Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 01:05 PM UTC

PDB ID	:	4Y28 / pdb_00004y28
Title	:	The structure of plant photosystem I super-complex at 2.8 angstrom resolution.
Authors	:	Mazor, Y.; Brovikov, A.; Nelson, N.
Deposited on	:	2015-02-09
Resolution	:	2.80 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:

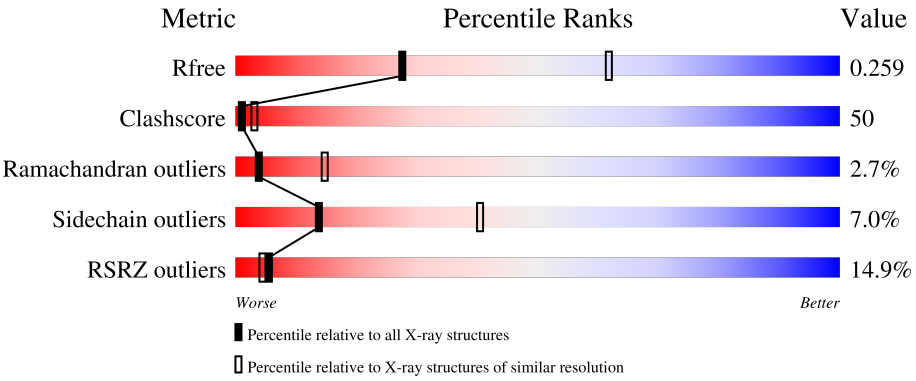
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	758	9% 73% 24% ••
2	B	733	9% 75% 24% •
3	I	30	17% 37% 47% 13% •
4	J	42	14% 36% 40% 17% 5% •
5	F	154	11% 64% 28% 6% •

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Mol	Chain	Length	Quality of chain
6	G	97	25% 33% 44% 13% 6%
7	L	167	21% 38% 41% 11% 5%
8	C	81	9% 56% 36% 7%
9	D	147	24% 41% 37% 14%
10	E	66	8% 45% 44% 9%
11	H	90	26% 49% 28% 12% 7%
12	K	129	14% 9% 26% 9% 56%
13	2	269	12% 18% 43% 12% 23%
14	4	252	9% 23% 43% 11% 21%
15	1	202	25% 27% 53% 14%
16	3	275	23% 12% 48% 15% 22%

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
17	CL0	A	1011	X	-	-	-
18	CLA	1	1001	X	-	X	-
18	CLA	1	1002	X	-	-	-
18	CLA	1	1003	X	-	X	-
18	CLA	1	1004	X	-	X	-
18	CLA	1	1005	X	-	-	-
18	CLA	1	1006	X	-	-	-
18	CLA	1	1007	X	-	-	-
18	CLA	1	1008	X	-	X	-
18	CLA	1	1011	X	-	-	-
18	CLA	1	1012	X	-	-	-
18	CLA	1	1013	X	-	-	-
18	CLA	1	1014	X	-	-	-
18	CLA	2	2001	X	-	X	-
18	CLA	2	2002	X	-	X	-
18	CLA	2	2003	X	-	X	-
18	CLA	2	2004	X	-	X	-
18	CLA	2	2005	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	2006	X	-	X	-
18	CLA	2	2007	X	-	X	-
18	CLA	2	2008	X	-	-	-
18	CLA	2	2009	X	-	-	-
18	CLA	2	2012	X	-	X	-
18	CLA	2	2016	X	-	X	-
18	CLA	2	2019	X	-	-	-
18	CLA	3	3001	X	-	X	-
18	CLA	3	3002	X	-	-	-
18	CLA	3	3003	X	-	X	-
18	CLA	3	3004	X	-	-	-
18	CLA	3	3005	X	-	-	-
18	CLA	3	3006	X	-	X	-
18	CLA	3	3007	X	-	-	-
18	CLA	3	3008	X	-	-	-
18	CLA	3	3010	X	-	X	-
18	CLA	3	3012	X	-	X	-
18	CLA	3	3013	X	-	X	-
18	CLA	3	3017	X	-	-	-
18	CLA	3	3018	X	-	-	-
18	CLA	3	3019	X	-	-	-
18	CLA	4	4001	X	-	X	-
18	CLA	4	4002	X	-	-	-
18	CLA	4	4003	X	-	-	-
18	CLA	4	4004	X	-	-	-
18	CLA	4	4005	X	-	-	-
18	CLA	4	4006	X	-	X	-
18	CLA	4	4007	X	-	-	-
18	CLA	4	4008	X	-	-	-
18	CLA	4	4009	X	-	-	-
18	CLA	4	4012	X	-	X	-
18	CLA	4	4016	X	-	X	-
18	CLA	4	4017	X	-	-	-
18	CLA	A	1013	X	-	-	-
18	CLA	A	1022	X	-	-	-
18	CLA	A	1101	X	-	-	-
18	CLA	A	1102	X	-	-	-
18	CLA	A	1103	X	-	-	-
18	CLA	A	1104	X	-	-	-
18	CLA	A	1105	X	-	-	-
18	CLA	A	1106	X	-	-	-
18	CLA	A	1107	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	1108	X	-	-	-
18	CLA	A	1109	X	-	-	-
18	CLA	A	1110	X	-	-	-
18	CLA	A	1111	X	-	-	-
18	CLA	A	1112	X	-	-	-
18	CLA	A	1113	X	-	-	-
18	CLA	A	1114	X	-	-	-
18	CLA	A	1115	X	-	-	-
18	CLA	A	1116	X	-	-	-
18	CLA	A	1117	X	-	-	-
18	CLA	A	1118	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1120	X	-	-	-
18	CLA	A	1121	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	-	-
18	CLA	A	1124	X	-	-	-
18	CLA	A	1125	X	-	-	-
18	CLA	A	1126	X	-	-	-
18	CLA	A	1127	X	-	-	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1131	X	-	-	-
18	CLA	A	1132	X	-	-	-
18	CLA	A	1134	X	-	-	-
18	CLA	A	1135	X	-	-	-
18	CLA	A	1136	X	-	-	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1138	X	-	-	-
18	CLA	A	1139	X	-	-	-
18	CLA	A	1140	X	-	-	-
18	CLA	A	1151	X	-	-	-
18	CLA	A	1237	X	-	-	-
18	CLA	B	1012	X	-	-	-
18	CLA	B	1021	X	-	-	-
18	CLA	B	1023	X	-	-	-
18	CLA	B	1201	X	-	-	-
18	CLA	B	1202	X	-	-	-
18	CLA	B	1203	X	-	-	-
18	CLA	B	1204	X	-	-	-
18	CLA	B	1205	X	-	-	-
18	CLA	B	1206	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	-	-
18	CLA	B	1210	X	-	-	-
18	CLA	B	1211	X	-	-	-
18	CLA	B	1212	X	-	-	-
18	CLA	B	1214	X	-	-	-
18	CLA	B	1215	X	-	-	-
18	CLA	B	1216	X	-	-	-
18	CLA	B	1217	X	-	-	-
18	CLA	B	1218	X	-	-	-
18	CLA	B	1219	X	-	-	-
18	CLA	B	1221	X	-	-	-
18	CLA	B	1222	X	-	-	-
18	CLA	B	1224	X	-	-	-
18	CLA	B	1225	X	-	-	-
18	CLA	B	1226	X	-	-	-
18	CLA	B	1227	X	-	-	-
18	CLA	B	1228	X	-	-	-
18	CLA	B	1229	X	-	-	-
18	CLA	B	1230	X	-	-	-
18	CLA	B	1231	X	-	-	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	X	-	-	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1236	X	-	-	-
18	CLA	B	1238	X	-	-	-
18	CLA	B	1239	X	-	-	-
18	CLA	B	1240	X	-	-	-
18	CLA	F	1301	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	G	1001	X	-	X	-
18	CLA	G	1002	X	-	X	-
18	CLA	G	1003	X	-	X	-
18	CLA	H	1000	X	-	-	-
18	CLA	J	1302	X	-	-	-
18	CLA	K	1001	X	-	-	-
18	CLA	L	1501	X	-	-	-
18	CLA	L	1502	X	-	-	-
18	CLA	L	1503	X	-	-	-
22	BCR	G	2011	-	-	X	-
22	BCR	L	6019	-	-	X	-
27	LUT	1	1501	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LUT	1	1502	X	-	-	-
27	LUT	2	2501	X	-	X	-
27	LUT	2	2502	X	-	X	-
27	LUT	3	3501	X	-	X	-
27	LUT	3	3502	X	-	X	-
27	LUT	4	4501	X	-	X	-
27	LUT	4	4502	X	-	X	-
27	LUT	4	4503	X	-	X	-
27	LUT	I	6018	X	-	-	-
28	CHL	1	1009	X	-	X	-
28	CHL	1	1010	X	-	-	-
28	CHL	2	2010	X	-	-	-
28	CHL	2	2011	X	-	-	-
28	CHL	2	2013	X	-	-	-
28	CHL	3	3011	X	-	X	-
28	CHL	4	4010	X	-	-	-
28	CHL	4	4011	X	-	-	-
28	CHL	4	4013	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35653 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	742	Total	C	N	O	S	0	0	0
			5852	3833	997	1004	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	LEU	engineered mutation	UNP P05310
A	22	LEU	VAL	engineered mutation	UNP P05310
A	117	ARG	GLY	engineered mutation	UNP P05310
A	220	GLY	ARG	engineered mutation	UNP P05310

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	732	Total	C	N	O	S	0	0	0
			5856	3851	995	996	14			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	LEU	ILE	engineered mutation	UNP P05311
B	115	ILE	ASN	engineered mutation	UNP P05311
B	273	MET	VAL	engineered mutation	UNP P05311
B	471	SER	THR	engineered mutation	UNP P05311
B	476	VAL	ILE	engineered mutation	UNP P05311
B	477	LEU	PRO	engineered mutation	UNP P05311
B	635	TYR	ILE	engineered mutation	UNP P05311

- Molecule 3 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	29	Total	C	N	O	S	0	0	0
			224	155	35	33	1			

- Molecule 4 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	41	Total	C	N	O	0	0	0
			321	217	50	54			

- Molecule 5 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	150	Total	C	N	O	S	0	0	0
			1187	770	207	208	2			

- Molecule 6 is a protein called photosystem I reaction center.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	91	Total	C	N	O	0	0	0
			689	444	117	128			

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	160	Total	C	N	O	S	0	0	0
			1197	791	190	215	1			

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	0
			1116	720	192	201	3			

- Molecule 10 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	E	66	Total	C	N	O	0	0	0
			530	337	93	100			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	H	84	Total	C	N	O	0	0	0
			642	425	97	120			

- Molecule 12 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	57	Total	C	N	O	S	0	0	0
			379	241	64	71	3			

- Molecule 13 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	2	207	Total	C	N	O	S	0	0	0
			1613	1057	263	289	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	133	LEU	ASN	engineered mutation	UNP Q41038

- Molecule 14 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	4	198	Total	C	N	O	S	0	0	0
			1544	1007	252	282	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	128	ASP	ALA	engineered mutation	UNP Q9SQL2

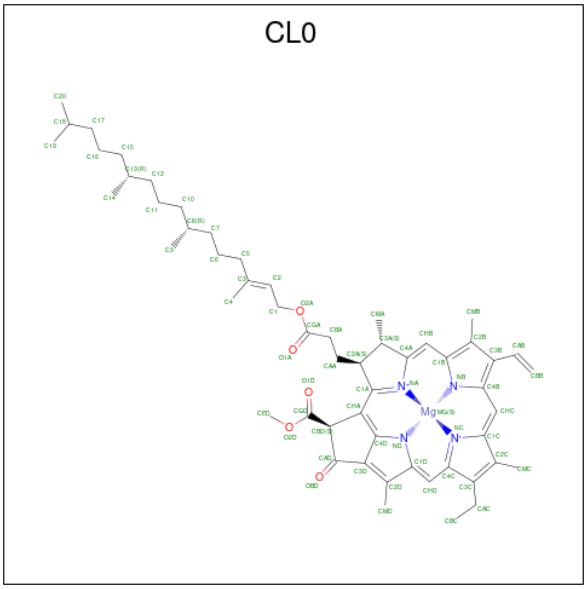
- Molecule 15 is a protein called Light-harvesting complex I chlorophyll A/B-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	194	Total	C	N	O	S	0	0	0
			1513	986	254	268	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

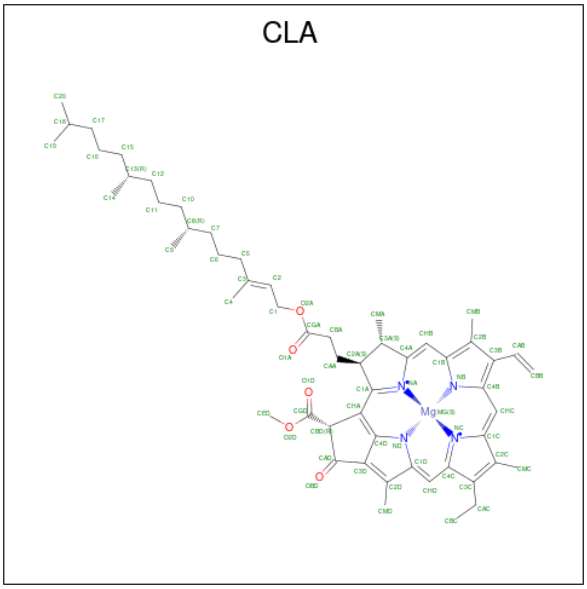
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	215	Total	C	N	O	S	0	0	0
			1619	1053	263	298	5			

- Molecule 17 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	H	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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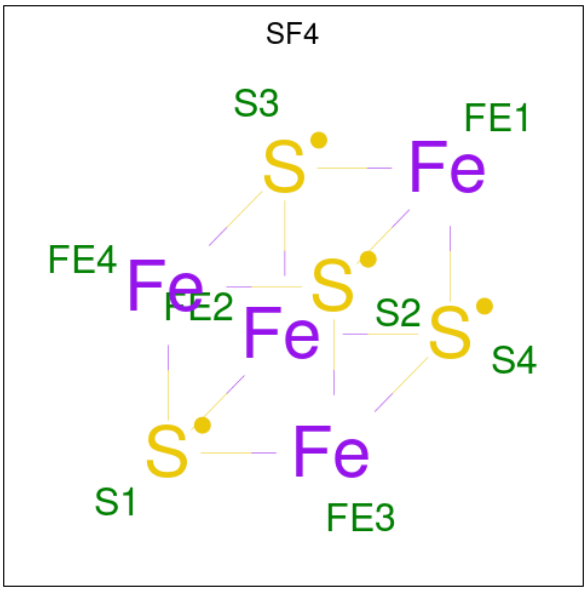
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	2	1	Total C Mg N 27 22 1 4	0	0
18	2	1	Total C Mg N O 50 40 1 4 5	0	0
18	4	1	Total C Mg N O 50 40 1 4 5	0	0
18	4	1	Total C Mg N O 60 50 1 4 5	0	0
18	4	1	Total C Mg N O 50 40 1 4 5	0	0
18	4	1	Total C Mg N O 65 55 1 4 5	0	0
18	4	1	Total C Mg N O 60 50 1 4 5	0	0
18	4	1	Total C Mg N O 60 50 1 4 5	0	0
18	4	1	Total C Mg N O 50 40 1 4 5	0	0
18	4	1	Total C Mg N O 60 50 1 4 5	0	0
18	4	1	Total C Mg N O 46 36 1 4 5	0	0
18	4	1	Total C Mg N O 65 55 1 4 5	0	0
18	4	1	Total C Mg N O 46 36 1 4 5	0	0
18	4	1	Total C Mg N O 65 55 1 4 5	0	0
18	1	1	Total C Mg N O 60 50 1 4 5	0	0
18	1	1	Total C Mg N O 46 36 1 4 5	0	0
18	1	1	Total C Mg N O 55 45 1 4 5	0	0
18	1	1	Total C Mg N O 65 55 1 4 5	0	0
18	1	1	Total C Mg N O 55 45 1 4 5	0	0
18	1	1	Total C Mg N O 50 40 1 4 5	0	0
18	1	1	Total C Mg N O 46 36 1 4 5	0	0

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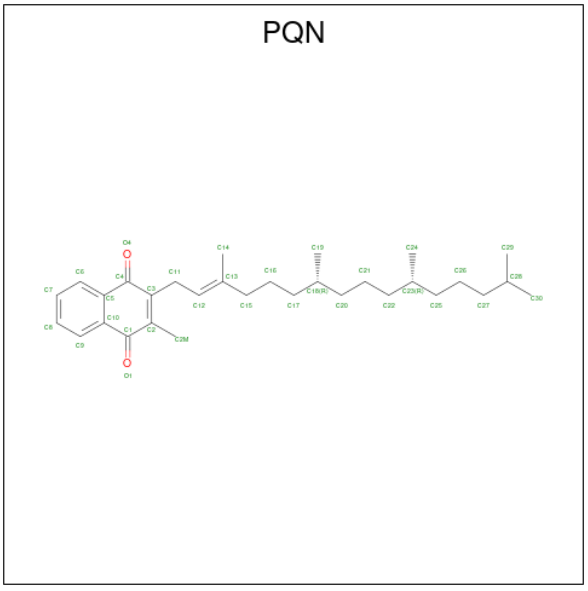
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N		0	0
			27	22	1	4			

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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



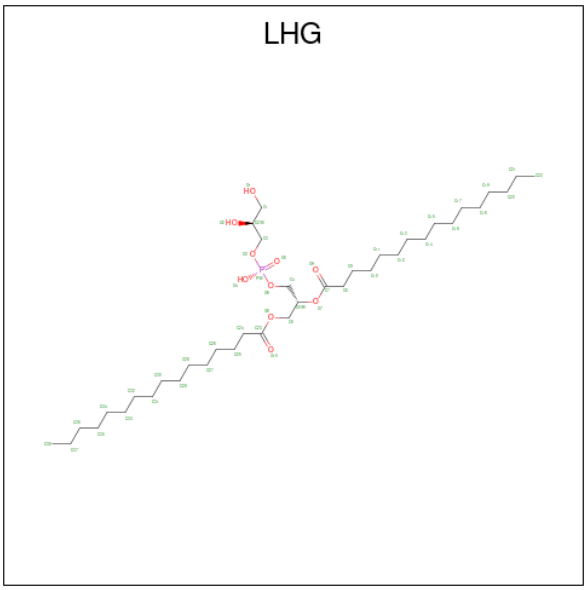
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 33 31 2	0	0

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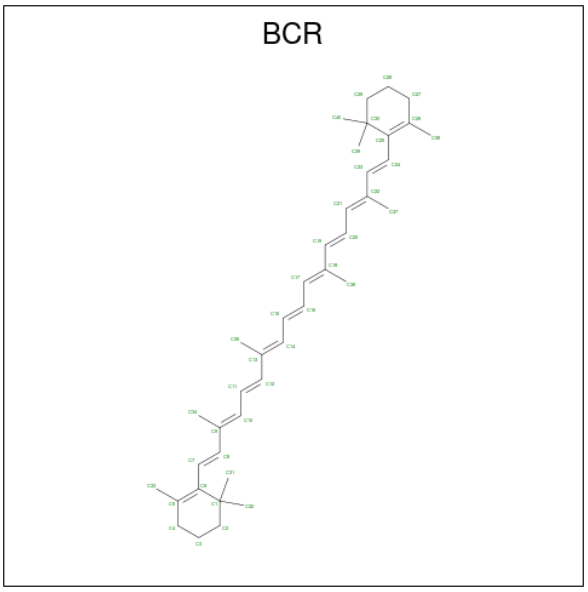
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total 33	C 31	O 2	0	0

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total 40	C 29	O 10	P 1	0	0
21	A	1	Total 49	C 38	O 10	P 1	0	0
21	B	1	Total 21	C 10	O 10	P 1	0	0
21	2	1	Total 24	C 13	O 10	P 1	0	0
21	1	1	Total 49	C 38	O 10	P 1	0	0

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



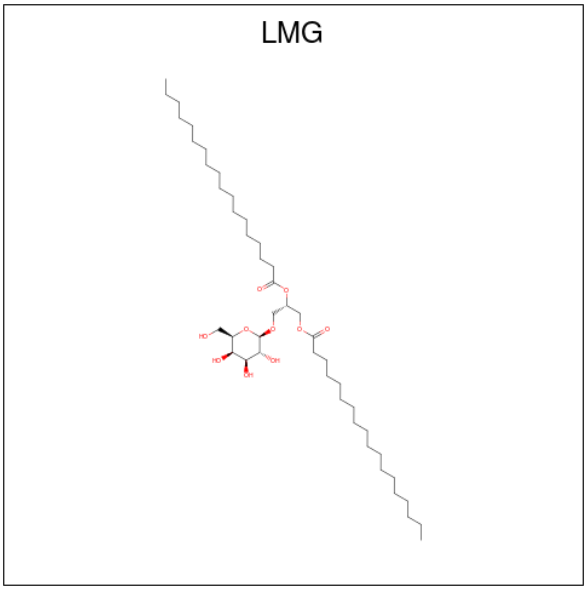
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	3	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 38 28 10	0	0
23	J	1	Total C O 55 45 10	0	0
23	F	1	Total C O 23 13 10	0	0
23	F	1	Total C O 37 27 10	0	0

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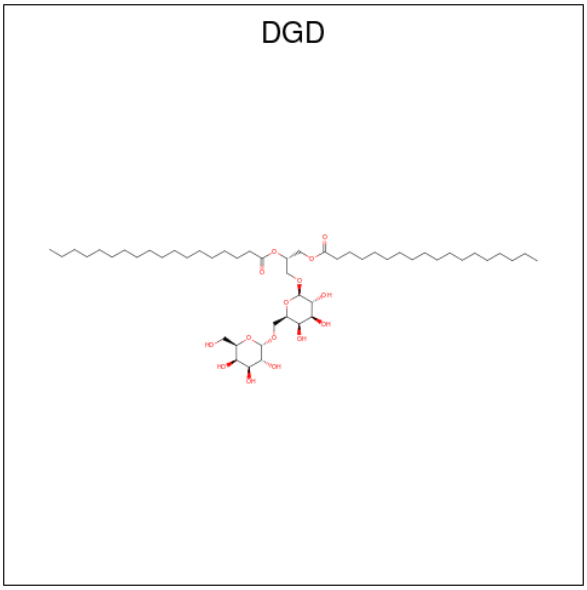
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	G	1	Total C O 41 31 10	0	0
23	2	1	Total C O 35 25 10	0	0
23	4	1	Total C O 35 25 10	0	0

- Molecule 24 is CALCIUM ION (CCD ID: CA) (formula: Ca).

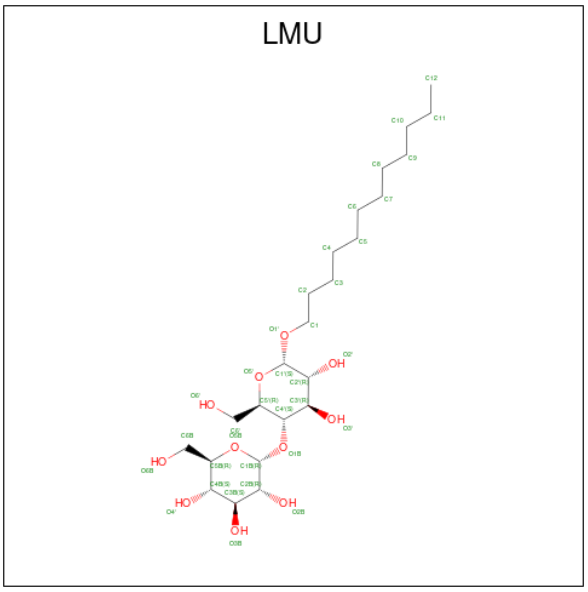
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Ca 1 1	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



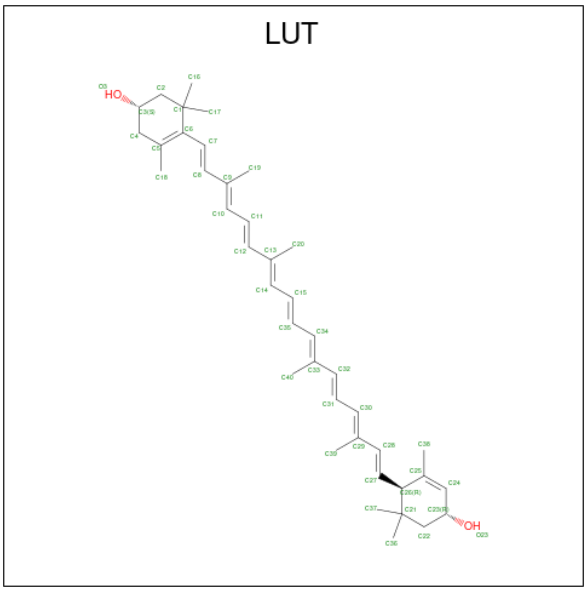
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 61 46 15	0	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	B	1	Total C O 35 24 11	0	0
26	B	1	Total C O 35 24 11	0	0

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



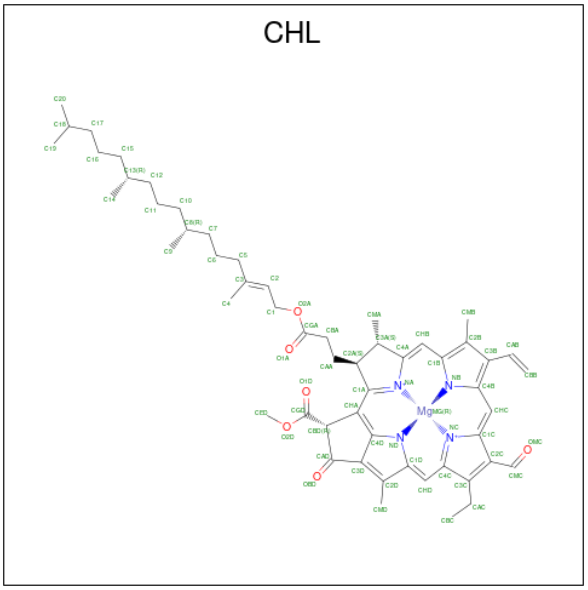
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	1	Total C O 42 40 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	2	1	Total C O 42 40 2	0	0
27	2	1	Total C O 42 40 2	0	0
27	4	1	Total C O 42 40 2	0	0
27	4	1	Total C O 42 40 2	0	0
27	4	1	Total C O 42 40 2	0	0
27	1	1	Total C O 42 40 2	0	0
27	1	1	Total C O 42 40 2	0	0
27	3	1	Total C O 42 40 2	0	0
27	3	1	Total C O 42 40 2	0	0

- Molecule 28 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



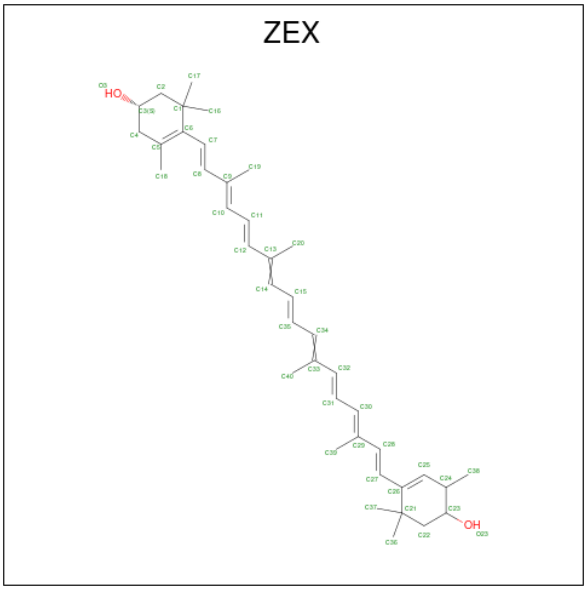
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	2	1	Total C Mg N O 47 36 1 4 6	0	0
28	2	1	Total C Mg N O 48 37 1 4 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	3	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 29 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).

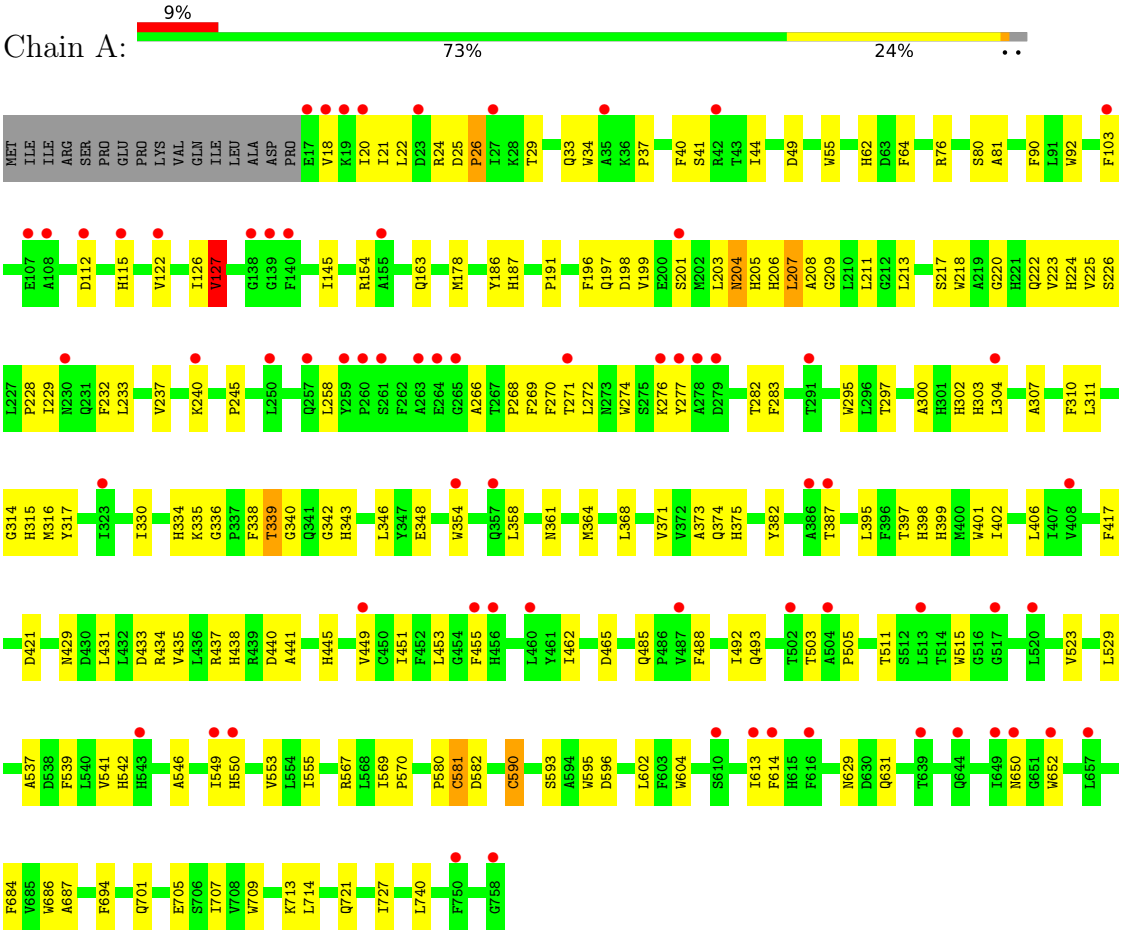


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	4	1	Total	C	O	0	0
			42	40	2		

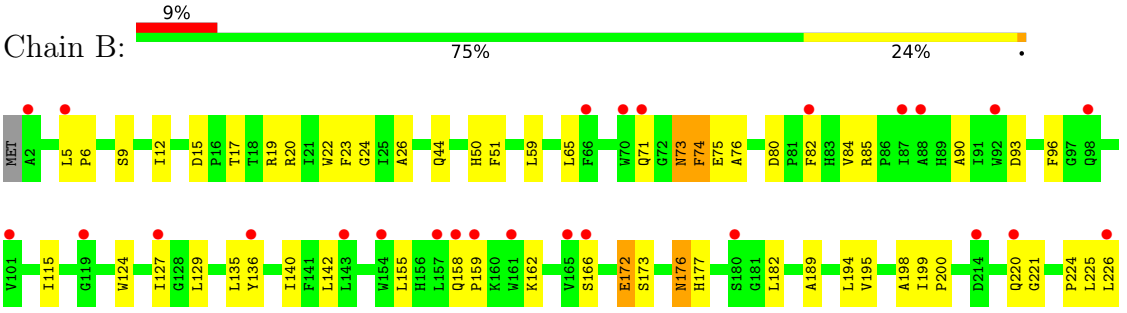
3 Residue-property plots (i)

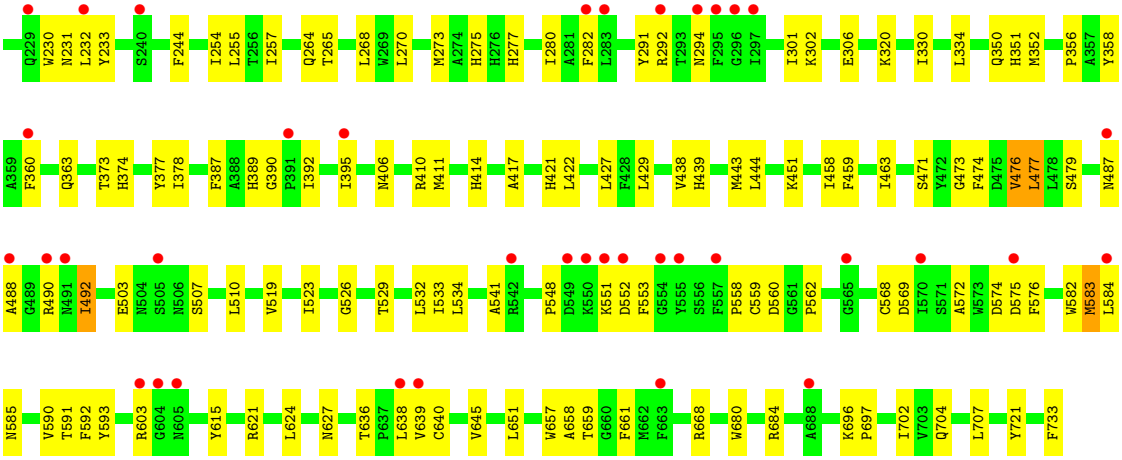
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



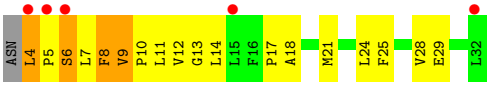
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





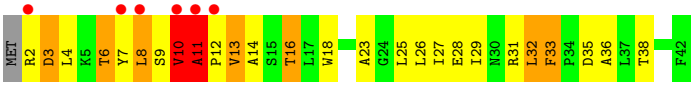
• Molecule 3: Photosystem I reaction center subunit VIII





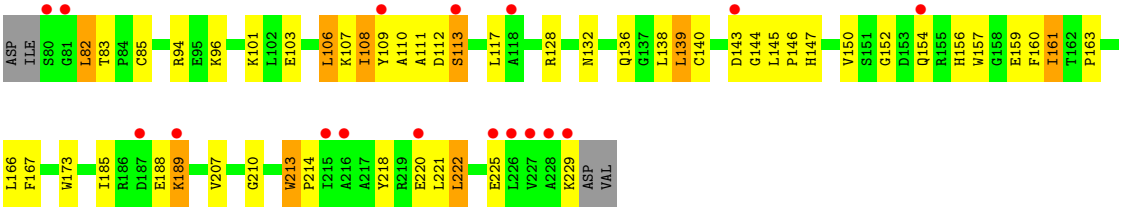
• Molecule 4: Photosystem I reaction center subunit IX





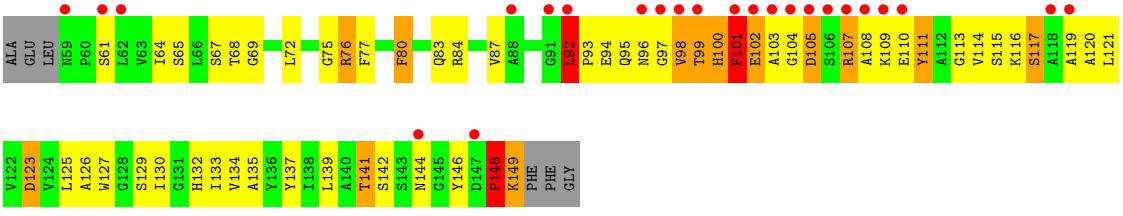
• Molecule 5: Photosystem I reaction center subunit III





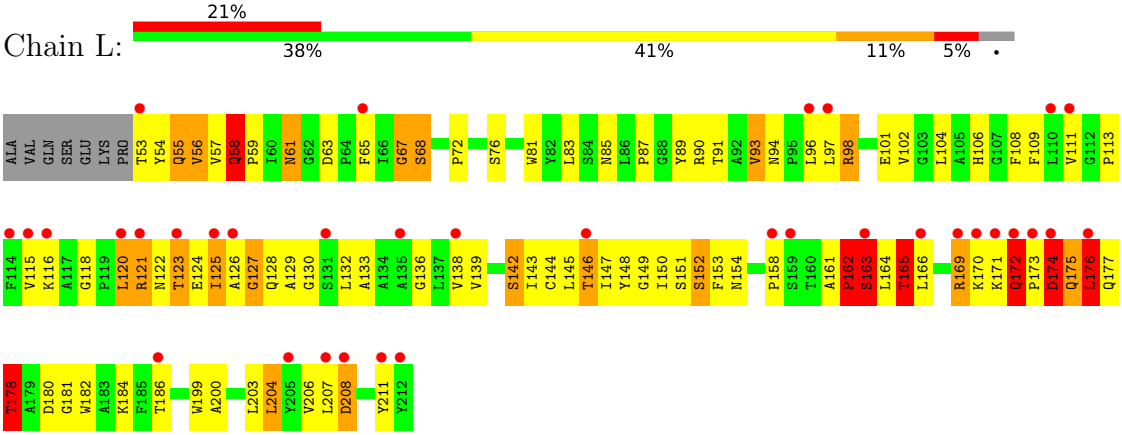
• Molecule 6: photosystem I reaction center





