C4B-C3B-C2B	-2.06	107.21	110.83
19	1	1303	CLA	C4D-C3D-CAD	2.06	110.34	108.11
19	H	1241	CLA	C4A-NA-C1A	2.06	107.62	106.68
19	B	1238	CLA	CMA-C3A-C2A	-2.06	106.02	113.98
22	B	7040	LMU	O5B-C1B-C2B	2.06	114.60	110.37
19	H	1505	CLA	O1D-CGD-CBD	-2.06	120.46	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	3001	CLA	CHD-C1D-ND	2.06	127.75	124.84
19	A	9011	CLA	C2A-C1A-CHA	-2.06	120.30	123.87
19	R	1144	CLA	CGD-CBD-CAD	-2.06	104.19	110.85
19	3	3015	CLA	C1C-NC-C4C	-2.06	105.74	106.68
19	A	1107	CLA	O2A-C1-C2	2.06	116.02	108.11
19	B	1213	CLA	C3D-C4D-ND	2.05	113.33	109.99
19	A	1140	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
22	A	7010	LMU	C3B-C4B-C5B	2.05	113.96	110.23
19	B	1228	CLA	C3D-C4D-ND	2.05	113.33	109.99
19	A	1111	CLA	CHC-C4B-NB	2.05	127.13	124.05
19	3	3001	CLA	C3D-C2D-C1D	2.05	109.84	107.35
19	3	3015	CLA	CHB-C1B-NB	-2.05	121.11	124.08
22	R	7007	LMU	C1B-O5B-C5B	2.05	117.73	113.72
19	B	1208	CLA	C4-C3-C5	2.05	118.79	115.23
19	A	1151	CLA	C2D-C1D-ND	-2.05	108.10	110.13
19	3	2009	CLA	CMB-C2B-C1B	2.05	128.54	125.42
19	3	3002	CLA	CHD-C1D-ND	2.05	127.74	124.84
19	A	1121	CLA	CED-O2D-CGD	2.05	120.57	115.92
19	A	1125	CLA	CHB-C1B-NB	-2.05	120.97	124.05
21	B	6020	BCR	C33-C5-C6	-2.05	122.25	124.48
19	3	3014	CLA	C3C-C4C-CHD	-2.05	119.91	125.23
19	3	3007	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
22	B	7038	LMU	O1B-C4'-C5'	2.05	114.85	109.48
19	A	1103	CLA	C6-C7-C8	-2.05	109.16	115.97
19	A	1140	CLA	C1D-ND-C4D	-2.05	104.88	106.31
19	L	1501	CLA	CHB-C1B-NB	-2.05	120.98	124.05
19	1	1013	CLA	CHC-C4B-C3B	-2.05	118.49	127.37
19	K	1143	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
21	B	6004	BCR	C32-C1-C31	2.05	114.49	108.63
19	4	4013	CLA	CHD-C1D-ND	2.04	127.73	124.84
19	B	1239	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
22	2	7027	LMU	O5'-C1'-C2'	2.04	114.57	110.37
19	1	1014	CLA	CHB-C1B-NB	-2.04	120.98	124.05
21	3	6022	BCR	C35-C13-C12	2.04	121.21	118.09
22	R	7021	LMU	O5B-C5B-C4B	2.04	113.38	109.70
19	B	1233	CLA	C3D-C4D-ND	2.04	113.30	109.99
21	J	6012	BCR	C37-C22-C23	2.04	121.20	118.09
19	F	1240	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
21	I	6021	BCR	C33-C5-C6	-2.04	122.26	124.48
22	E	7048	LMU	O5'-C5'-C6'	2.04	111.49	106.44
19	A	1132	CLA	CAC-C3C-C2C	-2.04	123.81	127.56
19	A	1103	CLA	O1A-CGA-CBA	-2.04	115.82	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	1209	CLA	O2A-CGA-CBA	2.04	118.04	111.83
19	A	9022	CLA	C6-C5-C3	2.04	118.43	113.47
19	A	1109	CLA	O2A-CGA-CBA	2.04	118.04	111.83
19	B	1217	CLA	CMC-C2C-C1C	2.03	128.21	125.03
22	B	7012	LMU	O1B-C4'-C3'	2.03	112.40	107.23
22	R	7024	LMU	O5B-C5B-C6B	2.03	111.48	106.44
19	B	1220	CLA	C9-C8-C10	2.03	118.52	111.27
21	A	6003	BCR	C32-C1-C31	2.03	114.45	108.63
19	A	1108	CLA	CMB-C2B-C1B	2.03	128.51	125.42
19	K	1143	CLA	C2A-C1A-CHA	-2.03	120.34	123.87
19	3	1147	CLA	C3D-C4D-ND	2.03	113.29	109.99
19	2	2011	CLA	CHD-C1D-ND	2.03	127.71	124.84
20	A	5001	PQN	C11-C3-C2	-2.03	121.41	124.89
21	B	6006	BCR	C7-C6-C5	-2.03	116.88	121.56
19	A	1126	CLA	C3D-C4D-ND	2.03	113.29	109.99
19	J	1308	CLA	C1D-ND-C4D	-2.03	104.89	106.31
19	A	1124	CLA	C4-C3-C5	2.03	118.75	115.23
19	A	1105	CLA	O2A-CGA-CBA	2.03	119.81	112.14
19	H	1505	CLA	CAC-C3C-C4C	2.03	127.43	124.79
19	A	1115	CLA	CAC-C3C-C4C	2.03	127.43	124.79
19	1	1007	CLA	CBC-CAC-C3C	2.03	117.92	112.42
19	A	1149	CLA	C3D-C4D-ND	2.03	113.28	109.99
22	2	7046	LMU	O5'-C5'-C6'	2.03	111.47	106.44
22	R	7021	LMU	C1B-O1B-C4'	2.03	122.79	117.98
19	H	1505	CLA	C1D-ND-C4D	-2.03	104.89	106.31
19	B	1301	CLA	CAC-C3C-C4C	2.03	128.20	125.03
21	F	6016	BCR	C28-C27-C26	-2.03	110.44	114.06
22	G	7051	LMU	O2B-C2B-C3B	-2.03	105.60	110.38
19	1	1303	CLA	C2D-C1D-ND	-2.03	108.12	110.13
19	2	2014	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	3	3013	CLA	CHB-C1B-NB	-2.03	121.01	124.05
19	4	4001	CLA	C5-C3-C4	2.03	119.25	114.59
19	A	1237	CLA	C2A-C1A-CHA	-2.02	120.35	123.87
19	4	4010	CLA	C3D-C4D-ND	2.02	112.27	109.50
21	A	6007	BCR	C1-C6-C7	2.02	121.14	115.65
19	K	3009	CLA	CAC-C3C-C4C	2.02	127.42	124.79
19	B	1210	CLA	CHB-C4A-NA	2.02	127.32	124.40
19	B	1215	CLA	O2A-C1-C2	2.02	115.88	108.11
21	B	6006	BCR	C32-C1-C6	-2.02	107.08	110.24
19	2	2002	CLA	CED-O2D-CGD	2.02	120.50	115.92
19	4	4013	CLA	C3D-C4D-ND	2.02	112.26	109.50
19	A	1124	CLA	O2A-CGA-O1A	-2.02	118.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	F	6016	BCR	C23-C24-C25	-2.02	121.61	127.00
19	A	1151	CLA	C4A-NA-C1A	2.02	107.60	106.68
19	4	4003	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
19	A	1140	CLA	CMB-C2B-C1B	2.02	128.49	125.42
19	A	1132	CLA	C3D-C4D-ND	2.02	113.27	109.99
22	R	7022	LMU	C1B-O1B-C4'	2.02	122.76	117.98
19	B	1202	CLA	C4B-C3B-C2B	2.02	109.81	107.30
22	A	7045	LMU	O6'-C6'-C5'	-2.02	104.47	111.33
19	K	1146	CLA	C2D-C1D-ND	-2.02	108.13	110.13
19	A	1129	CLA	CMB-C2B-C1B	2.02	128.49	125.42
21	A	6011	BCR	C23-C22-C21	-2.02	115.84	119.01
22	C	7015	LMU	O1B-C1B-C2B	2.02	113.05	108.09
19	4	4002	CLA	CAA-C2A-C3A	2.01	118.44	113.00
22	B	7012	LMU	C1'-C2'-C3'	2.01	114.25	110.01
19	1	1010	CLA	CAA-C2A-C3A	2.01	118.44	113.00
19	A	1131	CLA	C4-C3-C5	2.01	118.72	115.23
19	A	1124	CLA	C1D-ND-C4D	-2.01	104.90	106.31
19	A	1137	CLA	CHB-C1B-NB	-2.01	121.03	124.05
19	R	1144	CLA	CAA-C2A-C1A	2.01	118.57	111.97
19	A	1119	CLA	CGD-CBD-CAD	2.01	117.36	110.85
19	B	1202	CLA	CBC-CAC-C3C	-2.01	106.96	112.42
19	4	4015	CLA	C3D-C4D-ND	2.01	113.26	109.99
22	3	7003	LMU	C6B-C5B-C4B	-2.01	108.08	113.02
19	3	3013	CLA	C1-C2-C3	-2.01	122.90	126.20
21	3	6022	BCR	C36-C18-C17	-2.01	119.56	122.82
19	4	4003	CLA	C1-C2-C3	-2.01	122.90	126.20
19	2	4009	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
22	H	7030	LMU	C2'-C3'-C4'	2.01	114.24	109.68
22	F	7036	LMU	O5B-C5B-C6B	2.01	111.42	106.44
19	2	2001	CLA	CMB-C2B-C1B	2.01	128.48	125.42
19	B	1211	CLA	CAC-C3C-C2C	-2.01	123.87	127.56
19	A	9023	CLA	C6-C7-C8	-2.01	109.29	115.97
19	B	1202	CLA	CMA-C3A-C2A	-2.01	106.21	113.98
22	4	7008	LMU	O2'-C2'-C3'	-2.01	105.64	110.38
21	A	6002	BCR	C35-C13-C12	2.01	121.16	118.09
19	L	1503	CLA	C4A-NA-C1A	2.01	107.59	106.68
19	A	1120	CLA	C1D-ND-C4D	-2.01	104.91	106.31
19	A	1127	CLA	C2A-C1A-CHA	-2.00	120.39	123.87
19	1	1015	CLA	CHD-C1D-ND	2.00	127.67	124.84
19	B	1220	CLA	C1-C2-C3	-2.00	122.92	126.20
19	1	1303	CLA	CHA-C1A-NA	-2.00	121.86	126.39
19	B	1224	CLA	C2A-C1A-CHA	-2.00	120.39	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1119	CLA	C3D-C4D-ND	2.00	113.24	109.99
19	4	1004	CLA	C6-C5-C3	-2.00	108.59	113.47
19	F	1302	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
22	4	7009	LMU	C4B-C3B-C2B	2.00	114.34	110.83
21	I	6018	BCR	C37-C22-C21	-2.00	119.58	122.82
19	3	3017	CLA	CBA-CAA-C2A	-2.00	107.84	113.79

All (97) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1102	CLA	C8
19	A	1103	CLA	C8
19	A	1104	CLA	C8
19	A	1106	CLA	C8
19	A	1107	CLA	C8
19	A	1109	CLA	C8
19	A	1115	CLA	C8
19	A	1117	CLA	C8
19	A	1119	CLA	C8
19	A	1122	CLA	C8
19	A	1123	CLA	C8
19	A	1124	CLA	C8
19	A	1125	CLA	C8
19	A	1126	CLA	C8
19	A	1127	CLA	C8
19	A	1128	CLA	C8
19	A	1131	CLA	C8
19	A	1132	CLA	C8
19	A	1136	CLA	C8
19	A	1138	CLA	C8
19	A	1140	CLA	C8
19	A	1141	CLA	C8
19	A	1149	CLA	C2A
19	A	1149	CLA	CBD
19	A	1237	CLA	C8
19	A	9011	CLA	C8
19	A	9012	CLA	C8
19	A	9013	CLA	C8
19	A	9022	CLA	C8
19	A	9023	CLA	C8
19	B	1202	CLA	C8
19	B	1203	CLA	C8

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Mol	Chain	Res	Type	Atom
19	B	1205	CLA	C8
19	B	1206	CLA	C8
19	B	1208	CLA	C8
19	B	1209	CLA	C8
19	B	1210	CLA	C8
19	B	1211	CLA	C8
19	B	1212	CLA	C8
19	B	1214	CLA	C8
19	B	1215	CLA	C8
19	B	1216	CLA	C8
19	B	1219	CLA	C8
19	B	1222	CLA	C8
19	B	1223	CLA	C8
19	B	1224	CLA	C8
19	B	1225	CLA	C8
19	B	1226	CLA	C8
19	B	1229	CLA	C8
19	B	1234	CLA	C8
19	B	1235	CLA	C8
19	B	1238	CLA	C8
19	B	1239	CLA	C8
19	B	9010	CLA	C8
19	F	1305	CLA	C3A
19	F	1305	CLA	CBD
19	F	1305	CLA	C2A
19	H	1145	CLA	C8
19	H	1145	CLA	CBD
19	H	1207	CLA	C8
19	H	1241	CLA	C8
19	H	1505	CLA	C8
19	I	1204	CLA	C8
19	J	1308	CLA	C8
19	J	1311	CLA	C8
19	K	3009	CLA	C8
19	L	1130	CLA	C8
19	L	1148	CLA	C3A
19	L	1148	CLA	C2A
19	L	1503	CLA	CBD
19	L	1504	CLA	C8
19	R	1144	CLA	C8
19	R	1150	CLA	C8
19	1	1007	CLA	C8

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Mol	Chain	Res	Type	Atom
19	1	1008	CLA	C2A
19	1	1013	CLA	CBD
19	1	1014	CLA	C8
19	1	1303	CLA	C3A
19	1	1303	CLA	C2A
19	2	2002	CLA	C8
19	2	2006	CLA	C8
19	2	2007	CLA	C8
19	2	2014	CLA	C8
19	2	4009	CLA	C8
19	3	2009	CLA	C8
19	3	3011	CLA	C8
19	3	3013	CLA	C8
19	3	3016	CLA	C8
19	4	1004	CLA	C8
19	4	1304	CLA	C8
19	4	1304	CLA	CBD
19	4	1306	CLA	C8
19	4	4002	CLA	C2A
19	4	4003	CLA	C8
19	4	4006	CLA	C8
20	A	5001	PQN	C23
20	B	5002	PQN	C23

All (2930) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1101	CLA	C3A-C2A-CAA-CBA
19	A	1101	CLA	C2B-C3B-CAB-CBB
19	A	1102	CLA	C3A-C2A-CAA-CBA
19	A	1102	CLA	CBA-CGA-O2A-C1
19	A	1102	CLA	O1A-CGA-O2A-C1
19	A	1102	CLA	CBD-CGD-O2D-CED
19	A	1103	CLA	C1A-C2A-CAA-CBA
19	A	1103	CLA	C3A-C2A-CAA-CBA
19	A	1103	CLA	C2B-C3B-CAB-CBB
19	A	1104	CLA	CBA-CGA-O2A-C1
19	A	1104	CLA	O1A-CGA-O2A-C1
19	A	1104	CLA	CBD-CGD-O2D-CED
19	A	1105	CLA	C1A-C2A-CAA-CBA
19	A	1105	CLA	C3A-C2A-CAA-CBA
19	A	1105	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	1106	CLA	C1A-C2A-CAA-CBA
19	A	1106	CLA	C3A-C2A-CAA-CBA
19	A	1106	CLA	C4B-C3B-CAB-CBB
19	A	1106	CLA	CHA-CBD-CGD-O1D
19	A	1106	CLA	CHA-CBD-CGD-O2D
19	A	1107	CLA	C1A-C2A-CAA-CBA
19	A	1107	CLA	C2B-C3B-CAB-CBB
19	A	1108	CLA	C2B-C3B-CAB-CBB
19	A	1108	CLA	CBD-CGD-O2D-CED
19	A	1109	CLA	C4B-C3B-CAB-CBB
19	A	1109	CLA	CBD-CGD-O2D-CED
19	A	1110	CLA	C2B-C3B-CAB-CBB
19	A	1111	CLA	C2B-C3B-CAB-CBB
19	A	1111	CLA	CBD-CGD-O2D-CED
19	A	1112	CLA	C1A-C2A-CAA-CBA
19	A	1113	CLA	C1A-C2A-CAA-CBA
19	A	1113	CLA	CBA-CGA-O2A-C1
19	A	1113	CLA	O1A-CGA-O2A-C1
19	A	1113	CLA	CBD-CGD-O2D-CED
19	A	1115	CLA	CBA-CGA-O2A-C1
19	A	1115	CLA	O1A-CGA-O2A-C1
19	A	1115	CLA	C2-C3-C5-C6
19	A	1115	CLA	C4-C3-C5-C6
19	A	1116	CLA	C1A-C2A-CAA-CBA
19	A	1116	CLA	C3A-C2A-CAA-CBA
19	A	1116	CLA	CBD-CGD-O2D-CED
19	A	1117	CLA	C1A-C2A-CAA-CBA
19	A	1117	CLA	C3A-C2A-CAA-CBA
19	A	1117	CLA	CBA-CGA-O2A-C1
19	A	1117	CLA	O1A-CGA-O2A-C1
19	A	1117	CLA	C2B-C3B-CAB-CBB
19	A	1117	CLA	CAD-CBD-CGD-O1D
19	A	1117	CLA	CAD-CBD-CGD-O2D
19	A	1117	CLA	CBD-CGD-O2D-CED
19	A	1120	CLA	C2B-C3B-CAB-CBB
19	A	1120	CLA	CAD-CBD-CGD-O1D
19	A	1120	CLA	CAD-CBD-CGD-O2D
19	A	1121	CLA	C1A-C2A-CAA-CBA
19	A	1121	CLA	C3A-C2A-CAA-CBA
19	A	1122	CLA	C1A-C2A-CAA-CBA
19	A	1124	CLA	C2B-C3B-CAB-CBB
19	A	1124	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1125	CLA	C2B-C3B-CAB-CBB
19	A	1125	CLA	C11-C10-C8-C9
19	A	1126	CLA	C2B-C3B-CAB-CBB
19	A	1127	CLA	C2B-C3B-CAB-CBB
19	A	1128	CLA	C1A-C2A-CAA-CBA
19	A	1128	CLA	C3A-C2A-CAA-CBA
19	A	1128	CLA	C2B-C3B-CAB-CBB
19	A	1128	CLA	CHA-CBD-CGD-O1D
19	A	1128	CLA	CHA-CBD-CGD-O2D
19	A	1128	CLA	CBD-CGD-O2D-CED
19	A	1129	CLA	C4B-C3B-CAB-CBB
19	A	1131	CLA	CBD-CGD-O2D-CED
19	A	1132	CLA	C1A-C2A-CAA-CBA
19	A	1132	CLA	CHA-CBD-CGD-O1D
19	A	1132	CLA	CHA-CBD-CGD-O2D
19	A	1133	CLA	C1A-C2A-CAA-CBA
19	A	1133	CLA	C3A-C2A-CAA-CBA
19	A	1135	CLA	C1A-C2A-CAA-CBA
19	A	1135	CLA	CBD-CGD-O2D-CED
19	A	1136	CLA	C2B-C3B-CAB-CBB
19	A	1136	CLA	CAD-CBD-CGD-O1D
19	A	1136	CLA	CAD-CBD-CGD-O2D
19	A	1137	CLA	C1A-C2A-CAA-CBA
19	A	1137	CLA	C4B-C3B-CAB-CBB
19	A	1139	CLA	C1A-C2A-CAA-CBA
19	A	1139	CLA	CBD-CGD-O2D-CED
19	A	1140	CLA	C1A-C2A-CAA-CBA
19	A	1140	CLA	C3A-C2A-CAA-CBA
19	A	1149	CLA	C1A-C2A-CAA-CBA
19	A	1149	CLA	CAD-CBD-CGD-O1D
19	A	1149	CLA	CAD-CBD-CGD-O2D
19	A	1149	CLA	CBD-CGD-O2D-CED
19	A	1151	CLA	C3A-C2A-CAA-CBA
19	A	1151	CLA	C4B-C3B-CAB-CBB
19	A	1151	CLA	CBD-CGD-O2D-CED
19	A	1237	CLA	C11-C10-C8-C7
19	A	9011	CLA	C3A-C2A-CAA-CBA
19	A	9011	CLA	C2B-C3B-CAB-CBB
19	A	9011	CLA	C4B-C3B-CAB-CBB
19	A	9012	CLA	CBD-CGD-O2D-CED
19	A	9012	CLA	O1D-CGD-O2D-CED
19	A	9012	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	9013	CLA	C2B-C3B-CAB-CBB
19	A	9022	CLA	C2B-C3B-CAB-CBB
19	A	9022	CLA	C4-C3-C5-C6
19	B	1201	CLA	C1A-C2A-CAA-CBA
19	B	1201	CLA	C3A-C2A-CAA-CBA
19	B	1202	CLA	C1A-C2A-CAA-CBA
19	B	1202	CLA	C2-C1-O2A-CGA
19	B	1202	CLA	CAD-CBD-CGD-O1D
19	B	1202	CLA	CAD-CBD-CGD-O2D
19	B	1203	CLA	C2B-C3B-CAB-CBB
19	B	1203	CLA	CBD-CGD-O2D-CED
19	B	1205	CLA	CHA-CBD-CGD-O1D
19	B	1205	CLA	CHA-CBD-CGD-O2D
19	B	1205	CLA	C11-C10-C8-C9
19	B	1205	CLA	C12-C13-C15-C16
19	B	1206	CLA	C1A-C2A-CAA-CBA
19	B	1208	CLA	C1A-C2A-CAA-CBA
19	B	1208	CLA	C3A-C2A-CAA-CBA
19	B	1208	CLA	CBA-CGA-O2A-C1
19	B	1208	CLA	O1A-CGA-O2A-C1
19	B	1209	CLA	C4B-C3B-CAB-CBB
19	B	1210	CLA	C1A-C2A-CAA-CBA
19	B	1210	CLA	CAD-CBD-CGD-O1D
19	B	1210	CLA	CAD-CBD-CGD-O2D
19	B	1211	CLA	C1A-C2A-CAA-CBA
19	B	1211	CLA	C3A-C2A-CAA-CBA
19	B	1212	CLA	CAD-CBD-CGD-O1D
19	B	1212	CLA	CAD-CBD-CGD-O2D
19	B	1213	CLA	C4B-C3B-CAB-CBB
19	B	1213	CLA	C2C-C3C-CAC-CBC
19	B	1213	CLA	C4C-C3C-CAC-CBC
19	B	1213	CLA	CBD-CGD-O2D-CED
19	B	1214	CLA	C1A-C2A-CAA-CBA
19	B	1214	CLA	C3A-C2A-CAA-CBA
19	B	1214	CLA	CBD-CGD-O2D-CED
19	B	1215	CLA	C1A-C2A-CAA-CBA
19	B	1215	CLA	C3A-C2A-CAA-CBA
19	B	1216	CLA	C1A-C2A-CAA-CBA
19	B	1216	CLA	C3A-C2A-CAA-CBA
19	B	1216	CLA	CBD-CGD-O2D-CED
19	B	1217	CLA	C4B-C3B-CAB-CBB
19	B	1217	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	1218	CLA	CHA-CBD-CGD-O1D
19	B	1218	CLA	CHA-CBD-CGD-O2D
19	B	1218	CLA	CBD-CGD-O2D-CED
19	B	1219	CLA	C1A-C2A-CAA-CBA
19	B	1219	CLA	C3A-C2A-CAA-CBA
19	B	1219	CLA	C4B-C3B-CAB-CBB
19	B	1220	CLA	CBA-CGA-O2A-C1
19	B	1220	CLA	O1A-CGA-O2A-C1
19	B	1220	CLA	C4B-C3B-CAB-CBB
19	B	1222	CLA	C4B-C3B-CAB-CBB
19	B	1222	CLA	CBD-CGD-O2D-CED
19	B	1223	CLA	C1A-C2A-CAA-CBA
19	B	1223	CLA	C3A-C2A-CAA-CBA
19	B	1223	CLA	C4B-C3B-CAB-CBB
19	B	1223	CLA	C11-C12-C13-C14
19	B	1224	CLA	C3A-C2A-CAA-CBA
19	B	1224	CLA	CBD-CGD-O2D-CED
19	B	1225	CLA	C1A-C2A-CAA-CBA
19	B	1225	CLA	C3A-C2A-CAA-CBA
19	B	1225	CLA	C4B-C3B-CAB-CBB
19	B	1226	CLA	C2B-C3B-CAB-CBB
19	B	1226	CLA	CAD-CBD-CGD-O1D
19	B	1226	CLA	CAD-CBD-CGD-O2D
19	B	1227	CLA	C1A-C2A-CAA-CBA
19	B	1227	CLA	C3A-C2A-CAA-CBA
19	B	1227	CLA	CBD-CGD-O2D-CED
19	B	1228	CLA	C1A-C2A-CAA-CBA
19	B	1228	CLA	C3A-C2A-CAA-CBA
19	B	1228	CLA	C2C-C3C-CAC-CBC
19	B	1228	CLA	C4C-C3C-CAC-CBC
19	B	1228	CLA	CHA-CBD-CGD-O1D
19	B	1228	CLA	CHA-CBD-CGD-O2D
19	B	1229	CLA	C1A-C2A-CAA-CBA
19	B	1230	CLA	C1A-C2A-CAA-CBA
19	B	1230	CLA	C3A-C2A-CAA-CBA
19	B	1230	CLA	CBD-CGD-O2D-CED
19	B	1231	CLA	C1A-C2A-CAA-CBA
19	B	1231	CLA	C3A-C2A-CAA-CBA
19	B	1231	CLA	CAD-CBD-CGD-O1D
19	B	1231	CLA	CAD-CBD-CGD-O2D
19	B	1231	CLA	CBD-CGD-O2D-CED
19	B	1232	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	B	1232	CLA	CBD-CGD-O2D-CED
19	B	1233	CLA	C3A-C2A-CAA-CBA
19	B	1233	CLA	O1A-CGA-O2A-C1
19	B	1233	CLA	C2-C3-C5-C6
19	B	1235	CLA	C2B-C3B-CAB-CBB
19	B	1236	CLA	C4B-C3B-CAB-CBB
19	B	1238	CLA	C4B-C3B-CAB-CBB
19	B	1239	CLA	C3A-C2A-CAA-CBA
19	B	1239	CLA	C2B-C3B-CAB-CBB
19	B	1239	CLA	C4B-C3B-CAB-CBB
19	B	9010	CLA	C4B-C3B-CAB-CBB
19	B	9010	CLA	CBD-CGD-O2D-CED
19	F	1302	CLA	CBD-CGD-O2D-CED
19	F	1302	CLA	O1D-CGD-O2D-CED
19	F	1305	CLA	C1A-C2A-CAA-CBA
19	F	1305	CLA	CBD-CGD-O2D-CED
19	F	1305	CLA	O1D-CGD-O2D-CED
19	G	1242	CLA	CAD-CBD-CGD-O1D
19	G	1242	CLA	CAD-CBD-CGD-O2D
19	G	1242	CLA	CBD-CGD-O2D-CED
19	G	1242	CLA	C2-C3-C5-C6
19	G	1242	CLA	C4-C3-C5-C6
19	H	1145	CLA	C1A-C2A-CAA-CBA
19	H	1145	CLA	C3A-C2A-CAA-CBA
19	H	1145	CLA	CBD-CGD-O2D-CED
19	H	1145	CLA	O1D-CGD-O2D-CED
19	H	1207	CLA	O2A-C1-C2-C3
19	H	1241	CLA	C4B-C3B-CAB-CBB
19	H	1241	CLA	CAD-CBD-CGD-O1D
19	H	1241	CLA	CAD-CBD-CGD-O2D
19	H	1241	CLA	CBD-CGD-O2D-CED
19	H	1505	CLA	C4-C3-C5-C6
19	J	1308	CLA	C1A-C2A-CAA-CBA
19	J	1308	CLA	C2C-C3C-CAC-CBC
19	J	1308	CLA	C4C-C3C-CAC-CBC
19	J	1308	CLA	CAD-CBD-CGD-O1D
19	J	1308	CLA	CAD-CBD-CGD-O2D
19	J	1308	CLA	CBD-CGD-O2D-CED
19	J	1311	CLA	C3A-C2A-CAA-CBA
19	J	1311	CLA	C4B-C3B-CAB-CBB
19	J	1311	CLA	CHA-CBD-CGD-O1D
19	J	1311	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	J	1311	CLA	CBD-CGD-O2D-CED
19	K	1142	CLA	C2B-C3B-CAB-CBB
19	K	1146	CLA	C4B-C3B-CAB-CBB
19	K	3009	CLA	C3A-C2A-CAA-CBA
19	K	3009	CLA	C2-C1-O2A-CGA
19	K	3009	CLA	C2B-C3B-CAB-CBB
19	L	1130	CLA	C1A-C2A-CAA-CBA
19	L	1130	CLA	C4B-C3B-CAB-CBB
19	L	1130	CLA	CBD-CGD-O2D-CED
19	L	1130	CLA	O1D-CGD-O2D-CED
19	L	1148	CLA	C1A-C2A-CAA-CBA
19	L	1148	CLA	C2-C1-O2A-CGA
19	L	1148	CLA	C2C-C3C-CAC-CBC
19	L	1148	CLA	C4C-C3C-CAC-CBC
19	L	1501	CLA	C1A-C2A-CAA-CBA
19	L	1501	CLA	C3A-C2A-CAA-CBA
19	L	1501	CLA	C2B-C3B-CAB-CBB
19	L	1501	CLA	CBD-CGD-O2D-CED
19	L	1502	CLA	C1A-C2A-CAA-CBA
19	L	1502	CLA	CHA-CBD-CGD-O1D
19	L	1502	CLA	CHA-CBD-CGD-O2D
19	L	1502	CLA	CBD-CGD-O2D-CED
19	L	1503	CLA	C1A-C2A-CAA-CBA
19	L	1503	CLA	C4C-C3C-CAC-CBC
19	L	1504	CLA	C4B-C3B-CAB-CBB
19	L	1504	CLA	CBD-CGD-O2D-CED
19	R	1144	CLA	C1A-C2A-CAA-CBA
19	R	1144	CLA	O1A-CGA-O2A-C1
19	R	1144	CLA	CHA-CBD-CGD-O1D
19	R	1144	CLA	CHA-CBD-CGD-O2D
19	R	1144	CLA	CBD-CGD-O2D-CED
19	R	1150	CLA	C1A-C2A-CAA-CBA
19	R	1150	CLA	CAD-CBD-CGD-O1D
19	R	1150	CLA	CAD-CBD-CGD-O2D
19	R	1150	CLA	O2A-C1-C2-C3
19	1	1001	CLA	C1A-C2A-CAA-CBA
19	1	1001	CLA	C3A-C2A-CAA-CBA
19	1	1001	CLA	CBA-CGA-O2A-C1
19	1	1001	CLA	CHA-CBD-CGD-O1D
19	1	1001	CLA	CHA-CBD-CGD-O2D
19	1	1002	CLA	CBD-CGD-O2D-CED
19	1	1005	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	1	1005	CLA	C4B-C3B-CAB-CBB
19	1	1005	CLA	CBD-CGD-O2D-CED
19	1	1005	CLA	O1D-CGD-O2D-CED
19	1	1007	CLA	C1A-C2A-CAA-CBA
19	1	1007	CLA	C4B-C3B-CAB-CBB
19	1	1007	CLA	C2C-C3C-CAC-CBC
19	1	1007	CLA	C4C-C3C-CAC-CBC
19	1	1007	CLA	CHA-CBD-CGD-O1D
19	1	1007	CLA	CHA-CBD-CGD-O2D
19	1	1008	CLA	C2B-C3B-CAB-CBB
19	1	1008	CLA	C2-C3-C5-C6
19	1	1008	CLA	C4-C3-C5-C6
19	1	1010	CLA	C1A-C2A-CAA-CBA
19	1	1010	CLA	C2B-C3B-CAB-CBB
19	1	1010	CLA	CBD-CGD-O2D-CED
19	1	1013	CLA	C4B-C3B-CAB-CBB
19	1	1013	CLA	CBD-CGD-O2D-CED
19	1	1014	CLA	C4B-C3B-CAB-CBB
19	1	1014	CLA	CBD-CGD-O2D-CED
19	1	1303	CLA	C3A-C2A-CAA-CBA
19	1	1303	CLA	C4B-C3B-CAB-CBB
19	1	1303	CLA	C2-C3-C5-C6
19	2	2001	CLA	C1A-C2A-CAA-CBA
19	2	2001	CLA	C3A-C2A-CAA-CBA
19	2	2001	CLA	O2A-C1-C2-C3
19	2	2002	CLA	C1A-C2A-CAA-CBA
19	2	2002	CLA	C3A-C2A-CAA-CBA
19	2	2002	CLA	C4B-C3B-CAB-CBB
19	2	2002	CLA	CAD-CBD-CGD-O1D
19	2	2002	CLA	CAD-CBD-CGD-O2D
19	2	2004	CLA	C2-C1-O2A-CGA
19	2	2006	CLA	C1A-C2A-CAA-CBA
19	2	2006	CLA	CBD-CGD-O2D-CED
19	2	2007	CLA	CBA-CGA-O2A-C1
19	2	2007	CLA	O1A-CGA-O2A-C1
19	2	2013	CLA	CBA-CGA-O2A-C1
19	2	2013	CLA	O1A-CGA-O2A-C1
19	2	2014	CLA	C1A-C2A-CAA-CBA
19	2	2014	CLA	C3A-C2A-CAA-CBA
19	2	2014	CLA	C4B-C3B-CAB-CBB
19	2	2014	CLA	CAD-CBD-CGD-O1D
19	2	2014	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	2	2014	CLA	CBD-CGD-O2D-CED
19	2	4009	CLA	C2-C1-O2A-CGA
19	2	4009	CLA	C4B-C3B-CAB-CBB
19	2	4009	CLA	CHA-CBD-CGD-O1D
19	2	4009	CLA	CHA-CBD-CGD-O2D
19	2	4009	CLA	C14-C13-C15-C16
19	3	1147	CLA	CBD-CGD-O2D-CED
19	3	2009	CLA	C1A-C2A-CAA-CBA
19	3	3007	CLA	C1A-C2A-CAA-CBA
19	3	3008	CLA	C1A-C2A-CAA-CBA
19	3	3008	CLA	C4B-C3B-CAB-CBB
19	3	3011	CLA	CHA-CBD-CGD-O1D
19	3	3011	CLA	CHA-CBD-CGD-O2D
19	3	3013	CLA	C1A-C2A-CAA-CBA
19	3	3013	CLA	C3A-C2A-CAA-CBA
19	3	3013	CLA	C4B-C3B-CAB-CBB
19	3	3013	CLA	CAD-CBD-CGD-O1D
19	3	3013	CLA	CAD-CBD-CGD-O2D
19	3	3016	CLA	O1A-CGA-O2A-C1
19	3	3016	CLA	C2B-C3B-CAB-CBB
19	3	3016	CLA	CHA-CBD-CGD-O1D
19	3	3016	CLA	CHA-CBD-CGD-O2D
19	4	1004	CLA	C2B-C3B-CAB-CBB
19	4	1004	CLA	C4C-C3C-CAC-CBC
19	4	1304	CLA	C3A-C2A-CAA-CBA
19	4	1304	CLA	C6-C7-C8-C9
19	4	1306	CLA	CHA-CBD-CGD-O1D
19	4	1306	CLA	CHA-CBD-CGD-O2D
19	4	4002	CLA	C2-C1-O2A-CGA
19	4	4003	CLA	C1A-C2A-CAA-CBA
19	4	4003	CLA	C3A-C2A-CAA-CBA
19	4	4003	CLA	CBD-CGD-O2D-CED
19	4	4003	CLA	O1D-CGD-O2D-CED
19	4	4006	CLA	CBD-CGD-O2D-CED
19	4	4014	CLA	C3A-C2A-CAA-CBA
19	4	4014	CLA	C2B-C3B-CAB-CBB
19	4	4014	CLA	C2C-C3C-CAC-CBC
19	4	4014	CLA	C4C-C3C-CAC-CBC
19	4	4014	CLA	CBD-CGD-O2D-CED
19	4	4015	CLA	C1A-C2A-CAA-CBA
19	4	4015	CLA	C4B-C3B-CAB-CBB
21	A	6002	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	A	6002	BCR	C11-C10-C9-C34
21	A	6002	BCR	C10-C11-C12-C13
21	A	6002	BCR	C18-C19-C20-C21
21	A	6002	BCR	C19-C20-C21-C22
21	A	6002	BCR	C20-C21-C22-C23
21	A	6002	BCR	C20-C21-C22-C37
21	A	6002	BCR	C21-C22-C23-C24
21	A	6002	BCR	C37-C22-C23-C24
21	A	6003	BCR	C5-C6-C7-C8
21	A	6003	BCR	C7-C8-C9-C10
21	A	6003	BCR	C7-C8-C9-C34
21	A	6003	BCR	C21-C22-C23-C24
21	A	6003	BCR	C23-C24-C25-C26
21	A	6003	BCR	C23-C24-C25-C30
21	A	6007	BCR	C21-C22-C23-C24
21	A	6007	BCR	C37-C22-C23-C24
21	A	6007	BCR	C23-C24-C25-C26
21	A	6007	BCR	C23-C24-C25-C30
21	A	6008	BCR	C5-C6-C7-C8
21	A	6008	BCR	C7-C8-C9-C10
21	A	6008	BCR	C7-C8-C9-C34
21	A	6008	BCR	C11-C12-C13-C14
21	A	6008	BCR	C17-C18-C19-C20
21	A	6008	BCR	C36-C18-C19-C20
21	A	6011	BCR	C7-C8-C9-C10
21	A	6011	BCR	C7-C8-C9-C34
21	B	6004	BCR	C7-C8-C9-C10
21	B	6004	BCR	C10-C11-C12-C13
21	B	6004	BCR	C17-C18-C19-C20
21	B	6004	BCR	C36-C18-C19-C20
21	B	6004	BCR	C23-C24-C25-C26
21	B	6004	BCR	C23-C24-C25-C30
21	B	6005	BCR	C5-C6-C7-C8
21	B	6005	BCR	C18-C19-C20-C21
21	B	6006	BCR	C11-C10-C9-C8
21	B	6006	BCR	C11-C10-C9-C34
21	B	6006	BCR	C11-C12-C13-C14
21	B	6010	BCR	C9-C10-C11-C12
21	B	6017	BCR	C5-C6-C7-C8
21	B	6017	BCR	C21-C22-C23-C24
21	B	6017	BCR	C37-C22-C23-C24
21	B	6020	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	B	6020	BCR	C11-C10-C9-C34
21	B	6020	BCR	C11-C12-C13-C14
21	B	6020	BCR	C11-C12-C13-C35
21	B	6020	BCR	C13-C14-C15-C16
21	B	6020	BCR	C37-C22-C23-C24
21	F	6014	BCR	C9-C10-C11-C12
21	F	6014	BCR	C18-C19-C20-C21
21	F	6014	BCR	C19-C20-C21-C22
21	F	6016	BCR	C11-C10-C9-C8
21	F	6016	BCR	C11-C10-C9-C34
21	F	6016	BCR	C11-C12-C13-C14
21	F	6016	BCR	C11-C12-C13-C35
21	I	6018	BCR	C21-C22-C23-C24
21	I	6021	BCR	C10-C11-C12-C13
21	I	6021	BCR	C17-C18-C19-C20
21	I	6021	BCR	C36-C18-C19-C20
21	I	6021	BCR	C21-C22-C23-C24
21	I	6021	BCR	C37-C22-C23-C24
21	J	6012	BCR	C7-C8-C9-C10
21	J	6012	BCR	C17-C18-C19-C20
21	J	6012	BCR	C18-C19-C20-C21
21	J	6012	BCR	C20-C21-C22-C23
21	J	6012	BCR	C20-C21-C22-C37
21	J	6012	BCR	C37-C22-C23-C24
21	L	6019	BCR	C11-C10-C9-C8
21	L	6019	BCR	C11-C10-C9-C34
21	L	6019	BCR	C10-C11-C12-C13
21	L	6019	BCR	C20-C21-C22-C37
21	1	6023	BCR	C1-C6-C7-C8
21	1	6023	BCR	C5-C6-C7-C8
21	1	6023	BCR	C11-C10-C9-C8
21	1	6023	BCR	C11-C10-C9-C34
21	1	6023	BCR	C10-C11-C12-C13
21	1	6023	BCR	C21-C22-C23-C24
21	1	6023	BCR	C37-C22-C23-C24
21	3	6022	BCR	C1-C6-C7-C8
21	3	6022	BCR	C5-C6-C7-C8
21	3	6022	BCR	C15-C16-C17-C18
21	3	6022	BCR	C17-C18-C19-C20
21	3	6022	BCR	C36-C18-C19-C20
21	3	6022	BCR	C18-C19-C20-C21
21	3	6022	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
21	3	6022	BCR	C20-C21-C22-C23
21	3	6022	BCR	C20-C21-C22-C37
21	3	6022	BCR	C37-C22-C23-C24
22	A	7010	LMU	O5'-C1'-O1'-C1
22	A	7010	LMU	C2-C1-O1'-C1'
22	A	7045	LMU	C2-C1-O1'-C1'
22	B	7040	LMU	C2'-C1'-O1'-C1
22	D	7050	LMU	C2B-C1B-O1B-C4'
22	E	7037	LMU	C2'-C1'-O1'-C1
22	E	7037	LMU	O5'-C1'-O1'-C1
22	E	7037	LMU	C2-C1-O1'-C1'
22	F	7036	LMU	C2B-C1B-O1B-C4'
22	F	7036	LMU	O5'-C1'-O1'-C1
22	F	7036	LMU	C2-C1-O1'-C1'
22	G	7026	LMU	C2'-C1'-O1'-C1
22	G	7026	LMU	O5'-C1'-O1'-C1
22	H	7002	LMU	C2'-C1'-O1'-C1
22	H	7002	LMU	C2-C1-O1'-C1'
22	H	7011	LMU	O5'-C1'-O1'-C1
22	H	7028	LMU	C2-C1-O1'-C1'
22	H	7030	LMU	C2-C1-O1'-C1'
22	H	7032	LMU	O5'-C1'-O1'-C1
22	H	7043	LMU	O5'-C1'-O1'-C1
22	K	7041	LMU	C2B-C1B-O1B-C4'
22	K	7042	LMU	O5'-C1'-O1'-C1
22	K	7047	LMU	C2-C1-O1'-C1'
22	L	7029	LMU	O5'-C1'-O1'-C1
22	R	7007	LMU	C2'-C1'-O1'-C1
22	R	7007	LMU	O5'-C1'-O1'-C1
22	R	7020	LMU	C2-C1-O1'-C1'
22	R	7022	LMU	O5'-C1'-O1'-C1
22	R	7022	LMU	C2-C1-O1'-C1'
22	1	7004	LMU	C2'-C1'-O1'-C1
22	1	7013	LMU	C2-C1-O1'-C1'
22	2	7006	LMU	O5'-C1'-O1'-C1
22	2	7027	LMU	O5'-C1'-O1'-C1
22	2	7031	LMU	C2B-C1B-O1B-C4'
22	2	7046	LMU	O5'-C1'-O1'-C1
22	3	7003	LMU	C2'-C1'-O1'-C1
22	3	7005	LMU	O5'-C1'-O1'-C1
22	4	7008	LMU	O5'-C1'-O1'-C1
22	4	7009	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
22	4	7009	LMU	O5'-C1'-O1'-C1
22	4	7019	LMU	O5'-C1'-O1'-C1
22	4	7034	LMU	C2'-C1'-O1'-C1
22	4	7034	LMU	O5'-C1'-O1'-C1
22	4	7053	LMU	C2'-C1'-O1'-C1
22	4	7053	LMU	O5'-C1'-O1'-C1
24	B	7101	LMG	C2-C1-O1-C7
24	B	7101	LMG	O6-C1-O1-C7
24	B	7101	LMG	C11-C10-O7-C8
22	G	7051	LMU	C3'-C4'-O1B-C1B
22	H	7002	LMU	C3'-C4'-O1B-C1B
22	1	7013	LMU	C3'-C4'-O1B-C1B
22	2	7006	LMU	C5'-C4'-O1B-C1B
19	B	1239	CLA	C4C-C3C-CAC-CBC
19	3	3016	CLA	C4C-C3C-CAC-CBC
19	4	1306	CLA	C4C-C3C-CAC-CBC
19	4	4003	CLA	C4C-C3C-CAC-CBC
19	L	1503	CLA	C2C-C3C-CAC-CBC
19	4	1004	CLA	C2C-C3C-CAC-CBC
19	A	1104	CLA	O1D-CGD-O2D-CED
19	A	1115	CLA	O1D-CGD-O2D-CED
19	A	1116	CLA	O1D-CGD-O2D-CED
19	A	1123	CLA	O1D-CGD-O2D-CED
19	A	1151	CLA	O1D-CGD-O2D-CED
19	B	1213	CLA	O1D-CGD-O2D-CED
19	B	1217	CLA	O1D-CGD-O2D-CED
19	B	1222	CLA	O1D-CGD-O2D-CED
19	H	1505	CLA	O1D-CGD-O2D-CED
19	L	1501	CLA	O1D-CGD-O2D-CED
19	R	1144	CLA	O1D-CGD-O2D-CED
19	1	1001	CLA	O1D-CGD-O2D-CED
19	1	1303	CLA	O1D-CGD-O2D-CED
19	3	3007	CLA	O1D-CGD-O2D-CED
19	4	4007	CLA	O1D-CGD-O2D-CED
22	H	7011	LMU	O5B-C1B-O1B-C4'
22	R	7007	LMU	O5B-C1B-O1B-C4'
22	3	7005	LMU	O5B-C1B-O1B-C4'
22	H	7011	LMU	C2B-C1B-O1B-C4'
22	B	7012	LMU	C3'-C4'-O1B-C1B
22	H	7043	LMU	C3'-C4'-O1B-C1B
22	K	7042	LMU	C3'-C4'-O1B-C1B
22	R	7014	LMU	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
22	R	7021	LMU	C3'-C4'-O1B-C1B
22	3	7005	LMU	C3'-C4'-O1B-C1B
22	4	7008	LMU	C5'-C4'-O1B-C1B
22	4	7034	LMU	C5'-C4'-O1B-C1B
22	4	7053	LMU	C5'-C4'-O1B-C1B
19	A	1115	CLA	C4C-C3C-CAC-CBC
19	B	1220	CLA	C4C-C3C-CAC-CBC
19	B	1224	CLA	C4C-C3C-CAC-CBC
19	1	1303	CLA	C4C-C3C-CAC-CBC
19	3	3008	CLA	C4C-C3C-CAC-CBC
19	A	1124	CLA	C2C-C3C-CAC-CBC
19	A	1125	CLA	C2C-C3C-CAC-CBC
19	B	1220	CLA	C2C-C3C-CAC-CBC
19	4	1306	CLA	C2C-C3C-CAC-CBC
19	A	1105	CLA	O1D-CGD-O2D-CED
19	A	1109	CLA	O1D-CGD-O2D-CED
19	A	1113	CLA	O1D-CGD-O2D-CED
19	A	1117	CLA	O1D-CGD-O2D-CED
19	A	1131	CLA	O1D-CGD-O2D-CED
19	A	1139	CLA	O1D-CGD-O2D-CED
19	A	1149	CLA	O1D-CGD-O2D-CED
19	B	1208	CLA	O1D-CGD-O2D-CED
19	B	1214	CLA	O1D-CGD-O2D-CED
19	B	1218	CLA	O1D-CGD-O2D-CED
19	B	1224	CLA	O1D-CGD-O2D-CED
19	B	1230	CLA	O1D-CGD-O2D-CED
19	G	1242	CLA	O1D-CGD-O2D-CED
19	L	1502	CLA	O1D-CGD-O2D-CED
19	1	1002	CLA	O1D-CGD-O2D-CED
19	1	1007	CLA	O1D-CGD-O2D-CED
19	1	1008	CLA	O1D-CGD-O2D-CED
19	1	1010	CLA	O1D-CGD-O2D-CED
19	2	2006	CLA	O1D-CGD-O2D-CED
19	2	2014	CLA	O1D-CGD-O2D-CED
19	3	1147	CLA	O1D-CGD-O2D-CED
19	4	4014	CLA	O1D-CGD-O2D-CED
19	A	1105	CLA	CBD-CGD-O2D-CED
19	A	1107	CLA	CBD-CGD-O2D-CED
19	A	1112	CLA	CBD-CGD-O2D-CED
19	A	1115	CLA	CBD-CGD-O2D-CED
19	A	1122	CLA	CBD-CGD-O2D-CED
19	A	1123	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1125	CLA	CBD-CGD-O2D-CED
19	A	1126	CLA	CBD-CGD-O2D-CED
19	A	1138	CLA	CBD-CGD-O2D-CED
19	B	1202	CLA	CBD-CGD-O2D-CED
19	B	1208	CLA	CBD-CGD-O2D-CED
19	B	1212	CLA	CBD-CGD-O2D-CED
19	B	1220	CLA	CBD-CGD-O2D-CED
19	B	1226	CLA	CBD-CGD-O2D-CED
19	B	1229	CLA	CBD-CGD-O2D-CED
19	B	1234	CLA	CBD-CGD-O2D-CED
19	H	1505	CLA	CBD-CGD-O2D-CED
19	I	1204	CLA	CBD-CGD-O2D-CED
19	K	3009	CLA	CBD-CGD-O2D-CED
19	L	1503	CLA	CBD-CGD-O2D-CED
19	1	1001	CLA	CBD-CGD-O2D-CED
19	1	1003	CLA	CBD-CGD-O2D-CED
19	1	1007	CLA	CBD-CGD-O2D-CED
19	1	1008	CLA	CBD-CGD-O2D-CED
19	1	1303	CLA	CBD-CGD-O2D-CED
19	2	2013	CLA	CBD-CGD-O2D-CED
19	2	4009	CLA	CBD-CGD-O2D-CED
19	3	3007	CLA	CBD-CGD-O2D-CED
19	4	4001	CLA	CBD-CGD-O2D-CED
19	4	4007	CLA	CBD-CGD-O2D-CED
19	4	4015	CLA	CBD-CGD-O2D-CED
22	4	7052	LMU	O5B-C1B-O1B-C4'
22	3	7005	LMU	C2B-C1B-O1B-C4'
19	A	1133	CLA	O1A-CGA-O2A-C1
19	A	9011	CLA	O1A-CGA-O2A-C1
19	B	1206	CLA	O1A-CGA-O2A-C1
19	B	1214	CLA	O1A-CGA-O2A-C1
19	B	1236	CLA	O1A-CGA-O2A-C1
19	H	1505	CLA	O1A-CGA-O2A-C1
19	R	1150	CLA	O1A-CGA-O2A-C1
19	3	3011	CLA	O1A-CGA-O2A-C1
19	1	1003	CLA	C2-C1-O2A-CGA
22	R	7022	LMU	C3'-C4'-O1B-C1B
19	A	1113	CLA	C4C-C3C-CAC-CBC
19	A	1125	CLA	C4C-C3C-CAC-CBC
19	1	1002	CLA	C4C-C3C-CAC-CBC
19	A	1115	CLA	C2C-C3C-CAC-CBC
19	A	1133	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	B	1222	CLA	C2C-C3C-CAC-CBC
19	B	1239	CLA	C2C-C3C-CAC-CBC
19	1	1303	CLA	C2C-C3C-CAC-CBC
19	2	2002	CLA	C2C-C3C-CAC-CBC
19	3	3008	CLA	C2C-C3C-CAC-CBC
19	3	3016	CLA	C2C-C3C-CAC-CBC
19	4	4003	CLA	C2C-C3C-CAC-CBC
19	A	1124	CLA	O1D-CGD-O2D-CED
19	B	1203	CLA	O1D-CGD-O2D-CED
19	B	1227	CLA	O1D-CGD-O2D-CED
19	J	1308	CLA	O1D-CGD-O2D-CED
19	1	1013	CLA	O1D-CGD-O2D-CED
22	A	7045	LMU	O5B-C1B-O1B-C4'
22	B	7038	LMU	O5B-C1B-O1B-C4'
22	E	7037	LMU	O5B-C1B-O1B-C4'
22	K	7042	LMU	O5B-C1B-O1B-C4'
22	R	7020	LMU	O5B-C1B-O1B-C4'
22	R	7024	LMU	O5B-C1B-O1B-C4'
22	1	7004	LMU	O5B-C1B-O1B-C4'
22	B	7038	LMU	C2B-C1B-O1B-C4'
22	E	7037	LMU	C2B-C1B-O1B-C4'
19	1	1010	CLA	CBA-CGA-O2A-C1
24	B	7101	LMG	C8-C9-O8-C28
19	A	1124	CLA	C4C-C3C-CAC-CBC
19	H	1145	CLA	C4C-C3C-CAC-CBC
19	2	2013	CLA	C4C-C3C-CAC-CBC
19	B	1224	CLA	C2C-C3C-CAC-CBC
19	H	1145	CLA	C2C-C3C-CAC-CBC
19	2	2013	CLA	C2C-C3C-CAC-CBC
19	A	1112	CLA	O1D-CGD-O2D-CED
19	A	1138	CLA	O1D-CGD-O2D-CED
19	B	1212	CLA	O1D-CGD-O2D-CED
19	B	1220	CLA	O1D-CGD-O2D-CED
19	J	1311	CLA	O1D-CGD-O2D-CED
19	L	1504	CLA	O1D-CGD-O2D-CED
19	1	1003	CLA	O1D-CGD-O2D-CED
19	4	4001	CLA	O1D-CGD-O2D-CED
19	A	1133	CLA	CBA-CGA-O2A-C1
19	A	9011	CLA	CBA-CGA-O2A-C1
19	B	1214	CLA	CBA-CGA-O2A-C1
19	B	1221	CLA	CBA-CGA-O2A-C1
19	B	1233	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	1236	CLA	CBA-CGA-O2A-C1
19	H	1505	CLA	CBA-CGA-O2A-C1
19	3	3011	CLA	CBA-CGA-O2A-C1
19	A	1132	CLA	CBD-CGD-O2D-CED
19	4	1306	CLA	CBD-CGD-O2D-CED
22	2	7046	LMU	O5B-C1B-O1B-C4'
19	A	1116	CLA	O1A-CGA-O2A-C1
19	A	1126	CLA	O1A-CGA-O2A-C1
19	A	1151	CLA	O1A-CGA-O2A-C1
19	A	1237	CLA	O1A-CGA-O2A-C1
19	A	9013	CLA	O1A-CGA-O2A-C1
19	B	1217	CLA	O1A-CGA-O2A-C1
19	B	1221	CLA	O1A-CGA-O2A-C1
19	B	1228	CLA	O1A-CGA-O2A-C1
19	B	9010	CLA	O1A-CGA-O2A-C1
19	J	1311	CLA	O1A-CGA-O2A-C1
19	K	1143	CLA	O1A-CGA-O2A-C1
19	1	1007	CLA	O1A-CGA-O2A-C1
19	1	1008	CLA	O1A-CGA-O2A-C1
19	2	4009	CLA	O1A-CGA-O2A-C1
19	3	3017	CLA	O1A-CGA-O2A-C1
19	4	4007	CLA	O1A-CGA-O2A-C1
19	A	1105	CLA	O1A-CGA-O2A-C1
19	1	1001	CLA	O1A-CGA-O2A-C1
19	A	1119	CLA	C4C-C3C-CAC-CBC
19	A	1133	CLA	C4C-C3C-CAC-CBC
19	B	1234	CLA	C4C-C3C-CAC-CBC
19	1	1005	CLA	C4C-C3C-CAC-CBC
19	2	2002	CLA	C4C-C3C-CAC-CBC
19	B	1218	CLA	C2C-C3C-CAC-CBC
19	3	1147	CLA	C2C-C3C-CAC-CBC
22	E	7048	LMU	C4'-C5'-C6'-O6'
22	2	7027	LMU	C4B-C5B-C6B-O6B
19	A	1107	CLA	O1D-CGD-O2D-CED
19	A	1126	CLA	O1D-CGD-O2D-CED
19	B	1202	CLA	O1D-CGD-O2D-CED
19	B	1232	CLA	O1D-CGD-O2D-CED
19	K	3009	CLA	O1D-CGD-O2D-CED
19	4	4015	CLA	O1D-CGD-O2D-CED
22	K	7041	LMU	O5B-C1B-O1B-C4'
22	K	7042	LMU	C2B-C1B-O1B-C4'
22	L	7029	LMU	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
22	A	7035	LMU	C3'-C4'-O1B-C1B
22	K	7001	LMU	C5'-C4'-O1B-C1B
22	K	7047	LMU	C5'-C4'-O1B-C1B
19	B	1222	CLA	C4C-C3C-CAC-CBC
19	B	1226	CLA	C4C-C3C-CAC-CBC
19	2	2001	CLA	C4C-C3C-CAC-CBC
19	3	1147	CLA	C4C-C3C-CAC-CBC
19	A	1113	CLA	C2C-C3C-CAC-CBC
19	A	1119	CLA	C2C-C3C-CAC-CBC
19	1	1005	CLA	C2C-C3C-CAC-CBC
19	A	1108	CLA	O1D-CGD-O2D-CED
19	A	1128	CLA	O1D-CGD-O2D-CED
19	A	1135	CLA	O1D-CGD-O2D-CED
19	B	1216	CLA	O1D-CGD-O2D-CED
19	B	1231	CLA	O1D-CGD-O2D-CED
19	4	4006	CLA	O1D-CGD-O2D-CED
22	G	7039	LMU	O5B-C1B-O1B-C4'
22	A	7045	LMU	C5'-C4'-O1B-C1B
19	A	9023	CLA	C4C-C3C-CAC-CBC
19	A	9023	CLA	C2C-C3C-CAC-CBC
19	B	1226	CLA	C2C-C3C-CAC-CBC
19	B	1234	CLA	C2C-C3C-CAC-CBC
19	1	1002	CLA	C2C-C3C-CAC-CBC
19	1	1014	CLA	C2C-C3C-CAC-CBC
19	2	2001	CLA	C2C-C3C-CAC-CBC
24	B	7101	LMG	O9-C10-O7-C8
19	B	1213	CLA	CBA-CGA-O2A-C1
19	4	4015	CLA	CBA-CGA-O2A-C1
19	B	1213	CLA	O1A-CGA-O2A-C1
22	R	7021	LMU	C4B-C5B-C6B-O6B
19	A	1103	CLA	C3-C5-C6-C7
19	A	1117	CLA	C3-C5-C6-C7
19	A	1126	CLA	C3-C5-C6-C7
19	A	1128	CLA	C3-C5-C6-C7
19	A	1131	CLA	C3-C5-C6-C7
19	A	9022	CLA	C3-C5-C6-C7
19	B	1202	CLA	C3-C5-C6-C7
19	B	1238	CLA	C3-C5-C6-C7
19	H	1505	CLA	C3-C5-C6-C7
19	J	1308	CLA	C3-C5-C6-C7
19	L	1504	CLA	C3-C5-C6-C7
19	4	1306	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	3	2009	CLA	C5-C6-C7-C8
19	B	1218	CLA	C4C-C3C-CAC-CBC
19	A	1102	CLA	O1D-CGD-O2D-CED
19	A	1126	CLA	CBA-CGA-O2A-C1
19	A	1137	CLA	CBA-CGA-O2A-C1
19	A	1237	CLA	CBA-CGA-O2A-C1
19	B	1206	CLA	CBA-CGA-O2A-C1
19	B	1209	CLA	CBA-CGA-O2A-C1
19	B	9010	CLA	CBA-CGA-O2A-C1
19	F	1305	CLA	CBA-CGA-O2A-C1
19	K	1143	CLA	CBA-CGA-O2A-C1
19	L	1503	CLA	CBA-CGA-O2A-C1
19	R	1144	CLA	CBA-CGA-O2A-C1
19	R	1150	CLA	CBA-CGA-O2A-C1
19	1	1007	CLA	CBA-CGA-O2A-C1
19	1	1008	CLA	CBA-CGA-O2A-C1
19	3	3016	CLA	CBA-CGA-O2A-C1
19	3	3017	CLA	CBA-CGA-O2A-C1
22	4	7018	LMU	O5'-C5'-C6'-O6'
22	B	7040	LMU	C3'-C4'-O1B-C1B
22	A	7044	LMU	C4B-C5B-C6B-O6B
19	A	1110	CLA	CBD-CGD-O2D-CED
19	A	1120	CLA	CBD-CGD-O2D-CED
19	A	1133	CLA	CBD-CGD-O2D-CED
19	A	1136	CLA	CBD-CGD-O2D-CED
19	A	1140	CLA	CBD-CGD-O2D-CED
19	A	9022	CLA	CBD-CGD-O2D-CED
19	A	9023	CLA	CBD-CGD-O2D-CED
19	B	1211	CLA	CBD-CGD-O2D-CED
19	H	1207	CLA	CBD-CGD-O2D-CED
19	3	2009	CLA	CBD-CGD-O2D-CED
19	3	3011	CLA	CBD-CGD-O2D-CED
19	A	1116	CLA	C4C-C3C-CAC-CBC
19	A	1137	CLA	C2C-C3C-CAC-CBC
19	A	1111	CLA	O1D-CGD-O2D-CED
19	B	1226	CLA	O1D-CGD-O2D-CED
19	H	1241	CLA	O1D-CGD-O2D-CED
19	1	1014	CLA	O1D-CGD-O2D-CED
19	4	4015	CLA	O1A-CGA-O2A-C1
19	4	4014	CLA	C2-C1-O2A-CGA
19	A	1137	CLA	C4C-C3C-CAC-CBC
19	A	1116	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	A	1149	CLA	C2C-C3C-CAC-CBC
19	1	1001	CLA	C2C-C3C-CAC-CBC
22	4	7019	LMU	O5B-C1B-O1B-C4'
19	A	1103	CLA	C4-C3-C5-C6
19	A	1141	CLA	C4-C3-C5-C6
19	B	1222	CLA	C4-C3-C5-C6
19	L	1130	CLA	C4-C3-C5-C6
19	L	1504	CLA	C4-C3-C5-C6
19	R	1144	CLA	C4-C3-C5-C6
19	1	1014	CLA	C4-C3-C5-C6
19	2	2002	CLA	C4-C3-C5-C6
19	3	2009	CLA	C4-C3-C5-C6
20	A	5001	PQN	C14-C13-C15-C16
20	B	5002	PQN	C14-C13-C15-C16
19	A	1103	CLA	C2-C3-C5-C6
19	A	1141	CLA	C2-C3-C5-C6
19	A	9022	CLA	C2-C3-C5-C6
19	B	1222	CLA	C2-C3-C5-C6
19	H	1505	CLA	C2-C3-C5-C6
19	L	1130	CLA	C2-C3-C5-C6
19	L	1504	CLA	C2-C3-C5-C6
19	R	1144	CLA	C2-C3-C5-C6
19	1	1014	CLA	C2-C3-C5-C6
19	2	2002	CLA	C2-C3-C5-C6
19	3	2009	CLA	C2-C3-C5-C6
19	A	1122	CLA	O1D-CGD-O2D-CED
19	B	9010	CLA	O1D-CGD-O2D-CED
22	R	7024	LMU	O5B-C5B-C6B-O6B
22	4	7009	LMU	O5B-C5B-C6B-O6B
19	A	1141	CLA	C2A-CAA-CBA-CGA
19	B	1211	CLA	C2A-CAA-CBA-CGA
19	B	1214	CLA	C2A-CAA-CBA-CGA
19	H	1207	CLA	C2A-CAA-CBA-CGA
19	4	4007	CLA	C3-C5-C6-C7
22	4	7019	LMU	C2B-C1B-O1B-C4'
19	A	1127	CLA	C3-C5-C6-C7
19	A	1140	CLA	C3-C5-C6-C7
19	B	1219	CLA	C3-C5-C6-C7
19	B	1234	CLA	C3-C5-C6-C7
19	B	1239	CLA	C3-C5-C6-C7
22	4	7033	LMU	C3'-C4'-O1B-C1B
19	A	1116	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	1138	CLA	CBA-CGA-O2A-C1
19	A	1149	CLA	CBA-CGA-O2A-C1
19	A	1151	CLA	CBA-CGA-O2A-C1
19	A	9013	CLA	CBA-CGA-O2A-C1
19	B	1216	CLA	CBA-CGA-O2A-C1
19	B	1217	CLA	CBA-CGA-O2A-C1
19	B	1228	CLA	CBA-CGA-O2A-C1
19	H	1241	CLA	CBA-CGA-O2A-C1
19	J	1311	CLA	CBA-CGA-O2A-C1
19	2	4009	CLA	CBA-CGA-O2A-C1
19	3	2009	CLA	CBA-CGA-O2A-C1
19	4	4007	CLA	CBA-CGA-O2A-C1
19	1	1014	CLA	C4C-C3C-CAC-CBC
22	G	7051	LMU	O5'-C5'-C6'-O6'
22	H	7002	LMU	O5B-C5B-C6B-O6B
22	R	7022	LMU	O5'-C5'-C6'-O6'
22	K	7041	LMU	C4'-C5'-C6'-O6'
22	R	7014	LMU	C4'-C5'-C6'-O6'
21	B	6020	BCR	C15-C16-C17-C18
21	I	6018	BCR	C19-C20-C21-C22
21	I	6021	BCR	C9-C10-C11-C12
21	J	6012	BCR	C19-C20-C21-C22
21	1	6023	BCR	C9-C10-C11-C12
21	3	6022	BCR	C9-C10-C11-C12
19	A	1107	CLA	O1A-CGA-O2A-C1
19	B	1216	CLA	O1A-CGA-O2A-C1
19	H	1241	CLA	O1A-CGA-O2A-C1
19	3	2009	CLA	O1A-CGA-O2A-C1
19	K	1146	CLA	C2C-C3C-CAC-CBC
19	1	1010	CLA	O1A-CGA-O2A-C1
22	E	7048	LMU	O5'-C5'-C6'-O6'
22	R	7014	LMU	O5'-C5'-C6'-O6'
22	4	7052	LMU	O5B-C5B-C6B-O6B
22	B	7038	LMU	C4B-C5B-C6B-O6B
22	K	7042	LMU	C4B-C5B-C6B-O6B
19	A	1119	CLA	C3-C5-C6-C7
19	A	1122	CLA	C3-C5-C6-C7
19	B	1208	CLA	C3-C5-C6-C7
19	B	1215	CLA	C3-C5-C6-C7
19	K	3009	CLA	C3-C5-C6-C7
19	2	2007	CLA	C3-C5-C6-C7
19	3	3016	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	A	5001	PQN	C13-C15-C16-C17
19	2	2004	CLA	CBD-CGD-O2D-CED
19	A	1125	CLA	O1D-CGD-O2D-CED
19	B	1229	CLA	O1D-CGD-O2D-CED
19	2	2013	CLA	O1D-CGD-O2D-CED
19	2	4009	CLA	O1D-CGD-O2D-CED
19	H	1207	CLA	CBA-CGA-O2A-C1
22	E	7037	LMU	O5'-C5'-C6'-O6'
22	H	7028	LMU	O5'-C5'-C6'-O6'
22	N	7049	LMU	O5B-C5B-C6B-O6B
22	R	7022	LMU	O5B-C5B-C6B-O6B
22	R	7025	LMU	O5B-C5B-C6B-O6B
22	4	7033	LMU	O5'-C5'-C6'-O6'
22	4	7053	LMU	O5B-C5B-C6B-O6B
19	A	1137	CLA	O1A-CGA-O2A-C1
19	F	1305	CLA	O1A-CGA-O2A-C1
19	L	1503	CLA	O1A-CGA-O2A-C1
22	A	7010	LMU	C4'-C5'-C6'-O6'
22	L	7029	LMU	C4B-C5B-C6B-O6B
22	4	7008	LMU	C4'-C5'-C6'-O6'
22	D	7050	LMU	O5B-C5B-C6B-O6B
22	A	7044	LMU	C3'-C4'-O1B-C1B
22	2	7046	LMU	C5'-C4'-O1B-C1B
22	B	7012	LMU	C4'-C5'-C6'-O6'
22	2	7006	LMU	C4'-C5'-C6'-O6'
22	4	7018	LMU	C4'-C5'-C6'-O6'
19	3	3016	CLA	CBD-CGD-O2D-CED
19	B	1218	CLA	CBA-CGA-O2A-C1
19	2	2007	CLA	C2C-C3C-CAC-CBC
22	G	7051	LMU	O5B-C5B-C6B-O6B
22	H	7032	LMU	O5'-C5'-C6'-O6'
22	N	7049	LMU	O5'-C5'-C6'-O6'
22	4	7019	LMU	O5'-C5'-C6'-O6'
22	H	7002	LMU	C4B-C5B-C6B-O6B
19	I	1204	CLA	O1D-CGD-O2D-CED
22	2	7006	LMU	O5B-C1B-O1B-C4'
19	2	4009	CLA	C3-C5-C6-C7
19	A	1119	CLA	CBD-CGD-O2D-CED
19	B	1209	CLA	CBD-CGD-O2D-CED
19	B	1215	CLA	CBD-CGD-O2D-CED
19	R	1150	CLA	CBD-CGD-O2D-CED
22	2	7006	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
19	B	1238	CLA	C2C-C3C-CAC-CBC
22	G	7051	LMU	C4'-C5'-C6'-O6'
22	N	7049	LMU	C4B-C5B-C6B-O6B
22	R	7024	LMU	C4B-C5B-C6B-O6B
19	A	1132	CLA	O1D-CGD-O2D-CED
19	A	1107	CLA	CBA-CGA-O2A-C1
19	A	1128	CLA	CBA-CGA-O2A-C1
19	4	4006	CLA	CBA-CGA-O2A-C1
19	A	9012	CLA	C4-C3-C5-C6
19	B	1223	CLA	C4-C3-C5-C6
19	3	3011	CLA	C4-C3-C5-C6
19	3	3016	CLA	C4-C3-C5-C6
19	A	1132	CLA	C2-C3-C5-C6
19	A	9012	CLA	C2-C3-C5-C6
19	B	1223	CLA	C2-C3-C5-C6
19	3	3016	CLA	C2-C3-C5-C6
20	A	5001	PQN	C12-C13-C15-C16
20	B	5002	PQN	C12-C13-C15-C16
19	2	2006	CLA	C15-C16-C17-C18
19	A	1149	CLA	O1A-CGA-O2A-C1
19	B	1209	CLA	O1A-CGA-O2A-C1
19	A	9013	CLA	C2C-C3C-CAC-CBC
22	H	7017	LMU	O5B-C5B-C6B-O6B
22	4	7053	LMU	C4B-C5B-C6B-O6B
19	A	1134	CLA	CBD-CGD-O2D-CED
19	B	1228	CLA	CBD-CGD-O2D-CED
19	B	1239	CLA	CBD-CGD-O2D-CED
22	A	7035	LMU	O5'-C5'-C6'-O6'
22	B	7038	LMU	O5B-C5B-C6B-O6B
22	2	7046	LMU	O5'-C5'-C6'-O6'
22	A	7023	LMU	C4B-C5B-C6B-O6B
22	A	7044	LMU	C4'-C5'-C6'-O6'
22	H	7028	LMU	C4'-C5'-C6'-O6'
19	A	1103	CLA	C2A-CAA-CBA-CGA
19	H	1505	CLA	C2A-CAA-CBA-CGA
19	J	1311	CLA	C2A-CAA-CBA-CGA
19	R	1144	CLA	C2A-CAA-CBA-CGA
19	A	1138	CLA	O1A-CGA-O2A-C1
19	H	1207	CLA	O1A-CGA-O2A-C1
24	B	7101	LMG	O10-C28-O8-C9
22	A	7010	LMU	C3'-C4'-O1B-C1B
22	A	7016	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
22	A	7023	LMU	O5'-C1'-O1'-C1
22	B	7040	LMU	O5'-C1'-O1'-C1
22	C	7015	LMU	O5'-C1'-O1'-C1
22	D	7050	LMU	O5'-C1'-O1'-C1
22	G	7051	LMU	O5'-C1'-O1'-C1
22	H	7002	LMU	O5'-C1'-O1'-C1
22	K	7041	LMU	O5'-C1'-O1'-C1
22	R	7014	LMU	O5'-C1'-O1'-C1
22	R	7024	LMU	O5'-C1'-O1'-C1
22	1	7004	LMU	O5'-C1'-O1'-C1
22	3	7003	LMU	O5'-C1'-O1'-C1
22	4	7018	LMU	O5'-C1'-O1'-C1
22	4	7052	LMU	O5'-C1'-O1'-C1
22	3	7005	LMU	C2-C3-C4-C5
22	A	7010	LMU	O5'-C5'-C6'-O6'
22	4	7008	LMU	O5'-C5'-C6'-O6'
22	R	7022	LMU	C4'-C5'-C6'-O6'
22	4	7009	LMU	C4B-C5B-C6B-O6B
22	4	7033	LMU	C4'-C5'-C6'-O6'
19	B	1234	CLA	O1D-CGD-O2D-CED
19	2	2004	CLA	CBA-CGA-O2A-C1
19	2	2012	CLA	CBA-CGA-O2A-C1
19	4	4014	CLA	CBA-CGA-O2A-C1
24	B	7101	LMG	C29-C28-O8-C9
19	A	9013	CLA	CBD-CGD-O2D-CED
19	B	1236	CLA	CBD-CGD-O2D-CED
22	A	7044	LMU	O5B-C5B-C6B-O6B
22	H	7028	LMU	O5B-C5B-C6B-O6B
22	H	7030	LMU	O5B-C5B-C6B-O6B
22	K	7041	LMU	O5'-C5'-C6'-O6'
22	2	7027	LMU	O5B-C5B-C6B-O6B
19	1	1010	CLA	C2C-C3C-CAC-CBC
22	H	7030	LMU	C3-C4-C5-C6
22	R	7025	LMU	C4B-C5B-C6B-O6B
19	A	1128	CLA	O1A-CGA-O2A-C1
22	G	7039	LMU	O5'-C5'-C6'-O6'
22	H	7011	LMU	O5'-C5'-C6'-O6'
22	H	7030	LMU	O5'-C5'-C6'-O6'
22	K	7042	LMU	O5B-C5B-C6B-O6B
22	R	7021	LMU	O5B-C5B-C6B-O6B
22	R	7024	LMU	O5'-C5'-C6'-O6'
22	3	7003	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
22	4	7019	LMU	O5B-C5B-C6B-O6B
22	L	7029	LMU	C4'-C5'-C6'-O6'
22	4	7052	LMU	C4B-C5B-C6B-O6B
22	E	7037	LMU	C1-C2-C3-C4
19	4	4002	CLA	CBD-CGD-O2D-CED
19	A	1149	CLA	C4C-C3C-CAC-CBC
22	E	7048	LMU	C3'-C4'-O1B-C1B
22	A	7010	LMU	C4B-C5B-C6B-O6B
22	A	7035	LMU	C4'-C5'-C6'-O6'
22	A	7016	LMU	C2-C3-C4-C5
22	E	7048	LMU	C5-C6-C7-C8
22	K	7001	LMU	C5-C6-C7-C8
22	R	7020	LMU	C6-C7-C8-C9
21	B	6020	BCR	C9-C10-C11-C12
21	F	6016	BCR	C15-C16-C17-C18
21	1	6023	BCR	C13-C14-C15-C16
19	2	2004	CLA	O1A-CGA-O2A-C1
19	2	2012	CLA	O1A-CGA-O2A-C1
19	4	4006	CLA	O1A-CGA-O2A-C1
19	4	4014	CLA	O1A-CGA-O2A-C1
19	A	1109	CLA	C2C-C3C-CAC-CBC
19	4	1306	CLA	O1D-CGD-O2D-CED
19	A	1110	CLA	CBA-CGA-O2A-C1
19	A	1139	CLA	CBA-CGA-O2A-C1
19	A	1140	CLA	CBA-CGA-O2A-C1
19	K	1146	CLA	CBA-CGA-O2A-C1
19	L	1501	CLA	CBA-CGA-O2A-C1
19	1	1013	CLA	CBA-CGA-O2A-C1
19	2	2001	CLA	CBA-CGA-O2A-C1
19	4	1306	CLA	CBA-CGA-O2A-C1
22	E	7037	LMU	C3-C4-C5-C6
22	H	7011	LMU	C6-C7-C8-C9
22	R	7007	LMU	C7-C8-C9-C10
22	R	7022	LMU	C11-C10-C9-C8
22	H	7030	LMU	C4B-C5B-C6B-O6B
22	4	7019	LMU	C4B-C5B-C6B-O6B
22	E	7048	LMU	C11-C10-C9-C8
22	3	7005	LMU	C4-C5-C6-C7
22	A	7044	LMU	C5'-C4'-O1B-C1B
19	A	1133	CLA	O1D-CGD-O2D-CED
19	L	1503	CLA	O1D-CGD-O2D-CED
22	B	7038	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	2	7027	LMU	C3-C4-C5-C6
19	1	1008	CLA	C2C-C3C-CAC-CBC
22	H	7017	LMU	C4B-C5B-C6B-O6B
22	H	7030	LMU	C4'-C5'-C6'-O6'
22	R	7024	LMU	C4'-C5'-C6'-O6'
22	H	7011	LMU	C11-C10-C9-C8
22	K	7042	LMU	C3-C4-C5-C6
22	1	7013	LMU	C1-C2-C3-C4
19	A	1132	CLA	C4-C3-C5-C6
19	B	1216	CLA	C4-C3-C5-C6
19	B	1216	CLA	C2-C3-C5-C6
19	A	1132	CLA	C2C-C3C-CAC-CBC
19	A	1115	CLA	C14-C13-C15-C16
19	A	1117	CLA	C6-C7-C8-C9
19	A	1123	CLA	C14-C13-C15-C16
19	A	1132	CLA	C14-C13-C15-C16
19	A	1138	CLA	C11-C10-C8-C9
19	A	1138	CLA	C14-C13-C15-C16
19	A	9013	CLA	C11-C10-C8-C9
19	A	9023	CLA	C14-C13-C15-C16
19	B	1206	CLA	C11-C10-C8-C9
19	B	1211	CLA	C14-C13-C15-C16
19	B	1220	CLA	C14-C13-C15-C16
19	B	1222	CLA	C11-C10-C8-C9
19	B	1224	CLA	C6-C7-C8-C9
19	B	1226	CLA	C11-C10-C8-C9
19	B	1229	CLA	C11-C10-C8-C9
19	B	1229	CLA	C14-C13-C15-C16
19	B	9010	CLA	C11-C12-C13-C14
19	J	1311	CLA	C11-C12-C13-C14
19	R	1150	CLA	C11-C10-C8-C9
19	R	1150	CLA	C11-C12-C13-C14
19	1	1014	CLA	C11-C12-C13-C14
19	3	2009	CLA	C6-C7-C8-C9
20	A	5001	PQN	C21-C22-C23-C24
22	E	7037	LMU	C4'-C5'-C6'-O6'
22	2	7046	LMU	C4'-C5'-C6'-O6'
22	3	7003	LMU	C4'-C5'-C6'-O6'
19	A	1136	CLA	O1D-CGD-O2D-CED
19	H	1207	CLA	O1D-CGD-O2D-CED
22	A	7010	LMU	C2'-C1'-O1'-C1
22	A	7023	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
22	C	7015	LMU	C2'-C1'-O1'-C1
22	D	7050	LMU	C2'-C1'-O1'-C1
22	G	7051	LMU	C2'-C1'-O1'-C1
22	H	7030	LMU	C2'-C1'-O1'-C1
22	H	7032	LMU	C2'-C1'-O1'-C1
22	K	7041	LMU	C2'-C1'-O1'-C1
22	R	7014	LMU	C2'-C1'-O1'-C1
22	R	7024	LMU	C2'-C1'-O1'-C1
22	R	7025	LMU	C2'-C1'-O1'-C1
22	2	7006	LMU	C2'-C1'-O1'-C1
22	4	7018	LMU	C2'-C1'-O1'-C1
22	4	7019	LMU	C2'-C1'-O1'-C1
22	4	7052	LMU	C2'-C1'-O1'-C1
22	H	7032	LMU	C5-C6-C7-C8
19	3	2009	CLA	O1D-CGD-O2D-CED
19	2	2006	CLA	CBA-CGA-O2A-C1
19	A	1140	CLA	O1A-CGA-O2A-C1
22	G	7051	LMU	C4B-C5B-C6B-O6B
22	H	7028	LMU	C4B-C5B-C6B-O6B
19	B	1211	CLA	O1D-CGD-O2D-CED
21	A	6003	BCR	C11-C12-C13-C35
21	A	6003	BCR	C37-C22-C23-C24
21	A	6008	BCR	C11-C12-C13-C35
21	A	6008	BCR	C37-C22-C23-C24
21	B	6004	BCR	C7-C8-C9-C34
21	B	6004	BCR	C11-C12-C13-C35
21	B	6004	BCR	C37-C22-C23-C24
21	B	6006	BCR	C11-C12-C13-C35
21	B	6006	BCR	C37-C22-C23-C24
21	B	6017	BCR	C7-C8-C9-C34
21	F	6014	BCR	C37-C22-C23-C24
21	I	6018	BCR	C11-C12-C13-C35
21	I	6018	BCR	C37-C22-C23-C24
21	J	6012	BCR	C7-C8-C9-C34
21	J	6012	BCR	C36-C18-C19-C20
21	L	6019	BCR	C7-C8-C9-C34
21	3	6022	BCR	C11-C12-C13-C35
22	A	7023	LMU	O5B-C5B-C6B-O6B
22	B	7012	LMU	O5'-C5'-C6'-O6'
22	L	7029	LMU	O5B-C5B-C6B-O6B
22	L	7029	LMU	O5'-C5'-C6'-O6'
21	A	6003	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	6004	BCR	C21-C22-C23-C24
21	B	6006	BCR	C21-C22-C23-C24
21	B	6017	BCR	C7-C8-C9-C10
21	B	6020	BCR	C21-C22-C23-C24
21	F	6014	BCR	C21-C22-C23-C24
21	J	6012	BCR	C21-C22-C23-C24
21	L	6019	BCR	C7-C8-C9-C10
21	L	6019	BCR	C21-C22-C23-C24
21	3	6022	BCR	C11-C12-C13-C14
21	3	6022	BCR	C21-C22-C23-C24
19	A	1116	CLA	C3-C5-C6-C7
22	G	7039	LMU	C11-C10-C9-C8
22	H	7043	LMU	C7-C8-C9-C10
22	2	7027	LMU	C1-C2-C3-C4
22	A	7023	LMU	O5'-C5'-C6'-O6'
22	4	7018	LMU	O5B-C5B-C6B-O6B
19	A	1106	CLA	C5-C6-C7-C8
19	K	1146	CLA	C4C-C3C-CAC-CBC
22	G	7039	LMU	C4'-C5'-C6'-O6'
22	H	7011	LMU	C4'-C5'-C6'-O6'
22	R	7022	LMU	C4B-C5B-C6B-O6B
22	3	7005	LMU	O1'-C1-C2-C3
19	1	1001	CLA	C4C-C3C-CAC-CBC
19	A	9013	CLA	C8-C10-C11-C12
19	L	1130	CLA	C5-C6-C7-C8
22	4	7052	LMU	C5'-C4'-O1B-C1B
19	A	1103	CLA	C2-C1-O2A-CGA
19	A	1123	CLA	C2-C1-O2A-CGA
19	A	1124	CLA	C2-C1-O2A-CGA
19	A	1139	CLA	C2-C1-O2A-CGA
19	1	1007	CLA	C2-C1-O2A-CGA
19	A	1110	CLA	O1D-CGD-O2D-CED
19	A	9023	CLA	O1D-CGD-O2D-CED
19	2	2004	CLA	O1D-CGD-O2D-CED
19	3	3011	CLA	O1D-CGD-O2D-CED
22	R	7007	LMU	C4B-C5B-C6B-O6B
19	A	1141	CLA	CBD-CGD-O2D-CED
22	A	7044	LMU	C2-C3-C4-C5
22	2	7031	LMU	C2-C3-C4-C5
22	4	7019	LMU	C7-C8-C9-C10
19	A	1138	CLA	C13-C15-C16-C17
19	B	1223	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	C	7015	LMU	O5'-C5'-C6'-O6'
22	R	7007	LMU	O5B-C5B-C6B-O6B
19	B	1220	CLA	C3-C5-C6-C7
19	B	1226	CLA	C3-C5-C6-C7
19	B	1238	CLA	C4C-C3C-CAC-CBC
19	A	1140	CLA	O1D-CGD-O2D-CED
19	A	1139	CLA	O1A-CGA-O2A-C1
19	4	1306	CLA	O1A-CGA-O2A-C1
22	R	7025	LMU	O1'-C1-C2-C3
19	A	1127	CLA	CBD-CGD-O2D-CED
22	H	7017	LMU	O5'-C5'-C6'-O6'
22	H	7032	LMU	C4'-C5'-C6'-O6'
19	A	1106	CLA	C12-C13-C15-C16
19	A	9011	CLA	C12-C13-C15-C16
19	B	1211	CLA	C11-C10-C8-C7
19	B	1220	CLA	C11-C12-C13-C15
19	L	1130	CLA	C12-C13-C15-C16
19	2	2014	CLA	C11-C12-C13-C15
19	3	3011	CLA	C11-C10-C8-C7
19	4	1304	CLA	C12-C13-C15-C16
22	H	7028	LMU	O1'-C1-C2-C3
19	A	1107	CLA	C5-C6-C7-C8
21	F	6016	BCR	C9-C10-C11-C12
21	L	6019	BCR	C15-C16-C17-C18
19	A	1107	CLA	C2C-C3C-CAC-CBC
22	R	7021	LMU	O5'-C5'-C6'-O6'
19	A	9022	CLA	O1D-CGD-O2D-CED
22	H	7043	LMU	C4B-C5B-C6B-O6B
22	K	7042	LMU	C4'-C5'-C6'-O6'
19	A	9011	CLA	C3-C5-C6-C7
19	B	1224	CLA	C8-C10-C11-C12
19	B	1214	CLA	C10-C11-C12-C13
22	1	7013	LMU	O1'-C1-C2-C3
19	A	1110	CLA	O1A-CGA-O2A-C1
19	K	1146	CLA	O1A-CGA-O2A-C1
19	L	1501	CLA	O1A-CGA-O2A-C1
19	2	2001	CLA	O1A-CGA-O2A-C1
19	A	1120	CLA	O1D-CGD-O2D-CED
19	A	1109	CLA	C5-C6-C7-C8
19	B	1220	CLA	C13-C15-C16-C17
19	J	1311	CLA	C8-C10-C11-C12
19	L	1130	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	3	3016	CLA	C13-C15-C16-C17
20	B	5002	PQN	C15-C16-C17-C18
20	B	5002	PQN	C18-C20-C21-C22
20	B	5002	PQN	C20-C21-C22-C23
19	A	1105	CLA	C2A-CAA-CBA-CGA
19	A	1112	CLA	C2A-CAA-CBA-CGA
19	A	1115	CLA	C2A-CAA-CBA-CGA
19	A	1116	CLA	C2A-CAA-CBA-CGA
19	A	1122	CLA	C2A-CAA-CBA-CGA
19	A	1124	CLA	C2A-CAA-CBA-CGA
19	A	1131	CLA	C2A-CAA-CBA-CGA
19	A	1133	CLA	C2A-CAA-CBA-CGA
19	A	1138	CLA	C2A-CAA-CBA-CGA
19	A	1139	CLA	C2A-CAA-CBA-CGA
19	A	9011	CLA	C2A-CAA-CBA-CGA
19	B	1210	CLA	C2A-CAA-CBA-CGA
19	B	1218	CLA	C2A-CAA-CBA-CGA
19	B	1219	CLA	C2A-CAA-CBA-CGA
19	B	1226	CLA	C2A-CAA-CBA-CGA
19	B	1227	CLA	C2A-CAA-CBA-CGA
19	B	1238	CLA	C2A-CAA-CBA-CGA
19	L	1130	CLA	C2A-CAA-CBA-CGA
19	2	2006	CLA	C2A-CAA-CBA-CGA
21	A	6008	BCR	C10-C11-C12-C13
21	B	6006	BCR	C10-C11-C12-C13
21	B	6020	BCR	C10-C11-C12-C13
21	I	6018	BCR	C10-C11-C12-C13
19	A	1119	CLA	C10-C11-C12-C13
19	A	1126	CLA	C15-C16-C17-C18
19	A	1140	CLA	C10-C11-C12-C13
19	A	9011	CLA	C10-C11-C12-C13
19	B	1206	CLA	C5-C6-C7-C8
19	B	1206	CLA	C15-C16-C17-C18
19	B	1214	CLA	C8-C10-C11-C12
19	B	1216	CLA	C10-C11-C12-C13
19	B	1229	CLA	C10-C11-C12-C13
19	B	1234	CLA	C5-C6-C7-C8
19	B	1235	CLA	C8-C10-C11-C12
19	B	1238	CLA	C10-C11-C12-C13
19	I	1204	CLA	C8-C10-C11-C12
19	L	1130	CLA	C13-C15-C16-C17
19	1	1007	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	4	4006	CLA	C5-C6-C7-C8
20	A	5001	PQN	C20-C21-C22-C23
22	3	7005	LMU	O5'-C5'-C6'-O6'
19	B	1218	CLA	O1A-CGA-O2A-C1
19	L	1502	CLA	C2C-C3C-CAC-CBC
22	E	7048	LMU	O5'-C1'-O1'-C1
22	H	7030	LMU	O5'-C1'-O1'-C1
22	R	7025	LMU	O5'-C1'-O1'-C1
22	G	7026	LMU	O5'-C5'-C6'-O6'
22	2	7046	LMU	O1'-C1-C2-C3
22	N	7049	LMU	C4'-C5'-C6'-O6'
19	A	1117	CLA	C10-C11-C12-C13
19	A	1127	CLA	C5-C6-C7-C8
19	A	1138	CLA	C15-C16-C17-C18
19	A	1140	CLA	C5-C6-C7-C8
19	A	1140	CLA	C13-C15-C16-C17
19	A	1237	CLA	C8-C10-C11-C12
19	A	9011	CLA	C5-C6-C7-C8
19	A	9023	CLA	C10-C11-C12-C13
19	A	9023	CLA	C13-C15-C16-C17
19	B	1206	CLA	C10-C11-C12-C13
19	B	1209	CLA	C5-C6-C7-C8
19	B	1211	CLA	C5-C6-C7-C8
19	B	1229	CLA	C13-C15-C16-C17
19	B	1235	CLA	C13-C15-C16-C17
19	B	1239	CLA	C15-C16-C17-C18
19	H	1207	CLA	C8-C10-C11-C12
19	I	1204	CLA	C5-C6-C7-C8
19	R	1150	CLA	C8-C10-C11-C12
22	K	7042	LMU	C5-C6-C7-C8
19	1	1013	CLA	O1A-CGA-O2A-C1
22	G	7026	LMU	C1-C2-C3-C4
19	B	1215	CLA	C10-C11-C12-C13
22	K	7042	LMU	O1'-C1-C2-C3
22	R	7007	LMU	C3'-C4'-O1B-C1B
19	A	9013	CLA	C4C-C3C-CAC-CBC
22	A	7023	LMU	O1'-C1-C2-C3
19	A	1132	CLA	C3-C5-C6-C7
22	4	7009	LMU	C5'-C4'-O1B-C1B
19	A	1123	CLA	C10-C11-C12-C13
19	A	9023	CLA	C15-C16-C17-C18
19	B	1205	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	B	1210	CLA	C15-C16-C17-C18
19	B	1226	CLA	C5-C6-C7-C8
19	2	2006	CLA	O1A-CGA-O2A-C1
19	3	3011	CLA	C2-C3-C5-C6
22	H	7032	LMU	O1'-C1-C2-C3
22	A	7010	LMU	C5'-C4'-O1B-C1B
19	B	1215	CLA	O1D-CGD-O2D-CED
19	A	1104	CLA	C5-C6-C7-C8
19	B	1219	CLA	C5-C6-C7-C8
19	B	1222	CLA	C5-C6-C7-C8
19	3	3011	CLA	C8-C10-C11-C12
19	A	1125	CLA	CBA-CGA-O2A-C1
19	B	1215	CLA	CBA-CGA-O2A-C1
19	G	1242	CLA	CBA-CGA-O2A-C1
19	3	1147	CLA	CBA-CGA-O2A-C1
19	A	1109	CLA	C3-C5-C6-C7
19	B	1221	CLA	C3-C5-C6-C7
19	4	4006	CLA	C3-C5-C6-C7
22	2	7006	LMU	O1'-C1-C2-C3
22	4	7033	LMU	O1'-C1-C2-C3
21	A	6011	BCR	C19-C20-C21-C22
21	F	6016	BCR	C13-C14-C15-C16
21	I	6018	BCR	C9-C10-C11-C12
21	1	6023	BCR	C19-C20-C21-C22
19	A	1141	CLA	C5-C6-C7-C8
19	A	1134	CLA	C2A-CAA-CBA-CGA
19	B	1222	CLA	C2A-CAA-CBA-CGA
19	3	2009	CLA	C2A-CAA-CBA-CGA
19	2	2014	CLA	CBA-CGA-O2A-C1
19	2	2007	CLA	C4C-C3C-CAC-CBC
19	A	1117	CLA	C5-C6-C7-C8
19	A	1117	CLA	C15-C16-C17-C18
19	A	9013	CLA	C15-C16-C17-C18
19	B	1202	CLA	C15-C16-C17-C18
19	B	1225	CLA	C10-C11-C12-C13
19	2	4009	CLA	C10-C11-C12-C13
19	3	3016	CLA	C5-C6-C7-C8
19	4	1304	CLA	C8-C10-C11-C12
19	B	1221	CLA	CBD-CGD-O2D-CED
19	B	1228	CLA	O1D-CGD-O2D-CED
19	A	1132	CLA	C8-C10-C11-C12
19	B	1205	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	B	1226	CLA	C15-C16-C17-C18
19	1	1014	CLA	C10-C11-C12-C13
19	A	1109	CLA	C10-C11-C12-C13
19	A	1119	CLA	C5-C6-C7-C8
19	A	1131	CLA	C15-C16-C17-C18
19	A	1136	CLA	C5-C6-C7-C8
19	A	1237	CLA	C15-C16-C17-C18
19	A	9022	CLA	C13-C15-C16-C17
19	B	1206	CLA	C8-C10-C11-C12
19	B	1210	CLA	C10-C11-C12-C13
19	B	1211	CLA	C10-C11-C12-C13
19	R	1150	CLA	C10-C11-C12-C13
19	2	4009	CLA	C8-C10-C11-C12
19	1	1003	CLA	CBA-CGA-O2A-C1
19	R	1144	CLA	C8-C10-C11-C12
22	N	7049	LMU	C1-C2-C3-C4
19	R	1150	CLA	O1D-CGD-O2D-CED
19	4	4002	CLA	O1D-CGD-O2D-CED
19	A	1123	CLA	C15-C16-C17-C18
19	2	4009	CLA	C5-C6-C7-C8
19	A	1123	CLA	C11-C10-C8-C9
22	A	7044	LMU	O5'-C5'-C6'-O6'
19	B	1239	CLA	O1D-CGD-O2D-CED
22	A	7016	LMU	C4-C5-C6-C7
19	B	1201	CLA	C2C-C3C-CAC-CBC
22	A	7035	LMU	C2'-C1'-O1'-C1
22	H	7043	LMU	C2'-C1'-O1'-C1
22	N	7049	LMU	C2'-C1'-O1'-C1
22	3	7005	LMU	C2'-C1'-O1'-C1
22	1	7004	LMU	C4'-C5'-C6'-O6'
19	3	3016	CLA	O1D-CGD-O2D-CED
19	A	1135	CLA	CBA-CGA-O2A-C1
19	A	1109	CLA	C16-C17-C18-C19
19	A	1136	CLA	C16-C17-C18-C19
20	B	5002	PQN	C26-C27-C28-C30
19	A	9013	CLA	C10-C11-C12-C13
22	H	7032	LMU	C5'-C4'-O1B-C1B
19	B	1215	CLA	O1A-CGA-O2A-C1
22	H	7030	LMU	C2B-C1B-O1B-C4'
21	A	6003	BCR	C11-C10-C9-C34
21	B	6004	BCR	C11-C10-C9-C34
21	B	6005	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
21	B	6006	BCR	C20-C21-C22-C37
21	B	6010	BCR	C11-C10-C9-C34
21	B	6020	BCR	C20-C21-C22-C37
21	F	6016	BCR	C20-C21-C22-C37
21	I	6021	BCR	C20-C21-C22-C37
21	3	6022	BCR	C11-C10-C9-C34
19	1	1010	CLA	C4C-C3C-CAC-CBC
22	A	7010	LMU	O5B-C5B-C6B-O6B
22	K	7001	LMU	O5'-C5'-C6'-O6'
22	R	7025	LMU	C6-C7-C8-C9
21	A	6007	BCR	C7-C8-C9-C34
21	A	6007	BCR	C11-C12-C13-C35
21	A	6007	BCR	C36-C18-C19-C20
21	L	6019	BCR	C37-C22-C23-C24
22	4	7052	LMU	O1'-C1-C2-C3
21	A	6007	BCR	C7-C8-C9-C10
21	A	6007	BCR	C17-C18-C19-C20
21	A	6008	BCR	C21-C22-C23-C24
22	H	7043	LMU	C6-C7-C8-C9
22	R	7024	LMU	O1'-C1-C2-C3
19	A	1123	CLA	C2A-CAA-CBA-CGA
19	A	1129	CLA	C2A-CAA-CBA-CGA
19	B	1231	CLA	C2A-CAA-CBA-CGA
19	G	1242	CLA	C2A-CAA-CBA-CGA
19	J	1308	CLA	C2A-CAA-CBA-CGA
19	K	1142	CLA	C2A-CAA-CBA-CGA
19	K	1146	CLA	C2A-CAA-CBA-CGA
19	1	1013	CLA	C2A-CAA-CBA-CGA
19	3	3013	CLA	C2A-CAA-CBA-CGA
19	A	9012	CLA	C13-C15-C16-C17
19	4	1304	CLA	C5-C6-C7-C8
19	A	1107	CLA	O2A-C1-C2-C3
19	A	1125	CLA	O2A-C1-C2-C3
19	A	1139	CLA	O2A-C1-C2-C3
19	K	1143	CLA	O2A-C1-C2-C3
21	A	6003	BCR	C9-C10-C11-C12
19	A	1237	CLA	C16-C17-C18-C20
19	B	1234	CLA	C11-C12-C13-C14
19	H	1145	CLA	C16-C17-C18-C19
19	I	1204	CLA	C11-C12-C13-C14
19	3	3011	CLA	C16-C17-C18-C19
20	A	5001	PQN	C26-C27-C28-C30

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Mol	Chain	Res	Type	Atoms
22	B	7038	LMU	O1'-C1-C2-C3
19	B	1209	CLA	O1D-CGD-O2D-CED
19	A	1125	CLA	O1A-CGA-O2A-C1
19	A	1111	CLA	C3-C5-C6-C7
19	A	1124	CLA	C3-C5-C6-C7
19	4	1004	CLA	C3-C5-C6-C7
22	F	7036	LMU	O5'-C5'-C6'-O6'
19	A	1131	CLA	C13-C15-C16-C17
20	A	5001	PQN	C25-C26-C27-C28
21	A	6003	BCR	C11-C10-C9-C8
21	B	6004	BCR	C11-C10-C9-C8
21	B	6006	BCR	C20-C21-C22-C23
21	B	6010	BCR	C11-C10-C9-C8
21	B	6020	BCR	C20-C21-C22-C23
21	I	6021	BCR	C20-C21-C22-C23
21	L	6019	BCR	C20-C21-C22-C23
21	3	6022	BCR	C11-C10-C9-C8
22	N	7049	LMU	O5'-C1'-O1'-C1
19	B	1211	CLA	C13-C15-C16-C17
22	A	7016	LMU	C11-C10-C9-C8
19	B	1236	CLA	O1D-CGD-O2D-CED
22	H	7002	LMU	O5'-C5'-C6'-O6'
22	L	7029	LMU	O5B-C1B-O1B-C4'
22	H	7011	LMU	O1'-C1-C2-C3
19	A	1119	CLA	O1D-CGD-O2D-CED
19	A	1123	CLA	CBA-CGA-O2A-C1
22	R	7020	LMU	C1-C2-C3-C4
22	R	7024	LMU	C1-C2-C3-C4
19	B	1210	CLA	C5-C6-C7-C8
22	H	7032	LMU	C3'-C4'-O1B-C1B
22	R	7007	LMU	C5'-C4'-O1B-C1B
19	J	1311	CLA	C2C-C3C-CAC-CBC
19	A	9022	CLA	C2-C1-O2A-CGA
19	B	1229	CLA	C2-C1-O2A-CGA
19	3	3013	CLA	C2-C1-O2A-CGA
19	A	1106	CLA	C16-C17-C18-C19
19	A	1127	CLA	C6-C7-C8-C9
19	B	1235	CLA	C16-C17-C18-C19
19	B	1238	CLA	C16-C17-C18-C19
19	H	1207	CLA	C16-C17-C18-C20
19	I	1204	CLA	C11-C12-C13-C15
19	2	2007	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
19	3	3011	CLA	C16-C17-C18-C20
19	3	3016	CLA	C16-C17-C18-C20
19	4	4006	CLA	C6-C7-C8-C9
22	G	7051	LMU	C1-C2-C3-C4
22	H	7002	LMU	C1-C2-C3-C4
22	H	7011	LMU	C1-C2-C3-C4
19	A	1103	CLA	C13-C15-C16-C17
19	3	3013	CLA	C5-C6-C7-C8
22	F	7036	LMU	O5B-C5B-C6B-O6B
22	C	7015	LMU	C7-C8-C9-C10
22	C	7015	LMU	C11-C10-C9-C8
22	3	7005	LMU	C7-C8-C9-C10
22	4	7052	LMU	C3-C4-C5-C6
22	D	7050	LMU	C4'-C5'-C6'-O6'
22	R	7021	LMU	C1-C2-C3-C4
22	A	7035	LMU	C6-C7-C8-C9
22	E	7048	LMU	C2-C3-C4-C5
22	2	7046	LMU	C6-C7-C8-C9
22	4	7008	LMU	C3-C4-C5-C6
24	B	7101	LMG	C33-C34-C35-C36
19	A	1119	CLA	C13-C15-C16-C17
19	A	1128	CLA	C13-C15-C16-C17
19	A	9011	CLA	C8-C10-C11-C12
19	H	1145	CLA	C8-C10-C11-C12
22	K	7041	LMU	C4-C5-C6-C7
22	3	7005	LMU	C5-C6-C7-C8
22	H	7030	LMU	C4-C5-C6-C7
22	R	7014	LMU	C2-C3-C4-C5
22	R	7024	LMU	C2-C3-C4-C5
22	1	7013	LMU	C5-C6-C7-C8
22	2	7031	LMU	C3-C4-C5-C6
22	4	7034	LMU	C3-C4-C5-C6
22	G	7026	LMU	C2-C1-O1'-C1'
19	2	2007	CLA	CBD-CGD-O2D-CED
19	2	2012	CLA	CBD-CGD-O2D-CED
22	K	7042	LMU	C6-C7-C8-C9
22	N	7049	LMU	C11-C10-C9-C8
22	3	7003	LMU	C4-C5-C6-C7
19	B	1203	CLA	C13-C15-C16-C17
19	H	1505	CLA	C5-C6-C7-C8
19	A	1101	CLA	C4B-C3B-CAB-CBB
19	A	1108	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A	1121	CLA	C4B-C3B-CAB-CBB
19	A	1122	CLA	C4B-C3B-CAB-CBB
19	A	1123	CLA	C4B-C3B-CAB-CBB
19	B	1214	CLA	C4B-C3B-CAB-CBB
19	B	1230	CLA	C4B-C3B-CAB-CBB
19	H	1505	CLA	C4B-C3B-CAB-CBB
19	1	1003	CLA	C4B-C3B-CAB-CBB
19	2	2001	CLA	C4B-C3B-CAB-CBB
19	2	2006	CLA	C4B-C3B-CAB-CBB
19	2	2007	CLA	C4B-C3B-CAB-CBB
19	4	1306	CLA	C4B-C3B-CAB-CBB
19	4	4001	CLA	C4B-C3B-CAB-CBB
22	H	7032	LMU	C4-C5-C6-C7
22	4	7019	LMU	C3-C4-C5-C6
19	A	1109	CLA	C16-C17-C18-C20
19	A	1128	CLA	C16-C17-C18-C19
19	A	1237	CLA	C16-C17-C18-C19
19	A	9012	CLA	C16-C17-C18-C19
19	A	9012	CLA	C16-C17-C18-C20
19	B	1211	CLA	C16-C17-C18-C19
19	B	1229	CLA	C16-C17-C18-C20
19	H	1145	CLA	C16-C17-C18-C20
19	4	4006	CLA	C6-C7-C8-C10
19	A	1134	CLA	O1D-CGD-O2D-CED
19	B	1223	CLA	C2A-CAA-CBA-CGA
19	A	1111	CLA	C5-C6-C7-C8
19	B	1223	CLA	C8-C10-C11-C12
19	R	1150	CLA	C5-C6-C7-C8
22	F	7036	LMU	C11-C10-C9-C8
19	R	1150	CLA	C6-C7-C8-C10
19	1	1014	CLA	C6-C7-C8-C10
22	A	7045	LMU	C6-C7-C8-C9
24	B	7101	LMG	C32-C33-C34-C35
22	4	7052	LMU	C3'-C4'-O1B-C1B
19	L	1148	CLA	CBA-CGA-O2A-C1
19	4	4015	CLA	C2C-C3C-CAC-CBC
19	B	9010	CLA	C10-C11-C12-C13
22	B	7040	LMU	C1-C2-C3-C4
22	B	7040	LMU	O5B-C5B-C6B-O6B
22	A	7010	LMU	C5-C6-C7-C8
22	D	7050	LMU	C6-C7-C8-C9
22	K	7042	LMU	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	1	7004	LMU	C5-C6-C7-C8
22	1	7013	LMU	C6-C7-C8-C9
19	G	1242	CLA	O1A-CGA-O2A-C1
19	A	1110	CLA	C3-C5-C6-C7
19	A	1104	CLA	C3A-C2A-CAA-CBA
19	A	1107	CLA	C3A-C2A-CAA-CBA
19	A	1111	CLA	C3A-C2A-CAA-CBA
19	A	1112	CLA	C3A-C2A-CAA-CBA
19	A	1113	CLA	C3A-C2A-CAA-CBA
19	A	1125	CLA	C3A-C2A-CAA-CBA
19	A	1132	CLA	C3A-C2A-CAA-CBA
19	A	1139	CLA	C3A-C2A-CAA-CBA
19	B	1206	CLA	C3A-C2A-CAA-CBA
19	B	1210	CLA	C3A-C2A-CAA-CBA
19	B	1212	CLA	C3A-C2A-CAA-CBA
19	B	1213	CLA	C3A-C2A-CAA-CBA
19	F	1305	CLA	C3A-C2A-CAA-CBA
19	L	1130	CLA	C3A-C2A-CAA-CBA
19	L	1148	CLA	C3A-C2A-CAA-CBA
19	L	1502	CLA	C3A-C2A-CAA-CBA
19	R	1144	CLA	C3A-C2A-CAA-CBA
19	1	1003	CLA	C3A-C2A-CAA-CBA
19	1	1007	CLA	C3A-C2A-CAA-CBA
19	2	2006	CLA	C3A-C2A-CAA-CBA
19	2	4009	CLA	C3A-C2A-CAA-CBA
19	3	2009	CLA	C3A-C2A-CAA-CBA
19	4	4006	CLA	C3A-C2A-CAA-CBA
22	A	7044	LMU	C5-C6-C7-C8
22	C	7015	LMU	C6-C7-C8-C9
24	B	7101	LMG	C35-C36-C37-C38
22	A	7010	LMU	C1-C2-C3-C4
22	1	7013	LMU	C3-C4-C5-C6
19	B	1203	CLA	C10-C11-C12-C13
20	B	5002	PQN	C23-C25-C26-C27
22	F	7036	LMU	C4'-C5'-C6'-O6'
19	A	9013	CLA	O1D-CGD-O2D-CED
21	B	6005	BCR	C19-C20-C21-C22
21	B	6017	BCR	C13-C14-C15-C16
19	A	1124	CLA	C16-C17-C18-C19
19	A	1128	CLA	C16-C17-C18-C20
19	B	1234	CLA	C11-C12-C13-C15
19	L	1148	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	K	7042	LMU	O5'-C5'-C6'-O6'
22	4	7052	LMU	O5'-C5'-C6'-O6'
22	4	7008	LMU	C1-C2-C3-C4
22	4	7009	LMU	C1-C2-C3-C4
19	2	2014	CLA	O1A-CGA-O2A-C1
22	A	7035	LMU	C11-C10-C9-C8
22	4	7034	LMU	C4-C5-C6-C7
22	N	7049	LMU	C7-C8-C9-C10
24	B	7101	LMG	C37-C38-C39-C40
19	B	1223	CLA	CBA-CGA-O2A-C1
22	D	7050	LMU	C4B-C5B-C6B-O6B
22	G	7026	LMU	C3-C4-C5-C6
22	L	7029	LMU	C11-C10-C9-C8
22	2	7006	LMU	C7-C8-C9-C10
22	2	7027	LMU	C2-C3-C4-C5
19	B	1216	CLA	C5-C6-C7-C8
19	B	1225	CLA	C5-C6-C7-C8
22	E	7037	LMU	C11-C10-C9-C8
22	G	7051	LMU	C6-C7-C8-C9
22	H	7017	LMU	C6-C7-C8-C9
22	L	7029	LMU	C7-C8-C9-C10
22	R	7007	LMU	C11-C10-C9-C8
22	4	7018	LMU	C4-C5-C6-C7
22	4	7052	LMU	C5-C6-C7-C8
19	A	1135	CLA	O1A-CGA-O2A-C1
19	1	1003	CLA	O1A-CGA-O2A-C1
22	R	7021	LMU	O1'-C1-C2-C3
22	H	7011	LMU	C5'-C4'-O1B-C1B
22	N	7049	LMU	C3'-C4'-O1B-C1B
24	B	7101	LMG	C17-C18-C19-C20
22	A	7010	LMU	C4-C5-C6-C7
22	4	7018	LMU	C2-C3-C4-C5
22	2	7046	LMU	C1-C2-C3-C4
22	R	7014	LMU	C4B-C5B-C6B-O6B
22	4	7018	LMU	C7-C8-C9-C10
19	H	1207	CLA	C16-C17-C18-C19
22	E	7037	LMU	O5B-C5B-C6B-O6B
22	1	7013	LMU	O5'-C5'-C6'-O6'
19	A	1106	CLA	C2B-C3B-CAB-CBB
19	A	1109	CLA	C2B-C3B-CAB-CBB
19	A	1121	CLA	C2B-C3B-CAB-CBB
19	A	1135	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A	1138	CLA	C2B-C3B-CAB-CBB
19	A	1140	CLA	C2B-C3B-CAB-CBB
19	B	1225	CLA	C2B-C3B-CAB-CBB
19	B	1227	CLA	C2B-C3B-CAB-CBB
19	B	1236	CLA	C2B-C3B-CAB-CBB
19	B	1238	CLA	C2B-C3B-CAB-CBB
19	B	9010	CLA	C2B-C3B-CAB-CBB
19	F	1305	CLA	C2B-C3B-CAB-CBB
19	3	3017	CLA	C2B-C3B-CAB-CBB
19	4	4002	CLA	C2B-C3B-CAB-CBB
19	4	4007	CLA	C2B-C3B-CAB-CBB
21	A	6002	BCR	C23-C24-C25-C26
21	A	6002	BCR	C23-C24-C25-C30
21	A	6003	BCR	C1-C6-C7-C8
21	A	6007	BCR	C1-C6-C7-C8
21	A	6008	BCR	C1-C6-C7-C8
21	A	6008	BCR	C23-C24-C25-C26
21	A	6008	BCR	C23-C24-C25-C30
21	A	6011	BCR	C1-C6-C7-C8
21	A	6011	BCR	C5-C6-C7-C8
21	A	6011	BCR	C23-C24-C25-C26
21	A	6011	BCR	C23-C24-C25-C30
21	B	6005	BCR	C1-C6-C7-C8
21	B	6010	BCR	C1-C6-C7-C8
21	B	6010	BCR	C5-C6-C7-C8
21	B	6017	BCR	C1-C6-C7-C8
21	F	6014	BCR	C1-C6-C7-C8
21	F	6014	BCR	C5-C6-C7-C8
21	I	6018	BCR	C1-C6-C7-C8
21	I	6018	BCR	C5-C6-C7-C8
21	J	6012	BCR	C1-C6-C7-C8
19	B	1221	CLA	C5-C6-C7-C8
22	A	7016	LMU	C5-C6-C7-C8
19	A	1109	CLA	CBA-CGA-O2A-C1
19	B	1226	CLA	CBA-CGA-O2A-C1
19	L	1504	CLA	CBA-CGA-O2A-C1
19	B	1202	CLA	C10-C11-C12-C13
19	H	1145	CLA	C3-C5-C6-C7
19	2	2006	CLA	C3-C5-C6-C7
22	A	7045	LMU	C2-C3-C4-C5
22	2	7046	LMU	C2-C3-C4-C5
22	A	7045	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
19	A	1110	CLA	C2A-CAA-CBA-CGA
19	B	1228	CLA	C2A-CAA-CBA-CGA
19	A	1119	CLA	C8-C10-C11-C12
19	B	9010	CLA	C5-C6-C7-C8
22	R	7007	LMU	C9-C10-C11-C12
22	A	7045	LMU	C11-C10-C9-C8
19	A	1123	CLA	O1A-CGA-O2A-C1
19	F	1302	CLA	C2C-C3C-CAC-CBC
22	A	7016	LMU	O1'-C1-C2-C3
22	R	7007	LMU	C2-C3-C4-C5
22	E	7048	LMU	C5'-C4'-O1B-C1B
19	A	1141	CLA	C2C-C3C-CAC-CBC
19	3	3017	CLA	C2C-C3C-CAC-CBC
22	4	7034	LMU	C2-C3-C4-C5
21	B	6010	BCR	C10-C11-C12-C13
21	B	6017	BCR	C18-C19-C20-C21
19	A	1132	CLA	C13-C15-C16-C17
19	A	1127	CLA	C6-C7-C8-C10
19	2	2007	CLA	C16-C17-C18-C19
22	A	7045	LMU	C5-C6-C7-C8
22	H	7017	LMU	C7-C8-C9-C10
22	K	7047	LMU	C6-C7-C8-C9
22	N	7049	LMU	C6-C7-C8-C9
19	B	1202	CLA	CBA-CGA-O2A-C1
19	B	1210	CLA	CBA-CGA-O2A-C1
19	A	1109	CLA	C6-C7-C8-C9
19	A	1125	CLA	C14-C13-C15-C16
19	B	1235	CLA	C11-C12-C13-C14
22	A	7010	LMU	C7-C8-C9-C10
22	B	7038	LMU	C11-C10-C9-C8
22	F	7036	LMU	C2-C3-C4-C5
22	H	7032	LMU	C7-C8-C9-C10
22	K	7001	LMU	C7-C8-C9-C10
22	4	7008	LMU	C5-C6-C7-C8
19	B	1203	CLA	C8-C10-C11-C12
19	J	1308	CLA	C5-C6-C7-C8
19	1	1008	CLA	C4C-C3C-CAC-CBC
22	A	7023	LMU	C4-C5-C6-C7
22	K	7001	LMU	C6-C7-C8-C9
22	4	7009	LMU	C6-C7-C8-C9
22	4	7009	LMU	C3'-C4'-O1B-C1B
22	R	7007	LMU	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	H	7028	LMU	C2-C3-C4-C5
22	H	7028	LMU	C2'-C1'-O1'-C1
22	2	7031	LMU	C2'-C1'-O1'-C1
22	4	7008	LMU	C2'-C1'-O1'-C1
19	B	1238	CLA	C8-C10-C11-C12
19	K	3009	CLA	C13-C15-C16-C17
22	A	7023	LMU	C3-C4-C5-C6
22	H	7017	LMU	C11-C10-C9-C8
19	A	1110	CLA	C5-C6-C7-C8
22	E	7037	LMU	C7-C8-C9-C10
22	4	7033	LMU	C5'-C4'-O1B-C1B
22	4	7019	LMU	C6-C7-C8-C9
22	R	7022	LMU	O1'-C1-C2-C3
19	B	1211	CLA	C3-C5-C6-C7
22	K	7001	LMU	C1-C2-C3-C4
21	A	6007	BCR	C19-C20-C21-C22
19	B	1238	CLA	C16-C17-C18-C20
19	3	3016	CLA	C16-C17-C18-C19
19	4	1306	CLA	C6-C7-C8-C10
22	B	7040	LMU	C11-C10-C9-C8
22	N	7049	LMU	C2-C3-C4-C5
19	4	1306	CLA	C5-C6-C7-C8
22	K	7041	LMU	C3-C4-C5-C6
22	K	7042	LMU	C11-C10-C9-C8
22	K	7042	LMU	C9-C10-C11-C12
22	4	7053	LMU	C11-C10-C9-C8
22	2	7031	LMU	C5-C6-C7-C8
19	B	1223	CLA	O1A-CGA-O2A-C1
21	B	6010	BCR	C36-C18-C19-C20
22	G	7026	LMU	C6-C7-C8-C9
22	1	7004	LMU	C7-C8-C9-C10
22	3	7003	LMU	C11-C10-C9-C8
21	B	6004	BCR	C11-C12-C13-C14
22	K	7001	LMU	C11-C10-C9-C8
22	4	7033	LMU	C6-C7-C8-C9
19	J	1311	CLA	C14-C13-C15-C16
19	A	1117	CLA	C16-C17-C18-C19
19	B	1229	CLA	C16-C17-C18-C19
22	A	7035	LMU	C4-C5-C6-C7
22	A	7035	LMU	C7-C8-C9-C10
22	2	7027	LMU	C4-C5-C6-C7
24	B	7101	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	1205	CLA	C4-C3-C5-C6
19	1	1007	CLA	C4-C3-C5-C6
22	H	7017	LMU	C4-C5-C6-C7
22	H	7028	LMU	C6-C7-C8-C9
24	B	7101	LMG	C40-C41-C42-C43
19	H	1145	CLA	C15-C16-C17-C18
22	A	7044	LMU	C3-C4-C5-C6
22	R	7021	LMU	C7-C8-C9-C10
22	L	7029	LMU	C1-C2-C3-C4
22	A	7010	LMU	C6-C7-C8-C9
19	B	1203	CLA	C15-C16-C17-C18
19	B	1224	CLA	C10-C11-C12-C13
22	A	7016	LMU	C1-C2-C3-C4
22	A	7023	LMU	C7-C8-C9-C10
22	L	7029	LMU	C6-C7-C8-C9
22	1	7004	LMU	C2-C3-C4-C5
19	A	1115	CLA	C5-C6-C7-C8
19	A	1128	CLA	C8-C10-C11-C12
19	B	1226	CLA	C8-C10-C11-C12
19	A	1136	CLA	C16-C17-C18-C20
19	A	1109	CLA	C4C-C3C-CAC-CBC
19	B	1226	CLA	O1A-CGA-O2A-C1
22	D	7050	LMU	O5'-C5'-C6'-O6'
22	N	7049	LMU	C5-C6-C7-C8
22	G	7039	LMU	C1-C2-C3-C4
19	A	1103	CLA	C15-C16-C17-C18
19	A	1125	CLA	C8-C10-C11-C12
19	A	9012	CLA	C15-C16-C17-C18
19	3	3016	CLA	C8-C10-C11-C12
22	B	7038	LMU	O5'-C5'-C6'-O6'
22	R	7020	LMU	O5'-C5'-C6'-O6'
22	4	7052	LMU	C2B-C1B-O1B-C4'
19	A	1132	CLA	C4C-C3C-CAC-CBC
22	G	7039	LMU	C5-C6-C7-C8
22	1	7004	LMU	C11-C10-C9-C8
22	H	7017	LMU	C4'-C5'-C6'-O6'
19	B	1238	CLA	CBA-CGA-O2A-C1
19	B	1210	CLA	O1A-CGA-O2A-C1
22	A	7044	LMU	O1'-C1-C2-C3
22	R	7014	LMU	C11-C10-C9-C8
22	4	7008	LMU	C4-C5-C6-C7
22	4	7034	LMU	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	A	9013	CLA	C13-C15-C16-C17
21	A	6002	BCR	C9-C10-C11-C12
22	B	7040	LMU	O5'-C5'-C6'-O6'
22	2	7031	LMU	O5'-C5'-C6'-O6'
19	B	1211	CLA	C16-C17-C18-C20
19	B	1216	CLA	C8-C10-C11-C12
19	B	1235	CLA	C15-C16-C17-C18
22	A	7016	LMU	C6-C7-C8-C9
22	A	7044	LMU	C11-C10-C9-C8
22	K	7047	LMU	C2-C3-C4-C5
22	2	7046	LMU	C4-C5-C6-C7
22	H	7028	LMU	C7-C8-C9-C10
19	A	1131	CLA	C4-C3-C5-C6
19	L	1148	CLA	C4-C3-C5-C6
19	B	1205	CLA	C2-C3-C5-C6
19	F	1305	CLA	C2-C3-C5-C6
22	B	7040	LMU	C5'-C4'-O1B-C1B
19	A	1135	CLA	C2A-CAA-CBA-CGA
19	A	1140	CLA	C2A-CAA-CBA-CGA
19	B	1201	CLA	C2A-CAA-CBA-CGA
19	4	1004	CLA	C2A-CAA-CBA-CGA
19	A	1137	CLA	CBD-CGD-O2D-CED
19	A	1132	CLA	CBA-CGA-O2A-C1
22	R	7025	LMU	O5'-C5'-C6'-O6'
22	3	7005	LMU	O5B-C5B-C6B-O6B
22	G	7039	LMU	C2-C3-C4-C5
22	4	7033	LMU	C11-C10-C9-C8
19	A	1123	CLA	C5-C6-C7-C8
19	B	1208	CLA	C5-C6-C7-C8
22	R	7025	LMU	C9-C10-C11-C12
22	R	7024	LMU	C5'-C4'-O1B-C1B
22	4	7034	LMU	C1-C2-C3-C4
22	4	7053	LMU	C1-C2-C3-C4
22	2	7046	LMU	C11-C10-C9-C8
24	B	7101	LMG	C15-C16-C17-C18
19	A	9022	CLA	C16-C17-C18-C19
19	3	3013	CLA	C16-C17-C18-C20
22	K	7047	LMU	O5B-C5B-C6B-O6B
19	L	1148	CLA	O1A-CGA-O2A-C1
19	L	1504	CLA	O1A-CGA-O2A-C1
19	A	1106	CLA	C3-C5-C6-C7
19	A	1101	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A	1102	CLA	C1A-C2A-CAA-CBA
19	A	1111	CLA	C1A-C2A-CAA-CBA
19	A	1125	CLA	C1A-C2A-CAA-CBA
19	A	1134	CLA	C1A-C2A-CAA-CBA
19	A	1151	CLA	C1A-C2A-CAA-CBA
19	A	9011	CLA	C1A-C2A-CAA-CBA
19	A	9022	CLA	C1A-C2A-CAA-CBA
19	B	1212	CLA	C1A-C2A-CAA-CBA
19	B	1213	CLA	C1A-C2A-CAA-CBA
19	B	1224	CLA	C1A-C2A-CAA-CBA
19	B	1233	CLA	C1A-C2A-CAA-CBA
19	B	1236	CLA	C1A-C2A-CAA-CBA
19	B	1239	CLA	C1A-C2A-CAA-CBA
19	J	1311	CLA	C1A-C2A-CAA-CBA
19	K	3009	CLA	C1A-C2A-CAA-CBA
19	1	1003	CLA	C1A-C2A-CAA-CBA
19	1	1303	CLA	C1A-C2A-CAA-CBA
19	2	4009	CLA	C1A-C2A-CAA-CBA
19	4	1304	CLA	C1A-C2A-CAA-CBA
19	4	4006	CLA	C1A-C2A-CAA-CBA
19	4	4014	CLA	C1A-C2A-CAA-CBA
19	A	1129	CLA	CBA-CGA-O2A-C1
22	L	7029	LMU	C2-C3-C4-C5
22	2	7046	LMU	C7-C8-C9-C10
22	H	7028	LMU	C5-C6-C7-C8
22	4	7052	LMU	C6-C7-C8-C9
19	A	1109	CLA	C8-C10-C11-C12
19	2	2004	CLA	C2C-C3C-CAC-CBC
22	H	7030	LMU	O5B-C1B-O1B-C4'
19	A	1115	CLA	C12-C13-C15-C16
19	A	1123	CLA	C11-C12-C13-C15
19	A	1126	CLA	C6-C7-C8-C10
19	A	1132	CLA	C11-C12-C13-C15
19	A	1138	CLA	C12-C13-C15-C16
19	A	1141	CLA	C11-C10-C8-C7
19	A	9013	CLA	C12-C13-C15-C16
19	B	1203	CLA	C12-C13-C15-C16
19	B	1205	CLA	C11-C10-C8-C7
19	B	1206	CLA	C11-C10-C8-C7
19	B	1206	CLA	C12-C13-C15-C16
19	B	1216	CLA	C11-C12-C13-C15
19	B	1222	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	B	1226	CLA	C6-C7-C8-C10
19	B	1234	CLA	C6-C7-C8-C10
19	B	9010	CLA	C11-C10-C8-C7
19	H	1145	CLA	C12-C13-C15-C16
19	H	1207	CLA	C12-C13-C15-C16
19	K	3009	CLA	C11-C10-C8-C7
19	K	3009	CLA	C12-C13-C15-C16
19	R	1150	CLA	C11-C10-C8-C7
19	1	1014	CLA	C11-C12-C13-C15
19	2	2006	CLA	C11-C10-C8-C7
19	2	2014	CLA	C11-C10-C8-C7
19	3	3013	CLA	C11-C12-C13-C15
19	3	3016	CLA	C11-C10-C8-C7
22	2	7027	LMU	C7-C8-C9-C10
19	B	1209	CLA	C6-C7-C8-C10
22	4	7009	LMU	O5'-C5'-C6'-O6'
22	4	7018	LMU	C11-C10-C9-C8
19	3	3007	CLA	C3A-C2A-CAA-CBA
22	A	7045	LMU	C3-C4-C5-C6
19	3	3013	CLA	C13-C15-C16-C17
22	2	7006	LMU	C5-C6-C7-C8
19	B	1202	CLA	O1A-CGA-O2A-C1
22	A	7016	LMU	C7-C8-C9-C10
19	A	1141	CLA	O1D-CGD-O2D-CED
19	A	1106	CLA	C2A-CAA-CBA-CGA
19	L	1502	CLA	C2A-CAA-CBA-CGA
19	L	1503	CLA	C2A-CAA-CBA-CGA
19	A	1109	CLA	C14-C13-C15-C16
19	A	1123	CLA	C11-C12-C13-C14
19	A	9013	CLA	C14-C13-C15-C16
19	B	1203	CLA	C14-C13-C15-C16
19	B	1216	CLA	C11-C10-C8-C9
19	B	1225	CLA	C6-C7-C8-C9
19	B	1229	CLA	C11-C12-C13-C14
19	K	3009	CLA	C11-C12-C13-C14
19	K	3009	CLA	C14-C13-C15-C16
19	2	2006	CLA	C11-C12-C13-C14
19	2	2014	CLA	C11-C10-C8-C9
19	3	3011	CLA	C11-C10-C8-C9
19	3	3013	CLA	C11-C12-C13-C14
19	4	1304	CLA	C14-C13-C15-C16
22	2	7006	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
21	B	6006	BCR	C19-C20-C21-C22
22	4	7018	LMU	C1-C2-C3-C4
22	B	7040	LMU	C4-C5-C6-C7
19	B	1239	CLA	CBA-CGA-O2A-C1
22	G	7026	LMU	C2-C3-C4-C5
22	H	7011	LMU	O5B-C5B-C6B-O6B
22	K	7001	LMU	O5B-C5B-C6B-O6B
22	N	7049	LMU	C5'-C4'-O1B-C1B
22	A	7023	LMU	C4'-C5'-C6'-O6'
22	E	7048	LMU	O1'-C1-C2-C3
22	F	7036	LMU	C2'-C1'-O1'-C1
22	2	7027	LMU	C2'-C1'-O1'-C1
19	1	1007	CLA	C14-C13-C15-C16
24	B	7101	LMG	O1-C7-C8-C9
19	B	1211	CLA	C8-C10-C11-C12
19	B	1239	CLA	C10-C11-C12-C13
22	E	7037	LMU	O1'-C1-C2-C3
19	A	1120	CLA	CBA-CGA-O2A-C1
19	B	1219	CLA	CBA-CGA-O2A-C1
19	K	3009	CLA	CBA-CGA-O2A-C1
19	4	4002	CLA	CBA-CGA-O2A-C1
19	A	1117	CLA	C16-C17-C18-C20
19	A	1138	CLA	C16-C17-C18-C19
19	B	1209	CLA	C6-C7-C8-C9
19	B	1235	CLA	C16-C17-C18-C20
19	3	3013	CLA	C16-C17-C18-C19
22	4	7009	LMU	C5-C6-C7-C8
22	H	7017	LMU	C1-C2-C3-C4
22	G	7039	LMU	C5'-C4'-O1B-C1B
22	R	7025	LMU	C3-C4-C5-C6
21	F	6014	BCR	C11-C10-C9-C34
19	L	1148	CLA	C5-C6-C7-C8
19	3	3011	CLA	C5-C6-C7-C8
19	A	1109	CLA	O1A-CGA-O2A-C1
19	F	1305	CLA	C4-C3-C5-C6
19	A	1125	CLA	C2-C3-C5-C6
19	A	1131	CLA	C2-C3-C5-C6
19	L	1148	CLA	C2-C3-C5-C6
22	G	7039	LMU	C3'-C4'-O1B-C1B
19	3	3013	CLA	C10-C11-C12-C13
21	A	6002	BCR	C7-C8-C9-C34
21	B	6010	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	I	6018	BCR	C36-C18-C19-C20
21	I	6021	BCR	C7-C8-C9-C34
22	C	7015	LMU	C5-C6-C7-C8
22	R	7025	LMU	C4-C5-C6-C7
19	B	1225	CLA	C16-C17-C18-C20
22	2	7031	LMU	C4-C5-C6-C7
22	3	7005	LMU	C6-C7-C8-C9
21	A	6002	BCR	C7-C8-C9-C10
21	I	6018	BCR	C11-C12-C13-C14
21	I	6018	BCR	C17-C18-C19-C20
21	I	6021	BCR	C7-C8-C9-C10
21	1	6023	BCR	C7-C8-C9-C10
19	A	1129	CLA	O1A-CGA-O2A-C1
19	B	1238	CLA	O1A-CGA-O2A-C1
19	K	3009	CLA	O1A-CGA-O2A-C1
19	H	1145	CLA	C13-C15-C16-C17
19	3	3013	CLA	C15-C16-C17-C18
22	A	7045	LMU	C7-C8-C9-C10
22	R	7024	LMU	C7-C8-C9-C10
19	B	1225	CLA	C2A-CAA-CBA-CGA
19	A	1123	CLA	C3-C5-C6-C7
22	R	7014	LMU	O1'-C1-C2-C3
22	B	7038	LMU	C3-C4-C5-C6
22	1	7004	LMU	C3-C4-C5-C6
22	G	7051	LMU	C7-C8-C9-C10
22	H	7002	LMU	C6-C7-C8-C9
19	H	1145	CLA	CBA-CGA-O2A-C1
19	A	1237	CLA	O2A-C1-C2-C3
19	A	9013	CLA	O2A-C1-C2-C3
19	B	1206	CLA	O2A-C1-C2-C3
24	B	7101	LMG	C13-C14-C15-C16
22	B	7038	LMU	C5-C6-C7-C8
22	R	7020	LMU	C11-C10-C9-C8
22	2	7027	LMU	C5-C6-C7-C8
22	4	7009	LMU	C2-C3-C4-C5
22	K	7041	LMU	O1'-C1-C2-C3
19	A	1132	CLA	O1A-CGA-O2A-C1
21	B	6005	BCR	C20-C21-C22-C23
22	R	7024	LMU	C5-C6-C7-C8
19	A	1106	CLA	C15-C16-C17-C18
19	A	9023	CLA	CBA-CGA-O2A-C1
19	1	1002	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	B	7101	LMG	C39-C40-C41-C42
22	A	7023	LMU	C2-C3-C4-C5
22	H	7032	LMU	C11-C10-C9-C8
22	K	7041	LMU	C6-C7-C8-C9
22	K	7047	LMU	C7-C8-C9-C10
22	3	7003	LMU	C2-C3-C4-C5
22	H	7002	LMU	C11-C10-C9-C8
22	A	7045	LMU	C1-C2-C3-C4
22	H	7002	LMU	C9-C10-C11-C12
22	2	7006	LMU	C9-C10-C11-C12
22	G	7039	LMU	C4-C5-C6-C7
22	R	7007	LMU	C5-C6-C7-C8
19	B	1201	CLA	C4C-C3C-CAC-CBC
19	A	1141	CLA	C3-C5-C6-C7
19	R	1150	CLA	C3-C5-C6-C7
19	1	1007	CLA	C3-C5-C6-C7
22	4	7053	LMU	C2-C3-C4-C5
22	A	7044	LMU	C9-C10-C11-C12
22	G	7026	LMU	C4B-C5B-C6B-O6B
22	G	7039	LMU	C9-C10-C11-C12
22	4	7033	LMU	C2-C3-C4-C5
22	3	7003	LMU	C4B-C5B-C6B-O6B
22	G	7026	LMU	C9-C10-C11-C12
22	H	7043	LMU	C9-C10-C11-C12
19	2	2014	CLA	C8-C10-C11-C12
19	A	1111	CLA	C6-C7-C8-C9
19	A	1107	CLA	C4C-C3C-CAC-CBC
22	R	7024	LMU	C3'-C4'-O1B-C1B
22	K	7047	LMU	C4-C5-C6-C7
22	4	7008	LMU	C2-C3-C4-C5
19	B	1221	CLA	C6-C7-C8-C9
22	G	7051	LMU	C9-C10-C11-C12
19	A	1132	CLA	C10-C11-C12-C13
19	B	1224	CLA	C5-C6-C7-C8
19	2	2006	CLA	C10-C11-C12-C13
19	A	1110	CLA	C4-C3-C5-C6
19	A	1125	CLA	C4-C3-C5-C6
19	B	1209	CLA	C4-C3-C5-C6
22	4	7034	LMU	C4B-C5B-C6B-O6B
22	H	7002	LMU	C4-C5-C6-C7
22	R	7022	LMU	C2-C3-C4-C5
22	4	7034	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	7044	LMU	C2-C1-O1'-C1'
22	E	7048	LMU	C2-C1-O1'-C1'
22	G	7039	LMU	C2-C1-O1'-C1'
22	H	7011	LMU	C2-C1-O1'-C1'
22	K	7042	LMU	C2-C1-O1'-C1'
22	L	7029	LMU	C2-C1-O1'-C1'
22	N	7049	LMU	C2-C1-O1'-C1'
22	R	7007	LMU	C2-C1-O1'-C1'
22	R	7021	LMU	C2-C1-O1'-C1'
22	R	7025	LMU	C2-C1-O1'-C1'
22	2	7006	LMU	C2-C1-O1'-C1'
22	2	7031	LMU	C2-C1-O1'-C1'
22	2	7046	LMU	C2-C1-O1'-C1'
22	3	7005	LMU	C2-C1-O1'-C1'
22	4	7052	LMU	C2-C1-O1'-C1'
22	A	7044	LMU	C1-C2-C3-C4
19	A	1126	CLA	C6-C7-C8-C9
19	A	1128	CLA	C11-C10-C8-C9
19	A	1132	CLA	C11-C12-C13-C14
19	A	9013	CLA	C6-C7-C8-C9
19	B	1203	CLA	C6-C7-C8-C9
19	B	1206	CLA	C14-C13-C15-C16
19	B	1214	CLA	C11-C10-C8-C9
19	B	1216	CLA	C11-C12-C13-C14
19	B	1224	CLA	C11-C10-C8-C9
19	B	1225	CLA	C11-C12-C13-C14
19	B	1226	CLA	C6-C7-C8-C9
19	B	1234	CLA	C6-C7-C8-C9
19	H	1207	CLA	C14-C13-C15-C16
19	K	3009	CLA	C11-C10-C8-C9
19	2	2006	CLA	C6-C7-C8-C9
19	2	2014	CLA	C11-C12-C13-C14
19	3	3016	CLA	C11-C10-C8-C9
19	4	1304	CLA	C11-C12-C13-C14
19	A	1103	CLA	C5-C6-C7-C8
19	B	1203	CLA	C4B-C3B-CAB-CBB
19	B	1210	CLA	C4B-C3B-CAB-CBB
19	F	1302	CLA	C4B-C3B-CAB-CBB
19	1	1002	CLA	C4B-C3B-CAB-CBB
19	4	4007	CLA	C4B-C3B-CAB-CBB
19	A	9022	CLA	C15-C16-C17-C18
19	B	1226	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	2	2007	CLA	C13-C15-C16-C17
22	3	7003	LMU	C9-C10-C11-C12
19	A	1120	CLA	O1A-CGA-O2A-C1
22	L	7029	LMU	C2'-C1'-O1'-C1
22	2	7031	LMU	C9-C10-C11-C12
22	B	7012	LMU	C4B-C5B-C6B-O6B
22	R	7021	LMU	C4'-C5'-C6'-O6'
22	E	7037	LMU	C9-C10-C11-C12
19	A	1101	CLA	CAA-CBA-CGA-O2A
19	3	3008	CLA	CAA-CBA-CGA-O2A
19	A	1132	CLA	C12-C13-C15-C16
19	A	1136	CLA	C12-C13-C15-C16
19	B	1202	CLA	C6-C7-C8-C10
19	B	1203	CLA	C6-C7-C8-C10
19	B	1211	CLA	C6-C7-C8-C10
19	B	1214	CLA	C11-C10-C8-C7
19	B	1216	CLA	C11-C10-C8-C7
19	B	1220	CLA	C6-C7-C8-C10
19	B	1223	CLA	C11-C12-C13-C15
19	B	1225	CLA	C6-C7-C8-C10
19	B	1225	CLA	C11-C12-C13-C15
19	B	1238	CLA	C11-C10-C8-C7
19	B	1239	CLA	C12-C13-C15-C16
19	J	1311	CLA	C11-C12-C13-C15
19	K	3009	CLA	C11-C12-C13-C15
19	2	2006	CLA	C11-C12-C13-C15
19	2	2007	CLA	C11-C10-C8-C7
19	2	4009	CLA	C12-C13-C15-C16
19	B	1223	CLA	C13-C15-C16-C17
19	B	9010	CLA	C8-C10-C11-C12
22	R	7020	LMU	C9-C10-C11-C12
22	H	7032	LMU	C4B-C5B-C6B-O6B
19	A	1124	CLA	C16-C17-C18-C20
19	A	1138	CLA	C16-C17-C18-C20
22	K	7047	LMU	C9-C10-C11-C12
19	A	1110	CLA	C3A-C2A-CAA-CBA
19	A	1120	CLA	C3A-C2A-CAA-CBA
19	A	1134	CLA	C3A-C2A-CAA-CBA
19	B	1202	CLA	C3A-C2A-CAA-CBA
19	B	1222	CLA	C3A-C2A-CAA-CBA
19	B	1226	CLA	C4-C3-C5-C6
19	L	1503	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	L	1502	CLA	C4C-C3C-CAC-CBC
19	A	1112	CLA	C2C-C3C-CAC-CBC
22	A	7010	LMU	C2B-C1B-O1B-C4'
19	1	1014	CLA	C8-C10-C11-C12
21	A	6008	BCR	C19-C20-C21-C22
21	F	6016	BCR	C19-C20-C21-C22
21	1	6023	BCR	C7-C8-C9-C34
22	1	7004	LMU	O5'-C5'-C6'-O6'
22	3	7003	LMU	O5B-C5B-C6B-O6B
22	R	7014	LMU	C9-C10-C11-C12
19	B	1233	CLA	C4-C3-C5-C6
19	1	1303	CLA	C4-C3-C5-C6
19	B	1219	CLA	O1A-CGA-O2A-C1
19	B	1239	CLA	O1A-CGA-O2A-C1
22	H	7030	LMU	C7-C8-C9-C10
22	4	7033	LMU	C9-C10-C11-C12
19	3	3011	CLA	C10-C11-C12-C13
22	A	7045	LMU	C9-C10-C11-C12
22	C	7015	LMU	C9-C10-C11-C12
22	1	7013	LMU	C9-C10-C11-C12
22	2	7046	LMU	C9-C10-C11-C12
22	C	7015	LMU	C3-C4-C5-C6
22	3	7003	LMU	C5-C6-C7-C8
19	A	1103	CLA	C16-C17-C18-C19
19	A	1103	CLA	C16-C17-C18-C20
19	A	1119	CLA	C16-C17-C18-C20
19	4	1306	CLA	C6-C7-C8-C9
19	B	1220	CLA	C5-C6-C7-C8
19	A	9023	CLA	O1A-CGA-O2A-C1
22	B	7040	LMU	C5-C6-C7-C8
19	A	1132	CLA	C5-C6-C7-C8
19	4	4002	CLA	O1A-CGA-O2A-C1
22	H	7043	LMU	O5'-C5'-C6'-O6'
19	A	1131	CLA	C16-C17-C18-C19
22	F	7036	LMU	C5-C6-C7-C8
22	4	7018	LMU	C4B-C5B-C6B-O6B
22	4	7052	LMU	C4'-C5'-C6'-O6'
19	B	1230	CLA	C2B-C3B-CAB-CBB
21	B	6017	BCR	C23-C24-C25-C26
21	F	6014	BCR	C23-C24-C25-C30
21	I	6021	BCR	C5-C6-C7-C8
21	L	6019	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	1	6023	BCR	C23-C24-C25-C30
22	4	7019	LMU	C4'-C5'-C6'-O6'
19	A	1109	CLA	C13-C15-C16-C17
19	B	1203	CLA	C5-C6-C7-C8
22	R	7025	LMU	C1-C2-C3-C4
22	A	7045	LMU	C4-C5-C6-C7
22	R	7014	LMU	C5-C6-C7-C8
19	A	1106	CLA	C13-C15-C16-C17
19	A	1140	CLA	C15-C16-C17-C18
22	R	7021	LMU	C4-C5-C6-C7
22	R	7022	LMU	C9-C10-C11-C12
19	A	1149	CLA	CAA-CBA-CGA-O2A
19	A	1127	CLA	C2A-CAA-CBA-CGA
19	1	1002	CLA	O1A-CGA-O2A-C1
22	1	7004	LMU	C3'-C4'-O1B-C1B
19	B	1225	CLA	C3-C5-C6-C7
19	K	1143	CLA	C2C-C3C-CAC-CBC
19	A	1127	CLA	O1D-CGD-O2D-CED
19	2	2012	CLA	O1D-CGD-O2D-CED
19	2	2014	CLA	C12-C13-C15-C16
22	E	7048	LMU	C6-C7-C8-C9
21	3	6022	BCR	C10-C11-C12-C13
19	B	1238	CLA	C5-C6-C7-C8
19	4	4003	CLA	C5-C6-C7-C8
19	A	1110	CLA	C2-C3-C5-C6
19	B	1226	CLA	C2-C3-C5-C6
22	A	7023	LMU	C1-C2-C3-C4
22	2	7046	LMU	C3'-C4'-O1B-C1B
19	1	1014	CLA	CBA-CGA-O2A-C1
19	A	1125	CLA	C6-C7-C8-C9
19	A	1136	CLA	C14-C13-C15-C16
19	B	1202	CLA	C6-C7-C8-C9
19	B	1202	CLA	C11-C10-C8-C9
19	B	1211	CLA	C6-C7-C8-C9
19	B	1238	CLA	C11-C10-C8-C9
19	2	2007	CLA	C11-C10-C8-C9
19	2	2007	CLA	C14-C13-C15-C16
24	B	7101	LMG	C41-C42-C43-C44
22	R	7021	LMU	C9-C10-C11-C12
19	A	1106	CLA	C16-C17-C18-C20
22	A	7044	LMU	C6-C7-C8-C9
22	E	7037	LMU	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	R	7022	LMU	C2'-C1'-O1'-C1
22	A	7035	LMU	C5-C6-C7-C8
22	R	7020	LMU	C7-C8-C9-C10
22	3	7003	LMU	O1'-C1-C2-C3
19	A	1124	CLA	C10-C11-C12-C13
19	B	1215	CLA	C4-C3-C5-C6
21	A	6008	BCR	C13-C14-C15-C16
21	B	6017	BCR	C19-C20-C21-C22
19	B	1209	CLA	C2-C3-C5-C6
22	R	7007	LMU	O1'-C1-C2-C3
21	I	6018	BCR	C11-C10-C9-C34
19	A	1111	CLA	CBA-CGA-O2A-C1
19	A	1119	CLA	CBA-CGA-O2A-C1
19	A	9022	CLA	C16-C17-C18-C20
19	B	1225	CLA	C16-C17-C18-C19
19	A	1103	CLA	C11-C12-C13-C15
19	A	1106	CLA	C11-C10-C8-C7
19	A	1117	CLA	C12-C13-C15-C16
19	A	1125	CLA	C6-C7-C8-C10
19	A	1128	CLA	C6-C7-C8-C10
19	A	1131	CLA	C11-C10-C8-C7
19	A	9012	CLA	C6-C7-C8-C10
19	A	9013	CLA	C11-C10-C8-C7
19	B	1211	CLA	C12-C13-C15-C16
19	B	1239	CLA	C11-C12-C13-C15
19	2	2006	CLA	C6-C7-C8-C10
19	2	2007	CLA	C12-C13-C15-C16
19	3	3013	CLA	C11-C10-C8-C7
19	4	1304	CLA	C11-C12-C13-C15
19	A	9012	CLA	C5-C6-C7-C8
21	A	6007	BCR	C11-C12-C13-C14
19	4	1004	CLA	CBA-CGA-O2A-C1
19	H	1145	CLA	O1A-CGA-O2A-C1
19	1	1014	CLA	O1A-CGA-O2A-C1
22	4	7052	LMU	C2-C3-C4-C5
19	A	9022	CLA	C2A-CAA-CBA-CGA
19	4	1304	CLA	C16-C17-C18-C20
19	B	9010	CLA	C4-C3-C5-C6
19	H	1207	CLA	C4-C3-C5-C6
19	3	1147	CLA	O1A-CGA-O2A-C1
19	B	1211	CLA	C2-C3-C5-C6
22	B	7038	LMU	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
19	A	9011	CLA	C13-C15-C16-C17
19	B	1230	CLA	O2A-C1-C2-C3
24	B	7101	LMG	C9-C8-O7-C10
22	K	7001	LMU	C3'-C4'-O1B-C1B
19	A	1138	CLA	C5-C6-C7-C8
21	I	6018	BCR	C11-C10-C9-C8
22	R	7022	LMU	C5-C6-C7-C8
19	A	1124	CLA	C5-C6-C7-C8
19	4	1004	CLA	C5-C6-C7-C8
22	C	7015	LMU	C4'-C5'-C6'-O6'
19	J	1308	CLA	C6-C7-C8-C9
19	A	1141	CLA	CBA-CGA-O2A-C1
19	A	1125	CLA	C5-C6-C7-C8
19	B	1206	CLA	C2A-CAA-CBA-CGA
19	1	1007	CLA	C2-C3-C5-C6
22	R	7021	LMU	C3-C4-C5-C6
19	B	1210	CLA	C13-C15-C16-C17
19	2	4009	CLA	C13-C15-C16-C17
22	H	7043	LMU	C11-C10-C9-C8
19	B	1223	CLA	C5-C6-C7-C8
19	A	1103	CLA	C11-C10-C8-C9
19	B	1239	CLA	C11-C12-C13-C14
22	A	7023	LMU	O5B-C1B-O1B-C4'
19	A	1119	CLA	C16-C17-C18-C19
22	G	7039	LMU	O5B-C5B-C6B-O6B
22	K	7041	LMU	C9-C10-C11-C12
22	B	7040	LMU	C2-C3-C4-C5
19	A	1119	CLA	O1A-CGA-O2A-C1
22	K	7047	LMU	C3-C4-C5-C6
19	A	1135	CLA	C2-C1-O2A-CGA
19	J	1311	CLA	C2-C1-O2A-CGA
22	G	7039	LMU	C2'-C1'-O1'-C1
19	B	1220	CLA	C16-C17-C18-C20
19	J	1308	CLA	C6-C7-C8-C10
19	B	1212	CLA	C10-C11-C12-C13
22	2	7031	LMU	C1-C2-C3-C4
22	G	7026	LMU	C2B-C1B-O1B-C4'
19	J	1311	CLA	C4-C3-C5-C6
19	B	1224	CLA	C3-C5-C6-C7
19	L	1148	CLA	C3-C5-C6-C7
19	H	1207	CLA	C2-C3-C5-C6
19	B	1211	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	H	1207	CLA	C13-C15-C16-C17
19	A	1151	CLA	C2A-CAA-CBA-CGA
19	B	1236	CLA	C2A-CAA-CBA-CGA
19	J	1311	CLA	C4C-C3C-CAC-CBC
19	A	1132	CLA	C16-C17-C18-C19
19	A	1140	CLA	C16-C17-C18-C20
19	A	1115	CLA	C3-C5-C6-C7
19	B	1205	CLA	C3-C5-C6-C7
19	B	1229	CLA	C3-C5-C6-C7
19	2	2014	CLA	C14-C13-C15-C16
22	H	7028	LMU	C1-C2-C3-C4
22	A	7010	LMU	O1'-C1-C2-C3
22	A	7035	LMU	C9-C10-C11-C12
22	C	7015	LMU	C2-C1-O1'-C1'
22	3	7003	LMU	C2-C1-O1'-C1'
21	A	6002	BCR	C36-C18-C19-C20
22	1	7004	LMU	C5'-C4'-O1B-C1B
19	A	1131	CLA	C4B-C3B-CAB-CBB
19	B	1205	CLA	C4B-C3B-CAB-CBB
19	B	1206	CLA	C4B-C3B-CAB-CBB
19	B	1234	CLA	C1A-C2A-CAA-CBA
19	K	1143	CLA	C4B-C3B-CAB-CBB
19	3	3017	CLA	C1A-C2A-CAA-CBA
19	4	4002	CLA	C1A-C2A-CAA-CBA
19	A	1127	CLA	CBA-CGA-O2A-C1
19	B	1211	CLA	C4-C3-C5-C6
22	H	7017	LMU	C5-C6-C7-C8
22	H	7043	LMU	O5B-C5B-C6B-O6B
19	2	2004	CLA	C4C-C3C-CAC-CBC
21	B	6017	BCR	C15-C16-C17-C18
19	4	1304	CLA	C16-C17-C18-C19
19	A	1127	CLA	O1A-CGA-O2A-C1
22	G	7026	LMU	C7-C8-C9-C10
19	A	1120	CLA	C2-C3-C5-C6
19	1	1013	CLA	C2-C3-C5-C6
19	2	2001	CLA	C2-C3-C5-C6
19	A	1131	CLA	C8-C10-C11-C12
19	A	1103	CLA	C11-C10-C8-C7
19	A	1124	CLA	C11-C10-C8-C7
19	A	1138	CLA	C11-C10-C8-C7
19	A	9013	CLA	C11-C12-C13-C15
19	A	9023	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	B	1202	CLA	C11-C12-C13-C15
19	B	1210	CLA	C11-C10-C8-C7
19	B	1220	CLA	C12-C13-C15-C16
19	B	1226	CLA	C11-C12-C13-C15
19	B	1226	CLA	C12-C13-C15-C16
19	B	1229	CLA	C11-C10-C8-C7
19	B	1235	CLA	C11-C10-C8-C7
19	H	1145	CLA	C11-C12-C13-C15
19	I	1204	CLA	C11-C10-C8-C7
19	K	3009	CLA	C6-C7-C8-C10
19	3	3011	CLA	C11-C12-C13-C15
20	A	5001	PQN	C21-C22-C23-C25
20	A	5001	PQN	C22-C23-C25-C26
20	A	5001	PQN	C26-C27-C28-C29
22	A	7023	LMU	C5-C6-C7-C8
19	1	1303	CLA	CBA-CGA-O2A-C1
22	G	7051	LMU	C3-C4-C5-C6
22	C	7015	LMU	C5'-C4'-O1B-C1B
22	E	7048	LMU	C1-C2-C3-C4
19	A	1111	CLA	O1A-CGA-O2A-C1
19	3	3011	CLA	C13-C15-C16-C17
22	3	7003	LMU	C3-C4-C5-C6
22	2	7027	LMU	O5B-C1B-O1B-C4'
19	A	1135	CLA	C3A-C2A-CAA-CBA
19	1	1002	CLA	C3A-C2A-CAA-CBA
19	4	4015	CLA	C3A-C2A-CAA-CBA
19	A	1131	CLA	C16-C17-C18-C20
19	B	1215	CLA	C2-C3-C5-C6
19	4	1004	CLA	O1A-CGA-O2A-C1
19	A	1103	CLA	C11-C12-C13-C14
19	A	1117	CLA	C14-C13-C15-C16
19	A	1131	CLA	C11-C10-C8-C9
19	B	1211	CLA	C11-C10-C8-C9
19	I	1204	CLA	C11-C10-C8-C9
19	J	1311	CLA	C6-C7-C8-C9
19	3	3013	CLA	C11-C10-C8-C9
21	A	6003	BCR	C19-C20-C21-C22
21	B	6004	BCR	C19-C20-C21-C22
19	A	1137	CLA	O1D-CGD-O2D-CED
22	1	7004	LMU	C6-C7-C8-C9
19	B	1206	CLA	C3-C5-C6-C7
22	B	7040	LMU	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	1141	CLA	O1A-CGA-O2A-C1
24	B	7101	LMG	O1-C7-C8-O7
22	R	7020	LMU	C4-C5-C6-C7
19	A	1123	CLA	C8-C10-C11-C12
19	B	1219	CLA	C6-C7-C8-C9
19	L	1130	CLA	C16-C17-C18-C20
22	H	7030	LMU	O1'-C1-C2-C3
19	A	1126	CLA	C10-C11-C12-C13
19	B	9010	CLA	C2-C3-C5-C6
19	A	1102	CLA	C2C-C3C-CAC-CBC
22	2	7006	LMU	O5B-C5B-C6B-O6B
19	A	1126	CLA	CAD-CBD-CGD-O2D
19	A	1133	CLA	CAD-CBD-CGD-O2D
19	A	9012	CLA	CAD-CBD-CGD-O2D
19	A	9022	CLA	CAD-CBD-CGD-O2D
19	B	1203	CLA	CAD-CBD-CGD-O2D
19	B	1232	CLA	CAD-CBD-CGD-O2D
19	B	1234	CLA	CAD-CBD-CGD-O2D
19	4	1004	CLA	CAD-CBD-CGD-O2D
19	4	4003	CLA	CAD-CBD-CGD-O2D
19	4	4014	CLA	CAD-CBD-CGD-O2D
19	A	9022	CLA	C5-C6-C7-C8
19	B	1229	CLA	CBA-CGA-O2A-C1
19	4	4003	CLA	CBA-CGA-O2A-C1
19	B	1235	CLA	C3-C5-C6-C7
19	4	4003	CLA	O1A-CGA-O2A-C1
22	A	7010	LMU	O5B-C1B-O1B-C4'
22	4	7019	LMU	C9-C10-C11-C12
19	B	1229	CLA	O1A-CGA-O2A-C1
19	A	1112	CLA	CHA-CBD-CGD-O1D
19	A	1112	CLA	CHA-CBD-CGD-O2D
19	A	1126	CLA	CAD-CBD-CGD-O1D
19	A	1133	CLA	CAD-CBD-CGD-O1D
19	A	9012	CLA	CAD-CBD-CGD-O1D
19	A	9022	CLA	CAD-CBD-CGD-O1D
19	B	1203	CLA	CAD-CBD-CGD-O1D
19	B	1216	CLA	CHA-CBD-CGD-O1D
19	B	1216	CLA	CHA-CBD-CGD-O2D
19	B	1230	CLA	CHA-CBD-CGD-O1D
19	B	1230	CLA	CHA-CBD-CGD-O2D
19	B	1232	CLA	CAD-CBD-CGD-O1D
19	B	1234	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	F	1302	CLA	CAD-CBD-CGD-O1D
19	1	1003	CLA	CHA-CBD-CGD-O1D
19	2	2007	CLA	CAD-CBD-CGD-O1D
19	3	2009	CLA	CHA-CBD-CGD-O1D
19	3	2009	CLA	CHA-CBD-CGD-O2D
19	4	1004	CLA	CAD-CBD-CGD-O1D
19	4	4003	CLA	CAD-CBD-CGD-O1D
19	4	4006	CLA	CHA-CBD-CGD-O1D
19	4	4006	CLA	CHA-CBD-CGD-O2D
19	4	4007	CLA	CHA-CBD-CGD-O1D
19	4	4014	CLA	CAD-CBD-CGD-O1D
21	A	6007	BCR	C13-C14-C15-C16
21	F	6014	BCR	C13-C14-C15-C16
19	L	1130	CLA	C16-C17-C18-C19
19	A	1126	CLA	C13-C15-C16-C17
19	A	1115	CLA	C2B-C3B-CAB-CBB
19	A	1119	CLA	C2B-C3B-CAB-CBB
19	A	1123	CLA	C2B-C3B-CAB-CBB
19	A	1134	CLA	C2B-C3B-CAB-CBB
19	A	9023	CLA	C2B-C3B-CAB-CBB
19	B	1202	CLA	C2B-C3B-CAB-CBB
19	B	1228	CLA	C2B-C3B-CAB-CBB
19	B	1233	CLA	C2B-C3B-CAB-CBB
19	I	1204	CLA	C2B-C3B-CAB-CBB
19	1	1002	CLA	C2B-C3B-CAB-CBB
19	2	2004	CLA	C2B-C3B-CAB-CBB
19	2	2006	CLA	C2B-C3B-CAB-CBB
19	2	2007	CLA	C2B-C3B-CAB-CBB
19	3	3011	CLA	C2B-C3B-CAB-CBB
21	B	6017	BCR	C23-C24-C25-C30
22	D	7050	LMU	C4-C5-C6-C7
21	B	6020	BCR	C7-C8-C9-C34
22	N	7049	LMU	C3-C4-C5-C6
19	B	1212	CLA	C11-C12-C13-C14
22	4	7018	LMU	C6-C7-C8-C9
21	B	6010	BCR	C17-C18-C19-C20
22	A	7016	LMU	C9-C10-C11-C12
22	R	7020	LMU	C5-C6-C7-C8
22	4	7053	LMU	C4-C5-C6-C7
22	4	7053	LMU	O5B-C1B-O1B-C4'
19	1	1007	CLA	C12-C13-C15-C16
19	A	1237	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A	6011	BCR	C18-C19-C20-C21
21	B	6010	BCR	C18-C19-C20-C21
21	1	6023	BCR	C18-C19-C20-C21
19	4	4003	CLA	CAA-CBA-CGA-O2A
19	A	1141	CLA	C13-C15-C16-C17
19	F	1302	CLA	C4C-C3C-CAC-CBC
22	4	7052	LMU	C7-C8-C9-C10
21	A	6011	BCR	C13-C14-C15-C16
19	A	1112	CLA	C4C-C3C-CAC-CBC
19	F	1305	CLA	C5-C6-C7-C8
22	A	7023	LMU	C2B-C1B-O1B-C4'
19	A	1106	CLA	C11-C10-C8-C9
19	A	1106	CLA	C14-C13-C15-C16
19	A	1237	CLA	C11-C12-C13-C14
19	A	9011	CLA	C14-C13-C15-C16
19	A	9013	CLA	C11-C12-C13-C14
19	A	9023	CLA	C6-C7-C8-C9
19	B	1210	CLA	C11-C10-C8-C9
19	B	1210	CLA	C14-C13-C15-C16
19	B	1215	CLA	C6-C7-C8-C9
19	B	1220	CLA	C11-C12-C13-C14
19	B	1235	CLA	C11-C10-C8-C9
19	K	3009	CLA	C6-C7-C8-C9
22	H	7011	LMU	C3'-C4'-O1B-C1B
19	A	1123	CLA	C12-C13-C15-C16
19	B	1229	CLA	C11-C12-C13-C15
19	B	1229	CLA	C12-C13-C15-C16
19	B	1238	CLA	C6-C7-C8-C10
19	J	1311	CLA	C6-C7-C8-C10
21	F	6014	BCR	C11-C10-C9-C8
19	A	1141	CLA	C4C-C3C-CAC-CBC
22	K	7042	LMU	C2'-C1'-O1'-C1
19	A	1102	CLA	C4-C3-C5-C6
19	A	9011	CLA	C4-C3-C5-C6
19	A	1140	CLA	C16-C17-C18-C19
22	H	7032	LMU	C3-C4-C5-C6
22	3	7005	LMU	C4'-C5'-C6'-O6'
19	4	1004	CLA	C6-C7-C8-C10
22	L	7029	LMU	C3-C4-C5-C6
19	4	4015	CLA	C4C-C3C-CAC-CBC
22	K	7001	LMU	C4-C5-C6-C7
19	A	1131	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	1222	CLA	CBA-CGA-O2A-C1
19	B	1206	CLA	C2-C1-O2A-CGA
19	A	1109	CLA	C4-C3-C5-C6
19	B	1210	CLA	C4-C3-C5-C6
19	B	1210	CLA	CAA-CBA-CGA-O2A
19	B	1224	CLA	CAA-CBA-CGA-O2A
22	H	7011	LMU	C4-C5-C6-C7
22	C	7015	LMU	C3'-C4'-O1B-C1B
21	F	6014	BCR	C7-C8-C9-C34
22	4	7053	LMU	C2B-C1B-O1B-C4'
19	B	1222	CLA	O1A-CGA-O2A-C1
22	A	7023	LMU	C9-C10-C11-C12
21	B	6010	BCR	C21-C22-C23-C24
19	B	1213	CLA	CAA-CBA-CGA-O2A
19	A	1131	CLA	O1A-CGA-O2A-C1
19	A	1136	CLA	C13-C15-C16-C17
19	A	1137	CLA	C2A-CAA-CBA-CGA
19	A	9012	CLA	C2A-CAA-CBA-CGA
19	1	1014	CLA	C2A-CAA-CBA-CGA
21	J	6012	BCR	C15-C16-C17-C18
22	H	7017	LMU	C3'-C4'-O1B-C1B
19	A	9011	CLA	C2-C3-C5-C6
19	B	1210	CLA	C2-C3-C5-C6
19	J	1311	CLA	C2-C3-C5-C6
22	A	7035	LMU	O1'-C1-C2-C3
22	A	7016	LMU	C2-C1-O1'-C1'
22	H	7017	LMU	C2-C1-O1'-C1'
22	4	7019	LMU	C2-C1-O1'-C1'
19	A	1102	CLA	C6-C7-C8-C10
19	A	1109	CLA	C11-C12-C13-C14
19	A	1124	CLA	C11-C10-C8-C9
19	A	1128	CLA	C6-C7-C8-C9
19	B	1239	CLA	C14-C13-C15-C16
19	A	1124	CLA	CBA-CGA-O2A-C1
19	A	1134	CLA	C4B-C3B-CAB-CBB
19	B	1226	CLA	C4B-C3B-CAB-CBB
19	R	1150	CLA	C4B-C3B-CAB-CBB
19	1	1008	CLA	C4B-C3B-CAB-CBB
19	B	1238	CLA	CBD-CGD-O2D-CED
19	A	1115	CLA	C16-C17-C18-C19
19	A	9013	CLA	C16-C17-C18-C20
22	A	7035	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
19	A	1124	CLA	O1A-CGA-O2A-C1
19	1	1303	CLA	O1A-CGA-O2A-C1
19	3	3017	CLA	C4C-C3C-CAC-CBC
19	A	1109	CLA	C11-C10-C8-C7
19	A	1237	CLA	C11-C12-C13-C15
19	A	9023	CLA	C6-C7-C8-C10
19	B	1226	CLA	C11-C10-C8-C7
22	H	7032	LMU	O5B-C5B-C6B-O6B
22	B	7038	LMU	C4-C5-C6-C7
19	B	9010	CLA	CAA-CBA-CGA-O2A
19	A	9013	CLA	C16-C17-C18-C19
19	A	9022	CLA	C10-C11-C12-C13
19	H	1207	CLA	C10-C11-C12-C13
22	2	7006	LMU	C3-C4-C5-C6
19	A	1138	CLA	C3A-C2A-CAA-CBA
19	K	1146	CLA	C3A-C2A-CAA-CBA
19	1	1005	CLA	C3A-C2A-CAA-CBA
19	3	3008	CLA	C3A-C2A-CAA-CBA
19	3	3017	CLA	C3A-C2A-CAA-CBA
19	B	1227	CLA	CAA-CBA-CGA-O2A
22	4	7052	LMU	C11-C10-C9-C8
21	A	6011	BCR	C35-C13-C14-C15
21	F	6014	BCR	C20-C21-C22-C37
21	F	6016	BCR	C16-C17-C18-C36
19	A	1108	CLA	CAA-CBA-CGA-O2A
19	A	1102	CLA	C2-C1-O2A-CGA
19	A	1106	CLA	C2-C1-O2A-CGA
19	4	4001	CLA	C2-C1-O2A-CGA
21	B	6004	BCR	C13-C14-C15-C16
19	B	1223	CLA	C10-C11-C12-C13
19	B	1226	CLA	C10-C11-C12-C13
19	1	1013	CLA	C4-C3-C5-C6
19	2	2001	CLA	C4-C3-C5-C6
19	A	1103	CLA	CBD-CGD-O2D-CED
21	F	6014	BCR	C7-C8-C9-C10
19	B	1212	CLA	C4-C3-C5-C6
19	4	4007	CLA	C4-C3-C5-C6
19	J	1308	CLA	CAA-CBA-CGA-O2A
19	A	1237	CLA	C2-C3-C5-C6
22	2	7031	LMU	O5B-C1B-O1B-C4'
19	A	1132	CLA	C16-C17-C18-C20
19	H	1145	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	4	7009	LMU	O5B-C1B-O1B-C4'
19	A	1108	CLA	CAA-CBA-CGA-O1A
22	4	7019	LMU	C4-C5-C6-C7
19	A	1131	CLA	C6-C7-C8-C9
19	B	1203	CLA	C11-C10-C8-C9
19	B	1206	CLA	C6-C7-C8-C9
19	B	1220	CLA	C6-C7-C8-C9
19	B	9010	CLA	C11-C10-C8-C9
19	L	1130	CLA	C14-C13-C15-C16
20	B	5002	PQN	C21-C22-C23-C24
22	4	7019	LMU	C2-C3-C4-C5
22	4	7034	LMU	C4'-C5'-C6'-O6'
19	H	1145	CLA	CAA-CBA-CGA-O2A
22	G	7026	LMU	O5B-C5B-C6B-O6B
19	L	1501	CLA	C2A-CAA-CBA-CGA
19	A	1104	CLA	C1A-C2A-CAA-CBA
19	A	1110	CLA	C1A-C2A-CAA-CBA
19	A	1120	CLA	C1A-C2A-CAA-CBA
19	A	1141	CLA	C1A-C2A-CAA-CBA
19	B	1222	CLA	C1A-C2A-CAA-CBA
19	K	1146	CLA	C1A-C2A-CAA-CBA
19	3	3016	CLA	C1A-C2A-CAA-CBA
21	A	6011	BCR	C12-C13-C14-C15
21	F	6014	BCR	C20-C21-C22-C23
21	F	6016	BCR	C16-C17-C18-C19
22	H	7032	LMU	O5B-C1B-O1B-C4'
22	K	7001	LMU	O1'-C1-C2-C3
22	K	7001	LMU	C2-C3-C4-C5
19	A	1131	CLA	C10-C11-C12-C13
19	A	1102	CLA	C2B-C3B-CAB-CBB
19	A	1105	CLA	C2B-C3B-CAB-CBB
19	A	1122	CLA	C2B-C3B-CAB-CBB
19	B	1211	CLA	C2B-C3B-CAB-CBB
19	B	1215	CLA	C2B-C3B-CAB-CBB
19	L	1148	CLA	C2B-C3B-CAB-CBB
19	R	1144	CLA	C2B-C3B-CAB-CBB
19	3	2009	CLA	C2B-C3B-CAB-CBB
19	4	1306	CLA	C2B-C3B-CAB-CBB
19	4	4015	CLA	C2B-C3B-CAB-CBB
21	A	6007	BCR	C5-C6-C7-C8
21	F	6014	BCR	C23-C24-C25-C26
21	I	6021	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	J	6012	BCR	C5-C6-C7-C8
21	L	6019	BCR	C5-C6-C7-C8
21	1	6023	BCR	C23-C24-C25-C26
22	4	7033	LMU	C3-C4-C5-C6
22	4	7033	LMU	C7-C8-C9-C10
19	A	1134	CLA	CAA-CBA-CGA-O1A
19	B	1225	CLA	C4-C3-C5-C6
22	H	7032	LMU	C9-C10-C11-C12
22	H	7011	LMU	C7-C8-C9-C10
19	4	1304	CLA	CBA-CGA-O2A-C1
19	A	9012	CLA	C8-C10-C11-C12
19	A	1125	CLA	C11-C10-C8-C7
19	A	9011	CLA	C11-C10-C8-C7
19	B	1203	CLA	C11-C10-C8-C7
19	B	1211	CLA	C11-C12-C13-C15
19	B	1212	CLA	C11-C10-C8-C7
19	B	1224	CLA	C11-C10-C8-C7
19	H	1207	CLA	C11-C10-C8-C7
19	4	1304	CLA	C6-C7-C8-C10
19	A	9011	CLA	C16-C17-C18-C19
19	4	4003	CLA	C6-C7-C8-C9
19	B	1224	CLA	C2A-CAA-CBA-CGA
22	H	7030	LMU	C6-C7-C8-C9
22	C	7015	LMU	O1'-C1-C2-C3
19	A	1149	CLA	C2-C1-O2A-CGA
22	G	7051	LMU	C5-C6-C7-C8
22	G	7039	LMU	C4B-C5B-C6B-O6B
19	A	1112	CLA	CAA-CBA-CGA-O1A
19	J	1311	CLA	C12-C13-C15-C16
19	K	1143	CLA	C4C-C3C-CAC-CBC
22	B	7038	LMU	C2-C3-C4-C5
19	A	1102	CLA	C2-C3-C5-C6
19	A	1109	CLA	C2-C3-C5-C6
19	4	4007	CLA	C2-C3-C5-C6
22	H	7002	LMU	C3-C4-C5-C6
22	B	7040	LMU	C9-C10-C11-C12
24	B	7101	LMG	C38-C39-C40-C41
22	1	7004	LMU	C9-C10-C11-C12
22	4	7034	LMU	O5'-C5'-C6'-O6'
19	3	1147	CLA	C2A-CAA-CBA-CGA
19	A	1112	CLA	CAA-CBA-CGA-O2A
19	A	1103	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	1141	CLA	C14-C13-C15-C16
19	A	1237	CLA	C11-C10-C8-C9
22	R	7021	LMU	C11-C10-C9-C8
19	B	1225	CLA	CBD-CGD-O2D-CED
22	R	7025	LMU	C2-C3-C4-C5
19	A	1125	CLA	C10-C11-C12-C13
22	H	7028	LMU	O5'-C1'-O1'-C1
24	B	7101	LMG	C14-C15-C16-C17
19	A	1126	CLA	C4-C3-C5-C6
19	A	9023	CLA	C4-C3-C5-C6
19	4	1304	CLA	C4-C3-C5-C6
19	R	1150	CLA	CAA-CBA-CGA-O2A
22	D	7050	LMU	C3-C4-C5-C6
19	A	1122	CLA	O1A-CGA-O2A-C1
19	A	1134	CLA	CAA-CBA-CGA-O2A
19	A	1101	CLA	CAA-CBA-CGA-O1A
19	A	9013	CLA	C2A-CAA-CBA-CGA
19	I	1204	CLA	C2A-CAA-CBA-CGA
22	2	7046	LMU	C5-C6-C7-C8
19	B	1232	CLA	CAA-CBA-CGA-O2A
22	H	7043	LMU	C1-C2-C3-C4
19	B	1229	CLA	C4-C3-C5-C6
19	A	1141	CLA	C4B-C3B-CAB-CBB
19	L	1503	CLA	C4B-C3B-CAB-CBB
19	A	1128	CLA	C10-C11-C12-C13
22	4	7008	LMU	C3'-C4'-O1B-C1B
19	2	2007	CLA	O1D-CGD-O2D-CED
19	A	1122	CLA	CBA-CGA-O2A-C1
19	B	1202	CLA	CAA-CBA-CGA-O2A
19	B	1223	CLA	C16-C17-C18-C20
22	R	7014	LMU	C1-C2-C3-C4
21	B	6010	BCR	C20-C21-C22-C37
21	B	6017	BCR	C20-C21-C22-C37
19	A	1117	CLA	C8-C10-C11-C12
22	R	7021	LMU	C6-C7-C8-C9
22	H	7011	LMU	C2-C3-C4-C5
19	B	1224	CLA	C6-C7-C8-C10
19	4	1304	CLA	C11-C10-C8-C7
22	A	7045	LMU	C3'-C4'-O1B-C1B
19	2	2006	CLA	CAA-CBA-CGA-O2A
19	A	1237	CLA	C5-C6-C7-C8
24	B	7101	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	G	7026	LMU	C4-C5-C6-C7
19	B	1236	CLA	C2-C1-O2A-CGA
19	A	1119	CLA	C14-C13-C15-C16
19	A	1124	CLA	C11-C12-C13-C14
19	A	9012	CLA	C11-C12-C13-C14
19	B	1202	CLA	C14-C13-C15-C16
19	B	1203	CLA	C11-C12-C13-C14
22	K	7001	LMU	C4'-C5'-C6'-O6'
19	1	1007	CLA	C2A-CAA-CBA-CGA
19	4	4014	CLA	C2A-CAA-CBA-CGA
19	A	1237	CLA	C2-C1-O2A-CGA
19	B	1230	CLA	C2-C1-O2A-CGA
19	B	1235	CLA	C2-C1-O2A-CGA
19	R	1144	CLA	C2-C1-O2A-CGA
19	A	1125	CLA	C16-C17-C18-C20
19	4	4003	CLA	C6-C7-C8-C10
19	A	1122	CLA	C3A-C2A-CAA-CBA
19	A	1141	CLA	C3A-C2A-CAA-CBA
19	B	1221	CLA	C4-C3-C5-C6
19	B	1234	CLA	C3A-C2A-CAA-CBA
19	2	2004	CLA	C3A-C2A-CAA-CBA
19	3	3016	CLA	C3A-C2A-CAA-CBA
19	3	3008	CLA	CAA-CBA-CGA-O1A
19	B	1210	CLA	C4C-C3C-CAC-CBC
19	A	1149	CLA	CAA-CBA-CGA-O1A
19	B	1221	CLA	O1D-CGD-O2D-CED
22	4	7053	LMU	O1'-C1-C2-C3
22	H	7011	LMU	C3-C4-C5-C6
22	F	7036	LMU	C4-C5-C6-C7
22	1	7004	LMU	C4-C5-C6-C7
19	B	1232	CLA	CAA-CBA-CGA-O1A
22	K	7041	LMU	C1-C2-C3-C4
19	J	1311	CLA	C3-C5-C6-C7
22	R	7022	LMU	C6-C7-C8-C9
19	A	1124	CLA	C8-C10-C11-C12
21	B	6010	BCR	C20-C21-C22-C23
21	B	6017	BCR	C20-C21-C22-C23
21	F	6016	BCR	C20-C21-C22-C23
22	D	7050	LMU	C7-C8-C9-C10
19	4	1304	CLA	O1A-CGA-O2A-C1
19	A	1125	CLA	C16-C17-C18-C19
19	A	1109	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	3	3016	CLA	C10-C11-C12-C13
19	A	1119	CLA	C2A-CAA-CBA-CGA
21	I	6018	BCR	C15-C16-C17-C18
19	A	9023	CLA	C16-C17-C18-C20
22	A	7023	LMU	C11-C10-C9-C8
19	L	1130	CLA	CBA-CGA-O2A-C1
19	1	1002	CLA	C2-C1-O2A-CGA
19	A	1106	CLA	C11-C12-C13-C14
19	B	1205	CLA	C14-C13-C15-C16
19	B	1210	CLA	C6-C7-C8-C9
19	H	1145	CLA	C11-C12-C13-C14
19	3	3011	CLA	C11-C12-C13-C14
20	A	5001	PQN	C24-C23-C25-C26
19	A	9011	CLA	C16-C17-C18-C20
19	A	1138	CLA	CAA-CBA-CGA-O2A
19	B	1217	CLA	CAA-CBA-CGA-O2A
19	A	9011	CLA	CAA-CBA-CGA-O2A
19	B	1223	CLA	CAA-CBA-CGA-O2A
19	H	1505	CLA	CAA-CBA-CGA-O2A
19	I	1204	CLA	CAA-CBA-CGA-O2A
19	A	1106	CLA	C6-C7-C8-C10
19	A	1109	CLA	C6-C7-C8-C10
19	A	1109	CLA	C12-C13-C15-C16
19	A	1119	CLA	C12-C13-C15-C16
19	A	1123	CLA	C11-C10-C8-C7
19	A	1141	CLA	C12-C13-C15-C16
19	A	9012	CLA	C11-C12-C13-C15
19	B	1203	CLA	C11-C12-C13-C15
19	B	1210	CLA	C12-C13-C15-C16
19	B	9010	CLA	C6-C7-C8-C10
19	B	9010	CLA	C11-C12-C13-C15
19	R	1150	CLA	C11-C12-C13-C15
19	3	2009	CLA	C6-C7-C8-C10
20	B	5002	PQN	C21-C22-C23-C25
19	B	1210	CLA	C2C-C3C-CAC-CBC
19	A	9012	CLA	C2B-C3B-CAB-CBB
19	B	1201	CLA	C2B-C3B-CAB-CBB
19	K	1143	CLA	C2B-C3B-CAB-CBB
19	4	1304	CLA	C2B-C3B-CAB-CBB
21	B	6005	BCR	C23-C24-C25-C26
21	B	6005	BCR	C23-C24-C25-C30
21	F	6016	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	L	6019	BCR	C23-C24-C25-C30
21	3	6022	BCR	C23-C24-C25-C26
21	3	6022	BCR	C23-C24-C25-C30
22	H	7017	LMU	C5'-C4'-O1B-C1B
19	B	1218	CLA	CAA-CBA-CGA-O2A
22	4	7008	LMU	C6-C7-C8-C9
19	A	1151	CLA	C2-C1-O2A-CGA
19	A	9012	CLA	C2-C1-O2A-CGA
19	B	1223	CLA	C2-C1-O2A-CGA
19	B	1226	CLA	C2-C1-O2A-CGA
19	F	1305	CLA	C2-C1-O2A-CGA
19	2	2014	CLA	C2-C1-O2A-CGA
19	A	1110	CLA	C6-C7-C8-C9
22	4	7053	LMU	C7-C8-C9-C10
22	L	7029	LMU	C5-C6-C7-C8
19	A	1103	CLA	CAA-CBA-CGA-O2A
19	3	3013	CLA	CAA-CBA-CGA-O2A
19	A	1103	CLA	O1D-CGD-O2D-CED
22	B	7012	LMU	C2-C1-O1'-C1'
19	2	2002	CLA	C3-C5-C6-C7
19	1	1002	CLA	CAA-CBA-CGA-O2A
19	4	4015	CLA	CAA-CBA-CGA-O2A
19	A	1139	CLA	CAA-CBA-CGA-O2A
19	B	1233	CLA	CAA-CBA-CGA-O2A
19	K	3009	CLA	CAA-CBA-CGA-O2A
19	4	1304	CLA	CAA-CBA-CGA-O2A
22	A	7010	LMU	C11-C10-C9-C8
22	G	7026	LMU	C11-C10-C9-C8
19	B	1212	CLA	C2-C3-C5-C6
19	B	1231	CLA	CAA-CBA-CGA-O1A
19	4	4001	CLA	C2A-CAA-CBA-CGA
22	1	7004	LMU	C4B-C5B-C6B-O6B
19	B	1226	CLA	C11-C12-C13-C14
19	B	1238	CLA	C6-C7-C8-C9
19	A	1111	CLA	CAA-CBA-CGA-O2A
19	A	1125	CLA	CAA-CBA-CGA-O2A
19	1	1007	CLA	CAA-CBA-CGA-O2A
19	2	2013	CLA	CAA-CBA-CGA-O2A
22	G	7039	LMU	O1'-C1-C2-C3
19	B	1218	CLA	C1A-C2A-CAA-CBA
19	B	1232	CLA	C1A-C2A-CAA-CBA
19	K	1142	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	2	2004	CLA	C1A-C2A-CAA-CBA
19	3	1147	CLA	C4B-C3B-CAB-CBB
19	A	1111	CLA	C4-C3-C5-C6
19	A	1124	CLA	C4-C3-C5-C6
22	A	7035	LMU	O5'-C1'-O1'-C1
22	G	7039	LMU	O5'-C1'-O1'-C1
19	A	1141	CLA	CAA-CBA-CGA-O2A
22	E	7037	LMU	C2-C3-C4-C5
21	A	6002	BCR	C17-C18-C19-C20
21	B	6006	BCR	C17-C18-C19-C20
21	B	6020	BCR	C7-C8-C9-C10
21	B	6004	BCR	C15-C16-C17-C18
21	F	6014	BCR	C15-C16-C17-C18
19	A	1106	CLA	C10-C11-C12-C13
19	A	1107	CLA	C2-C1-O2A-CGA
19	A	1133	CLA	C2-C1-O2A-CGA
19	B	1227	CLA	C2-C1-O2A-CGA
19	B	1228	CLA	C2-C1-O2A-CGA
19	H	1207	CLA	C2-C1-O2A-CGA
19	A	1140	CLA	CAA-CBA-CGA-O2A
19	3	1147	CLA	CAA-CBA-CGA-O2A
19	A	1106	CLA	C11-C12-C13-C15
19	A	1124	CLA	C11-C12-C13-C15
19	A	9011	CLA	C6-C7-C8-C10
19	A	9012	CLA	C12-C13-C15-C16
19	B	1210	CLA	C6-C7-C8-C10
19	B	1220	CLA	C11-C10-C8-C7
19	3	3011	CLA	C15-C16-C17-C18
22	1	7013	LMU	C7-C8-C9-C10
19	B	1239	CLA	C8-C10-C11-C12
19	B	1213	CLA	C2A-CAA-CBA-CGA
19	B	1233	CLA	C2A-CAA-CBA-CGA
19	A	1123	CLA	C13-C15-C16-C17
22	R	7007	LMU	C3-C4-C5-C6
19	B	1231	CLA	CAA-CBA-CGA-O2A
19	A	1116	CLA	C4-C3-C5-C6
19	A	1137	CLA	C3A-C2A-CAA-CBA
19	A	9022	CLA	C3A-C2A-CAA-CBA
19	J	1308	CLA	C3A-C2A-CAA-CBA
19	R	1150	CLA	C3A-C2A-CAA-CBA
19	B	1208	CLA	C6-C7-C8-C10
19	1	1007	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	4	7009	LMU	C2B-C1B-O1B-C4'
22	K	7042	LMU	C2-C3-C4-C5
19	A	9011	CLA	C6-C7-C8-C9
19	B	1202	CLA	C11-C12-C13-C14
19	B	1212	CLA	C11-C10-C8-C9
19	B	9010	CLA	C14-C13-C15-C16
19	H	1145	CLA	C14-C13-C15-C16
19	H	1207	CLA	C11-C10-C8-C9
22	H	7002	LMU	C2-C3-C4-C5
19	A	1138	CLA	CAA-CBA-CGA-O1A
19	B	1233	CLA	CAA-CBA-CGA-O1A
19	4	1304	CLA	CAA-CBA-CGA-O1A
19	G	1242	CLA	C2C-C3C-CAC-CBC
19	A	9022	CLA	C8-C10-C11-C12
19	B	1223	CLA	CAA-CBA-CGA-O1A
22	H	7032	LMU	C2B-C1B-O1B-C4'
19	L	1130	CLA	O1A-CGA-O2A-C1
22	B	7040	LMU	O5B-C1B-O1B-C4'
19	4	4007	CLA	CAA-CBA-CGA-O2A
22	4	7034	LMU	O5B-C5B-C6B-O6B
19	A	1103	CLA	CAA-CBA-CGA-O1A
19	A	1139	CLA	CAA-CBA-CGA-O1A
19	B	1218	CLA	CAA-CBA-CGA-O1A
19	H	1505	CLA	CAA-CBA-CGA-O1A
19	I	1204	CLA	CAA-CBA-CGA-O1A
19	A	1125	CLA	CAA-CBA-CGA-O1A
19	A	9011	CLA	CAA-CBA-CGA-O1A
19	B	1215	CLA	C5-C6-C7-C8
19	A	1141	CLA	CAA-CBA-CGA-O1A
19	B	1217	CLA	CAA-CBA-CGA-O1A
19	K	3009	CLA	CAA-CBA-CGA-O1A
19	2	2013	CLA	CAA-CBA-CGA-O1A
22	H	7032	LMU	C2-C3-C4-C5
19	B	1219	CLA	CAA-CBA-CGA-O2A
19	B	1225	CLA	C2-C3-C5-C6
19	B	1213	CLA	CAD-CBD-CGD-O2D
19	B	1235	CLA	CAD-CBD-CGD-O2D
19	B	1236	CLA	CAD-CBD-CGD-O2D
19	B	1238	CLA	CAD-CBD-CGD-O2D
19	F	1302	CLA	CAD-CBD-CGD-O2D
19	F	1305	CLA	CAD-CBD-CGD-O2D
19	3	2009	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	1140	CLA	CAA-CBA-CGA-O1A
19	4	4015	CLA	CAA-CBA-CGA-O1A
19	2	2014	CLA	C5-C6-C7-C8
19	A	1138	CLA	C2C-C3C-CAC-CBC
19	3	3016	CLA	C2-C1-O2A-CGA
19	A	1111	CLA	CAA-CBA-CGA-O1A
19	3	3017	CLA	CAA-CBA-CGA-O2A
22	4	7018	LMU	O1'-C1-C2-C3
19	4	4007	CLA	CAA-CBA-CGA-O1A
22	A	7044	LMU	C4-C5-C6-C7
19	A	1109	CLA	CAA-CBA-CGA-O2A
19	A	1131	CLA	CAA-CBA-CGA-O2A
19	A	9023	CLA	CAA-CBA-CGA-O2A
19	2	2007	CLA	CAA-CBA-CGA-O2A
19	B	1235	CLA	CAA-CBA-CGA-O2A
19	B	1239	CLA	CAA-CBA-CGA-O2A
22	R	7020	LMU	C3-C4-C5-C6

There are no ring outliers.