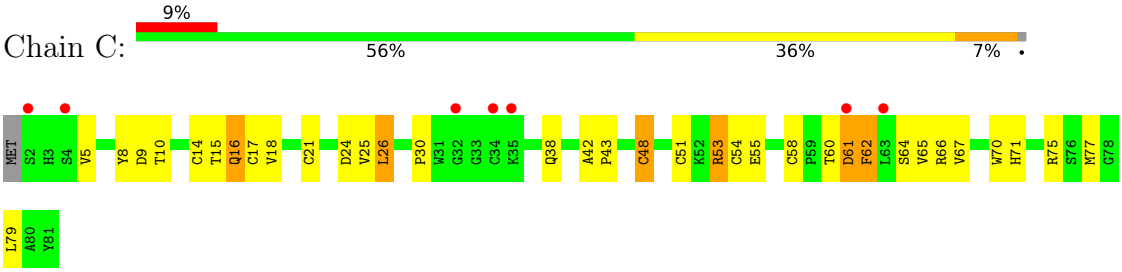
• Molecule 7: Putative uncharacterized protein

Chain L:



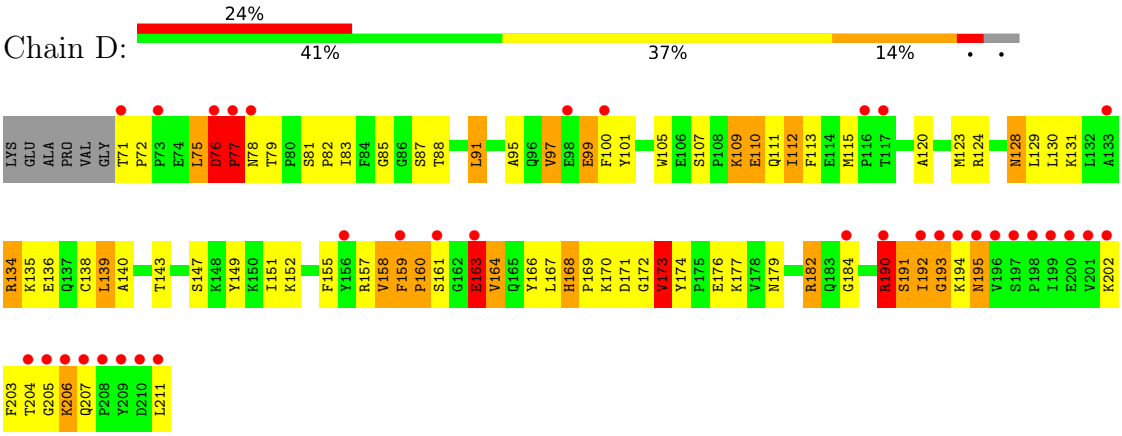
• Molecule 8: Photosystem I iron-sulfur center

Chain C:



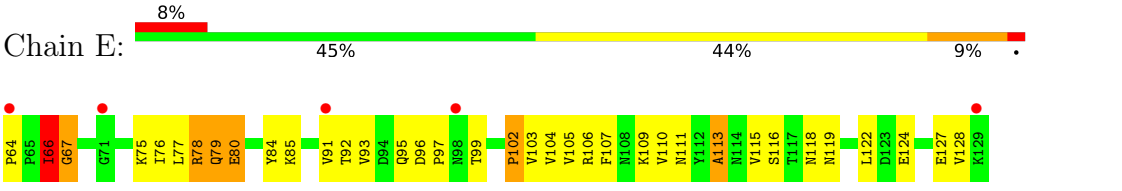
• Molecule 9: Photosystem I reaction center subunit II, chloroplastic

Chain D:



• Molecule 10: Photosystem I reaction center subunit IV A, chloroplastic

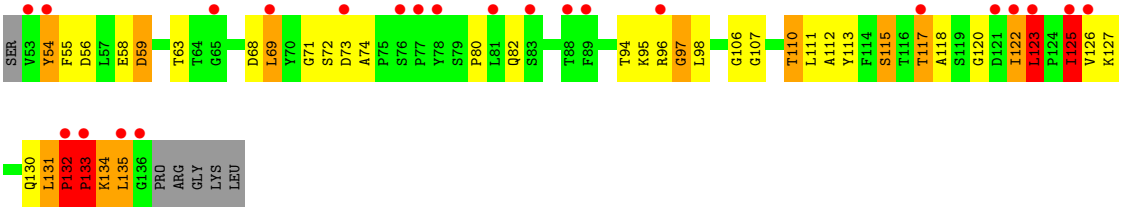
Chain E:



• Molecule 11: Photosystem I reaction center subunit VI

Chain H:

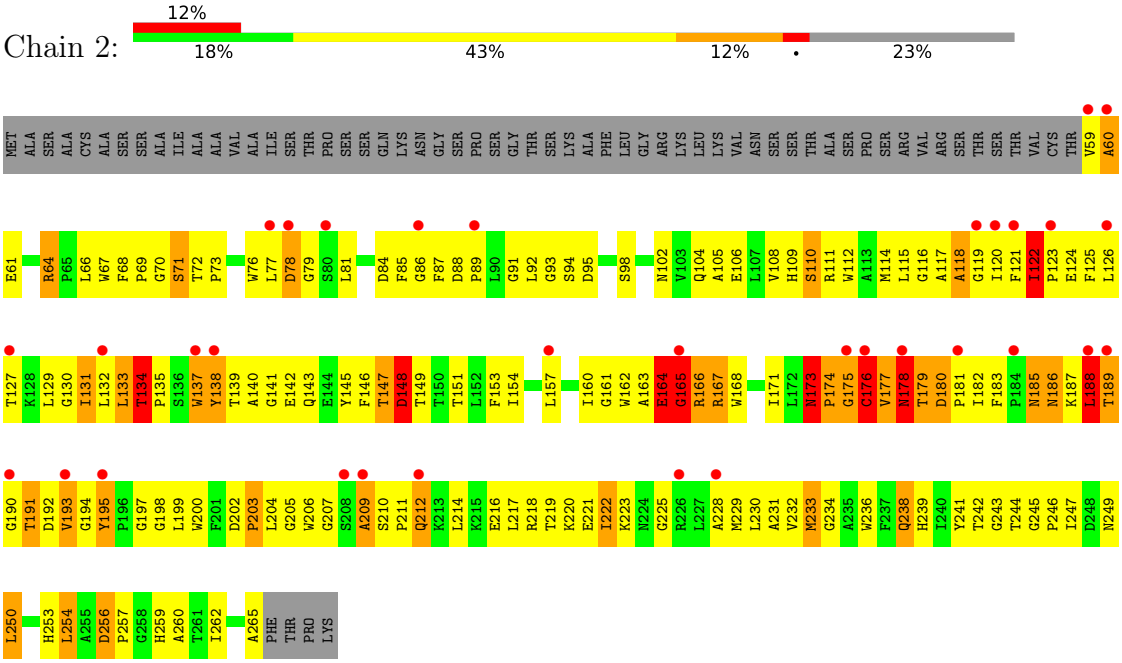




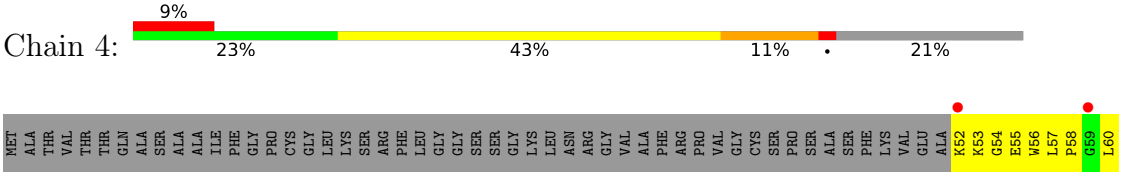
• Molecule 12: Photosystem I reaction center subunit X psaK

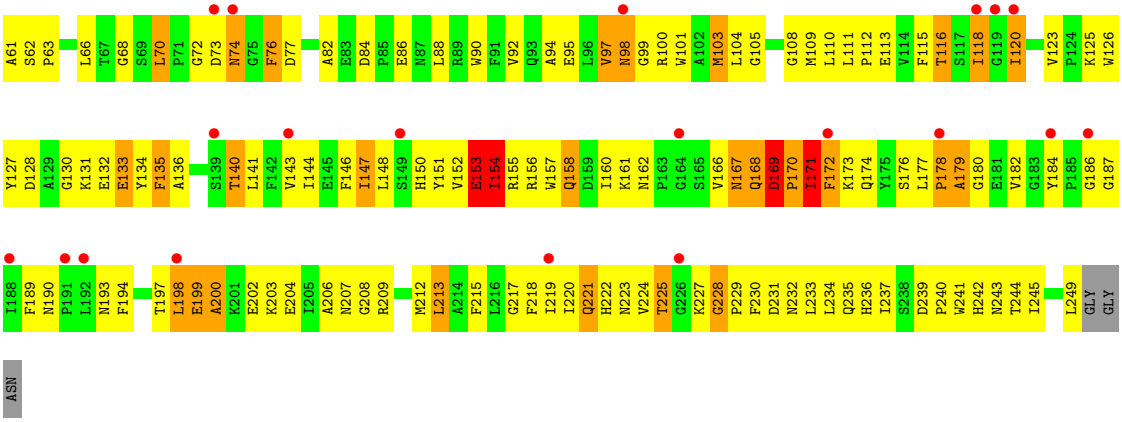


• Molecule 13: Type II chlorophyll a/b binding protein from photosystem I



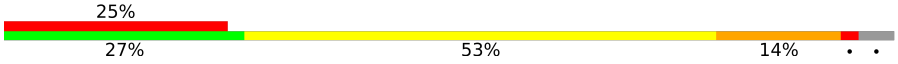
• Molecule 14: Chlorophyll a-b binding protein P4, chloroplastic

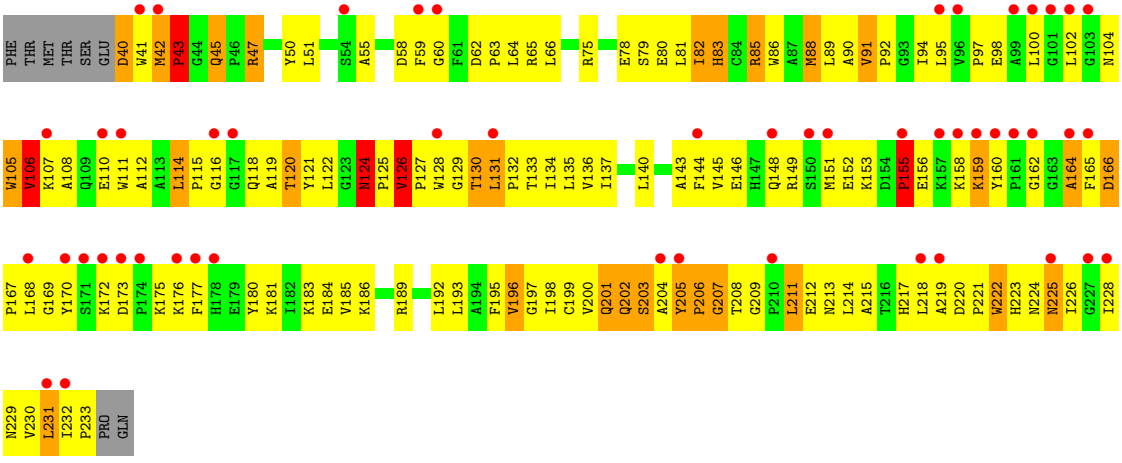




• Molecule 15: Light-harvesting complex I chlorophyll A/B-binding protein

Chain 1:

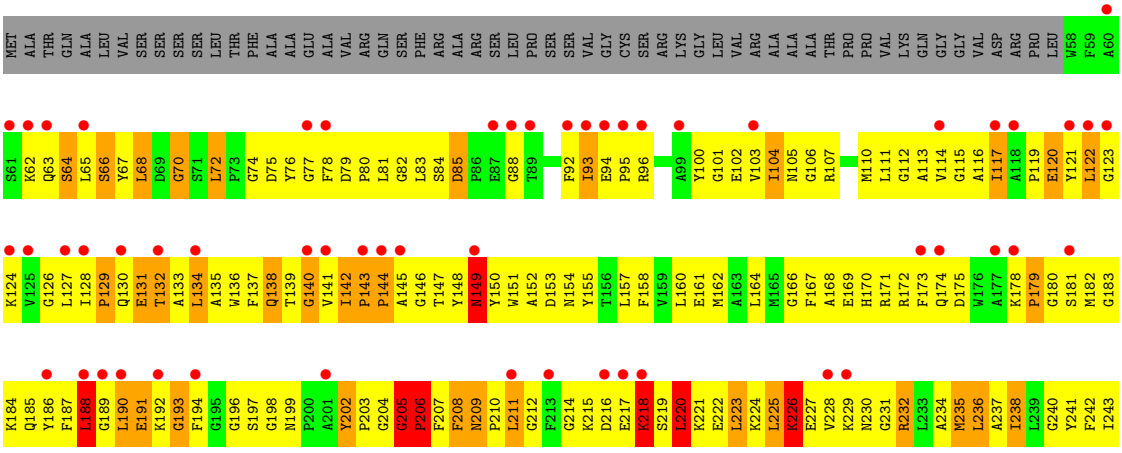


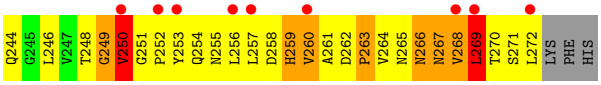


• Molecule 16: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:






Q244
G245
L246
V247
T248
G249
V250
G251
P252
Y253
Q254
N255
L256
L257
D258
H259
V260
A261
D262
P263
V264
N265
M266
N267
V268
L269
T270
S271
L272
LYS
PHE
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	189.00Å 201.90Å 213.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.80 48.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.65-2.80) 89.2 (48.65-2.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.268 0.246 , 0.259	Depositor DCC
R_{free} test set	3977 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å^2)	78.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	35653	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LUT, LMG, CLA, ZEX, PQN, SF4, LMU, CHL, CL0, BCR, DGD, CA, LHG

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	0.30	0/6049	0.72	2/8253 (0.0%)
2	B	0.30	0/6067	0.72	3/8287 (0.0%)
3	I	1.37	0/230	1.42	3/313 (1.0%)
4	J	1.15	0/330	1.47	6/452 (1.3%)
5	F	0.85	0/1214	1.06	10/1638 (0.6%)
6	G	1.11	0/705	1.56	12/956 (1.3%)
7	L	1.05	0/1233	1.37	17/1690 (1.0%)
8	C	1.11	2/625 (0.3%)	1.14	5/846 (0.6%)
9	D	1.29	0/1146	1.53	24/1550 (1.5%)
10	E	1.14	0/542	1.46	11/737 (1.5%)
11	H	0.84	2/662 (0.3%)	1.31	14/902 (1.6%)
12	K	0.70	0/381	1.28	7/517 (1.4%)
13	2	1.31	3/1672 (0.2%)	1.56	41/2292 (1.8%)
14	4	1.31	3/1592 (0.2%)	1.45	34/2174 (1.6%)
15	1	1.17	1/1563 (0.1%)	1.50	32/2132 (1.5%)
16	3	1.16	5/1666 (0.3%)	1.60	46/2265 (2.0%)
All	All	0.86	16/25677 (0.1%)	1.16	267/35004 (0.8%)

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
6	G	0	1
7	L	0	1
13	2	0	1
14	4	0	1
16	3	0	1
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	164	GLU	C-O	-15.54	1.03	1.24
14	4	153	GLU	C-O	-14.60	1.03	1.23
14	4	154	ILE	C-N	9.56	1.47	1.33
16	3	205	GLY	C-O	-8.79	1.12	1.24
16	3	208	PHE	C-N	8.31	1.43	1.33
14	4	153	GLU	C-N	7.68	1.44	1.33
13	2	164	GLU	C-N	7.45	1.44	1.33
8	C	42	ALA	C-N	6.44	1.41	1.34
16	3	205	GLY	C-N	6.43	1.48	1.33
16	3	85	ASP	C-N	6.35	1.38	1.33
13	2	165	GLY	C-N	6.07	1.42	1.33
11	H	123	LEU	C-N	5.69	1.42	1.33
11	H	74	ALA	C-N	5.66	1.40	1.33
8	C	58	CYS	C-N	5.62	1.38	1.33
15	1	91	VAL	CA-CB	-5.25	1.51	1.54
16	3	209	ASN	N-CA	5.08	1.52	1.46

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	66	ILE	N-CA-C	16.27	126.04	110.42
6	G	100	HIS	N-CA-C	-15.45	83.33	108.52
7	L	174	ASP	N-CA-C	14.88	132.29	109.23
6	G	101	PHE	CA-C-N	14.51	149.25	121.54
6	G	101	PHE	C-N-CA	14.51	149.25	121.54
9	D	158	VAL	N-CA-C	12.87	125.03	111.00
4	J	11	ALA	CA-C-N	-12.47	108.11	120.83
4	J	11	ALA	C-N-CA	-12.47	108.11	120.83
13	2	147	THR	N-CA-C	12.16	126.58	112.72
9	D	173	VAL	CB-CA-C	-11.70	98.35	111.45
13	2	180	ASP	N-CA-C	-11.13	90.56	109.15
13	2	190	GLY	N-CA-C	-10.96	92.06	110.80
16	3	208	PHE	CA-C-N	-10.79	107.23	122.66
16	3	208	PHE	C-N-CA	-10.79	107.23	122.66
10	E	113	ALA	N-CA-C	-10.59	92.17	109.96
16	3	64	SER	N-CA-C	10.32	125.24	108.41
7	L	55	GLN	N-CA-C	10.27	127.07	113.72
14	4	198	LEU	N-CA-C	-10.27	96.02	110.50
16	3	134	LEU	N-CA-C	-10.14	94.14	109.86
14	4	110	LEU	N-CA-C	10.09	122.03	111.14
13	2	165	GLY	N-CA-C	-10.00	89.48	113.18
6	G	105	ASP	N-CA-C	9.87	124.35	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	165	GLY	CA-C-N	-9.73	102.95	121.54
13	2	165	GLY	C-N-CA	-9.73	102.95	121.54
15	1	95	LEU	N-CA-C	9.54	121.76	111.36
11	H	134	LYS	N-CA-C	-9.48	101.48	113.23
15	1	129	GLY	N-CA-C	9.35	123.95	112.73
16	3	143	PRO	N-CA-C	9.22	121.94	110.70
11	H	120	GLY	N-CA-C	-9.19	91.41	113.18
16	3	205	GLY	CA-C-O	9.07	134.49	121.52
14	4	213	LEU	N-CA-C	-8.97	100.66	111.69
16	3	206	PRO	CA-N-CD	-8.95	99.47	112.00
16	3	66	SER	N-CA-C	8.73	120.88	111.36
15	1	90	ALA	N-CA-C	8.72	120.78	111.28
16	3	138	GLN	N-CA-C	8.60	121.79	111.82
13	2	165	GLY	O-C-N	8.59	133.86	122.70
14	4	153	GLU	O-C-N	-8.57	110.37	122.03
15	1	155	PRO	CA-N-CD	-8.50	100.10	112.00
14	4	154	ILE	CA-C-N	-8.34	107.45	122.46
14	4	154	ILE	C-N-CA	-8.34	107.45	122.46
12	K	87	PRO	N-CA-C	8.25	125.00	113.53
13	2	179	THR	N-CA-C	8.19	121.52	109.07
16	3	122	LEU	N-CA-C	8.19	119.83	111.07
7	L	178	THR	N-CA-C	-8.13	96.72	109.07
14	4	130	GLY	N-CA-C	8.06	122.41	112.73
14	4	154	ILE	N-CA-C	-8.05	92.60	109.34
13	2	164	GLU	N-CA-C	7.99	123.16	113.41
13	2	148	ASP	N-CA-C	7.95	127.72	110.80
16	3	205	GLY	O-C-N	-7.87	110.42	123.00
15	1	43	PRO	N-CA-C	7.79	128.52	112.47
16	3	249	GLY	N-CA-C	-7.76	96.14	112.45
14	4	153	GLU	N-CA-C	7.69	123.15	112.93
15	1	43	PRO	CA-N-CD	-7.67	101.27	112.00
16	3	140	GLY	N-CA-C	7.62	121.87	112.73
16	3	189	GLY	N-CA-C	-7.57	100.92	112.51
9	D	149	TYR	N-CA-C	-7.56	97.80	109.52
15	1	207	GLY	N-CA-C	-7.52	95.35	113.18
9	D	134	ARG	N-CA-C	7.51	124.93	113.51
9	D	75	LEU	N-CA-C	7.50	122.17	112.12
13	2	164	GLU	O-C-N	-7.43	111.81	122.36
16	3	259	HIS	N-CA-C	-7.42	103.19	111.28
6	G	98	VAL	N-CA-C	7.38	124.69	109.34
16	3	142	ILE	CB-CA-C	-7.36	106.54	114.35
14	4	133	GLU	N-CA-C	7.28	121.71	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	9	VAL	CB-CA-C	-7.27	104.48	114.00
14	4	169	ASP	C-N-CD	7.23	136.51	120.60
4	J	8	LEU	N-CA-C	-7.21	103.36	111.07
7	L	175	GLN	N-CA-C	7.20	126.14	110.80
12	K	79	PHE	N-CA-C	-7.20	97.94	109.39
7	L	68	SER	N-CA-C	7.18	119.24	110.41
16	3	260	VAL	N-CA-C	7.14	117.94	110.72
7	L	176	LEU	N-CA-C	-7.14	95.60	110.80
16	3	208	PHE	CA-C-O	-7.11	113.29	120.90
16	3	191	GLU	N-CA-C	-7.10	103.54	111.28
15	1	106	VAL	CB-CA-C	-7.09	102.57	112.14
15	1	222	TRP	N-CA-C	7.00	118.91	111.28
10	E	96	ASP	N-CA-C	6.99	119.76	109.42
15	1	110	GLU	N-CA-C	6.95	119.74	111.33
13	2	191	THR	N-CA-C	-6.93	99.71	110.17
6	G	119	ALA	N-CA-C	6.92	119.66	110.53
14	4	200	ALA	N-CA-C	-6.91	103.83	111.36
15	1	82	ILE	CB-CA-C	-6.91	103.13	111.97
13	2	177	VAL	N-CA-C	-6.91	103.58	110.62
16	3	142	ILE	N-CA-C	6.87	122.58	112.61
5	F	161	ILE	N-CA-C	6.85	117.61	110.62
9	D	168	HIS	C-N-CD	6.84	135.65	120.60
2	B	668	ARG	N-CA-C	6.82	118.51	111.14
15	1	126	VAL	C-N-CD	6.81	135.58	120.60
15	1	91	VAL	O-C-N	6.74	124.73	120.42
6	G	80	PHE	N-CA-C	6.71	118.25	111.07
5	F	107	LYS	N-CA-C	6.69	118.57	111.28
11	H	74	ALA	CA-C-N	-6.62	112.70	120.11
11	H	74	ALA	C-N-CA	-6.62	112.70	120.11
16	3	192	LYS	N-CA-C	-6.61	104.08	111.28
10	E	66	ILE	CB-CA-C	-6.60	103.52	111.97
12	K	82	ARG	N-CA-C	6.60	118.55	109.18
14	4	131	LYS	N-CA-C	6.55	118.83	108.67
14	4	172	PHE	N-CA-C	-6.54	101.27	110.50
14	4	135	PHE	N-CA-C	-6.50	100.21	109.96
14	4	56	TRP	N-CA-C	-6.49	104.62	112.54
15	1	91	VAL	CB-CA-C	-6.46	105.54	114.00
7	L	127	GLY	N-CA-C	6.44	123.20	110.77
4	J	33	PHE	CA-C-N	-6.40	113.69	120.66
4	J	33	PHE	C-N-CA	-6.40	113.69	120.66
9	D	163	GLU	N-CA-C	-6.33	102.18	110.53
13	2	166	ARG	CA-C-N	6.32	129.27	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	166	ARG	C-N-CA	6.32	129.27	120.29
5	F	154	GLN	N-CA-C	6.30	118.96	111.71
4	J	6	THR	N-CA-C	-6.30	104.41	111.28
11	H	117	THR	N-CA-C	6.29	117.70	108.14
13	2	138	TYR	N-CA-C	-6.29	100.53	109.96
16	3	199	ASN	N-CA-C	6.25	118.69	109.62
13	2	60	ALA	N-CA-C	6.24	119.52	110.28
9	D	97	VAL	N-CA-C	6.24	120.23	113.43
6	G	76	ARG	N-CA-C	6.22	118.06	111.28
6	G	113	GLY	N-CA-C	6.22	119.74	111.03
7	L	120	LEU	N-CA-C	6.22	118.86	111.71
9	D	190	ARG	N-CA-C	-6.19	95.56	107.57
11	H	115	SER	N-CA-C	-6.18	104.54	111.28
12	K	84	GLY	N-CA-C	-6.15	101.00	111.27
3	I	8	PHE	N-CA-C	-6.14	105.61	113.23
11	H	133	PRO	CA-N-CD	-6.03	103.56	112.00
16	3	193	GLY	N-CA-C	-6.01	105.52	112.73
13	2	72	THR	CA-C-N	-5.99	114.21	120.38
13	2	72	THR	C-N-CA	-5.99	114.21	120.38
3	I	9	VAL	O-C-N	5.95	124.22	120.42
11	H	123	LEU	N-CA-C	5.90	120.78	108.39
9	D	193	GLY	N-CA-C	-5.89	99.23	113.18
16	3	269	LEU	N-CA-C	-5.86	104.90	111.28
9	D	184	GLY	N-CA-C	5.84	119.49	111.54
14	4	123	VAL	CA-C-N	-5.82	114.27	120.03
14	4	123	VAL	C-N-CA	-5.82	114.27	120.03
9	D	78	ASN	N-CA-C	-5.82	105.55	114.16
15	1	203	SER	N-CA-C	-5.81	102.71	110.55
9	D	120	ALA	N-CA-C	5.79	118.83	109.40
13	2	73	PRO	CA-C-N	-5.79	114.42	120.38
13	2	73	PRO	C-N-CA	-5.79	114.42	120.38
13	2	186	ASN	N-CA-C	-5.79	104.97	111.28
9	D	71	THR	CA-C-N	-5.79	114.42	120.38
9	D	71	THR	C-N-CA	-5.79	114.42	120.38
8	C	16	GLN	N-CA-C	5.78	117.58	111.28
13	2	210	SER	CA-C-N	-5.78	113.83	119.78
13	2	210	SER	C-N-CA	-5.78	113.83	119.78
11	H	110	THR	N-CA-C	-5.78	105.06	111.36
16	3	208	PHE	CB-CA-C	5.76	120.03	110.81
13	2	137	TRP	N-CA-C	-5.76	105.00	111.28
9	D	110	GLU	N-CA-C	-5.76	100.44	109.25
16	3	149	ASN	N-CA-C	-5.75	103.33	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	76	ASP	C-N-CD	5.75	133.25	120.60
5	F	213	TRP	CA-C-N	-5.75	113.74	120.12
5	F	213	TRP	C-N-CA	-5.75	113.74	120.12
13	2	78	ASP	N-CA-C	5.75	118.49	111.82
9	D	147	SER	N-CA-C	-5.68	101.03	109.94
14	4	98	ASN	N-CA-C	-5.66	105.11	111.28
13	2	167	ARG	N-CA-C	-5.65	105.20	111.36
10	E	96	ASP	CA-C-N	-5.64	112.79	119.84
10	E	96	ASP	C-N-CA	-5.64	112.79	119.84
13	2	64	ARG	CA-C-N	-5.62	114.17	119.85
13	2	64	ARG	C-N-CA	-5.62	114.17	119.85
11	H	54	TYR	N-CA-C	5.62	118.77	110.46
15	1	130	THR	N-CA-C	5.59	117.90	110.53
13	2	81	LEU	CA-C-N	-5.58	113.96	119.99
13	2	81	LEU	C-N-CA	-5.58	113.96	119.99
14	4	194	PHE	N-CA-C	-5.58	102.14	110.23
16	3	123	GLY	N-CA-C	-5.57	106.86	113.99
14	4	62	SER	CA-C-N	-5.55	114.53	120.03
14	4	62	SER	C-N-CA	-5.55	114.53	120.03
9	D	77	PRO	CA-N-CD	-5.55	103.73	111.50
11	H	132	PRO	CA-N-CD	-5.54	103.74	111.50
14	4	76	PHE	N-CA-C	5.54	117.70	107.73
15	1	83	HIS	N-CA-C	-5.54	105.33	111.36
11	H	131	LEU	C-N-CD	5.53	132.77	120.60
16	3	142	ILE	CA-C-N	-5.53	114.68	120.38
16	3	142	ILE	C-N-CA	-5.53	114.68	120.38
14	4	180	GLY	N-CA-C	5.53	126.28	113.18
7	L	200	ALA	N-CA-C	-5.51	105.35	111.36
9	D	72	PRO	CA-C-N	-5.50	115.07	120.52
9	D	72	PRO	C-N-CA	-5.50	115.07	120.52
15	1	105	TRP	N-CA-C	-5.50	105.28	111.28
13	2	134	THR	CA-C-N	-5.48	113.91	119.83
13	2	134	THR	C-N-CA	-5.48	113.91	119.83
11	H	123	LEU	CA-C-N	-5.46	113.14	119.47
11	H	123	LEU	C-N-CA	-5.46	113.14	119.47
13	2	175	GLY	N-CA-C	5.46	119.59	111.18
8	C	62	PHE	N-CA-CB	5.46	119.58	110.85
15	1	47	ARG	CA-C-N	-5.45	114.08	119.92
15	1	47	ARG	C-N-CA	-5.45	114.08	119.92
15	1	231	LEU	N-CA-C	5.44	122.39	110.80
14	4	77	ASP	CA-C-N	-5.44	114.07	119.56
14	4	77	ASP	C-N-CA	-5.44	114.07	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	63	ASP	CA-C-N	-5.43	114.42	120.45
7	L	63	ASP	C-N-CA	-5.43	114.42	120.45
9	D	182	ARG	N-CA-C	5.42	118.09	110.23
10	E	64	PRO	CA-C-N	-5.41	114.38	119.85
10	E	64	PRO	C-N-CA	-5.41	114.38	119.85
10	E	78	ARG	N-CA-C	5.40	118.08	111.82
16	3	70	GLY	N-CA-C	-5.38	107.79	115.64
15	1	45	GLN	CA-C-N	-5.37	114.23	119.76
15	1	45	GLN	C-N-CA	-5.37	114.23	119.76
13	2	122	ILE	CA-C-N	-5.36	114.09	119.56
13	2	122	ILE	C-N-CA	-5.36	114.09	119.56
15	1	124	ASN	CA-C-N	-5.36	114.44	119.85
15	1	124	ASN	C-N-CA	-5.36	114.44	119.85
16	3	72	LEU	CA-C-N	-5.36	114.26	119.78
16	3	72	LEU	C-N-CA	-5.36	114.26	119.78
16	3	220	LEU	N-CA-C	-5.36	105.85	112.38
16	3	206	PRO	CA-C-N	5.35	131.33	121.70
16	3	206	PRO	C-N-CA	5.35	131.33	121.70
13	2	118	ALA	N-CA-C	-5.35	105.45	111.28
16	3	268	VAL	N-CA-C	5.35	115.55	110.42
14	4	70	LEU	CA-C-N	-5.35	114.27	119.78
14	4	70	LEU	C-N-CA	-5.35	114.27	119.78
14	4	171	ILE	N-CA-C	-5.34	105.17	110.62
10	E	67	GLY	CA-C-N	-5.33	114.46	119.85
10	E	67	GLY	C-N-CA	-5.33	114.46	119.85
16	3	85	ASP	CA-C-N	-5.33	114.81	121.00
16	3	85	ASP	C-N-CA	-5.33	114.81	121.00
15	1	114	LEU	CA-C-N	-5.33	114.30	119.78
15	1	114	LEU	C-N-CA	-5.33	114.30	119.78
1	A	49	ASP	N-CA-C	-5.31	107.45	114.04
13	2	177	VAL	CB-CA-C	-5.31	104.97	112.14
12	K	86	ALA	N-CA-C	5.31	121.54	109.81
13	2	256	ASP	CA-C-N	-5.30	113.57	119.19
13	2	256	ASP	C-N-CA	-5.30	113.57	119.19
5	F	145	LEU	CA-C-N	-5.30	114.32	119.78
5	F	145	LEU	C-N-CA	-5.30	114.32	119.78
15	1	164	ALA	N-CA-C	-5.29	105.62	111.71
16	3	226	LYS	N-CA-C	-5.29	105.51	111.28
2	B	390	GLY	CA-C-N	5.28	124.46	118.97
2	B	390	GLY	C-N-CA	5.28	124.46	118.97
15	1	91	VAL	CA-C-N	-5.28	113.48	118.97
15	1	91	VAL	C-N-CA	-5.28	113.48	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	276	LYS	N-CA-C	-5.27	106.44	112.92
16	3	223	LEU	N-CA-C	-5.26	106.19	113.18
16	3	205	GLY	N-CA-C	-5.25	101.62	112.34
8	C	58	CYS	CA-C-N	-5.25	114.68	121.04
8	C	58	CYS	C-N-CA	-5.25	114.68	121.04
15	1	201	GLN	N-CA-C	-5.24	105.57	111.28
16	3	218	LYS	N-CA-C	-5.24	106.58	112.87
5	F	83	THR	CA-C-N	-5.22	114.40	119.78
5	F	83	THR	C-N-CA	-5.22	114.40	119.78
16	3	117	ILE	CB-CA-C	-5.21	105.20	110.88
14	4	147	ILE	CB-CA-C	-5.20	105.31	111.97
8	C	61	ASP	N-CA-CB	5.20	117.73	109.82
12	K	83	PHE	N-CA-C	5.19	117.76	110.23
12	K	63	GLY	N-CA-C	-5.19	106.51	112.73
7	L	172	GLN	CA-C-N	-5.17	113.38	119.84
7	L	172	GLN	C-N-CA	-5.17	113.38	119.84
16	3	266	ASN	N-CA-C	5.16	117.52	110.55
9	D	173	VAL	N-CA-C	5.15	116.03	110.21
14	4	97	VAL	N-CA-C	5.14	115.86	110.62
6	G	92	LEU	CA-C-N	-5.13	114.67	119.85
6	G	92	LEU	C-N-CA	-5.13	114.67	119.85
7	L	165	THR	N-CA-C	-5.13	103.92	110.53
7	L	58	GLN	O-C-N	5.12	124.99	121.71
16	3	202	TYR	CA-C-N	-5.12	114.44	120.12
16	3	202	TYR	C-N-CA	-5.12	114.44	120.12
15	1	50	TYR	N-CA-C	5.11	116.85	111.28
14	4	218	PHE	CB-CA-C	-5.11	102.86	110.88
9	D	105	TRP	N-CA-C	5.10	116.05	108.60
5	F	108	ILE	N-CA-C	5.09	115.81	110.62
14	4	228	GLY	CA-C-N	-5.08	113.68	118.97
14	4	228	GLY	C-N-CA	-5.08	113.68	118.97
13	2	195	TYR	N-CA-C	-5.07	100.46	108.82
7	L	153	PHE	N-CA-C	5.03	117.72	110.28
6	G	148	PRO	CA-N-CD	-5.02	104.97	112.00
7	L	163	SER	N-CA-C	5.00	117.63	111.82

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	2	164	GLU	Mainchain
16	3	205	GLY	Mainchain

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Mol	Chain	Res	Type	Group
14	4	153	GLU	Mainchain
6	G	101	PHE	Peptide
7	L	98	ARG	Sidechain

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	5852	0	5710	167	0
2	B	5856	0	5666	146	0
3	I	224	0	247	37	0
4	J	321	0	328	47	0
5	F	1187	0	1226	42	3
6	G	689	0	676	114	0
7	L	1197	0	1187	168	3
8	C	612	0	594	38	0
9	D	1116	0	1126	109	0
10	E	530	0	530	44	0
11	H	642	0	637	49	0
12	K	379	0	386	92	0
13	2	1613	0	1554	378	0
14	4	1544	0	1489	236	0
15	1	1513	0	1495	384	0
16	3	1619	0	1554	490	0
17	A	65	0	72	5	0
18	1	615	0	511	221	0
18	2	628	0	538	251	0
18	3	698	0	559	252	0
18	4	677	0	635	187	0
18	A	2583	0	2555	177	0
18	B	2519	0	2617	199	0
18	F	95	0	72	16	0
18	G	161	0	141	87	0
18	H	46	0	33	5	0
18	J	50	0	39	7	0
18	K	46	0	33	12	0
18	L	160	0	137	37	0
19	A	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	16	0	0	0	0
20	A	33	0	46	3	0
20	B	33	0	46	5	0
21	1	49	0	74	15	0
21	2	24	0	18	6	0
21	A	89	0	127	12	0
21	B	21	0	12	1	0
22	3	40	0	48	20	0
22	A	240	0	292	23	0
22	B	200	0	245	25	0
22	F	80	0	98	17	0
22	G	40	0	49	28	0
22	I	40	0	49	3	0
22	J	80	0	98	15	0
22	K	40	0	49	17	0
22	L	80	0	98	27	0
23	2	35	0	40	9	0
23	4	35	0	40	6	0
23	B	38	0	46	3	0
23	F	60	0	60	13	0
23	G	41	0	52	20	0
23	J	55	0	86	10	0
24	B	1	0	0	0	0
25	B	61	0	83	4	0
26	B	70	0	92	4	0
27	1	84	0	110	49	0
27	2	84	0	110	53	0
27	3	84	0	110	62	0
27	4	126	0	165	81	0
27	I	42	0	55	12	0
28	1	103	0	78	36	0
28	2	141	0	95	37	0
28	3	56	0	47	22	0
28	4	145	0	99	43	0
29	4	42	0	56	12	0
All	All	35653	0	35120	3545	3

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 50.

All (3545) 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)
16:3:138:GLN:HB2	16:3:145:ALA:HB2	1.25	1.18
16:3:268:VAL:HG21	18:3:3003:CLA:H43	1.17	1.16
16:3:111:LEU:HD22	18:3:3006:CLA:CBB	1.74	1.15
16:3:127:LEU:HB2	18:3:3018:CLA:HBC1	1.29	1.15
7:L:85:ASN:HB3	18:L:1501:CLA:HAC1	1.26	1.14
18:4:4009:CLA:HHC	18:4:4009:CLA:HBB1	1.28	1.14
27:4:4502:LUT:H381	27:4:4502:LUT:H28	1.27	1.13
13:2:122:ILE:HG23	13:2:133:LEU:HB2	1.31	1.12
12:K:69:ILE:HA	18:K:1001:CLA:O1A	1.50	1.12
13:2:139:THR:H	28:2:2010:CHL:CED	1.61	1.12
18:2:2001:CLA:H42	18:2:2002:CLA:HBA1	1.30	1.12
22:K:2011:BCR:H321	22:K:2011:BCR:HC8	1.31	1.12
18:4:4007:CLA:HHC	18:4:4007:CLA:HBB1	1.30	1.12
14:4:118:ILE:HD13	14:4:120:ILE:HD11	1.33	1.11
7:L:113:PRO:HG3	18:L:1503:CLA:HBB1	1.21	1.11
13:2:126:LEU:HB3	13:2:133:LEU:HD13	1.32	1.11
14:4:103:MET:HE1	14:4:207:ASN:HB3	1.13	1.11
18:2:2004:CLA:H52	27:2:2502:LUT:H383	1.32	1.10
16:3:162:MET:HA	16:3:162:MET:HE2	1.31	1.10
13:2:131:ILE:HD12	13:2:133:LEU:HD21	1.15	1.10
18:4:4001:CLA:H12	27:4:4501:LUT:H373	1.24	1.10
16:3:206:PRO:HD2	16:3:207:PHE:HB2	1.17	1.10
14:4:170:PRO:HB2	18:4:4016:CLA:HMA3	1.34	1.09
18:3:3004:CLA:HMB3	18:3:3004:CLA:HBB1	1.34	1.09
7:L:58:GLN:HG3	7:L:59:PRO:HD2	1.35	1.09
18:1:1003:CLA:H92	18:1:1003:CLA:HBB1	1.11	1.09
4:J:2:ARG:HE	4:J:4:LEU:HD12	1.17	1.08
7:L:145:LEU:HD11	22:L:6019:BCR:H392	1.34	1.08
18:2:2016:CLA:HBB1	18:2:2016:CLA:HHC	1.33	1.08
27:4:4503:LUT:H181	27:4:4503:LUT:H8	1.31	1.08
18:G:1001:CLA:H62	22:G:2011:BCR:H343	1.28	1.08
18:G:1001:CLA:HHC	18:G:1001:CLA:HBB1	1.31	1.07
15:1:114:LEU:HD23	15:1:115:PRO:HD2	1.25	1.07
13:2:223:LYS:NZ	21:2:2801:LHG:O5	1.88	1.07
18:2:2009:CLA:HHC	18:2:2009:CLA:HBB1	1.27	1.07
16:3:94:GLU:OE2	16:3:96:ARG:N	1.86	1.07
11:H:96:ARG:HG2	11:H:97:GLY:H	1.19	1.06
13:2:87:PHE:CZ	27:2:2502:LUT:H372	1.89	1.06
13:2:70:GLY:O	16:3:178:LYS:NZ	1.88	1.06
13:2:166:ARG:NH1	18:4:4009:CLA:OBD	1.88	1.06
15:1:149:ARG:NH2	18:1:1012:CLA:O1D	1.87	1.06
6:G:92:LEU:H	6:G:92:LEU:HD12	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2006:CLA:HBD	18:2:2006:CLA:H43	1.35	1.05
28:1:1010:CHL:HBC3	28:1:1010:CHL:HMC	1.38	1.05
16:3:111:LEU:CD2	18:3:3006:CLA:HBB2	1.84	1.05
16:3:111:LEU:CD2	18:3:3006:CLA:CBB	2.34	1.05
12:K:78:LEU:HD22	12:K:82:ARG:HG2	1.06	1.05
12:K:137:VAL:HA	12:K:140:LEU:HD22	1.35	1.05
18:F:1302:CLA:HBC2	18:F:1302:CLA:HHD	1.35	1.04
7:L:94:ASN:HB2	7:L:97:LEU:HD12	1.34	1.04
13:2:114:MET:HE3	18:2:2001:CLA:HMC2	1.37	1.03
18:2:2008:CLA:HHD	18:2:2008:CLA:HBC3	1.38	1.03
7:L:176:LEU:HD12	7:L:177:GLN:H	1.23	1.03
13:2:188:LEU:HD23	13:2:198:GLY:HA3	1.39	1.03
18:2:2001:CLA:C4	18:2:2002:CLA:HBA1	1.89	1.03
18:4:4007:CLA:HHD	18:4:4007:CLA:HBC2	1.37	1.03
15:1:97:PRO:HB2	15:1:102:LEU:HB2	1.35	1.03
18:3:3003:CLA:H42	18:3:3003:CLA:C1D	1.88	1.03
13:2:186:ASN:ND2	18:2:2016:CLA:O1D	1.90	1.03
16:3:164:LEU:HB3	22:3:3503:BCR:H351	1.41	1.02
12:K:72:ALA:HB3	18:K:1001:CLA:O2A	1.60	1.02
18:4:4002:CLA:H12	18:4:4002:CLA:HMA2	1.38	1.02
14:4:150:HIS:HA	18:4:4012:CLA:HAB	1.40	1.02
14:4:103:MET:HE1	14:4:207:ASN:CB	1.90	1.02
18:3:3002:CLA:HHC	18:3:3002:CLA:HBB1	1.42	1.02
18:3:3012:CLA:HBB1	18:3:3012:CLA:HMB3	1.38	1.02
15:1:85:ARG:HB3	18:1:1001:CLA:HBC3	1.04	1.01
15:1:114:LEU:CD2	15:1:115:PRO:HD2	1.90	1.01
18:3:3008:CLA:HBB1	18:3:3008:CLA:HHC	1.42	1.01
27:3:3501:LUT:H161	27:3:3501:LUT:H8	1.35	1.01
14:4:169:ASP:HB3	18:4:4016:CLA:C3D	1.90	1.01
13:2:188:LEU:HD23	13:2:198:GLY:CA	1.89	1.01
21:1:1801:LHG:H223	21:1:1801:LHG:C38	1.90	1.00
10:E:66:ILE:HG22	10:E:95:GLN:HE22	1.25	1.00
14:4:63:PRO:HD2	14:4:66:LEU:HD12	1.40	1.00
7:L:94:ASN:CB	7:L:97:LEU:HD12	1.91	1.00
8:C:8:TYR:HB3	9:D:191:SER:CB	1.90	1.00
13:2:200:TRP:NE1	18:2:2016:CLA:HAA2	1.76	1.00
13:2:244:THR:HG22	13:2:245:GLY:H	1.25	1.00
13:2:122:ILE:CG2	13:2:133:LEU:HB2	1.90	1.00
18:G:1003:CLA:H51	23:G:2021:LMG:H311	1.42	1.00
15:1:209:GLY:HA3	15:1:212:GLU:HB3	1.44	1.00
16:3:65:LEU:HD13	16:3:67:TYR:CE1	1.96	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3008:CLA:HBC2	18:3:3008:CLA:HHD	1.41	0.99
12:K:78:LEU:HD22	12:K:82:ARG:CG	1.91	0.99
18:2:2001:CLA:H11	27:2:2501:LUT:H173	1.44	0.99
28:4:4010:CHL:HHD	28:4:4010:CHL:HBC2	1.42	0.99
15:1:183:LYS:HG3	18:1:1007:CLA:HED2	1.41	0.99
15:1:183:LYS:HD3	18:1:1002:CLA:HAA2	1.40	0.99
16:3:205:GLY:HA3	16:3:208:PHE:CA	1.89	0.99
16:3:241:TYR:CE1	27:3:3501:LUT:H162	1.97	0.99
18:2:2016:CLA:HBD	18:2:2016:CLA:HBA2	1.43	0.99
18:3:3005:CLA:H93	18:3:3012:CLA:H43	1.44	0.99
15:1:85:ARG:CB	18:1:1001:CLA:HBC3	1.93	0.99
15:1:183:LYS:HD3	18:1:1002:CLA:CAA	1.92	0.99
6:G:108:ALA:HB1	6:G:111:TYR:CD1	1.98	0.98
13:2:262:ILE:HD11	18:2:2003:CLA:H11	1.45	0.98
16:3:268:VAL:HG23	18:3:3003:CLA:H12	1.41	0.98
10:E:122:LEU:H	10:E:122:LEU:HD12	1.25	0.98
13:2:139:THR:H	28:2:2010:CHL:HED1	1.29	0.97
13:2:219:THR:HG22	18:2:2007:CLA:HED3	1.43	0.97
12:K:124:ALA:HB1	22:K:2011:BCR:HC7	1.46	0.97
15:1:97:PRO:CB	15:1:102:LEU:HB2	1.93	0.97
22:G:2011:BCR:H403	22:G:2011:BCR:H23C	1.43	0.97
15:1:221:PRO:HG2	15:1:222:TRP:CE3	1.98	0.97
16:3:138:GLN:CB	16:3:145:ALA:HB2	1.94	0.97
18:4:4003:CLA:HHC	18:4:4003:CLA:HBB1	1.46	0.97
15:1:88:MET:HB2	18:1:1001:CLA:HMC2	1.44	0.97
7:L:87:PRO:CD	18:L:1502:CLA:HED2	1.94	0.97
7:L:145:LEU:HD21	22:L:6019:BCR:H403	1.44	0.97
13:2:220:LYS:HD3	18:2:2002:CLA:HED2	1.44	0.97
15:1:88:MET:HE3	18:1:1001:CLA:HHC	1.43	0.96
13:2:114:MET:HE3	18:2:2001:CLA:CMC	1.93	0.96
18:1:1008:CLA:HHC	18:1:1008:CLA:HBB1	1.47	0.96
16:3:205:GLY:HA3	16:3:208:PHE:CB	1.95	0.96
29:4:4505:ZEX:H362	29:4:4505:ZEX:H382	1.46	0.96
14:4:153:GLU:OE2	14:4:156:ARG:NH1	1.98	0.96
15:1:98:GLU:CB	15:1:211:LEU:HD21	1.94	0.96
18:3:3010:CLA:HMB3	18:3:3013:CLA:HAB	1.43	0.96
7:L:138:VAL:O	7:L:142:SER:OG	1.84	0.96
2:B:50:HIS:HB3	18:B:1210:CLA:HED3	1.48	0.95
13:2:126:LEU:HB3	13:2:133:LEU:CD1	1.96	0.95
18:2:2006:CLA:H43	18:2:2006:CLA:CBD	1.96	0.95
16:3:111:LEU:HD22	18:3:3006:CLA:HBB2	0.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4:LEU:HD11	3:I:6:SER:HB2	1.48	0.95
13:2:186:ASN:HB3	18:2:2016:CLA:HMA2	1.48	0.95
9:D:192:ILE:HG22	9:D:193:GLY:H	1.29	0.95
18:4:4008:CLA:C1	18:4:4008:CLA:HAA1	1.96	0.95
16:3:205:GLY:HA3	16:3:208:PHE:HB2	1.47	0.95
13:2:116:GLY:HA2	27:2:2502:LUT:H181	1.48	0.95
13:2:126:LEU:HD12	13:2:127:THR:N	1.82	0.94
13:2:87:PHE:CE2	27:2:2502:LUT:H363	2.03	0.94
13:2:188:LEU:HD22	13:2:189:THR:N	1.82	0.94
18:4:4001:CLA:C1	27:4:4501:LUT:H373	1.97	0.94
18:1:1005:CLA:HBB1	18:1:1005:CLA:HMB3	1.50	0.94
18:4:4007:CLA:H2A	18:4:4007:CLA:CED	1.98	0.93
15:1:230:VAL:C	15:1:231:LEU:HD23	1.93	0.93
13:2:106:GLU:O	13:2:110:SER:OG	1.85	0.93
5:F:221:LEU:C	5:F:222:LEU:HD23	1.94	0.93
18:3:3010:CLA:CMB	18:3:3013:CLA:HAB	1.97	0.93
12:K:137:VAL:HA	12:K:140:LEU:CD2	1.97	0.93
13:2:220:LYS:N	18:2:2007:CLA:HED1	1.83	0.93
15:1:232:ILE:HG23	15:1:233:PRO:HD2	1.46	0.93
13:2:193:VAL:HG23	13:2:194:GLY:H	1.30	0.93
14:4:170:PRO:HB2	18:4:4016:CLA:CMA	1.99	0.93
15:1:202:GLN:NE2	15:1:208:THR:HB	1.84	0.93
13:2:115:LEU:HB3	18:2:2006:CLA:HBB2	1.51	0.93
28:4:4011:CHL:HBC2	28:4:4011:CHL:HHD	1.48	0.93
16:3:136:TRP:O	27:3:3502:LUT:O3	1.85	0.92
6:G:77:PHE:HE1	18:G:1002:CLA:HAB	1.33	0.92
12:K:70:MET:HE2	12:K:71:VAL:N	1.84	0.92
16:3:209:ASN:OD1	27:3:3501:LUT:O23	1.85	0.92
14:4:118:ILE:HD13	14:4:120:ILE:CD1	2.00	0.92
4:J:28:GLU:OE1	18:J:1302:CLA:C4D	2.17	0.92
16:3:241:TYR:HE1	27:3:3501:LUT:H162	1.28	0.92
15:1:121:TYR:CD2	15:1:122:LEU:HG	2.04	0.92
16:3:182:MET:HE2	16:3:182:MET:HA	1.51	0.92
12:K:71:VAL:HG11	12:K:129:GLY:O	1.70	0.91
18:2:2003:CLA:HHB	18:2:2008:CLA:HBC3	1.53	0.91
18:1:1011:CLA:C3	27:1:1501:LUT:H23	2.00	0.91
27:4:4501:LUT:H371	27:4:4501:LUT:H28	1.53	0.91
16:3:206:PRO:HD2	16:3:207:PHE:CB	2.00	0.91
18:3:3010:CLA:HHC	18:3:3010:CLA:HBB1	1.51	0.91
18:2:2007:CLA:H51	18:2:2007:CLA:H92	1.53	0.91
9:D:76:ASP:HB3	9:D:77:PRO:HB3	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:131:ILE:CD1	13:2:133:LEU:HD21	2.00	0.91
18:1:1004:CLA:CBB	27:1:1502:LUT:H12	2.01	0.91
18:1:1003:CLA:H92	18:1:1003:CLA:CBB	2.00	0.90
15:1:126:VAL:HG23	15:1:127:PRO:HA	1.53	0.90
16:3:184:LYS:HG2	16:3:185:GLN:HG2	1.54	0.90
18:2:2005:CLA:HBC1	18:2:2012:CLA:HBC1	1.52	0.90
15:1:152:GLU:C	15:1:153:LYS:HD3	1.96	0.90
18:1:1008:CLA:C3D	18:1:1008:CLA:HED2	2.00	0.90
22:J:6012:BCR:H23C	22:J:6012:BCR:H383	1.51	0.90
13:2:163:ALA:O	13:2:166:ARG:HB3	1.72	0.90
13:2:211:PRO:O	13:2:212:GLN:HG3	1.70	0.90
14:4:125:LYS:NZ	14:4:231:ASP:OD1	2.03	0.90
15:1:127:PRO:HG2	15:1:128:TRP:CD1	2.07	0.90
18:1:1003:CLA:CGA	18:1:1008:CLA:HED1	2.00	0.90
16:3:102:GLU:OE2	16:3:232:ARG:NH2	2.04	0.90
18:2:2004:CLA:H8	27:2:2502:LUT:C38	2.00	0.90
18:1:1001:CLA:HHC	27:1:1501:LUT:H32	1.54	0.90
18:2:2004:CLA:H8	27:2:2502:LUT:H381	1.53	0.90
13:2:115:LEU:CB	18:2:2006:CLA:HBB2	2.02	0.89
27:4:4503:LUT:H363	28:1:1009:CHL:H8	1.53	0.89
16:3:225:LEU:HB3	16:3:226:LYS:NZ	1.87	0.89
18:4:4017:CLA:HED1	21:1:1801:LHG:H151	1.54	0.89
15:1:146:GLU:HG2	15:1:149:ARG:HH11	1.35	0.89
28:4:4013:CHL:HBC2	28:4:4013:CHL:HHD	1.54	0.89
16:3:248:THR:HG22	16:3:250:VAL:HG23	1.54	0.89
14:4:158:GLN:HE22	14:4:161:LYS:HE3	1.36	0.89
6:G:103:ALA:O	6:G:105:ASP:N	2.04	0.89
11:H:96:ARG:O	11:H:98:LEU:N	2.05	0.89
13:2:70:GLY:HA3	16:3:174:GLN:HE21	1.36	0.89
16:3:268:VAL:CG2	18:3:3003:CLA:H43	2.03	0.89
18:3:3012:CLA:HBB1	18:3:3012:CLA:CMB	2.03	0.89
13:2:120:ILE:HG21	27:2:2501:LUT:C37	2.03	0.89
15:1:120:THR:HG22	15:1:124:ASN:C	1.98	0.89
18:3:3004:CLA:C2	27:3:3502:LUT:H363	2.02	0.89
18:G:1001:CLA:C6	22:G:2011:BCR:H343	2.03	0.88
18:2:2004:CLA:H52	27:2:2502:LUT:C38	2.03	0.88
14:4:220:ILE:HD12	18:4:4003:CLA:HAC2	1.52	0.88
3:I:13:GLY:O	3:I:14:LEU:HD23	1.73	0.88
12:K:124:ALA:HB1	22:K:2011:BCR:H331	1.54	0.88
12:K:141:LYS:O	12:K:142:THR:OG1	1.91	0.88
12:K:128:VAL:O	12:K:132:ILE:HG13	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:220:LYS:CD	18:2:2002:CLA:HED2	2.02	0.88
14:4:94:ALA:CA	18:4:4012:CLA:HED2	2.03	0.88
15:1:183:LYS:CG	18:1:1007:CLA:HED2	2.03	0.88
18:1:1008:CLA:HED2	18:1:1008:CLA:C4D	2.03	0.88
13:2:139:THR:N	28:2:2010:CHL:CED	2.37	0.88
15:1:232:ILE:HG23	15:1:233:PRO:CD	2.02	0.88
16:3:110:MET:CE	16:3:230:ASN:HB3	2.02	0.88
15:1:88:MET:HE3	18:1:1001:CLA:CHC	2.02	0.88
15:1:183:LYS:HD3	18:1:1002:CLA:CBA	2.04	0.88
27:3:3502:LUT:H161	27:3:3502:LUT:H8	1.55	0.88
18:2:2003:CLA:C2B	27:2:2501:LUT:H383	2.03	0.88
16:3:127:LEU:HB2	18:3:3018:CLA:CBC	2.02	0.88
18:3:3003:CLA:H42	18:3:3003:CLA:C2D	2.04	0.88
7:L:121:ARG:CG	7:L:127:GLY:HA2	2.04	0.88
12:K:70:MET:HE2	12:K:71:VAL:CA	2.04	0.88
15:1:130:THR:HG22	15:1:132:PRO:CD	2.03	0.87
18:3:3003:CLA:HMB1	27:3:3501:LUT:H173	1.56	0.87
13:2:219:THR:HG22	18:2:2007:CLA:CED	2.03	0.87
16:3:65:LEU:CB	16:3:68:LEU:HD21	2.03	0.87
10:E:66:ILE:HG22	10:E:95:GLN:NE2	1.88	0.87
18:2:2001:CLA:C1	27:2:2501:LUT:H173	2.04	0.87
15:1:186:LYS:NZ	21:1:1801:LHG:O5	2.06	0.87
18:3:3003:CLA:H11	18:3:3003:CLA:C4D	2.03	0.87
4:J:2:ARG:HE	4:J:4:LEU:CD1	1.88	0.87
9:D:134:ARG:NH2	9:D:136:GLU:OE2	2.05	0.87
18:2:2005:CLA:H72	18:2:2005:CLA:H41	1.56	0.87
28:2:2013:CHL:HHC	28:2:2013:CHL:HBB1	1.57	0.87
3:I:14:LEU:C	3:I:17:PRO:HD2	2.00	0.87
18:L:1502:CLA:C4C	22:L:6019:BCR:H282	2.04	0.87
13:2:124:GLU:O	13:2:127:THR:HG22	1.75	0.87
15:1:111:TRP:CZ3	18:1:1006:CLA:HED1	2.10	0.87
15:1:183:LYS:HG3	18:1:1007:CLA:CED	2.04	0.87
13:2:70:GLY:HA3	16:3:174:GLN:NE2	1.90	0.86
14:4:115:PHE:O	14:4:118:ILE:HG22	1.73	0.86
5:F:138:LEU:HD23	5:F:159:GLU:OE2	1.74	0.86
18:2:2005:CLA:H41	18:2:2005:CLA:C7	2.03	0.86
14:4:94:ALA:HA	18:4:4012:CLA:HED2	1.57	0.86
15:1:152:GLU:O	15:1:153:LYS:HD3	1.75	0.86
15:1:226:ILE:HG21	18:1:1003:CLA:H42	1.56	0.86
13:2:120:ILE:O	13:2:123:PRO:HD2	1.74	0.86
28:4:4011:CHL:HAA1	28:4:4011:CHL:HBD	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1001:CLA:H61	27:1:1501:LUT:C30	2.06	0.86
28:3:3011:CHL:HBD	28:3:3011:CHL:HBA2	1.58	0.86
18:3:3018:CLA:HMB1	18:3:3018:CLA:HBB1	1.57	0.86
12:K:65:SER:O	12:K:69:ILE:HG22	1.74	0.86
16:3:140:GLY:HA2	18:3:3013:CLA:HBC2	1.57	0.86
1:A:220:GLY:HA3	18:A:1113:CLA:HBB1	1.55	0.86
18:A:1104:CLA:HED1	18:A:1128:CLA:H2	1.58	0.86
15:1:132:PRO:O	15:1:136:VAL:HG23	1.75	0.86
16:3:206:PRO:HA	16:3:209:ASN:C	2.01	0.86
15:1:230:VAL:HG13	18:1:1014:CLA:C1B	2.05	0.85
16:3:220:LEU:HD23	16:3:221:LYS:N	1.91	0.85
2:B:733:PHE:HB3	11:H:134:LYS:HE2	1.58	0.85
27:2:2501:LUT:H28	27:2:2501:LUT:H371	1.55	0.85
7:L:146:THR:O	7:L:150:ILE:HG13	1.76	0.85
9:D:76:ASP:HB3	9:D:77:PRO:CB	2.07	0.85
18:3:3017:CLA:CGA	18:3:3017:CLA:H3A	2.03	0.85
6:G:65:SER:OG	18:G:1001:CLA:HBA1	1.75	0.85
28:2:2010:CHL:CBB	28:2:2013:CHL:HBB2	2.05	0.85
3:I:6:SER:C	3:I:7:LEU:HD22	2.02	0.85
18:G:1003:CLA:H13	18:G:1003:CLA:C9	2.06	0.85
13:2:148:ASP:O	13:2:149:THR:HB	1.74	0.85
18:3:3003:CLA:CMB	27:3:3501:LUT:H173	2.05	0.85
16:3:226:LYS:H	16:3:226:LYS:HZ2	1.20	0.85
7:L:85:ASN:HB3	18:L:1501:CLA:CAC	2.06	0.85
13:2:143:GLN:HB2	13:2:145:TYR:CE1	2.11	0.85
18:G:1003:CLA:H13	18:G:1003:CLA:H8	1.56	0.85
13:2:219:THR:C	18:2:2007:CLA:HED1	2.01	0.85
15:1:111:TRP:CH2	18:1:1006:CLA:HED1	2.12	0.85
16:3:248:THR:HG21	16:3:255:ASN:ND2	1.92	0.85
14:4:233:LEU:O	14:4:237:ILE:HG13	1.77	0.84
16:3:135:ALA:N	16:3:138:GLN:HG2	1.91	0.84
16:3:256:LEU:O	16:3:260:VAL:HG23	1.77	0.84
12:K:86:ALA:HB1	12:K:87:PRO:HD3	1.55	0.84
13:2:127:THR:HG21	13:2:247:ILE:CD1	2.07	0.84
3:I:6:SER:O	3:I:7:LEU:HD22	1.77	0.84
12:K:137:VAL:CA	12:K:140:LEU:HD22	2.07	0.84
14:4:152:VAL:C	14:4:155:ARG:HB3	2.03	0.84
14:4:177:LEU:HD13	18:4:4016:CLA:HMD3	1.59	0.84
14:4:217:GLY:O	14:4:221:GLN:HB2	1.77	0.84
16:3:267:ASN:O	16:3:270:THR:OG1	1.93	0.84
15:1:85:ARG:HB3	18:1:1001:CLA:CBC	1.99	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:71:VAL:CG1	12:K:129:GLY:O	2.25	0.84
6:G:149:LYS:HB2	6:G:149:LYS:NZ	1.91	0.84
13:2:116:GLY:HA2	27:2:2502:LUT:C18	2.07	0.84
18:4:4001:CLA:H52	27:4:4501:LUT:H371	1.58	0.84
27:1:1501:LUT:C8	27:1:1501:LUT:H181	2.05	0.84
15:1:148:GLN:O	15:1:151:MET:HG2	1.78	0.84
7:L:121:ARG:HG3	7:L:127:GLY:HA2	1.58	0.84
16:3:146:GLY:O	16:3:147:THR:OG1	1.94	0.84
7:L:120:LEU:HB3	7:L:126:ALA:CB	2.08	0.84
18:4:4006:CLA:C1B	27:4:4503:LUT:H172	2.07	0.84
15:1:126:VAL:CG2	15:1:127:PRO:HA	2.07	0.84
18:G:1003:CLA:H13	18:G:1003:CLA:C8	2.08	0.83
8:C:8:TYR:HD2	9:D:191:SER:HA	1.40	0.83
13:2:200:TRP:HE1	18:2:2016:CLA:HAA2	1.41	0.83
28:4:4013:CHL:CHB	27:4:4503:LUT:H192	2.08	0.83
16:3:164:LEU:HB3	22:3:3503:BCR:C35	2.09	0.83
18:2:2012:CLA:HMB1	18:2:2012:CLA:HBB1	1.59	0.83
9:D:192:ILE:HG23	10:E:80:GLU:OE2	1.77	0.83
18:3:3004:CLA:HBB1	18:3:3004:CLA:CMB	2.08	0.83
12:K:64:SER:O	12:K:68:VAL:HG23	1.79	0.83
18:4:4002:CLA:HHC	18:4:4002:CLA:HBB1	1.60	0.83
22:A:6003:BCR:H23C	18:A:1103:CLA:H61	1.61	0.83
16:3:269:LEU:HD11	18:3:3008:CLA:HED1	1.58	0.83
6:G:116:LYS:HG3	18:G:1002:CLA:ND	1.93	0.83
18:2:2002:CLA:C1	18:2:2002:CLA:HED1	2.09	0.83
18:2:2016:CLA:HBC2	18:2:2016:CLA:HHD	1.59	0.83
18:4:4005:CLA:OBD	18:4:4012:CLA:HBA2	1.78	0.83
15:1:230:VAL:O	15:1:231:LEU:HD23	1.78	0.83
13:2:186:ASN:HD21	18:2:2016:CLA:CGD	1.91	0.82
13:2:220:LYS:CE	18:2:2002:CLA:HED2	2.09	0.82
15:1:88:MET:HB2	18:1:1001:CLA:CMC	2.09	0.82
16:3:190:LEU:HB2	16:3:207:PHE:CZ	2.14	0.82
7:L:85:ASN:CB	18:L:1501:CLA:HAC1	2.07	0.82
13:2:233:MET:HA	13:2:233:MET:CE	2.08	0.82
18:2:2012:CLA:HBB1	18:2:2012:CLA:CMB	2.08	0.82
18:2:2016:CLA:HBD	18:2:2016:CLA:CBA	2.09	0.82
18:2:2009:CLA:HED3	16:3:171:ARG:CG	2.10	0.82
18:4:4007:CLA:HBB1	18:4:4007:CLA:CHC	2.09	0.82
15:1:164:ALA:O	15:1:167:PRO:HD3	1.80	0.82
13:2:151:THR:O	13:2:154:ILE:HG22	1.78	0.82
13:2:239:HIS:O	13:2:243:GLY:N	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:226:LYS:CE	18:3:3007:CLA:HED2	2.09	0.82
13:2:87:PHE:CE2	27:2:2502:LUT:H372	2.15	0.82
7:L:87:PRO:HD2	18:L:1502:CLA:HED2	1.61	0.82
28:4:4010:CHL:CBB	28:4:4013:CHL:HBB2	2.10	0.82
16:3:120:GLU:CD	16:3:253:TYR:HB3	2.04	0.82
18:3:3001:CLA:CGA	27:3:3501:LUT:H382	2.09	0.82
18:3:3001:CLA:HBA1	27:3:3501:LUT:H382	1.62	0.82
18:3:3006:CLA:HED2	18:3:3006:CLA:C1A	2.09	0.82
6:G:65:SER:CB	18:G:1001:CLA:HBA1	2.09	0.82
13:2:131:ILE:HG22	13:2:132:LEU:H	1.45	0.82
18:4:4002:CLA:H12	18:4:4002:CLA:CMA	2.09	0.82
6:G:139:LEU:O	6:G:142:SER:OG	1.98	0.82
18:2:2002:CLA:HMC3	18:2:2002:CLA:HBC2	1.62	0.82
16:3:222:GLU:C	16:3:226:LYS:HZ3	1.87	0.82
4:J:36:ALA:HB1	23:J:5001:LMG:H111	1.60	0.82
27:3:3502:LUT:H28	27:3:3502:LUT:H361	1.61	0.82
27:4:4503:LUT:H363	28:1:1009:CHL:C9	2.10	0.81
18:3:3004:CLA:O1A	18:3:3004:CLA:H3A	1.80	0.81
18:G:1001:CLA:H41	22:G:2011:BCR:H342	1.60	0.81
13:2:87:PHE:HE2	27:2:2502:LUT:H363	1.43	0.81
7:L:199:TRP:O	7:L:203:LEU:HD13	1.80	0.81
18:L:1501:CLA:HBA1	18:L:1501:CLA:CHA	2.08	0.81
13:2:139:THR:HG23	13:2:142:GLU:OE2	1.80	0.81
14:4:152:VAL:O	14:4:155:ARG:HB3	1.79	0.81
15:1:106:VAL:CG2	15:1:208:THR:HG21	2.11	0.81
15:1:226:ILE:HA	18:1:1003:CLA:OBD	1.80	0.81
16:3:248:THR:HG21	16:3:255:ASN:HD22	1.42	0.81
13:2:139:THR:H	28:2:2010:CHL:HED3	1.44	0.81
7:L:87:PRO:O	7:L:98:ARG:HD2	1.80	0.81
13:2:188:LEU:O	13:2:188:LEU:HD13	1.80	0.81
2:B:166:SER:HB3	6:G:102:GLU:HB2	1.63	0.81
6:G:61:SER:HB2	18:G:1001:CLA:OBD	1.81	0.81
18:G:1001:CLA:CAB	22:G:2011:BCR:H363	2.11	0.81
18:K:1001:CLA:HHC	18:K:1001:CLA:HBB1	1.62	0.81
13:2:131:ILE:HB	13:2:133:LEU:CD1	2.10	0.81
15:1:85:ARG:HH21	18:1:1001:CLA:C4D	1.93	0.81
15:1:111:TRP:CD1	15:1:119:ALA:HB2	2.16	0.81
4:J:6:THR:HG21	23:F:5001:LMG:HC72	1.62	0.81
18:2:2001:CLA:HMB3	18:2:2001:CLA:HBB1	1.63	0.81
18:2:2009:CLA:HBB1	18:2:2009:CLA:CHC	2.09	0.81
16:3:258:ASP:CB	16:3:266:ASN:HD21	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:176:LEU:O	7:L:178:THR:HG22	1.80	0.80
9:D:204:THR:HG22	9:D:206:LYS:HG2	1.62	0.80
15:1:88:MET:HE1	18:1:1001:CLA:HAB	1.62	0.80
15:1:202:GLN:NE2	15:1:202:GLN:O	2.12	0.80
13:2:66:LEU:H	16:3:186:TYR:HE2	1.25	0.80
15:1:106:VAL:HG21	15:1:208:THR:HG21	1.60	0.80
12:K:63:GLY:O	12:K:66:THR:HG22	1.82	0.80
13:2:68:PHE:HB3	13:2:71:SER:OG	1.81	0.80
13:2:123:PRO:HA	13:2:126:LEU:HD21	1.62	0.80
16:3:142:ILE:HD11	18:3:3010:CLA:HBC3	1.60	0.80
6:G:137:TYR:O	6:G:141:THR:HG23	1.81	0.80
18:2:2008:CLA:HBC3	18:2:2008:CLA:CHD	2.11	0.80
16:3:269:LEU:HD11	18:3:3008:CLA:CED	2.11	0.80
27:3:3502:LUT:C28	27:3:3502:LUT:H371	2.11	0.80
18:4:4008:CLA:HBC2	18:4:4008:CLA:HHD	1.63	0.80
18:3:3006:CLA:HHC	18:3:3006:CLA:HBB1	1.63	0.80
15:1:130:THR:HG22	15:1:132:PRO:HD2	1.63	0.80
18:3:3003:CLA:C3B	27:3:3501:LUT:H172	2.12	0.80
4:J:10:VAL:HG11	23:F:5001:LMG:O2	1.82	0.80
9:D:76:ASP:HB3	9:D:77:PRO:CA	2.12	0.80
13:2:137:TRP:HH2	13:2:236:TRP:HA	1.46	0.80
16:3:110:MET:HE1	16:3:230:ASN:HB3	1.63	0.80
23:J:5001:LMG:O3	5:F:128:ARG:NH2	2.15	0.80
15:1:126:VAL:CB	15:1:127:PRO:HA	2.12	0.80
18:1:1004:CLA:O1A	18:1:1004:CLA:H3A	1.80	0.80
16:3:107:ARG:HB2	28:3:3011:CHL:HED1	1.63	0.80
13:2:68:PHE:HD2	13:2:71:SER:HB3	1.47	0.79
16:3:206:PRO:CD	16:3:207:PHE:HB2	2.07	0.79
5:F:132:ASN:O	5:F:136:GLN:HG2	1.81	0.79
6:G:76:ARG:HE	6:G:116:LYS:HE2	1.46	0.79
6:G:144:ASN:ND2	18:G:1003:CLA:HED2	1.96	0.79
13:2:127:THR:HG21	13:2:247:ILE:HD13	1.63	0.79
15:1:111:TRP:CZ2	18:1:1013:CLA:HBC1	2.17	0.79
16:3:106:GLY:O	16:3:110:MET:HB2	1.83	0.79
6:G:76:ARG:HG3	6:G:77:PHE:CE1	2.17	0.79
13:2:120:ILE:HG21	27:2:2501:LUT:H373	1.63	0.79
13:2:126:LEU:HA	13:2:130:GLY:O	1.81	0.79
18:K:1001:CLA:HHD	18:K:1001:CLA:HBC2	1.62	0.79
16:3:267:ASN:CG	16:3:270:THR:HG23	2.07	0.79
18:2:2002:CLA:HBC2	18:2:2002:CLA:CMC	2.12	0.79
18:4:4012:CLA:H122	18:4:4012:CLA:H91	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:138:GLN:HB2	16:3:145:ALA:CB	2.09	0.79
18:3:3008:CLA:HBC2	18:3:3008:CLA:CHD	2.10	0.79
12:K:133:GLY:O	12:K:137:VAL:HG23	1.82	0.79
14:4:170:PRO:HB3	18:4:4016:CLA:C4A	2.13	0.79
15:1:225:ASN:O	15:1:228:ILE:HG22	1.83	0.79
6:G:144:ASN:HD22	18:G:1003:CLA:HED2	1.46	0.79
9:D:82:PRO:HG3	9:D:128:ASN:ND2	1.98	0.79
28:1:1010:CHL:CBB	18:1:1013:CLA:HBB2	2.11	0.79
7:L:120:LEU:HB3	7:L:126:ALA:HB3	1.63	0.79
15:1:133:THR:O	15:1:137:ILE:HG13	1.82	0.79
16:3:78:PHE:N	18:3:3004:CLA:OBD	2.16	0.79
27:3:3501:LUT:H171	27:3:3501:LUT:C8	2.12	0.79
15:1:85:ARG:HB2	18:1:1011:CLA:HED2	1.65	0.78
13:2:87:PHE:HZ	27:2:2502:LUT:H372	1.42	0.78
1:A:401:TRP:CD1	18:A:1126:CLA:HAB	2.19	0.78
9:D:191:SER:C	9:D:192:ILE:HD12	2.07	0.78
18:1:1003:CLA:HBA1	18:1:1008:CLA:CED	2.13	0.78
6:G:114:VAL:HG11	18:G:1002:CLA:HAA2	1.66	0.78
13:2:187:LYS:O	13:2:188:LEU:HB3	1.83	0.78
18:B:1238:CLA:HAB	20:B:5002:PQN:H162	1.66	0.78
14:4:169:ASP:HB3	18:4:4016:CLA:C2D	2.12	0.78
18:4:4016:CLA:HBA1	18:4:4016:CLA:HBD	1.65	0.78
18:1:1003:CLA:HBA1	18:1:1008:CLA:HED1	1.65	0.78
8:C:75:ARG:NH2	9:D:99:GLU:OE2	2.14	0.78
18:2:2001:CLA:HED2	18:2:2001:CLA:OBD	1.82	0.78
15:1:97:PRO:HB2	15:1:102:LEU:CB	2.12	0.78