234 monomers are involved in 3025 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	7021	LMU	9	0
19	A	1104	CLA	13	0
19	L	1130	CLA	26	0
22	B	7012	LMU	1	0
19	B	1217	CLA	10	0
19	A	1116	CLA	8	0
19	L	1502	CLA	26	0
19	1	1014	CLA	17	0
19	B	1223	CLA	36	0
19	3	3005	CLA	9	0
19	3	3012	CLA	11	0
19	A	1115	CLA	71	0
19	A	1106	CLA	27	0
21	F	6016	BCR	36	0
22	4	7034	LMU	36	0
19	B	1209	CLA	15	0
19	B	1213	CLA	20	0
19	B	1219	CLA	13	0
19	A	1129	CLA	6	0
19	B	1238	CLA	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	3008	CLA	14	0
19	3	3011	CLA	13	0
22	R	7025	LMU	1	0
19	H	1241	CLA	11	0
19	B	1234	CLA	8	0
19	4	4001	CLA	4	0
21	B	6005	BCR	7	0
21	I	6018	BCR	15	0
19	A	1110	CLA	1	0
19	3	2009	CLA	36	0
19	F	1302	CLA	10	0
19	4	4002	CLA	24	0
19	B	1206	CLA	17	0
19	B	1233	CLA	6	0
22	D	7050	LMU	21	0
19	A	1133	CLA	33	0
19	A	1126	CLA	40	0
22	B	7040	LMU	3	0
19	B	1222	CLA	42	0
19	B	1229	CLA	20	0
19	B	1228	CLA	15	0
19	4	4013	CLA	11	0
19	K	3009	CLA	3	5
19	3	3007	CLA	2	0
19	A	9011	CLA	13	0
19	A	1121	CLA	8	0
19	A	1103	CLA	17	0
22	H	7043	LMU	3	0
19	A	1135	CLA	24	0
19	2	2002	CLA	17	0
21	3	6022	BCR	6	0
19	A	1136	CLA	24	0
22	A	7016	LMU	12	0
22	H	7030	LMU	4	0
19	B	1220	CLA	43	0
19	A	1137	CLA	8	0
22	4	7009	LMU	3	0
19	A	1132	CLA	17	0
19	4	1004	CLA	32	0
19	J	1308	CLA	33	0
22	3	7003	LMU	20	0
21	I	6021	BCR	32	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	7020	LMU	10	0
22	K	7047	LMU	5	2
21	1	6023	BCR	6	0
19	L	1503	CLA	8	0
19	1	1013	CLA	14	0
22	G	7026	LMU	9	0
19	3	3006	CLA	9	0
19	H	1505	CLA	3	0
20	A	5001	PQN	6	0
19	A	1127	CLA	18	0
19	B	1227	CLA	10	0
19	B	1221	CLA	23	0
19	B	1301	CLA	7	0
19	A	1139	CLA	30	0
23	C	8003	SF4	3	0
19	1	1015	CLA	3	0
21	A	6007	BCR	32	0
21	A	6011	BCR	46	0
19	A	1119	CLA	44	0
19	A	1102	CLA	19	0
19	A	1107	CLA	38	0
19	1	1012	CLA	2	0
19	R	1150	CLA	3	0
22	A	7044	LMU	1	0
19	2	2011	CLA	1	0
19	A	1109	CLA	17	0
21	B	6006	BCR	12	0
19	A	9013	CLA	31	0
22	G	7051	LMU	1	0
19	B	1224	CLA	16	0
19	2	2014	CLA	34	0
19	A	1140	CLA	44	0
19	B	1235	CLA	61	0
19	B	1226	CLA	21	0
19	K	1142	CLA	15	1
19	2	2007	CLA	15	0
19	4	4014	CLA	8	0
19	2	2004	CLA	16	0
19	A	9012	CLA	37	0
22	G	7039	LMU	4	0
22	R	7022	LMU	5	0
22	F	7036	LMU	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	1207	CLA	23	0
22	E	7048	LMU	17	0
19	H	1145	CLA	25	0
22	H	7017	LMU	2	0
19	2	4009	CLA	6	0
19	4	4006	CLA	11	0
19	3	1147	CLA	14	0
19	B	1211	CLA	18	0
19	3	3010	CLA	5	0
19	2	2003	CLA	1	0
21	B	6020	BCR	24	0
21	L	6019	BCR	34	0
22	R	7007	LMU	5	0
22	2	7027	LMU	3	0
19	B	1202	CLA	28	0
22	R	7014	LMU	4	0
19	A	1124	CLA	60	0
22	B	7038	LMU	7	0
19	F	1305	CLA	12	0
19	3	3017	CLA	5	0
19	3	3013	CLA	18	0
19	L	1504	CLA	20	0
22	H	7002	LMU	3	0
19	K	1146	CLA	7	0
19	1	1001	CLA	11	0
19	1	1303	CLA	7	0
23	C	8002	SF4	6	0
22	A	7023	LMU	6	0
19	B	9010	CLA	15	0
24	B	7101	LMG	19	0
19	A	1120	CLA	8	0
22	3	7005	LMU	38	0
19	4	4011	CLA	2	0
22	4	7053	LMU	13	0
19	3	3004	CLA	7	0
21	A	6003	BCR	14	0
19	A	1237	CLA	28	0
19	2	2006	CLA	8	0
21	B	6010	BCR	21	0
22	4	7052	LMU	36	0
19	1	1003	CLA	4	0
19	B	1218	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1215	CLA	11	0
19	1	1005	CLA	4	0
21	J	6012	BCR	32	0
22	2	7046	LMU	1	0
21	A	6008	BCR	25	0
19	J	1311	CLA	18	0
19	K	1143	CLA	28	0
19	L	1148	CLA	21	0
19	4	1306	CLA	18	0
22	1	7004	LMU	6	0
19	A	1138	CLA	29	0
22	N	7049	LMU	9	0
20	B	5002	PQN	22	0
19	A	1125	CLA	66	0
19	A	1134	CLA	21	0
19	1	1002	CLA	9	0
19	4	4012	CLA	6	0
19	1	1008	CLA	6	1
19	I	1204	CLA	6	0
22	K	7001	LMU	11	0
19	2	2012	CLA	17	0
19	B	1236	CLA	25	0
19	B	1208	CLA	5	0
19	3	3003	CLA	8	0
22	H	7032	LMU	11	0
22	2	7006	LMU	8	0
19	B	1201	CLA	10	0
19	1	1006	CLA	15	0
19	B	1230	CLA	20	0
22	A	7045	LMU	2	0
19	2	2013	CLA	6	0
19	4	4004	CLA	2	0
22	H	7011	LMU	15	0
19	A	9022	CLA	38	0
22	L	7029	LMU	12	0
23	A	8001	SF4	2	0
19	A	9023	CLA	50	0
19	B	1232	CLA	18	0
19	4	1009	CLA	2	0
19	B	1212	CLA	14	0
19	4	4010	CLA	2	0
22	A	7010	LMU	6	0

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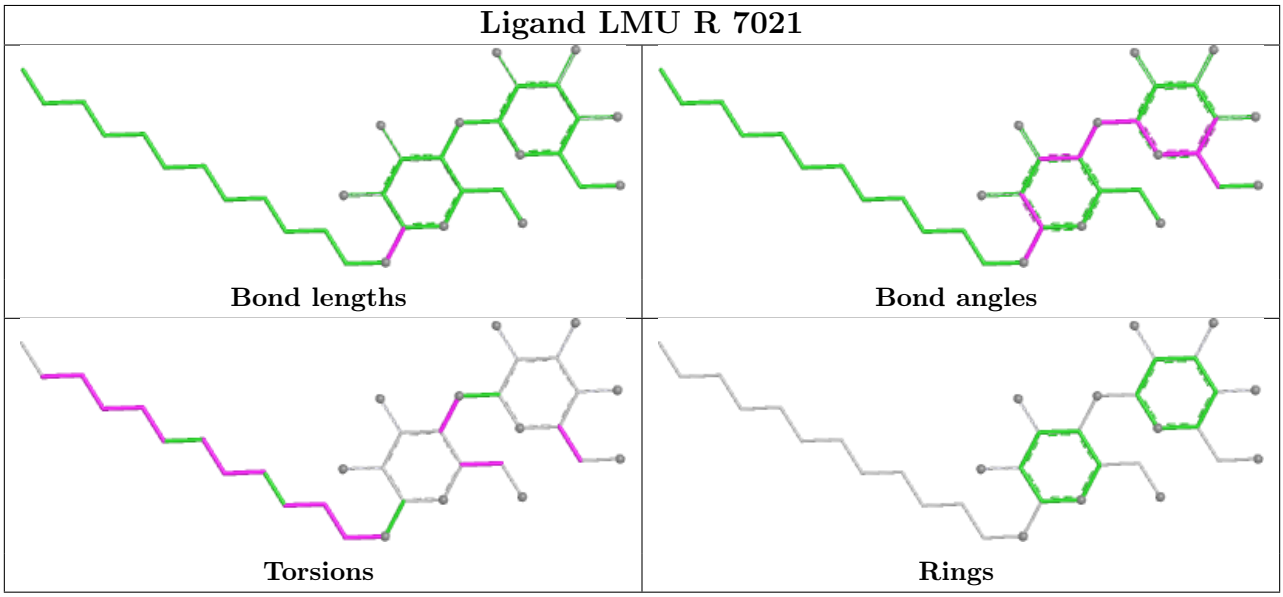
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	7033	LMU	7	0
19	A	1117	CLA	27	0
19	A	1123	CLA	30	0
19	A	1141	CLA	31	0
19	B	1205	CLA	25	0
19	4	4015	CLA	4	0
22	4	7019	LMU	1	0
19	A	1122	CLA	24	0
19	A	1128	CLA	18	0
19	B	1210	CLA	21	0
19	A	1151	CLA	18	0
22	K	7041	LMU	6	0
19	4	4003	CLA	3	0
19	2	2001	CLA	14	0
21	B	6017	BCR	43	0
19	B	1231	CLA	14	0
21	A	6002	BCR	44	0
19	G	1242	CLA	10	0
19	A	1112	CLA	31	0
19	A	1108	CLA	6	0
22	H	7028	LMU	2	0
22	2	7031	LMU	2	0
19	A	1149	CLA	7	0
19	B	1216	CLA	15	0
19	1	1011	CLA	5	0
19	A	1131	CLA	35	0
19	A	1105	CLA	25	0
19	A	1113	CLA	11	0
19	B	1203	CLA	18	0
19	3	3016	CLA	13	0
19	A	1111	CLA	20	0
19	A	1101	CLA	14	0
19	L	1501	CLA	16	0
21	B	6004	BCR	5	0
21	F	6014	BCR	25	0
19	B	1214	CLA	21	0
22	E	7037	LMU	7	0
22	4	7008	LMU	3	0
22	K	7042	LMU	16	0
19	R	1144	CLA	10	0
19	B	1239	CLA	21	0
19	1	1010	CLA	9	0

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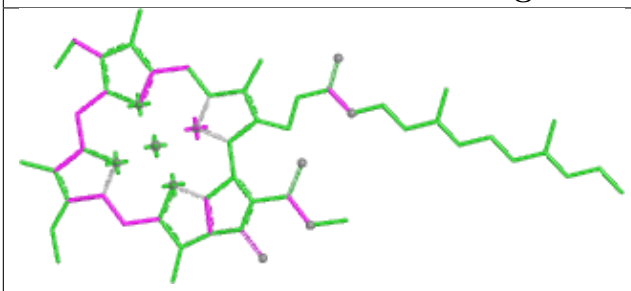
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	7013	LMU	4	0
19	1	1007	CLA	19	0
19	B	1225	CLA	28	0
19	4	1304	CLA	22	0

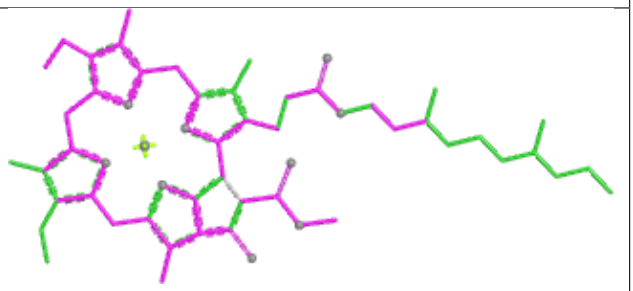
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



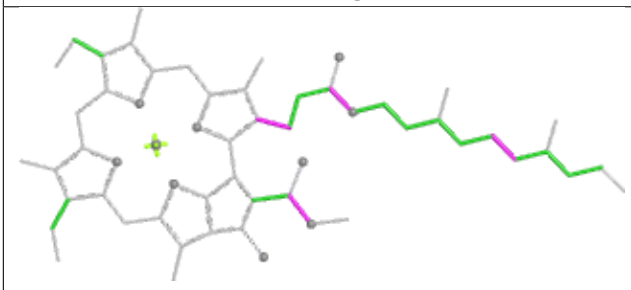
Ligand CLA A 1104



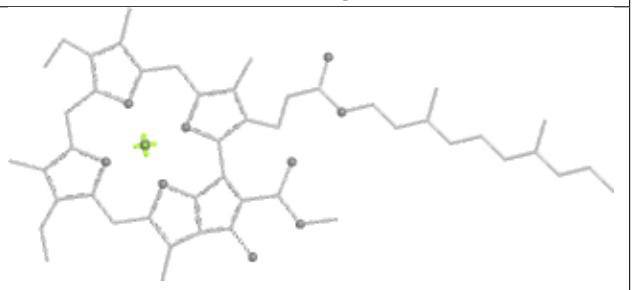
Bond lengths



Bond angles

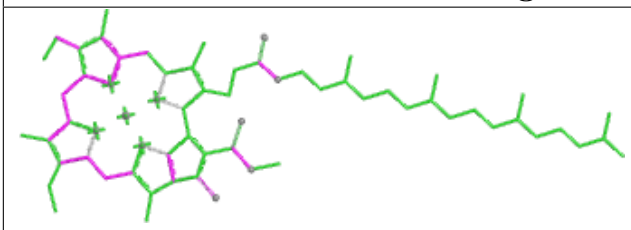


Torsions

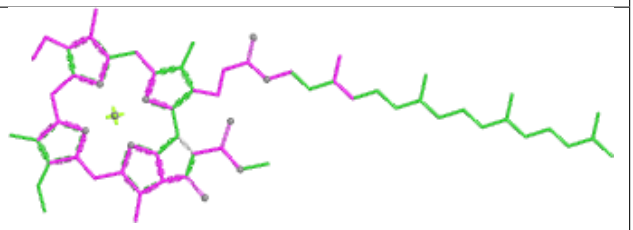


Rings

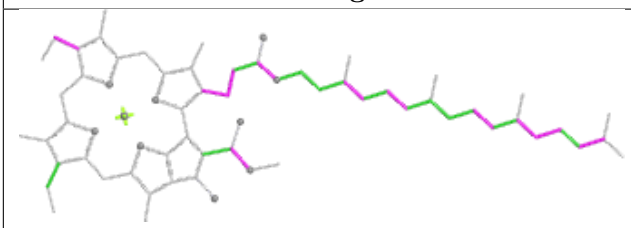
Ligand CLA L 1130



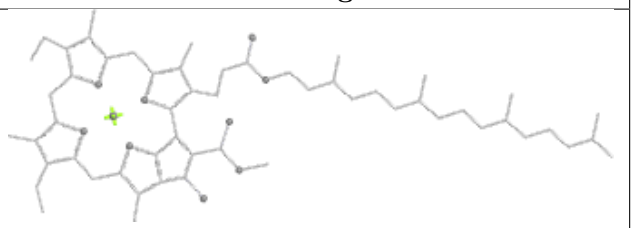
Bond lengths



Bond angles

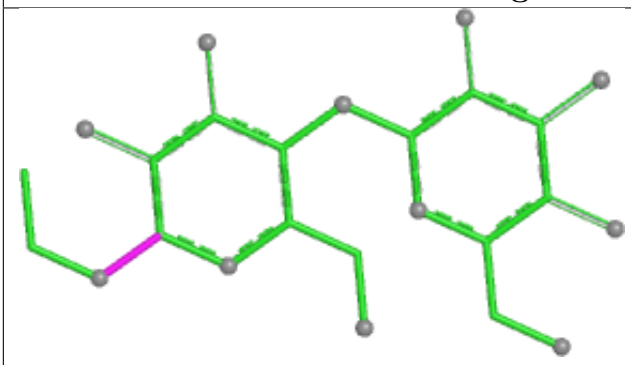


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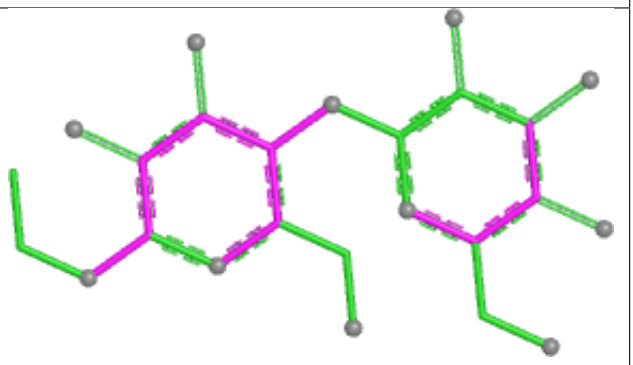


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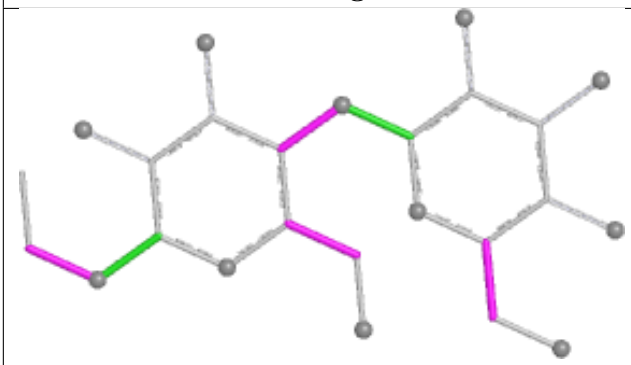
Ligand LMU B 7012



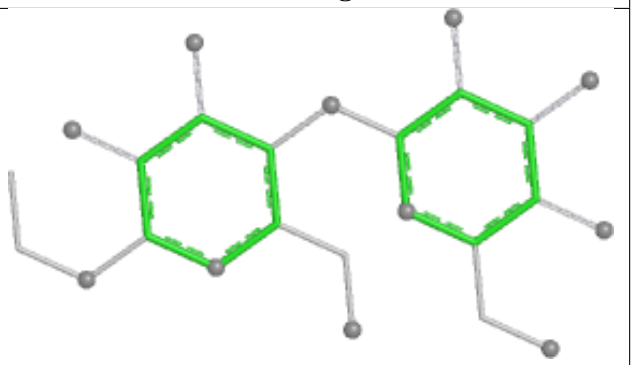
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Bond angles

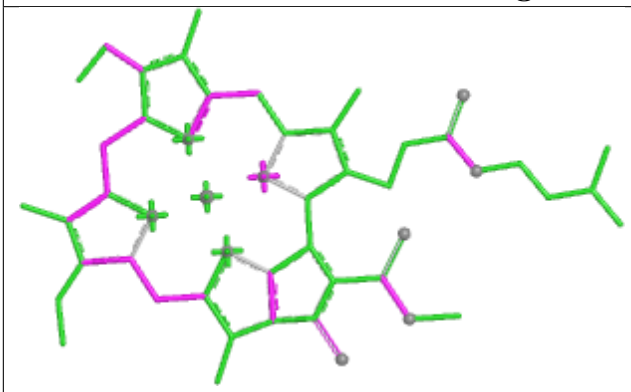


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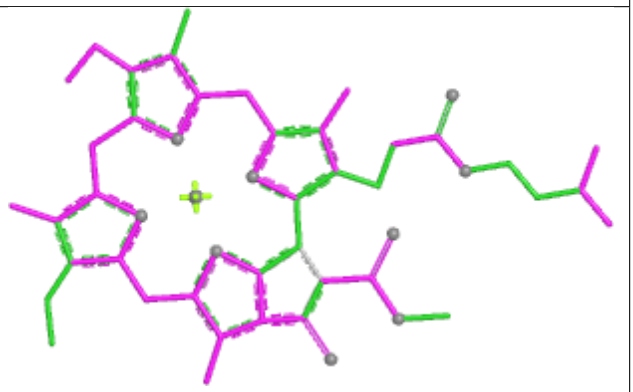


Rings

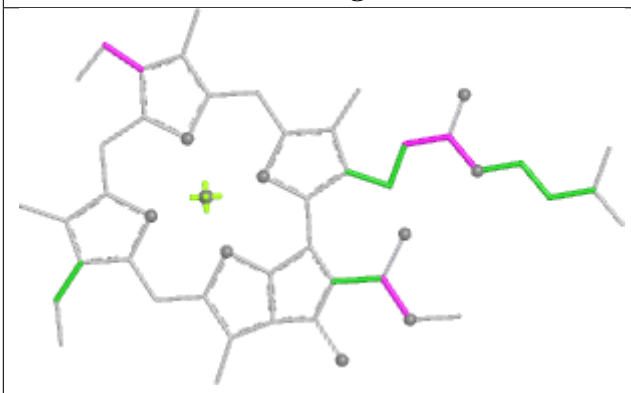
Ligand CLA B 1217



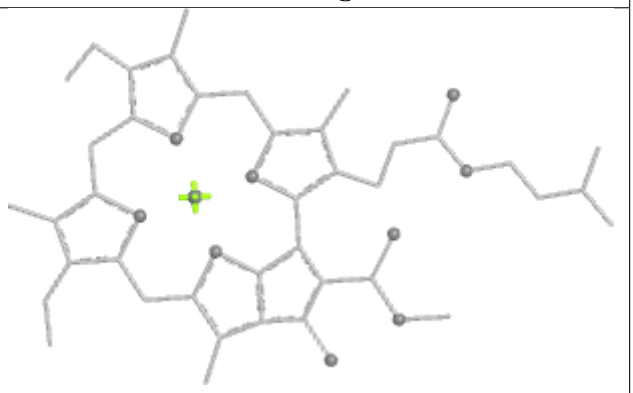
Bond lengths



Bond angles

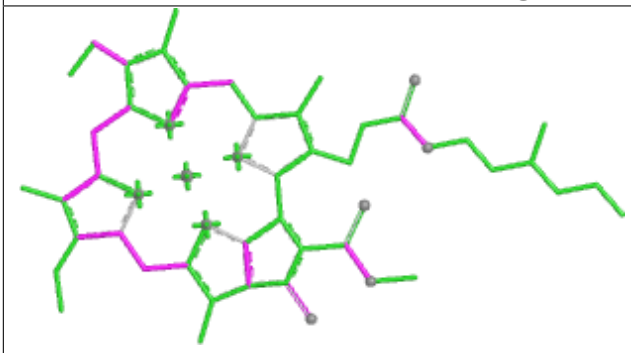


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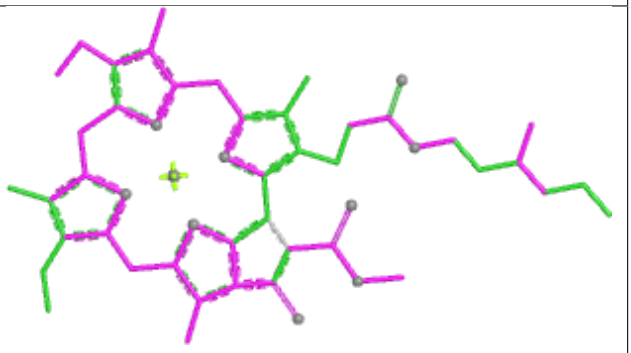


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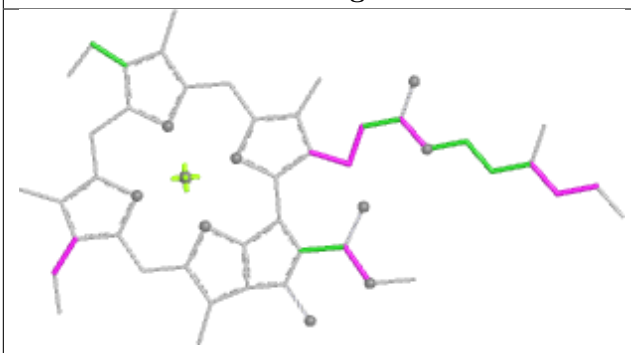
Ligand CLA A 1116



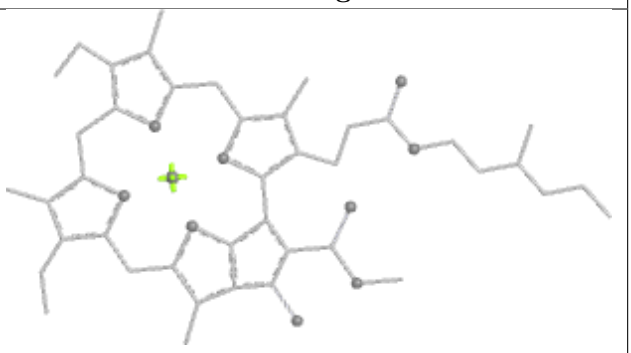
Bond lengths



Bond angles

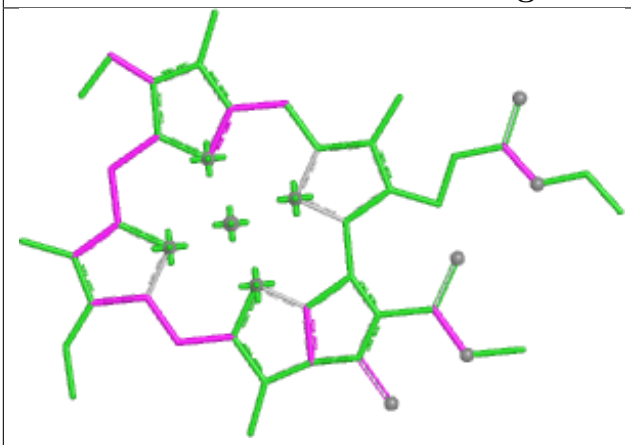


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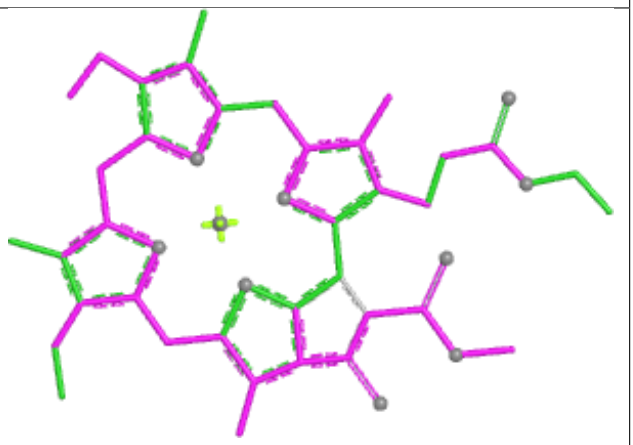


Rings

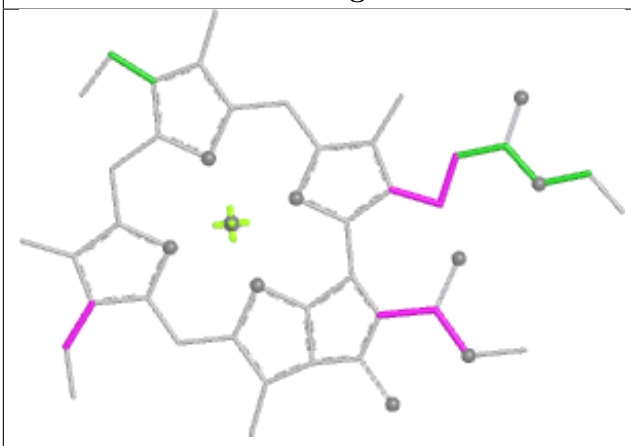
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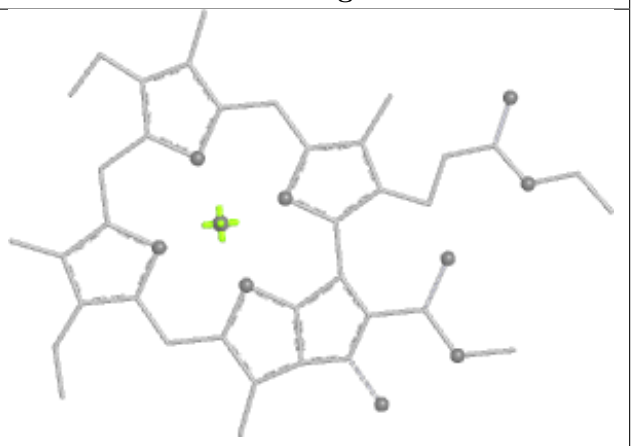
Bond lengths



Bond angles

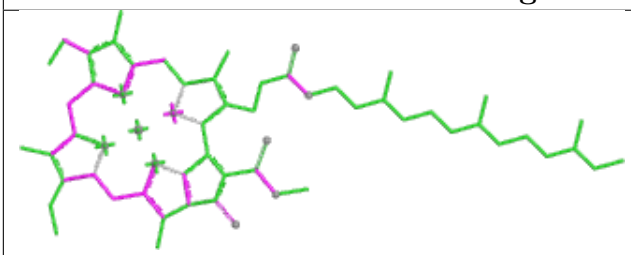


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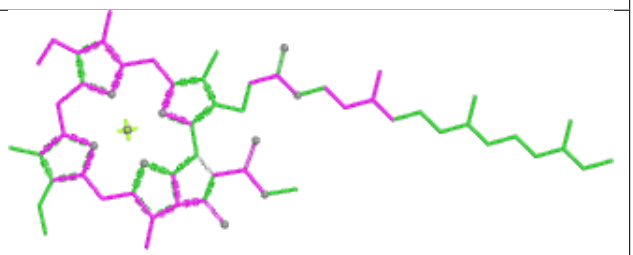


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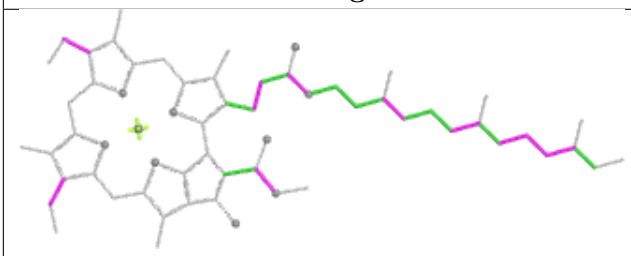
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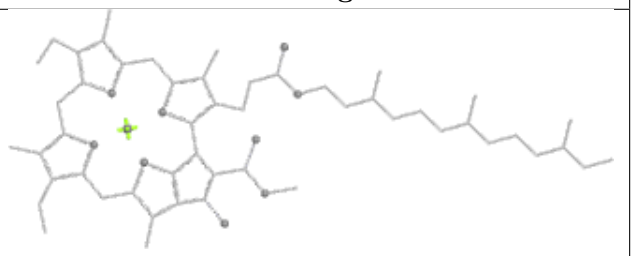
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Bond angles

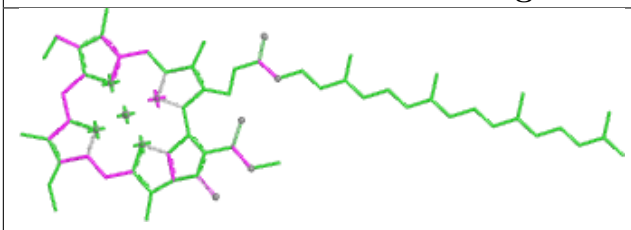


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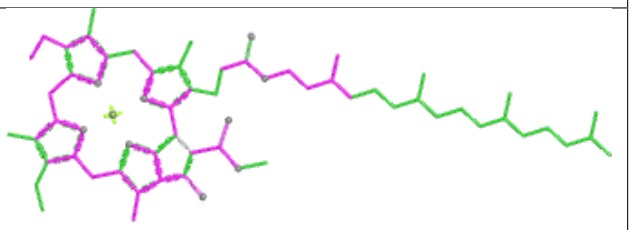


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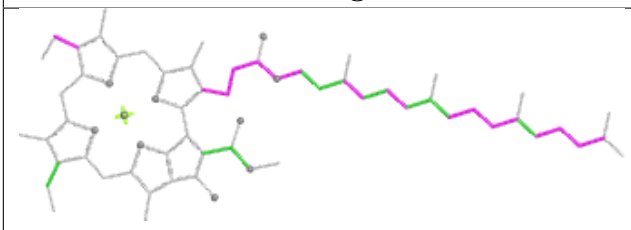
Ligand CLA B 1223



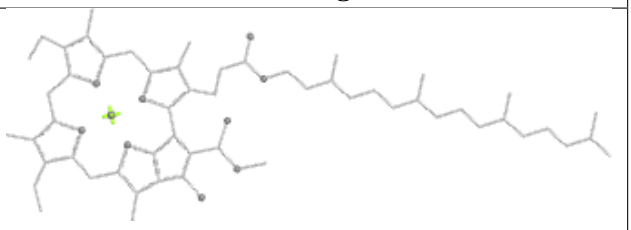
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Bond angles

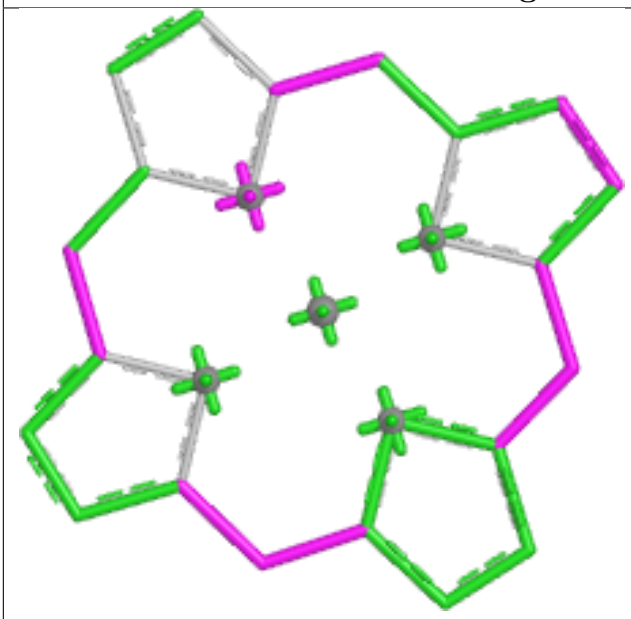


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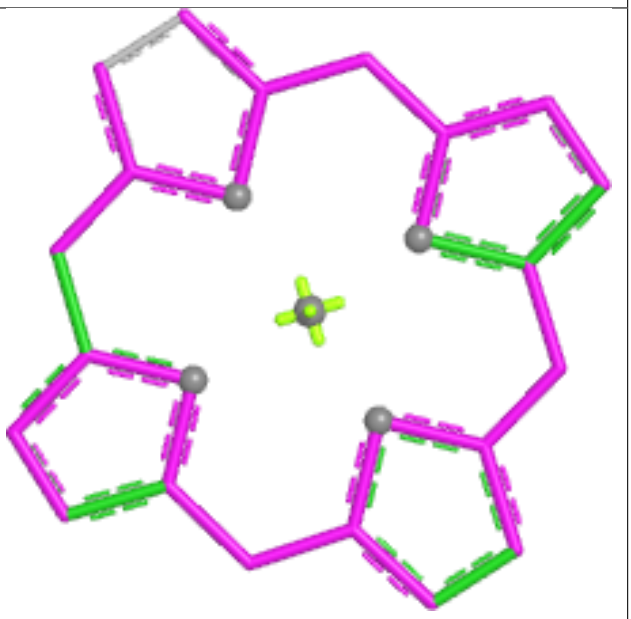


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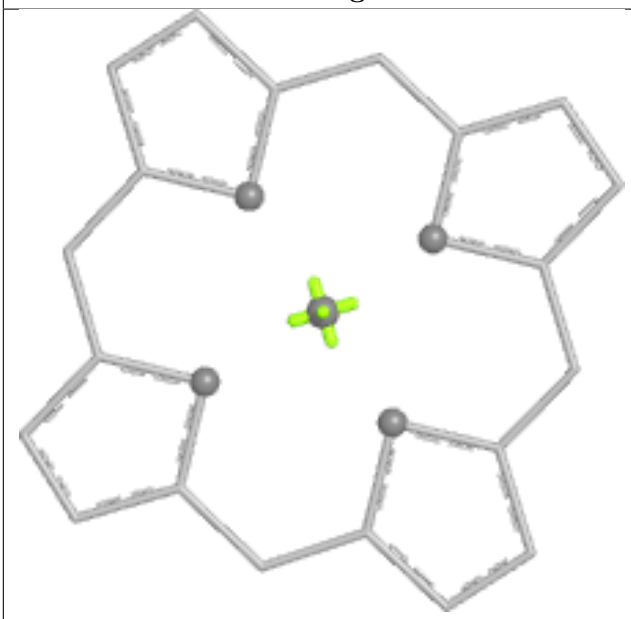
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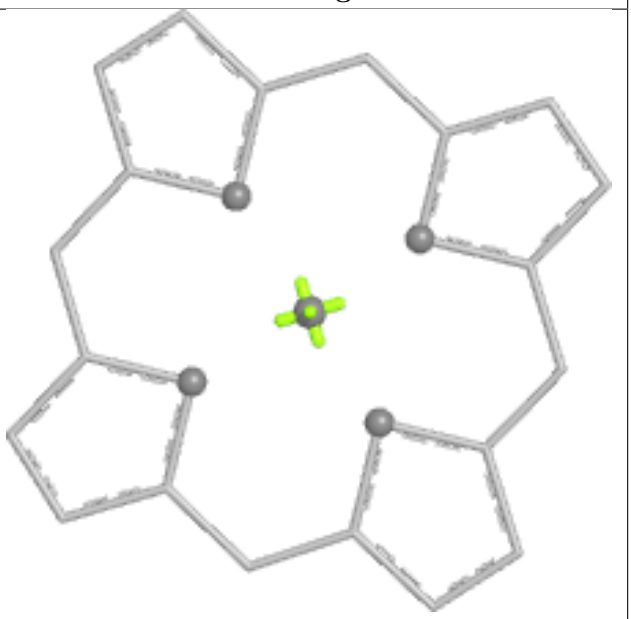
Bond lengths



Bond angles

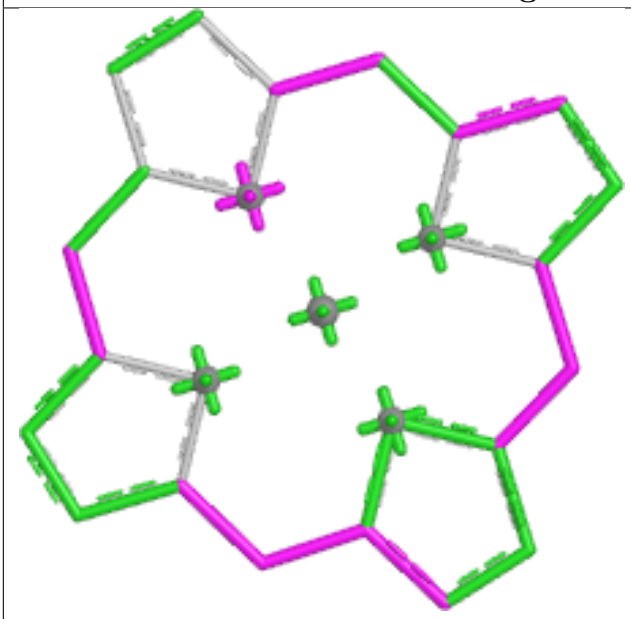


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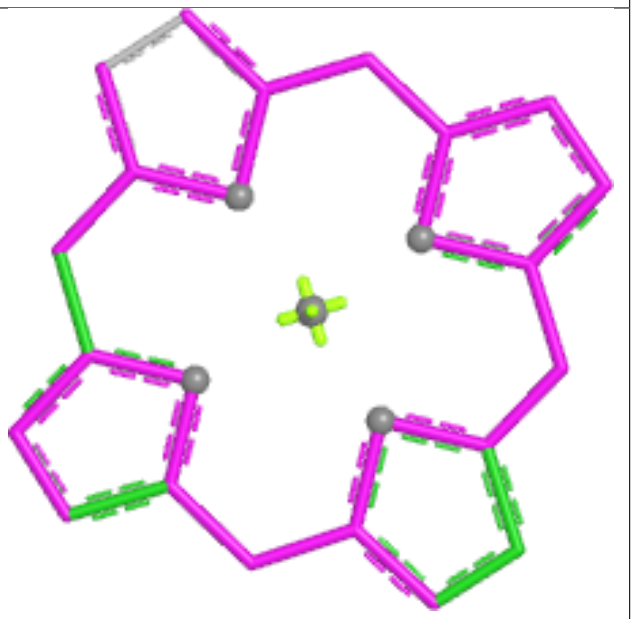


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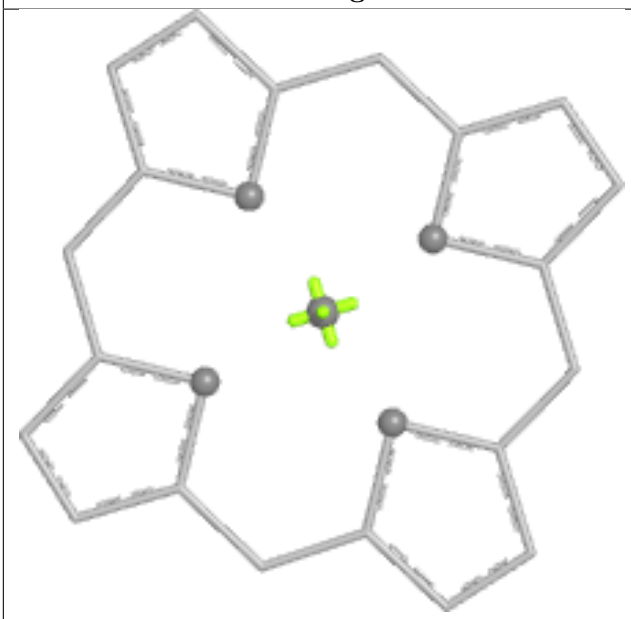
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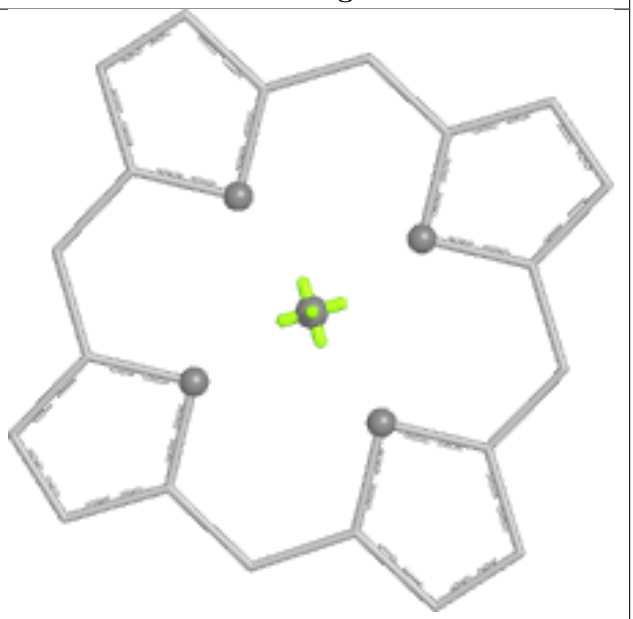
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Bond angles

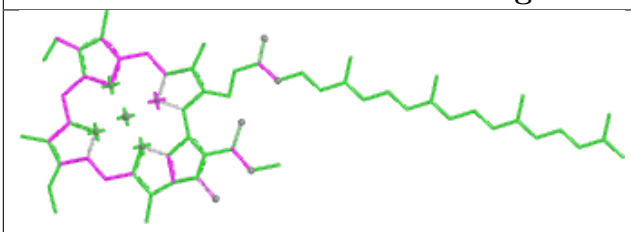


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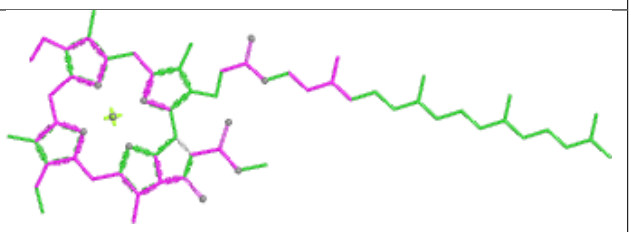


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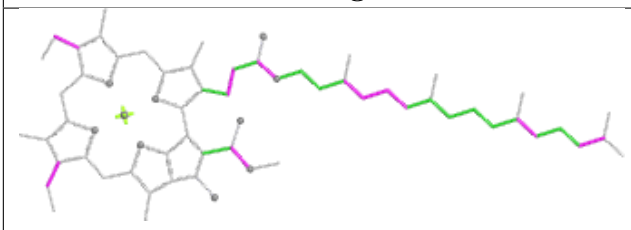
Ligand CLA A 1115



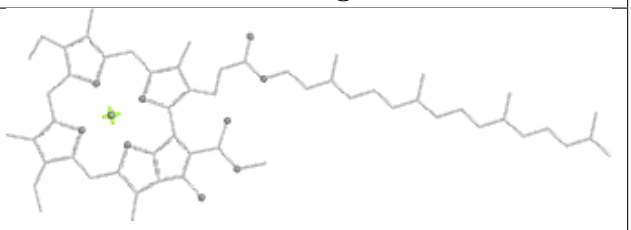
Bond lengths



Bond angles

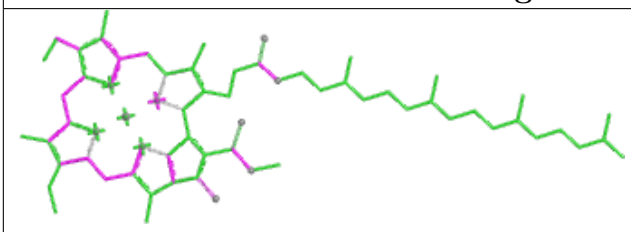


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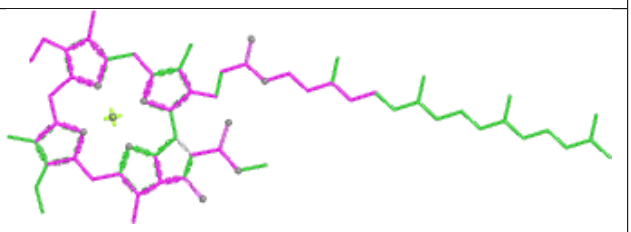


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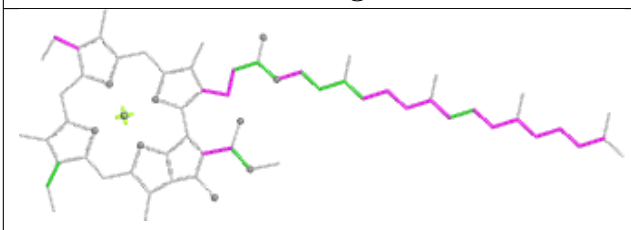
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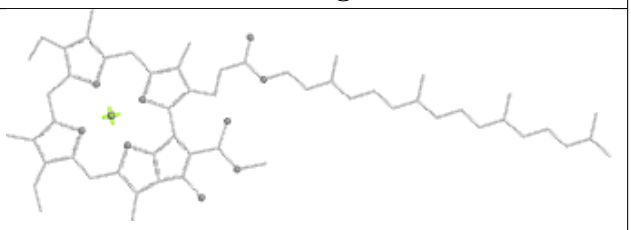
Bond lengths



Bond angles



Torsions

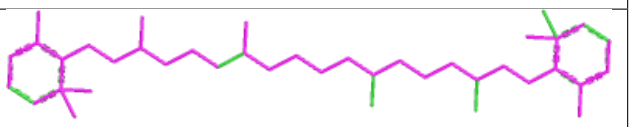


Rings

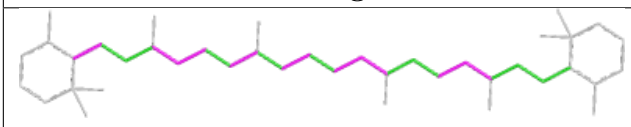
Ligand BCR F 6016



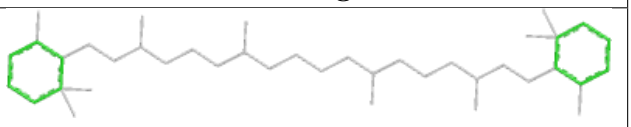
Bond lengths



Bond angles

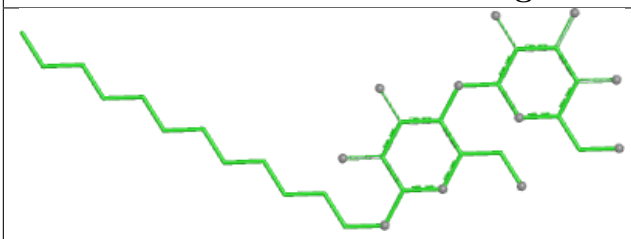


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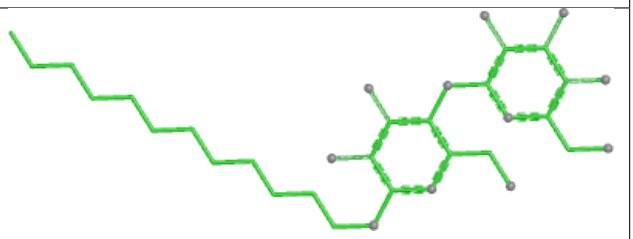


Rings

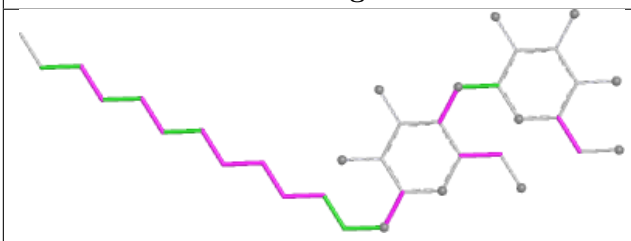
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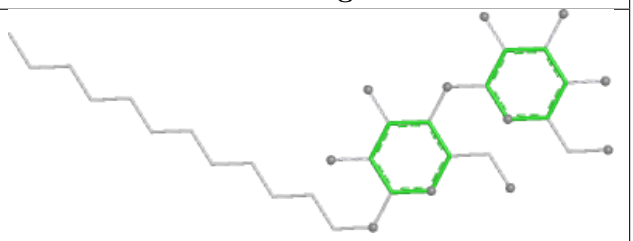
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Bond angles

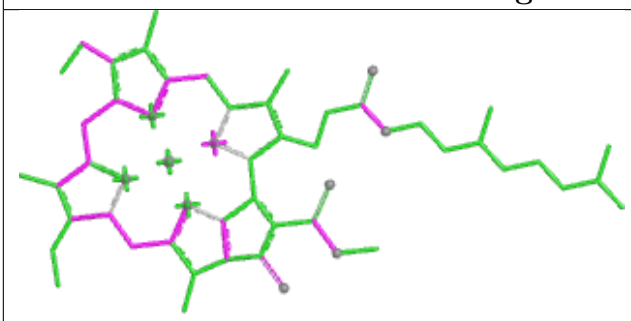


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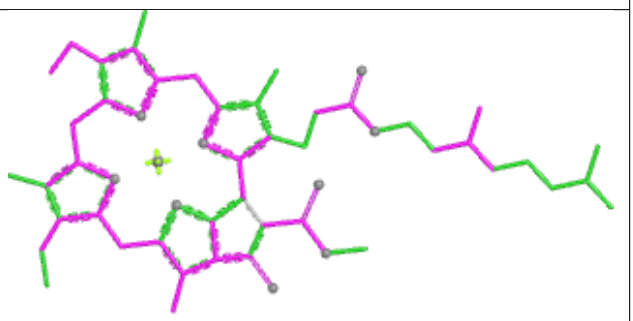


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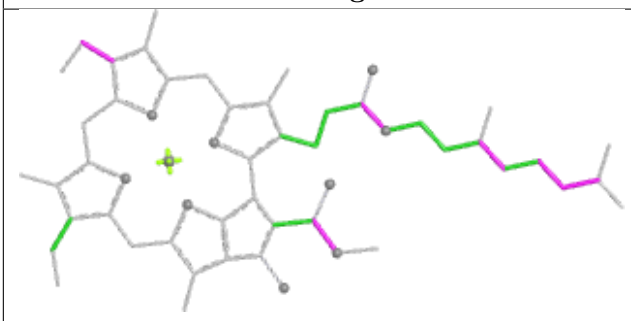
Ligand CLA B 1209



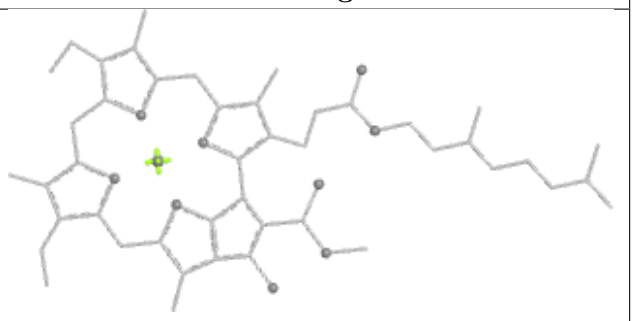
Bond lengths



Bond angles

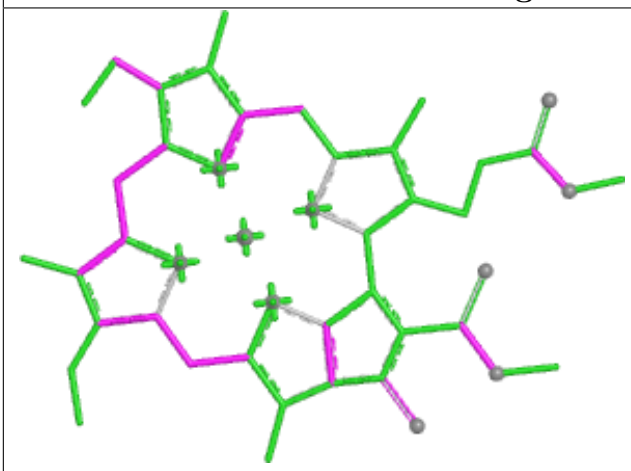


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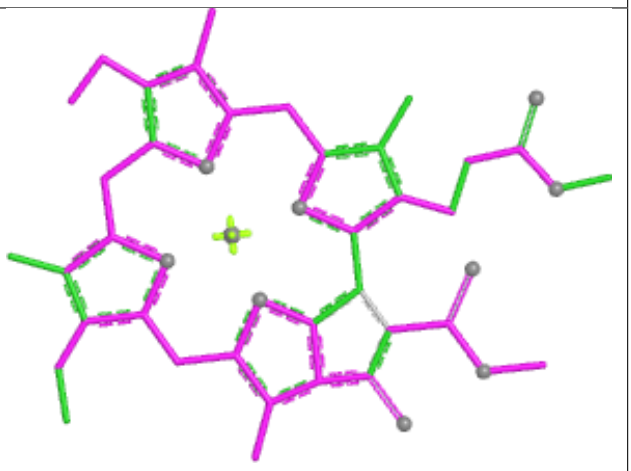


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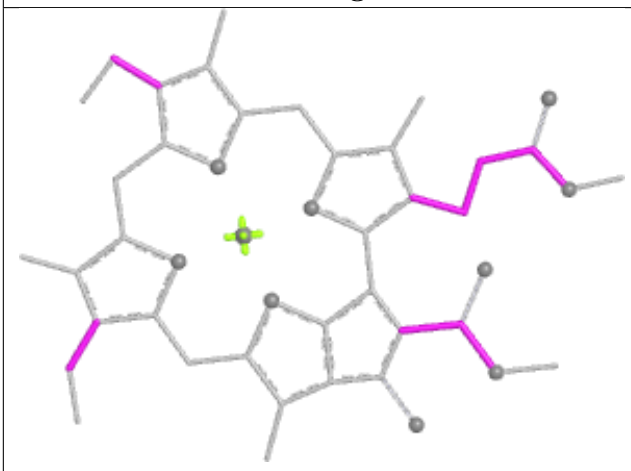
Ligand CLA B 1213



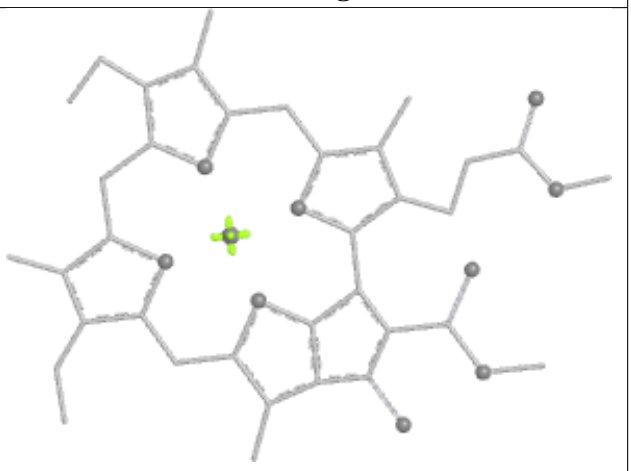
Bond lengths



Bond angles

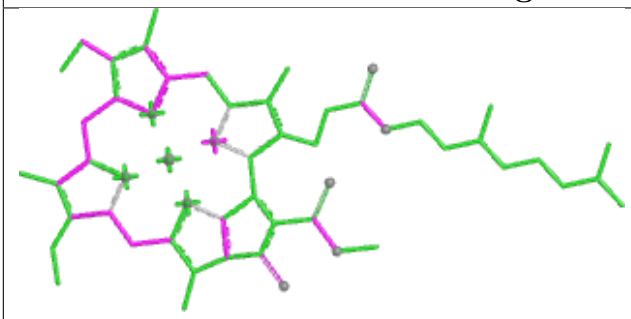


Torsions

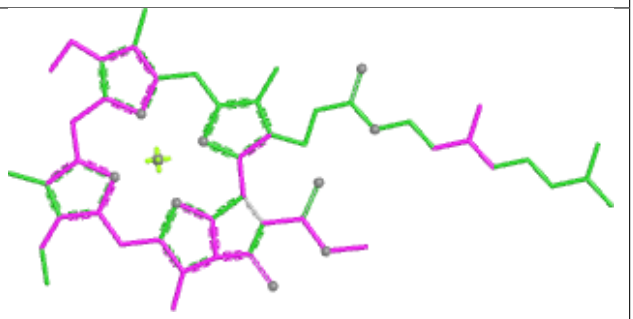


Rings

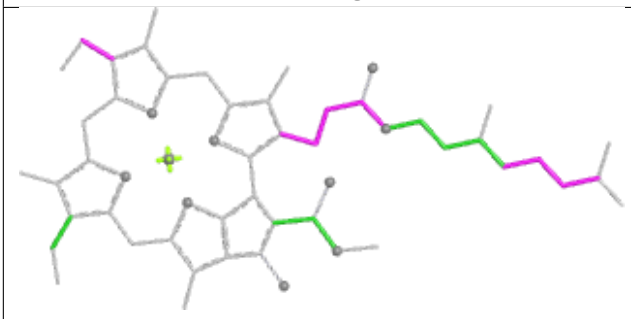
Ligand CLA B 1219



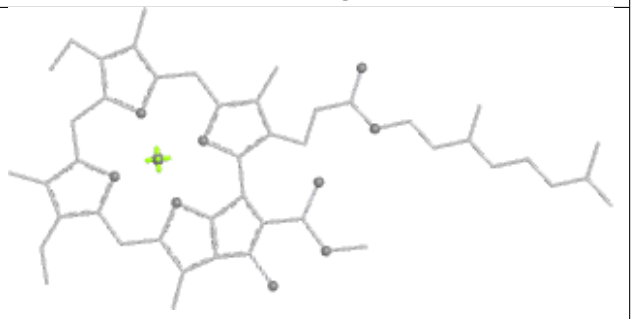
Bond lengths



Bond angles

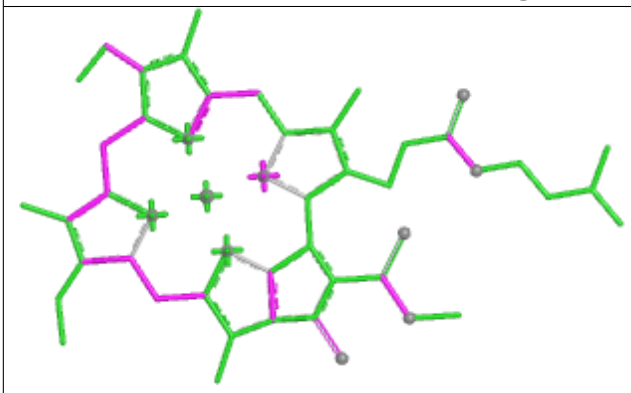


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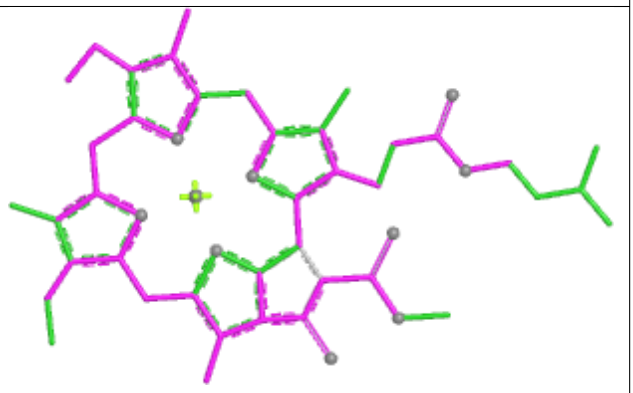


Rings

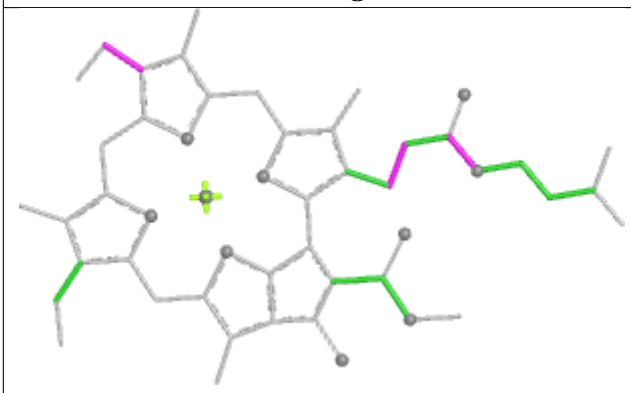
Ligand CLA A 1129



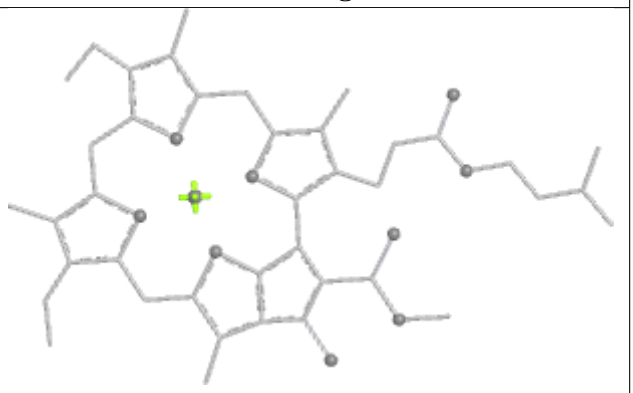
Bond lengths



Bond angles

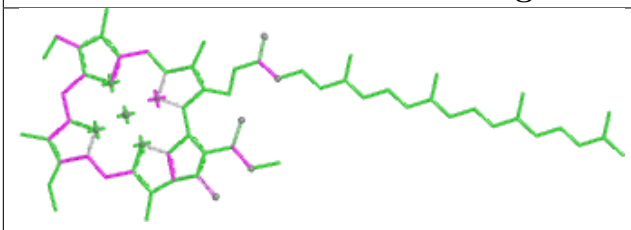


Torsions

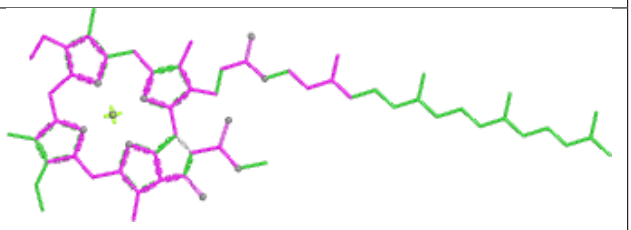


Rings

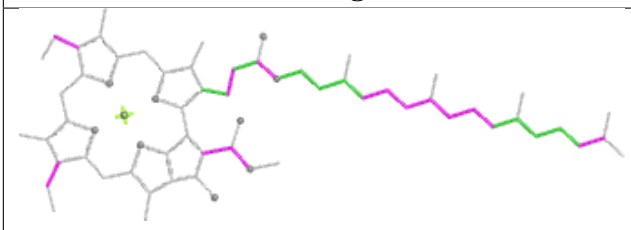
Ligand CLA B 1238



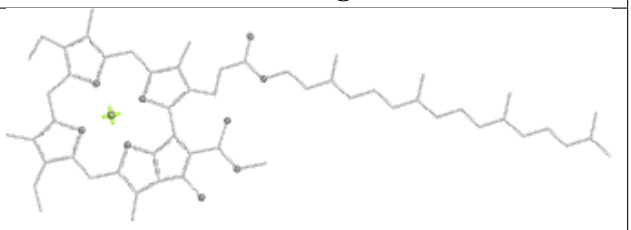
Bond lengths



Bond angles

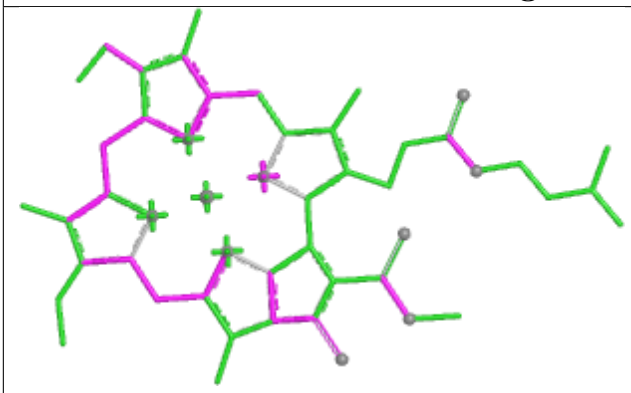


Torsions

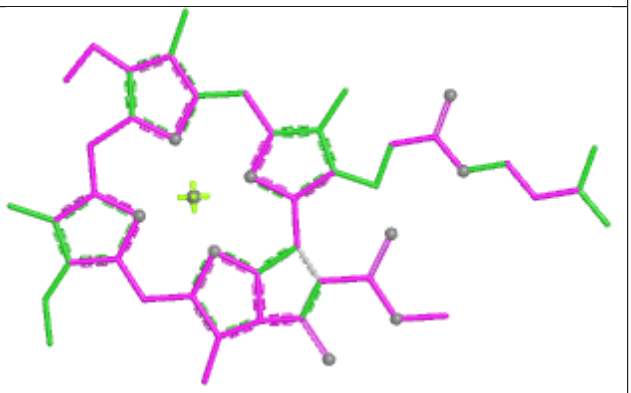


Rings

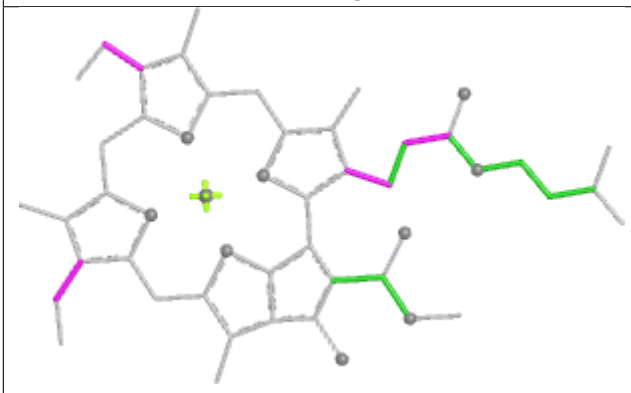
Ligand CLA 3 3008



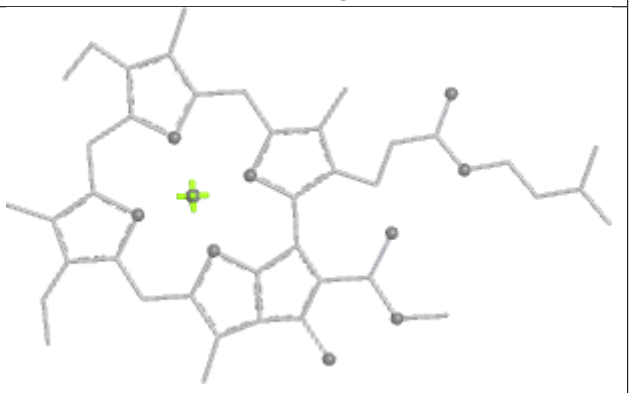
Bond lengths



Bond angles

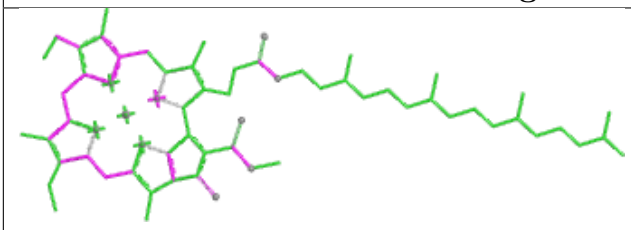


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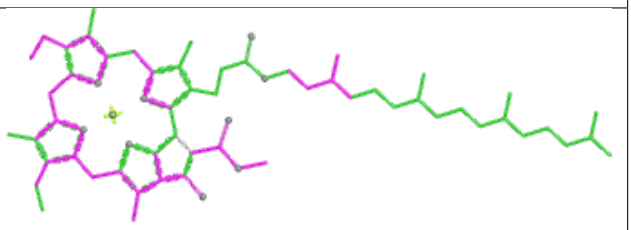


Rings

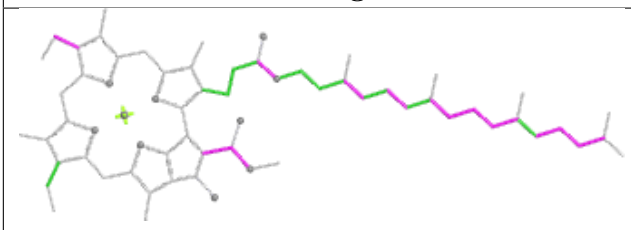
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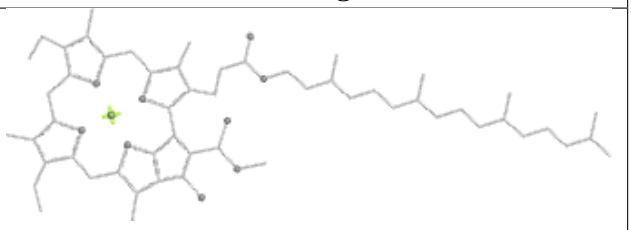
Bond lengths



Bond angles

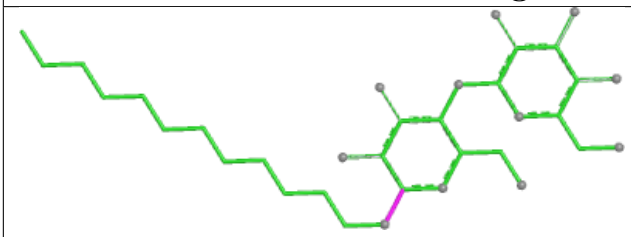


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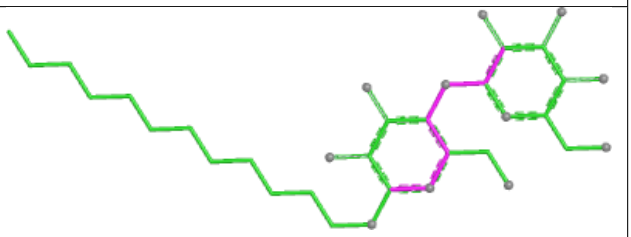


Rings

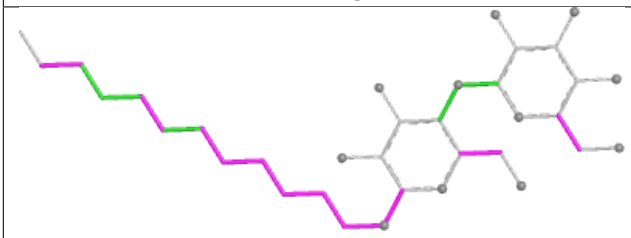
Ligand LMU R 7025



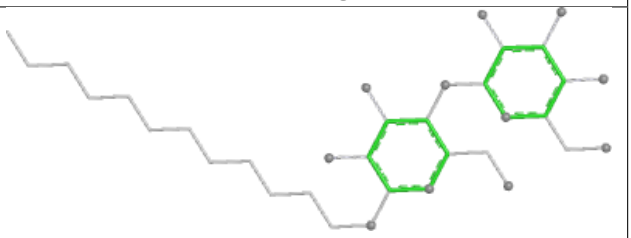
Bond lengths



Bond angles

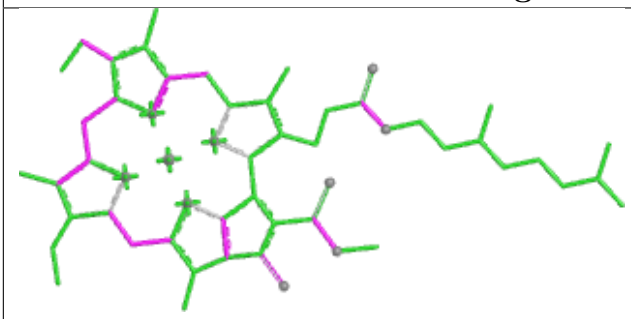


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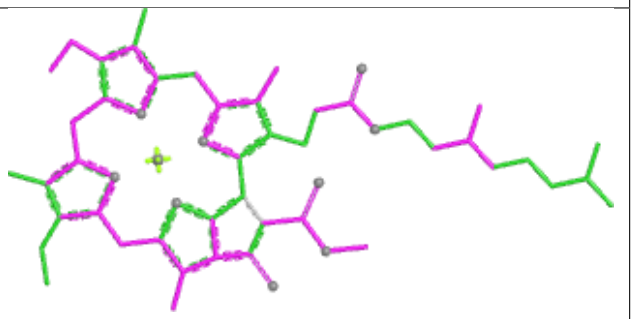


Rings

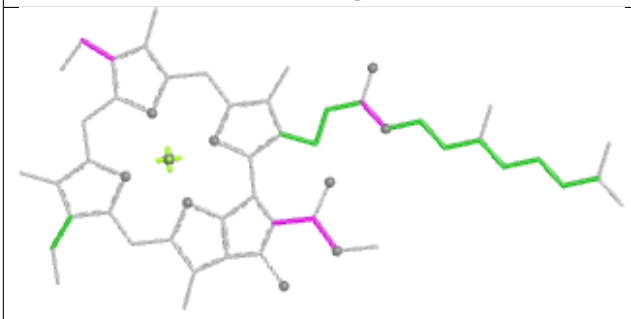
Ligand CLA H 1241



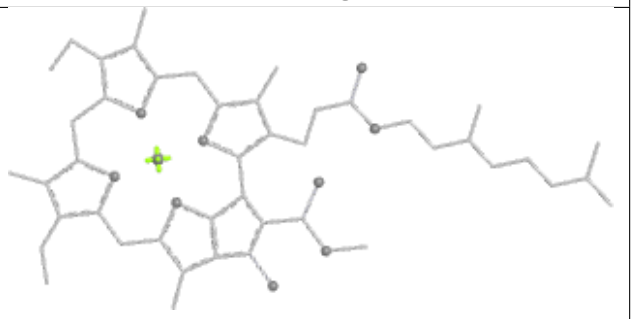
Bond lengths



Bond angles

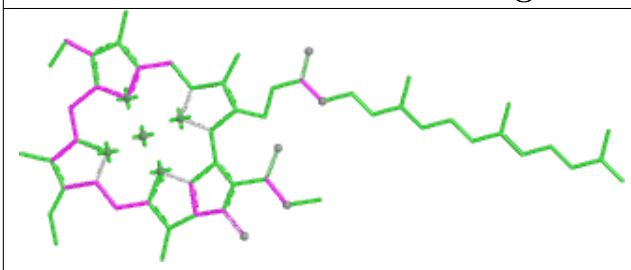


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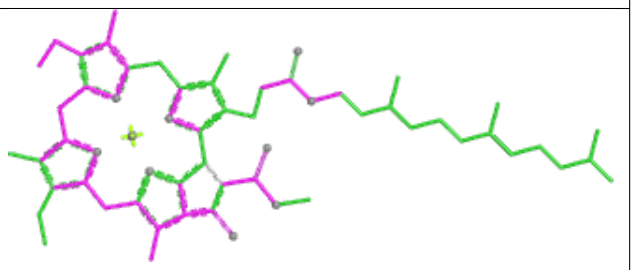


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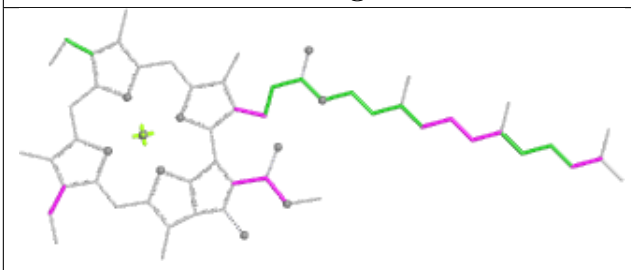
Ligand CLA B 1234



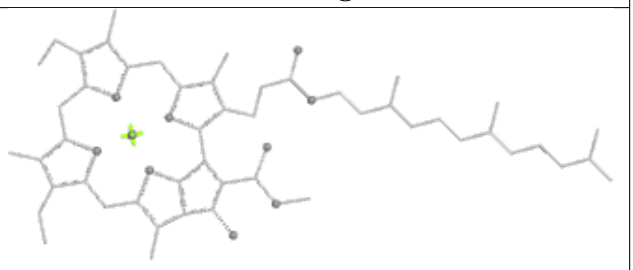
Bond lengths



Bond angles

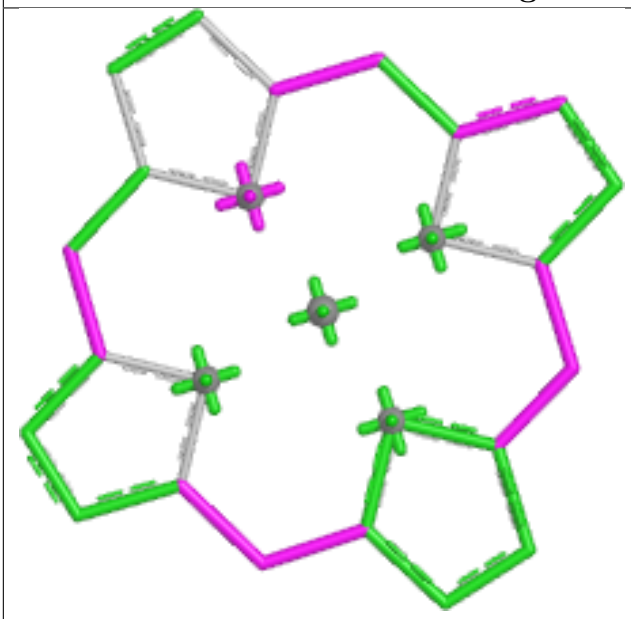


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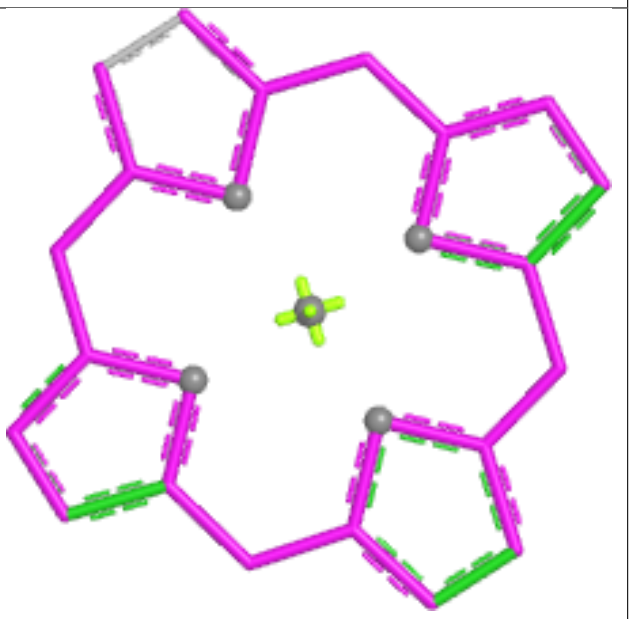


Rings

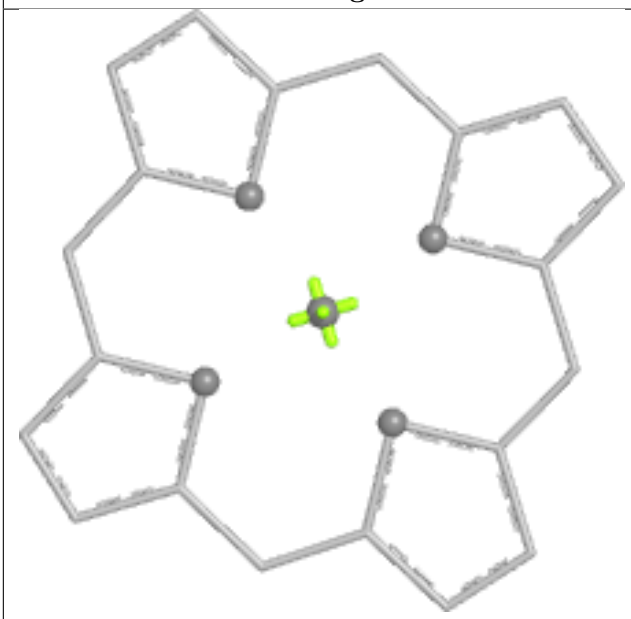
Ligand CLA 2 1307



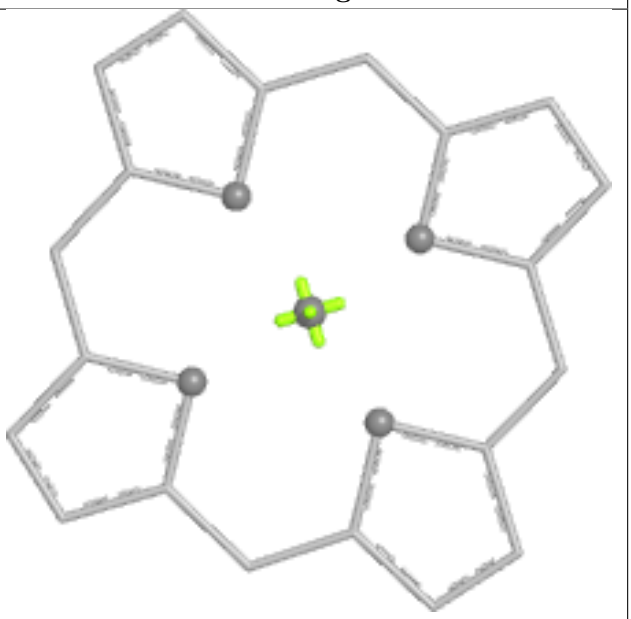
Bond lengths



Bond angles

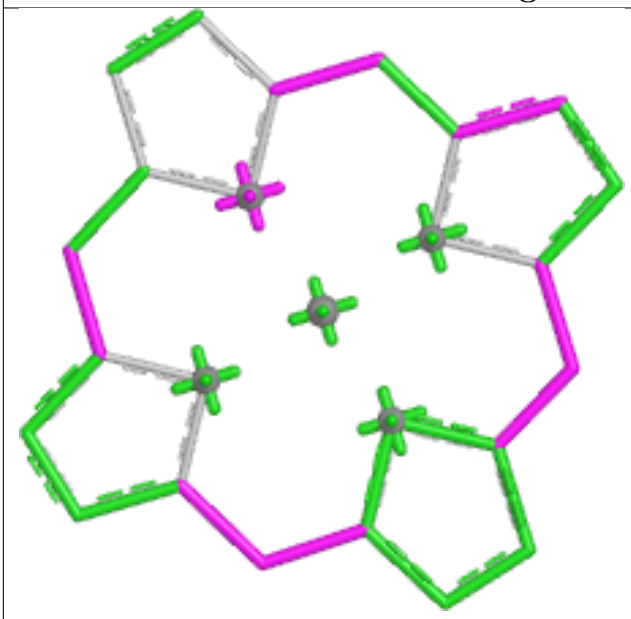


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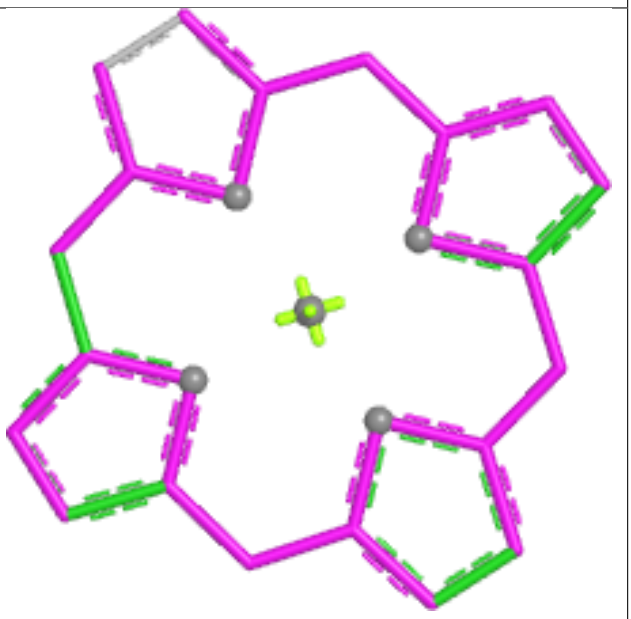


Rings

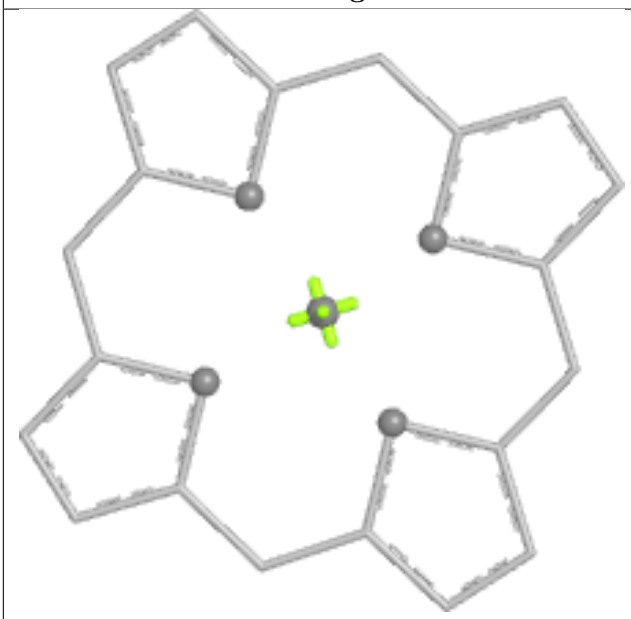
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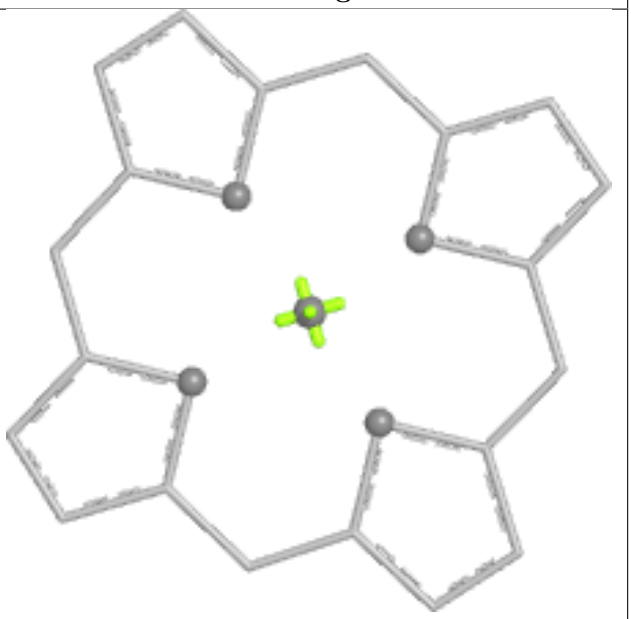
Bond lengths



Bond angles

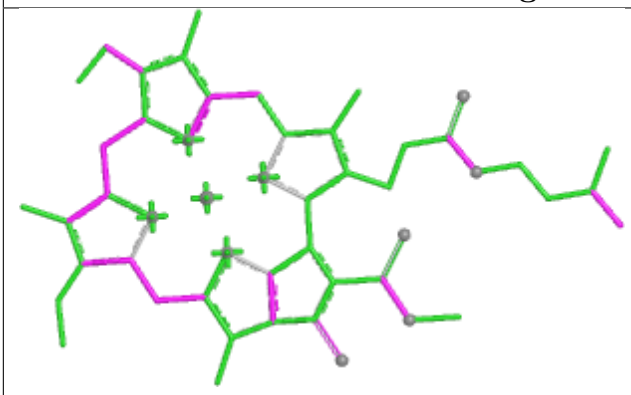


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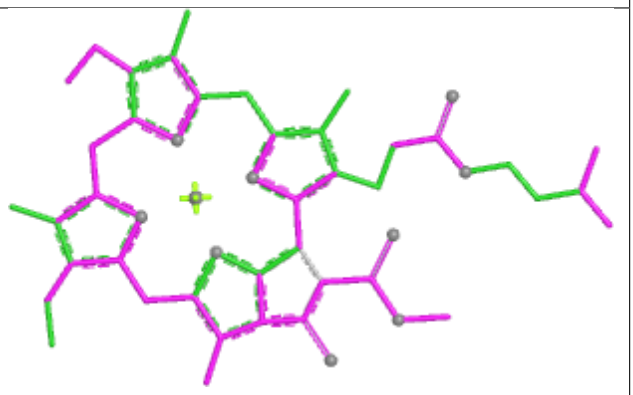


Rings

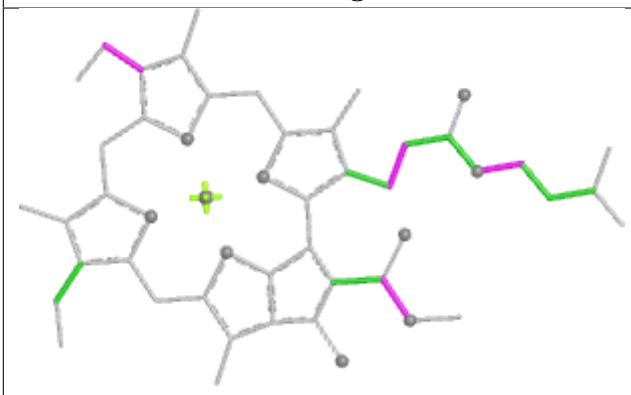
Ligand CLA 4 4001



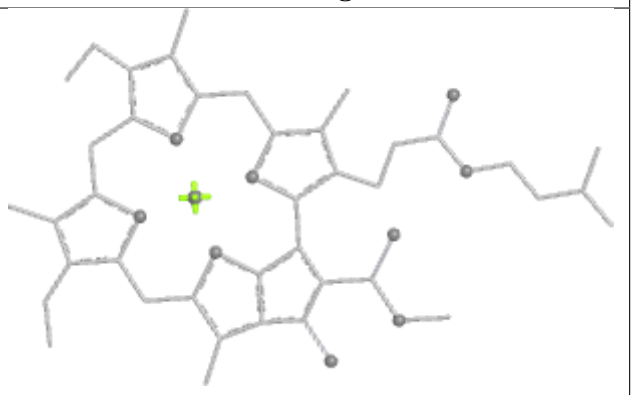
Bond lengths



Bond angles



Torsions

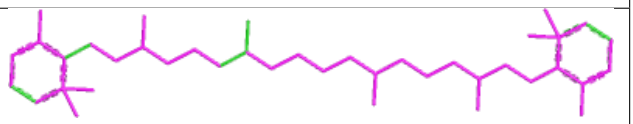


Rings

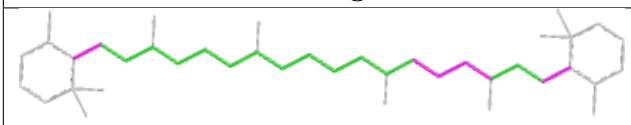
Ligand BCR B 6005



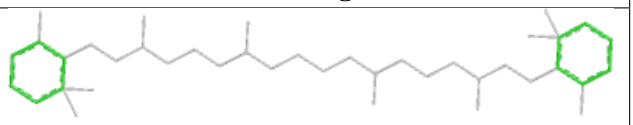
Bond lengths



Bond angles

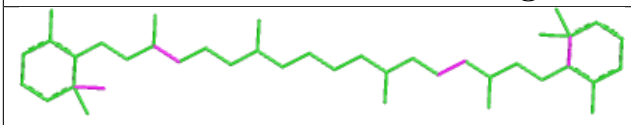


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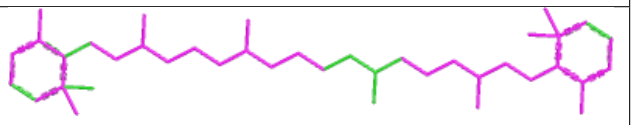


Rings

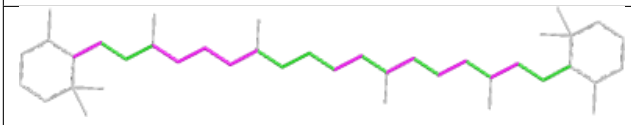
Ligand BCR I 6018



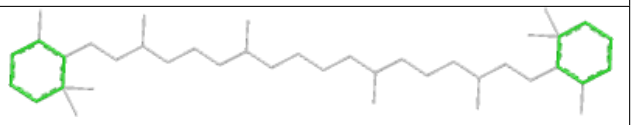
Bond lengths



Bond angles

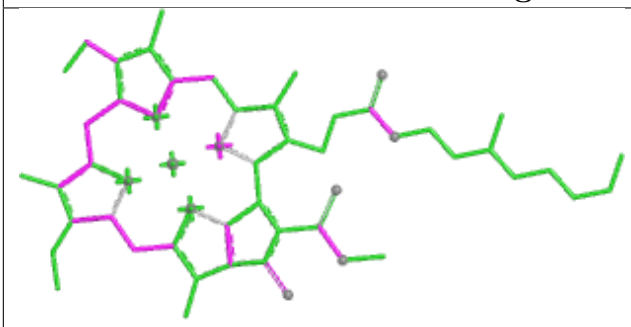


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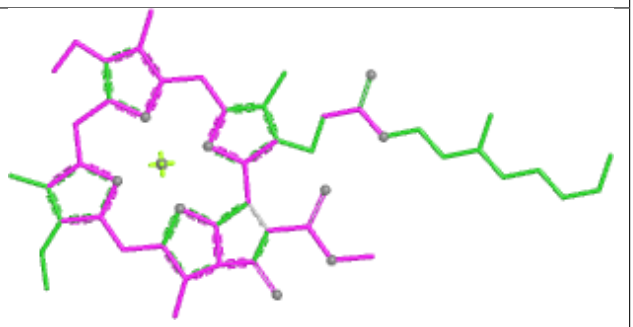


Rings

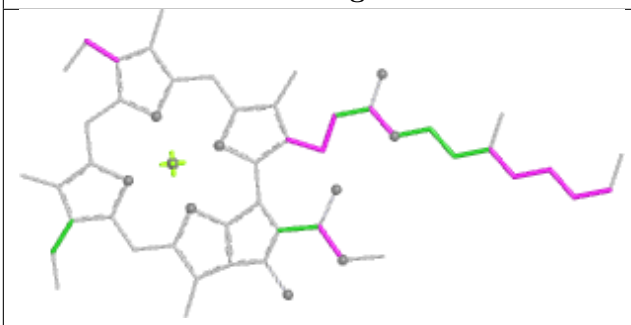
Ligand CLA A 1110



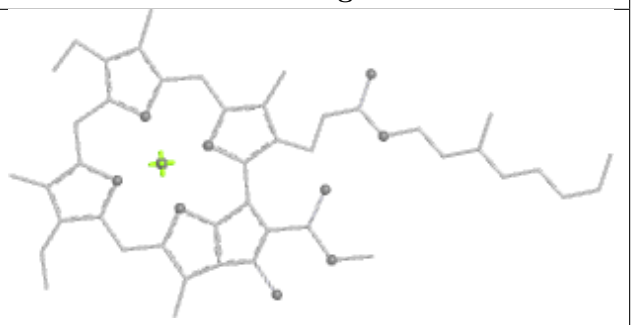
Bond lengths



Bond angles

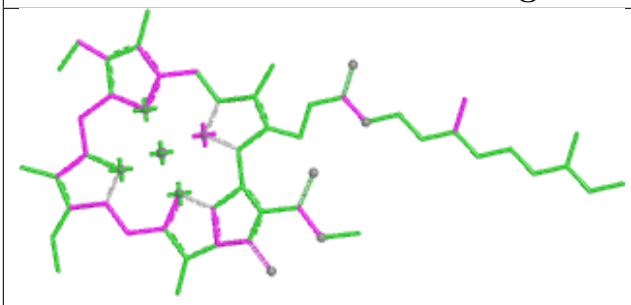


Torsions

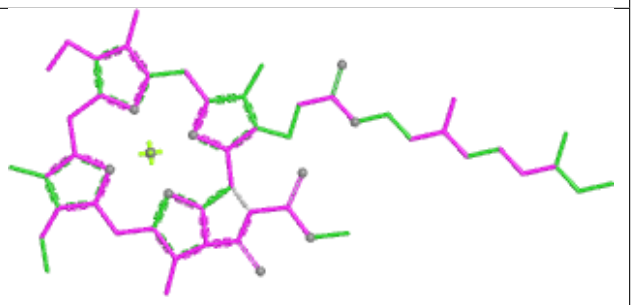


Rings

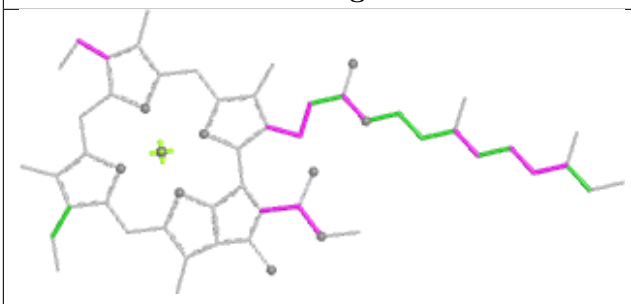
Ligand CLA 3 2009



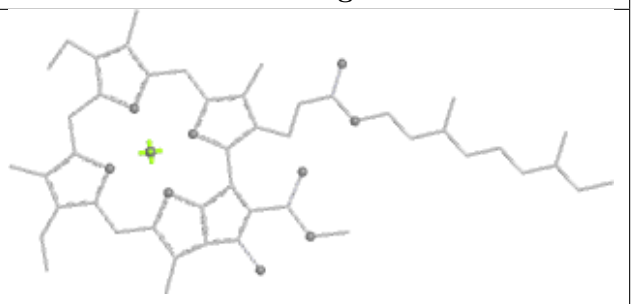
Bond lengths



Bond angles

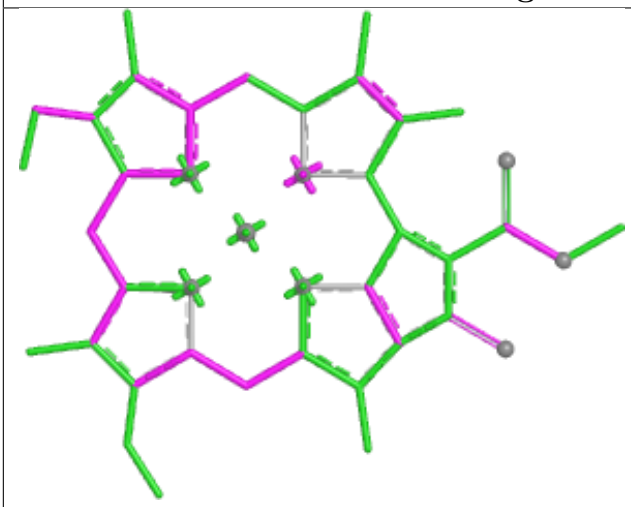


Torsions

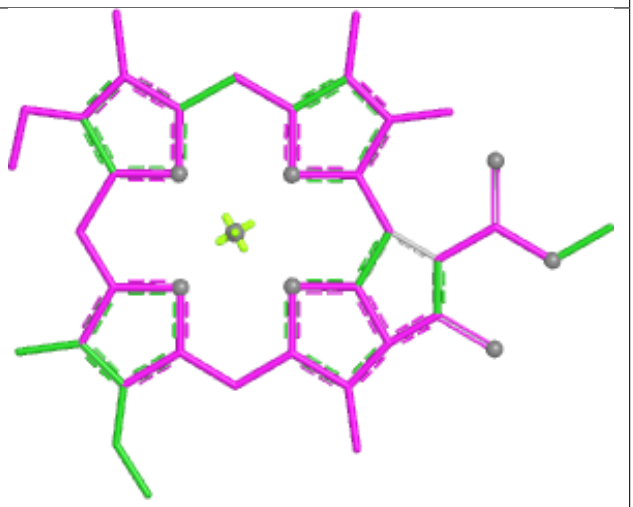


Rings

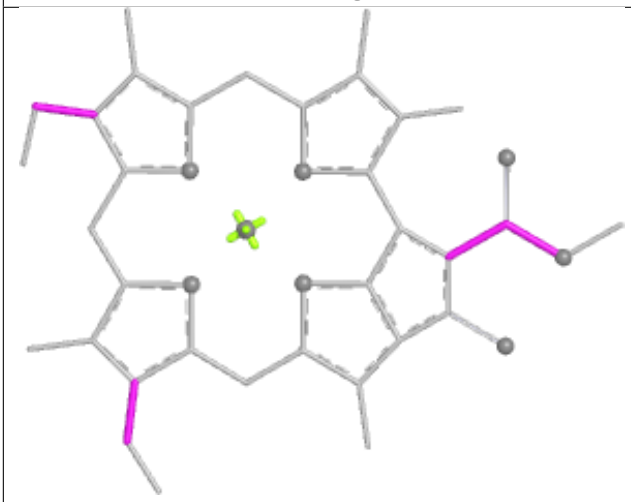
Ligand CLA F 1302



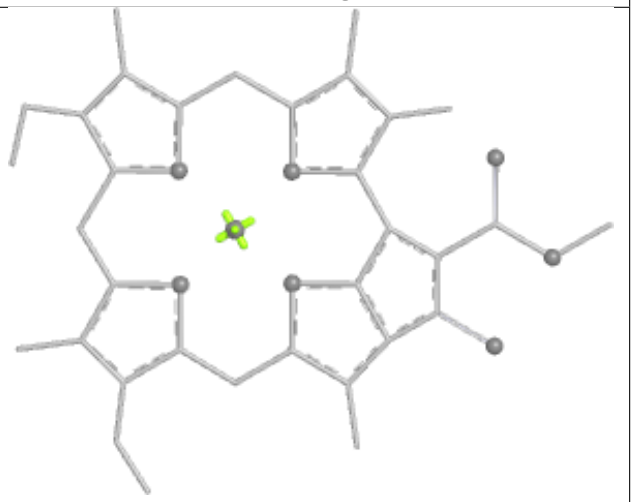
Bond lengths



Bond angles

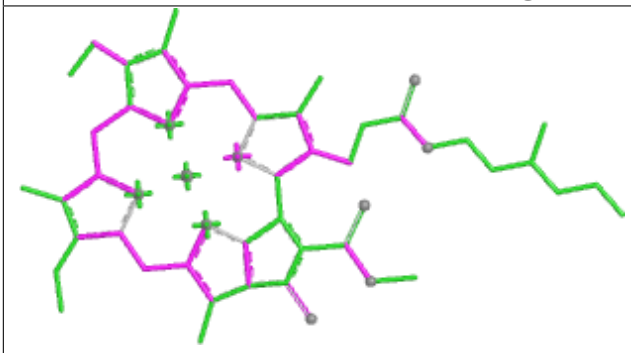


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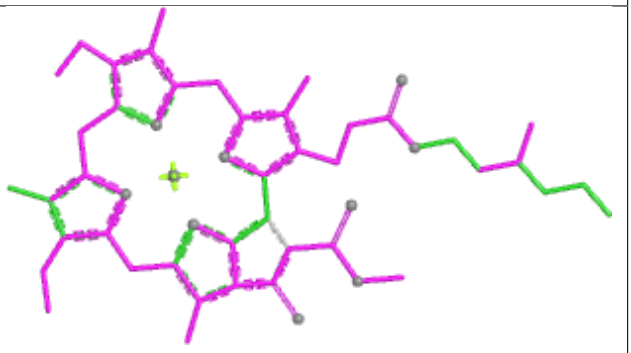


Rings

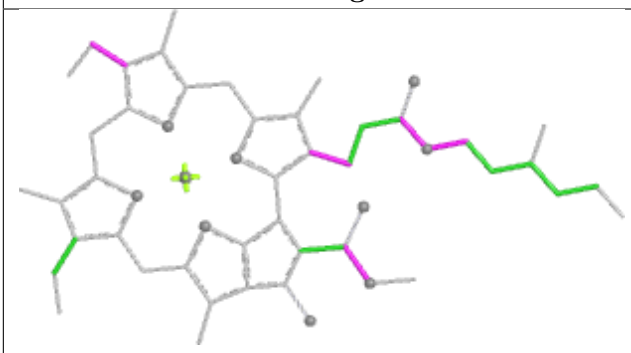
Ligand CLA 4 4002



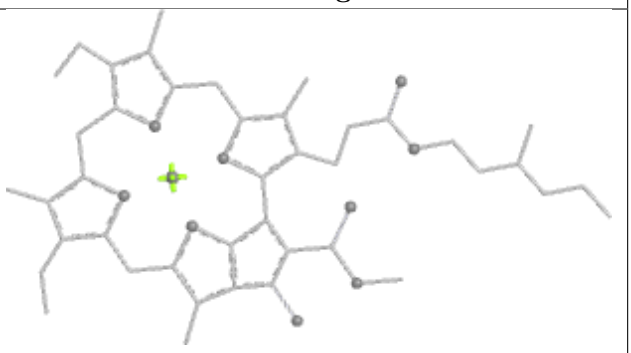
Bond lengths



Bond angles

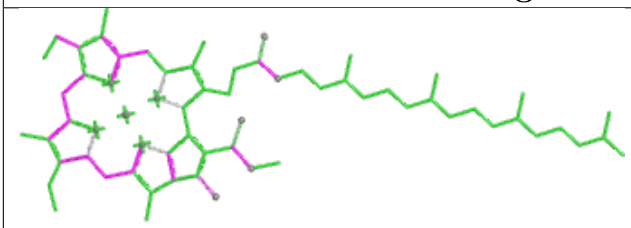


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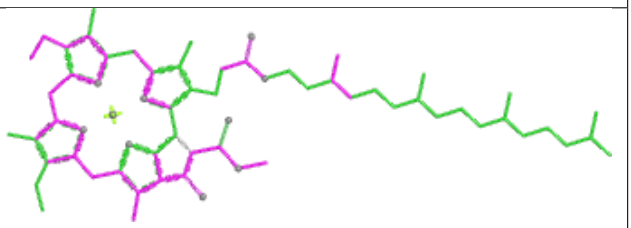


Rings

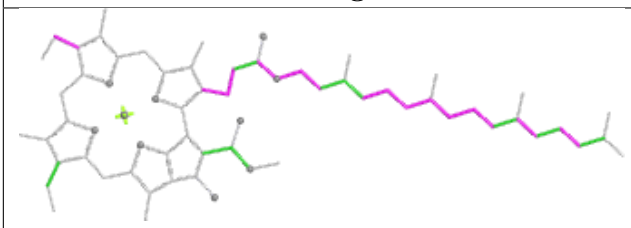
Ligand CLA B 1206



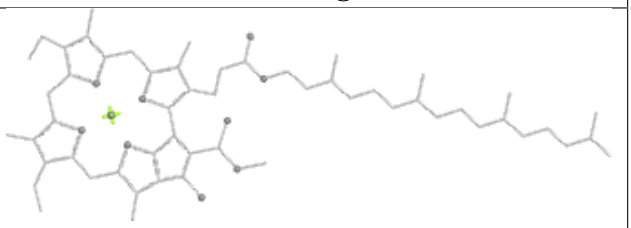
Bond lengths



Bond angles

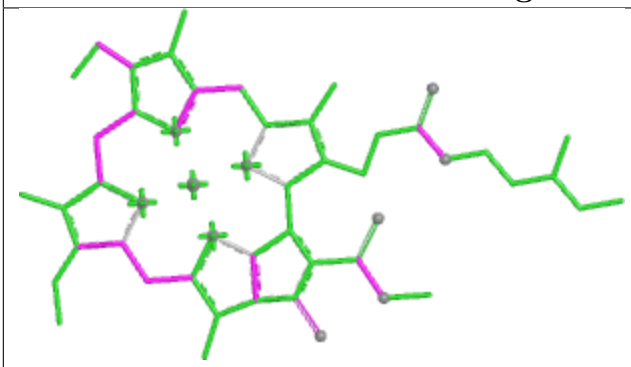


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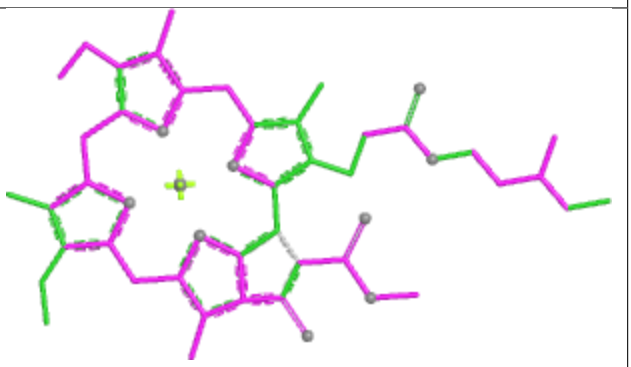


Rings

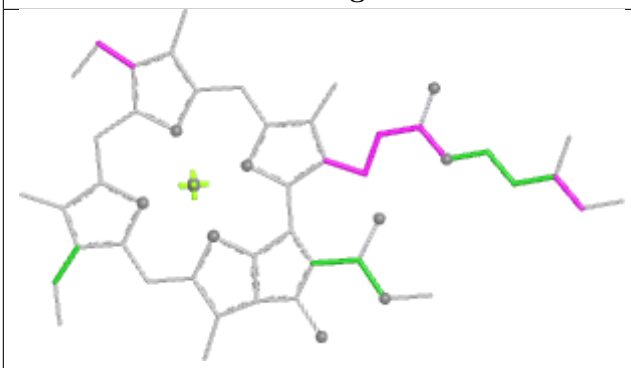
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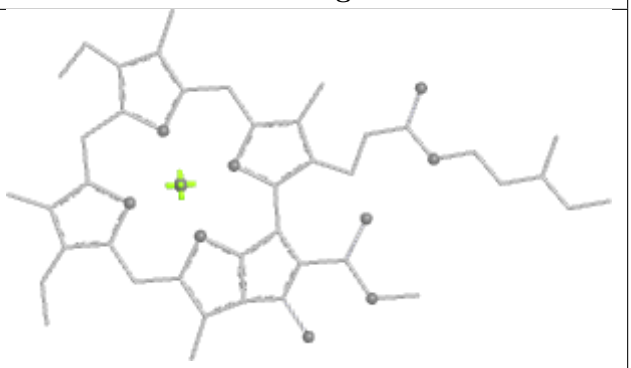
Bond lengths



Bond angles

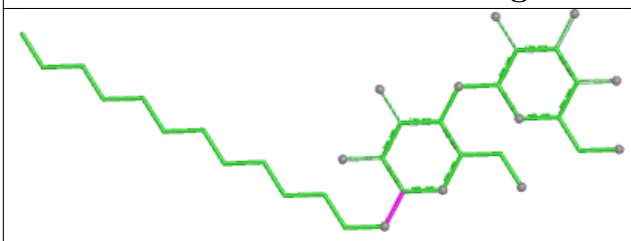


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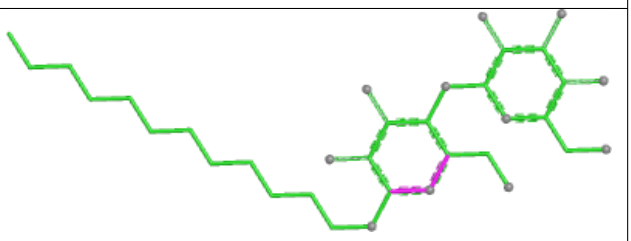


Rings

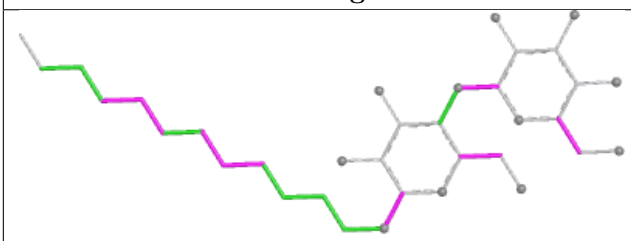
Ligand LMU D 7050



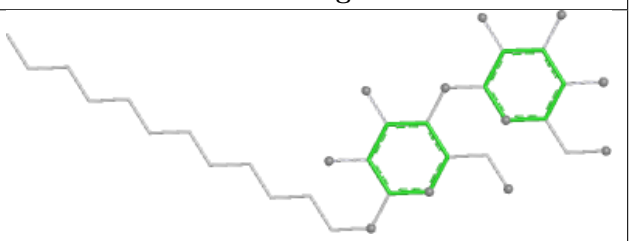
Bond lengths



Bond angles

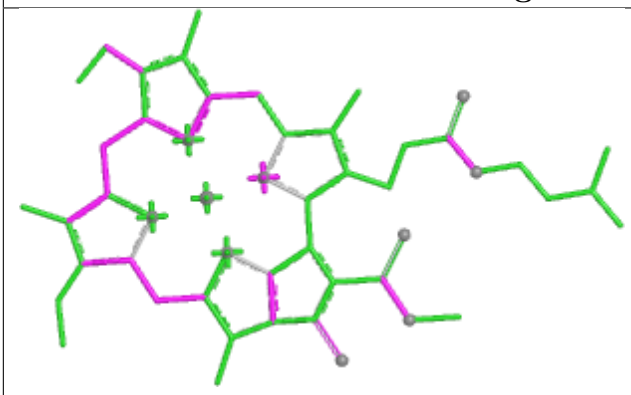


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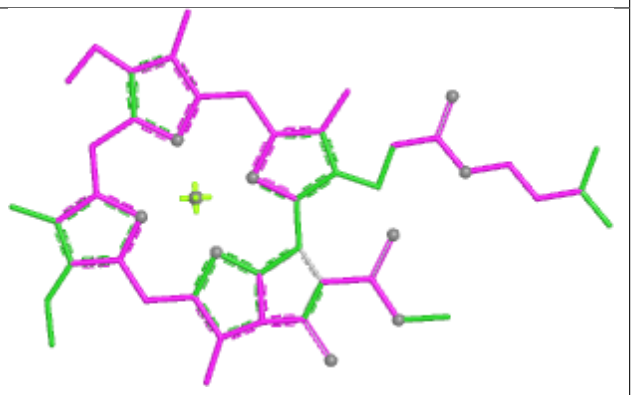


Rings

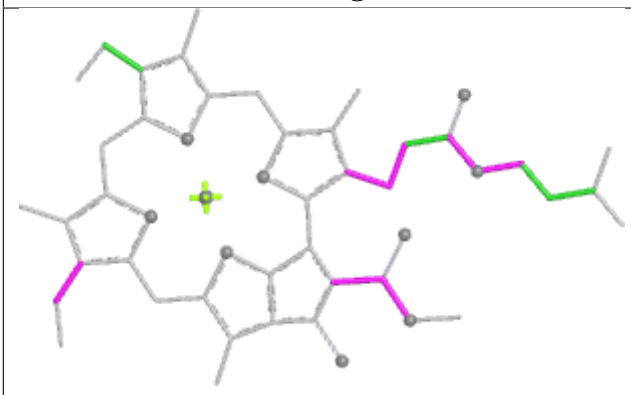
Ligand CLA A 1133



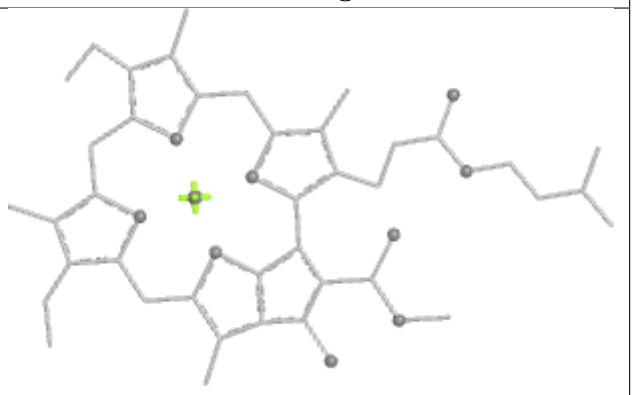
Bond lengths



Bond angles

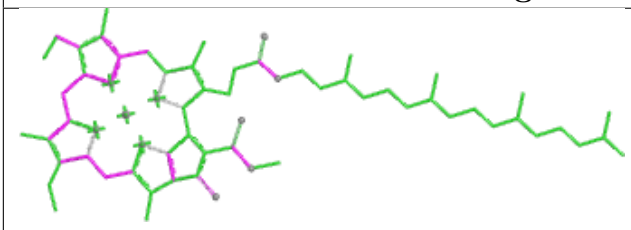


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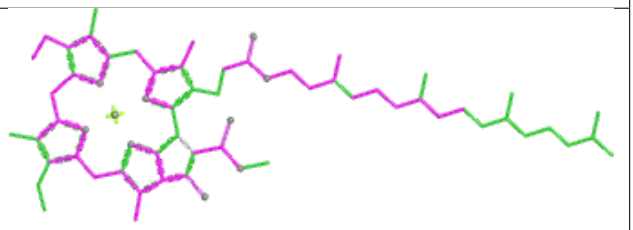


Rings

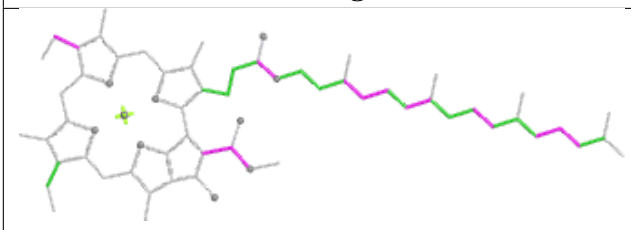
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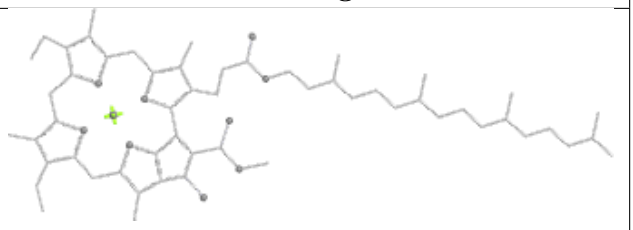
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Bond angles

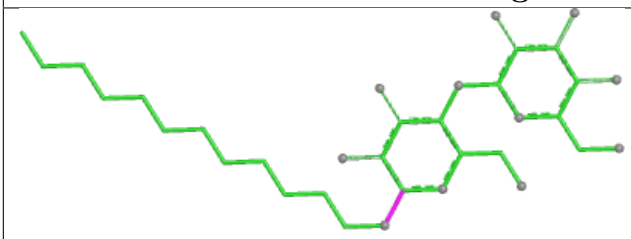


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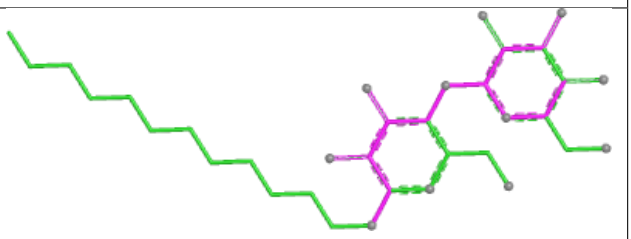


Rings

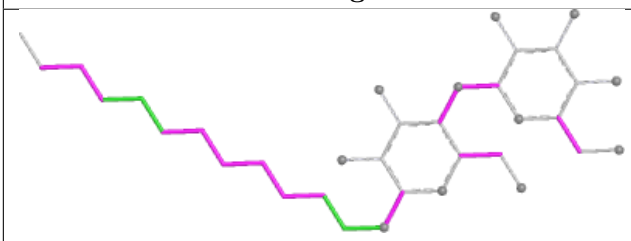
Ligand LMU B 7040



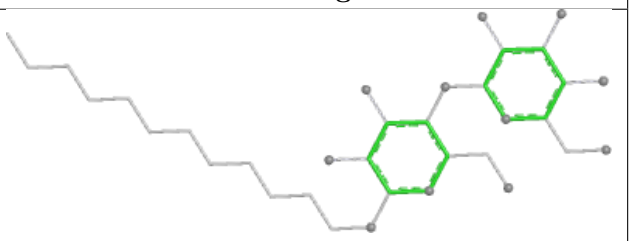
Bond lengths



Bond angles

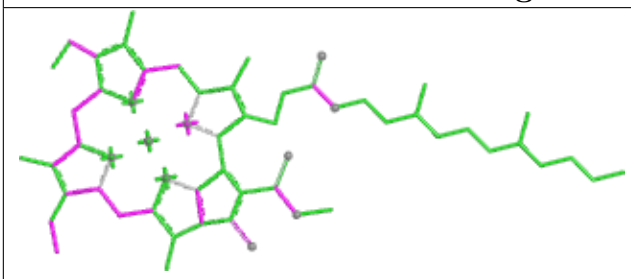


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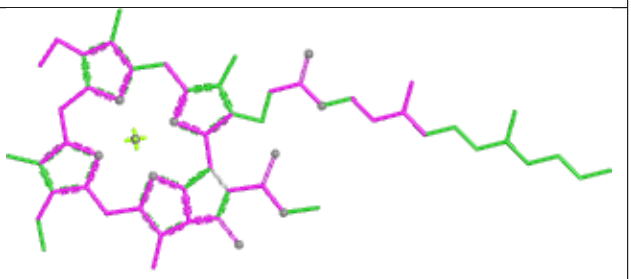


Rings

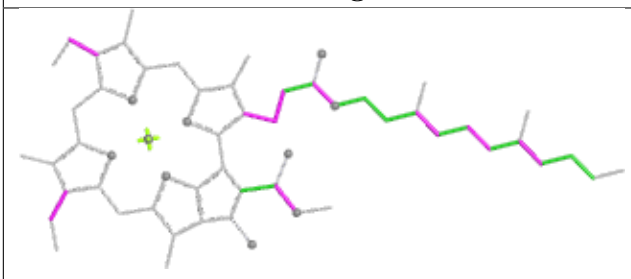
Ligand CLA B 1222



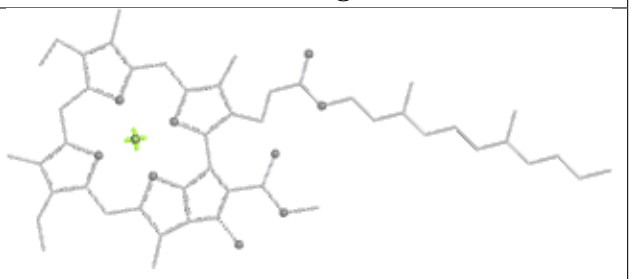
Bond lengths



Bond angles

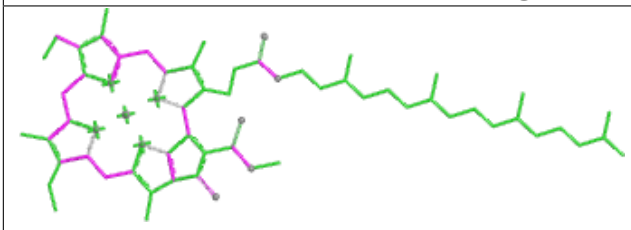


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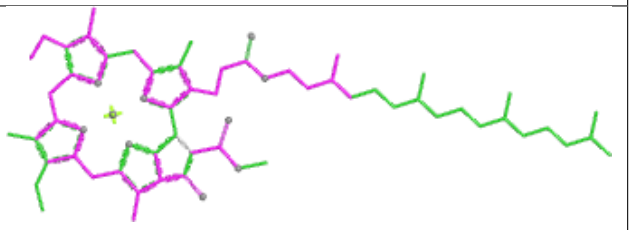


Rings

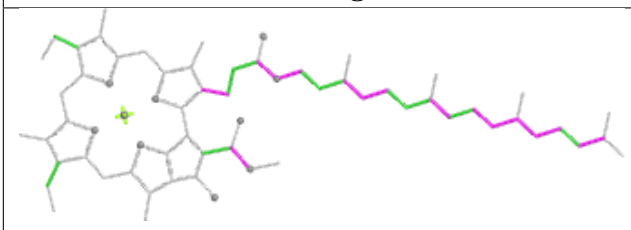
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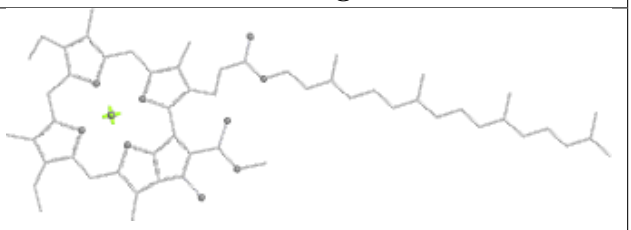
Bond lengths



Bond angles

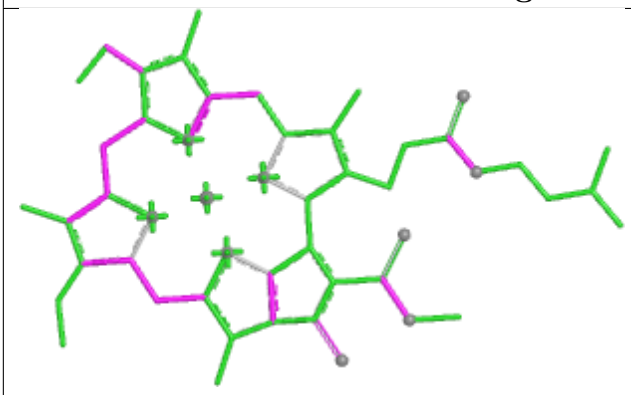


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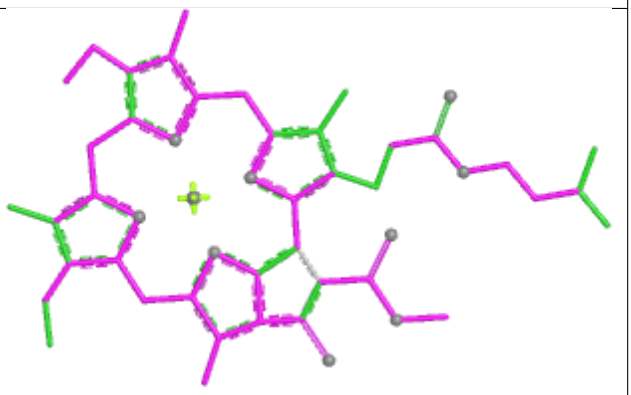


Rings

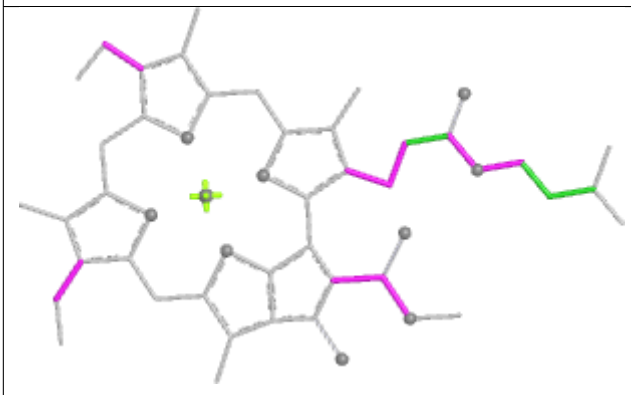
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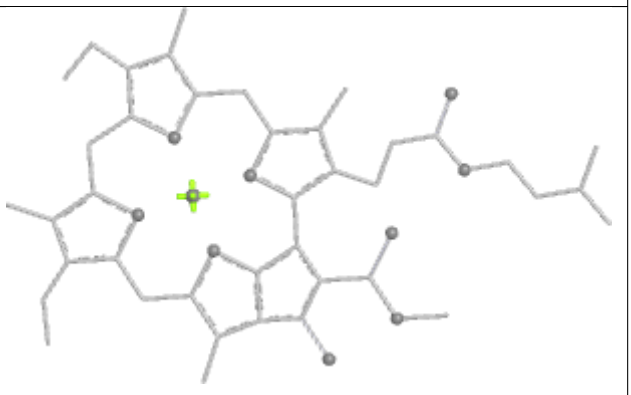
Bond lengths



Bond angles

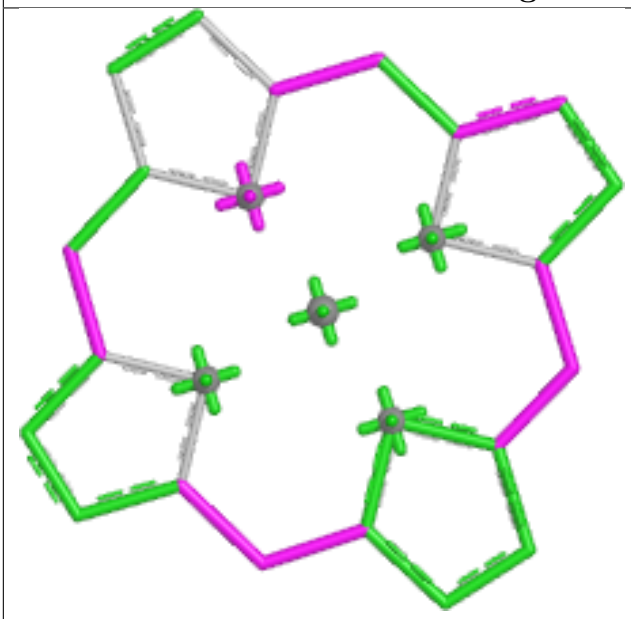


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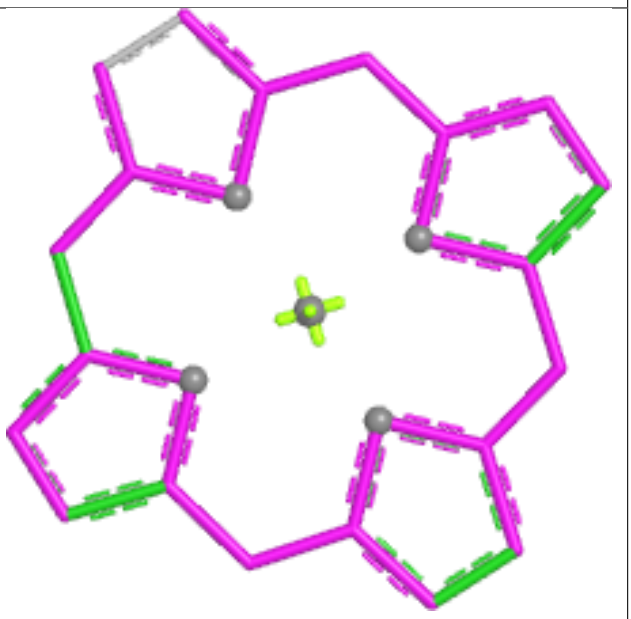


Rings

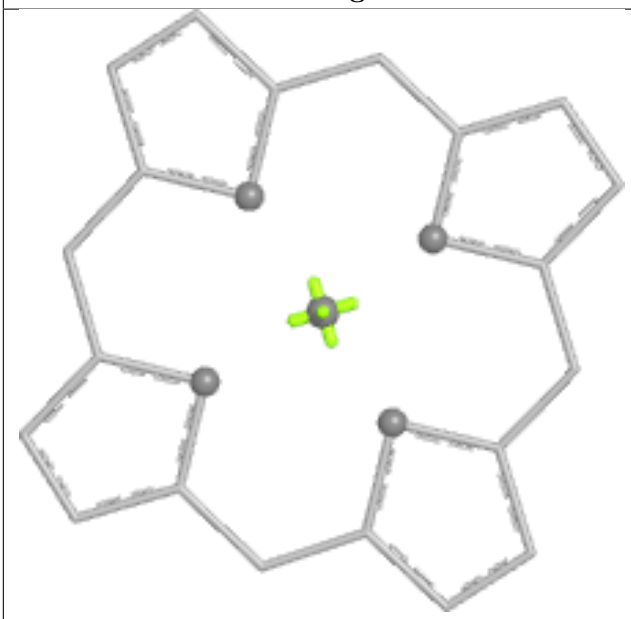
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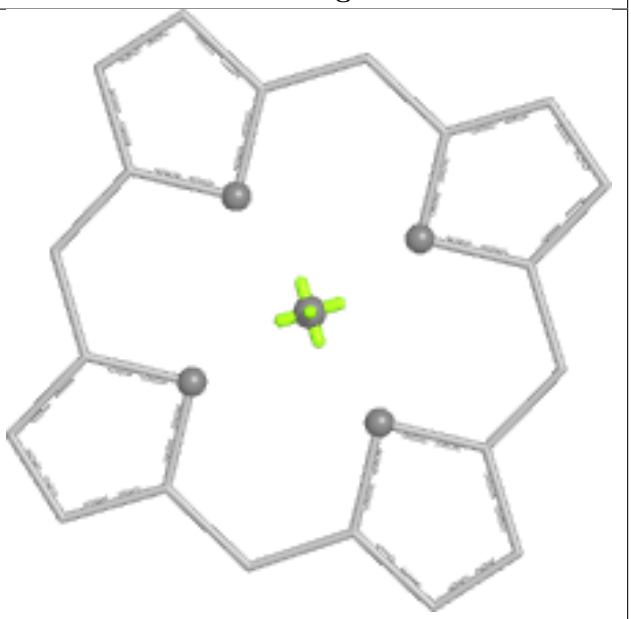
Bond lengths



Bond angles

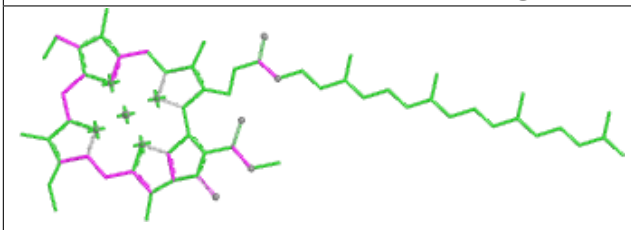


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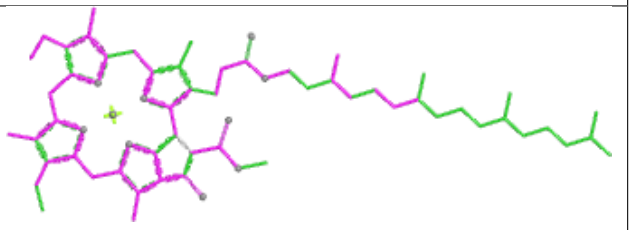


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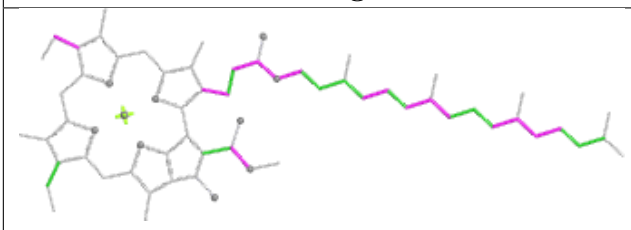
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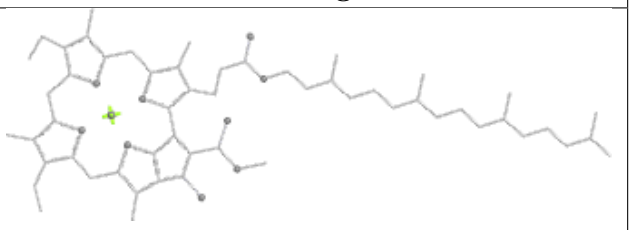
Bond lengths



Bond angles

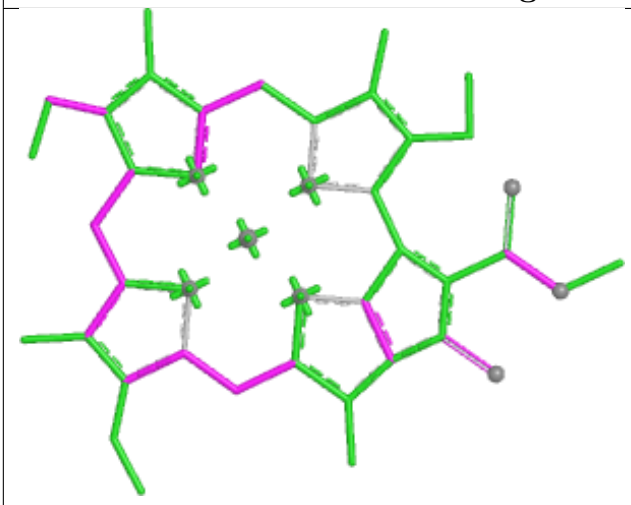


Torsions

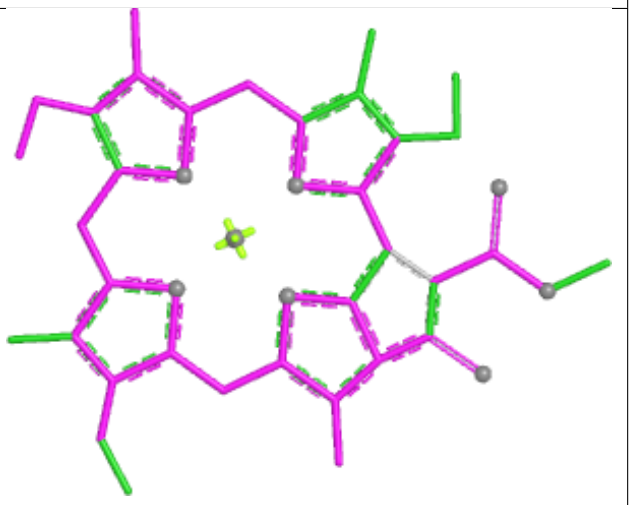


Rings

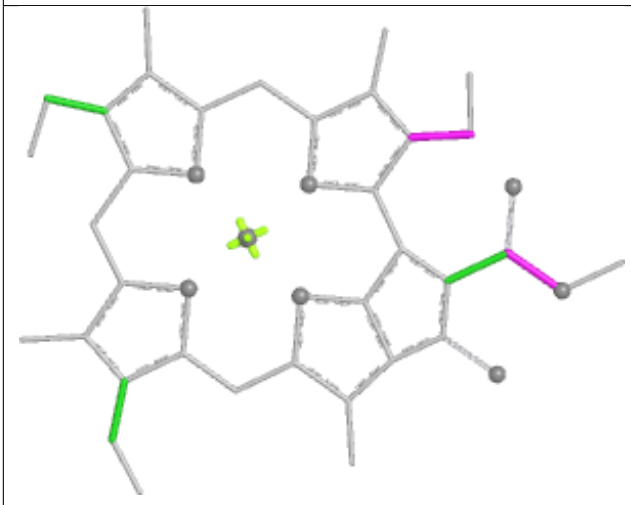
Ligand CLA 3 3007



Bond lengths



Bond angles

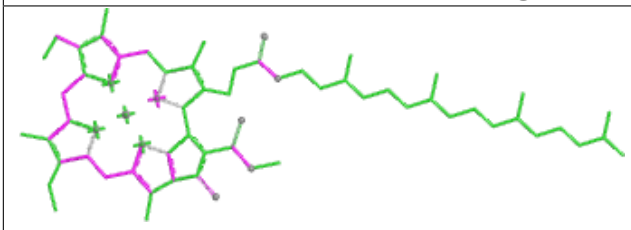


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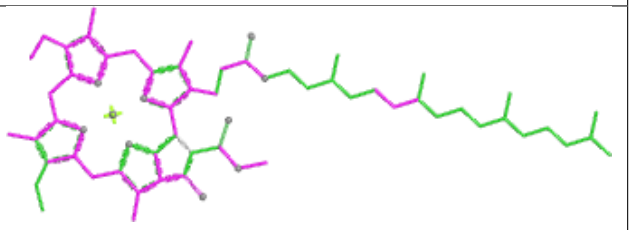


Rings

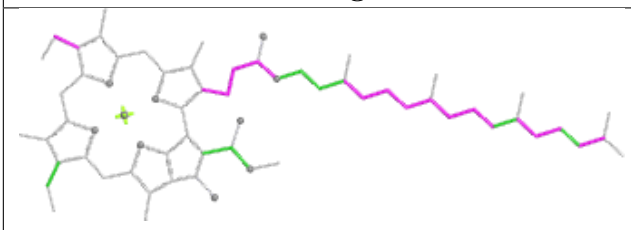
Ligand CLA A 9011



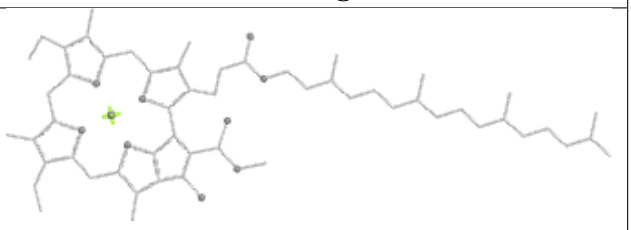
Bond lengths



Bond angles

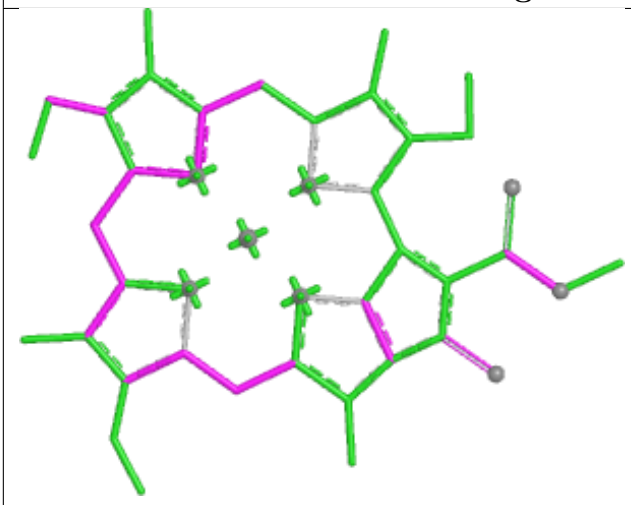


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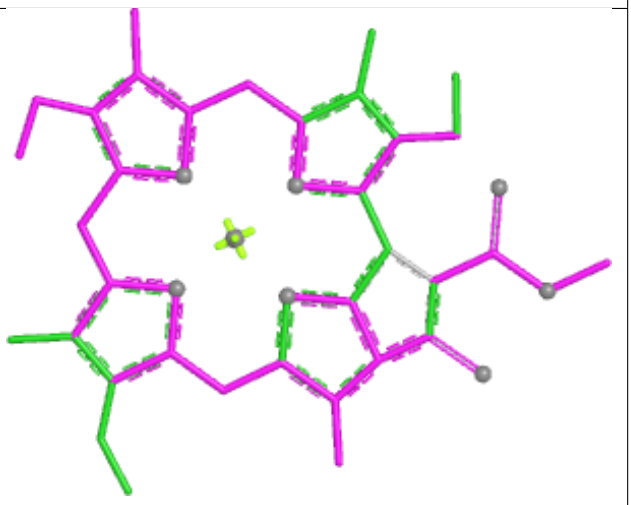


Rings

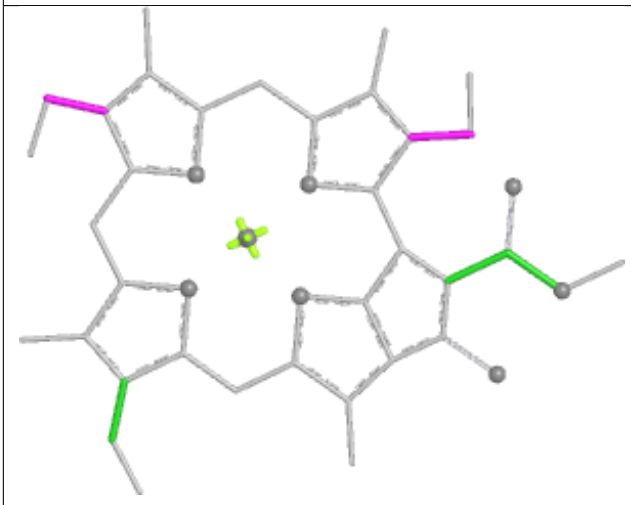
Ligand CLA A 1121



Bond lengths



Bond angles

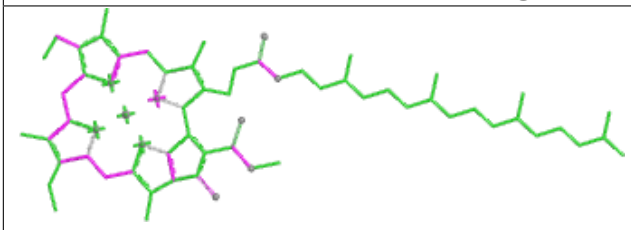


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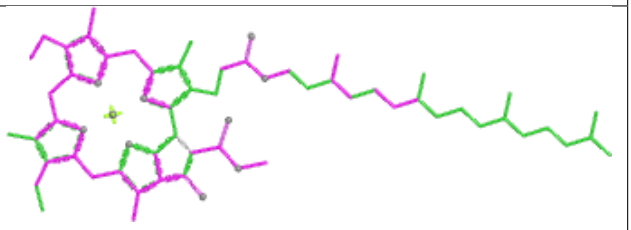


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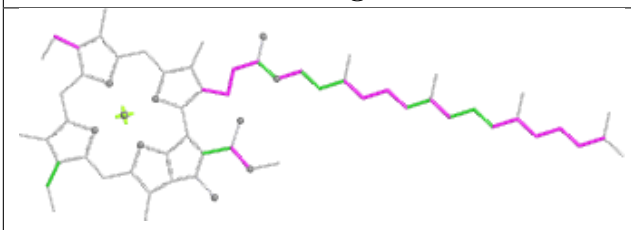
Ligand CLA A 1103



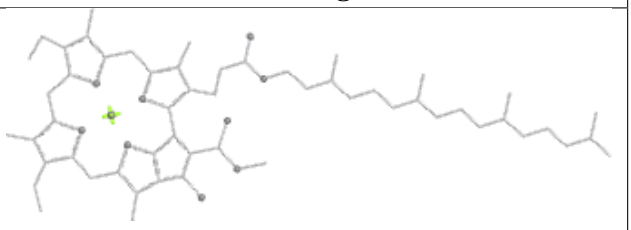
Bond lengths



Bond angles

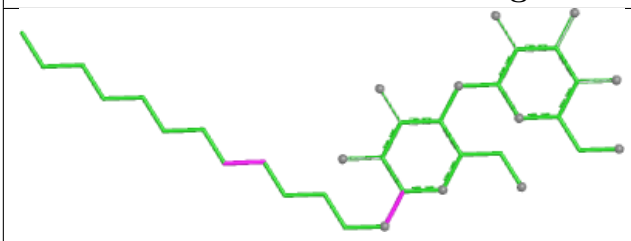


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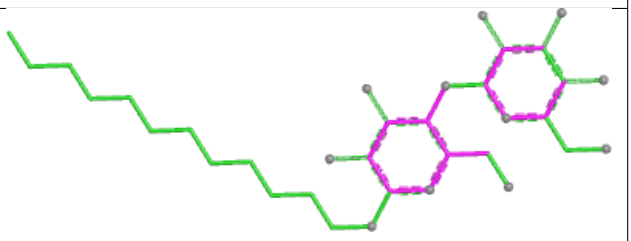


Rings

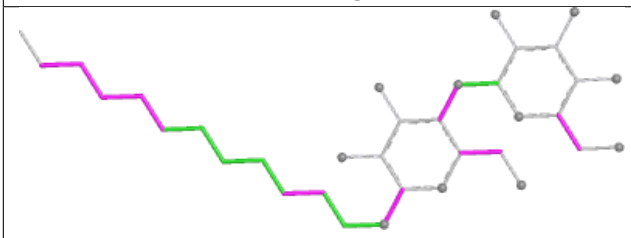
Ligand LMU H 7043



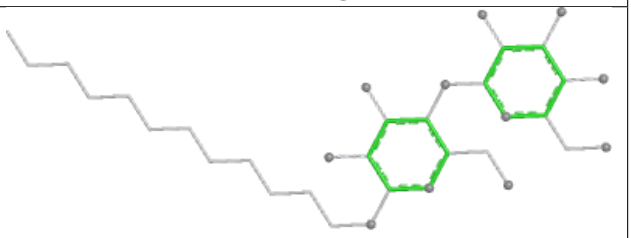
Bond lengths



Bond angles

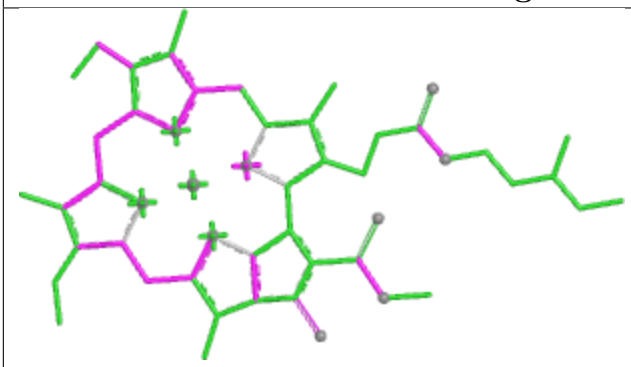


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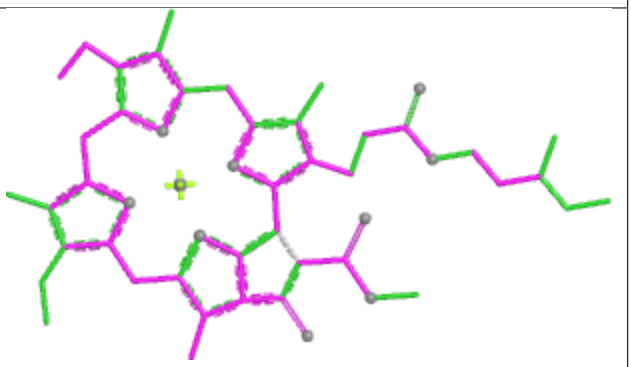


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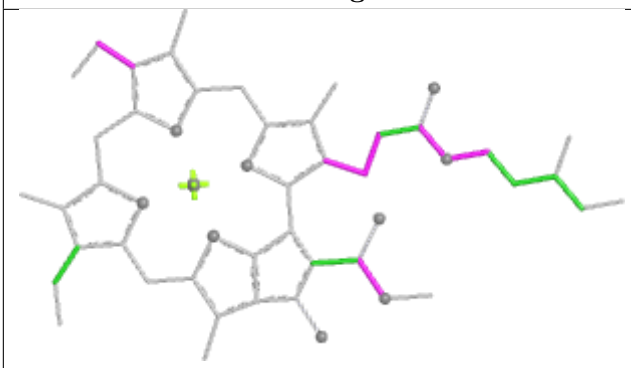
Ligand CLA A 1135



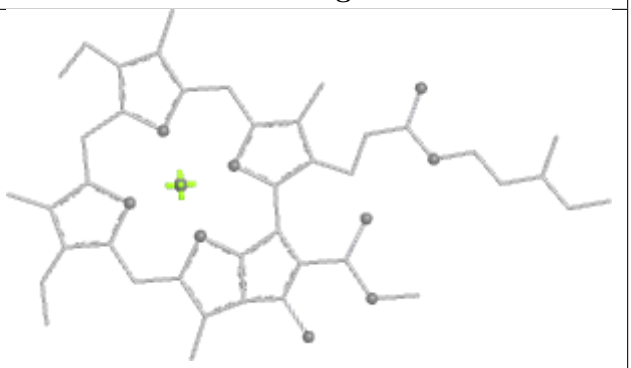
Bond lengths



Bond angles

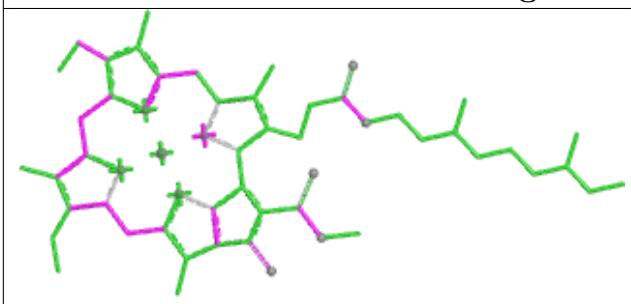


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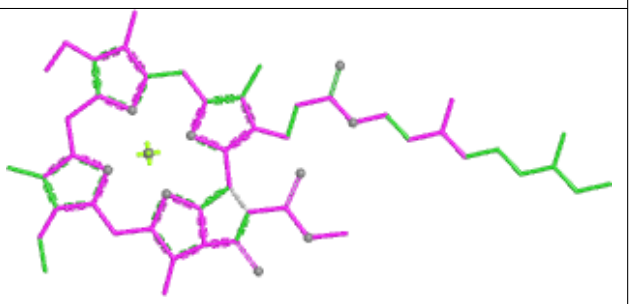


Rings

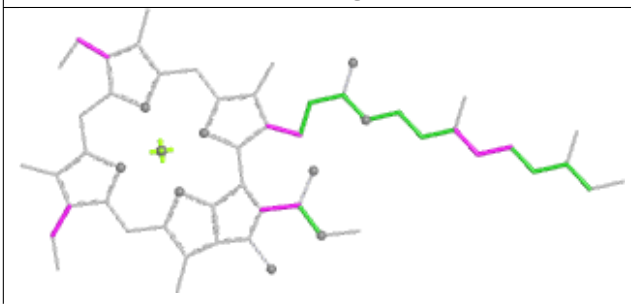
Ligand CLA 2 2002



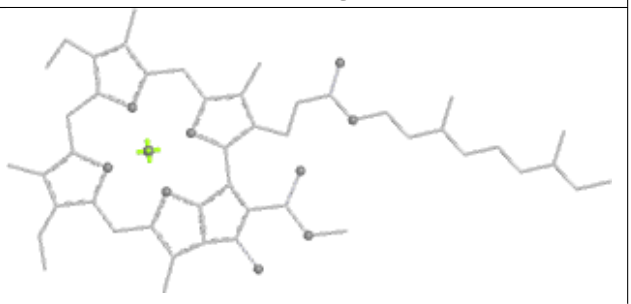
Bond lengths



Bond angles

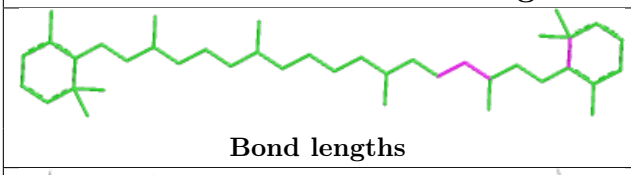


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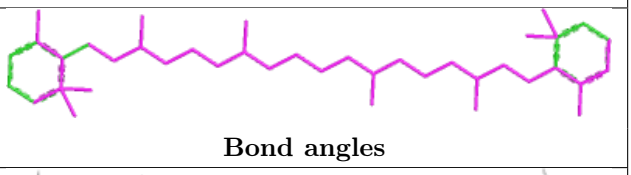


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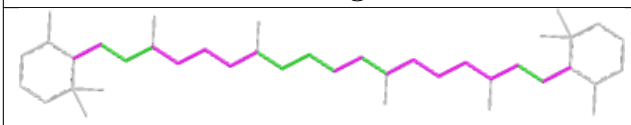
Ligand BCR 3 6022



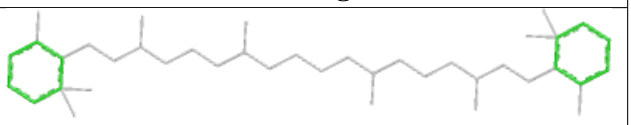
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Bond angles

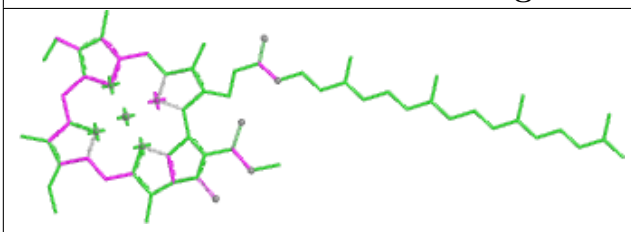


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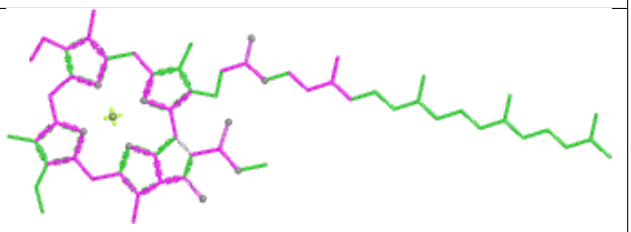


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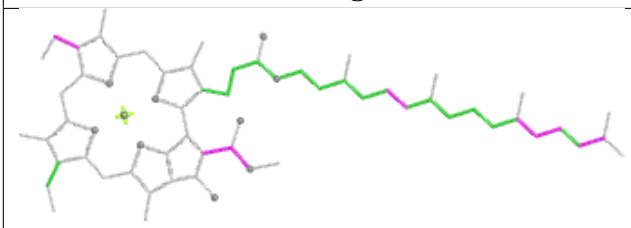
Ligand CLA A 1136



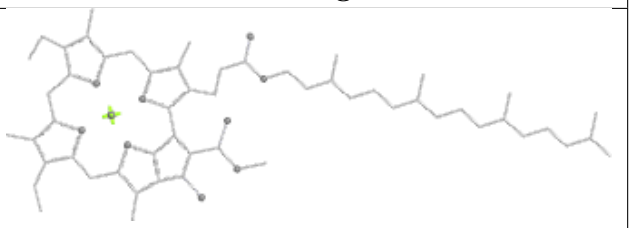
Bond lengths



Bond angles

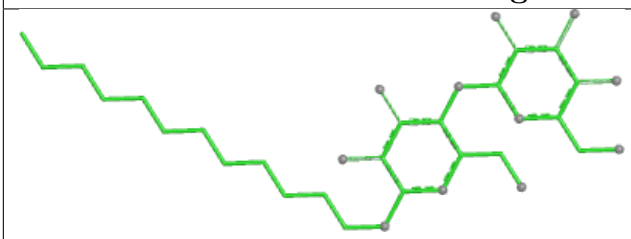


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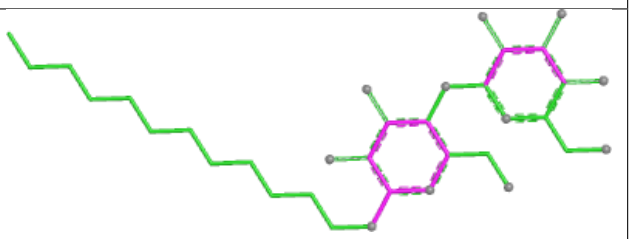


Rings

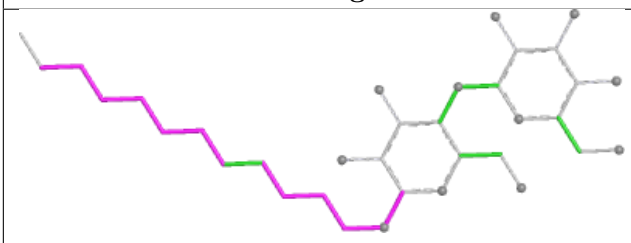
Ligand LMU A 7016



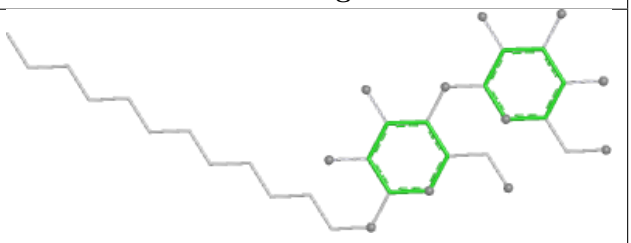
Bond lengths



Bond angles

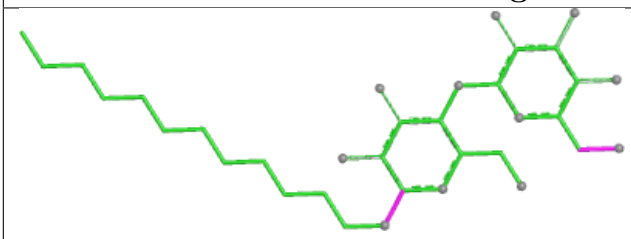


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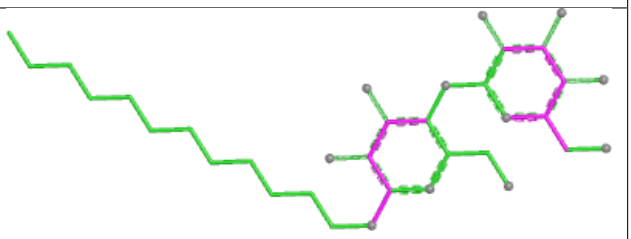


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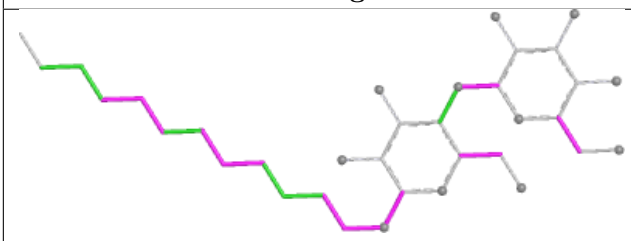
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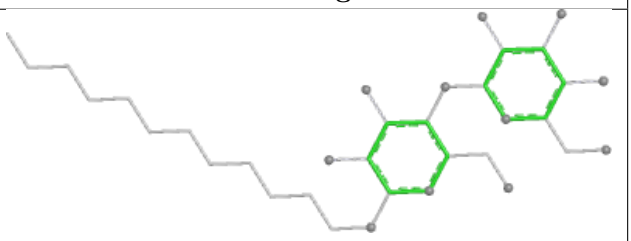
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Bond angles

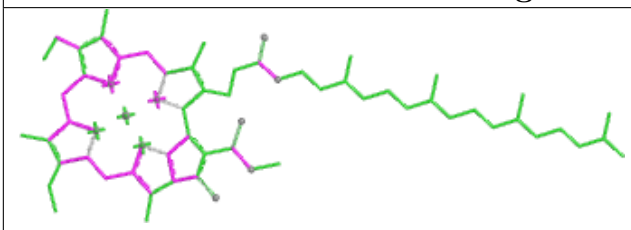


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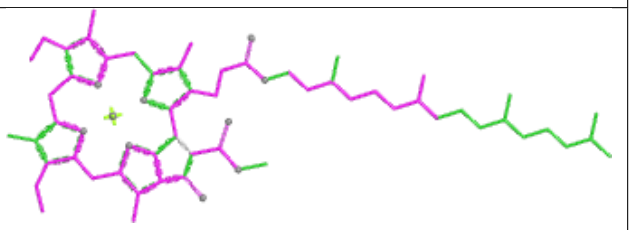


Rings

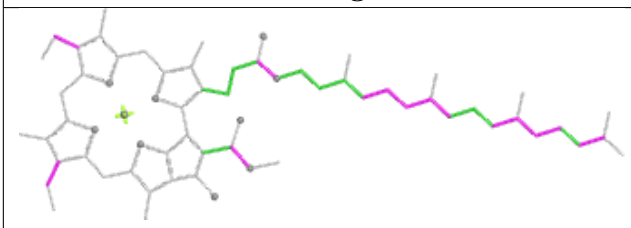
Ligand CLA B 1220



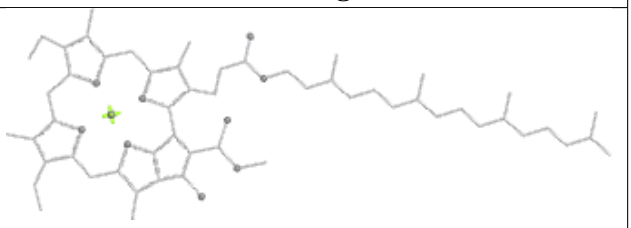
Bond lengths



Bond angles

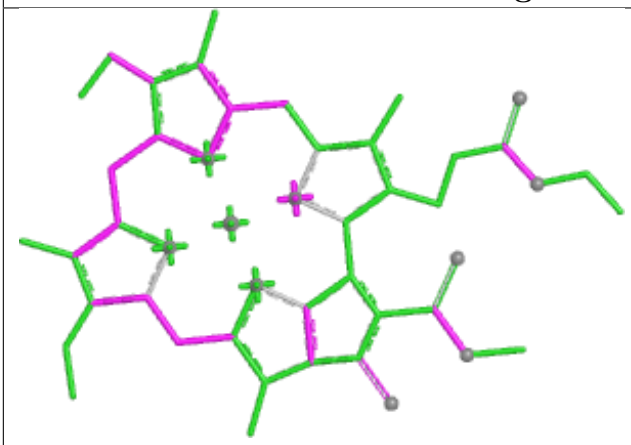


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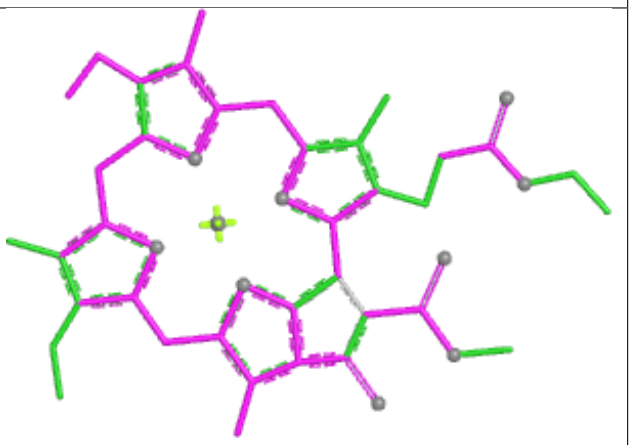