16:3:138:GLN:O	16:3:145:ALA:HB3	1.82	0.78
9:D:100:PHE:CE1	9:D:158:VAL:HB	2.19	0.78
13:2:123:PRO:HA	13:2:126:LEU:CD2	2.14	0.78
14:4:208:GLY:O	14:4:212:MET:HG3	1.83	0.78
15:1:202:GLN:HE22	15:1:208:THR:HB	1.48	0.78
18:3:3001:CLA:H43	18:3:3002:CLA:HBA1	1.65	0.78
7:L:132:LEU:O	7:L:132:LEU:HD12	1.82	0.78
13:2:262:ILE:HD11	18:2:2003:CLA:C1	2.14	0.78
15:1:146:GLU:HG2	15:1:149:ARG:NH1	1.98	0.78
2:B:73:ASN:HD22	2:B:74:PHE:H	1.28	0.78
12:K:71:VAL:HG21	12:K:133:GLY:HA2	1.66	0.78
18:2:2003:CLA:H42	18:2:2003:CLA:C1D	2.14	0.78
15:1:114:LEU:HD23	15:1:115:PRO:CD	2.11	0.78
13:2:139:THR:CA	28:2:2010:CHL:HED3	2.14	0.77
18:F:1302:CLA:HBC2	18:F:1302:CLA:CHD	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:96:ARG:HG2	11:H:97:GLY:N	1.97	0.77
13:2:139:THR:N	28:2:2010:CHL:HED3	2.00	0.77
13:2:182:ILE:CD1	18:4:4007:CLA:HAB	2.14	0.77
15:1:222:TRP:CH2	18:1:1008:CLA:HMB2	2.19	0.77
16:3:139:THR:HG23	16:3:140:GLY:H	1.49	0.77
18:3:3013:CLA:HMA3	22:3:3503:BCR:H353	1.67	0.77
18:B:1220:CLA:H42	18:B:1221:CLA:H13	1.65	0.77
6:G:121:LEU:HD23	6:G:121:LEU:O	1.83	0.77
7:L:139:VAL:O	7:L:143:ILE:HG13	1.85	0.77
13:2:233:MET:HA	13:2:233:MET:HE3	1.64	0.77
14:4:143:VAL:O	14:4:147:ILE:HG12	1.85	0.77
18:1:1005:CLA:H12	18:1:1005:CLA:HED1	1.64	0.77
6:G:77:PHE:CE1	18:G:1002:CLA:HAB	2.19	0.77
27:2:2502:LUT:H28	27:2:2502:LUT:H361	1.67	0.77
14:4:150:HIS:CA	18:4:4012:CLA:HAB	2.14	0.77
18:1:1003:CLA:CBA	18:1:1008:CLA:HED1	2.14	0.77
16:3:101:GLY:HA2	18:3:3012:CLA:HED2	1.64	0.77
12:K:71:VAL:HG12	12:K:129:GLY:HA2	1.67	0.77
18:1:1003:CLA:C2	18:1:1008:CLA:HMD2	2.15	0.77
16:3:205:GLY:CA	16:3:208:PHE:HB2	2.14	0.77
18:4:4012:CLA:H91	18:4:4012:CLA:C12	2.15	0.77
16:3:152:ALA:HB3	16:3:157:LEU:HD21	1.65	0.77
6:G:64:ILE:O	6:G:68:THR:HG22	1.85	0.77
7:L:87:PRO:HB3	7:L:101:GLU:OE1	1.85	0.77
12:K:124:ALA:CB	22:K:2011:BCR:H331	2.15	0.77
13:2:131:ILE:HD12	13:2:133:LEU:CD2	2.08	0.77
27:4:4503:LUT:H363	28:1:1009:CHL:C8	2.14	0.77
16:3:110:MET:SD	16:3:231:GLY:HA2	2.25	0.77
18:3:3006:CLA:HMA2	18:3:3013:CLA:C3C	2.14	0.77
6:G:115:SER:HB2	18:G:1002:CLA:OBD	1.84	0.77
16:3:162:MET:HA	16:3:162:MET:CE	2.14	0.77
3:I:4:LEU:HD12	3:I:6:SER:H	1.50	0.76
15:1:232:ILE:HG22	15:1:233:PRO:O	1.85	0.76
16:3:169:GLU:CD	16:3:172:ARG:HH11	1.92	0.76
4:J:2:ARG:HD3	4:J:4:LEU:HB2	1.65	0.76
18:3:3002:CLA:HBB1	18:3:3002:CLA:CHC	2.13	0.76
3:I:14:LEU:O	3:I:17:PRO:HD2	1.86	0.76
18:G:1001:CLA:HBB1	18:G:1001:CLA:CHC	2.09	0.76
12:K:72:ALA:CB	18:K:1001:CLA:O2A	2.32	0.76
13:2:131:ILE:HB	13:2:133:LEU:HG	1.67	0.76
16:3:68:LEU:HD13	16:3:68:LEU:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:178:THR:HG23	7:L:181:GLY:H	1.49	0.76
13:2:262:ILE:HD11	18:2:2003:CLA:H43	1.65	0.76
15:1:209:GLY:CA	15:1:212:GLU:HB3	2.14	0.76
16:3:155:TYR:CZ	18:3:3010:CLA:HAC1	2.20	0.76
18:3:3003:CLA:C1C	18:3:3003:CLA:H92	2.14	0.76
13:2:125:PHE:HB3	13:2:131:ILE:CD1	2.16	0.76
16:3:139:THR:HG23	16:3:140:GLY:N	2.01	0.76
1:A:539:PHE:HA	18:A:1136:CLA:HED1	1.65	0.76
6:G:149:LYS:C	6:G:149:LYS:HE3	2.11	0.76
13:2:163:ALA:C	13:2:166:ARG:HB3	2.10	0.76
13:2:191:THR:HG22	13:2:192:ASP:H	1.51	0.76
16:3:65:LEU:HD13	16:3:67:TYR:HE1	1.49	0.76
1:A:269:PHE:HA	1:A:274:TRP:HE1	1.50	0.76
7:L:176:LEU:HD12	7:L:177:GLN:N	2.00	0.76
13:2:115:LEU:HB3	18:2:2006:CLA:CBB	2.15	0.76
13:2:246:PRO:HA	13:2:249:ASN:OD1	1.84	0.76
18:2:2003:CLA:H42	18:2:2003:CLA:CHD	2.15	0.76
15:1:85:ARG:CB	18:1:1011:CLA:HED2	2.15	0.76
13:2:178:ASN:O	13:2:187:LYS:HD2	1.85	0.76
16:3:172:ARG:NH2	18:3:3012:CLA:O1D	2.12	0.76
15:1:192:LEU:O	15:1:196:VAL:HG23	1.86	0.76
16:3:205:GLY:HA3	16:3:208:PHE:N	2.00	0.76
6:G:94:GLU:HB2	6:G:98:VAL:H	1.51	0.76
14:4:221:GLN:O	14:4:225:THR:HB	1.86	0.76
18:4:4007:CLA:HHC	18:4:4007:CLA:CBB	2.15	0.76
28:3:3011:CHL:HBD	28:3:3011:CHL:CBA	2.16	0.76
18:B:1236:CLA:HED2	18:B:1235:CLA:HMA3	1.67	0.75
11:H:130:GLN:HB3	11:H:132:PRO:HB3	1.68	0.75
15:1:121:TYR:HD2	15:1:122:LEU:HG	1.50	0.75
15:1:126:VAL:HG23	15:1:127:PRO:CA	2.15	0.75
16:3:119:PRO:CB	16:3:133:ALA:HB2	2.17	0.75
16:3:161:GLU:OE1	18:3:3010:CLA:HAB	1.86	0.75
27:2:2501:LUT:H371	27:2:2501:LUT:C28	2.17	0.75
27:1:1502:LUT:H371	27:1:1502:LUT:H28	1.68	0.75
16:3:226:LYS:HE3	18:3:3007:CLA:HED2	1.67	0.75
6:G:149:LYS:HE3	6:G:149:LYS:O	1.86	0.75
7:L:176:LEU:CD1	7:L:177:GLN:H	1.97	0.75
16:3:137:PHE:O	16:3:141:VAL:HG12	1.86	0.75
11:H:133:PRO:HD2	11:H:135:LEU:H	1.52	0.75
16:3:131:GLU:HG3	16:3:131:GLU:O	1.87	0.75
16:3:185:GLN:HB2	16:3:186:TYR:CD1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:704:GLN:HG3	25:B:7101:DGD:HA22	1.67	0.75
7:L:130:GLY:O	7:L:133:ALA:N	2.19	0.75
13:2:199:LEU:O	13:2:199:LEU:HD23	1.87	0.75
18:2:2003:CLA:HHB	18:2:2008:CLA:CBC	2.15	0.75
14:4:156:ARG:NH2	18:4:4012:CLA:O1D	2.19	0.75
15:1:202:GLN:HE21	15:1:202:GLN:C	1.94	0.75
16:3:79:ASP:OD1	16:3:82:GLY:N	2.19	0.75
18:3:3010:CLA:HHC	18:3:3010:CLA:CBB	2.16	0.75
13:2:139:THR:HA	28:2:2010:CHL:HED3	1.68	0.75
15:1:58:ASP:HA	18:1:1004:CLA:HED2	1.69	0.75
13:2:130:GLY:O	13:2:133:LEU:HD11	1.87	0.75
16:3:120:GLU:OE1	16:3:252:PRO:HG2	1.87	0.75
1:A:440:ASP:HB2	9:D:88:THR:HG21	1.68	0.75
27:4:4503:LUT:C28	27:4:4503:LUT:H371	2.16	0.75
16:3:65:LEU:HB3	16:3:68:LEU:HD21	1.67	0.75
18:3:3010:CLA:H93	18:3:3010:CLA:C2C	2.17	0.75
16:3:120:GLU:CD	16:3:253:TYR:H	1.95	0.75
16:3:225:LEU:HB3	16:3:226:LYS:CE	2.16	0.75
4:J:38:THR:C	23:J:5001:LMG:H122	2.11	0.74
6:G:84:ARG:NH2	6:G:123:ASP:OD2	2.19	0.74
13:2:129:LEU:HD22	13:2:131:ILE:CG1	2.17	0.74
14:4:158:GLN:NE2	14:4:161:LYS:HE3	2.02	0.74
18:4:4005:CLA:HMD3	18:4:4012:CLA:ND	2.01	0.74
7:L:113:PRO:CG	18:L:1503:CLA:HBB1	2.12	0.74
14:4:82:ALA:HB1	14:4:88:LEU:HD13	1.68	0.74
18:3:3003:CLA:H92	18:3:3003:CLA:CHC	2.18	0.74
22:F:6016:BCR:H331	22:F:6016:BCR:C8	2.16	0.74
12:K:130:HIS:O	12:K:134:VAL:HG23	1.86	0.74
14:4:168:GLN:O	18:4:4016:CLA:HED3	1.87	0.74
15:1:160:TYR:HB3	18:1:1001:CLA:HED3	1.69	0.74
6:G:76:ARG:O	6:G:76:ARG:HD2	1.86	0.74
18:L:1501:CLA:HBA2	18:H:1000:CLA:HHB	1.69	0.74
15:1:104:ASN:CG	15:1:208:THR:HG23	2.11	0.74
15:1:226:ILE:N	18:1:1003:CLA:O1A	2.20	0.74
16:3:101:GLY:HA2	18:3:3012:CLA:CED	2.18	0.74
18:3:3001:CLA:HBA1	27:3:3501:LUT:C38	2.17	0.74
1:A:24:ARG:HH11	1:A:76:ARG:HH12	1.34	0.74
14:4:235:GLN:HB3	14:4:243:ASN:HD22	1.51	0.74
27:4:4501:LUT:H371	27:4:4501:LUT:C28	2.11	0.74
15:1:131:LEU:N	15:1:131:LEU:HD23	2.03	0.74
15:1:165:PHE:O	15:1:167:PRO:HD2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1003:CLA:HBB1	18:1:1003:CLA:C9	2.04	0.74
16:3:266:ASN:O	16:3:270:THR:HG21	1.87	0.74
27:3:3502:LUT:H161	27:3:3502:LUT:C8	2.12	0.74
28:1:1010:CHL:HBC3	28:1:1010:CHL:CMC	2.17	0.74
16:3:225:LEU:HB3	16:3:226:LYS:HZ1	1.51	0.74
2:B:488:ALA:O	6:G:146:TYR:OH	2.06	0.74
18:2:2005:CLA:H71	23:2:2802:LMG:H132	1.70	0.74
14:4:213:LEU:HD12	23:4:4801:LMG:H302	1.68	0.74
18:1:1003:CLA:H2	18:1:1008:CLA:HMD2	1.67	0.74
18:3:3002:CLA:HHC	18:3:3002:CLA:CBB	2.17	0.74
13:2:105:ALA:HB2	18:2:2012:CLA:HED2	1.68	0.74
13:2:174:PRO:HD2	13:2:175:GLY:H	1.52	0.74
13:2:254:LEU:N	13:2:254:LEU:HD23	2.01	0.74
16:3:259:HIS:NE2	18:3:3008:CLA:NC	2.36	0.74
1:A:217:SER:HA	18:A:1113:CLA:HBB2	1.70	0.74
6:G:116:LYS:HE3	18:G:1002:CLA:NC	2.02	0.74
18:G:1003:CLA:C5	23:G:2021:LMG:H311	2.17	0.74
14:4:215:PHE:CD2	27:4:4502:LUT:H14	2.22	0.74
28:4:4013:CHL:HHD	28:4:4013:CHL:CBC	2.18	0.74
15:1:202:GLN:CD	15:1:208:THR:HB	2.12	0.74
21:1:1801:LHG:HC81	21:1:1801:LHG:HC61	1.70	0.74
18:3:3013:CLA:CBB	27:3:3502:LUT:H181	2.17	0.74
18:G:1003:CLA:H93	23:G:2021:LMG:H162	1.70	0.73
8:C:10:THR:HG23	8:C:64:SER:OG	1.88	0.73
13:2:250:LEU:CD2	13:2:254:LEU:HD21	2.18	0.73
18:L:1501:CLA:HBA1	18:L:1501:CLA:CBD	2.18	0.73
12:K:75:THR:HG21	12:K:129:GLY:CA	2.18	0.73
18:2:2001:CLA:C4	18:2:2002:CLA:H3A	2.17	0.73
14:4:151:TYR:HB2	28:1:1009:CHL:H11	1.69	0.73
21:1:1801:LHG:H223	21:1:1801:LHG:H383	1.70	0.73
16:3:65:LEU:HD13	16:3:67:TYR:CZ	2.23	0.73
8:C:61:ASP:HB2	10:E:118:ASN:ND2	2.03	0.73
12:K:71:VAL:HG12	12:K:129:GLY:CA	2.18	0.73
12:K:76:LEU:O	12:K:79:PHE:HB2	1.89	0.73
28:1:1010:CHL:OMC	18:1:1013:CLA:HAB	1.89	0.73
10:E:66:ILE:HG23	10:E:67:GLY:N	2.03	0.73
12:K:72:ALA:O	12:K:76:LEU:HG	1.89	0.73
13:2:162:TRP:O	13:2:166:ARG:HB2	1.87	0.73
28:2:2010:CHL:HBB1	28:2:2013:CHL:HBB2	1.68	0.73
12:K:70:MET:HE2	12:K:71:VAL:HA	1.71	0.73
13:2:122:ILE:HG23	13:2:133:LEU:CB	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2016:CLA:HBA2	18:2:2016:CLA:CBD	2.17	0.73
18:4:4003:CLA:C4B	18:4:4003:CLA:H93	2.18	0.73
18:L:1501:CLA:HBA1	18:L:1501:CLA:HBD	1.71	0.73
16:3:103:VAL:O	16:3:107:ARG:HG3	1.89	0.73
4:J:2:ARG:O	4:J:4:LEU:N	2.20	0.73
4:J:6:THR:CG2	23:F:5001:LMG:HC1	2.19	0.73
11:H:59:ASP:OD1	11:H:59:ASP:N	2.22	0.73
18:4:4002:CLA:HHC	18:4:4002:CLA:CBB	2.19	0.73
18:B:1219:CLA:HBB2	22:B:6009:BCR:H343	1.70	0.73
7:L:121:ARG:HG2	7:L:127:GLY:H	1.53	0.73
18:1:1003:CLA:C2B	27:1:1501:LUT:H173	2.18	0.73
16:3:182:MET:HE2	16:3:182:MET:CA	2.19	0.73
7:L:91:THR:HG22	7:L:175:GLN:NE2	2.03	0.73
15:1:88:MET:HE1	18:1:1001:CLA:CAB	2.18	0.73
16:3:246:LEU:HD23	16:3:246:LEU:C	2.14	0.73
18:3:3008:CLA:HHC	18:3:3008:CLA:CBB	2.15	0.73
23:J:5001:LMG:HC8	23:J:5001:LMG:O10	1.87	0.73
18:2:2002:CLA:HED1	18:2:2002:CLA:O2A	1.89	0.73
14:4:169:ASP:HB3	18:4:4016:CLA:C4D	2.19	0.73
5:F:222:LEU:HD23	5:F:222:LEU:N	2.03	0.72
13:2:219:THR:CG2	18:2:2007:CLA:HED3	2.19	0.72
18:3:3001:CLA:CBA	27:3:3501:LUT:H382	2.19	0.72
6:G:76:ARG:HG2	6:G:116:LYS:HZ1	1.52	0.72
13:2:120:ILE:HD13	27:2:2501:LUT:H373	1.71	0.72
28:2:2011:CHL:HBD	28:2:2011:CHL:HAA1	1.69	0.72
16:3:187:PHE:O	16:3:188:LEU:HB2	1.88	0.72
7:L:87:PRO:HD3	18:L:1502:CLA:HED2	1.69	0.72
13:2:131:ILE:HB	13:2:133:LEU:CG	2.20	0.72
18:4:4016:CLA:OBD	18:4:4016:CLA:HED2	1.89	0.72
27:1:1501:LUT:H181	27:1:1501:LUT:H8	1.69	0.72
2:B:684:ARG:HH21	7:L:67:GLY:HA3	1.55	0.72
18:G:1001:CLA:HAB	22:G:2011:BCR:H363	1.71	0.72
7:L:166:LEU:HD23	7:L:166:LEU:O	1.90	0.72
11:H:132:PRO:CD	11:H:133:PRO:HD3	2.19	0.72
14:4:236:HIS:NE2	18:4:4008:CLA:NC	2.38	0.72
3:I:4:LEU:HD12	3:I:4:LEU:C	2.14	0.72
18:K:1001:CLA:HHC	18:K:1001:CLA:CBB	2.19	0.72
13:2:130:GLY:C	13:2:131:ILE:HG13	2.14	0.72
13:2:177:VAL:O	13:2:179:THR:N	2.22	0.72
14:4:225:THR:CG2	14:4:227:LYS:H	2.00	0.72
16:3:166:GLY:HA2	18:3:3012:CLA:CBB	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:182:MET:HA	16:3:182:MET:CE	2.14	0.72
7:L:128:GLN:CB	7:L:204:LEU:HG	2.19	0.72
13:2:129:LEU:HD23	13:2:129:LEU:C	2.15	0.72
16:3:184:LYS:CG	16:3:185:GLN:HE21	2.02	0.72
9:D:195:ASN:H	9:D:195:ASN:HD22	1.37	0.72
11:H:112:ALA:O	11:H:115:SER:HB3	1.88	0.72
16:3:244:GLN:O	16:3:248:THR:HB	1.90	0.72
7:L:121:ARG:HA	7:L:124:GLU:O	1.89	0.72
13:2:191:THR:HG22	13:2:192:ASP:N	2.03	0.72
18:2:2006:CLA:H43	18:2:2006:CLA:CAD	2.18	0.72
18:2:2009:CLA:HED3	16:3:171:ARG:HG3	1.70	0.72
16:3:122:LEU:O	16:3:126:GLY:N	2.23	0.72
16:3:268:VAL:CG2	18:3:3003:CLA:H12	2.19	0.72
18:2:2001:CLA:H42	18:2:2002:CLA:CBA	2.15	0.72
18:2:2016:CLA:HBB1	18:2:2016:CLA:CHC	2.12	0.72
15:1:82:ILE:HD12	15:1:149:ARG:NH2	2.05	0.72
27:1:1502:LUT:H371	27:1:1502:LUT:C28	2.18	0.72
7:L:96:LEU:HD23	7:L:96:LEU:C	2.15	0.71
14:4:151:TYR:O	14:4:155:ARG:HB2	1.89	0.71
15:1:211:LEU:HD12	15:1:212:GLU:H	1.55	0.71
18:1:1001:CLA:O1A	18:1:1001:CLA:H3A	1.88	0.71
16:3:202:TYR:HB3	18:3:3001:CLA:O1D	1.90	0.71
16:3:206:PRO:HA	16:3:209:ASN:O	1.90	0.71
16:3:218:LYS:C	16:3:218:LYS:HD3	2.15	0.71
18:A:1102:CLA:HBA2	18:A:1109:CLA:H51	1.72	0.71
7:L:166:LEU:HD23	7:L:166:LEU:C	2.15	0.71
9:D:129:LEU:C	9:D:129:LEU:HD23	2.14	0.71
13:2:188:LEU:HD22	13:2:188:LEU:C	2.15	0.71
15:1:200:VAL:HG11	18:1:1003:CLA:HAC2	1.71	0.71
13:2:230:LEU:HD21	18:2:2004:CLA:HMC1	1.72	0.71
21:2:2801:LHG:O4	21:2:2801:LHG:O2	2.07	0.71
14:4:140:THR:HB	15:1:225:ASN:OD1	1.90	0.71
1:A:37:PRO:HA	18:A:1101:CLA:HBC1	1.72	0.71
18:F:1301:CLA:HBB1	18:F:1301:CLA:HHC	1.72	0.71
9:D:112:ILE:N	9:D:112:ILE:HD12	2.04	0.71
10:E:122:LEU:HD12	10:E:122:LEU:N	2.02	0.71
16:3:223:LEU:CA	16:3:226:LYS:HG2	2.20	0.71
18:B:1204:CLA:H2	3:I:8:PHE:HD2	1.53	0.71
22:J:6013:BCR:H392	22:J:6013:BCR:H23C	1.71	0.71
18:G:1001:CLA:HED2	18:G:1001:CLA:C3D	2.21	0.71
13:2:148:ASP:O	13:2:149:THR:CB	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:168:GLN:OE1	14:4:171:ILE:HA	1.89	0.71
16:3:220:LEU:HD23	16:3:220:LEU:C	2.15	0.71
18:3:3003:CLA:CAB	27:3:3501:LUT:H172	2.20	0.71
13:2:177:VAL:HG23	13:2:178:ASN:N	2.05	0.71
16:3:169:GLU:OE2	16:3:172:ARG:NH1	2.22	0.71
14:4:118:ILE:CD1	14:4:120:ILE:HD11	2.06	0.71
18:1:1011:CLA:C5	27:1:1501:LUT:H23	2.18	0.71
16:3:141:VAL:HG22	16:3:143:PRO:HD2	1.72	0.71
18:B:1235:CLA:H72	18:B:1235:CLA:HBB1	1.71	0.71
7:L:102:VAL:HG13	7:L:106:HIS:CE1	2.26	0.71
13:2:109:HIS:CD2	18:2:2012:CLA:HMD1	2.25	0.71
15:1:186:LYS:HD3	18:1:1007:CLA:O1D	1.90	0.71
23:G:2021:LMG:HC61	15:1:115:PRO:HA	1.71	0.71
15:1:125:PRO:O	15:1:126:VAL:HG22	1.89	0.71
18:L:1502:CLA:HAC2	22:L:6019:BCR:H292	1.72	0.71
12:K:70:MET:HE1	12:K:71:VAL:HG22	1.73	0.71
14:4:60:LEU:HG	14:4:61:ALA:N	2.06	0.71
16:3:223:LEU:HA	16:3:226:LYS:HG2	1.73	0.71
4:J:28:GLU:OE1	18:J:1302:CLA:CHA	2.39	0.70
14:4:152:VAL:HG13	28:4:4011:CHL:NB	2.06	0.70
16:3:67:TYR:HE2	16:3:84:SER:CB	2.04	0.70
16:3:142:ILE:O	16:3:146:GLY:HA2	1.90	0.70
16:3:265:ASN:O	16:3:270:THR:HB	1.91	0.70
18:3:3006:CLA:H43	18:3:3018:CLA:O2A	1.90	0.70
18:A:1114:CLA:HBB1	18:A:1114:CLA:HHC	1.73	0.70
22:L:6019:BCR:C27	22:L:6019:BCR:H393	2.21	0.70
22:K:2011:BCR:HC8	22:K:2011:BCR:C32	2.16	0.70
18:2:2005:CLA:C7	23:2:2802:LMG:H132	2.21	0.70
18:3:3006:CLA:HMA2	18:3:3013:CLA:CAC	2.21	0.70
9:D:192:ILE:HG22	9:D:193:GLY:N	2.03	0.70
18:2:2016:CLA:HHC	18:2:2016:CLA:CBB	2.14	0.70
15:1:204:ALA:C	15:1:206:PRO:HD3	2.16	0.70
16:3:226:LYS:HZ2	16:3:226:LYS:N	1.89	0.70
18:3:3001:CLA:C4	18:3:3002:CLA:HBA1	2.20	0.70
13:2:200:TRP:CD1	18:2:2016:CLA:HAA2	2.25	0.70
28:2:2010:CHL:HBB1	28:2:2010:CHL:HHC	1.71	0.70
18:4:4003:CLA:HBB1	18:4:4003:CLA:CHC	2.19	0.70
16:3:226:LYS:NZ	16:3:226:LYS:H	1.88	0.70
6:G:75:GLY:O	6:G:80:PHE:HB2	1.90	0.70
18:1:1001:CLA:ND	27:1:1501:LUT:H383	2.06	0.70
18:1:1008:CLA:HHC	18:1:1008:CLA:CBB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:4002:CLA:OBD	18:4:4007:CLA:HBD	1.92	0.70
15:1:41:TRP:CD1	15:1:59:PHE:HA	2.26	0.70
18:3:3006:CLA:HED2	18:3:3006:CLA:CHA	2.21	0.70
13:2:77:LEU:CD1	13:2:86:GLY:HA2	2.22	0.70
28:4:4013:CHL:HHB	27:4:4503:LUT:H192	1.72	0.70
15:1:121:TYR:O	15:1:122:LEU:HD23	1.91	0.70
18:3:3012:CLA:H12	18:3:3017:CLA:CBB	2.22	0.70
2:B:582:TRP:CH2	18:B:1012:CLA:HAB	2.27	0.70
27:I:6018:LUT:C8	27:I:6018:LUT:H181	2.21	0.70
18:2:2003:CLA:C3B	27:2:2501:LUT:H383	2.21	0.70
28:4:4013:CHL:HHB	27:4:4503:LUT:C19	2.22	0.70
9:D:169:PRO:O	9:D:170:LYS:HB3	1.90	0.70
10:E:111:ASN:ND2	10:E:113:ALA:O	2.24	0.70
18:1:1008:CLA:HBB1	18:1:1008:CLA:CHC	2.19	0.70
28:2:2013:CHL:OMC	28:2:2013:CHL:HBC2	1.92	0.70
14:4:150:HIS:O	14:4:154:ILE:HG22	1.91	0.70
16:3:107:ARG:CB	28:3:3011:CHL:HED1	2.21	0.70
7:L:91:THR:HA	7:L:175:GLN:NE2	2.05	0.69
13:2:141:GLY:HA2	28:2:2013:CHL:HBC1	1.72	0.69
15:1:126:VAL:HB	15:1:127:PRO:HA	1.73	0.69
1:A:593:SER:OG	1:A:596:ASP:OD2	2.10	0.69
2:B:294:ASN:HB3	6:G:107:ARG:HA	1.74	0.69
7:L:83:LEU:O	7:L:89:TYR:HD2	1.75	0.69
15:1:167:PRO:HD2	27:1:1501:LUT:O23	1.91	0.69
27:2:2501:LUT:C37	27:2:2501:LUT:H28	2.22	0.69
14:4:104:LEU:C	18:4:4006:CLA:HBB2	2.17	0.69
16:3:135:ALA:H	16:3:138:GLN:HG2	1.55	0.69
16:3:166:GLY:O	16:3:170:HIS:ND1	2.23	0.69
27:3:3502:LUT:H28	27:3:3502:LUT:H371	1.73	0.69
15:1:89:LEU:O	15:1:92:PRO:HD2	1.92	0.69
18:3:3008:CLA:HBB1	18:3:3008:CLA:CHC	2.16	0.69
10:E:111:ASN:HD22	10:E:113:ALA:H	1.40	0.69
11:H:68:ASP:OD1	11:H:71:GLY:HA3	1.92	0.69
18:2:2002:CLA:HED1	18:2:2002:CLA:CGA	2.22	0.69
18:2:2016:CLA:HBD	18:2:2016:CLA:CGA	2.22	0.69
14:4:94:ALA:N	18:4:4012:CLA:HED2	2.07	0.69
16:3:155:TYR:CE1	18:3:3010:CLA:HAC1	2.27	0.69
16:3:259:HIS:CG	18:3:3003:CLA:HAA2	2.28	0.69
5:F:106:LEU:HD13	5:F:106:LEU:O	1.91	0.69
14:4:120:ILE:HD12	14:4:120:ILE:N	2.07	0.69
16:3:117:ILE:HD11	16:3:252:PRO:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:1011:CL0:H15	17:A:1011:CL0:H2	1.75	0.69
8:C:14:CYS:C	8:C:15:THR:HG23	2.16	0.69
14:4:136:ALA:HB1	14:4:140:THR:HG21	1.75	0.69
14:4:197:THR:OG1	14:4:200:ALA:HB2	1.93	0.69
18:3:3003:CLA:C9	18:3:3003:CLA:H122	2.23	0.69
18:G:1001:CLA:HHC	18:G:1001:CLA:CBB	2.15	0.69
13:2:123:PRO:HA	13:2:126:LEU:CG	2.22	0.69
28:4:4011:CHL:HAA1	28:4:4011:CHL:CBD	2.21	0.69
16:3:184:LYS:C	16:3:185:GLN:HG2	2.18	0.69
18:3:3004:CLA:H3A	18:3:3004:CLA:CGA	2.22	0.69
18:A:1013:CLA:H203	18:A:1140:CLA:H51	1.74	0.69
18:2:2005:CLA:HBC1	18:2:2012:CLA:CBC	2.23	0.69
18:2:2008:CLA:HAA2	16:3:160:LEU:HB2	1.74	0.69
15:1:75:ARG:NH1	18:1:1005:CLA:O1A	2.26	0.69
16:3:110:MET:HA	16:3:234:ALA:CB	2.23	0.69
13:2:77:LEU:HD12	13:2:86:GLY:HA2	1.75	0.69
27:2:2502:LUT:H361	27:2:2502:LUT:C28	2.22	0.69
18:4:4007:CLA:H2A	18:4:4007:CLA:O2D	1.93	0.69
15:1:209:GLY:O	15:1:213:ASN:N	2.19	0.69
16:3:259:HIS:HA	16:3:266:ASN:CB	2.23	0.69
6:G:76:ARG:HE	6:G:116:LYS:CE	2.04	0.68
13:2:233:MET:HE3	13:2:233:MET:CA	2.23	0.68
15:1:193:LEU:O	15:1:193:LEU:HD23	1.93	0.68
18:1:1004:CLA:H2	27:1:1502:LUT:H182	1.74	0.68
16:3:258:ASP:HB2	16:3:266:ASN:HD21	1.58	0.68
22:A:6017:BCR:H362	18:B:1023:CLA:H112	1.75	0.68
12:K:124:ALA:O	12:K:128:VAL:HG23	1.94	0.68
18:4:4002:CLA:HBB1	18:4:4002:CLA:CHC	2.23	0.68
18:4:4007:CLA:HBC2	18:4:4007:CLA:CHD	2.13	0.68
15:1:144:PHE:O	15:1:148:GLN:HG2	1.93	0.68
16:3:155:TYR:CE1	18:3:3010:CLA:CAC	2.76	0.68
18:3:3005:CLA:HMD3	18:3:3012:CLA:ND	2.08	0.68
18:3:3006:CLA:CBB	18:3:3006:CLA:HHC	2.22	0.68
7:L:98:ARG:HH22	7:L:175:GLN:HE22	1.41	0.68
12:K:71:VAL:HG21	12:K:133:GLY:CA	2.23	0.68
13:2:117:ALA:HB1	27:2:2501:LUT:H32	1.75	0.68
13:2:131:ILE:CG2	13:2:133:LEU:HG	2.23	0.68
13:2:186:ASN:OD1	18:2:2016:CLA:H2A	1.93	0.68
18:4:4006:CLA:C3B	27:4:4502:LUT:H183	2.23	0.68
27:3:3501:LUT:H161	27:3:3501:LUT:C8	2.17	0.68
22:L:6019:BCR:C38	22:L:6019:BCR:H23C	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:125:PHE:HB3	13:2:131:ILE:HD11	1.75	0.68
18:1:1002:CLA:HED2	18:1:1002:CLA:O1A	1.94	0.68
18:A:1022:CLA:H122	22:A:6017:BCR:H352	1.75	0.68
7:L:91:THR:HA	7:L:98:ARG:NH2	2.08	0.68
12:K:66:THR:O	12:K:69:ILE:HG23	1.94	0.68
13:2:68:PHE:CD2	13:2:71:SER:HB3	2.29	0.68
13:2:69:PRO:HD2	18:2:2009:CLA:O1D	1.93	0.68
14:4:132:GLU:HB2	14:4:133:GLU:OE2	1.94	0.68
27:4:4502:LUT:H381	27:4:4502:LUT:C28	2.06	0.68
15:1:177:PHE:CE2	15:1:181:LYS:HE2	2.28	0.68
18:3:3010:CLA:HBB1	18:3:3010:CLA:CHC	2.20	0.68
11:H:132:PRO:HD2	11:H:133:PRO:CD	2.23	0.68
18:2:2008:CLA:HHC	18:2:2008:CLA:HBB1	1.75	0.68
15:1:58:ASP:HA	18:1:1004:CLA:CED	2.23	0.68
16:3:110:MET:HE1	16:3:230:ASN:C	2.19	0.68
4:J:2:ARG:NE	4:J:4:LEU:HD12	2.01	0.68
7:L:162:PRO:HG2	11:H:68:ASP:HB2	1.75	0.68
13:2:211:PRO:O	13:2:212:GLN:CG	2.42	0.68
14:4:213:LEU:CD1	23:4:4801:LMG:H302	2.24	0.68
29:4:4505:ZEX:H362	29:4:4505:ZEX:C38	2.22	0.68
5:F:139:LEU:N	5:F:139:LEU:HD23	2.07	0.68
7:L:109:PHE:HE1	18:L:1503:CLA:C2C	2.06	0.68
10:E:111:ASN:ND2	10:E:113:ALA:H	1.91	0.68
13:2:168:TRP:CD2	18:2:2012:CLA:HMA2	2.29	0.68
18:4:4005:CLA:HMB3	27:4:4502:LUT:H403	1.75	0.68
18:G:1001:CLA:H41	22:G:2011:BCR:C34	2.22	0.68
14:4:203:LYS:HA	18:4:4007:CLA:O1D	1.92	0.68
15:1:106:VAL:HG21	15:1:202:GLN:OE1	1.94	0.68
16:3:236:LEU:HD23	18:3:3004:CLA:HMC1	1.76	0.68
1:A:387:THR:HG21	1:A:523:VAL:HB	1.75	0.68
22:L:6019:BCR:H393	22:L:6019:BCR:H271	1.76	0.68
13:2:177:VAL:HG23	13:2:178:ASN:H	1.59	0.68
16:3:237:ALA:HB1	27:3:3501:LUT:H161	1.76	0.68
18:3:3013:CLA:CMA	22:3:3503:BCR:H353	2.23	0.68
7:L:161:ALA:HB3	7:L:174:ASP:OD1	1.94	0.67
11:H:106:GLY:O	11:H:110:THR:HG22	1.94	0.67
12:K:78:LEU:HB3	12:K:82:ARG:HB2	1.75	0.67
18:K:1001:CLA:HBB1	18:K:1001:CLA:CHC	2.24	0.67
18:2:2009:CLA:HED3	16:3:171:ARG:HG2	1.76	0.67
15:1:80:GLU:HG3	18:1:1004:CLA:C1B	2.24	0.67
15:1:130:THR:HG22	15:1:132:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:1003:CLA:H13	18:G:1003:CLA:H91	1.73	0.67
9:D:160:PRO:HD2	9:D:161:SER:H	1.60	0.67
13:2:175:GLY:O	13:2:176:CYS:HB3	1.92	0.67
14:4:209:ARG:HD3	18:4:4004:CLA:CHD	2.24	0.67
15:1:221:PRO:HG2	15:1:222:TRP:CZ3	2.30	0.67
15:1:158:LYS:C	15:1:159:LYS:HD3	2.19	0.67
15:1:193:LEU:HD23	15:1:193:LEU:C	2.18	0.67
2:B:15:ASP:HB3	2:B:20:ARG:HB3	1.76	0.67
18:K:1001:CLA:O2D	18:K:1001:CLA:H2A	1.93	0.67
13:2:131:ILE:HG22	13:2:132:LEU:N	2.09	0.67
16:3:183:GLY:HA2	16:3:194:PHE:CB	2.23	0.67
18:2:2001:CLA:H11	27:2:2501:LUT:C17	2.24	0.67
14:4:197:THR:O	14:4:200:ALA:HB3	1.95	0.67
14:4:198:LEU:O	14:4:199:GLU:HB2	1.94	0.67
15:1:85:ARG:HH11	15:1:85:ARG:CG	2.08	0.67
18:B:1206:CLA:HMA3	18:B:1207:CLA:HBB1	1.77	0.67
6:G:120:ALA:HB3	6:G:123:ASP:OD1	1.95	0.67
22:G:2011:BCR:H403	22:G:2011:BCR:C23	2.19	0.67
15:1:131:LEU:HD23	15:1:131:LEU:H	1.58	0.67