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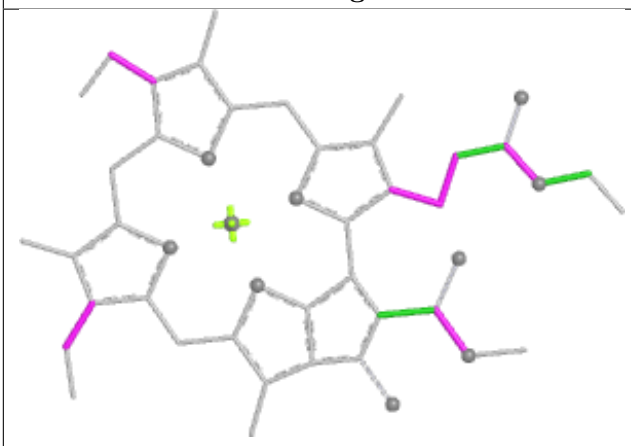
Ligand CLA A 1137



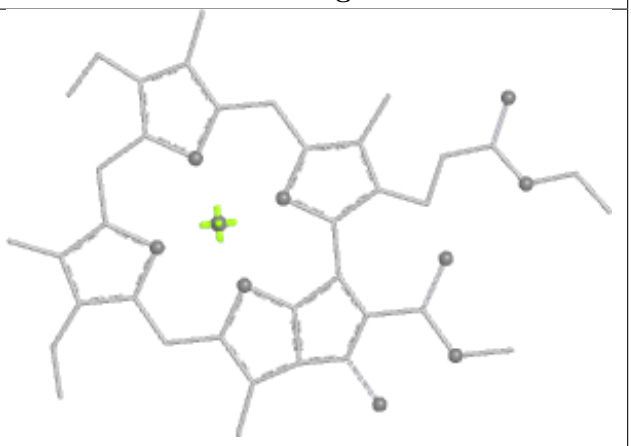
Bond lengths



Bond angles

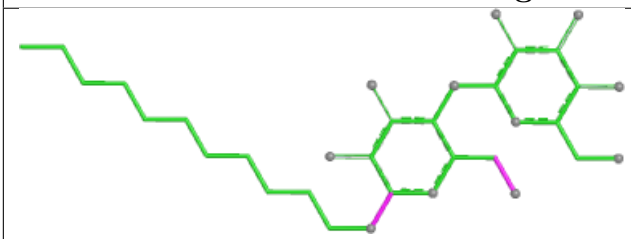


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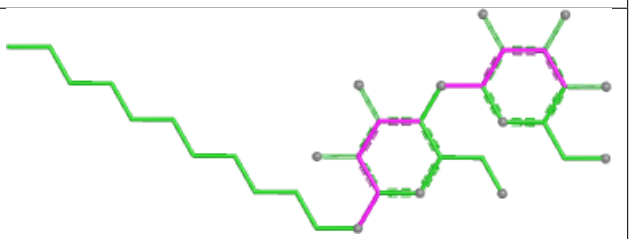


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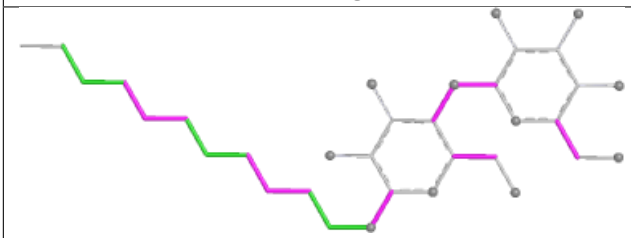
Ligand LMU 4 7009



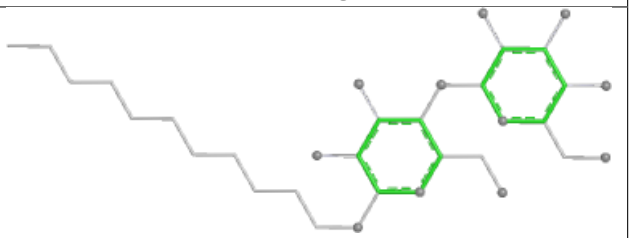
Bond lengths



Bond angles

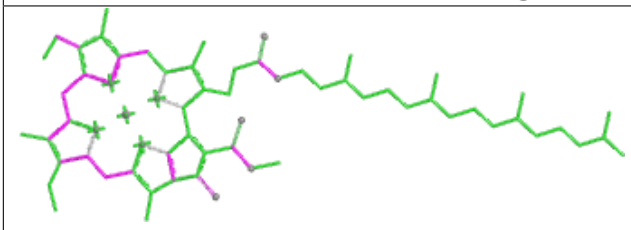


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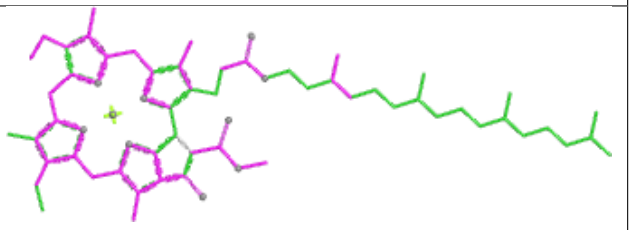


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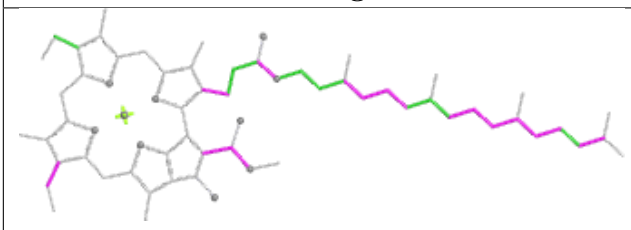
Ligand CLA A 1132



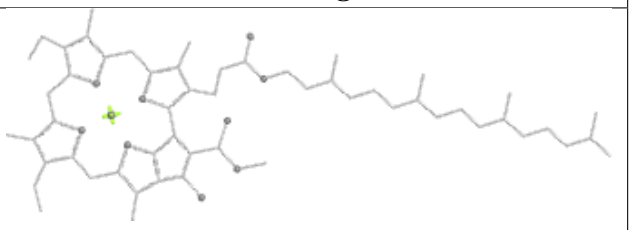
Bond lengths



Bond angles

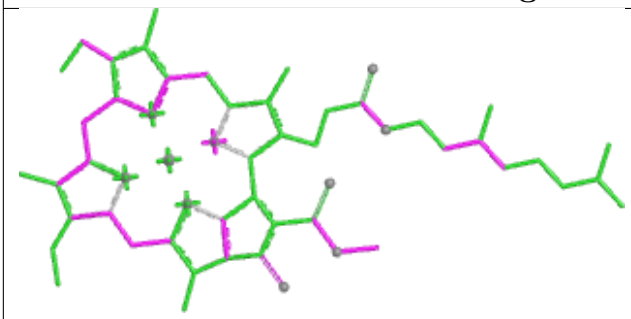


Torsions

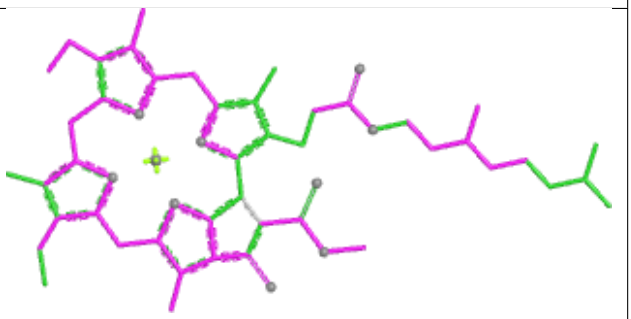


Rings

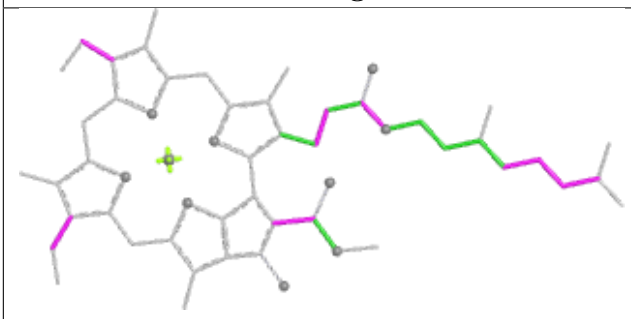
Ligand CLA 4 1004



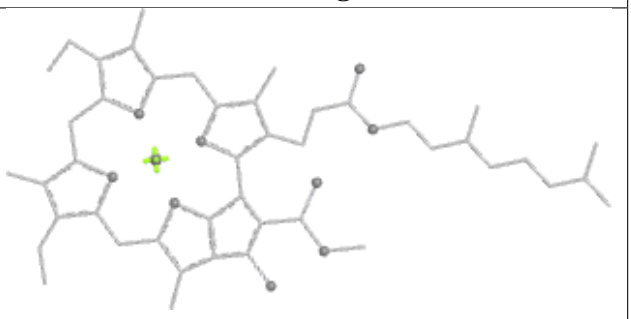
Bond lengths



Bond angles

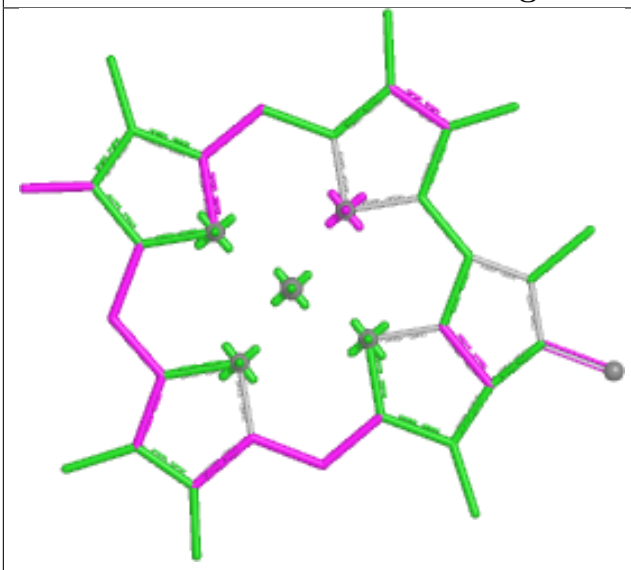


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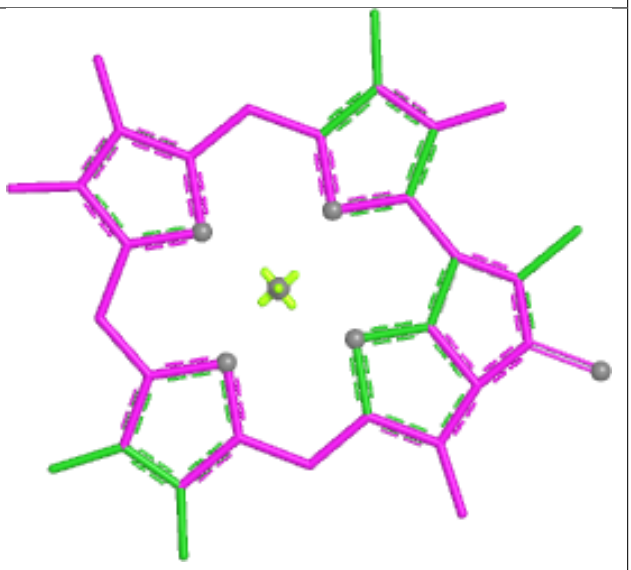


Rings

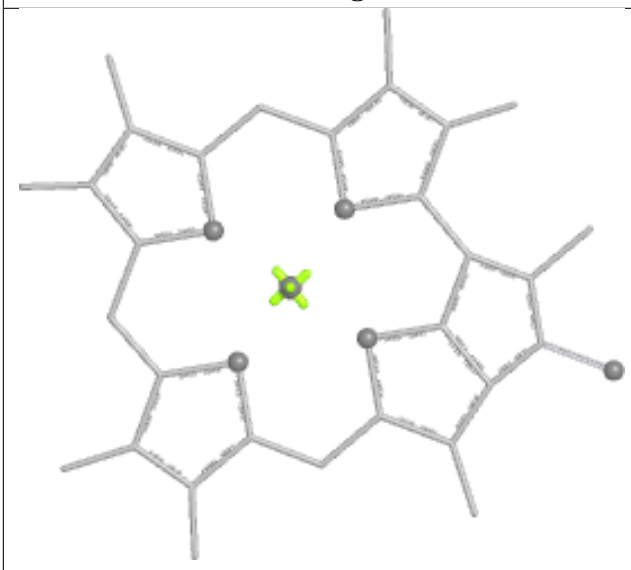
Ligand CLA 3 1118



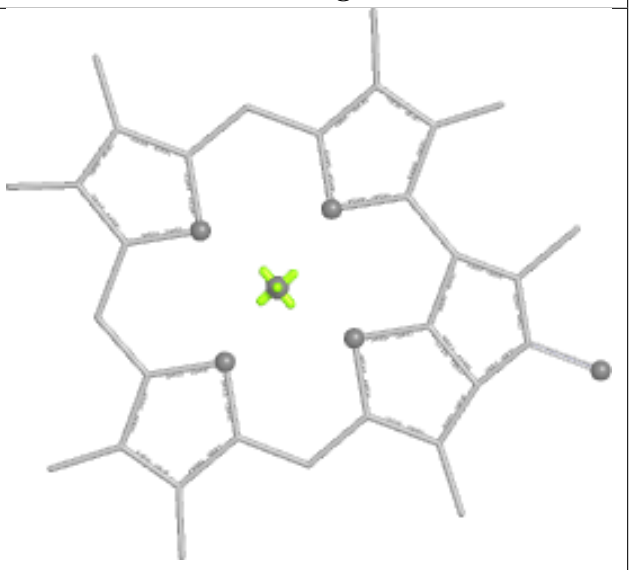
Bond lengths



Bond angles

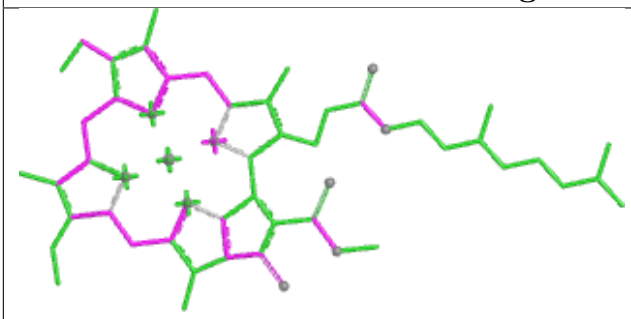


Torsions

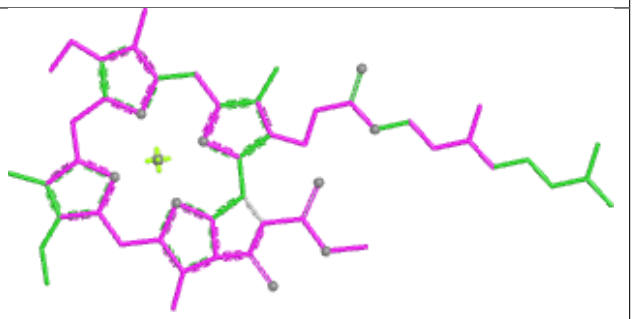


Rings

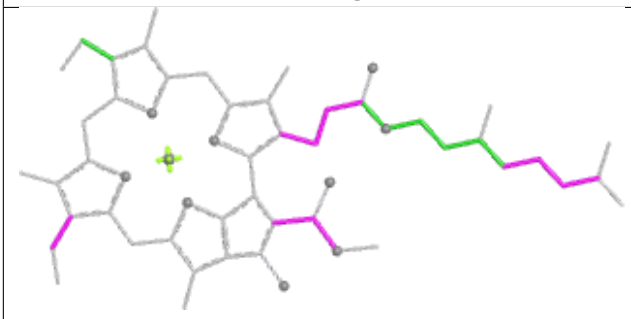
Ligand CLA J 1308



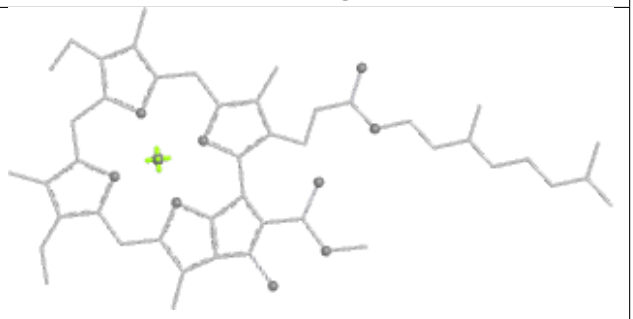
Bond lengths



Bond angles

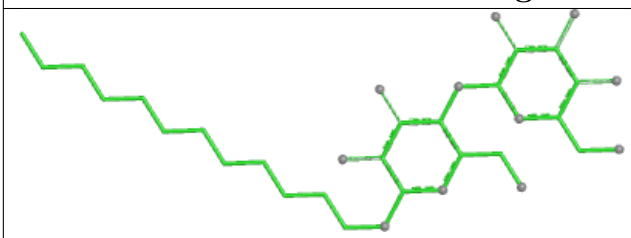


Torsions

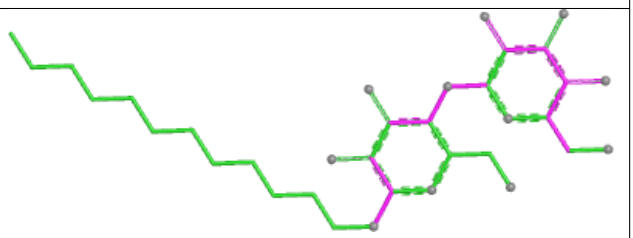


Rings

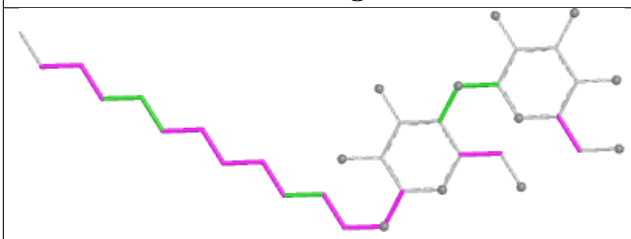
Ligand LMU 3 7003



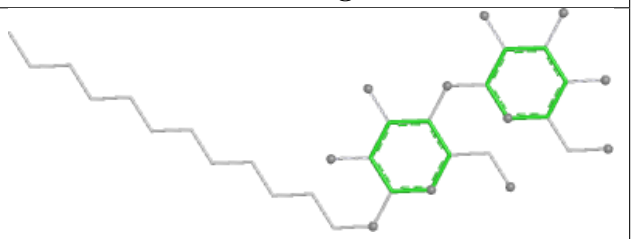
Bond lengths



Bond angles



Torsions

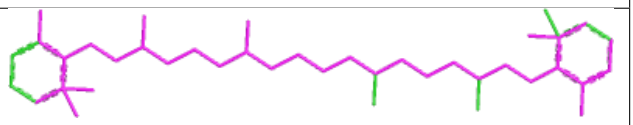


Rings

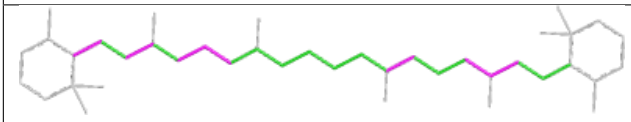
Ligand BCR I 6021



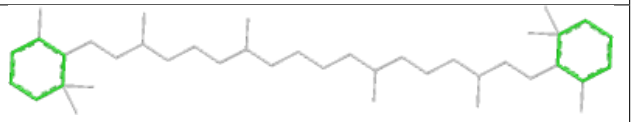
Bond lengths



Bond angles

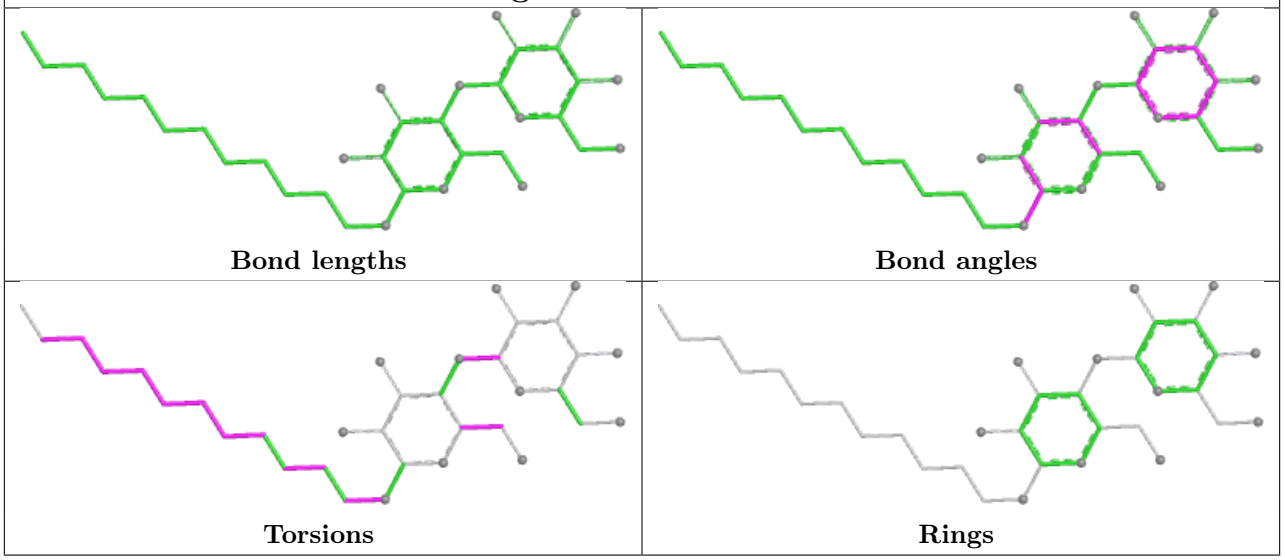


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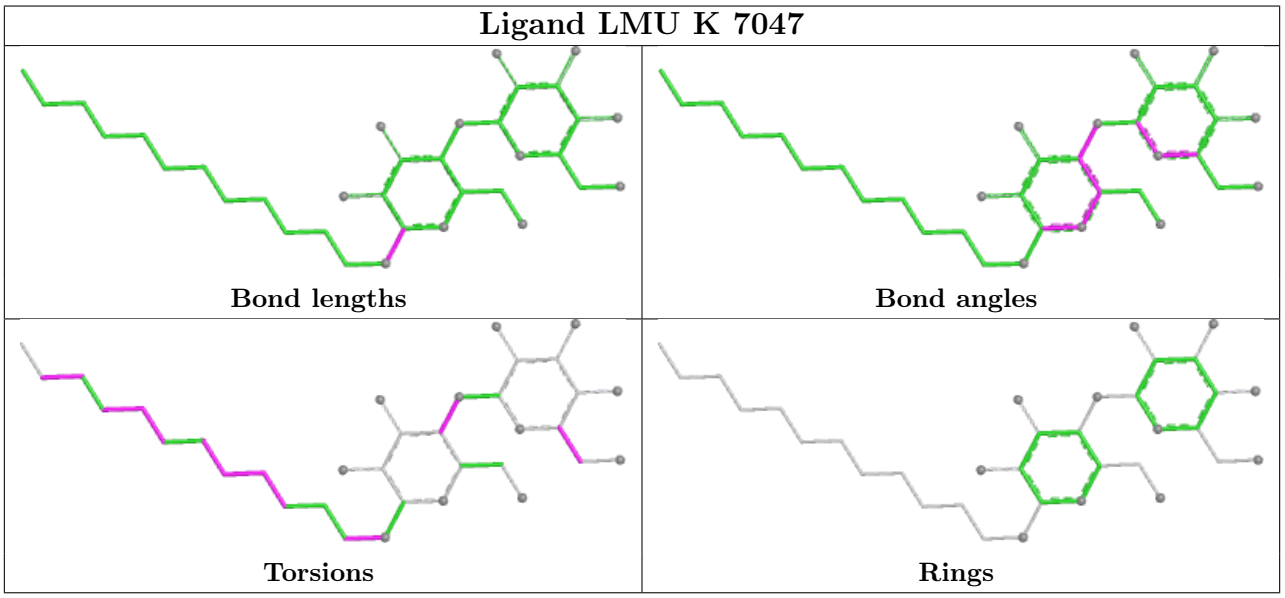


Rings

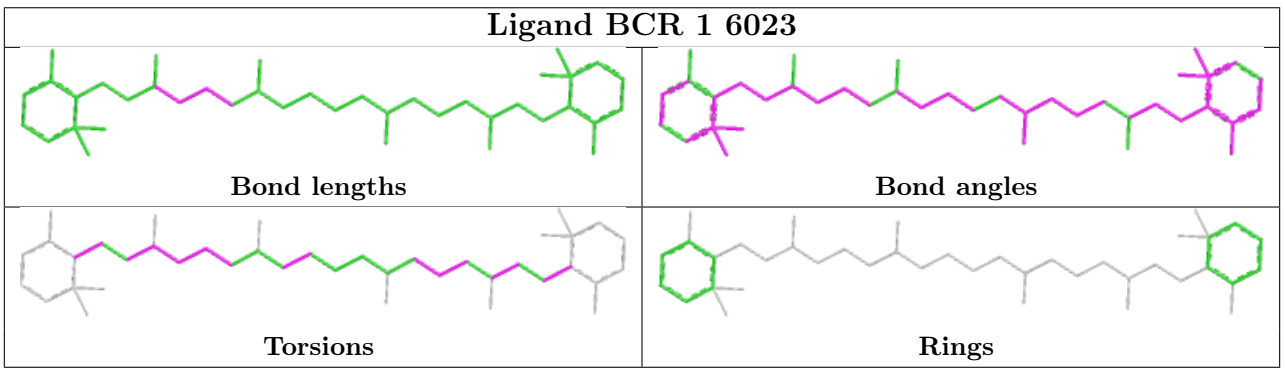
Ligand LMU R 7020



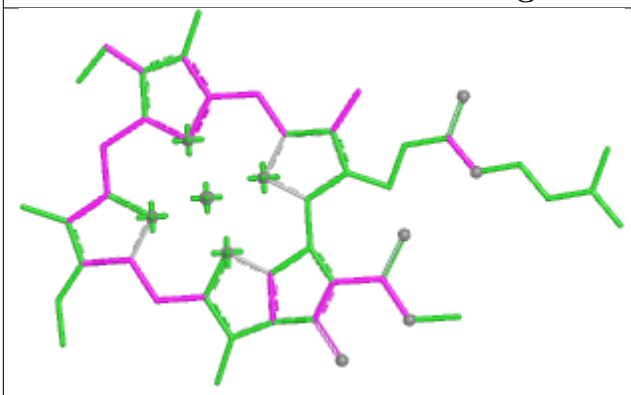
Ligand LMU K 7047



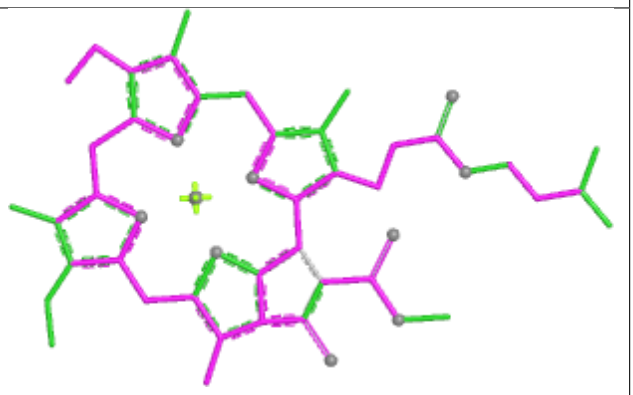
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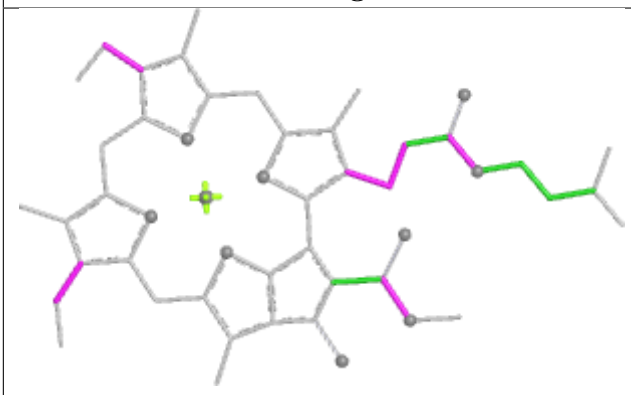
Ligand CLA L 1503



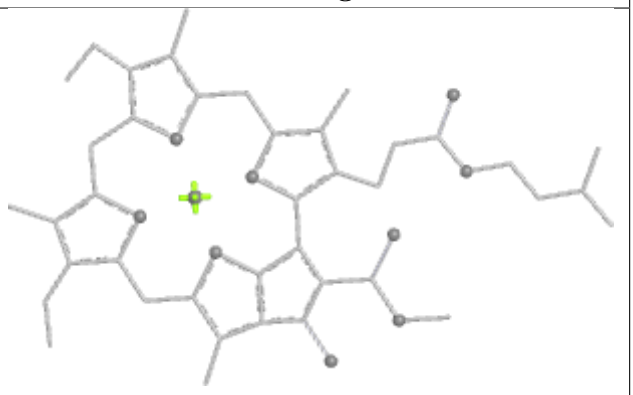
Bond lengths



Bond angles

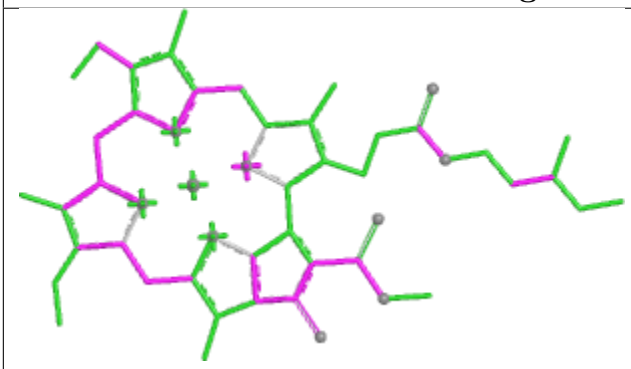


Torsions

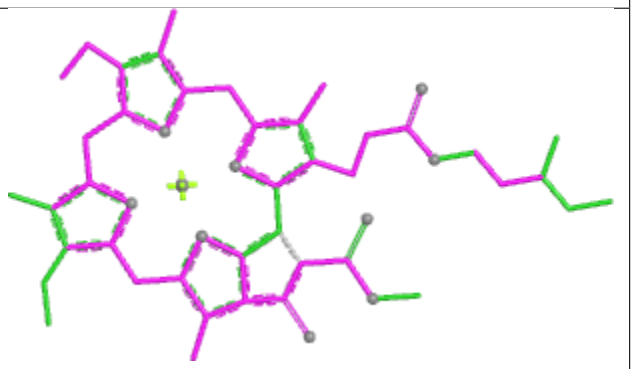


Rings

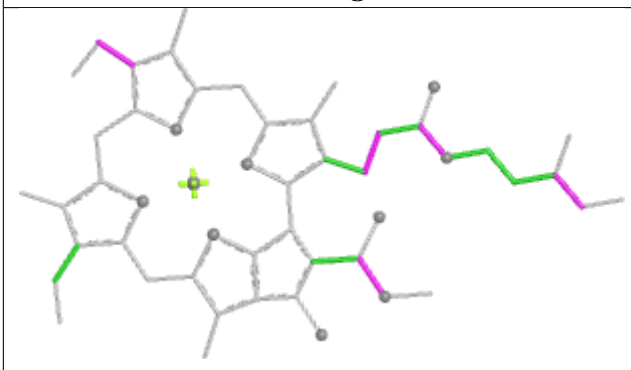
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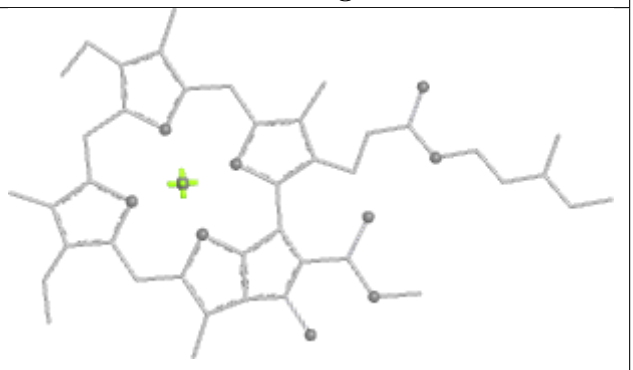
Bond lengths



Bond angles

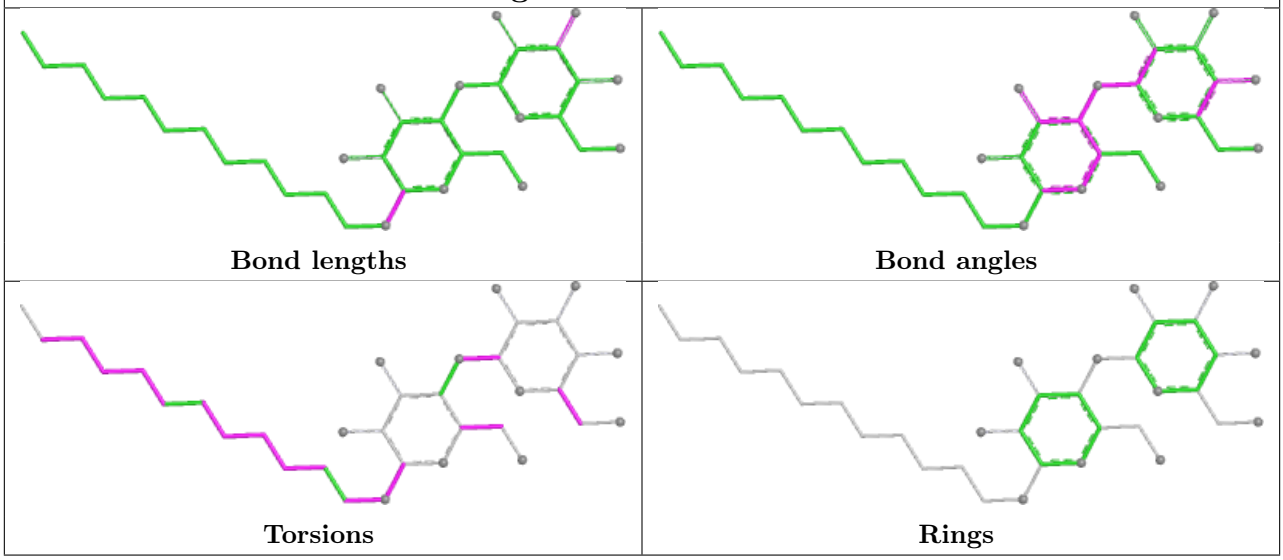


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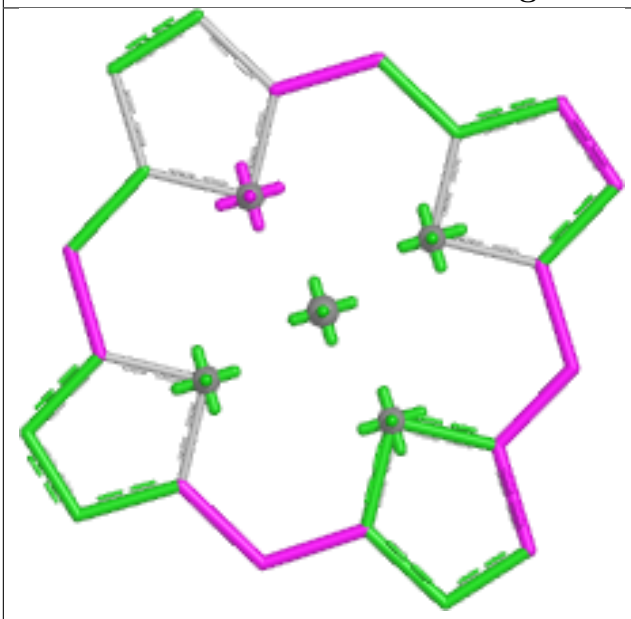


Rings

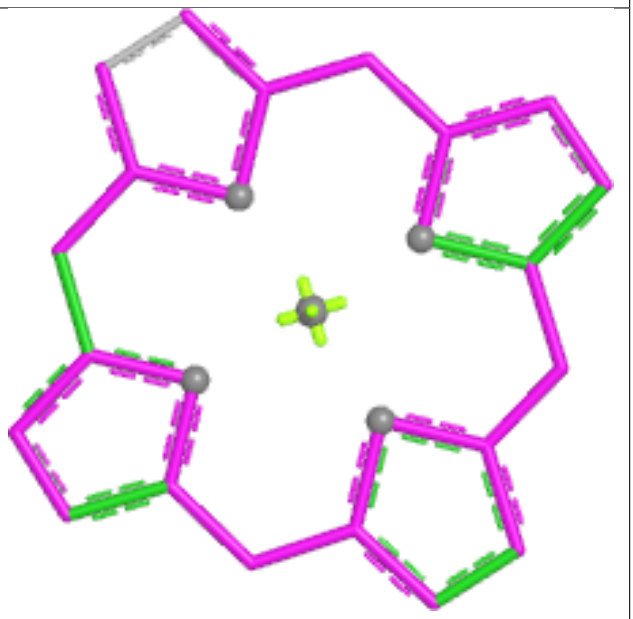
Ligand LMU G 7026



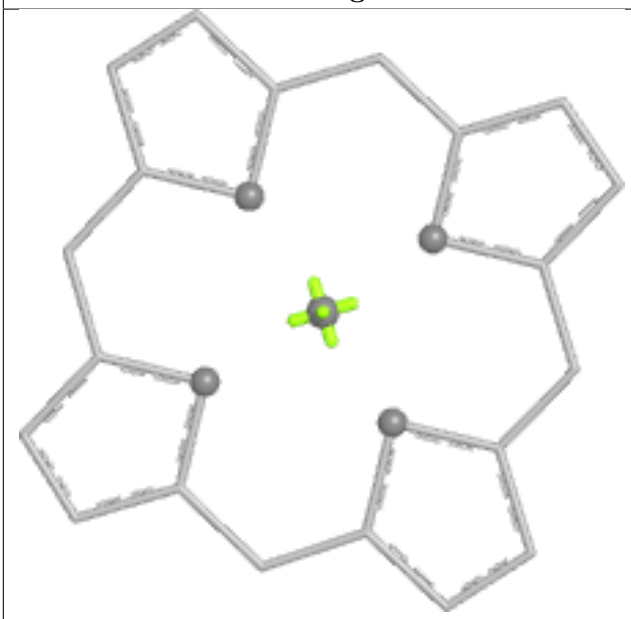
Ligand CLA 3 3006



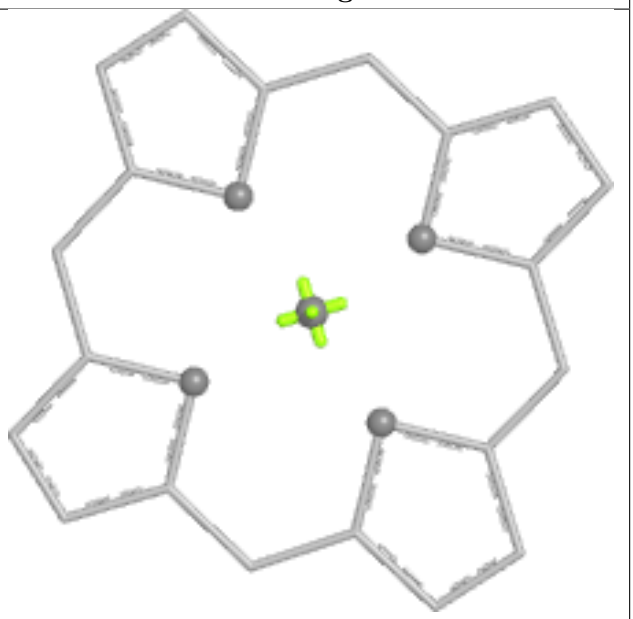
Bond lengths



Bond angles

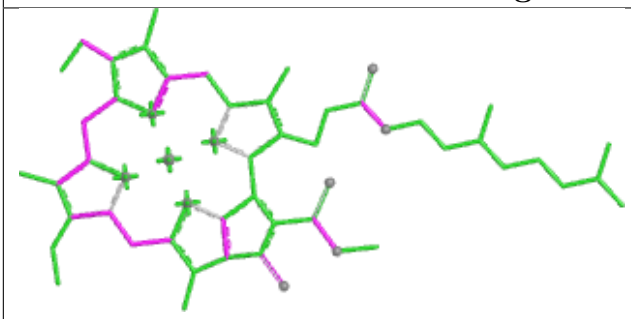


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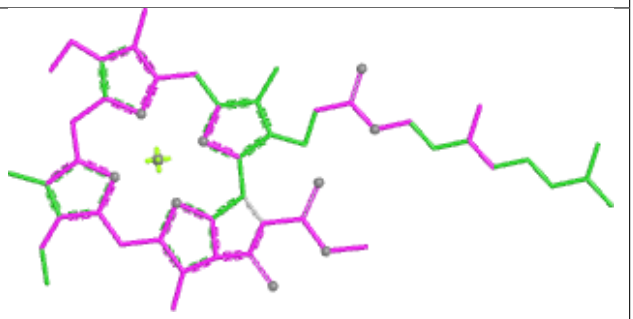


Rings

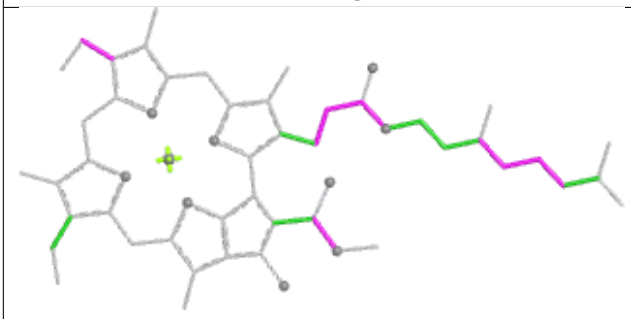
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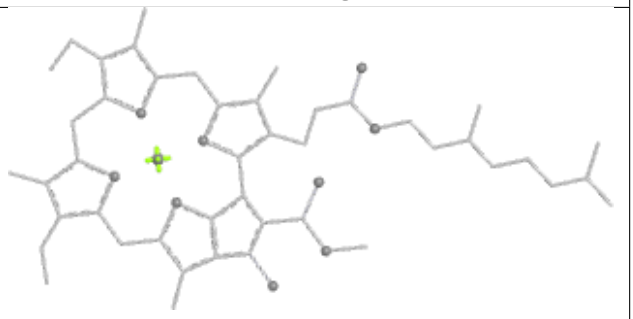
Bond lengths



Bond angles

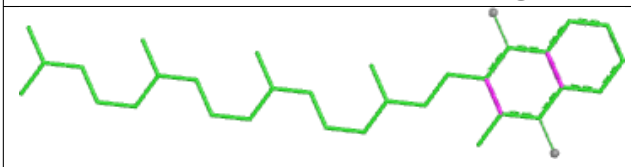


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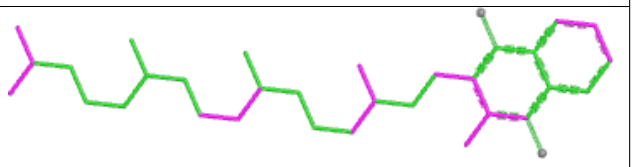


Rings

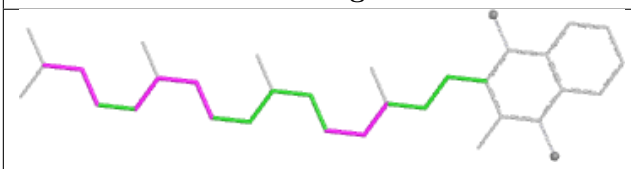
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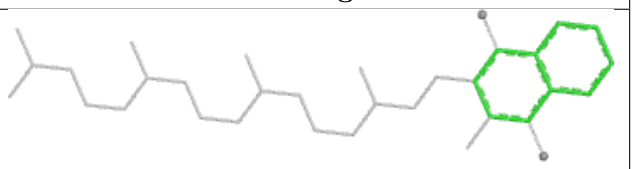
Bond lengths



Bond angles

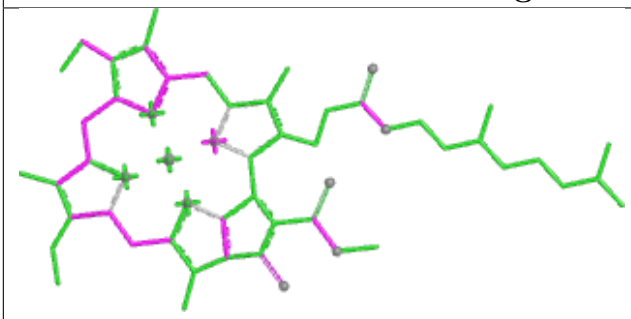


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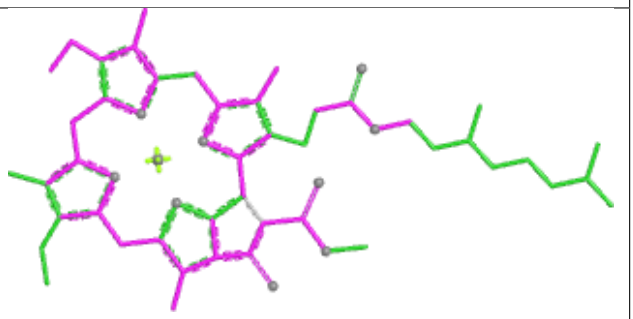


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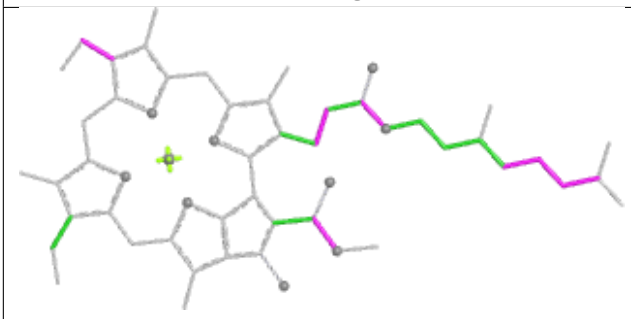
Ligand CLA A 1127



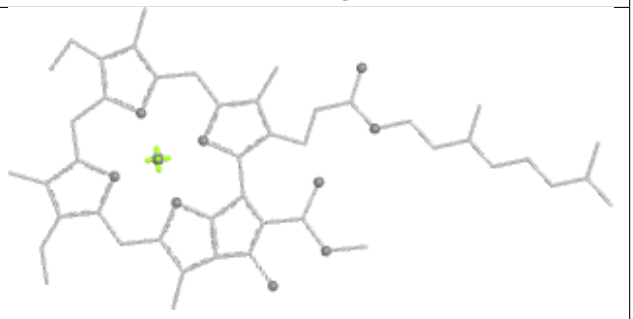
Bond lengths



Bond angles

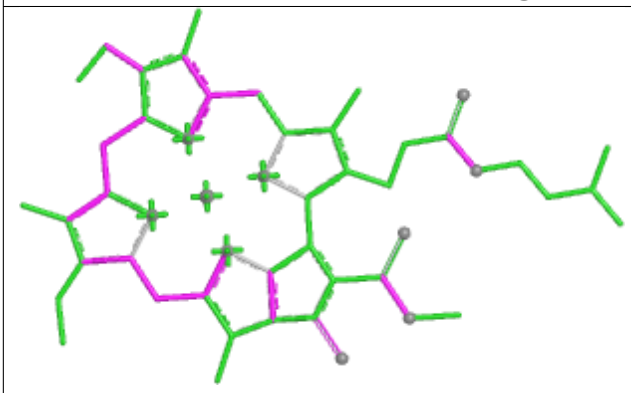


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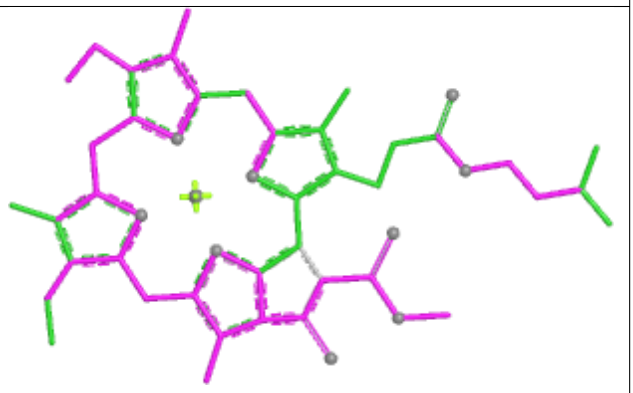


Rings

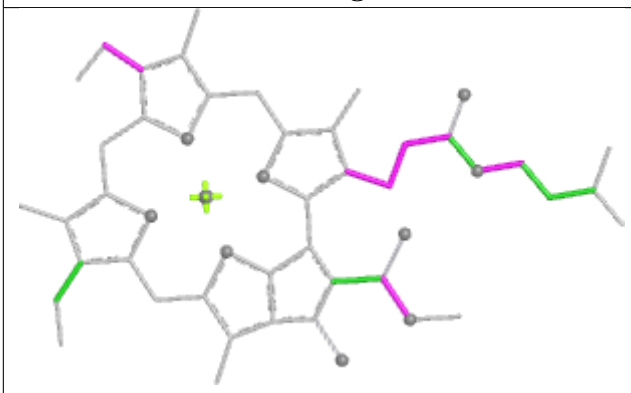
Ligand CLA B 1227



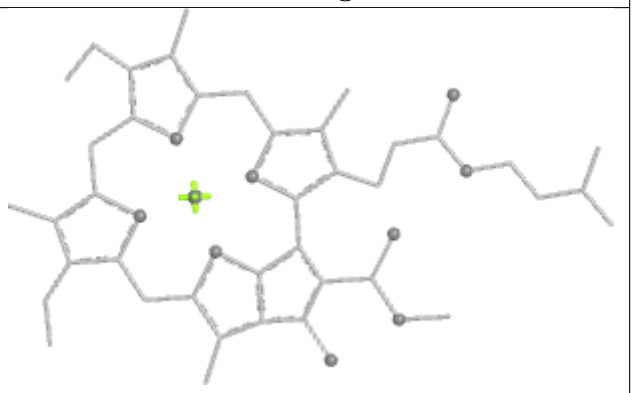
Bond lengths



Bond angles

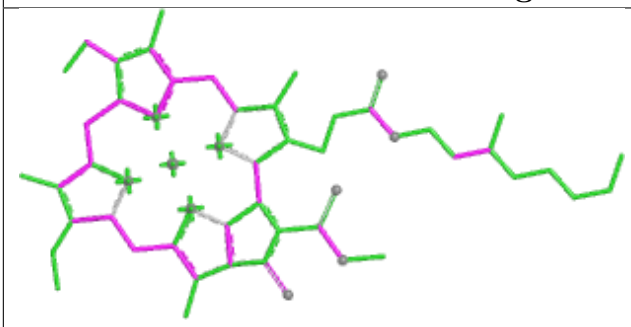


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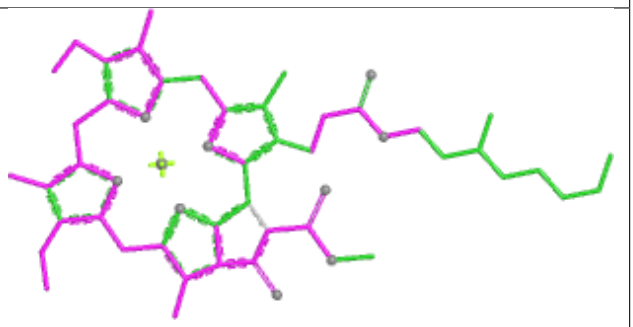


Rings

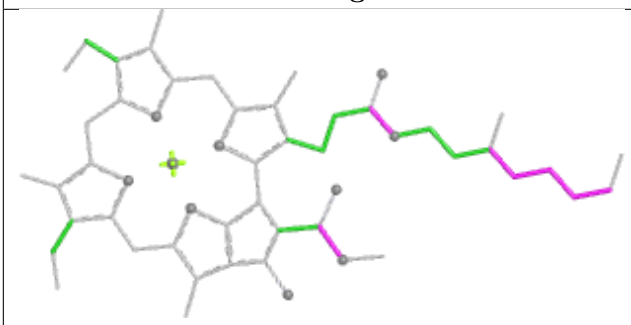
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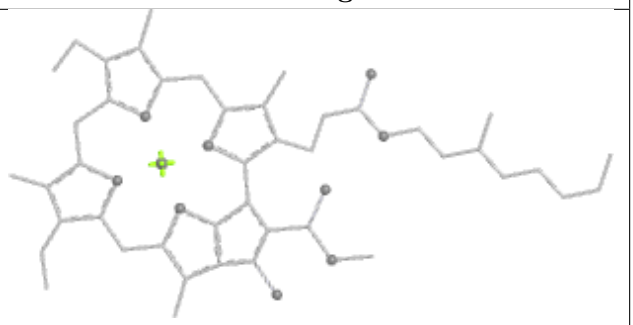
Bond lengths



Bond angles

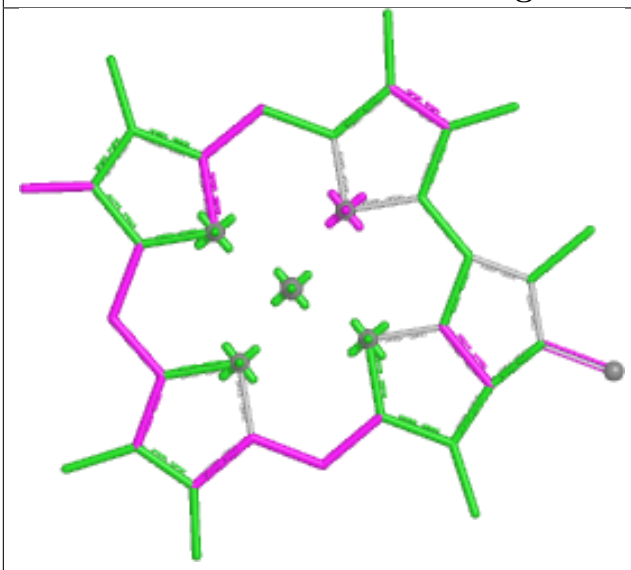


Torsions

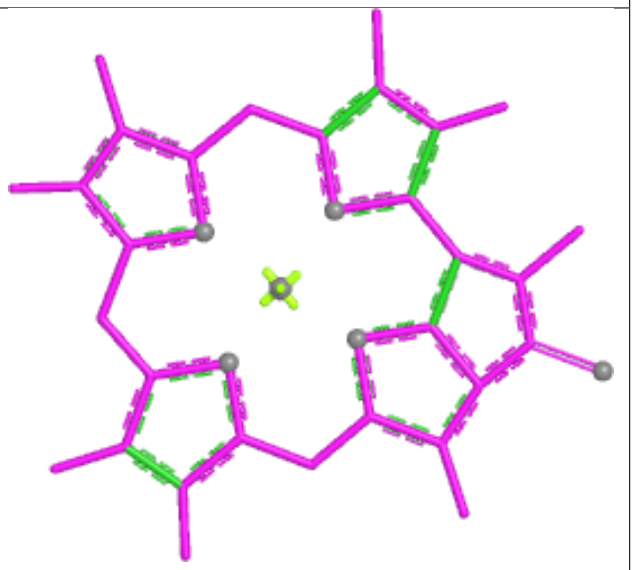


Rings

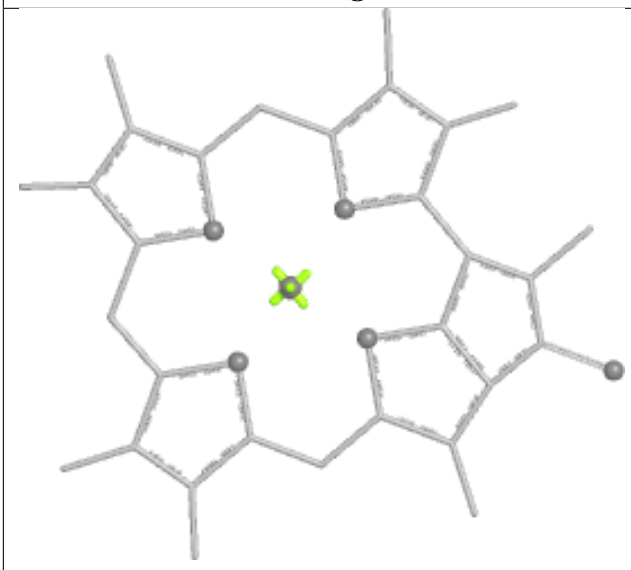
Ligand CLA B 1301



Bond lengths



Bond angles

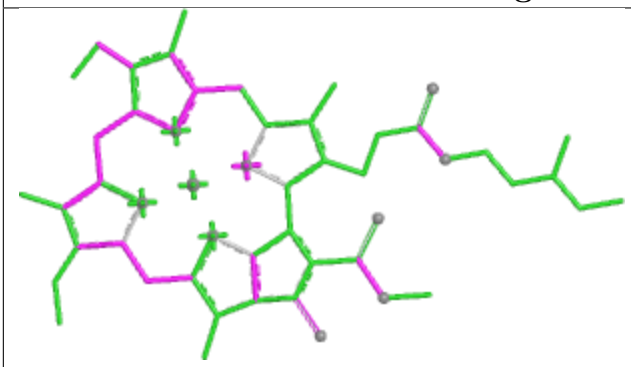


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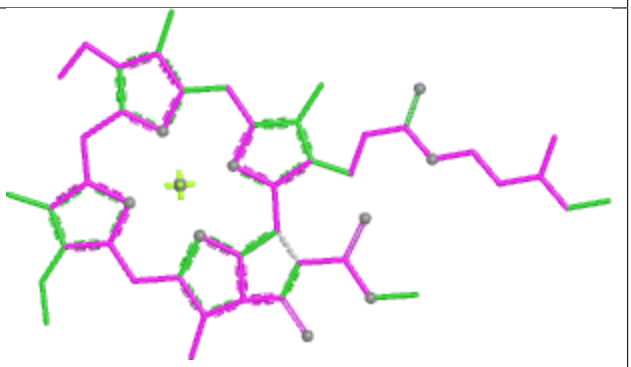


Rings

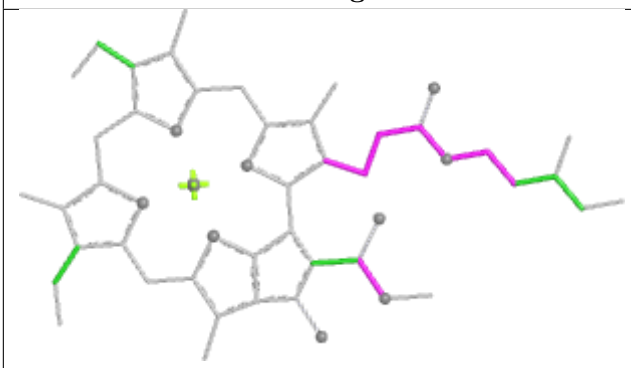
Ligand CLA A 1139



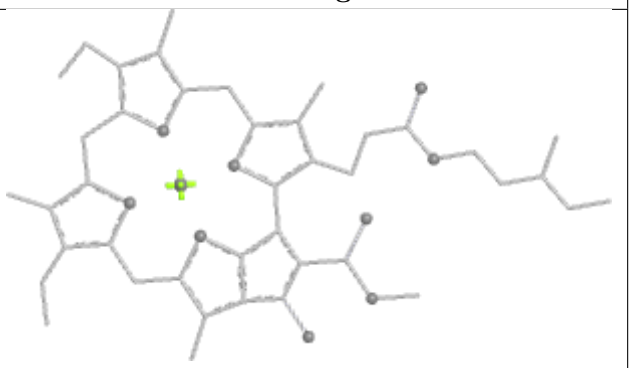
Bond lengths



Bond angles

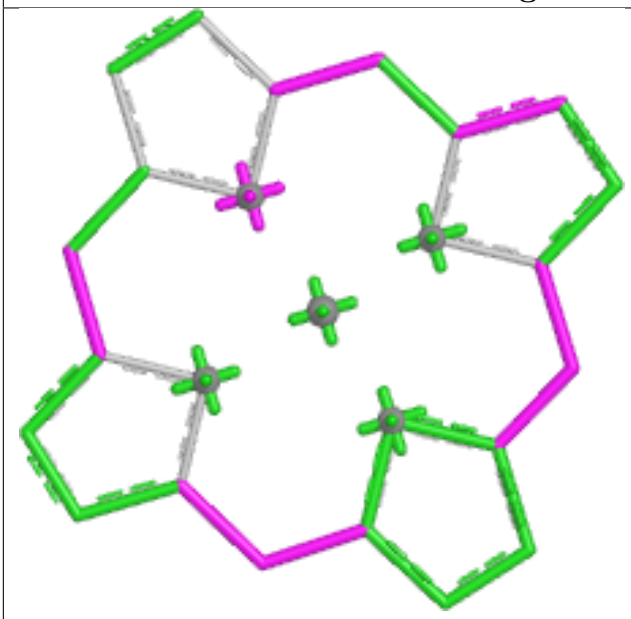


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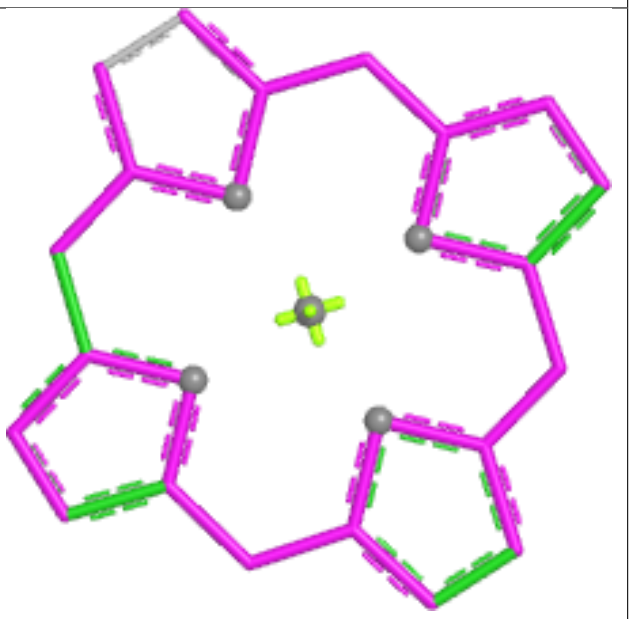


Rings

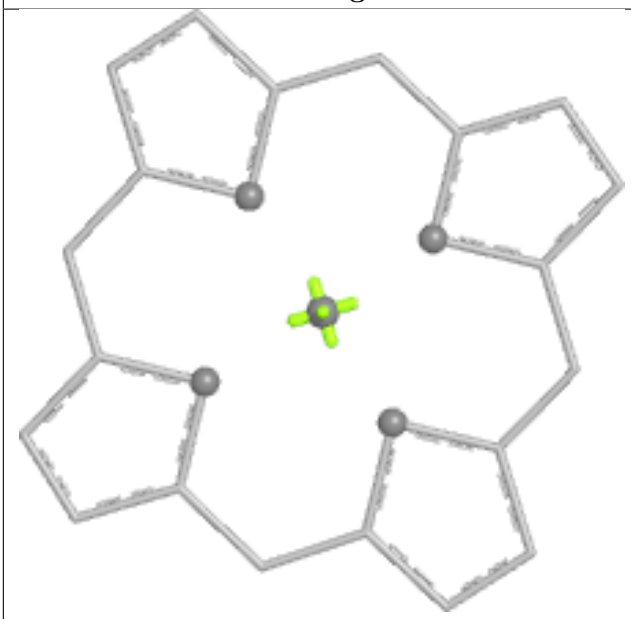
Ligand CLA 1 1015



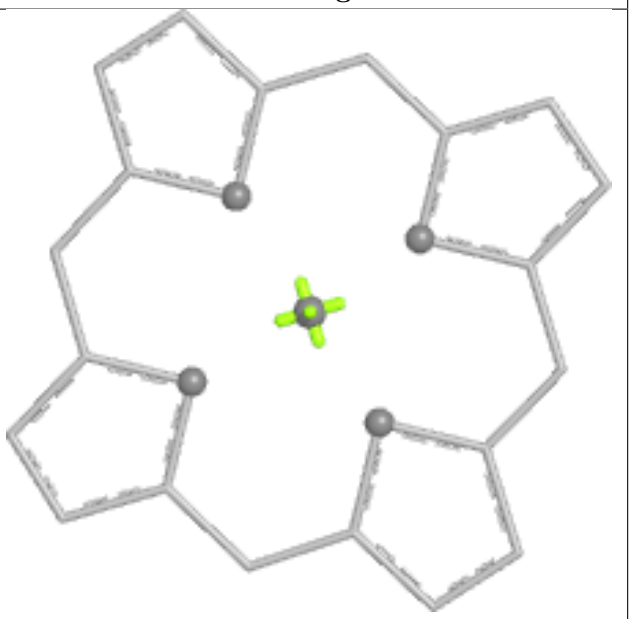
Bond lengths



Bond angles

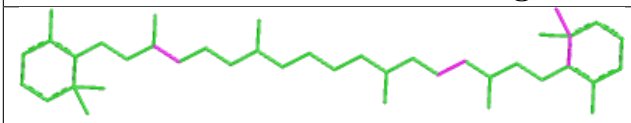


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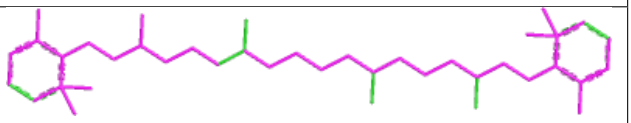


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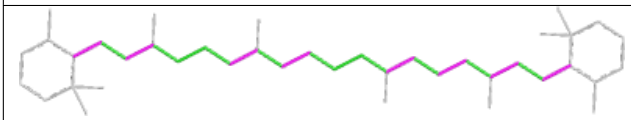
Ligand BCR A 6007



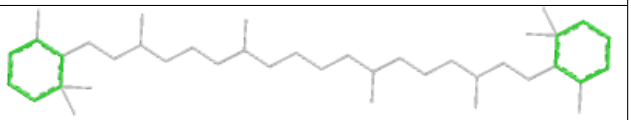
Bond lengths



Bond angles

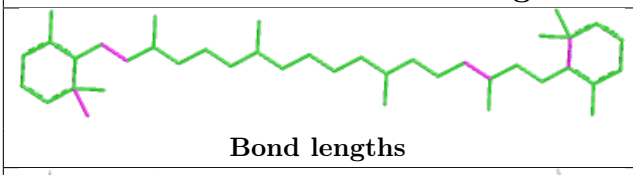


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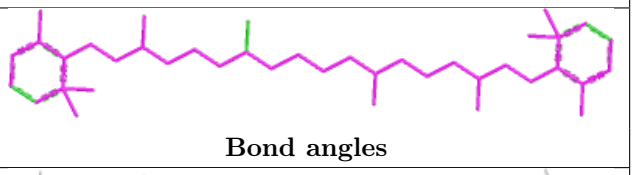


Rings

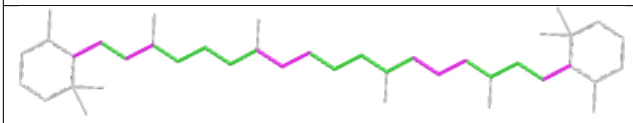
Ligand BCR A 6011



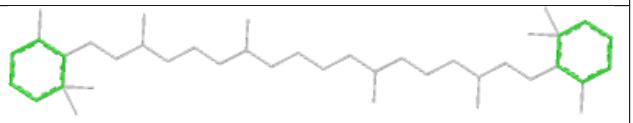
Bond lengths



Bond angles

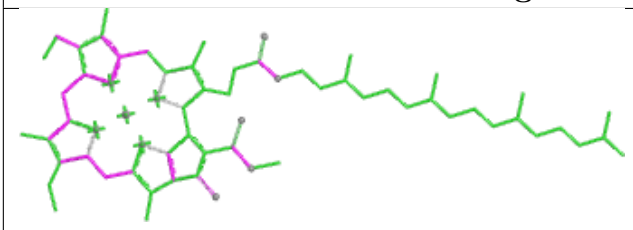


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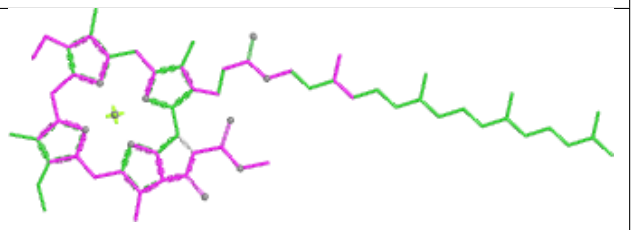


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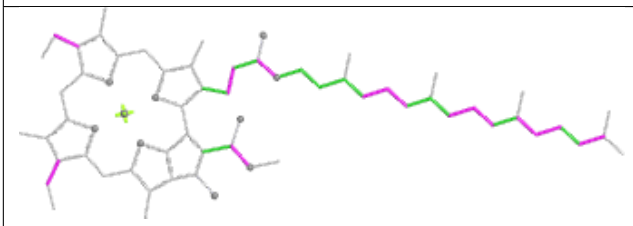
Ligand CLA A 1119



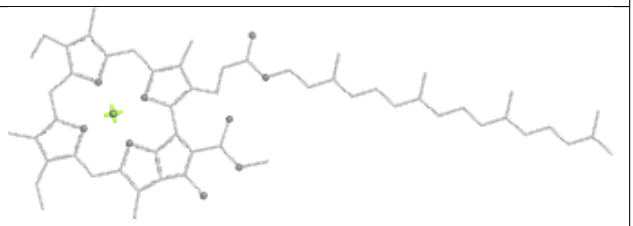
Bond lengths



Bond angles

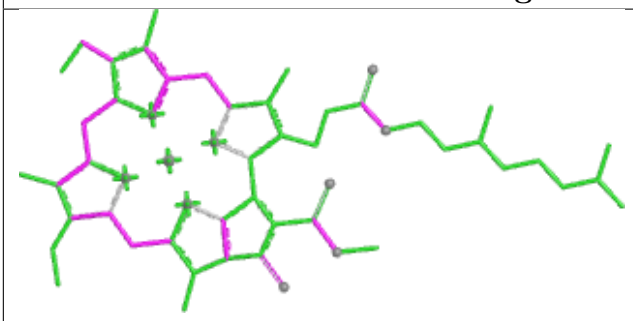


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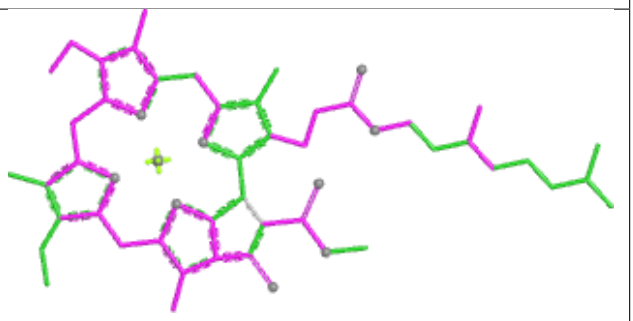


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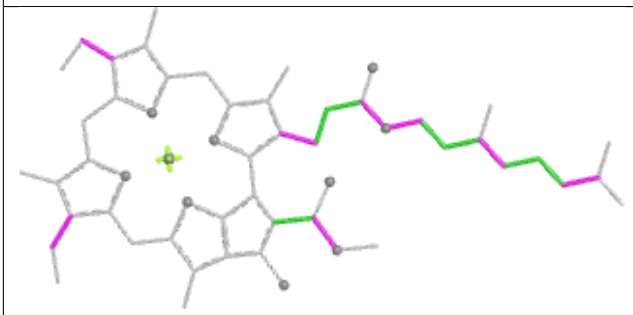
Ligand CLA A 1102



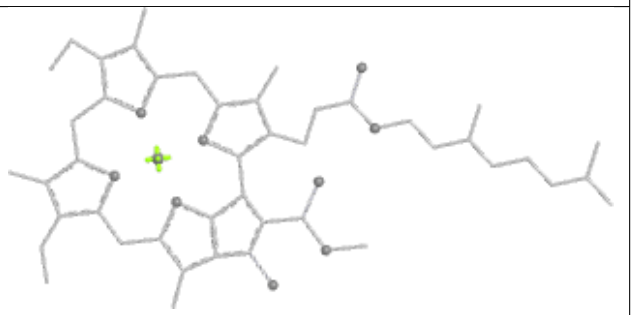
Bond lengths



Bond angles

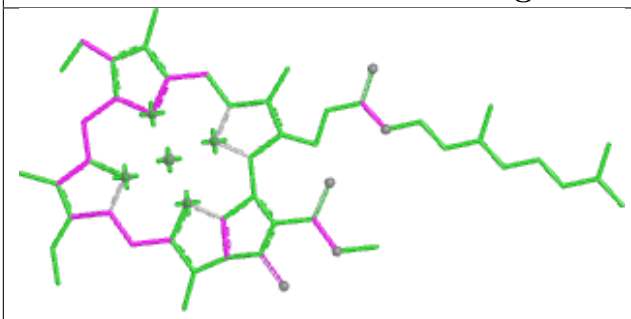


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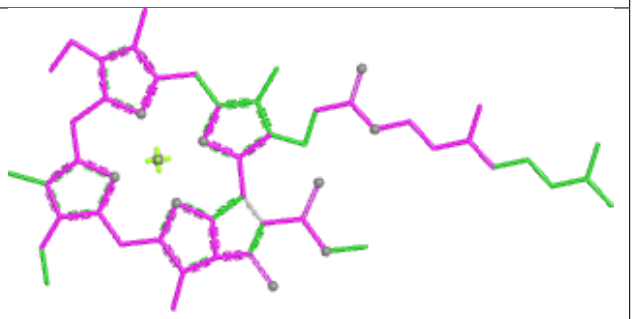


Rings

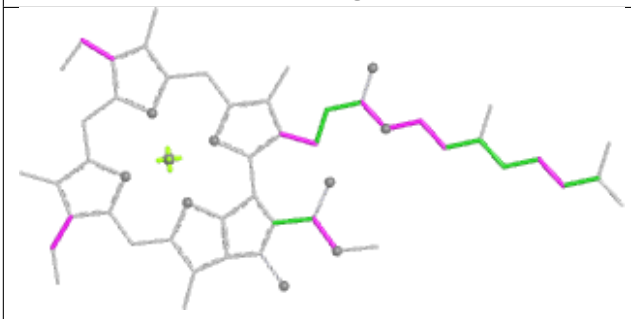
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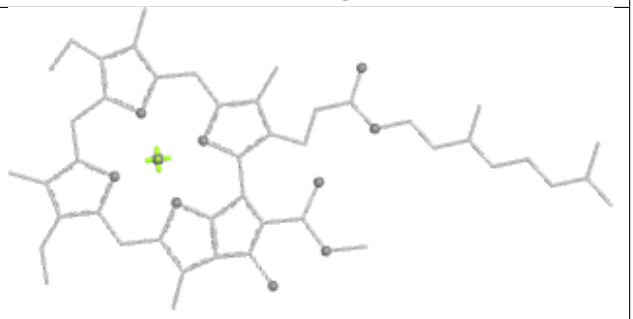
Bond lengths



Bond angles

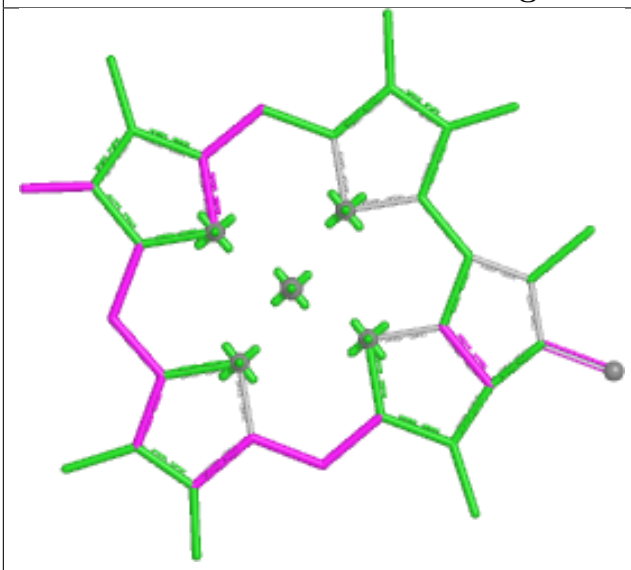


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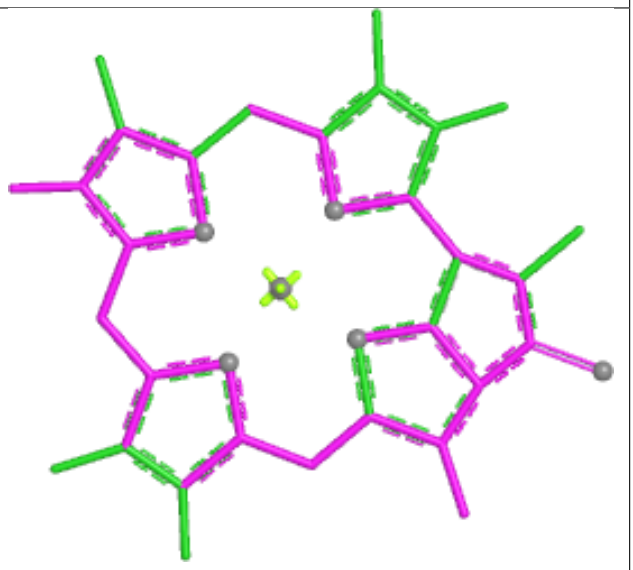


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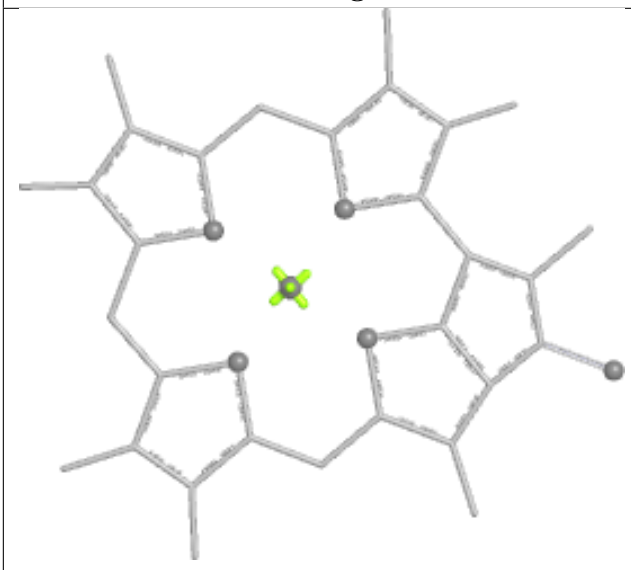
Ligand CLA 1 1012



Bond lengths



Bond angles

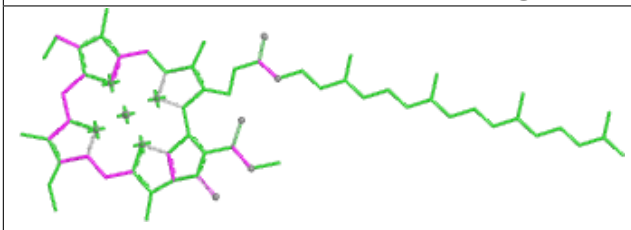


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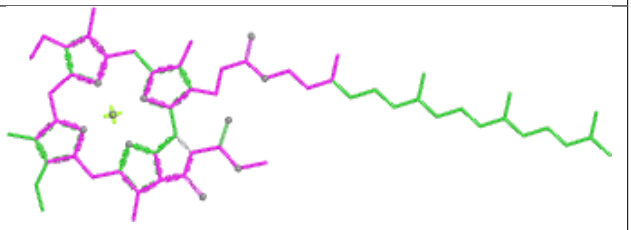


Rings

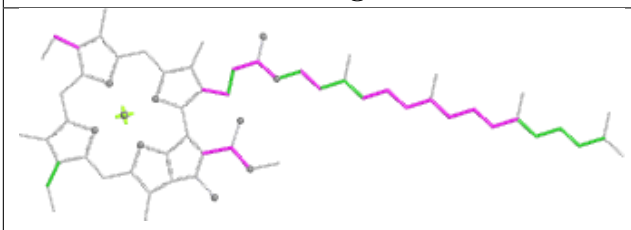
Ligand CLA R 1150



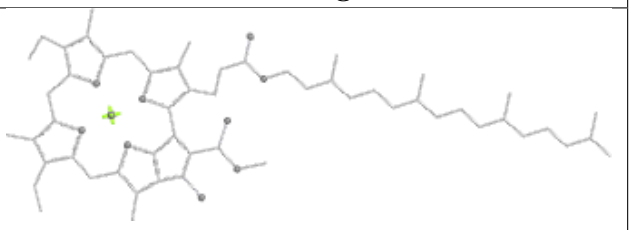
Bond lengths



Bond angles

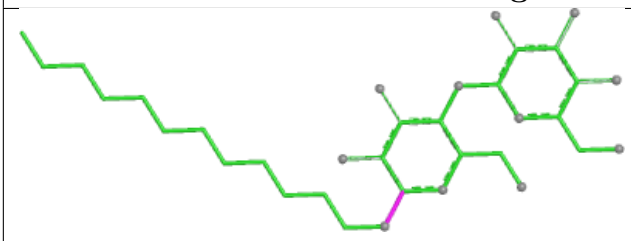


Torsions



Rings

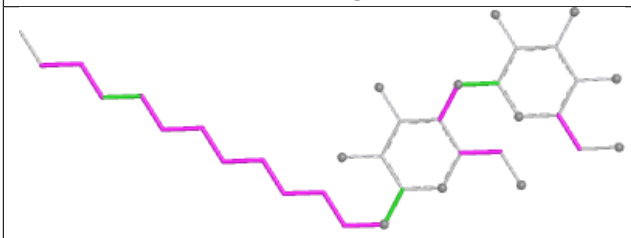
Ligand LMU A 7044



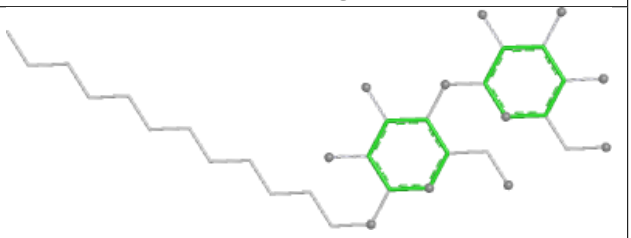
Bond lengths



Bond angles

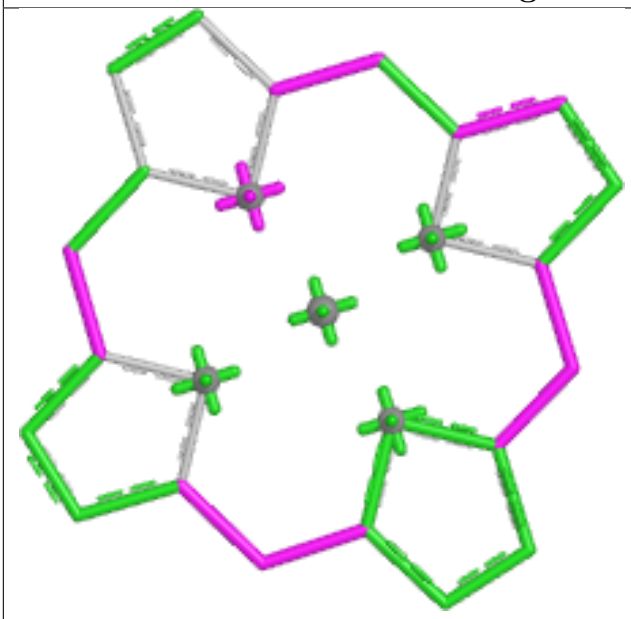


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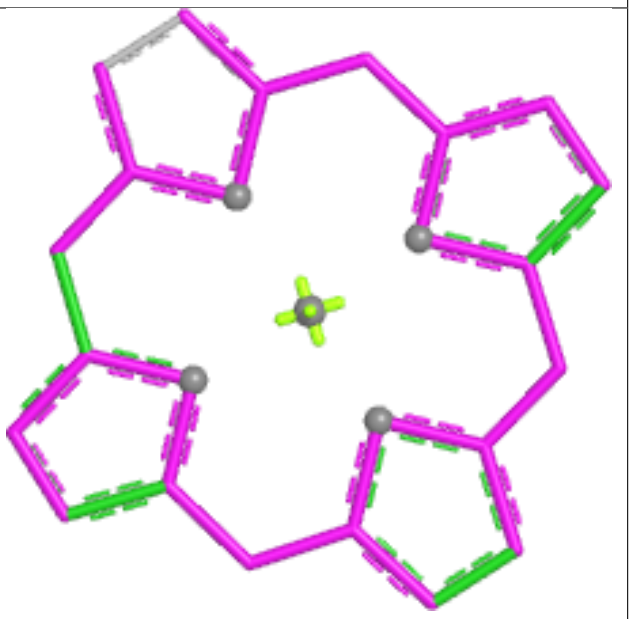


Rings

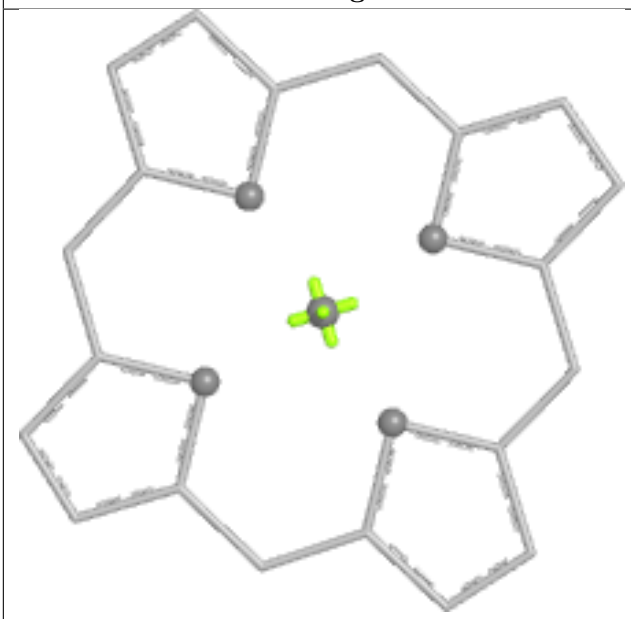
Ligand CLA 2 2011



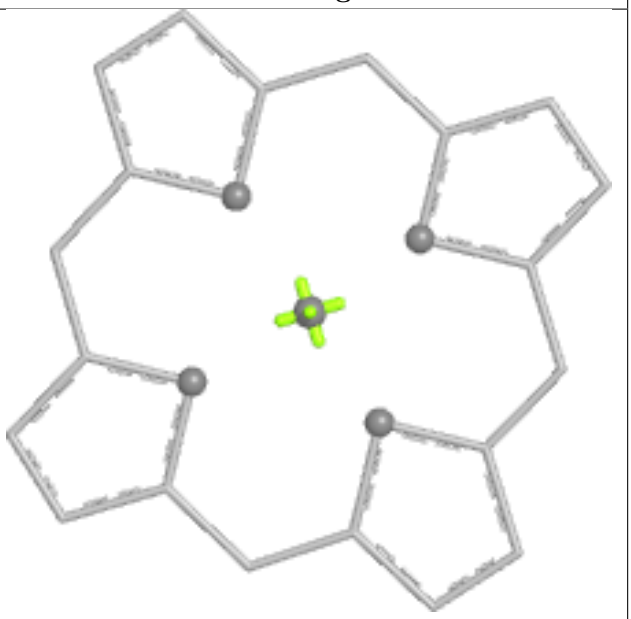
Bond lengths



Bond angles

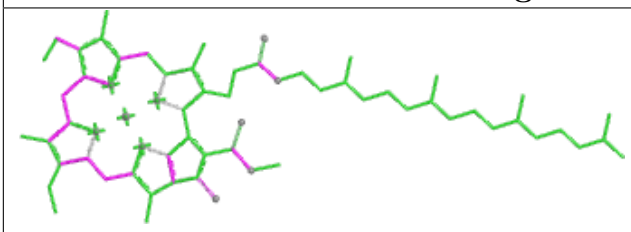


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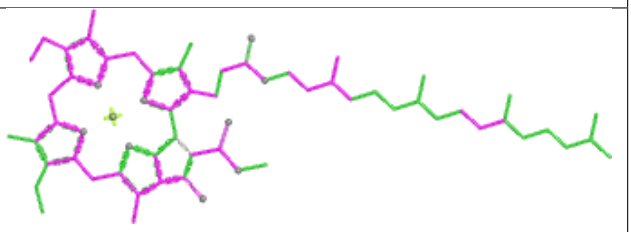


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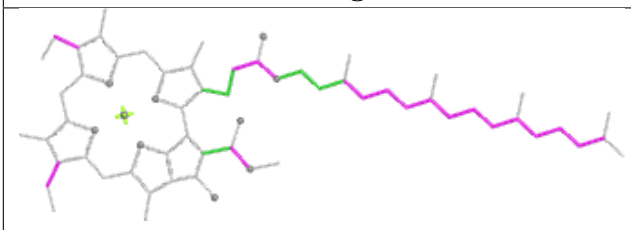
Ligand CLA A 1109



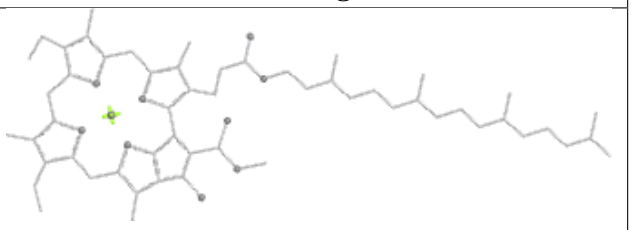
Bond lengths



Bond angles



Torsions

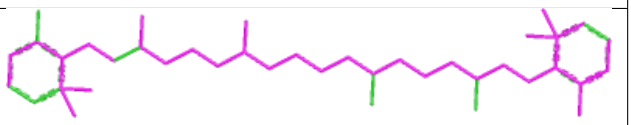


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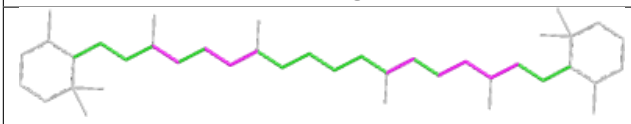
Ligand BCR B 6006



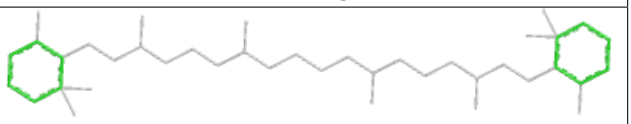
Bond lengths



Bond angles

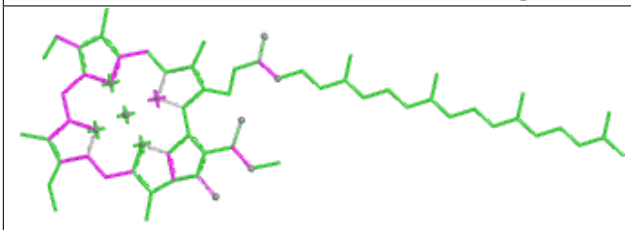


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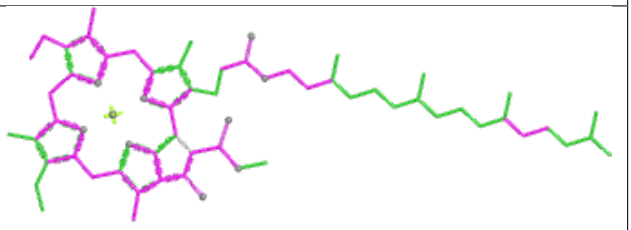


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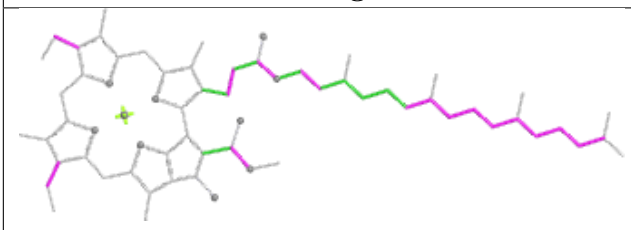
Ligand CLA A 9013



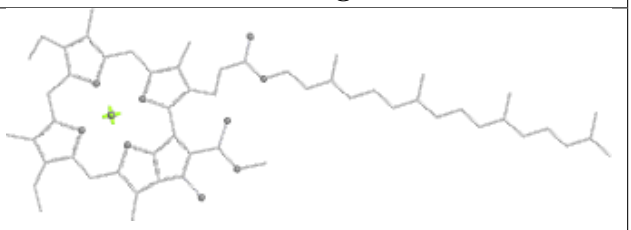
Bond lengths



Bond angles

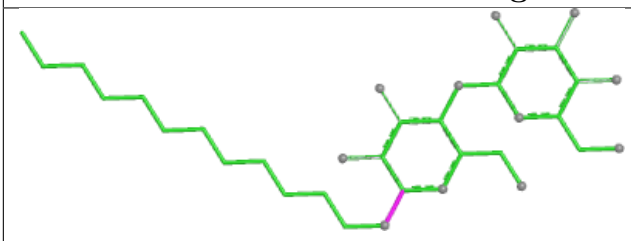


Torsions

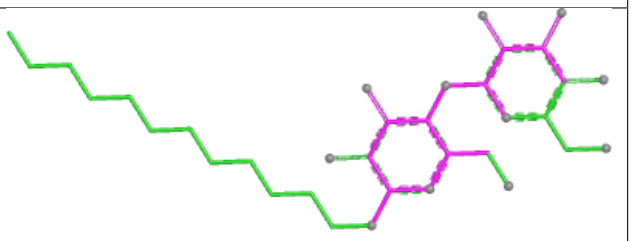


Rings

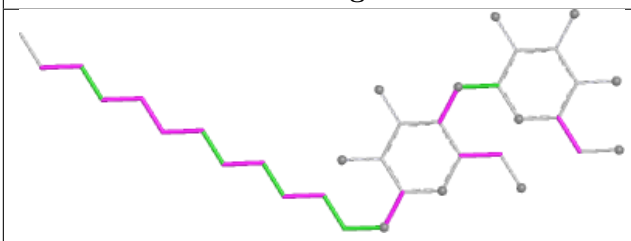
Ligand LMU G 7051



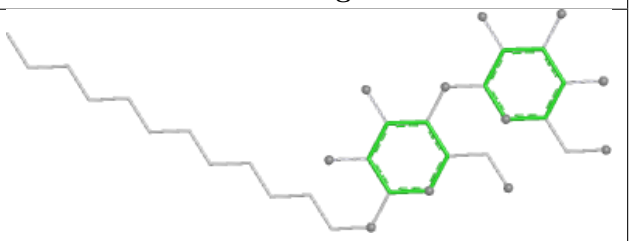
Bond lengths



Bond angles

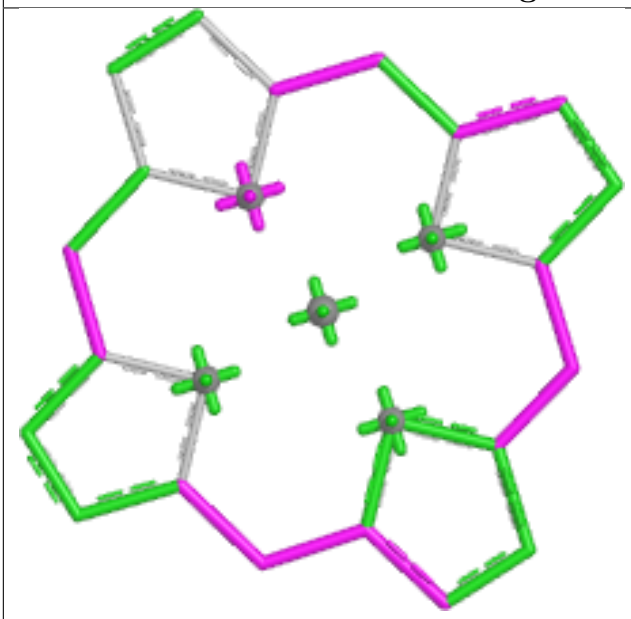


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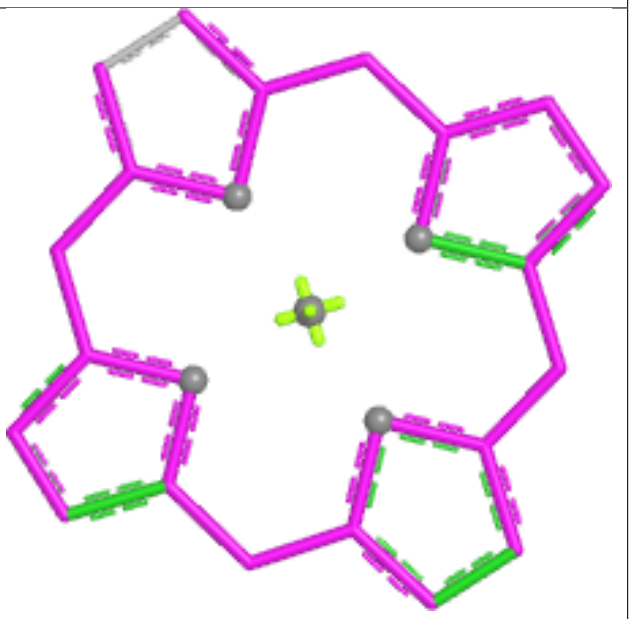


Rings

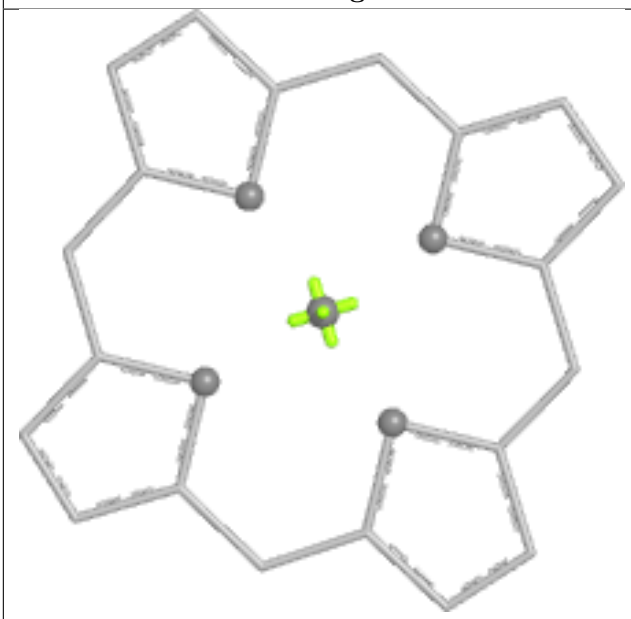
Ligand CLA 3 3014



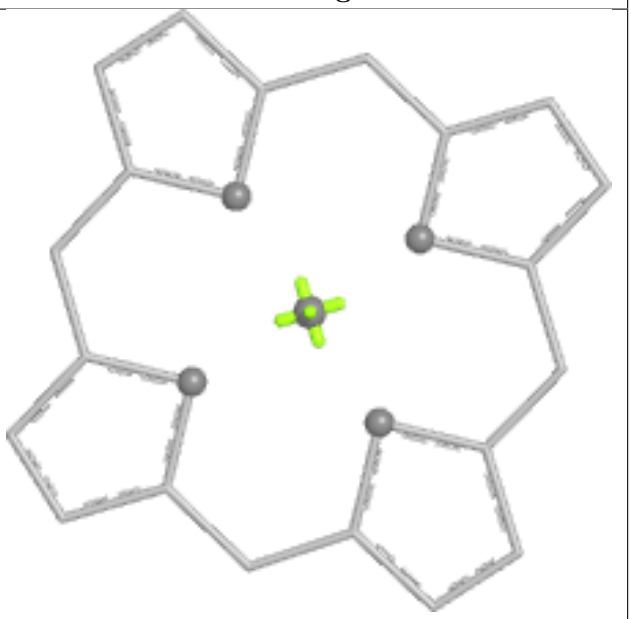
Bond lengths



Bond angles

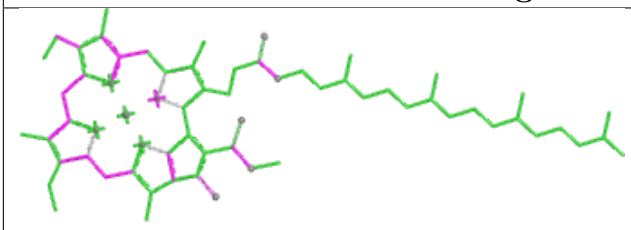


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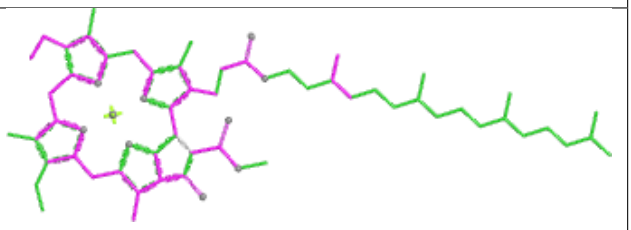


Rings

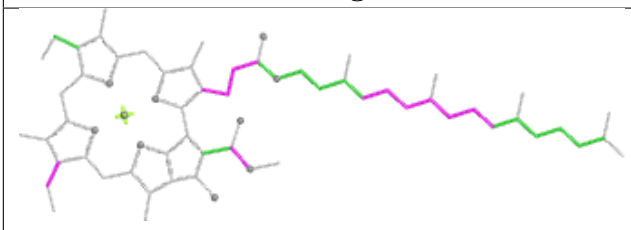
Ligand CLA B 1224



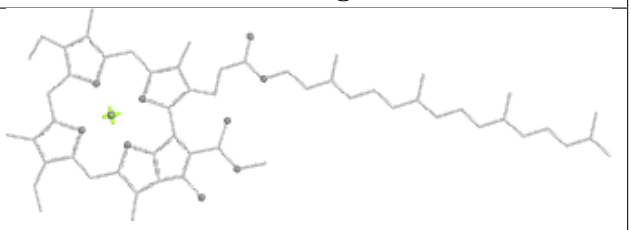
Bond lengths



Bond angles

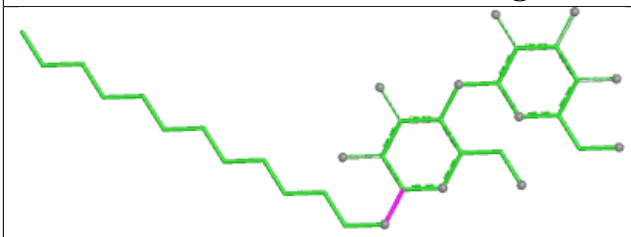


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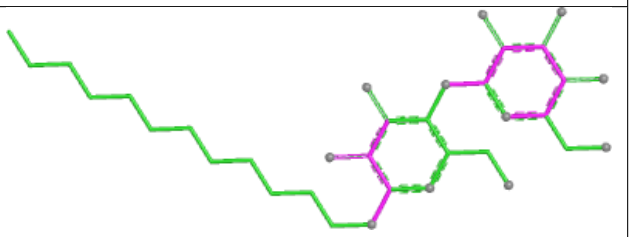


Rings

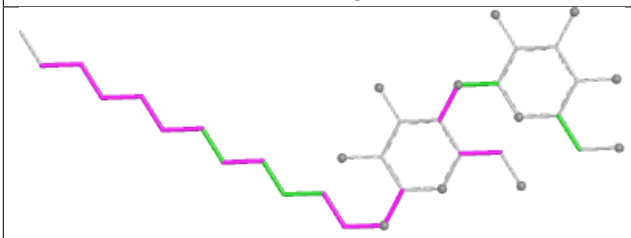
Ligand LMU C 7015



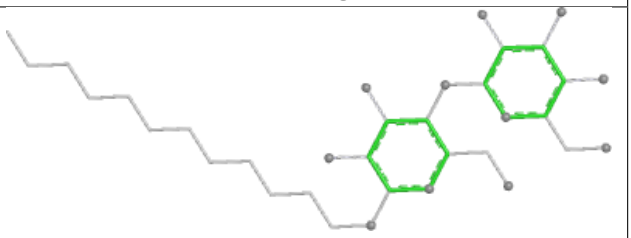
Bond lengths



Bond angles

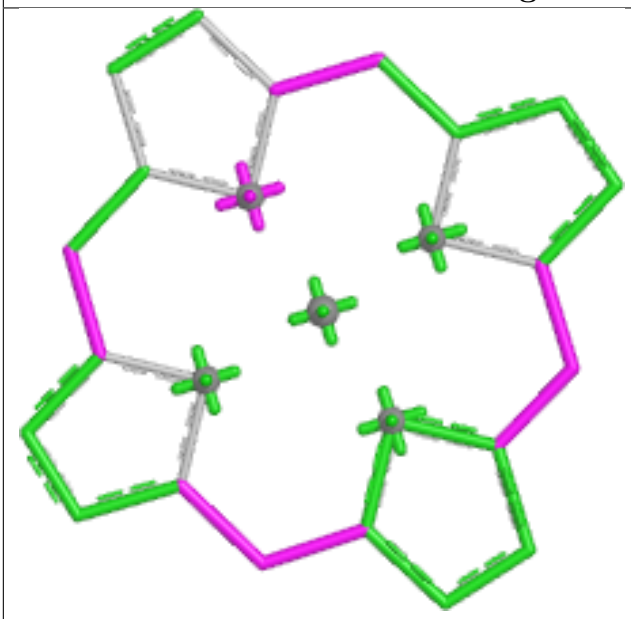


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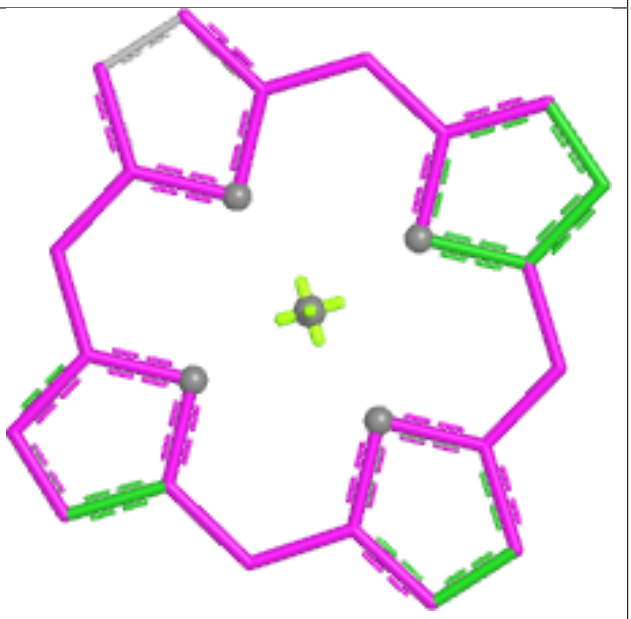


Rings

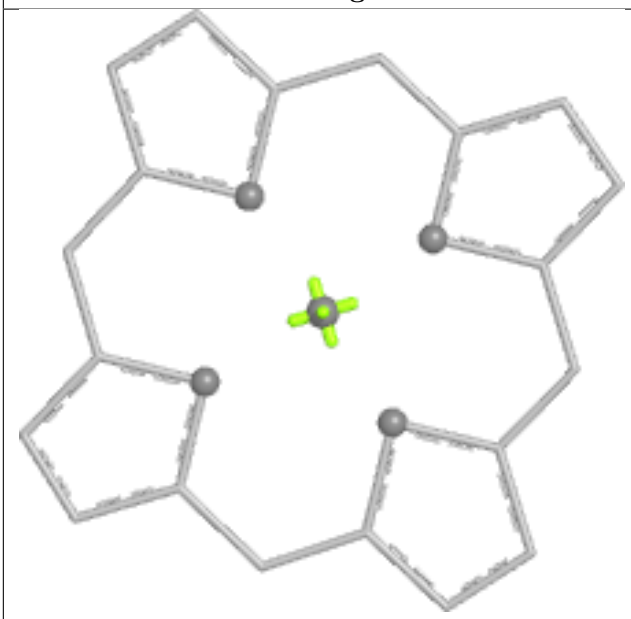
Ligand CLA 2 2010



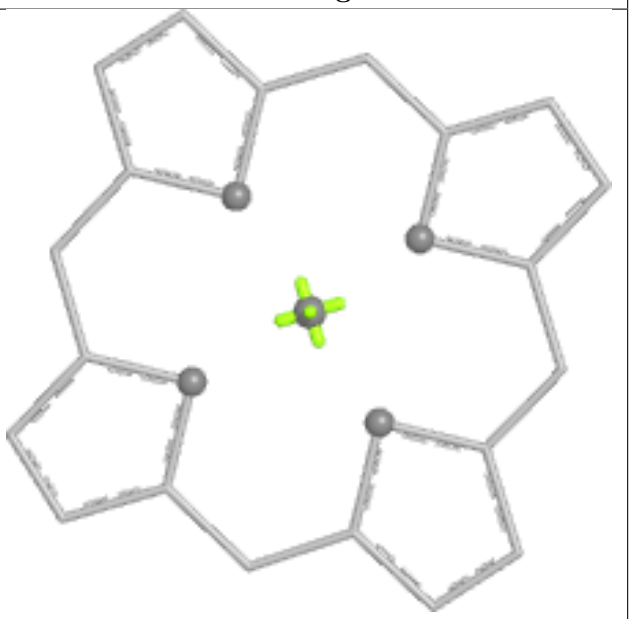
Bond lengths



Bond angles

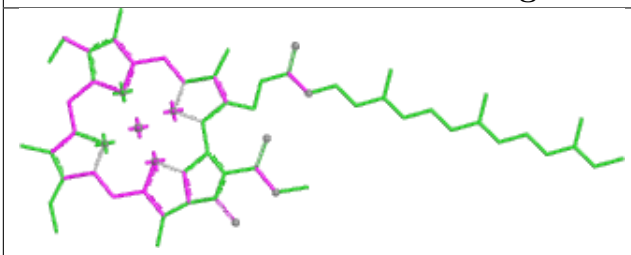


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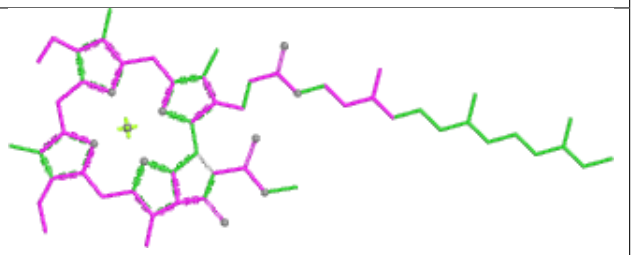


Rings

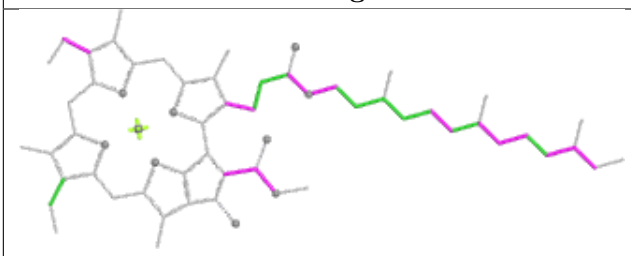
Ligand CLA 2 2014



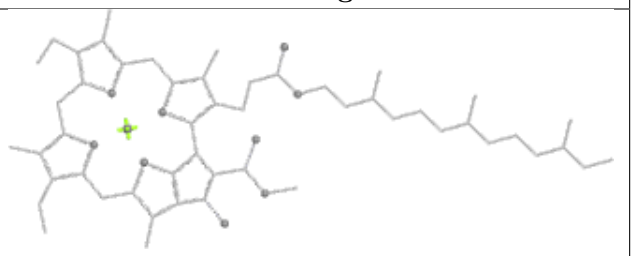
Bond lengths



Bond angles

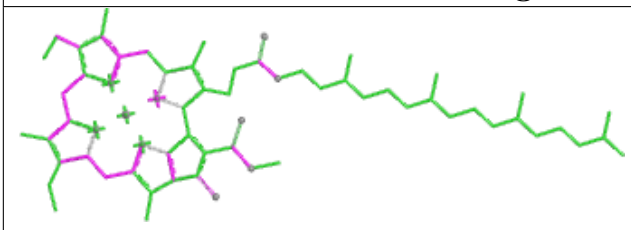


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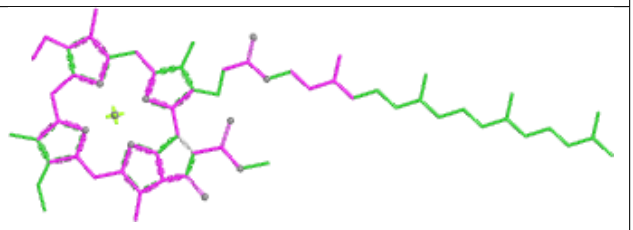


Rings

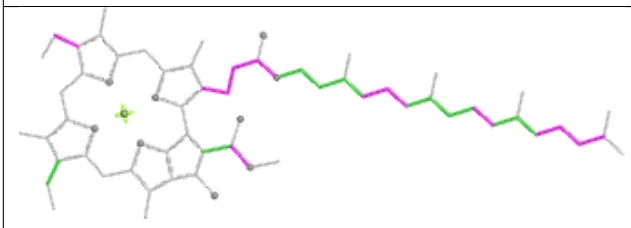
Ligand CLA A 1140



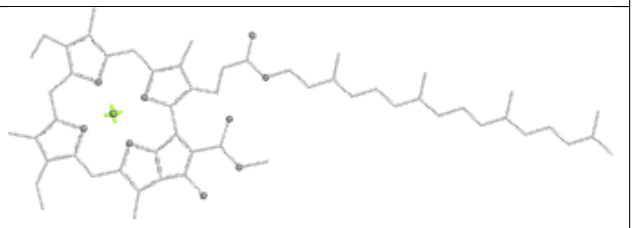
Bond lengths



Bond angles

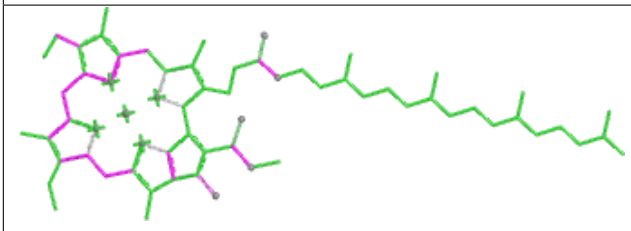


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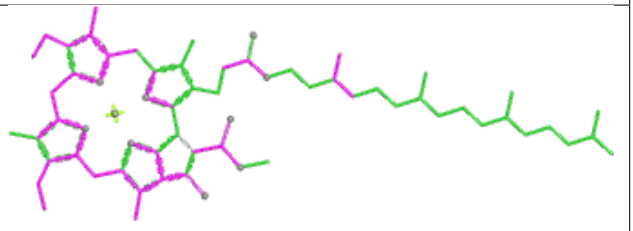


Rings

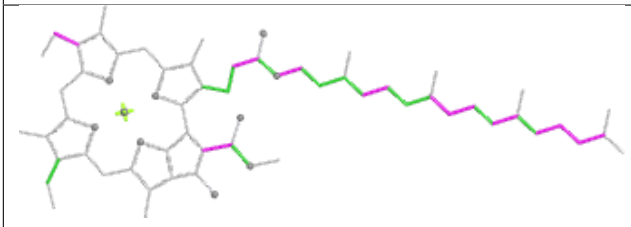
Ligand CLA B 1235



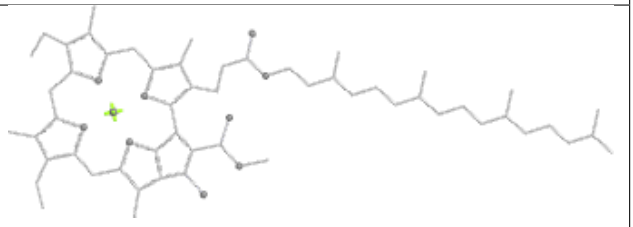
Bond lengths



Bond angles

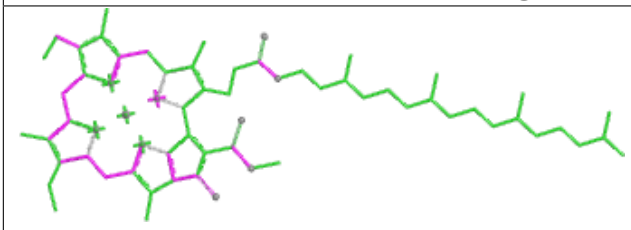


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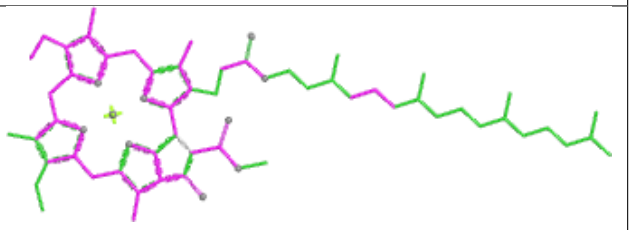


Rings

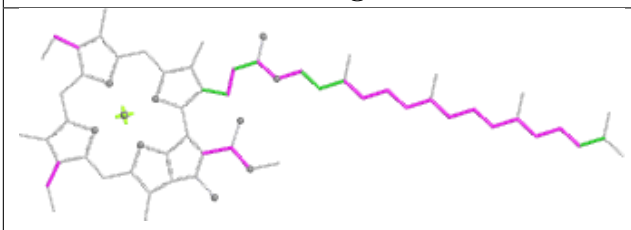
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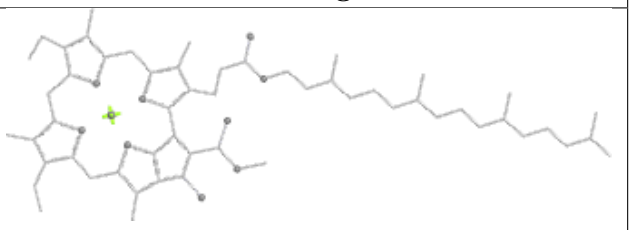
Bond lengths



Bond angles

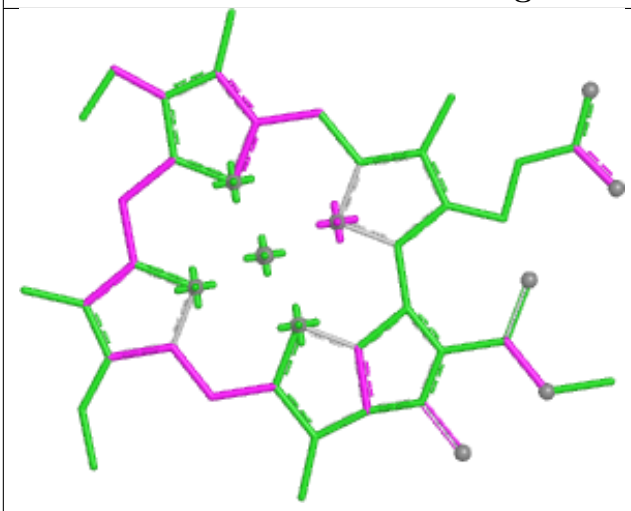


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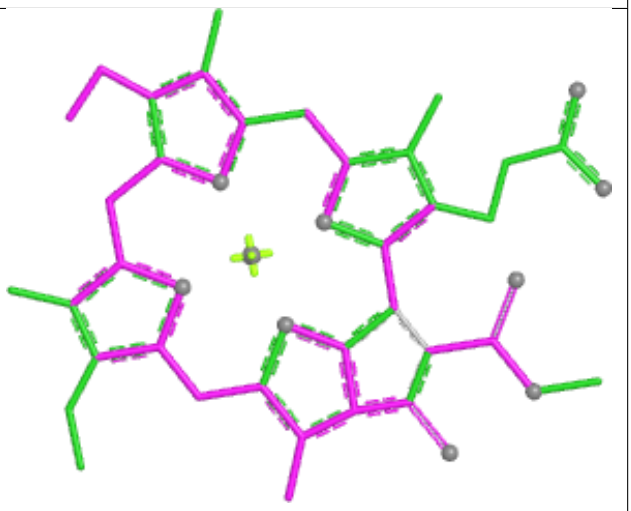


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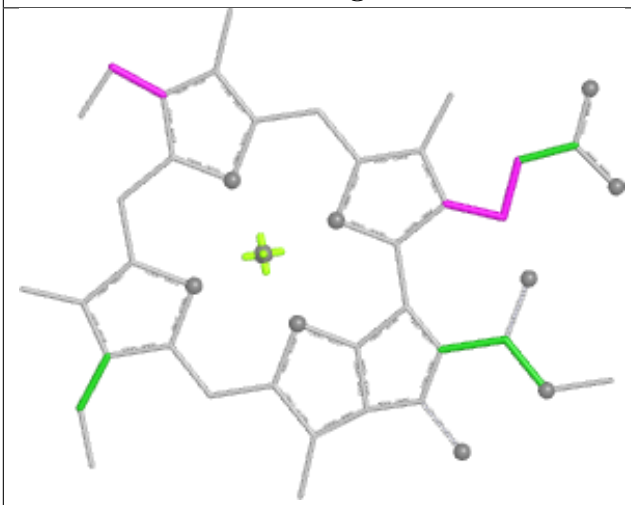
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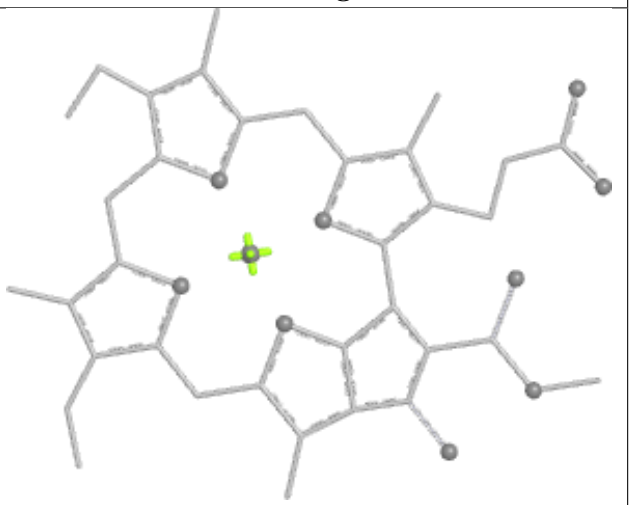
Bond lengths



Bond angles

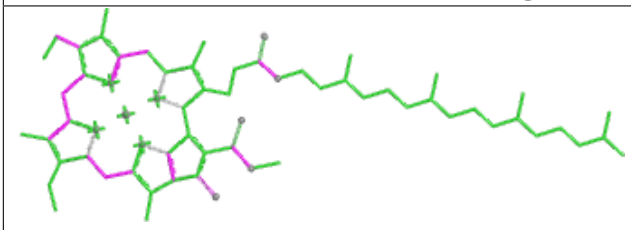


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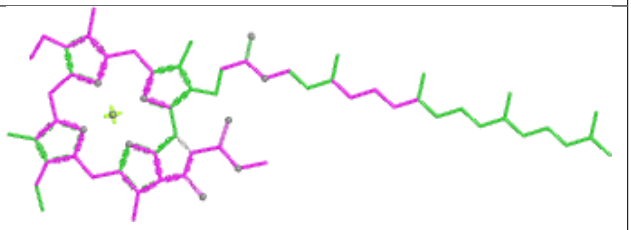


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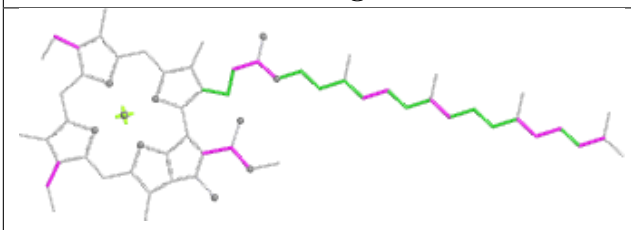
Ligand CLA 2 2007



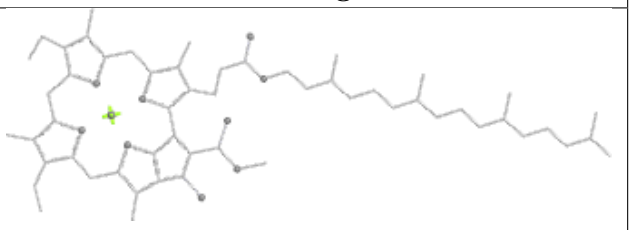
Bond lengths



Bond angles

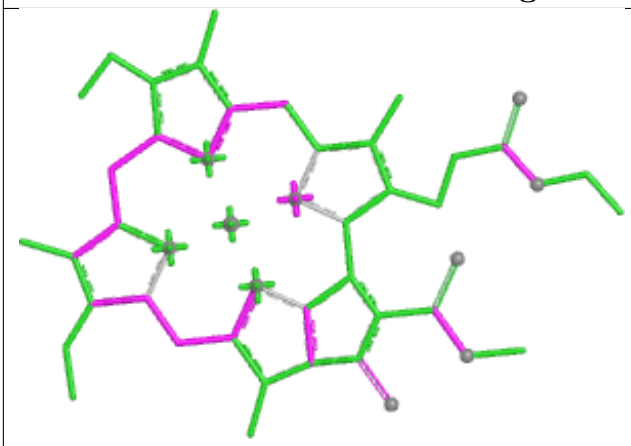


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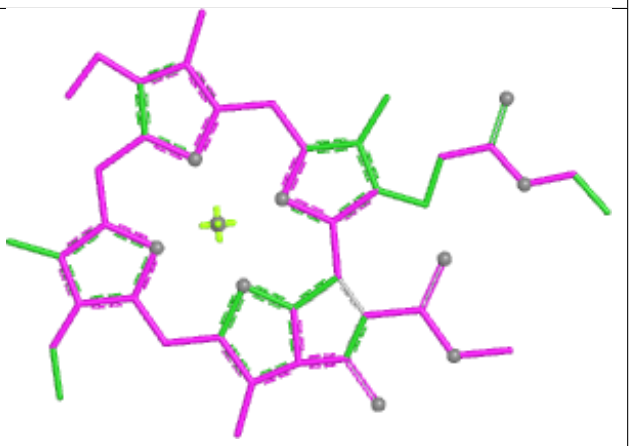


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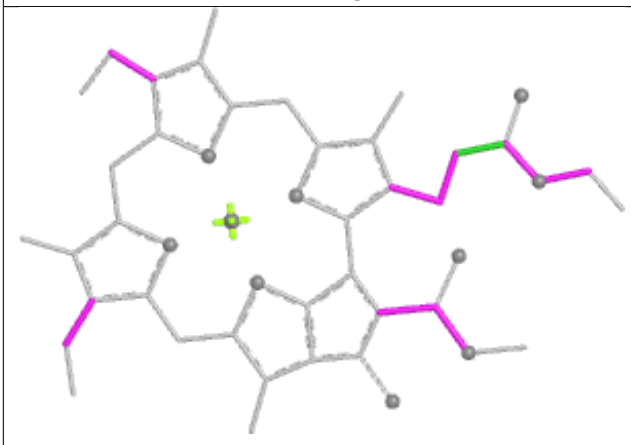
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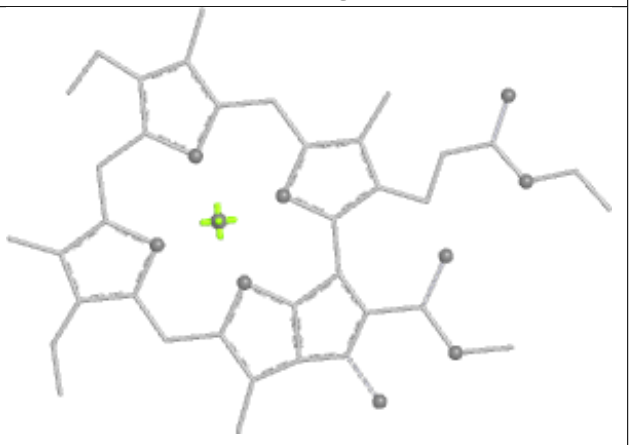
Bond lengths



Bond angles

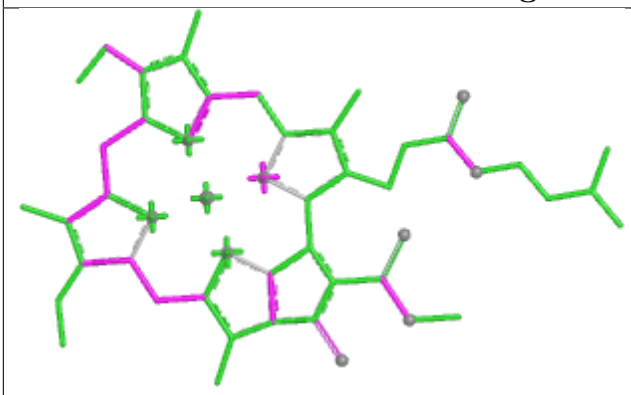


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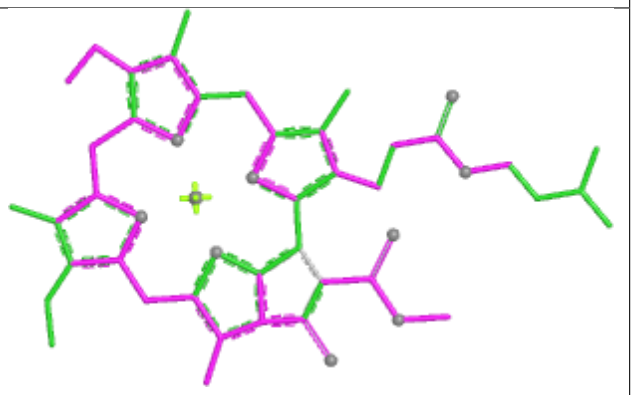


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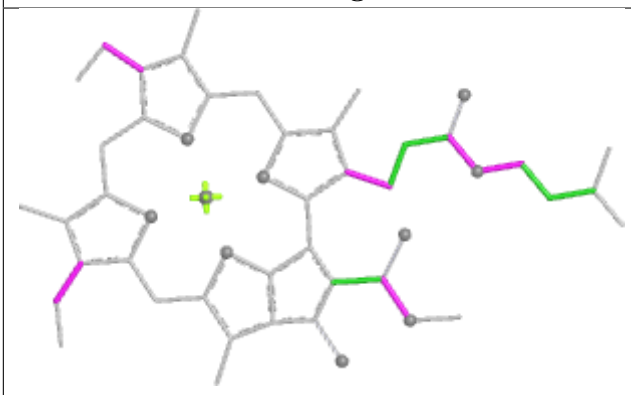
Ligand CLA 2 2004



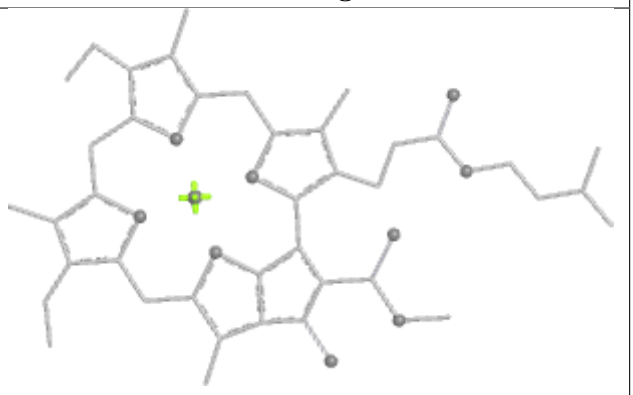
Bond lengths



Bond angles

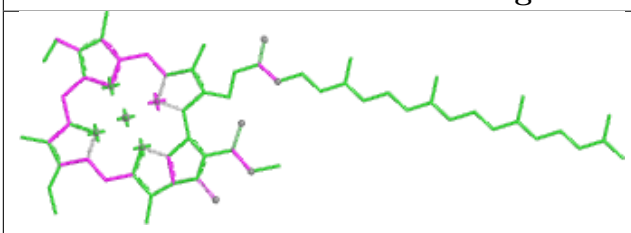


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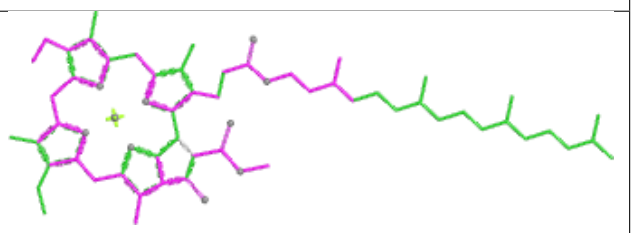


Rings

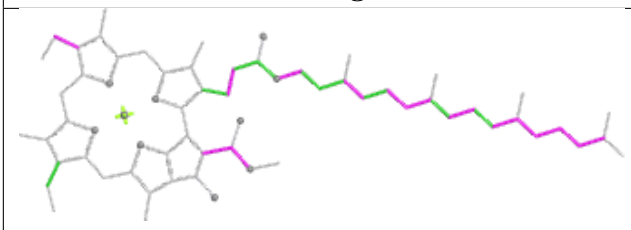
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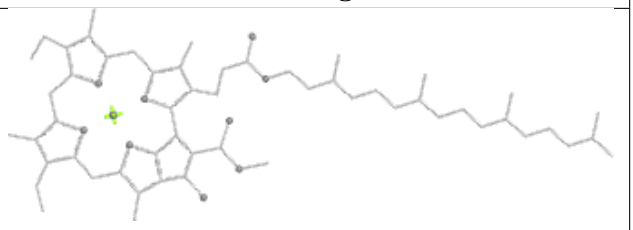
Bond lengths



Bond angles

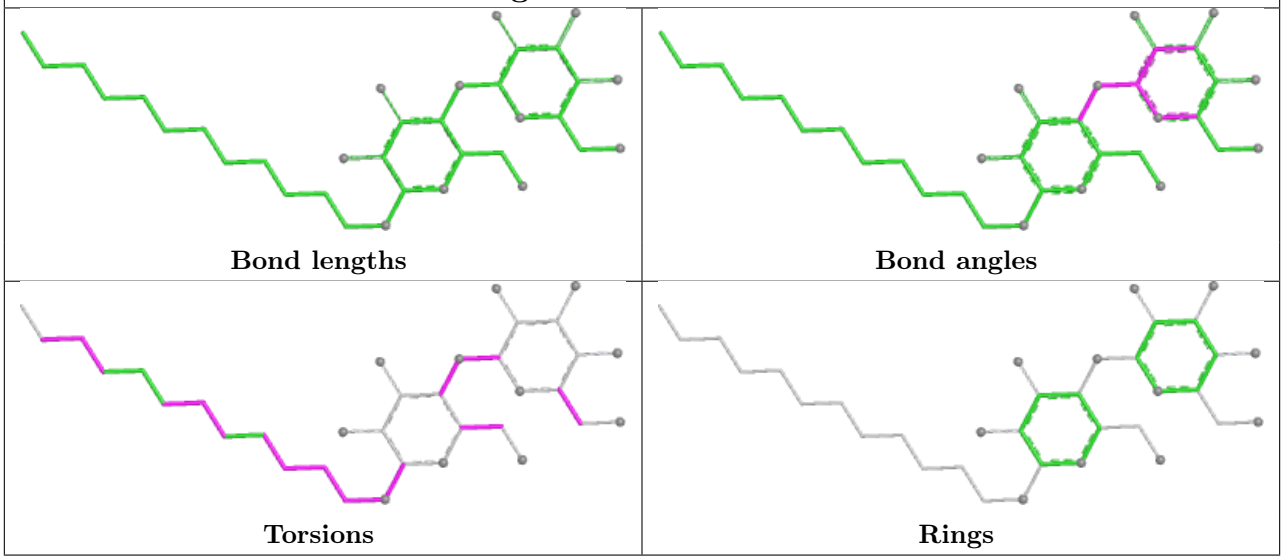


Torsions

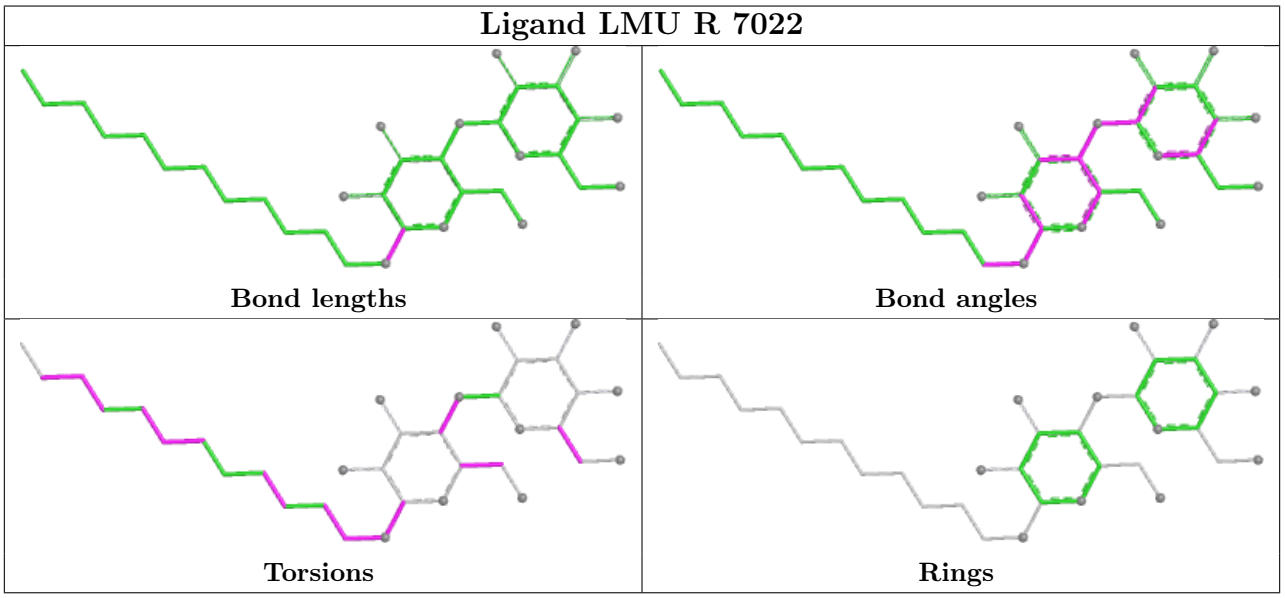


Rings

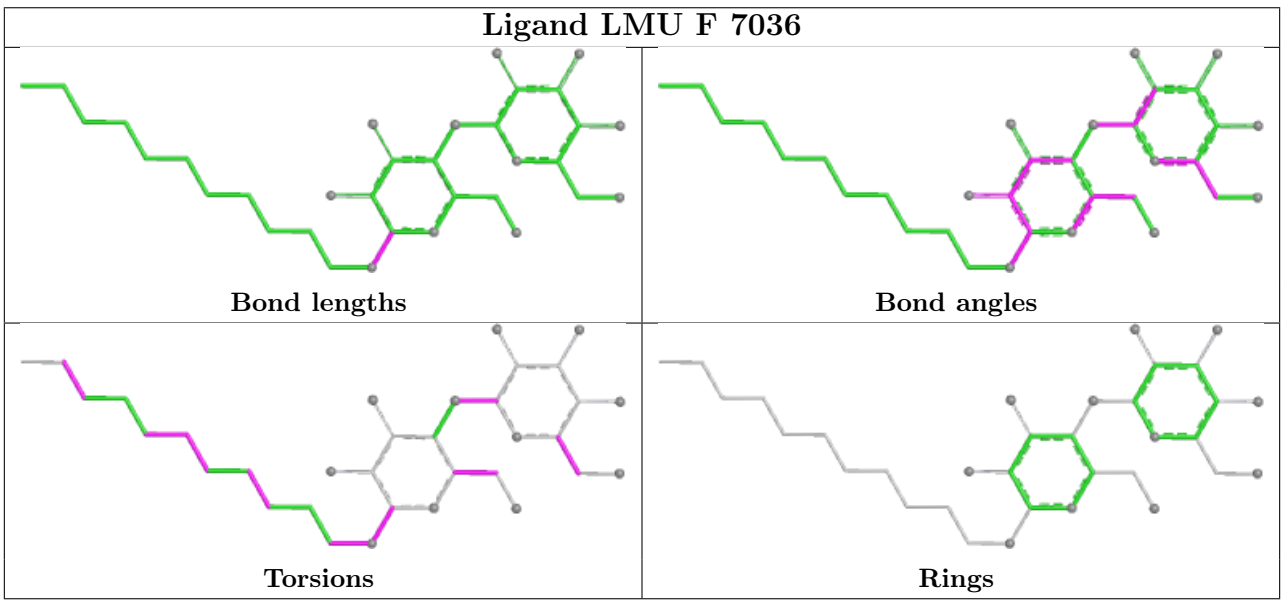
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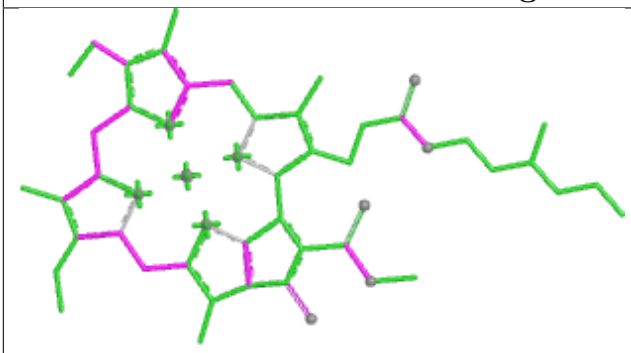
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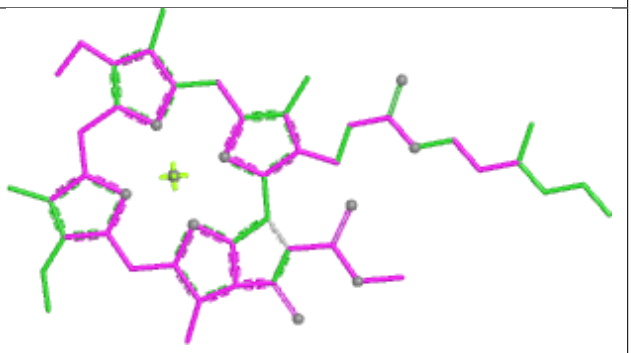
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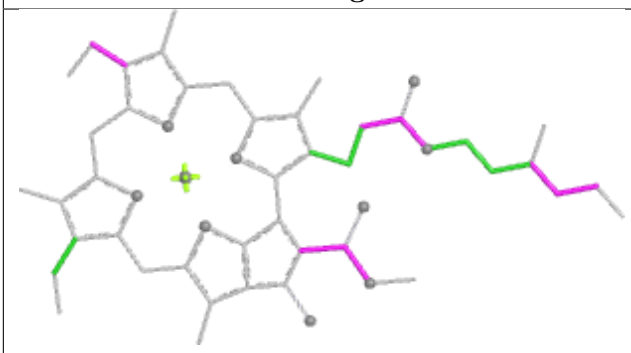
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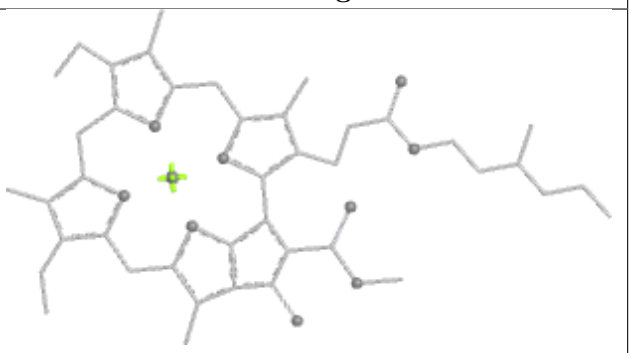
Bond lengths



Bond angles

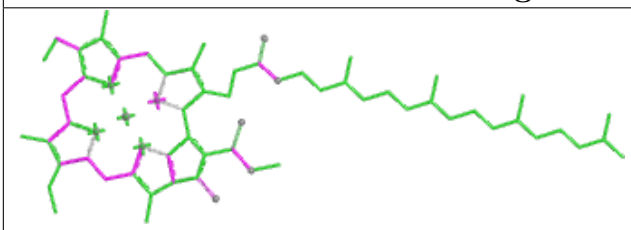


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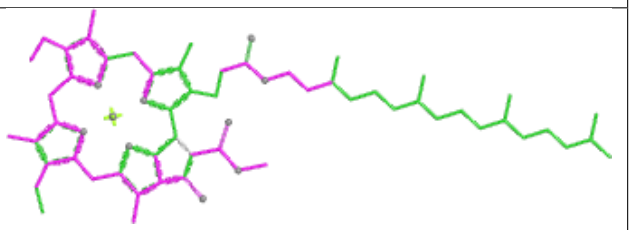


Rings

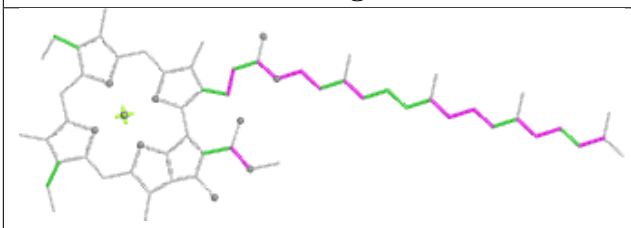
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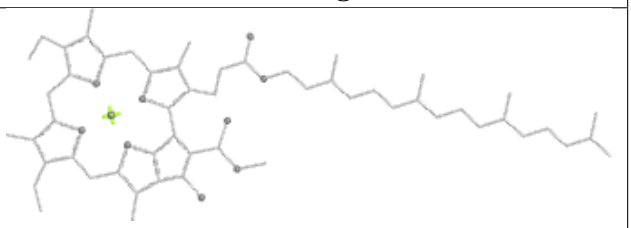
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Bond angles

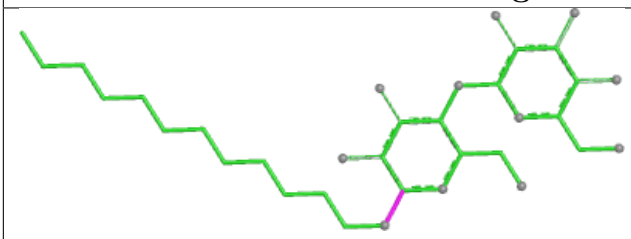


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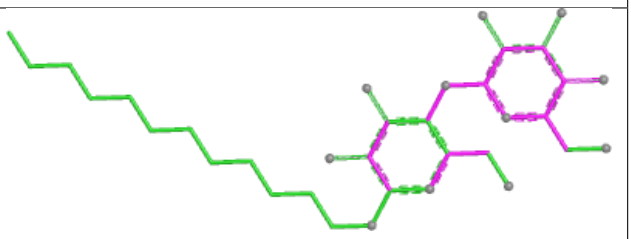


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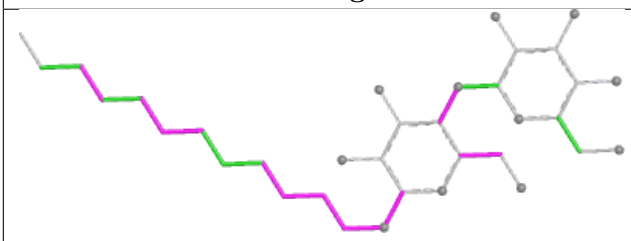
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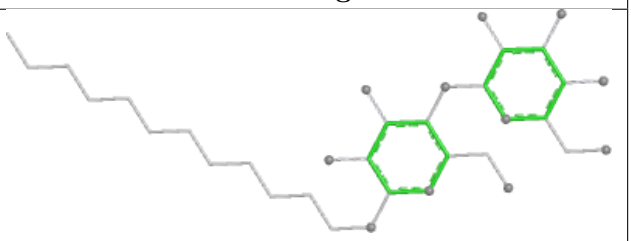
Bond lengths



Bond angles

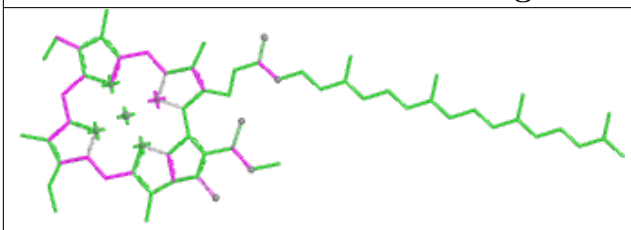


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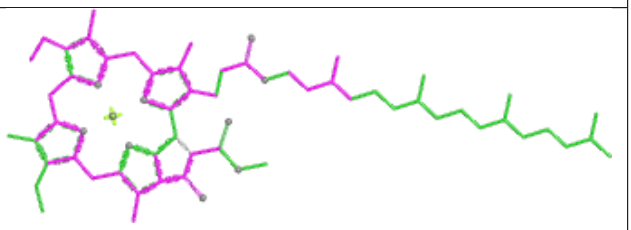


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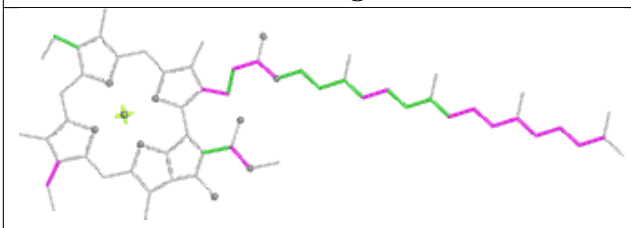
Ligand CLA H 1145



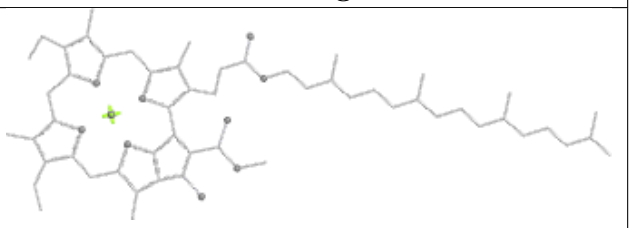
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Bond angles

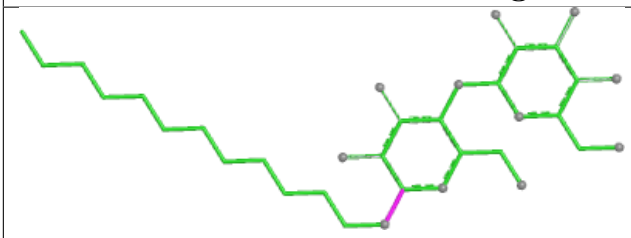


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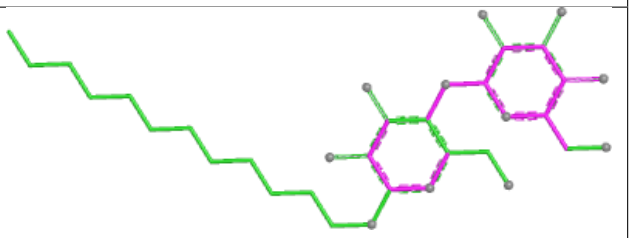


Rings

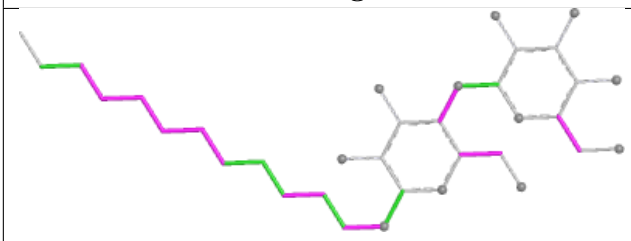
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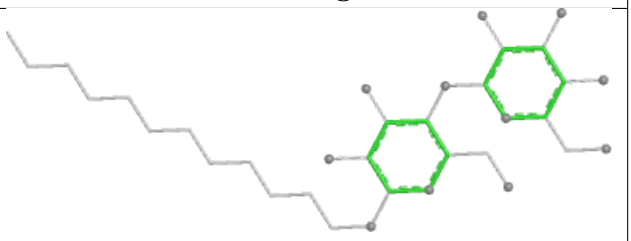
Bond lengths



Bond angles

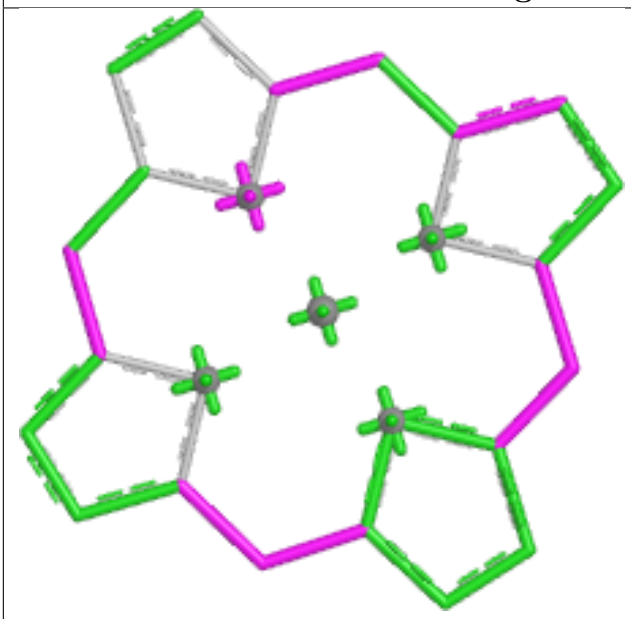


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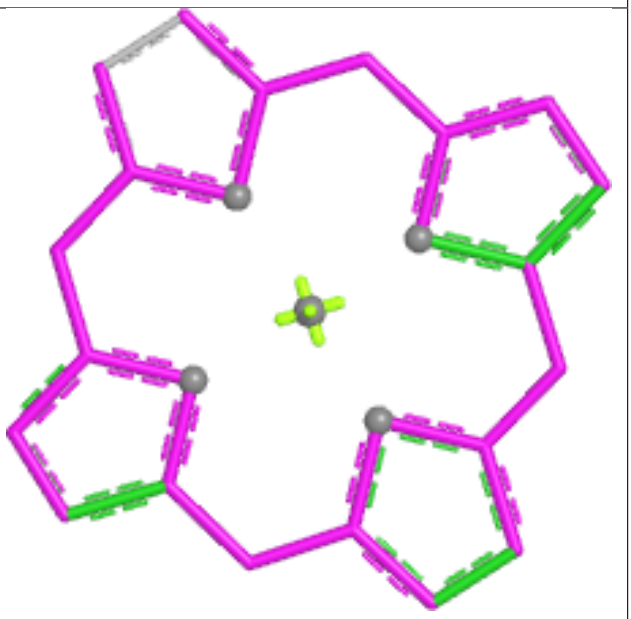


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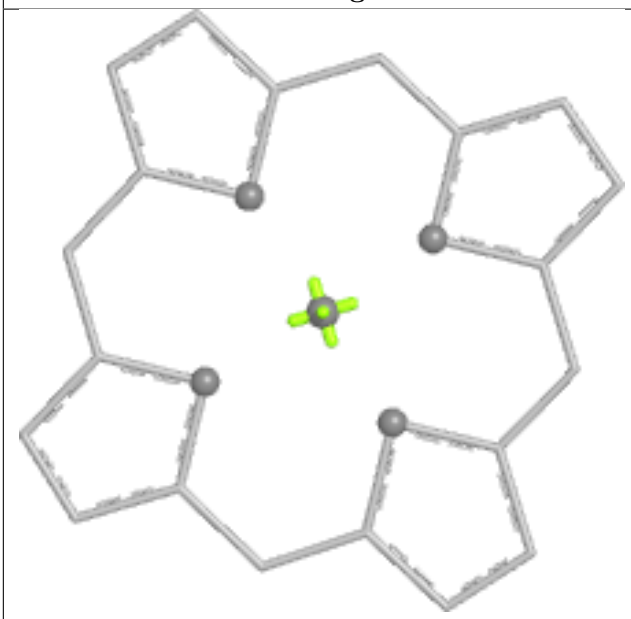
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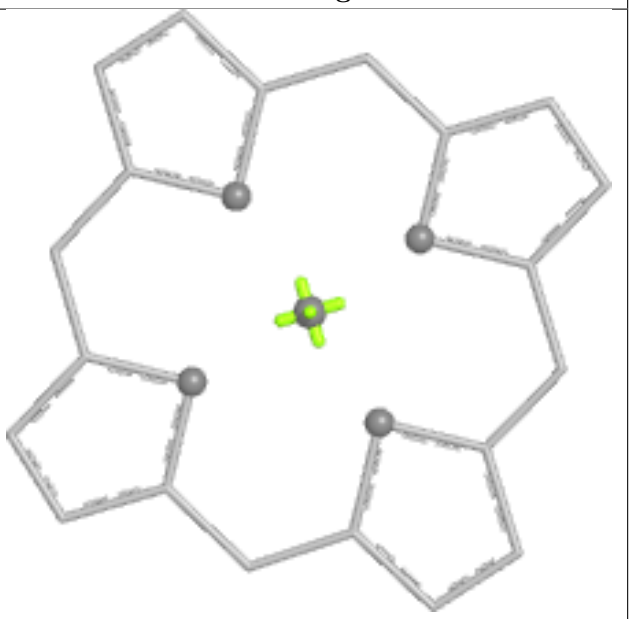
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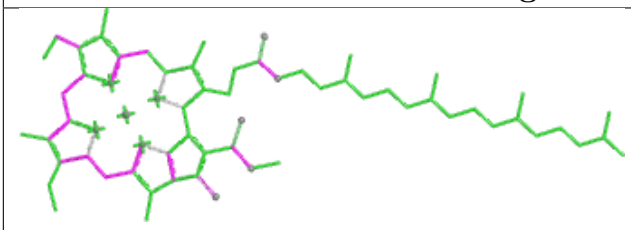


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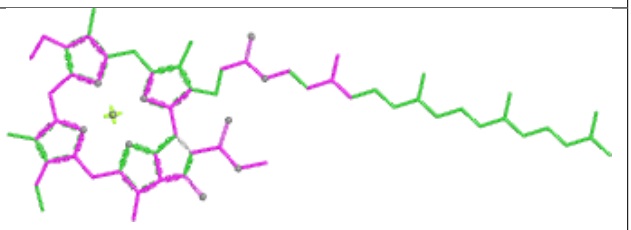


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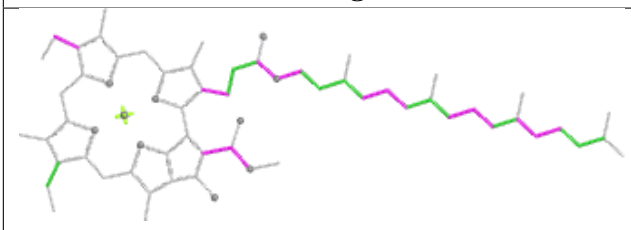
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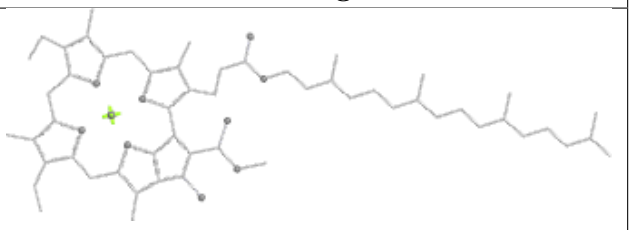
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Bond angles

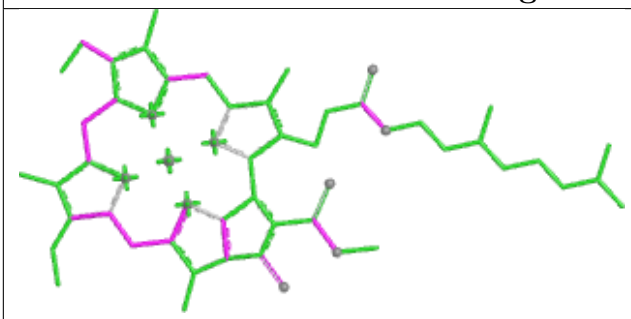


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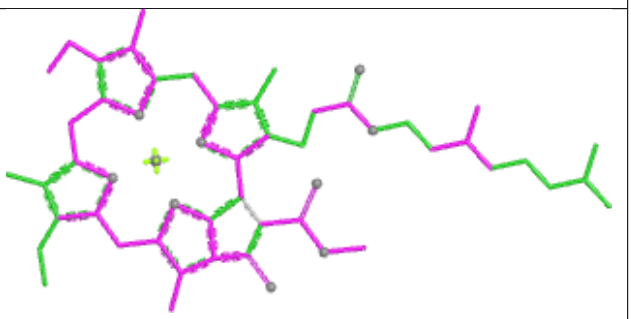


Rings

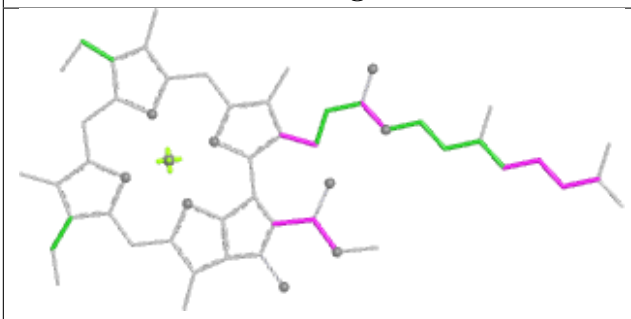
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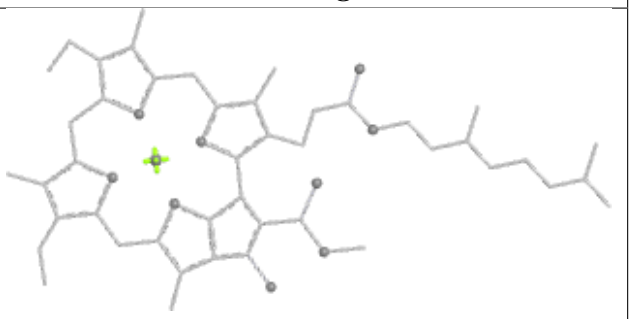
Bond lengths



Bond angles

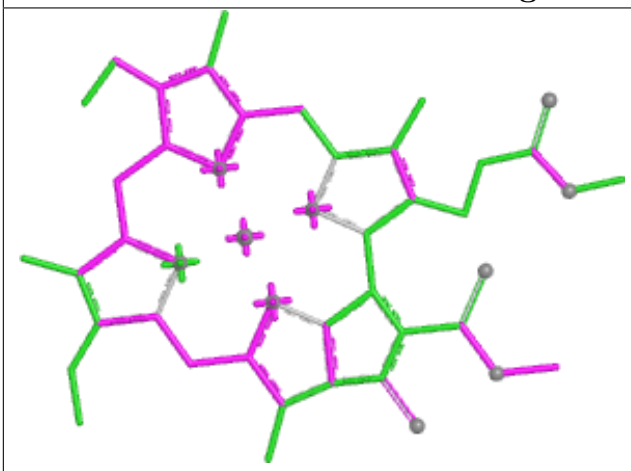


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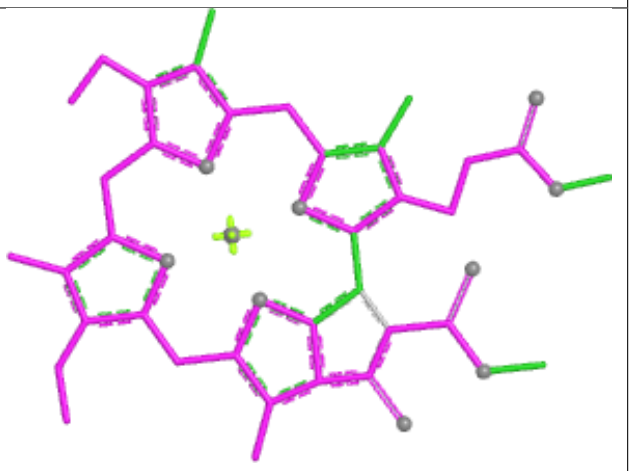


Rings

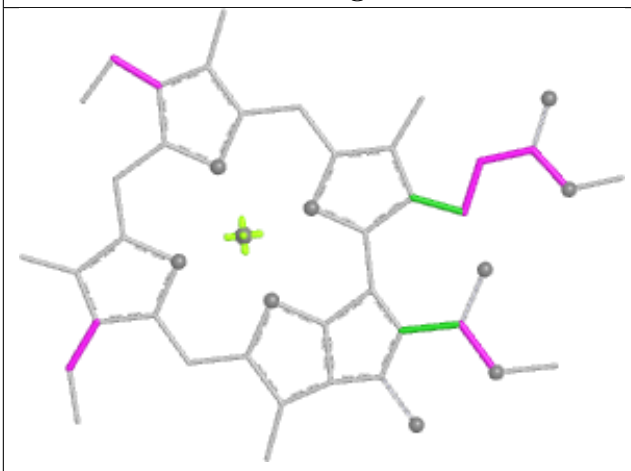
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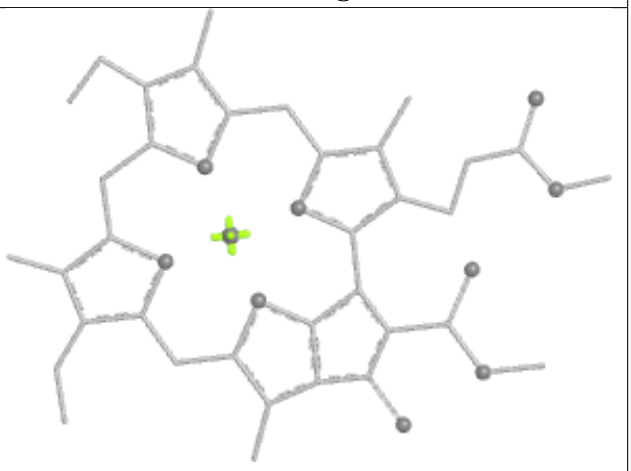
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Bond angles

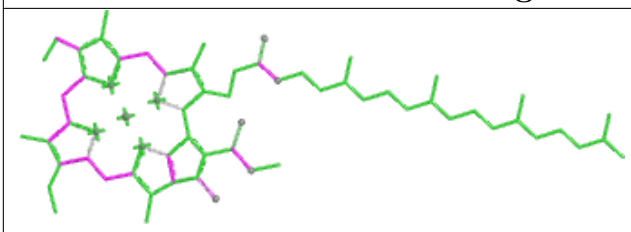


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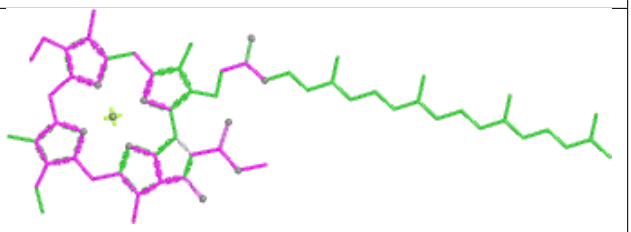


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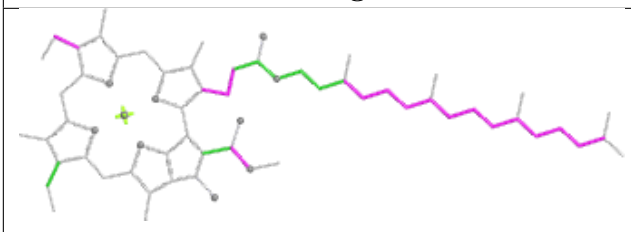
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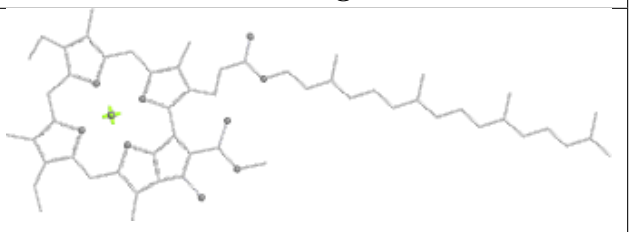
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Bond angles

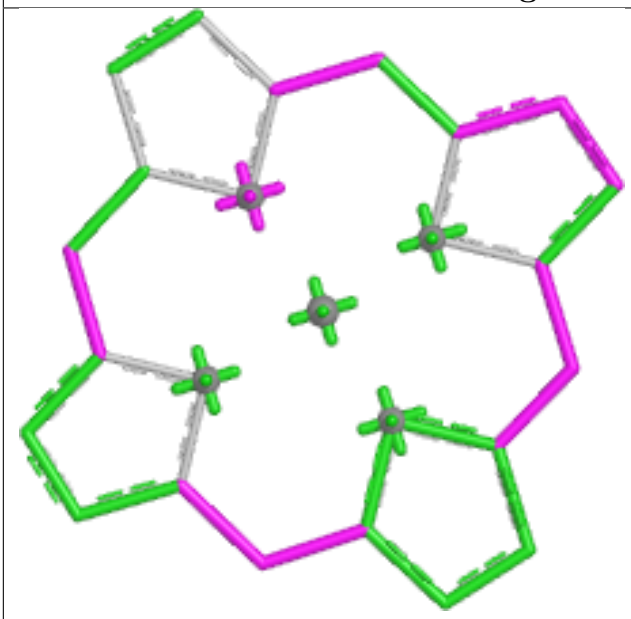


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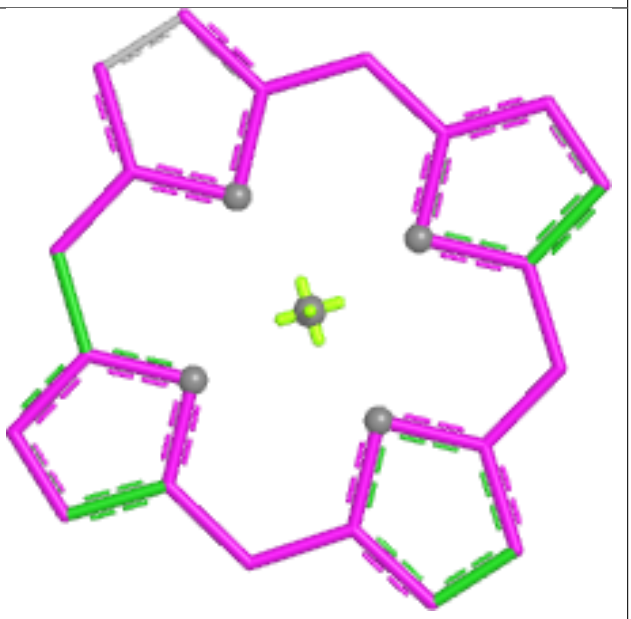


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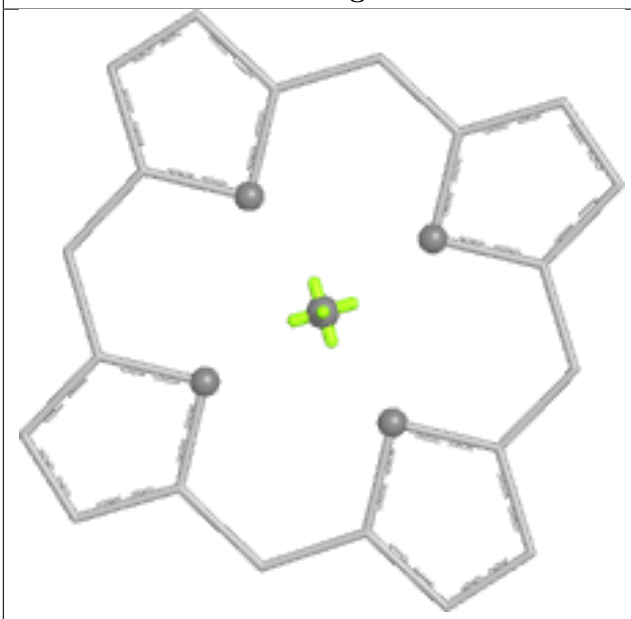
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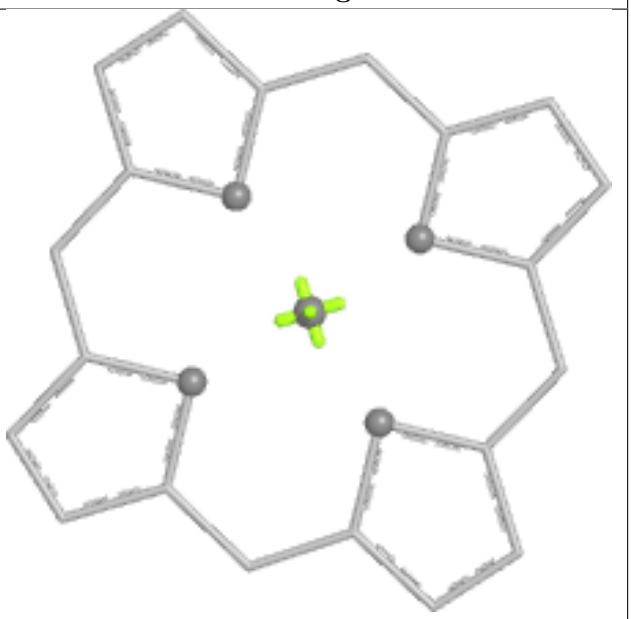
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Bond angles

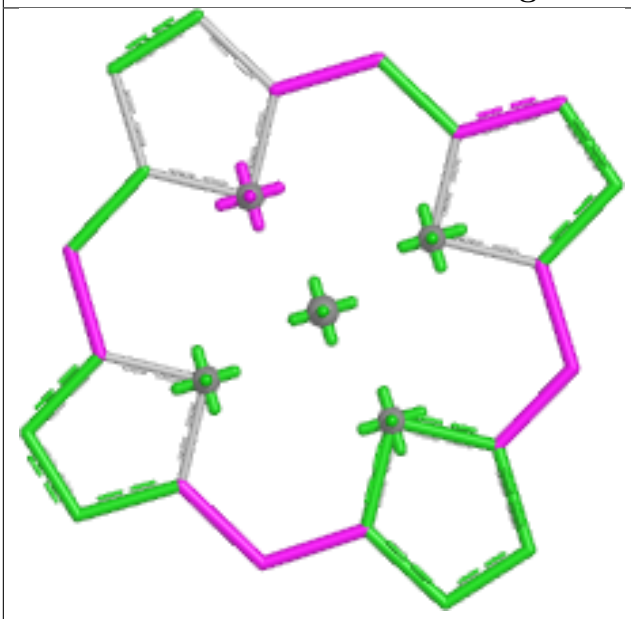


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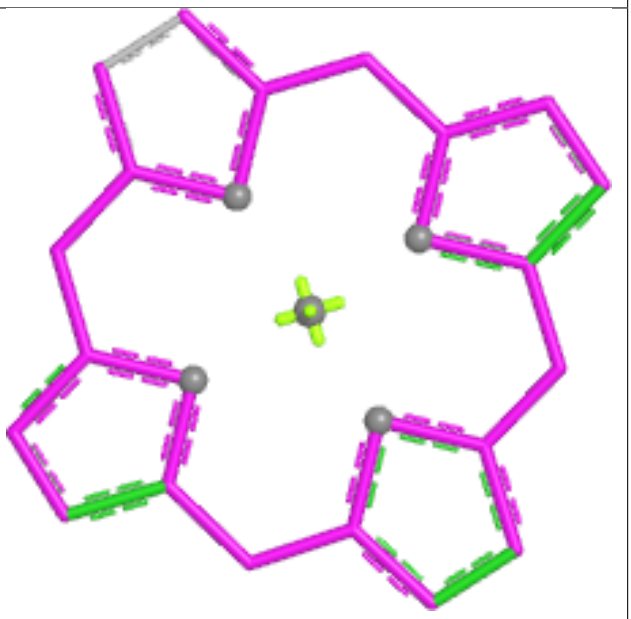