16:3:119:PRO:HB2	16:3:133:ALA:CB	2.25	0.67
16:3:249:GLY:O	16:3:250:VAL:HG23	1.94	0.67
7:L:90:ARG:O	7:L:98:ARG:NH2	2.27	0.67
12:K:86:ALA:CB	12:K:87:PRO:HD3	2.25	0.67
13:2:64:ARG:NH2	13:2:77:LEU:O	2.28	0.67
14:4:170:PRO:HA	18:4:4016:CLA:O1D	1.95	0.67
18:4:4001:CLA:H52	27:4:4501:LUT:H28	1.75	0.67
18:4:4003:CLA:HHD	18:4:4003:CLA:HBC2	1.77	0.67
15:1:152:GLU:CG	15:1:156:GLU:HA	2.25	0.67
16:3:138:GLN:CG	16:3:145:ALA:HB2	2.24	0.67
23:2:2802:LMG:HO4	23:2:2802:LMG:HO5	1.42	0.67
14:4:220:ILE:HD12	18:4:4003:CLA:CAC	2.23	0.67
14:4:229:PRO:HA	14:4:232:ASN:HD22	1.59	0.67
15:1:195:PHE:O	15:1:198:ILE:HB	1.95	0.67
16:3:251:GLY:O	16:3:255:ASN:N	2.24	0.67
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.76	0.67
12:K:66:THR:HA	12:K:69:ILE:CG2	2.23	0.67
12:K:76:LEU:N	12:K:76:LEU:HD23	2.10	0.67
13:2:203:PRO:HD2	27:2:2501:LUT:O3	1.95	0.67
18:4:4003:CLA:H11	18:4:4008:CLA:OBD	1.94	0.67
15:1:130:THR:HG22	15:1:131:LEU:N	2.10	0.67
18:1:1001:CLA:CHC	27:1:1501:LUT:H32	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3004:CLA:H2	27:3:3502:LUT:H363	1.77	0.67
6:G:116:LYS:HE3	18:G:1002:CLA:C1C	2.23	0.66
12:K:136:VAL:O	12:K:140:LEU:HD22	1.94	0.66
13:2:262:ILE:HA	18:2:2003:CLA:OBD	1.94	0.66
18:2:2009:CLA:CED	16:3:171:ARG:HG3	2.25	0.66
16:3:267:ASN:O	16:3:271:SER:N	2.28	0.66
18:B:1204:CLA:H2	3:I:8:PHE:CD2	2.31	0.66
18:B:1210:CLA:HHC	18:B:1210:CLA:HBB1	1.76	0.66
9:D:192:ILE:CG2	9:D:193:GLY:H	2.07	0.66
14:4:112:PRO:O	14:4:116:THR:OG1	2.13	0.66
15:1:85:ARG:HB2	18:1:1011:CLA:CED	2.25	0.66
18:3:3001:CLA:HBB2	27:3:3501:LUT:H34	1.77	0.66
1:A:34:TRP:CE3	4:J:8:LEU:HD22	2.30	0.66
7:L:102:VAL:HG22	18:L:1502:CLA:O1D	1.94	0.66
13:2:70:GLY:CA	16:3:174:GLN:HE21	2.05	0.66
18:1:1003:CLA:C3B	27:1:1501:LUT:H173	2.26	0.66
6:G:132:HIS:CE1	22:G:2011:BCR:H19C	2.29	0.66
7:L:90:ARG:C	7:L:98:ARG:HH21	2.04	0.66
9:D:157:ARG:HB2	9:D:167:LEU:HD11	1.76	0.66
13:2:222:ILE:HD12	13:2:222:ILE:N	2.09	0.66
18:4:4003:CLA:HHC	18:4:4003:CLA:CBB	2.23	0.66
1:A:462:ILE:HG22	18:A:1132:CLA:HBC2	1.78	0.66
4:J:6:THR:HG22	23:F:5001:LMG:HC1	1.76	0.66
7:L:204:LEU:O	7:L:204:LEU:HD13	1.95	0.66
7:L:129:ALA:O	7:L:132:LEU:HB3	1.96	0.66
11:H:131:LEU:HB2	11:H:132:PRO:HA	1.78	0.66
13:2:188:LEU:HD23	13:2:198:GLY:N	2.09	0.66
14:4:105:GLY:HA2	18:4:4006:CLA:CBB	2.25	0.66
21:1:1801:LHG:O3	21:1:1801:LHG:O1	2.10	0.66
16:3:223:LEU:N	16:3:226:LYS:HZ3	1.93	0.66
16:3:258:ASP:HB3	16:3:266:ASN:HD21	1.61	0.66
16:3:268:VAL:HG23	18:3:3003:CLA:C1	2.21	0.66
3:I:13:GLY:C	3:I:14:LEU:HD23	2.21	0.66
5:F:94:ARG:NH1	5:F:143:ASP:O	2.26	0.66
10:E:76:ILE:C	10:E:77:LEU:HD12	2.20	0.66
13:2:119:GLY:O	13:2:123:PRO:HD3	1.96	0.66
14:4:235:GLN:HB3	14:4:243:ASN:ND2	2.10	0.66
15:1:94:ILE:HG13	27:1:1502:LUT:H382	1.78	0.66
16:3:155:TYR:CD1	18:3:3010:CLA:HAC2	2.31	0.66
16:3:268:VAL:HG21	18:3:3003:CLA:C4	2.11	0.66
2:B:12:ILE:HD11	2:B:23:PHE:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:8:TYR:CD2	9:D:191:SER:HA	2.27	0.66
9:D:195:ASN:H	9:D:195:ASN:ND2	1.92	0.66
13:2:244:THR:HG22	13:2:245:GLY:N	2.03	0.66
14:4:212:MET:HB3	27:4:4502:LUT:C34	2.26	0.66
18:4:4001:CLA:HBC2	28:4:4011:CHL:O1A	1.96	0.66
15:1:43:PRO:HB2	28:1:1009:CHL:O1D	1.96	0.66
15:1:120:THR:HG22	15:1:124:ASN:O	1.94	0.66
18:1:1004:CLA:H3A	18:1:1004:CLA:CGA	2.26	0.66
28:1:1009:CHL:O2D	28:1:1009:CHL:H2A	1.96	0.66
16:3:223:LEU:HA	16:3:226:LYS:CG	2.26	0.66
6:G:76:ARG:NE	6:G:116:LYS:HE2	2.11	0.66
8:C:25:VAL:HG21	8:C:48:CYS:HB2	1.77	0.66
18:4:4001:CLA:H52	27:4:4501:LUT:C37	2.26	0.66
15:1:98:GLU:HA	15:1:102:LEU:HB3	1.77	0.66
16:3:267:ASN:OD1	16:3:270:THR:HG23	1.94	0.66
18:3:3008:CLA:HBD	18:3:3008:CLA:HBA1	1.77	0.66
5:F:138:LEU:CD2	5:F:159:GLU:OE2	2.44	0.65
18:G:1003:CLA:H91	18:G:1003:CLA:C13	2.26	0.65
7:L:91:THR:HG22	7:L:175:GLN:HE21	1.61	0.65
12:K:136:VAL:C	12:K:140:LEU:HD22	2.21	0.65
14:4:212:MET:HE3	18:4:4004:CLA:HMC3	1.78	0.65
1:A:453:LEU:HD21	18:A:1136:CLA:HAB	1.78	0.65
6:G:121:LEU:HD23	6:G:121:LEU:C	2.22	0.65
18:1:1014:CLA:O2D	18:1:1014:CLA:HBA2	1.94	0.65
16:3:94:GLU:OE2	16:3:95:PRO:HD2	1.96	0.65
16:3:178:LYS:HB2	16:3:181:SER:OG	1.96	0.65
16:3:184:LYS:HG2	16:3:185:GLN:HE21	1.59	0.65
2:B:603:ARG:HH22	2:B:627:ASN:HD21	1.43	0.65
10:E:111:ASN:HD21	10:E:113:ALA:HB3	1.60	0.65
13:2:174:PRO:CD	13:2:175:GLY:H	2.08	0.65
13:2:256:ASP:OD1	13:2:259:HIS:HD2	1.79	0.65
16:3:78:PHE:HB3	18:3:3004:CLA:OBD	1.96	0.65
16:3:267:ASN:OD1	16:3:269:LEU:HG	1.95	0.65
1:A:567:ARG:NH2	9:D:88:THR:O	2.29	0.65
2:B:487:ASN:HB3	6:G:149:LYS:HB3	1.77	0.65
13:2:111:ARG:NH1	28:2:2011:CHL:OBD	2.27	0.65
18:2:2016:CLA:HBC2	18:2:2016:CLA:CHD	2.25	0.65
22:B:6006:BCR:H362	18:B:1211:CLA:H2	1.79	0.65
3:I:5:PRO:O	3:I:7:LEU:N	2.29	0.65
23:2:2802:LMG:O5	23:2:2802:LMG:O4	2.10	0.65
14:4:167:ASN:CG	14:4:168:GLN:H	2.03	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ASN:HD21	2:B:291:TYR:H	1.43	0.65
18:2:2002:CLA:O1D	18:2:2007:CLA:H42	1.97	0.65
18:3:3001:CLA:HBA2	27:3:3501:LUT:H24	1.78	0.65
12:K:72:ALA:HB3	18:K:1001:CLA:CGA	2.26	0.65
13:2:191:THR:O	13:2:192:ASP:HB2	1.96	0.65
15:1:85:ARG:HD2	18:1:1001:CLA:C3C	2.26	0.65
15:1:146:GLU:OE2	15:1:149:ARG:NH1	2.29	0.65
18:1:1003:CLA:O1A	18:1:1003:CLA:HBD	1.97	0.65
1:A:441:ALA:O	1:A:445:HIS:ND1	2.30	0.65
12:K:70:MET:CE	12:K:71:VAL:HA	2.26	0.65
13:2:199:LEU:HD23	13:2:199:LEU:C	2.22	0.65
13:2:239:HIS:ND1	13:2:244:THR:O	2.29	0.65
14:4:140:THR:O	14:4:144:ILE:HG13	1.96	0.65
16:3:65:LEU:O	16:3:68:LEU:HD22	1.97	0.65
22:L:6019:BCR:H311	22:L:6019:BCR:HC8	1.79	0.65
9:D:115:MET:HE1	9:D:130:LEU:HD11	1.78	0.65
12:K:75:THR:HG21	12:K:129:GLY:N	2.12	0.65
18:2:2004:CLA:H13	27:2:2502:LUT:H393	1.78	0.65
15:1:41:TRP:HD1	15:1:59:PHE:C	2.04	0.65
16:3:267:ASN:C	16:3:270:THR:HG1	2.02	0.65
18:3:3005:CLA:H93	18:3:3012:CLA:C4	2.25	0.65
3:I:6:SER:O	3:I:9:VAL:HG23	1.97	0.65
13:2:262:ILE:CD1	18:2:2003:CLA:H43	2.27	0.65
27:4:4503:LUT:H28	27:4:4503:LUT:H361	1.79	0.65
15:1:166:ASP:CG	15:1:169:GLY:HA2	2.21	0.65
16:3:234:ALA:O	16:3:238:ILE:HG22	1.97	0.65
2:B:560:ASP:CG	8:C:66:ARG:HH12	2.05	0.64
18:F:1302:CLA:HBB1	18:F:1302:CLA:HHC	1.79	0.64
14:4:223:ASN:O	14:4:225:THR:N	2.30	0.64
18:4:4009:CLA:H2A	18:4:4009:CLA:O2D	1.98	0.64
16:3:63:GLN:OE1	16:3:78:PHE:HD2	1.80	0.64
16:3:74:GLY:HA2	16:3:225:LEU:CD2	2.27	0.64
16:3:231:GLY:O	16:3:235:MET:HG3	1.97	0.64
18:3:3005:CLA:HED1	18:3:3005:CLA:H12	1.79	0.64
15:1:98:GLU:CA	15:1:102:LEU:HB3	2.26	0.64
16:3:121:TYR:O	16:3:124:LYS:HB2	1.96	0.64
1:A:629:ASN:ND2	1:A:631:GLN:OE1	2.30	0.64
2:B:373:THR:HB	18:B:1224:CLA:HMB1	1.78	0.64
28:4:4010:CHL:HBB1	28:4:4013:CHL:HBB2	1.79	0.64
6:G:114:VAL:HG11	18:G:1002:CLA:CAA	2.26	0.64
18:2:2002:CLA:H2A	18:2:2002:CLA:O1A	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:2010:CHL:O2D	28:2:2010:CHL:H2A	1.96	0.64
15:1:105:TRP:H	15:1:105:TRP:CD1	2.13	0.64
15:1:202:GLN:HE21	15:1:202:GLN:CA	2.10	0.64
18:B:1229:CLA:H61	22:F:6016:BCR:H393	1.79	0.64
9:D:176:GLU:H	9:D:176:GLU:CD	2.06	0.64
18:4:4006:CLA:NB	27:4:4503:LUT:H172	2.13	0.64
16:3:75:ASP:OD1	16:3:77:GLY:N	2.30	0.64
16:3:117:ILE:HD13	16:3:252:PRO:HG2	1.78	0.64
16:3:216:ASP:N	16:3:216:ASP:OD1	2.27	0.64
7:L:169:ARG:HD2	7:L:171:LYS:CB	2.28	0.64
13:2:218:ARG:O	13:2:222:ILE:HD13	1.98	0.64
18:2:2007:CLA:H2A	18:2:2007:CLA:O1D	1.98	0.64
18:4:4008:CLA:HHC	18:4:4008:CLA:HBB1	1.78	0.64
28:4:4010:CHL:HBB1	28:4:4013:CHL:CBB	2.27	0.64
16:3:105:ASN:ND2	18:3:3012:CLA:OBD	2.30	0.64
16:3:225:LEU:N	16:3:226:LYS:HZ2	1.94	0.64
5:F:207:VAL:HB	18:F:1301:CLA:HED2	1.79	0.64
22:L:6019:BCR:H23C	22:L:6019:BCR:H382	1.79	0.64
15:1:98:GLU:N	15:1:102:LEU:HB3	2.12	0.64
16:3:144:PRO:HG2	16:3:145:ALA:H	1.61	0.64
11:H:132:PRO:HD2	11:H:133:PRO:HD3	1.79	0.64
21:2:2801:LHG:HC42	22:3:3503:BCR:H281	1.80	0.64
14:4:72:GLY:HA2	23:4:4801:LMG:O5	1.97	0.64
14:4:225:THR:HG22	14:4:227:LYS:H	1.61	0.64
18:1:1002:CLA:O2D	18:1:1002:CLA:H2A	1.98	0.64
1:A:24:ARG:HD3	1:A:76:ARG:HH22	1.63	0.64
7:L:176:LEU:C	7:L:178:THR:HG22	2.23	0.64
13:2:186:ASN:OD1	18:2:2016:CLA:HMA1	1.98	0.64
29:4:4505:ZEX:H41	18:1:1014:CLA:O1A	1.98	0.64
18:A:1151:CLA:HAB	18:A:1122:CLA:HHB	1.80	0.64
18:A:1131:CLA:HAB	18:A:1132:CLA:HHB	1.79	0.64
13:2:135:PRO:HG2	18:2:2006:CLA:CED	2.27	0.64
16:3:259:HIS:HA	16:3:266:ASN:HB2	1.80	0.64
18:3:3003:CLA:H122	18:3:3003:CLA:H91	1.80	0.64
4:J:10:VAL:HA	4:J:14:ALA:HB2	1.79	0.63
7:L:211:TYR:HE2	18:L:1503:CLA:C2	2.12	0.63
13:2:131:ILE:HB	13:2:133:LEU:HD11	1.78	0.63
16:3:110:MET:HE1	16:3:230:ASN:O	1.98	0.63
1:A:34:TRP:HE3	4:J:8:LEU:HD22	1.63	0.63
27:4:4501:LUT:H28	27:4:4501:LUT:C37	2.28	0.63
15:1:79:SER:HB2	18:1:1012:CLA:HED2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:111:LEU:CD2	18:3:3006:CLA:HBB1	2.27	0.63
18:3:3001:CLA:HBB1	27:3:3501:LUT:H32	1.79	0.63
7:L:211:TYR:HE2	18:L:1503:CLA:C3	2.12	0.63
18:4:4009:CLA:HBB1	18:4:4009:CLA:CHC	2.11	0.63
18:4:4005:CLA:HMD1	18:4:4012:CLA:C4C	2.29	0.63
15:1:130:THR:CG2	15:1:132:PRO:HD2	2.26	0.63
28:1:1010:CHL:HHC	28:1:1010:CHL:HBB1	1.78	0.63
7:L:96:LEU:HD12	11:H:94:THR:HG21	1.81	0.63
11:H:72:SER:OG	11:H:73:ASP:N	2.25	0.63
13:2:202:ASP:OD2	13:2:205:GLY:HA2	1.99	0.63
15:1:97:PRO:HB2	15:1:102:LEU:HD22	1.79	0.63
27:1:1502:LUT:H28	27:1:1502:LUT:C37	2.28	0.63
16:3:136:TRP:CG	16:3:137:PHE:N	2.66	0.63
18:B:1204:CLA:H51	27:I:6018:LUT:O23	1.99	0.63
18:B:1229:CLA:HAB	18:B:1230:CLA:CMB	2.27	0.63
13:2:186:ASN:CB	18:2:2016:CLA:HMA2	2.25	0.63
13:2:204:LEU:HB3	13:2:206:TRP:NE1	2.14	0.63
15:1:146:GLU:CG	15:1:149:ARG:HH11	2.10	0.63
15:1:169:GLY:O	15:1:172:LYS:HG3	1.99	0.63
18:L:1502:CLA:HBA1	18:L:1502:CLA:CHA	2.27	0.63
12:K:71:VAL:CG1	12:K:132:ILE:HB	2.29	0.63
13:2:131:ILE:CB	13:2:133:LEU:HG	2.28	0.63
16:3:110:MET:HE2	27:3:3501:LUT:H15	1.81	0.63
18:A:1139:CLA:H43	18:A:1138:CLA:H171	1.80	0.63
18:B:1220:CLA:HAB	18:B:1227:CLA:HMD2	1.80	0.63
3:I:5:PRO:C	3:I:7:LEU:H	2.07	0.63
6:G:94:GLU:HB2	6:G:98:VAL:N	2.13	0.63
8:C:54:CYS:SG	8:C:55:GLU:N	2.72	0.63
16:3:65:LEU:HD23	16:3:66:SER:H	1.63	0.63
18:3:3003:CLA:H92	18:3:3003:CLA:C2C	2.29	0.63
2:B:351:HIS:HB3	18:B:1214:CLA:HED2	1.80	0.63
4:J:16:THR:HG21	22:J:6013:BCR:C40	2.29	0.63
7:L:133:ALA:O	7:L:136:GLY:N	2.30	0.63
7:L:145:LEU:CD2	22:L:6019:BCR:H403	2.26	0.63
7:L:163:SER:O	7:L:172:GLN:HG2	1.99	0.63
13:2:193:VAL:HG23	13:2:194:GLY:N	2.04	0.63
15:1:211:LEU:CD1	15:1:212:GLU:H	2.12	0.63
1:A:604:TRP:CH2	18:A:1022:CLA:HAB	2.34	0.62
6:G:95:GLN:HG3	6:G:95:GLN:O	1.98	0.62
13:2:186:ASN:CG	18:2:2016:CLA:H2A	2.24	0.62
14:4:105:GLY:N	18:4:4006:CLA:HBB2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:170:PRO:HB3	18:4:4016:CLA:NA	2.12	0.62
15:1:151:MET:O	15:1:151:MET:HG3	1.97	0.62
16:3:257:LEU:O	16:3:261:ALA:N	2.30	0.62
18:3:3006:CLA:HBB1	18:3:3006:CLA:CHC	2.27	0.62
18:3:3012:CLA:HBC2	18:3:3012:CLA:HMC1	1.81	0.62
9:D:139:LEU:O	9:D:139:LEU:HD23	1.99	0.62
12:K:85:LEU:CB	12:K:118:THR:HG21	2.29	0.62
18:2:2003:CLA:C1B	27:2:2501:LUT:H383	2.28	0.62
18:2:2006:CLA:C4	18:2:2006:CLA:H71	2.28	0.62
23:2:2802:LMG:O2	23:2:2802:LMG:H292	1.98	0.62
16:3:193:GLY:HA3	16:3:207:PHE:CD2	2.33	0.62
1:A:205:HIS:CD2	18:A:1111:CLA:HMC2	2.34	0.62
6:G:76:ARG:HG3	6:G:77:PHE:CD1	2.34	0.62
6:G:149:LYS:HB2	6:G:149:LYS:HZ2	1.64	0.62
7:L:121:ARG:C	7:L:124:GLU:H	2.07	0.62
18:L:1501:CLA:HBD	18:L:1501:CLA:CBA	2.29	0.62
15:1:111:TRP:NE1	15:1:119:ALA:HB2	2.14	0.62
15:1:127:PRO:HG2	15:1:128:TRP:NE1	2.14	0.62
15:1:143:ALA:HA	18:1:1012:CLA:HAB	1.79	0.62
16:3:190:LEU:HB2	16:3:207:PHE:HZ	1.63	0.62
6:G:116:LYS:HB2	18:G:1002:CLA:C4D	2.29	0.62
13:2:197:GLY:CA	18:2:2001:CLA:HED1	2.29	0.62
28:4:4013:CHL:HHC	28:4:4013:CHL:HBB1	1.80	0.62
15:1:146:GLU:O	15:1:149:ARG:HB2	1.98	0.62
16:3:94:GLU:CD	16:3:96:ARG:H	2.01	0.62
18:3:3010:CLA:HMB2	18:3:3013:CLA:HAB	1.81	0.62
18:A:1237:CLA:HMD3	22:A:6017:BCR:H393	1.81	0.62
18:A:1110:CLA:HBC3	18:A:1111:CLA:HAB	1.81	0.62
2:B:5:LEU:HD22	3:I:28:VAL:HG22	1.82	0.62
13:2:88:ASP:OD1	27:2:2502:LUT:O23	2.16	0.62
13:2:104:GLN:NE2	13:2:193:VAL:HB	2.15	0.62
18:2:2005:CLA:H41	18:2:2005:CLA:H92	1.79	0.62
15:1:155:PRO:O	15:1:158:LYS:N	2.33	0.62
15:1:162:GLY:N	18:1:1001:CLA:HED2	2.14	0.62
15:1:183:LYS:CD	18:1:1002:CLA:HAA2	2.23	0.62
16:3:225:LEU:O	16:3:225:LEU:HD13	1.99	0.62
16:3:262:ASP:HB3	16:3:265:ASN:ND2	2.15	0.62
18:3:3003:CLA:H11	18:3:3003:CLA:C3D	2.27	0.62
6:G:133:ILE:HA	22:G:2011:BCR:H401	1.81	0.62
14:4:177:LEU:CD1	18:4:4016:CLA:HMD3	2.30	0.62
16:3:134:LEU:CB	16:3:138:GLN:HG3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3003:CLA:HAB	27:3:3501:LUT:H172	1.82	0.62
18:3:3017:CLA:HHC	18:3:3017:CLA:HBB1	1.82	0.62
9:D:173:VAL:HG12	9:D:174:TYR:N	2.14	0.62
13:2:87:PHE:HB3	18:2:2004:CLA:CAD	2.29	0.62
18:4:4016:CLA:HBA1	18:4:4016:CLA:CBD	2.29	0.62
18:A:1110:CLA:CBC	18:A:1111:CLA:HAB	2.29	0.62
18:2:2006:CLA:O1A	28:2:2013:CHL:HMD2	2.00	0.62
14:4:239:ASP:OD2	14:4:242:HIS:HD2	1.82	0.62
13:2:220:LYS:HG2	18:2:2007:CLA:O2D	1.99	0.62
18:3:3001:CLA:O1A	18:3:3001:CLA:H3A	1.99	0.62
28:3:3011:CHL:HAA1	28:3:3011:CHL:CGD	2.29	0.62
18:A:1138:CLA:H111	18:A:1138:CLA:HAB	1.82	0.62
2:B:85:ARG:HD2	2:B:115:ILE:HD13	1.82	0.62
5:F:163:PRO:O	5:F:166:LEU:HB3	1.99	0.62
5:F:218:TYR:HH	14:4:90:TRP:CG	2.17	0.62
7:L:109:PHE:CE1	18:L:1503:CLA:C2C	2.83	0.62
10:E:66:ILE:HG23	10:E:93:VAL:HG11	1.81	0.62
13:2:104:GLN:HE22	13:2:193:VAL:CG2	2.13	0.62
13:2:220:LYS:HA	18:2:2007:CLA:CED	2.30	0.62
13:2:220:LYS:CA	18:2:2007:CLA:HED1	2.30	0.62
16:3:169:GLU:OE2	16:3:169:GLU:HA	1.99	0.62
13:2:123:PRO:HA	13:2:126:LEU:HG	1.82	0.61
14:4:105:GLY:O	14:4:109:MET:HE3	2.00	0.61
18:4:4003:CLA:H93	18:4:4003:CLA:CHC	2.30	0.61
16:3:164:LEU:HD13	22:3:3503:BCR:C35	2.30	0.61
16:3:164:LEU:CB	22:3:3503:BCR:H351	2.26	0.61
9:D:75:LEU:O	9:D:76:ASP:HB2	1.98	0.61
9:D:111:GLN:O	9:D:123:MET:N	2.31	0.61
9:D:158:VAL:O	9:D:159:PHE:HB2	1.99	0.61
11:H:123:LEU:H	11:H:123:LEU:HD12	1.64	0.61
13:2:68:PHE:HB3	13:2:71:SER:HG	1.65	0.61
13:2:165:GLY:O	18:4:4009:CLA:HED2	1.99	0.61
8:C:14:CYS:O	8:C:15:THR:OG1	2.15	0.61
13:2:89:PRO:HD2	27:2:2502:LUT:H221	1.82	0.61
18:2:2001:CLA:H41	18:2:2002:CLA:H3A	1.81	0.61
15:1:158:LYS:HD3	15:1:159:LYS:NZ	2.15	0.61
1:A:354:TRP:HB3	18:A:1103:CLA:HAC1	1.81	0.61
18:B:1222:CLA:H41	18:B:1234:CLA:H43	1.82	0.61
18:2:2005:CLA:H72	18:2:2005:CLA:C4	2.29	0.61
15:1:205:TYR:OH	18:1:1003:CLA:OBD	2.18	0.61
16:3:203:PRO:HD3	28:3:3011:CHL:CMD	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASN:ND2	18:A:1103:CLA:OBD	2.29	0.61
1:A:590:CYS:HB3	19:A:3001:SF4:S2	2.41	0.61
22:B:6005:BCR:H311	18:B:1202:CLA:H42	1.83	0.61
18:B:1206:CLA:H18	27:I:6018:LUT:H403	1.82	0.61
10:E:95:GLN:OE1	10:E:95:GLN:HA	2.00	0.61
18:B:1205:CLA:H102	18:B:1205:CLA:H2	1.83	0.61
11:H:122:ILE:O	11:H:122:ILE:HG22	1.99	0.61
15:1:85:ARG:HD2	18:1:1001:CLA:C4C	2.30	0.61
6:G:98:VAL:O	6:G:99:THR:HG22	2.00	0.61
13:2:105:ALA:CB	18:2:2012:CLA:HED2	2.31	0.61
18:2:2009:CLA:HED1	16:3:167:PHE:O	2.01	0.61
15:1:230:VAL:HG12	15:1:231:LEU:HD23	1.82	0.61
1:A:222:GLN:HA	1:A:226:SER:HB2	1.83	0.61
9:D:134:ARG:O	9:D:135:LYS:HB3	2.01	0.61
18:2:2012:CLA:H12	23:2:2802:LMG:C36	2.30	0.61
18:3:3003:CLA:C2B	27:3:3501:LUT:H173	2.29	0.61
2:B:173:SER:O	2:B:177:HIS:ND1	2.20	0.61
13:2:127:THR:HG21	13:2:247:ILE:HD11	1.83	0.61
16:3:184:LYS:HG2	16:3:185:GLN:CG	2.29	0.61
1:A:358:LEU:HD11	18:A:1128:CLA:HBB1	1.82	0.61
4:J:7:TYR:CZ	23:F:5001:LMG:HC4	2.36	0.61
9:D:140:ALA:O	9:D:143:THR:HG22	2.00	0.61
12:K:81:GLY:O	12:K:82:ARG:HD3	1.99	0.61
15:1:111:TRP:CE2	15:1:119:ALA:CB	2.84	0.61
18:L:1502:CLA:CHD	22:L:6019:BCR:H282	2.31	0.60
13:2:115:LEU:HB2	18:2:2006:CLA:HBB2	1.82	0.60
15:1:211:LEU:HD12	15:1:211:LEU:N	2.16	0.60
16:3:67:TYR:HE2	16:3:84:SER:HB2	1.66	0.60
16:3:155:TYR:CZ	18:3:3010:CLA:CAC	2.83	0.60
2:B:451:LYS:NZ	18:B:1230:CLA:O1D	2.35	0.60
18:G:1001:CLA:HED2	18:G:1001:CLA:CAD	2.31	0.60
18:2:2001:CLA:HBB1	18:2:2001:CLA:CMB	2.31	0.60
18:2:2004:CLA:CMB	18:2:2004:CLA:HBB1	2.31	0.60
16:3:120:GLU:OE2	16:3:253:TYR:N	2.33	0.60
16:3:175:ASP:HB2	28:3:3011:CHL:HAC2	1.82	0.60
18:3:3005:CLA:HBA2	18:3:3005:CLA:O2D	2.00	0.60
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.83	0.60
22:F:6016:BCR:H382	22:F:6016:BCR:C23	2.32	0.60
12:K:83:PHE:HB2	22:K:2011:BCR:C4	2.31	0.60
18:B:1218:CLA:H41	18:B:1218:CLA:H92	1.84	0.60
5:F:150:VAL:HG12	5:F:160:PHE:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:1302:CLA:HHD	18:F:1302:CLA:CBC	2.23	0.60
6:G:116:LYS:HG3	18:G:1002:CLA:C1D	2.30	0.60
7:L:172:GLN:O	7:L:172:GLN:HG3	2.00	0.60
13:2:105:ALA:CA	18:2:2012:CLA:HED2	2.31	0.60
15:1:217:HIS:CE1	15:1:221:PRO:CB	2.85	0.60
2:B:273:MET:O	2:B:277:HIS:ND1	2.34	0.60
7:L:72:PRO:O	7:L:76:SER:OG	2.19	0.60
27:4:4503:LUT:C36	28:1:1009:CHL:H93	2.32	0.60
18:3:3018:CLA:HBB1	18:3:3018:CLA:CMB	2.29	0.60
1:A:274:TRP:O	12:K:141:LYS:HD2	2.01	0.60
2:B:422:LEU:HG	18:B:1236:CLA:HAB	1.82	0.60
13:2:230:LEU:CD2	18:2:2004:CLA:HMC1	2.31	0.60
16:3:105:ASN:ND2	18:3:3012:CLA:HMD1	2.17	0.60
16:3:137:PHE:CE1	16:3:138:GLN:HB3	2.37	0.60
2:B:411:MET:HE1	18:B:1227:CLA:C1D	2.32	0.60
18:B:1205:CLA:HAB	18:B:1206:CLA:HAA2	1.83	0.60
22:J:6013:BCR:C23	22:J:6013:BCR:H403	2.31	0.60
13:2:154:ILE:HG21	18:4:4008:CLA:HED1	1.83	0.60
28:2:2011:CHL:HAA1	28:2:2011:CHL:CBD	2.30	0.60
27:4:4503:LUT:H8	27:4:4503:LUT:C18	2.19	0.60
28:1:1009:CHL:HHC	28:1:1009:CHL:HBB1	1.83	0.60
16:3:74:GLY:CA	16:3:225:LEU:HD22	2.31	0.60
27:3:3501:LUT:H8	27:3:3501:LUT:H171	1.82	0.60
15:1:55:ALA:HB3	15:1:58:ASP:HB2	1.84	0.60
15:1:226:ILE:HG13	18:1:1003:CLA:CMD	2.32	0.60
18:3:3001:CLA:O2A	27:3:3501:LUT:H382	2.01	0.60
18:3:3017:CLA:H2A	18:3:3017:CLA:O2D	2.02	0.60
20:A:5001:PQN:H141	18:A:1139:CLA:HBB2	1.83	0.60
22:A:6008:BCR:C23	18:A:1124:CLA:HAB	2.31	0.60
22:B:6004:BCR:H14C	18:B:1217:CLA:HBB1	1.83	0.60
3:I:24:LEU:HD22	22:L:6019:BCR:H333	1.82	0.60
12:K:70:MET:CE	12:K:71:VAL:HG22	2.31	0.60
14:4:154:ILE:HG13	28:1:1009:CHL:HED1	1.82	0.60
28:4:4011:CHL:HHD	28:4:4011:CHL:CBC	2.28	0.60
15:1:120:THR:HG22	15:1:125:PRO:HA	1.84	0.60
2:B:73:ASN:O	2:B:75:GLU:N	2.35	0.60
2:B:172:GLU:HG3	6:G:93:PRO:HG2	1.84	0.60
16:3:107:ARG:NH1	16:3:227:GLU:OE1	2.35	0.60
18:3:3006:CLA:HMA2	18:3:3013:CLA:HAC2	1.84	0.60
13:2:181:PRO:HD2	18:2:2016:CLA:CBB	2.32	0.59
28:4:4010:CHL:HHD	28:4:4010:CHL:CBC	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:41:TRP:CD1	15:1:59:PHE:CA	2.85	0.59
15:1:80:GLU:HG3	18:1:1004:CLA:NB	2.17	0.59
15:1:88:MET:CB	18:1:1001:CLA:HMC2	2.26	0.59
27:3:3502:LUT:H361	27:3:3502:LUT:C28	2.32	0.59
18:A:1106:CLA:HAB	18:A:1126:CLA:H13	1.83	0.59
2:B:51:PHE:CE1	18:B:1208:CLA:HBB1	2.36	0.59
9:D:100:PHE:CE1	9:D:158:VAL:CB	2.85	0.59
16:3:74:GLY:O	16:3:232:ARG:NH1	2.35	0.59
22:3:3503:BCR:C23	22:3:3503:BCR:H403	2.32	0.59
13:2:85:PHE:HZ	13:2:223:LYS:HE3	1.66	0.59
15:1:58:ASP:CA	18:1:1004:CLA:HED2	2.32	0.59
1:A:546:ALA:O	1:A:550:HIS:ND1	2.34	0.59
22:B:6004:BCR:H311	18:B:1212:CLA:H8	1.84	0.59
13:2:114:MET:HE1	18:2:2001:CLA:CHC	2.32	0.59
28:2:2013:CHL:HAA2	28:2:2013:CHL:HBD	1.85	0.59
14:4:84:ASP:OD1	14:4:86:GLU:N	2.35	0.59
14:4:104:LEU:C	18:4:4006:CLA:CBB	2.74	0.59
14:4:170:PRO:HD2	14:4:172:PHE:O	2.02	0.59
18:4:4004:CLA:H3A	18:4:4004:CLA:O1A	2.01	0.59
15:1:111:TRP:HZ3	18:1:1006:CLA:HED1	1.66	0.59
11:H:72:SER:O	11:H:73:ASP:HB3	2.01	0.59
18:4:4001:CLA:C5	27:4:4501:LUT:H28	2.31	0.59
6:G:114:VAL:HG12	6:G:116:LYS:H	1.68	0.59
13:2:256:ASP:CG	13:2:259:HIS:HD2	2.10	0.59
18:2:2016:CLA:H2A	18:2:2016:CLA:O2A	2.01	0.59
16:3:67:TYR:CE2	16:3:84:SER:CB	2.86	0.59
16:3:135:ALA:H	16:3:138:GLN:CG	2.15	0.59
16:3:268:VAL:HA	16:3:271:SER:HB3	1.84	0.59
2:B:377:TYR:CD2	18:B:1224:CLA:HAB	2.37	0.59
18:4:4005:CLA:HMD1	18:4:4012:CLA:CHD	2.33	0.59
16:3:137:PHE:CD1	16:3:138:GLN:N	2.71	0.59
16:3:155:TYR:CE1	18:3:3010:CLA:HAC2	2.38	0.59
16:3:183:GLY:HA3	16:3:194:PHE:C	2.28	0.59
4:J:25:LEU:O	4:J:29:ILE:HG12	2.02	0.59
9:D:100:PHE:CE1	9:D:158:VAL:CG1	2.85	0.59
15:1:80:GLU:OE2	15:1:189:ARG:NE	2.35	0.59
15:1:183:LYS:HD3	18:1:1002:CLA:HBA2	1.83	0.59
15:1:222:TRP:CH2	18:1:1008:CLA:CMB	2.85	0.59
16:3:104:ILE:HD12	16:3:172:ARG:CZ	2.33	0.59
2:B:334:LEU:HD11	18:B:1226:CLA:HBB1	1.85	0.59
18:B:1222:CLA:HAA2	18:B:1223:CLA:OBD	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:1001:CLA:HBC2	18:K:1001:CLA:CHD	2.30	0.59
15:1:85:ARG:O	18:1:1001:CLA:HBC2	2.03	0.59
15:1:160:TYR:CZ	15:1:181:LYS:HD3	2.38	0.59
16:3:100:TYR:OH	16:3:172:ARG:HD2	2.03	0.59
6:G:129:SER:O	6:G:133:ILE:HG13	2.03	0.59
7:L:124:GLU:O	7:L:126:ALA:N	2.36	0.59
9:D:91:LEU:N	9:D:91:LEU:HD23	2.18	0.59
10:E:111:ASN:OD1	10:E:115:VAL:HG22	2.02	0.59
13:2:139:THR:O	13:2:139:THR:HG22	2.01	0.59
14:4:126:TRP:C	14:4:128:ASP:H	2.11	0.59
15:1:111:TRP:CZ2	18:1:1013:CLA:CBC	2.85	0.59
18:1:1005:CLA:HMD1	18:1:1012:CLA:CHD	2.33	0.59
16:3:127:LEU:O	18:3:3018:CLA:HBC3	2.02	0.59
16:3:246:LEU:HD23	16:3:246:LEU:O	2.03	0.59
18:B:1211:CLA:CMC	18:B:1212:CLA:HAB	2.33	0.58
7:L:211:TYR:CE2	18:L:1503:CLA:C2	2.85	0.58
13:2:110:SER:HB3	13:2:225:GLY:HA3	1.85	0.58
14:4:225:THR:HG23	14:4:227:LYS:H	1.68	0.58
15:1:221:PRO:CG	15:1:222:TRP:CZ3	2.86	0.58
18:1:1001:CLA:HBA1	27:1:1501:LUT:H382	1.85	0.58
16:3:134:LEU:HB3	16:3:138:GLN:HG3	1.85	0.58
2:B:582:TRP:HH2	18:B:1012:CLA:HAB	1.68	0.58
5:F:82:LEU:HB3	5:F:140:CYS:O	2.02	0.58
13:2:262:ILE:HG23	18:2:2003:CLA:HMD2	1.85	0.58
18:2:2007:CLA:H51	18:2:2007:CLA:C9	2.31	0.58
18:1:1001:CLA:H61	27:1:1501:LUT:H30	1.82	0.58
16:3:141:VAL:HG22	16:3:143:PRO:CD	2.32	0.58
16:3:267:ASN:ND2	16:3:270:THR:HG23	2.18	0.58
6:G:76:ARG:CG	6:G:77:PHE:CE1	2.86	0.58
12:K:83:PHE:HB2	22:K:2011:BCR:HC42	1.84	0.58
12:K:86:ALA:HB1	12:K:87:PRO:CD	2.28	0.58
23:4:4801:LMG:O5	23:4:4801:LMG:O4	2.14	0.58
15:1:186:LYS:CE	21:1:1801:LHG:HC41	2.33	0.58
16:3:248:THR:HG22	16:3:249:GLY:O	2.03	0.58
1:A:41:SER:HB3	1:A:44:ILE:HG22	1.84	0.58
6:G:123:ASP:OD1	6:G:123:ASP:N	2.31	0.58
18:G:1001:CLA:H51	22:G:2011:BCR:H341	1.85	0.58
12:K:71:VAL:HG11	12:K:132:ILE:HB	1.85	0.58
13:2:125:PHE:O	13:2:130:GLY:N	2.30	0.58
14:4:95:GLU:HG3	18:4:4004:CLA:C4B	2.33	0.58
6:G:111:TYR:CD1	6:G:111:TYR:N	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:26:LEU:H	8:C:26:LEU:HD22	1.68	0.58
13:2:126:LEU:HD23	13:2:133:LEU:O	2.04	0.58
1:A:218:TRP:HD1	1:A:303:HIS:CD2	2.21	0.58
14:4:120:ILE:HD12	14:4:120:ILE:H	1.68	0.58
27:4:4501:LUT:C8	27:4:4501:LUT:H171	2.34	0.58
2:B:492:ILE:HD11	6:G:146:TYR:CE1	2.38	0.58
18:B:1203:CLA:HHB	18:B:1226:CLA:HAB	1.86	0.58
16:3:161:GLU:CD	18:3:3010:CLA:HAB	2.29	0.58
18:G:1003:CLA:C4B	23:G:2021:LMG:H151	2.33	0.58
13:2:145:TYR:CB	18:2:2006:CLA:H92	2.34	0.58
14:4:223:ASN:O	14:4:224:VAL:HB	2.03	0.58
15:1:41:TRP:CE3	28:1:1009:CHL:HBC3	2.38	0.58
16:3:142:ILE:HD11	18:3:3010:CLA:CBC	2.33	0.58
28:3:3011:CHL:HBB1	28:3:3011:CHL:HHC	1.84	0.58
13:2:135:PRO:HG2	18:2:2006:CLA:HED1	1.86	0.58
15:1:134:ILE:HD11	18:1:1013:CLA:C2D	2.34	0.58
15:1:183:LYS:HZ2	18:1:1002:CLA:CGD	2.17	0.58
18:1:1002:CLA:HMD3	18:1:1007:CLA:C4D	2.33	0.58
22:3:3503:BCR:HC8	22:3:3503:BCR:H323	1.85	0.58
2:B:659:THR:HA	18:B:1023:CLA:HAB	1.85	0.58
18:B:1236:CLA:HED1	18:B:1234:CLA:HMB1	1.84	0.58
5:F:109:TYR:O	5:F:110:ALA:HB3	2.04	0.58
5:F:160:PHE:O	5:F:163:PRO:HD2	2.04	0.58
6:G:92:LEU:HD12	6:G:92:LEU:N	2.02	0.58
7:L:143:ILE:O	7:L:146:THR:HG22	2.04	0.58
12:K:72:ALA:CB	18:K:1001:CLA:CGA	2.81	0.58
14:4:153:GLU:CG	14:4:156:ARG:HH11	2.17	0.58
15:1:58:ASP:CG	18:1:1004:CLA:HED2	2.29	0.58
15:1:165:PHE:O	27:1:1501:LUT:H24	2.04	0.58
15:1:177:PHE:CD2	15:1:181:LYS:HE2	2.38	0.58
18:3:3001:CLA:CBA	27:3:3501:LUT:H24	2.34	0.58
16:3:162:MET:HE2	16:3:162:MET:CA	2.21	0.57
16:3:185:GLN:C	16:3:186:TYR:HD1	2.12	0.57
28:4:4011:CHL:HHC	28:4:4011:CHL:HBB1	1.85	0.57
15:1:85:ARG:HE	18:1:1001:CLA:C4C	2.17	0.57
16:3:146:GLY:C	16:3:147:THR:HG1	2.04	0.57
16:3:197:SER:OG	16:3:198:GLY:N	2.37	0.57
16:3:210:PRO:HB2	16:3:211:LEU:CD1	2.34	0.57
2:B:707:LEU:HD23	25:B:7101:DGD:HA21	1.85	0.57
7:L:91:THR:HA	7:L:175:GLN:HE22	1.69	0.57
9:D:88:THR:O	9:D:88:THR:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2008:CLA:HHC	18:2:2008:CLA:CBB	2.34	0.57
14:4:158:GLN:NE2	14:4:158:GLN:HA	2.17	0.57
14:4:178:PRO:O	14:4:179:ALA:HB2	2.04	0.57
16:3:94:GLU:OE1	16:3:96:ARG:HB2	2.04	0.57
16:3:119:PRO:HB2	16:3:133:ALA:HB2	1.86	0.57
1:A:707:ILE:HD13	18:A:1138:CLA:HMD2	1.85	0.57
4:J:36:ALA:CB	23:J:5001:LMG:H111	2.30	0.57
18:G:1003:CLA:H91	18:G:1003:CLA:C14	2.35	0.57
10:E:104:VAL:HG12	10:E:119:ASN:OD1	2.03	0.57
12:K:90:ASN:O	16:3:64:SER:HB3	2.04	0.57
13:2:110:SER:O	13:2:114:MET:HG3	2.04	0.57
14:4:57:LEU:HD11	18:4:4009:CLA:CED	2.35	0.57
14:4:103:MET:HB2	18:4:4001:CLA:CMC	2.34	0.57
16:3:62:LYS:O	16:3:63:GLN:HB2	2.04	0.57
16:3:62:LYS:HB2	16:3:63:GLN:OE1	2.04	0.57
18:B:1216:CLA:HAA2	18:B:1221:CLA:HBB1	1.86	0.57
22:J:6012:BCR:H383	22:J:6012:BCR:C23	2.28	0.57
7:L:121:ARG:HG2	7:L:127:GLY:N	2.20	0.57
7:L:204:LEU:HD13	7:L:204:LEU:C	2.28	0.57
18:L:1502:CLA:HHD	22:L:6019:BCR:H292	1.87	0.57
9:D:155:PHE:CZ	9:D:168:HIS:HB3	2.39	0.57
11:H:132:PRO:N	11:H:133:PRO:HD3	2.18	0.57
12:K:136:VAL:HG12	12:K:140:LEU:HD21	1.86	0.57
15:1:58:ASP:CB	18:1:1004:CLA:HED2	2.35	0.57
16:3:267:ASN:HA	18:3:3003:CLA:O1A	2.05	0.57
18:A:1138:CLA:HAA2	18:B:1228:CLA:HMB2	1.86	0.57
18:G:1003:CLA:H62	23:G:2021:LMG:H132	1.84	0.57
9:D:76:ASP:CB	9:D:77:PRO:HB3	2.30	0.57
18:4:4017:CLA:HMC1	29:4:4505:ZEX:H393	1.85	0.57
16:3:110:MET:CE	27:3:3501:LUT:H201	2.35	0.57
1:A:24:ARG:NH1	1:A:76:ARG:HH12	2.03	0.57
3:I:4:LEU:CD1	3:I:6:SER:H	2.15	0.57
11:H:107:GLY:C	11:H:110:THR:HG22	2.30	0.57
13:2:87:PHE:HE2	27:2:2502:LUT:C36	2.14	0.57
14:4:101:TRP:CE2	28:4:4011:CHL:HED3	2.39	0.57
14:4:184:TYR:O	18:4:4001:CLA:HED2	2.04	0.57
18:4:4006:CLA:C1B	27:4:4503:LUT:C17	2.83	0.57
15:1:124:ASN:N	15:1:124:ASN:OD1	2.38	0.57
16:3:100:TYR:O	16:3:100:TYR:HD1	1.87	0.57
16:3:136:TRP:CD2	16:3:137:PHE:N	2.72	0.57
18:3:3010:CLA:H93	18:3:3010:CLA:C3C	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:PHE:HB2	21:A:5003:LHG:HC42	1.86	0.57
18:A:1127:CLA:H91	18:A:1117:CLA:H92	1.86	0.57
18:B:1211:CLA:HHC	18:B:1211:CLA:HBB1	1.85	0.57
18:2:2005:CLA:O1D	18:2:2012:CLA:H61	2.05	0.57
18:4:4003:CLA:H121	18:4:4003:CLA:H91	1.85	0.57
18:4:4008:CLA:HBC2	18:4:4008:CLA:CHD	2.34	0.57
28:4:4013:CHL:HBB1	27:4:4502:LUT:H161	1.86	0.57
15:1:127:PRO:CG	15:1:128:TRP:CD1	2.85	0.57
16:3:101:GLY:CA	18:3:3012:CLA:HED2	2.35	0.57
9:D:167:LEU:O	9:D:170:LYS:HB2	2.04	0.57
15:1:111:TRP:CD1	15:1:112:ALA:N	2.72	0.57
18:1:1011:CLA:H43	27:1:1501:LUT:O23	2.04	0.57
16:3:65:LEU:HB3	16:3:68:LEU:CD2	2.34	0.57
16:3:253:TYR:O	16:3:256:LEU:HB3	2.04	0.57
1:A:204:ASN:HB3	18:A:1118:CLA:HMD2	1.86	0.57
18:B:1240:CLA:HED3	18:B:1220:CLA:HHB	1.86	0.57
6:G:102:GLU:O	6:G:103:ALA:HB3	2.05	0.57
18:G:1003:CLA:H51	23:G:2021:LMG:C31	2.25	0.57
7:L:115:VAL:HG13	7:L:127:GLY:O	2.05	0.57
13:2:197:GLY:HA2	18:2:2001:CLA:HED1	1.86	0.57
18:2:2005:CLA:HED2	18:2:2012:CLA:O1A	2.05	0.57
15:1:205:TYR:HE2	18:1:1003:CLA:O1D	1.88	0.57
15:1:223:HIS:CD2	15:1:223:HIS:N	2.73	0.57
7:L:171:LYS:O	7:L:172:GLN:HB3	2.04	0.56
18:L:1501:CLA:HED2	11:H:82:GLN:NE2	2.20	0.56
18:2:2001:CLA:CGA	18:2:2001:CLA:H3A	2.35	0.56
14:4:147:ILE:HD11	21:1:1801:LHG:C36	2.35	0.56
14:4:240:PRO:HG2	18:4:4008:CLA:C2B	2.34	0.56
15:1:133:THR:HG22	15:1:137:ILE:HD11	1.87	0.56
15:1:167:PRO:HD2	27:1:1501:LUT:H1	1.70	0.56
16:3:136:TRP:CE2	16:3:137:PHE:HB3	2.38	0.56
1:A:493:GLN:HG3	1:A:515:TRP:HD1	1.68	0.56
13:2:143:GLN:CB	13:2:145:TYR:CE1	2.85	0.56
13:2:164:GLU:HA	13:2:167:ARG:H	1.70	0.56
13:2:211:PRO:O	13:2:212:GLN:CB	2.52	0.56
28:4:4013:CHL:CBB	27:4:4502:LUT:H161	2.34	0.56
16:3:185:GLN:HB2	16:3:186:TYR:CE1	2.39	0.56
1:A:310:PHE:HZ	18:A:1117:CLA:H121	1.70	0.56
27:I:6018:LUT:H162	22:I:6020:BCR:H353	1.87	0.56
18:G:1003:CLA:C3	23:G:2021:LMG:H331	2.35	0.56
18:G:1003:CLA:H52	23:G:2021:LMG:C33	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:1003:CLA:C4	23:G:2021:LMG:H332	2.36	0.56
9:D:97:VAL:O	9:D:97:VAL:HG12	2.05	0.56
18:2:2009:CLA:HHC	18:2:2009:CLA:CBB	2.18	0.56
14:4:88:LEU:O	14:4:92:VAL:HG23	2.05	0.56
18:4:4005:CLA:HAB	27:4:4502:LUT:H35	1.86	0.56
15:1:41:TRP:HD1	15:1:59:PHE:O	1.87	0.56
15:1:83:HIS:HD2	27:1:1502:LUT:H35	1.69	0.56
18:1:1005:CLA:HMD3	18:1:1012:CLA:ND	2.20	0.56
16:3:110:MET:SD	16:3:231:GLY:CA	2.92	0.56
16:3:259:HIS:ND1	18:3:3003:CLA:HAA2	2.20	0.56
1:A:40:PHE:HB3	18:A:1102:CLA:HED2	1.87	0.56
1:A:364:MET:HE3	18:A:1119:CLA:H93	1.87	0.56
13:2:125:PHE:HB3	13:2:131:ILE:HD12	1.88	0.56
16:3:65:LEU:HB2	16:3:68:LEU:HD21	1.83	0.56
18:G:1001:CLA:C4	22:G:2011:BCR:H342	2.35	0.56
11:H:133:PRO:HD2	11:H:135:LEU:N	2.21	0.56
13:2:129:LEU:HD22	13:2:131:ILE:HG13	1.87	0.56
15:1:111:TRP:CE2	15:1:119:ALA:HB1	2.40	0.56
15:1:170:TYR:HE2	27:1:1501:LUT:H372	1.70	0.56
16:3:263:PRO:HG3	18:3:3008:CLA:HMB1	1.86	0.56
2:B:476:VAL:HG12	2:B:477:LEU:H	1.71	0.56
7:L:116:LYS:HD3	18:L:1503:CLA:CMB	2.35	0.56
9:D:168:HIS:HA	9:D:169:PRO:C	2.30	0.56
9:D:192:ILE:HG23	10:E:80:GLU:CD	2.31	0.56
10:E:102:PRO:HG2	10:E:103:VAL:HG23	1.88	0.56
18:2:2002:CLA:HBB1	18:2:2002:CLA:CMB	2.34	0.56
18:4:4017:CLA:H3A	29:4:4505:ZEX:H202	1.88	0.56
15:1:127:PRO:C	15:1:128:TRP:CD1	2.83	0.56
16:3:226:LYS:HE2	18:3:3007:CLA:HED2	1.84	0.56
18:3:3003:CLA:H42	18:3:3003:CLA:CHD	2.35	0.56
13:2:141:GLY:HA2	28:2:2013:CHL:CBC	2.35	0.56
14:4:215:PHE:CE1	27:4:4502:LUT:H10	2.40	0.56
18:4:4005:CLA:CMD	18:4:4012:CLA:C1D	2.83	0.56
27:4:4503:LUT:H371	27:4:4503:LUT:H28	1.86	0.56
15:1:160:TYR:CE2	15:1:181:LYS:HD3	2.40	0.56
15:1:203:SER:O	15:1:204:ALA:HB3	2.05	0.56
28:1:1010:CHL:HBB2	18:1:1013:CLA:HBB2	1.88	0.56
1:A:373:ALA:HB2	1:A:399:HIS:HB2	1.88	0.56
18:B:1238:CLA:H13	27:I:6018:LUT:C19	2.36	0.56
9:D:202:LYS:O	9:D:203:PHE:HB2	2.04	0.56
12:K:70:MET:HE2	12:K:71:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:97:VAL:HG21	14:4:156:ARG:NH2	2.21	0.56
16:3:167:PHE:O	16:3:171:ARG:HG3	2.05	0.56
22:B:6004:BCR:H292	18:B:1218:CLA:C4D	2.36	0.56
11:H:107:GLY:HA2	11:H:110:THR:CG2	2.36	0.56
12:K:86:ALA:CB	12:K:87:PRO:CD	2.84	0.56
18:2:2005:CLA:OBD	18:2:2012:CLA:HBA2	2.05	0.56
16:3:225:LEU:HB3	16:3:226:LYS:HE3	1.88	0.56
10:E:78:ARG:O	10:E:79:GLN:HB2	2.05	0.56
18:2:2001:CLA:CGA	18:2:2001:CLA:C3A	2.83	0.56
14:4:113:GLU:CD	14:4:230:PHE:HB3	2.30	0.56
16:3:190:LEU:O	16:3:194:PHE:N	2.38	0.56
18:B:1204:CLA:O2A	3:I:12:VAL:HG21	2.05	0.55
18:B:1219:CLA:HMB2	18:1:1005:CLA:H41	1.87	0.55
18:G:1001:CLA:HED3	18:G:1001:CLA:CHA	2.35	0.55
7:L:145:LEU:HD11	22:L:6019:BCR:C39	2.20	0.55
13:2:126:LEU:HB2	13:2:134:THR:HA	1.87	0.55
18:2:2004:CLA:HHC	27:2:2502:LUT:H32	1.88	0.55
14:4:169:ASP:HA	18:4:4016:CLA:O1D	2.06	0.55
16:3:197:SER:HB2	16:3:203:PRO:C	2.32	0.55
16:3:235:MET:O	16:3:238:ILE:HG23	2.06	0.55
16:3:263:PRO:HG3	18:3:3008:CLA:CMB	2.36	0.55
18:3:3003:CLA:C3B	27:3:3501:LUT:C17	2.84	0.55
1:A:21:ILE:HD13	18:A:1108:CLA:HAA2	1.87	0.55
21:A:5003:LHG:H302	18:A:1122:CLA:H152	1.89	0.55
22:F:6014:BCR:H23C	22:F:6014:BCR:C40	2.36	0.55
7:L:90:ARG:O	7:L:98:ARG:HD3	2.06	0.55
11:H:95:LYS:O	11:H:96:ARG:HB3	2.06	0.55
14:4:52:LYS:O	14:4:53:LYS:HB3	2.06	0.55
28:4:4011:CHL:HBC2	28:4:4011:CHL:CHD	2.29	0.55
18:A:1105:CLA:HHC	18:A:1105:CLA:HBB1	1.89	0.55
18:A:1134:CLA:H92	18:A:1134:CLA:H2	1.87	0.55
2:B:26:ALA:HB2	25:B:7101:DGD:HA32	1.89	0.55
2:B:292:ARG:HH21	6:G:107:ARG:NH1	2.04	0.55
22:K:2011:BCR:H321	22:K:2011:BCR:C8	2.15	0.55
13:2:120:ILE:C	13:2:123:PRO:HD2	2.31	0.55
18:4:4007:CLA:H2A	18:4:4007:CLA:HED2	1.87	0.55
15:1:118:GLN:O	15:1:119:ALA:HB3	2.06	0.55
18:1:1001:CLA:H3A	18:1:1001:CLA:CGA	2.35	0.55
16:3:135:ALA:H	16:3:138:GLN:CD	2.14	0.55
1:A:92:TRP:HE1	18:A:1106:CLA:HBA1	1.72	0.55
18:A:1022:CLA:H161	22:A:6017:BCR:H321	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:6017:BCR:H292	20:B:5002:PQN:H142	1.89	0.55
4:J:28:GLU:CD	18:J:1302:CLA:ND	2.64	0.55
4:J:38:THR:O	23:J:5001:LMG:H122	2.05	0.55
13:2:142:GLU:HG3	13:2:142:GLU:O	2.06	0.55
16:3:134:LEU:CB	16:3:138:GLN:CG	2.84	0.55
1:A:223:VAL:HG23	1:A:224:HIS:CD2	2.42	0.55
18:G:1003:CLA:H91	18:G:1003:CLA:H142	1.88	0.55
7:L:169:ARG:CZ	7:L:171:LYS:CB	2.85	0.55
13:2:197:GLY:HA2	18:2:2001:CLA:CED	2.36	0.55
18:2:2016:CLA:CAD	18:2:2016:CLA:HED2	2.36	0.55
18:4:4001:CLA:H51	27:4:4501:LUT:H30	1.89	0.55
16:3:65:LEU:CD2	16:3:66:SER:H	2.19	0.55
16:3:74:GLY:HA2	16:3:225:LEU:HD22	1.87	0.55
16:3:221:LYS:C	16:3:223:LEU:H	2.14	0.55
18:3:3006:CLA:C1D	18:3:3018:CLA:CBB	2.84	0.55
18:3:3010:CLA:H93	18:3:3010:CLA:C1C	2.37	0.55
9:D:100:PHE:CE1	9:D:158:VAL:HG11	2.41	0.55
9:D:109:LYS:HG2	9:D:110:GLU:N	2.22	0.55
11:H:134:LYS:O	11:H:135:LEU:HG	2.06	0.55
13:2:139:THR:HA	28:2:2010:CHL:CED	2.35	0.55
16:3:140:GLY:HA2	18:3:3013:CLA:CBC	2.32	0.55
18:B:1204:CLA:H11	27:I:6018:LUT:O23	2.07	0.55
18:B:1206:CLA:HBB1	18:B:1206:CLA:HMB1	1.88	0.55
22:J:6012:BCR:H23C	22:J:6012:BCR:C38	2.30	0.55
18:2:2004:CLA:HBC2	18:2:2004:CLA:HHD	1.88	0.55
14:4:103:MET:HE2	27:4:4501:LUT:H15	1.87	0.55
27:4:4503:LUT:H361	28:1:1009:CHL:H62	1.89	0.55
15:1:126:VAL:CB	15:1:127:PRO:CA	2.83	0.55
16:3:110:MET:CE	27:3:3501:LUT:C20	2.85	0.55
16:3:267:ASN:HB2	18:3:3003:CLA:O1A	2.07	0.55
12:K:132:ILE:O	12:K:136:VAL:HG23	2.07	0.55
18:4:4004:CLA:CBB	27:4:4502:LUT:H32	2.36	0.55
16:3:131:GLU:OE2	18:3:3018:CLA:HMA3	2.06	0.55
1:A:555:ILE:HG12	18:B:1023:CLA:HMD3	1.89	0.55
22:G:2011:BCR:C23	22:G:2011:BCR:C40	2.85	0.55
11:H:110:THR:HG23	11:H:111:LEU:N	2.20	0.55
18:2:2003:CLA:C3B	27:2:2501:LUT:C38	2.85	0.55
27:4:4501:LUT:C8	27:4:4501:LUT:C17	2.85	0.55
15:1:89:LEU:C	15:1:92:PRO:HD2	2.32	0.55
18:1:1001:CLA:CBB	27:1:1501:LUT:C32	2.85	0.55
16:3:65:LEU:CD1	16:3:67:TYR:HE1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:203:PRO:HD3	28:3:3011:CHL:HMD3	1.88	0.55
18:3:3003:CLA:C2B	27:3:3501:LUT:C17	2.84	0.55
18:3:3005:CLA:CMD	18:3:3012:CLA:C1D	2.84	0.55
18:3:3006:CLA:CHA	18:3:3006:CLA:CED	2.85	0.55
22:F:6014:BCR:C40	22:F:6014:BCR:C23	2.85	0.55
7:L:94:ASN:HB3	7:L:97:LEU:HD12	1.83	0.55
9:D:100:PHE:CD1	9:D:158:VAL:HB	2.41	0.55
18:2:2001:CLA:H3A	18:2:2001:CLA:O1A	2.06	0.55
16:3:134:LEU:HB3	16:3:138:GLN:CG	2.36	0.55
1:A:434:ARG:O	1:A:438:HIS:ND1	2.33	0.54
18:G:1001:CLA:CHA	18:G:1001:CLA:CED	2.85	0.54
7:L:121:ARG:O	7:L:124:GLU:N	2.38	0.54
18:2:2002:CLA:CGA	18:2:2002:CLA:CED	2.84	0.54
14:4:186:GLY:O	14:4:189:PHE:HB2	2.07	0.54
27:4:4502:LUT:C17	27:4:4502:LUT:C8	2.86	0.54
15:1:134:ILE:CD1	18:1:1013:CLA:C2D	2.85	0.54
15:1:230:VAL:HG12	15:1:231:LEU:CD2	2.36	0.54
18:1:1005:CLA:HMD1	18:1:1012:CLA:C1D	2.37	0.54
16:3:208:PHE:HB3	18:3:3001:CLA:CMD	2.37	0.54
16:3:232:ARG:HD2	18:3:3004:CLA:C4C	2.37	0.54
18:3:3003:CLA:CHC	18:3:3003:CLA:C9	2.85	0.54
18:3:3013:CLA:CMA	22:3:3503:BCR:C35	2.85	0.54
8:C:14:CYS:SG	8:C:16:GLN:HG2	2.48	0.54
10:E:78:ARG:NH1	10:E:124:GLU:OE1	2.40	0.54
12:K:75:THR:HG21	12:K:129:GLY:HA2	1.88	0.54
13:2:118:ALA:CB	18:2:2006:CLA:CMC	2.85	0.54
14:4:118:ILE:HG23	14:4:120:ILE:H	1.72	0.54
18:4:4006:CLA:C4B	27:4:4503:LUT:C17	2.86	0.54
18:1:1001:CLA:CGA	18:1:1001:CLA:C3A	2.85	0.54
16:3:104:ILE:HD12	16:3:172:ARG:NH2	2.21	0.54
16:3:129:PRO:O	16:3:132:THR:HG22	2.07	0.54
16:3:141:VAL:HG13	16:3:144:PRO:HD2	1.88	0.54
16:3:185:GLN:C	16:3:186:TYR:CD1	2.85	0.54
16:3:196:GLY:O	16:3:197:SER:HB3	2.06	0.54
28:3:3011:CHL:CBD	28:3:3011:CHL:CAA	2.85	0.54
18:3:3017:CLA:H3A	18:3:3017:CLA:O2A	2.06	0.54
1:A:274:TRP:CH2	18:A:1115:CLA:HBB1	2.42	0.54
2:B:254:ILE:HG13	2:B:255:LEU:HG	1.88	0.54
13:2:125:PHE:CB	13:2:131:ILE:HD12	2.37	0.54
14:4:241:TRP:CE3	18:4:4008:CLA:HMA2	2.42	0.54
18:4:4007:CLA:HED2	18:4:4007:CLA:CAA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:85:ARG:NE	18:1:1001:CLA:C4C	2.71	0.54
18:B:1207:CLA:H92	7:L:132:LEU:HG	1.90	0.54
6:G:95:GLN:O	6:G:96:ASN:HB2	2.07	0.54
18:G:1001:CLA:C5	22:G:2011:BCR:C34	2.85	0.54
7:L:102:VAL:CG1	7:L:106:HIS:HD1	2.21	0.54
13:2:92:LEU:CD1	27:2:2502:LUT:C24	2.85	0.54
18:2:2016:CLA:CBD	18:2:2016:CLA:CGA	2.85	0.54
14:4:133:GLU:C	14:4:134:TYR:CD1	2.86	0.54
18:4:4003:CLA:C1C	18:4:4003:CLA:H61	2.38	0.54
16:3:101:GLY:CA	18:3:3012:CLA:CED	2.85	0.54
18:3:3003:CLA:C9	18:3:3003:CLA:C12	2.85	0.54
1:A:213:LEU:HD22	22:A:6002:BCR:H361	1.89	0.54
18:A:1106:CLA:H62	18:A:1126:CLA:H92	1.89	0.54
18:B:1224:CLA:CGA	18:B:1224:CLA:H3A	2.37	0.54
23:F:5002:LMG:H292	18:1:1014:CLA:C1D	2.38	0.54
8:C:61:ASP:HB2	10:E:118:ASN:CG	2.32	0.54
18:2:2003:CLA:CHD	18:2:2003:CLA:C4	2.85	0.54
28:2:2011:CHL:CBB	18:2:2016:CLA:CAB	2.86	0.54
14:4:198:LEU:HD12	14:4:198:LEU:N	2.21	0.54
15:1:80:GLU:OE2	15:1:189:ARG:NH2	2.39	0.54
15:1:183:LYS:HG2	18:1:1007:CLA:HED2	1.89	0.54
18:1:1005:CLA:CMD	18:1:1012:CLA:C1D	2.85	0.54
12:K:70:MET:CE	12:K:71:VAL:CG2	2.85	0.54
13:2:197:GLY:CA	18:2:2001:CLA:CED	2.85	0.54
14:4:152:VAL:CG1	28:4:4011:CHL:C1B	2.85	0.54
14:4:155:ARG:NH1	28:1:1009:CHL:OBD	2.41	0.54
15:1:88:MET:CE	18:1:1001:CLA:CAB	2.85	0.54
15:1:134:ILE:HD11	18:1:1013:CLA:C3D	2.38	0.54
18:1:1003:CLA:H12	18:1:1008:CLA:CMD	2.37	0.54
16:3:117:ILE:CD1	16:3:252:PRO:HB2	2.38	0.54
18:3:3002:CLA:HBC2	18:3:3002:CLA:CMC	2.37	0.54
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.90	0.54
2:B:225:LEU:O	2:B:230:TRP:NE1	2.35	0.54
13:2:178:ASN:HD22	13:2:179:THR:N	2.05	0.54
13:2:211:PRO:C	13:2:212:GLN:HG3	2.32	0.54
16:3:67:TYR:HE2	16:3:84:SER:HB3	1.72	0.54
16:3:120:GLU:OE2	16:3:254:GLN:N	2.31	0.54
16:3:179:PRO:HG2	16:3:180:GLY:H	1.71	0.54
18:3:3010:CLA:C1C	18:3:3010:CLA:C9	2.85	0.54
1:A:268:PRO:HD2	1:A:277:TYR:CZ	2.43	0.54
3:I:4:LEU:HD11	3:I:6:SER:CB	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:1002:CLA:HBD	18:G:1002:CLA:HBA2	1.89	0.54
18:G:1003:CLA:C5	23:G:2021:LMG:C33	2.85	0.54
18:2:2005:CLA:CBC	18:2:2012:CLA:CBC	2.85	0.54
18:2:2007:CLA:CBB	22:3:3503:BCR:C26	2.85	0.54
14:4:152:VAL:HG11	28:4:4011:CHL:CHB	2.38	0.54
18:4:4016:CLA:C4D	18:4:4016:CLA:C1	2.86	0.54
15:1:120:THR:HG22	15:1:125:PRO:N	2.23	0.54
18:3:3013:CLA:CBB	27:3:3502:LUT:C18	2.86	0.54
22:3:3503:BCR:C32	22:3:3503:BCR:C8	2.86	0.54
22:J:6012:BCR:C23	22:J:6012:BCR:C38	2.85	0.54
18:G:1001:CLA:H51	22:G:2011:BCR:C34	2.38	0.54
12:K:79:PHE:O	12:K:80:ALA:HB2	2.07	0.54
13:2:125:PHE:CB	13:2:131:ILE:CD1	2.86	0.54
13:2:188:LEU:HD13	13:2:188:LEU:C	2.32	0.54
13:2:225:GLY:O	13:2:229:MET:HG3	2.08	0.54
13:2:233:MET:HG2	18:2:2004:CLA:H193	1.89	0.54
28:2:2013:CHL:O2A	28:2:2013:CHL:H2A	2.07	0.54
14:4:169:ASP:CB	18:4:4016:CLA:C2D	2.85	0.54
14:4:170:PRO:CB	18:4:4016:CLA:C4A	2.85	0.54
18:4:4007:CLA:CHD	18:4:4007:CLA:CBC	2.86	0.54
15:1:40:ASP:N	15:1:47:ARG:HD2	2.23	0.54
15:1:225:ASN:C	15:1:225:ASN:HD22	2.15	0.54
1:A:266:ALA:HB3	16:3:272:LEU:HD13	1.90	0.54
2:B:306:GLU:HA	2:B:320:LYS:HG2	1.90	0.54
18:B:1240:CLA:HED1	22:B:6009:BCR:H353	1.89	0.54
22:F:6014:BCR:H23C	22:F:6014:BCR:H402	1.88	0.54
28:2:2011:CHL:HBB2	18:2:2016:CLA:CBB	2.38	0.54
18:2:2012:CLA:HMB1	18:2:2012:CLA:CBB	2.34	0.54
16:3:132:THR:O	16:3:134:LEU:HD23	2.07	0.54
16:3:134:LEU:HB3	16:3:138:GLN:OE1	2.07	0.54
2:B:6:PRO:HG3	2:B:24:GLY:HA2	1.88	0.53
2:B:523:ILE:HD13	18:B:1234:CLA:HAB	1.90	0.53
6:G:114:VAL:HG11	18:G:1002:CLA:CBA	2.38	0.53
7:L:102:VAL:HG12	7:L:106:HIS:HD1	1.72	0.53
14:4:151:TYR:CD1	14:4:151:TYR:C	2.85	0.53
18:4:4006:CLA:C3B	27:4:4502:LUT:C18	2.85	0.53
18:4:4008:CLA:HHC	18:4:4008:CLA:CBB	2.37	0.53
18:G:1003:CLA:C3	23:G:2021:LMG:C33	2.85	0.53
7:L:116:LYS:HD3	18:L:1503:CLA:HMB1	1.88	0.53
7:L:169:ARG:HD2	7:L:171:LYS:H	1.72	0.53
13:2:104:GLN:NE2	13:2:193:VAL:CG2	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:101:TRP:CZ2	28:4:4011:CHL:HED3	2.43	0.53
14:4:225:THR:HG21	14:4:232:ASN:OD1	2.09	0.53
18:4:4001:CLA:HBC2	18:4:4001:CLA:HHD	1.89	0.53
28:1:1009:CHL:H2A	28:1:1009:CHL:CED	2.39	0.53
1:A:126:ILE:HB	22:J:6013:BCR:H322	1.90	0.53
7:L:94:ASN:HB2	7:L:97:LEU:CD1	2.23	0.53
13:2:67:TRP:NE1	13:2:86:GLY:O	2.41	0.53
18:2:2008:CLA:CHD	18:2:2008:CLA:CBC	2.85	0.53
27:4:4503:LUT:H181	27:4:4503:LUT:C8	2.10	0.53
15:1:58:ASP:CB	18:1:1004:CLA:CED	2.86	0.53
15:1:112:ALA:HB3	28:1:1010:CHL:HMD2	1.91	0.53
18:1:1003:CLA:C2	18:1:1008:CLA:CMD	2.85	0.53
18:3:3006:CLA:CMD	18:3:3018:CLA:CAB	2.87	0.53
21:A:7001:LHG:H252	18:A:1128:CLA:H42	1.89	0.53
7:L:91:THR:HA	7:L:98:ARG:HH21	1.71	0.53
13:2:188:LEU:CD2	13:2:198:GLY:HA3	2.24	0.53
16:3:119:PRO:C	16:3:133:ALA:CB	2.82	0.53
28:3:3011:CHL:CBA	28:3:3011:CHL:CBD	2.85	0.53
1:A:269:PHE:HD2	1:A:270:PHE:HD1	1.55	0.53
22:A:6002:BCR:H331	18:A:1112:CLA:HHB	1.90	0.53
18:B:1229:CLA:HAB	18:B:1230:CLA:HMB1	1.90	0.53
9:D:82:PRO:HG3	9:D:128:ASN:HD21	1.72	0.53
18:2:2001:CLA:H43	18:2:2002:CLA:HBA1	1.85	0.53
18:2:2002:CLA:CMC	18:2:2002:CLA:CBC	2.86	0.53
14:4:120:ILE:CD1	14:4:120:ILE:H	2.22	0.53
14:4:199:GLU:HA	14:4:202:GLU:HG3	1.90	0.53
18:4:4004:CLA:H3A	18:4:4004:CLA:CGA	2.38	0.53
18:3:3008:CLA:HBA1	18:3:3008:CLA:CBD	2.38	0.53
18:B:1209:CLA:HBB1	18:B:1209:CLA:HMB1	1.89	0.53
7:L:90:ARG:HA	11:H:72:SER:OG	2.09	0.53
7:L:206:VAL:O	7:L:207:LEU:HB2	2.09	0.53
9:D:76:ASP:HB3	9:D:77:PRO:HA	1.88	0.53
13:2:220:LYS:CE	18:2:2002:CLA:CED	2.85	0.53
13:2:242:THR:HG22	13:2:242:THR:O	2.08	0.53
13:2:246:PRO:O	13:2:249:ASN:HB2	2.09	0.53
14:4:135:PHE:O	14:4:136:ALA:HB3	2.09	0.53
18:4:4016:CLA:HBA1	18:4:4016:CLA:CHA	2.39	0.53
23:4:4801:LMG:HC72	23:4:4801:LMG:O2	2.07	0.53
15:1:152:GLU:HG3	15:1:156:GLU:HA	1.91	0.53
16:3:67:TYR:CE2	16:3:84:SER:HB2	2.43	0.53
16:3:110:MET:SD	16:3:231:GLY:N	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLY:HA2	18:A:1118:CLA:HBC1	1.91	0.53
1:A:493:GLN:HG3	1:A:515:TRP:CD1	2.43	0.53
27:I:6018:LUT:H181	27:I:6018:LUT:H8	1.90	0.53