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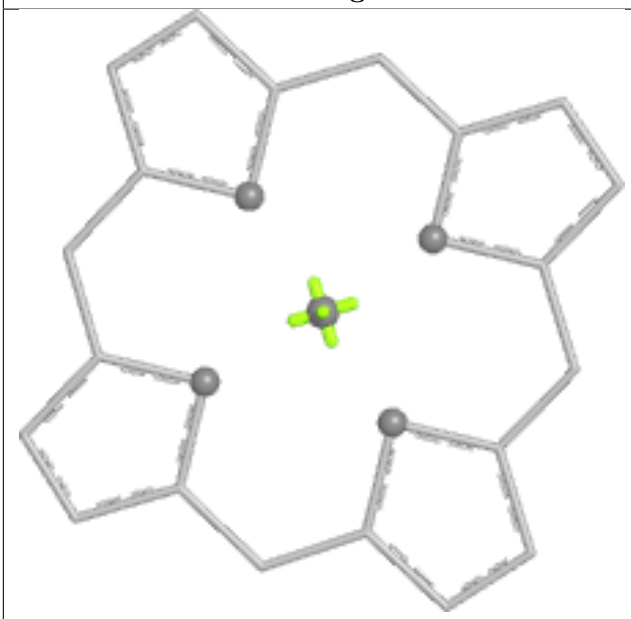
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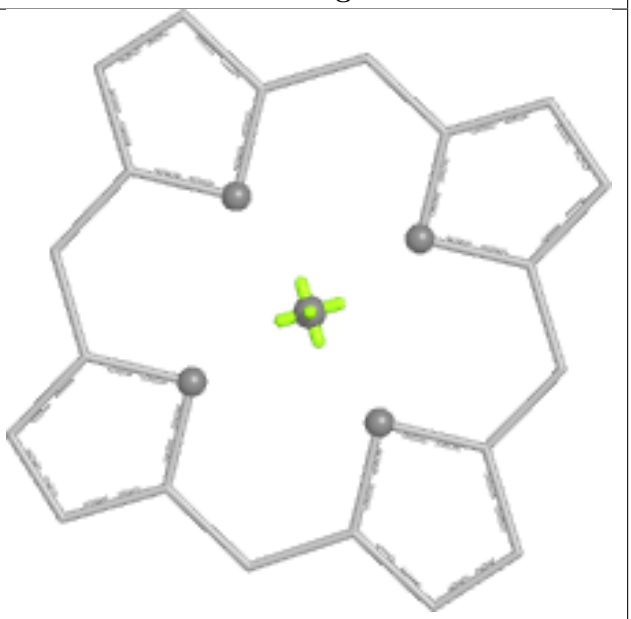
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Bond angles

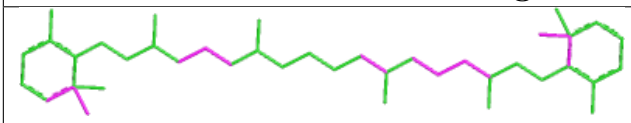


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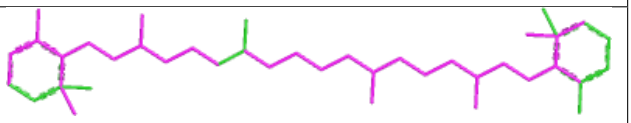


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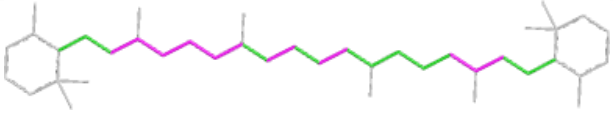
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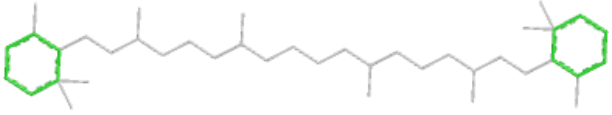
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Bond angles

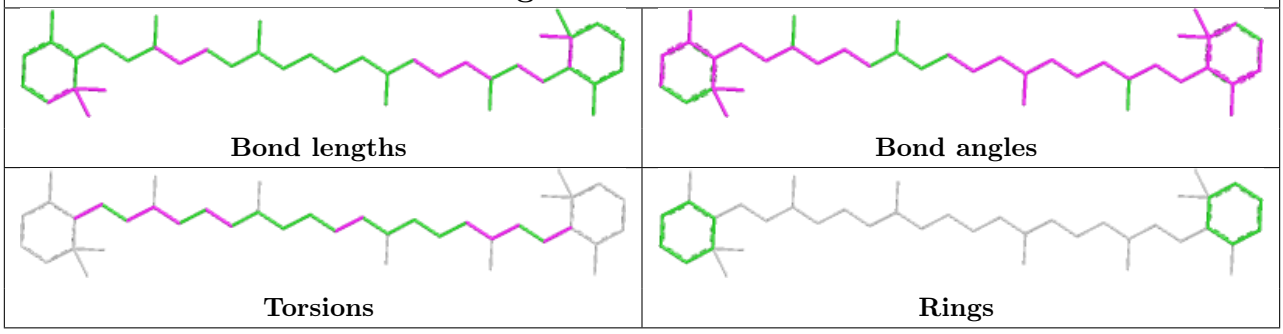


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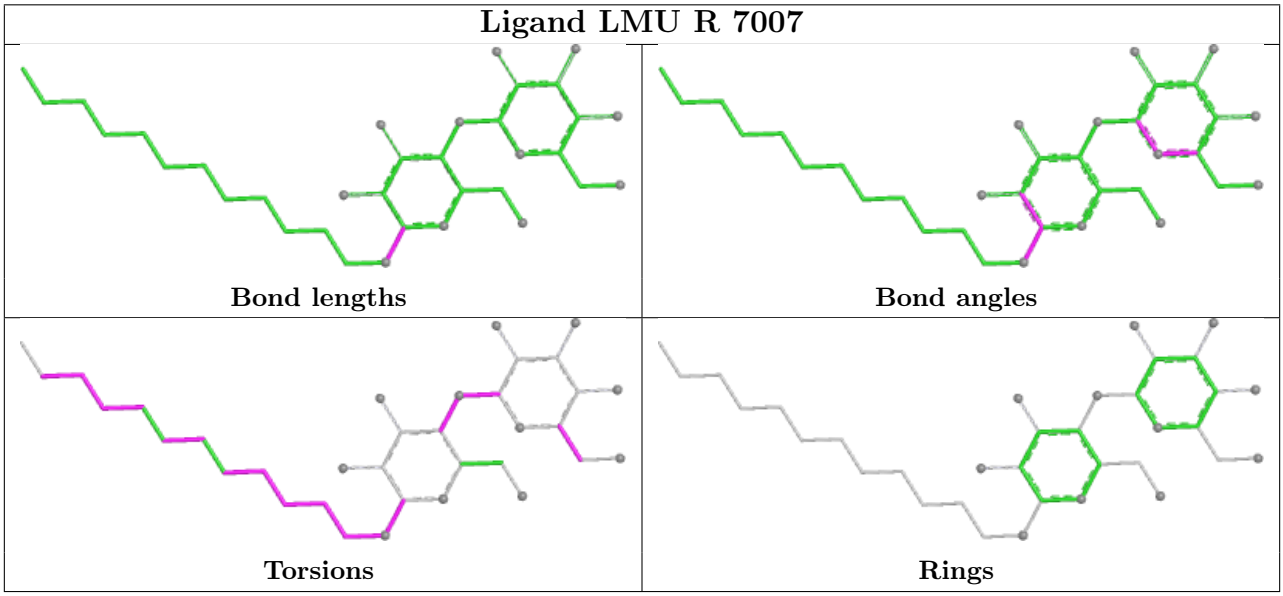


Rings

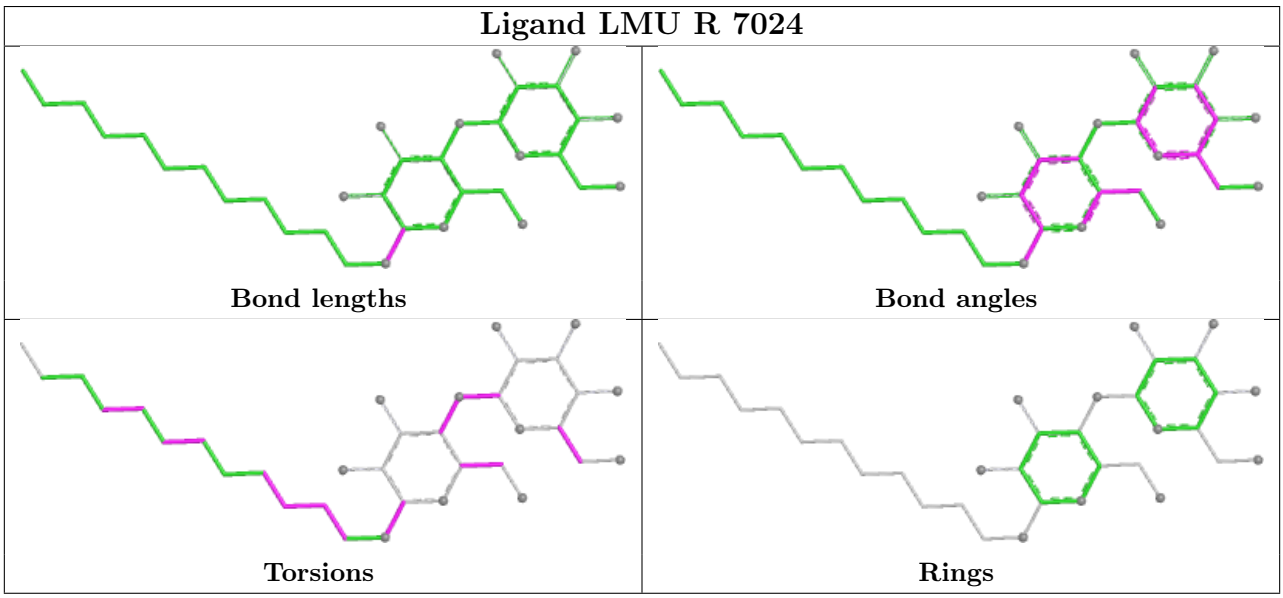
Ligand BCR L 6019



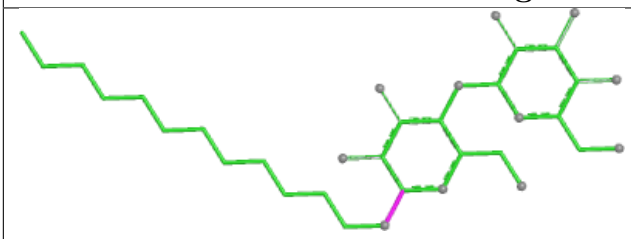
Ligand LMU R 7007



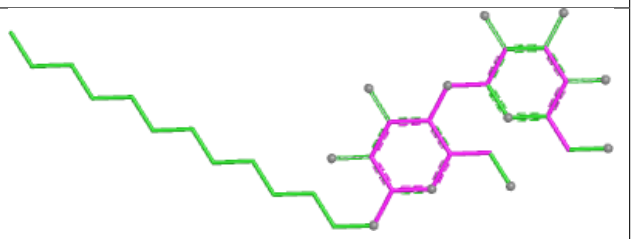
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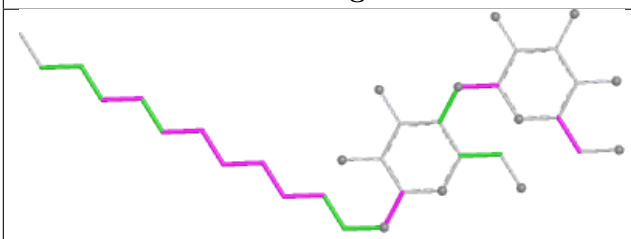
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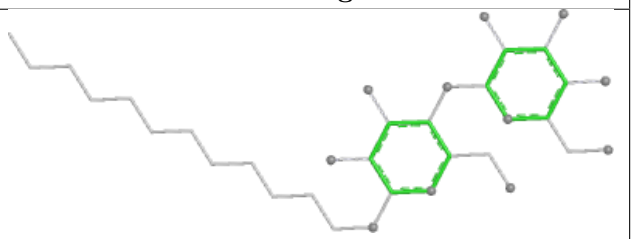
Bond lengths



Bond angles

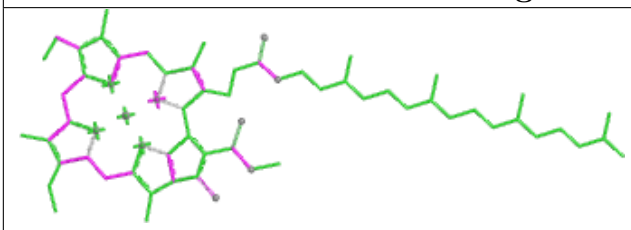


Torsions

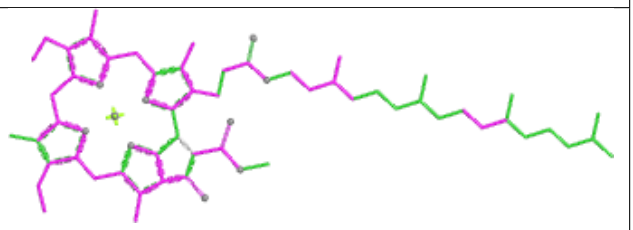


Rings

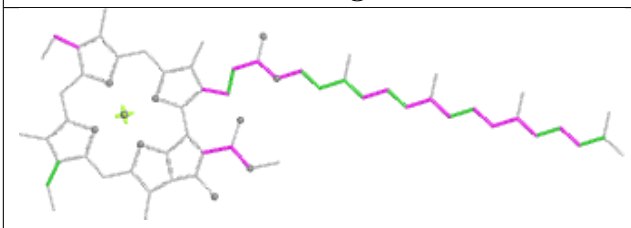
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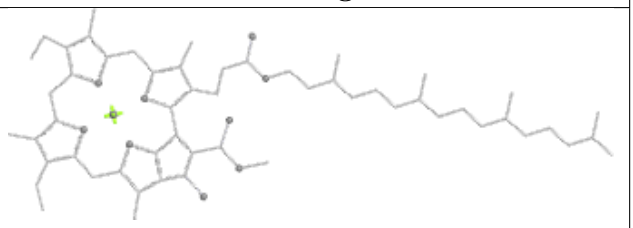
Bond lengths



Bond angles

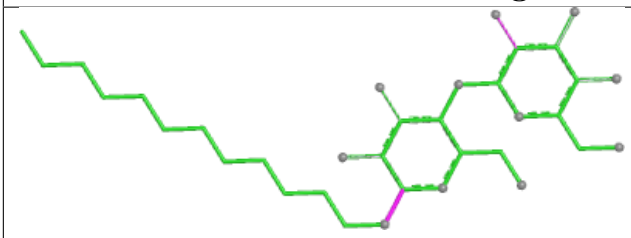


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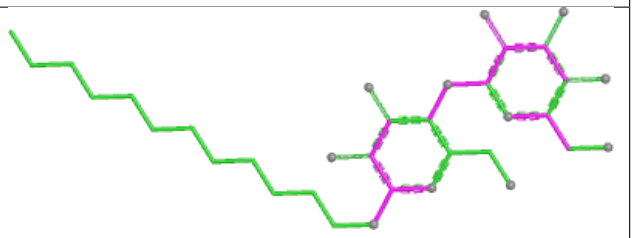


Rings

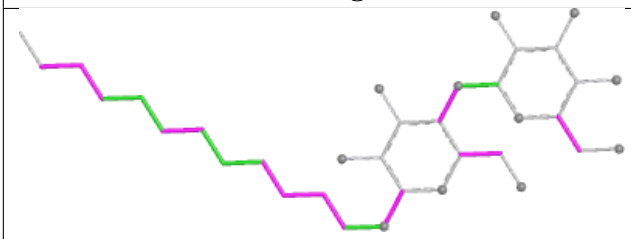
Ligand LMU R 7014



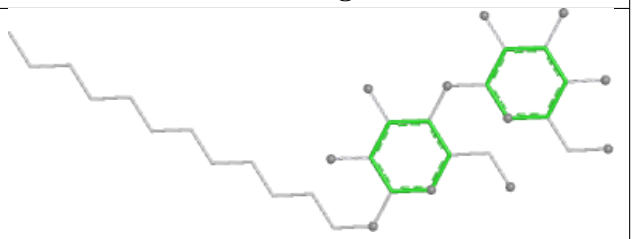
Bond lengths



Bond angles

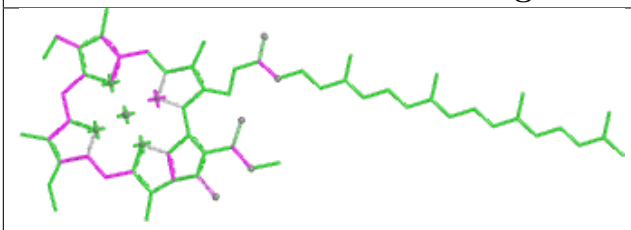


Torsions

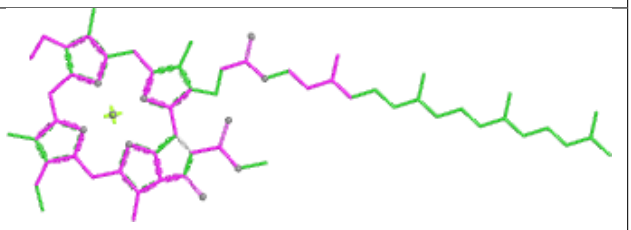


Rings

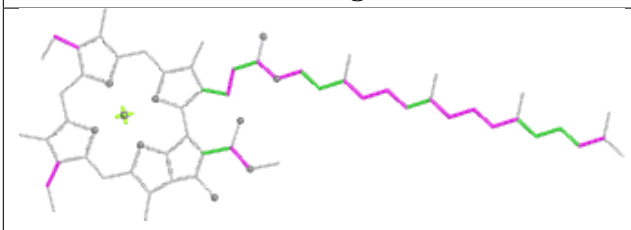
Ligand CLA A 1124



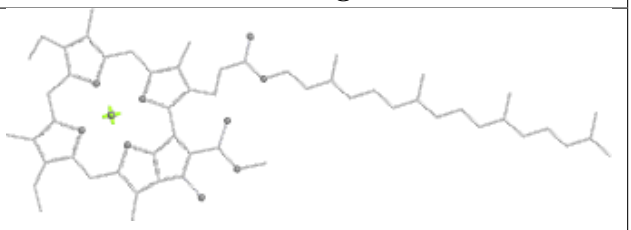
Bond lengths



Bond angles

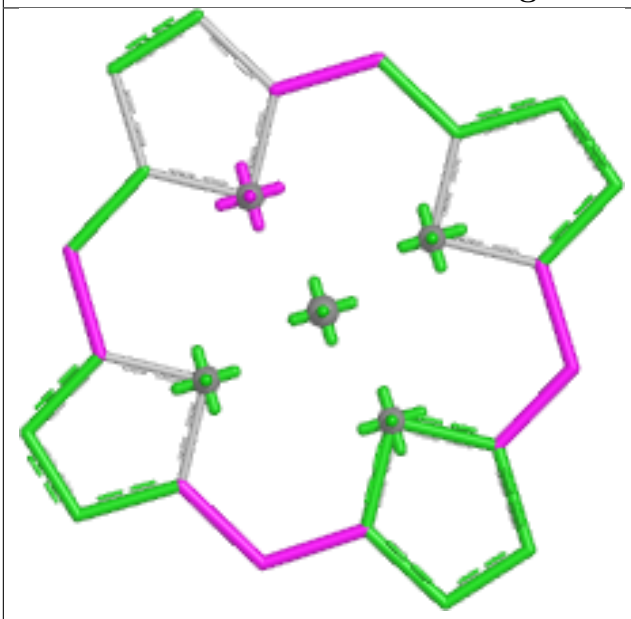


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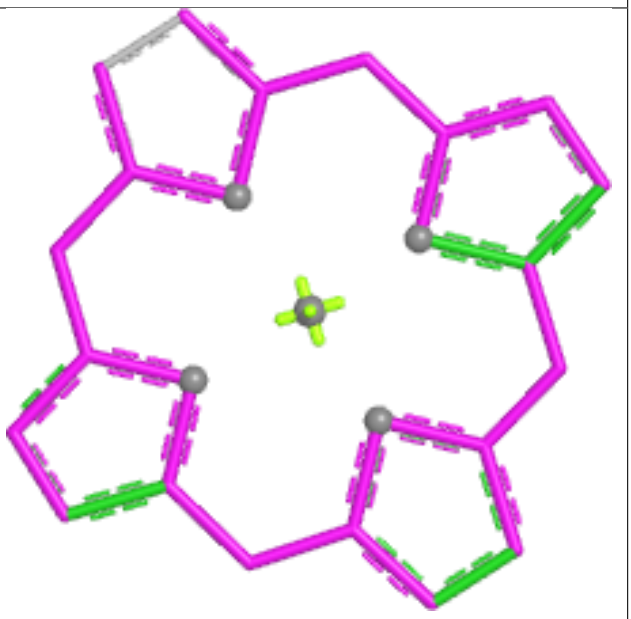


Rings

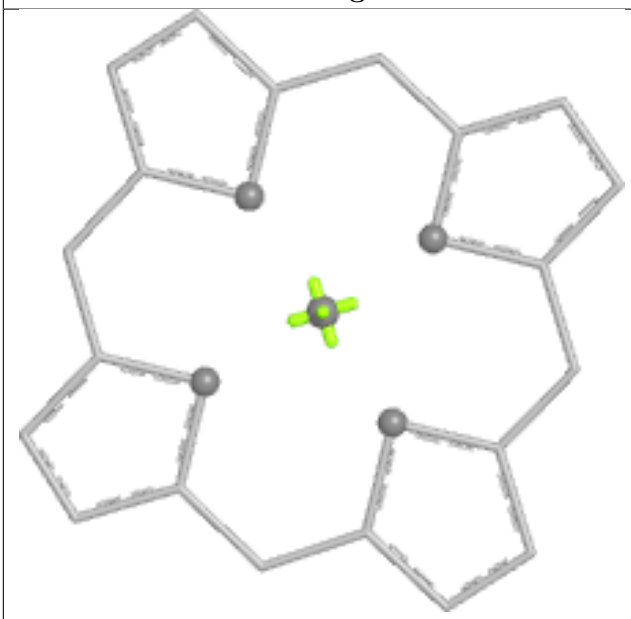
Ligand CLA 3 3015



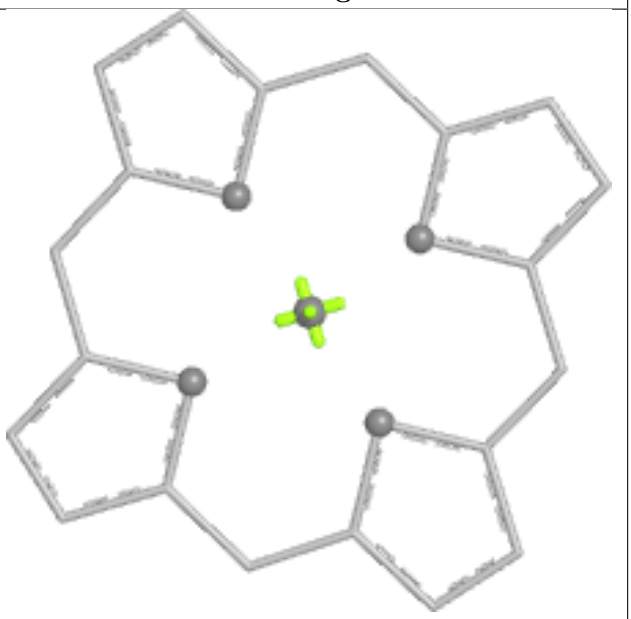
Bond lengths



Bond angles

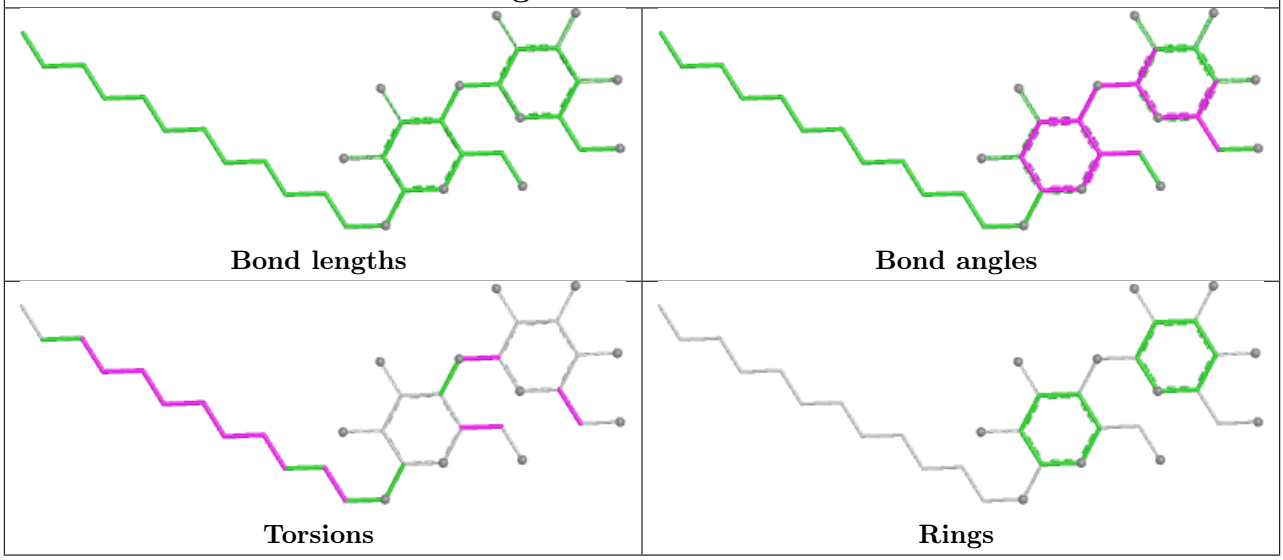


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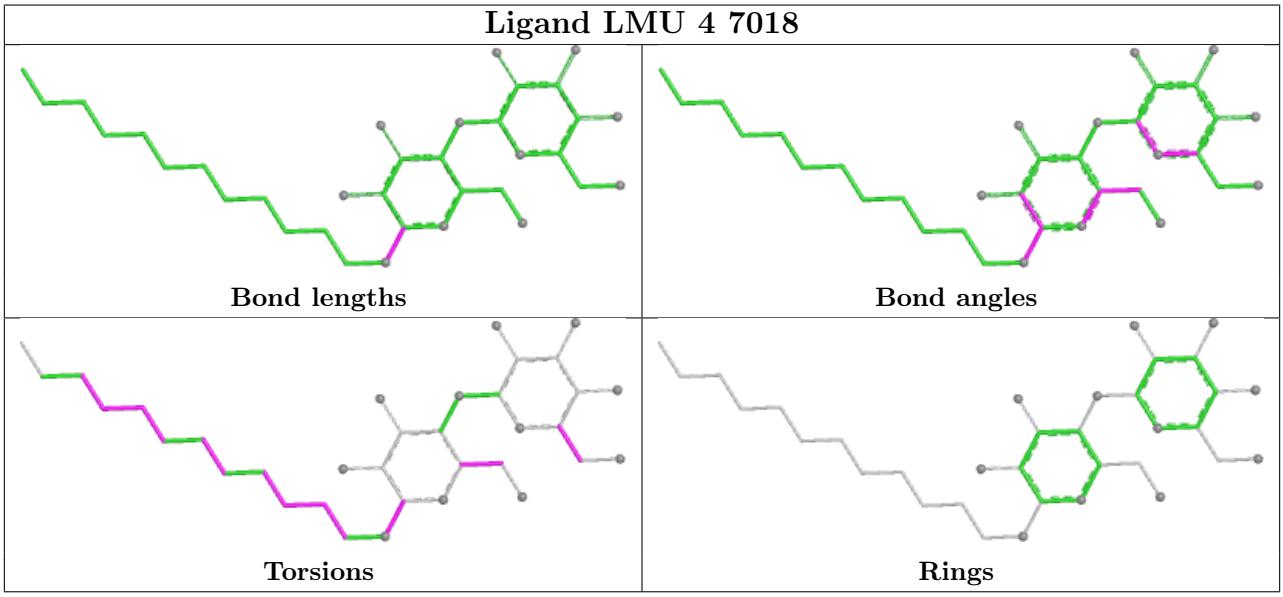


Rings

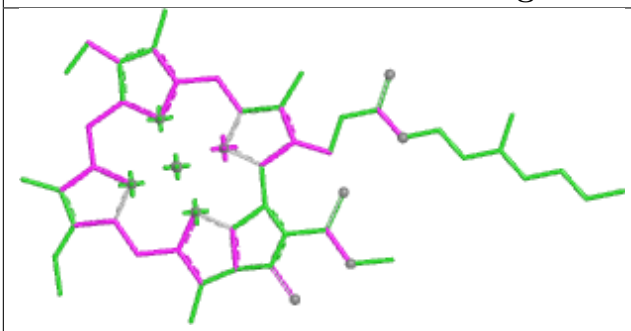
Ligand LMU B 7038



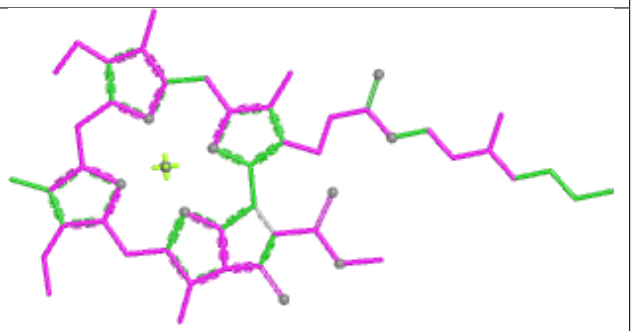
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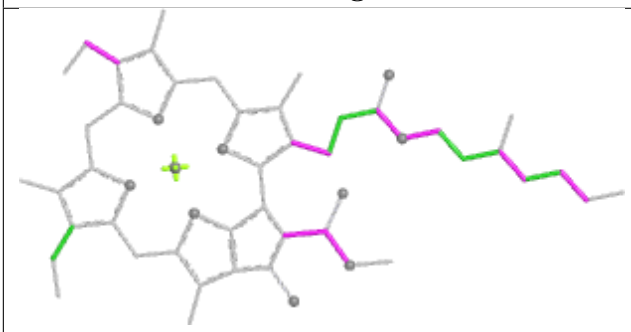
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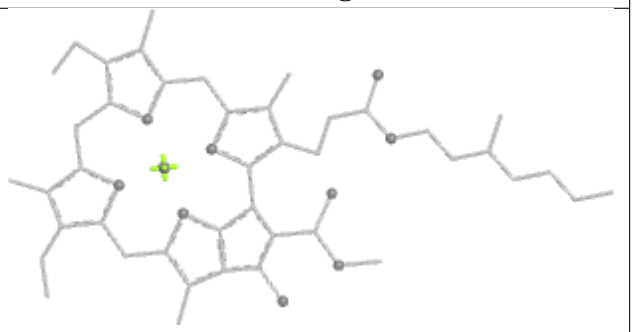
Bond lengths



Bond angles

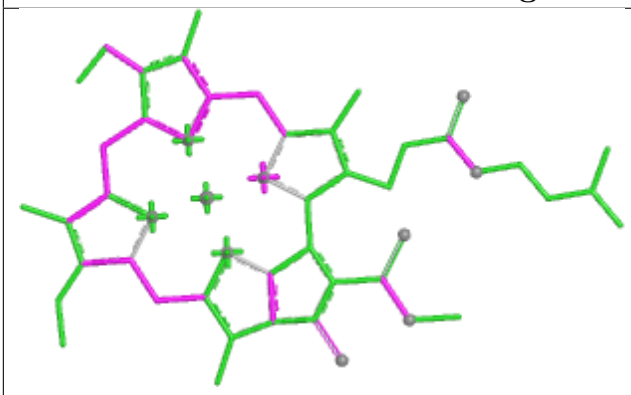


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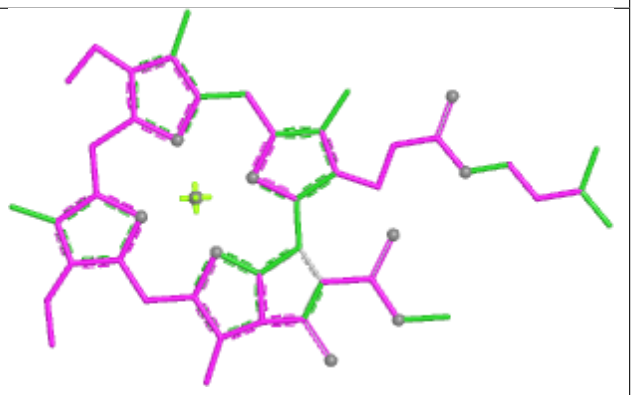


Rings

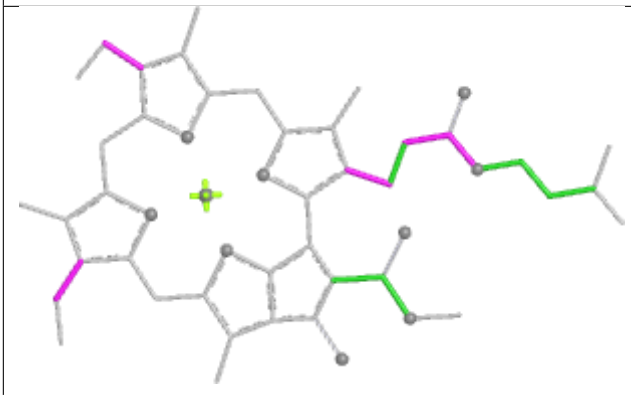
Ligand CLA 3 3017



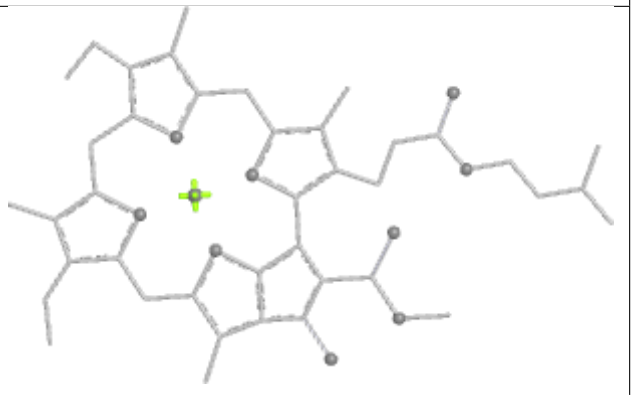
Bond lengths



Bond angles

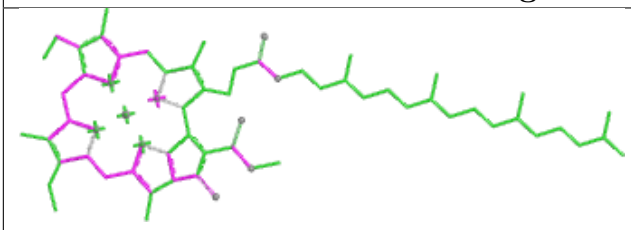


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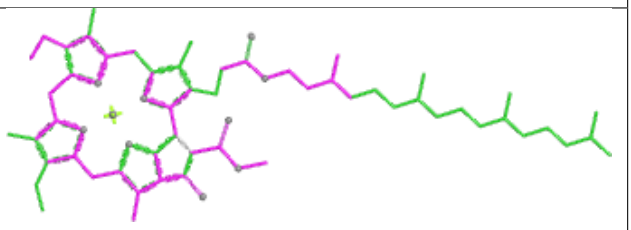


Rings

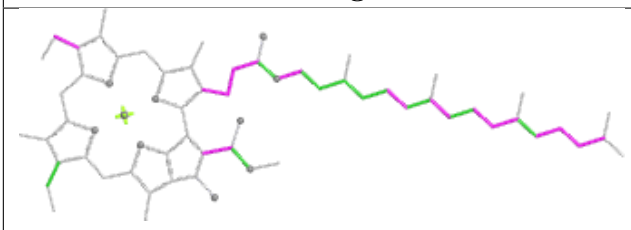
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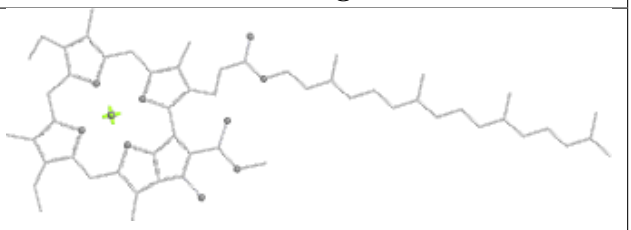
Bond lengths



Bond angles

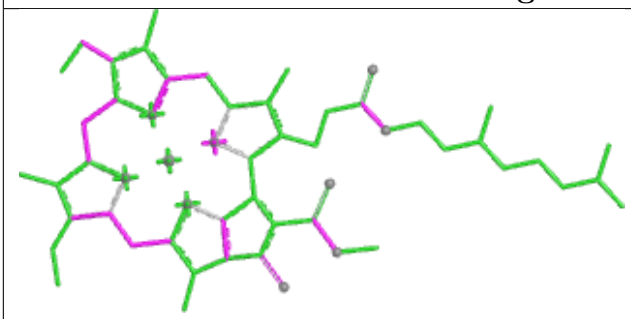


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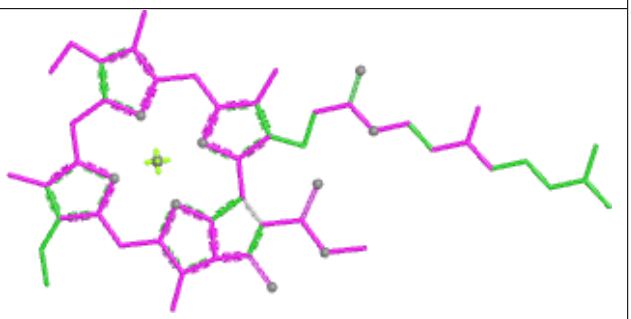


Rings

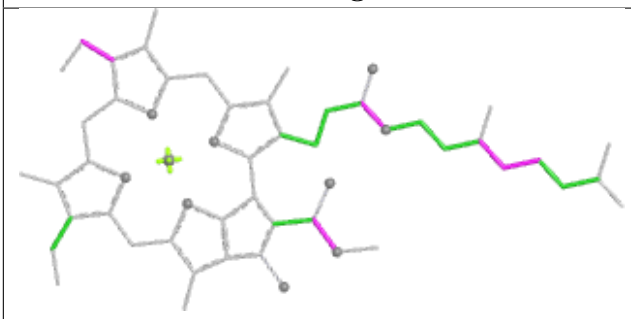
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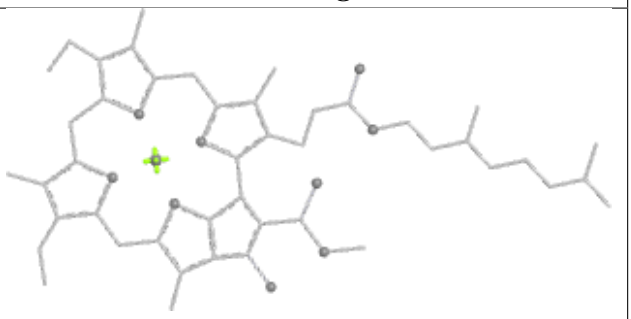
Bond lengths



Bond angles

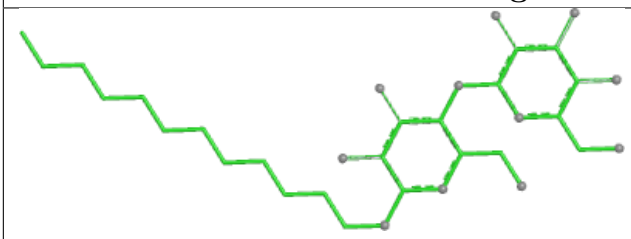


Torsions

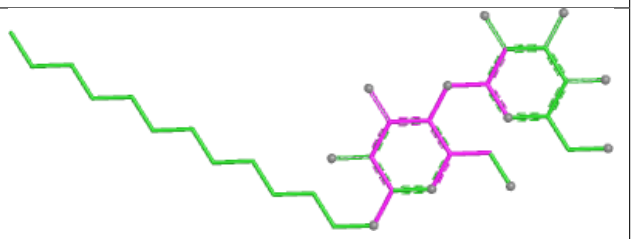


Rings

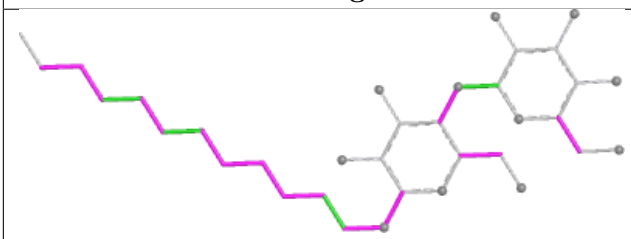
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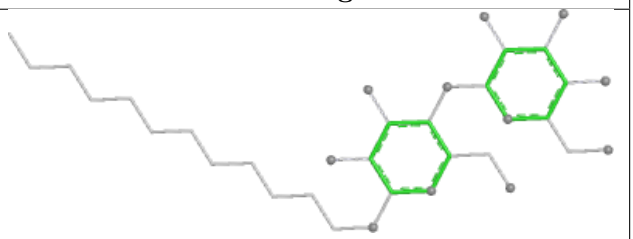
Bond lengths



Bond angles

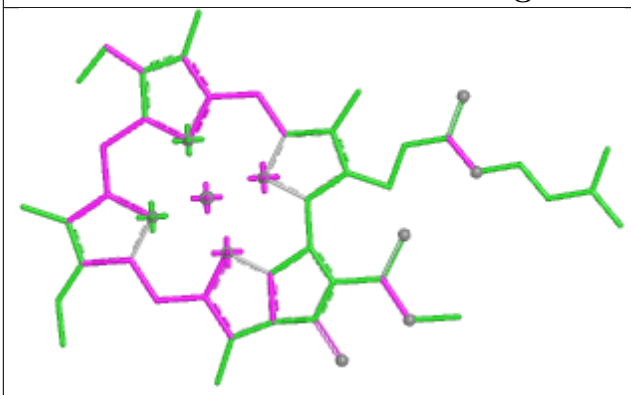


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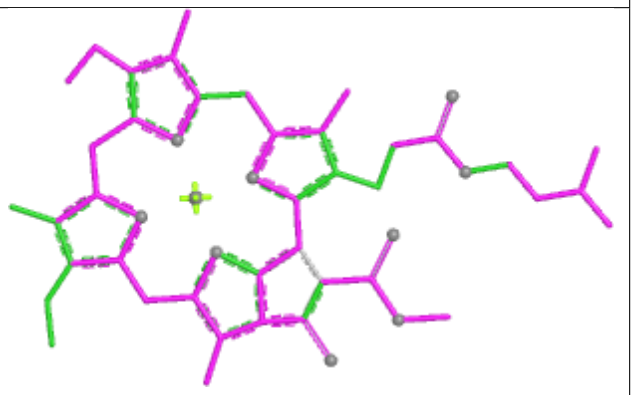


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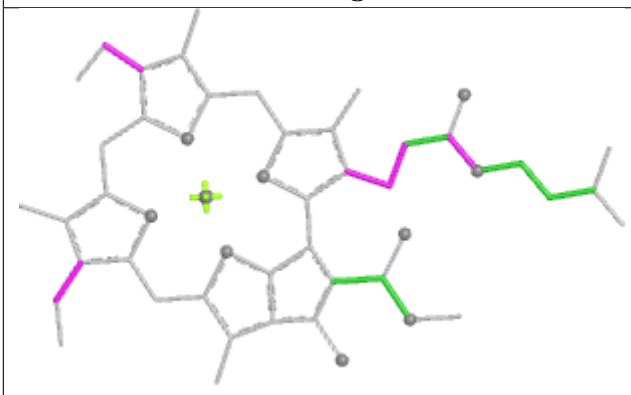
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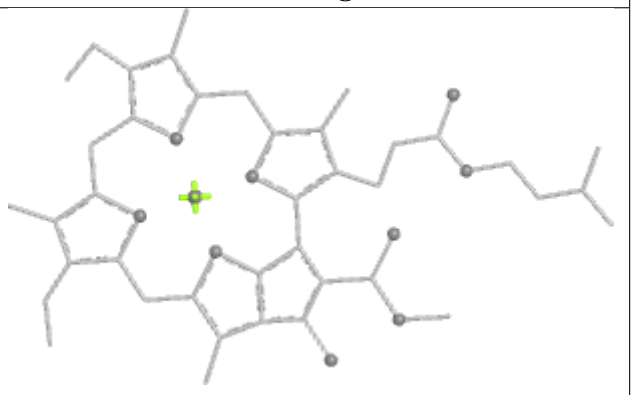
Bond lengths



Bond angles

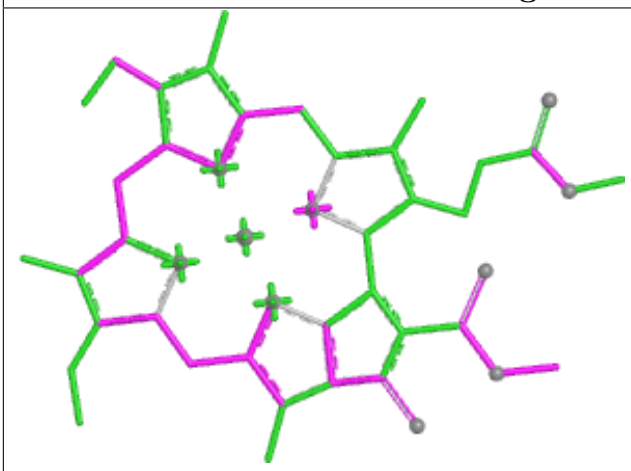


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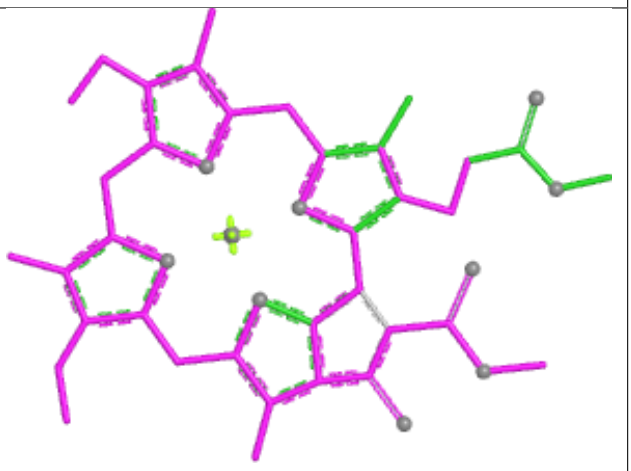


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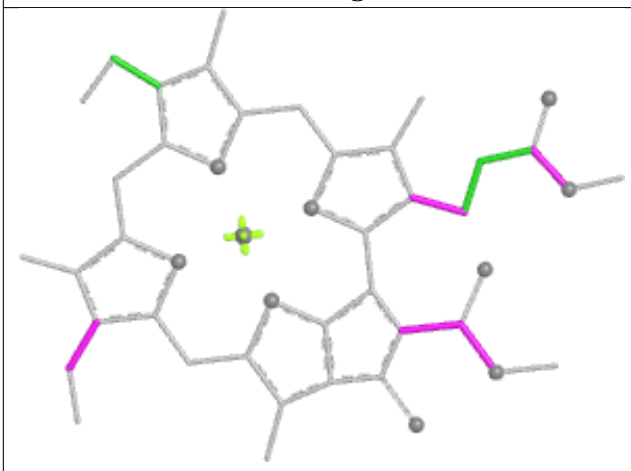
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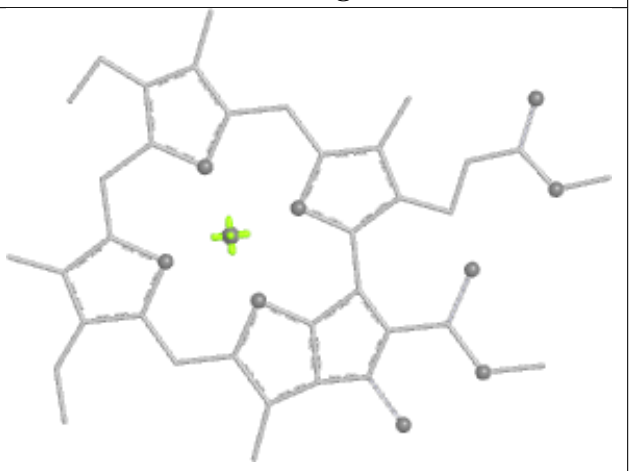
Bond lengths



Bond angles

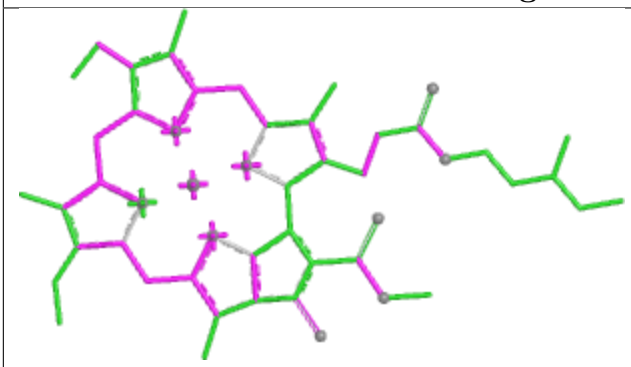


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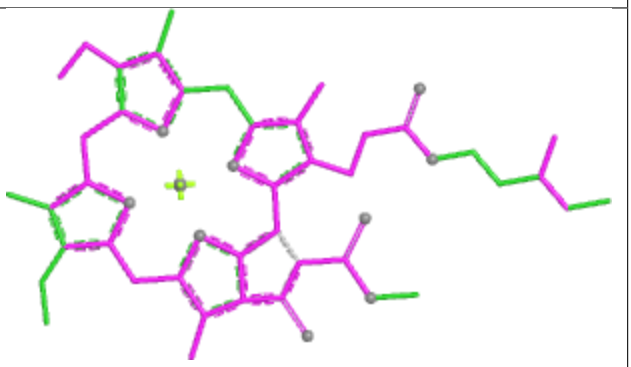


Rings

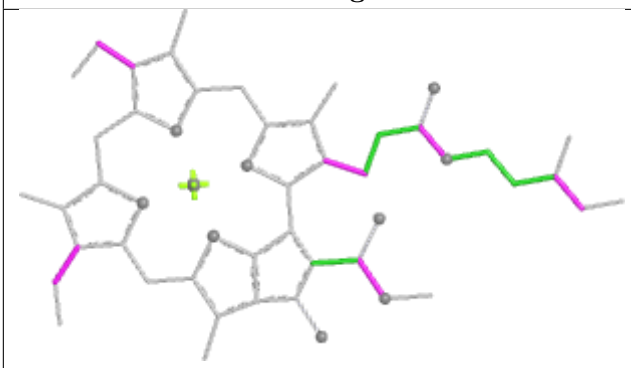
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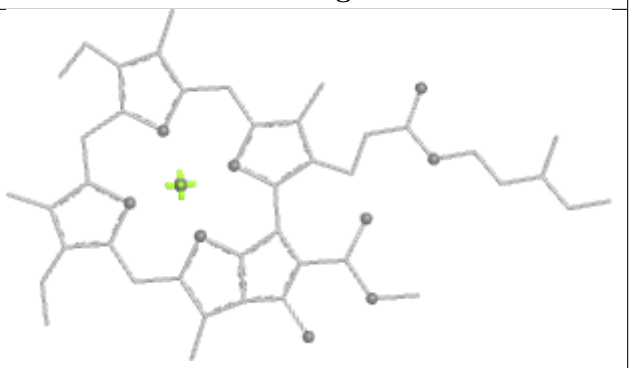
Bond lengths



Bond angles

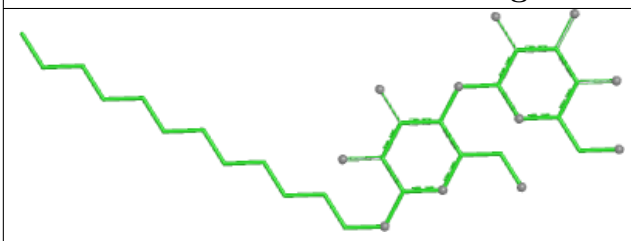


Torsions

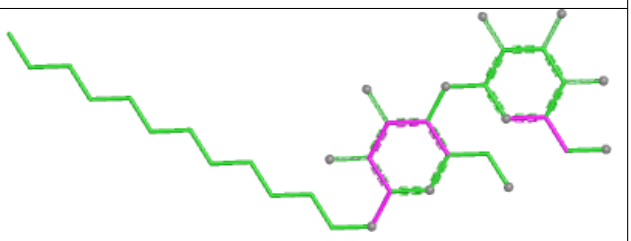


Rings

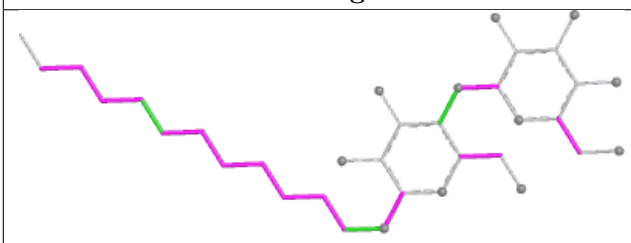
Ligand LMU A 7023



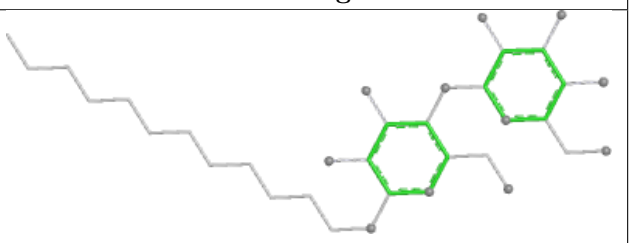
Bond lengths



Bond angles

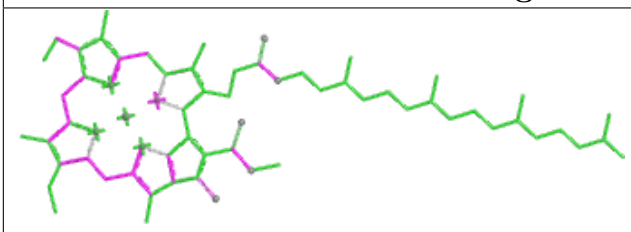


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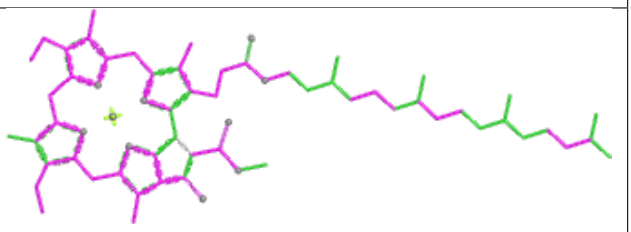


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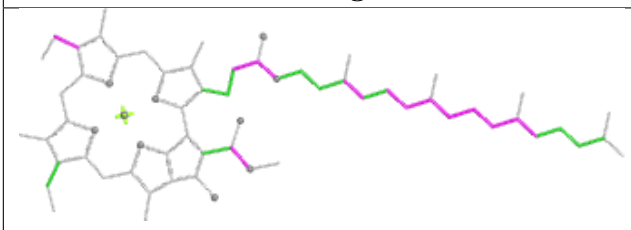
Ligand CLA B 9010



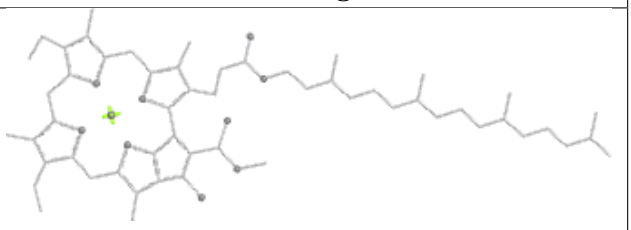
Bond lengths



Bond angles

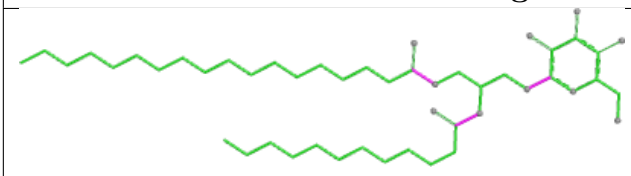


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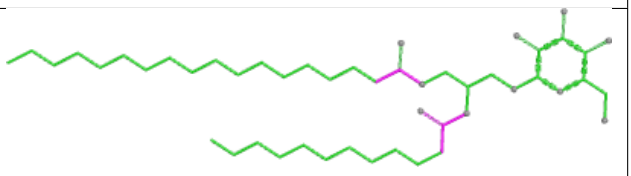


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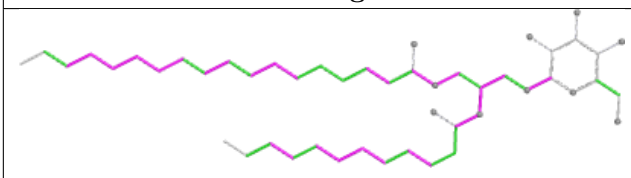
Ligand LMG B 7101



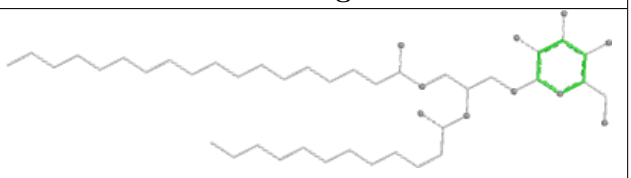
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Bond angles

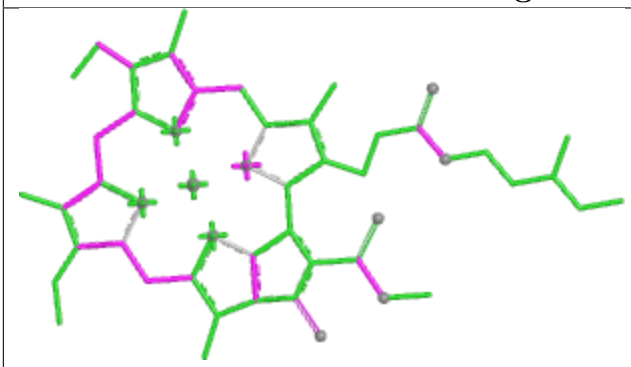


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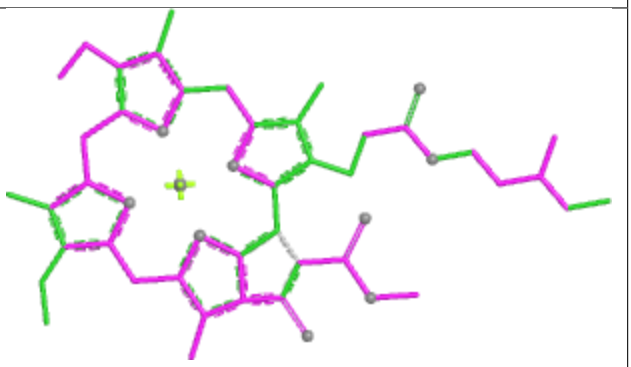


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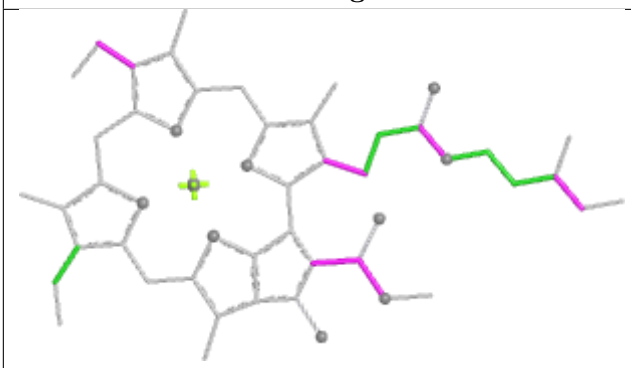
Ligand CLA A 1120



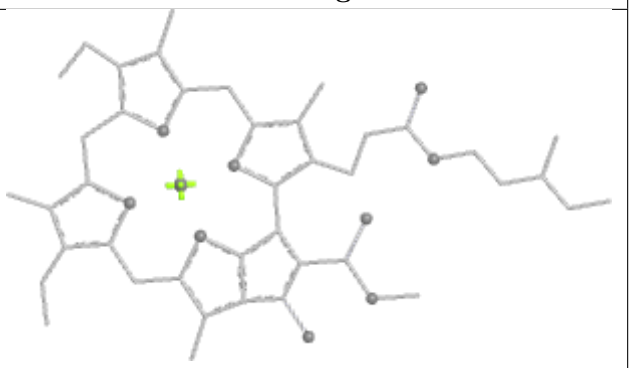
Bond lengths



Bond angles

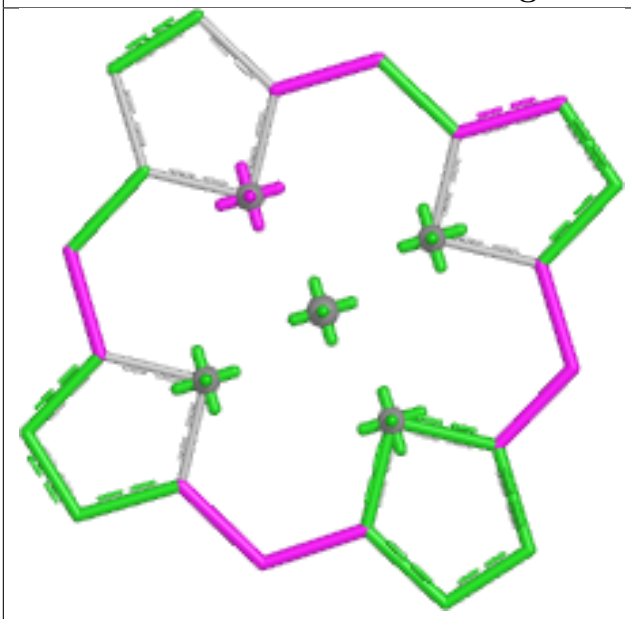


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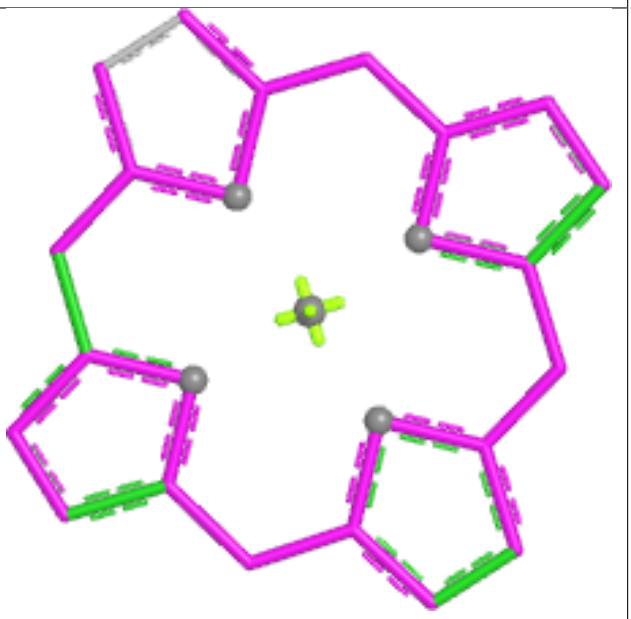


Rings

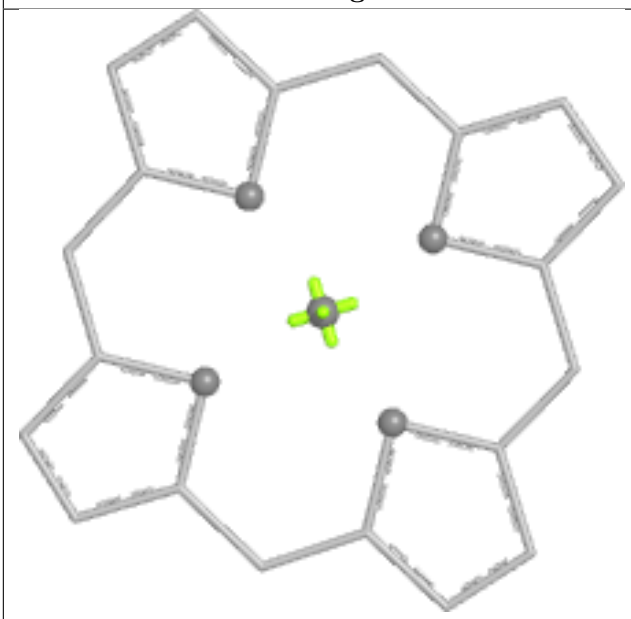
Ligand CLA 2 2008



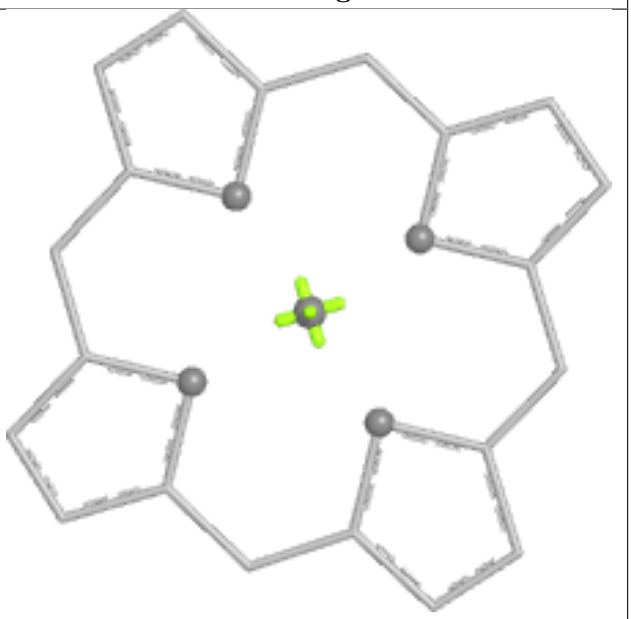
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Bond angles

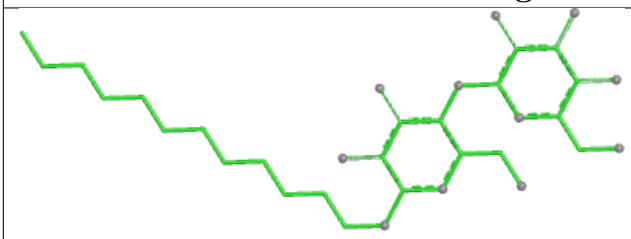


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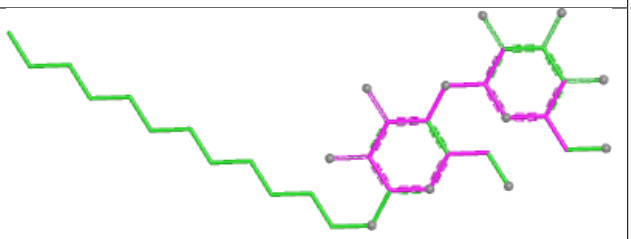


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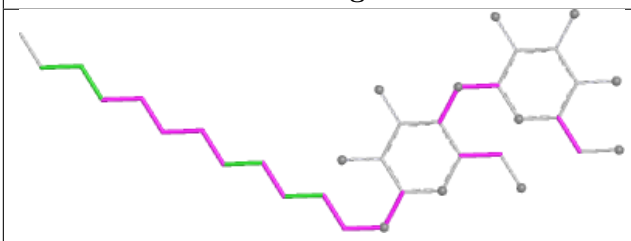
Ligand LMU 3 7005



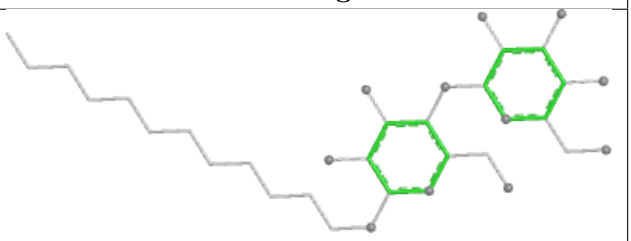
Bond lengths



Bond angles

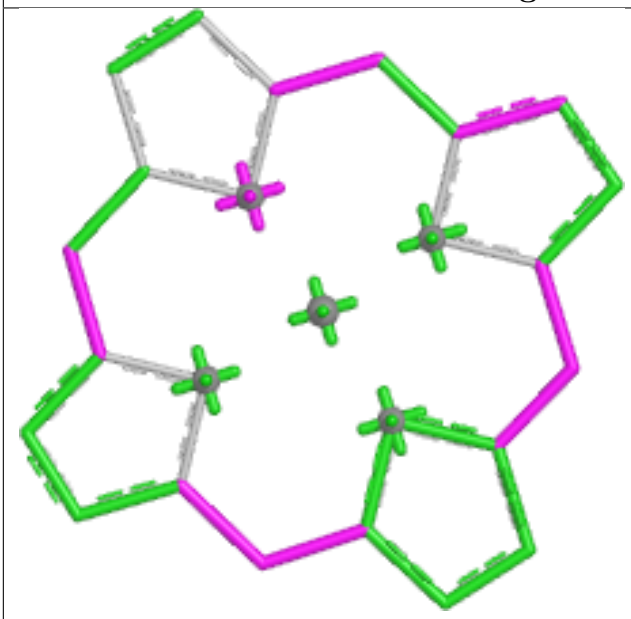


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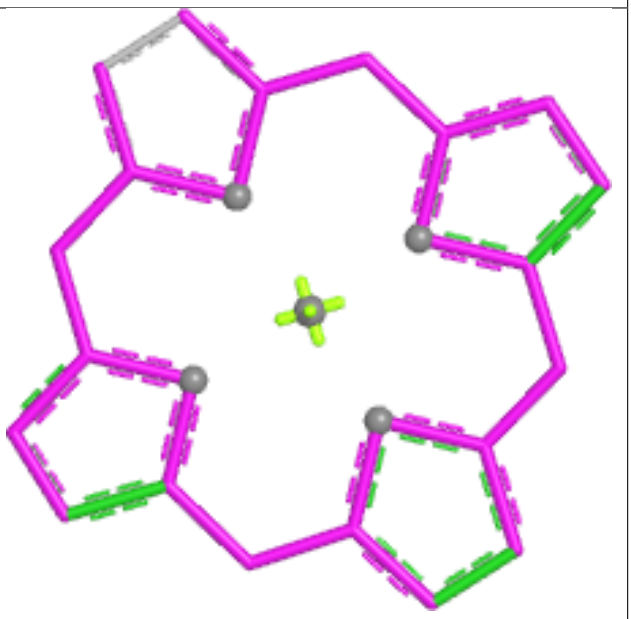


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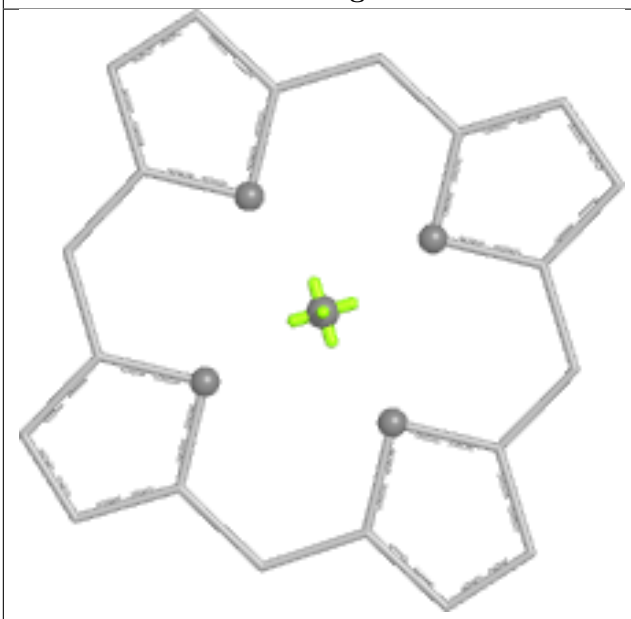
Ligand CLA 4 4011



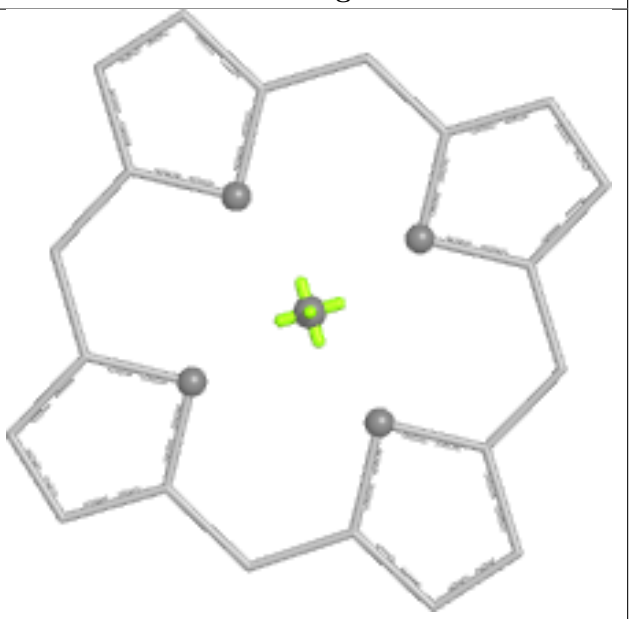
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Bond angles

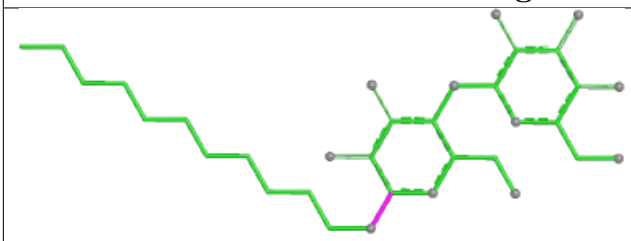


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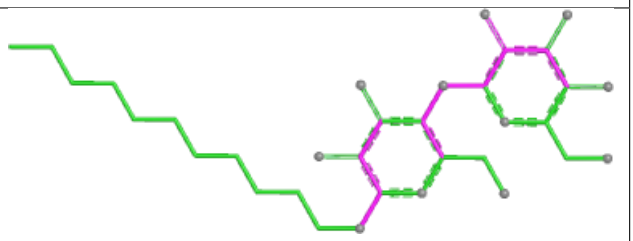


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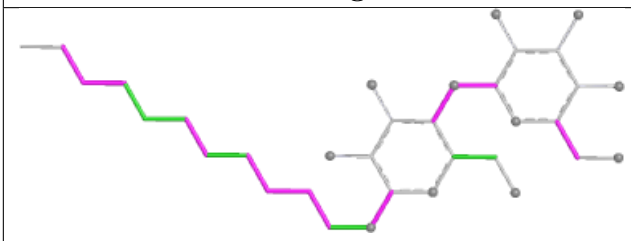
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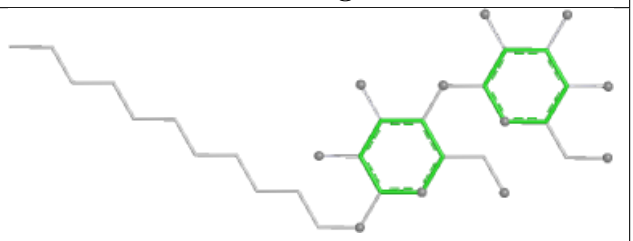
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Bond angles

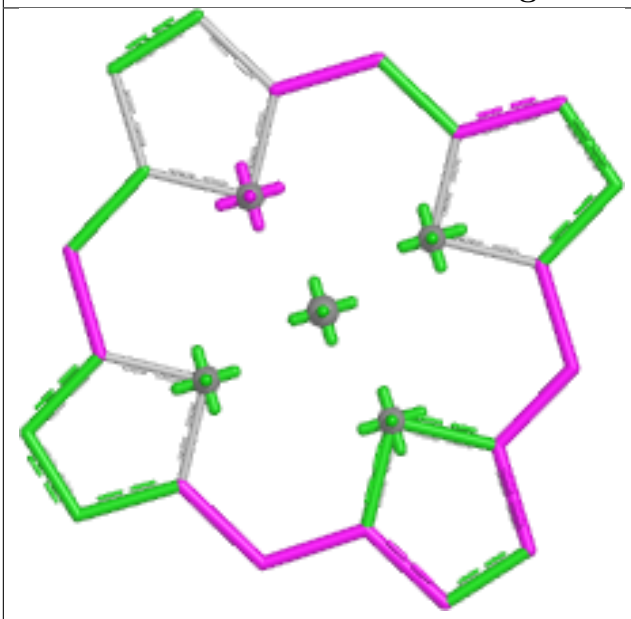


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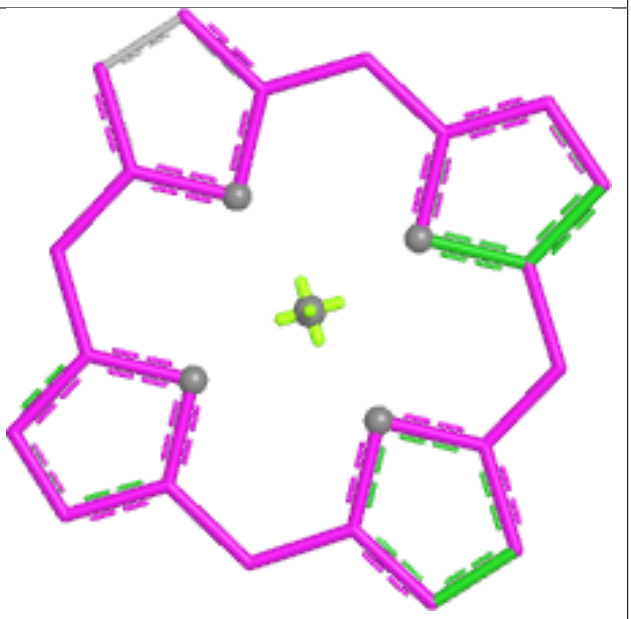


Rings

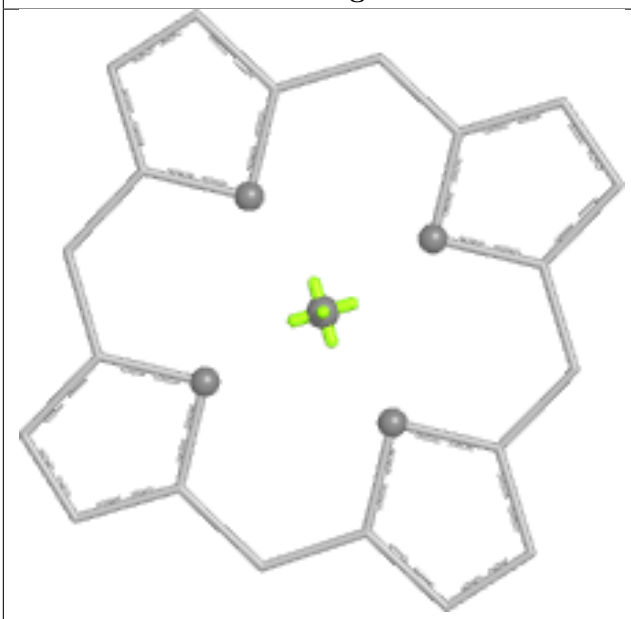
Ligand CLA 3 3004



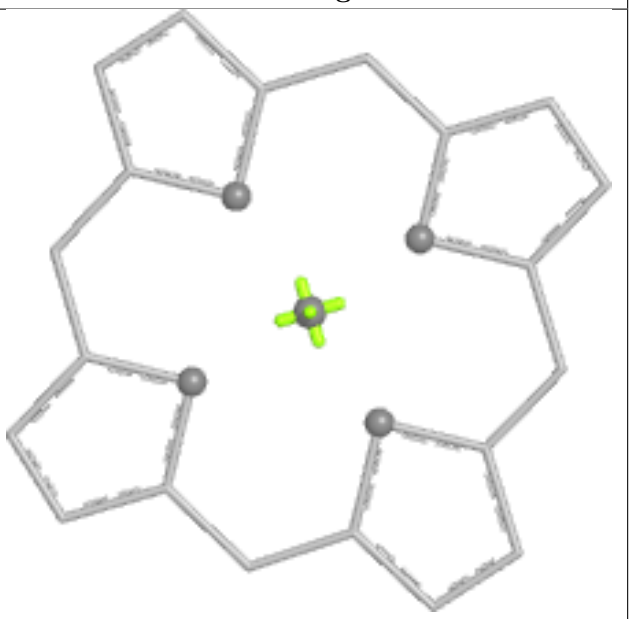
Bond lengths



Bond angles

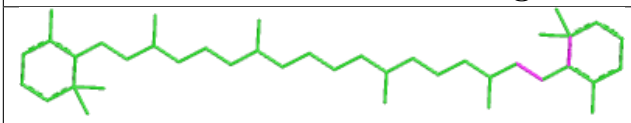


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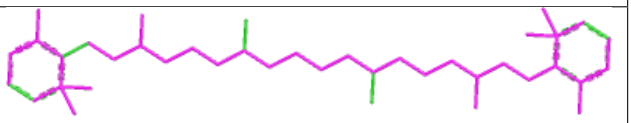


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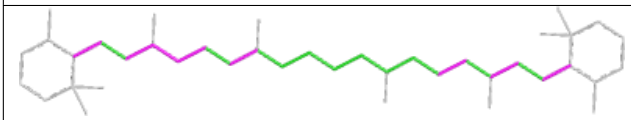
Ligand BCR A 6003



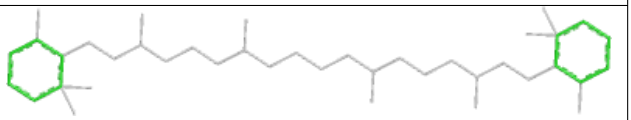
Bond lengths



Bond angles

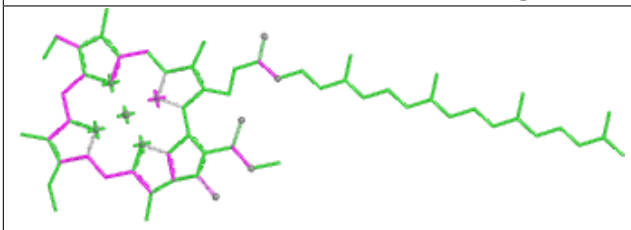


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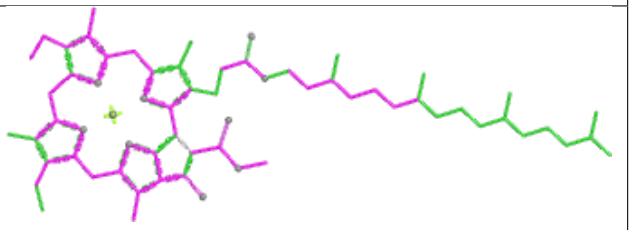


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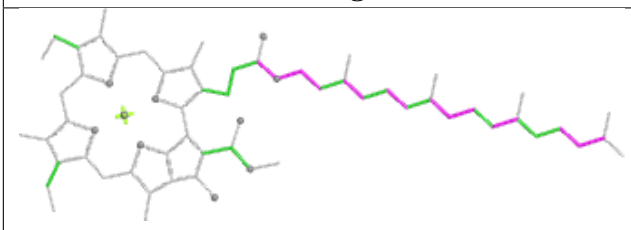
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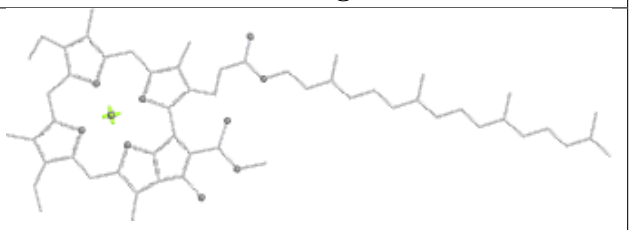
Bond lengths



Bond angles

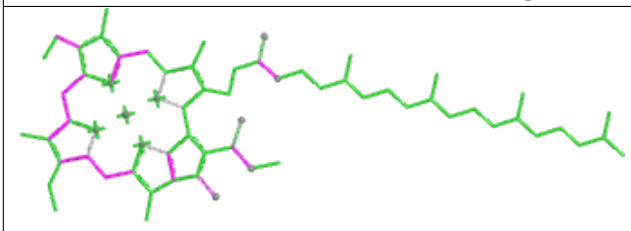


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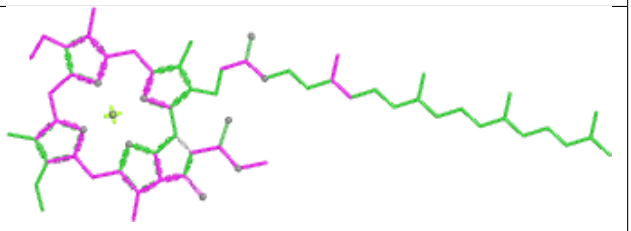


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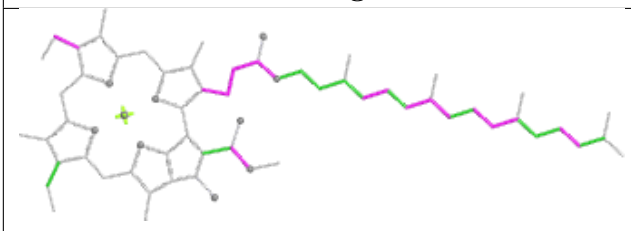
Ligand CLA 2 2006



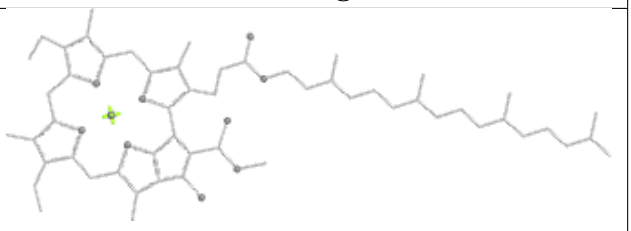
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Bond angles

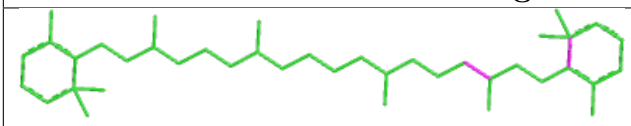


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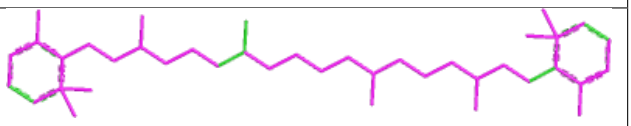


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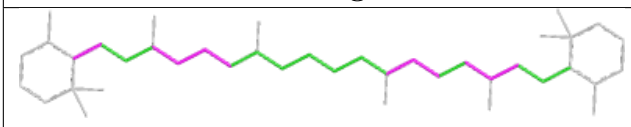
Ligand BCR B 6010



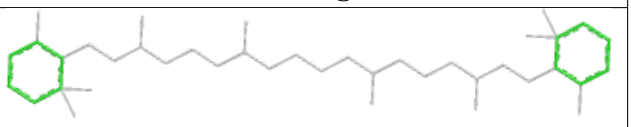
Bond lengths



Bond angles

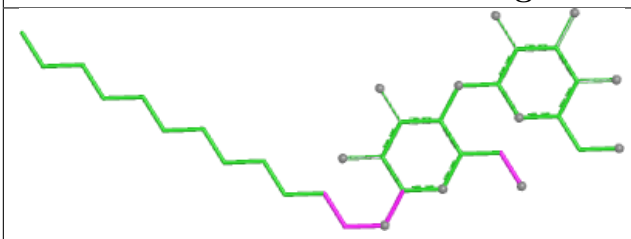


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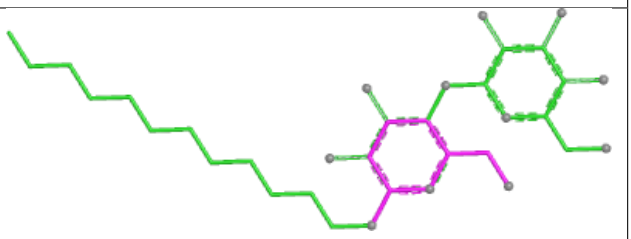


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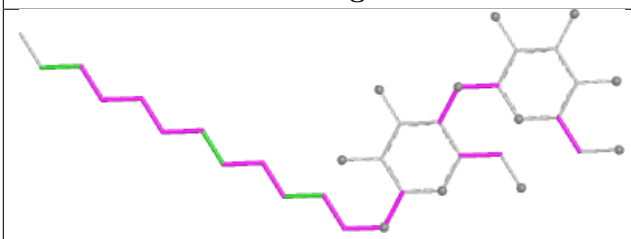
Ligand LMU 4 7052



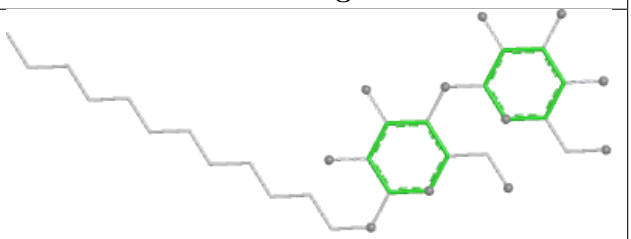
Bond lengths



Bond angles

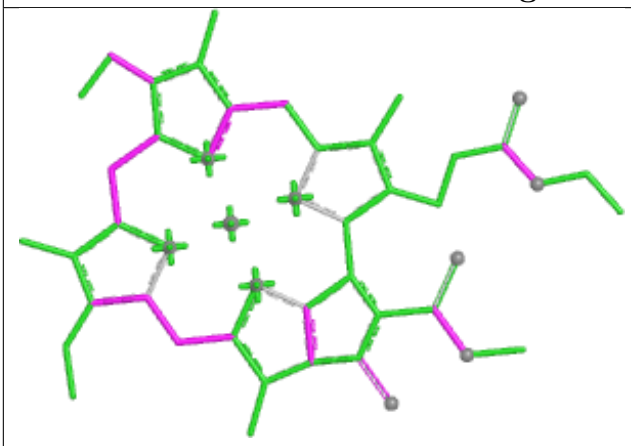


Torsions

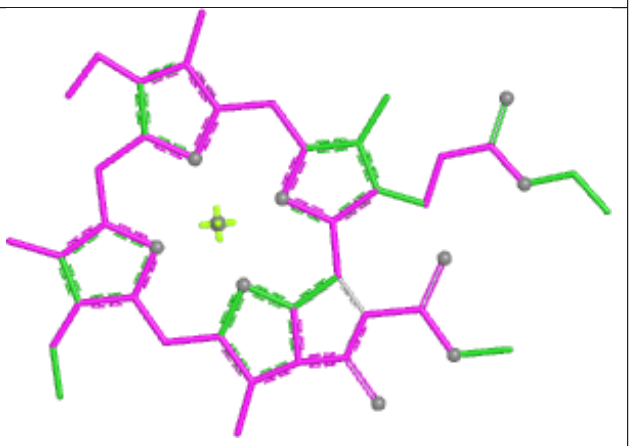


Rings

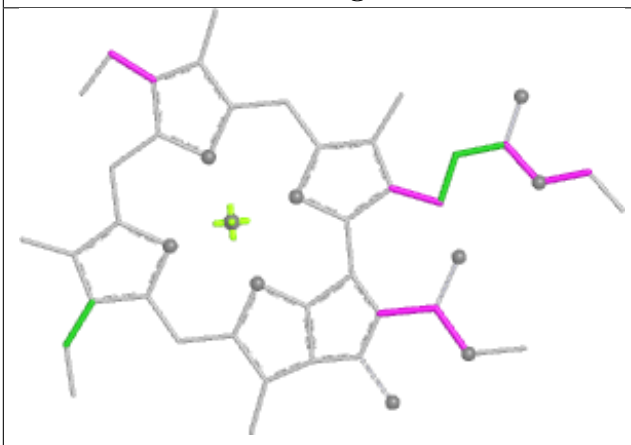
Ligand CLA 1 1003



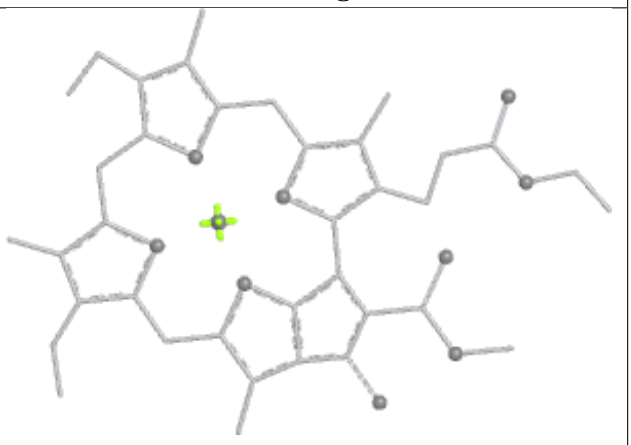
Bond lengths



Bond angles

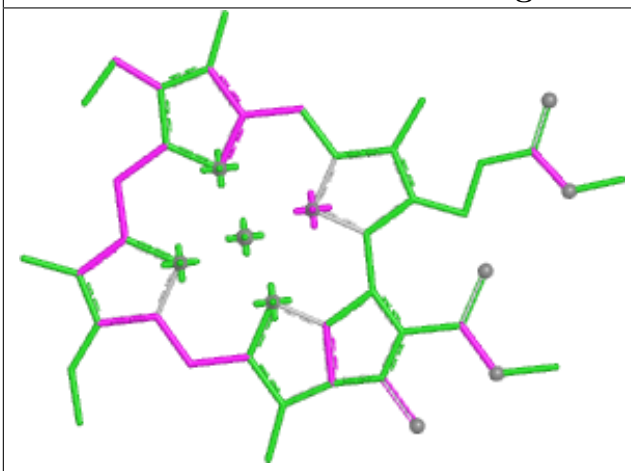


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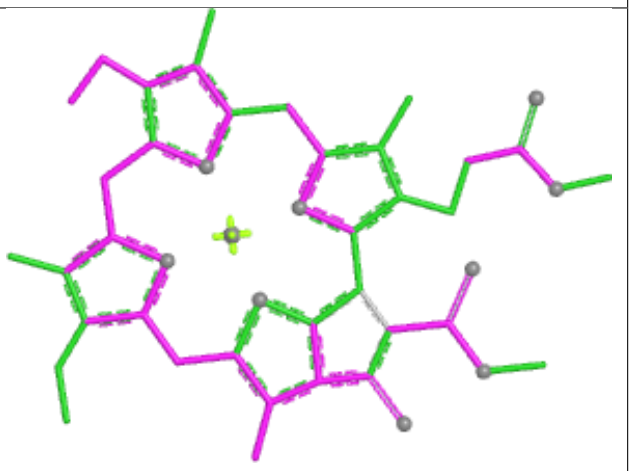


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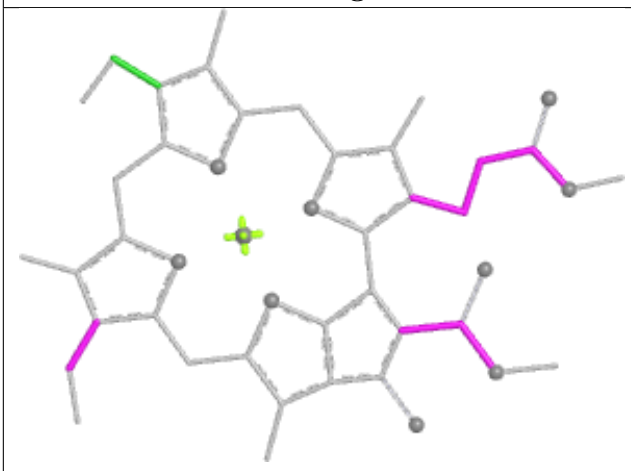
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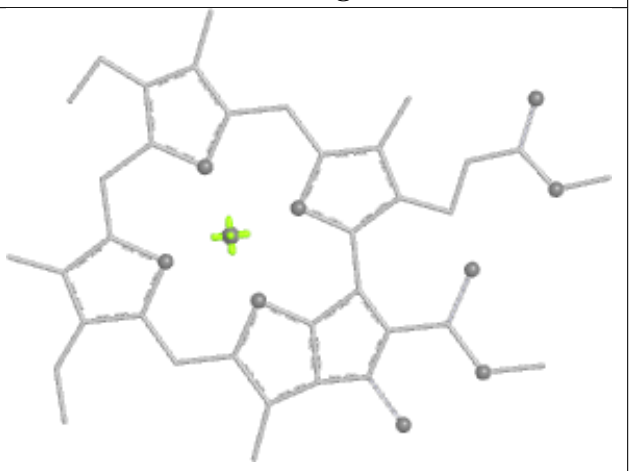
Bond lengths



Bond angles

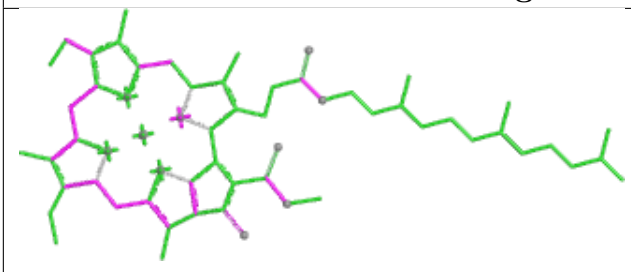


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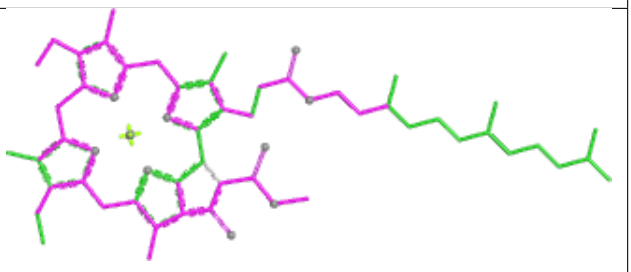


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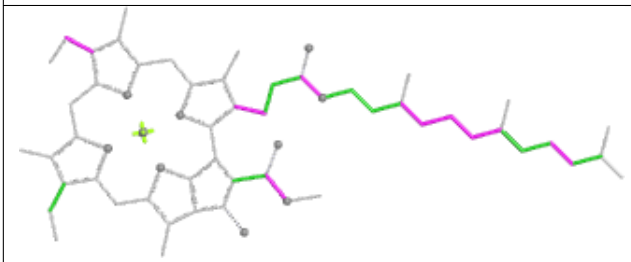
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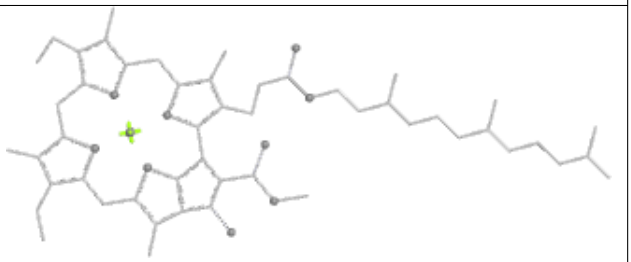
Bond lengths



Bond angles

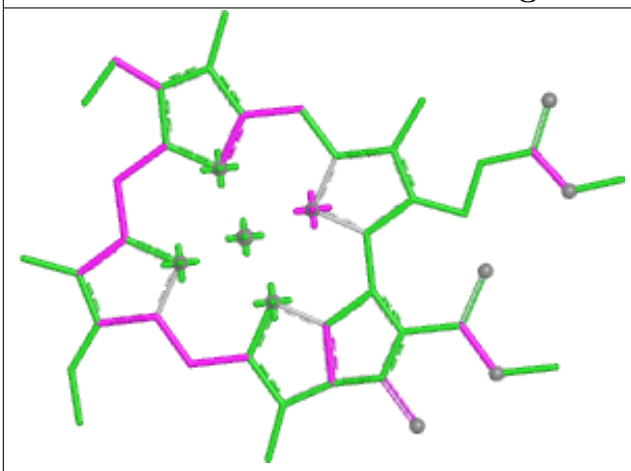


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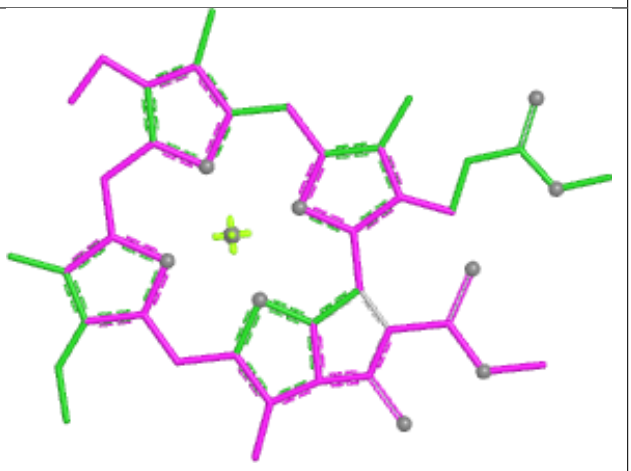


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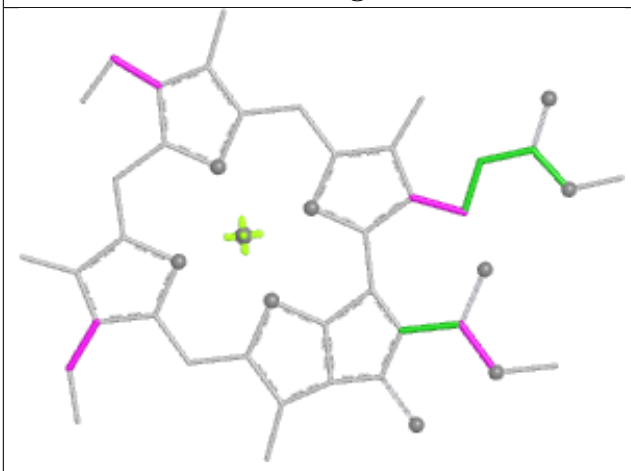
Ligand CLA 1 1005



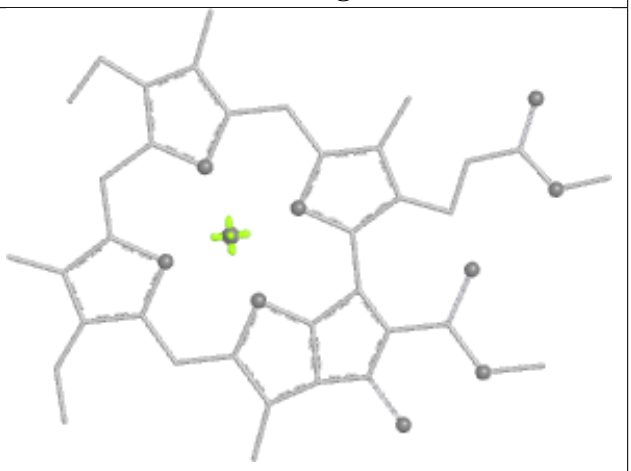
Bond lengths



Bond angles



Torsions



Rings

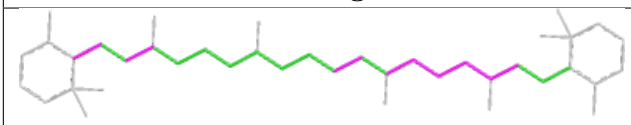
Ligand BCR J 6012



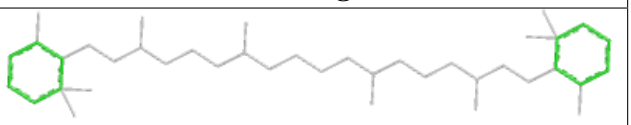
Bond lengths



Bond angles

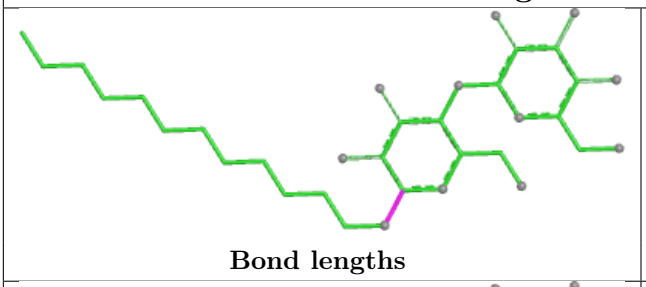


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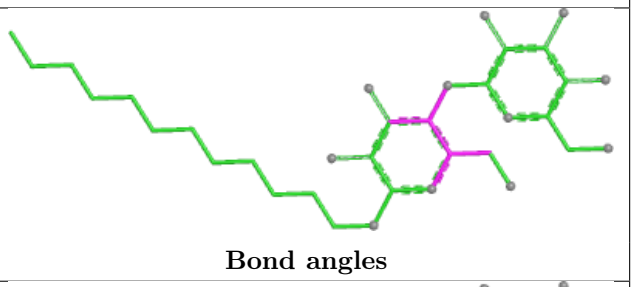


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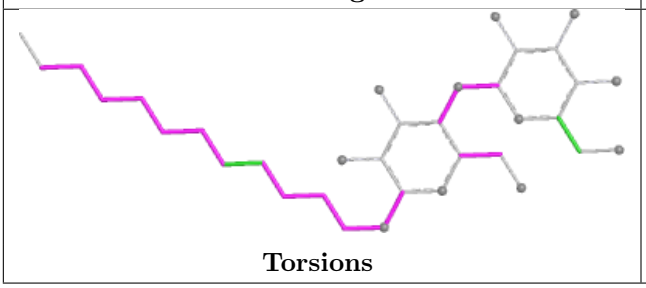
Ligand LMU 2 7046



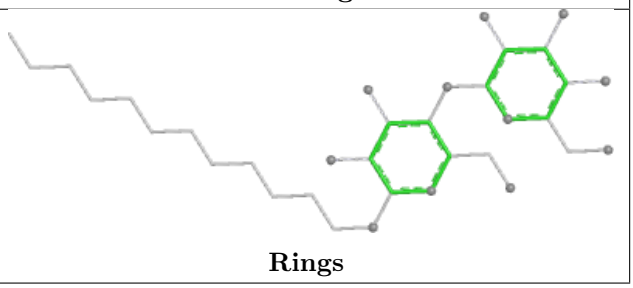
Bond lengths



Bond angles

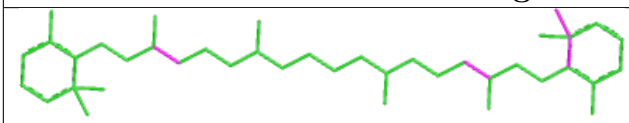


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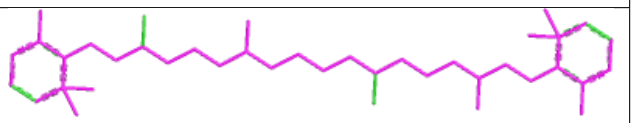


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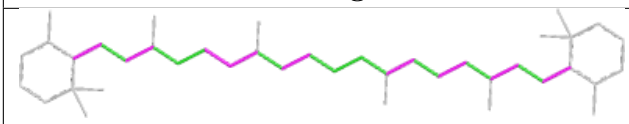
Ligand BCR A 6008



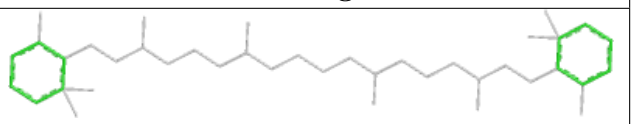
Bond lengths



Bond angles

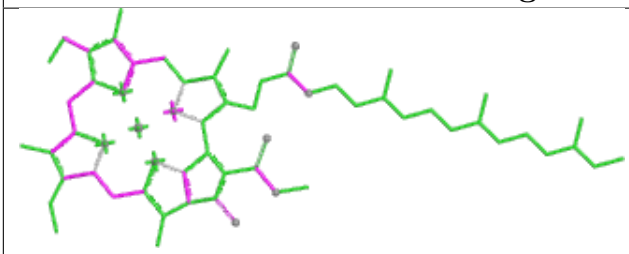


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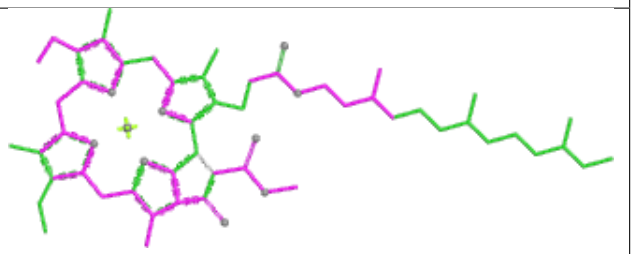


Rings

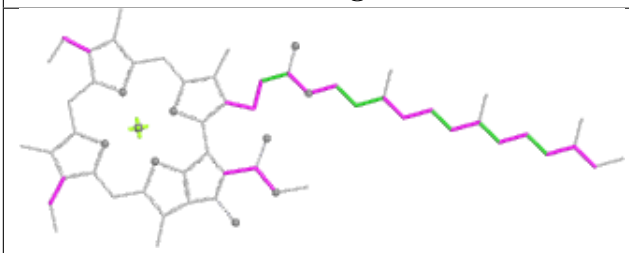
Ligand CLA J 1311



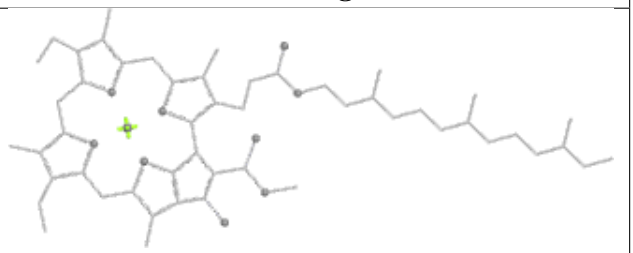
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Bond angles

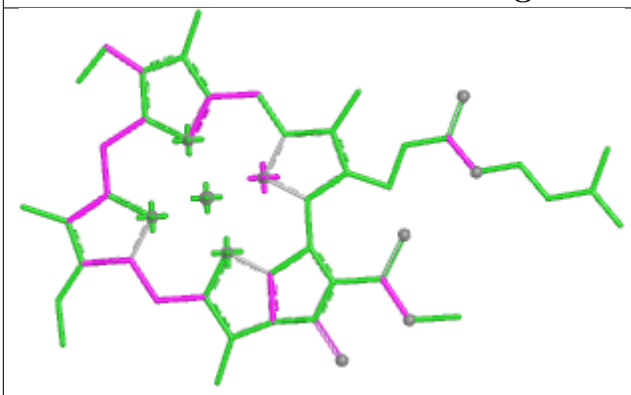


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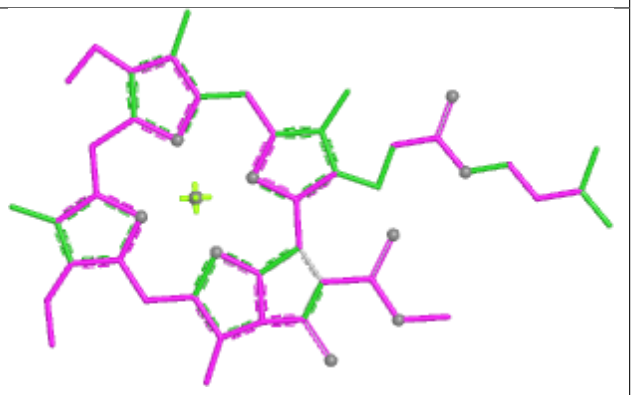


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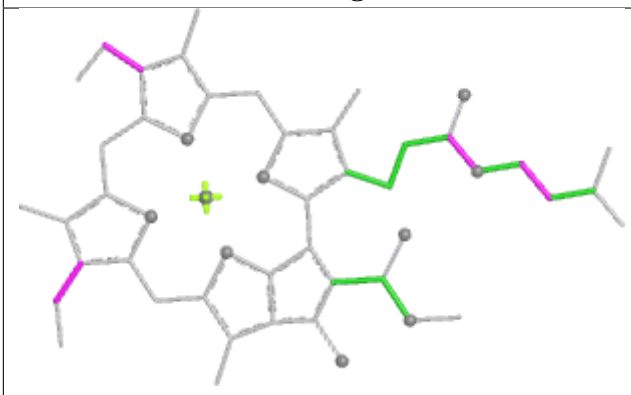
Ligand CLA K 1143



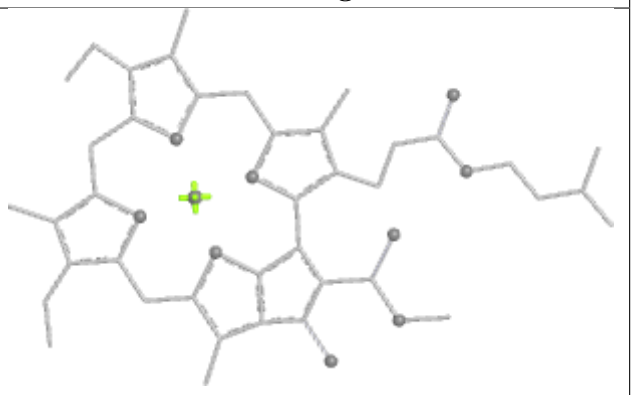
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Bond angles

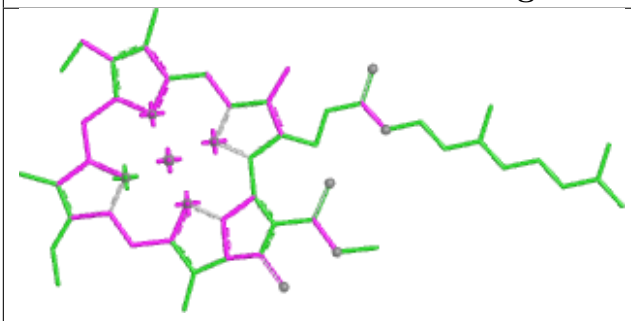


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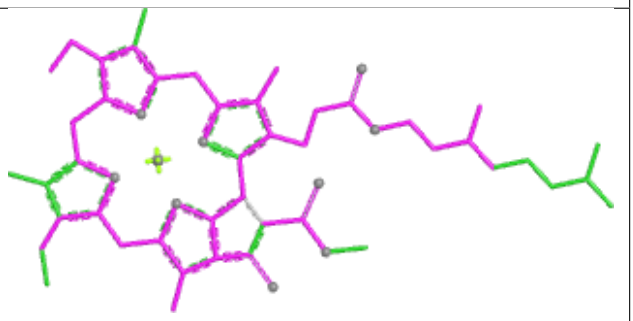


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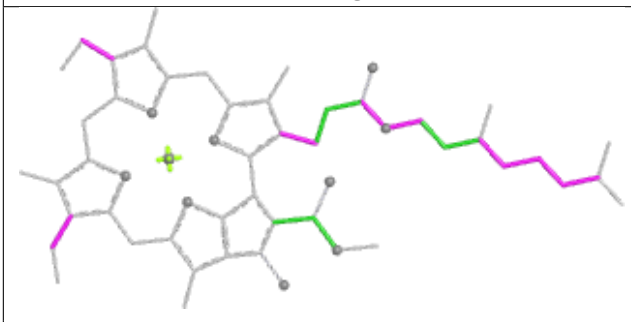
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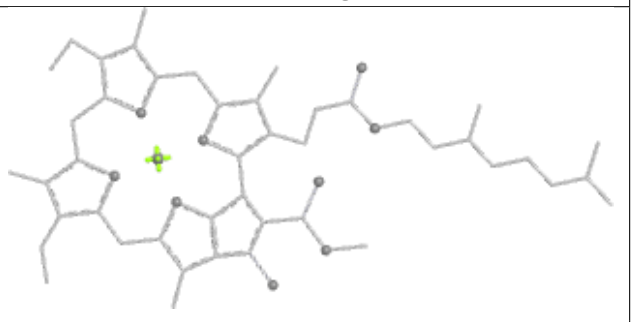
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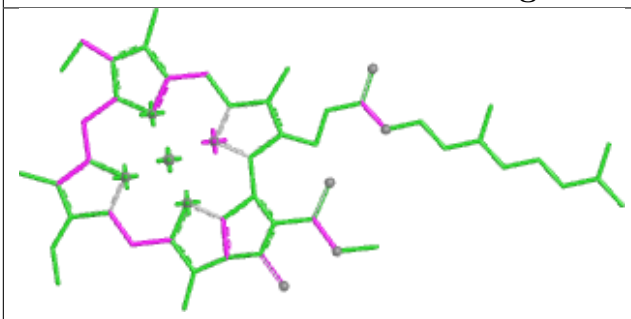


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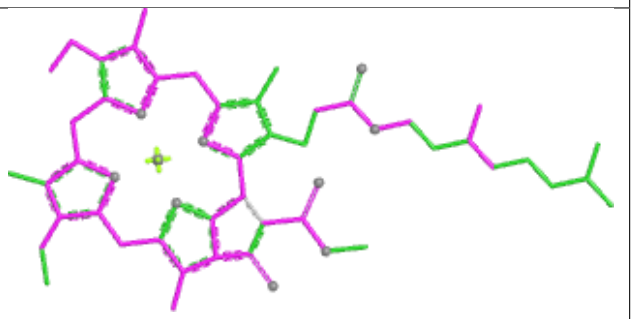


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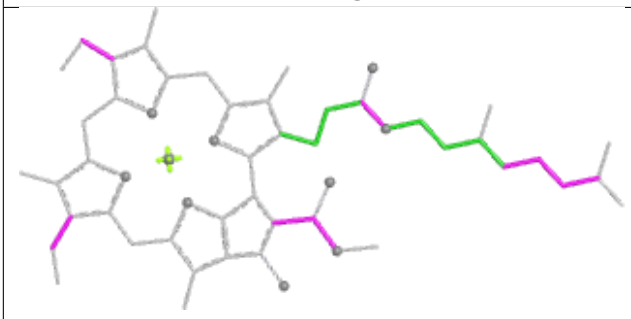
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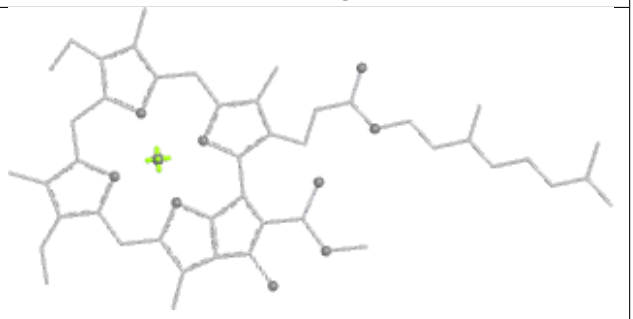
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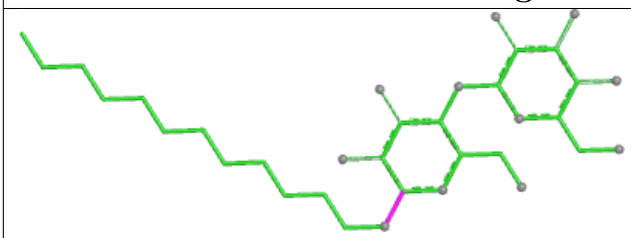


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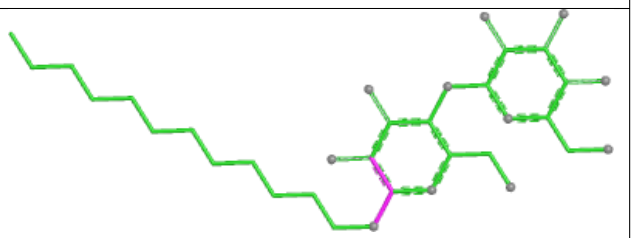


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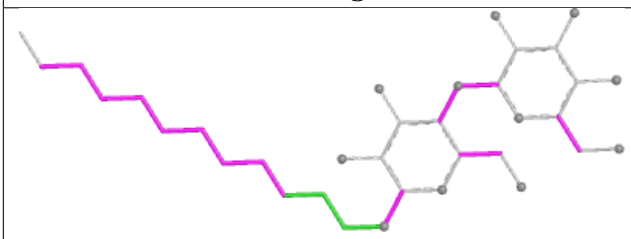
Ligand LMU 1 7004



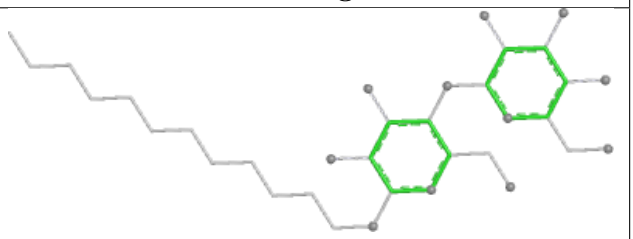
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Bond angles

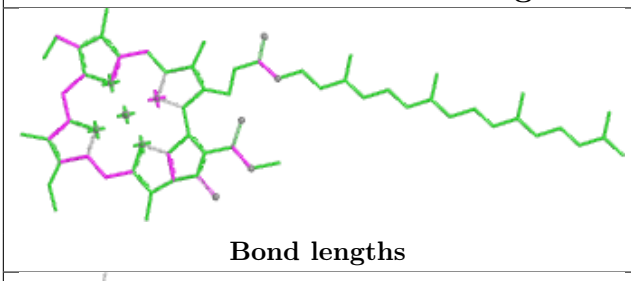


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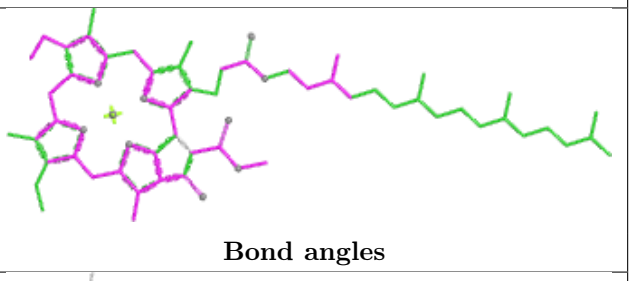


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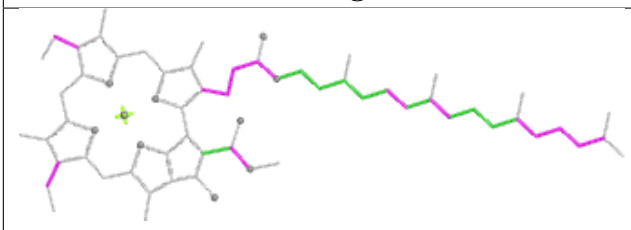
Ligand CLA A 1138



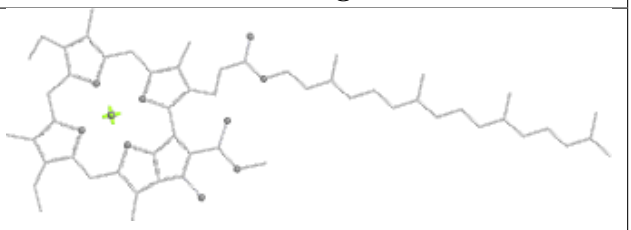
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Bond angles

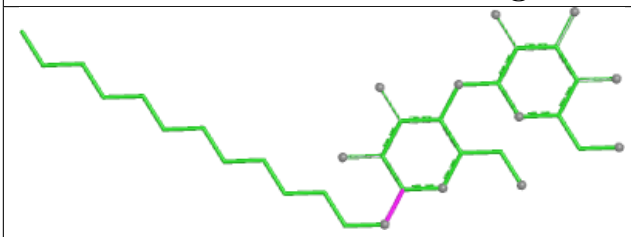


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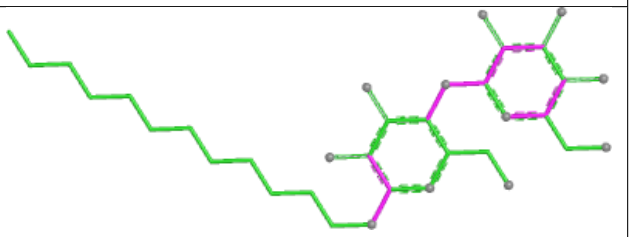


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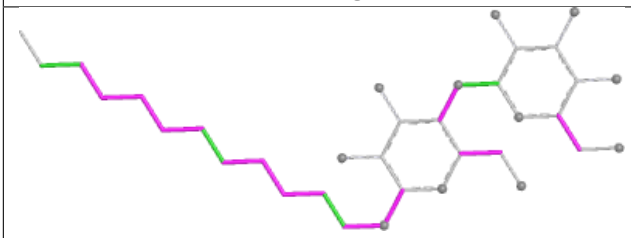
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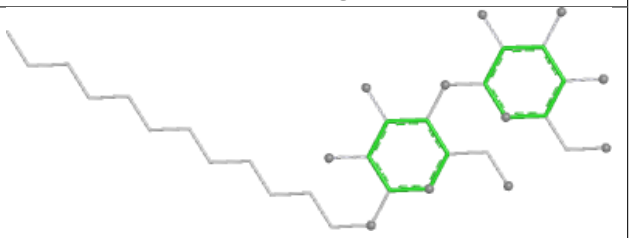
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Bond angles

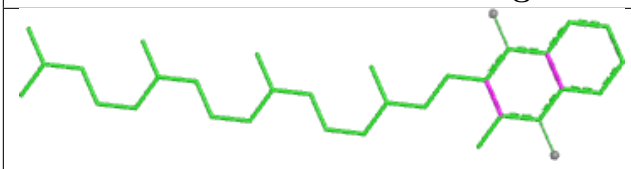


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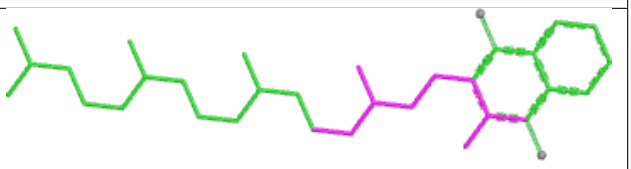


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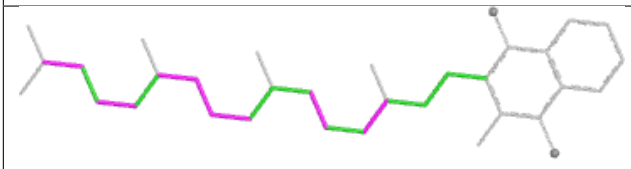
Ligand PQN B 5002



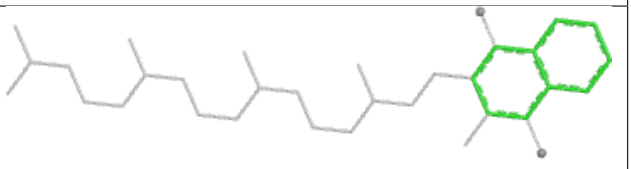
Bond lengths



Bond angles

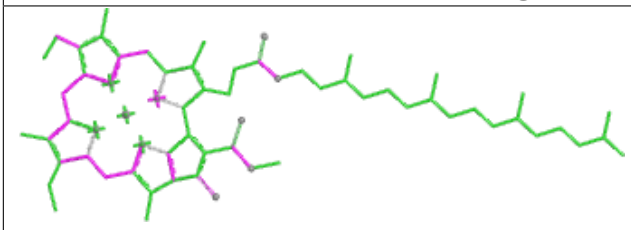


Torsions

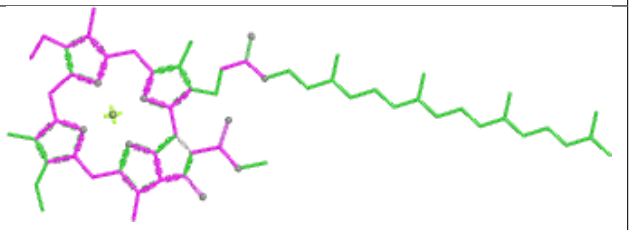


Rings

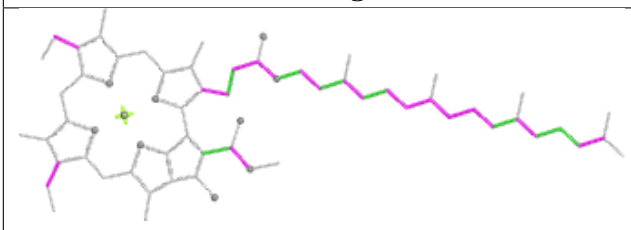
Ligand CLA A 1125



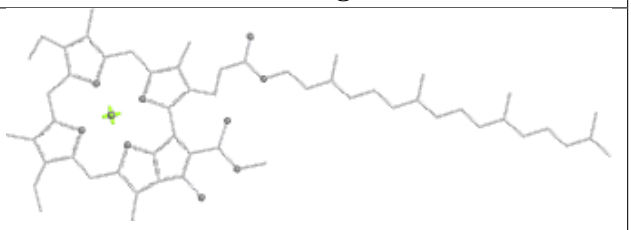
Bond lengths



Bond angles

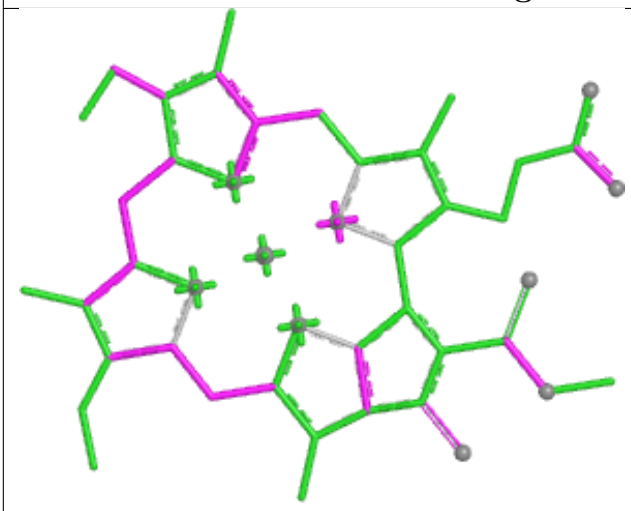


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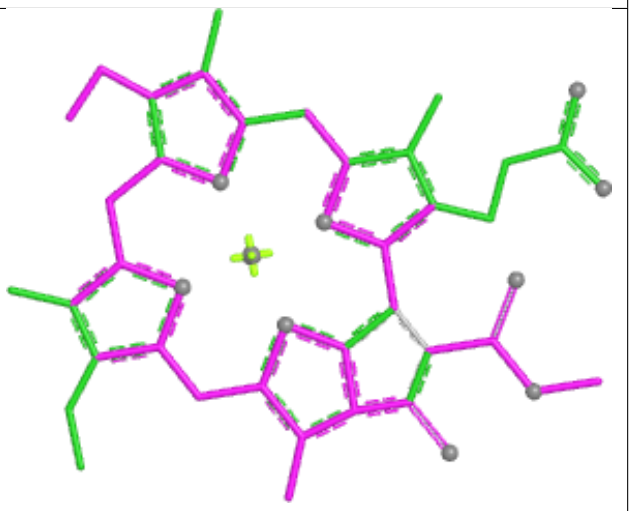


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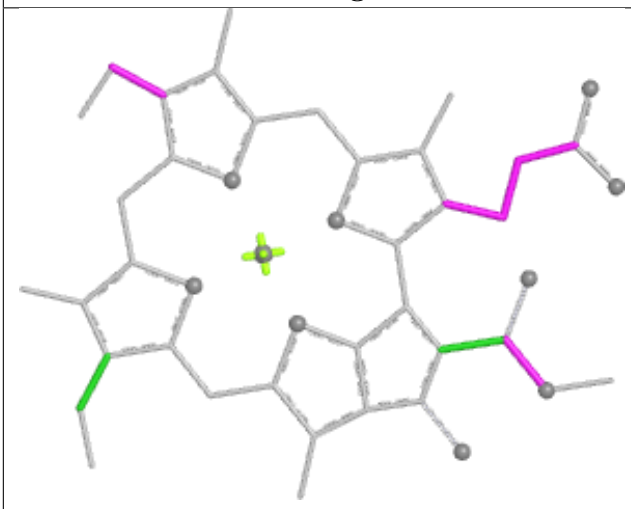
Ligand CLA A 1134



Bond lengths



Bond angles

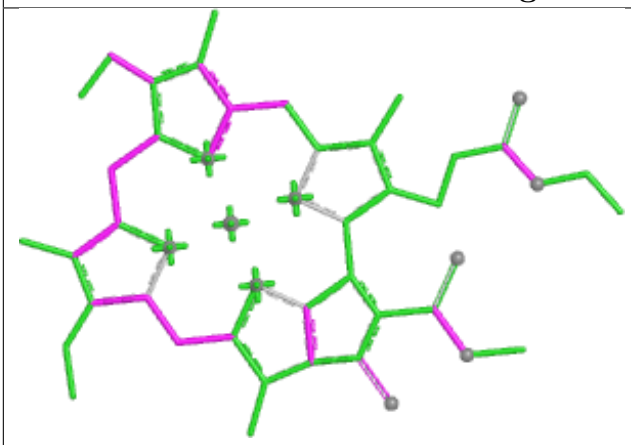


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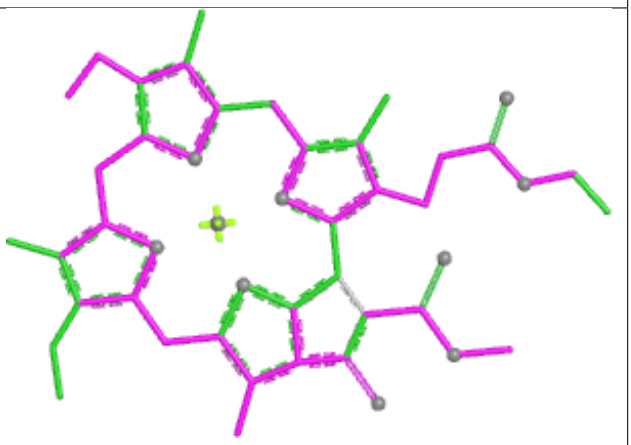


Rings

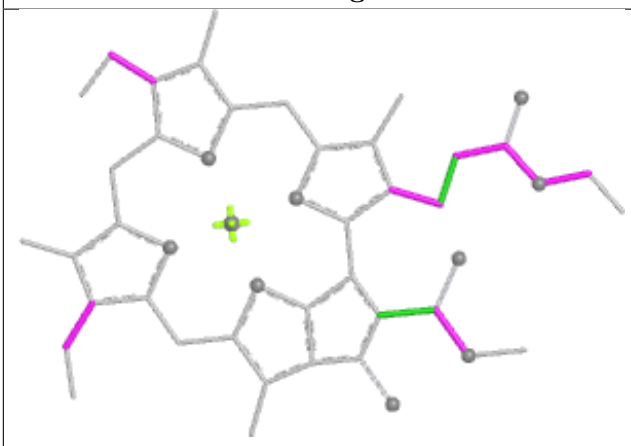
Ligand CLA 1 1002



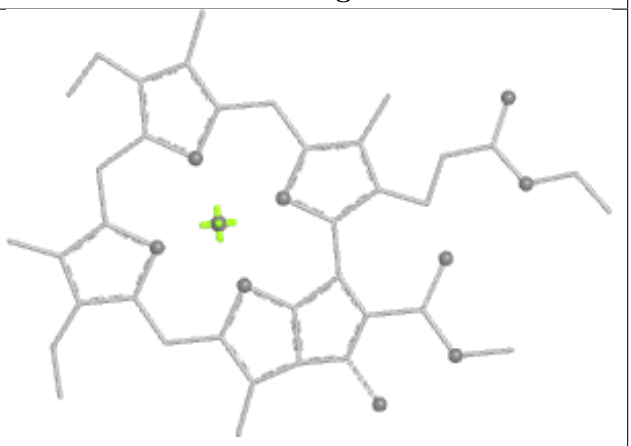
Bond lengths



Bond angles

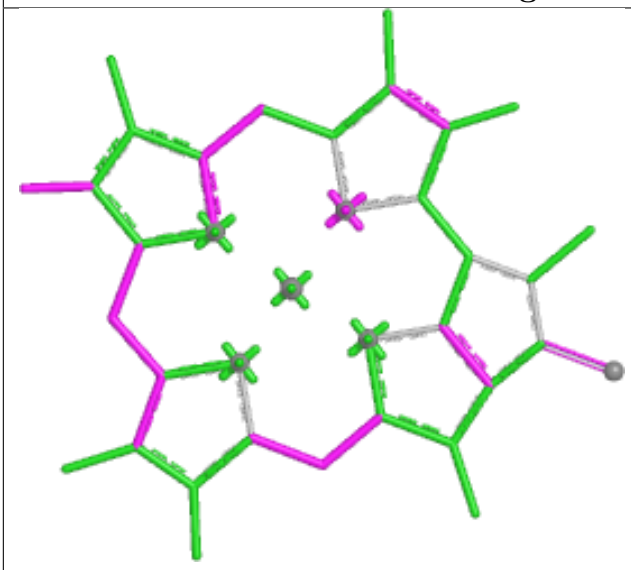


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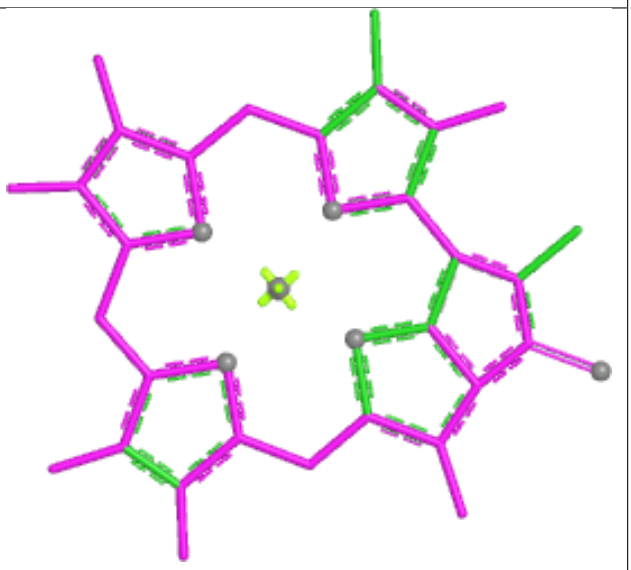


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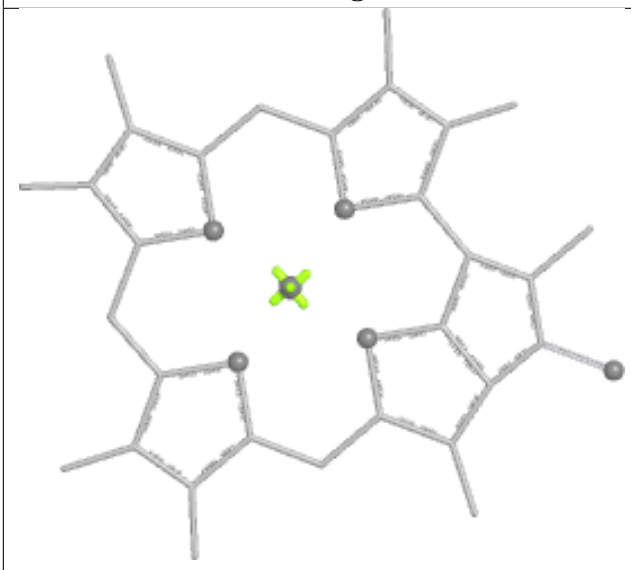
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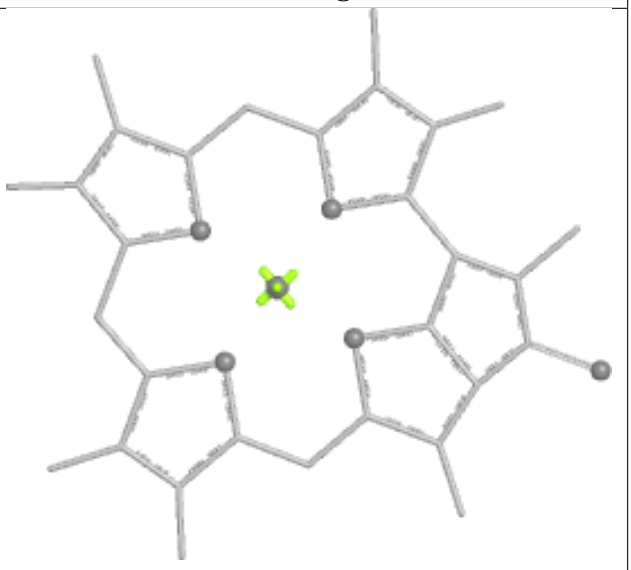
Bond lengths



Bond angles

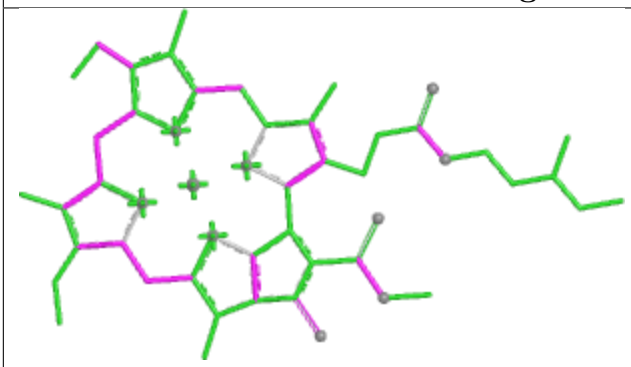


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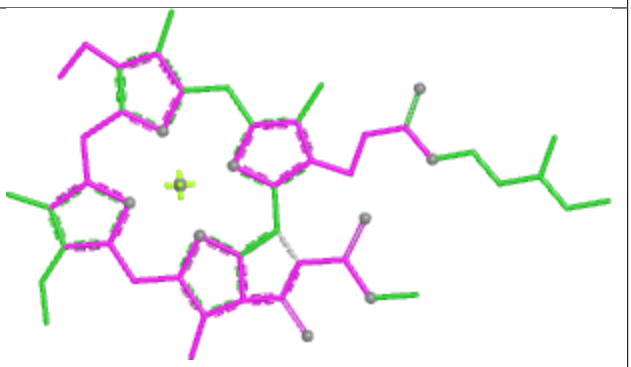


Rings

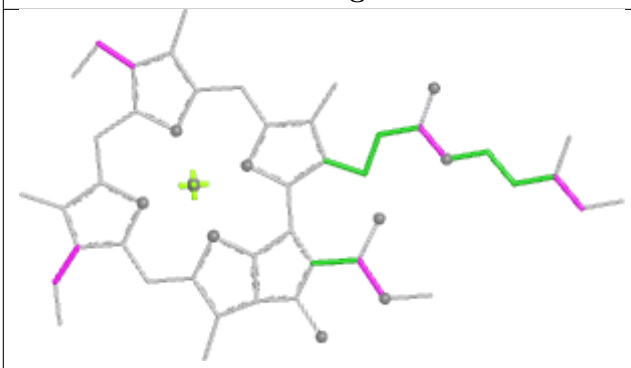
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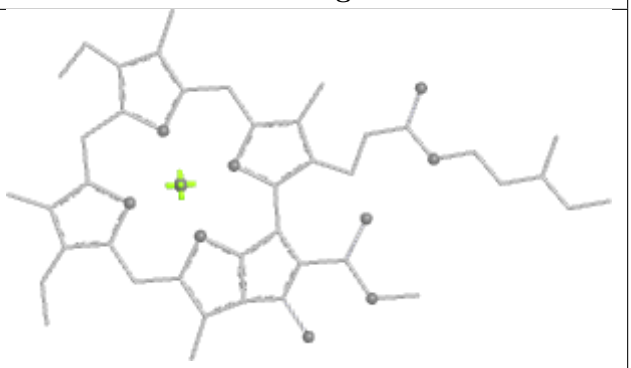
Bond lengths



Bond angles

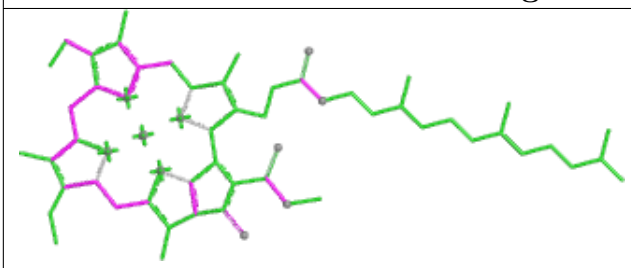


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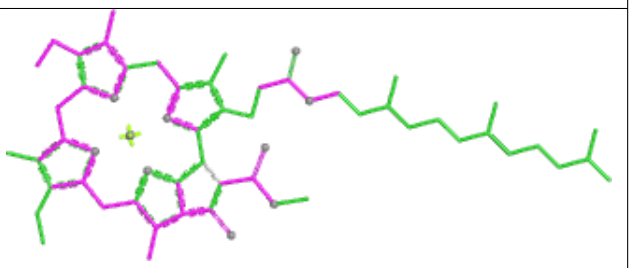


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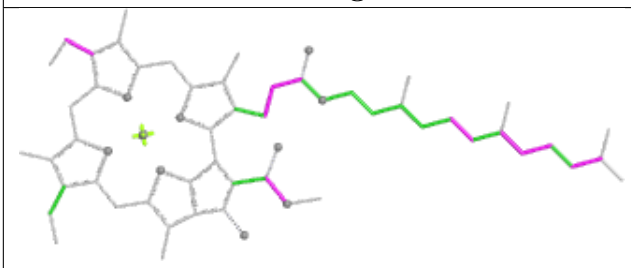
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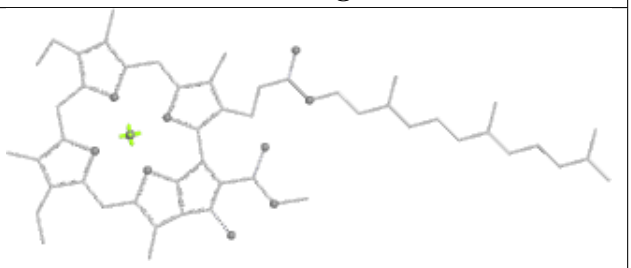
Bond lengths



Bond angles

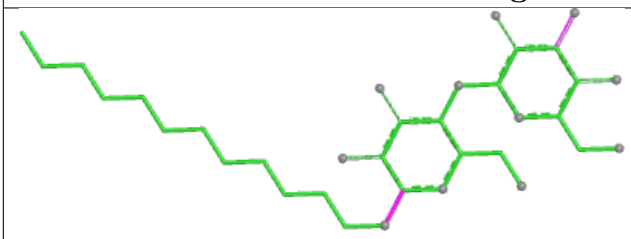


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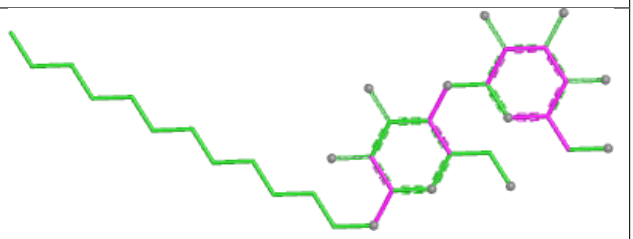


Rings

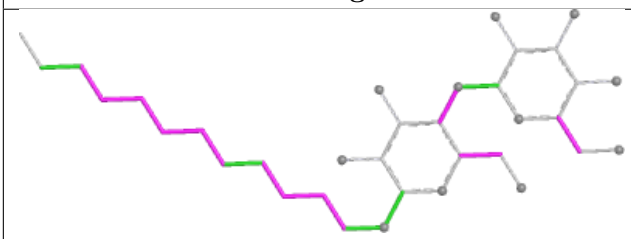
Ligand LMU K 7001



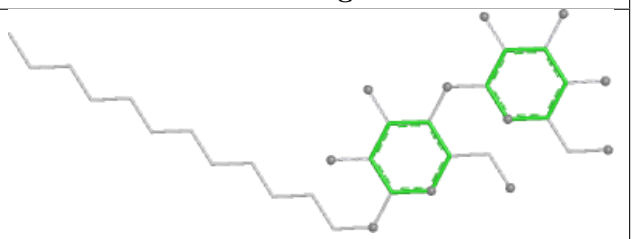
Bond lengths



Bond angles

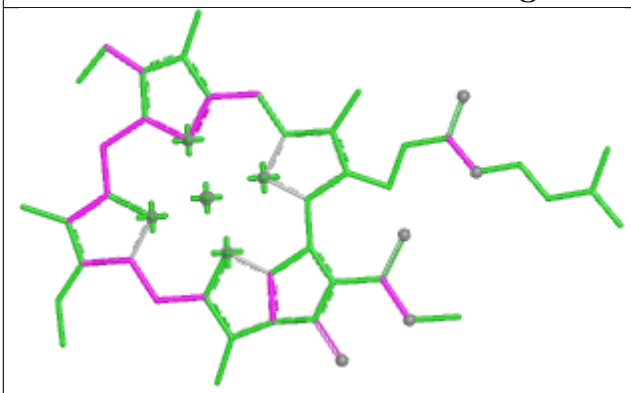


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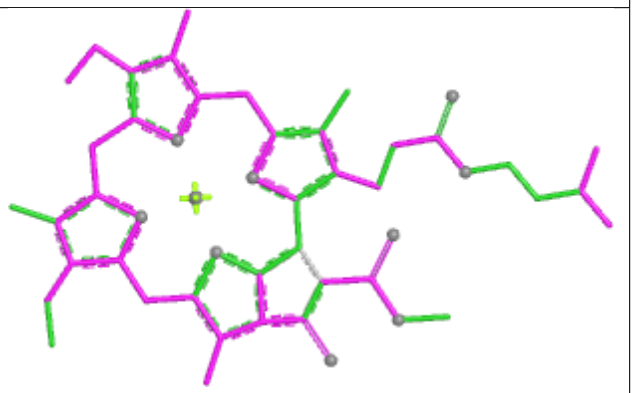


Rings

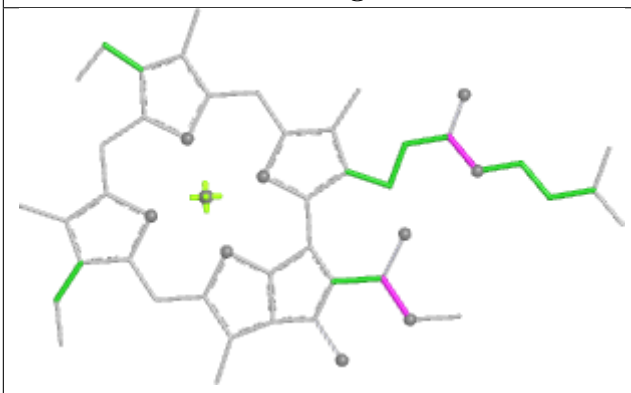
Ligand CLA 2 2012



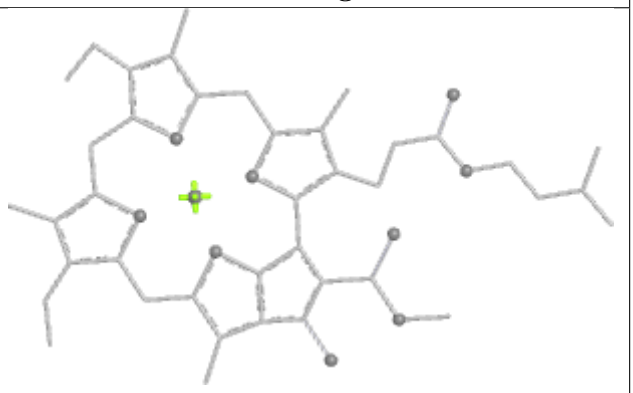
Bond lengths



Bond angles

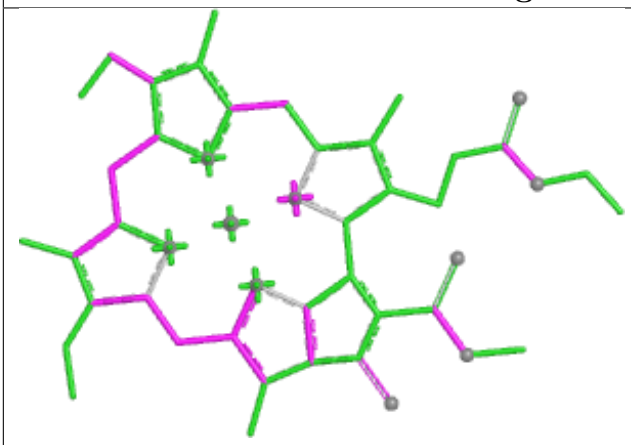


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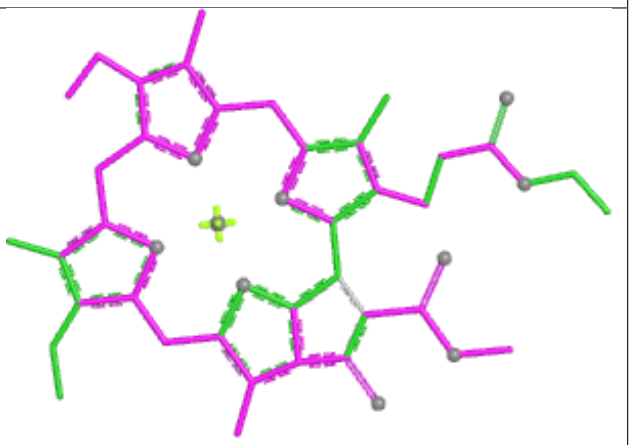


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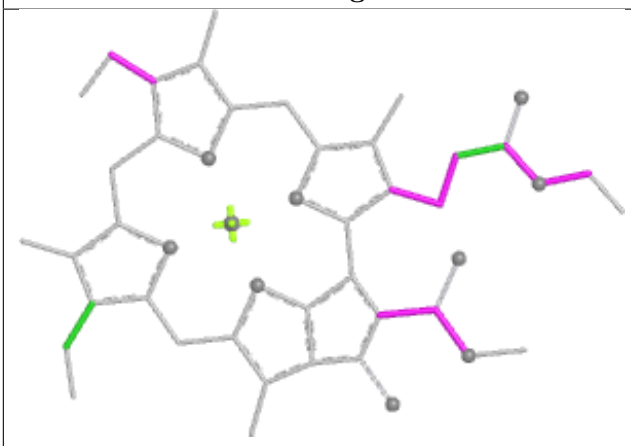
Ligand CLA B 1236



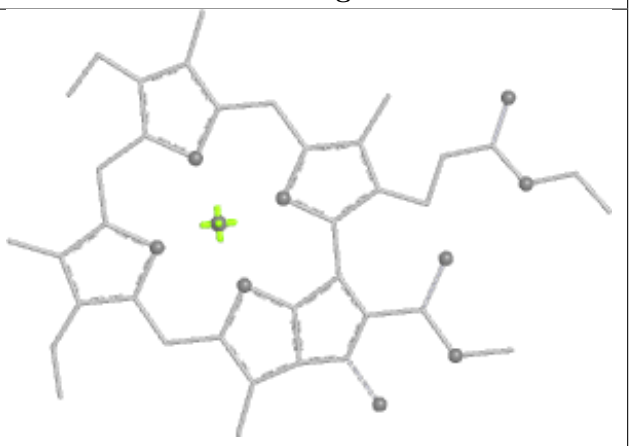
Bond lengths



Bond angles

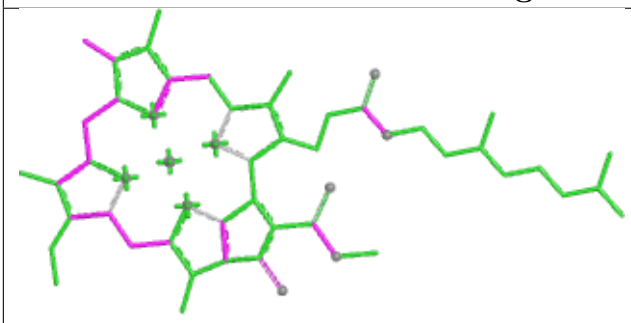


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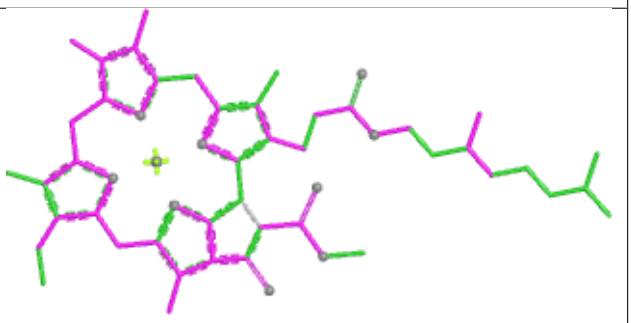


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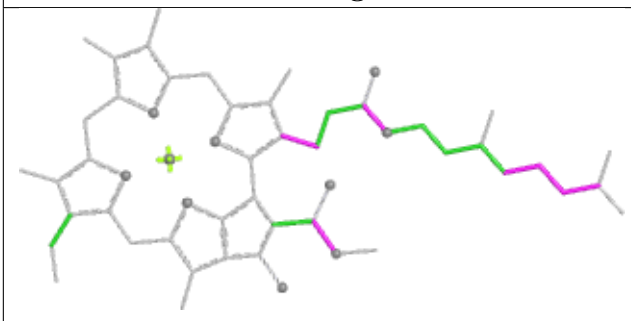
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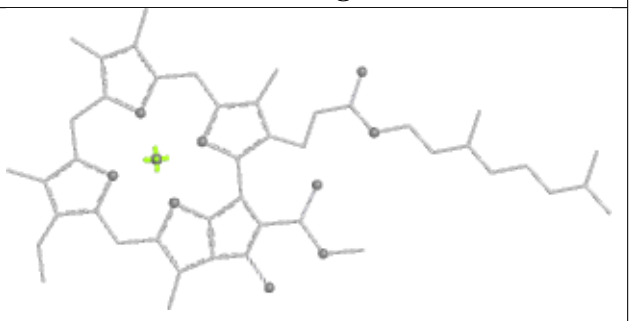
Bond lengths



Bond angles

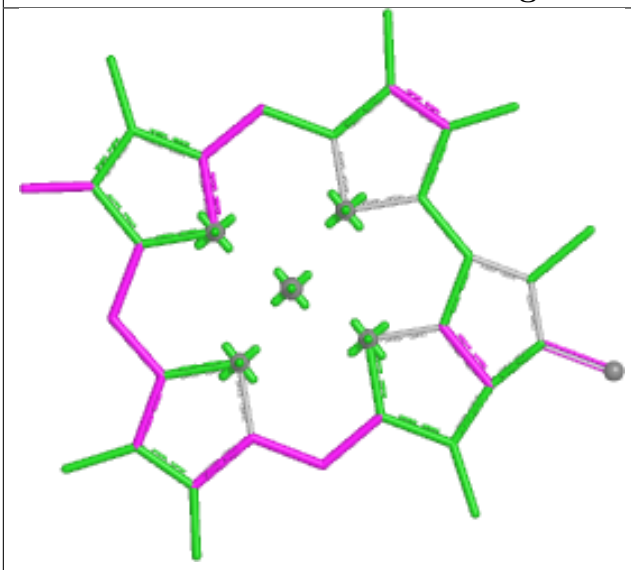


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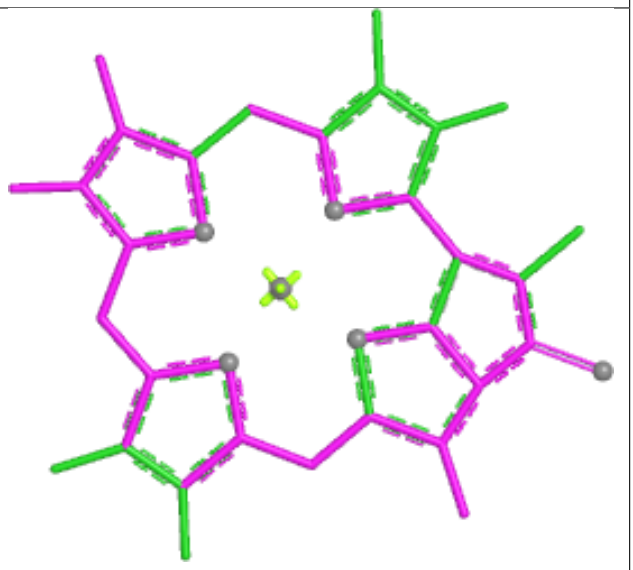


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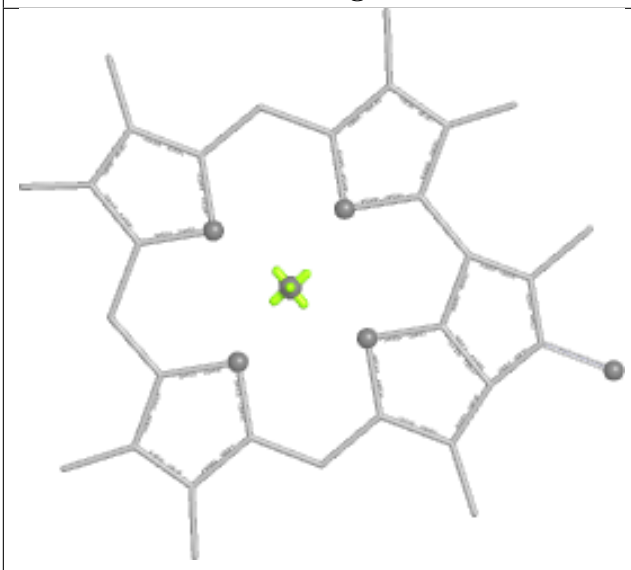
Ligand CLA 3 3003



Bond lengths



Bond angles

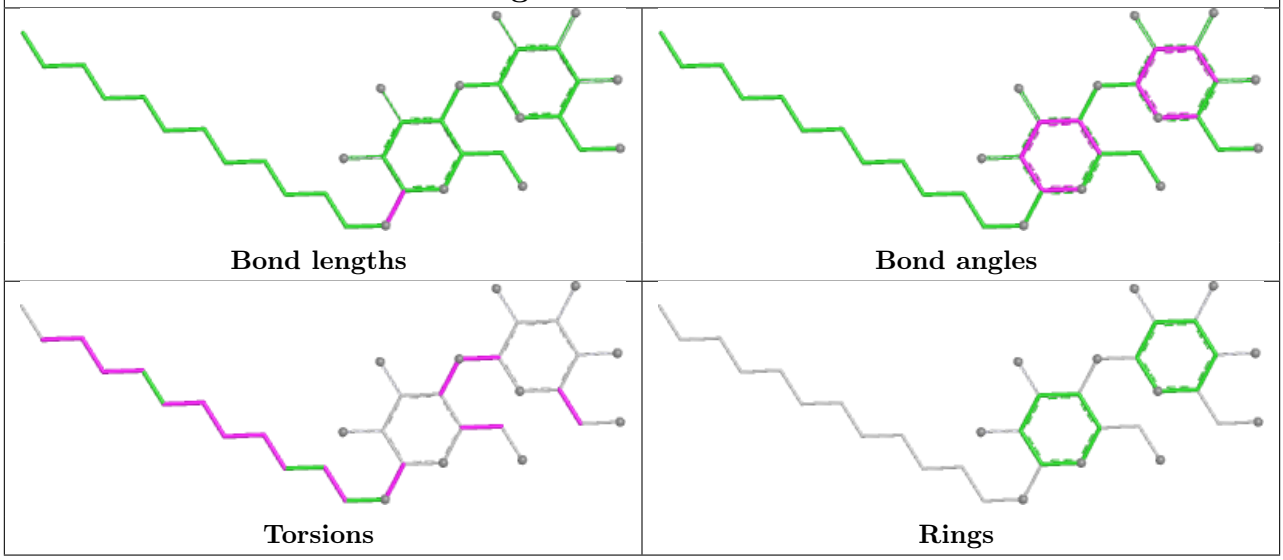


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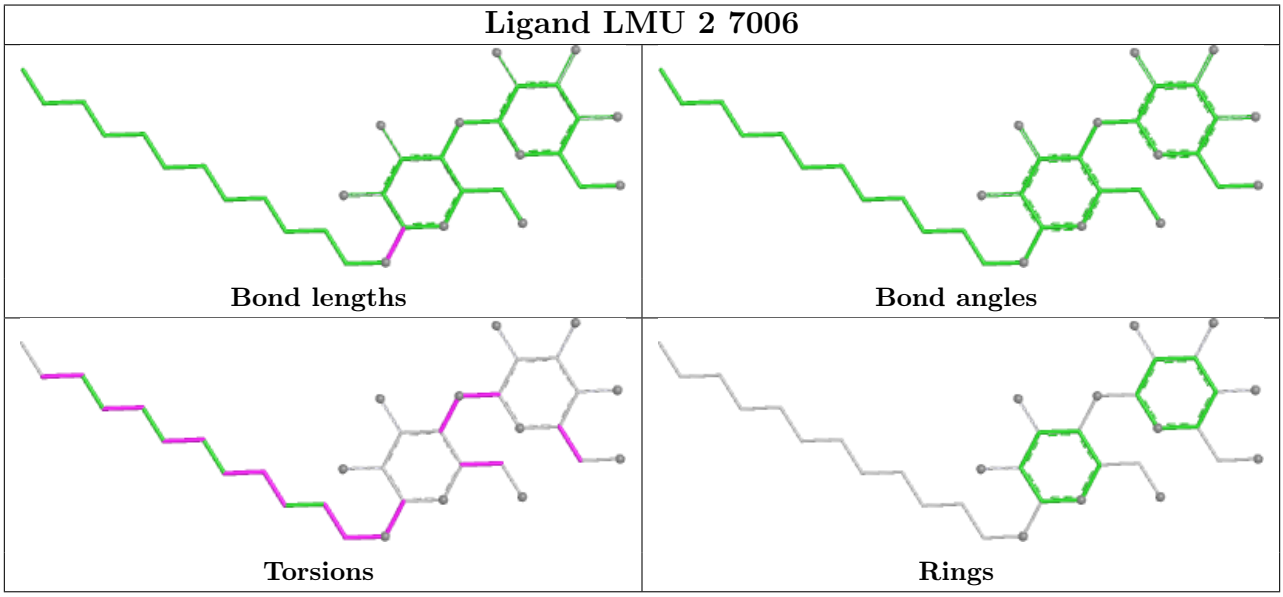


Rings

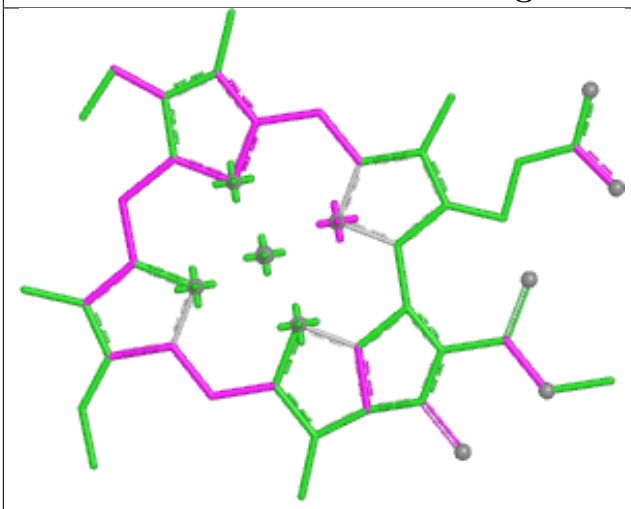
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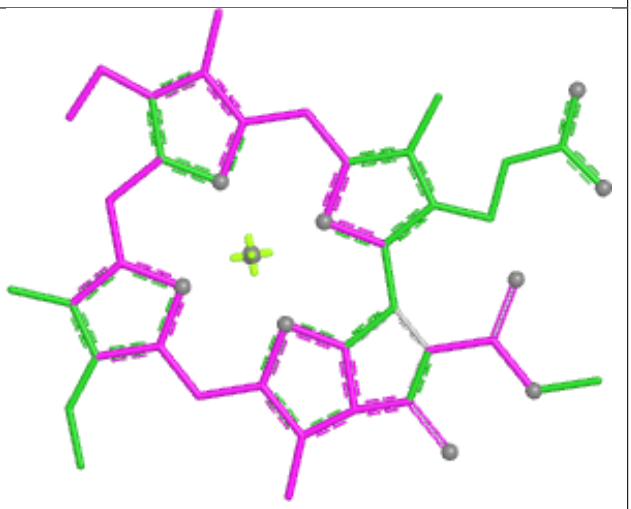
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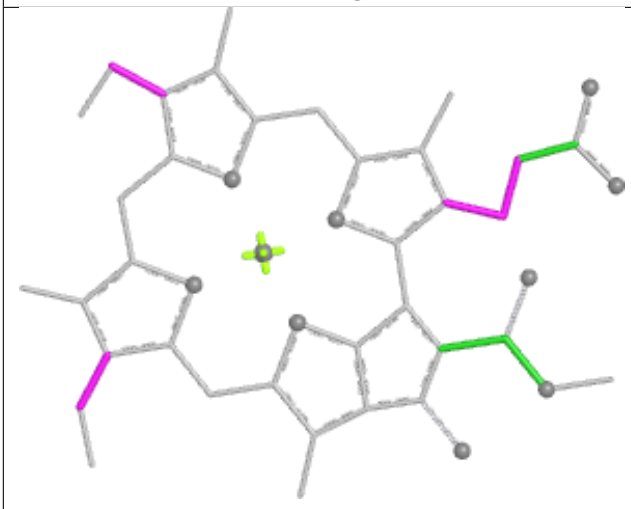
Ligand CLA B 1201



Bond lengths



Bond angles

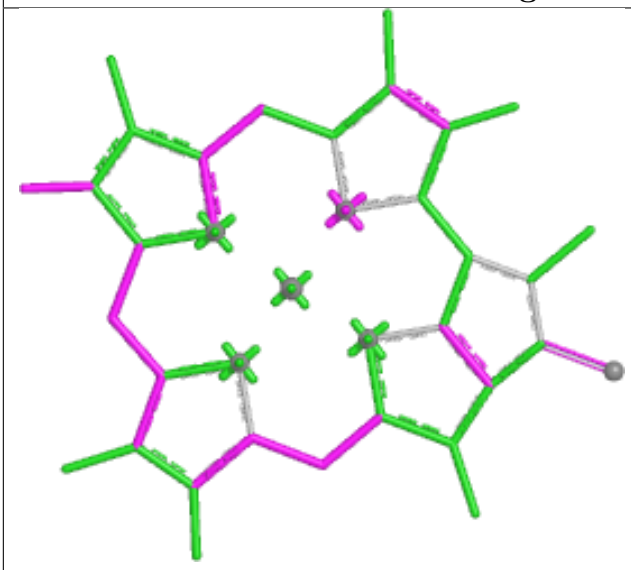


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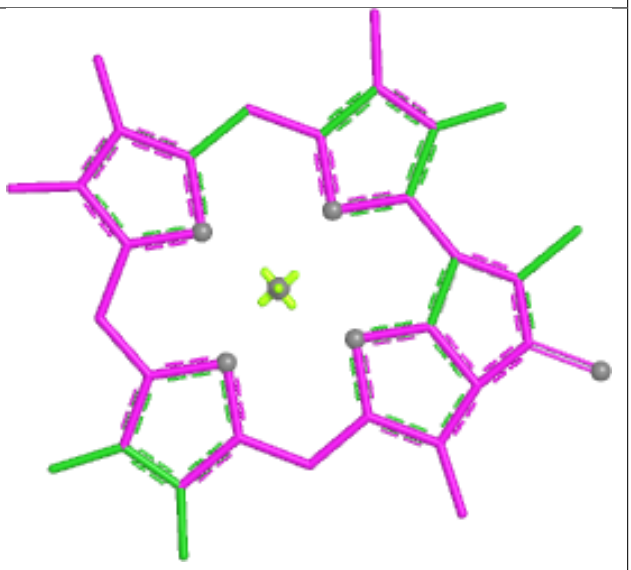


Rings

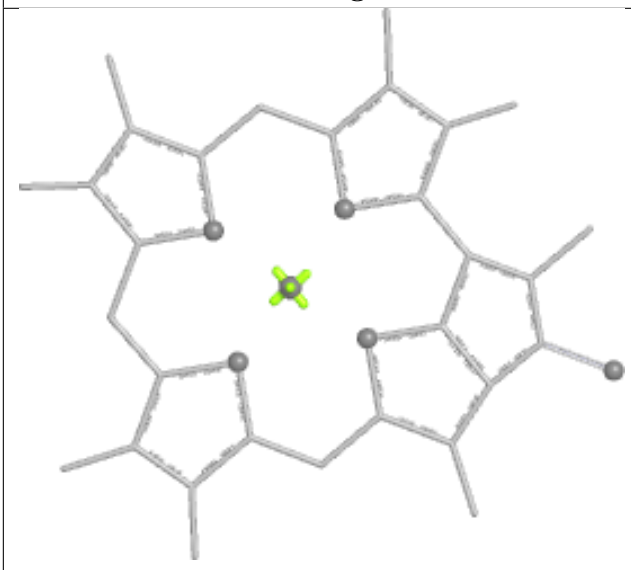
Ligand CLA 1 1006



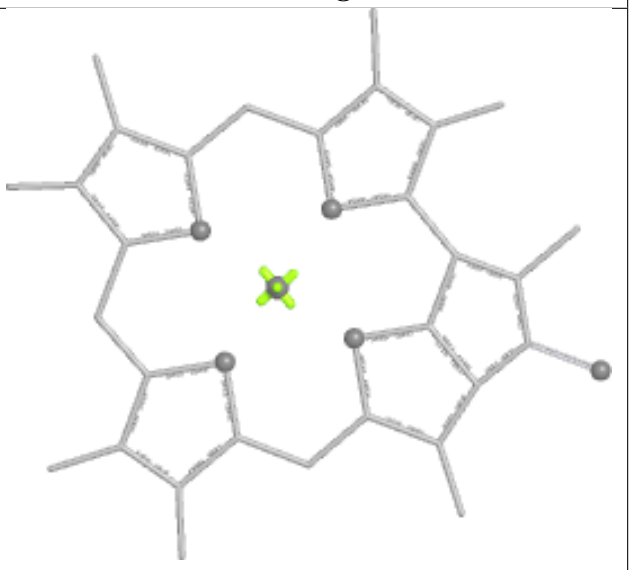
Bond lengths



Bond angles

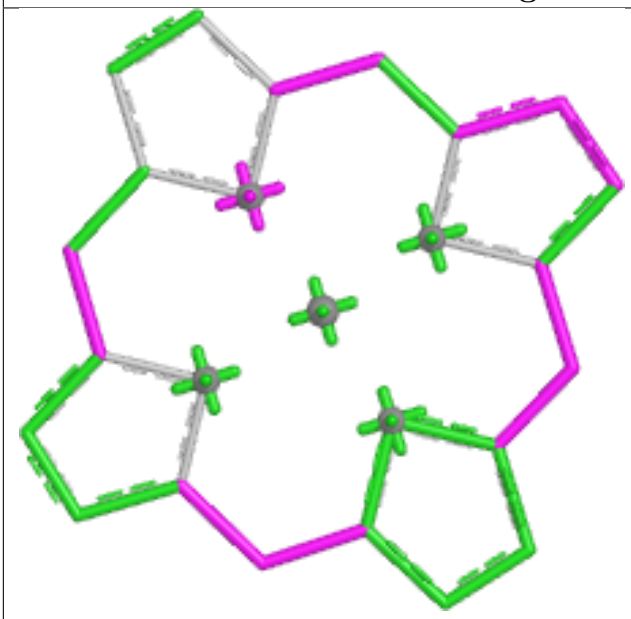


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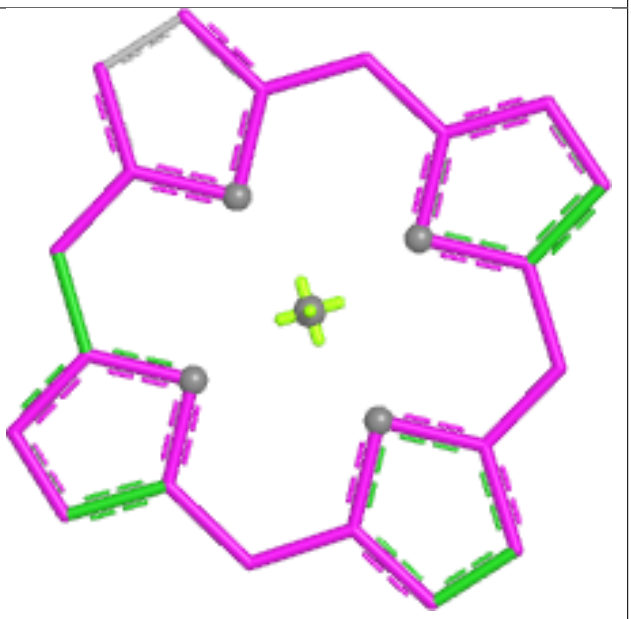