13:2:122:ILE:HG23	13:2:133:LEU:HD22	1.90	0.53
13:2:177:VAL:CG2	13:2:178:ASN:N	2.72	0.53
13:2:197:GLY:N	18:2:2001:CLA:CED	2.72	0.53
18:2:2005:CLA:H41	18:2:2005:CLA:C9	2.39	0.53
18:4:4002:CLA:CMA	18:4:4002:CLA:C1	2.85	0.53
15:1:221:PRO:CG	15:1:222:TRP:CE3	2.85	0.53
16:3:94:GLU:CD	16:3:96:ARG:N	2.65	0.53
16:3:119:PRO:HB2	16:3:133:ALA:HB1	1.89	0.53
16:3:193:GLY:HA3	16:3:207:PHE:CE2	2.44	0.53
16:3:227:GLU:HB2	18:3:3001:CLA:C1B	2.39	0.53
16:3:259:HIS:N	16:3:266:ASN:ND2	2.57	0.53
13:2:181:PRO:HD2	18:2:2016:CLA:HBB1	1.91	0.53
18:2:2003:CLA:CGA	18:2:2003:CLA:C1A	2.87	0.53
14:4:245:ILE:HG12	14:4:249:LEU:HD12	1.89	0.53
15:1:104:ASN:ND2	15:1:208:THR:HG23	2.24	0.53
15:1:120:THR:HG22	15:1:125:PRO:CA	2.38	0.53
18:1:1001:CLA:C4D	27:1:1501:LUT:H383	2.39	0.53
18:1:1004:CLA:HBB2	27:1:1502:LUT:H12	1.86	0.53
18:A:1106:CLA:H42	18:A:1126:CLA:HMD2	1.90	0.53
18:A:1121:CLA:C2D	22:K:2011:BCR:H323	2.38	0.53
2:B:389:HIS:HA	2:B:392:ILE:HD12	1.91	0.53
18:B:1238:CLA:H18	27:I:6018:LUT:H203	1.90	0.53
18:F:1301:CLA:HHC	18:F:1301:CLA:CBB	2.37	0.53
6:G:149:LYS:HB2	6:G:149:LYS:HZ1	1.71	0.53
18:L:1502:CLA:C3C	22:L:6019:BCR:H282	2.39	0.53
22:L:6019:BCR:C38	22:L:6019:BCR:C23	2.85	0.53
8:C:26:LEU:HD22	8:C:26:LEU:N	2.23	0.53
10:E:66:ILE:HB	10:E:95:GLN:OE1	2.08	0.53
16:3:226:LYS:CE	16:3:226:LYS:N	2.72	0.53
16:3:253:TYR:CD1	16:3:253:TYR:C	2.85	0.53
3:I:29:GLU:HB2	7:L:151:SER:OG	2.08	0.53
4:J:9:SER:O	4:J:10:VAL:HG22	2.09	0.53
9:D:173:VAL:HG12	9:D:174:TYR:H	1.72	0.53
13:2:87:PHE:CE2	27:2:2502:LUT:C36	2.86	0.53
13:2:250:LEU:HD23	13:2:254:LEU:HD21	1.89	0.53
18:3:3006:CLA:CMA	18:3:3013:CLA:C3C	2.85	0.53
18:A:1134:CLA:H3A	18:A:1116:CLA:H93	1.91	0.52
10:E:104:VAL:HG12	10:E:119:ASN:CG	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:145:VAL:O	15:1:148:GLN:HB2	2.08	0.52
15:1:202:GLN:NE2	15:1:202:GLN:CA	2.71	0.52
18:3:3018:CLA:HBC2	18:3:3018:CLA:CMC	2.39	0.52
1:A:90:PHE:HE2	1:A:178:MET:HE3	1.73	0.52
1:A:268:PRO:HA	1:A:271:THR:HG22	1.91	0.52
2:B:422:LEU:HG	18:B:1236:CLA:CAB	2.39	0.52
6:G:108:ALA:HB1	6:G:111:TYR:CE1	2.41	0.52
13:2:139:THR:CA	28:2:2010:CHL:CED	2.84	0.52
13:2:230:LEU:HD21	18:2:2004:CLA:CMC	2.39	0.52
18:2:2006:CLA:HMA3	28:2:2013:CHL:HAC2	1.91	0.52
14:4:239:ASP:CG	14:4:242:HIS:HD2	2.17	0.52
15:1:42:MET:SD	15:1:45:GLN:HG3	2.50	0.52
15:1:97:PRO:C	15:1:102:LEU:HB2	2.34	0.52
18:1:1003:CLA:H12	18:1:1008:CLA:HMD2	1.90	0.52
16:3:217:GLU:C	16:3:219:SER:N	2.68	0.52
16:3:223:LEU:C	16:3:226:LYS:HG2	2.34	0.52
28:3:3011:CHL:O1D	28:3:3011:CHL:H2A	2.09	0.52
1:A:401:TRP:NE1	18:A:1126:CLA:HAB	2.24	0.52
18:A:1101:CLA:ND	4:J:12:PRO:HG3	2.24	0.52
2:B:373:THR:HG23	2:B:591:THR:HG21	1.91	0.52
2:B:636:THR:HG22	2:B:638:LEU:H	1.75	0.52
18:G:1001:CLA:CAB	22:G:2011:BCR:C36	2.86	0.52
8:C:8:TYR:C	8:C:10:THR:H	2.17	0.52
8:C:21:CYS:SG	8:C:24:ASP:N	2.83	0.52
13:2:149:THR:HG21	28:2:2010:CHL:HMD1	1.91	0.52
18:2:2012:CLA:C1	23:2:2802:LMG:C36	2.87	0.52
18:4:4001:CLA:HBC2	18:4:4001:CLA:CHD	2.40	0.52
18:4:4003:CLA:O1A	18:4:4003:CLA:HBD	2.08	0.52
18:3:3004:CLA:CGA	18:3:3004:CLA:C3A	2.87	0.52
18:3:3006:CLA:CMB	18:3:3013:CLA:C4B	2.87	0.52
18:A:1138:CLA:H121	18:F:1301:CLA:HAC1	1.90	0.52
23:B:5005:LMG:H111	18:B:1227:CLA:HAA2	1.91	0.52
7:L:90:ARG:HB3	7:L:93:VAL:HG23	1.91	0.52
8:C:51:CYS:SG	8:C:53:ARG:HD3	2.49	0.52
10:E:66:ILE:CG2	10:E:67:GLY:N	2.72	0.52
13:2:85:PHE:CD2	18:2:2009:CLA:HBC2	2.44	0.52
13:2:186:ASN:ND2	18:2:2016:CLA:C1A	2.73	0.52
18:2:2006:CLA:CAD	18:2:2006:CLA:C4	2.85	0.52
18:2:2008:CLA:HBB1	18:2:2008:CLA:CHC	2.38	0.52
28:2:2010:CHL:HBB2	18:2:2012:CLA:HBC1	1.91	0.52
27:2:2501:LUT:C37	27:2:2501:LUT:C28	2.85	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:171:ARG:HD3	28:3:3011:CHL:OMC	2.09	0.52
18:3:3008:CLA:HBA1	18:3:3008:CLA:CHA	2.38	0.52
22:A:6011:BCR:H24C	18:B:1230:CLA:HMC2	1.91	0.52
13:2:204:LEU:HB3	13:2:206:TRP:CD1	2.45	0.52
14:4:94:ALA:HB2	18:4:4012:CLA:CED	2.40	0.52
15:1:41:TRP:CE3	28:1:1009:CHL:CBC	2.91	0.52
15:1:94:ILE:HG23	15:1:105:TRP:HB3	1.91	0.52
18:1:1005:CLA:CMD	18:1:1012:CLA:ND	2.72	0.52
16:3:120:GLU:CD	16:3:253:TYR:CB	2.81	0.52
16:3:121:TYR:HA	16:3:253:TYR:CD2	2.44	0.52
16:3:249:GLY:C	16:3:250:VAL:HG23	2.35	0.52
2:B:182:LEU:HD13	18:B:1210:CLA:HHB	1.92	0.52
18:B:1232:CLA:O1A	18:G:1003:CLA:HHB	2.09	0.52
4:J:38:THR:OG1	5:F:136:GLN:NE2	2.42	0.52
22:L:6020:BCR:H342	18:H:1000:CLA:HAB	1.92	0.52
9:D:204:THR:O	9:D:206:LYS:N	2.42	0.52
10:E:79:GLN:HG3	10:E:84:TYR:CZ	2.45	0.52
13:2:89:PRO:HD2	27:2:2502:LUT:C22	2.40	0.52
14:4:94:ALA:N	18:4:4012:CLA:CED	2.73	0.52
15:1:134:ILE:CD1	18:1:1013:CLA:C3D	2.88	0.52
15:1:211:LEU:HD12	15:1:211:LEU:H	1.75	0.52
15:1:226:ILE:O	15:1:229:ASN:N	2.43	0.52
16:3:104:ILE:CD1	16:3:172:ARG:NH2	2.72	0.52
16:3:164:LEU:HD13	22:3:3503:BCR:H352	1.91	0.52
16:3:184:LYS:HG2	16:3:185:GLN:NE2	2.25	0.52
16:3:262:ASP:CB	16:3:265:ASN:ND2	2.73	0.52
16:3:263:PRO:HD2	16:3:264:VAL:H	1.75	0.52
16:3:267:ASN:ND2	16:3:270:THR:CG2	2.73	0.52
18:3:3017:CLA:HAA2	18:3:3017:CLA:CED	2.38	0.52
2:B:680:TRP:NE1	9:D:88:THR:HG23	2.25	0.52
9:D:135:LYS:O	9:D:138:CYS:N	2.43	0.52
9:D:155:PHE:CZ	9:D:168:HIS:CB	2.93	0.52
11:H:113:TYR:C	11:H:115:SER:H	2.16	0.52
12:K:118:THR:HG1	12:K:121:ASP:HB3	1.74	0.52
12:K:120:ALA:HA	12:K:123:LEU:HD12	1.92	0.52
13:2:134:THR:N	13:2:135:PRO:HD2	2.25	0.52
13:2:177:VAL:C	13:2:179:THR:H	2.17	0.52
14:4:105:GLY:C	14:4:109:MET:HE3	2.34	0.52
14:4:147:ILE:HD11	21:1:1801:LHG:H361	1.92	0.52
15:1:130:THR:CG2	15:1:131:LEU:N	2.73	0.52
15:1:222:TRP:NE1	18:1:1008:CLA:CMA	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:94:GLU:OE2	16:3:95:PRO:CD	2.57	0.52
16:3:139:THR:CG2	16:3:140:GLY:N	2.73	0.52
18:3:3013:CLA:HMA3	22:3:3503:BCR:C35	2.39	0.52
1:A:342:GLY:O	1:A:343:HIS:HB2	2.09	0.52
26:B:8002:LMU:O3'	26:B:8002:LMU:O2B	2.19	0.52
6:G:77:PHE:CD1	6:G:77:PHE:N	2.78	0.52
6:G:116:LYS:NZ	18:G:1002:CLA:C4B	2.73	0.52
18:G:1003:CLA:H52	23:G:2021:LMG:C32	2.39	0.52
7:L:176:LEU:CG	7:L:177:GLN:N	2.73	0.52
10:E:122:LEU:H	10:E:122:LEU:CD1	2.05	0.52
18:2:2003:CLA:H2	18:2:2008:CLA:OBD	2.09	0.52
18:2:2005:CLA:OBD	18:2:2012:CLA:H2	2.09	0.52
18:2:2007:CLA:C4C	21:2:2801:LHG:HC62	2.40	0.52
14:4:100:ARG:HA	14:4:103:MET:HG3	1.91	0.52
15:1:82:ILE:CD1	15:1:149:ARG:NH2	2.73	0.52
15:1:85:ARG:CB	18:1:1011:CLA:CED	2.85	0.52
18:1:1001:CLA:CBB	27:1:1501:LUT:H32	2.40	0.52
16:3:210:PRO:HB2	16:3:211:LEU:HD13	1.90	0.52
18:3:3010:CLA:HBD	18:3:3010:CLA:HAA1	1.92	0.52
1:A:397:THR:HG22	18:A:1126:CLA:HAB	1.91	0.52
18:B:1220:CLA:H13	22:B:6009:BCR:H312	1.92	0.52
3:I:9:VAL:O	3:I:13:GLY:N	2.34	0.52
8:C:17:CYS:SG	8:C:18:VAL:N	2.83	0.52
13:2:122:ILE:HG21	13:2:133:LEU:HB2	1.89	0.52
13:2:177:VAL:CG2	13:2:178:ASN:H	2.22	0.52
13:2:220:LYS:HD3	18:2:2002:CLA:CED	2.29	0.52
13:2:234:GLY:O	13:2:238:GLN:HB2	2.10	0.52
15:1:108:ALA:HA	15:1:111:TRP:CZ3	2.45	0.52
18:1:1003:CLA:H11	18:1:1008:CLA:OBD	2.09	0.52
16:3:110:MET:SD	16:3:230:ASN:C	2.93	0.52
16:3:115:GLY:O	16:3:119:PRO:CD	2.57	0.52
18:3:3006:CLA:H12	22:3:3503:BCR:H313	1.91	0.52
18:3:3013:CLA:O2D	18:3:3013:CLA:H2A	2.09	0.52
1:A:272:LEU:HD13	18:K:1001:CLA:HBC1	1.92	0.52
4:J:36:ALA:CB	23:J:5001:LMG:HC72	2.40	0.52
8:C:10:THR:HG23	8:C:64:SER:CB	2.40	0.52
13:2:188:LEU:HD22	13:2:189:THR:CA	2.39	0.52
13:2:216:GLU:O	13:2:220:LYS:HG3	2.09	0.52
15:1:83:HIS:CE1	18:1:1012:CLA:HMD2	2.45	0.52
15:1:116:GLY:O	15:1:118:GLN:HG2	2.10	0.52
16:3:110:MET:HE1	16:3:230:ASN:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:164:LEU:CB	22:3:3503:BCR:C35	2.85	0.52
18:3:3003:CLA:CGA	18:3:3003:CLA:CHA	2.88	0.52
18:3:3006:CLA:C1A	18:3:3006:CLA:CED	2.85	0.52
1:A:33:GLN:HB2	18:A:1109:CLA:HBA1	1.91	0.51
7:L:98:ARG:HH22	7:L:175:GLN:NE2	2.08	0.51
9:D:204:THR:HG22	9:D:206:LYS:CG	2.38	0.51
28:4:4013:CHL:HBC2	28:4:4013:CHL:CHD	2.32	0.51
15:1:104:ASN:ND2	15:1:208:THR:CG2	2.73	0.51
15:1:111:TRP:CE2	15:1:119:ALA:HB2	2.43	0.51
15:1:211:LEU:CD1	15:1:212:GLU:N	2.73	0.51
16:3:174:GLN:OE1	16:3:174:GLN:HA	2.10	0.51
18:3:3003:CLA:C2D	18:3:3003:CLA:C4	2.85	0.51
18:3:3005:CLA:H12	18:3:3005:CLA:CED	2.39	0.51
18:3:3005:CLA:HMD1	18:3:3012:CLA:CHD	2.40	0.51
27:3:3501:LUT:H8	27:3:3501:LUT:C16	2.13	0.51
1:A:686:TRP:CD2	17:A:1011:CL0:H5	2.45	0.51
1:A:686:TRP:HZ3	18:B:1012:CLA:HMD3	1.75	0.51
18:A:1013:CLA:HMD3	2:B:533:ILE:HG12	1.92	0.51
18:A:1139:CLA:H61	4:J:18:TRP:CG	2.45	0.51
18:G:1003:CLA:C5	23:G:2021:LMG:C31	2.85	0.51
7:L:121:ARG:CG	7:L:127:GLY:CA	2.84	0.51
7:L:169:ARG:NH1	7:L:171:LYS:CB	2.73	0.51
22:L:6020:BCR:H19C	18:L:1501:CLA:HMB1	1.92	0.51
9:D:163:GLU:OE2	9:D:164:VAL:N	2.42	0.51
14:4:199:GLU:HG2	14:4:202:GLU:OE1	2.10	0.51
14:4:219:ILE:HG23	14:4:220:ILE:N	2.25	0.51
15:1:127:PRO:CG	15:1:128:TRP:NE1	2.73	0.51
15:1:196:VAL:O	15:1:199:CYS:N	2.43	0.51
18:3:3005:CLA:CMD	18:3:3012:CLA:ND	2.72	0.51
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.39	0.51
18:F:1302:CLA:HHC	18:F:1302:CLA:CBB	2.40	0.51
9:D:211:LEU:N	9:D:211:LEU:CD1	2.72	0.51
13:2:131:ILE:CG2	13:2:132:LEU:H	2.20	0.51
13:2:178:ASN:O	13:2:179:THR:HG23	2.11	0.51
13:2:232:VAL:HG11	27:2:2502:LUT:H12	1.92	0.51
14:4:148:LEU:HB3	27:4:4503:LUT:H15	1.91	0.51
14:4:171:ILE:N	14:4:171:ILE:CD1	2.73	0.51
15:1:232:ILE:CG2	15:1:233:PRO:N	2.73	0.51
16:3:211:LEU:CD1	16:3:211:LEU:N	2.72	0.51
6:G:92:LEU:H	6:G:92:LEU:CD1	1.98	0.51
7:L:91:THR:CB	7:L:175:GLN:NE2	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:174:PRO:CD	13:2:175:GLY:N	2.70	0.51
13:2:220:LYS:NZ	18:2:2002:CLA:CED	2.73	0.51
13:2:222:ILE:N	13:2:222:ILE:CD1	2.73	0.51
18:2:2002:CLA:OBD	18:2:2007:CLA:HBD	2.10	0.51
27:2:2502:LUT:H181	27:2:2502:LUT:C8	2.40	0.51
14:4:120:ILE:CD1	14:4:120:ILE:N	2.72	0.51
14:4:147:ILE:HD13	21:1:1801:LHG:H351	1.92	0.51
27:4:4503:LUT:H363	28:1:1009:CHL:H93	1.86	0.51
15:1:226:ILE:HG13	18:1:1003:CLA:HMD3	1.92	0.51
16:3:153:ASP:OD1	16:3:154:ASN:N	2.44	0.51
22:A:6017:BCR:H353	18:B:1239:CLA:HMB2	1.93	0.51
2:B:255:LEU:HD11	18:B:1212:CLA:HBC1	1.91	0.51
2:B:429:LEU:HD11	18:B:1235:CLA:HMB2	1.91	0.51
6:G:64:ILE:HD12	18:G:1001:CLA:C3D	2.40	0.51
13:2:129:LEU:CD2	13:2:131:ILE:CG1	2.86	0.51
13:2:241:TYR:CE1	13:2:265:ALA:HB3	2.46	0.51
13:2:262:ILE:CD1	18:2:2003:CLA:H11	2.29	0.51
18:2:2016:CLA:HBA2	18:2:2016:CLA:CHA	2.40	0.51
14:4:101:TRP:CE2	28:4:4011:CHL:CED	2.94	0.51
14:4:171:ILE:N	14:4:171:ILE:HD12	2.25	0.51
18:4:4005:CLA:HBC1	18:4:4012:CLA:HBC1	1.92	0.51
16:3:249:GLY:C	16:3:250:VAL:CG2	2.83	0.51
1:A:208:ALA:HB1	18:A:1118:CLA:HBC3	1.93	0.51
1:A:346:LEU:HG	1:A:429:ASN:ND2	2.25	0.51
18:A:1110:CLA:HBD	18:A:1110:CLA:HBA1	1.93	0.51
2:B:177:HIS:HB3	18:B:1210:CLA:HBB1	1.93	0.51
4:J:6:THR:CG2	23:F:5001:LMG:HC72	2.39	0.51
18:F:1301:CLA:HBB1	18:F:1301:CLA:CHC	2.39	0.51
9:D:135:LYS:O	9:D:138:CYS:HB2	2.10	0.51
9:D:191:SER:O	9:D:192:ILE:HB	2.11	0.51
13:2:85:PHE:HD2	18:2:2009:CLA:HBC2	1.75	0.51
13:2:137:TRP:CD1	13:2:137:TRP:H	2.27	0.51
18:2:2004:CLA:H12	18:2:2004:CLA:CHB	2.40	0.51
14:4:113:GLU:OE1	14:4:229:PRO:HG2	2.11	0.51
16:3:65:LEU:HD13	16:3:67:TYR:OH	2.09	0.51
27:3:3501:LUT:H371	27:3:3501:LUT:H28	1.92	0.51
6:G:116:LYS:HE3	18:G:1002:CLA:CHC	2.40	0.51
13:2:108:VAL:HG12	13:2:112:TRP:HD1	1.76	0.51
14:4:206:ALA:HB2	23:4:4801:LMG:HC62	1.92	0.51
15:1:81:LEU:CD1	15:1:159:LYS:HG3	2.41	0.51
16:3:217:GLU:C	16:3:219:SER:H	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:ASN:HD21	1:A:631:GLN:HB2	1.75	0.51
10:E:91:VAL:HB	10:E:104:VAL:HG23	1.92	0.51
13:2:122:ILE:N	13:2:122:ILE:CD1	2.73	0.51
18:2:2005:CLA:H92	18:2:2005:CLA:C4	2.40	0.51
14:4:135:PHE:C	14:4:135:PHE:CD1	2.89	0.51
15:1:97:PRO:C	15:1:102:LEU:CB	2.84	0.51
15:1:202:GLN:HE21	15:1:202:GLN:HA	1.75	0.51
18:1:1008:CLA:CED	18:1:1008:CLA:CHA	2.89	0.51
16:3:183:GLY:HA3	16:3:194:PHE:O	2.11	0.51
18:3:3012:CLA:C1	18:3:3017:CLA:CBB	2.89	0.51
27:3:3502:LUT:C8	27:3:3502:LUT:C16	2.86	0.51
6:G:76:ARG:NE	6:G:116:LYS:NZ	2.59	0.51
6:G:114:VAL:CG1	18:G:1002:CLA:HBA1	2.41	0.51
7:L:207:LEU:O	7:L:208:ASP:HB3	2.11	0.51
11:H:132:PRO:CD	11:H:133:PRO:CD	2.84	0.51
13:2:186:ASN:CG	18:2:2016:CLA:CMA	2.84	0.51
13:2:187:LYS:CG	13:2:188:LEU:H	2.23	0.51
18:2:2002:CLA:C1	18:2:2002:CLA:CED	2.85	0.51
14:4:169:ASP:OD2	18:4:4016:CLA:HMD1	2.10	0.51
15:1:83:HIS:CE1	18:1:1012:CLA:CMD	2.94	0.51
15:1:166:ASP:OD2	15:1:169:GLY:HA2	2.10	0.51
16:3:134:LEU:HB2	16:3:138:GLN:HG3	1.92	0.51
16:3:248:THR:CG2	16:3:255:ASN:HD22	2.17	0.51
16:3:266:ASN:O	16:3:267:ASN:ND2	2.44	0.51
27:3:3502:LUT:H28	27:3:3502:LUT:C36	2.37	0.51
18:B:1216:CLA:CGA	18:B:1221:CLA:HBB1	2.41	0.51
11:H:123:LEU:O	11:H:123:LEU:HD13	2.10	0.51
13:2:130:GLY:O	13:2:131:ILE:HG13	2.10	0.51
18:2:2001:CLA:CGA	18:2:2001:CLA:C4A	2.89	0.51
18:2:2002:CLA:H2A	18:2:2002:CLA:O2D	2.11	0.51
15:1:152:GLU:OE1	15:1:152:GLU:HA	2.11	0.51
16:3:115:GLY:O	16:3:119:PRO:HD3	2.11	0.51
16:3:171:ARG:HD3	28:3:3011:CHL:HBB1	1.93	0.51
16:3:184:LYS:CG	16:3:185:GLN:NE2	2.73	0.51
18:A:1105:CLA:H12	22:J:6013:BCR:H14C	1.93	0.50
12:K:127:THR:O	12:K:131:ILE:HG12	2.11	0.50
13:2:126:LEU:HD12	13:2:126:LEU:C	2.36	0.50
14:4:55:GLU:OE1	14:4:58:PRO:HA	2.11	0.50
14:4:171:ILE:HD13	18:4:4016:CLA:HMA3	1.93	0.50
14:4:228:GLY:O	14:4:232:ASN:ND2	2.45	0.50
15:1:230:VAL:CG1	18:1:1014:CLA:C1B	2.86	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:268:VAL:HG22	18:3:3003:CLA:HMD3	1.93	0.50
1:A:330:ILE:O	1:A:334:HIS:ND1	2.40	0.50
18:G:1003:CLA:H8	18:G:1003:CLA:C13	2.33	0.50
7:L:96:LEU:HD23	7:L:96:LEU:O	2.11	0.50
22:L:6019:BCR:C8	22:L:6019:BCR:H321	2.41	0.50
13:2:85:PHE:CZ	13:2:223:LYS:HE3	2.47	0.50
14:4:152:VAL:HG13	28:4:4011:CHL:C1B	2.41	0.50
18:4:4001:CLA:H3A	18:4:4001:CLA:CGA	2.41	0.50
28:4:4013:CHL:HBA1	27:4:4503:LUT:C10	2.40	0.50
1:A:25:ASP:HB3	1:A:26:PRO:HD2	1.94	0.50
18:B:1238:CLA:H191	3:I:18:ALA:HB2	1.93	0.50
7:L:96:LEU:C	7:L:96:LEU:CD2	2.85	0.50
12:K:137:VAL:N	12:K:140:LEU:HD22	2.26	0.50
13:2:188:LEU:CD2	13:2:197:GLY:C	2.84	0.50
28:4:4013:CHL:CBC	28:4:4013:CHL:CHD	2.85	0.50
18:1:1011:CLA:HBA1	18:1:1011:CLA:CHA	2.39	0.50
16:3:225:LEU:HD13	16:3:225:LEU:C	2.36	0.50
16:3:232:ARG:NH2	18:3:3004:CLA:ND	2.60	0.50
1:A:604:TRP:HH2	18:A:1022:CLA:HAB	1.74	0.50
2:B:71:GLN:OE1	2:B:90:ALA:N	2.37	0.50
9:D:171:ASP:O	9:D:173:VAL:N	2.44	0.50
13:2:92:LEU:HD12	27:2:2502:LUT:C24	2.41	0.50
18:2:2004:CLA:HBB1	18:2:2004:CLA:HMB1	1.94	0.50
18:2:2009:CLA:HBD	18:2:2009:CLA:HAA1	1.92	0.50
14:4:60:LEU:HG	14:4:61:ALA:O	2.10	0.50
18:1:1005:CLA:C3B	27:1:1502:LUT:C14	2.90	0.50
16:3:182:MET:HB3	28:3:3011:CHL:HMC	1.94	0.50
16:3:224:LYS:O	16:3:228:VAL:HG23	2.10	0.50
18:A:1013:CLA:H3A	18:A:1013:CLA:CGA	2.41	0.50
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.92	0.50
7:L:65:PHE:O	9:D:91:LEU:HG	2.11	0.50
13:2:118:ALA:CB	18:2:2006:CLA:HMC1	2.42	0.50
15:1:218:LEU:O	15:1:221:PRO:HD3	2.12	0.50
16:3:110:MET:HE2	27:3:3501:LUT:H201	1.94	0.50
16:3:152:ALA:HB3	16:3:157:LEU:CD2	2.38	0.50
16:3:205:GLY:CA	16:3:208:PHE:N	2.73	0.50
18:3:3003:CLA:CGA	18:3:3003:CLA:C1A	2.89	0.50
18:A:1101:CLA:C4D	4:J:12:PRO:HG3	2.41	0.50
2:B:377:TYR:HD2	18:B:1224:CLA:HAB	1.75	0.50
2:B:438:VAL:HG13	18:B:1012:CLA:H61	1.94	0.50
2:B:572:ALA:HA	2:B:575:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:F:5002:LMG:H292	18:1:1014:CLA:C4D	2.42	0.50
6:G:94:GLU:CB	6:G:98:VAL:H	2.21	0.50
12:K:118:THR:OG1	12:K:121:ASP:HB3	2.12	0.50
13:2:180:ASP:HB3	13:2:183:PHE:O	2.11	0.50
13:2:220:LYS:HE2	18:2:2002:CLA:HED2	1.91	0.50
14:4:236:HIS:CE1	14:4:240:PRO:HB3	2.46	0.50
28:4:4010:CHL:HBB1	28:4:4010:CHL:HHC	1.94	0.50
16:3:67:TYR:CZ	16:3:84:SER:C	2.89	0.50
22:A:6008:BCR:H402	18:A:1119:CLA:H122	1.93	0.50
2:B:65:LEU:HD21	22:B:6006:BCR:H291	1.93	0.50
2:B:551:LYS:C	2:B:553:PHE:H	2.20	0.50
11:H:58:GLU:OE1	11:H:58:GLU:HA	2.10	0.50
18:4:4006:CLA:C2B	27:4:4502:LUT:H183	2.41	0.50
15:1:158:LYS:C	15:1:159:LYS:CD	2.85	0.50
18:1:1003:CLA:HBA1	18:1:1008:CLA:HED2	1.93	0.50
16:3:121:TYR:CD1	16:3:121:TYR:C	2.89	0.50
1:A:511:THR:HG23	18:A:1116:CLA:O1A	2.11	0.50
23:B:5005:LMG:H172	18:B:1228:CLA:HBD	1.93	0.50
18:B:1221:CLA:HBA2	18:B:1202:CLA:H8	1.92	0.50
3:I:29:GLU:HA	3:I:29:GLU:OE2	2.11	0.50
6:G:121:LEU:C	6:G:121:LEU:CD2	2.84	0.50
12:K:78:LEU:O	12:K:80:ALA:N	2.42	0.50
13:2:126:LEU:CB	13:2:133:LEU:HD13	2.24	0.50
13:2:138:TYR:O	13:2:139:THR:HB	2.11	0.50
13:2:161:GLY:HA2	18:2:2012:CLA:CBB	2.42	0.50
18:2:2007:CLA:CMC	18:2:2007:CLA:HBC2	2.42	0.50
14:4:74:ASN:N	14:4:74:ASN:ND2	2.60	0.50
15:1:114:LEU:HD22	15:1:115:PRO:HD2	1.88	0.50
15:1:202:GLN:NE2	15:1:202:GLN:HA	2.27	0.50
16:3:269:LEU:HD11	18:3:3008:CLA:HED3	1.92	0.50
18:3:3003:CLA:O1A	18:3:3003:CLA:HBD	2.10	0.50
21:A:7001:LHG:H331	18:A:1104:CLA:H92	1.93	0.50
18:A:1122:CLA:H71	18:A:1122:CLA:H41	1.93	0.50
18:A:1123:CLA:HBB1	18:A:1119:CLA:H2	1.94	0.50
7:L:91:THR:CA	7:L:175:GLN:NE2	2.73	0.50
7:L:204:LEU:C	7:L:204:LEU:CD1	2.85	0.50
9:D:160:PRO:CD	9:D:161:SER:H	2.25	0.50
18:2:2009:CLA:CED	16:3:171:ARG:CG	2.86	0.50
28:4:4013:CHL:HBD	28:4:4013:CHL:HAA2	1.93	0.50
15:1:102:LEU:O	15:1:104:ASN:N	2.41	0.50
15:1:104:ASN:CG	15:1:208:THR:CG2	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:127:LEU:CB	18:3:3018:CLA:CBC	2.85	0.50
16:3:225:LEU:C	16:3:225:LEU:CD1	2.84	0.50
16:3:225:LEU:HD12	16:3:226:LYS:HE3	1.94	0.50
18:3:3003:CLA:C4D	18:3:3003:CLA:C1	2.85	0.50
18:A:1106:CLA:H2A	18:A:1106:CLA:HED2	1.94	0.49
2:B:529:THR:HG21	2:B:582:TRP:CE2	2.47	0.49
2:B:721:TYR:HB2	18:B:1021:CLA:HED3	1.94	0.49
6:G:76:ARG:NE	6:G:116:LYS:CE	2.73	0.49
7:L:91:THR:CG2	7:L:175:GLN:NE2	2.73	0.49
12:K:61:PHE:O	12:K:64:SER:HB3	2.12	0.49
13:2:79:GLY:HA2	13:2:84:ASP:OD2	2.11	0.49
14:4:103:MET:CE	14:4:207:ASN:C	2.85	0.49
18:4:4001:CLA:C4	18:4:4002:CLA:HMA2	2.41	0.49
18:4:4004:CLA:H111	27:4:4502:LUT:H393	1.94	0.49
18:4:4005:CLA:CMD	18:4:4012:CLA:ND	2.72	0.49
16:3:137:PHE:CD1	16:3:137:PHE:C	2.90	0.49
2:B:592:PHE:HE2	18:B:1021:CLA:H62	1.76	0.49
22:B:6006:BCR:H392	18:B:1211:CLA:H3A	1.94	0.49
9:D:112:ILE:N	9:D:112:ILE:CD1	2.72	0.49
9:D:163:GLU:OE1	9:D:164:VAL:O	2.30	0.49
9:D:195:ASN:ND2	9:D:195:ASN:N	2.60	0.49
14:4:103:MET:HE3	14:4:207:ASN:C	2.36	0.49
16:3:130:GLN:C	16:3:132:THR:H	2.18	0.49
16:3:183:GLY:CA	16:3:194:PHE:C	2.85	0.49
1:A:304:LEU:HD21	18:A:1113:CLA:HMC2	1.95	0.49
22:F:6016:BCR:H382	22:F:6016:BCR:H23C	1.94	0.49
7:L:111:VAL:O	7:L:115:VAL:HG23	2.12	0.49
13:2:77:LEU:HD13	13:2:86:GLY:HA2	1.93	0.49
13:2:250:LEU:CD2	13:2:250:LEU:C	2.85	0.49
18:2:2002:CLA:O2D	18:2:2002:CLA:HAA2	2.13	0.49
18:2:2006:CLA:HMA3	28:2:2013:CHL:C3C	2.41	0.49
18:A:1110:CLA:C4C	18:A:1110:CLA:H42	2.42	0.49
18:B:1238:CLA:H13	27:I:6018:LUT:H193	1.94	0.49
23:G:2021:LMG:O9	23:G:2021:LMG:HC92	2.13	0.49
7:L:90:ARG:HB2	7:L:98:ARG:HD3	1.95	0.49
11:H:123:LEU:HD12	11:H:123:LEU:N	2.26	0.49
22:K:2011:BCR:C32	22:K:2011:BCR:C8	2.85	0.49
13:2:177:VAL:C	13:2:179:THR:N	2.70	0.49
18:2:2004:CLA:H3A	18:2:2004:CLA:CGA	2.42	0.49
18:2:2016:CLA:CBA	18:2:2016:CLA:CBD	2.85	0.49
14:4:57:LEU:HD11	18:4:4009:CLA:HED1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:4003:CLA:HBC2	18:4:4003:CLA:CHD	2.41	0.49
15:1:202:GLN:OE1	15:1:208:THR:HB	2.11	0.49
18:1:1008:CLA:HED2	18:1:1008:CLA:CAD	2.43	0.49
2:B:439:HIS:O	2:B:443:MET:HG2	2.12	0.49
7:L:81:TRP:O	7:L:85:ASN:ND2	2.43	0.49
22:L:6020:BCR:H342	18:H:1000:CLA:CAB	2.42	0.49
9:D:134:ARG:HH22	9:D:136:GLU:CD	2.12	0.49
11:H:131:LEU:HB3	11:H:135:LEU:HD22	1.94	0.49
12:K:124:ALA:CB	22:K:2011:BCR:H343	2.42	0.49
13:2:238:GLN:NE2	18:2:2003:CLA:NA	2.60	0.49
18:2:2003:CLA:HMB1	18:2:2008:CLA:CBC	2.42	0.49
15:1:111:TRP:CG	15:1:119:ALA:HB2	2.47	0.49
1:A:336:GLY:N	21:A:5003:LHG:HC32	2.27	0.49
4:J:2:ARG:O	4:J:3:ASP:HB2	2.11	0.49
4:J:36:ALA:HB1	23:J:5001:LMG:HC72	1.94	0.49
13:2:66:LEU:N	16:3:186:TYR:HE2	2.03	0.49
13:2:147:THR:HG21	14:4:241:TRP:HE3	1.78	0.49
15:1:140:LEU:O	15:1:140:LEU:HD23	2.12	0.49
15:1:226:ILE:HG12	15:1:230:VAL:HG23	1.94	0.49
6:G:130:ILE:O	6:G:134:VAL:HG23	2.12	0.49
9:D:173:VAL:HG21	9:D:179:ASN:OD1	2.13	0.49
13:2:145:TYR:HB2	18:2:2006:CLA:H92	1.95	0.49
13:2:198:GLY:O	13:2:202:ASP:N	2.42	0.49
18:2:2005:CLA:H72	23:2:2802:LMG:H132	1.93	0.49
18:2:2007:CLA:C9	18:2:2007:CLA:C5	2.90	0.49
15:1:158:LYS:O	15:1:159:LYS:HE2	2.13	0.49
15:1:217:HIS:ND1	15:1:221:PRO:HA	2.28	0.49
16:3:151:TRP:NE1	18:3:3013:CLA:OBD	2.37	0.49
16:3:225:LEU:N	16:3:226:LYS:NZ	2.60	0.49
16:3:267:ASN:C	18:3:3003:CLA:HED2	2.37	0.49
18:B:1222:CLA:CAD	18:B:1234:CLA:HBB1	2.43	0.49
9:D:131:LYS:NZ	11:H:63:THR:O	2.46	0.49
18:2:2007:CLA:HBC2	18:2:2007:CLA:HMC3	1.95	0.49
14:4:147:ILE:CD1	21:1:1801:LHG:C36	2.91	0.49
28:4:4010:CHL:HBC2	28:4:4010:CHL:CHD	2.26	0.49
15:1:193:LEU:C	15:1:193:LEU:CD2	2.85	0.49
15:1:205:TYR:C	15:1:207:GLY:N	2.71	0.49
16:3:187:PHE:CZ	18:3:3019:CLA:C4B	2.95	0.49
1:A:80:SER:OG	1:A:186:TYR:HB2	2.12	0.49