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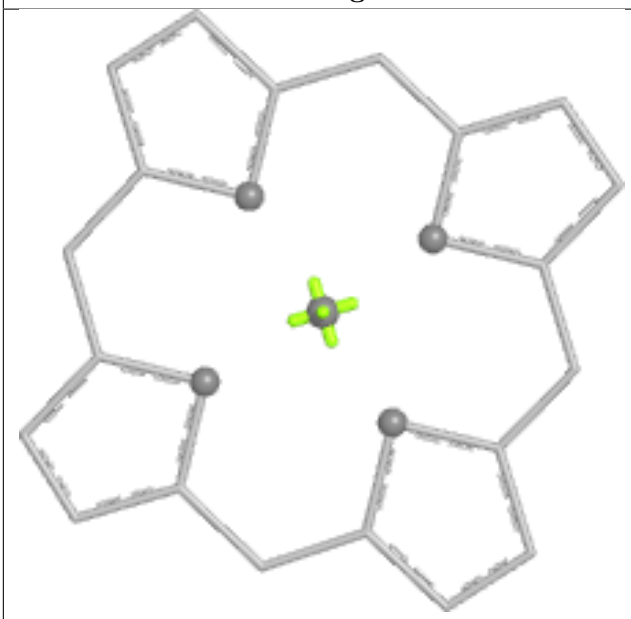
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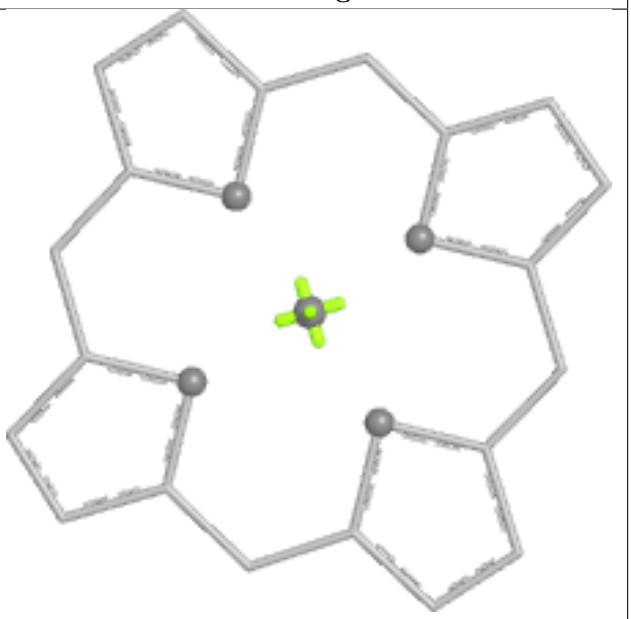
Bond lengths



Bond angles

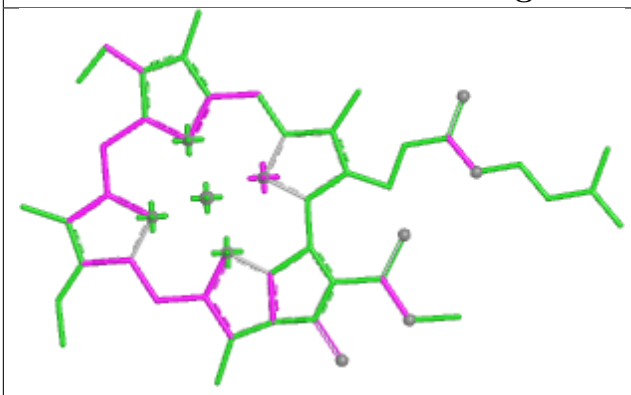


Torsions

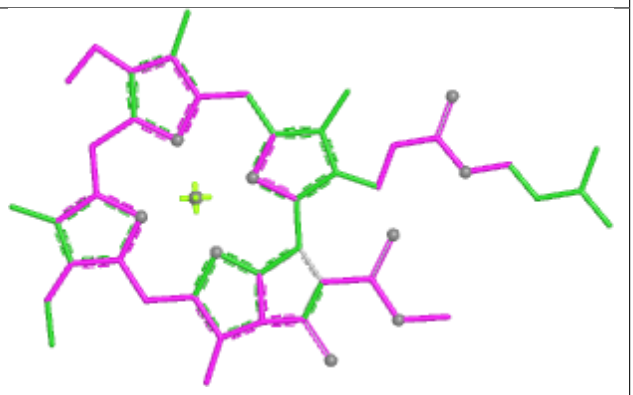


Rings

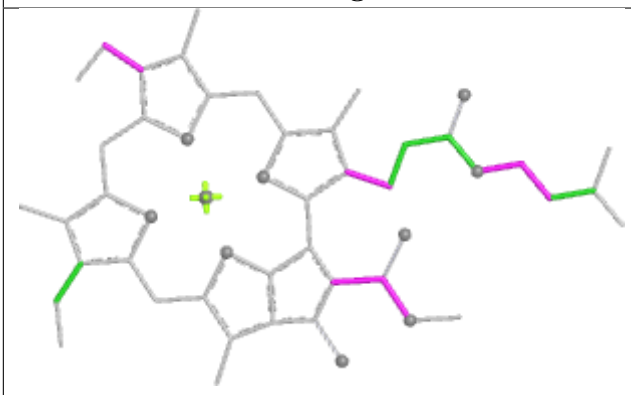
Ligand CLA B 1230



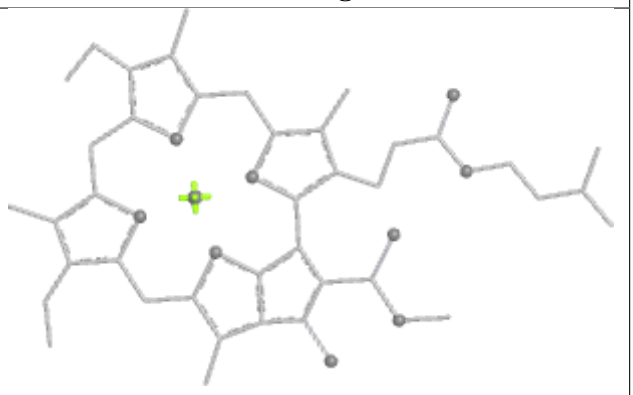
Bond lengths



Bond angles

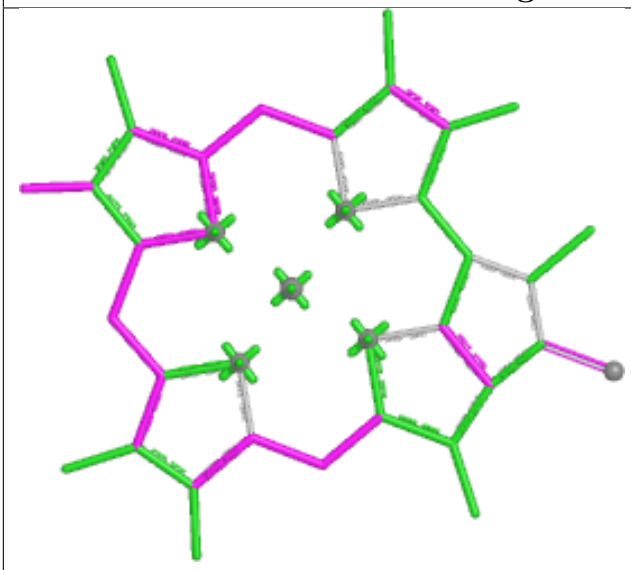


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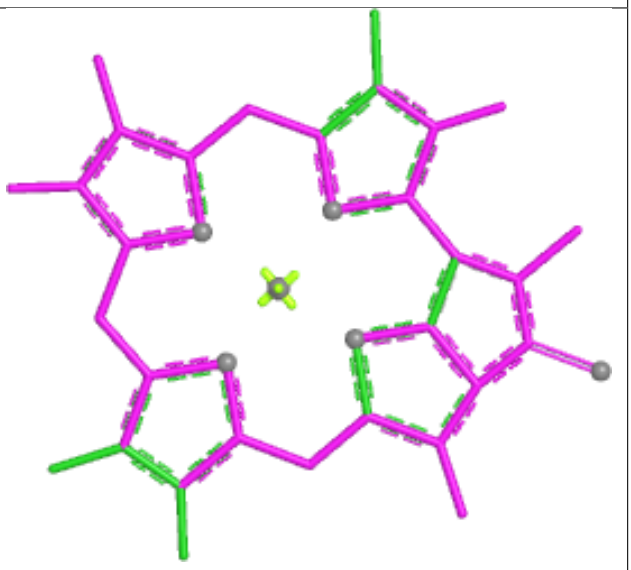


Rings

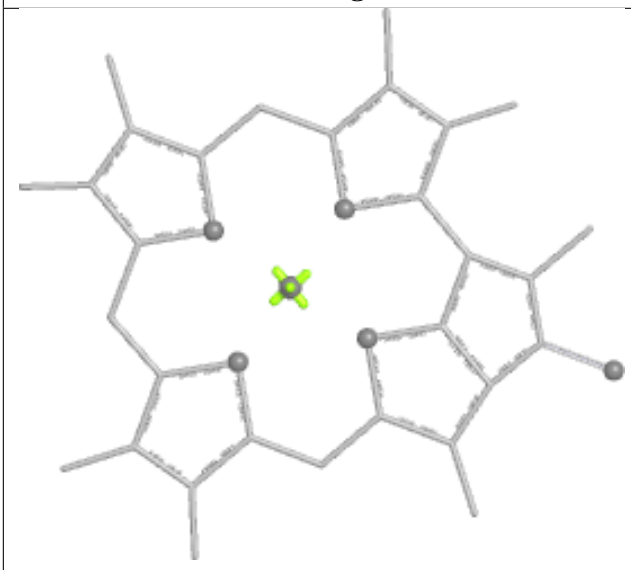
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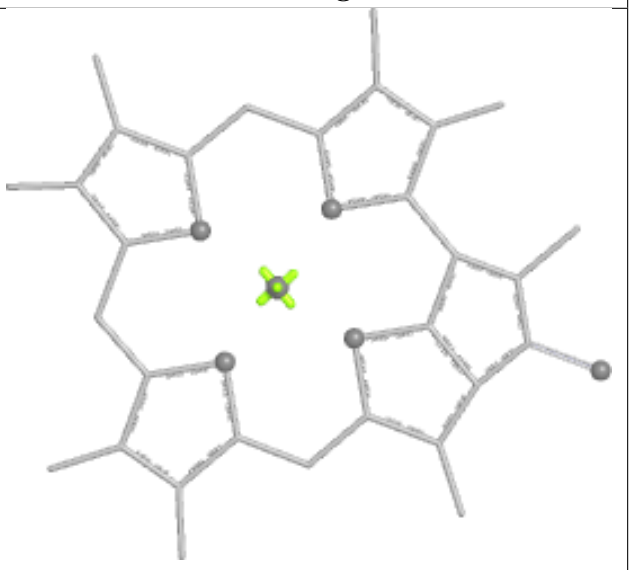
Bond lengths



Bond angles

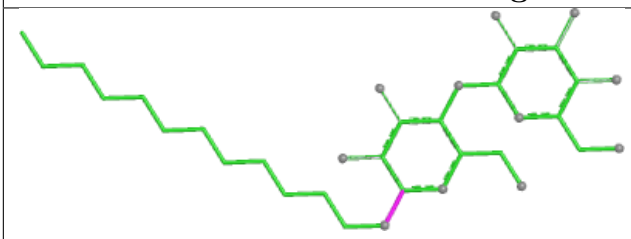


Torsions

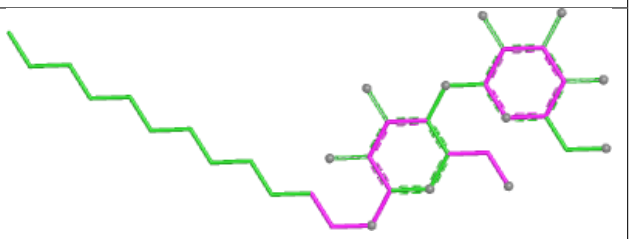


Rings

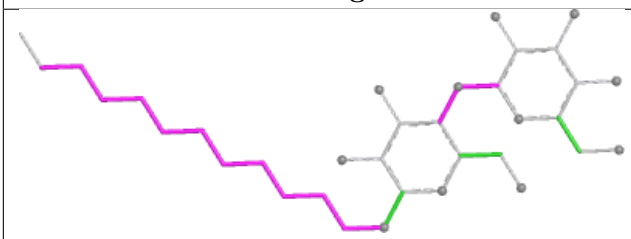
Ligand LMU A 7045



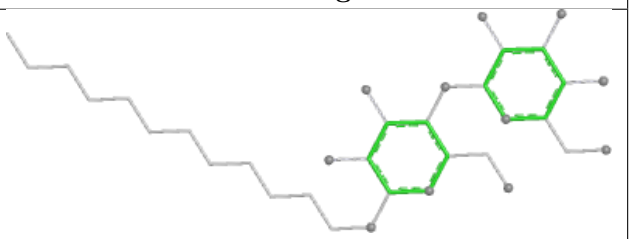
Bond lengths



Bond angles

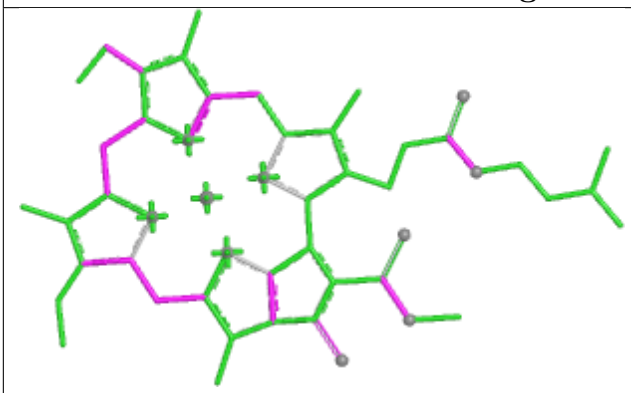


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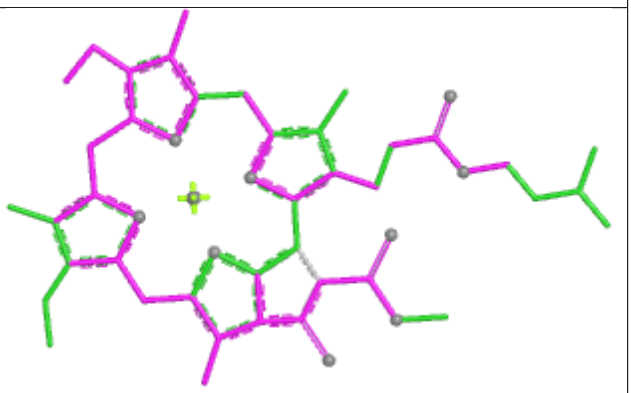


Rings

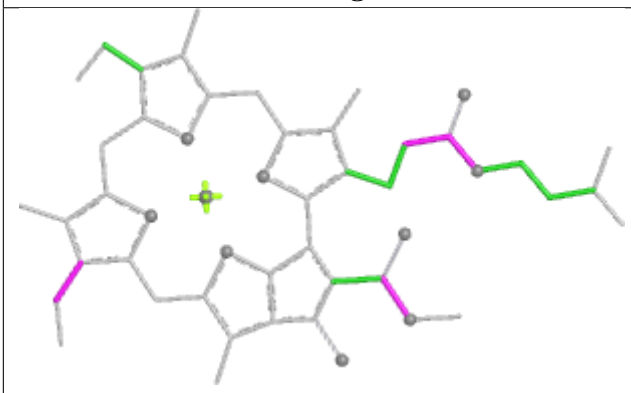
Ligand CLA 2 2013



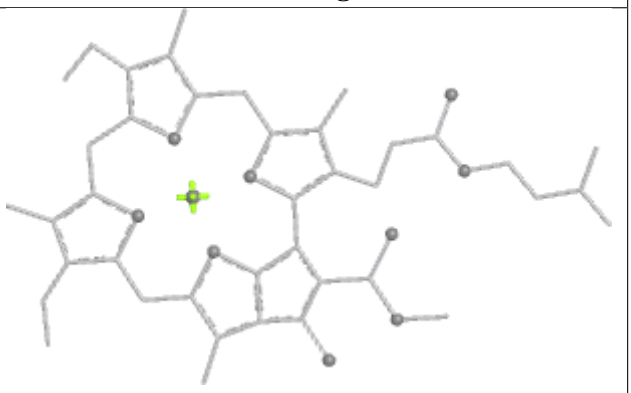
Bond lengths



Bond angles

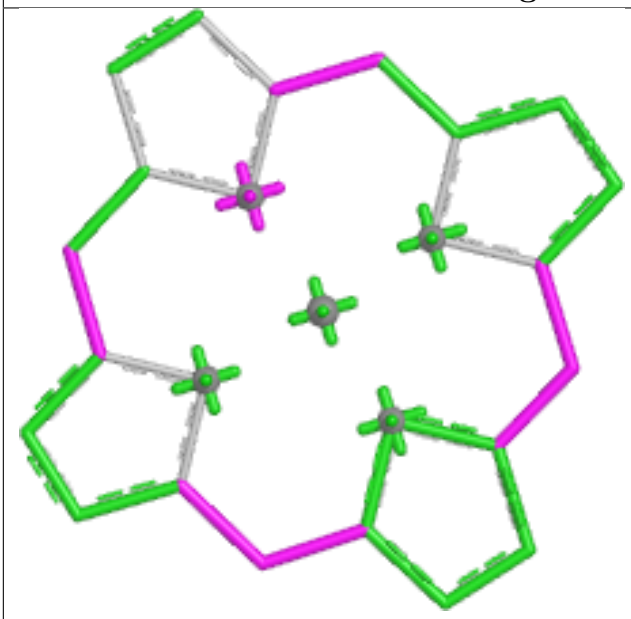


Torsions

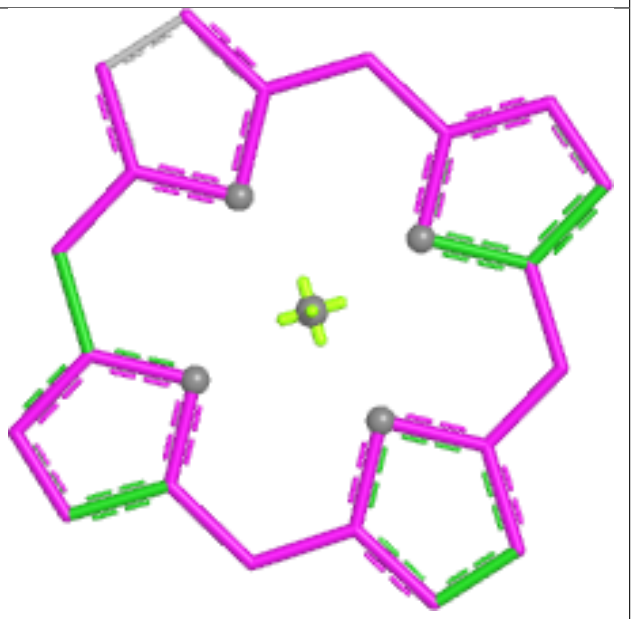


Rings

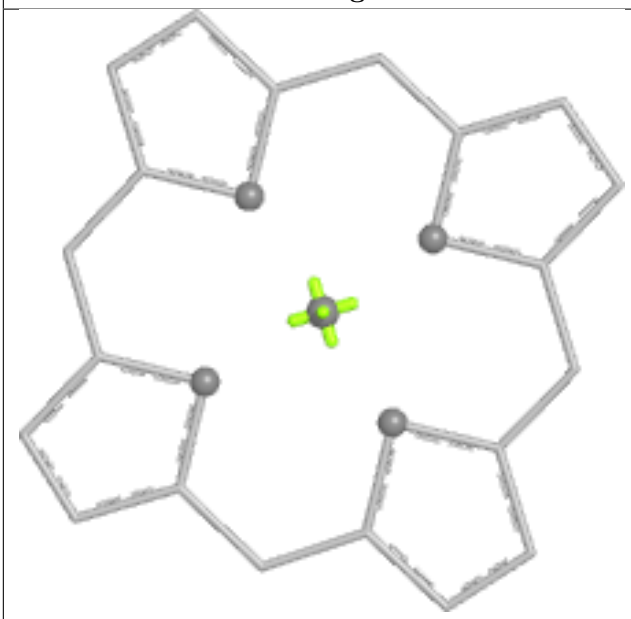
Ligand CLA 4 4004



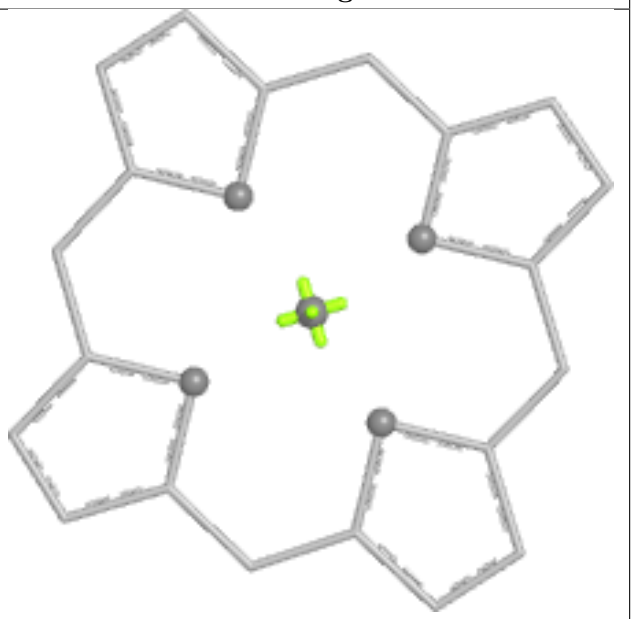
Bond lengths



Bond angles

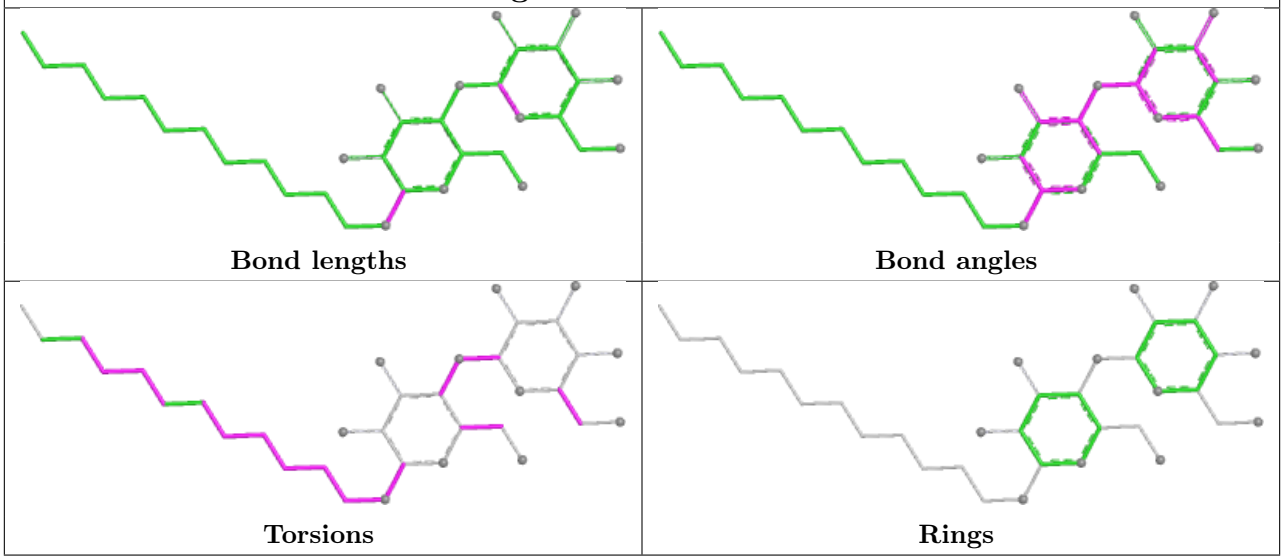


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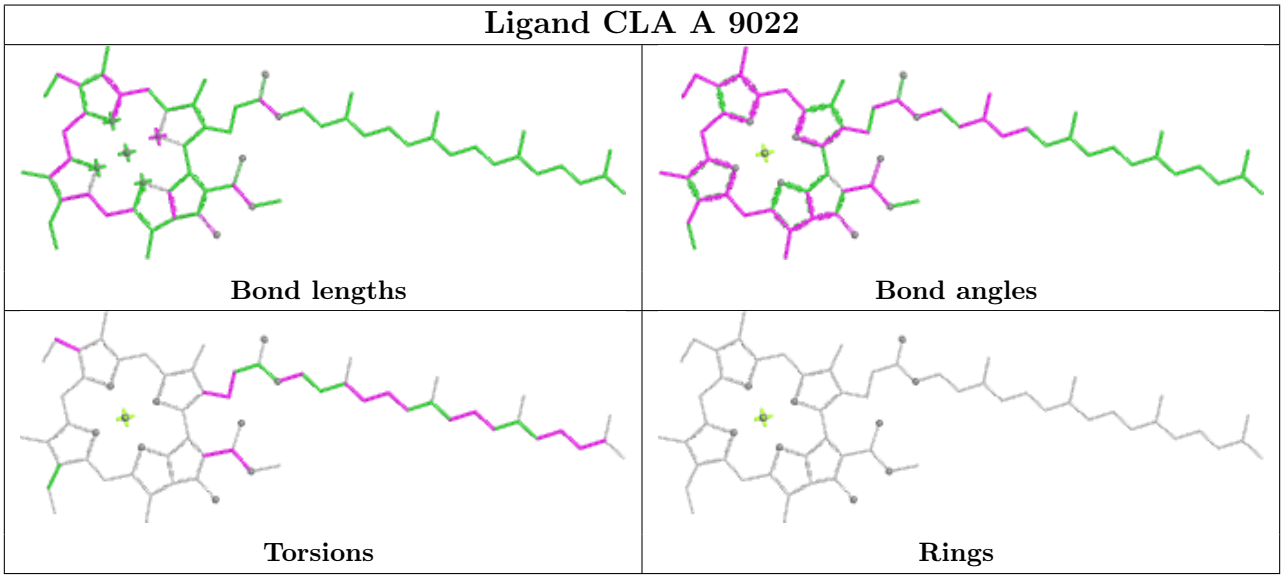


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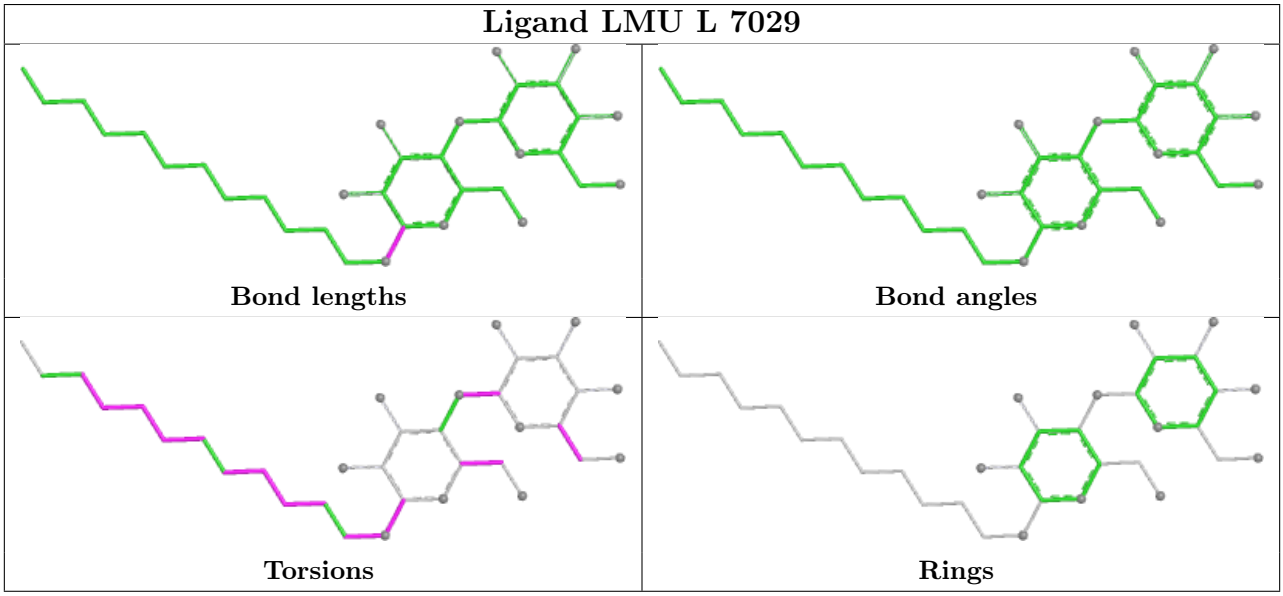
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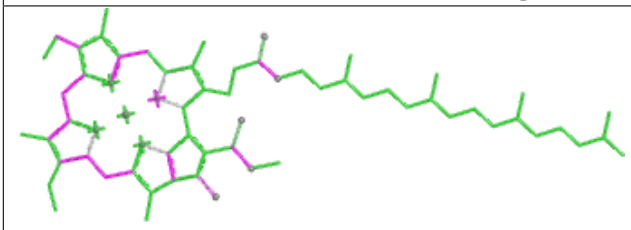
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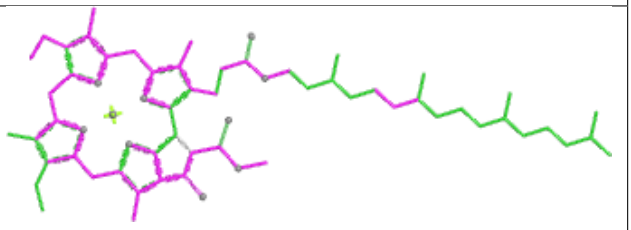
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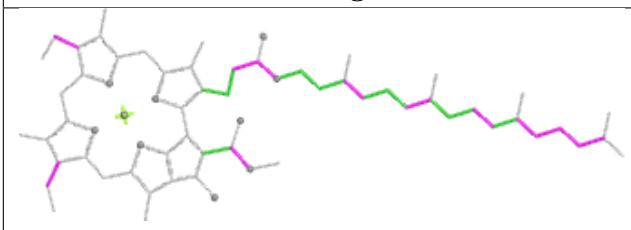
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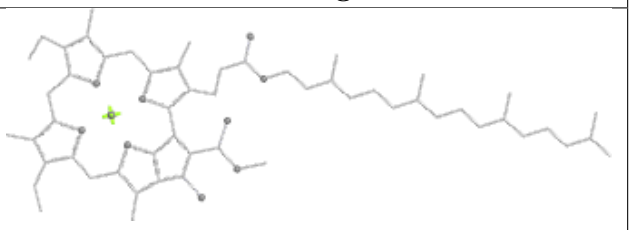
Bond lengths



Bond angles

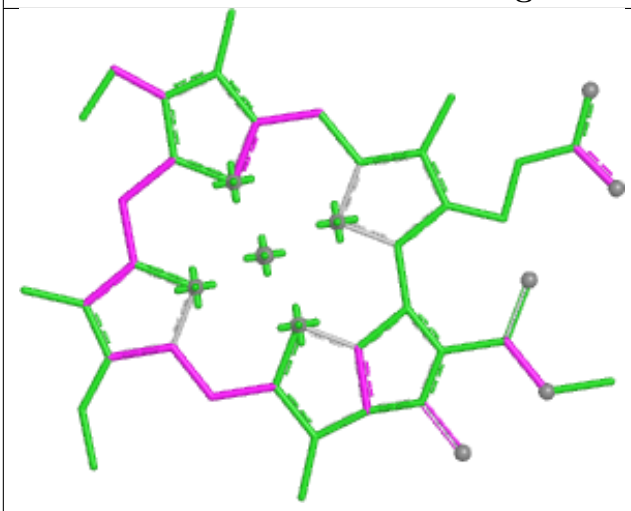


Torsions

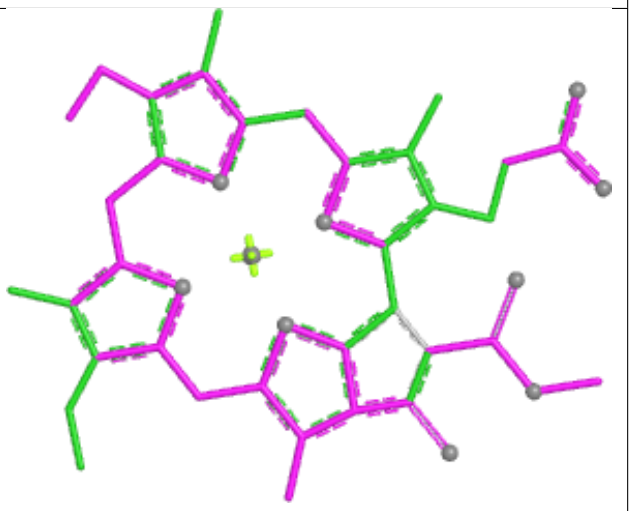


Rings

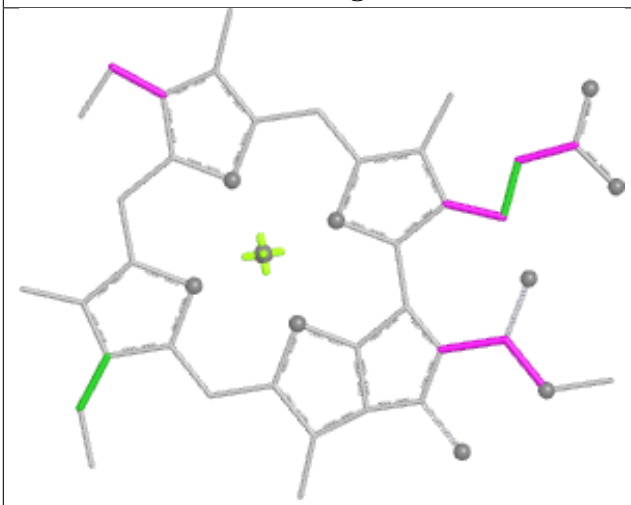
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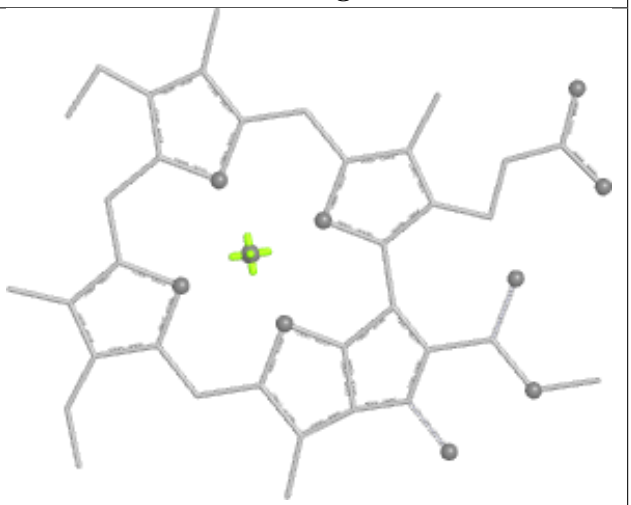
Bond lengths



Bond angles

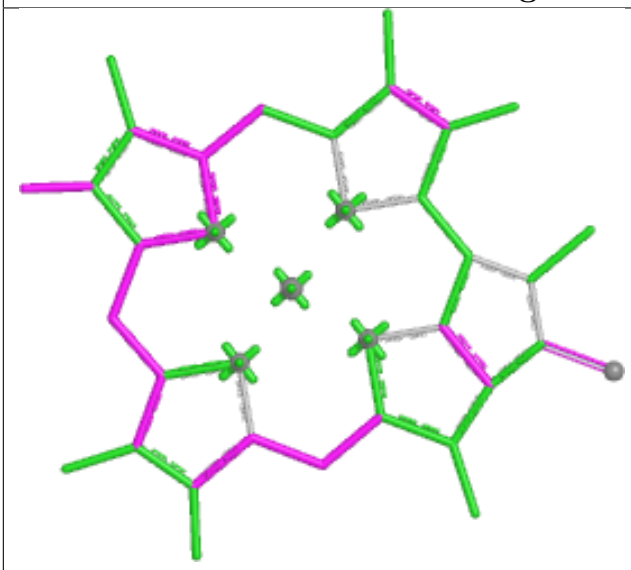


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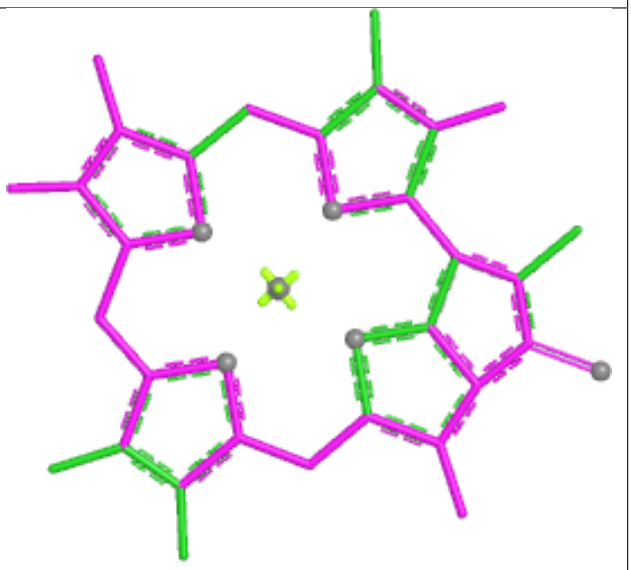


Rings

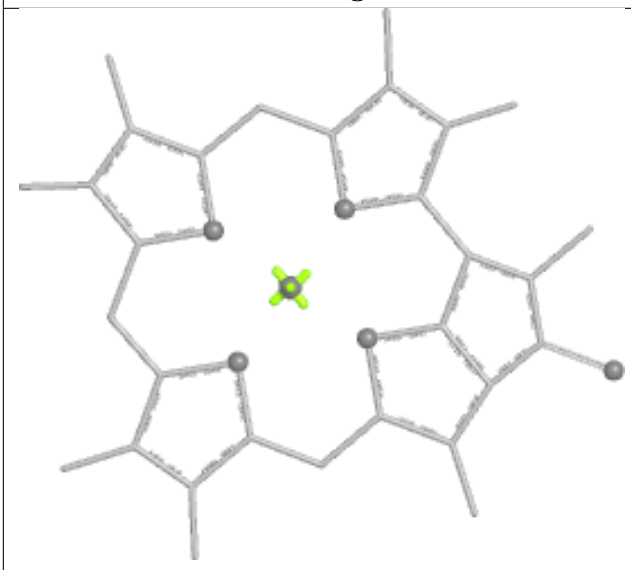
Ligand CLA 4 1009



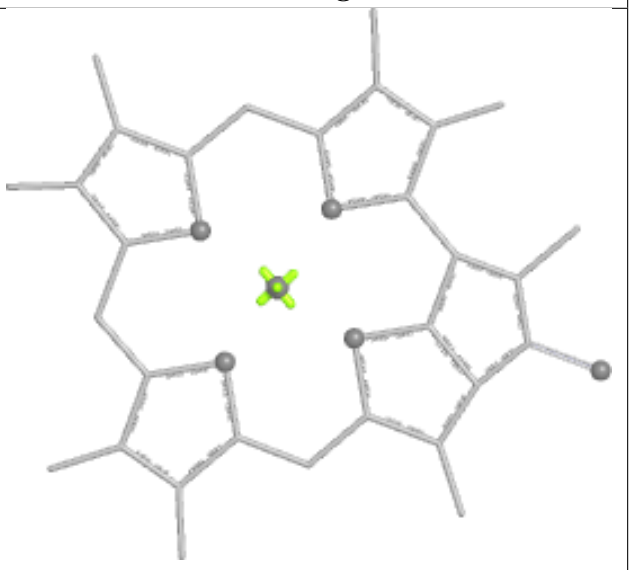
Bond lengths



Bond angles

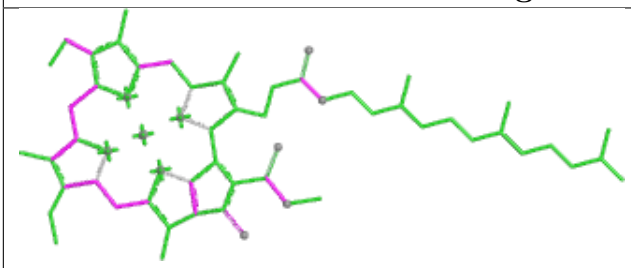


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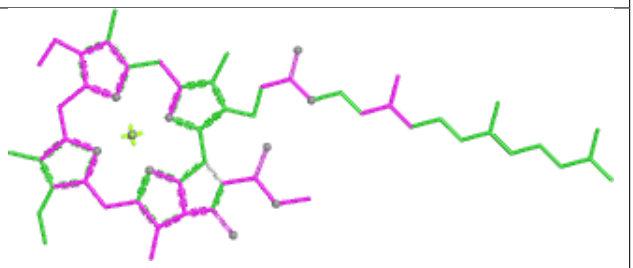


Rings

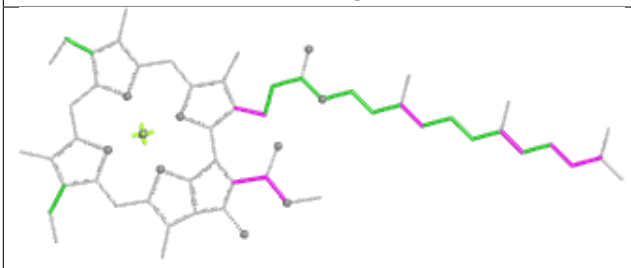
Ligand CLA B 1212



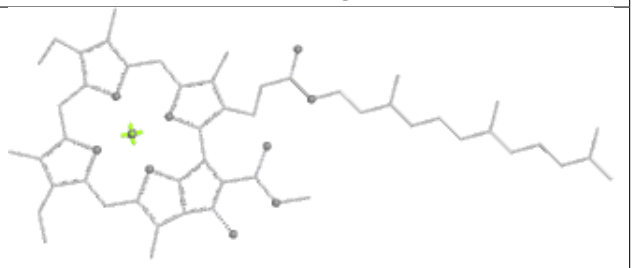
Bond lengths



Bond angles

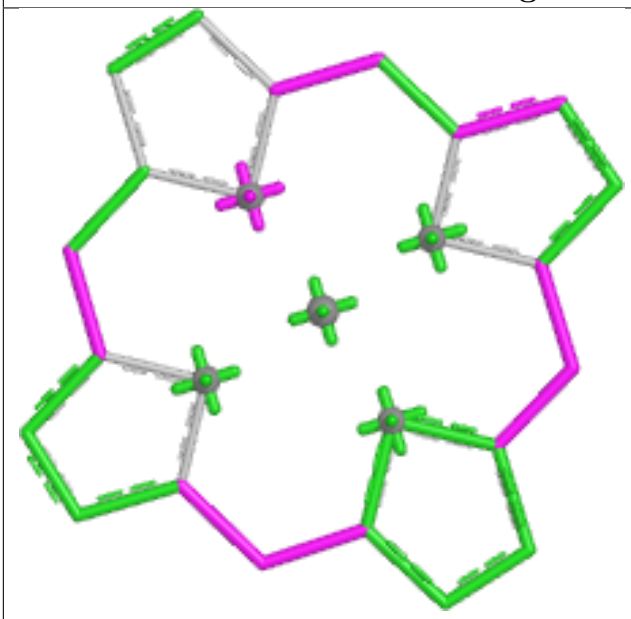


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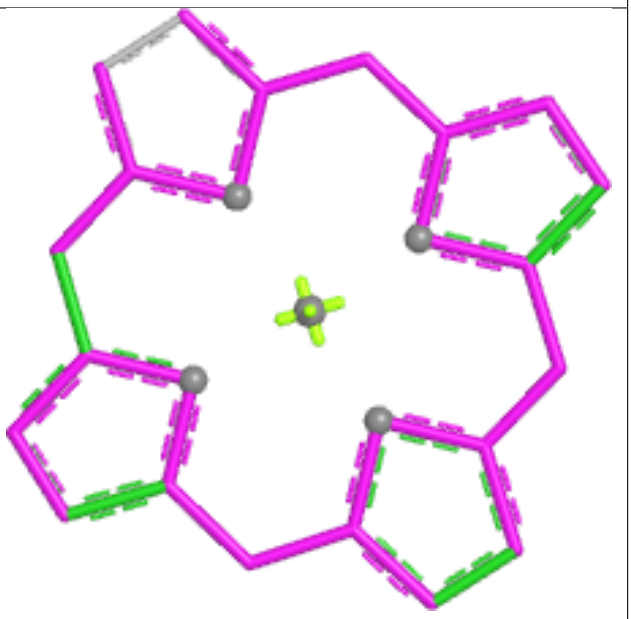


Rings

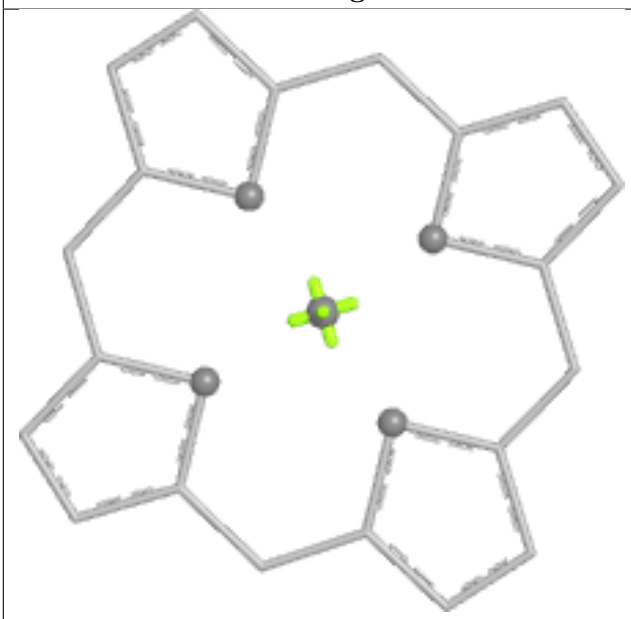
Ligand CLA 4 4010



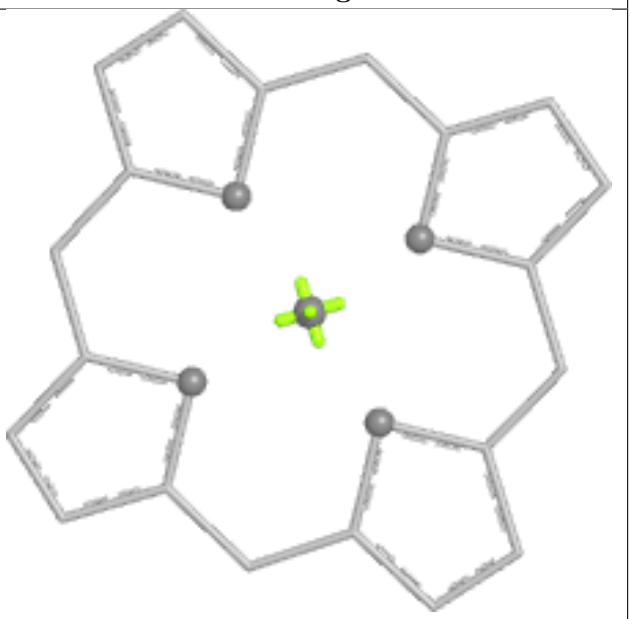
Bond lengths



Bond angles

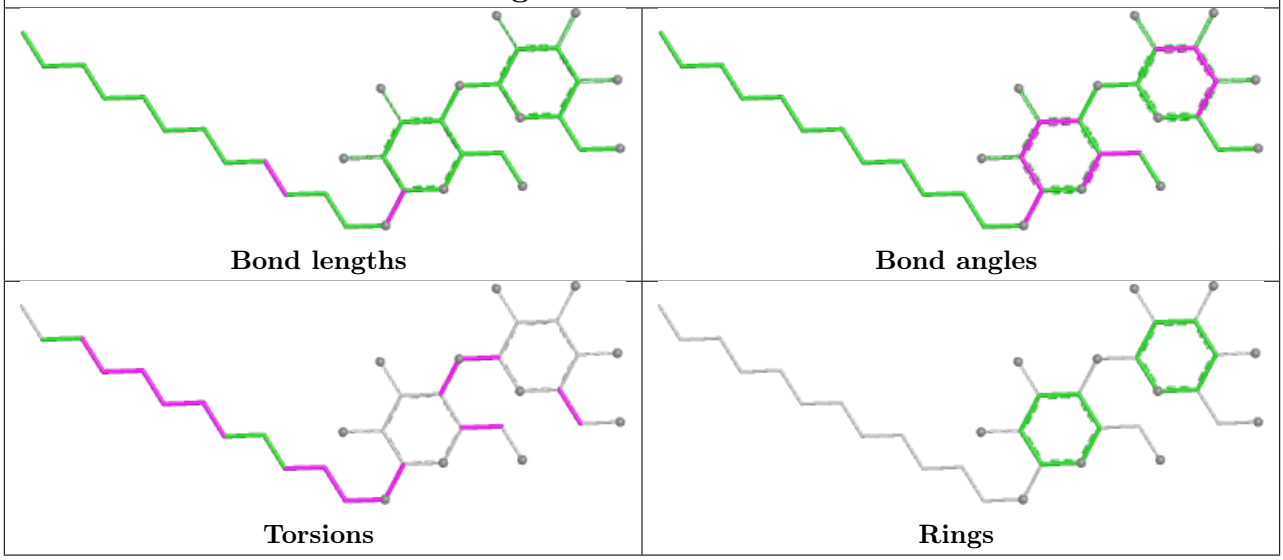


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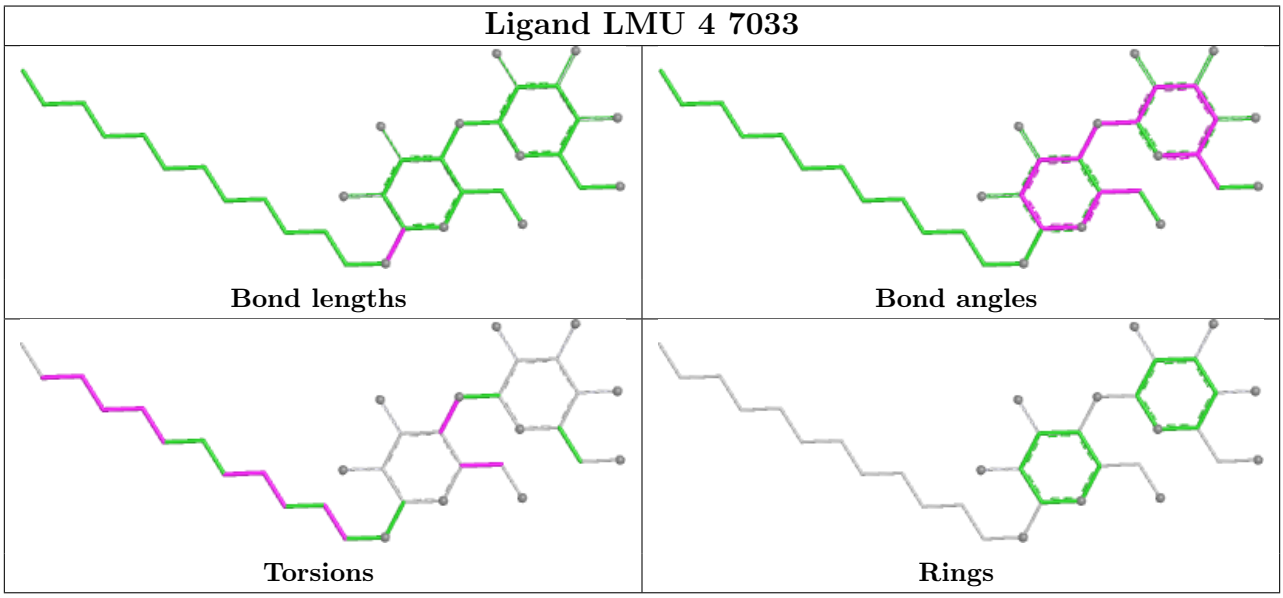


Rings

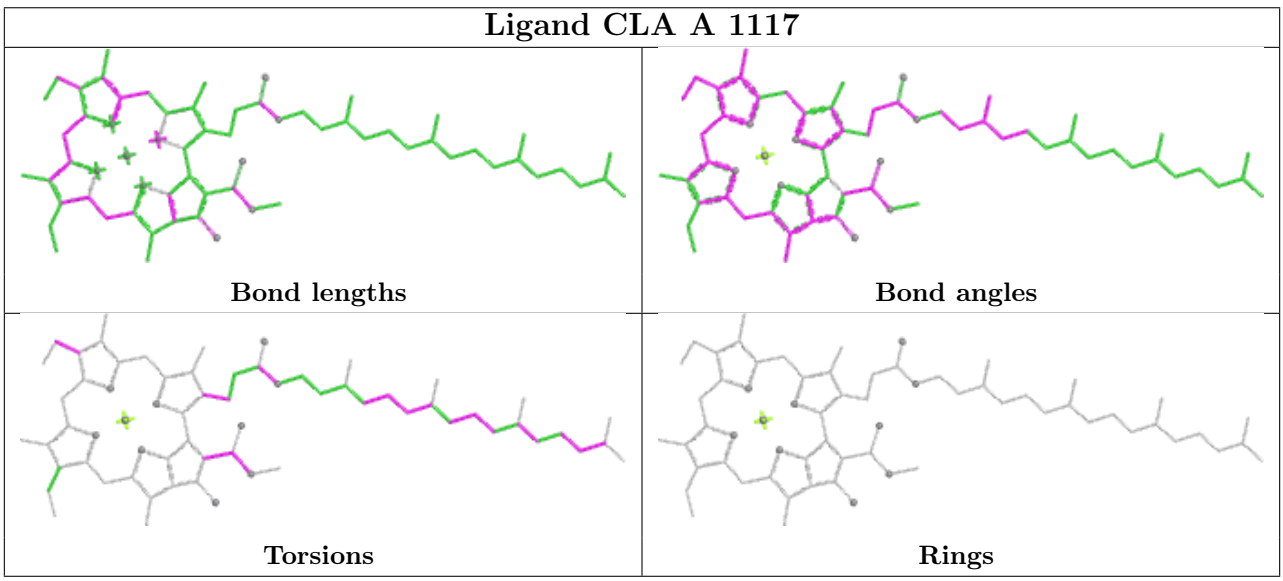
Ligand LMU A 7010



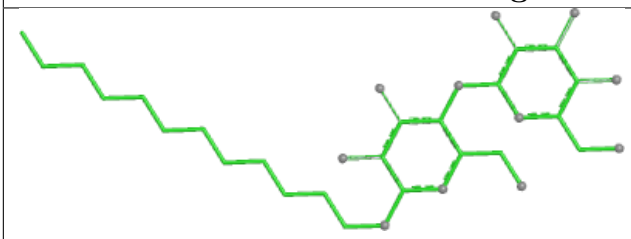
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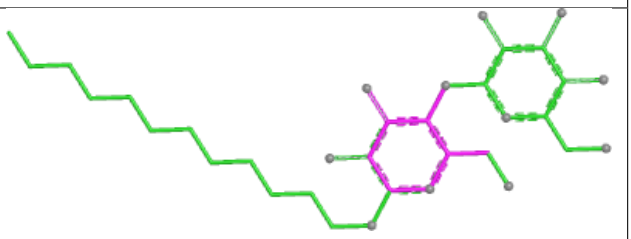
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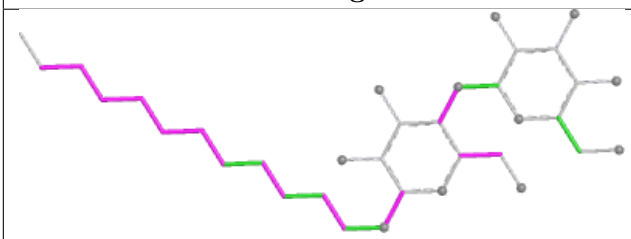
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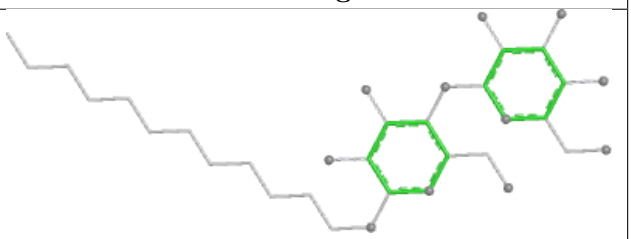
Bond lengths



Bond angles

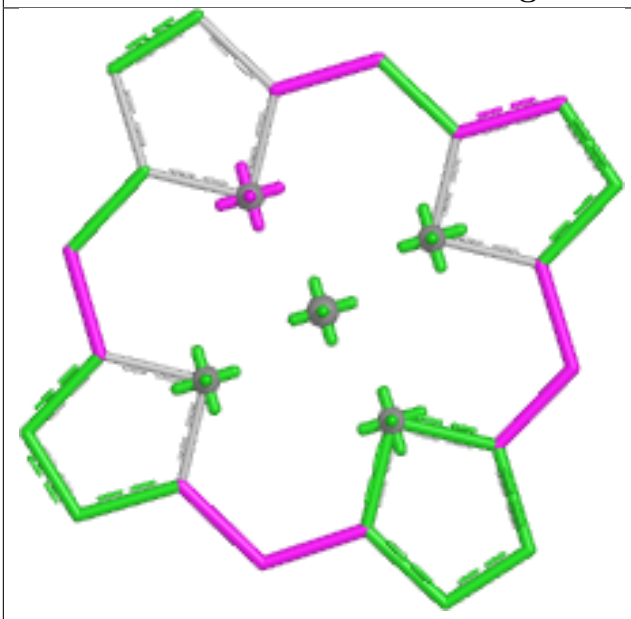


Torsions

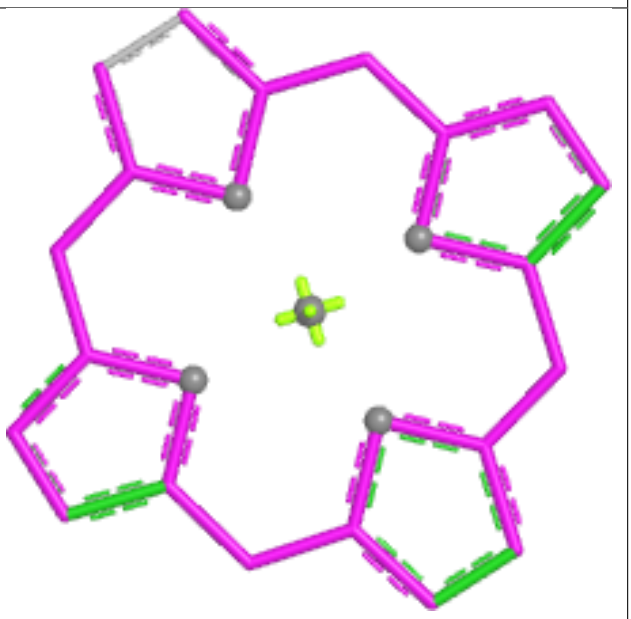


Rings

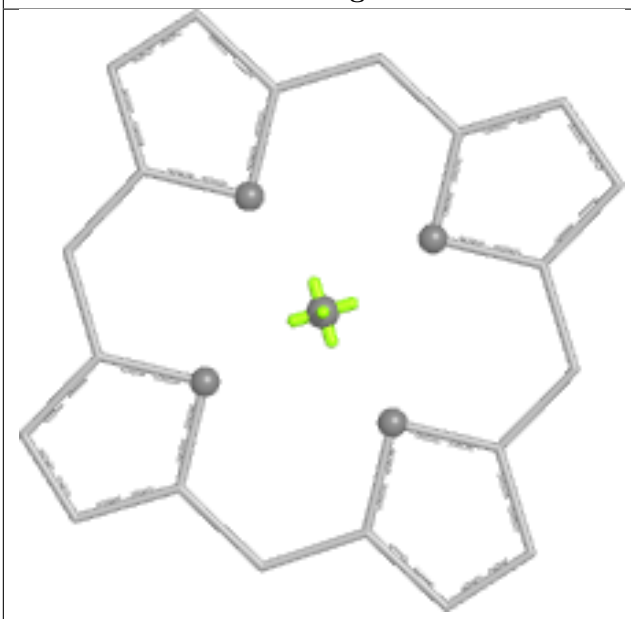
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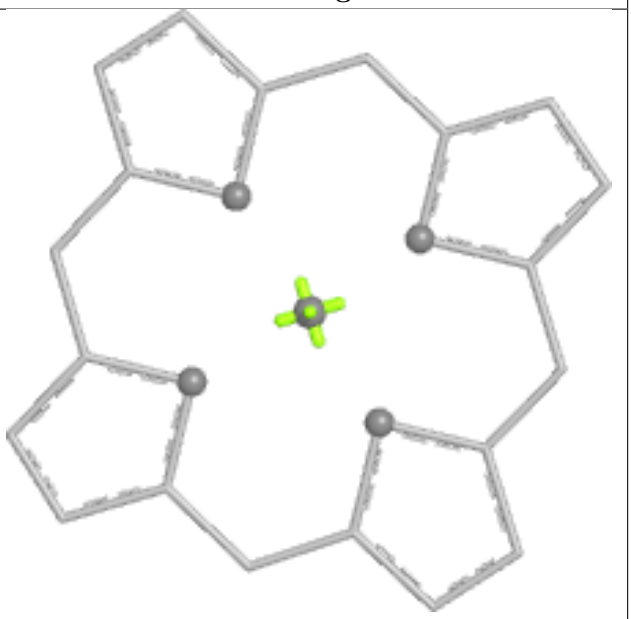
Bond lengths



Bond angles

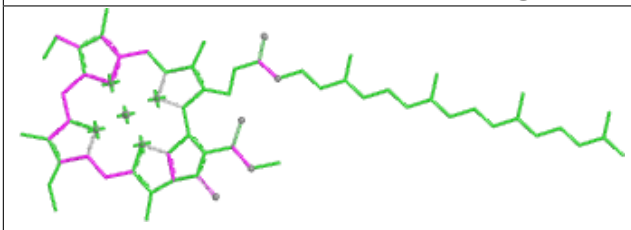


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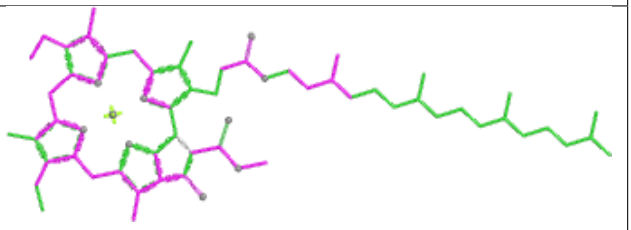


Rings

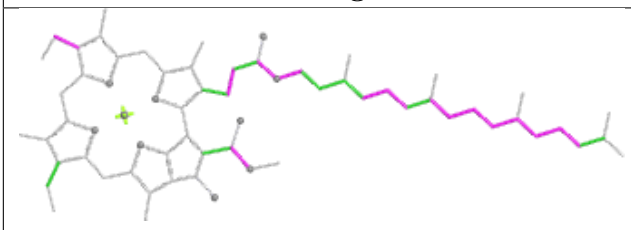
Ligand CLA A 1123



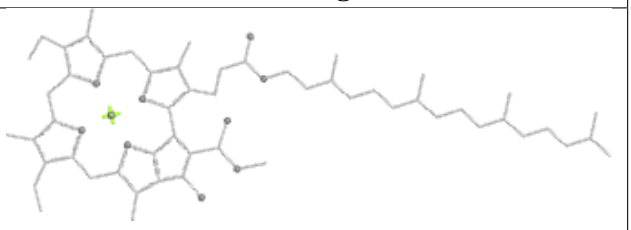
Bond lengths



Bond angles

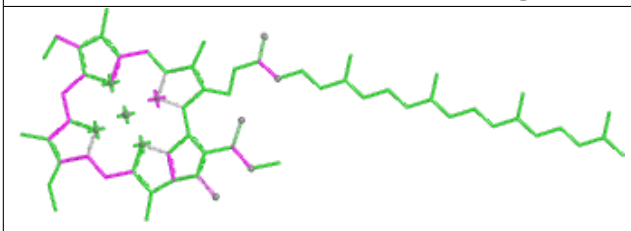


Torsions

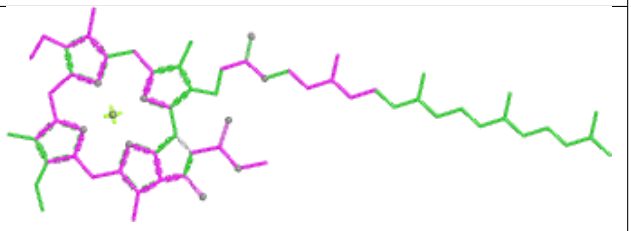


Rings

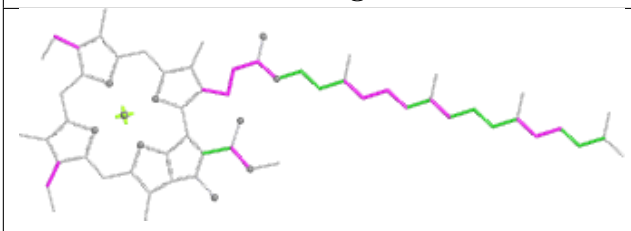
Ligand CLA A 1141



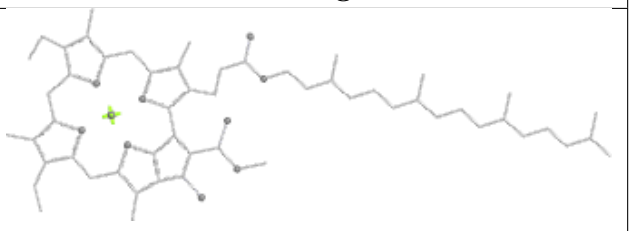
Bond lengths



Bond angles

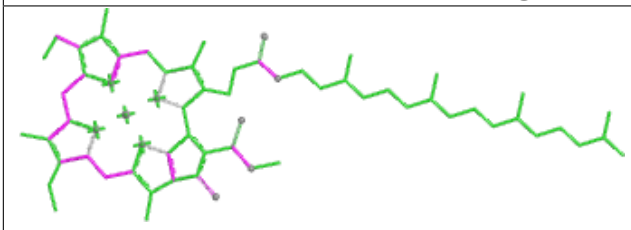


Torsions

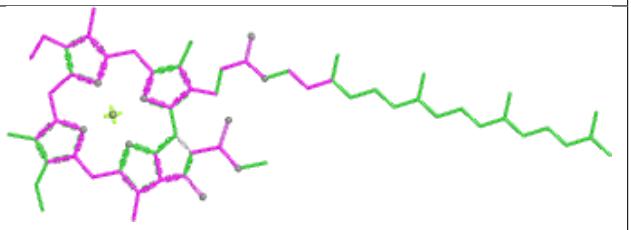


Rings

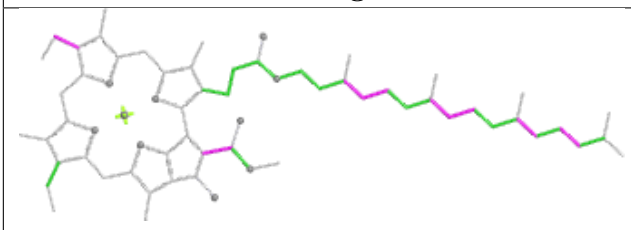
Ligand CLA B 1205



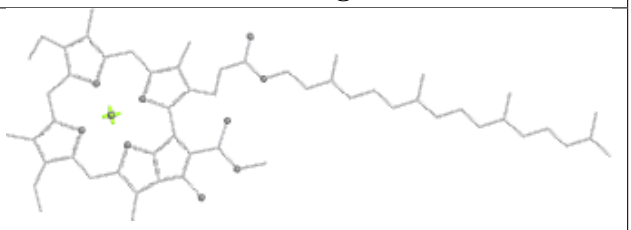
Bond lengths



Bond angles

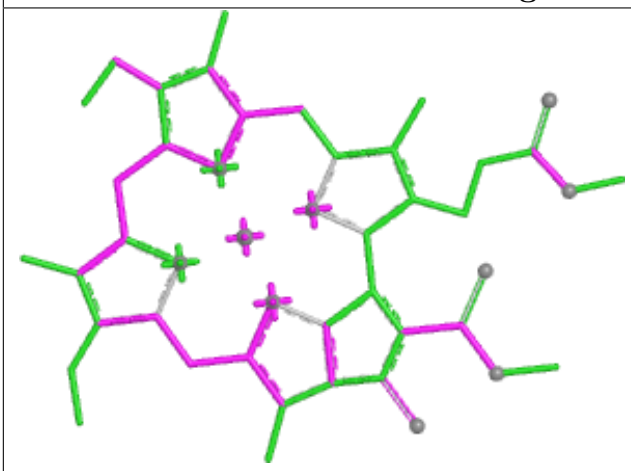


Torsions

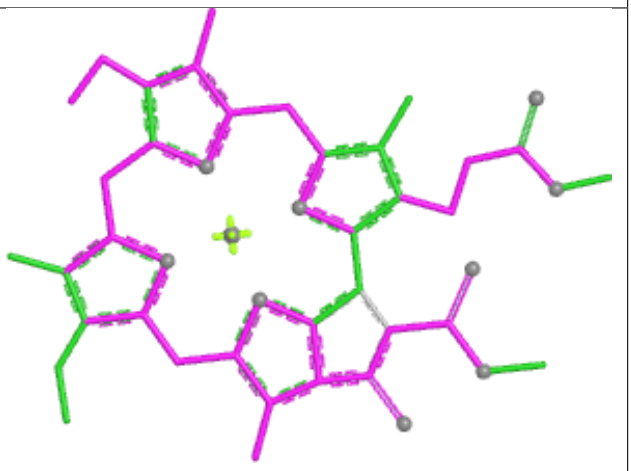


Rings

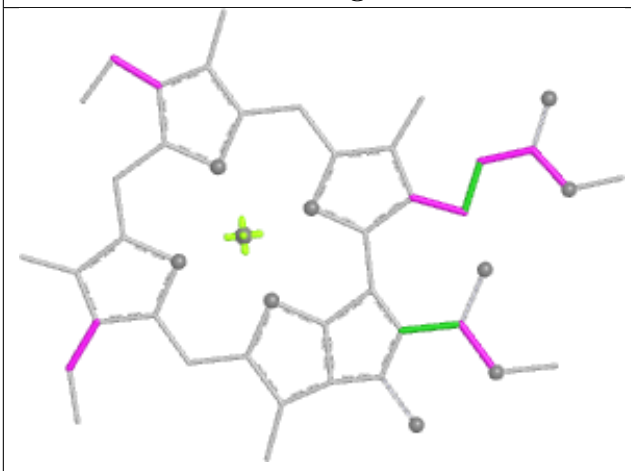
Ligand CLA 4 4015



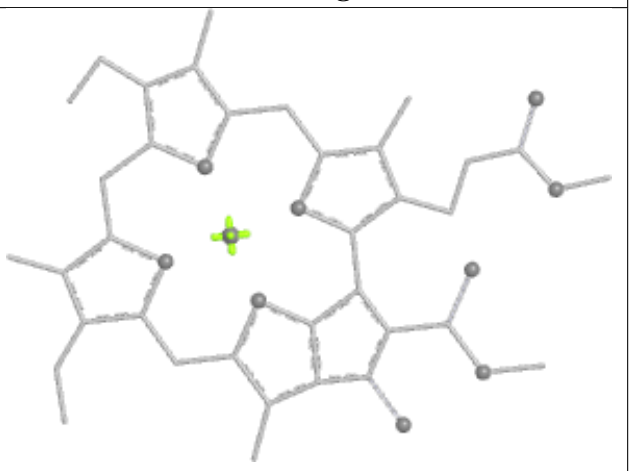
Bond lengths



Bond angles

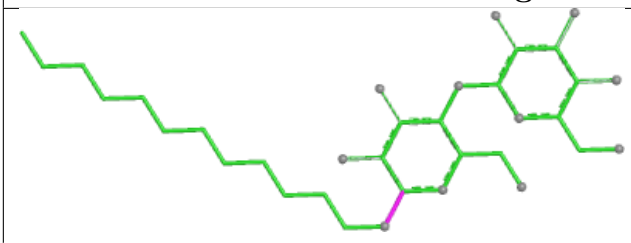


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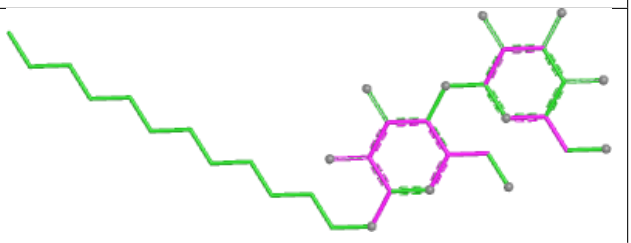


Rings

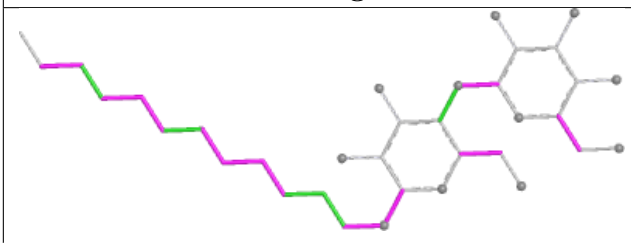
Ligand LMU 4 7019



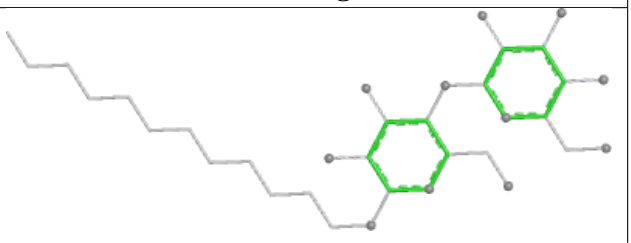
Bond lengths



Bond angles

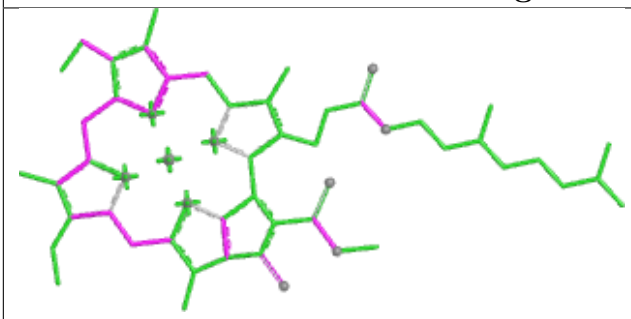


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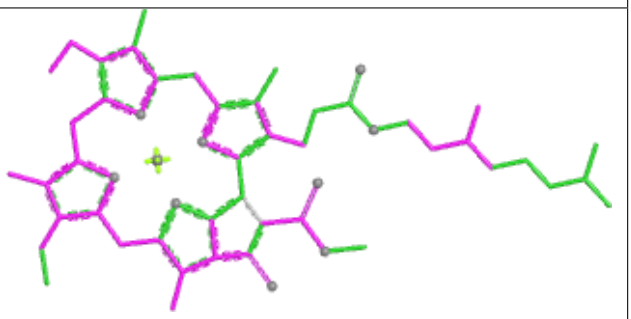


Rings

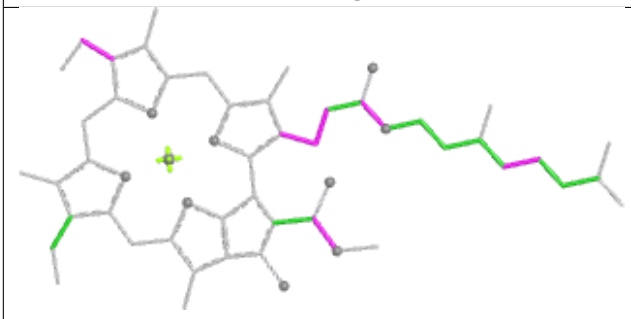
Ligand CLA A 1122



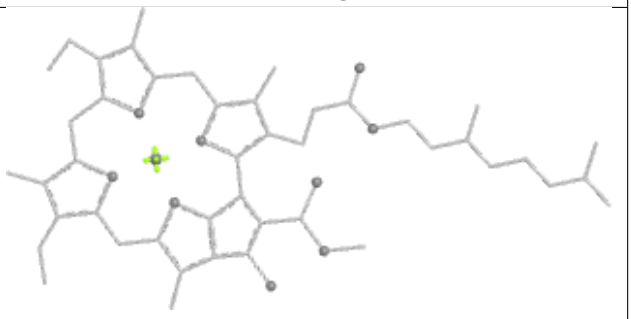
Bond lengths



Bond angles

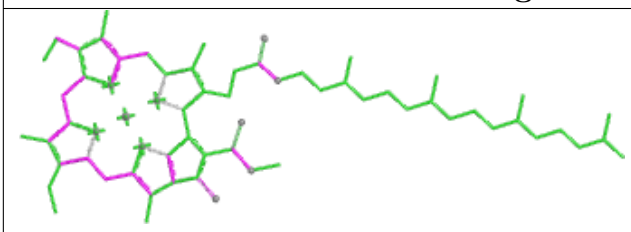


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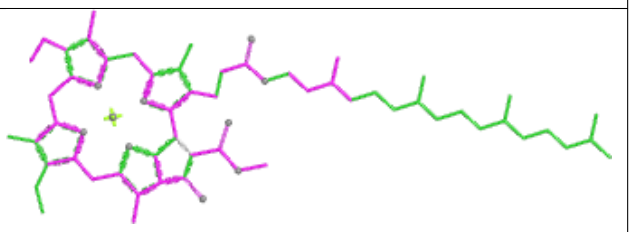


Rings

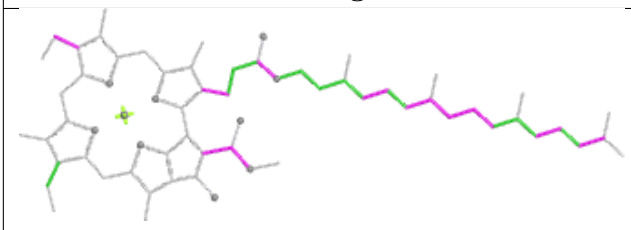
Ligand CLA A 1128



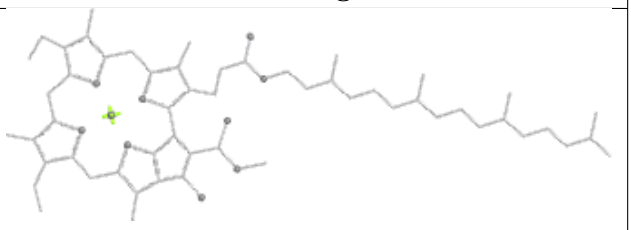
Bond lengths



Bond angles

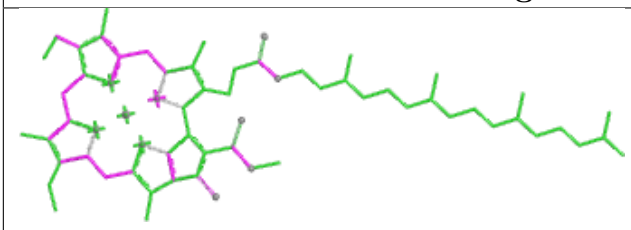


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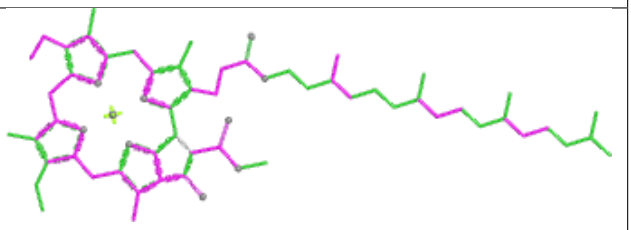


Rings

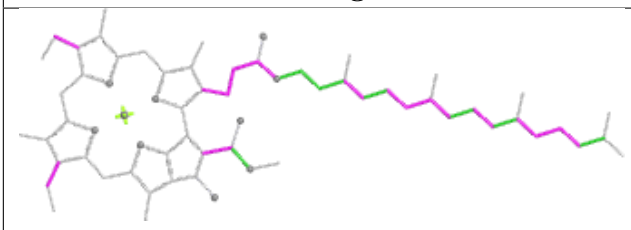
Ligand CLA B 1210



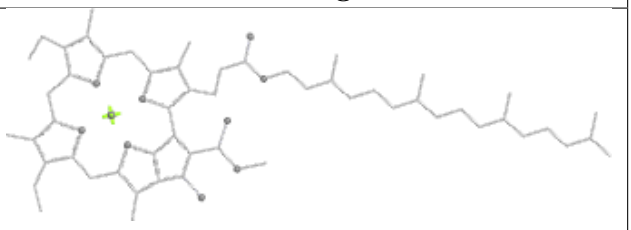
Bond lengths



Bond angles

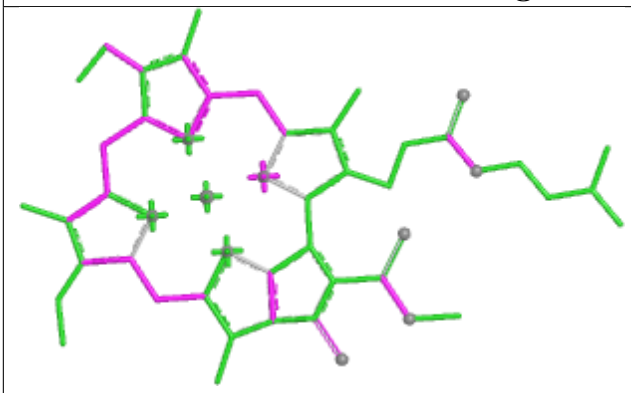


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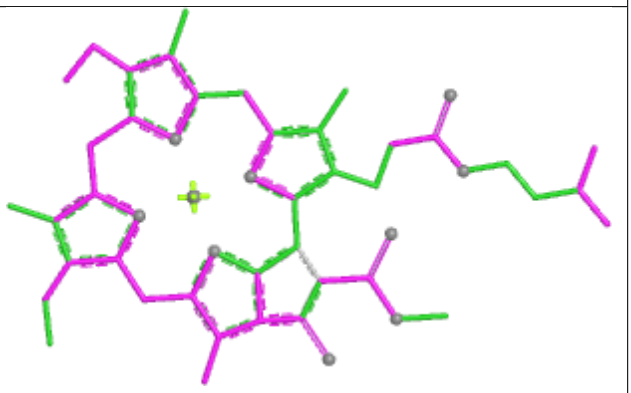


Rings

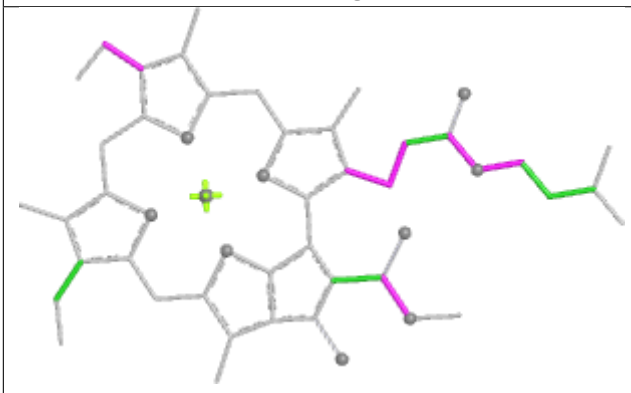
Ligand CLA A 1151



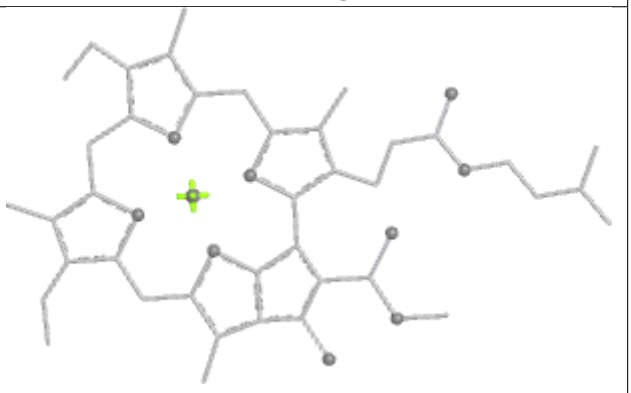
Bond lengths



Bond angles

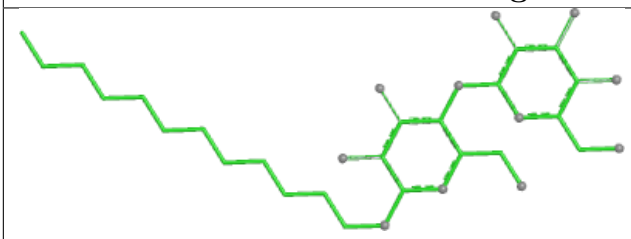


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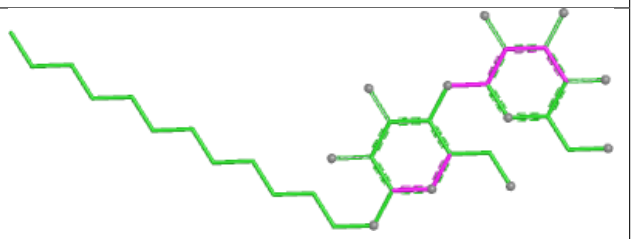


Rings

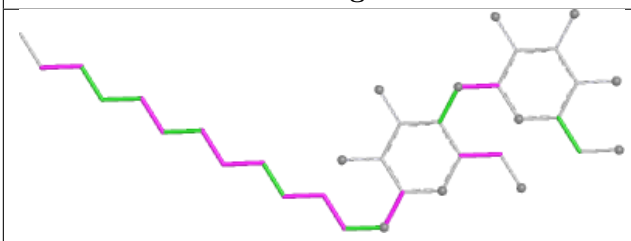
Ligand LMU K 7041



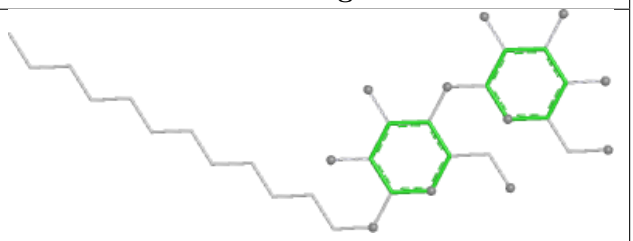
Bond lengths



Bond angles

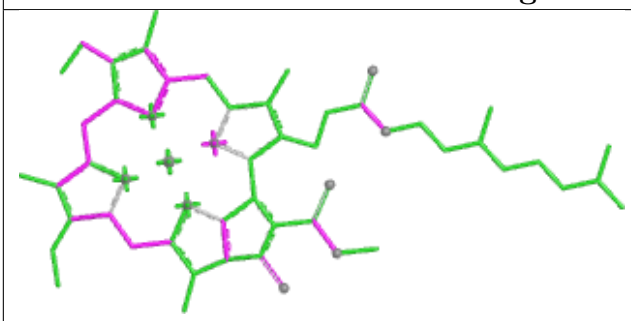


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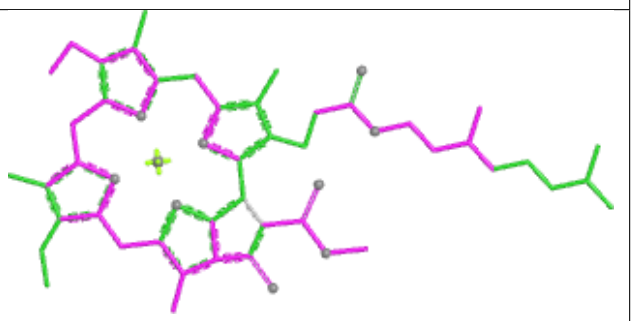


Rings

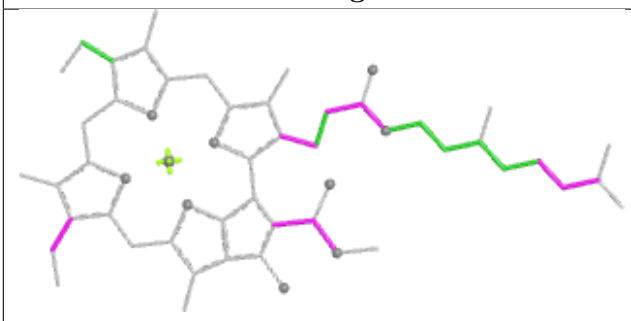
Ligand CLA 4 4003



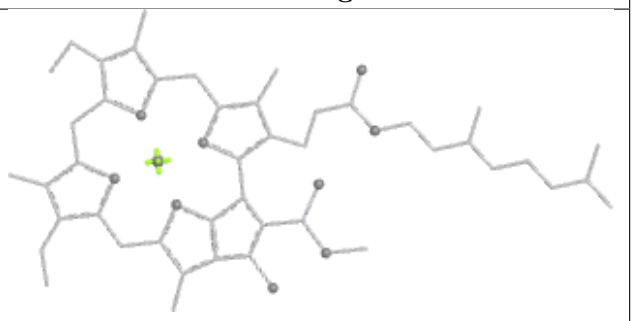
Bond lengths



Bond angles

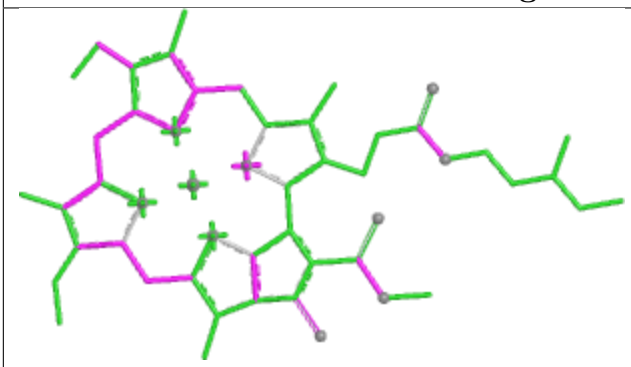


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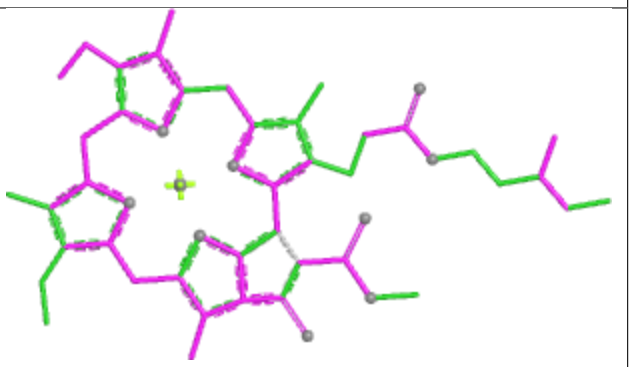


Rings

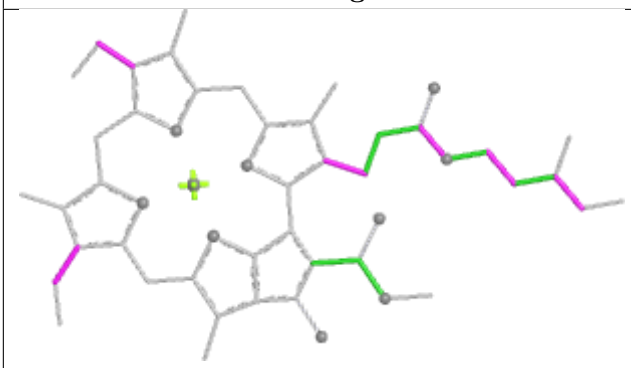
Ligand CLA 2 2001



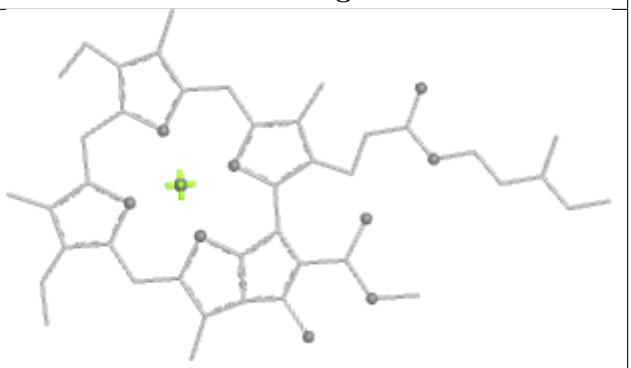
Bond lengths



Bond angles

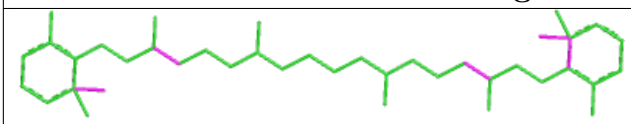


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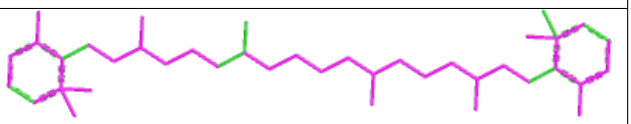


Rings

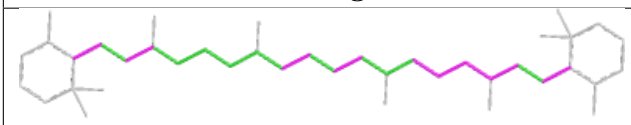
Ligand BCR B 6017



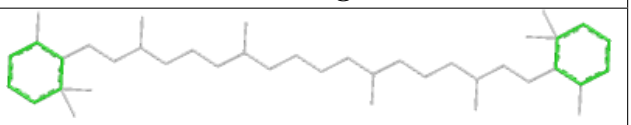
Bond lengths



Bond angles

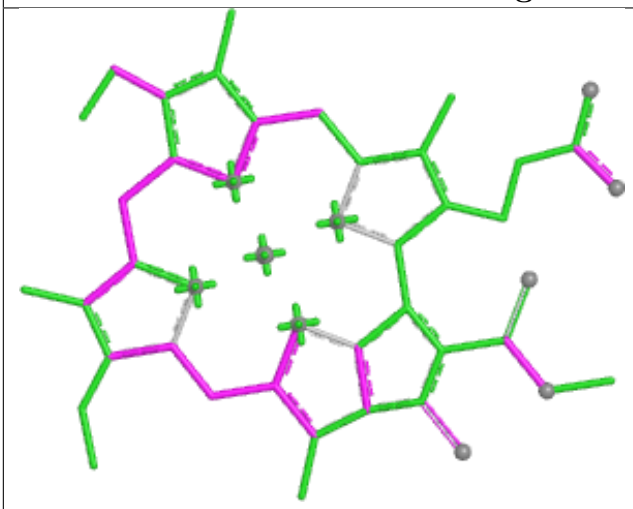


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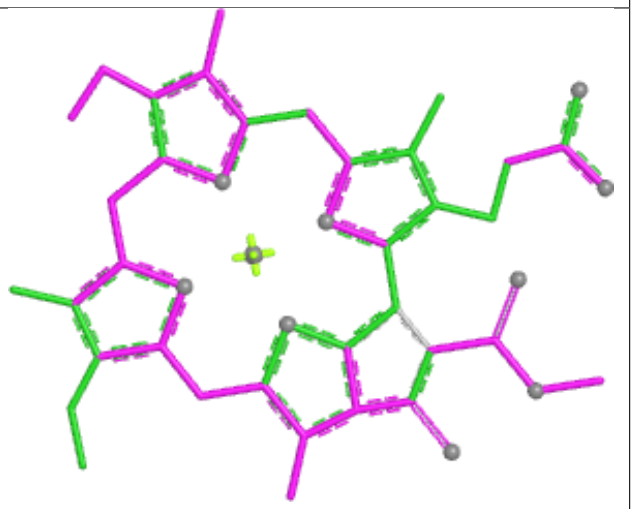


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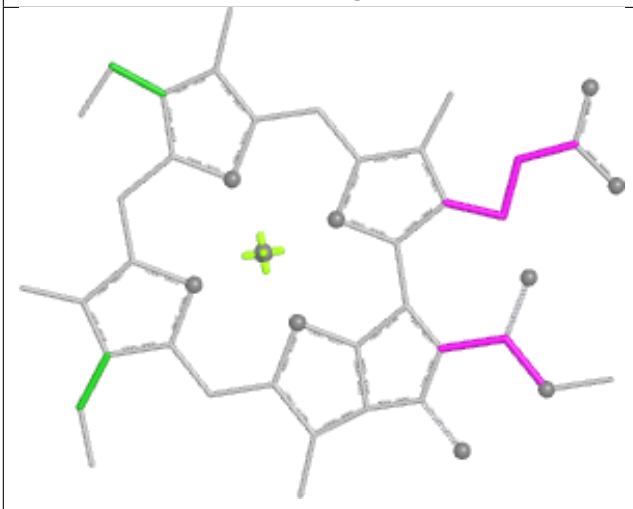
Ligand CLA B 1231



Bond lengths



Bond angles

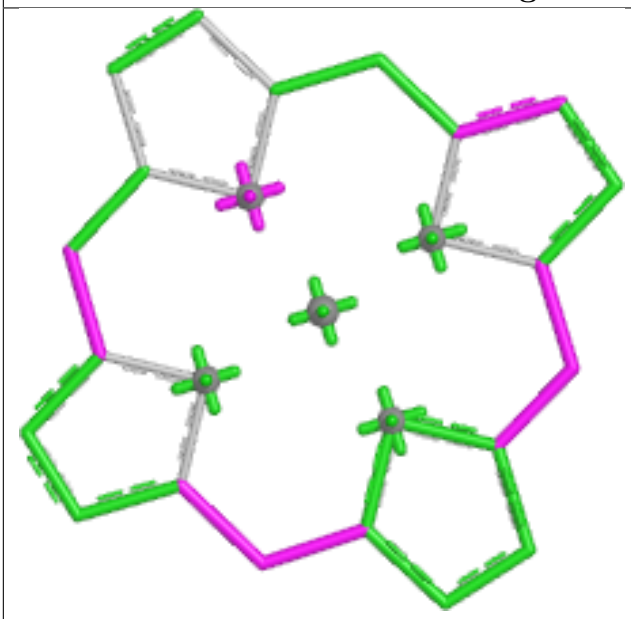


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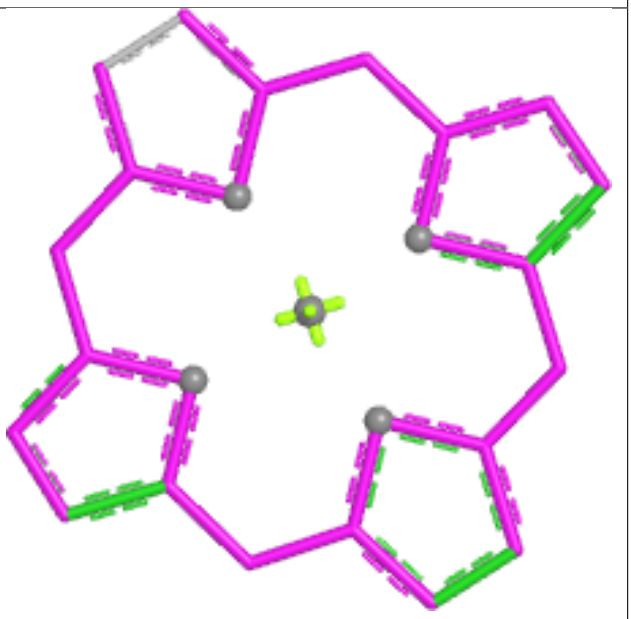


Rings

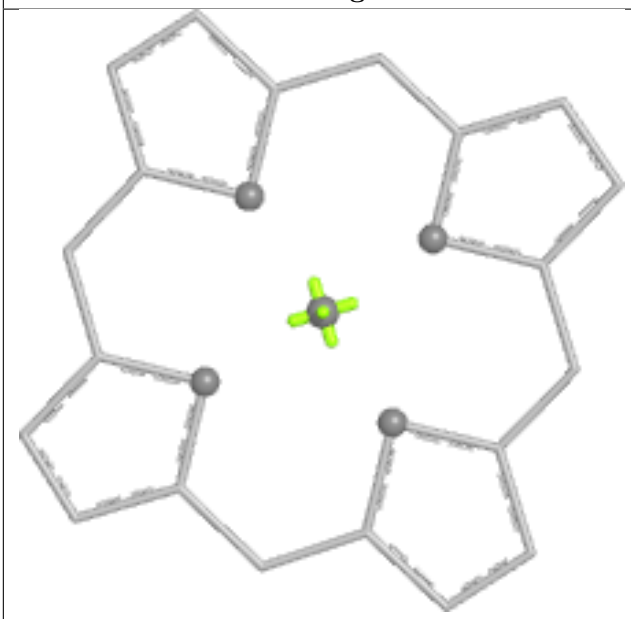
Ligand CLA 1 1310



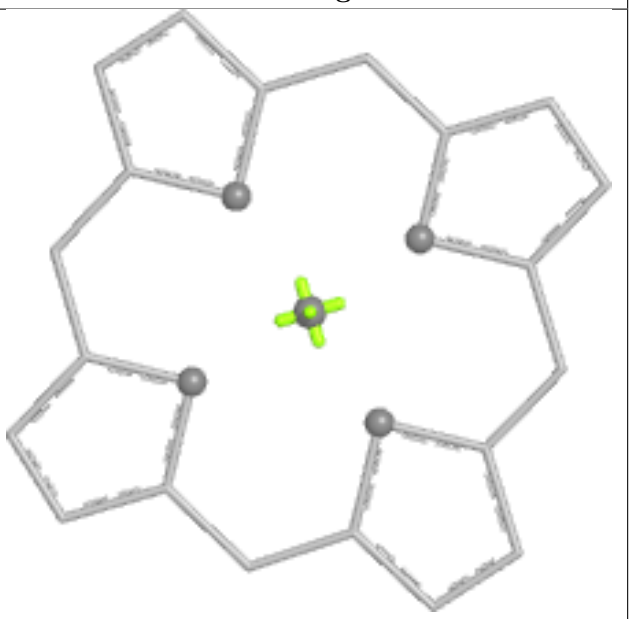
Bond lengths



Bond angles

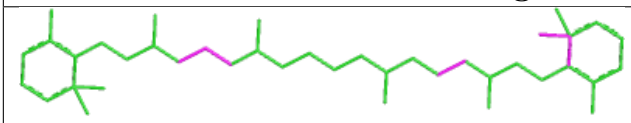


Torsions

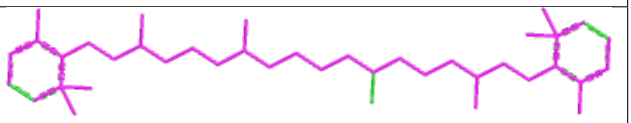


Rings

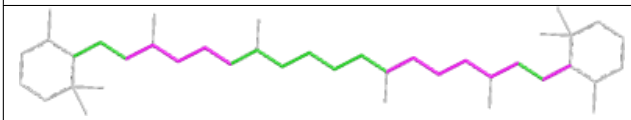
Ligand BCR A 6002



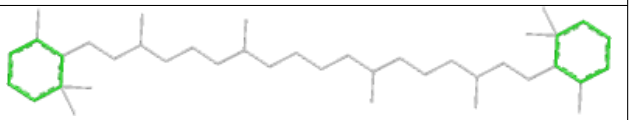
Bond lengths



Bond angles

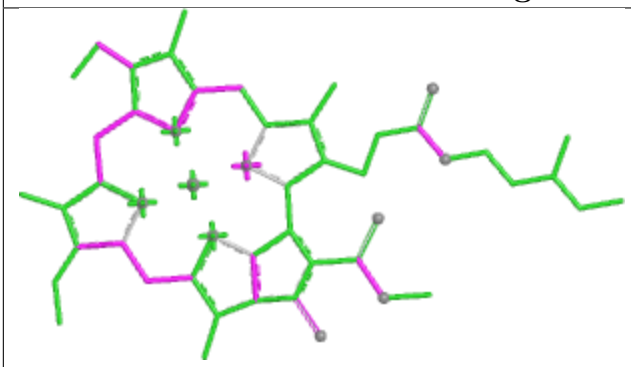


Torsions

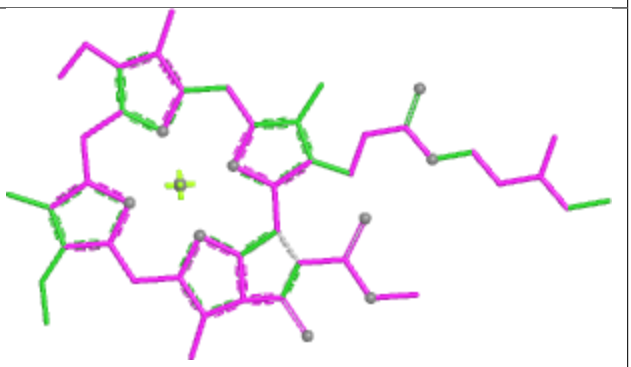


Rings

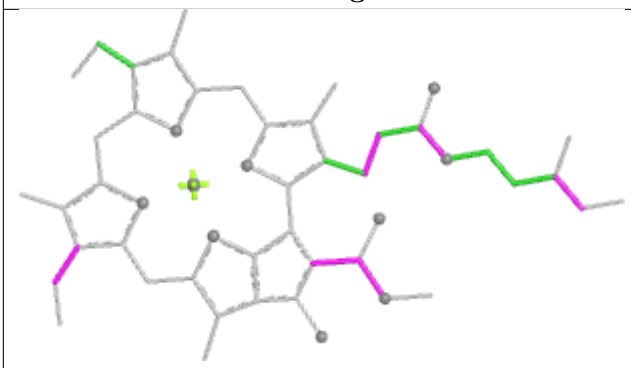
Ligand CLA G 1242



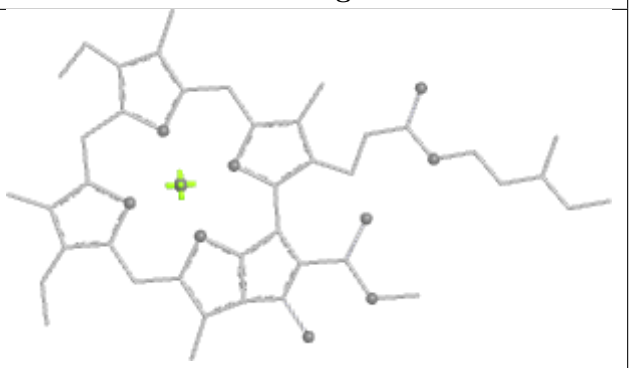
Bond lengths



Bond angles

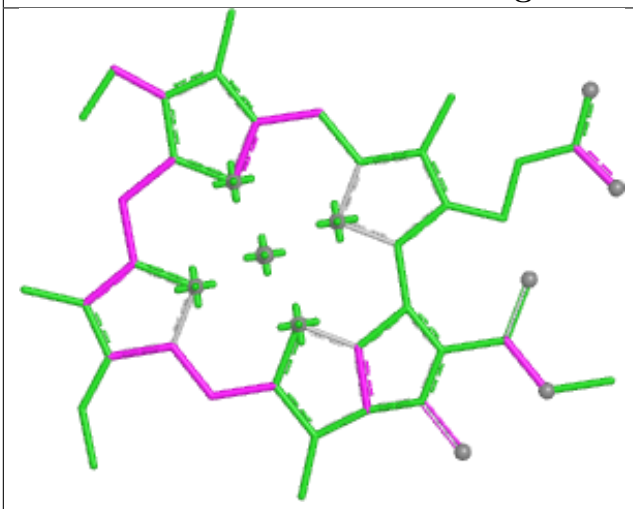


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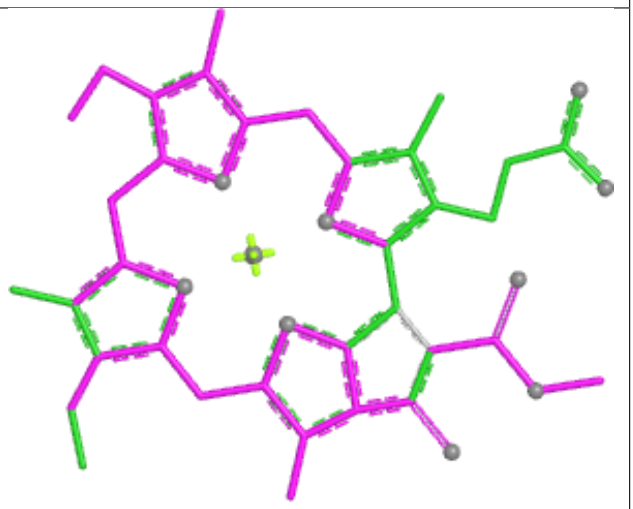


Rings

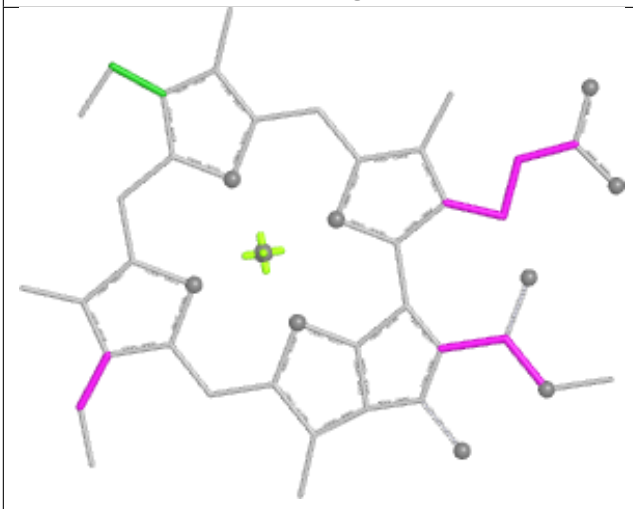
Ligand CLA A 1112



Bond lengths



Bond angles

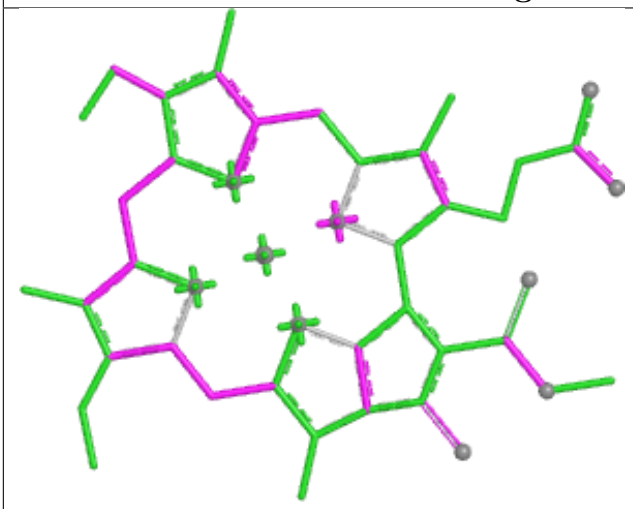


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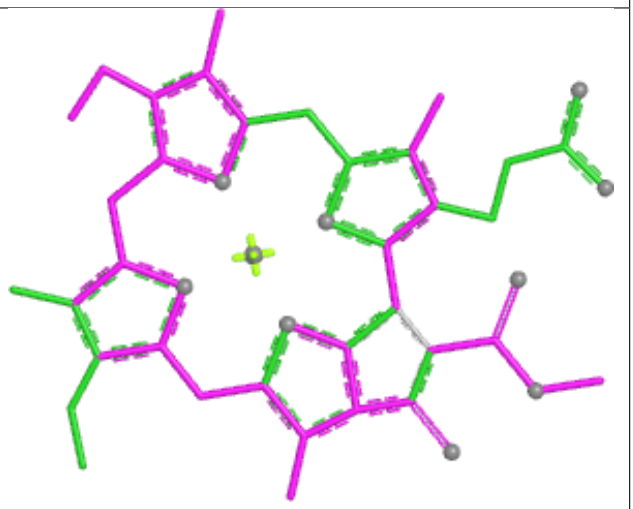


Rings

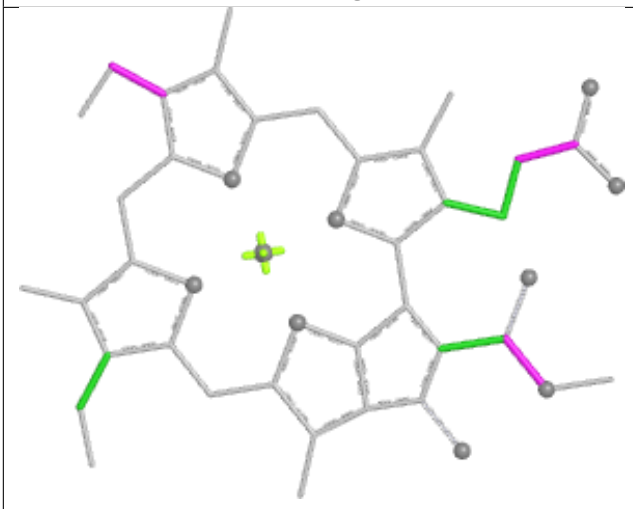
Ligand CLA A 1108



Bond lengths



Bond angles

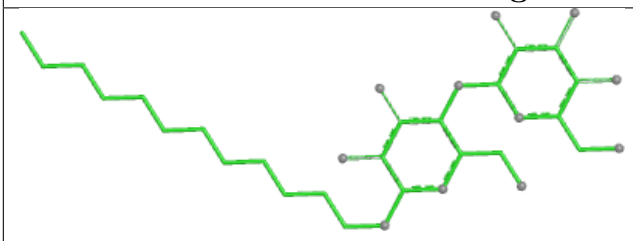


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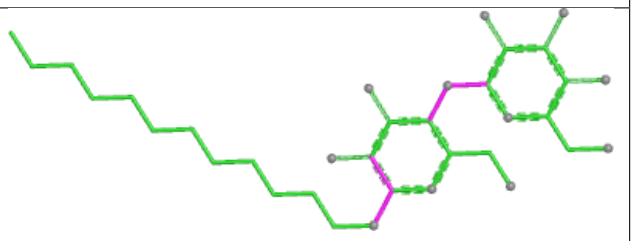


Rings

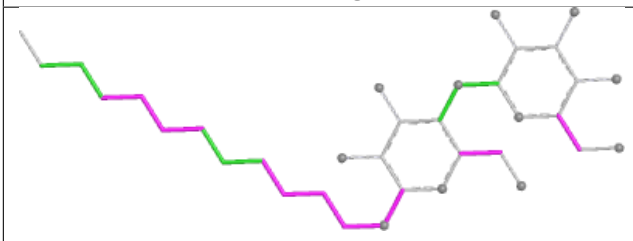
Ligand LMU H 7028



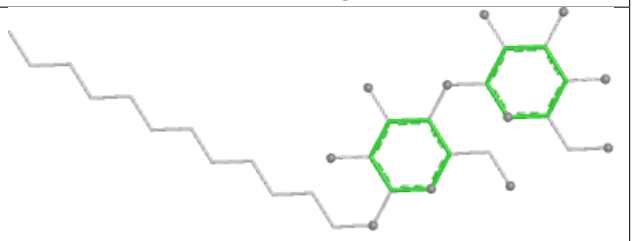
Bond lengths



Bond angles

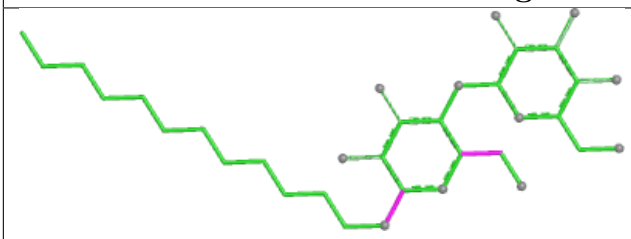


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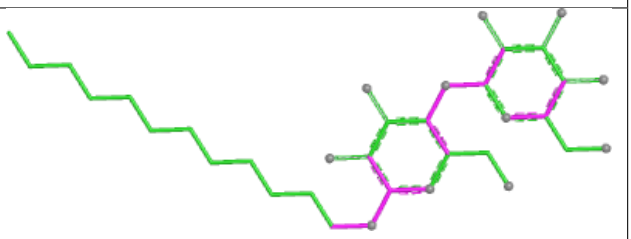


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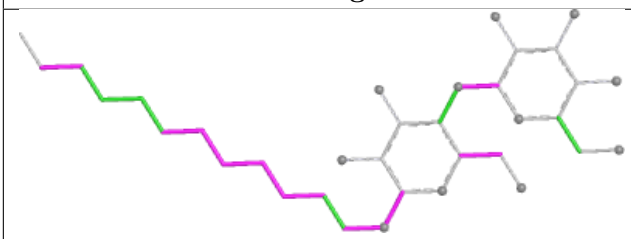
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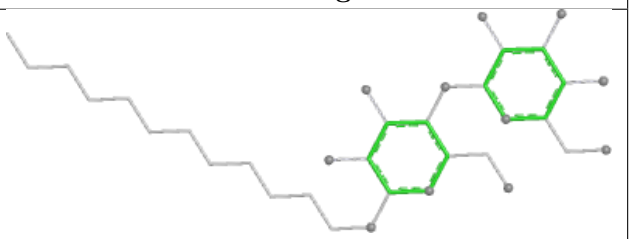
Bond lengths



Bond angles

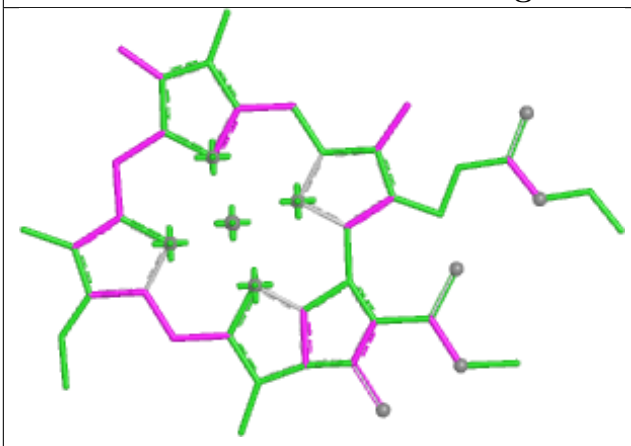


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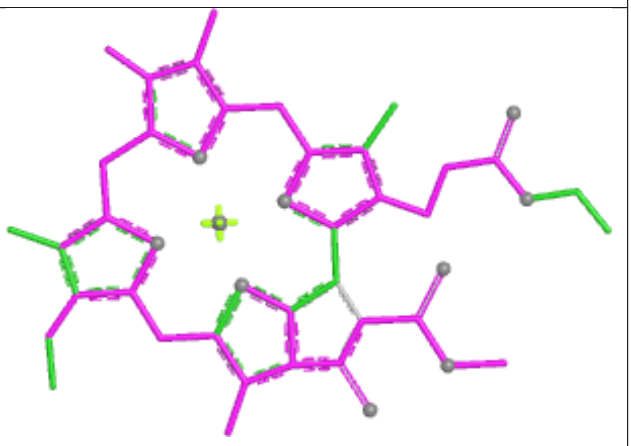


Rings

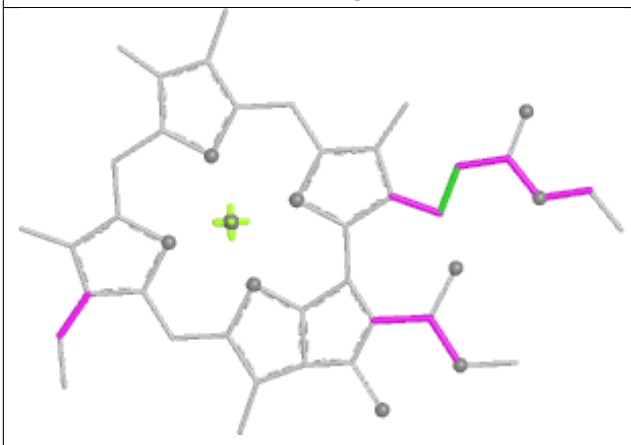
Ligand CLA A 1149



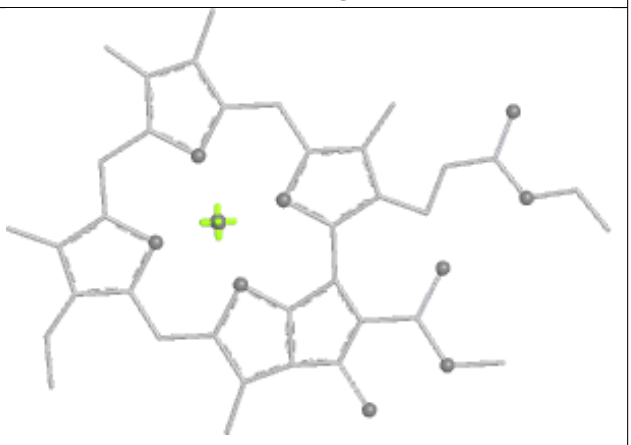
Bond lengths



Bond angles

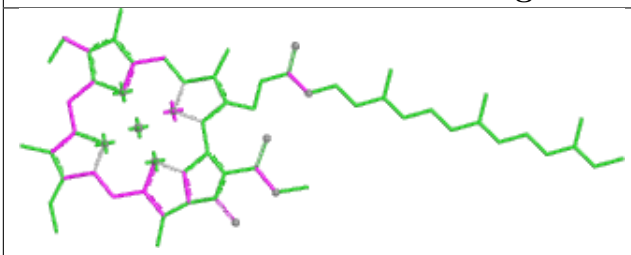


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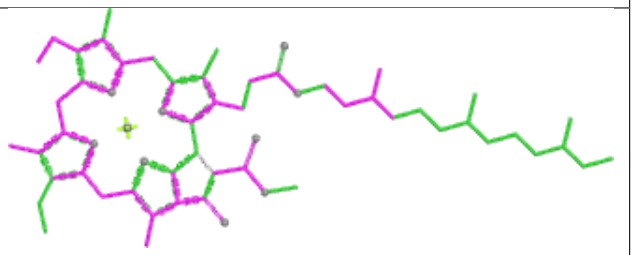


Rings

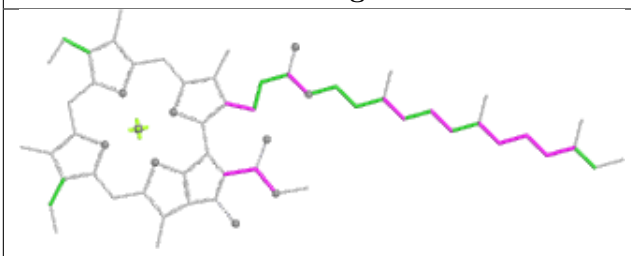
Ligand CLA B 1216



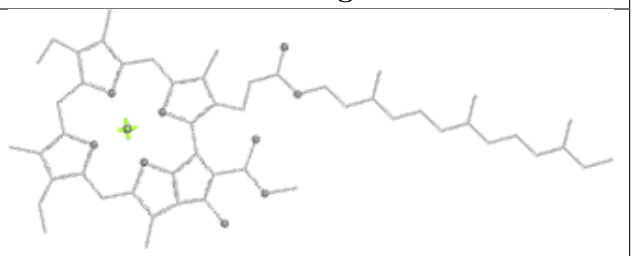
Bond lengths



Bond angles

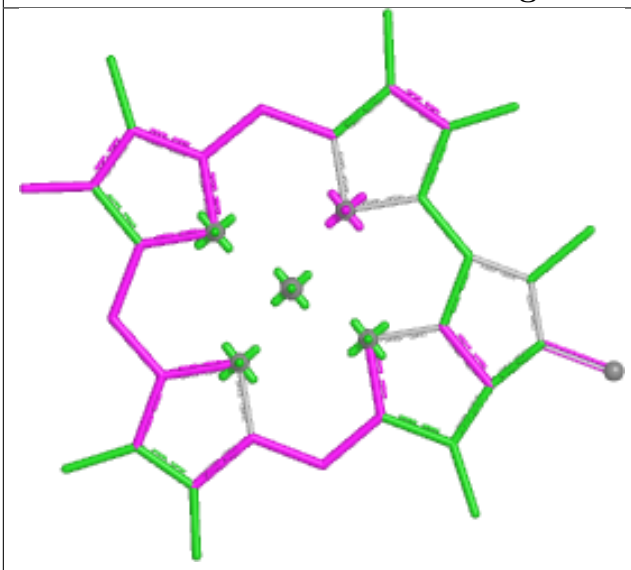


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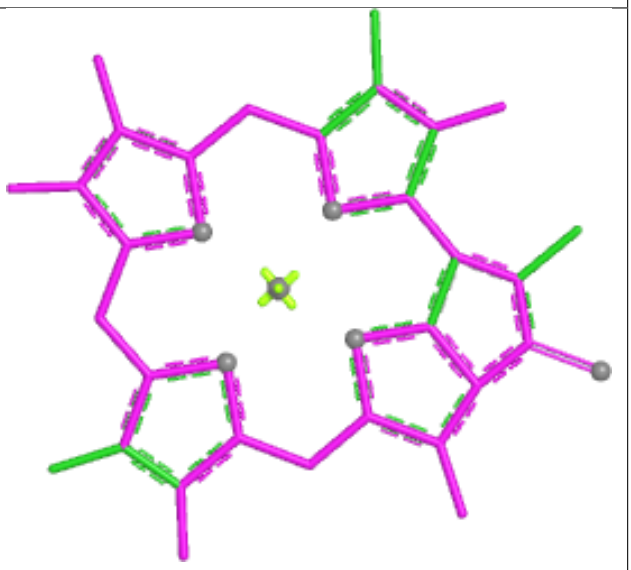


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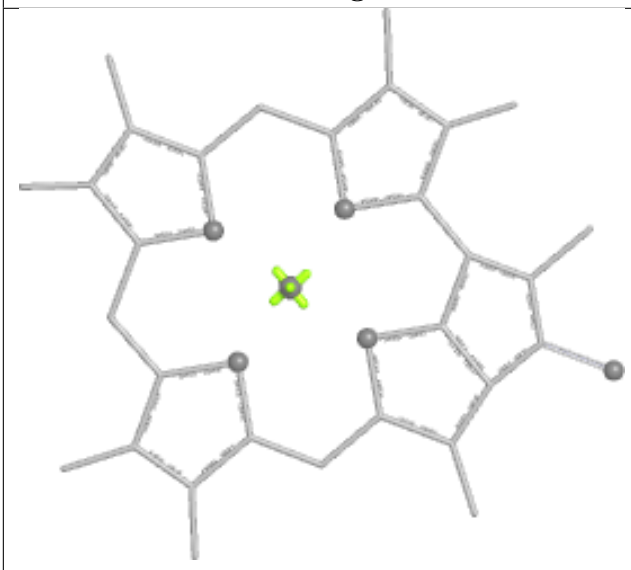
Ligand CLA 1 1011



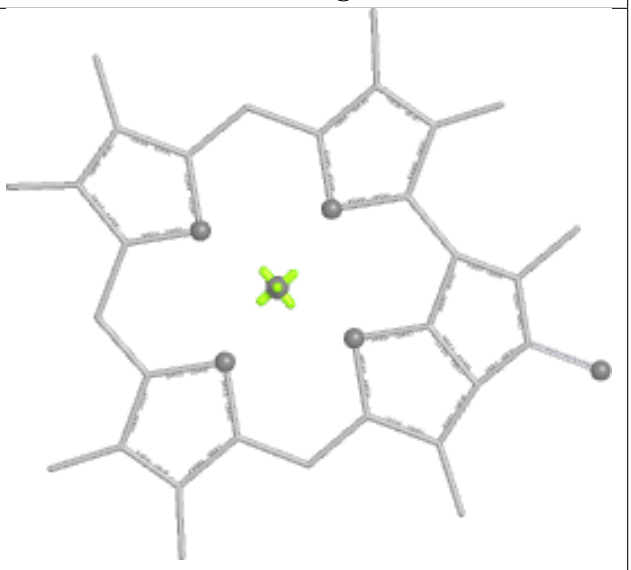
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Bond angles

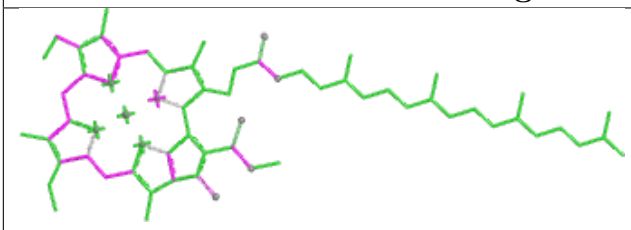


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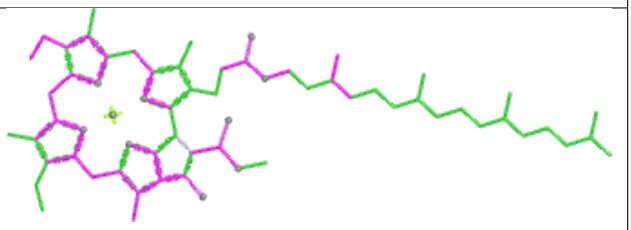


Rings

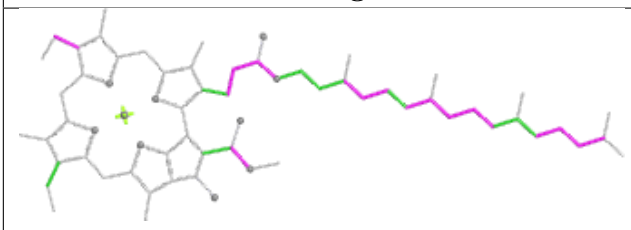
Ligand CLA A 1131



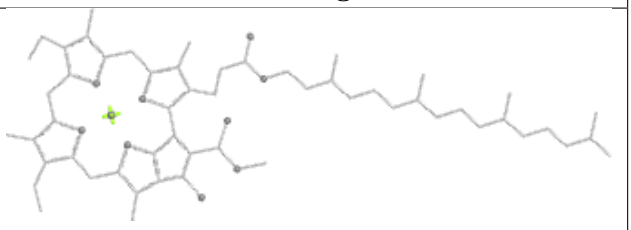
Bond lengths



Bond angles

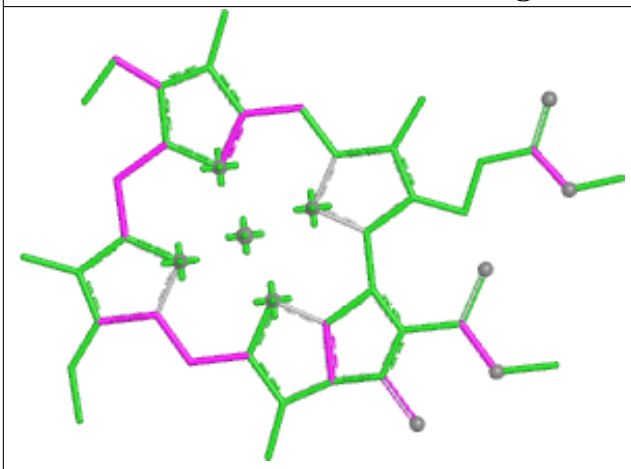


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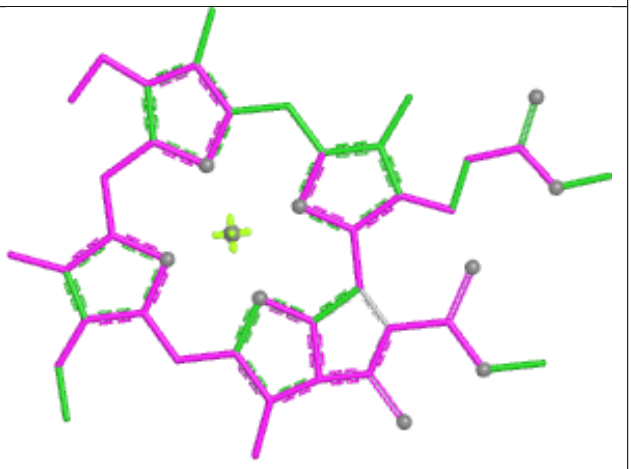


Rings

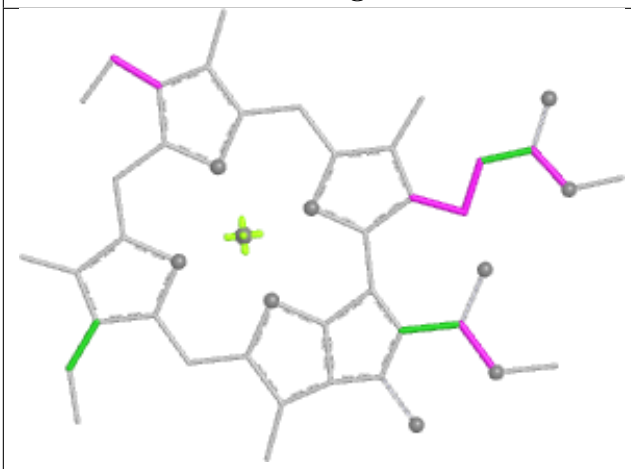
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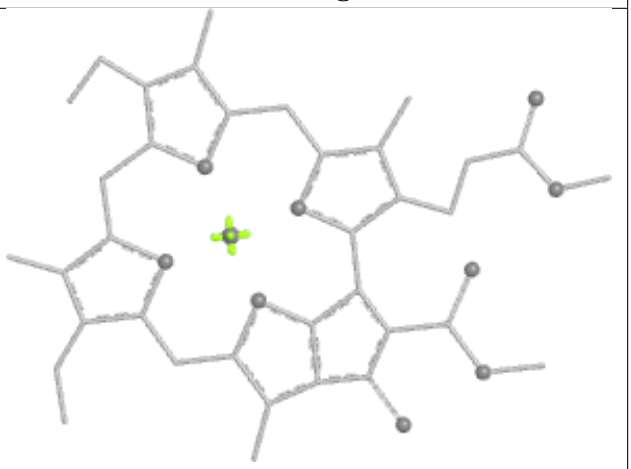
Bond lengths



Bond angles

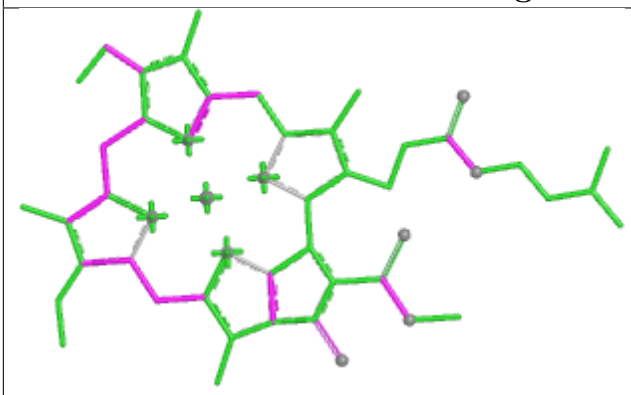


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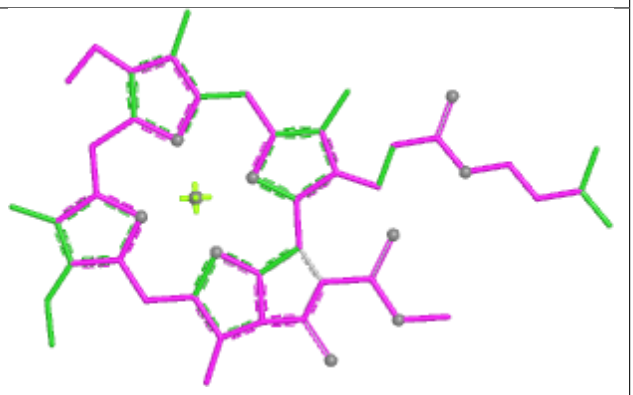


Rings

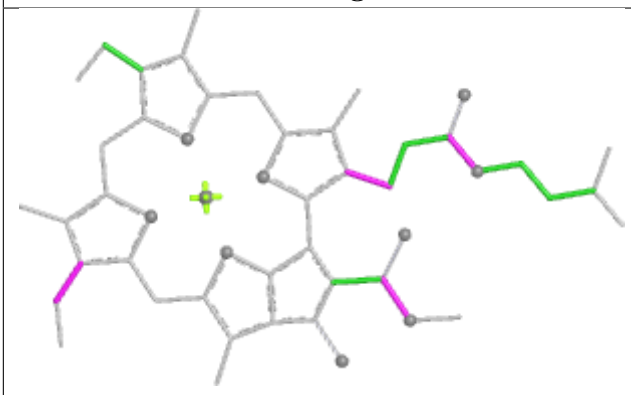
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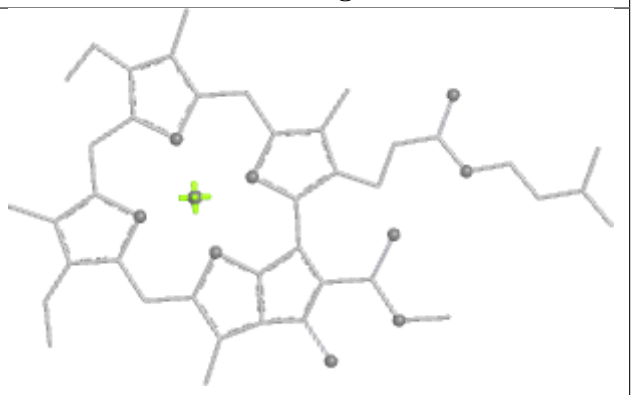
Bond lengths



Bond angles

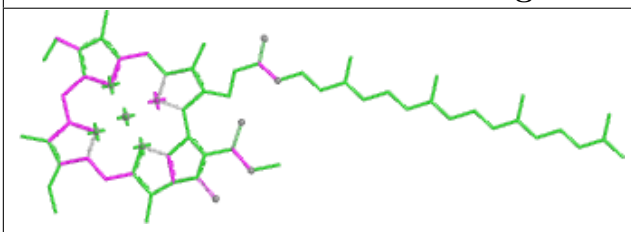


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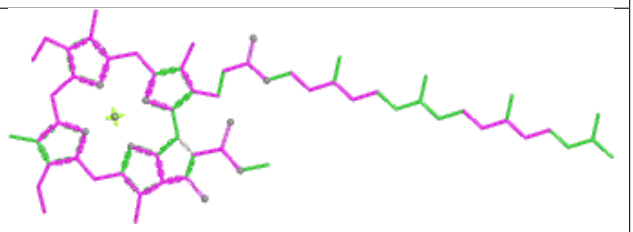


Rings

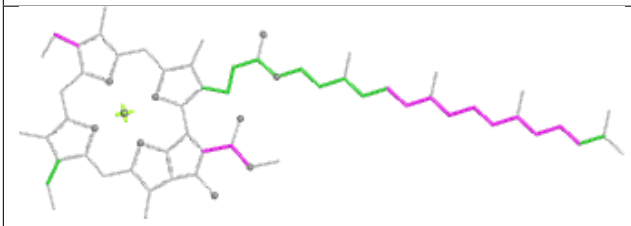
Ligand CLA B 1203



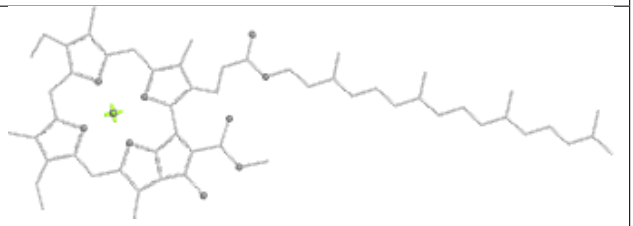
Bond lengths



Bond angles

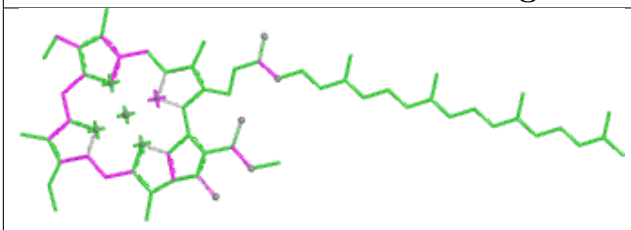


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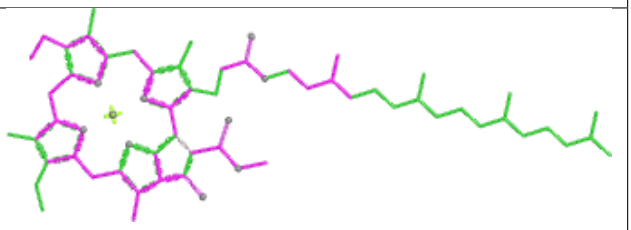


Rings

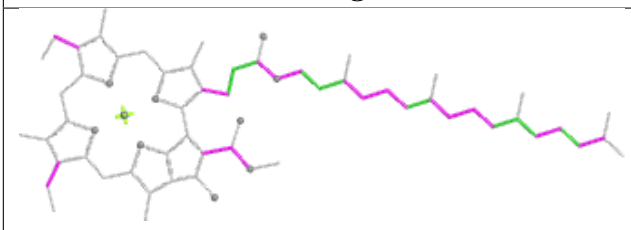
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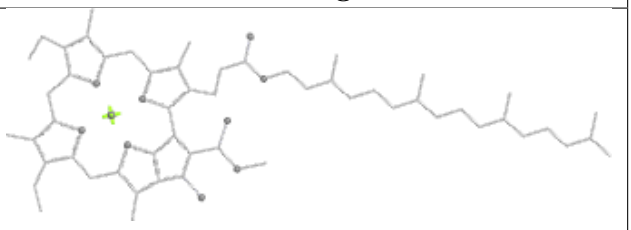
Bond lengths



Bond angles

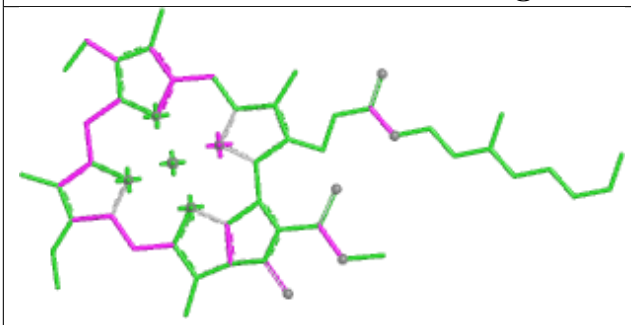


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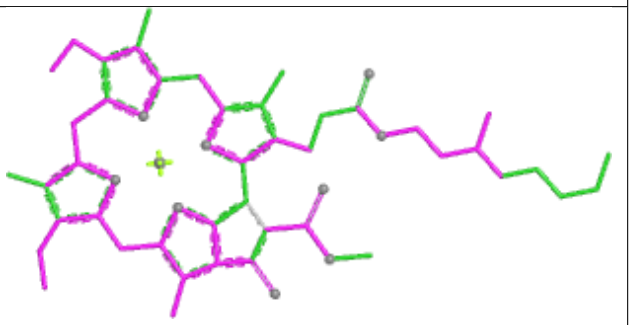


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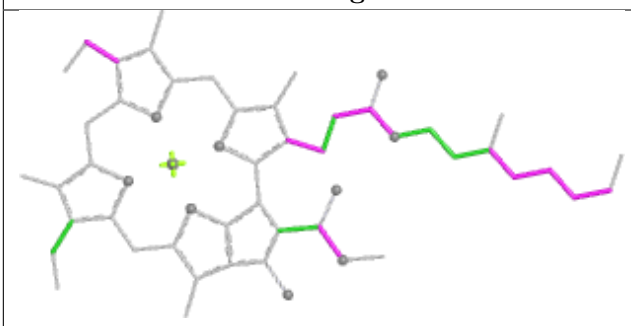
Ligand CLA A 1111



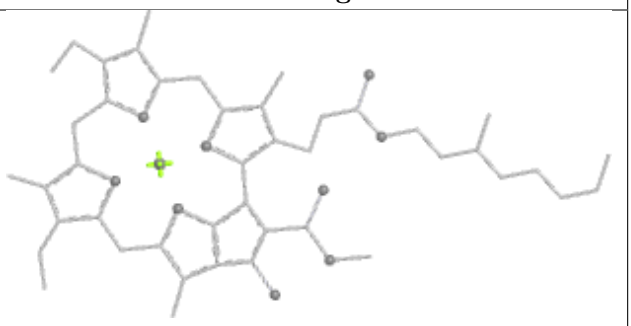
Bond lengths



Bond angles

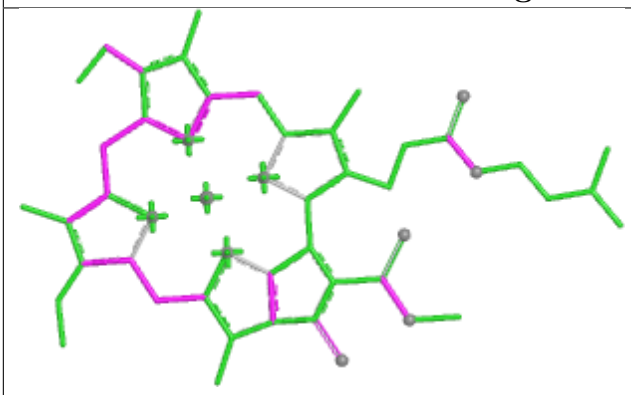


Torsions

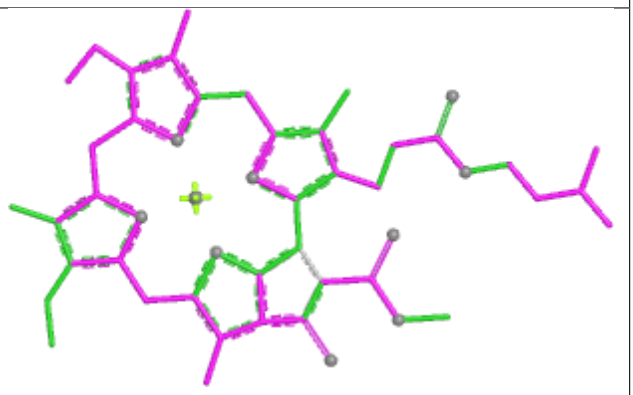


Rings

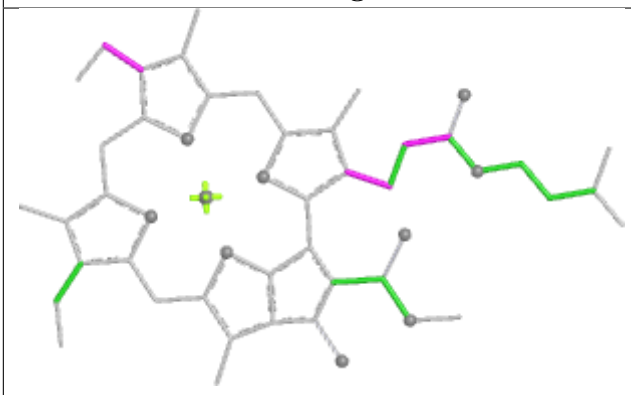
Ligand CLA A 1101



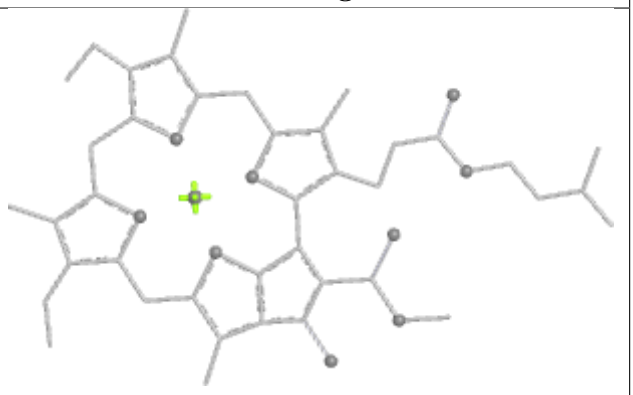
Bond lengths



Bond angles

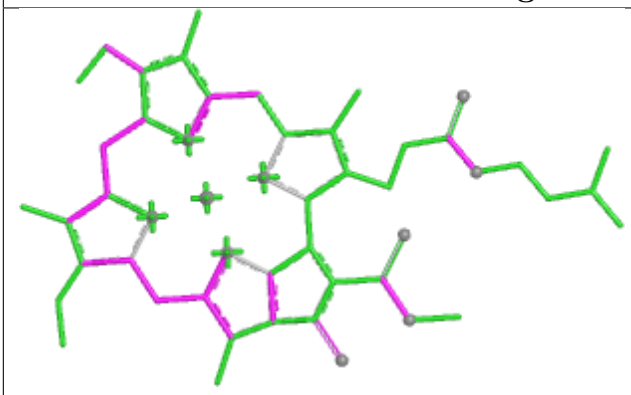


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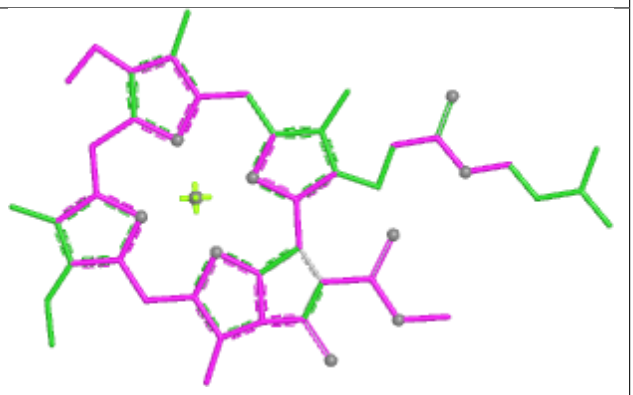


Rings

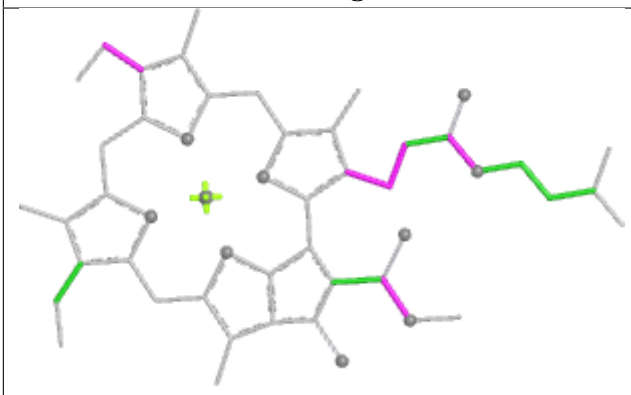
Ligand CLA L 1501



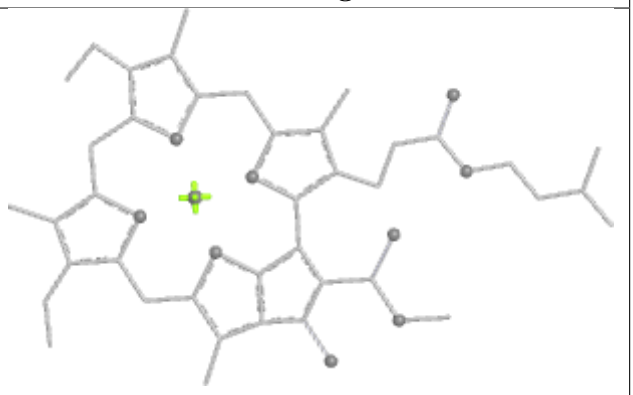
Bond lengths



Bond angles

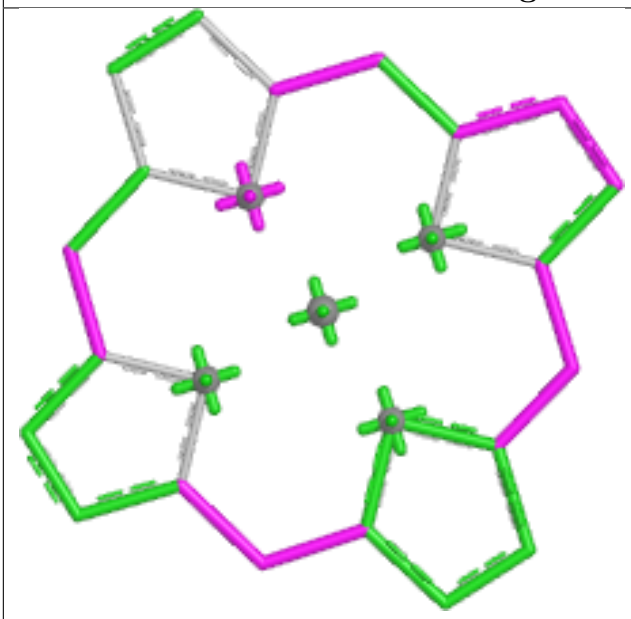


Torsions

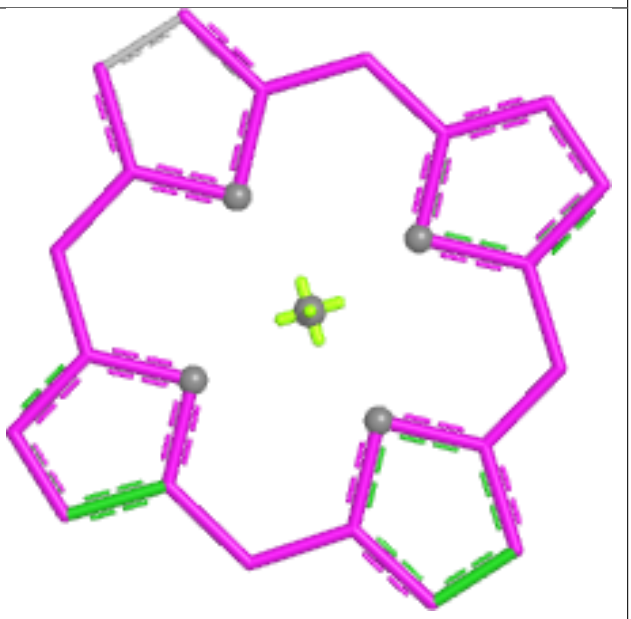


Rings

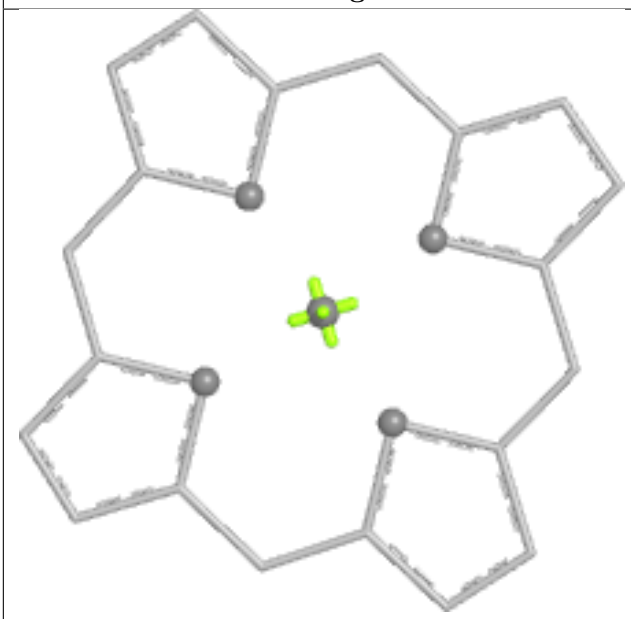
Ligand CLA 3 3001



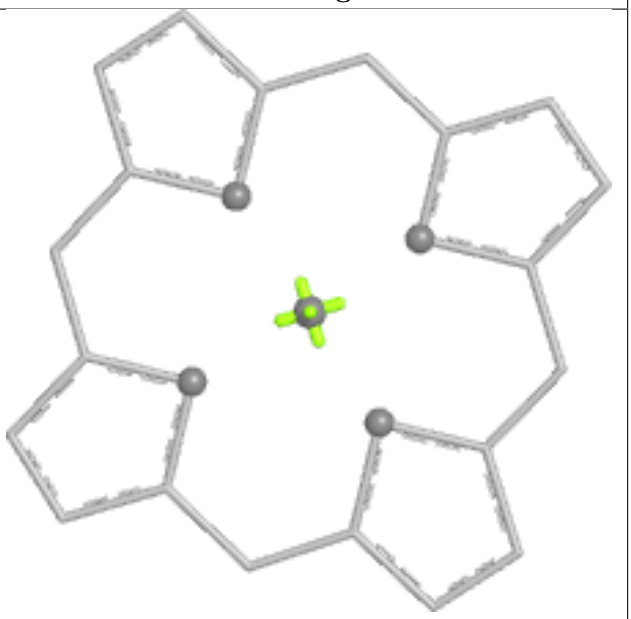
Bond lengths



Bond angles

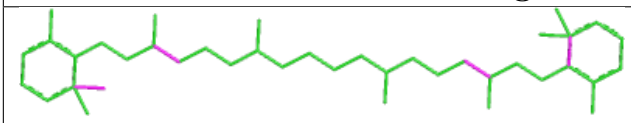


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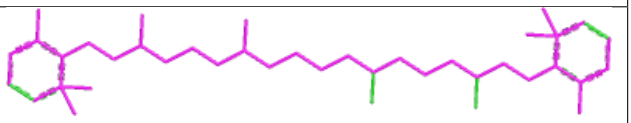


Rings

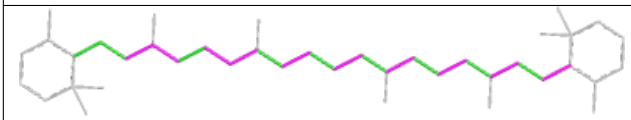
Ligand BCR B 6004



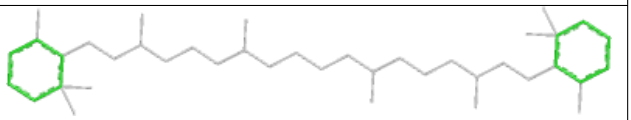
Bond lengths



Bond angles

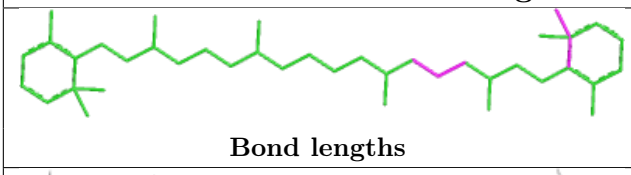


Torsions

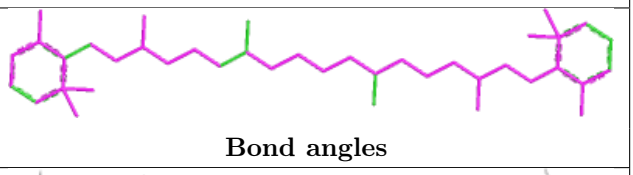


Rings

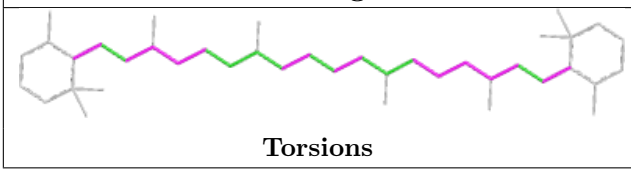
Ligand BCR F 6014



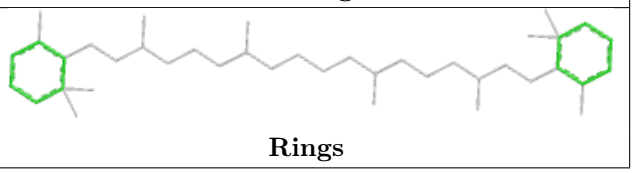
Bond lengths



Bond angles

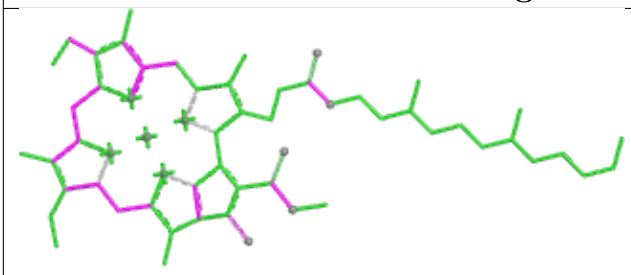


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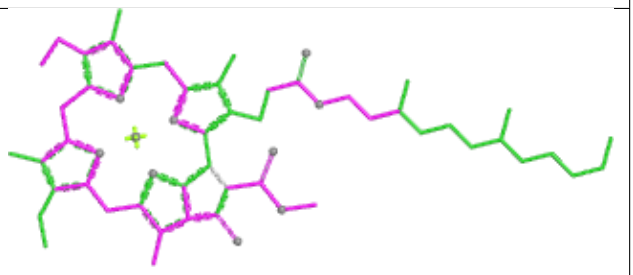


Rings

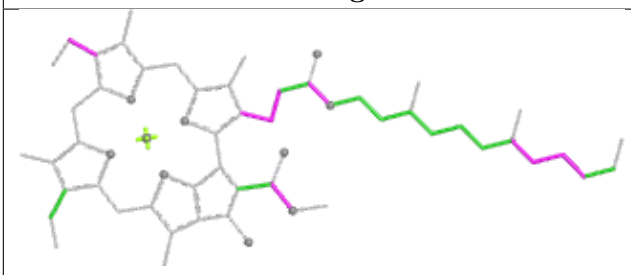
Ligand CLA B 1214



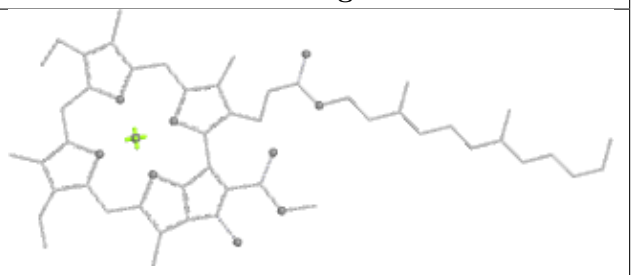
Bond lengths



Bond angles

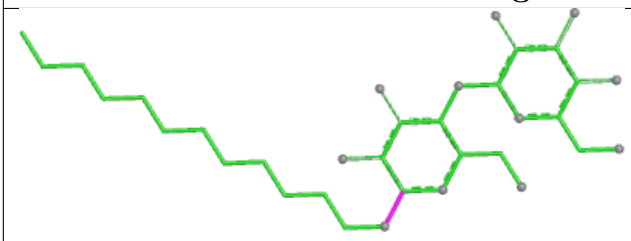


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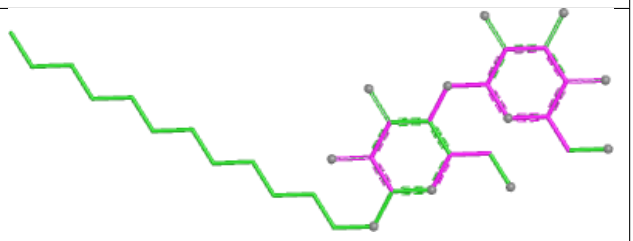


Rings

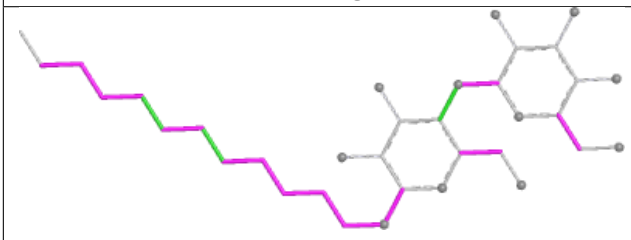
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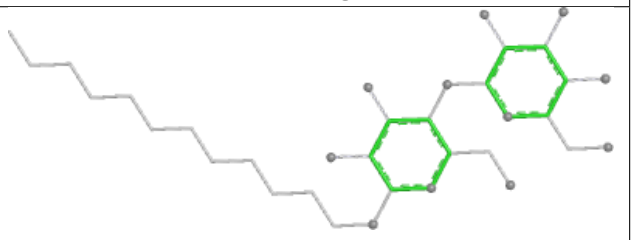
Bond lengths



Bond angles

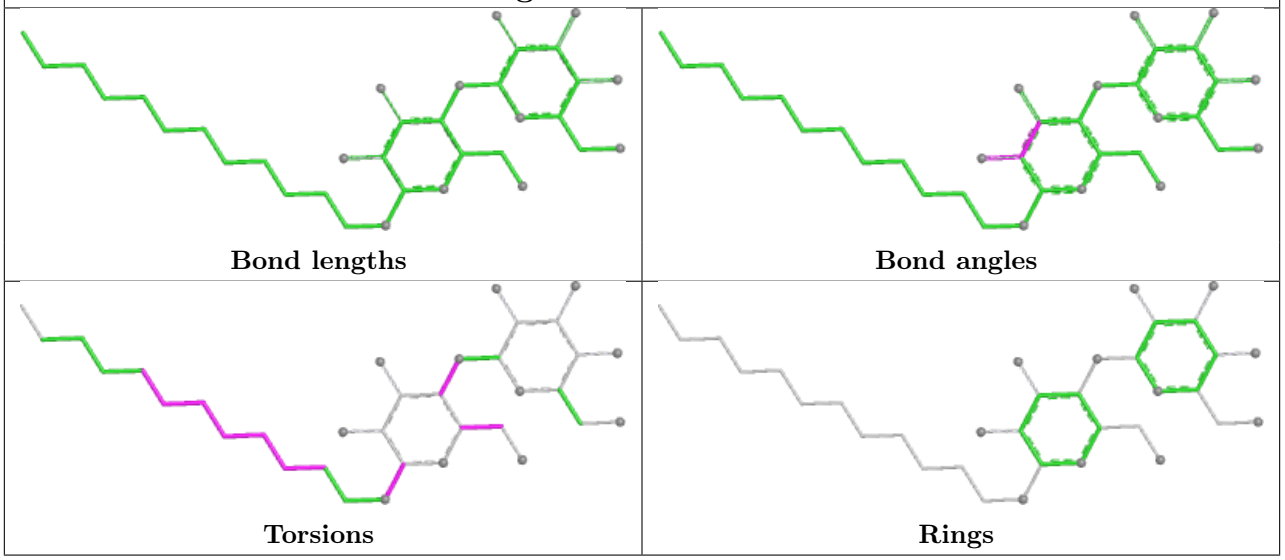


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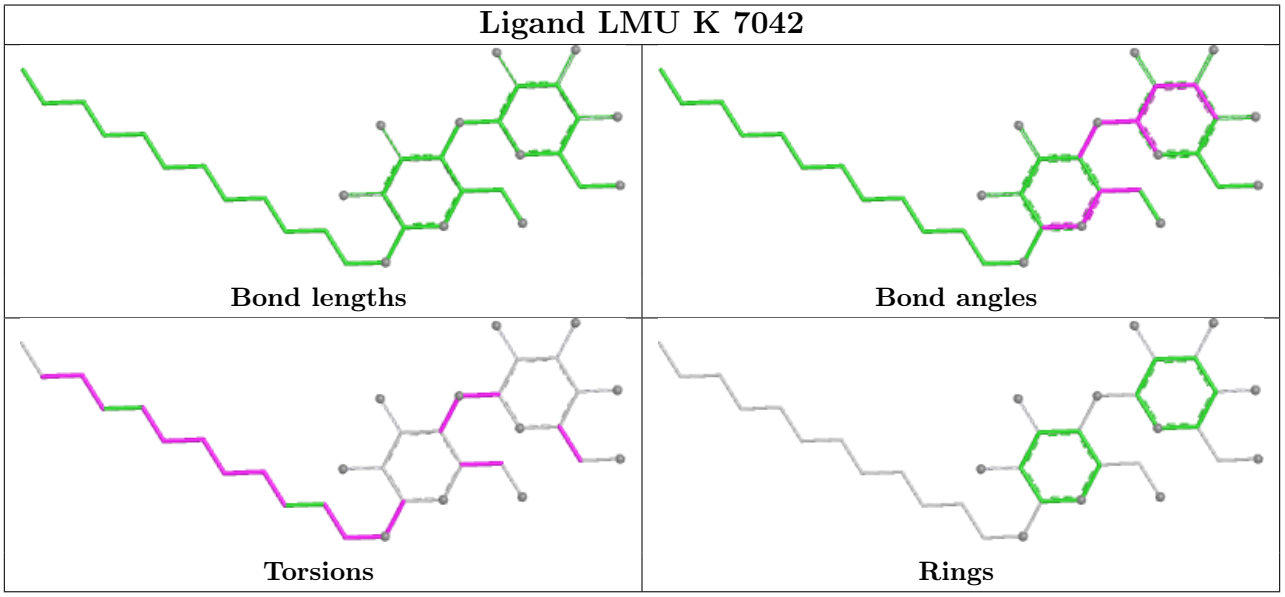


Rings

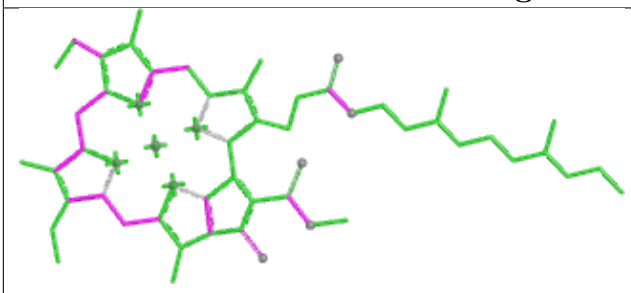
Ligand LMU 4 7008



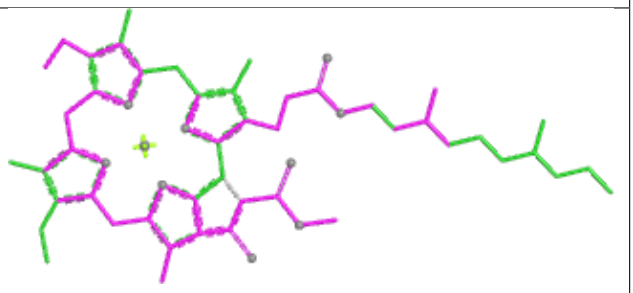
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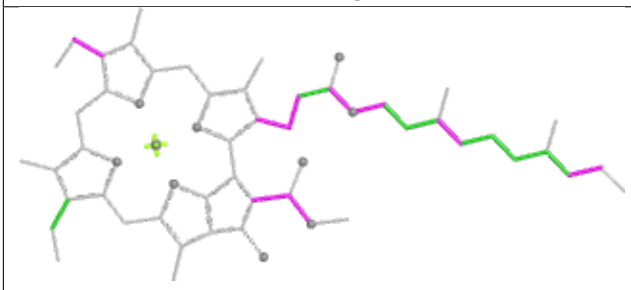
Ligand CLA R 1144



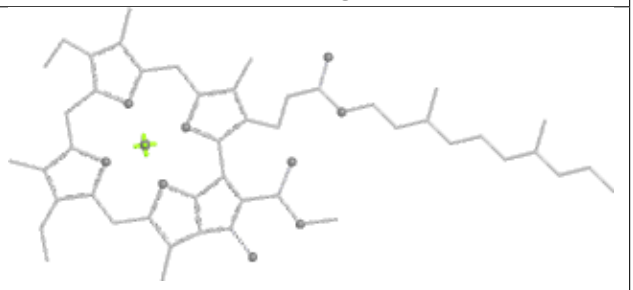
Bond lengths



Bond angles

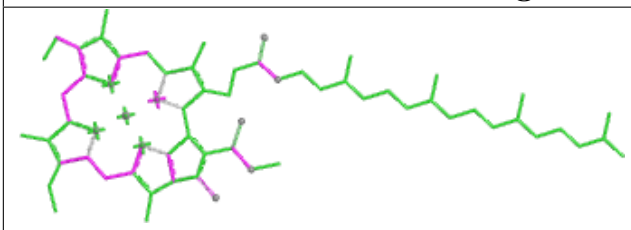


Torsions

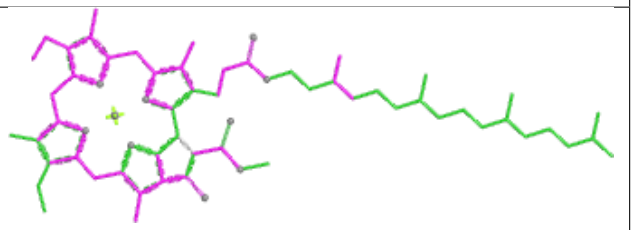


Rings

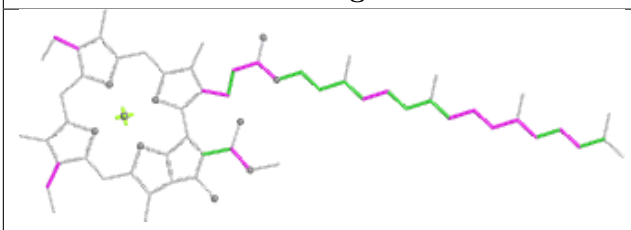
Ligand CLA B 1239



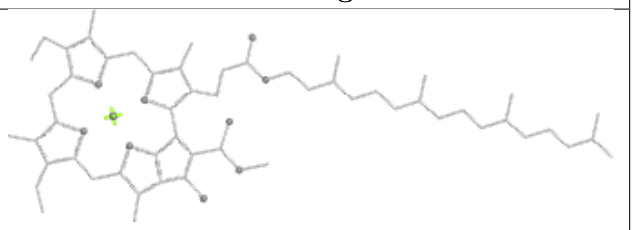
Bond lengths



Bond angles

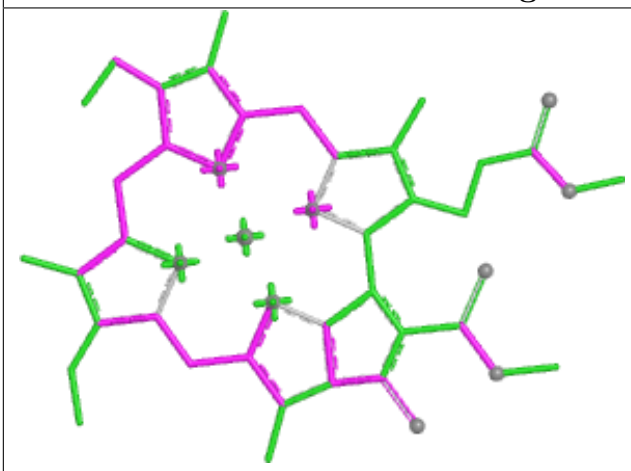


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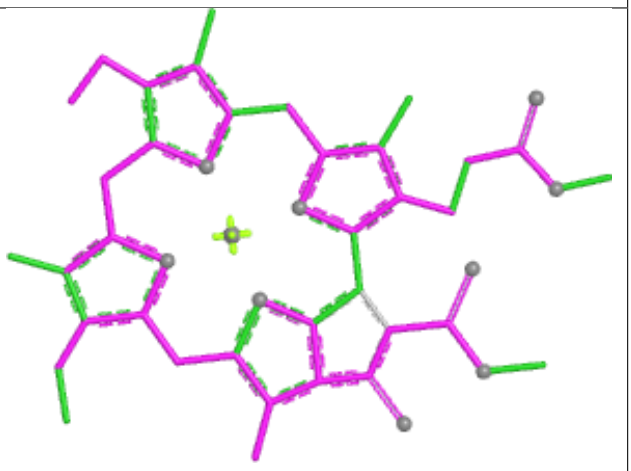


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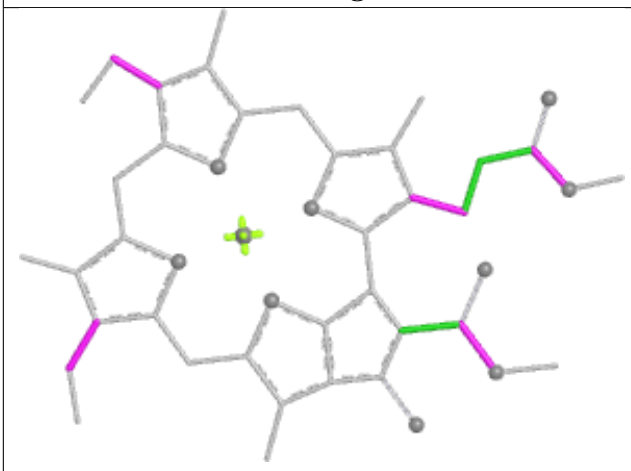
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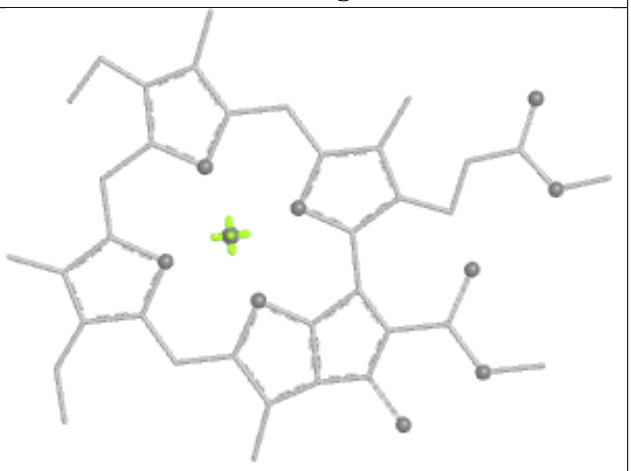
Bond lengths



Bond angles

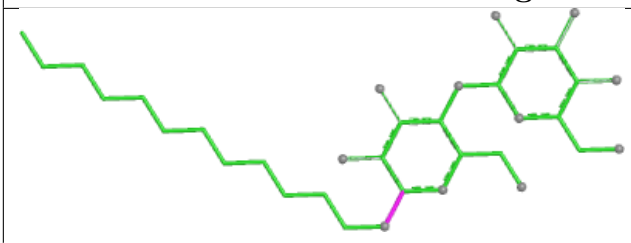


Torsions

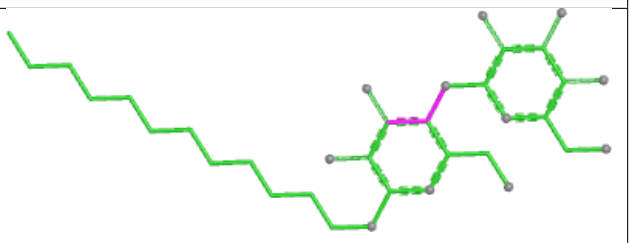


Rings

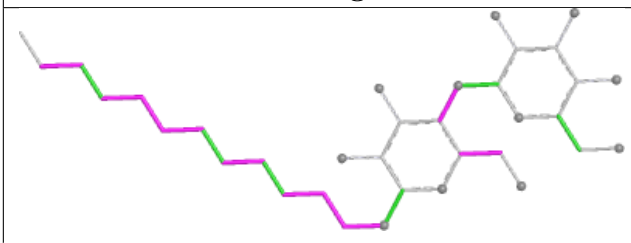
Ligand LMU 1 7013



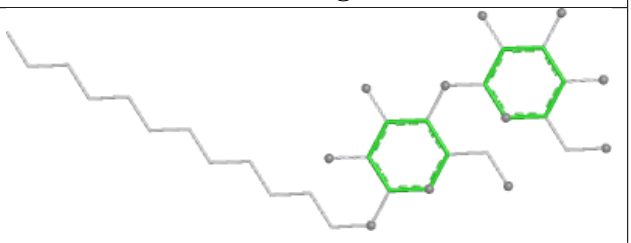
Bond lengths



Bond angles

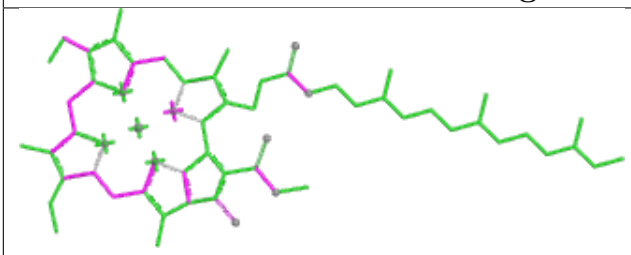


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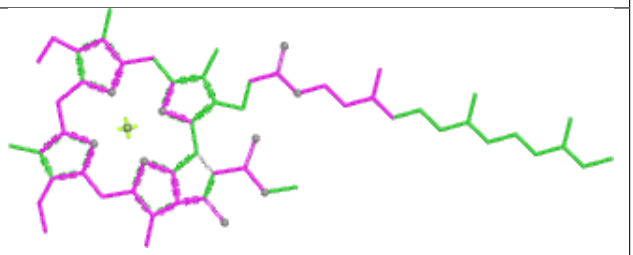


Rings

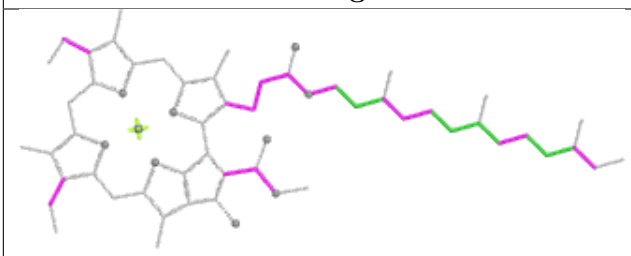
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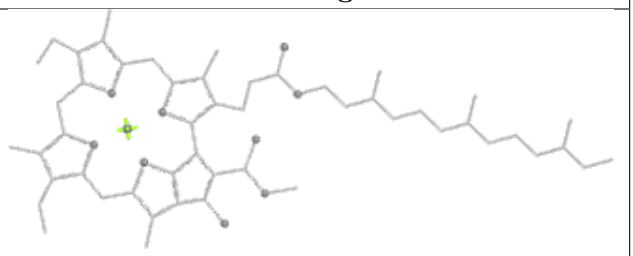
Bond lengths



Bond angles

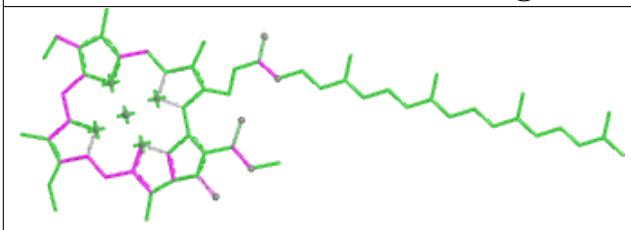


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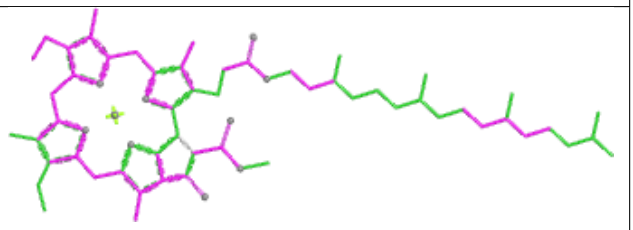


Rings

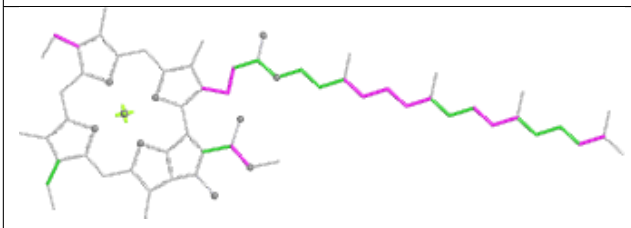
Ligand CLA B 1225



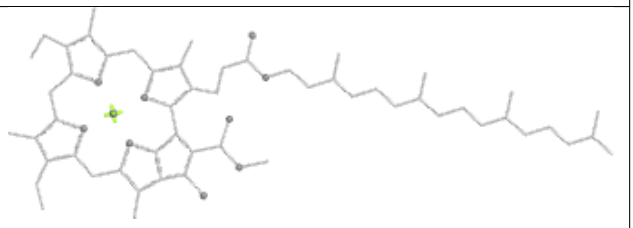
Bond lengths



Bond angles

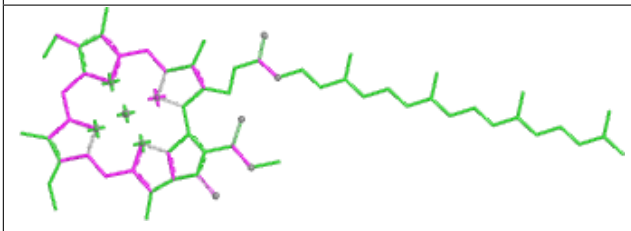


Torsions

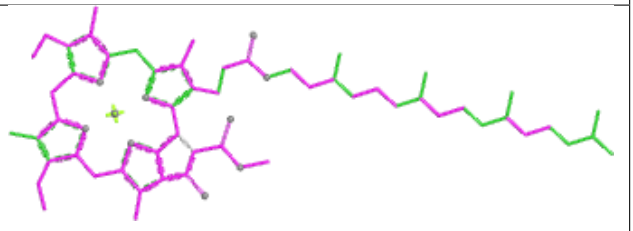


Rings

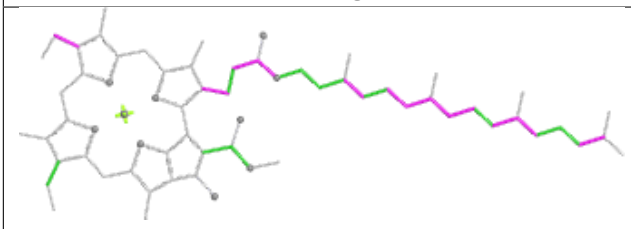
Ligand CLA 4 1304



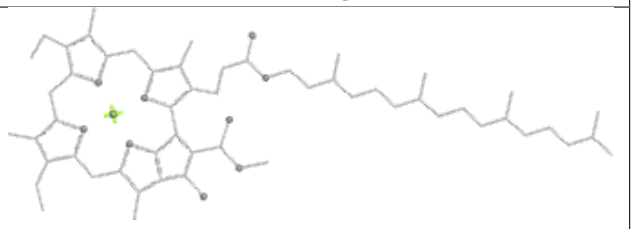
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	730/738 (98%)	1.34	157 (21%) 2 2	12, 19, 25, 27	0
2	B	733/733 (100%)	1.39	150 (20%) 2 2	8, 18, 26, 28	0
3	C	81/81 (100%)	1.81	32 (39%) 1 1	17, 21, 23, 24	0
4	D	138/138 (100%)	1.20	24 (17%) 4 4	18, 22, 25, 27	0
5	E	64/64 (100%)	1.08	10 (15%) 5 4	17, 21, 24, 25	0
6	F	154/154 (100%)	1.13	26 (16%) 4 4	17, 22, 25, 26	0
7	G	95/95 (100%)	1.06	7 (7%) 20 15	20, 25, 28, 29	0
8	H	69/69 (100%)	0.95	5 (7%) 21 15	22, 24, 29, 30	0
9	I	30/30 (100%)	0.87	5 (16%) 4 4	17, 19, 22, 22	0
10	J	42/42 (100%)	1.23	6 (14%) 6 5	17, 20, 25, 26	0
11	K	84/84 (100%)	0.89	6 (7%) 22 15	24, 27, 29, 30	0
12	L	161/161 (100%)	1.09	26 (16%) 4 4	16, 20, 26, 27	0
13	N	85/85 (100%)	0.49	5 (5%) 28 19	22, 25, 28, 29	0
14	R	0/53	-	-	-	-
15	1	165/170 (97%)	1.92	60 (36%) 1 1	32, 59, 69, 70	0
16	2	176/176 (100%)	1.50	41 (23%) 2 2	32, 52, 63, 66	0
17	3	156/172 (90%)	0.96	19 (12%) 8 7	25, 28, 32, 33	0
18	4	166/166 (100%)	1.63	53 (31%) 1 1	20, 44, 56, 57	0
All	All	3129/3211 (97%)	1.31	632 (20%) 3 2	8, 22, 57, 70	0

All (632) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	1	132	GLY	11.5
16	2	181	PRO	11.2
2	B	491	ASN	9.6

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Mol	Chain	Res	Type	RSRZ
11	K	62	SER	7.7
15	1	153	SER	7.4
18	4	230	ASP	7.4
18	4	119	GLY	7.2
1	A	388	ASP	7.2
16	2	168	TRP	7.0
15	1	79	TYR	6.8
15	1	81	GLU	6.8
2	B	258	LEU	6.5
15	1	174	SER	6.4
2	B	558	PRO	6.3
2	B	294	ASN	6.3
1	A	505	PRO	6.2
1	A	249	ILE	6.2
12	L	127	GLY	6.2
2	B	562	PRO	6.2
1	A	391	THR	6.2
1	A	251	ASN	6.1
1	A	344	LYS	6.1
2	B	676	GLU	6.1
16	2	197	GLY	6.0
1	A	376	MET	5.8
18	4	118	ILE	5.8
2	B	584	LEU	5.8
1	A	752	ALA	5.7
4	D	195	VAL	5.6
15	1	212	GLY	5.6
12	L	130	GLY	5.5
2	B	170	ASN	5.5
2	B	517	PHE	5.5
1	A	181	ALA	5.4
15	1	74	ALA	5.4
1	A	126	ILE	5.3
2	B	502	ASN	5.3
1	A	32	GLU	5.3
10	J	4	LEU	5.3
3	C	80	ALA	5.3
2	B	527	LEU	5.2
15	1	192	ARG	5.2
12	L	163	SER	5.2
3	C	9	ASP	5.2
1	A	385	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	124	TRP	5.1
12	L	126	ALA	5.1
1	A	266	ALA	5.0
4	D	86	SER	4.9
1	A	493	GLN	4.9
1	A	610	SER	4.9
15	1	72	VAL	4.9
18	4	165	SER	4.8
2	B	69	ALA	4.8
2	B	560	ASP	4.8
2	B	147	PHE	4.8
16	2	223	LYS	4.8
1	A	185	HIS	4.8
1	A	745	THR	4.8
1	A	33	GLN	4.7
2	B	252	THR	4.6
2	B	561	GLY	4.6
15	1	78	ARG	4.6
11	K	109	CYS	4.5
2	B	470	THR	4.5
1	A	433	ASP	4.5
1	A	220	ARG	4.4
15	1	215	GLU	4.4
15	1	135	PRO	4.4
2	B	563	GLY	4.4
2	B	679	ALA	4.4
4	D	170	ASP	4.4
1	A	484	LEU	4.3
15	1	82	SER	4.3
3	C	60	THR	4.3
15	1	217	LEU	4.3
16	2	198	GLY	4.2
2	B	5	ILE	4.2
2	B	212	PHE	4.1
1	A	509	ALA	4.1
1	A	203	LEU	4.1
1	A	750	PHE	4.1
15	1	85	ILE	4.1
1	A	494	ASN	4.1
16	2	225	GLY	4.1
1	A	548	THR	4.1
1	A	617	SER	4.1

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Mol	Chain	Res	Type	RSRZ
11	K	113	GLY	4.1
1	A	294	LEU	4.1
16	2	199	LEU	4.1
3	C	17	CYS	4.0
6	F	148	LEU	4.0
2	B	319	HIS	4.0
2	B	479	SER	4.0
2	B	590	VAL	4.0
1	A	635	THR	4.0
2	B	354	SER	4.0
7	G	130	TRP	3.9
11	K	90	ASP	3.9
3	C	78	GLY	3.9
2	B	93	ASP	3.9
2	B	682	HIS	3.9
2	B	181	GLY	3.9
2	B	683	GLU	3.8
3	C	8	TYR	3.8
10	J	13	VAL	3.8
6	F	201	PRO	3.8
18	4	187	GLY	3.8
2	B	724	PHE	3.8
2	B	423	SER	3.8
2	B	492	ILE	3.8
1	A	191	PRO	3.8
18	4	198	LEU	3.8
15	1	116	ALA	3.8
1	A	34	TRP	3.8
15	1	77	GLU	3.8
17	3	102	GLU	3.8
2	B	300	SER	3.7
2	B	292	ARG	3.7
18	4	89	ARG	3.7
1	A	751	LEU	3.7
2	B	204	GLY	3.7
2	B	645	VAL	3.7
15	1	86	HIS	3.7
1	A	122	VAL	3.7
6	F	229	ASN	3.7
1	A	587	GLY	3.7
12	L	162	PRO	3.7
15	1	73	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	208	ARG	3.7
2	B	667	TRP	3.7
16	2	227	LEU	3.7
16	2	171	ILE	3.7
2	B	124	TRP	3.7
6	F	215	VAL	3.6
5	E	112	TYR	3.6
2	B	222	LEU	3.6
2	B	6	PRO	3.6
15	1	127	ASN	3.6
4	D	205	LYS	3.6
18	4	208	GLY	3.6
9	I	28	VAL	3.6
2	B	346	SER	3.6
7	G	132	SER	3.6
2	B	453	ILE	3.5
3	C	52	LYS	3.5
2	B	582	TRP	3.5
2	B	255	LEU	3.5
16	2	237	PHE	3.5
2	B	493	TRP	3.5
8	H	91	PHE	3.5
2	B	271	THR	3.5
1	A	160	SER	3.5
4	D	106	SER	3.5
2	B	702	ILE	3.5
3	C	65	VAL	3.5
5	E	102	PRO	3.5
6	F	114	ALA	3.4
15	1	61	ASP	3.4
1	A	248	PHE	3.4
15	1	185	VAL	3.4
1	A	210	LEU	3.4
1	A	441	ALA	3.4
2	B	195	VAL	3.4
1	A	536	THR	3.4
1	A	304	LEU	3.4
1	A	196	PHE	3.3
2	B	484	PRO	3.3
2	B	343	VAL	3.3
3	C	67	VAL	3.3
2	B	221	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
10	J	7	TYR	3.3
17	3	86	PRO	3.3
3	C	11	CYS	3.3
15	1	87	CYS	3.3
2	B	690	LEU	3.2
3	C	5	VAL	3.2
17	3	135	ALA	3.2
17	3	166	GLY	3.2
1	A	66	SER	3.2
2	B	457	PRO	3.2
1	A	223	VAL	3.2
18	4	130	GLY	3.2
1	A	71	LEU	3.2
1	A	285	GLY	3.2
1	A	245	PRO	3.2
13	N	87	VAL	3.2
1	A	219	ALA	3.2
2	B	223	GLY	3.1
1	A	487	VAL	3.1
1	A	82	HIS	3.1
1	A	300	ALA	3.1
12	L	129	ALA	3.1
16	2	116	GLY	3.1
3	C	10	THR	3.1
3	C	34	CYS	3.1
1	A	384	TYR	3.1
1	A	105	ASN	3.1
18	4	158	GLN	3.1
1	A	742	GLY	3.1
6	F	199	ASP	3.1
17	3	224	LYS	3.1
8	H	120	ILE	3.1
10	J	38	ILE	3.1
1	A	506	GLY	3.1
18	4	120	ILE	3.1
2	B	233	TYR	3.1
2	B	722	ALA	3.0
1	A	471	GLY	3.0
1	A	470	LEU	3.0
13	N	162	CYS	3.0
1	A	182	GLY	3.0
2	B	313	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	153	GLN	3.0
16	2	165	GLY	3.0
16	2	234	GLY	3.0
1	A	735	VAL	3.0
1	A	329	ASP	3.0
6	F	187	ASP	3.0
4	D	169	LYS	3.0
17	3	112	GLY	3.0
1	A	153	TRP	3.0
1	A	662	SER	3.0
2	B	486	LEU	3.0
18	4	177	LEU	3.0
1	A	643	ALA	3.0
2	B	48	ALA	3.0
1	A	209	GLY	3.0
2	B	260	GLY	3.0
16	2	108	VAL	3.0
6	F	203	ALA	3.0
6	F	141	GLY	3.0
1	A	299	ILE	3.0
1	A	584	PRO	2.9
1	A	342	GLY	2.9
16	2	256	ASP	2.9
1	A	591	GLN	2.9
1	A	354	TRP	2.9
16	2	224	ASN	2.9
18	4	152	VAL	2.9
1	A	134	GLY	2.9
15	1	92	LEU	2.9
15	1	117	LEU	2.9
15	1	121	GLN	2.9
2	B	540	ASP	2.9
2	B	569	ASP	2.9
15	1	122	ALA	2.9
2	B	120	VAL	2.9
1	A	293	GLY	2.9
8	H	74	SER	2.9
18	4	109	MET	2.9
1	A	746	THR	2.9
3	C	36	ALA	2.9
2	B	568	CYS	2.9
1	A	100	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	707	ILE	2.9
1	A	217	SER	2.8
3	C	41	SER	2.8
11	K	60	SER	2.8
12	L	147	ILE	2.8
2	B	350	GLN	2.8
12	L	94	SER	2.8
18	4	168	GLN	2.8
2	B	274	ALA	2.8
15	1	115	ALA	2.8
4	D	105	ASP	2.8
15	1	89	TRP	2.8
1	A	98	PHE	2.8
1	A	143	ILE	2.8
2	B	458	ILE	2.8
12	L	55	GLN	2.8
1	A	724	ALA	2.8
12	L	119	PRO	2.8
1	A	607	ASN	2.8
17	3	183	GLY	2.8
1	A	211	LEU	2.8
12	L	204	LEU	2.8
15	1	172	GLY	2.8
18	4	129	ALA	2.8
2	B	263	PRO	2.8
2	B	420	SER	2.8
2	B	578	LEU	2.8
18	4	242	ASN	2.7
3	C	56	SER	2.7
18	4	144	ILE	2.7
4	D	89	GLY	2.7
18	4	222	ASN	2.7
2	B	186	SER	2.7
2	B	556	SER	2.7
1	A	225	VAL	2.7
2	B	94	PRO	2.7
2	B	533	ILE	2.7
1	A	593	SER	2.7
2	B	372	TYR	2.7
17	3	109	ALA	2.7
2	B	534	LEU	2.7
5	E	103	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
18	4	148	LEU	2.7
16	2	268	PRO	2.7
18	4	85	PRO	2.7
15	1	155	GLU	2.7
18	4	139	SER	2.7
17	3	113	ALA	2.7
12	L	205	TYR	2.7
18	4	182	VAL	2.7
1	A	63	ASP	2.7
1	A	485	GLN	2.6
4	D	114	MET	2.6
2	B	321	GLY	2.6
15	1	187	GLU	2.6
16	2	191	THR	2.6
1	A	685	VAL	2.6
1	A	733	VAL	2.6
2	B	507	SER	2.6
12	L	152	SER	2.6
2	B	364	ASP	2.6
2	B	418	ILE	2.6
3	C	7	ILE	2.6
2	B	641	ASN	2.6
3	C	15	THR	2.6
2	B	646	TRP	2.6
1	A	45	ALA	2.6
1	A	744	ALA	2.6
18	4	102	ALA	2.6
18	4	137	SER	2.6
12	L	148	TYR	2.6
6	F	115	PRO	2.6
6	F	214	PRO	2.6
17	3	95	PRO	2.6
18	4	122	ASN	2.6
6	F	160	PHE	2.6
15	1	169	ASP	2.6
2	B	513	GLY	2.6
2	B	273	VAL	2.6
3	C	70	TRP	2.6
18	4	101	TRP	2.6
3	C	12	ILE	2.6
12	L	79	ILE	2.6
18	4	160	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	68	TYR	2.6
16	2	109	HIS	2.6
5	E	68	PRO	2.6
18	4	196	PRO	2.6
17	3	130	GLN	2.6
2	B	610	ASN	2.6
1	A	272	LEU	2.6
15	1	84	LEU	2.6
2	B	133	GLU	2.6
1	A	514	THR	2.6
2	B	167	TRP	2.5
2	B	720	THR	2.6
18	4	90	TRP	2.5
1	A	555	ILE	2.5
2	B	419	ILE	2.5
18	4	154	ILE	2.5
16	2	110	SER	2.5
1	A	123	VAL	2.5
12	L	180	ASP	2.5
18	4	173	LYS	2.5
18	4	193	ASN	2.5
4	D	121	ILE	2.5
15	1	114	TRP	2.5
7	G	82	PHE	2.5
1	A	165	TYR	2.5
2	B	291	TYR	2.5
1	A	236	GLY	2.5
1	A	460	LEU	2.5
9	I	12	VAL	2.5
2	B	205	GLU	2.5
2	B	658	ALA	2.5
12	L	161	ALA	2.5
16	2	231	ALA	2.5
4	D	191	ILE	2.5
15	1	154	MET	2.5
15	1	211	THR	2.5
18	4	211	MET	2.5
2	B	67	HIS	2.5
6	F	84	PRO	2.5
2	B	732	LYS	2.5
6	F	189	LYS	2.5
15	1	88	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	444	SER	2.5
7	G	91	VAL	2.5
1	A	594	ALA	2.5
12	L	133	ALA	2.5
12	L	134	ALA	2.5
2	B	127	ILE	2.5
6	F	223	ASN	2.5
18	4	232	LEU	2.5
2	B	259	GLY	2.5
9	I	9	VAL	2.5
1	A	608	SER	2.5
1	A	705	GLU	2.5
17	3	238	ILE	2.5
5	E	108	ASN	2.5
10	J	35	ASP	2.5
16	2	170	ASP	2.5
2	B	620	LEU	2.5
18	4	124	PRO	2.5
17	3	115	GLY	2.5
17	3	228	VAL	2.5
1	A	374	GLN	2.5
7	G	107	ALA	2.4
1	A	53	TRP	2.4
18	4	157	TRP	2.4
1	A	381	PRO	2.4
1	A	449	VAL	2.4
1	A	551	VAL	2.4
15	1	68	GLY	2.4
1	A	703	LEU	2.4
2	B	272	ASP	2.4
18	4	178	PRO	2.4
16	2	262	ILE	2.4
17	3	235	MET	2.4
9	I	29	GLU	2.4
18	4	176	SER	2.4
2	B	454	LEU	2.4
2	B	237	PRO	2.4
18	4	225	GLY	2.4
2	B	632	ILE	2.4
18	4	128	ALA	2.4
1	A	151	GLN	2.4
8	H	64	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	643	LEU	2.4
15	1	76	LEU	2.4
18	4	212	LEU	2.4
1	A	486	PRO	2.4
1	A	708	VAL	2.4
4	D	142	THR	2.4
2	B	210	ASN	2.4
16	2	185	ASN	2.4
1	A	301	HIS	2.4
2	B	117	TYR	2.4
2	B	574	ASP	2.4
6	F	109	TYR	2.4
18	4	169	ASP	2.4
16	2	233	MET	2.4
18	4	88	LEU	2.4
1	A	512	SER	2.4
6	F	81	GLY	2.3
16	2	147	THR	2.3
1	A	569	ILE	2.3
2	B	437	TYR	2.3
15	1	222	ALA	2.3
2	B	74	PHE	2.3
2	B	183	PHE	2.3
1	A	69	SER	2.3
2	B	123	TRP	2.3
1	A	265	GLY	2.3
1	A	340	GLY	2.3
13	N	141	LYS	2.3
15	1	96	GLY	2.3
17	3	123	GLY	2.3
1	A	198	ASP	2.3
1	A	694	PHE	2.3
1	A	527	VAL	2.3
9	I	30	LYS	2.3
1	A	443	ILE	2.3
1	A	686	TRP	2.3
2	B	485	ALA	2.3
18	4	110	LEU	2.3
4	D	98	GLU	2.3
16	2	221	GLU	2.3
1	A	516	GLY	2.3
5	E	76	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
16	2	222	ILE	2.3
1	A	263	ALA	2.3
3	C	4	SER	2.3
3	C	45	THR	2.3
4	D	116	THR	2.3
4	D	203	THR	2.3
1	A	574	ASN	2.3
1	A	49	ASP	2.3
3	C	22	PRO	2.3
16	2	160	ILE	2.3
2	B	26	ALA	2.3
5	E	86	GLY	2.3
12	L	187	GLY	2.3
2	B	657	TRP	2.3
1	A	600	LEU	2.3
2	B	511	THR	2.3
2	B	674	LEU	2.3
3	C	69	LEU	2.3
1	A	303	HIS	2.3
18	4	134	TYR	2.3
2	B	580	VAL	2.3
5	E	94	ASP	2.3
18	4	114	VAL	2.3
1	A	130	GLU	2.2
3	C	46	GLU	2.2
4	D	88	GLY	2.2
12	L	157	ALA	2.2
16	2	194	GLY	2.2
2	B	427	LEU	2.2
16	2	253	HIS	2.2
6	F	212	SER	2.2
12	L	131	SER	2.2
12	L	201	TYR	2.2
15	1	113	GLU	2.2
18	4	84	ASP	2.2
1	A	345	GLY	2.2
1	A	741	GLY	2.2
15	1	91	MET	2.2
15	1	128	PRO	2.2
16	2	141	GLY	2.2
16	2	157	LEU	2.2
16	2	258	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	221	HIS	2.2
18	4	117	SER	2.2
3	C	63	LEU	2.2
8	H	119	ASP	2.2
12	L	193	GLY	2.2
1	A	753	ARG	2.2
11	K	59	THR	2.2
3	C	18	VAL	2.2
18	4	166	VAL	2.2
1	A	41	SER	2.2
2	B	571	SER	2.2
1	A	743	ILE	2.2
15	1	71	GLU	2.2
2	B	370	ALA	2.2
2	B	445	ALA	2.2
6	F	175	GLY	2.2
1	A	99	HIS	2.2
6	F	105	SER	2.2
13	N	140	GLN	2.2
15	1	137	ILE	2.2
2	B	508	LEU	2.2
6	F	230	ASN	2.2
2	B	734	GLY	2.2
17	3	106	GLY	2.2
1	A	102	ARG	2.2
2	B	137	THR	2.1
2	B	373	THR	2.1
7	G	105	THR	2.1
2	B	21	ILE	2.1
15	1	145	ILE	2.1
1	A	101	ALA	2.1
2	B	239	SER	2.1
7	G	69	GLY	2.1
15	1	60	GLY	2.1
18	4	216	GLY	2.1
1	A	655	ASP	2.1
2	B	95	HIS	2.1
6	F	177	VAL	2.1
2	B	567	THR	2.1
1	A	96	MET	2.1
2	B	307	ALA	2.1
17	3	234	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	758	GLY	2.1
16	2	135	PRO	2.1
17	3	240	GLY	2.1
5	E	98	ASN	2.1
15	1	157	ASP	2.1
16	2	180	ASP	2.1
2	B	595	HIS	2.1
2	B	309	ILE	2.1
5	E	77	LEU	2.1
1	A	659	ALA	2.1
1	A	663	GLN	2.1
6	F	184	ALA	2.1
15	1	218	ALA	2.1
1	A	500	PRO	2.1
4	D	84	GLY	2.1
4	D	113	GLU	2.1
4	D	125	GLY	2.1
15	1	213	PRO	2.1
1	A	510	SER	2.1
2	B	261	PHE	2.1
1	A	230	ASN	2.1
6	F	227	VAL	2.1
2	B	209	TRP	2.1
15	1	80	LYS	2.1
1	A	657	LEU	2.1
3	C	48	CYS	2.1
10	J	27	ILE	2.1
15	1	180	LEU	2.1
2	B	126	THR	2.1
18	4	197	THR	2.1
2	B	566	GLY	2.1
15	1	70	GLY	2.1
15	1	200	GLY	2.1
15	1	83	GLU	2.1
18	4	170	PRO	2.1
2	B	730	SER	2.1
1	A	395	LEU	2.1
16	2	217	LEU	2.1
2	B	397	ASP	2.1
2	B	717	TYR	2.1
4	D	95	GLN	2.1
4	D	204	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
6	F	178	GLY	2.1
2	B	576	PHE	2.1
3	C	25	VAL	2.0
3	C	37	LYS	2.0
1	A	359	SER	2.0
2	B	628	SER	2.0
1	A	697	ARG	2.0
2	B	174	ARG	2.0
2	B	347	LEU	2.0
2	B	412	LEU	2.0
4	D	102	ILE	2.0
12	L	132	LEU	2.0
15	1	221	LEU	2.0
1	A	218	TRP	2.0
1	A	425	THR	2.0
2	B	441	ASP	2.0
3	C	74	THR	2.0
16	2	235	ALA	2.0
1	A	232	PHE	2.0
1	A	518	GLY	2.0
15	1	126	GLY	2.0
1	A	570	PRO	2.0
4	D	79	PRO	2.0
12	L	113	PRO	2.0
16	2	266	PHE	2.0
1	A	76	ARG	2.0
2	B	175	LEU	2.0
2	B	616	LEU	2.0
1	A	755	ILE	2.0
2	B	262	HIS	2.0
2	B	448	THR	2.0
15	1	194	ALA	2.0
1	A	684	PHE	2.0
16	2	119	GLY	2.0
16	2	238	GLN	2.0
1	A	611	VAL	2.0
1	A	568	LEU	2.0
13	N	150	LEU	2.0
2	B	330	ILE	2.0
2	B	455	ILE	2.0
6	F	79	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	A	1309	25/65	0.49	0.16	25,46,54,54	0
19	CLA	3	3012	25/65	0.51	0.21	30,31,31,31	0
21	BCR	1	6023	40/40	0.54	0.17	21,28,29,30	0
21	BCR	A	6002	40/40	0.55	0.22	23,27,32,33	0
19	CLA	4	4003	55/65	0.55	0.18	15,34,47,50	0
19	CLA	1	1015	25/65	0.56	0.22	27,28,28,28	0
22	LMU	1	7004	35/35	0.56	0.15	17,44,50,52	0
19	CLA	L	1504	55/65	0.57	0.21	18,25,27,27	0
19	CLA	3	3016	65/65	0.57	0.18	23,26,29,31	0
19	CLA	3	3005	25/65	0.57	0.21	31,31,31,31	0
19	CLA	B	1233	51/65	0.58	0.18	24,27,27,28	0
19	CLA	2	2007	65/65	0.58	0.18	17,25,26,26	0
19	CLA	1	1006	36/65	0.58	0.16	29,30,30,31	0
22	LMU	1	7013	35/35	0.58	0.15	15,34,47,48	0
19	CLA	A	1141	65/65	0.59	0.16	28,30,31,32	0
22	LMU	A	7010	35/35	0.59	0.16	16,38,45,48	0
19	CLA	H	1505	55/65	0.59	0.17	18,27,28,29	0
19	CLA	3	3014	25/65	0.59	0.18	31,31,32,32	0
22	LMU	4	7053	34/35	0.59	0.16	21,41,47,48	0
19	CLA	3	3007	42/65	0.60	0.17	27,30,30,30	0
19	CLA	4	4014	47/65	0.60	0.17	21,35,46,48	0
19	CLA	2	2014	61/65	0.61	0.17	24,26,28,28	0
19	CLA	G	1242	51/65	0.61	0.16	26,28,29,29	0
21	BCR	3	6022	40/40	0.62	0.17	21,22,23,23	0
19	CLA	H	1241	55/65	0.62	0.16	23,25,26,26	0
22	LMU	L	7029	35/35	0.62	0.16	30,44,53,55	0
19	CLA	1	1001	46/65	0.63	0.16	28,29,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	2	2001	51/65	0.63	0.18	27,28,29,29	0
19	CLA	L	1148	55/65	0.63	0.15	21,25,26,27	0
22	LMU	G	7051	35/35	0.63	0.16	20,32,43,44	0
22	LMU	N	7049	35/35	0.64	0.14	15,28,40,41	0
19	CLA	4	4007	52/65	0.64	0.15	22,26,27,28	0
22	LMU	K	7041	35/35	0.64	0.15	15,31,45,45	0
22	LMU	4	7009	34/35	0.64	0.17	22,44,50,50	0
19	CLA	A	1151	50/65	0.64	0.15	24,27,29,29	0
19	CLA	K	1142	45/65	0.65	0.15	27,29,30,31	0
19	CLA	3	1118	36/65	0.65	0.17	28,29,30,30	0
19	CLA	1	1013	51/65	0.65	0.16	26,27,29,29	0
19	CLA	B	1212	60/65	0.65	0.18	20,23,25,26	0
19	CLA	A	1112	45/65	0.65	0.21	23,26,26,27	0
19	CLA	2	2005	25/65	0.65	0.18	30,31,32,32	0
19	CLA	B	1301	36/65	0.65	0.16	27,28,29,29	0
22	LMU	E	7048	35/35	0.65	0.15	19,30,44,46	0
19	CLA	B	1213	46/65	0.66	0.21	19,21,24,25	0
19	CLA	4	4001	50/65	0.66	0.19	21,23,25,25	0
21	BCR	J	6012	40/40	0.66	0.21	19,24,26,26	0
19	CLA	3	2009	56/65	0.67	0.16	13,35,50,50	0
19	CLA	B	1232	45/65	0.67	0.15	23,26,27,27	0
19	CLA	2	2004	50/65	0.67	0.17	23,25,25,25	0
22	LMU	H	7043	35/35	0.67	0.14	12,31,46,47	0
22	LMU	2	7046	35/35	0.67	0.15	4,27,42,42	0
22	LMU	K	7001	35/35	0.67	0.14	17,34,48,50	0
19	CLA	4	1306	55/65	0.67	0.16	20,26,27,27	0
19	CLA	K	3009	65/65	0.68	0.16	22,25,27,28	0
22	LMU	E	7037	35/35	0.68	0.17	8,21,40,40	0
19	CLA	1	1010	46/65	0.68	0.16	24,25,26,27	0
19	CLA	4	1304	65/65	0.68	0.17	21,23,25,25	0
22	LMU	H	7017	35/35	0.68	0.14	8,23,39,41	0
19	CLA	4	1004	55/65	0.69	0.17	22,25,26,27	0
19	CLA	4	4015	46/65	0.69	0.15	24,25,26,27	0
19	CLA	3	3006	25/65	0.69	0.16	26,27,28,28	0
19	CLA	1	1310	25/65	0.69	0.15	27,28,28,28	0
19	CLA	2	2013	50/65	0.69	0.22	20,22,24,26	0
19	CLA	3	3003	36/65	0.69	0.15	29,30,31,31	0
19	CLA	F	1305	53/65	0.69	0.15	22,23,25,25	0
19	CLA	3	3013	65/65	0.70	0.16	20,21,24,25	0
19	CLA	H	1145	65/65	0.70	0.14	12,24,33,39	0
19	CLA	K	1143	50/65	0.70	0.15	24,27,28,28	0
19	CLA	J	1311	61/65	0.70	0.14	19,26,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	3	3008	50/65	0.70	0.14	20,26,27,27	0
22	LMU	4	7052	35/35	0.70	0.14	18,30,48,75	0
19	CLA	2	2002	56/65	0.70	0.17	21,22,25,25	0
19	CLA	2	1307	25/65	0.71	0.14	29,30,31,31	0
19	CLA	3	3015	25/65	0.71	0.15	28,28,29,29	0
19	CLA	3	1147	46/65	0.71	0.15	25,27,28,28	0
19	CLA	3	3017	50/65	0.71	0.12	26,37,49,52	0
19	CLA	F	1302	41/65	0.71	0.17	24,26,26,26	0
19	CLA	3	3010	25/65	0.71	0.17	32,32,33,33	0
22	LMU	4	7034	35/35	0.71	0.16	14,30,42,47	0
19	CLA	A	1108	45/65	0.71	0.15	19,22,23,24	0
19	CLA	A	1134	45/65	0.71	0.17	22,26,27,28	0
22	LMU	H	7030	35/35	0.72	0.12	16,29,46,50	0
21	BCR	A	6007	40/40	0.72	0.22	19,23,28,28	0
19	CLA	2	2006	65/65	0.72	0.15	18,23,24,25	0
19	CLA	L	1503	50/65	0.72	0.20	19,21,23,24	0
22	LMU	K	7047	35/35	0.72	0.15	14,33,46,49	0
19	CLA	4	4004	25/65	0.72	0.18	29,30,30,30	0
19	CLA	4	4006	55/65	0.72	0.17	16,23,24,24	0
22	LMU	A	7045	35/35	0.72	0.14	11,23,41,43	0
19	CLA	1	1303	51/65	0.72	0.15	23,28,28,29	0
19	CLA	3	3004	25/65	0.72	0.15	27,28,28,28	0
19	CLA	A	1105	46/65	0.72	0.19	22,23,24,24	0
22	LMU	H	7011	35/35	0.72	0.14	17,32,38,43	0
19	CLA	A	1121	42/65	0.72	0.15	26,28,28,28	0
22	LMU	H	7028	35/35	0.72	0.14	7,21,40,40	0
22	LMU	C	7015	35/35	0.73	0.13	9,22,37,39	0
22	LMU	K	7042	35/35	0.73	0.15	13,23,42,43	0
22	LMU	D	7050	35/35	0.73	0.12	14,31,46,46	0
19	CLA	3	3011	65/65	0.73	0.15	23,25,26,26	0
19	CLA	1	1002	47/65	0.73	0.17	22,23,24,24	0
19	CLA	K	1146	50/65	0.73	0.14	25,28,30,30	0
19	CLA	1	1007	61/65	0.73	0.15	14,20,21,22	0
22	LMU	2	7031	35/35	0.73	0.12	17,37,45,48	0
19	CLA	R	1144	57/65	0.73	0.14	24,27,28,28	0
19	CLA	R	1150	65/65	0.73	0.14	22,24,25,25	0
19	CLA	1	1014	61/65	0.73	0.14	3,31,46,46	0
19	CLA	B	1218	46/65	0.73	0.19	20,20,22,23	0
22	LMU	B	7038	35/35	0.73	0.12	13,35,48,48	0
22	LMU	F	7036	34/35	0.74	0.12	19,32,42,45	0
19	CLA	A	1149	46/65	0.74	0.14	22,25,25,25	0
22	LMU	4	7008	35/35	0.74	0.13	11,29,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	H	1207	65/65	0.74	0.19	15,17,19,20	0
22	LMU	R	7021	35/35	0.74	0.12	17,28,45,46	0
19	CLA	A	1113	50/65	0.74	0.16	19,22,23,24	0
19	CLA	3	3002	25/65	0.74	0.15	28,28,28,28	0
22	LMU	R	7020	35/35	0.75	0.13	7,26,40,44	0
19	CLA	A	1115	65/65	0.75	0.16	10,28,41,42	0
22	LMU	B	7040	35/35	0.75	0.14	12,26,40,43	0
21	BCR	A	6008	40/40	0.75	0.19	21,24,27,27	0
19	CLA	A	1116	52/65	0.75	0.19	24,25,26,26	0
19	CLA	1	1008	51/65	0.75	0.13	24,26,27,27	0
19	CLA	A	1111	54/65	0.75	0.20	20,24,24,24	0
19	CLA	2	2008	25/65	0.75	0.15	24,24,25,25	0
22	LMU	4	7019	35/35	0.75	0.14	11,25,40,43	0
22	LMU	G	7026	35/35	0.75	0.11	12,35,46,51	0
22	LMU	A	7044	35/35	0.75	0.13	8,20,39,40	0
19	CLA	2	2003	25/65	0.75	0.14	23,24,25,25	0
22	LMU	2	7006	35/35	0.76	0.13	22,25,26,27	0
21	BCR	B	6006	40/40	0.76	0.18	15,19,20,21	0
21	BCR	I	6021	40/40	0.76	0.16	16,20,22,22	0
22	LMU	3	7003	35/35	0.76	0.13	8,25,41,41	0
22	LMU	3	7005	35/35	0.76	0.12	20,32,42,43	0
19	CLA	A	1119	65/65	0.76	0.18	13,18,19,20	0
19	CLA	2	4009	65/65	0.76	0.15	18,23,24,24	0
19	CLA	1	1003	47/65	0.76	0.15	17,19,19,20	0
19	CLA	1	1011	36/65	0.76	0.14	27,27,28,28	0
19	CLA	4	4010	25/65	0.76	0.19	26,27,27,27	0
21	BCR	B	6004	40/40	0.76	0.23	18,20,22,22	0
24	LMG	B	7101	49/55	0.76	0.22	14,18,26,27	0
19	CLA	4	4013	25/65	0.77	0.14	20,21,21,21	0
19	CLA	3	3001	25/65	0.77	0.12	24,25,25,25	0
19	CLA	L	1130	65/65	0.77	0.18	13,18,19,20	0
19	CLA	2	2011	25/65	0.77	0.16	24,25,25,25	0
22	LMU	H	7002	35/35	0.77	0.11	16,29,41,43	0
21	BCR	A	6003	40/40	0.77	0.19	21,24,26,26	0
19	CLA	B	1222	58/65	0.77	0.20	18,21,23,24	0
19	CLA	A	1109	65/65	0.77	0.18	13,20,22,23	0
21	BCR	B	6017	40/40	0.78	0.24	15,18,20,20	0
22	LMU	R	7025	35/35	0.78	0.13	5,22,39,42	0
19	CLA	B	1211	65/65	0.78	0.18	17,20,21,21	0
22	LMU	4	7018	35/35	0.78	0.11	9,23,41,42	0
22	LMU	A	7023	35/35	0.78	0.11	6,20,39,41	0
19	CLA	B	1223	65/65	0.78	0.19	13,18,19,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	BCR	L	6019	40/40	0.78	0.17	15,17,19,19	0
22	LMU	B	7012	25/35	0.78	0.11	22,32,44,49	0
19	CLA	B	1231	45/65	0.78	0.16	19,20,21,21	0
19	CLA	4	4005	25/65	0.79	0.15	20,21,22,22	0
19	CLA	1	1005	46/65	0.79	0.14	19,21,22,22	0
19	CLA	2	2012	50/65	0.79	0.16	20,22,23,23	0
19	CLA	A	1110	54/65	0.79	0.14	19,22,23,23	0
19	CLA	J	1308	55/65	0.79	0.12	12,30,44,45	0
22	LMU	2	7027	35/35	0.79	0.12	6,17,40,40	0
19	CLA	B	1209	55/65	0.79	0.17	18,19,20,21	0
19	CLA	A	1123	65/65	0.79	0.21	12,18,19,20	0
21	BCR	I	6018	40/40	0.79	0.18	14,15,18,18	0
22	LMU	R	7024	35/35	0.80	0.13	6,19,32,40	0
19	CLA	I	1204	60/65	0.80	0.16	13,17,18,18	0
19	CLA	4	1009	36/65	0.80	0.17	20,22,22,23	0
19	CLA	A	1102	55/65	0.80	0.18	13,19,20,20	0
22	LMU	A	7016	35/35	0.80	0.10	10,30,46,46	0
22	LMU	H	7032	35/35	0.80	0.12	8,25,36,45	0
22	LMU	R	7014	35/35	0.80	0.11	9,26,40,44	0
19	CLA	A	1117	65/65	0.80	0.20	10,20,21,22	0
19	CLA	B	1208	54/65	0.80	0.17	18,18,21,22	0
19	CLA	A	1124	65/65	0.81	0.18	18,21,23,24	0
19	CLA	L	1501	50/65	0.81	0.14	20,20,21,21	0
19	CLA	4	4002	52/65	0.81	0.13	21,22,24,25	0
22	LMU	4	7033	35/35	0.81	0.12	12,26,40,41	0
19	CLA	A	1120	51/65	0.81	0.13	22,24,24,26	0
19	CLA	1	1012	36/65	0.81	0.14	23,24,25,25	0
19	CLA	B	1201	45/65	0.81	0.19	19,21,22,22	0
21	BCR	B	6010	40/40	0.81	0.20	13,15,16,16	0
19	CLA	2	2010	25/65	0.82	0.14	23,23,24,24	0
19	CLA	A	1125	65/65	0.82	0.16	15,17,19,20	0
19	CLA	L	1502	47/65	0.82	0.16	17,19,20,20	0
19	CLA	F	1240	36/65	0.82	0.17	15,16,17,17	0
21	BCR	F	6014	40/40	0.82	0.20	9,11,15,15	0
19	CLA	B	1228	50/65	0.82	0.16	12,14,14,15	0
22	LMU	R	7022	35/35	0.82	0.12	5,21,33,35	0
19	CLA	B	1229	65/65	0.82	0.18	8,12,14,15	0
19	CLA	B	1230	50/65	0.82	0.19	17,18,19,20	0
19	CLA	B	1216	61/65	0.82	0.17	12,18,19,20	0
19	CLA	A	1103	65/65	0.82	0.20	13,14,21,22	0
19	CLA	A	1135	51/65	0.82	0.18	16,19,19,21	0
19	CLA	B	1234	60/65	0.82	0.19	13,14,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	LMU	R	7007	35/35	0.83	0.11	8,21,40,41	0
19	CLA	A	1101	50/65	0.83	0.16	17,18,18,19	0
21	BCR	F	6016	40/40	0.83	0.16	13,16,17,17	0
19	CLA	B	1206	65/65	0.83	0.17	10,12,17,18	0
21	BCR	A	6011	40/40	0.84	0.17	10,15,16,16	0
19	CLA	4	4011	25/65	0.84	0.15	10,11,12,12	0
21	BCR	B	6005	40/40	0.84	0.18	14,16,17,17	0
19	CLA	4	4012	36/65	0.84	0.15	14,15,16,16	0
19	CLA	B	1202	65/65	0.84	0.18	7,16,16,18	0
19	CLA	B	1214	59/65	0.84	0.16	18,20,22,23	0
19	CLA	A	1133	50/65	0.84	0.14	17,19,19,20	0
19	CLA	A	1107	55/65	0.84	0.18	15,16,24,24	0
19	CLA	A	1132	65/65	0.84	0.19	13,17,18,19	0
19	CLA	A	1138	65/65	0.84	0.20	15,18,19,20	0
19	CLA	A	1140	65/65	0.84	0.17	15,18,19,21	0
19	CLA	A	9013	65/65	0.85	0.17	2,10,29,32	0
19	CLA	A	1126	65/65	0.85	0.17	12,14,15,15	0
19	CLA	B	1210	65/65	0.85	0.17	16,20,21,22	0
19	CLA	B	1217	50/65	0.85	0.16	19,21,22,23	0
19	CLA	A	1237	65/65	0.85	0.18	8,17,18,18	0
19	CLA	B	1219	55/65	0.85	0.13	18,18,21,21	0
19	CLA	B	1220	65/65	0.85	0.14	13,15,20,21	0
19	CLA	A	1129	50/65	0.85	0.14	17,19,20,20	0
19	CLA	B	1225	65/65	0.86	0.20	9,12,13,14	0
22	LMU	G	7039	35/35	0.86	0.10	15,30,47,47	0
19	CLA	B	1226	65/65	0.86	0.18	11,12,19,19	0
19	CLA	A	1104	57/65	0.86	0.14	13,15,18,18	0
22	LMU	A	7035	35/35	0.86	0.11	6,18,32,40	0
19	CLA	B	1235	65/65	0.86	0.18	14,15,16,17	0
19	CLA	B	1236	47/65	0.86	0.18	14,15,17,17	0
19	CLA	B	1239	65/65	0.86	0.17	8,11,13,14	0
19	CLA	A	1128	65/65	0.87	0.16	14,16,17,18	0
19	CLA	A	1106	65/65	0.87	0.18	10,12,13,14	0
19	CLA	A	1131	65/65	0.87	0.14	12,14,16,16	0
19	CLA	A	1136	65/65	0.87	0.16	14,15,16,17	0
19	CLA	B	1224	65/65	0.87	0.16	9,13,14,15	0
19	CLA	B	1215	60/65	0.87	0.17	11,13,15,16	0
19	CLA	A	1122	55/65	0.87	0.15	13,14,18,18	0
19	CLA	B	1238	65/65	0.87	0.16	10,14,15,16	0
19	CLA	A	1139	51/65	0.87	0.17	16,16,17,18	0
21	BCR	B	6020	40/40	0.87	0.18	8,11,12,13	0
20	PQN	A	5001	33/33	0.87	0.19	12,13,14,15	0

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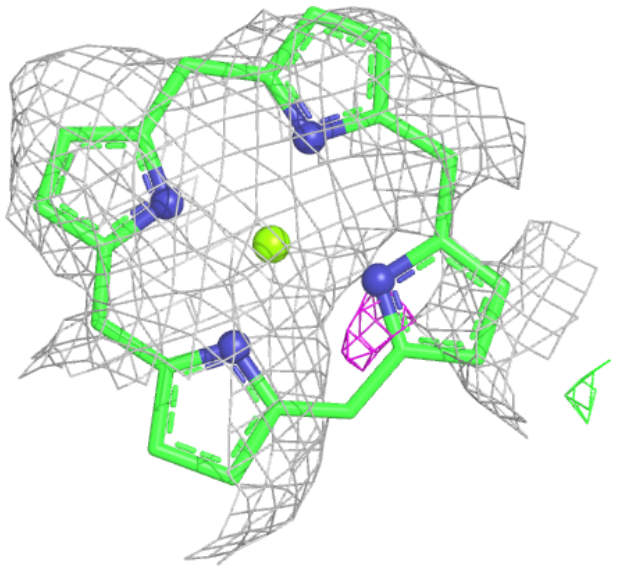
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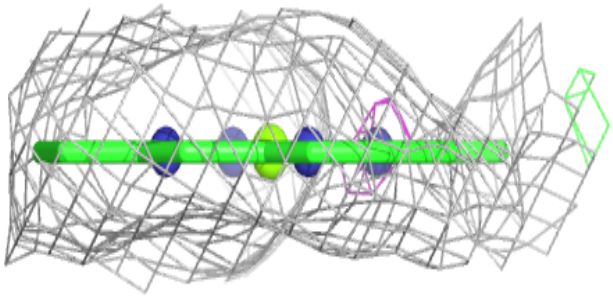
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	A	9012	65/65	0.87	0.16	2,14,28,36	0
19	CLA	A	1127	55/65	0.88	0.15	13,16,17,18	0
19	CLA	B	1205	65/65	0.88	0.18	9,13,14,14	0
19	CLA	A	9022	65/65	0.89	0.15	2,12,26,31	0
19	CLA	B	1221	54/65	0.89	0.17	13,13,16,16	0
19	CLA	B	1203	65/65	0.89	0.14	10,13,14,15	0
19	CLA	A	9023	65/65	0.89	0.17	2,14,29,38	0
20	PQN	B	5002	33/33	0.89	0.16	7,8,14,14	0
19	CLA	A	1137	47/65	0.89	0.14	13,14,15,17	0
19	CLA	B	1227	50/65	0.90	0.13	13,15,16,17	0
19	CLA	B	9010	65/65	0.90	0.16	2,12,34,40	0
19	CLA	A	9011	65/65	0.91	0.19	2,11,30,40	0
23	SF4	C	8002	8/8	0.98	0.07	14,16,24,28	0
23	SF4	C	8003	8/8	0.99	0.05	14,19,21,22	0
23	SF4	A	8001	8/8	0.99	0.07	12,17,19,21	0

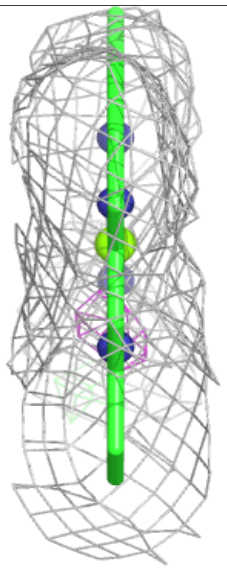
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CLA A 1309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

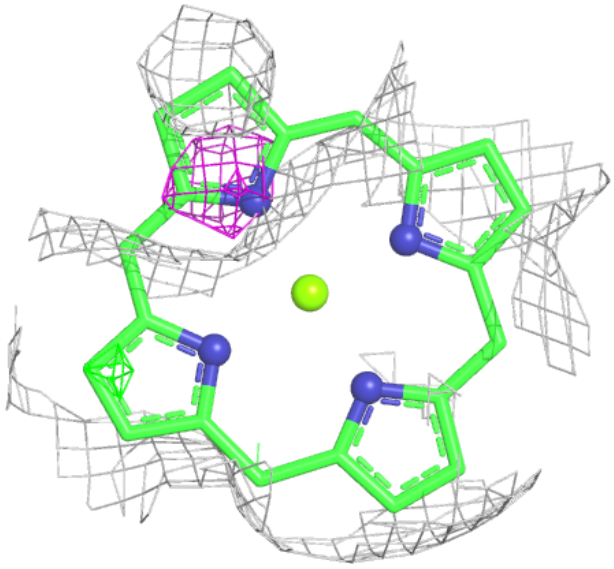


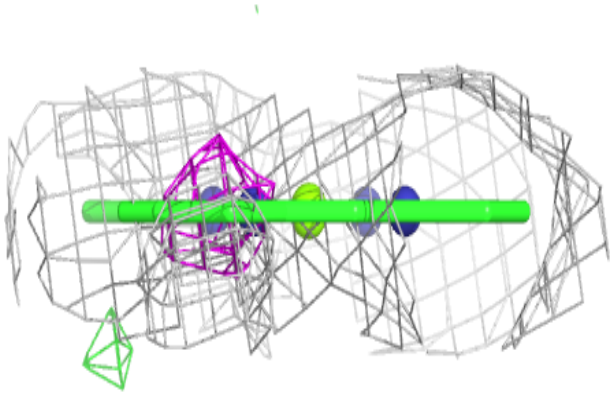


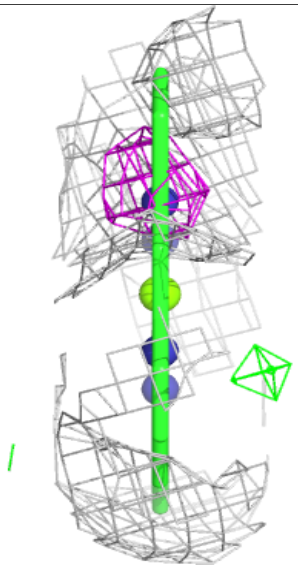


Electron density around CLA 3 3012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

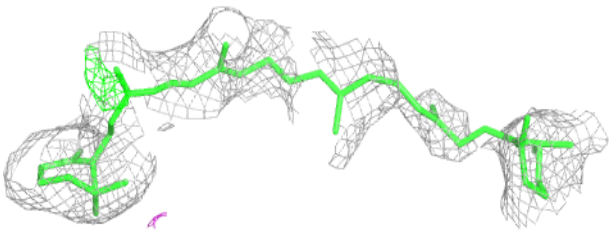


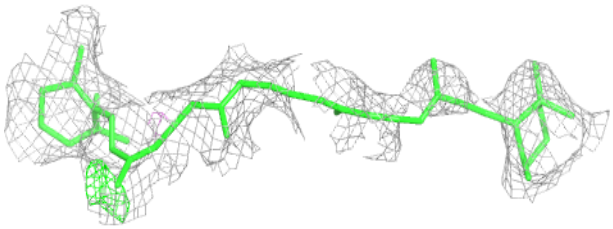


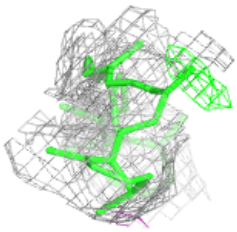


Electron density around BCR 1 6023:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

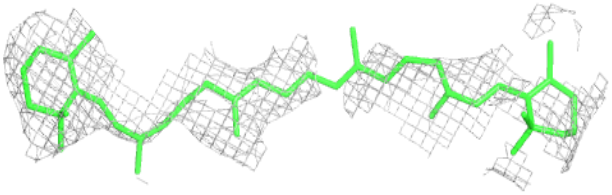


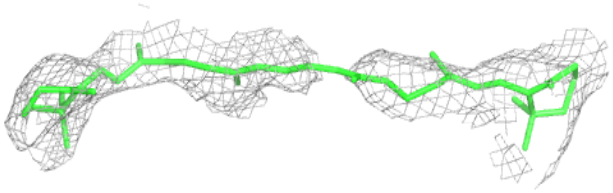


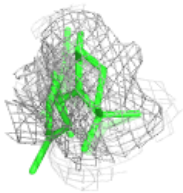


Electron density around BCR A 6002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

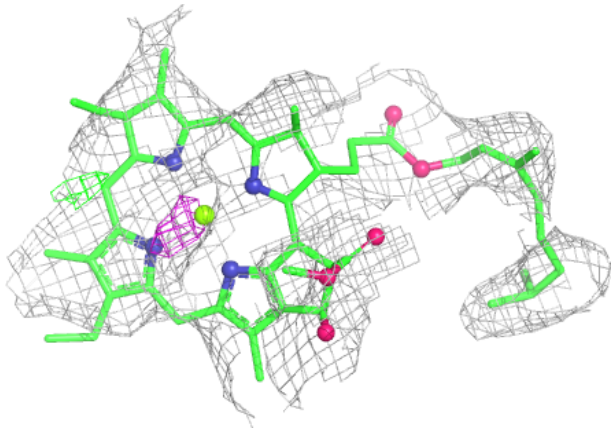


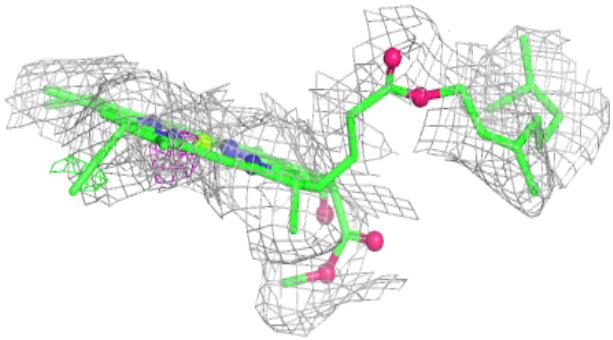


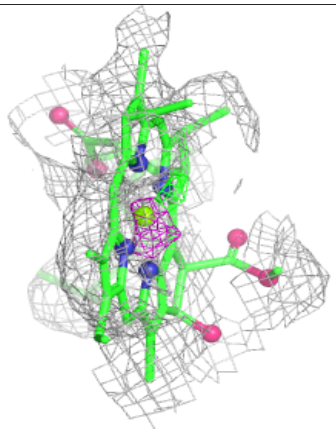


Electron density around CLA 4 4003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

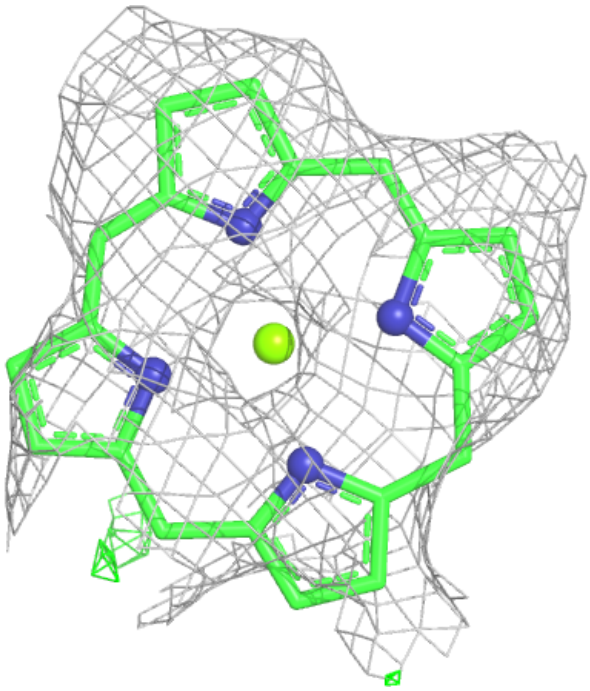


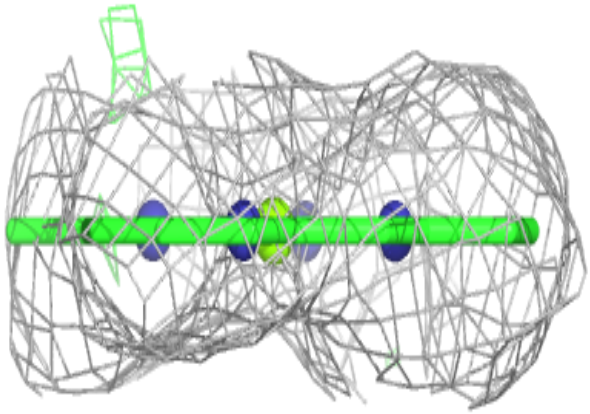


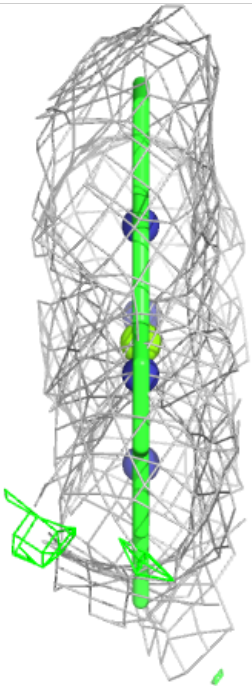


Electron density around CLA 1 1015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

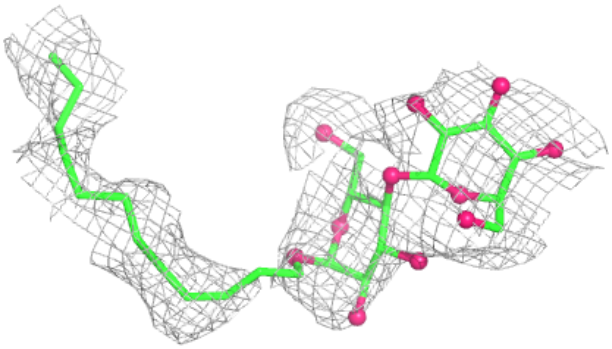


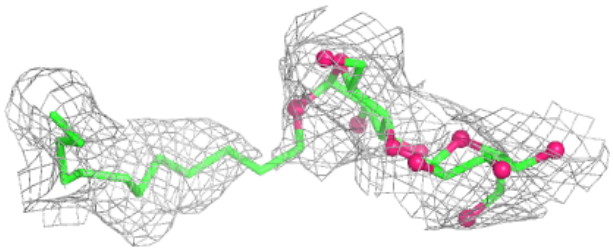


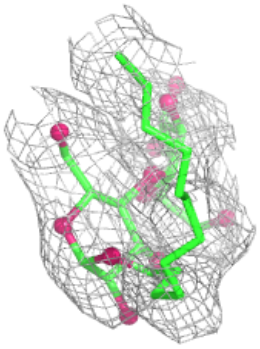


Electron density around LMU 1 7004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

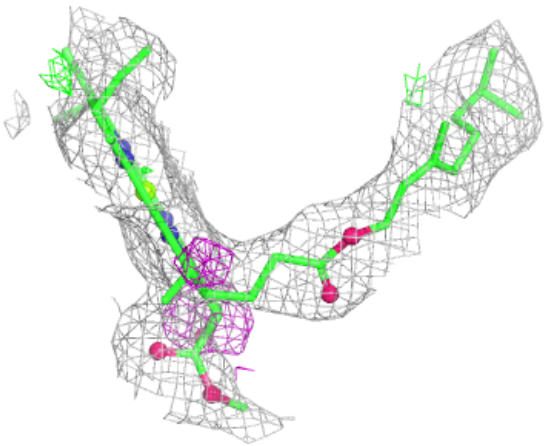


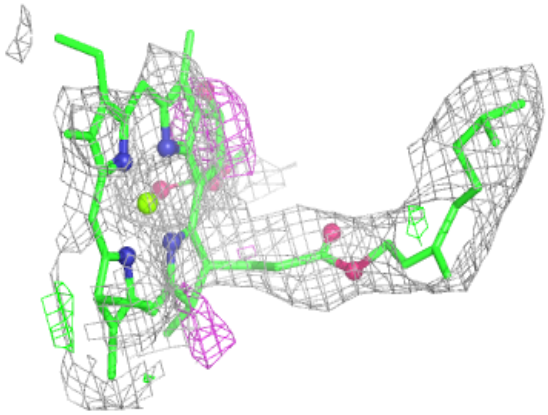


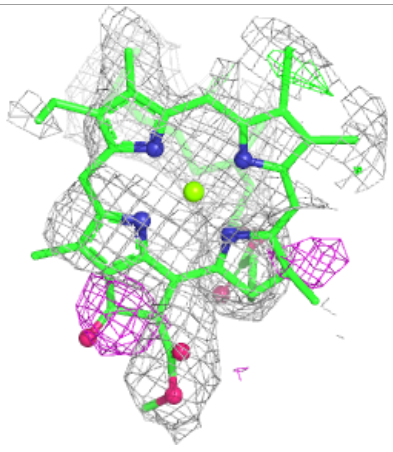


Electron density around CLA L 1504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

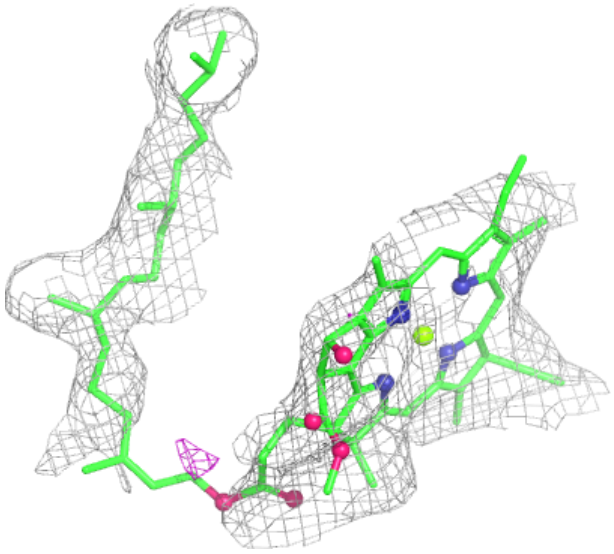


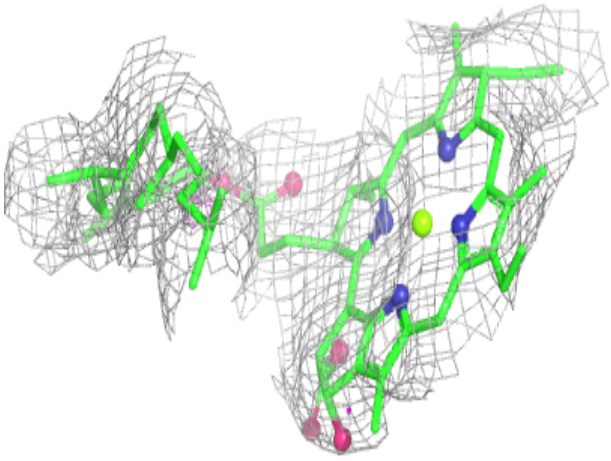


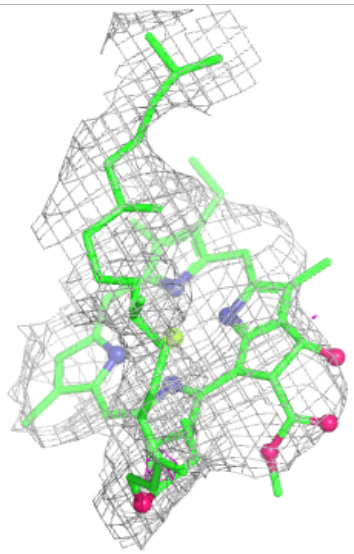


Electron density around CLA 3 3016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

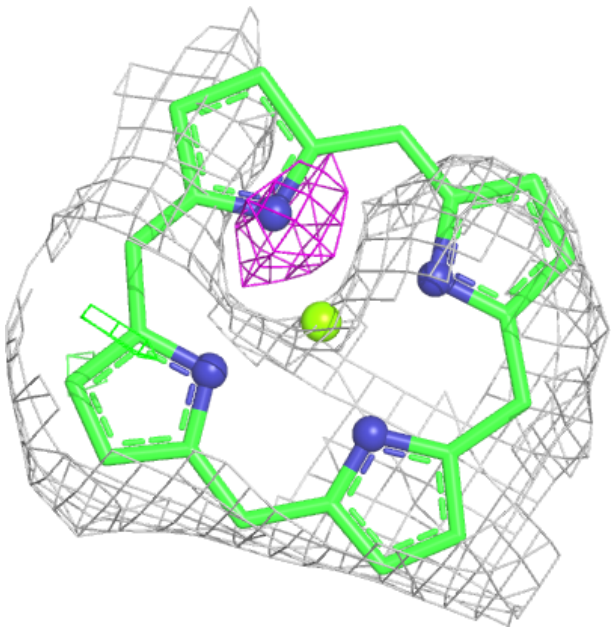


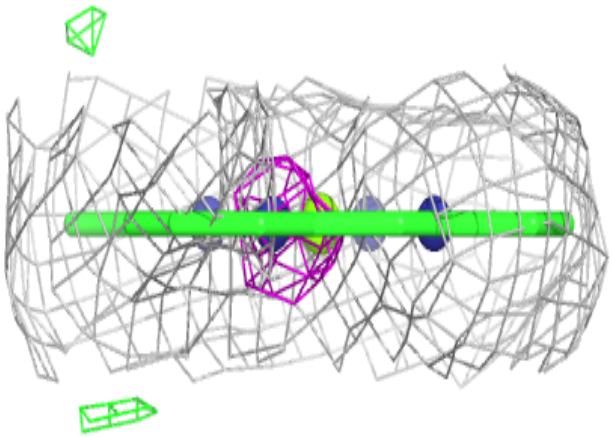


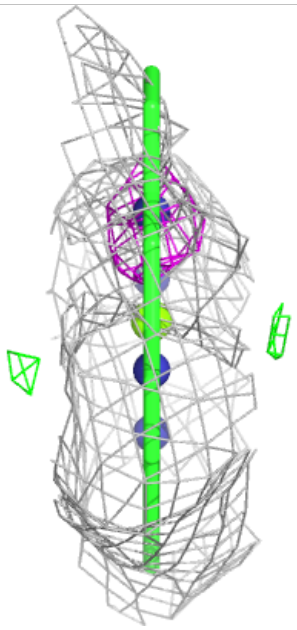


Electron density around CLA 3 3005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

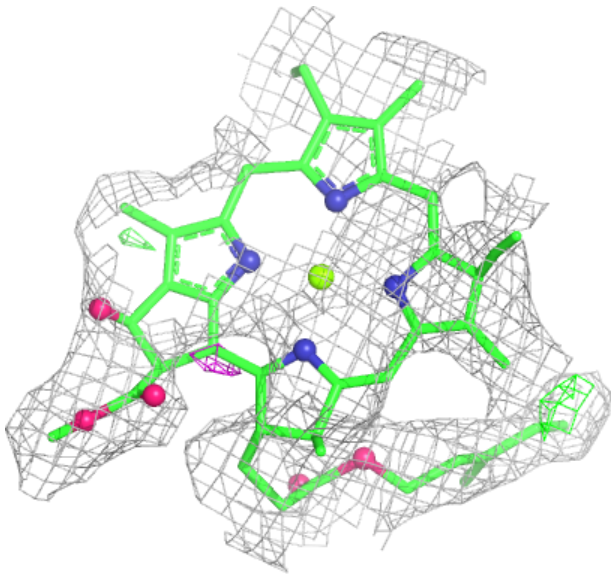


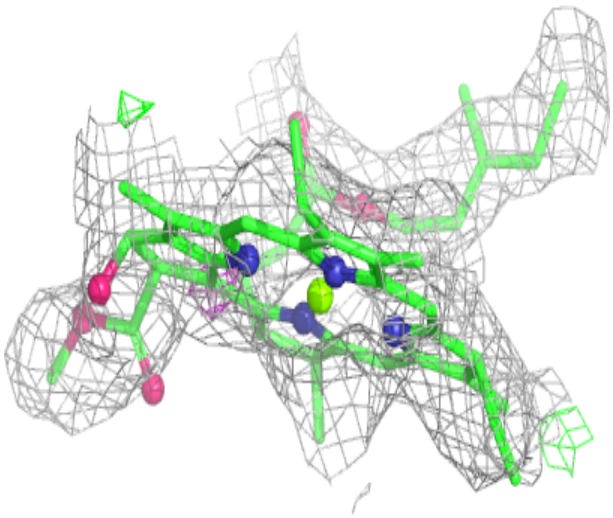


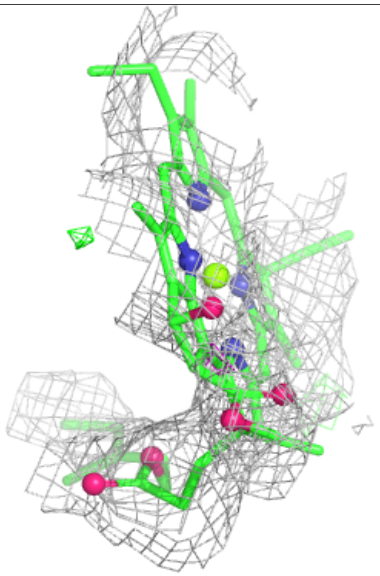


Electron density around CLA B 1233:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

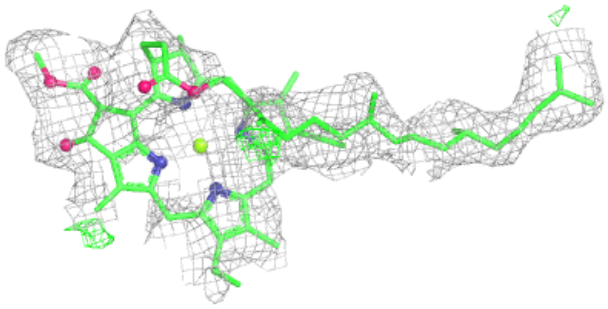


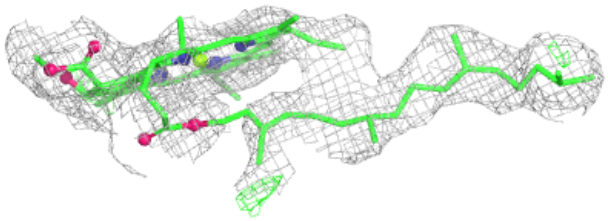


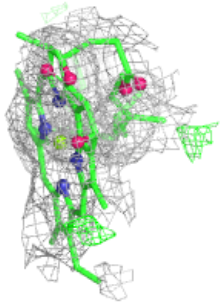


Electron density around CLA 2 2007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

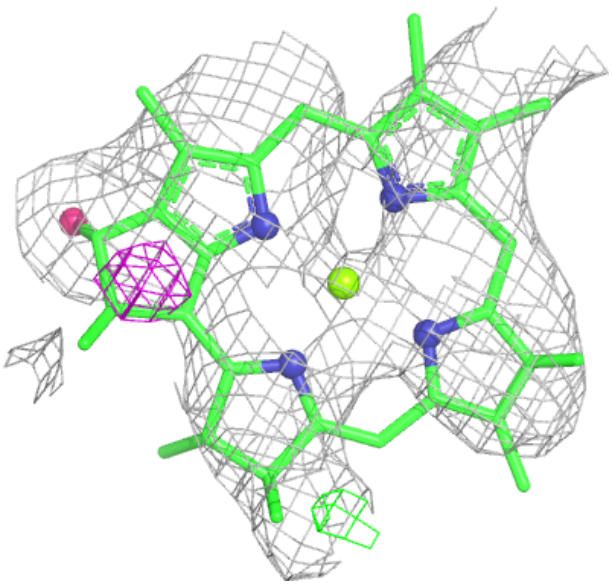


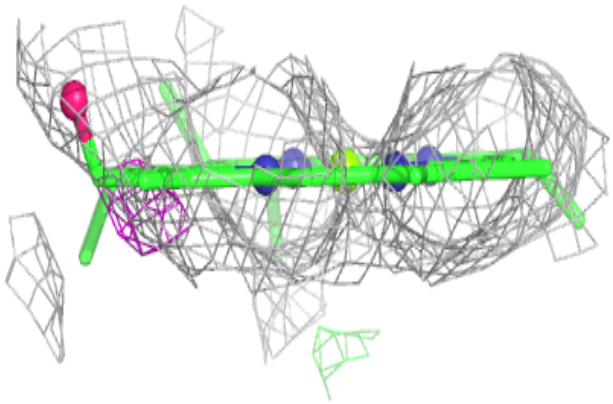




Electron density around CLA 1 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

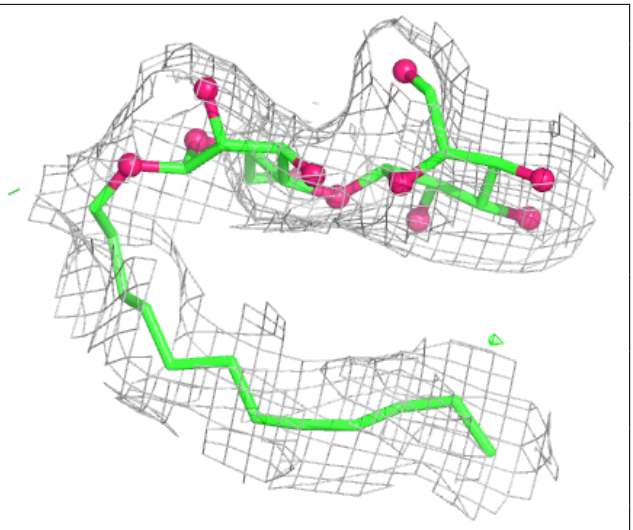


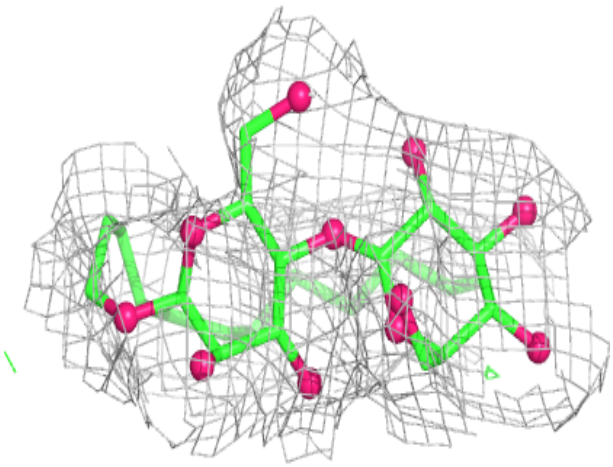


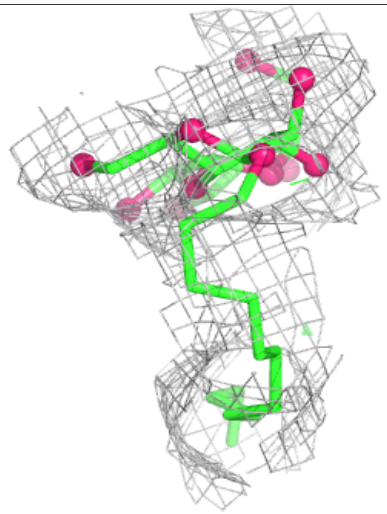


Electron density around LMU 1 7013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

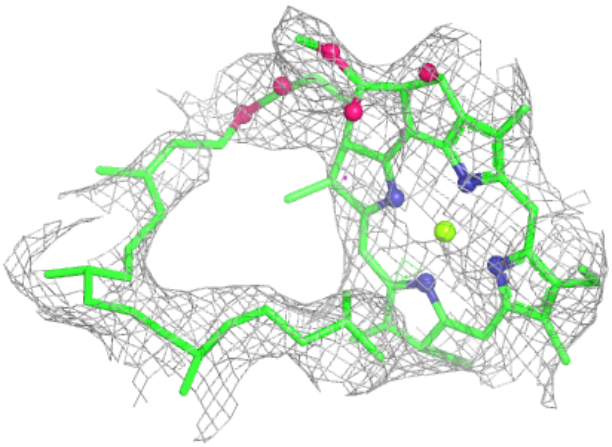


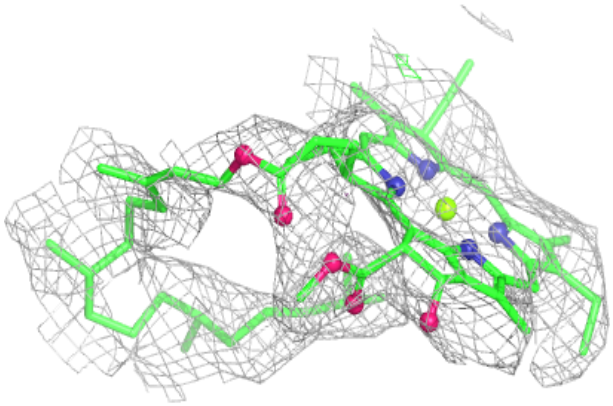




Electron density around CLA A 1141:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

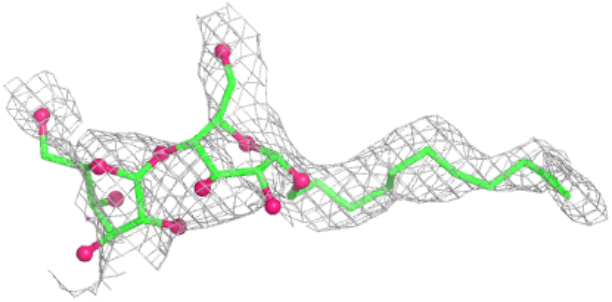


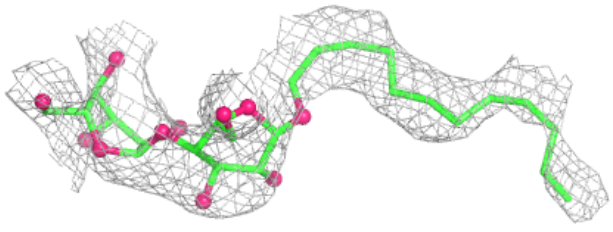


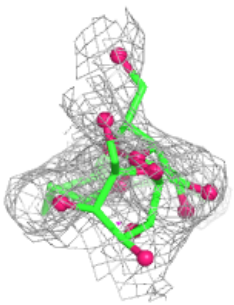


Electron density around LMU A 7010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

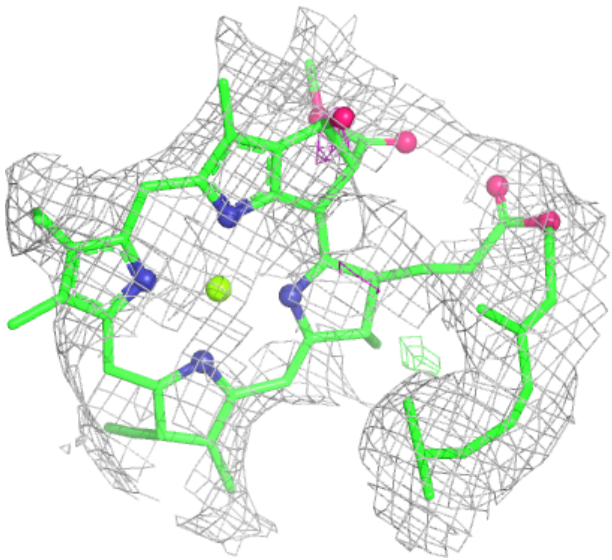


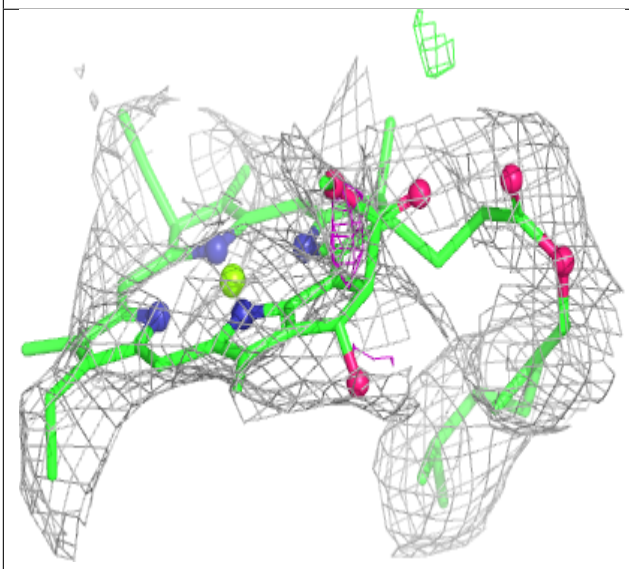


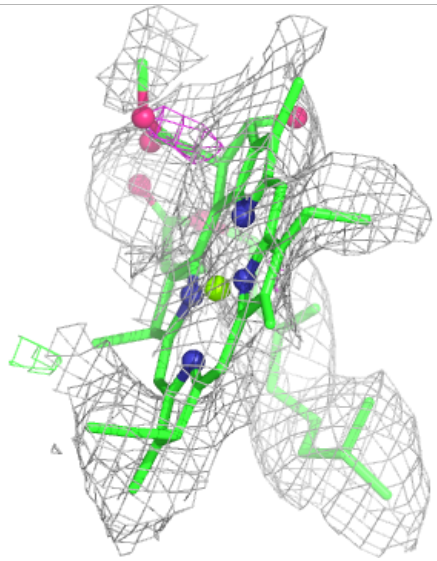


Electron density around CLA H 1505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

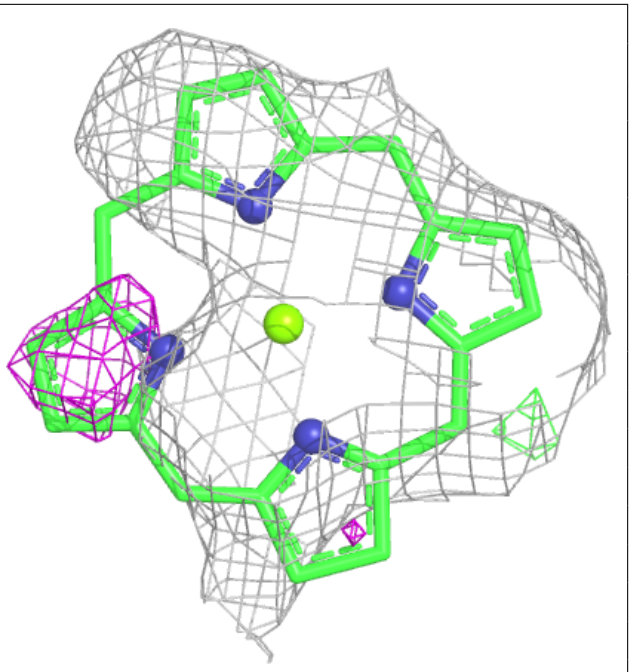


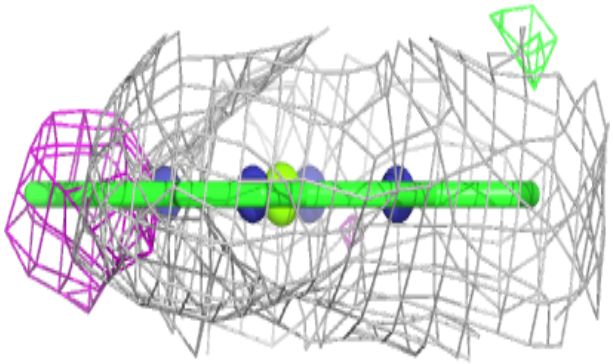


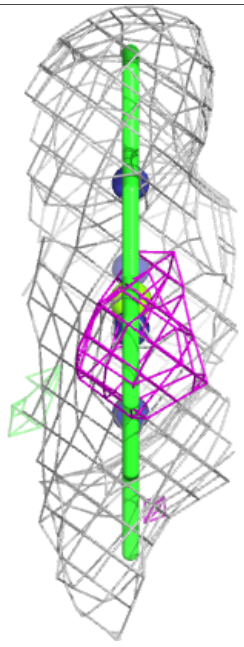


Electron density around CLA 3 3014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

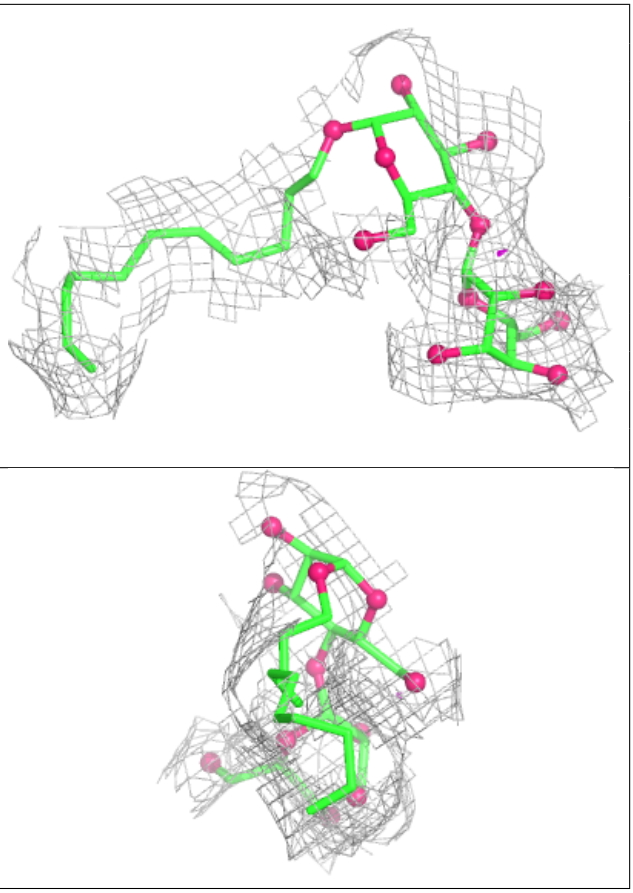






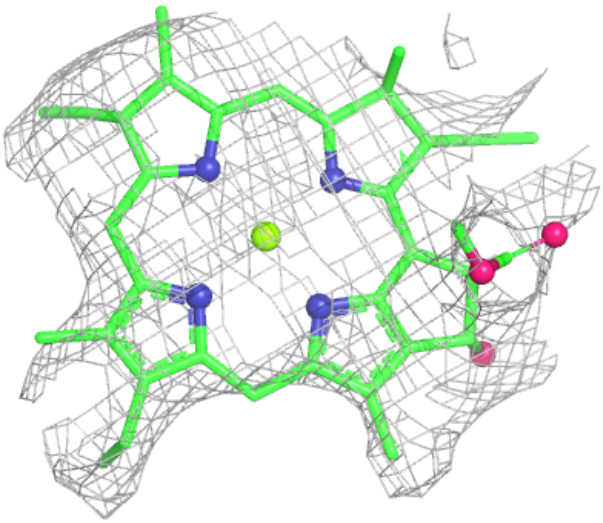
Electron density around LMU 4 7053:

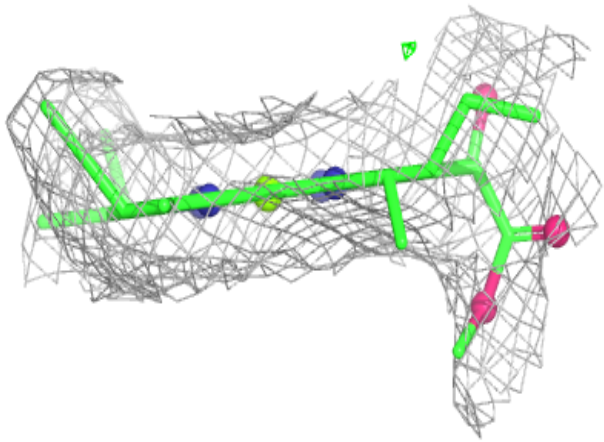
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

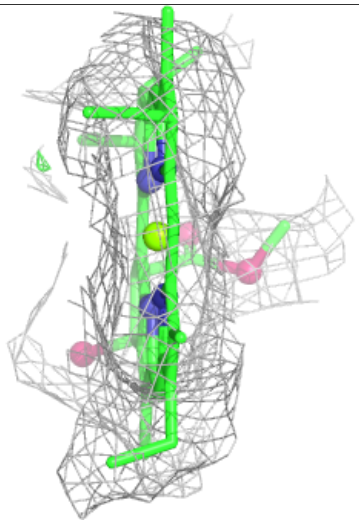


Electron density around CLA 3 3007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

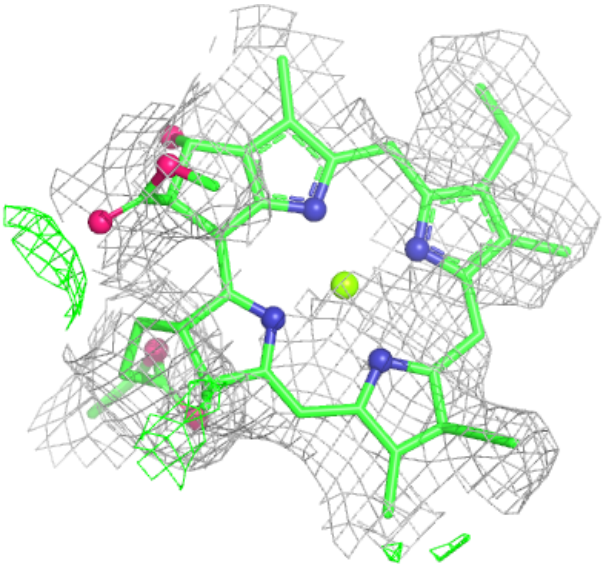


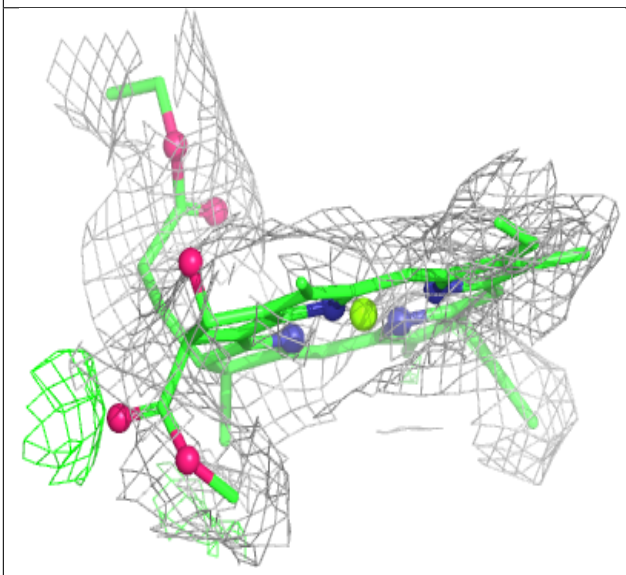


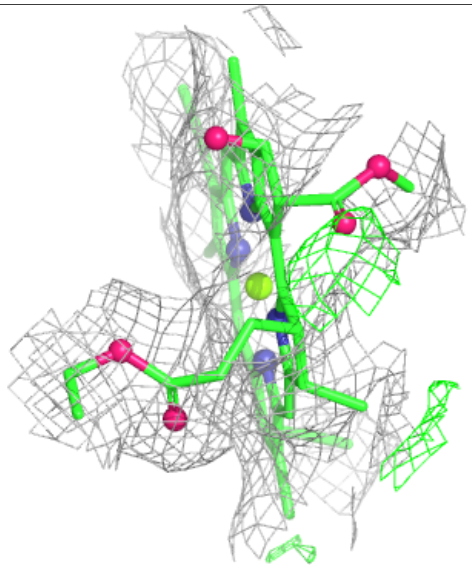


Electron density around CLA 4 4014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

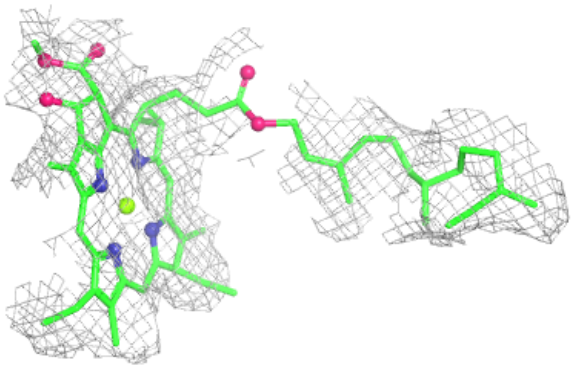


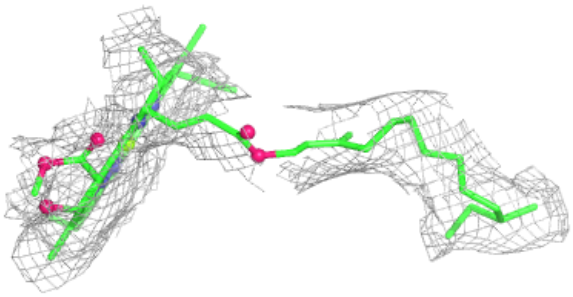


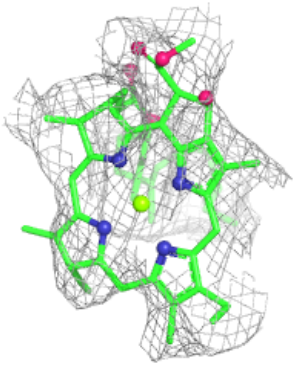


Electron density around CLA 2 2014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

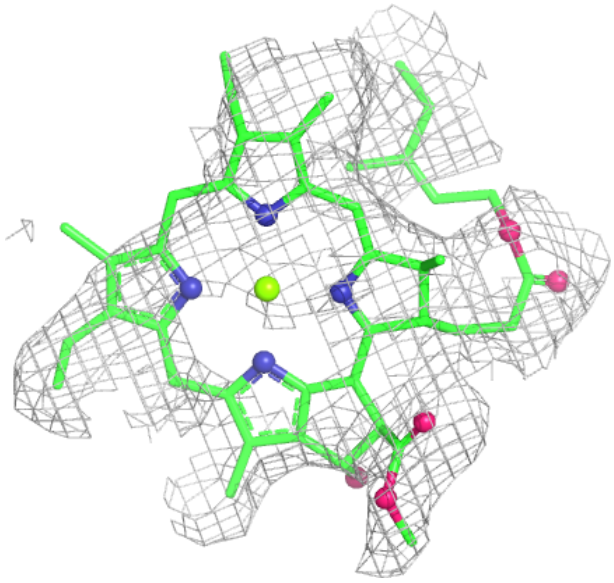


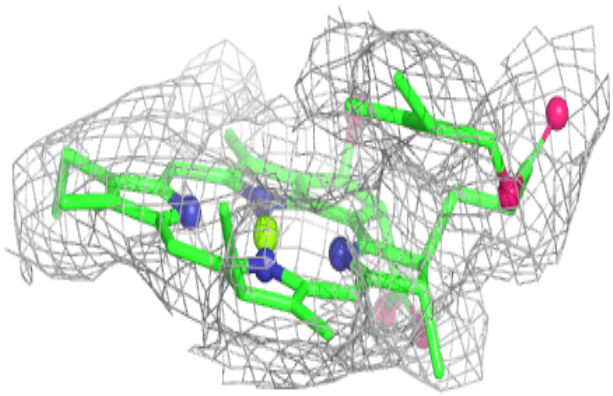


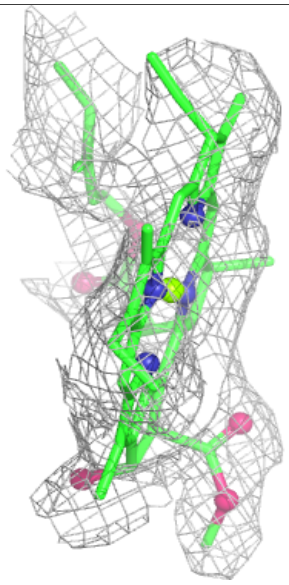


Electron density around CLA G 1242:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

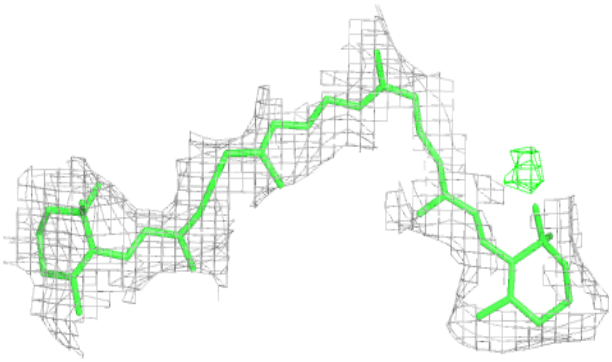


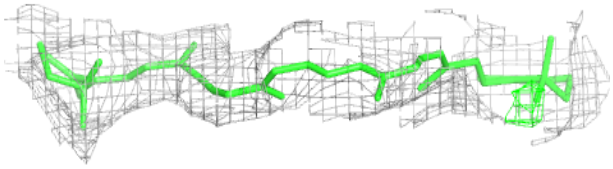




Electron density around BCR 3 6022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

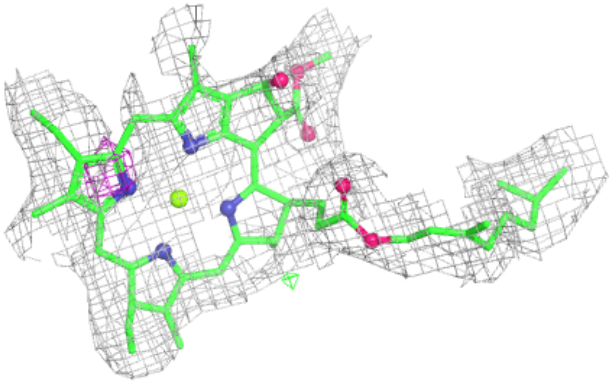


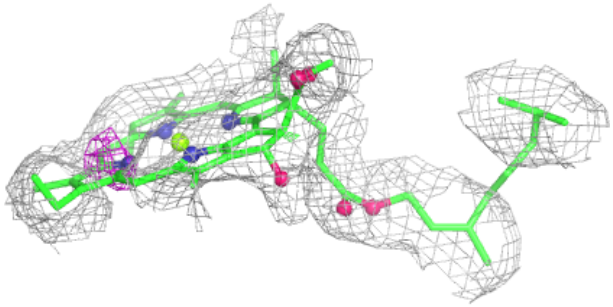


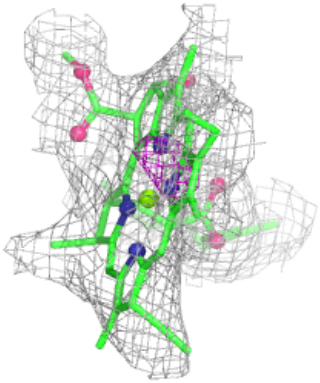


Electron density around CLA H 1241:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

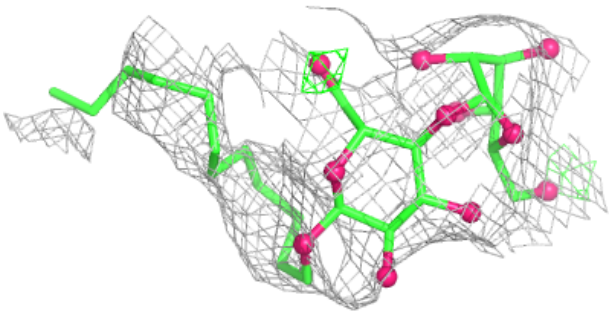


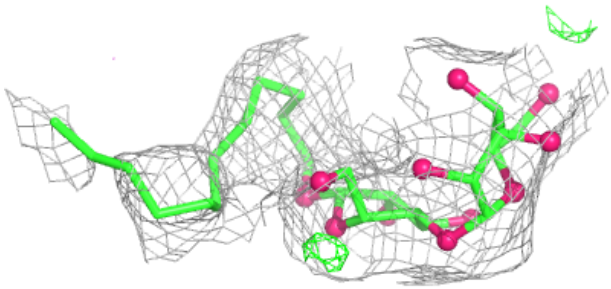


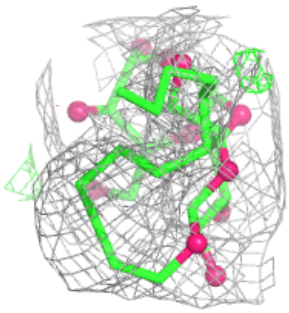


Electron density around LMU L 7029:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

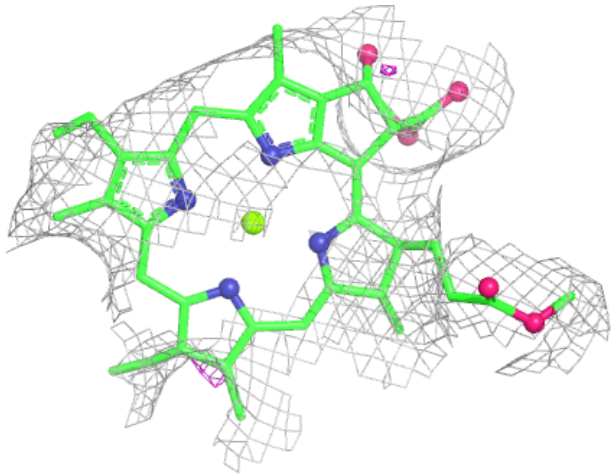


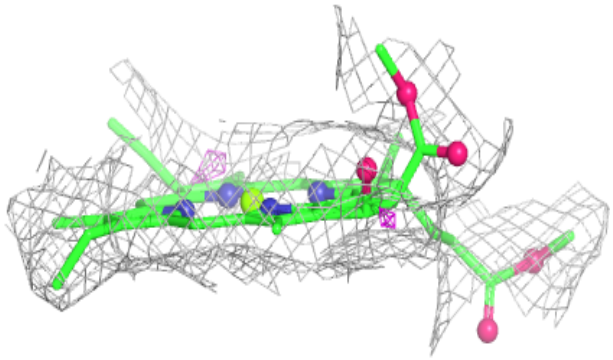


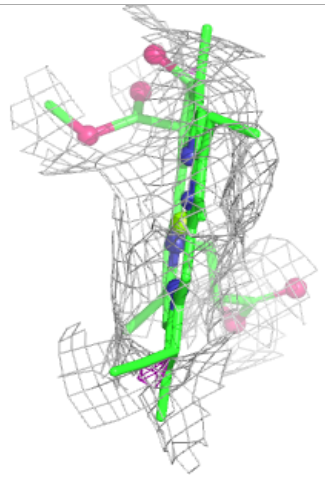


Electron density around CLA 1 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

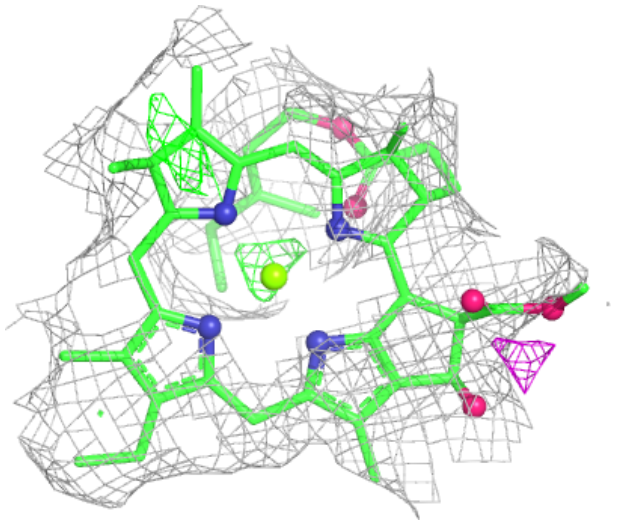


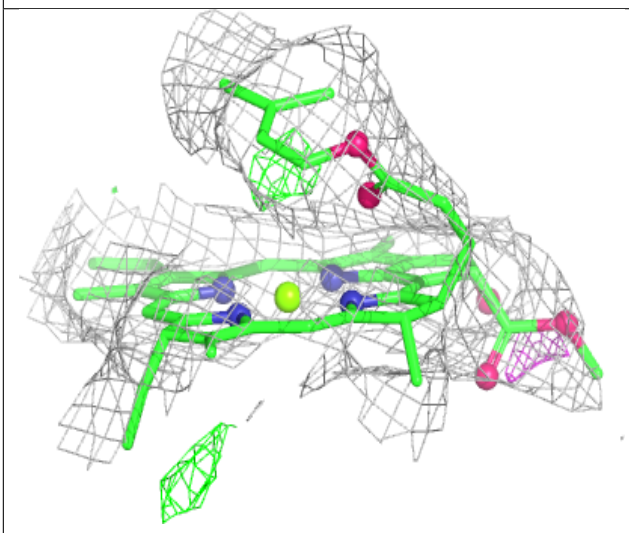


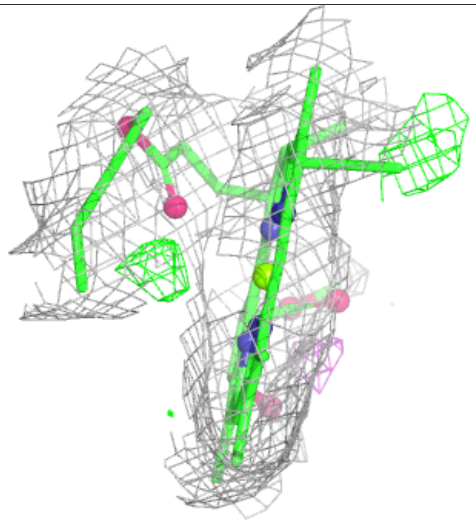


Electron density around CLA 2 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

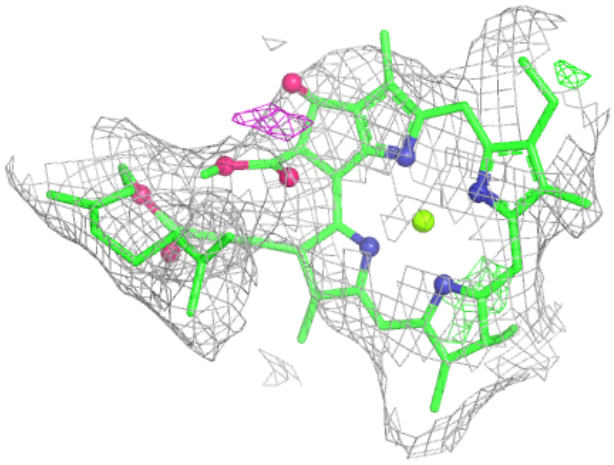


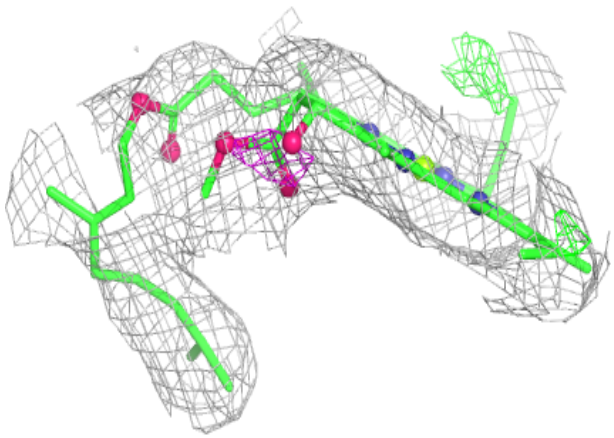


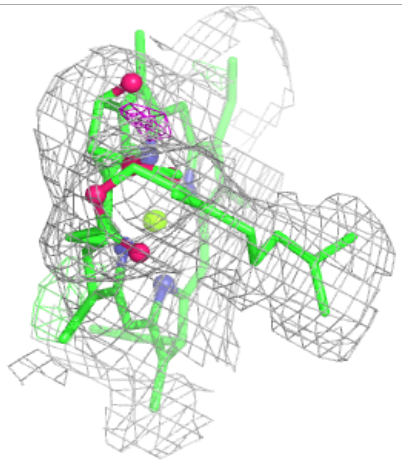


Electron density around CLA L 1148:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

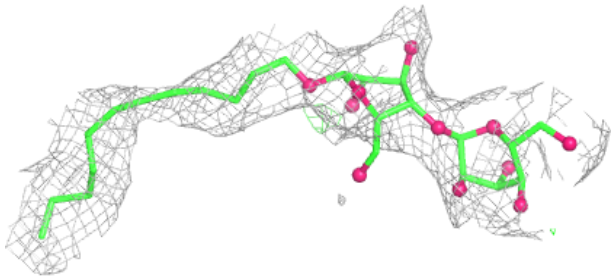


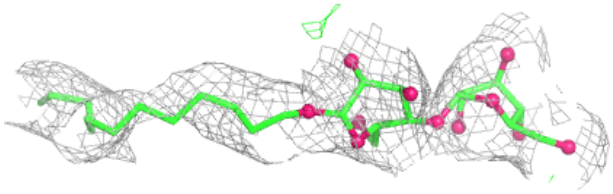


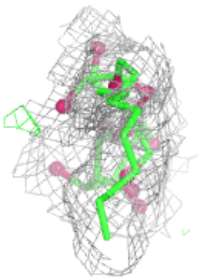


Electron density around LMU G 7051:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

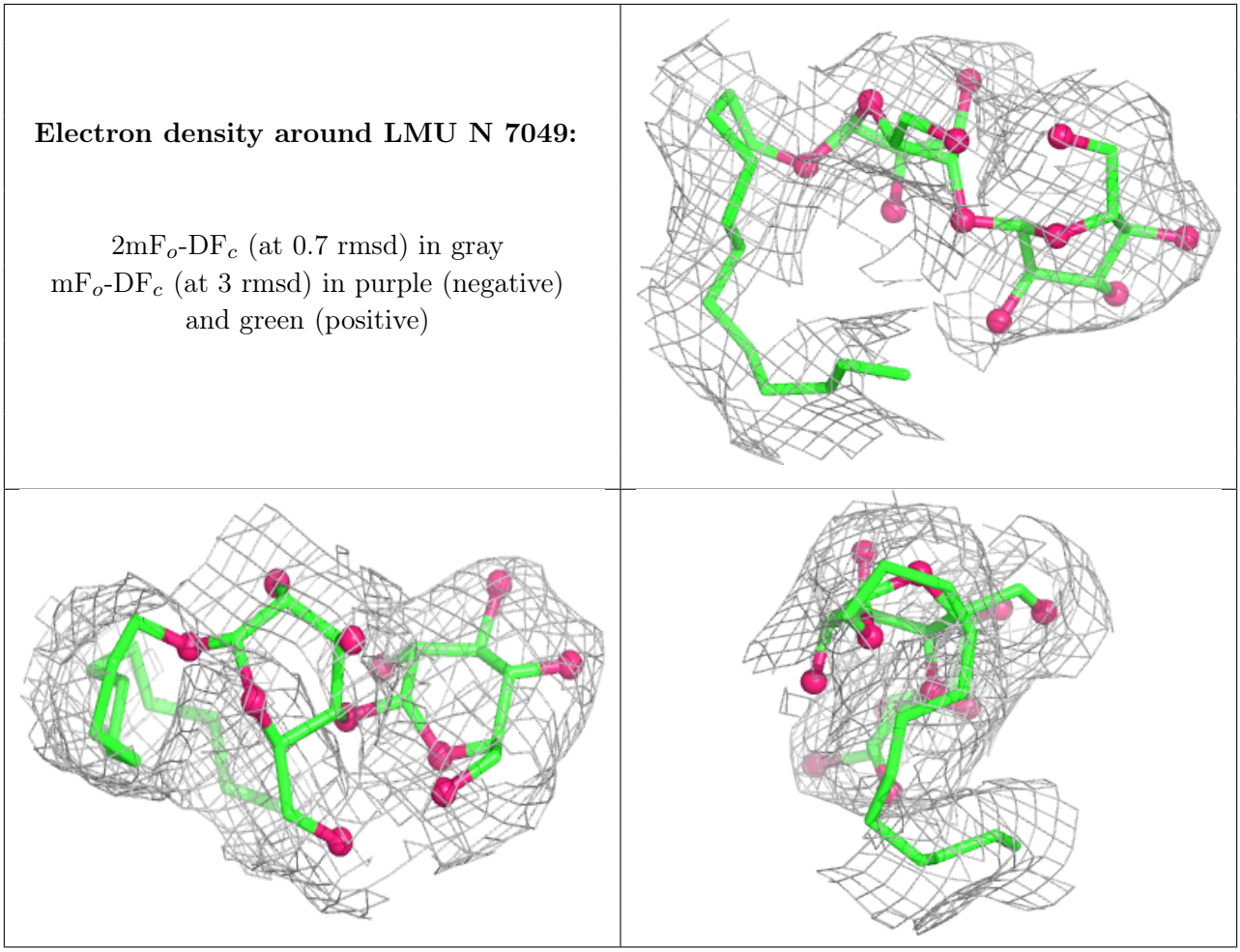






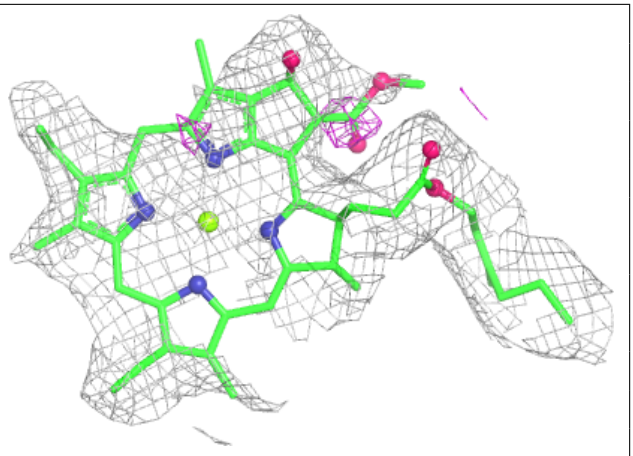
Electron density around LMU N 7049:

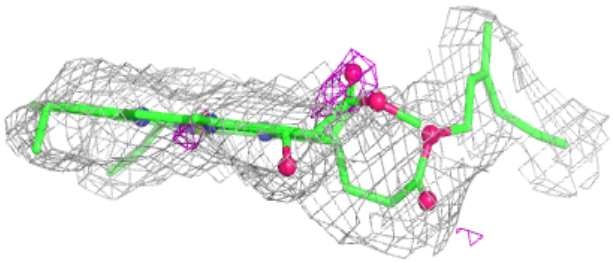
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

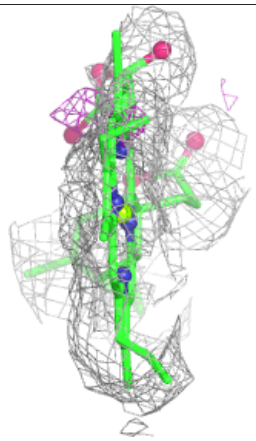


Electron density around CLA 4 4007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

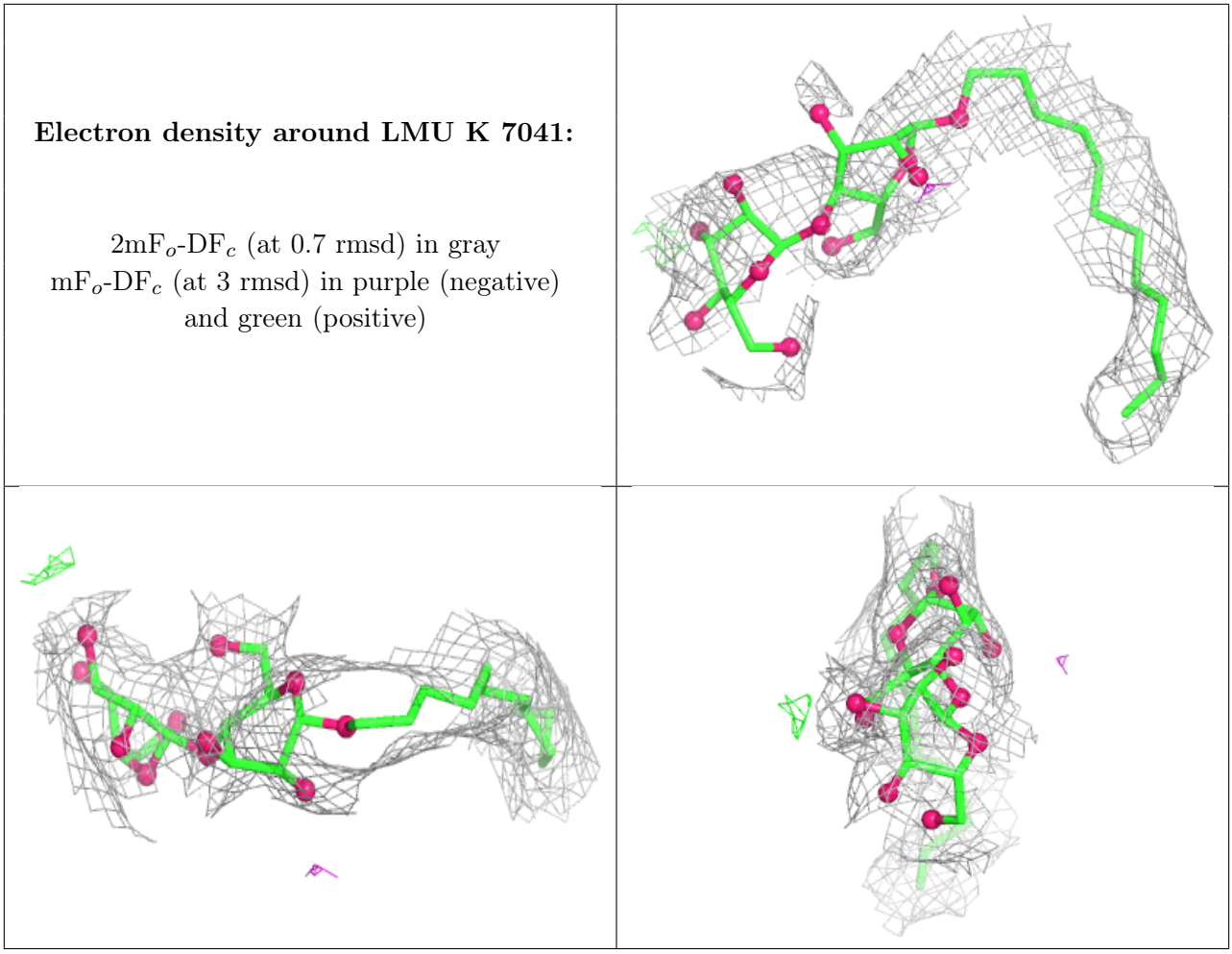






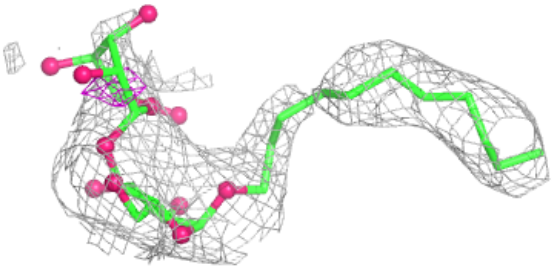
Electron density around LMU K 7041:

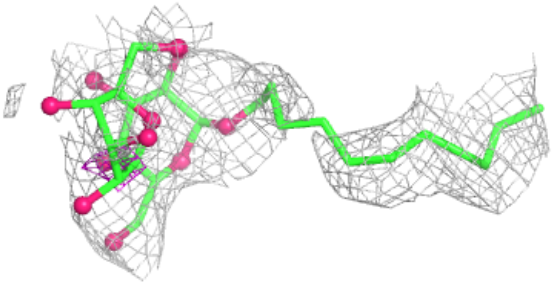
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

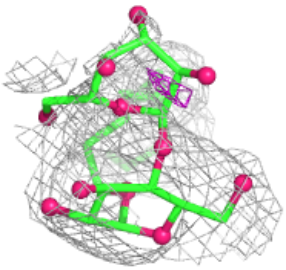


Electron density around LMU 4 7009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

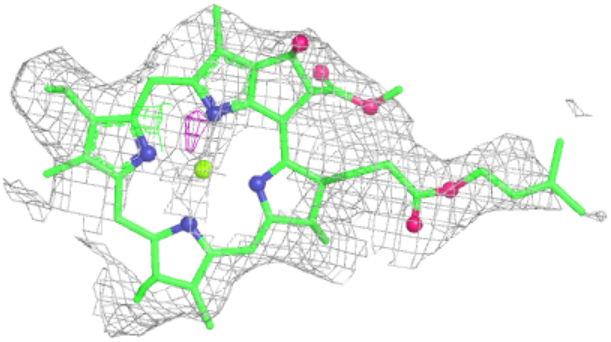


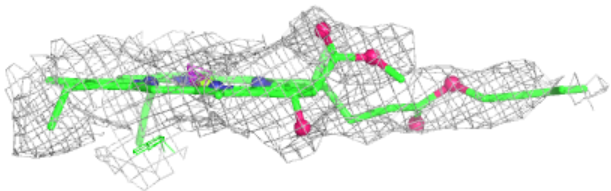




Electron density around CLA A 1151:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

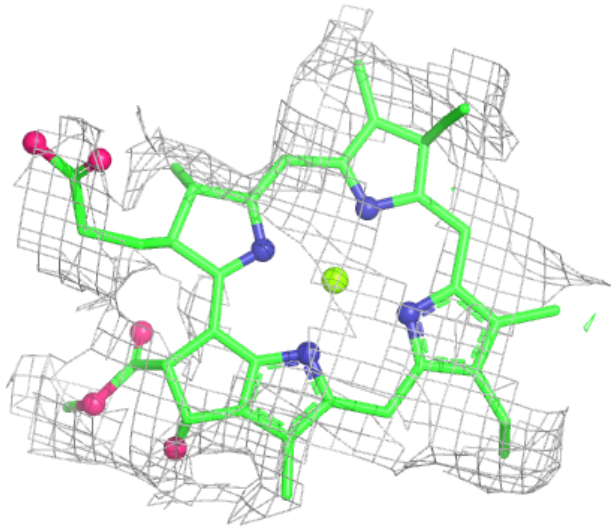


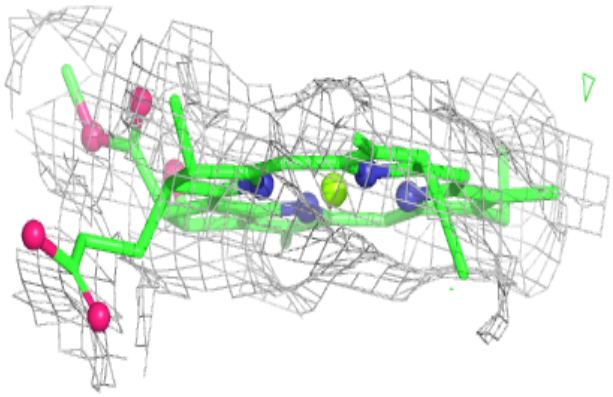


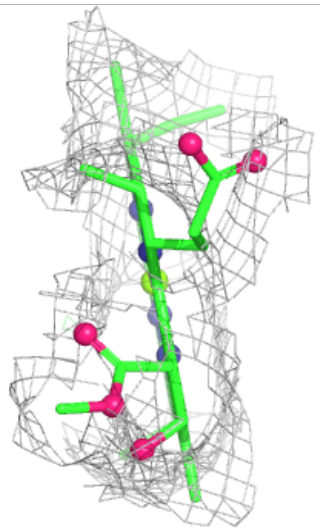


Electron density around CLA K 1142:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

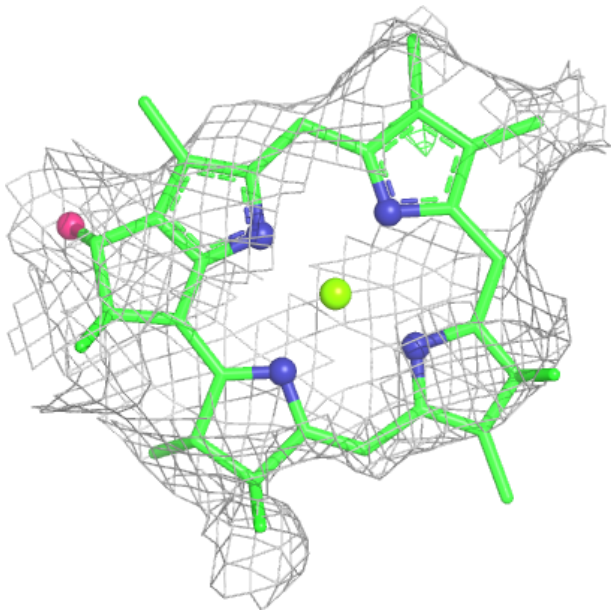


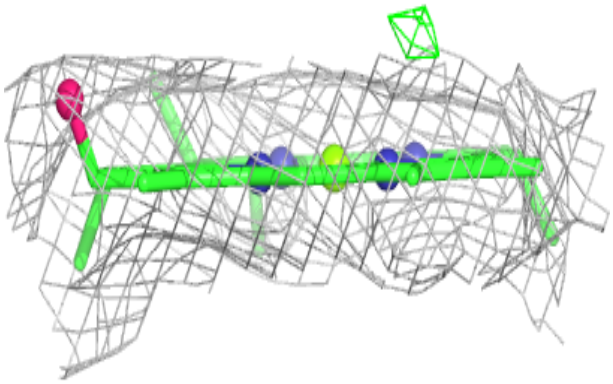


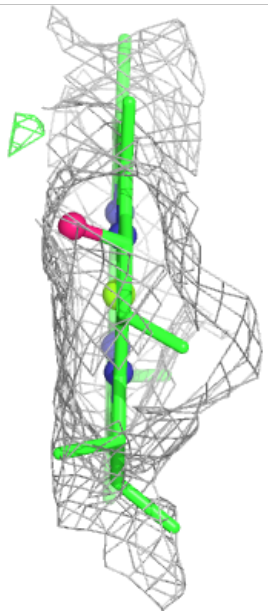


Electron density around CLA 3 1118:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

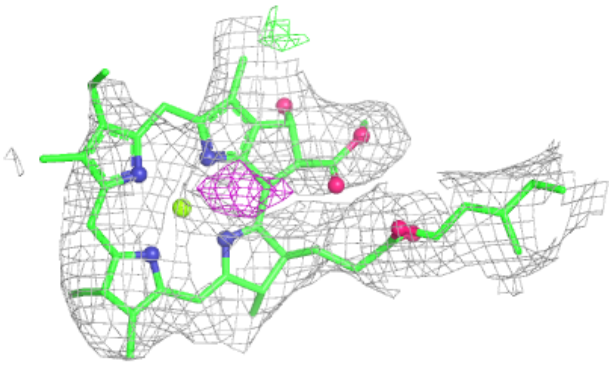


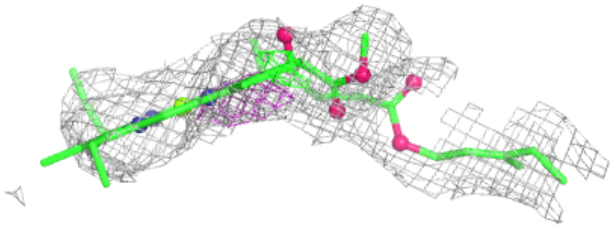


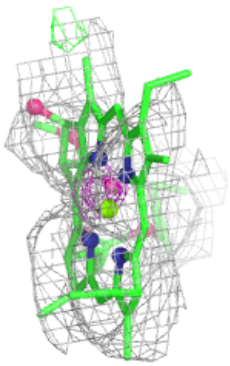


Electron density around CLA 1 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

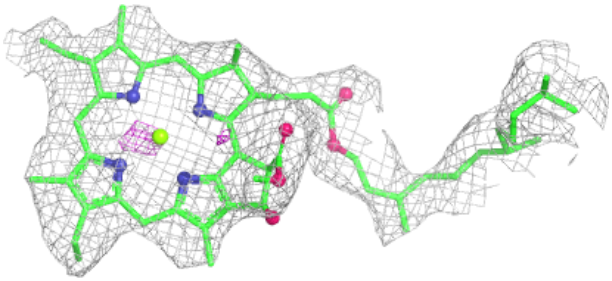


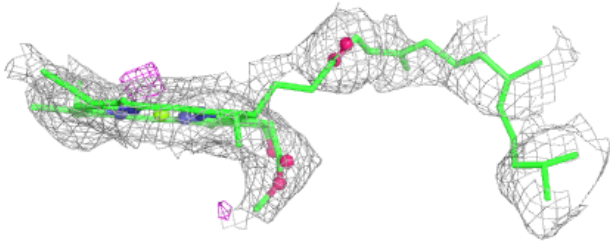


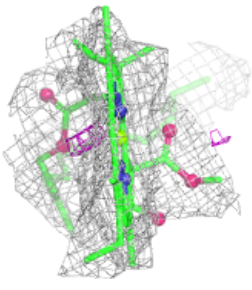


Electron density around CLA B 1212:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

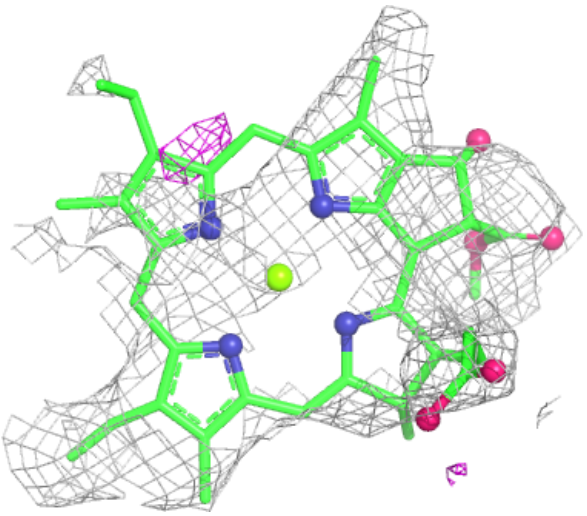


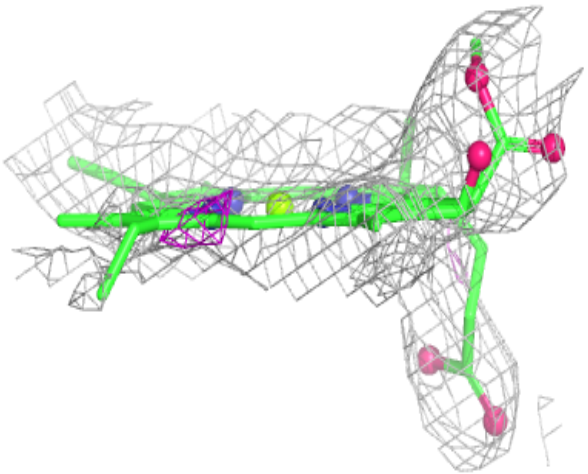




Electron density around CLA A 1112:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

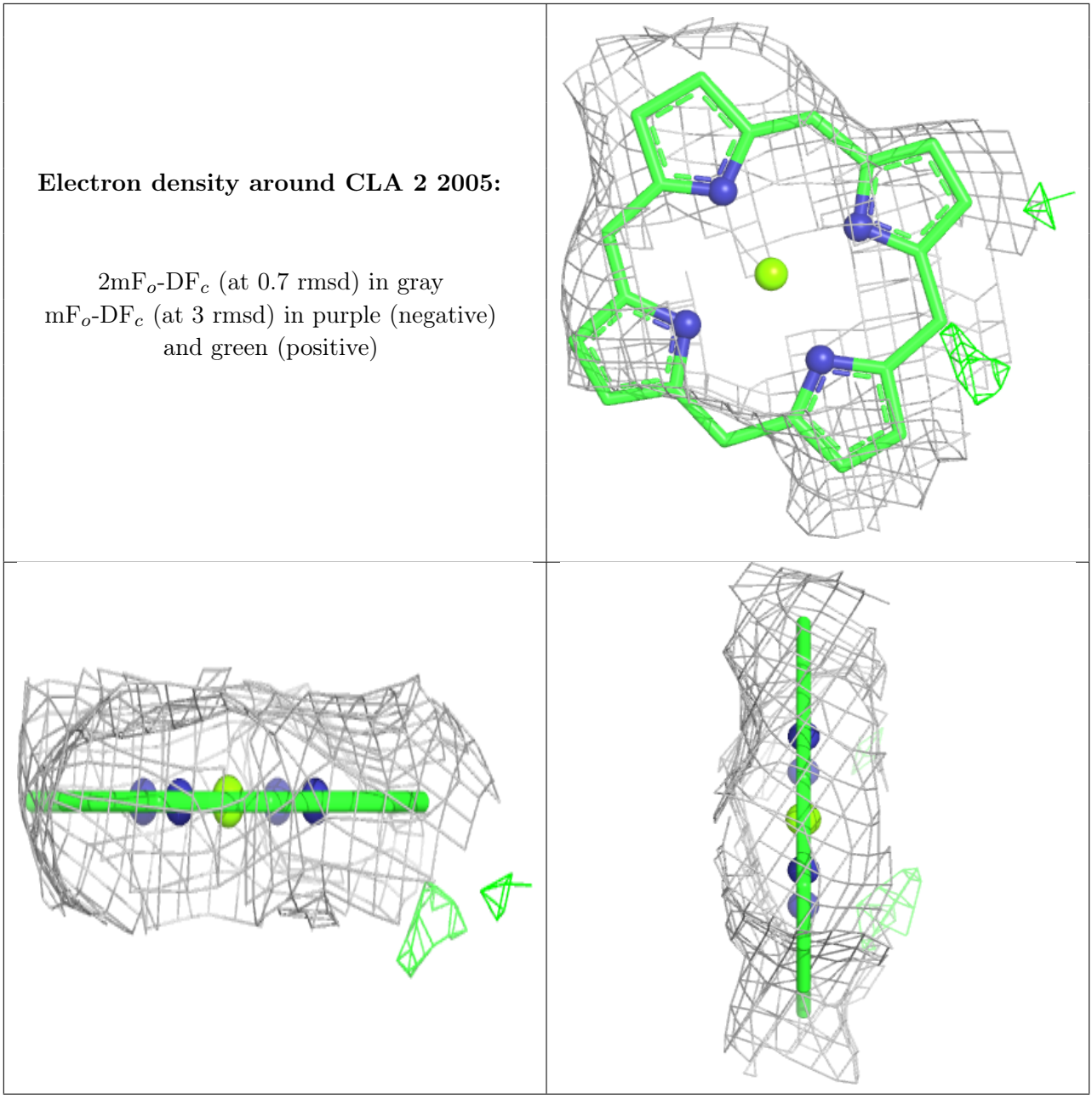






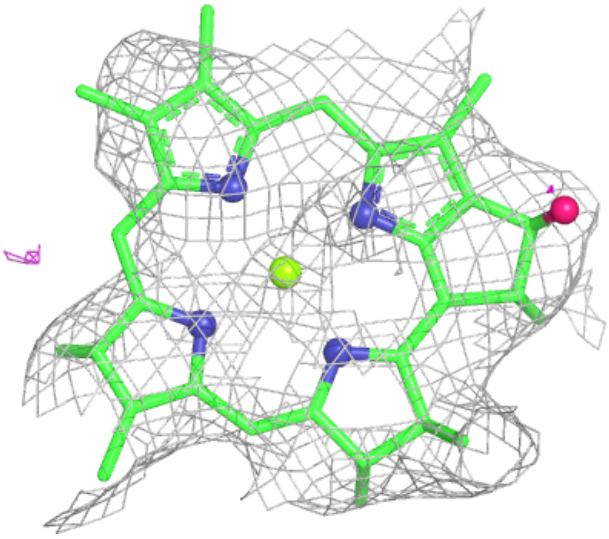
Electron density around CLA 2 2005:

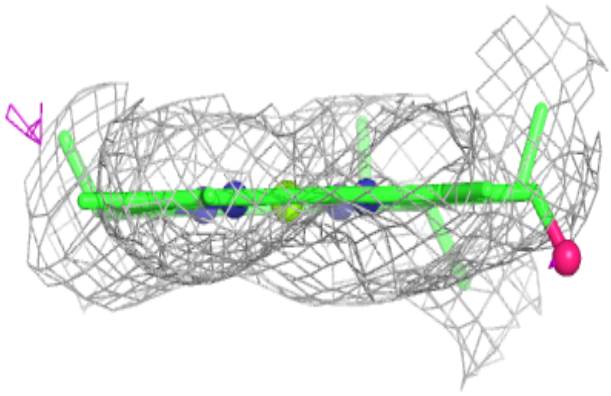
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

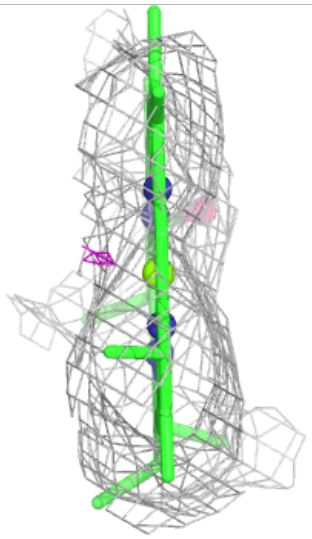


Electron density around CLA B 1301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

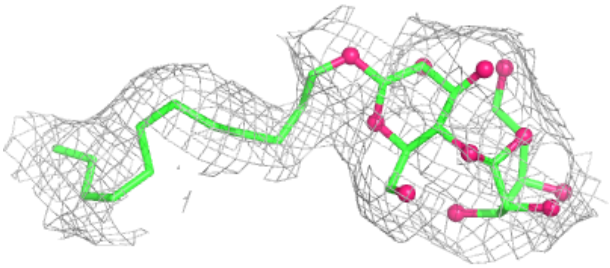


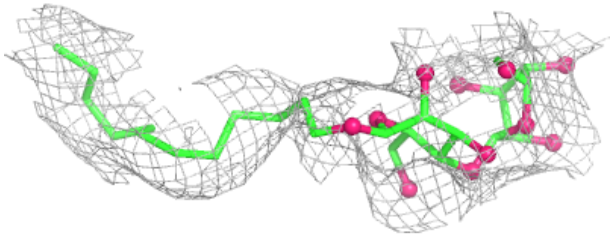


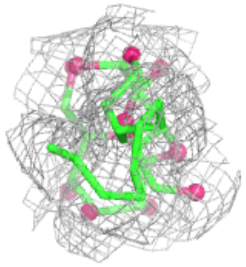


Electron density around LMU E 7048:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

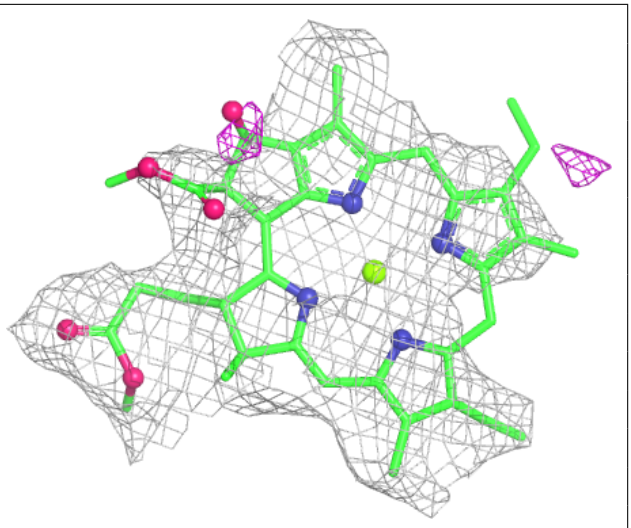


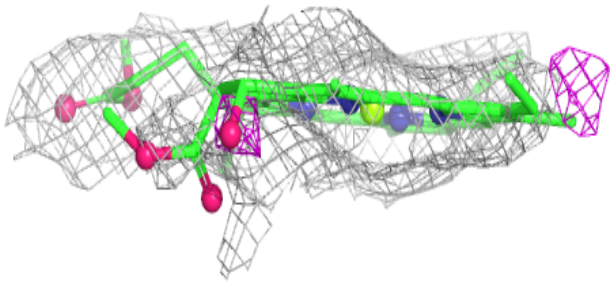


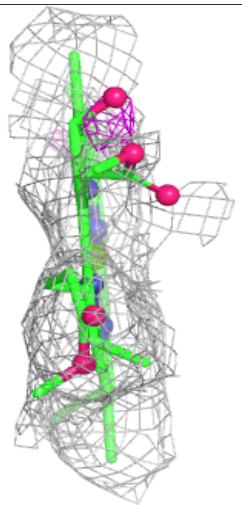


Electron density around CLA B 1213:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

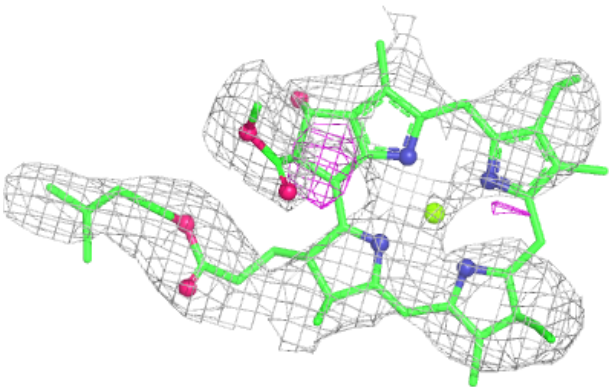


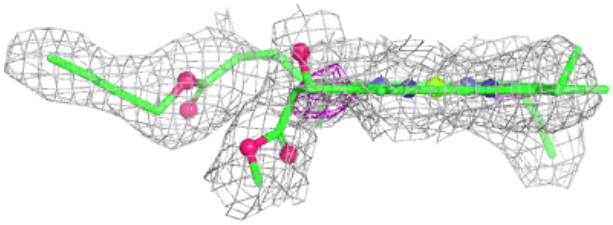


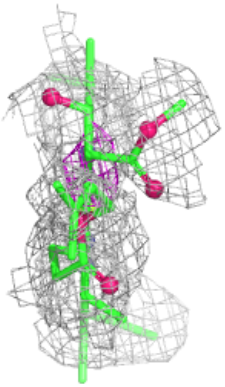


Electron density around CLA 4 4001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

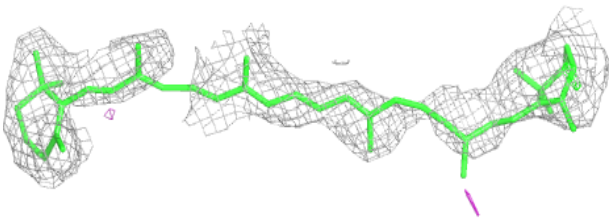


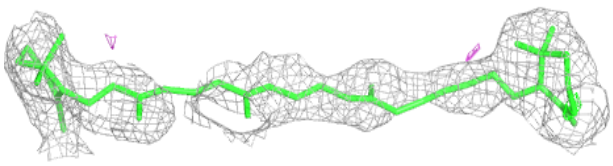


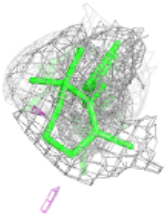


Electron density around BCR J 6012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

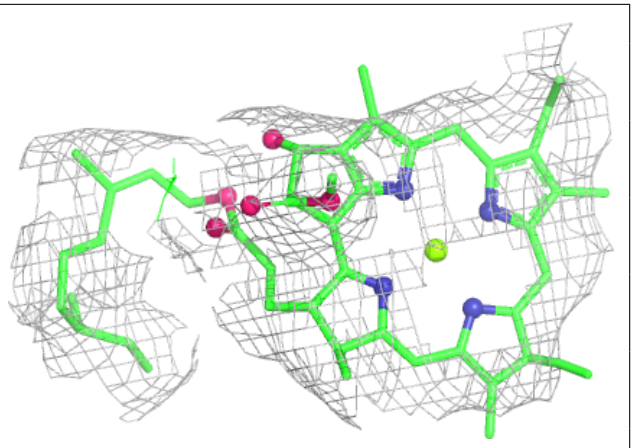


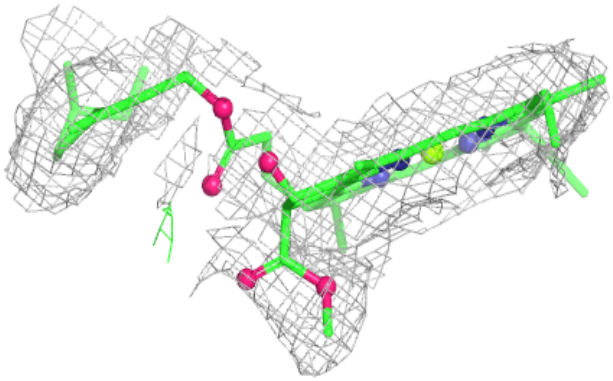


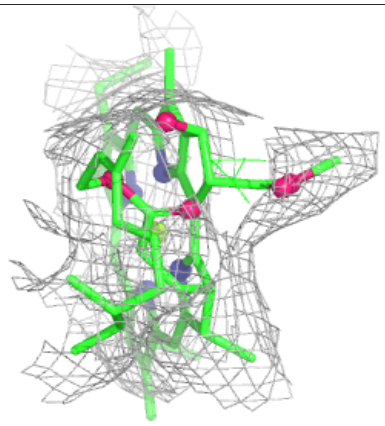


Electron density around CLA 3 2009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

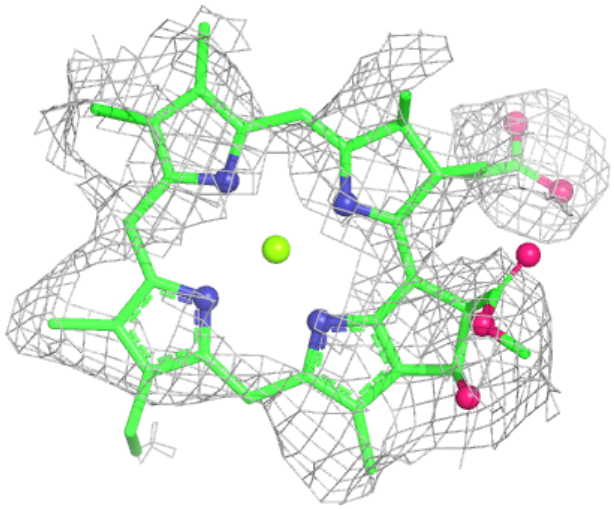


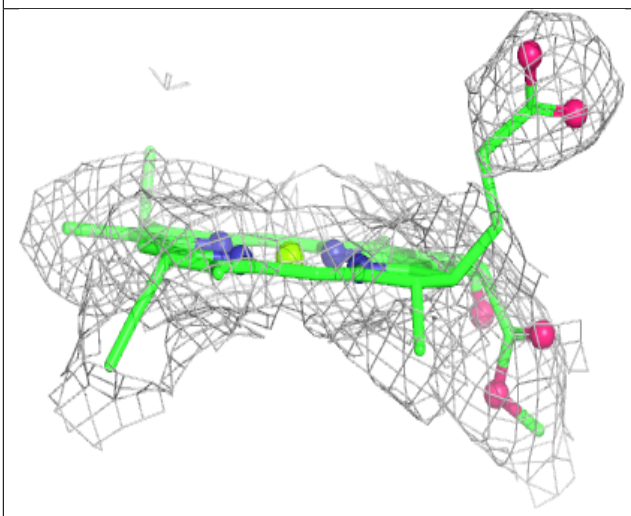


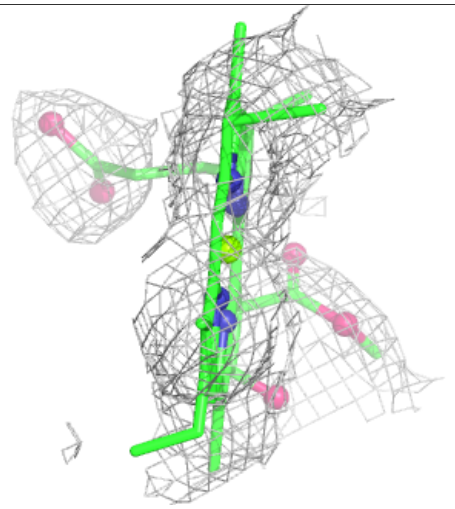


Electron density around CLA B 1232:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

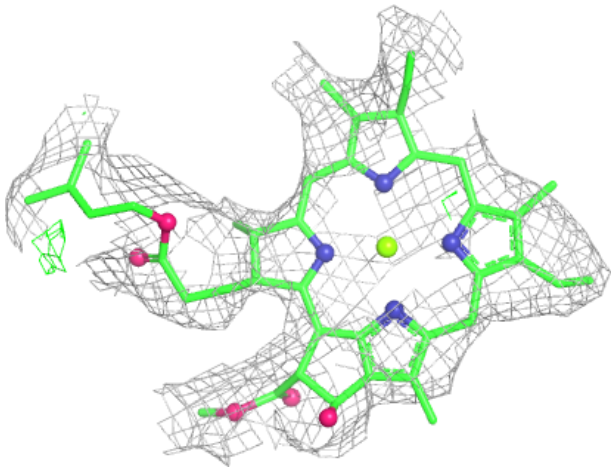


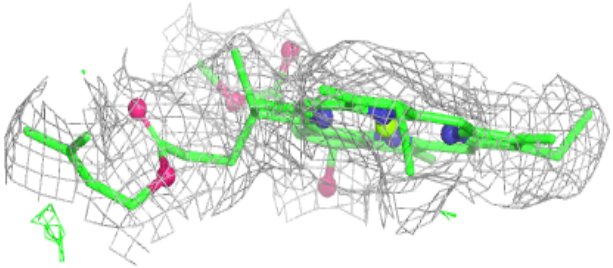


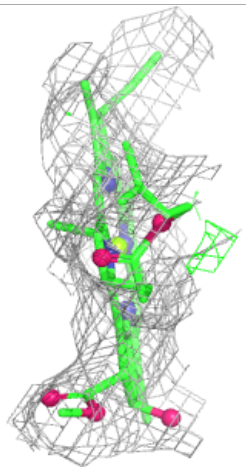


Electron density around CLA 2 2004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

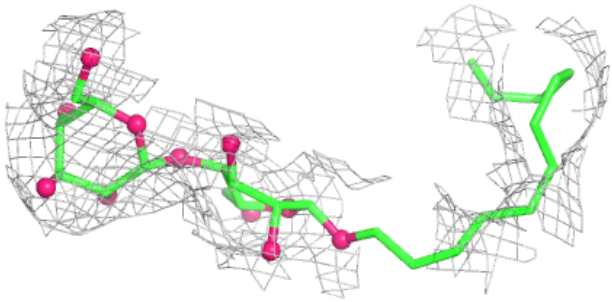


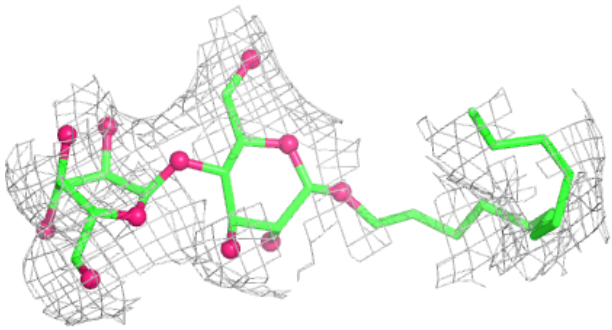


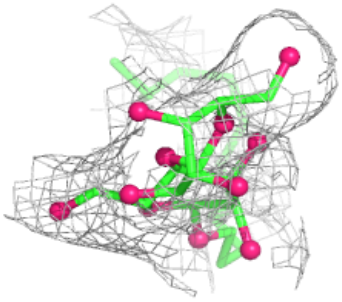


Electron density around LMU H 7043:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

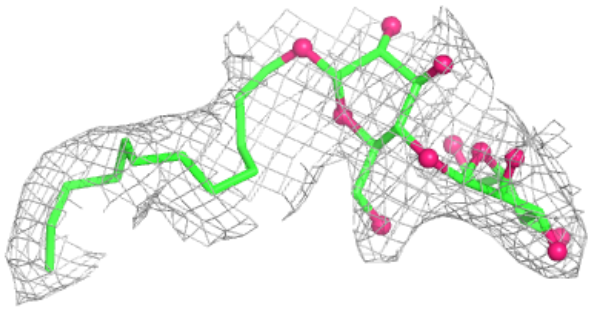


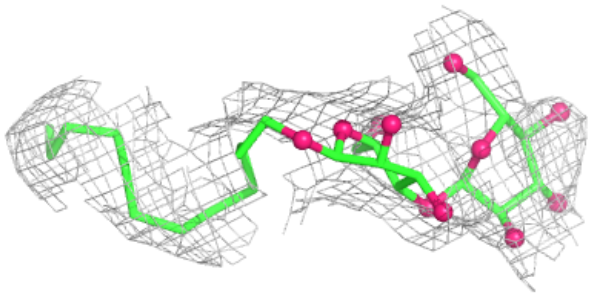


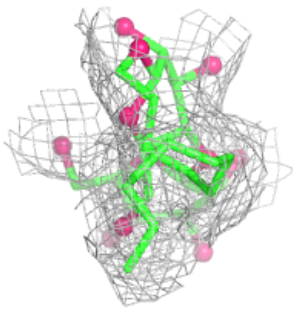


Electron density around LMU 2 7046:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

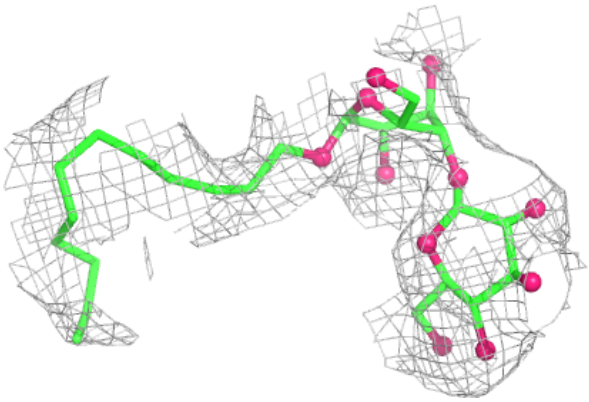


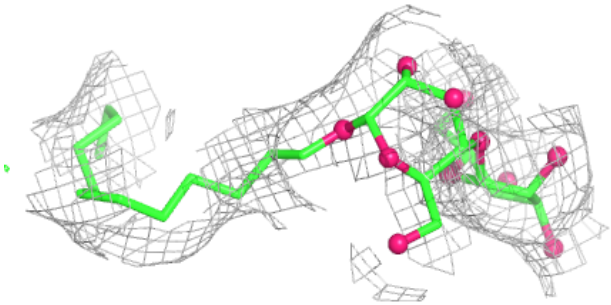


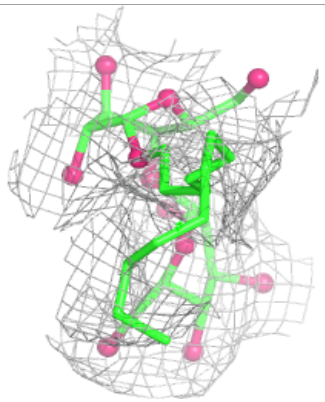


Electron density around LMU K 7001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

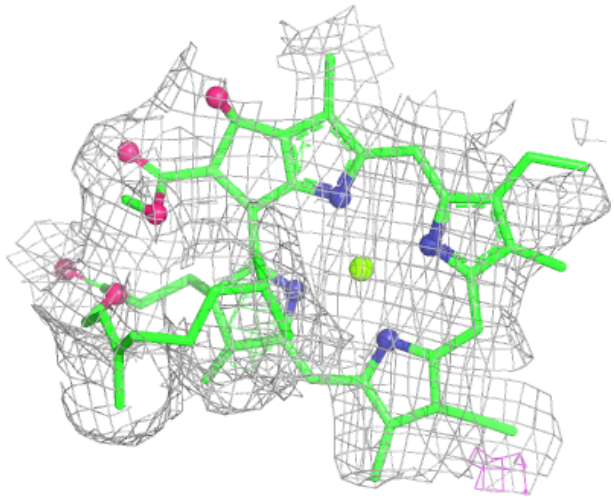


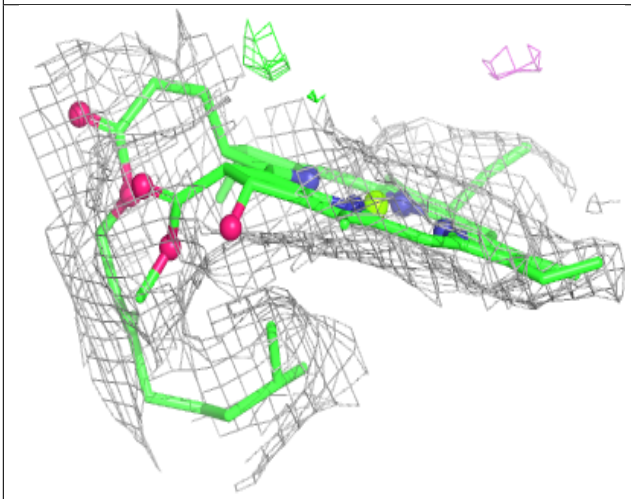




Electron density around CLA 4 1306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

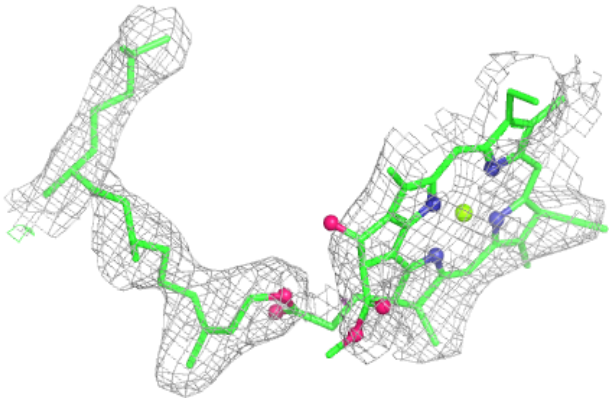


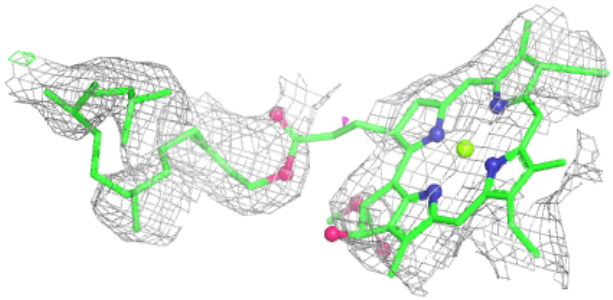


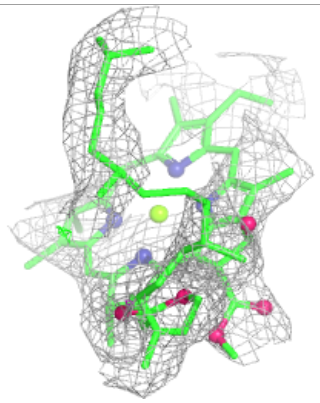


Electron density around CLA K 3009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

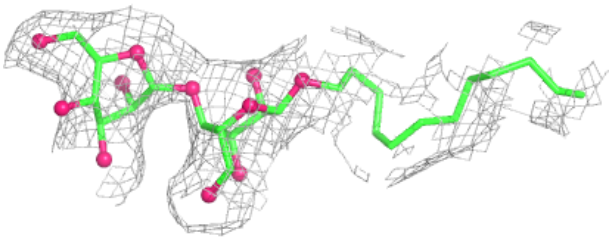


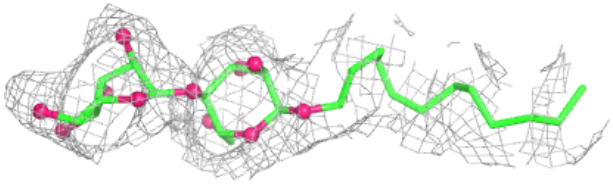


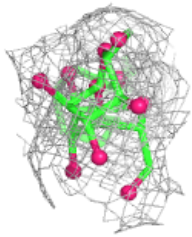


Electron density around LMU E 7037:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

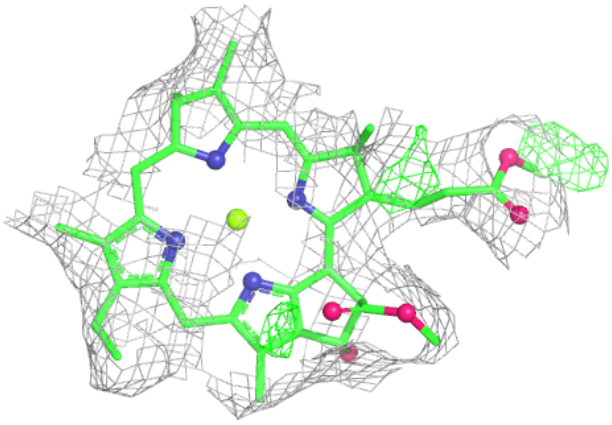


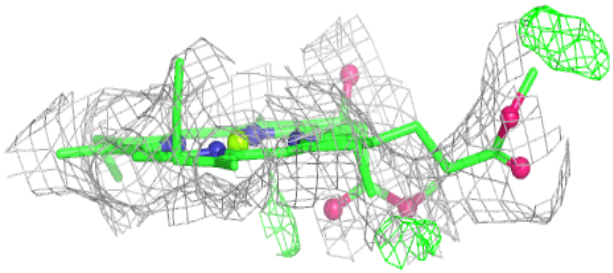


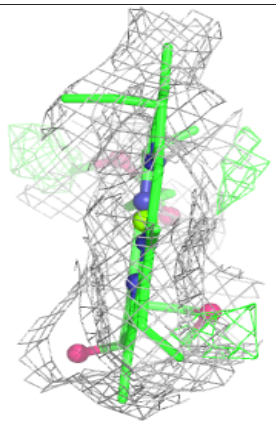


Electron density around CLA 1 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

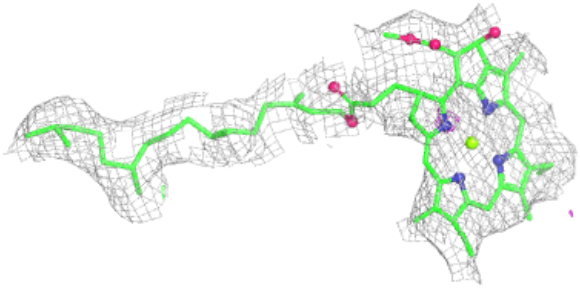


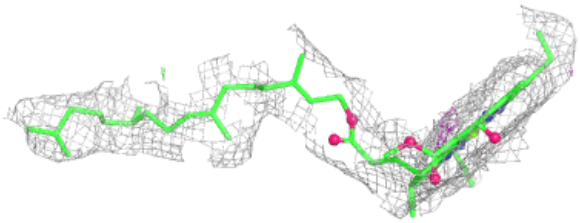


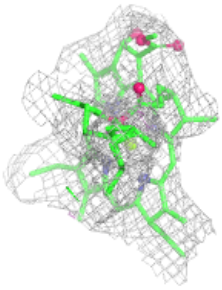


Electron density around CLA 4 1304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

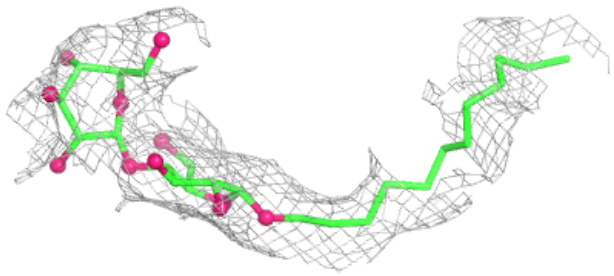


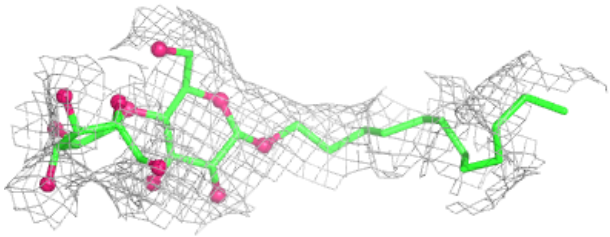


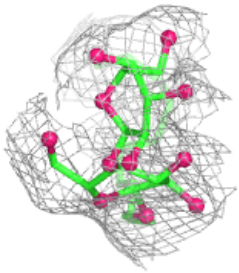


Electron density around LMU H 7017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

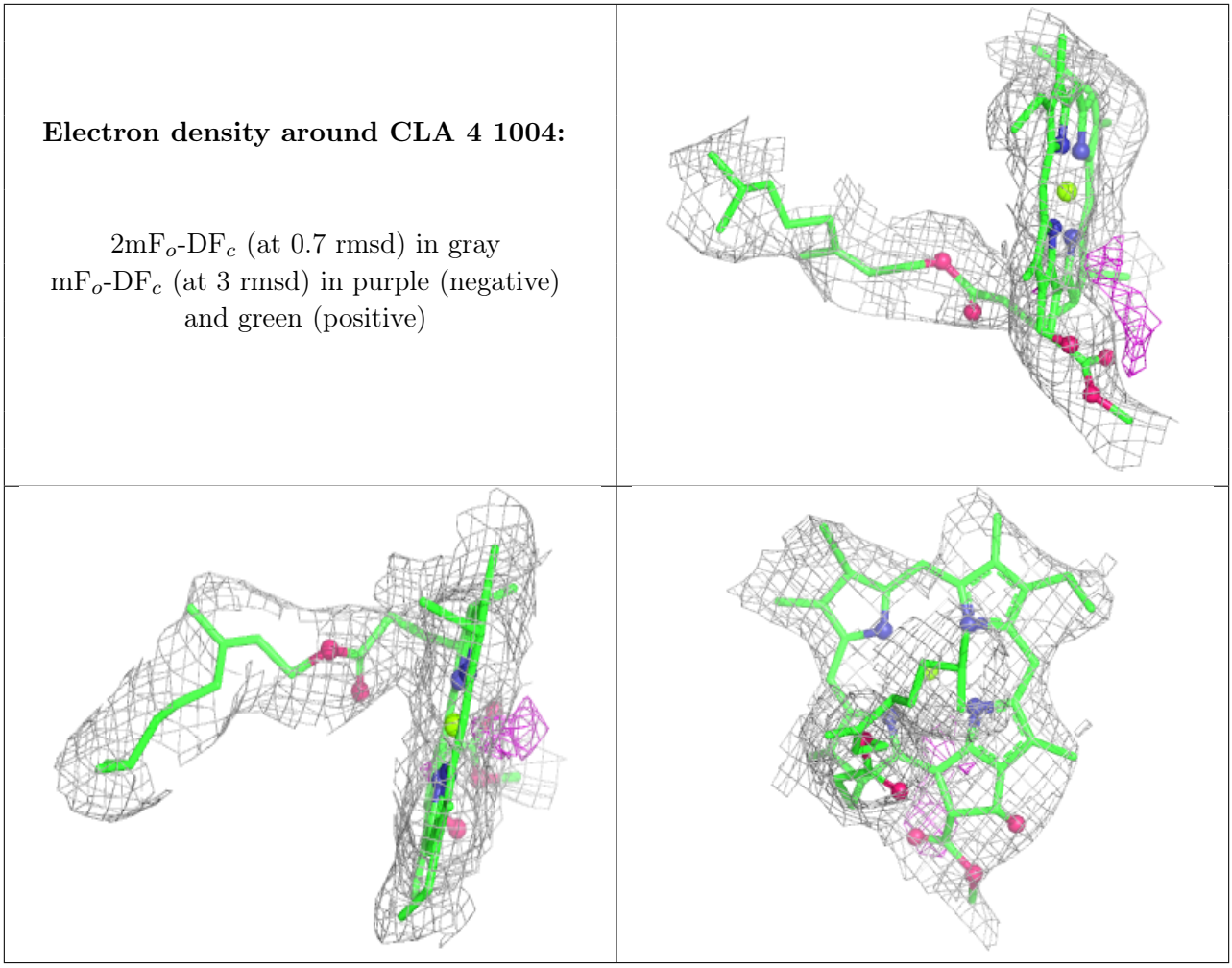






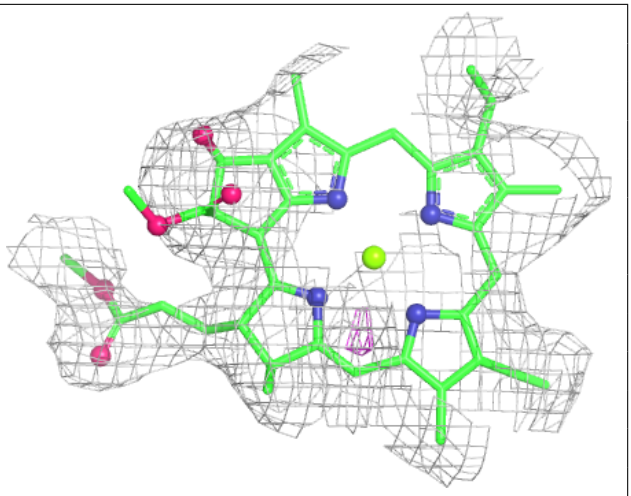
Electron density around CLA 4 1004:

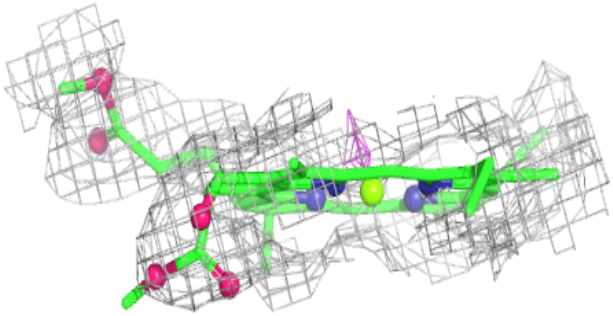
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

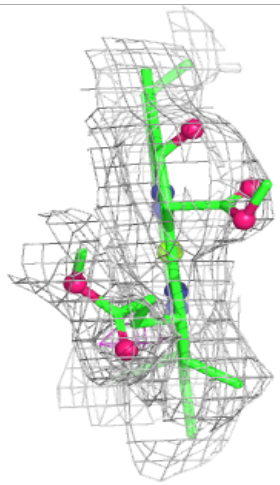


Electron density around CLA 4 4015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

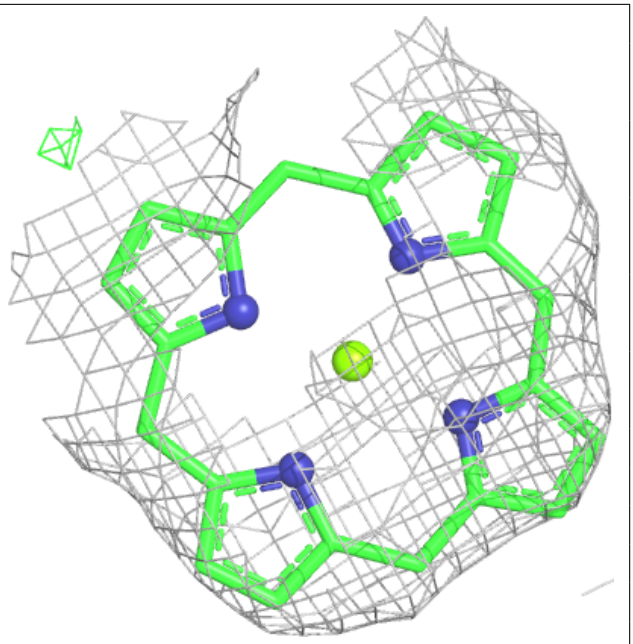


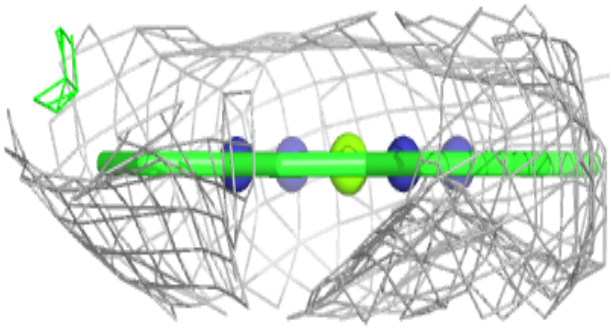


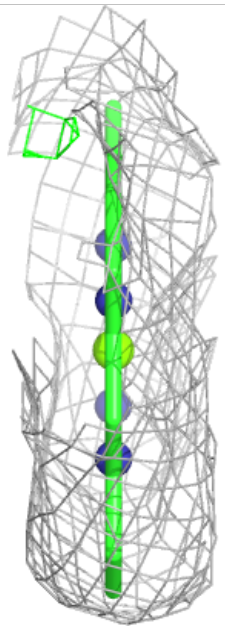


Electron density around CLA 3 3006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

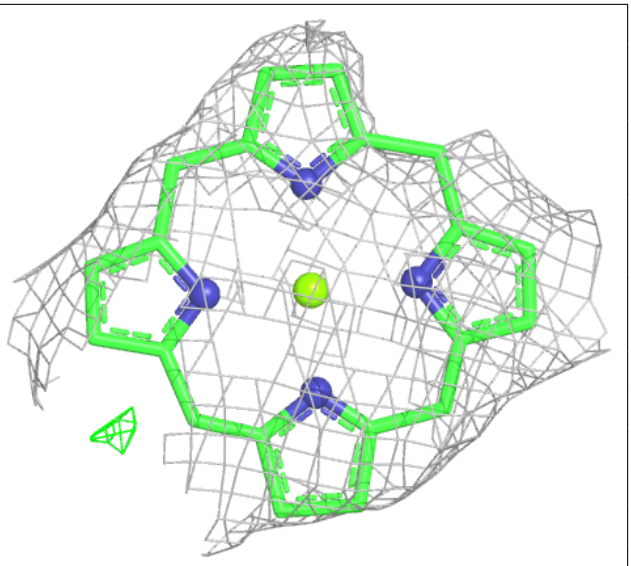


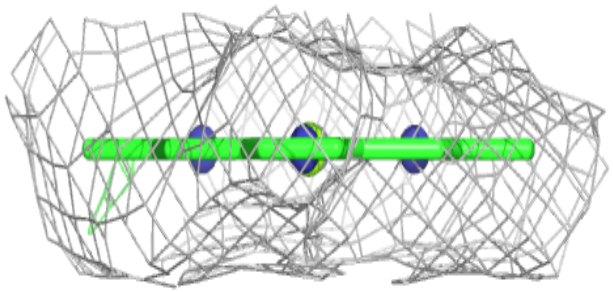


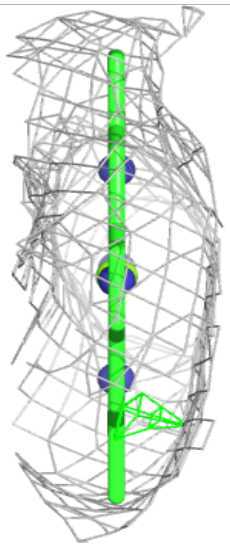


Electron density around CLA 1 1310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

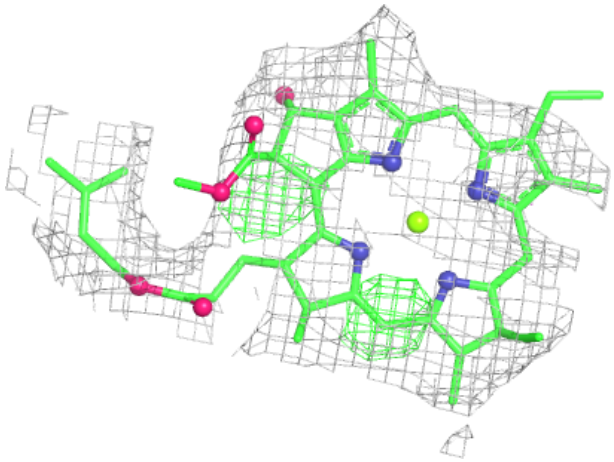


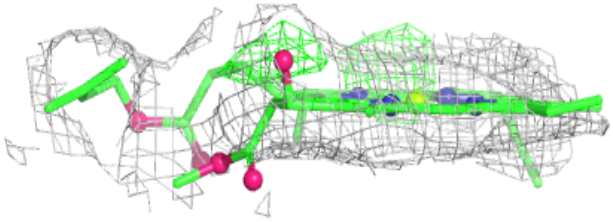


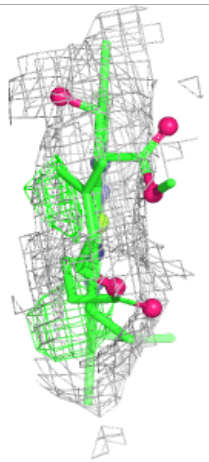


Electron density around CLA 2 2013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

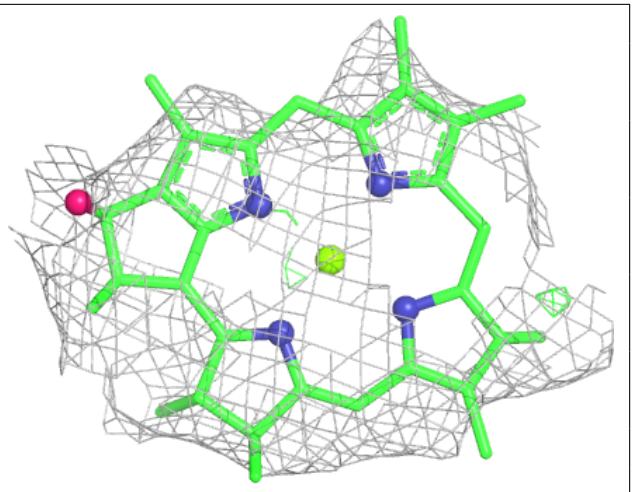


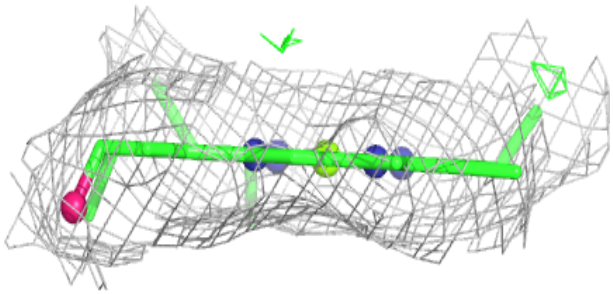


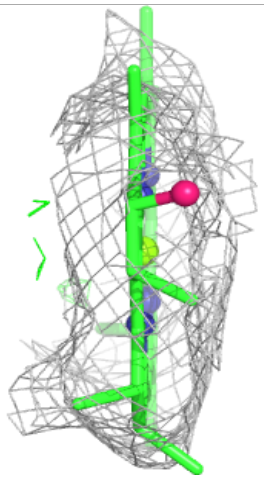


Electron density around CLA 3 3003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

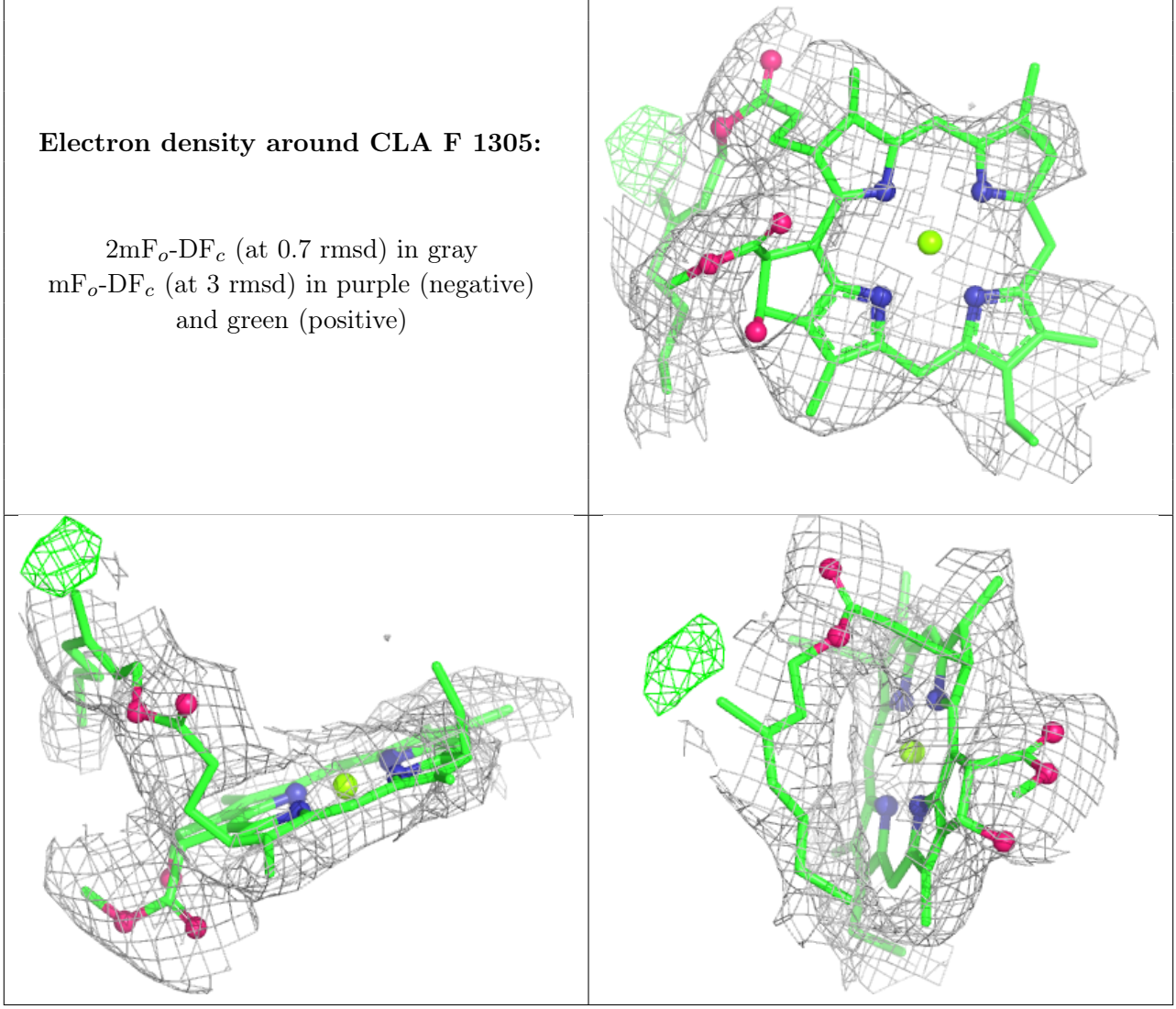






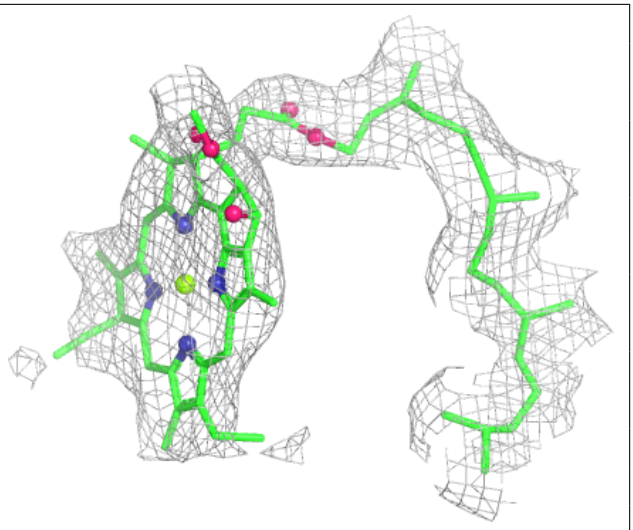
Electron density around CLA F 1305:

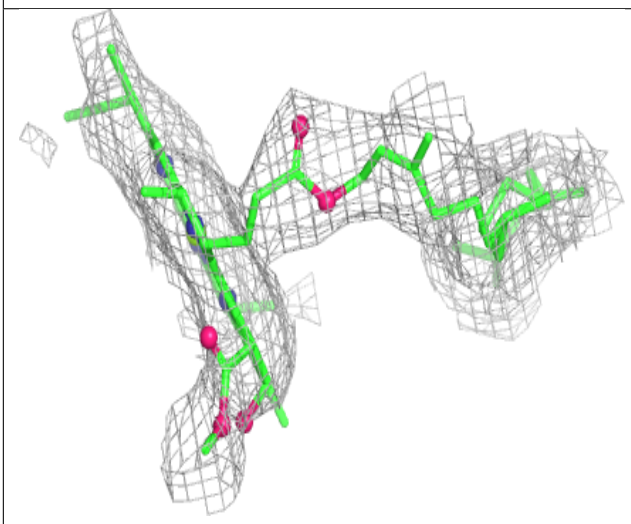
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

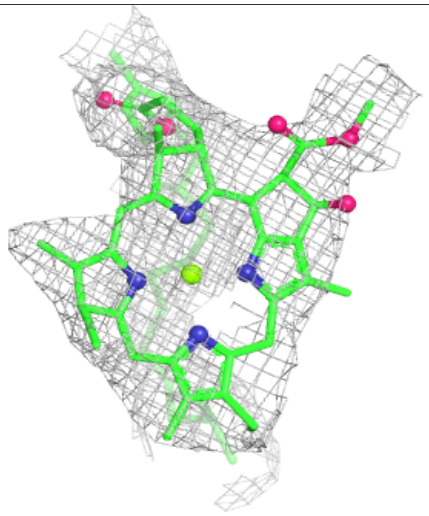


Electron density around CLA 3 3013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

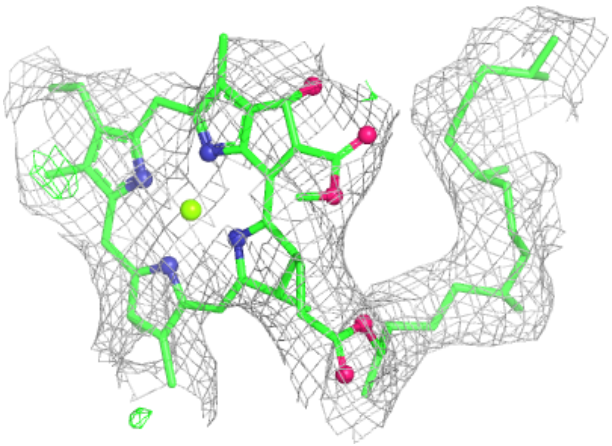


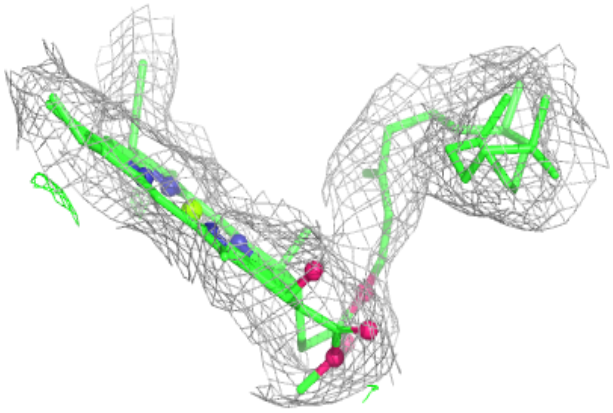


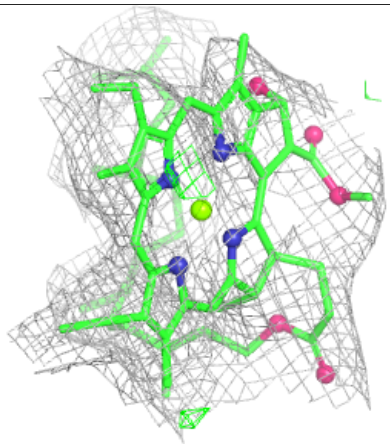


Electron density around CLA H 1145:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

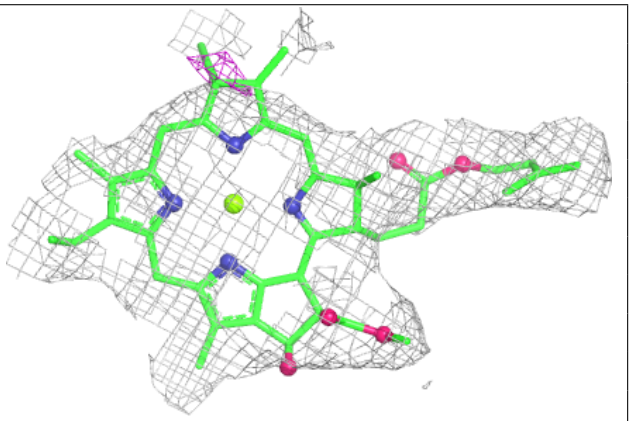


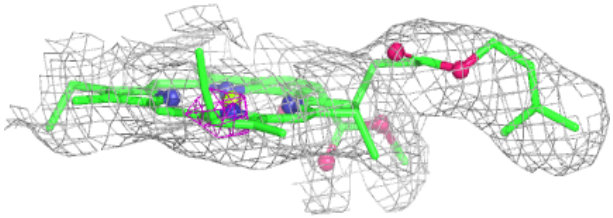


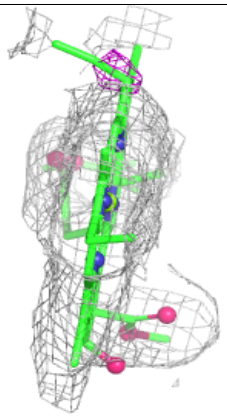


Electron density around CLA K 1143:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

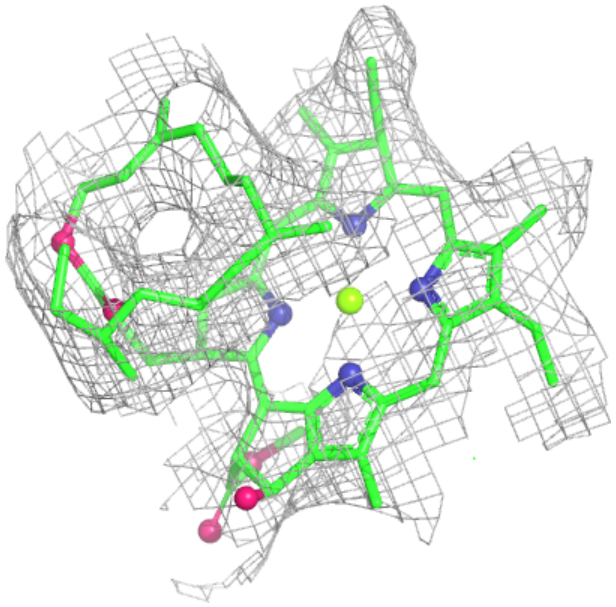


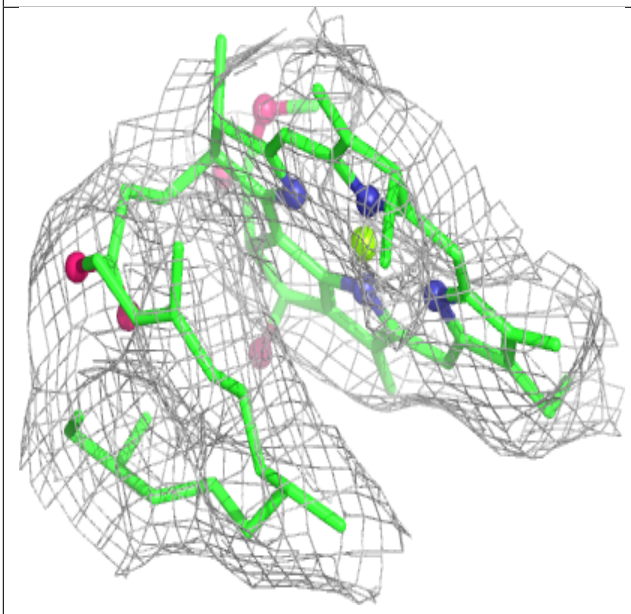


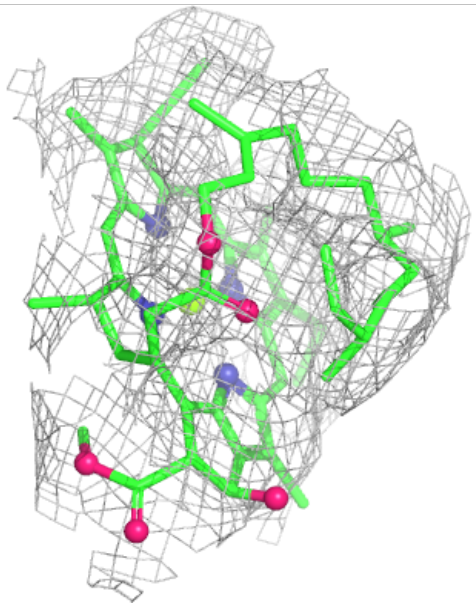


Electron density around CLA J 1311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

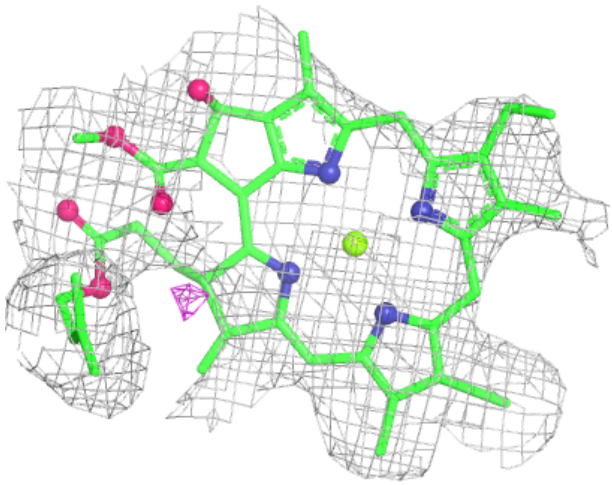


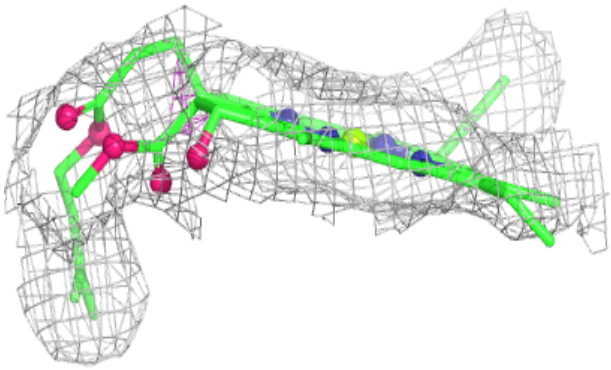


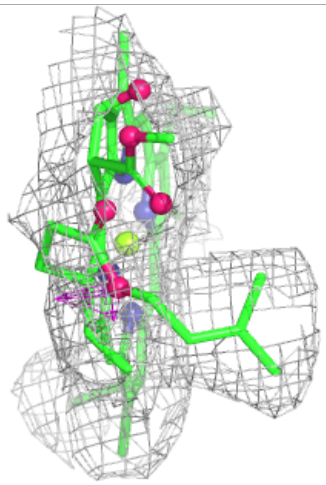


Electron density around CLA 3 3008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

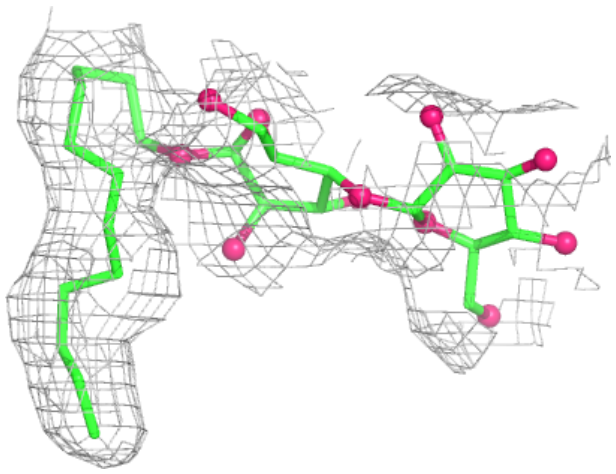


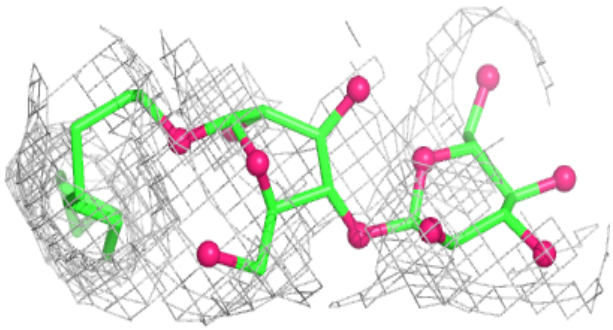


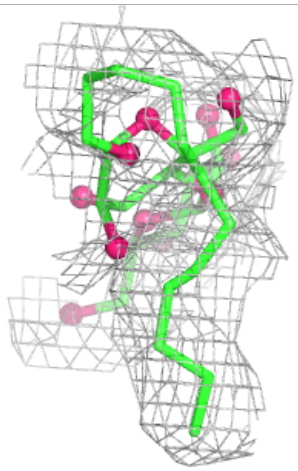


Electron density around LMU 4 7052:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

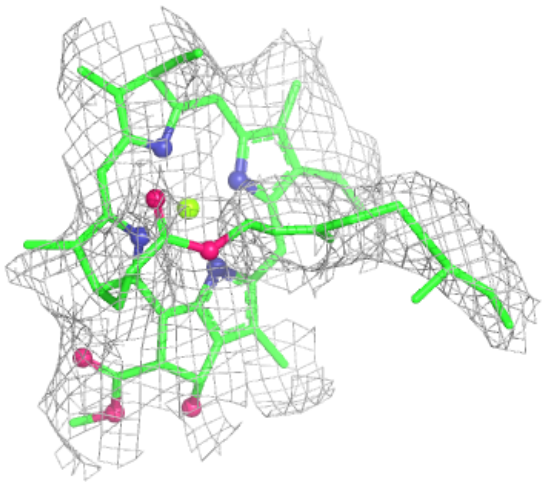


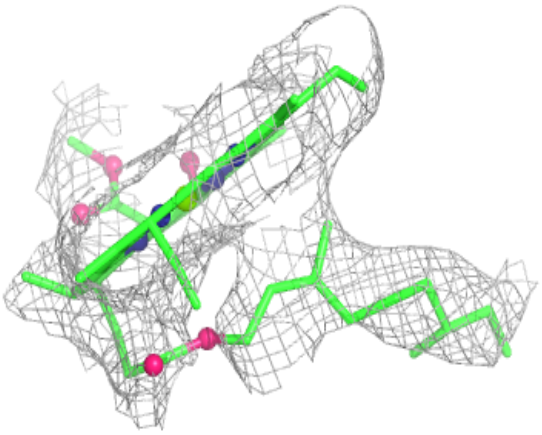


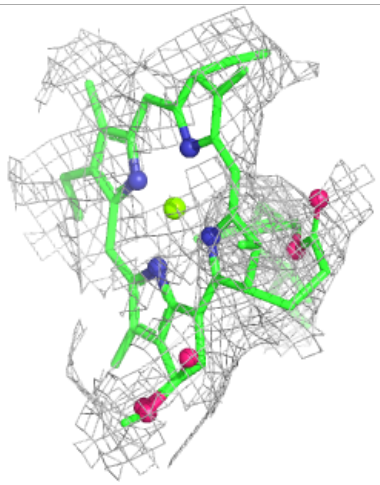


Electron density around CLA 2 2002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

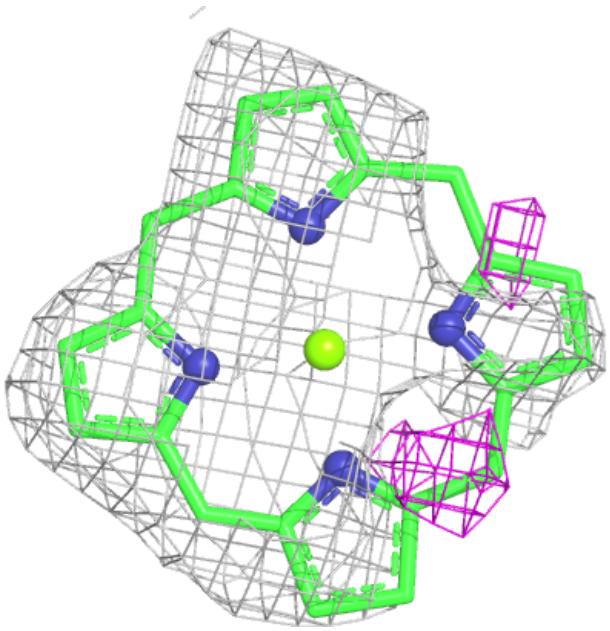


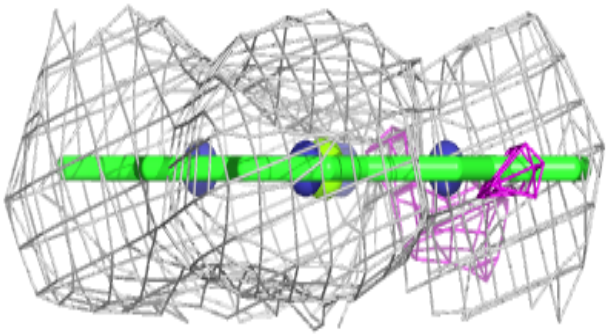


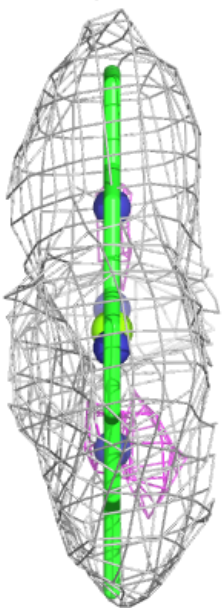


Electron density around CLA 2 1307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

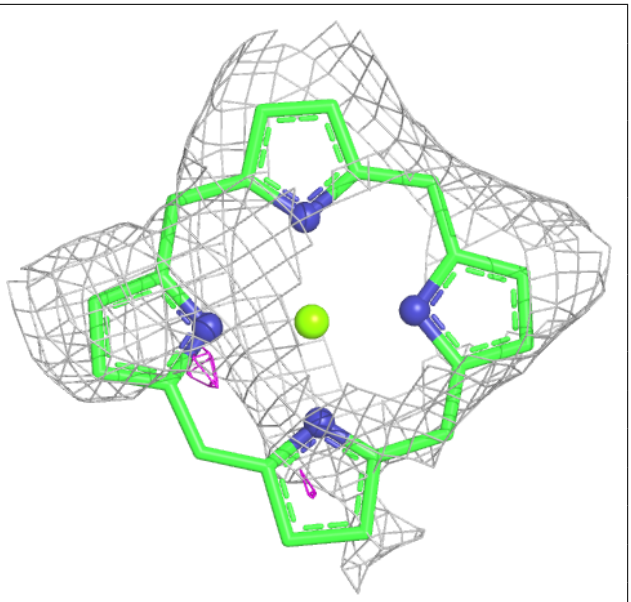


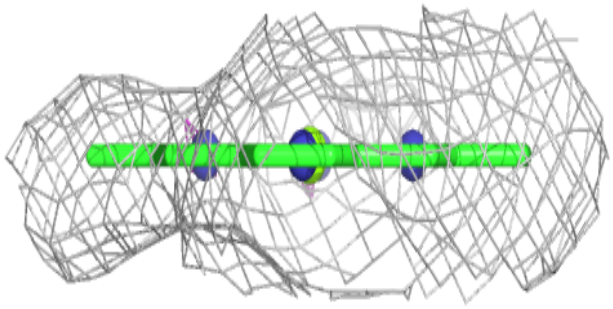


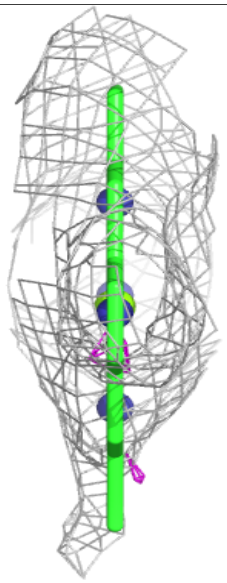


Electron density around CLA 3 3015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

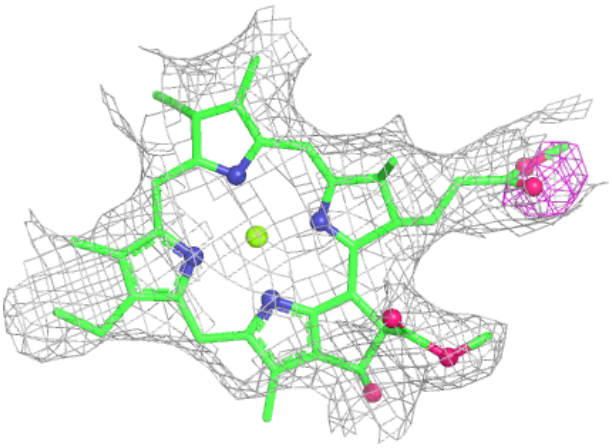


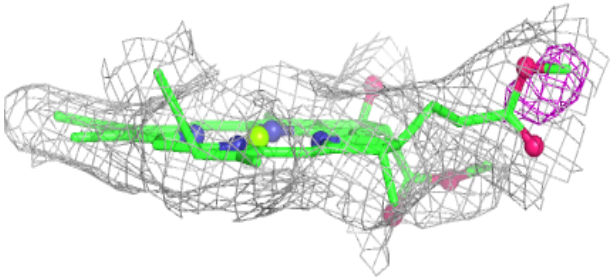


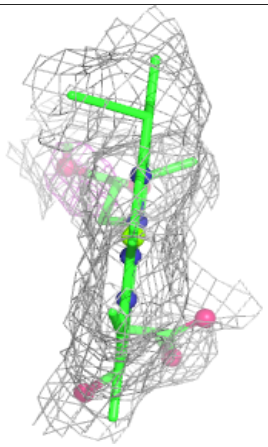


Electron density around CLA 3 1147:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

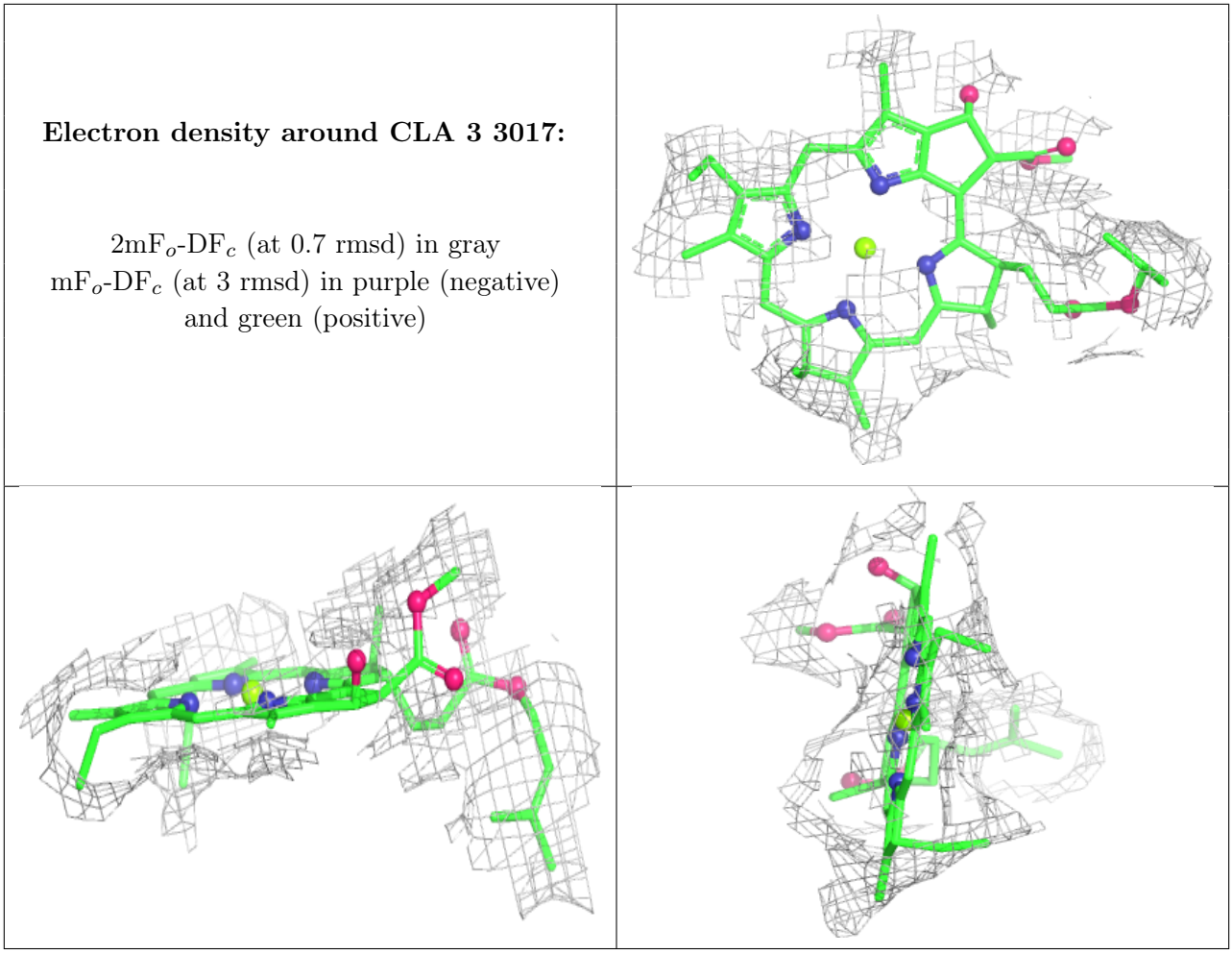






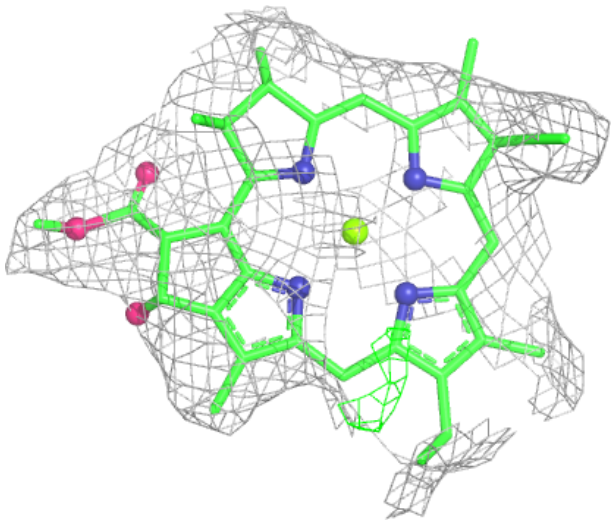
Electron density around CLA 3 3017:

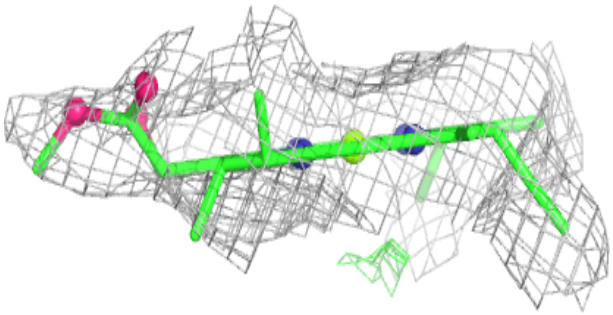
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

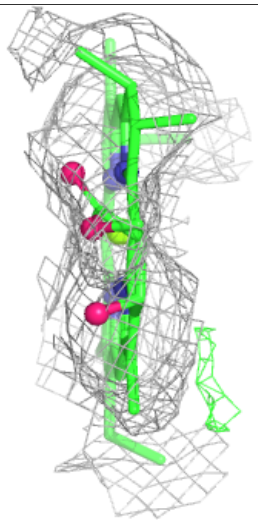


Electron density around CLA F 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

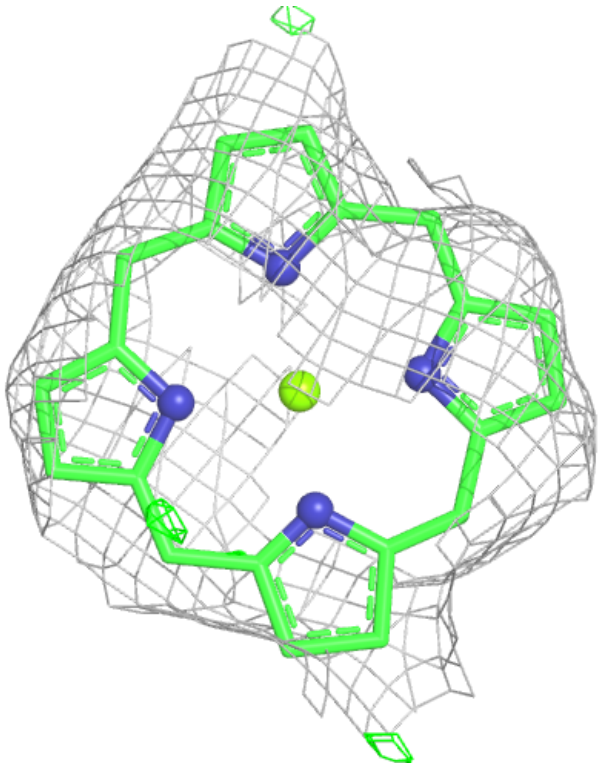


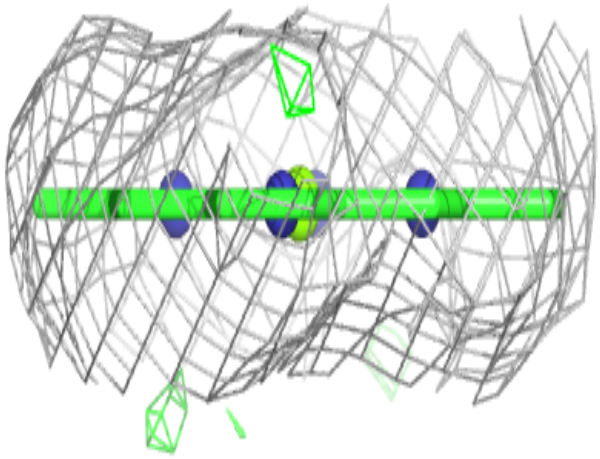


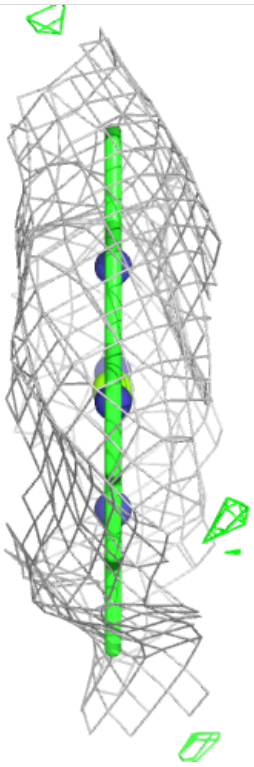


Electron density around CLA 3 3010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



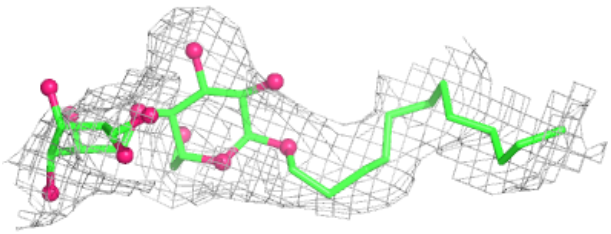


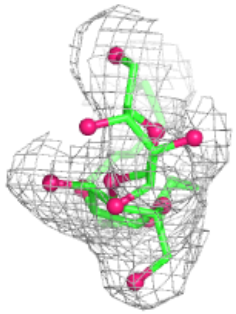


Electron density around LMU 4 7034:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

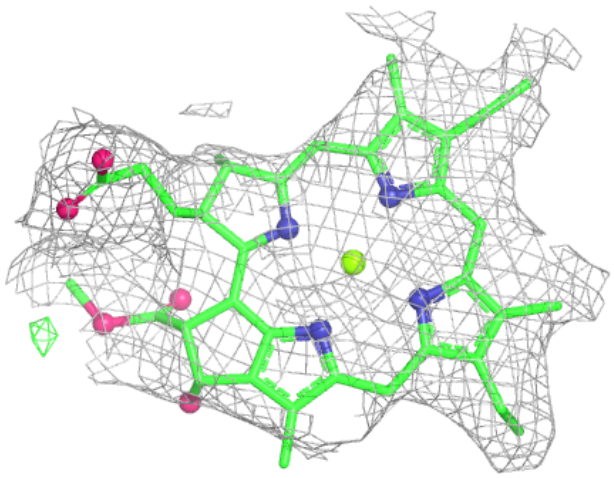


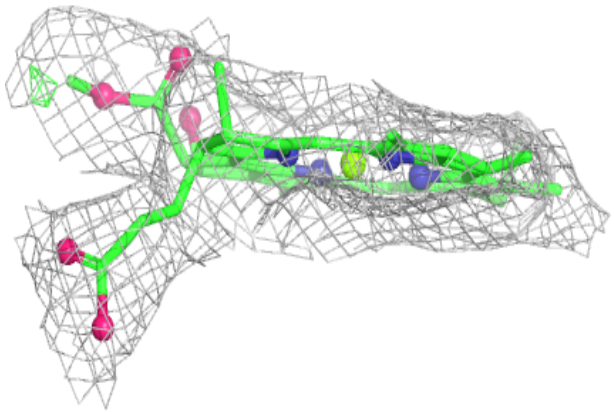


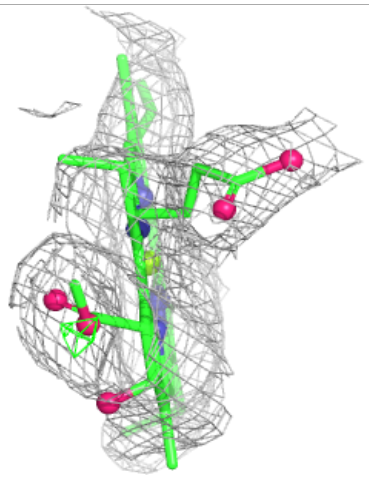


Electron density around CLA A 1108:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

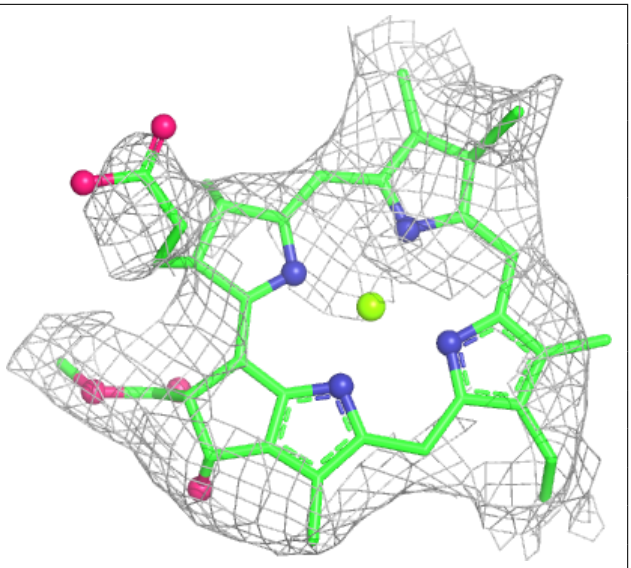


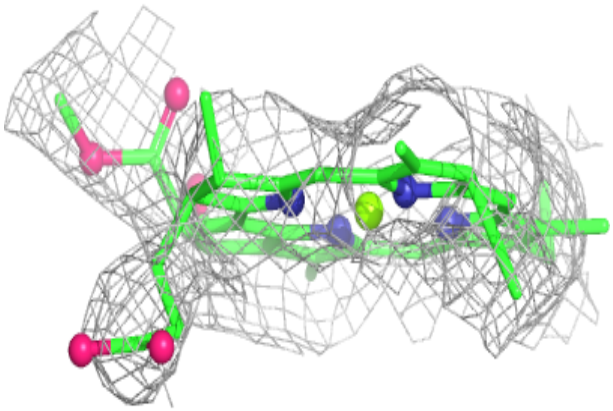


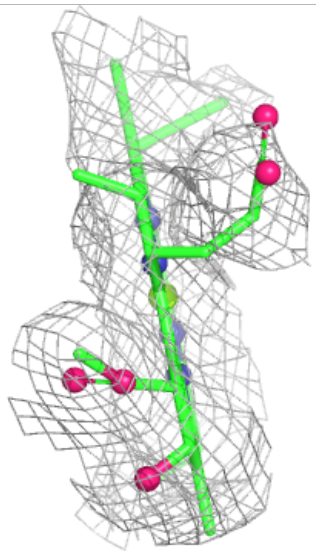


Electron density around CLA A 1134:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

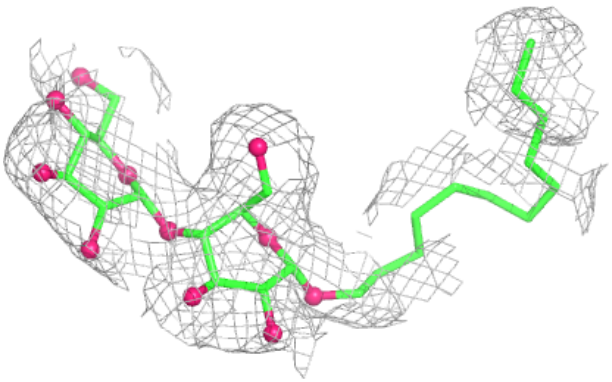


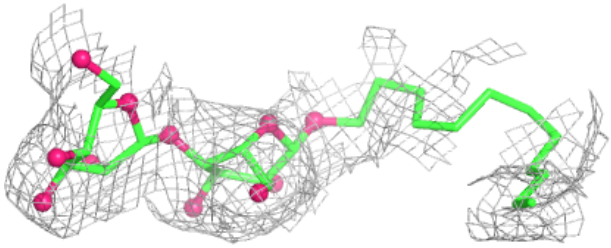




Electron density around LMU H 7030:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



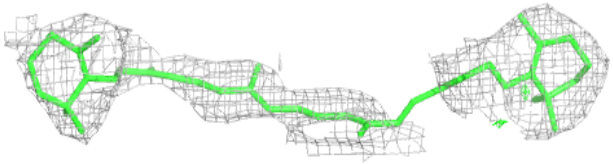


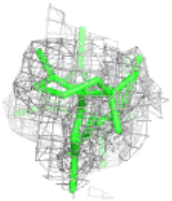


Electron density around BCR A 6007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

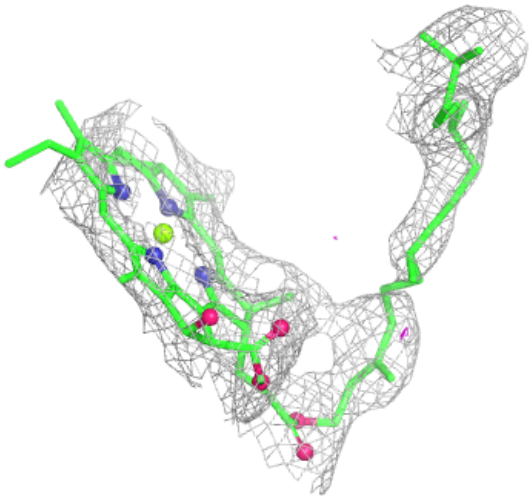


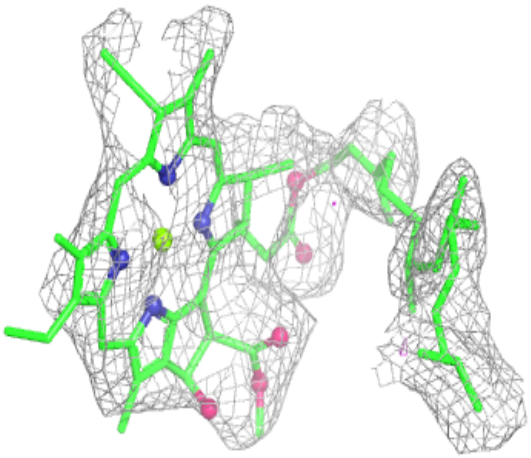


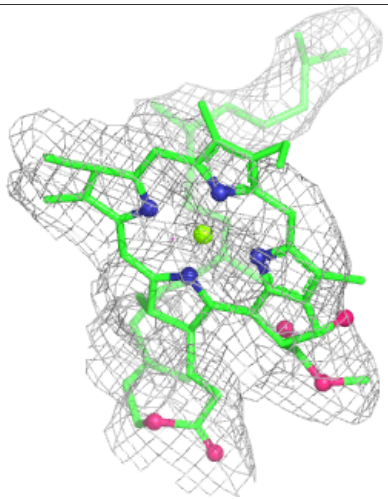


Electron density around CLA 2 2006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

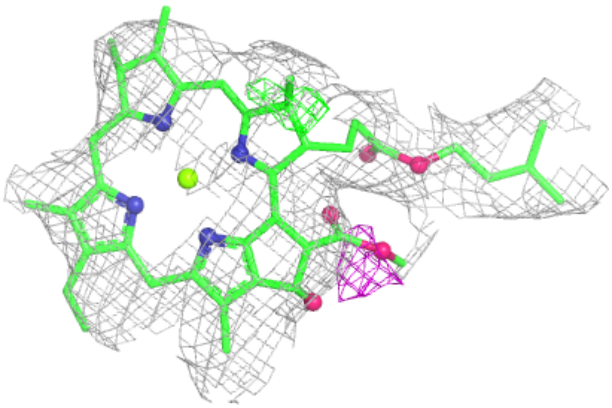


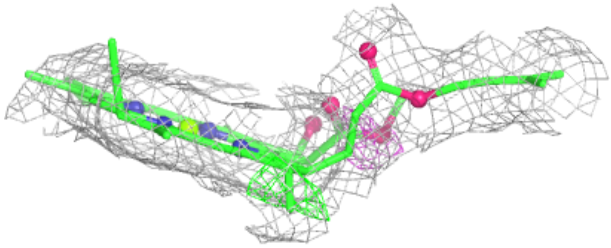


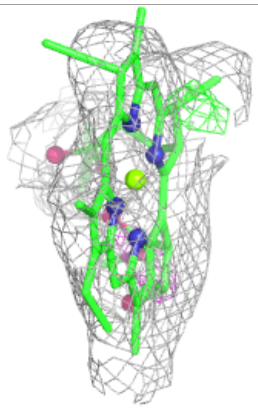


Electron density around CLA L 1503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

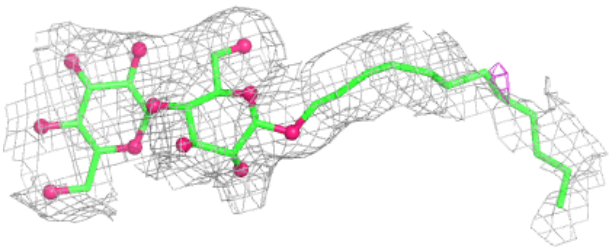


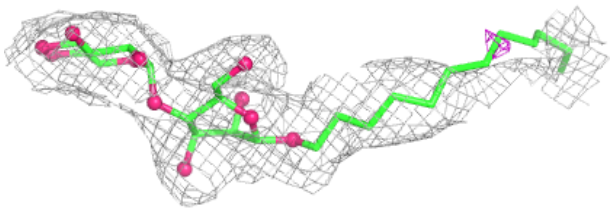


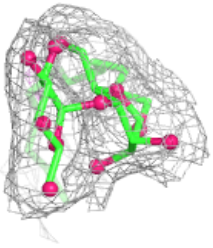


Electron density around LMU K 7047:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

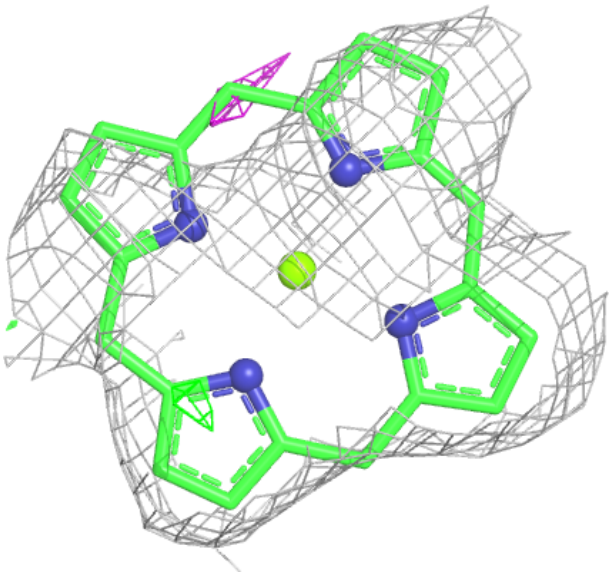


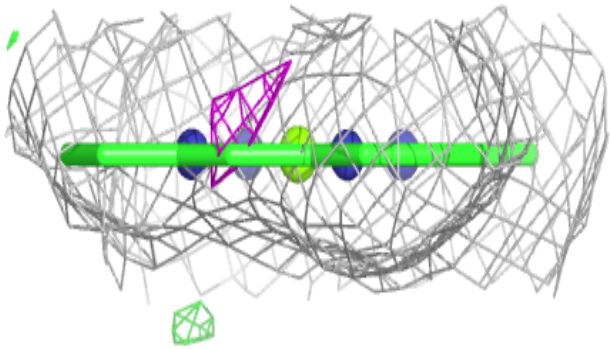


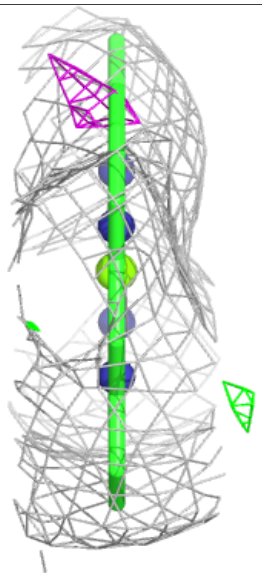


Electron density around CLA 4 4004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

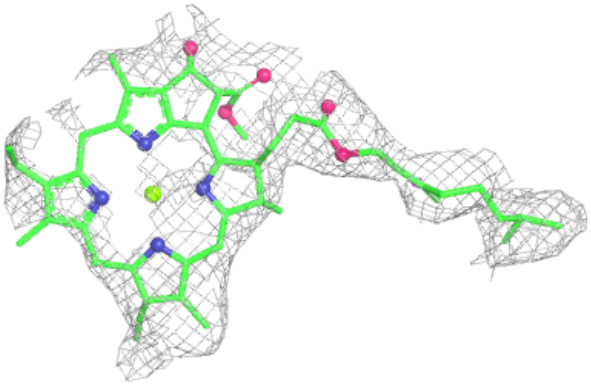


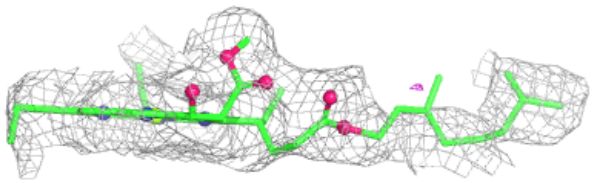


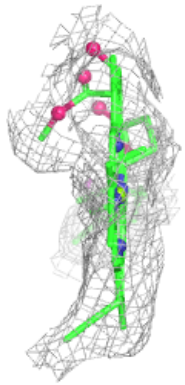


Electron density around CLA 4 4006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

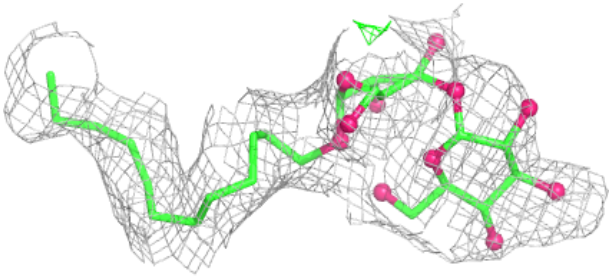


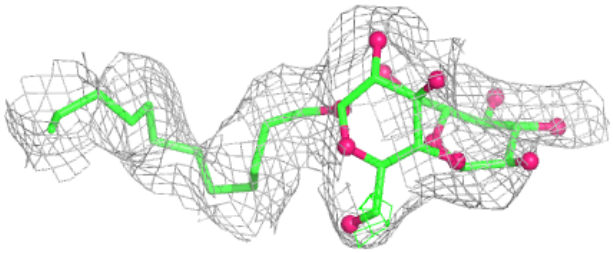


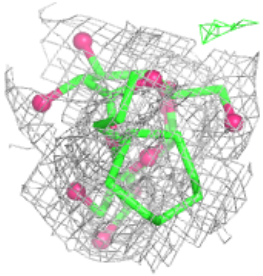


Electron density around LMU A 7045:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

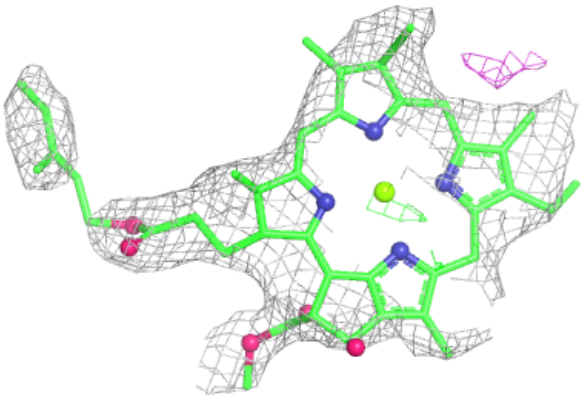


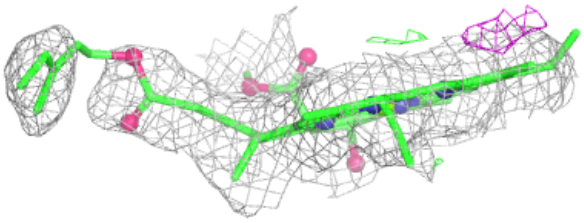


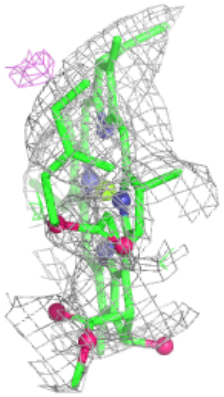


Electron density around CLA 1 1303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

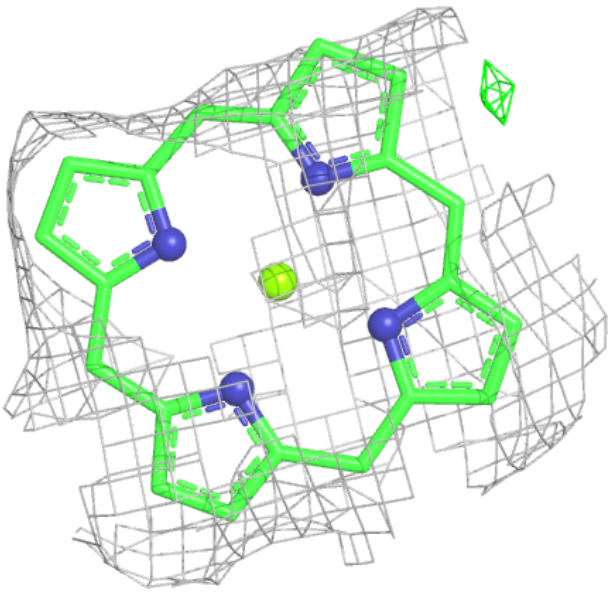


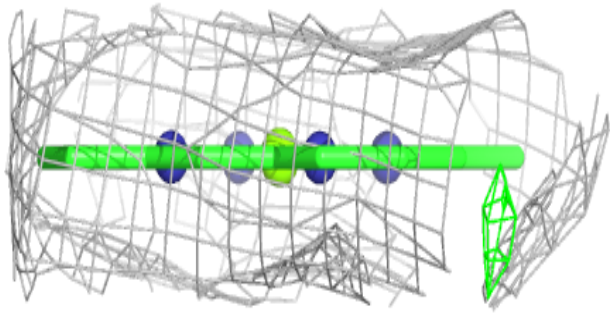


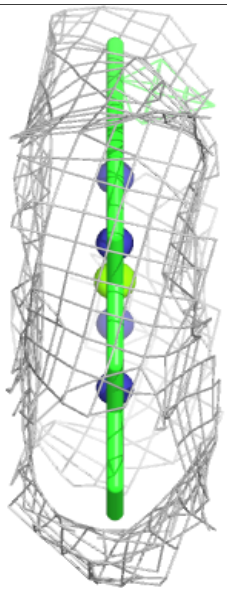


Electron density around CLA 3 3004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

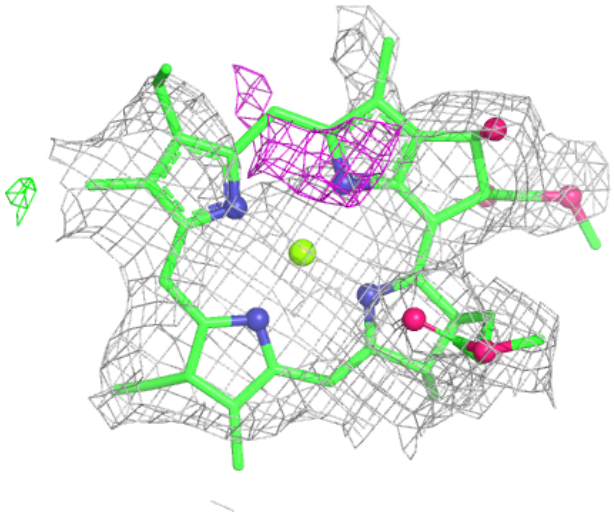


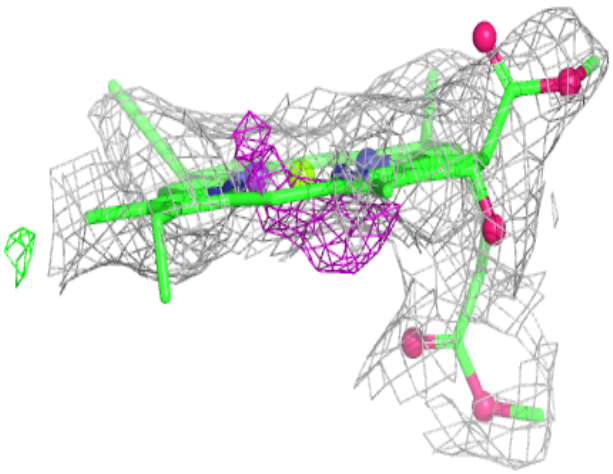


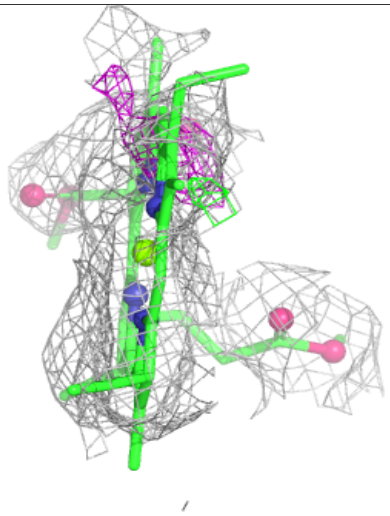


Electron density around CLA A 1105:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

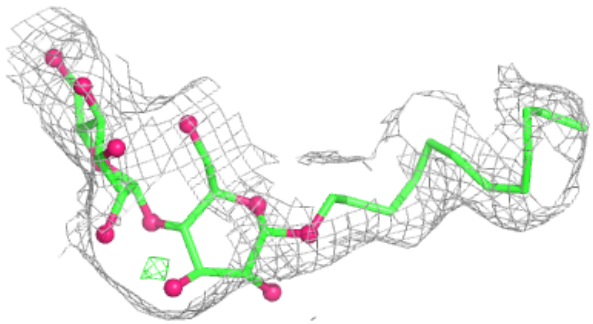


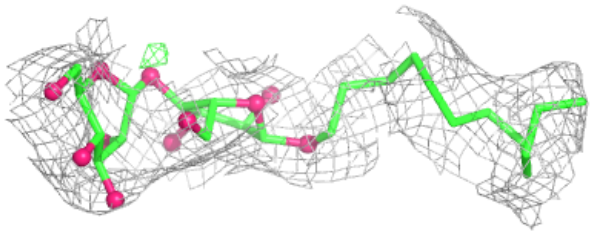


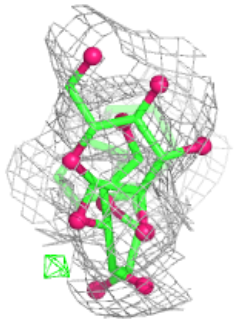


Electron density around LMU H 7011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

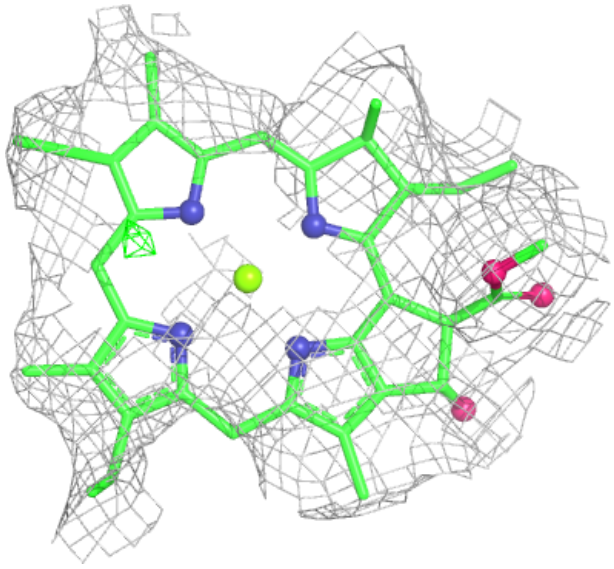


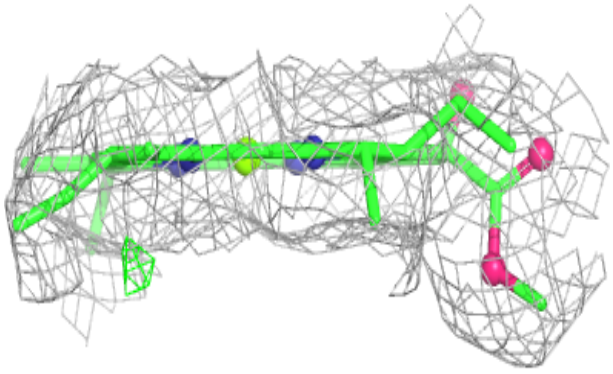




Electron density around CLA A 1121:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

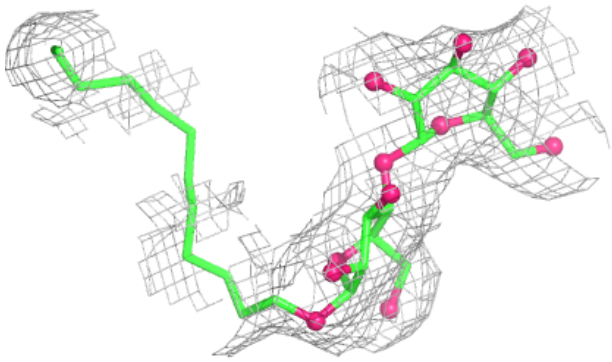


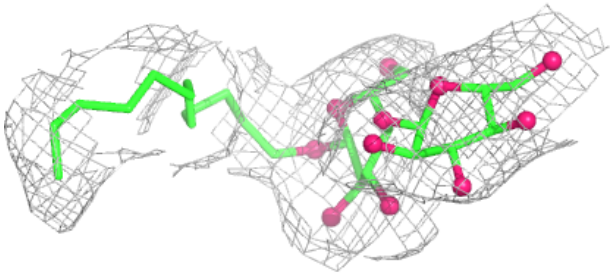


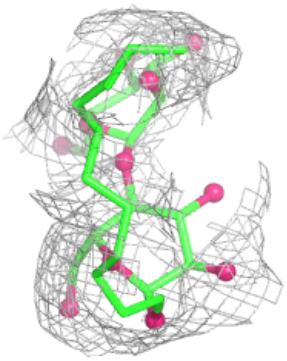


Electron density around LMU H 7028:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

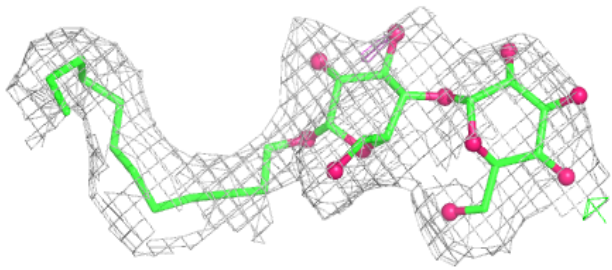


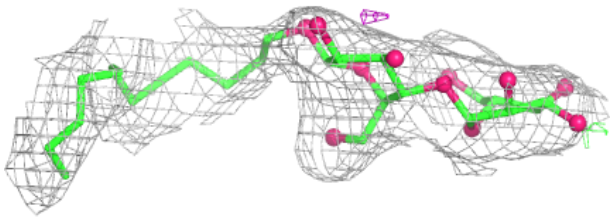


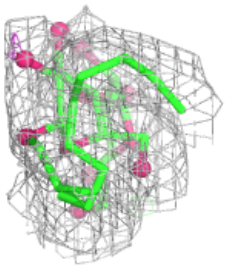


Electron density around LMU C 7015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

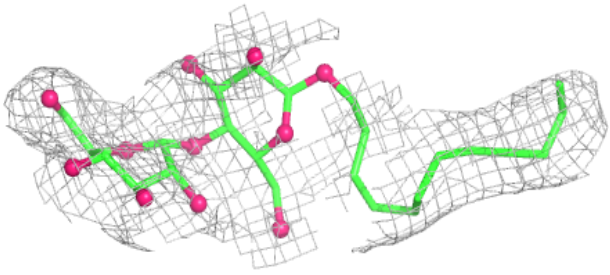


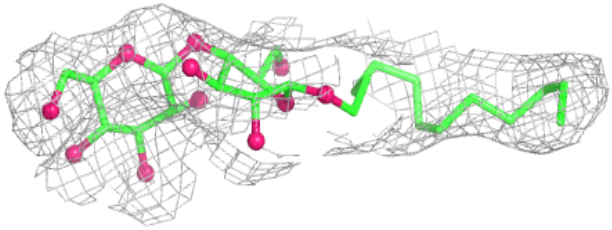


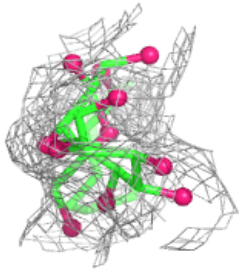


Electron density around LMU K 7042:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

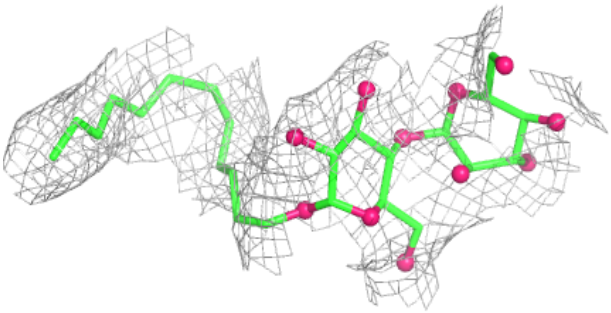


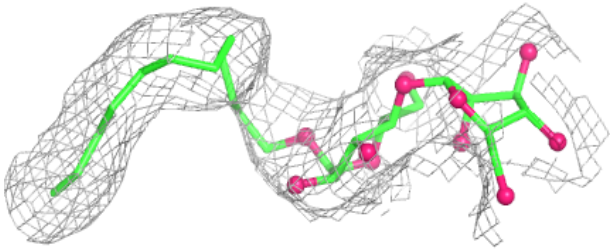


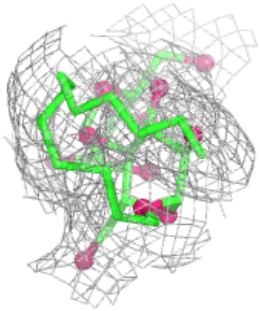


Electron density around LMU D 7050:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

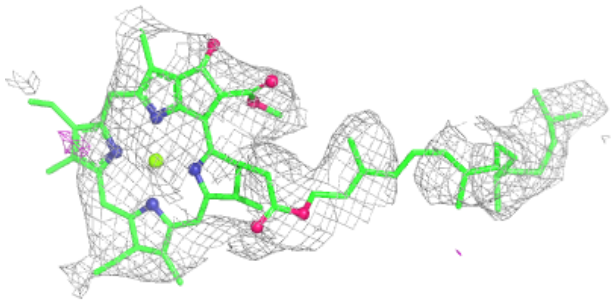


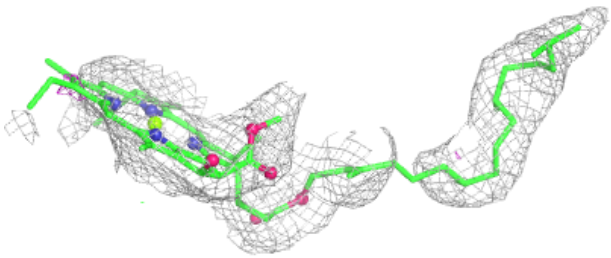


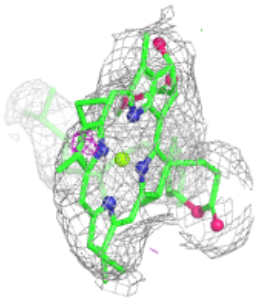


Electron density around CLA 3 3011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

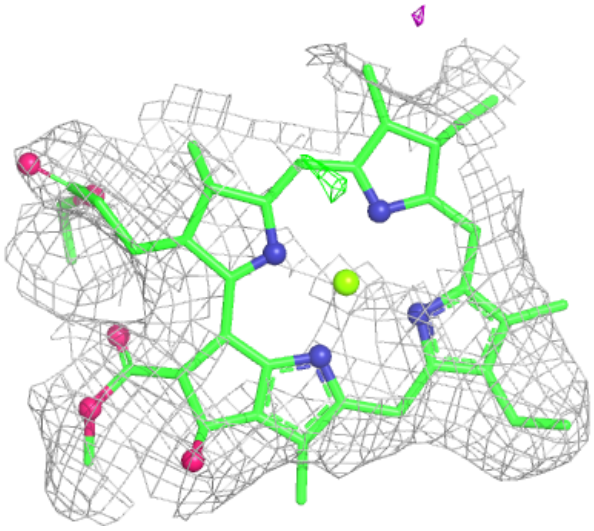


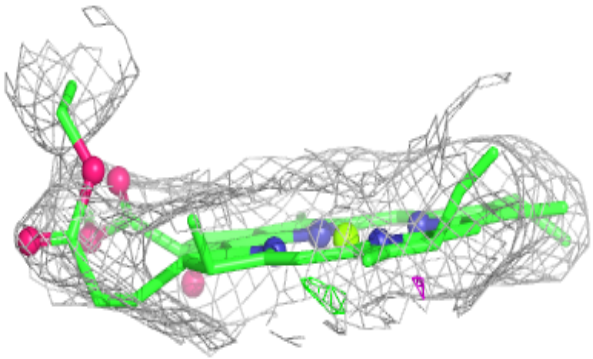


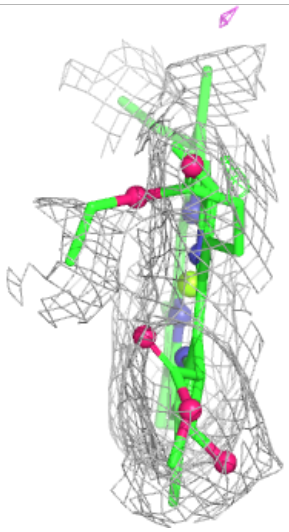


Electron density around CLA 1 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

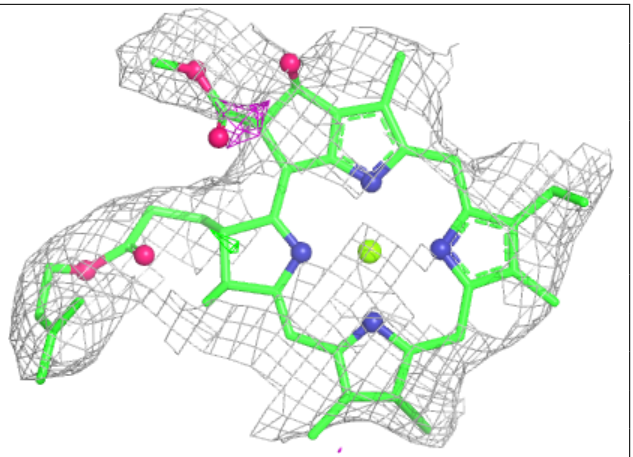


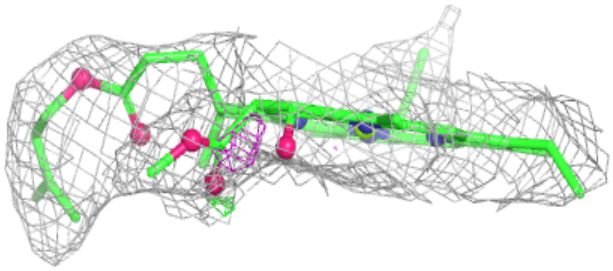


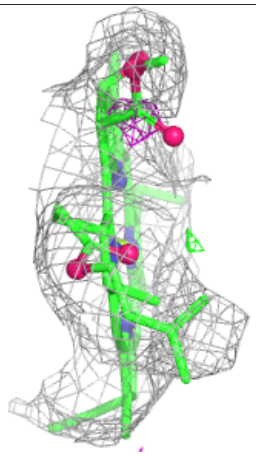


Electron density around CLA K 1146:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

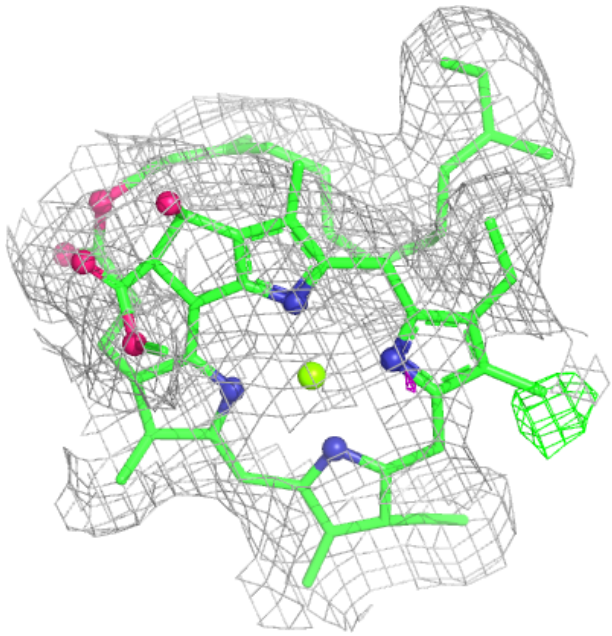


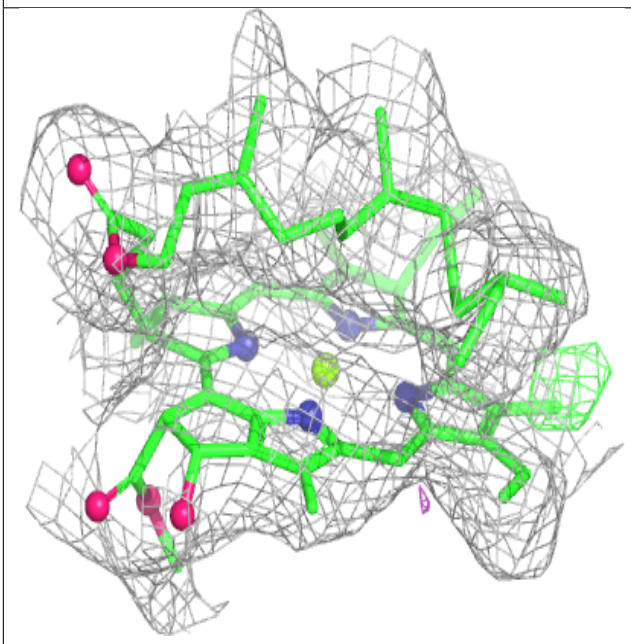


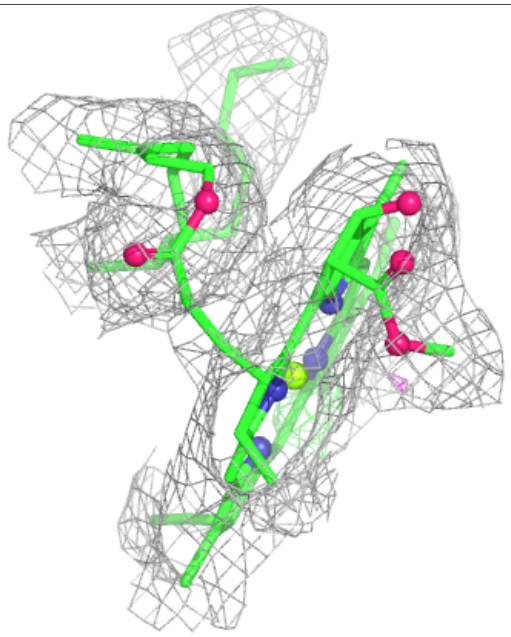


Electron density around CLA 1 1007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

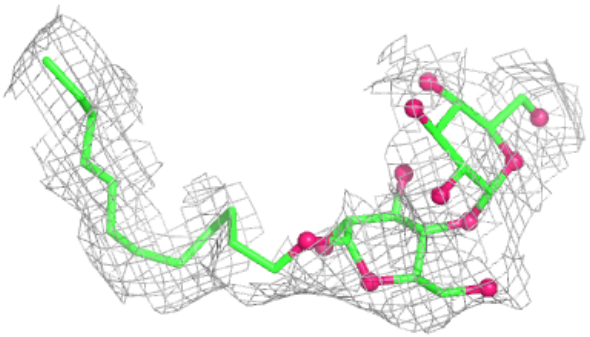


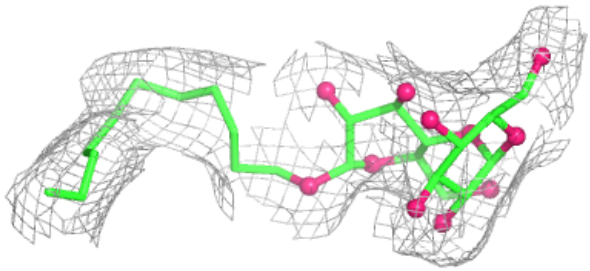




Electron density around LMU 2 7031:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

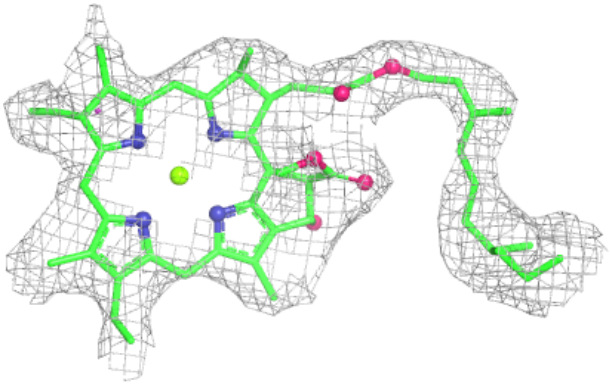


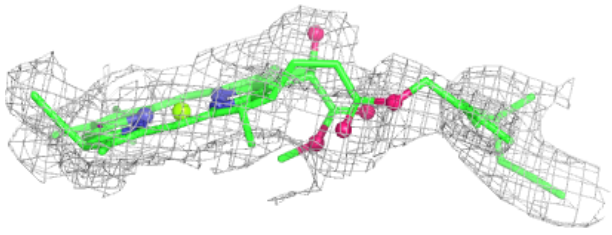


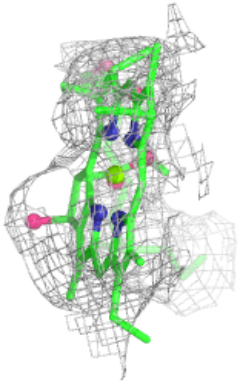


Electron density around CLA R 1144:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

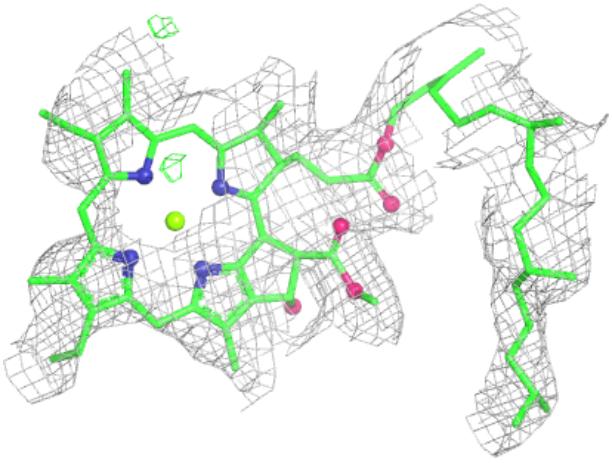


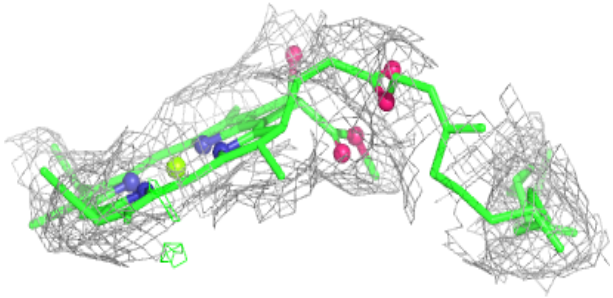


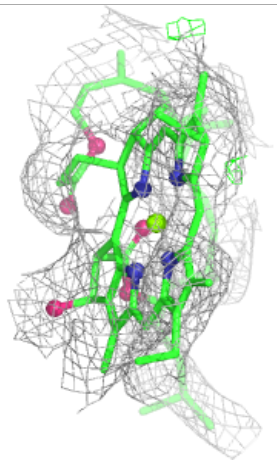


Electron density around CLA R 1150:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

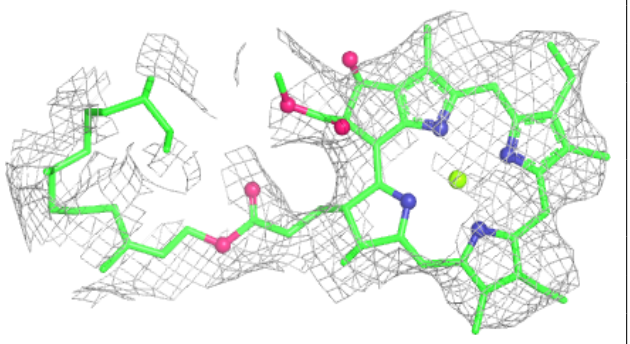


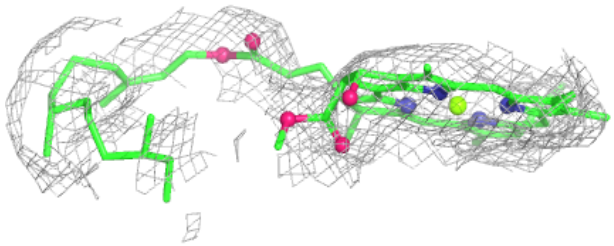


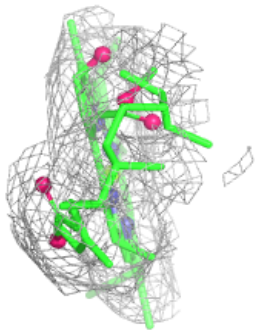


Electron density around CLA 1 1014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

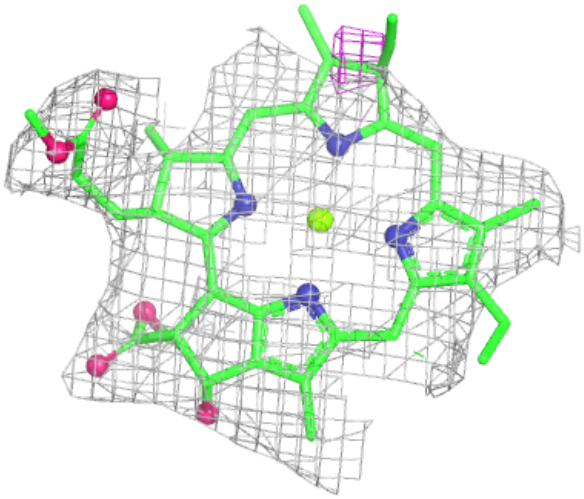


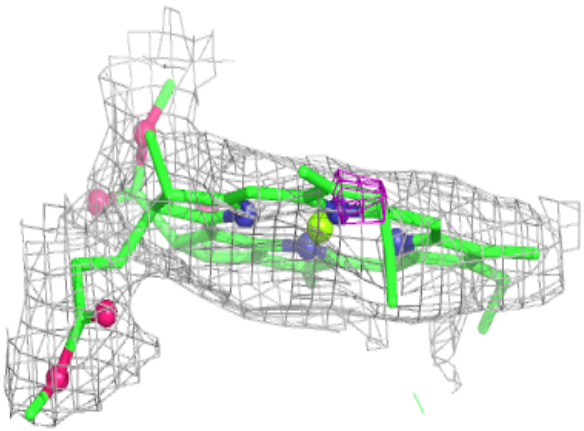


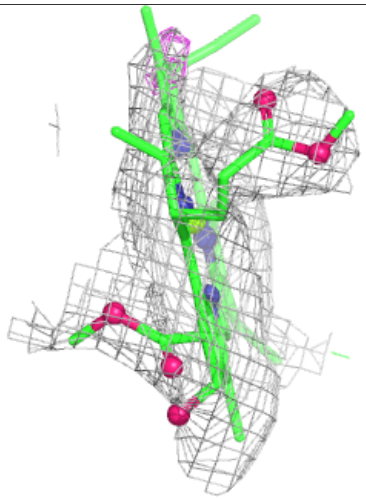


Electron density around CLA B 1218:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

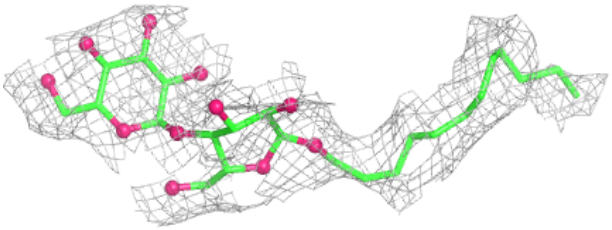


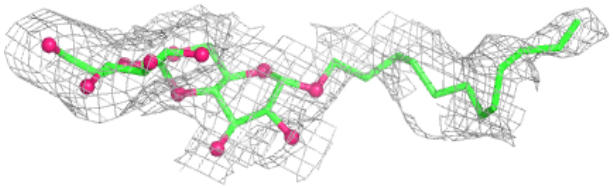


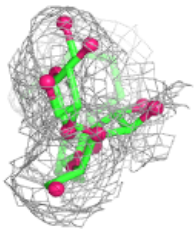


Electron density around LMU B 7038:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

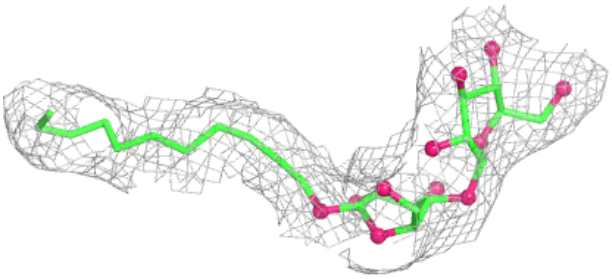


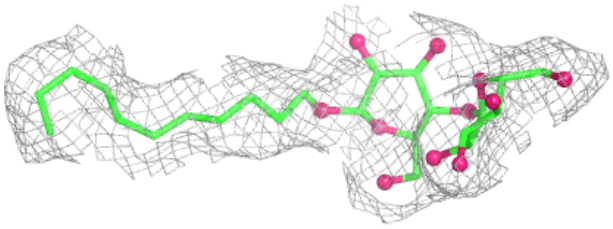


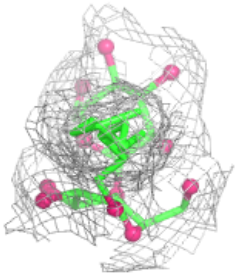


Electron density around LMU F 7036:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

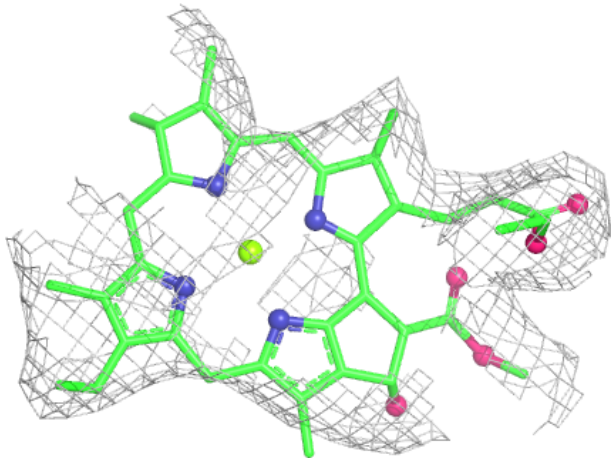


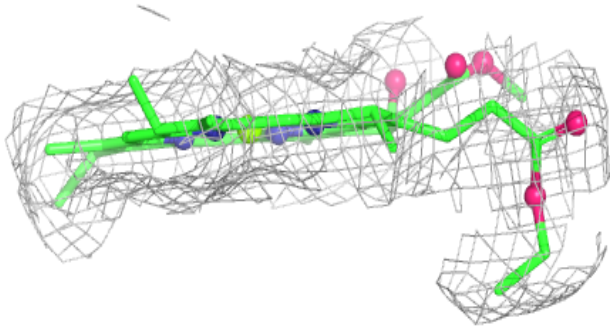


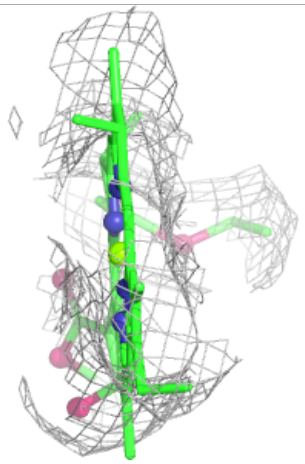


Electron density around CLA A 1149:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

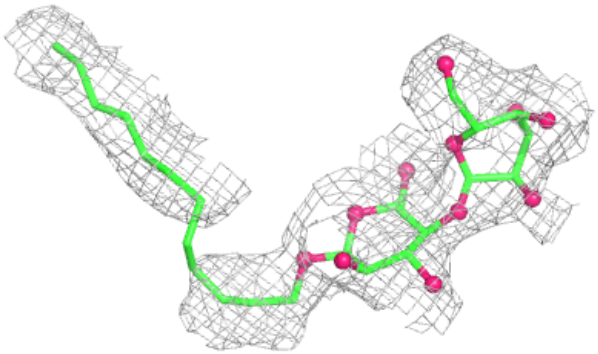


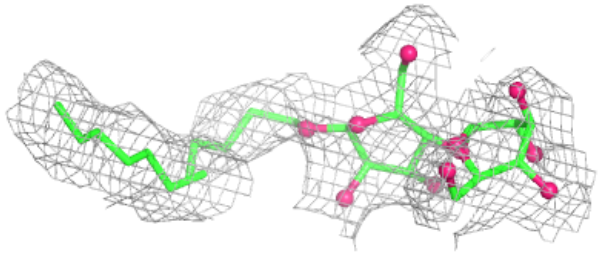


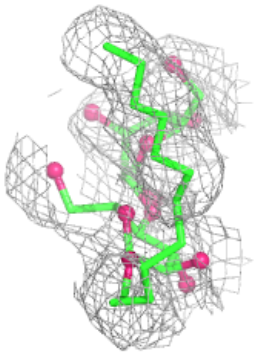


Electron density around LMU 4 7008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

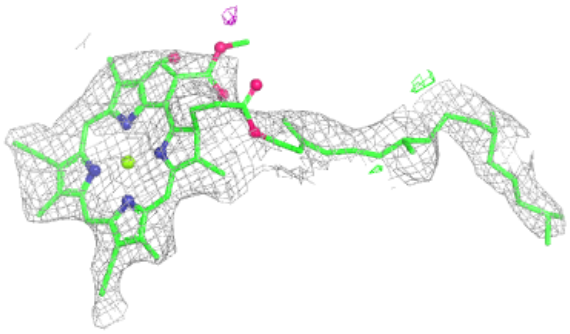


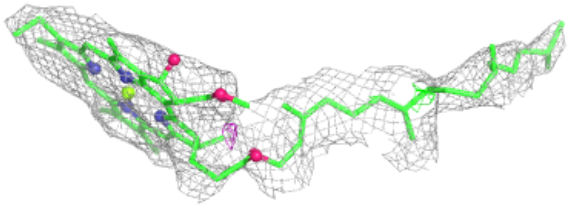


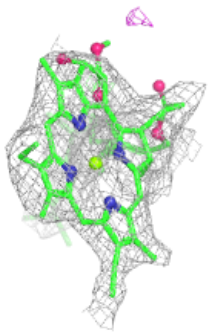


Electron density around CLA H 1207:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

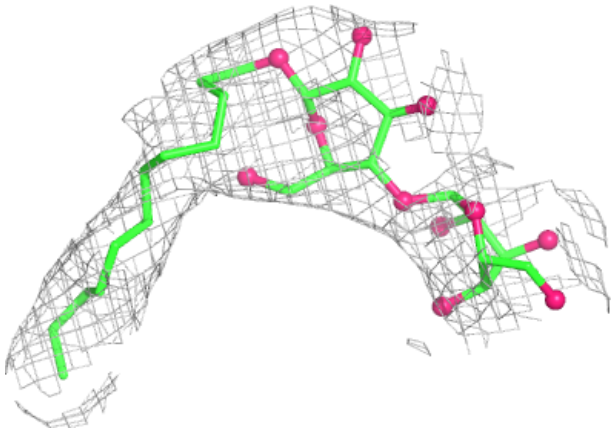


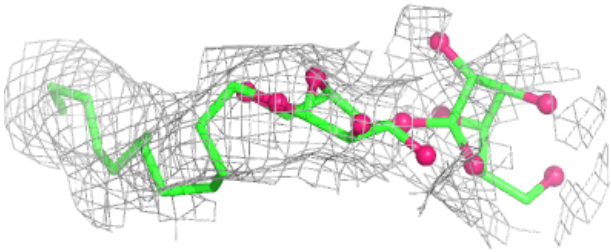




Electron density around LMU R 7021:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

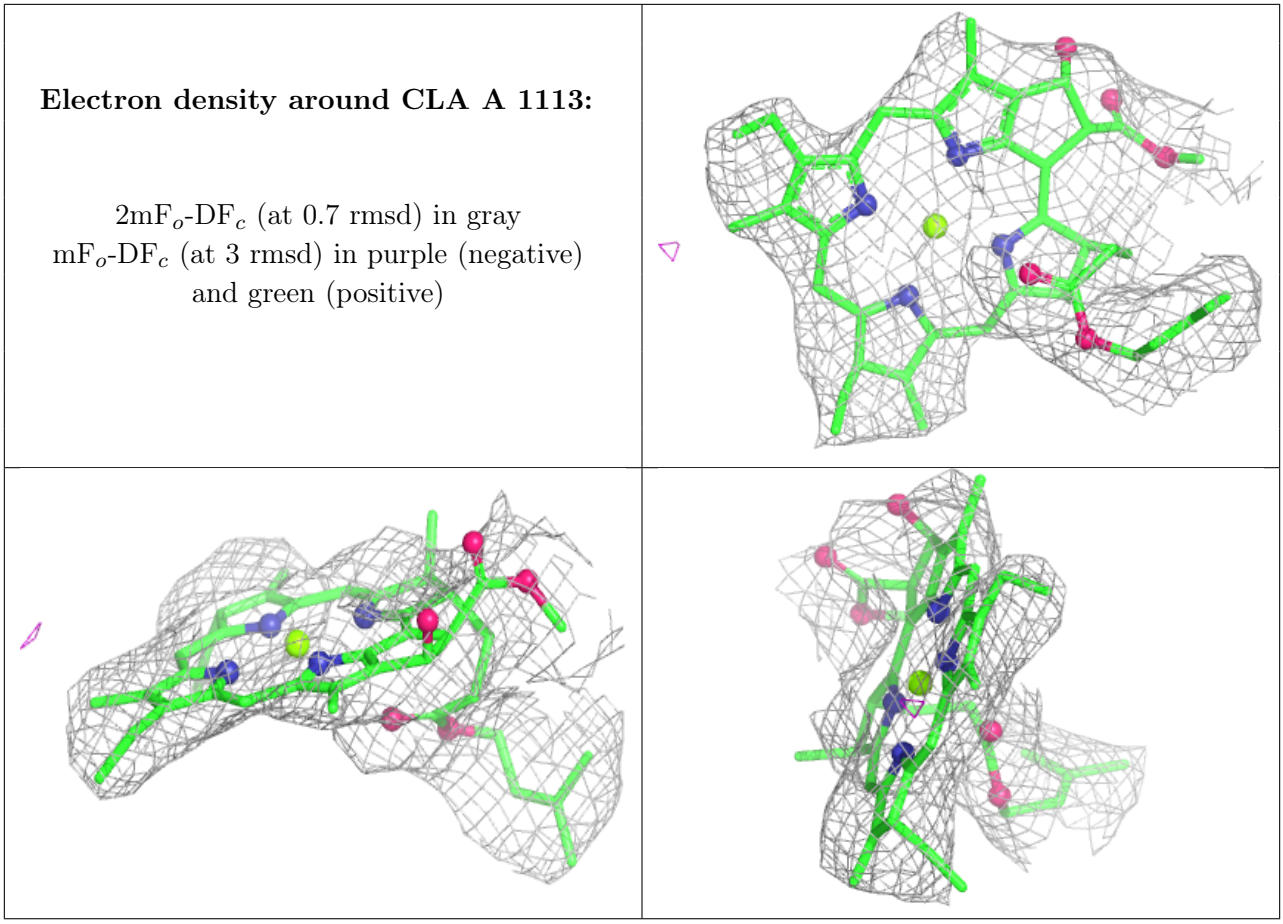






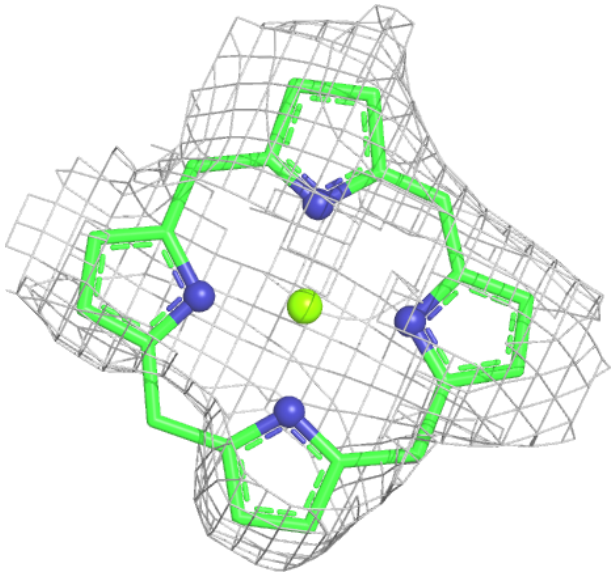
Electron density around CLA A 1113:

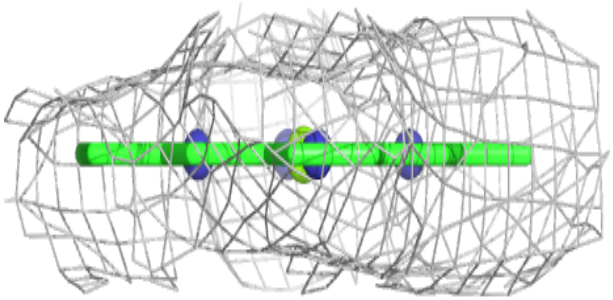
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

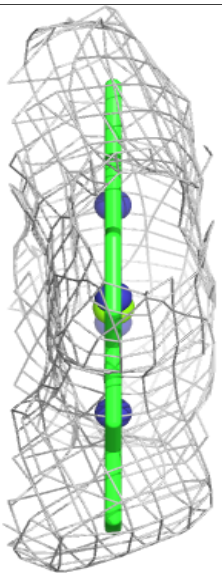


Electron density around CLA 3 3002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

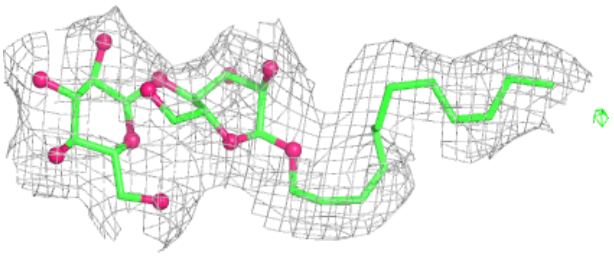


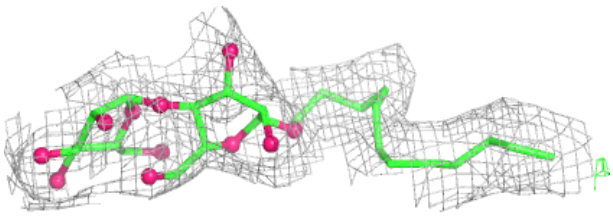


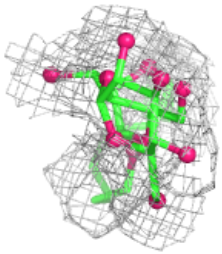


Electron density around LMU R 7020:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

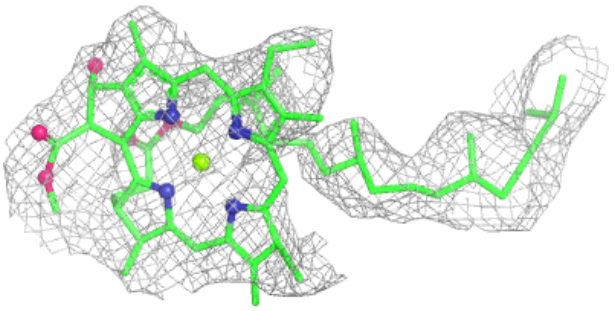


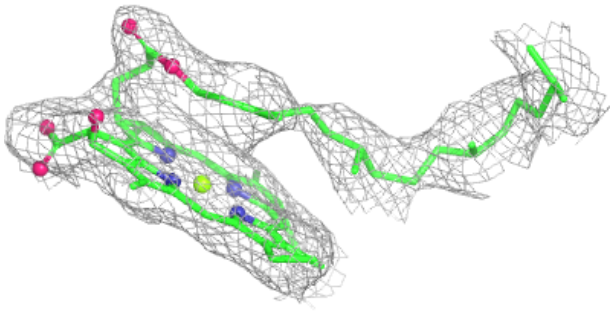


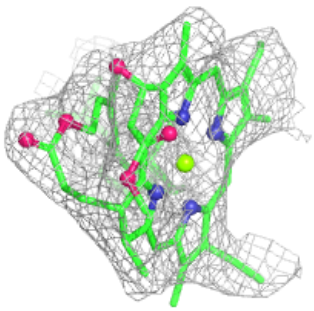


Electron density around CLA A 1115:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

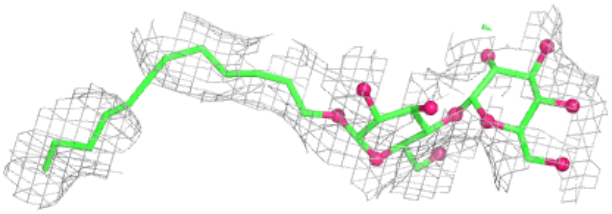


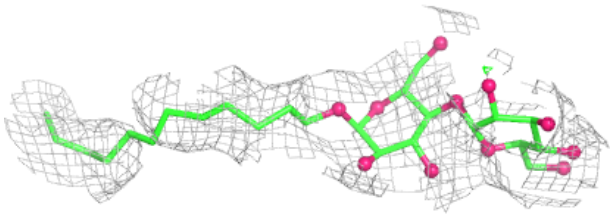


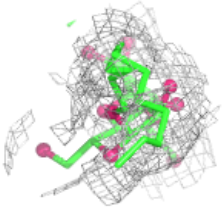


Electron density around LMU B 7040:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

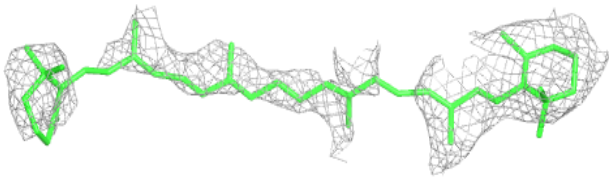


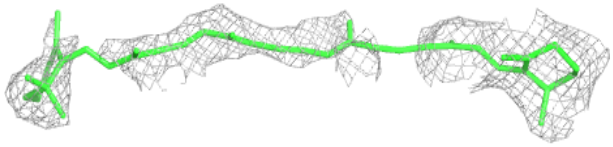


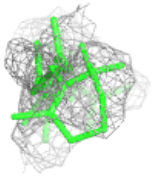


Electron density around BCR A 6008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

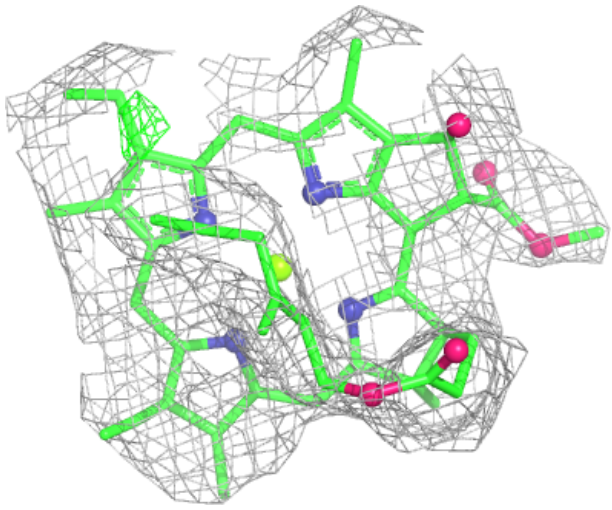


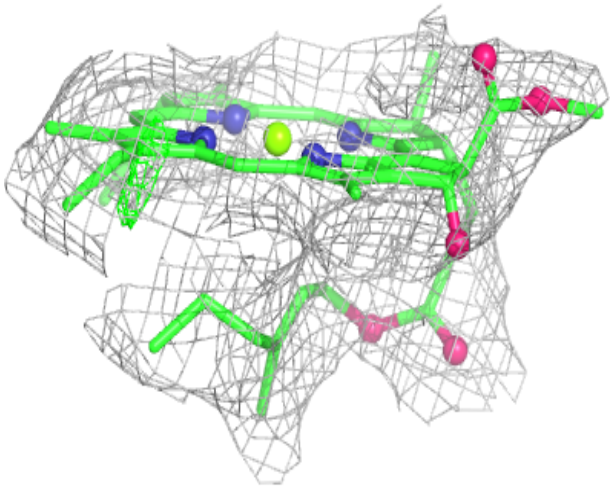




Electron density around CLA A 1116:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

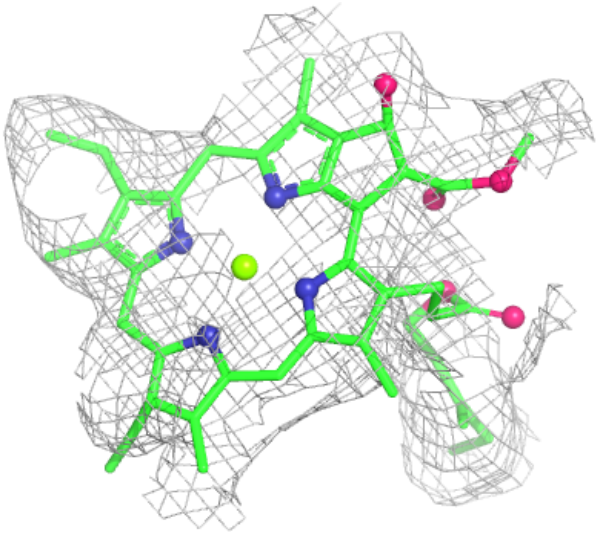


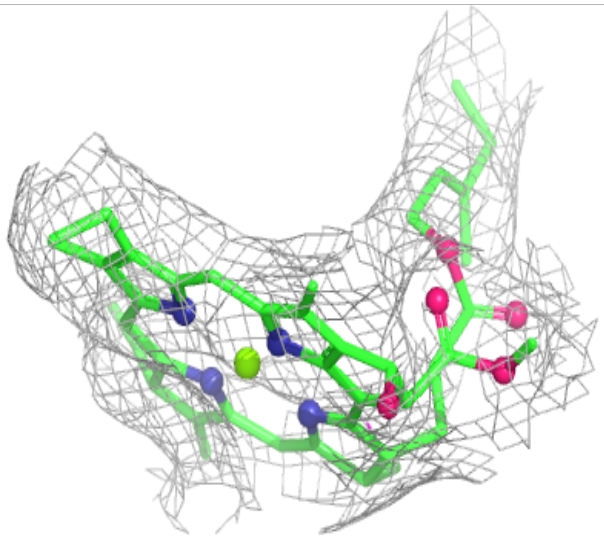


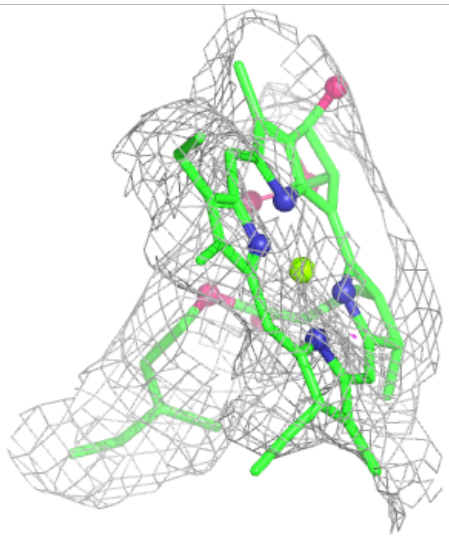


Electron density around CLA 1 1008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

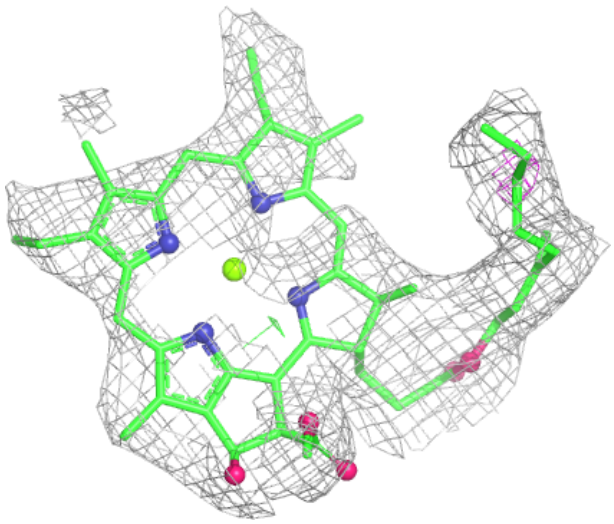






Electron density around CLA A 1111:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

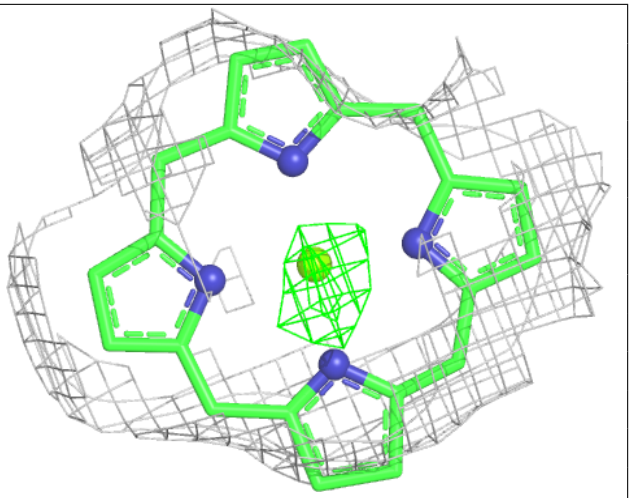


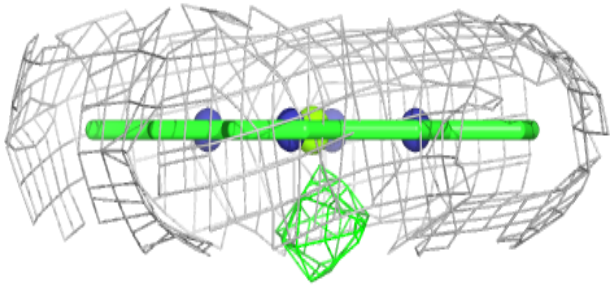


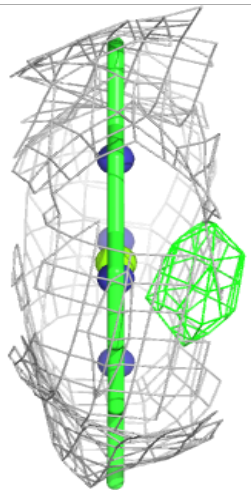


Electron density around CLA 2 2008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

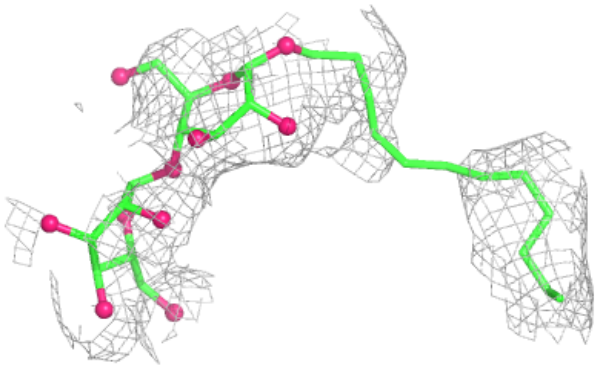


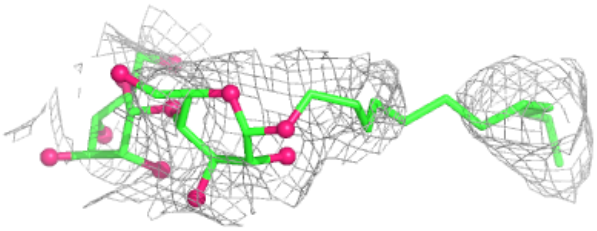


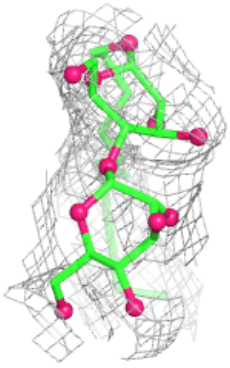


Electron density around LMU 4 7019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

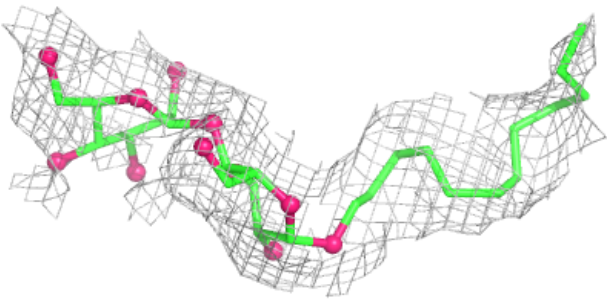


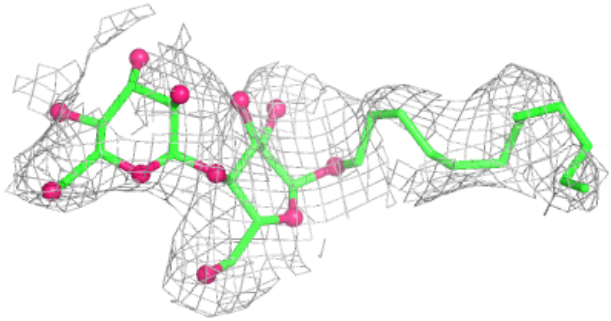


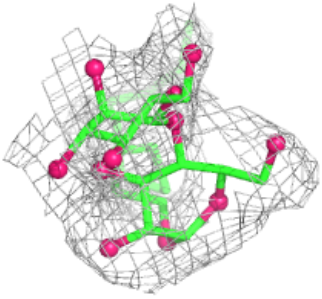


Electron density around LMU G 7026:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

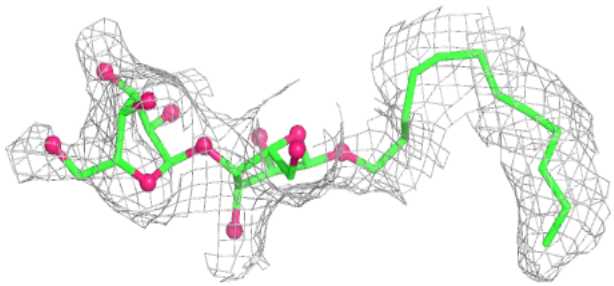


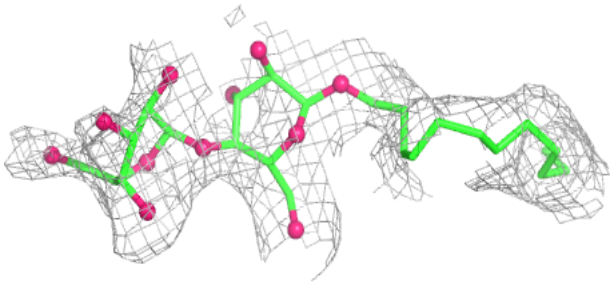


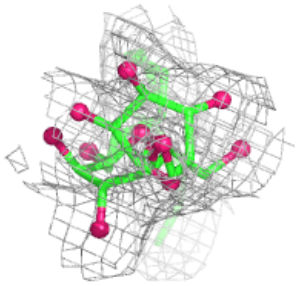


Electron density around LMU A 7044:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

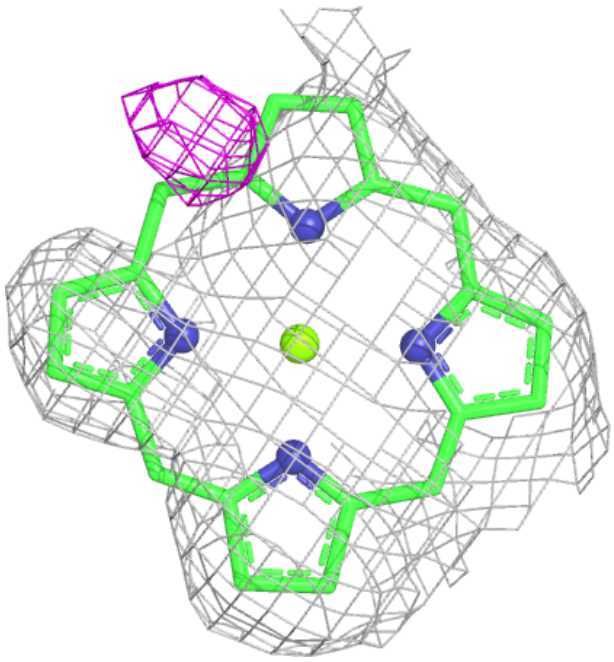


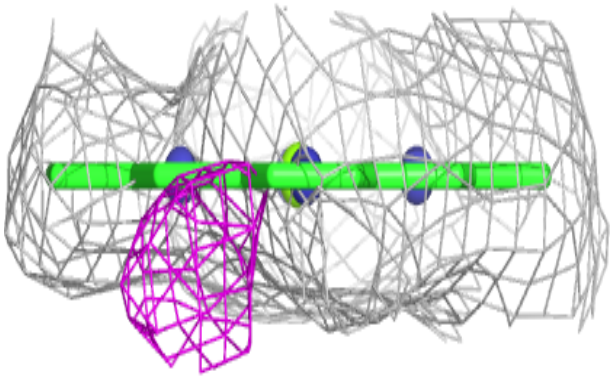


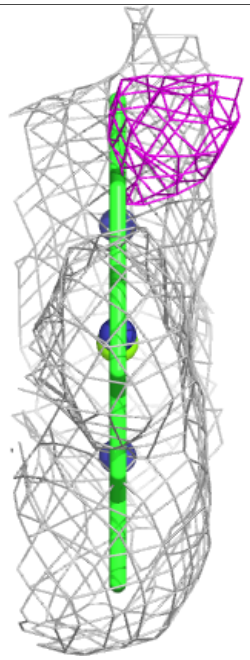


Electron density around CLA 2 2003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

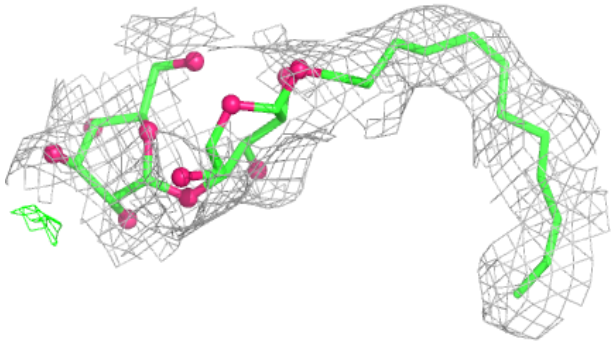


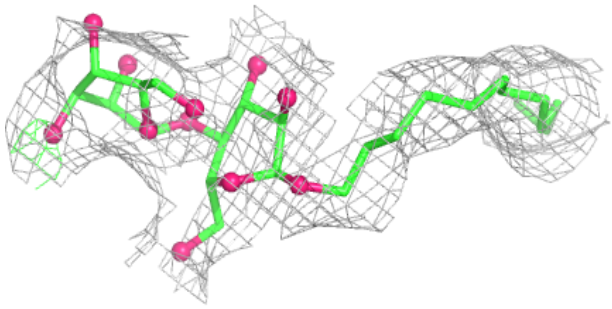


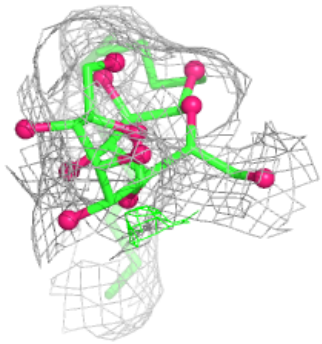


Electron density around LMU 2 7006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

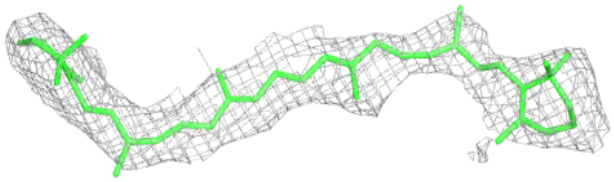


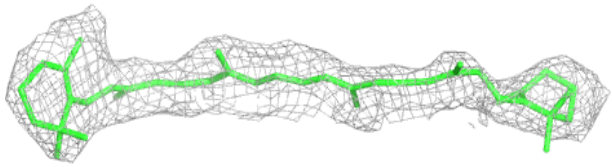


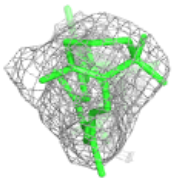


Electron density around BCR B 6006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

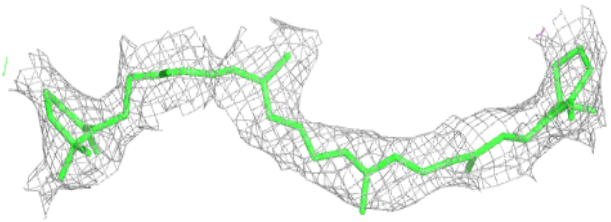


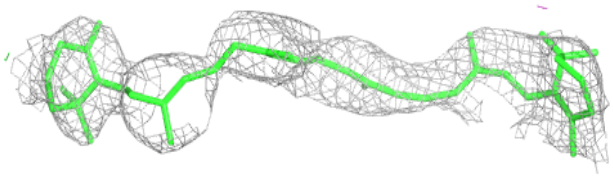


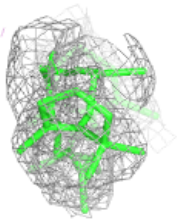


Electron density around BCR I 6021:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

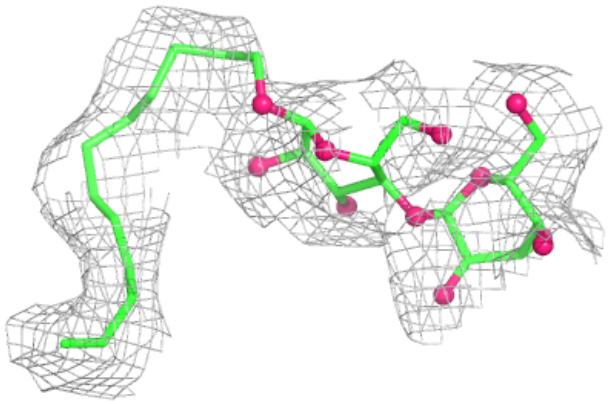


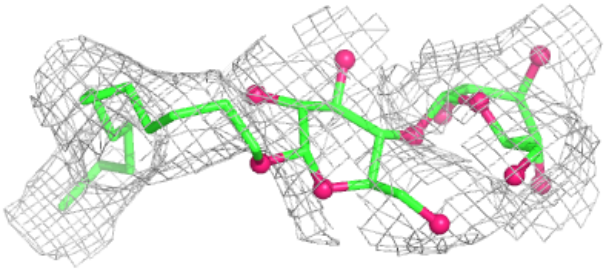


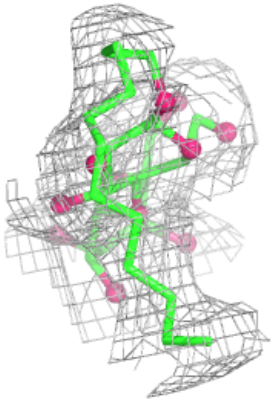


Electron density around LMU 3 7003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

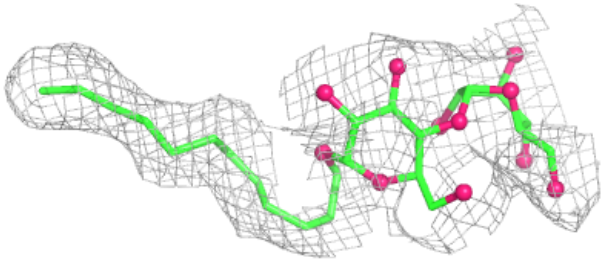


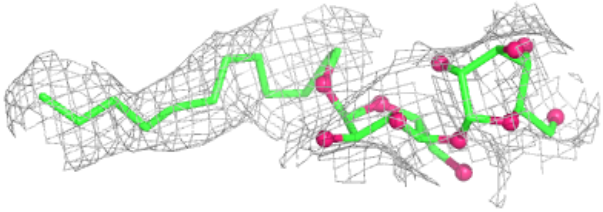


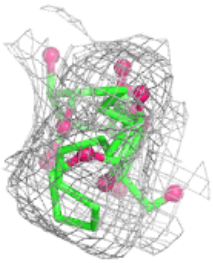


Electron density around LMU 3 7005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

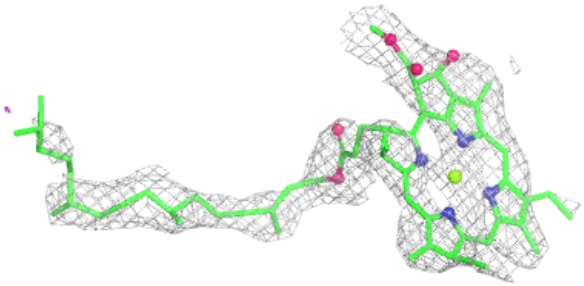


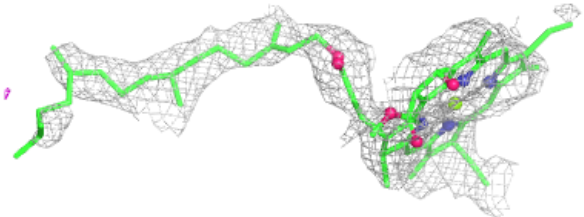


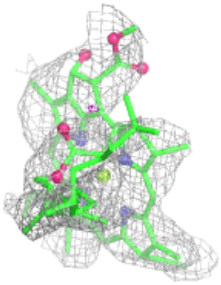


Electron density around CLA A 1119:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

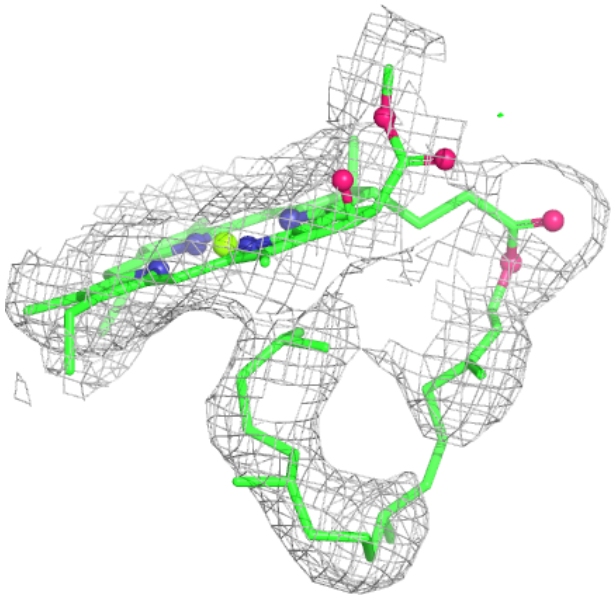


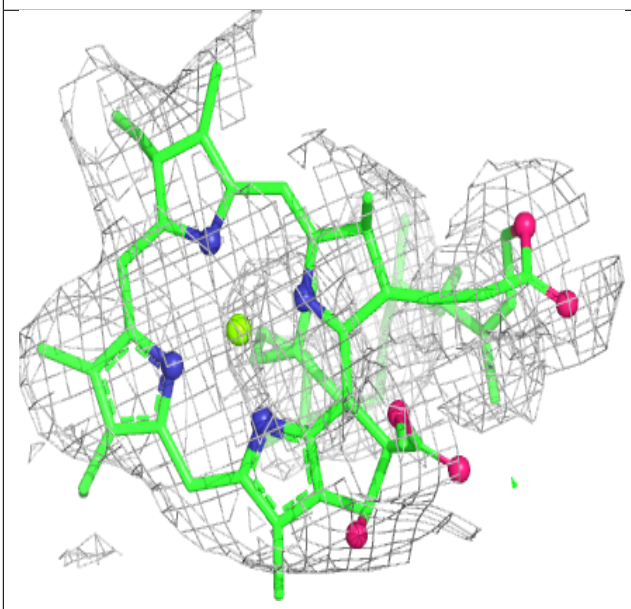


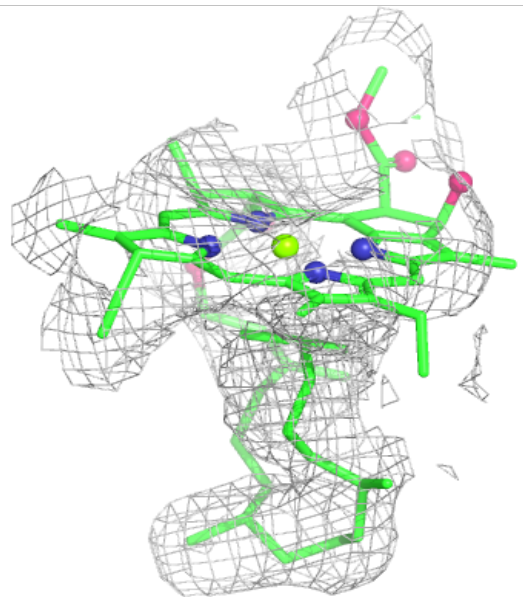


Electron density around CLA 2 4009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

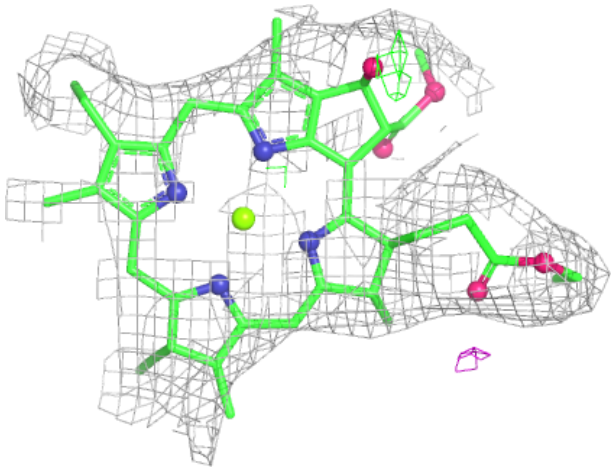


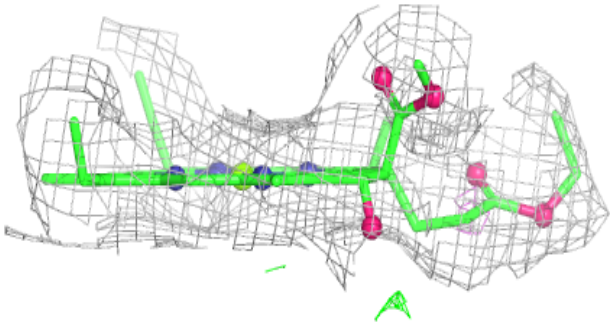


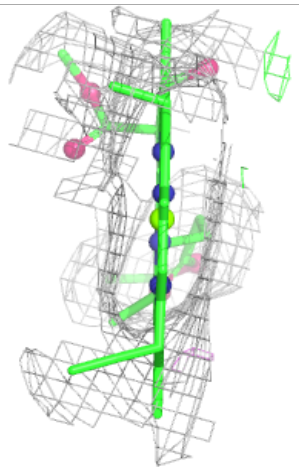


Electron density around CLA 1 1003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

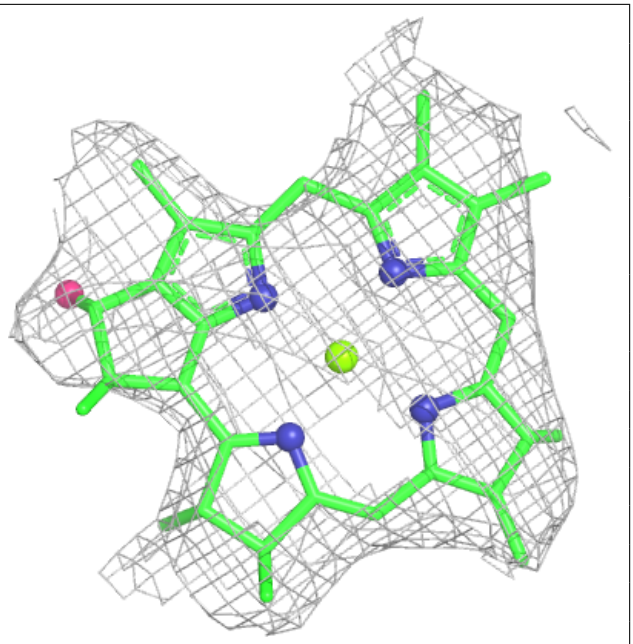


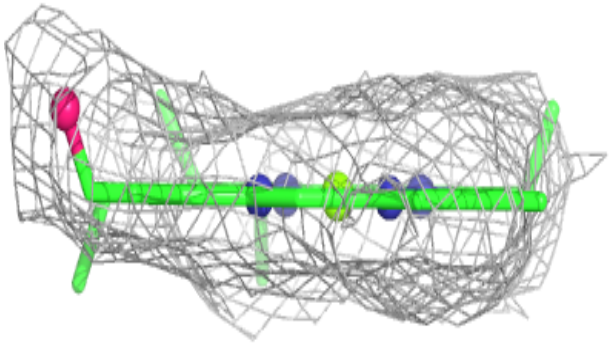


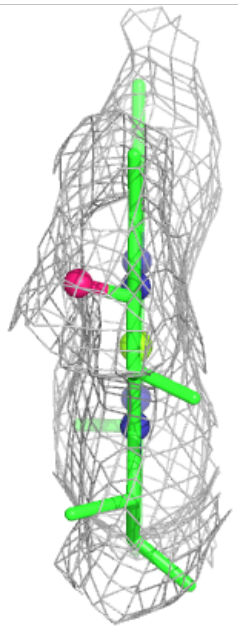


Electron density around CLA 1 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

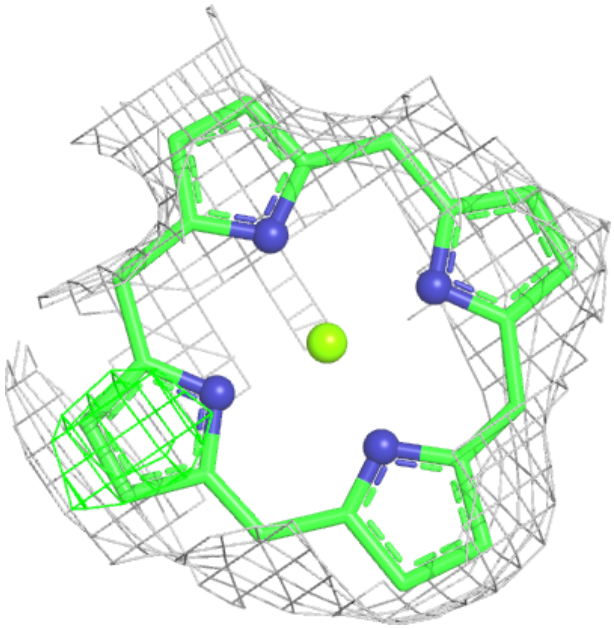


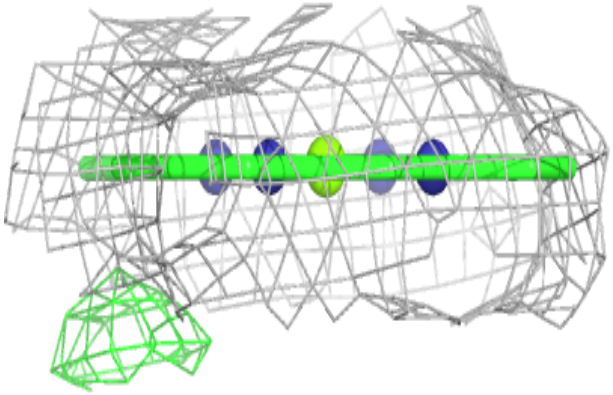


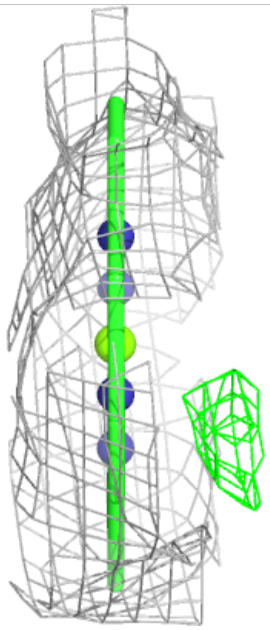


Electron density around CLA 4 4010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

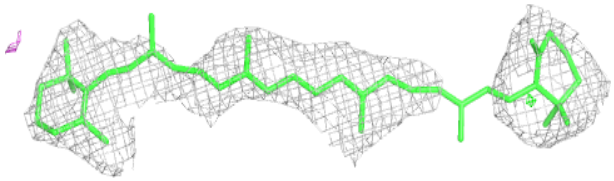


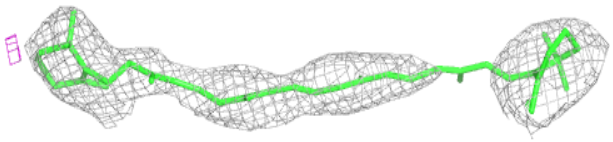


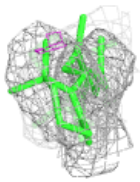


Electron density around BCR B 6004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

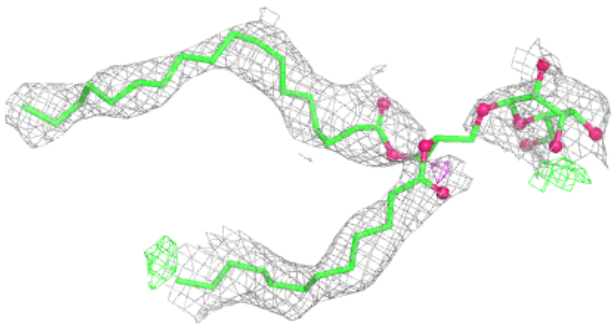


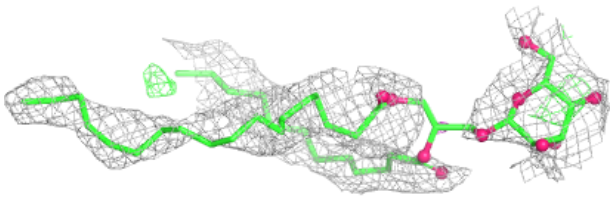


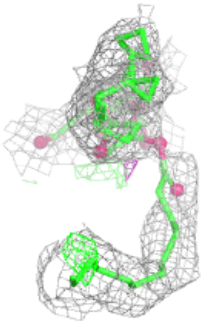


Electron density around LMG B 7101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

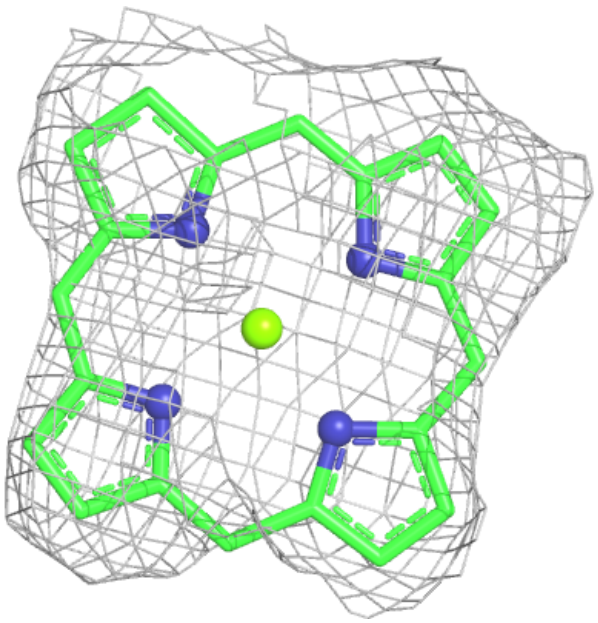


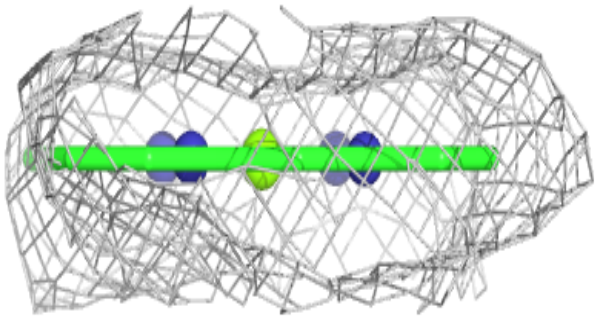


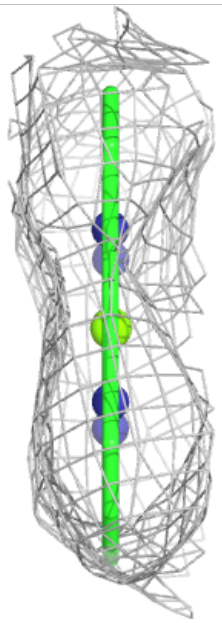


Electron density around CLA 4 4013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

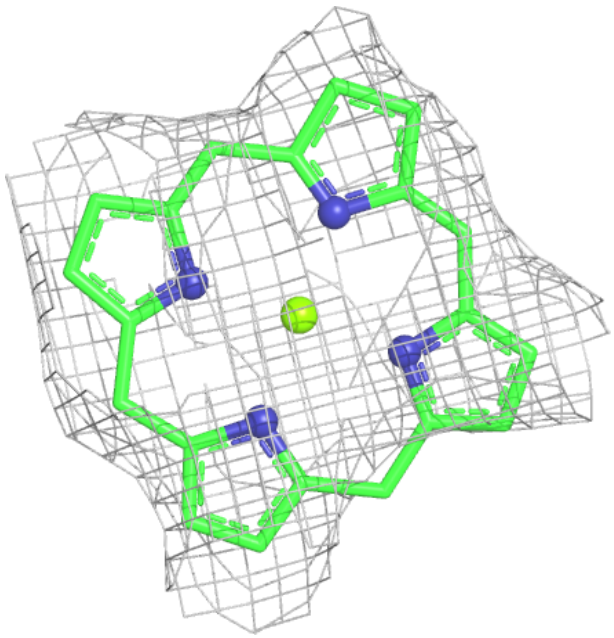


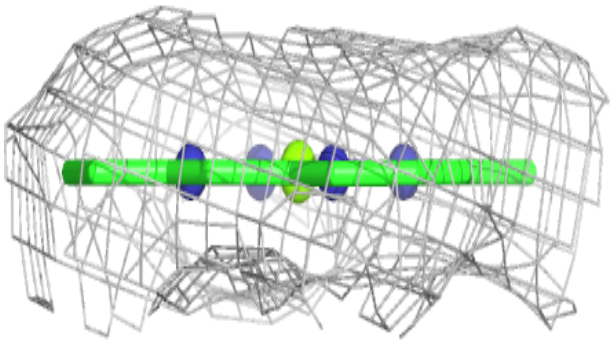


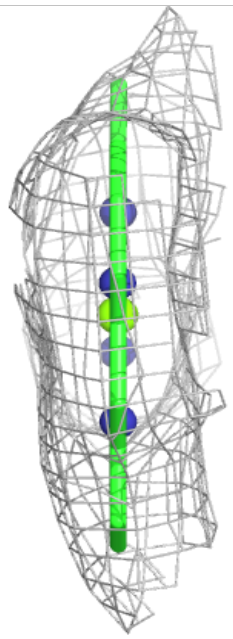


Electron density around CLA 3 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

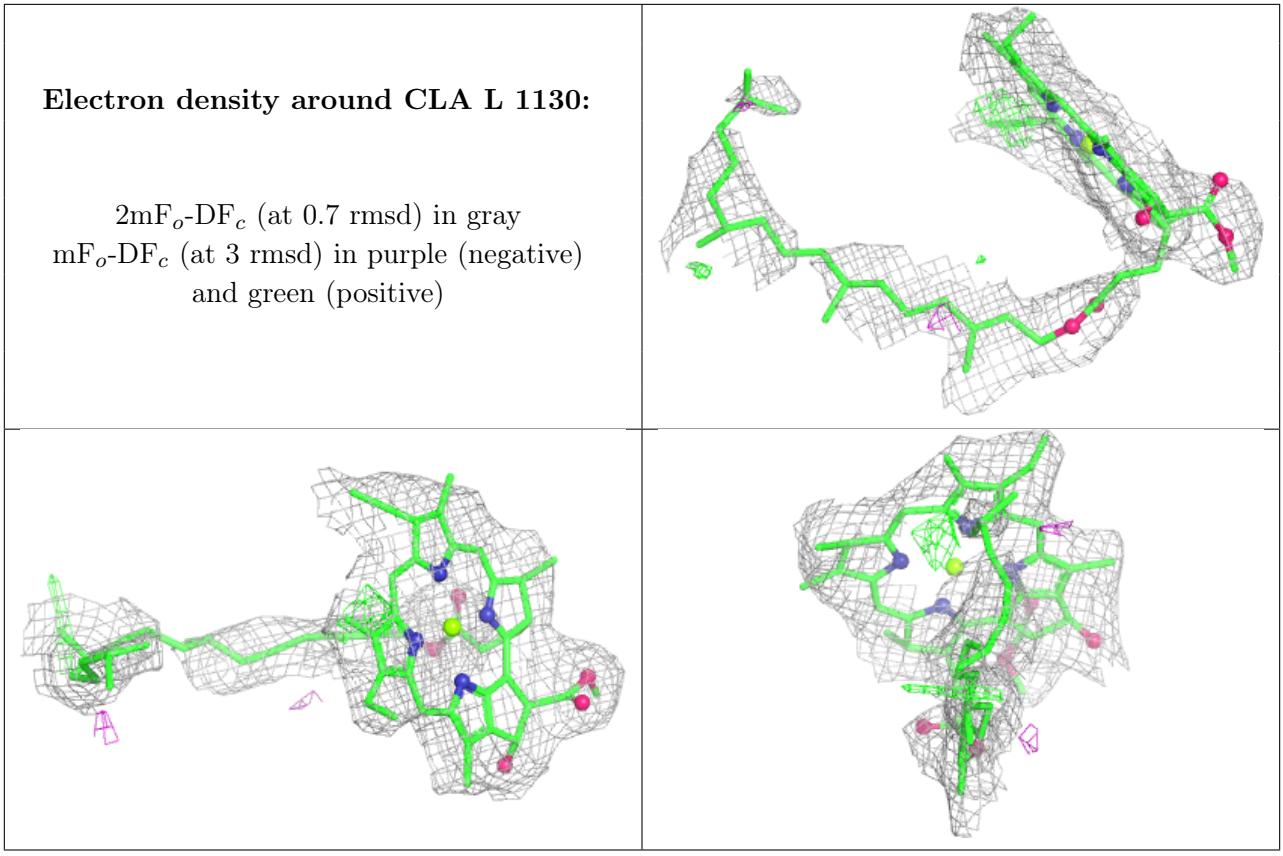






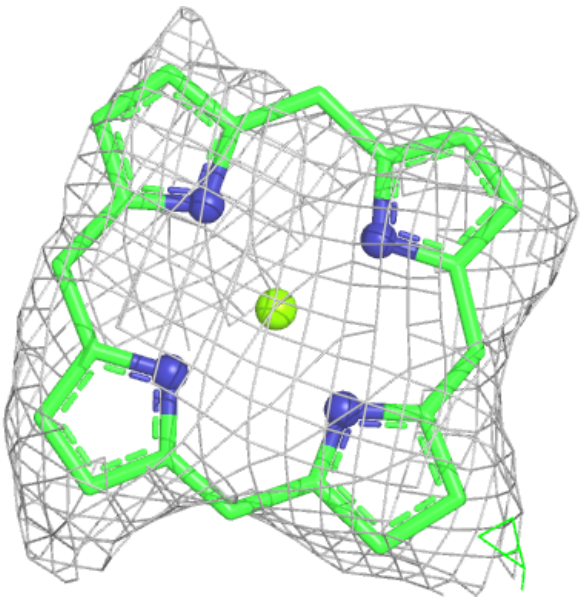
Electron density around CLA L 1130:

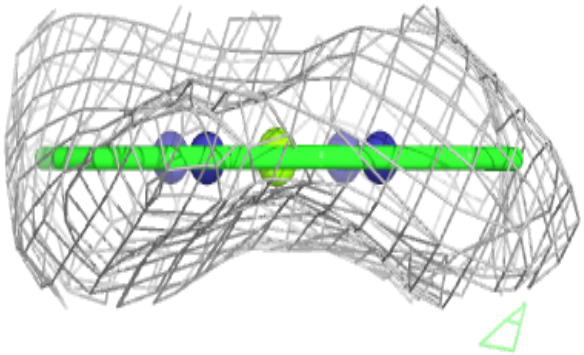
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

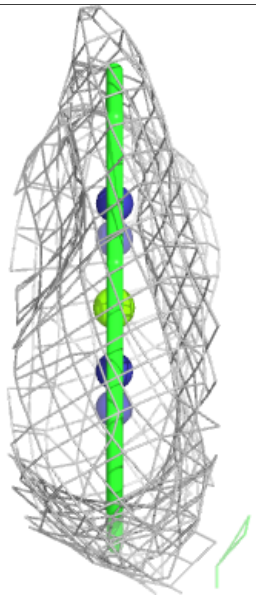


Electron density around CLA 2 2011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

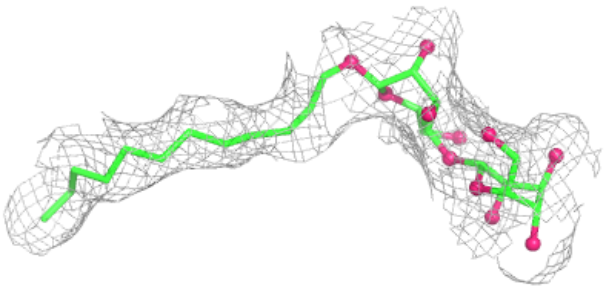


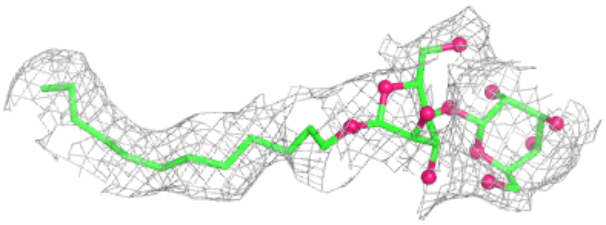


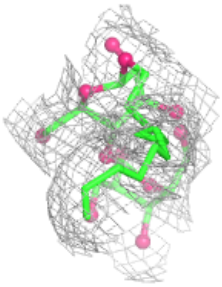


Electron density around LMU H 7002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

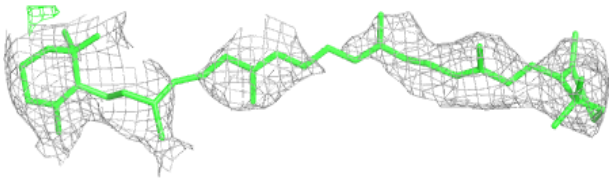


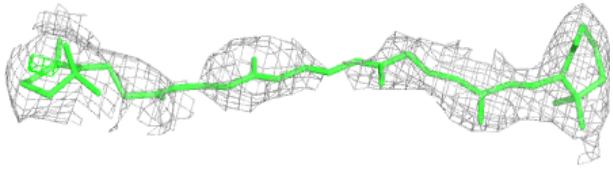


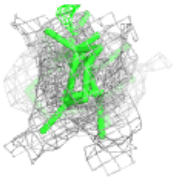


Electron density around BCR A 6003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

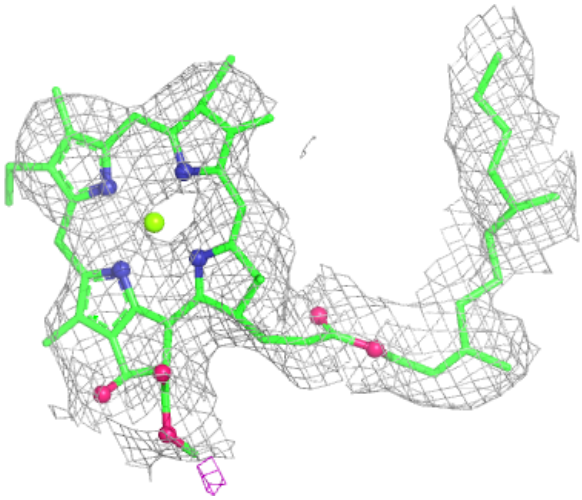


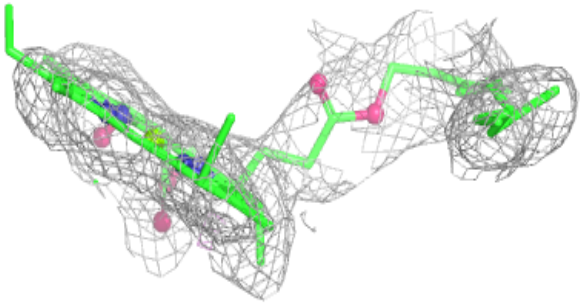


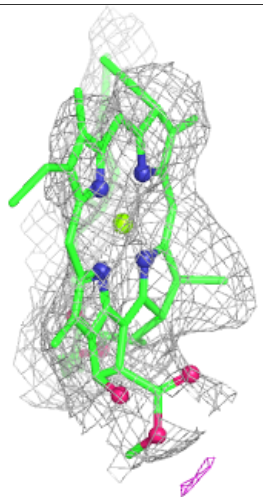


Electron density around CLA B 1222:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

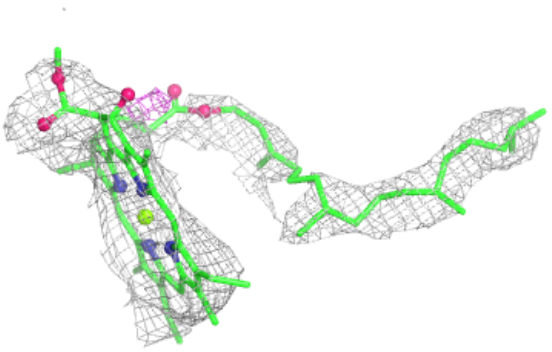


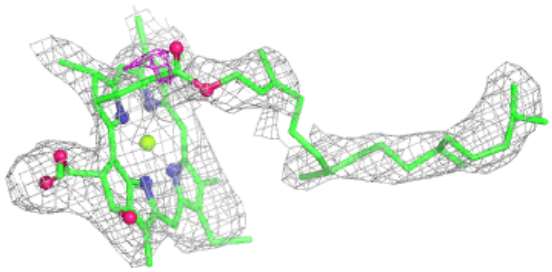


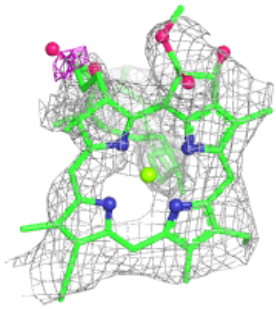


Electron density around CLA A 1109:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

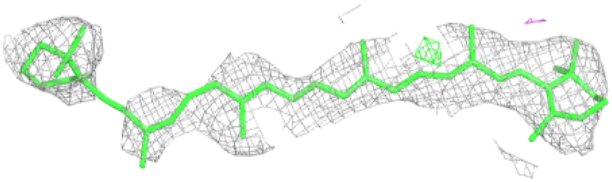


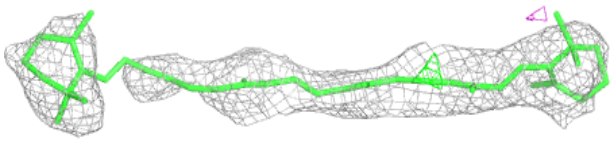


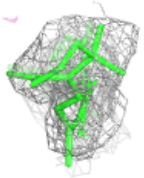


Electron density around BCR B 6017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

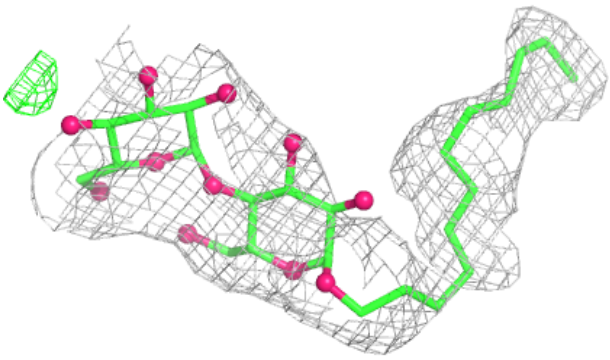


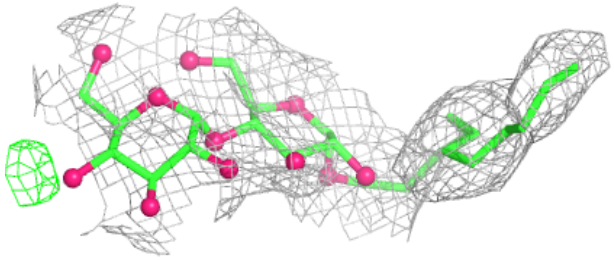


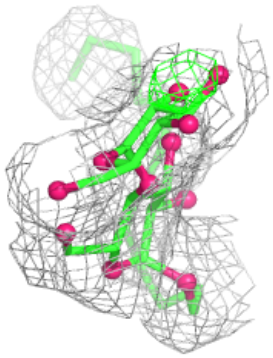


Electron density around LMU R 7025:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

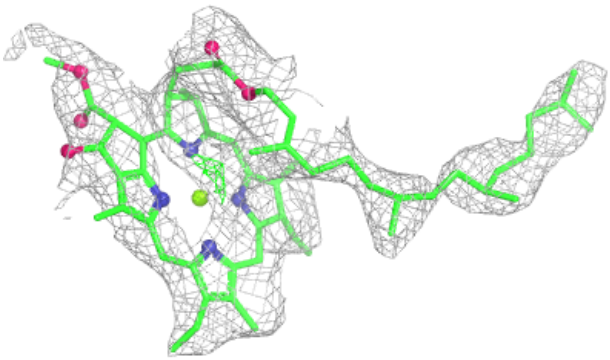


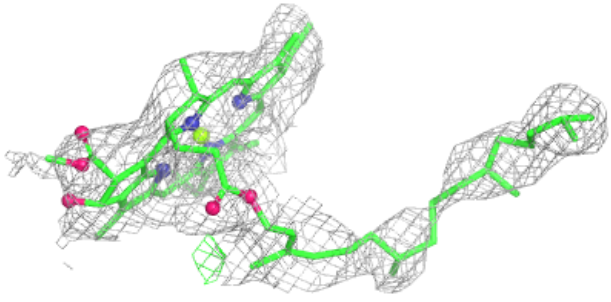


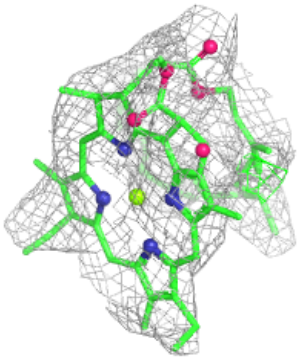


Electron density around CLA B 1211:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

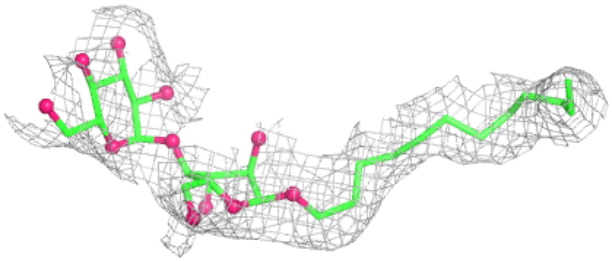




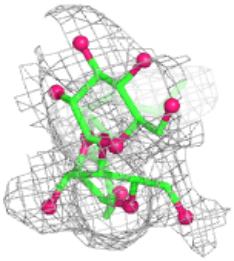


Electron density around LMU 4 7018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

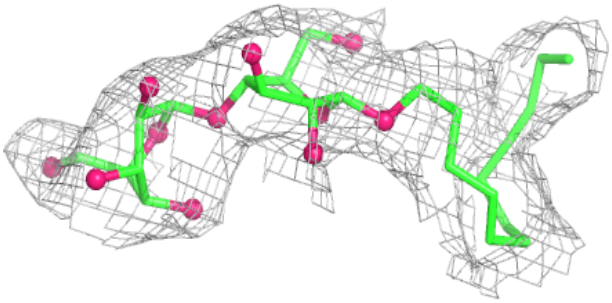


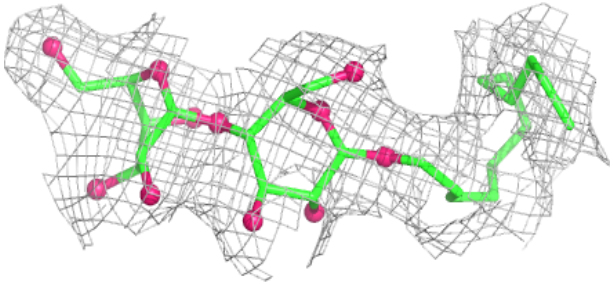


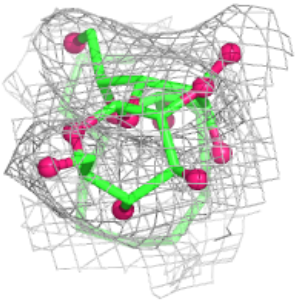


Electron density around LMU A 7023:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

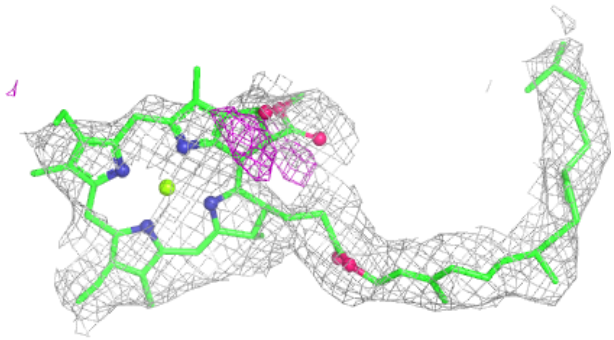


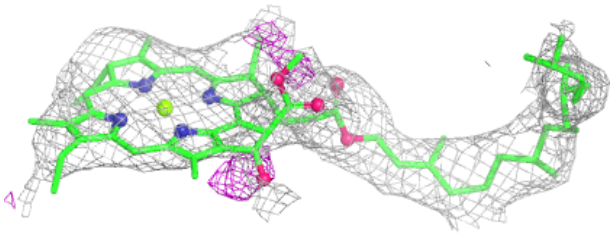


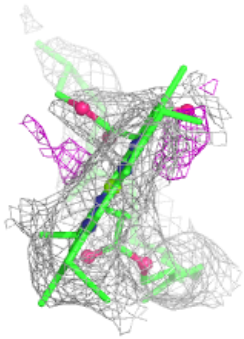


Electron density around CLA B 1223:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

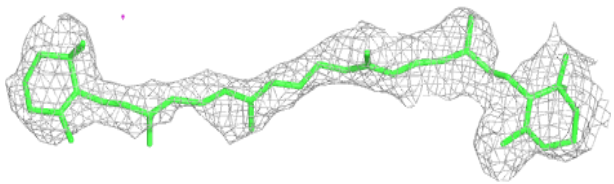


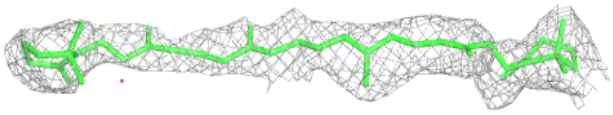


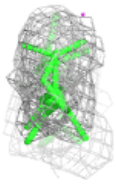


Electron density around BCR L 6019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

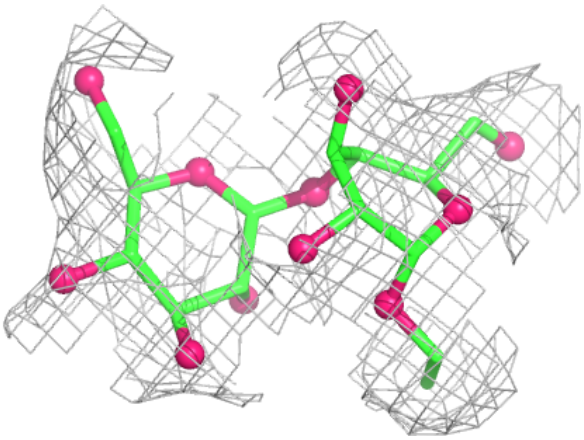


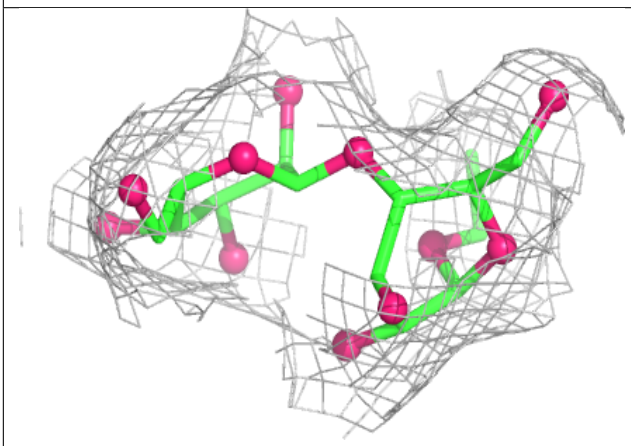


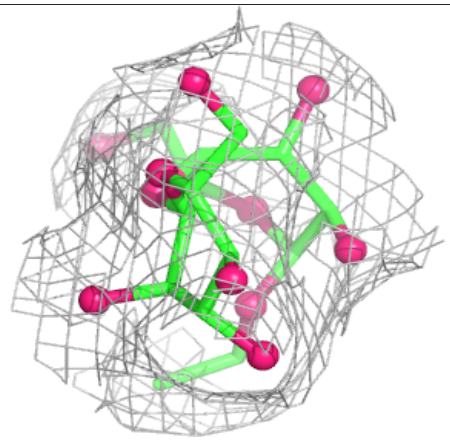


Electron density around LMU B 7012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

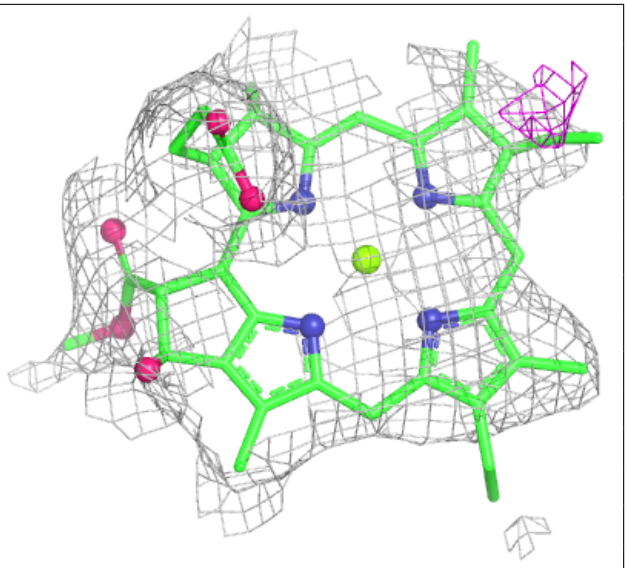


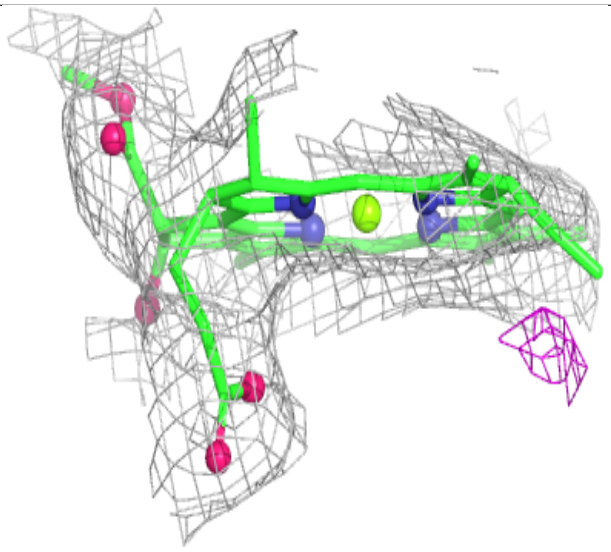


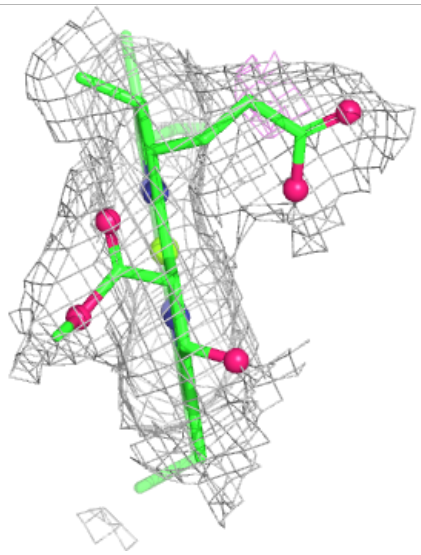


Electron density around CLA B 1231:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

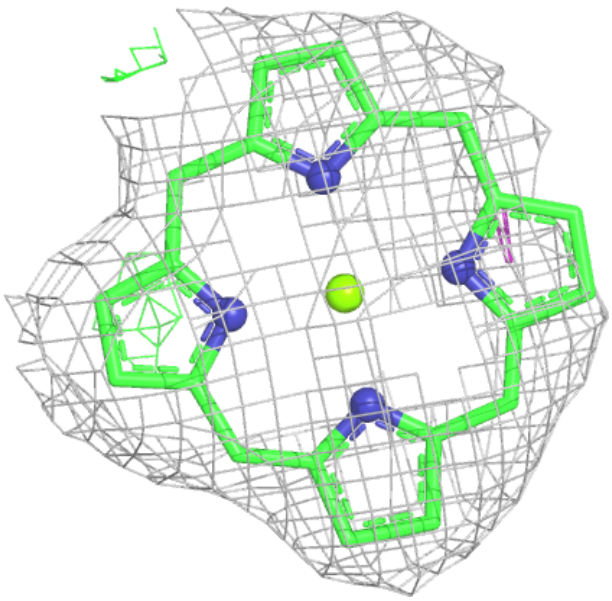


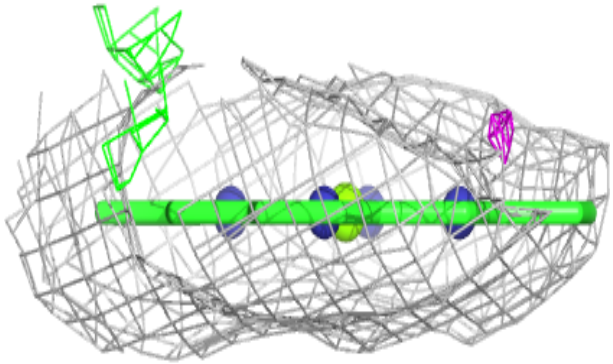


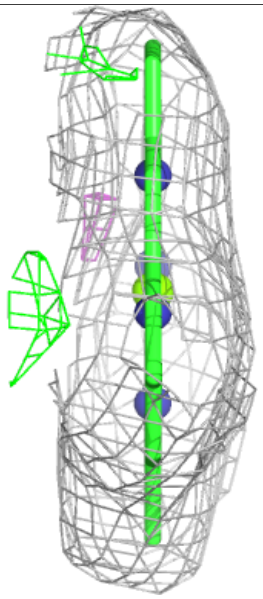


Electron density around CLA 4 4005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

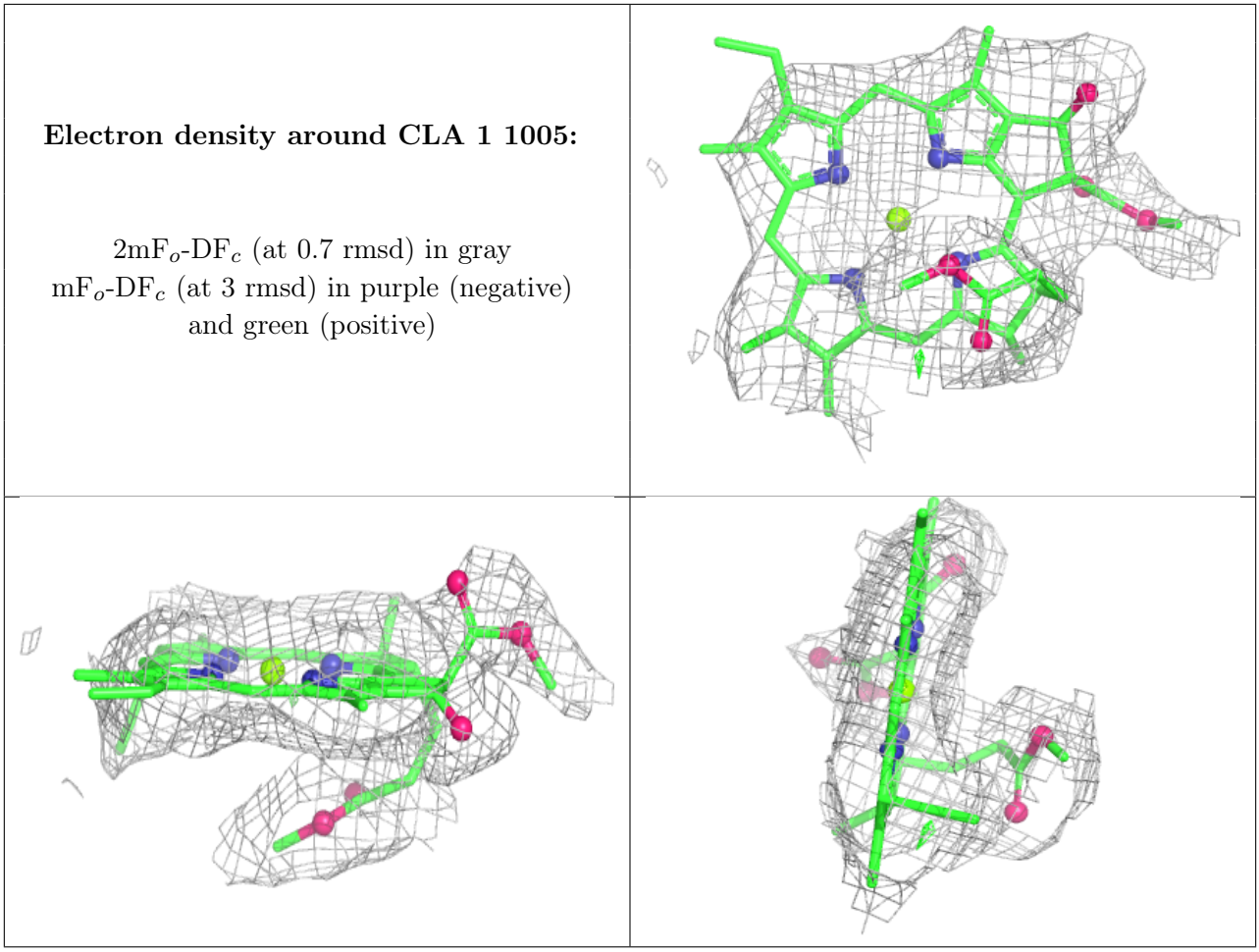






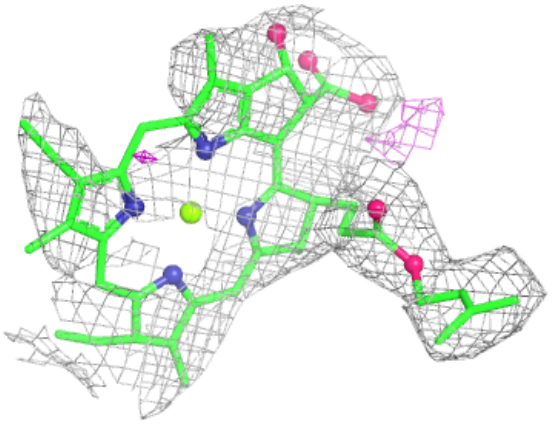
Electron density around CLA 1 1005:

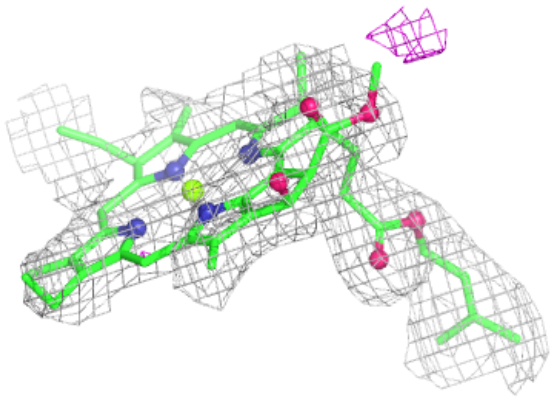
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

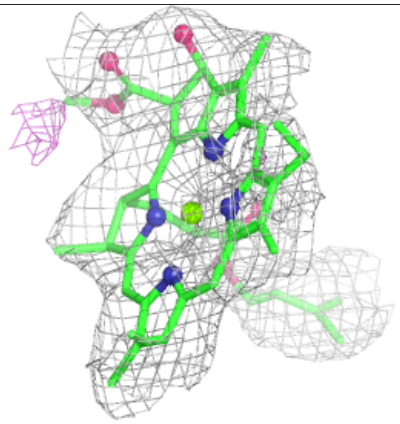


Electron density around CLA 2 2012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

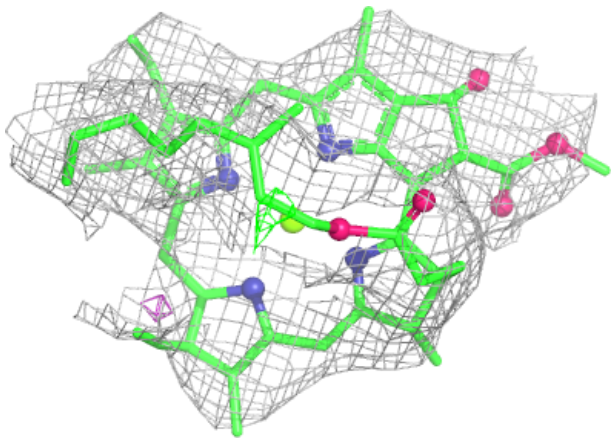


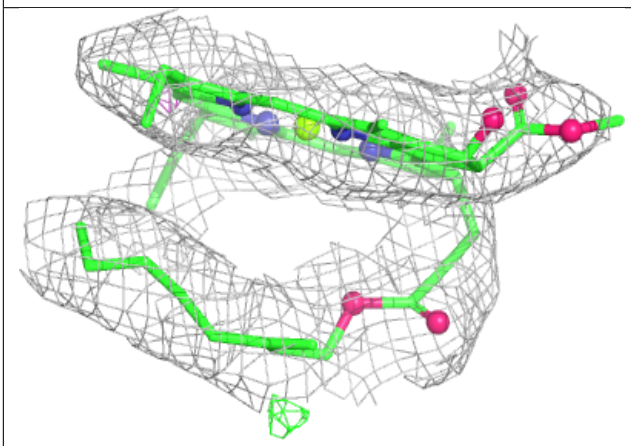




Electron density around CLA A 1110:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

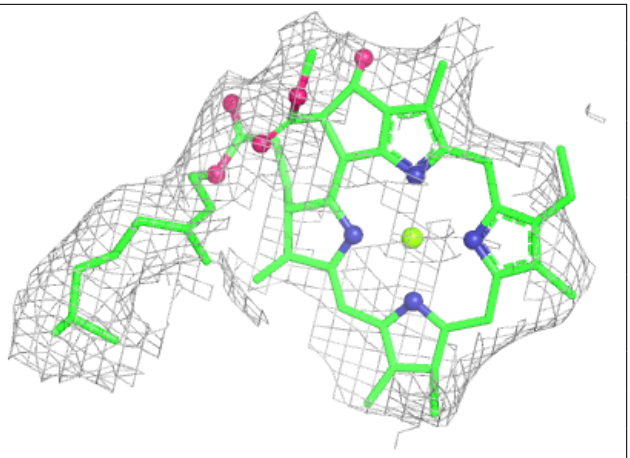


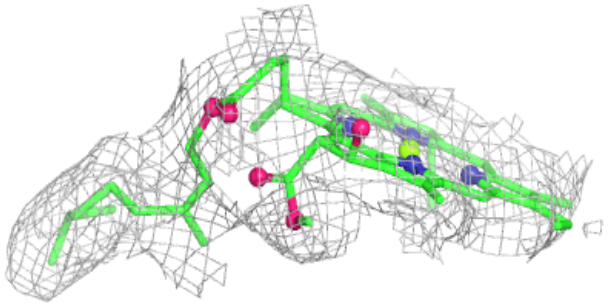




Electron density around CLA J 1308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

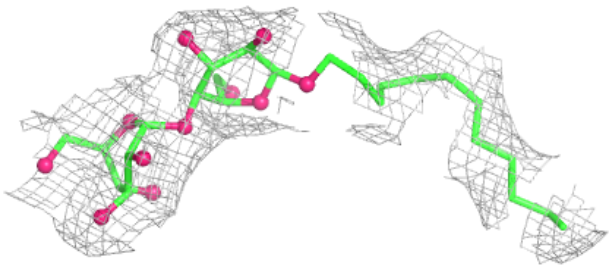


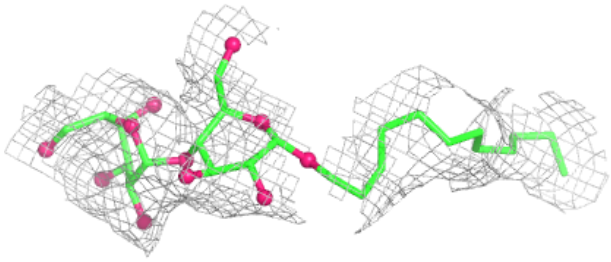


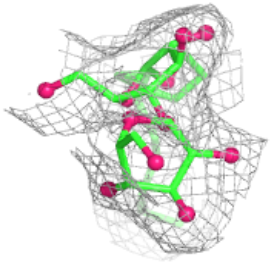


Electron density around LMU 2 7027:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

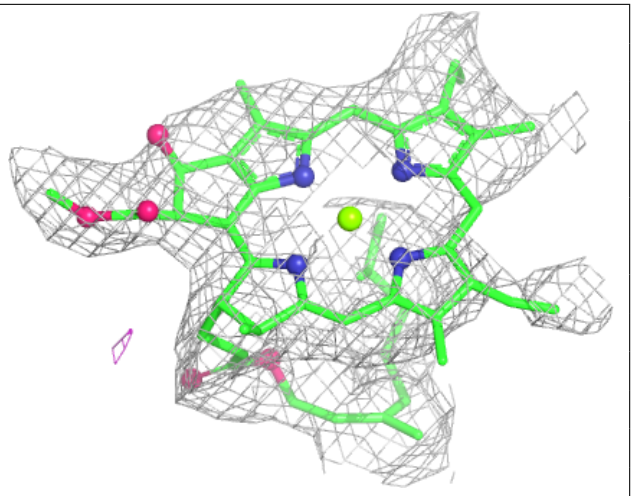


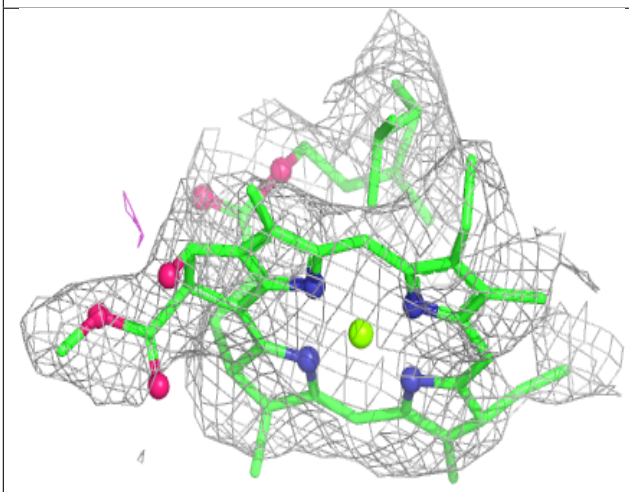


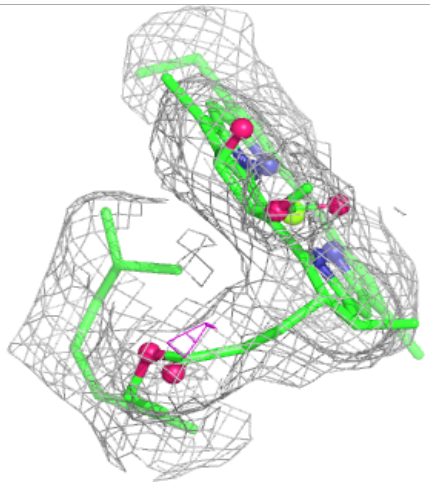


Electron density around CLA B 1209:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

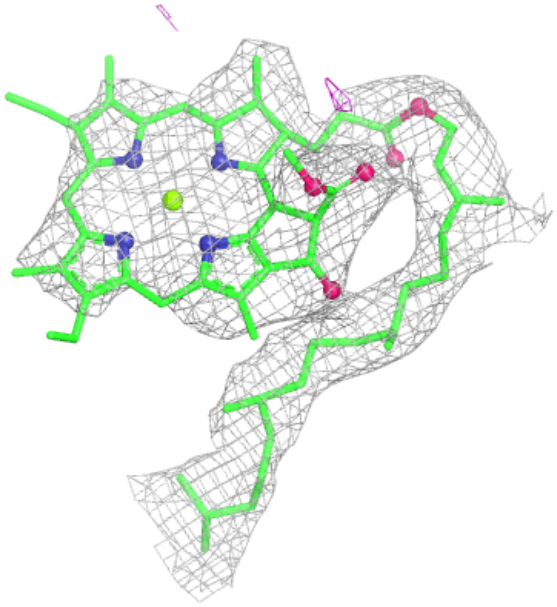


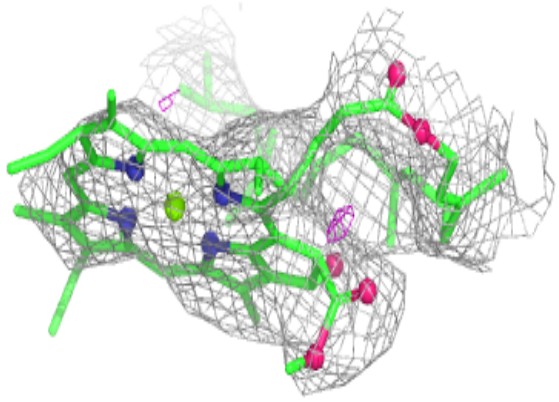


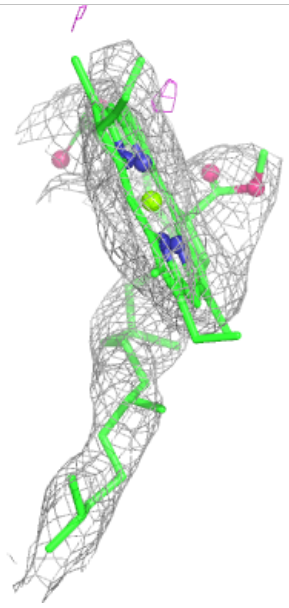


Electron density around CLA A 1123:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

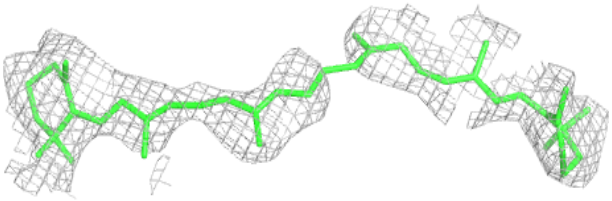


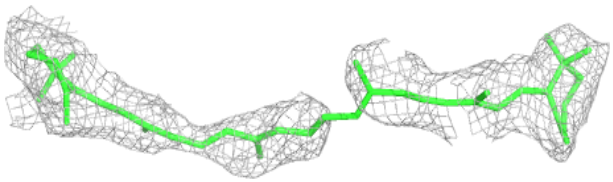


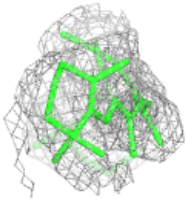


Electron density around BCR I 6018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

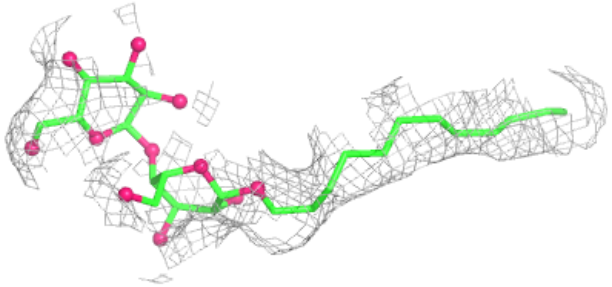


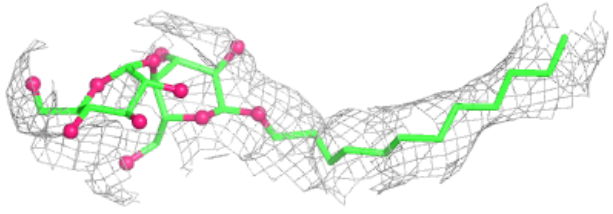


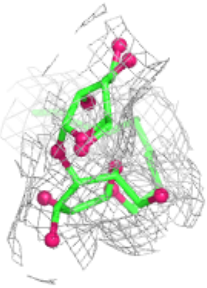


Electron density around LMU R 7024:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

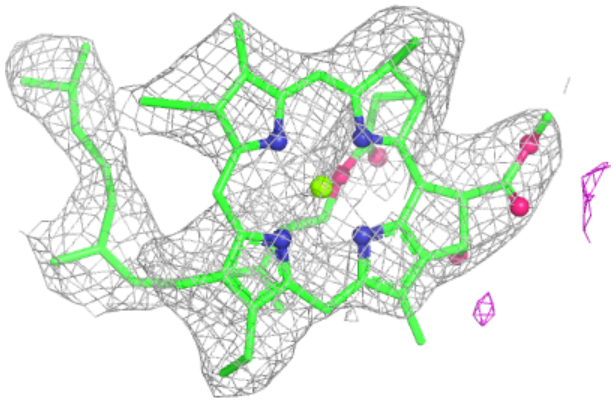


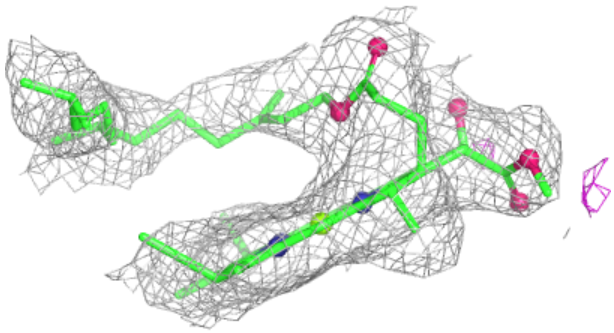




Electron density around CLA I 1204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

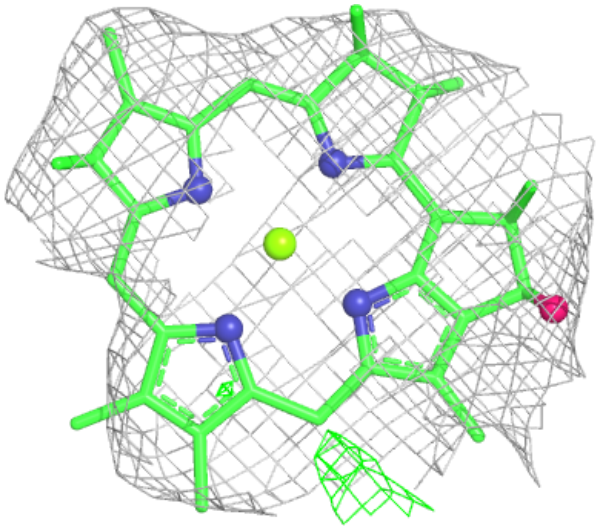


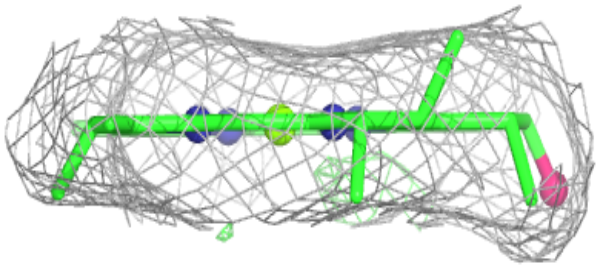


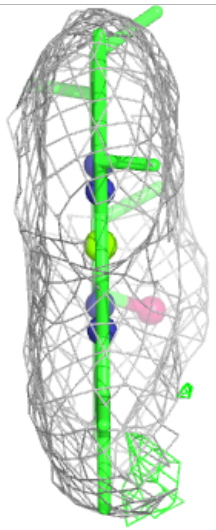


Electron density around CLA 4 1009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

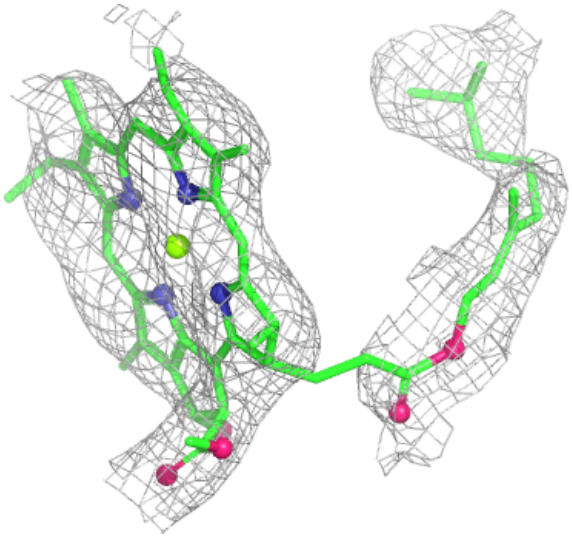


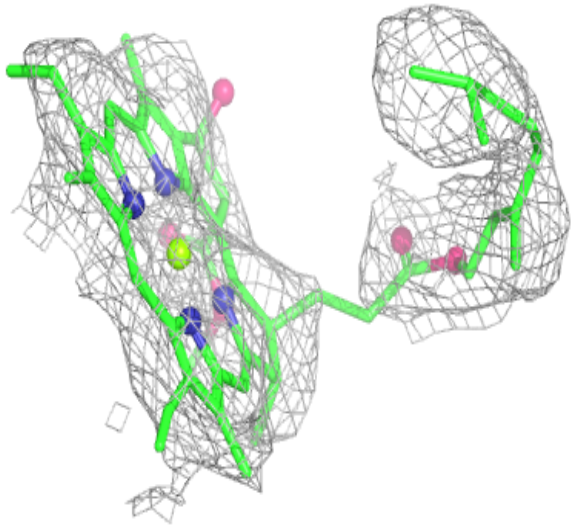


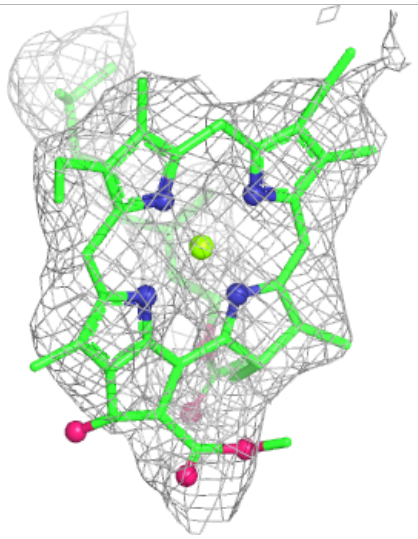


Electron density around CLA A 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

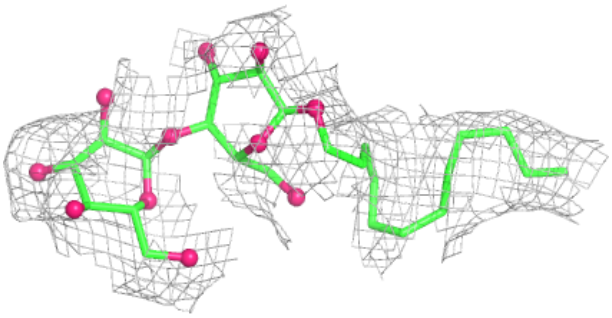


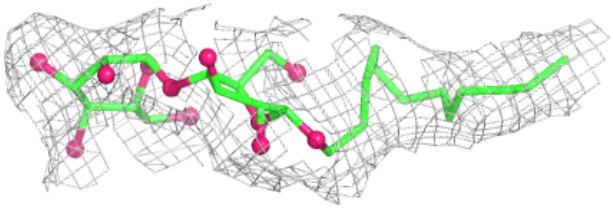


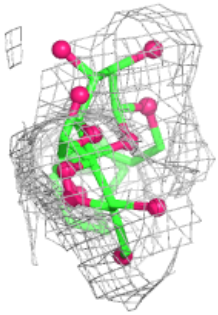


Electron density around LMU A 7016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

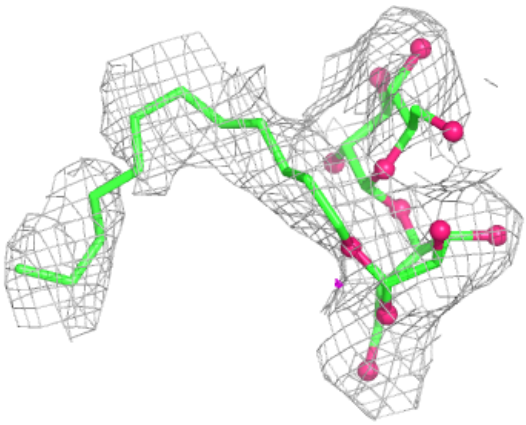


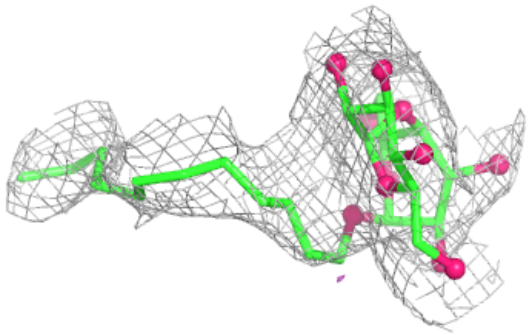




Electron density around LMU H 7032:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

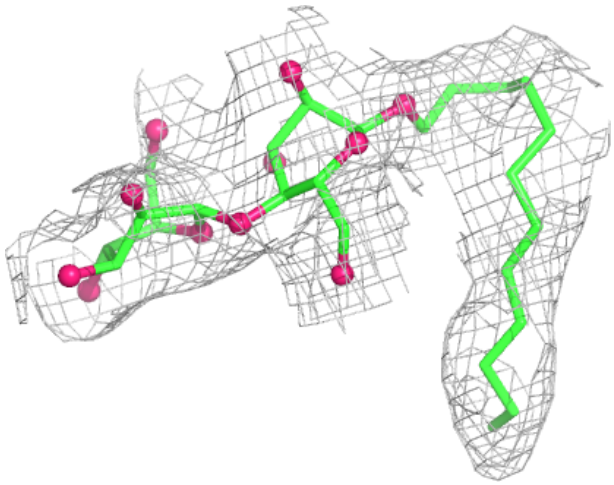


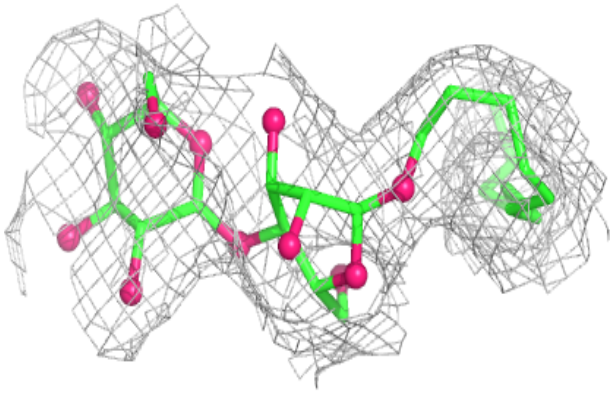




Electron density around LMU R 7014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

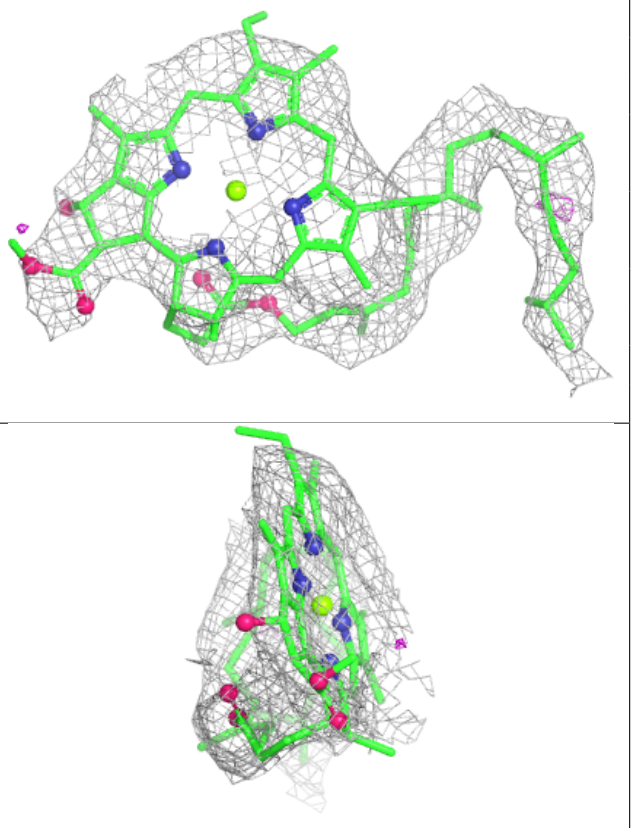


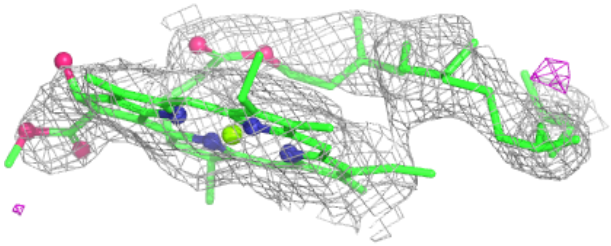




Electron density around CLA A 1117:

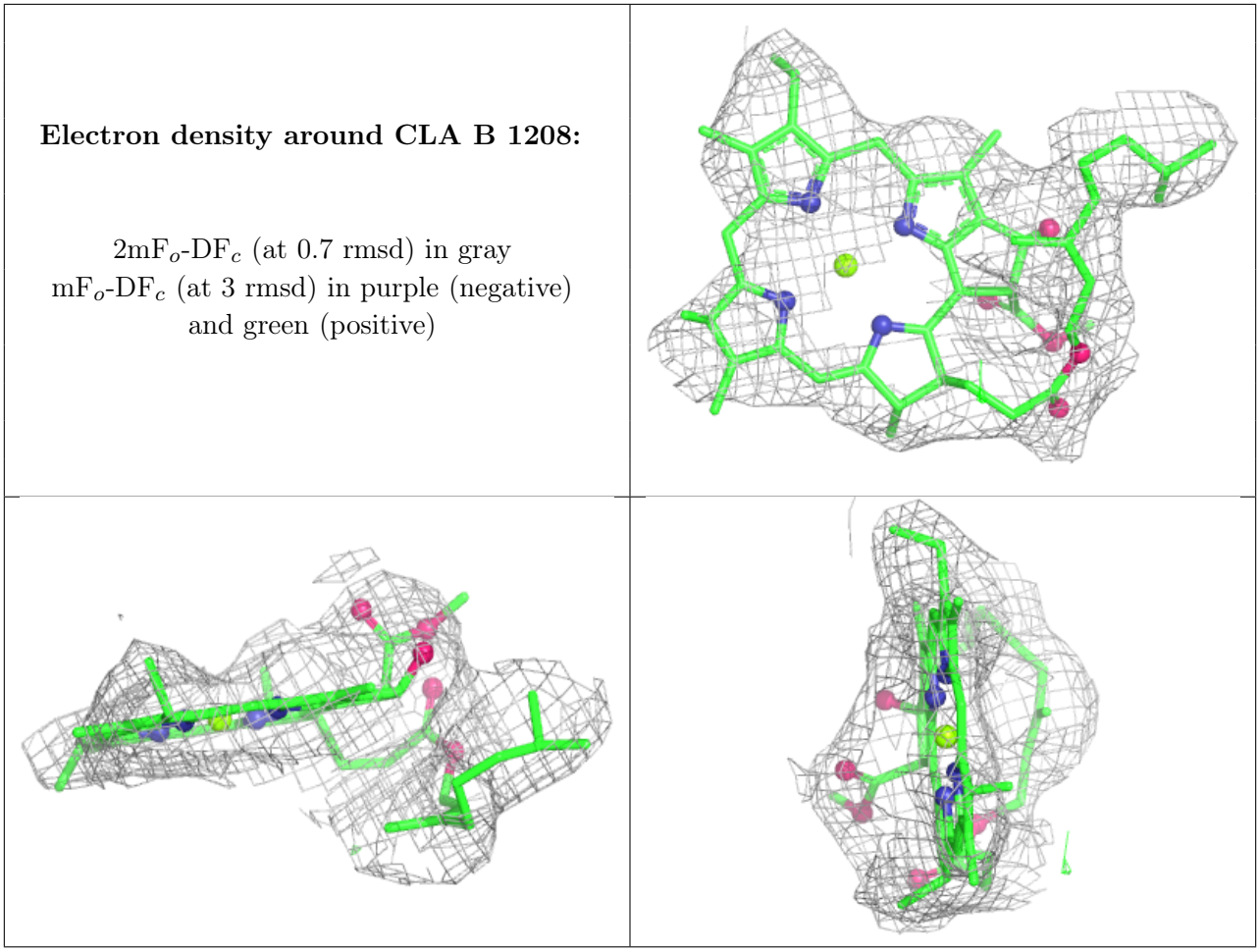
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





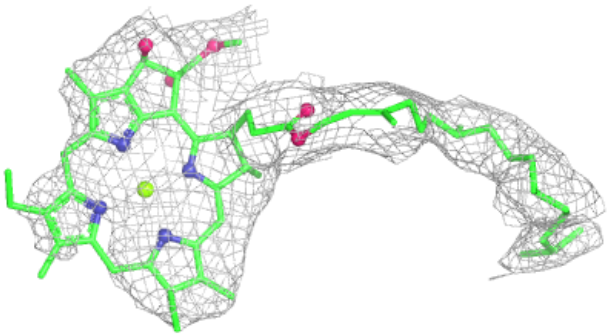
Electron density around CLA B 1208:

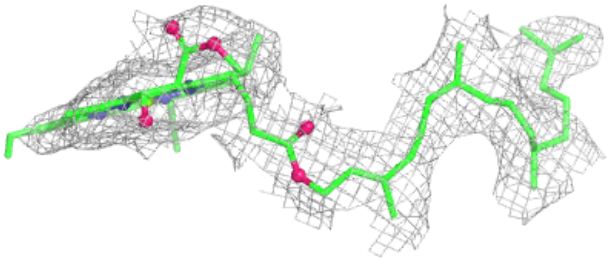
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 1124:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

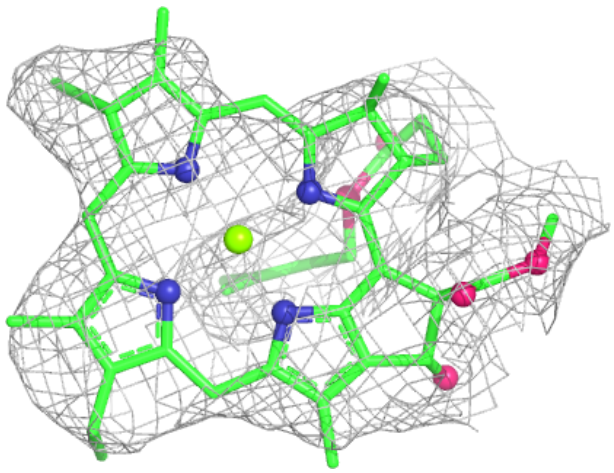


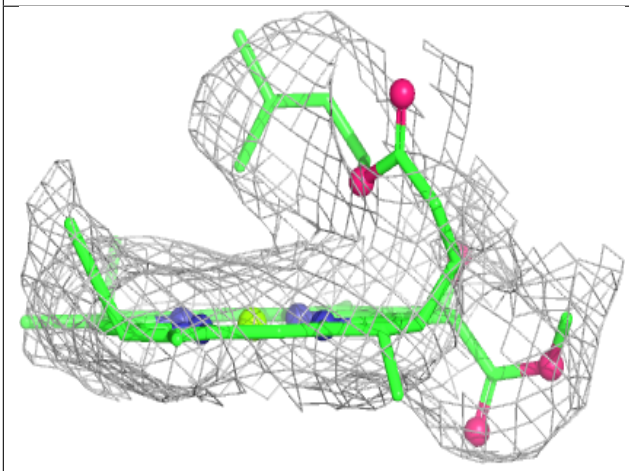


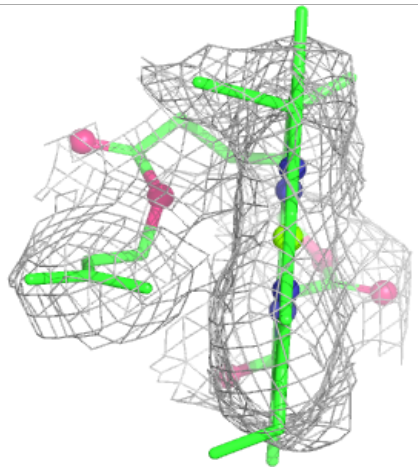


Electron density around CLA L 1501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

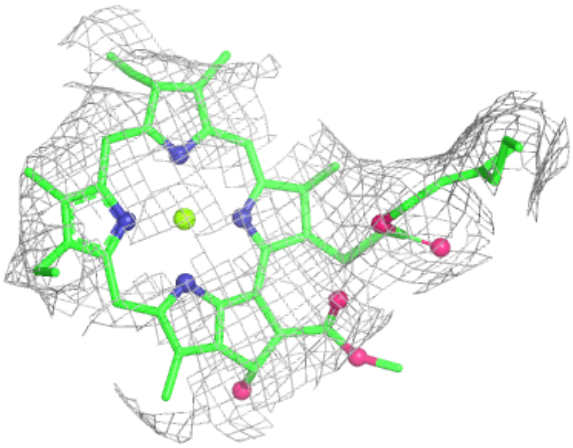


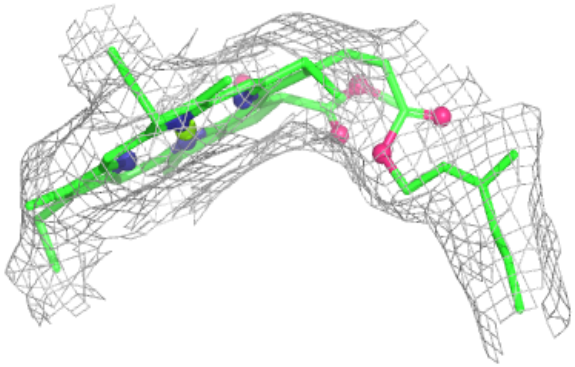


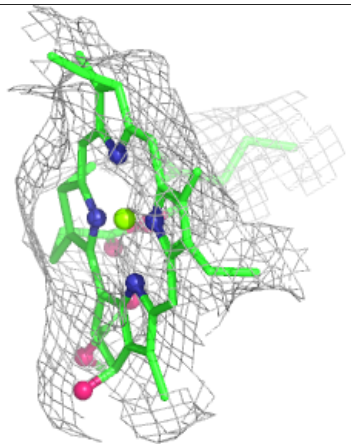


Electron density around CLA 4 4002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



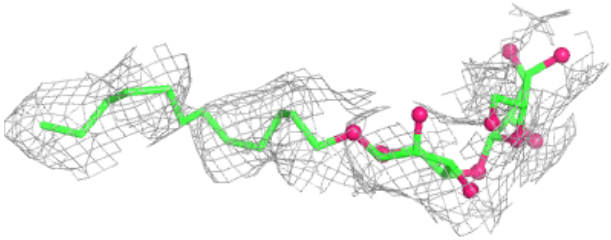


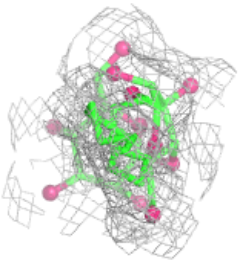


Electron density around LMU 4 7033:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

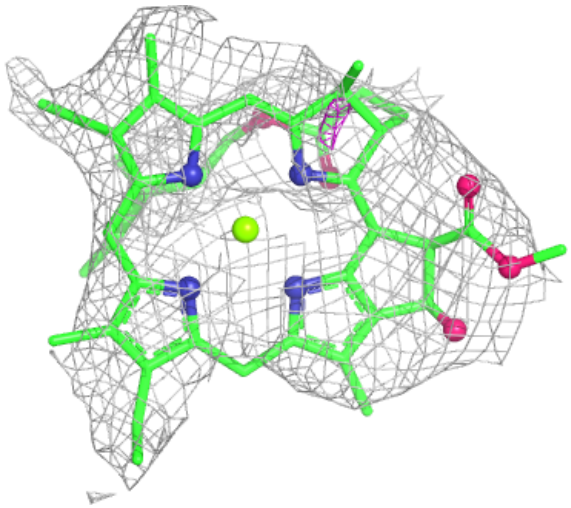


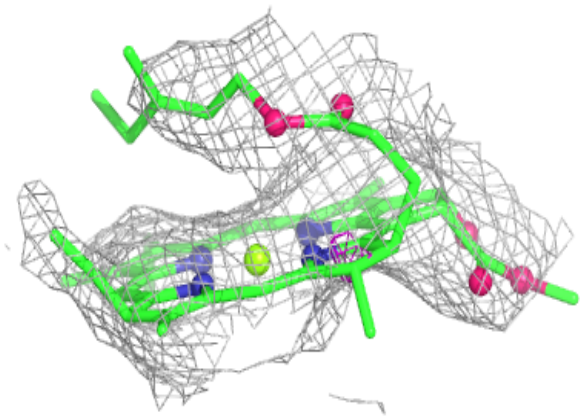


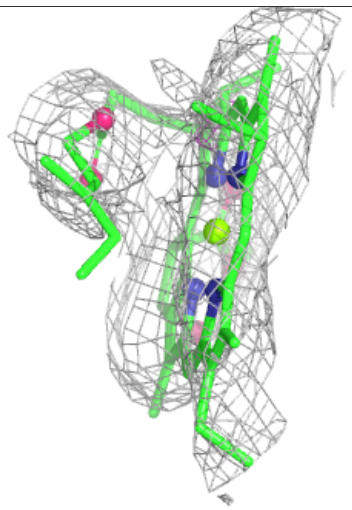


Electron density around CLA A 1120:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

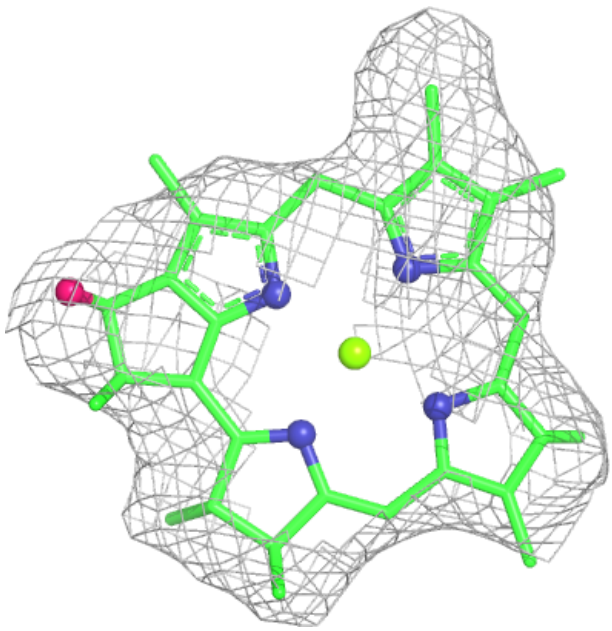


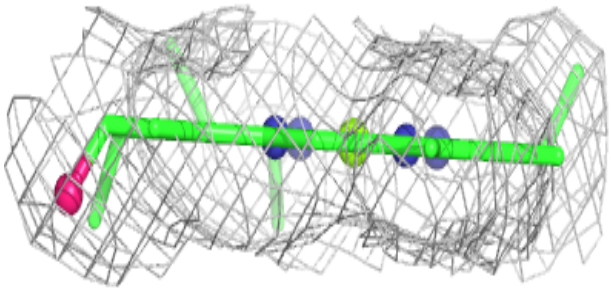


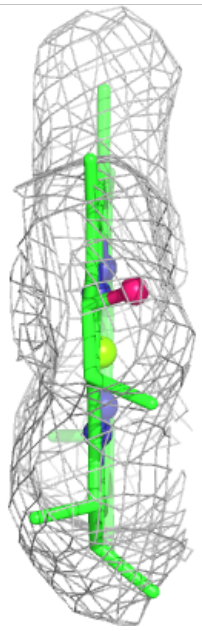


Electron density around CLA 1 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

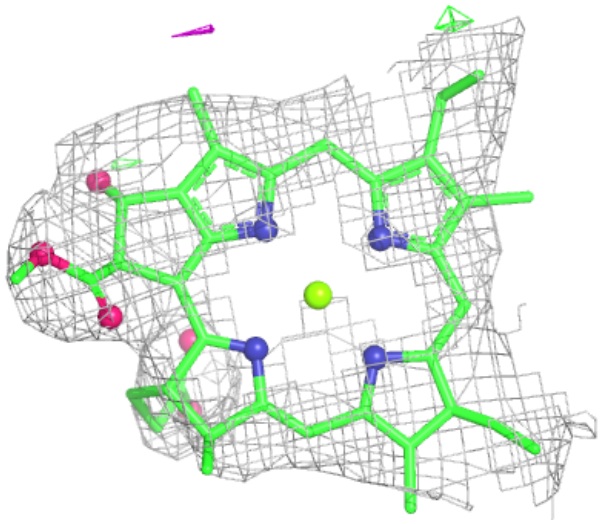


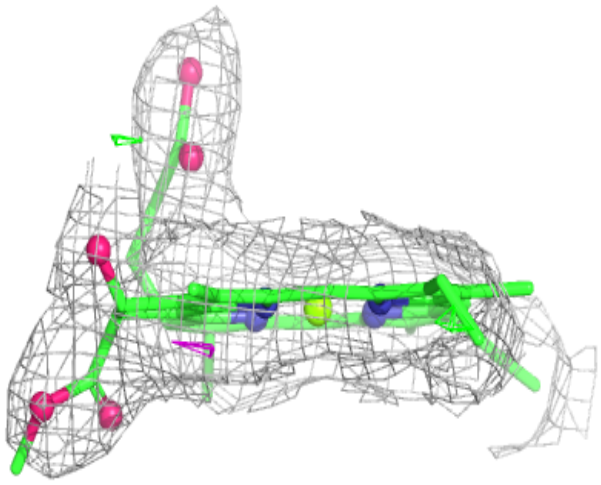




Electron density around CLA B 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

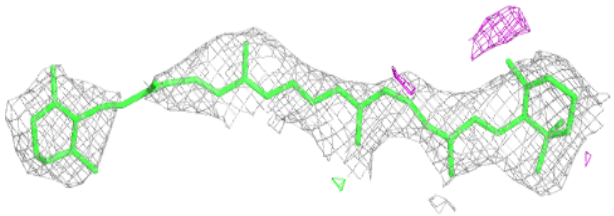


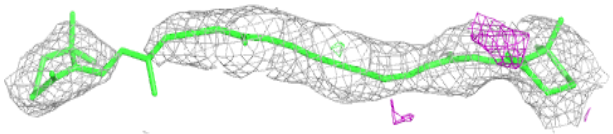


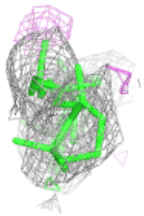


Electron density around BCR B 6010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

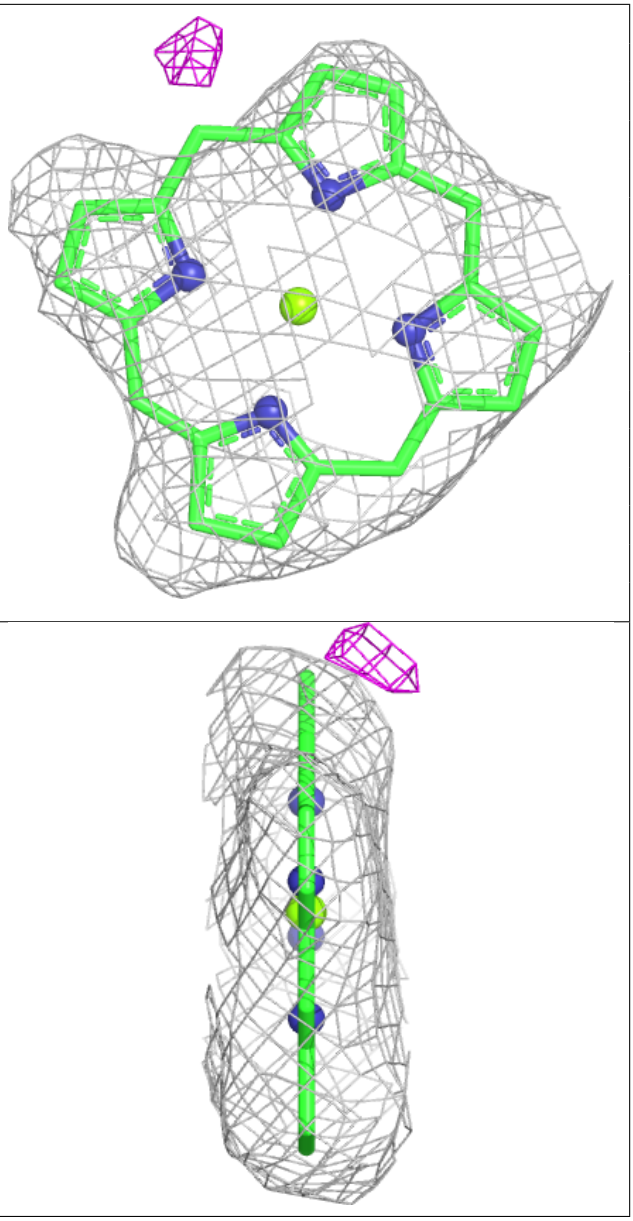


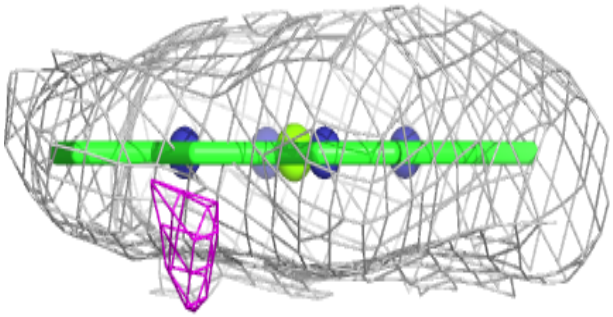




Electron density around CLA 2 2010:

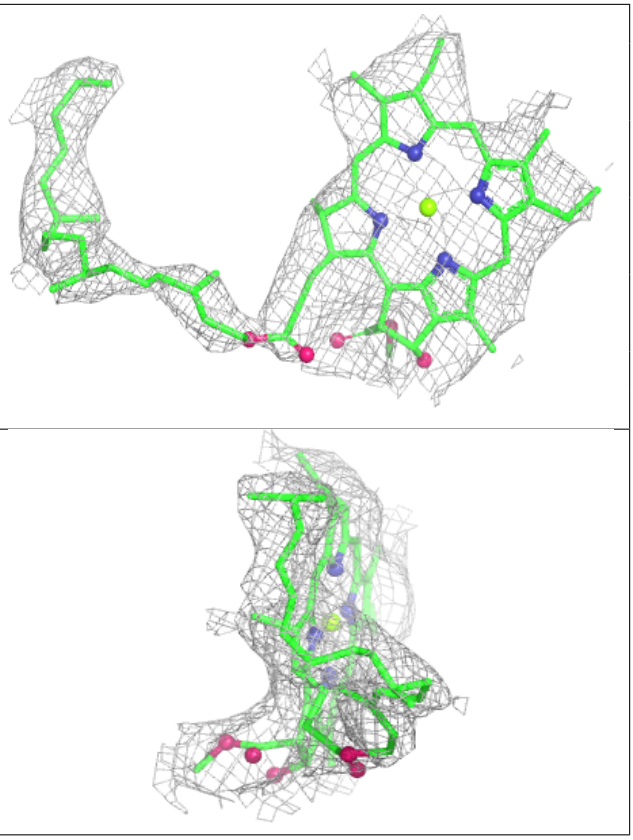
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

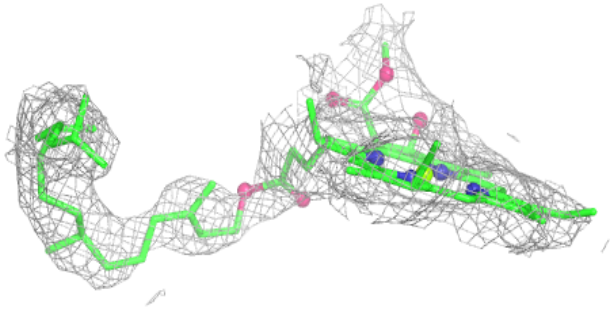




Electron density around CLA A 1125:

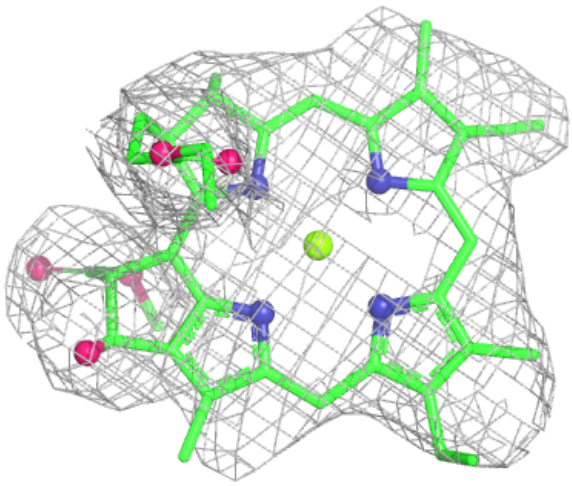
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

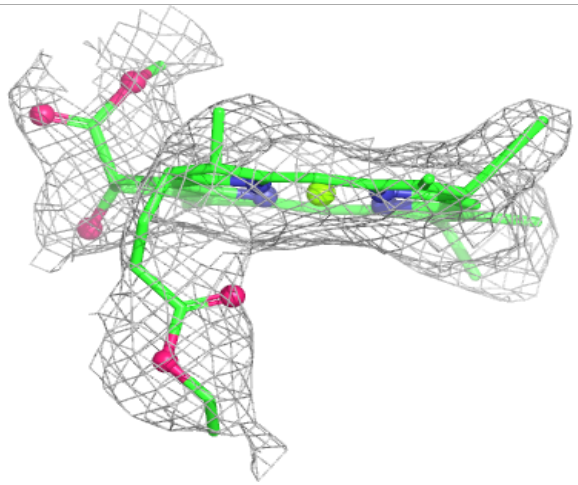


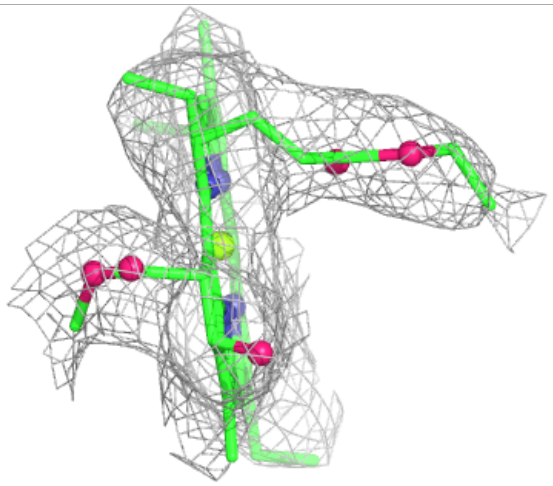


Electron density around CLA L 1502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

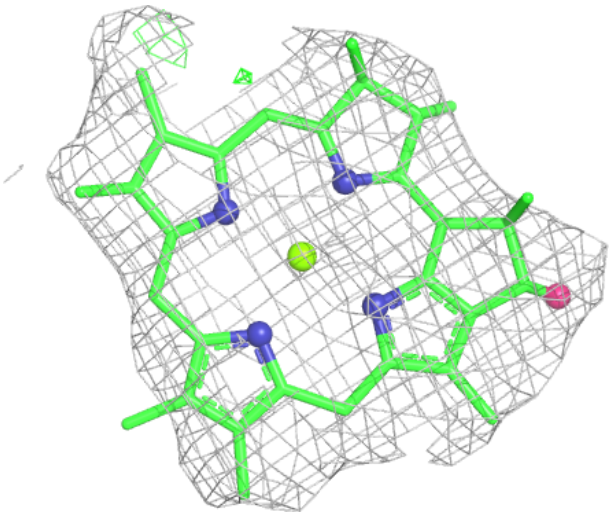


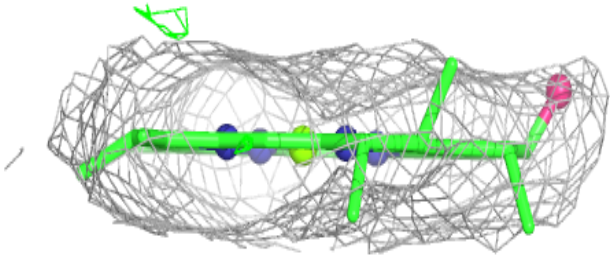


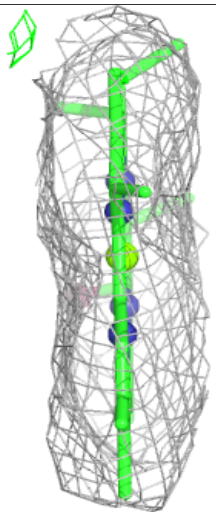


Electron density around CLA F 1240:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

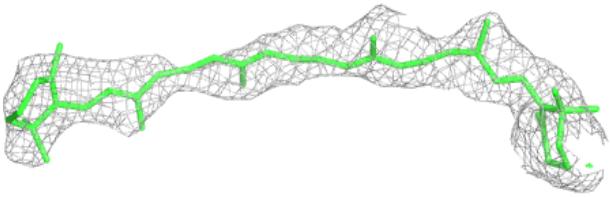


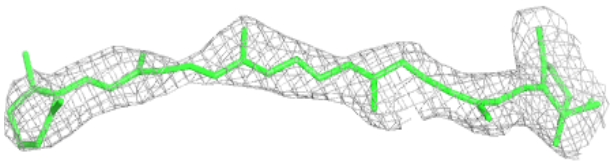


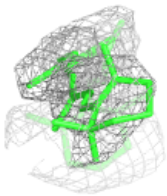


Electron density around BCR F 6014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

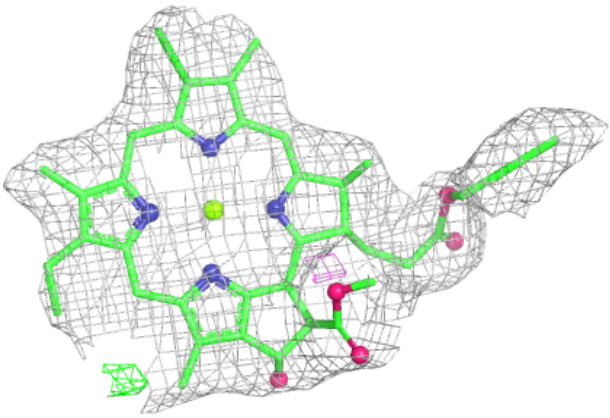


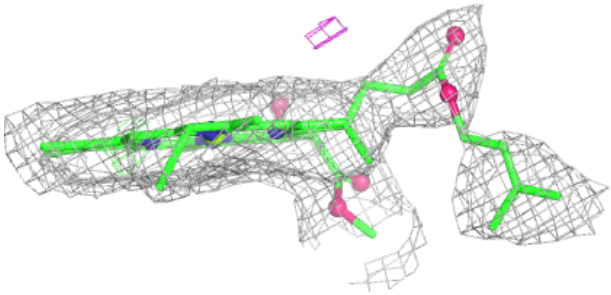




Electron density around CLA B 1228:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

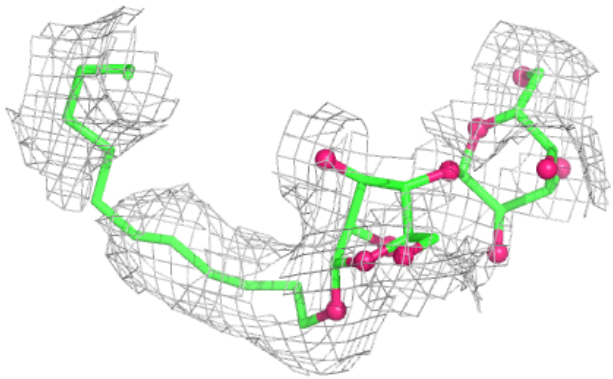


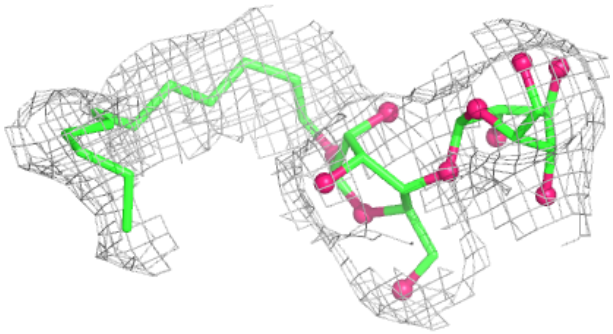


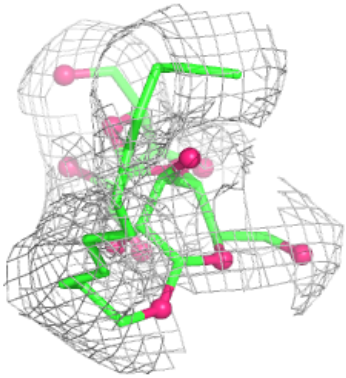


Electron density around LMU R 7022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

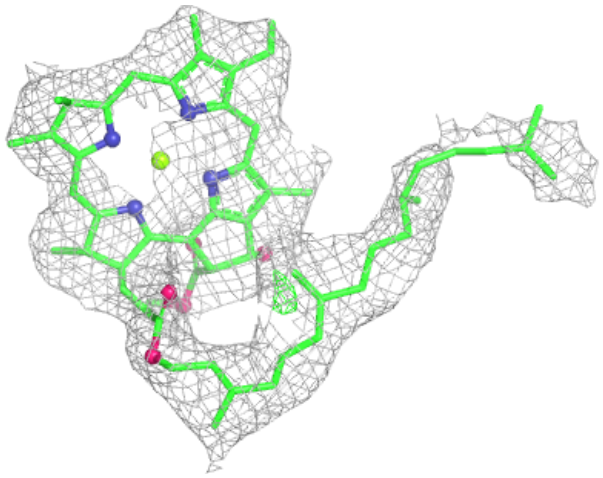


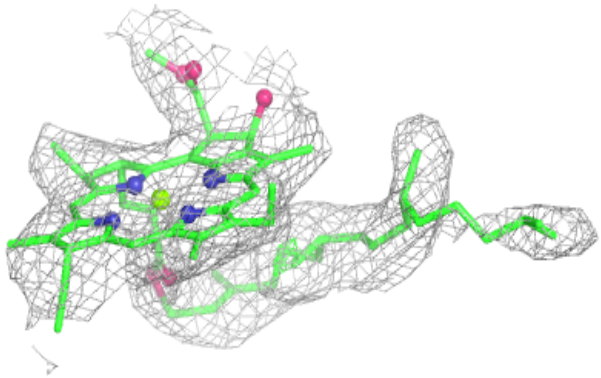


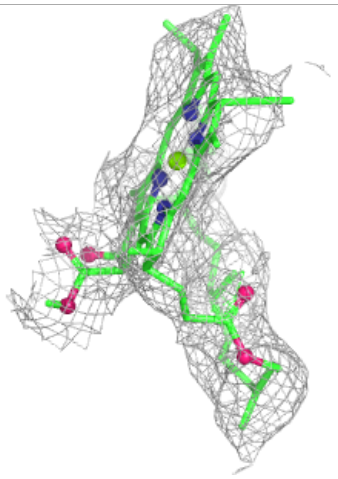


Electron density around CLA B 1229:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

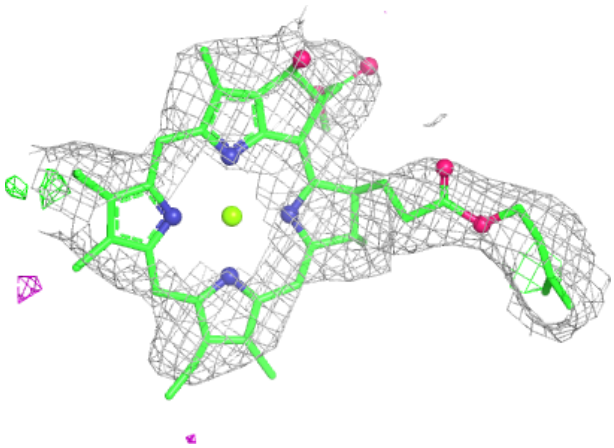


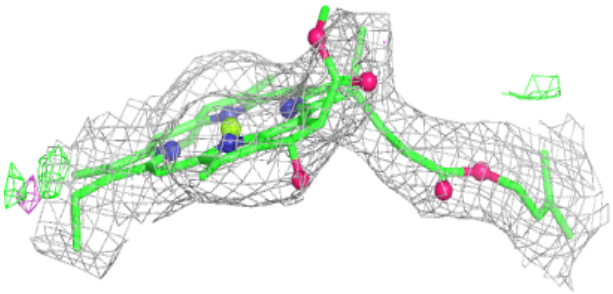


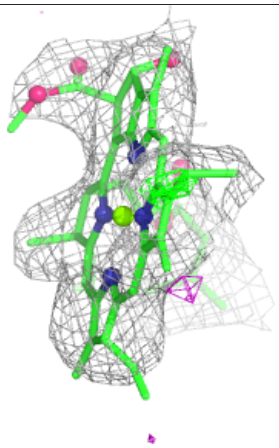


Electron density around CLA B 1230:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

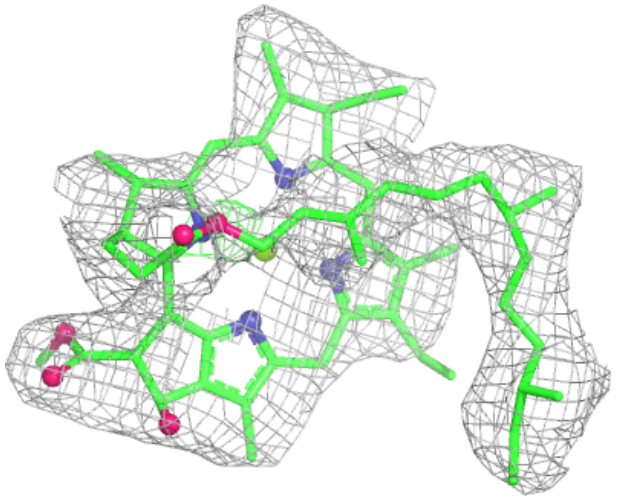


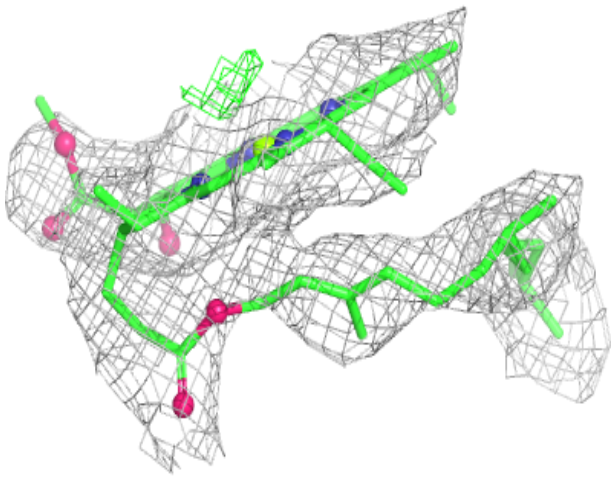


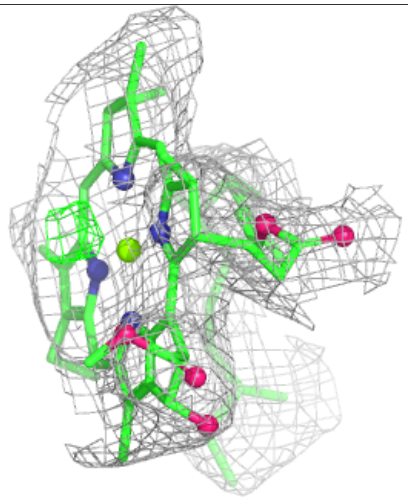


Electron density around CLA B 1216:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

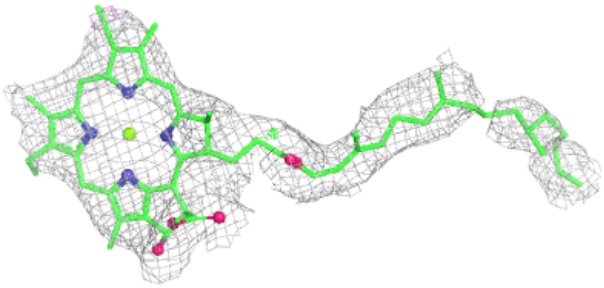


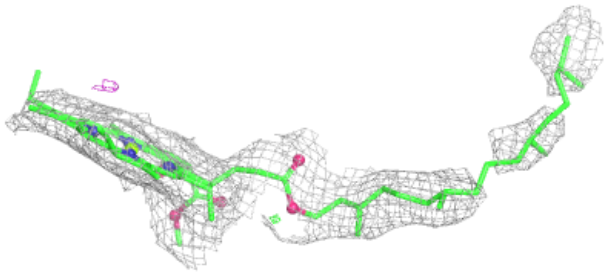


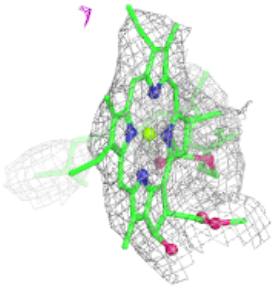


Electron density around CLA A 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

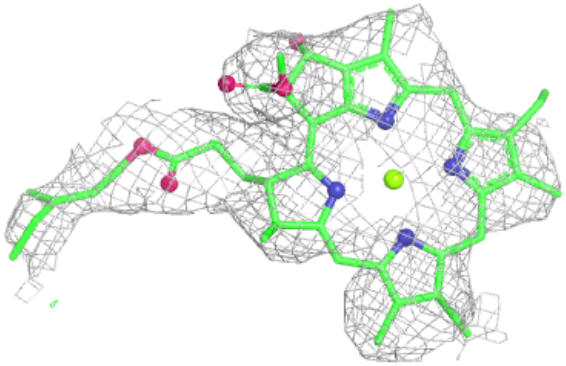


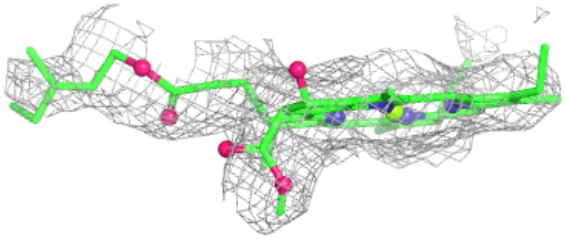


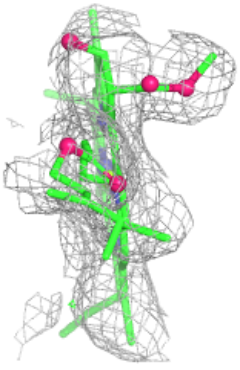


Electron density around CLA A 1135:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

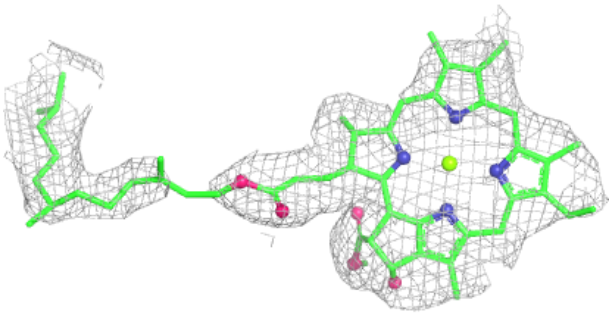


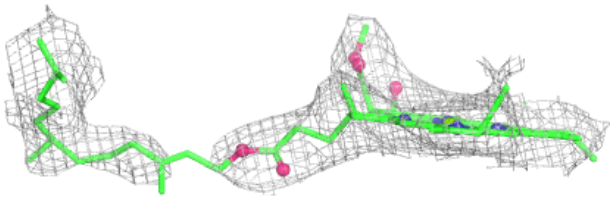




Electron density around CLA B 1234:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

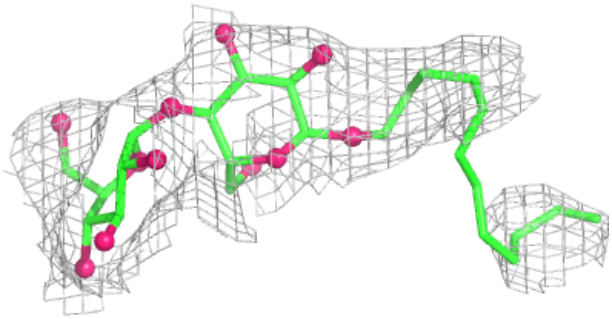


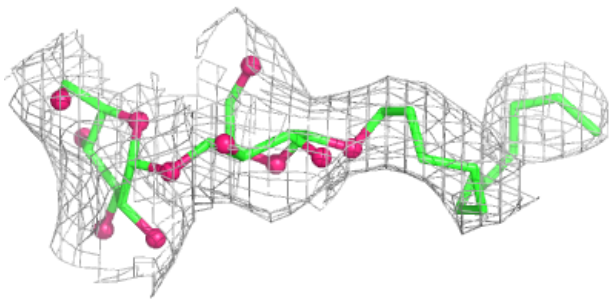


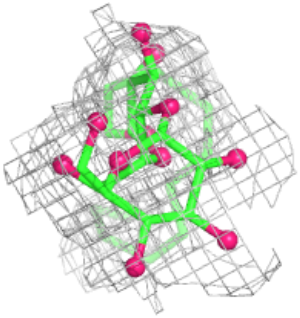


Electron density around LMU R 7007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

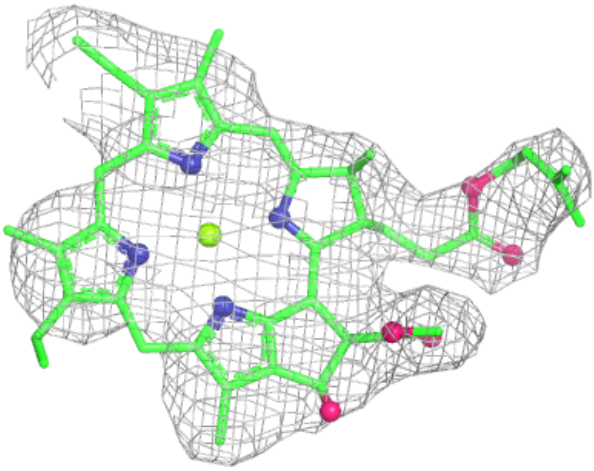


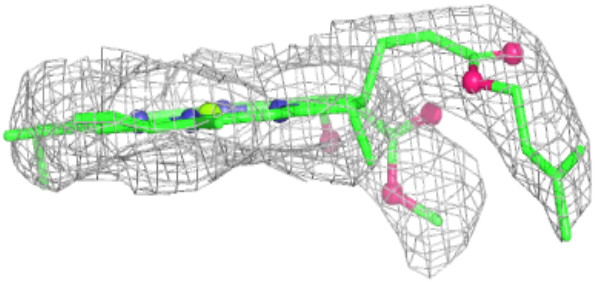


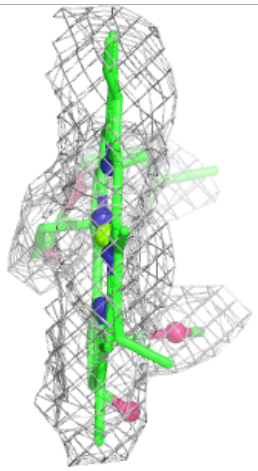


Electron density around CLA A 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

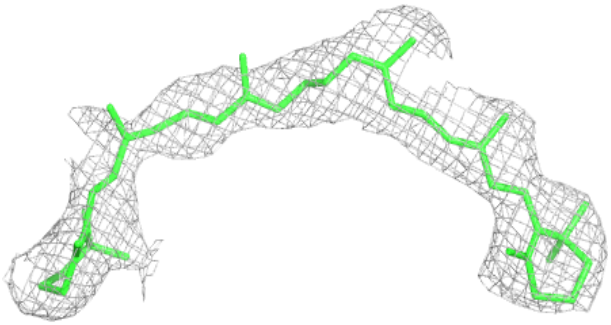


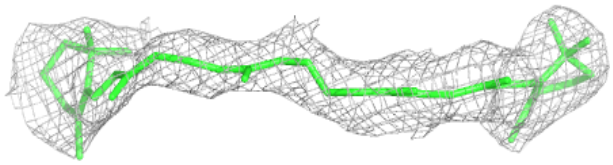


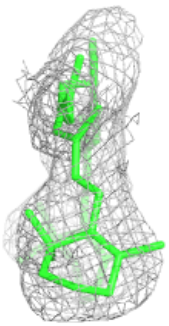


Electron density around BCR F 6016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

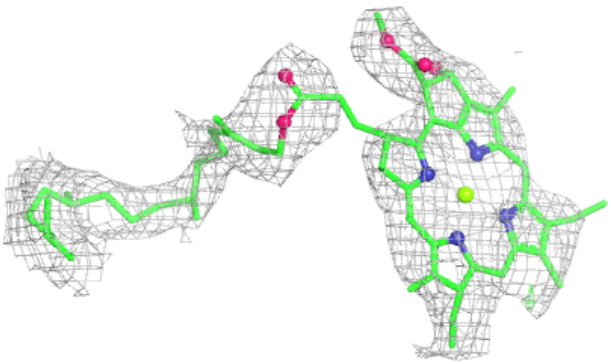


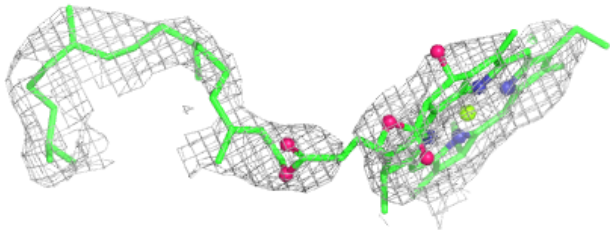


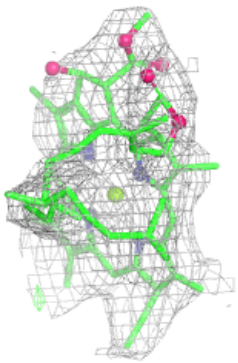


Electron density around CLA B 1206:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



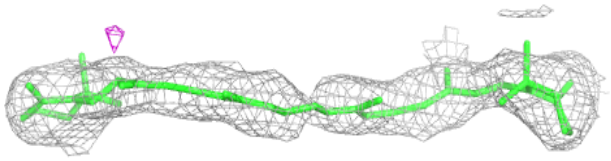


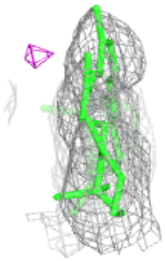


Electron density around BCR A 6011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

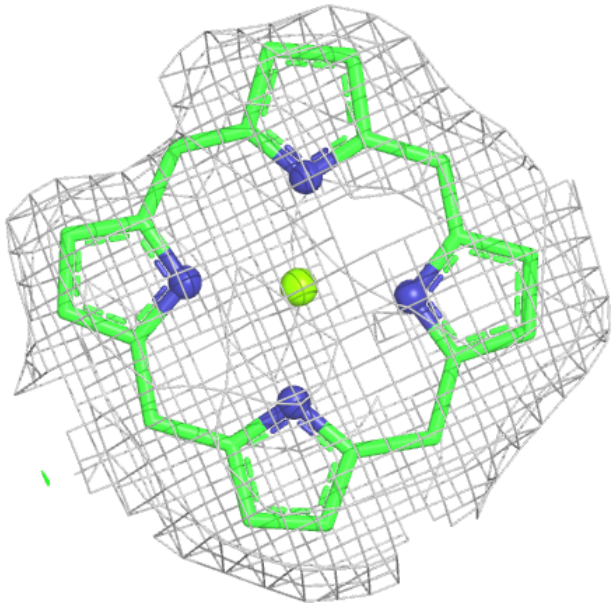


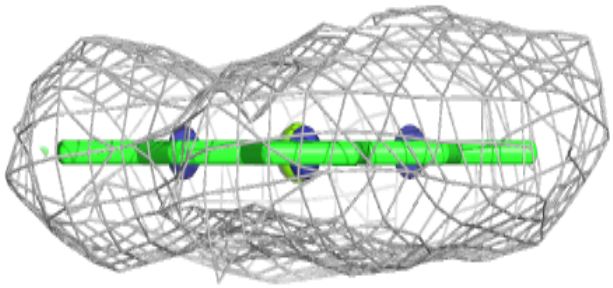


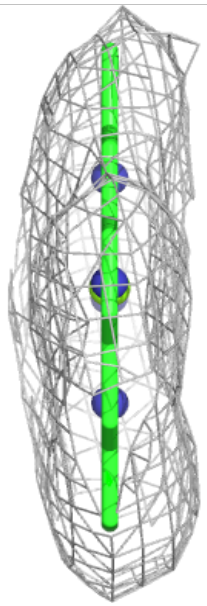


Electron density around CLA 4 4011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

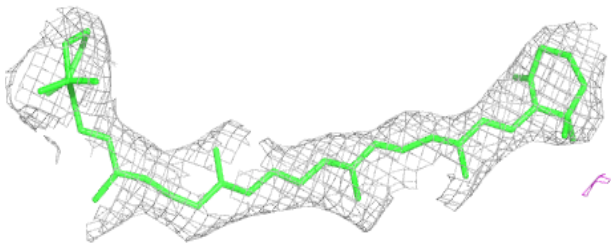


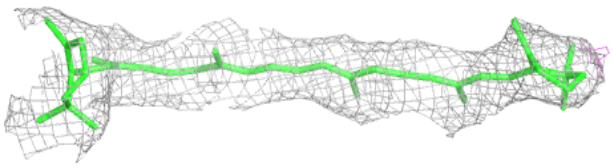




Electron density around BCR B 6005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

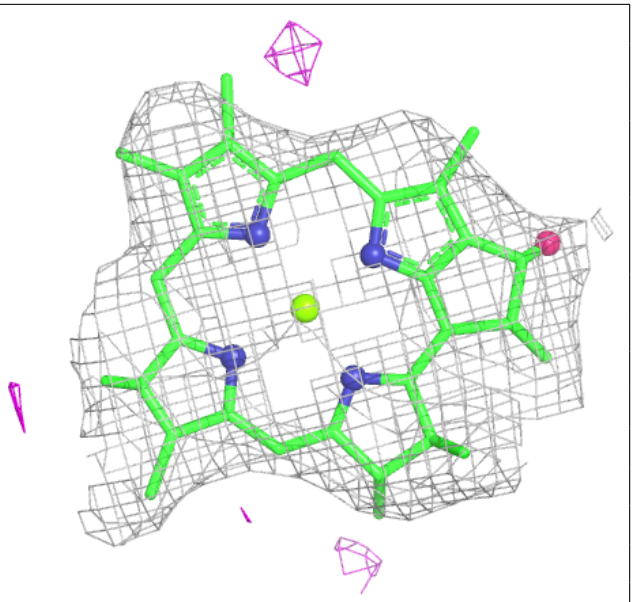


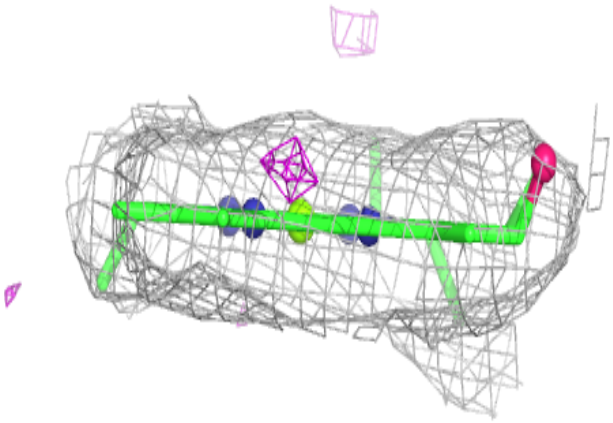


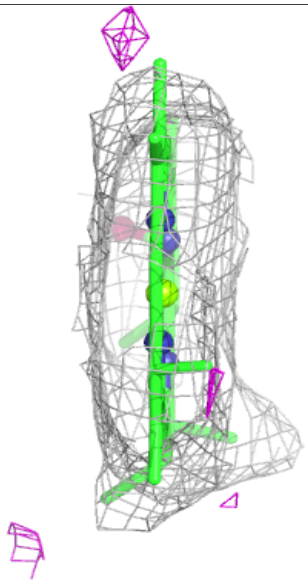


Electron density around CLA 4 4012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

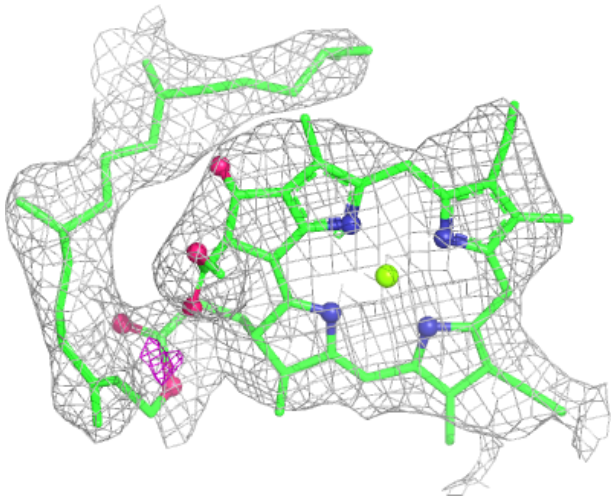


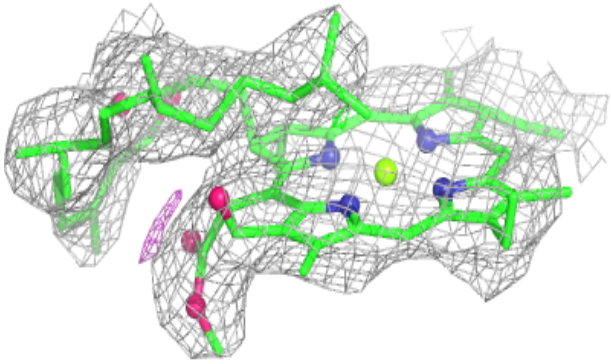


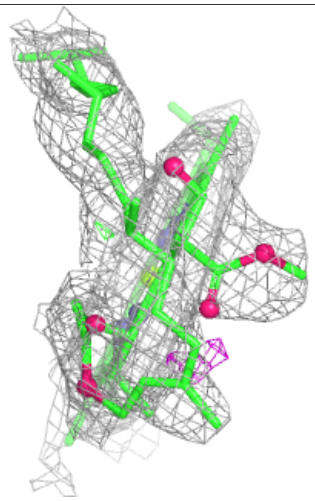


Electron density around CLA B 1202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

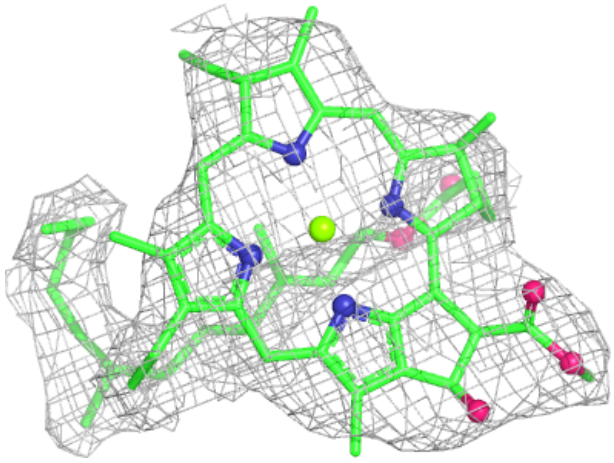


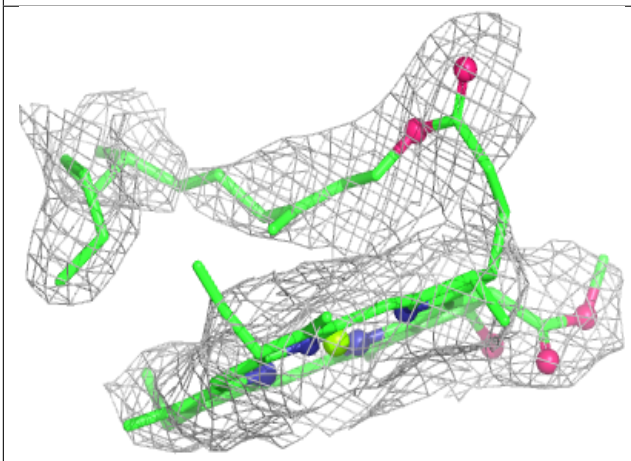


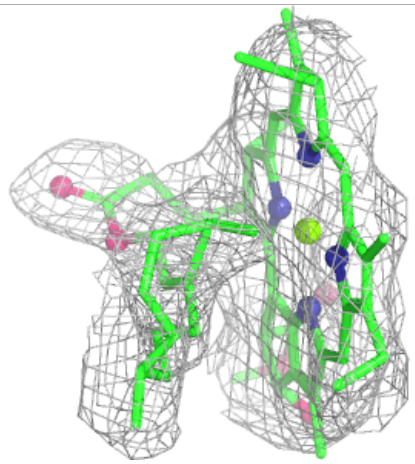


Electron density around CLA B 1214:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

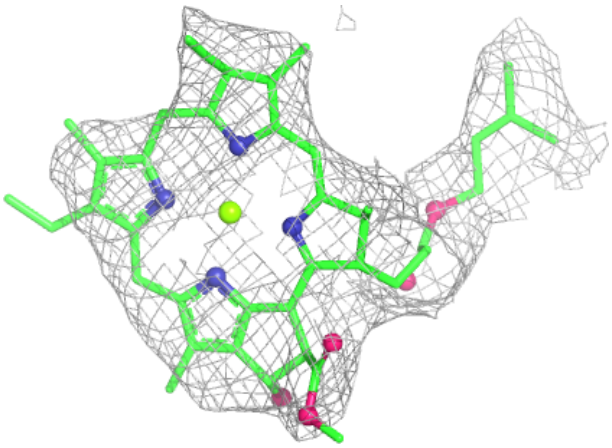


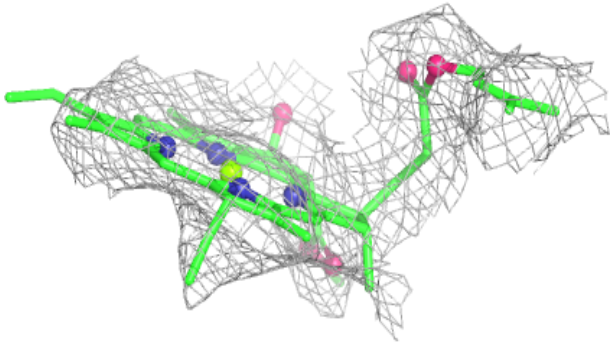


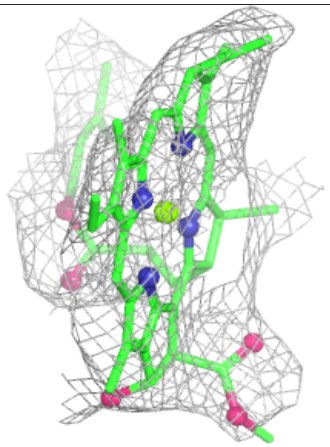


Electron density around CLA A 1133:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

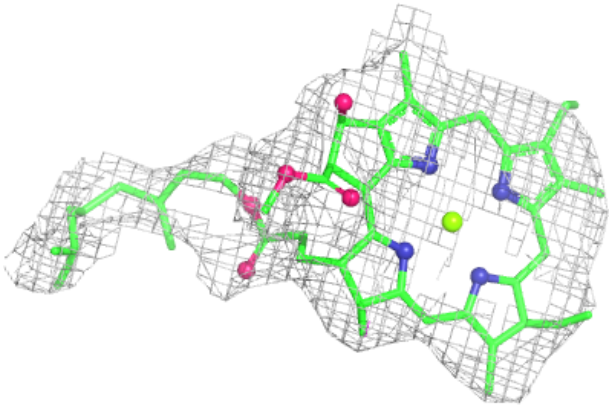


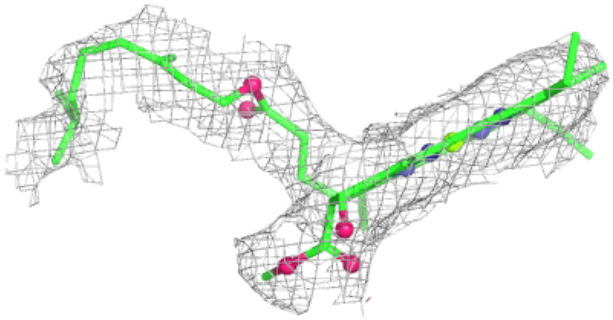


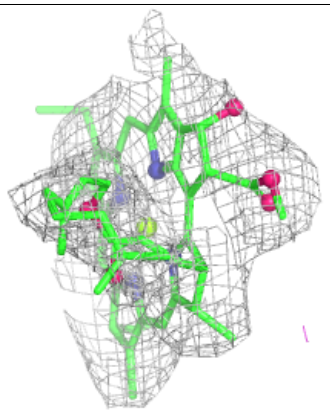


Electron density around CLA A 1107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

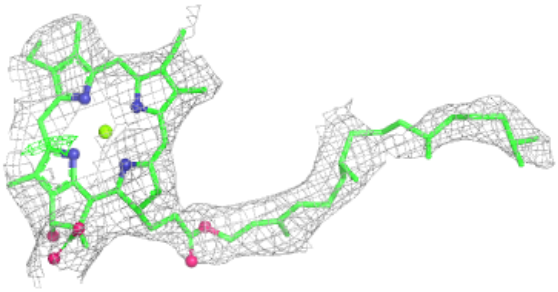


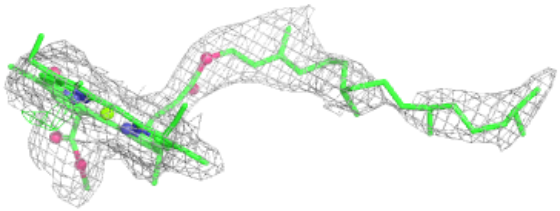


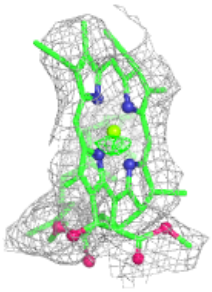


Electron density around CLA A 1132:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

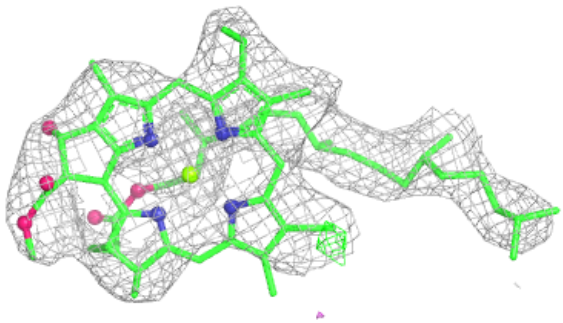


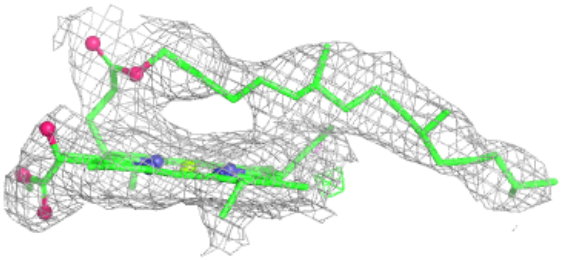


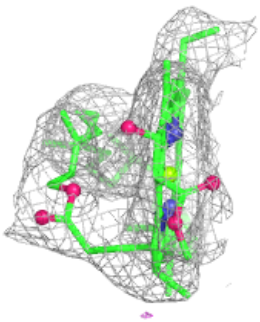


Electron density around CLA A 1138:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

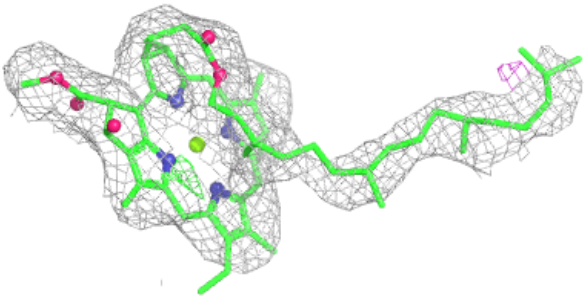


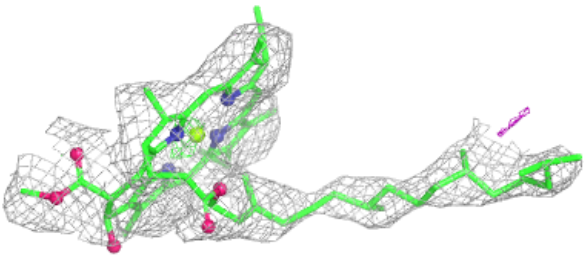


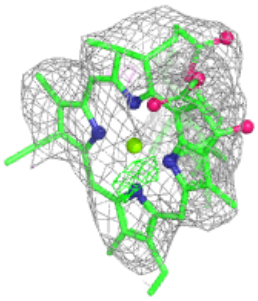


Electron density around CLA A 1140:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

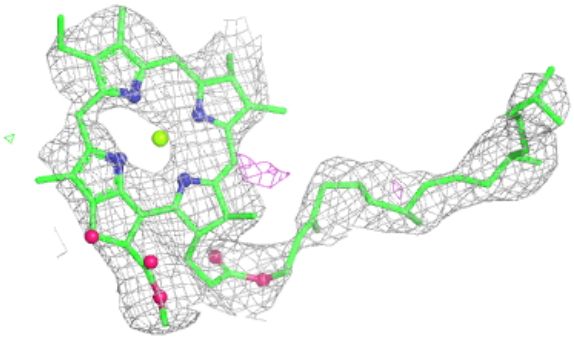


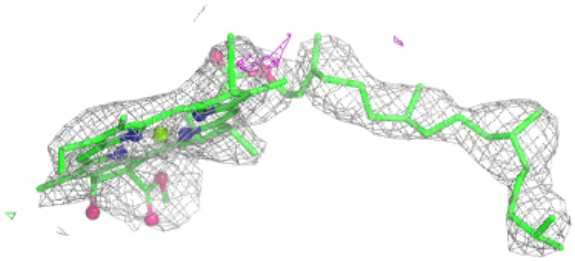


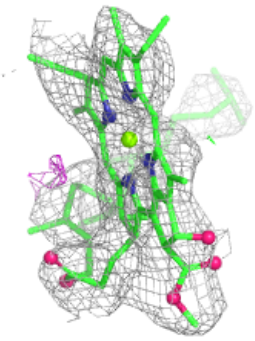


Electron density around CLA A 9013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

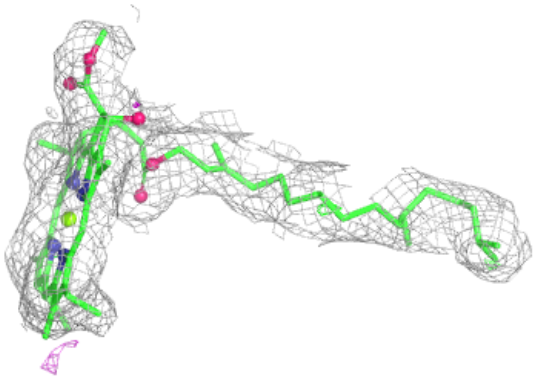


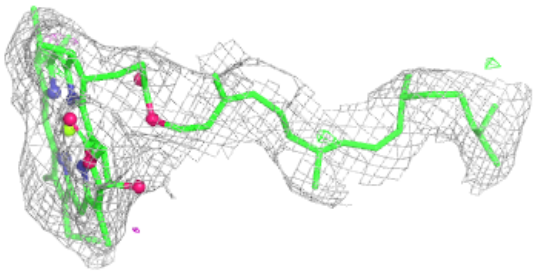


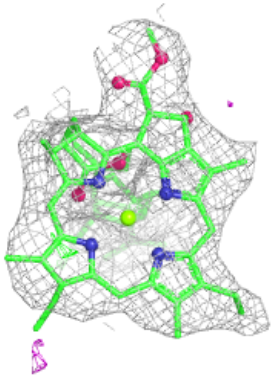


Electron density around CLA A 1126:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

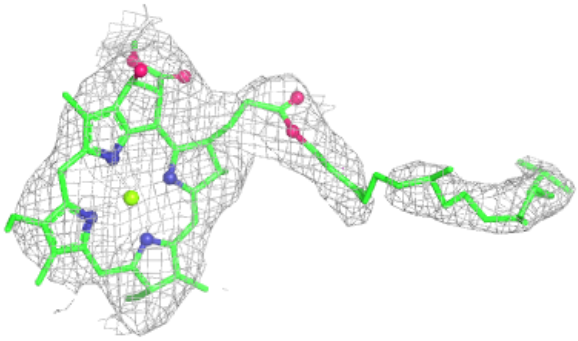


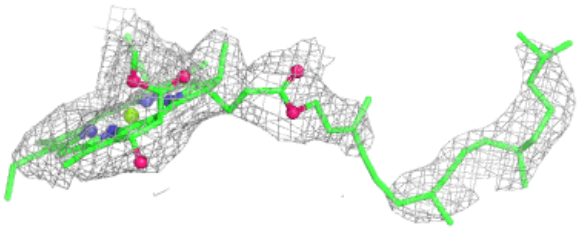


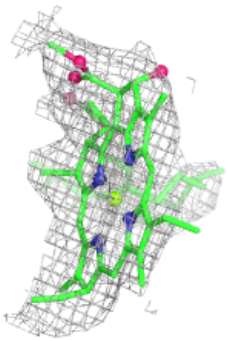


Electron density around CLA B 1210:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

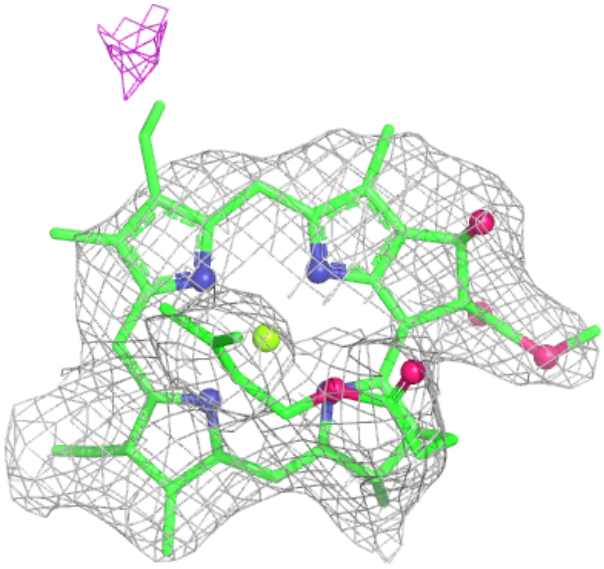


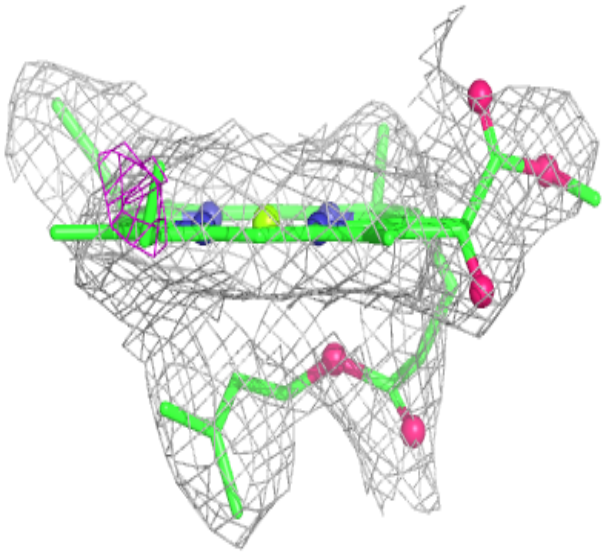


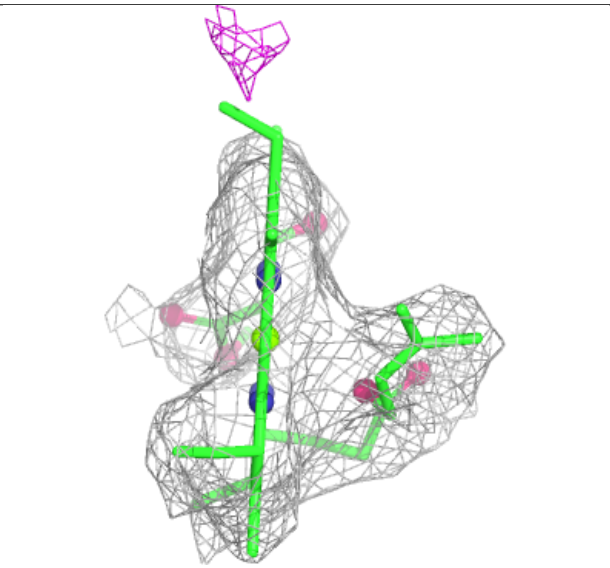


Electron density around CLA B 1217:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

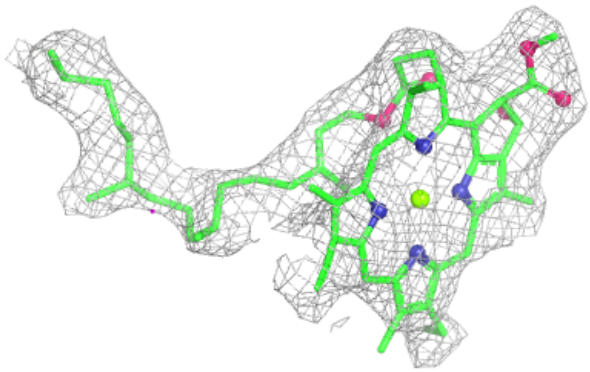


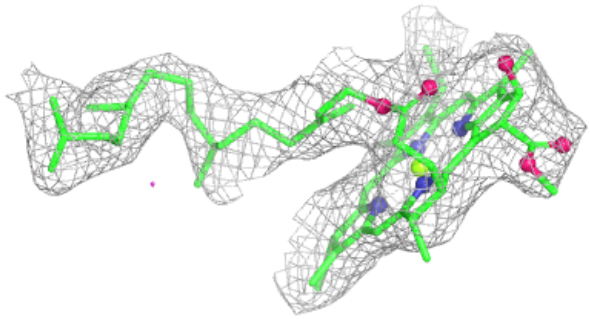




Electron density around CLA A 1237:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

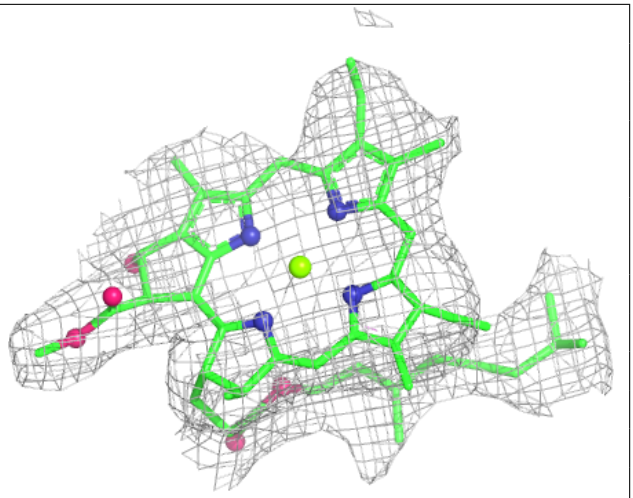


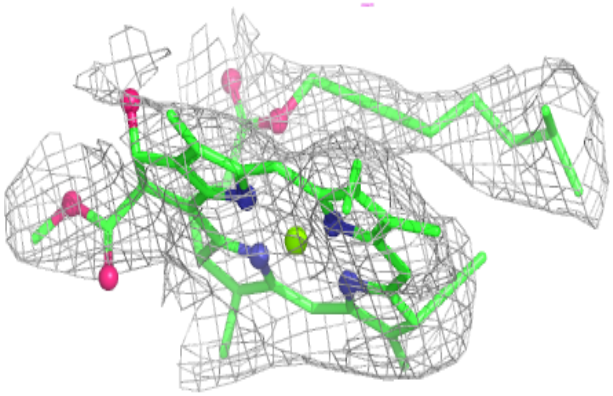


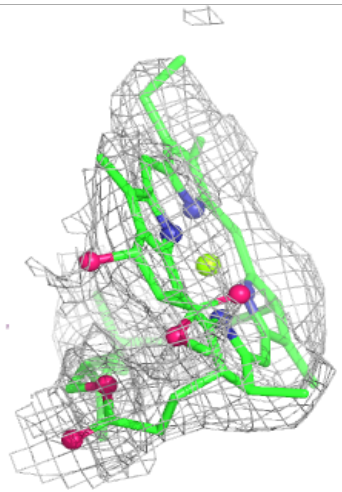


Electron density around CLA B 1219:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

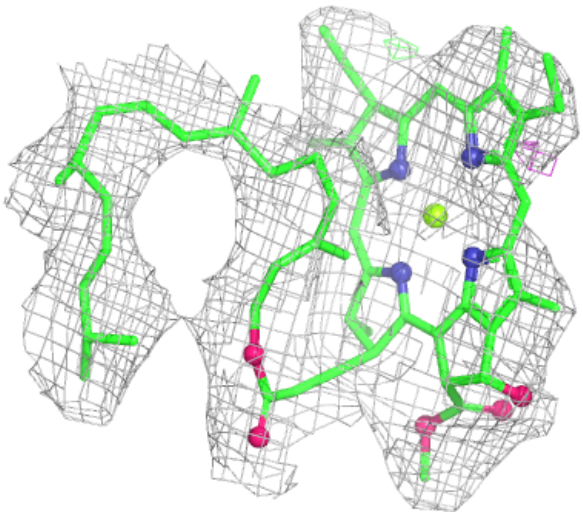


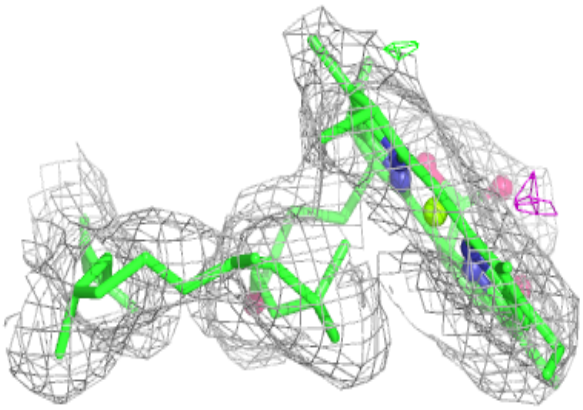




Electron density around CLA B 1220:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

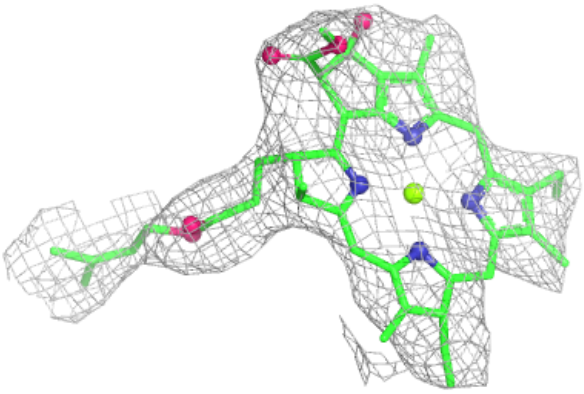


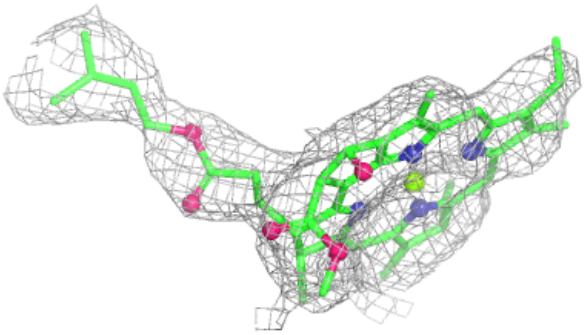


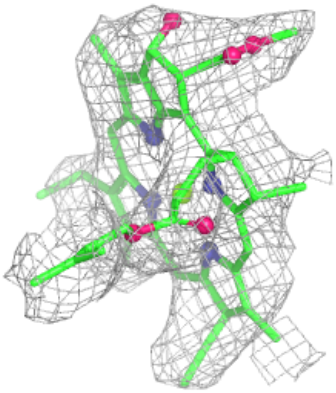


Electron density around CLA A 1129:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

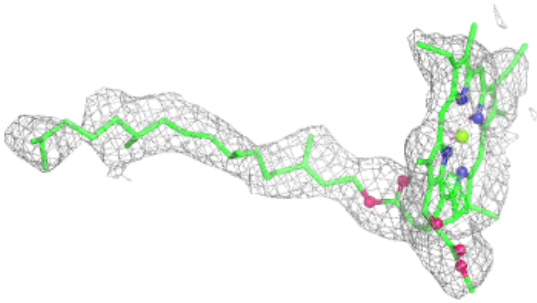


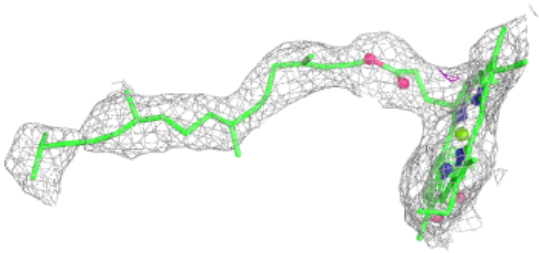


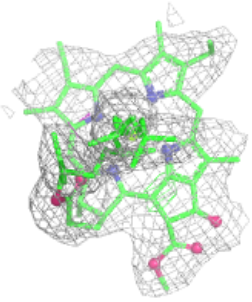


Electron density around CLA B 1225:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

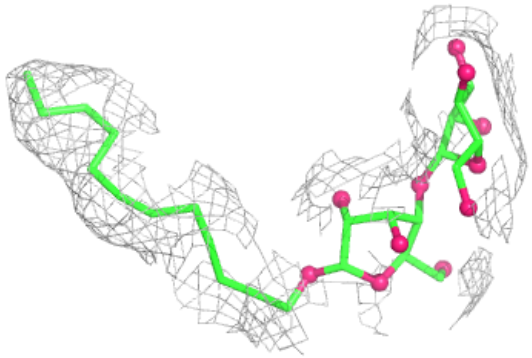


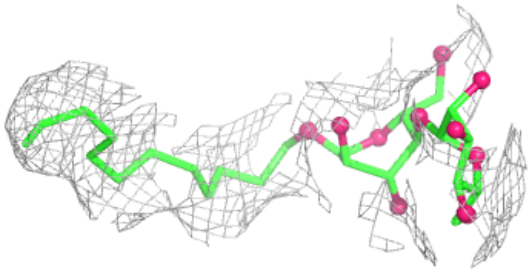


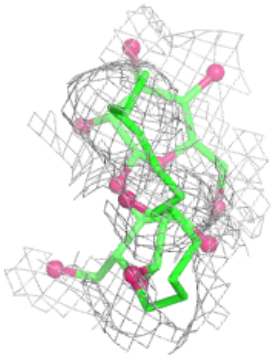


Electron density around LMU G 7039:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

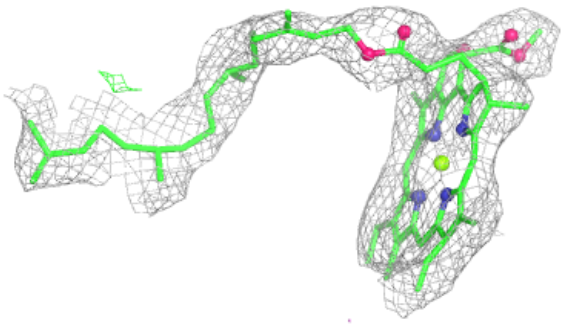


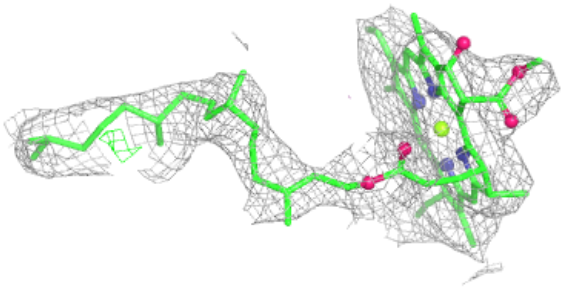


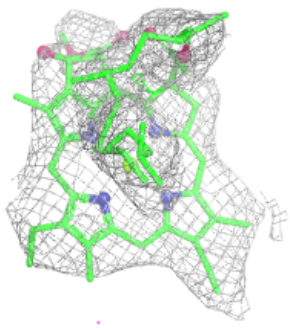


Electron density around CLA B 1226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

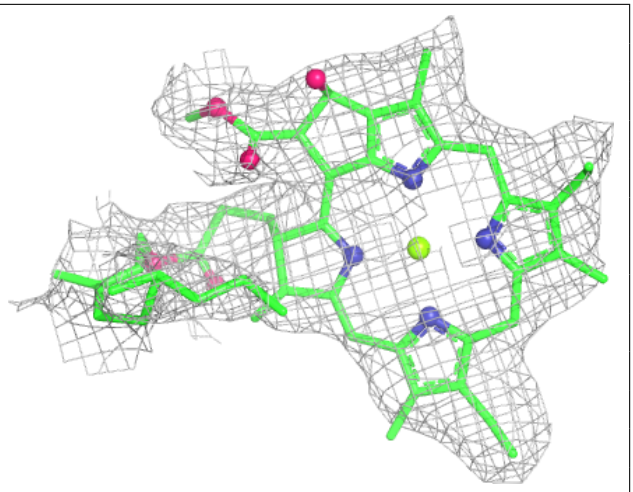


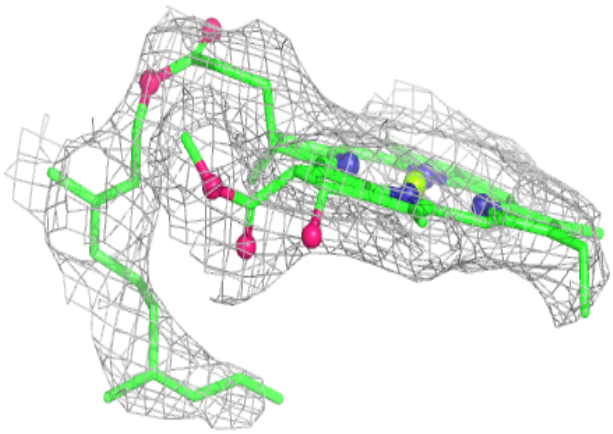


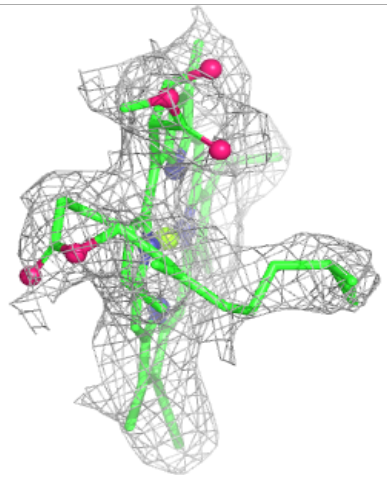


Electron density around CLA A 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

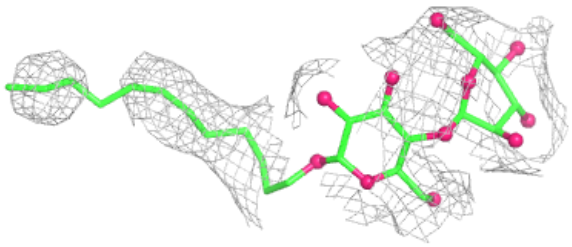


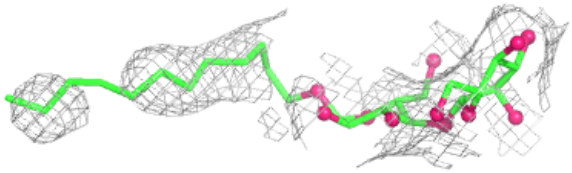




Electron density around LMU A 7035:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

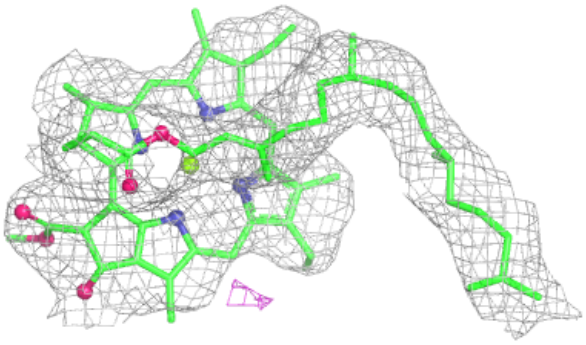


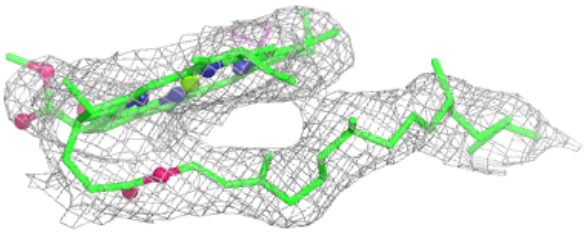


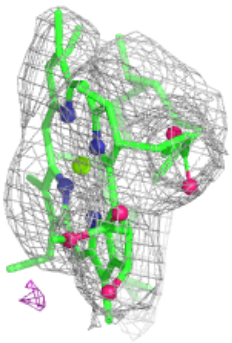


Electron density around CLA B 1235:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

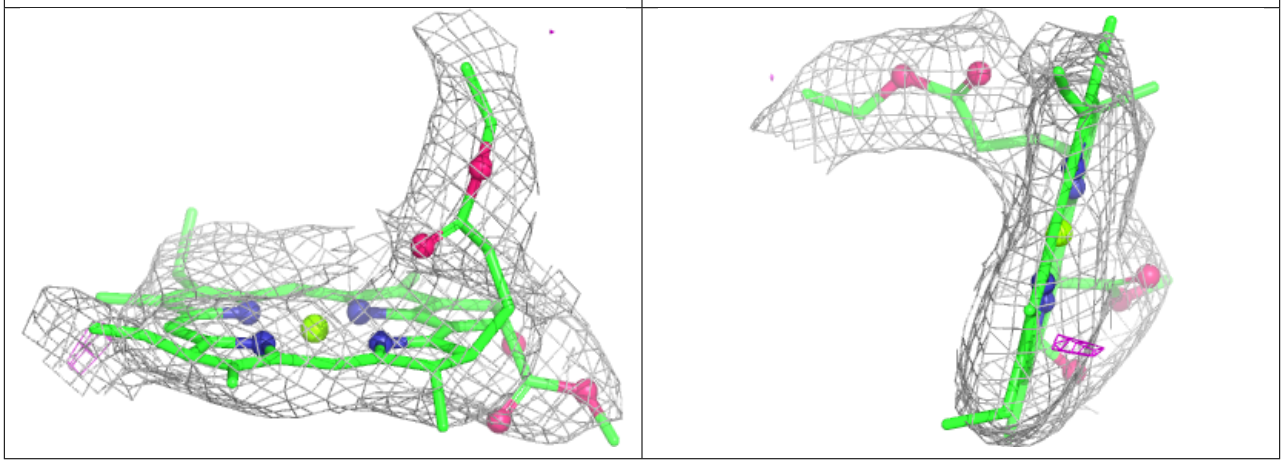






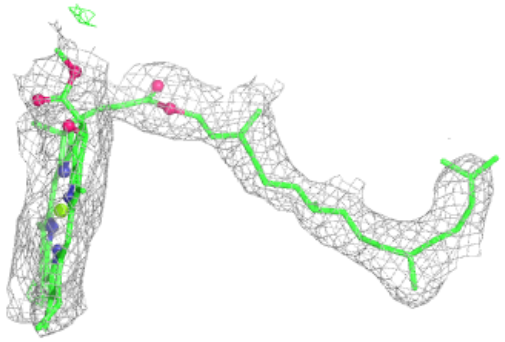
Electron density around CLA B 1236:

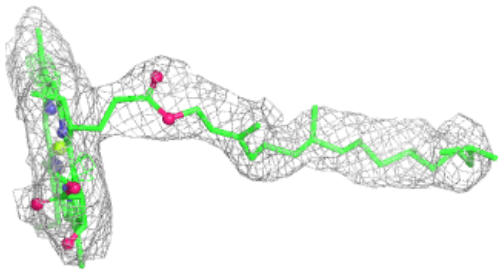
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

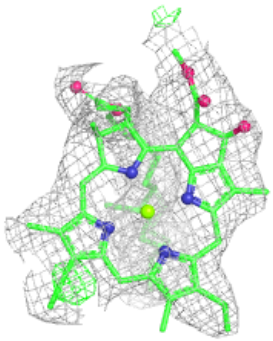


Electron density around CLA B 1239:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

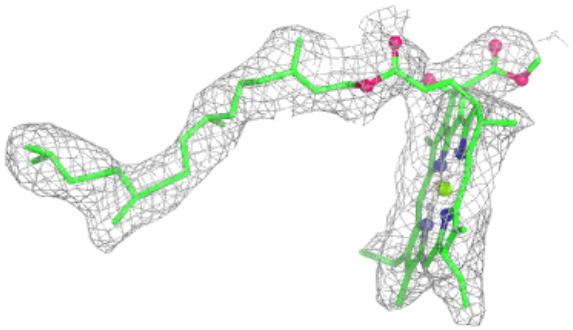


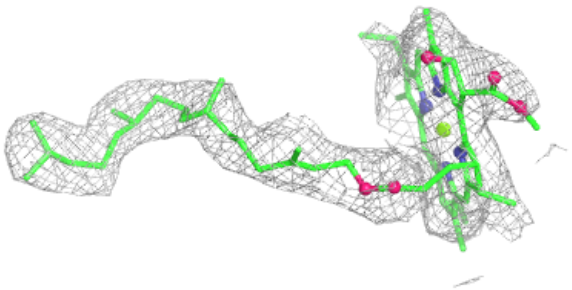


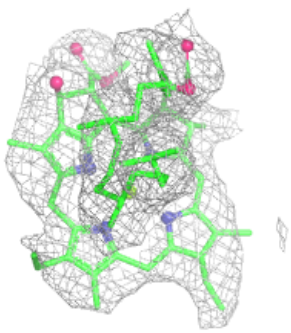


Electron density around CLA A 1128:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

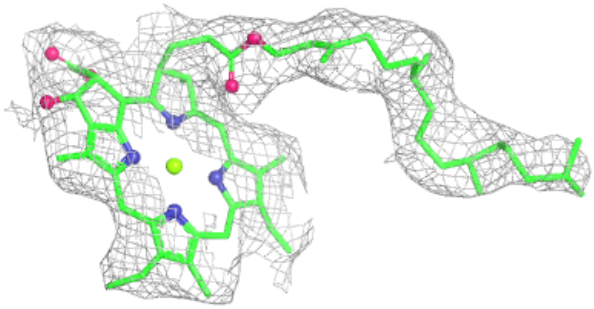


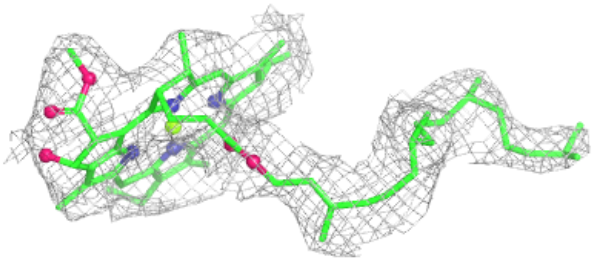


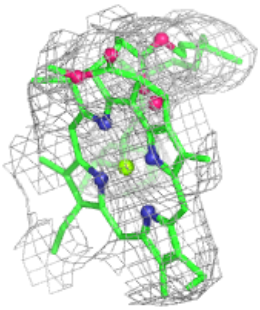


Electron density around CLA A 1106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

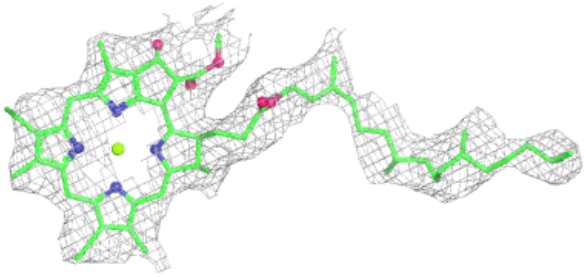


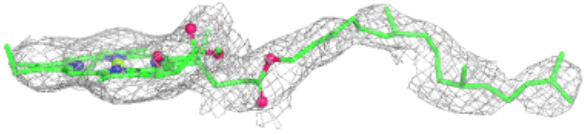


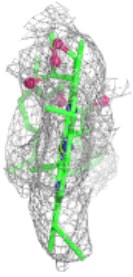


Electron density around CLA A 1131:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

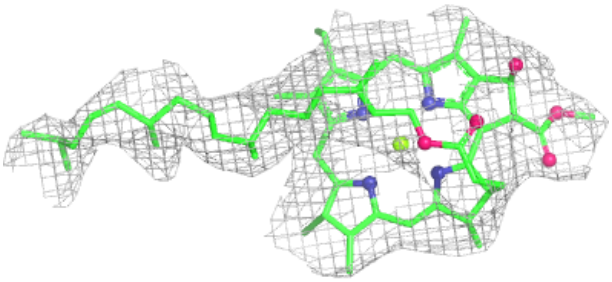


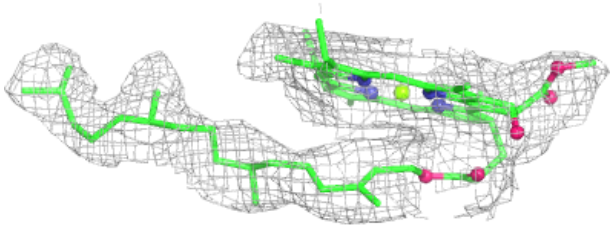


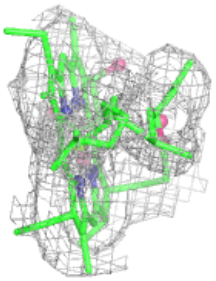


Electron density around CLA A 1136:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

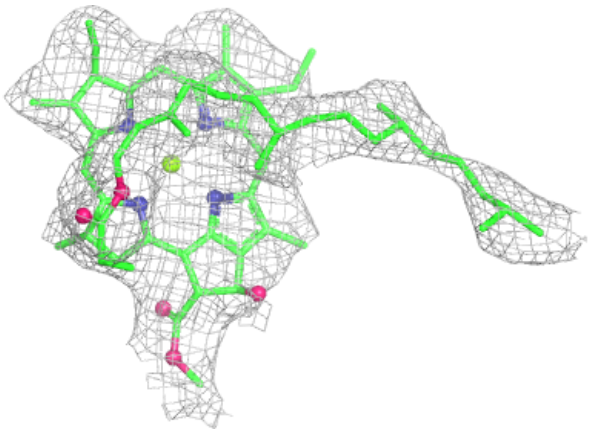


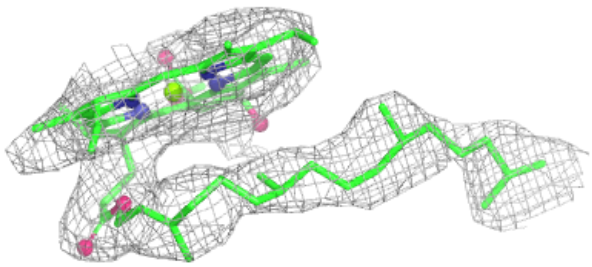


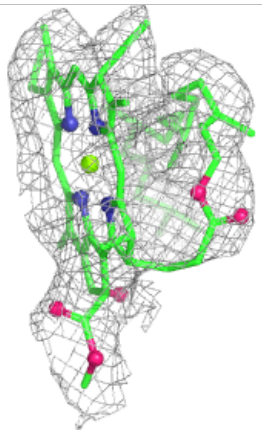


Electron density around CLA B 1224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

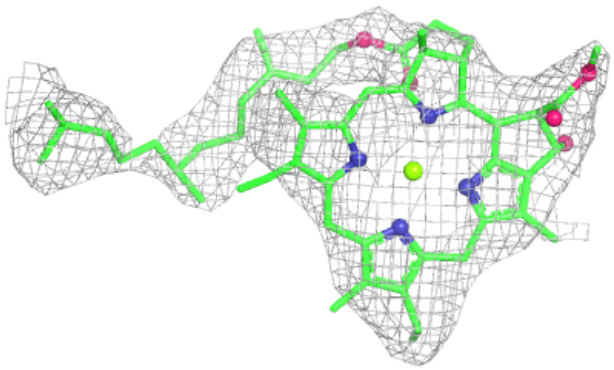


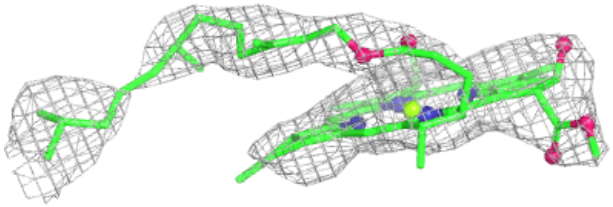


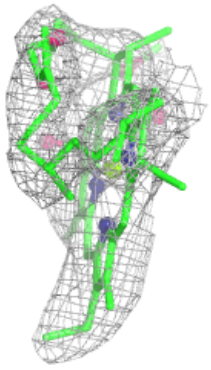


Electron density around CLA B 1215:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

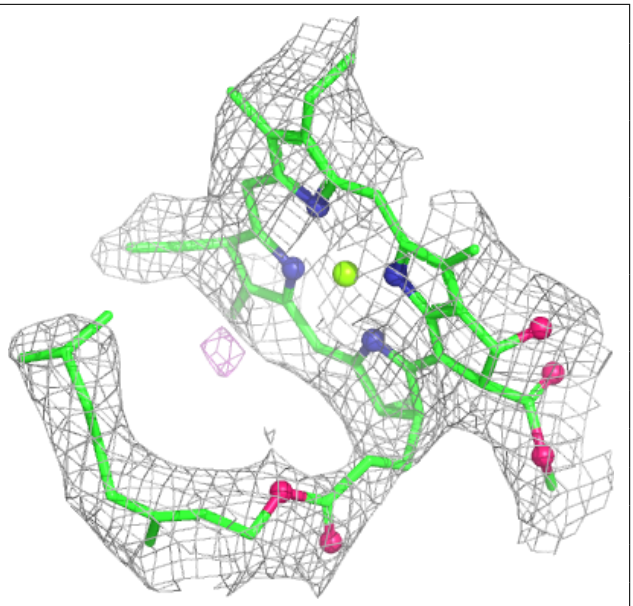


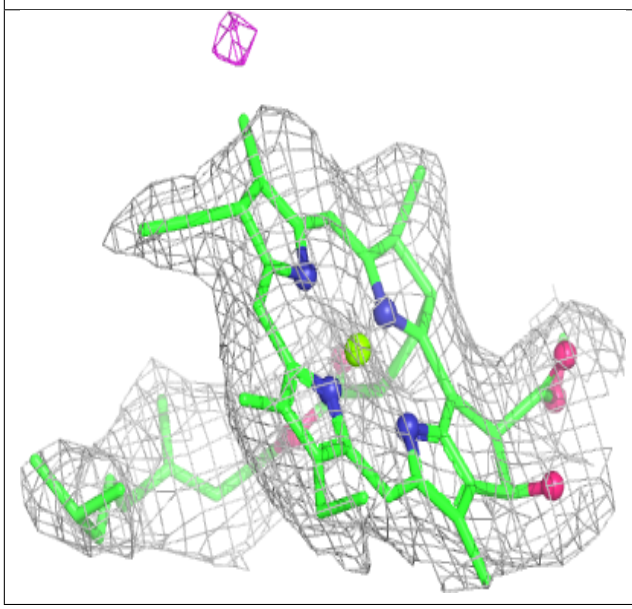


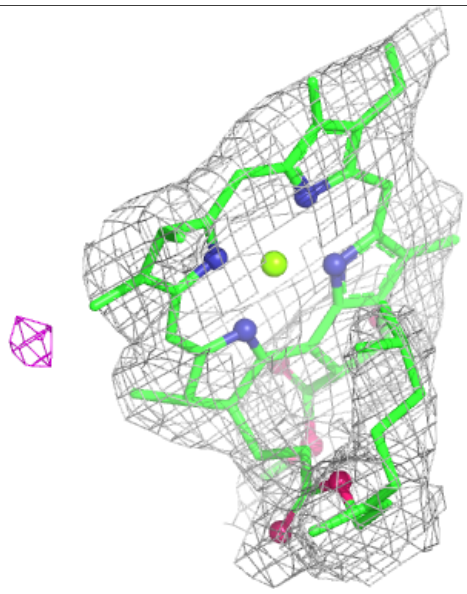


Electron density around CLA A 1122:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

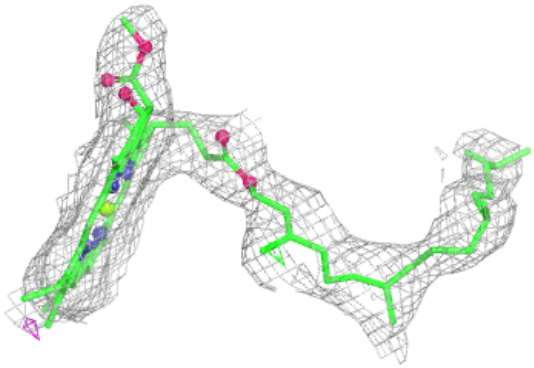


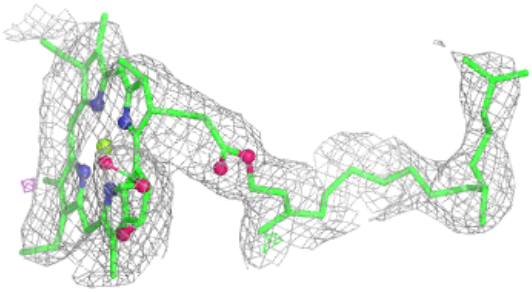


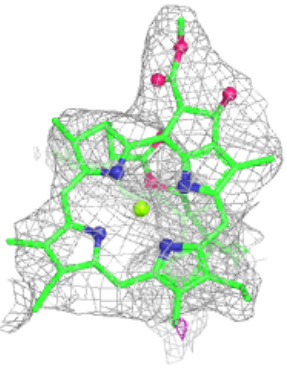


Electron density around CLA B 1238:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

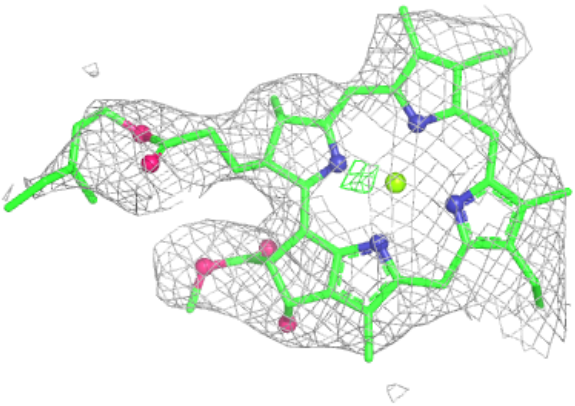


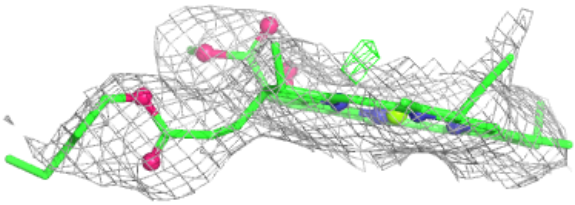


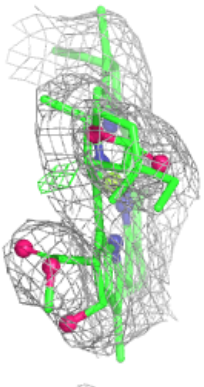


Electron density around CLA A 1139:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

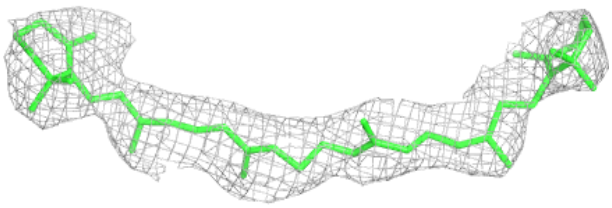


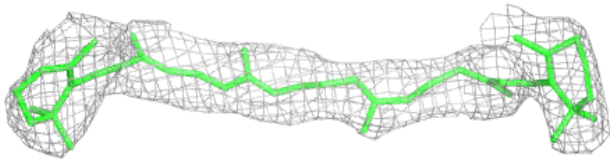


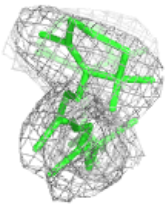


Electron density around BCR B 6020:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

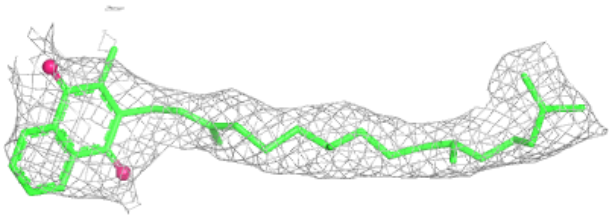


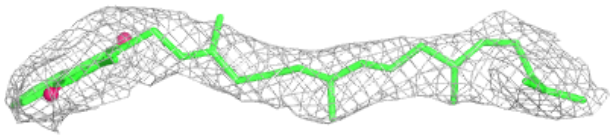


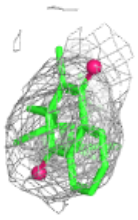


Electron density around PQN A 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

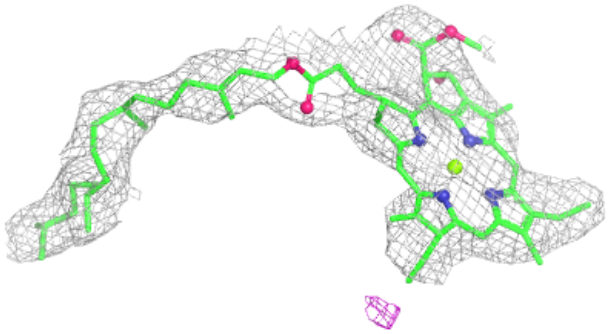


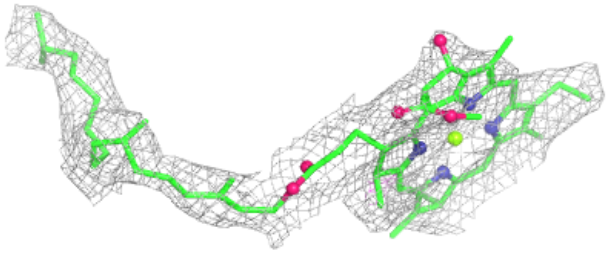


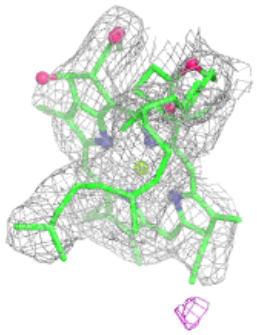


Electron density around CLA A 9012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

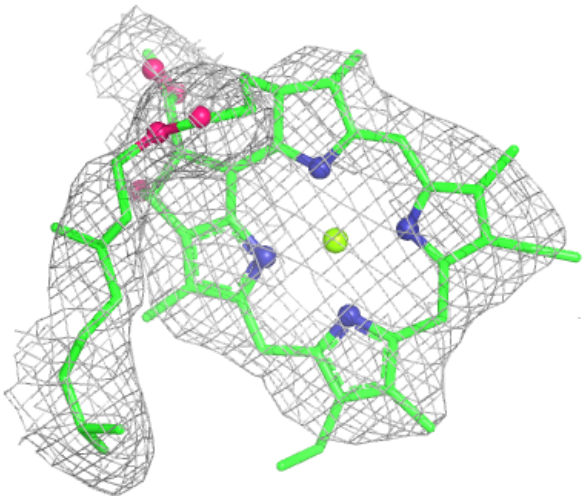


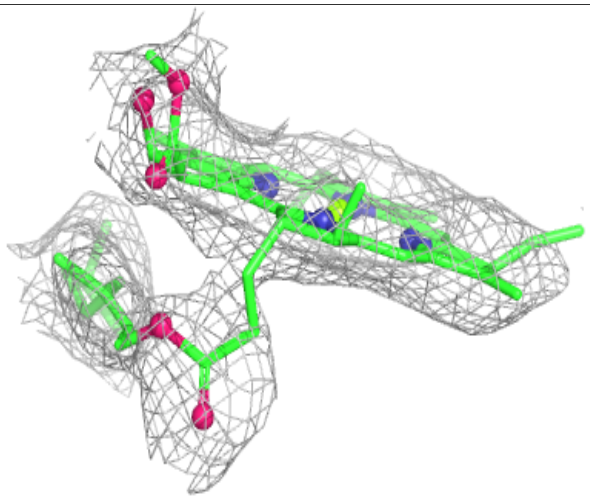


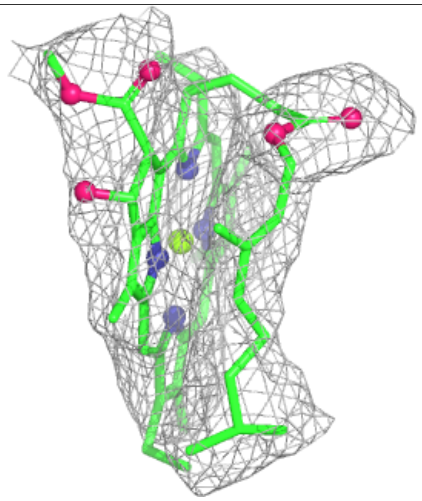


Electron density around CLA A 1127:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

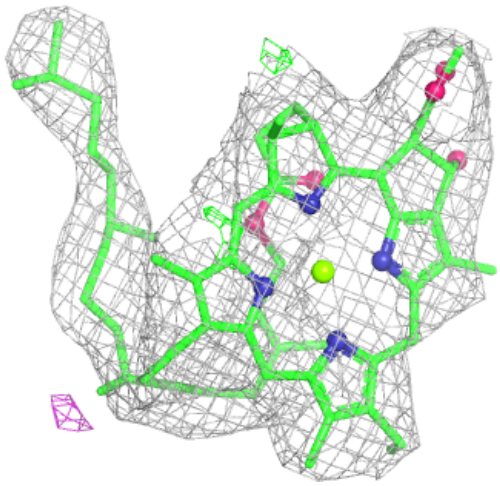


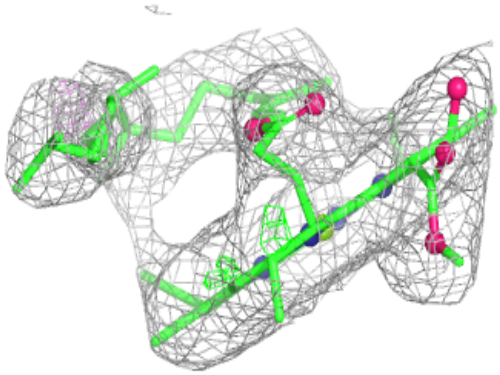


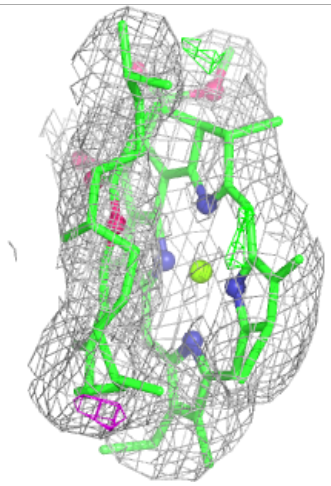


Electron density around CLA B 1205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

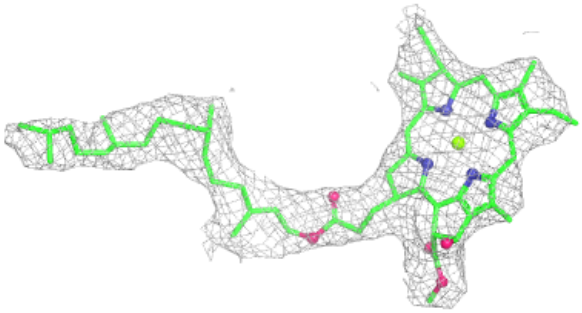


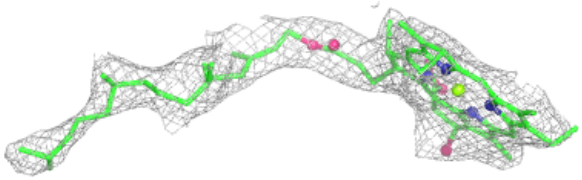


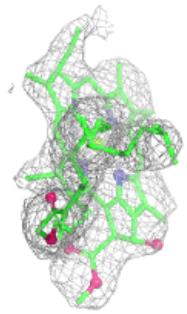


Electron density around CLA A 9022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

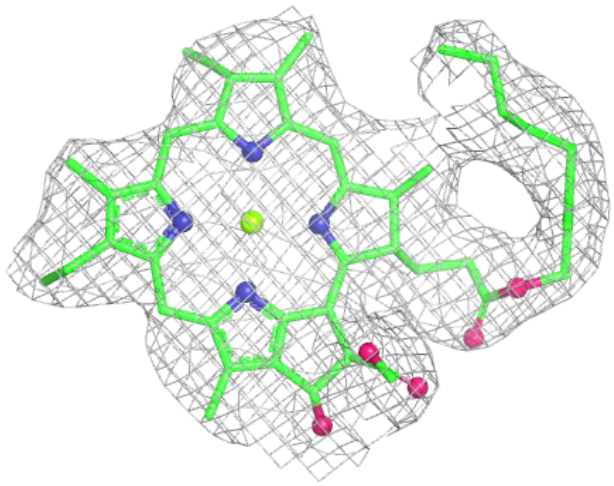


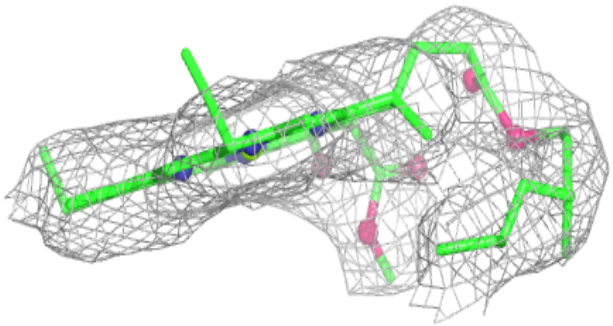


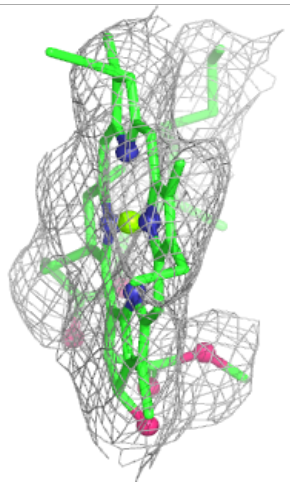


Electron density around CLA B 1221:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

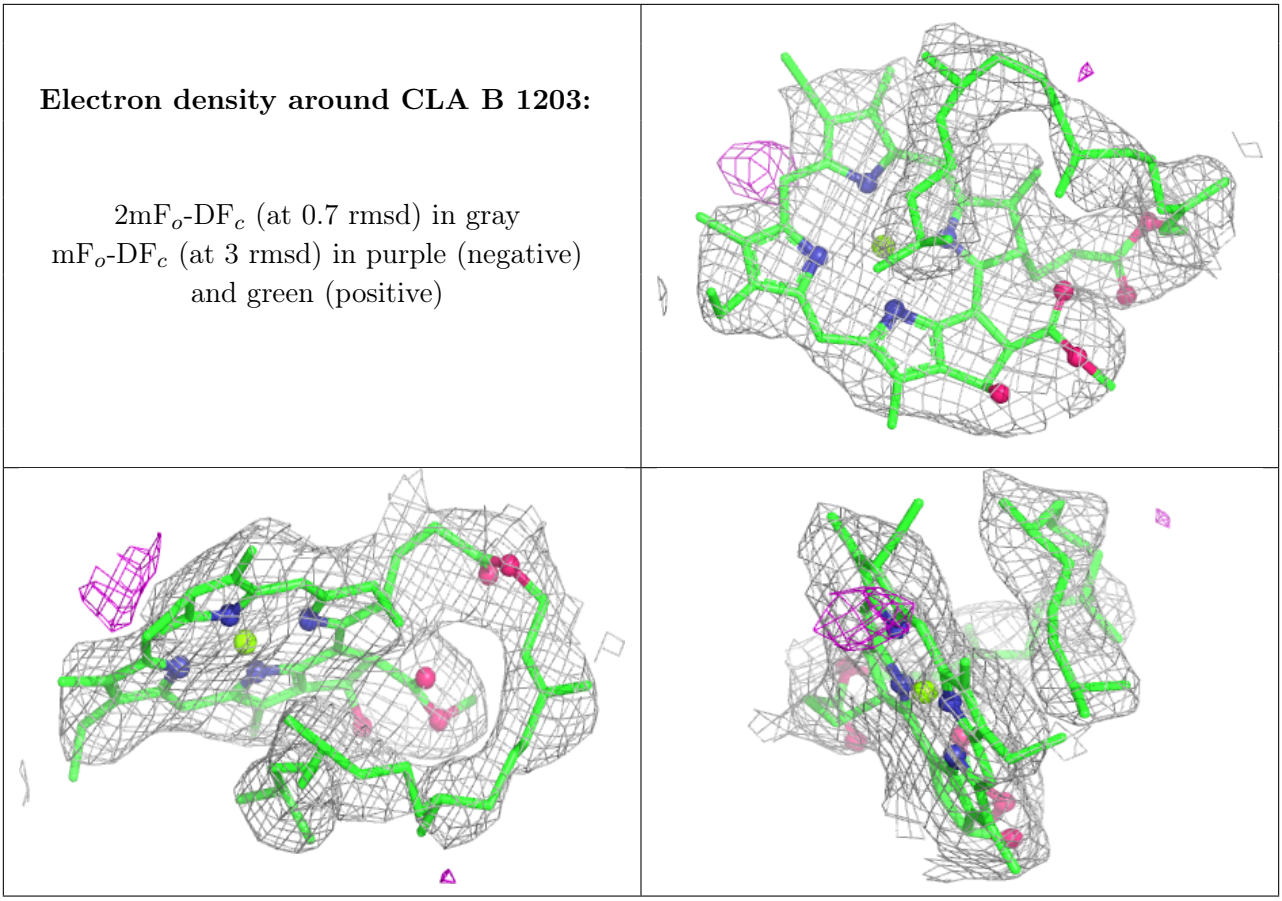






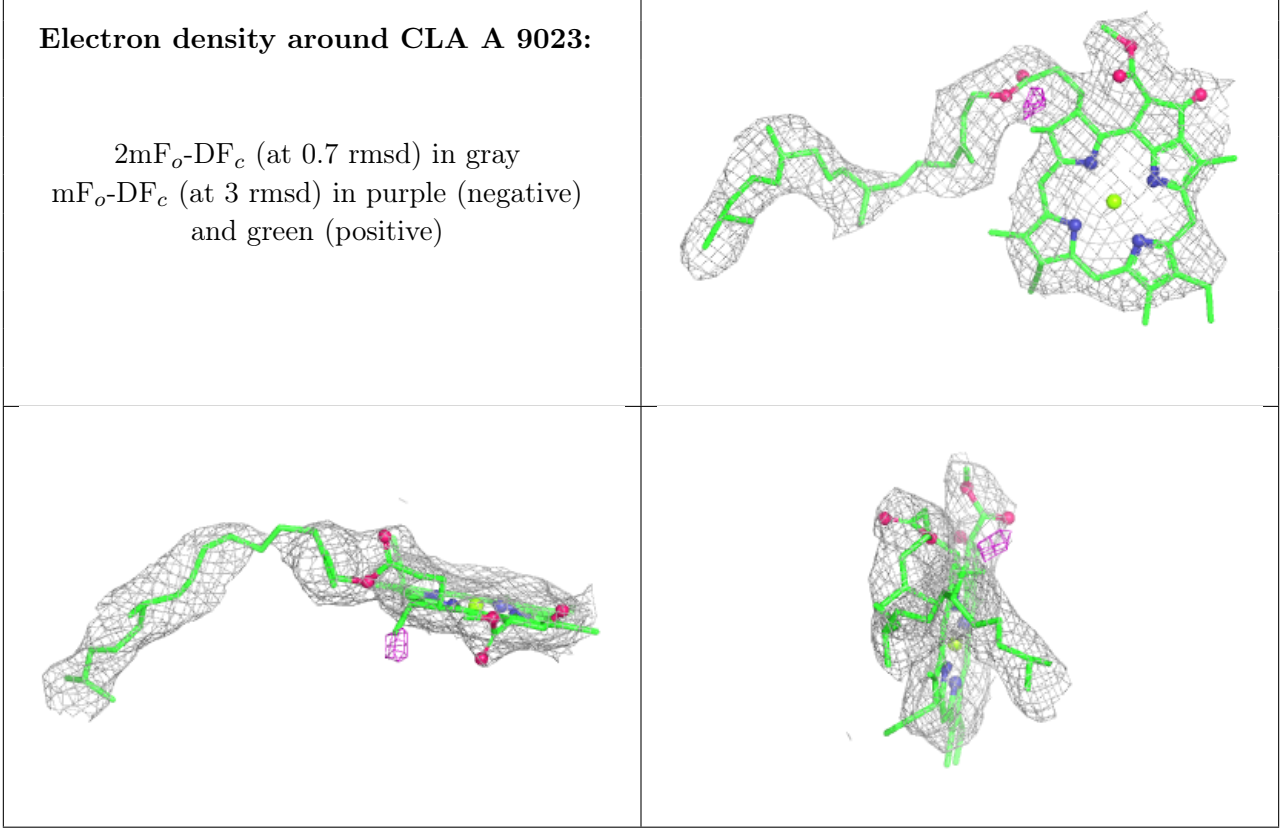
Electron density around CLA B 1203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



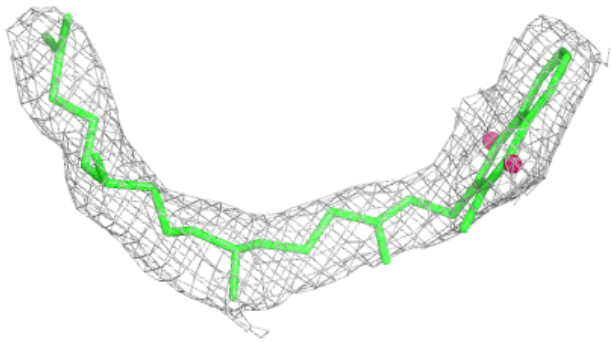
Electron density around CLA A 9023:

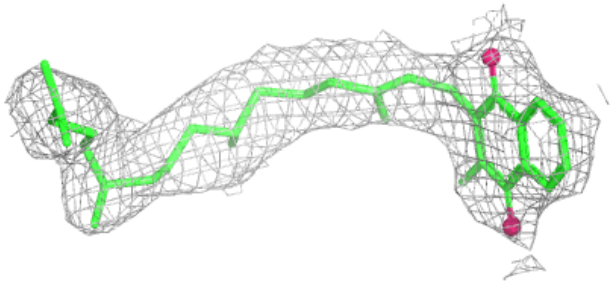
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

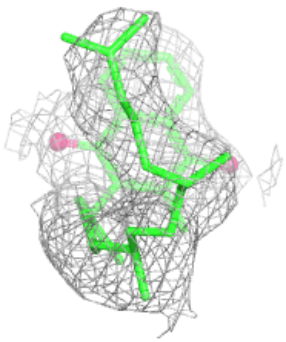


Electron density around PQN B 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

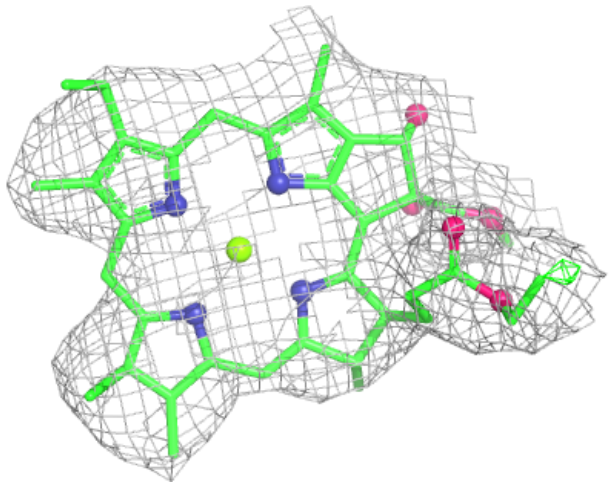


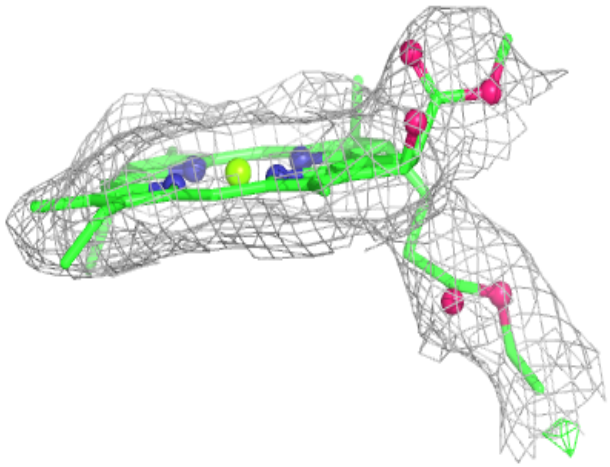


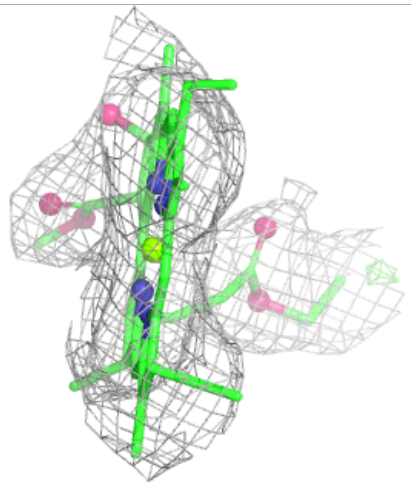


Electron density around CLA A 1137:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

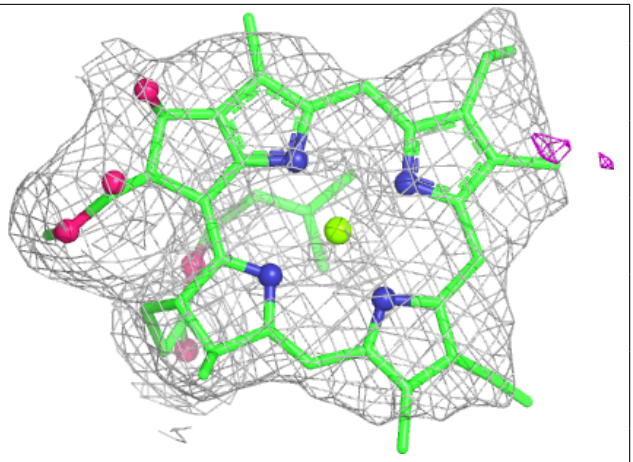


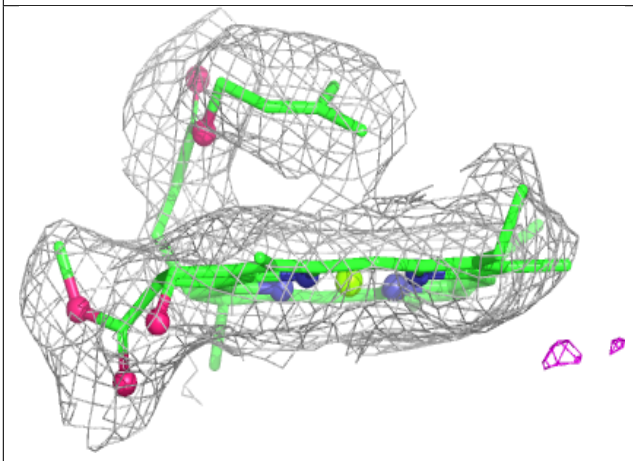




Electron density around CLA B 1227:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

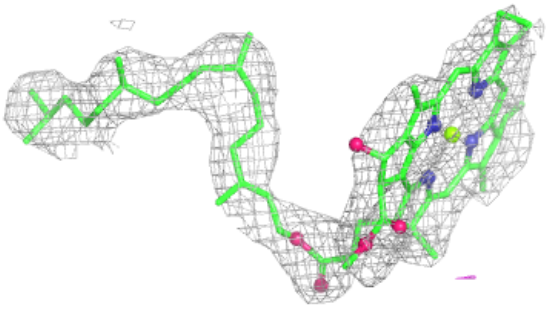


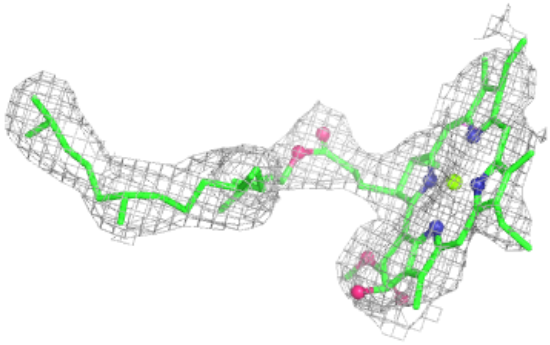


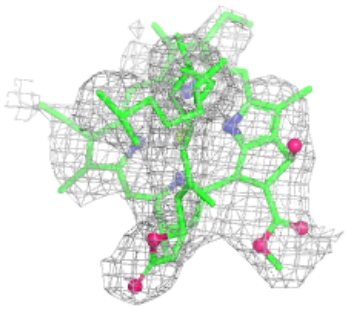


Electron density around CLA B 9010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

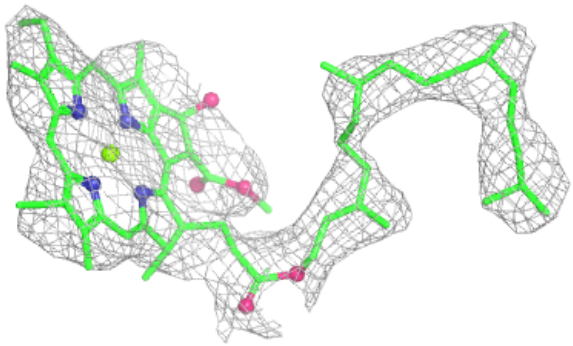


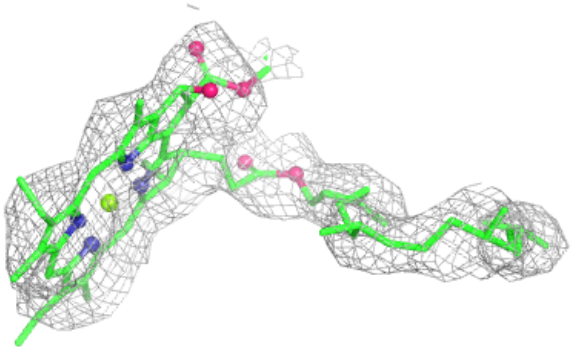


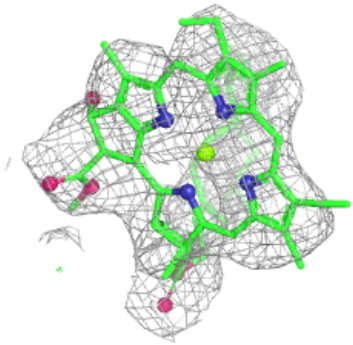


Electron density around CLA A 9011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.