1:A:368:LEU:HD11	18:A:1117:CLA:H71	1.95	0.49
1:A:684:PHE:CG	22:A:6011:BCR:H363	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LYS:NZ	5:F:229:LYS:O	2.40	0.49
18:A:1123:CLA:HBA1	18:A:1127:CLA:H191	1.94	0.49
18:B:1205:CLA:O1A	18:B:1224:CLA:HBD	2.13	0.49
13:2:133:LEU:CD1	13:2:133:LEU:C	2.85	0.49
13:2:232:VAL:HG11	27:2:2502:LUT:H10	1.94	0.49
28:2:2013:CHL:H2A	28:2:2013:CHL:O1D	2.12	0.49
14:4:94:ALA:CA	18:4:4012:CLA:CED	2.85	0.49
14:4:103:MET:HE2	27:4:4501:LUT:C15	2.42	0.49
18:4:4004:CLA:HBB1	27:4:4502:LUT:H30	1.95	0.49
28:4:4011:CHL:H11	27:4:4501:LUT:H383	1.93	0.49
15:1:222:TRP:CD1	18:1:1008:CLA:HMA2	2.48	0.49
16:3:67:TYR:CE1	16:3:85:ASP:HA	2.48	0.49
18:B:1208:CLA:H12	18:B:1209:CLA:C4D	2.43	0.49
6:G:95:GLN:C	6:G:97:GLY:H	2.20	0.49
7:L:65:PHE:CE1	9:D:115:MET:HE1	2.48	0.49
7:L:67:GLY:O	9:D:88:THR:HA	2.12	0.49
7:L:90:ARG:NH2	18:L:1501:CLA:HAC2	2.28	0.49
7:L:174:ASP:CG	7:L:175:GLN:HG2	2.38	0.49
13:2:118:ALA:O	13:2:121:PHE:N	2.46	0.49
14:4:109:MET:HE1	14:4:215:PHE:HD1	1.75	0.49
18:1:1008:CLA:C4D	18:1:1008:CLA:CED	2.85	0.49
16:3:68:LEU:N	16:3:68:LEU:CD1	2.73	0.49
16:3:169:GLU:HG3	18:3:3012:CLA:C4B	2.43	0.49
1:A:438:HIS:HA	9:D:88:THR:OG1	2.13	0.48
2:B:224:PRO:HB3	2:B:232:LEU:HD22	1.93	0.48
22:B:6004:BCR:H351	22:B:6004:BCR:H15C	1.59	0.48
18:B:1203:CLA:H8	25:B:7101:DGD:HBH2	1.95	0.48
7:L:118:GLY:O	7:L:122:ASN:ND2	2.46	0.48
7:L:125:ILE:O	7:L:125:ILE:HG22	2.12	0.48
10:E:76:ILE:HG22	10:E:78:ARG:H	1.78	0.48
11:H:107:GLY:HA2	11:H:110:THR:HG21	1.94	0.48
15:1:106:VAL:HG23	15:1:208:THR:HG21	1.89	0.48
15:1:222:TRP:CD1	18:1:1008:CLA:CMA	2.96	0.48
18:1:1003:CLA:C1	18:1:1008:CLA:HMD2	2.43	0.48
28:3:3011:CHL:HBD	28:3:3011:CHL:CAA	2.43	0.48
1:A:595:TRP:CD1	18:A:1128:CLA:HMD1	2.48	0.48
18:A:1110:CLA:O1A	16:3:81:LEU:HD22	2.13	0.48
18:B:1218:CLA:H41	18:B:1218:CLA:H61	1.67	0.48
7:L:90:ARG:HB3	7:L:93:VAL:CG2	2.43	0.48
7:L:132:LEU:HD12	7:L:132:LEU:C	2.35	0.48
18:L:1502:CLA:HAC2	22:L:6019:BCR:C29	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:70:TRP:CG	8:C:71:HIS:H	2.30	0.48
28:2:2013:CHL:HAA2	28:2:2013:CHL:CBD	2.43	0.48
23:2:2802:LMG:O9	23:2:2802:LMG:HC92	2.14	0.48
29:4:4505:ZEX:H173	15:1:200:VAL:HG13	1.95	0.48
18:3:3012:CLA:H12	18:3:3017:CLA:HBB2	1.94	0.48
18:B:1220:CLA:HMD3	18:B:1221:CLA:HHC	1.95	0.48
6:G:132:HIS:ND1	22:G:2011:BCR:H19C	2.27	0.48
18:G:1001:CLA:C6	22:G:2011:BCR:C34	2.85	0.48
13:2:220:LYS:HA	18:2:2007:CLA:HED2	1.94	0.48
14:4:113:GLU:CD	14:4:230:PHE:CB	2.86	0.48
18:A:1013:CLA:O2A	2:B:427:LEU:HA	2.12	0.48
2:B:350:GLN:HG3	18:B:1222:CLA:HED2	1.95	0.48
2:B:414:HIS:ND1	2:B:414:HIS:O	2.46	0.48
22:B:6006:BCR:H393	18:B:1211:CLA:HMA2	1.96	0.48
4:J:16:THR:HG21	22:J:6013:BCR:H401	1.95	0.48
9:D:129:LEU:HD23	9:D:129:LEU:O	2.12	0.48
9:D:166:TYR:CE2	9:D:170:LYS:HA	2.49	0.48
14:4:241:TRP:CD2	18:4:4008:CLA:HMA2	2.49	0.48
27:4:4503:LUT:C28	27:4:4503:LUT:C37	2.86	0.48
16:3:70:GLY:HA2	16:3:75:ASP:OD2	2.13	0.48
16:3:174:GLN:HB3	16:3:182:MET:HE3	1.94	0.48
18:3:3003:CLA:CAB	27:3:3501:LUT:C17	2.90	0.48
18:3:3006:CLA:HMB3	18:3:3013:CLA:CHC	2.43	0.48
1:A:218:TRP:HA	18:A:1112:CLA:HBB1	1.94	0.48
1:A:581:CYS:SG	2:B:562:PRO:HG3	2.53	0.48
18:B:1230:CLA:O1D	4:J:35:ASP:HA	2.13	0.48
4:J:23:ALA:O	4:J:27:ILE:HG13	2.13	0.48
18:F:1302:CLA:CHD	18:F:1302:CLA:CBC	2.86	0.48
7:L:102:VAL:HG13	7:L:106:HIS:ND1	2.29	0.48
12:K:137:VAL:HA	12:K:140:LEU:HD23	1.89	0.48
18:2:2004:CLA:C5	27:2:2502:LUT:C38	2.85	0.48
18:2:2005:CLA:H41	18:2:2005:CLA:C8	2.44	0.48
28:4:4011:CHL:CBC	28:4:4011:CHL:CHD	2.89	0.48
15:1:88:MET:CB	18:1:1001:CLA:CMC	2.88	0.48
15:1:88:MET:HB3	27:1:1501:LUT:C34	2.43	0.48
16:3:136:TRP:CZ2	16:3:137:PHE:HB3	2.49	0.48
16:3:182:MET:HE2	16:3:182:MET:N	2.28	0.48
18:3:3003:CLA:C12	18:3:3003:CLA:H93	2.44	0.48
18:3:3006:CLA:C2D	18:3:3018:CLA:CBB	2.91	0.48
1:A:81:ALA:HB1	18:A:1103:CLA:HBB1	1.96	0.48
7:L:149:GLY:HA3	7:L:182:TRP:CD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:102:ASN:OD1	18:2:2004:CLA:H11	2.12	0.48
16:3:158:PHE:HB2	18:3:3010:CLA:CMC	2.42	0.48
16:3:250:VAL:HG12	16:3:254:GLN:HG2	1.94	0.48
18:A:1022:CLA:H143	18:B:1207:CLA:HBC3	1.95	0.48
18:A:1125:CLA:H51	18:A:1125:CLA:H11	1.69	0.48
2:B:44:GLN:NE2	2:B:162:LYS:HD2	2.29	0.48
2:B:387:PHE:HB3	2:B:534:LEU:HB3	1.96	0.48
3:I:17:PRO:O	3:I:21:MET:HG3	2.13	0.48
9:D:163:GLU:CD	9:D:164:VAL:N	2.72	0.48
13:2:191:THR:CG2	13:2:192:ASP:H	2.24	0.48
16:3:197:SER:HB2	16:3:203:PRO:O	2.14	0.48
2:B:59:LEU:HG	18:B:1204:CLA:HBB2	1.96	0.48
6:G:109:LYS:HG3	6:G:110:GLU:HG3	1.96	0.48
6:G:144:ASN:ND2	18:G:1003:CLA:CED	2.73	0.48
18:G:1001:CLA:C5	22:G:2011:BCR:H343	2.44	0.48
10:E:107:PHE:N	10:E:107:PHE:CD1	2.82	0.48
12:K:71:VAL:HG12	12:K:129:GLY:O	2.09	0.48
13:2:120:ILE:CG2	27:2:2501:LUT:H373	2.38	0.48
13:2:238:GLN:NE2	18:2:2003:CLA:C4D	2.77	0.48
14:4:108:GLY:O	14:4:112:PRO:HD2	2.14	0.48
15:1:91:VAL:HB	15:1:92:PRO:HD3	1.96	0.48
15:1:127:PRO:C	15:1:128:TRP:CG	2.87	0.48
15:1:181:LYS:O	15:1:185:VAL:HG23	2.13	0.48
15:1:218:LEU:CD2	18:1:1008:CLA:HBB1	2.44	0.48
15:1:222:TRP:NE1	18:1:1008:CLA:HMA2	2.29	0.48
16:3:136:TRP:CG	16:3:137:PHE:H	2.32	0.48
16:3:139:THR:O	16:3:147:THR:HG22	2.14	0.48
16:3:208:PHE:HB3	18:3:3001:CLA:HMD2	1.95	0.48
2:B:583:MET:HE3	2:B:584:LEU:HD23	1.96	0.48
6:G:111:TYR:H	6:G:111:TYR:HD1	1.52	0.48
18:G:1001:CLA:CAD	18:G:1001:CLA:CED	2.92	0.48
9:D:211:LEU:N	9:D:211:LEU:HD12	2.28	0.48
13:2:117:ALA:O	13:2:120:ILE:HB	2.14	0.48
13:2:188:LEU:HD23	13:2:197:GLY:C	2.38	0.48
18:2:2003:CLA:HMB1	18:2:2008:CLA:HBC3	1.96	0.48
14:4:193:ASN:N	14:4:193:ASN:OD1	2.46	0.48
18:4:4006:CLA:CBB	27:4:4502:LUT:H181	2.44	0.48
15:1:94:ILE:HG12	27:1:1502:LUT:H24	1.95	0.48
16:3:203:PRO:HD3	28:3:3011:CHL:HMD1	1.96	0.48
16:3:268:VAL:CG2	18:3:3003:CLA:C1	2.87	0.48
13:2:176:CYS:HA	13:2:178:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:199:LEU:C	13:2:199:LEU:CD2	2.85	0.48
18:2:2005:CLA:HAB	27:2:2502:LUT:C40	2.43	0.48
14:4:95:GLU:HG3	18:4:4004:CLA:NB	2.29	0.48
14:4:144:ILE:HD13	18:1:1008:CLA:HAA2	1.94	0.48
16:3:65:LEU:CB	16:3:68:LEU:CD2	2.85	0.48
16:3:236:LEU:HD21	18:3:3004:CLA:HBC3	1.96	0.48
1:A:709:TRP:CD1	5:F:229:LYS:HD3	2.49	0.47
6:G:134:VAL:O	6:G:137:TYR:HB3	2.14	0.47
18:G:1001:CLA:C2B	22:G:2011:BCR:C17	2.91	0.47
7:L:176:LEU:CG	7:L:177:GLN:H	2.26	0.47
10:E:66:ILE:HG23	10:E:67:GLY:H	1.79	0.47
13:2:145:TYR:HB3	18:2:2006:CLA:C9	2.44	0.47
18:2:2016:CLA:HED2	18:2:2016:CLA:OBD	2.14	0.47
16:3:174:GLN:HB2	16:3:182:MET:HG2	1.96	0.47
22:3:3503:BCR:HC8	22:3:3503:BCR:C32	2.44	0.47
1:A:338:PHE:O	1:A:434:ARG:NH1	2.47	0.47
22:B:6010:BCR:H321	22:B:6010:BCR:HC8	1.95	0.47
7:L:108:PHE:HZ	18:L:1503:CLA:OBD	1.97	0.47
7:L:165:THR:OG1	7:L:169:ARG:HB3	2.14	0.47
18:2:2004:CLA:HBC2	18:2:2004:CLA:CHD	2.44	0.47
18:2:2005:CLA:H3A	18:2:2005:CLA:HBA1	1.70	0.47
15:1:111:TRP:HH2	18:1:1006:CLA:HED1	1.70	0.47
16:3:154:ASN:O	18:3:3010:CLA:HMC1	2.14	0.47
16:3:271:SER:HB2	18:3:3003:CLA:CED	2.44	0.47
18:3:3010:CLA:H2A	18:3:3010:CLA:CED	2.44	0.47
1:A:205:HIS:O	1:A:209:GLY:N	2.46	0.47
1:A:232:PHE:O	1:A:237:VAL:HG12	2.14	0.47
18:A:1125:CLA:HED1	18:A:1133:CLA:HAB	1.97	0.47
18:F:1302:CLA:HBB1	18:F:1302:CLA:CHC	2.44	0.47
22:F:6016:BCR:C8	22:F:6016:BCR:C33	2.85	0.47
6:G:68:THR:HG23	18:G:1001:CLA:O2A	2.14	0.47
7:L:121:ARG:HG2	7:L:127:GLY:HA2	1.93	0.47
8:C:77:MET:HB3	8:C:79:LEU:HG	1.97	0.47
13:2:246:PRO:HG2	13:2:247:ILE:H	1.80	0.47
15:1:158:LYS:O	15:1:159:LYS:HG2	2.15	0.47
15:1:226:ILE:HG22	18:1:1003:CLA:O2A	2.14	0.47
18:1:1006:CLA:H43	18:1:1013:CLA:HBD	1.96	0.47
16:3:102:GLU:CD	16:3:232:ARG:NH2	2.72	0.47
16:3:106:GLY:O	16:3:110:MET:N	2.42	0.47
1:A:22:LEU:HA	16:3:88:GLY:HA3	1.96	0.47
20:A:5001:PQN:H201	18:A:1138:CLA:HBC1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1122:CLA:H101	18:A:1122:CLA:H202	1.96	0.47
18:G:1001:CLA:O1A	22:G:2011:BCR:H352	2.15	0.47
9:D:101:TYR:CE2	9:D:135:LYS:HB2	2.50	0.47
14:4:190:ASN:OD1	27:4:4501:LUT:O23	2.23	0.47
18:1:1004:CLA:CGA	18:1:1004:CLA:C3A	2.92	0.47
18:3:3002:CLA:HAA2	18:3:3002:CLA:HBD	1.94	0.47
22:J:6013:BCR:H15C	22:J:6013:BCR:H351	1.67	0.47
12:K:71:VAL:HG12	12:K:129:GLY:C	2.40	0.47
13:2:68:PHE:HD2	13:2:71:SER:CB	2.23	0.47
14:4:158:GLN:NE2	14:4:158:GLN:CA	2.77	0.47
18:4:4017:CLA:HAC2	29:4:4505:ZEX:H373	1.96	0.47
15:1:166:ASP:OD1	15:1:169:GLY:N	2.48	0.47
15:1:180:TYR:HB3	18:1:1001:CLA:CMA	2.45	0.47
16:3:155:TYR:CE1	18:3:3010:CLA:H102	2.49	0.47
18:3:3006:CLA:HBD	18:3:3006:CLA:HAA1	1.97	0.47
18:3:3006:CLA:HMB2	18:3:3013:CLA:C4B	2.44	0.47
18:B:1213:CLA:NC	18:B:1213:CLA:H52	2.29	0.47
18:F:1302:CLA:O1D	23:F:5002:LMG:HC91	2.14	0.47
13:2:188:LEU:C	13:2:188:LEU:CD2	2.84	0.47
14:4:156:ARG:HB3	28:4:4011:CHL:CHD	2.45	0.47
14:4:167:ASN:CG	14:4:168:GLN:N	2.72	0.47
14:4:240:PRO:HG2	18:4:4008:CLA:C3B	2.44	0.47
15:1:43:PRO:HG2	28:1:1009:CHL:C3D	2.45	0.47
21:1:1801:LHG:H223	21:1:1801:LHG:H381	1.89	0.47
16:3:139:THR:CG2	16:3:140:GLY:H	2.23	0.47
1:A:64:PHE:CD2	18:A:1103:CLA:HMC2	2.49	0.47
18:A:1120:CLA:H91	18:A:1120:CLA:H112	1.73	0.47
22:A:6017:BCR:HC32	18:B:1205:CLA:HMC2	1.97	0.47
2:B:417:ALA:O	2:B:421:HIS:ND1	2.46	0.47
18:B:1218:CLA:H151	18:G:1003:CLA:C15	2.45	0.47
18:B:1213:CLA:C3D	18:G:1003:CLA:HED1	2.44	0.47
18:B:1234:CLA:H41	18:B:1234:CLA:H101	1.95	0.47
3:I:5:PRO:C	3:I:7:LEU:N	2.71	0.47
22:I:6020:BCR:H351	22:I:6020:BCR:H15C	1.68	0.47
4:J:2:ARG:C	4:J:4:LEU:N	2.71	0.47
6:G:65:SER:HB3	18:G:1001:CLA:HBA1	1.91	0.47
22:G:2011:BCR:H15C	22:G:2011:BCR:H351	1.69	0.47
9:D:83:ILE:HG12	9:D:124:ARG:HH11	1.80	0.47
12:K:71:VAL:HG13	12:K:132:ILE:HB	1.97	0.47
13:2:87:PHE:CE2	27:2:2502:LUT:C37	2.94	0.47
14:4:118:ILE:CD1	14:4:120:ILE:CD1	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:172:PHE:HD1	14:4:173:LYS:H	1.63	0.47
14:4:243:ASN:C	14:4:244:THR:HG23	2.39	0.47
18:4:4001:CLA:C4D	27:4:4501:LUT:H382	2.45	0.47
28:4:4013:CHL:HBA1	28:4:4013:CHL:H3A	1.70	0.47
15:1:62:ASP:OD2	15:1:65:ARG:HA	2.15	0.47
15:1:183:LYS:NZ	18:1:1002:CLA:O1D	2.44	0.47
18:1:1008:CLA:HED2	18:1:1008:CLA:CHA	2.45	0.47
16:3:62:LYS:NZ	16:3:76:TYR:CD2	2.83	0.47
16:3:136:TRP:HB2	27:3:3502:LUT:H22	1.97	0.47
18:3:3010:CLA:HMB2	18:3:3013:CLA:CAB	2.44	0.47
1:A:145:ILE:HA	18:A:1106:CLA:HMD2	1.97	0.47
18:A:1123:CLA:HBB1	18:A:1123:CLA:HMB1	1.97	0.47
2:B:73:ASN:HB2	2:B:76:ALA:HB3	1.96	0.47
18:B:1220:CLA:H62	18:B:1220:CLA:H101	1.64	0.47
22:L:6019:BCR:H24C	22:L:6019:BCR:H371	1.68	0.47
9:D:171:ASP:OD1	9:D:179:ASN:ND2	2.48	0.47
13:2:129:LEU:HD22	13:2:131:ILE:HD11	1.96	0.47
18:2:2001:CLA:H41	18:2:2002:CLA:CMA	2.45	0.47
14:4:222:HIS:C	14:4:222:HIS:HD1	2.23	0.47
18:1:1001:CLA:C4D	27:1:1501:LUT:C38	2.93	0.47
16:3:214:GLY:O	16:3:220:LEU:CB	2.62	0.47
1:A:316:MET:HE3	1:A:317:TYR:CZ	2.50	0.47
1:A:371:VAL:HG12	18:A:1124:CLA:HED3	1.96	0.47
1:A:582:ASP:OD1	8:C:53:ARG:HD2	2.15	0.47
21:A:7001:LHG:H191	18:A:1128:CLA:H111	1.97	0.47
2:B:576:PHE:CE1	18:B:1226:CLA:HAC2	2.49	0.47
18:B:1239:CLA:H3A	18:B:1239:CLA:HBA2	1.47	0.47
4:J:7:TYR:CE2	23:F:5001:LMG:HC4	2.50	0.47
13:2:256:ASP:O	13:2:260:ALA:HB3	2.14	0.47
15:1:85:ARG:HH11	15:1:85:ARG:HG2	1.79	0.47
15:1:85:ARG:NE	18:1:1001:CLA:CHD	2.78	0.47
18:1:1011:CLA:HBD	18:1:1011:CLA:HBA2	1.95	0.47
1:A:163:GLN:CD	18:A:1112:CLA:HED1	2.40	0.47
1:A:282:THR:OG1	1:A:283:PHE:N	2.48	0.47
1:A:602:LEU:HD21	18:A:1128:CLA:HBC1	1.95	0.47
18:A:1105:CLA:H3A	18:A:1105:CLA:HBA2	1.59	0.47
2:B:82:PHE:CZ	2:B:363:GLN:HG2	2.49	0.47
9:D:151:ILE:HG22	9:D:152:LYS:N	2.29	0.47
11:H:132:PRO:N	11:H:133:PRO:CD	2.78	0.47
12:K:78:LEU:C	12:K:80:ALA:N	2.72	0.47
13:2:114:MET:CE	18:2:2001:CLA:HHC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:133:LEU:C	13:2:135:PRO:HD2	2.39	0.47
27:4:4502:LUT:C8	27:4:4502:LUT:H171	2.45	0.47
15:1:85:ARG:CD	18:1:1001:CLA:C4C	2.93	0.47
16:3:70:GLY:N	16:3:75:ASP:OD2	2.48	0.47
16:3:80:PRO:CG	27:3:3502:LUT:H24	2.45	0.47
16:3:102:GLU:CD	16:3:232:ARG:HH21	2.23	0.47
16:3:111:LEU:HD21	18:3:3006:CLA:HBB1	1.97	0.47
18:3:3006:CLA:NC	22:3:3503:BCR:HC31	2.29	0.47
28:3:3011:CHL:CBA	28:3:3011:CHL:CHA	2.93	0.47
1:A:203:LEU:O	1:A:207:LEU:HB2	2.15	0.46
1:A:335:LYS:O	18:A:1151:CLA:HBC3	2.15	0.46
18:A:1107:CLA:H151	18:A:1109:CLA:H142	1.95	0.46
18:A:1110:CLA:H52	16:3:81:LEU:HD13	1.98	0.46
2:B:282:PHE:HE2	22:G:2011:BCR:H281	1.79	0.46
2:B:576:PHE:HE1	18:B:1226:CLA:HAC2	1.79	0.46
18:B:1240:CLA:H143	18:B:1240:CLA:H161	1.76	0.46
7:L:61:ASN:OD1	7:L:166:LEU:HD21	2.14	0.46
11:H:107:GLY:O	11:H:110:THR:CG2	2.63	0.46
13:2:69:PRO:HA	16:3:186:TYR:CZ	2.50	0.46
13:2:207:GLY:HA2	18:2:2001:CLA:HAA2	1.97	0.46
14:4:176:SER:OG	14:4:177:LEU:N	2.49	0.46
18:4:4006:CLA:C4B	27:4:4502:LUT:H183	2.45	0.46
15:1:111:TRP:HZ2	18:1:1013:CLA:CBC	2.26	0.46
15:1:149:ARG:HA	18:1:1011:CLA:HBC3	1.96	0.46
15:1:232:ILE:CG2	15:1:233:PRO:CD	2.84	0.46
18:1:1001:CLA:ND	27:1:1501:LUT:C38	2.75	0.46
16:3:92:PHE:HB3	18:3:3005:CLA:H11	1.97	0.46
2:B:657:TRP:CD2	18:B:1021:CLA:HMA2	2.50	0.46
22:B:6004:BCR:H282	18:B:1218:CLA:HBA2	1.96	0.46
18:B:1208:CLA:HED2	18:B:1208:CLA:H2A	1.97	0.46
7:L:120:LEU:HD23	7:L:120:LEU:HA	1.72	0.46
13:2:168:TRP:CG	18:2:2012:CLA:HMA2	2.49	0.46
14:4:68:GLY:HA2	14:4:73:ASP:OD2	2.16	0.46
16:3:141:VAL:HG13	16:3:141:VAL:O	2.15	0.46
16:3:267:ASN:N	16:3:270:THR:OG1	2.48	0.46
18:3:3010:CLA:H2A	18:3:3010:CLA:O2D	2.15	0.46
28:3:3011:CHL:CHA	28:3:3011:CHL:HBA1	2.44	0.46
2:B:294:ASN:HA	6:G:107:ARG:HG2	1.98	0.46
2:B:459:PHE:O	2:B:463:ILE:HG12	2.15	0.46
13:2:137:TRP:CH2	13:2:236:TRP:HA	2.38	0.46
14:4:166:VAL:HB	14:4:177:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:42:MET:HE2	15:1:42:MET:O	2.15	0.46
15:1:158:LYS:C	15:1:160:TYR:H	2.22	0.46
15:1:229:ASN:C	15:1:229:ASN:ND2	2.72	0.46
16:3:267:ASN:CG	16:3:270:THR:CG2	2.85	0.46
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.50	0.46
18:A:1121:CLA:H52	12:K:82:ARG:HG3	1.97	0.46
18:B:1236:CLA:HAC1	18:B:1228:CLA:HMC2	1.97	0.46
18:B:1021:CLA:HBA2	18:B:1021:CLA:H3A	1.68	0.46
18:B:1215:CLA:CGA	18:B:1215:CLA:H3A	2.42	0.46
5:F:213:TRP:CD1	5:F:214:PRO:HD3	2.51	0.46
18:2:2002:CLA:HAA2	18:2:2002:CLA:HBD	1.97	0.46
14:4:125:LYS:O	14:4:128:ASP:HB2	2.16	0.46
18:4:4001:CLA:H41	18:4:4001:CLA:H61	1.60	0.46
18:1:1002:CLA:HAA2	18:1:1002:CLA:HBD	1.98	0.46
18:1:1002:CLA:CMC	18:1:1002:CLA:HBC2	2.45	0.46
18:1:1011:CLA:CMB	18:1:1011:CLA:HBB1	2.45	0.46
16:3:80:PRO:HG2	27:3:3502:LUT:H24	1.96	0.46
18:A:1123:CLA:HMA2	18:A:1125:CLA:H92	1.98	0.46
18:B:1240:CLA:H62	18:B:1240:CLA:H41	1.74	0.46
3:I:4:LEU:C	3:I:4:LEU:CD1	2.85	0.46
6:G:100:HIS:O	6:G:101:PHE:CD2	2.69	0.46
9:D:151:ILE:CG2	9:D:152:LYS:N	2.79	0.46
13:2:129:LEU:HD22	13:2:131:ILE:CD1	2.46	0.46
13:2:173:ASN:HB3	13:2:174:PRO:CD	2.44	0.46
27:2:2502:LUT:H15	27:2:2502:LUT:H201	1.81	0.46
15:1:143:ALA:CA	18:1:1012:CLA:HAB	2.46	0.46
15:1:158:LYS:C	15:1:160:TYR:N	2.73	0.46
16:3:258:ASP:C	16:3:266:ASN:ND2	2.73	0.46
18:3:3004:CLA:H61	27:3:3502:LUT:C36	2.45	0.46
1:A:687:ALA:C	18:A:1013:CLA:HAB	2.41	0.46
2:B:224:PRO:HG2	2:B:233:TYR:CZ	2.51	0.46
6:G:149:LYS:O	6:G:149:LYS:HG3	2.14	0.46
9:D:166:TYR:OH	9:D:169:PRO:HD2	2.16	0.46
9:D:177:LYS:O	9:D:182:ARG:NH1	2.47	0.46
13:2:203:PRO:HD2	27:2:2501:LUT:C3	2.44	0.46
18:2:2002:CLA:HMD3	18:2:2007:CLA:C4D	2.44	0.46
18:4:4017:CLA:H3A	18:4:4017:CLA:HBA2	1.66	0.46
16:3:246:LEU:C	16:3:246:LEU:CD2	2.85	0.46
22:B:6005:BCR:H351	22:B:6005:BCR:H15C	1.74	0.46
18:B:1214:CLA:HBA2	18:B:1214:CLA:H3A	1.58	0.46
6:G:149:LYS:C	6:G:149:LYS:CE	2.85	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:85:ASN:HA	7:L:90:ARG:NH2	2.30	0.46
7:L:145:LEU:HB3	7:L:186:THR:CG2	2.45	0.46
9:D:81:SER:HB3	9:D:129:LEU:O	2.16	0.46
18:2:2004:CLA:HHD	18:2:2009:CLA:HBB2	1.98	0.46
27:2:2502:LUT:H28	27:2:2502:LUT:C36	2.42	0.46
14:4:132:GLU:O	14:4:134:TYR:CD1	2.69	0.46
15:1:80:GLU:CD	15:1:189:ARG:HH21	2.23	0.46
15:1:97:PRO:HB2	15:1:102:LEU:CG	2.45	0.46
15:1:167:PRO:C	15:1:169:GLY:N	2.72	0.46
28:1:1009:CHL:H3A	28:1:1009:CHL:HBA1	1.67	0.46
16:3:110:MET:CE	16:3:230:ASN:C	2.89	0.46
1:A:272:LEU:HD11	12:K:134:VAL:HG13	1.97	0.46
2:B:270:LEU:HD23	2:B:273:MET:HE3	1.98	0.46
5:F:146:PRO:O	5:F:147:HIS:HD2	1.99	0.46
18:G:1003:CLA:H52	23:G:2021:LMG:H332	1.98	0.46
13:2:91:GLY:O	13:2:94:SER:HB2	2.16	0.46
13:2:126:LEU:CB	13:2:134:THR:HA	2.45	0.46
13:2:127:THR:CG2	13:2:247:ILE:HD13	2.39	0.46
13:2:186:ASN:CG	18:2:2016:CLA:C2A	2.89	0.46
18:2:2001:CLA:H41	18:2:2001:CLA:H62	1.63	0.46
18:4:4006:CLA:C3B	27:4:4503:LUT:C17	2.93	0.46
15:1:41:TRP:HD1	15:1:59:PHE:CA	2.25	0.46
15:1:104:ASN:OD1	15:1:208:THR:HG23	2.15	0.46
15:1:173:ASP:HB3	15:1:176:LYS:HB3	1.97	0.46
9:D:204:THR:C	9:D:206:LYS:N	2.72	0.46
13:2:59:VAL:HG12	13:2:59:VAL:O	2.16	0.46
13:2:154:ILE:CG2	18:4:4008:CLA:HED1	2.46	0.46
13:2:195:TYR:C	18:2:2001:CLA:HED3	2.41	0.46
18:4:4006:CLA:C2B	27:4:4503:LUT:C17	2.93	0.46
15:1:97:PRO:HB2	15:1:102:LEU:CD2	2.43	0.46
16:3:225:LEU:CB	16:3:226:LYS:NZ	2.71	0.46
1:A:197:GLN:O	1:A:199:VAL:N	2.49	0.46
17:A:1011:CL0:H7	18:B:1021:CLA:HBB1	1.97	0.46
18:A:1104:CLA:H192	18:A:1104:CLA:H162	1.72	0.46
18:A:1122:CLA:H111	18:A:1122:CLA:H72	1.70	0.46
18:A:1132:CLA:H141	18:A:1132:CLA:H161	1.61	0.46
2:B:189:ALA:HB1	18:B:1211:CLA:HMC1	1.97	0.46
2:B:231:ASN:HA	18:B:1213:CLA:HAA2	1.98	0.46
18:G:1001:CLA:CED	18:G:1001:CLA:C4D	2.94	0.46
7:L:203:LEU:HD12	7:L:203:LEU:N	2.30	0.46
10:E:76:ILE:O	10:E:77:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:204:GLU:HG3	18:4:4001:CLA:NB	2.31	0.46
15:1:88:MET:CE	18:1:1001:CLA:CHC	2.86	0.46
15:1:183:LYS:HD3	18:1:1002:CLA:CGA	2.45	0.46
15:1:200:VAL:CG1	18:1:1003:CLA:HAC2	2.44	0.46
18:A:1140:CLA:H3A	18:A:1140:CLA:HBA2	1.69	0.45
2:B:142:LEU:HD21	22:B:6006:BCR:H24C	1.97	0.45
18:B:1230:CLA:HMA3	23:J:5001:LMG:H151	1.98	0.45
12:K:71:VAL:CG1	12:K:129:GLY:HA2	2.42	0.45
13:2:60:ALA:HB2	13:2:78:ASP:OD1	2.16	0.45
18:2:2002:CLA:HBB1	18:2:2002:CLA:HMB3	1.98	0.45
14:4:152:VAL:HG11	28:4:4011:CHL:C1B	2.45	0.45
14:4:204:GLU:HG3	18:4:4001:CLA:C4B	2.46	0.45
27:4:4503:LUT:C36	28:1:1009:CHL:H8	2.36	0.45
15:1:108:ALA:O	15:1:111:TRP:CZ3	2.69	0.45
15:1:183:LYS:HE3	18:1:1002:CLA:O1A	2.16	0.45
18:1:1005:CLA:HMB3	18:1:1005:CLA:CBB	2.33	0.45
21:1:1801:LHG:HC81	21:1:1801:LHG:C6	2.39	0.45
16:3:72:LEU:HD23	16:3:72:LEU:HA	1.73	0.45
16:3:135:ALA:HB1	16:3:137:PHE:CE2	2.52	0.45
18:A:1132:CLA:H193	18:A:1132:CLA:H162	1.70	0.45
18:A:1119:CLA:H111	18:A:1119:CLA:H143	1.67	0.45
2:B:9:SER:O	2:B:12:ILE:HG22	2.16	0.45
2:B:560:ASP:OD1	8:C:66:ARG:NH1	2.47	0.45
18:B:1229:CLA:H121	22:F:6016:BCR:H271	1.98	0.45
4:J:28:GLU:OE1	18:J:1302:CLA:ND	2.49	0.45
23:G:2021:LMG:O5	15:1:131:LEU:HD11	2.15	0.45
8:C:8:TYR:C	8:C:10:THR:N	2.72	0.45
13:2:131:ILE:HG21	13:2:133:LEU:HG	1.98	0.45
18:2:2016:CLA:CAD	18:2:2016:CLA:CED	2.94	0.45
14:4:54:GLY:O	14:4:74:ASN:HA	2.16	0.45
15:1:83:HIS:NE2	18:1:1012:CLA:HMD2	2.31	0.45
15:1:148:GLN:NE2	15:1:148:GLN:HA	2.31	0.45
15:1:230:VAL:CG1	18:1:1014:CLA:C4B	2.94	0.45
16:3:226:LYS:H	16:3:226:LYS:CE	2.29	0.45
18:3:3013:CLA:H3A	18:3:3013:CLA:HBA1	1.54	0.45
1:A:397:THR:HG23	1:A:613:ILE:HG21	1.97	0.45
18:B:1240:CLA:CED	18:B:1220:CLA:HHB	2.46	0.45
13:2:109:HIS:CD2	18:2:2012:CLA:CMD	2.98	0.45
14:4:154:ILE:O	28:1:1009:CHL:HED1	2.15	0.45
15:1:63:PRO:HD2	27:1:1502:LUT:C3	2.47	0.45
15:1:127:PRO:O	15:1:128:TRP:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:204:ALA:C	15:1:206:PRO:CD	2.87	0.45
15:1:212:GLU:O	15:1:215:ALA:HB3	2.16	0.45
15:1:225:ASN:N	15:1:225:ASN:ND2	2.60	0.45
16:3:190:LEU:HA	16:3:207:PHE:CE2	2.51	0.45
16:3:205:GLY:HA2	16:3:206:PRO:HD3	1.66	0.45
16:3:262:ASP:CB	16:3:265:ASN:HD22	2.29	0.45
1:A:503:THR:O	1:A:505:PRO:HD3	2.16	0.45
1:A:570:PRO:HD2	9:D:136:GLU:OE1	2.15	0.45
18:A:1110:CLA:H52	16:3:81:LEU:CD1	2.47	0.45
22:A:6017:BCR:H392	22:A:6017:BCR:H23C	1.99	0.45
2:B:265:THR:HG22	2:B:360:PHE:CE1	2.52	0.45
5:F:160:PHE:C	5:F:163:PRO:HD2	2.41	0.45
18:L:1501:CLA:O2A	18:H:1000:CLA:HMA2	2.16	0.45
9:D:211:LEU:CD1	9:D:211:LEU:H	2.28	0.45
18:2:2006:CLA:CMA	28:2:2013:CHL:HAC2	2.46	0.45
15:1:146:GLU:CG	15:1:149:ARG:NH1	2.73	0.45
18:1:1002:CLA:CMD	18:1:1007:CLA:C4D	2.95	0.45
18:1:1011:CLA:HBD	18:1:1011:CLA:CBA	2.46	0.45
16:3:114:VAL:HB	18:3:3006:CLA:HMC2	1.99	0.45
18:3:3008:CLA:CHD	18:3:3008:CLA:CBC	2.85	0.45
1:A:225:VAL:HG22	1:A:245:PRO:HB3	1.97	0.45
18:A:1151:CLA:HAB	18:A:1122:CLA:HMB1	1.97	0.45
18:A:1108:CLA:HED2	16:3:93:ILE:HB	1.98	0.45
2:B:282:PHE:CE2	22:G:2011:BCR:H281	2.51	0.45
18:B:1240:CLA:HBA1	21:B:5004:LHG:HC42	1.98	0.45
5:F:111:ALA:O	5:F:113:SER:N	2.50	0.45
22:F:6014:BCR:C8	22:F:6014:BCR:H331	2.46	0.45
10:E:111:ASN:ND2	10:E:113:ALA:N	2.60	0.45
13:2:164:GLU:O	13:2:168:TRP:HB2	2.16	0.45
14:4:74:ASN:N	14:4:74:ASN:HD22	2.14	0.45
18:4:4017:CLA:CMC	29:4:4505:ZEX:H393	2.47	0.45
16:3:149:ASN:O	16:3:150:TYR:CD1	2.70	0.45
16:3:157:LEU:O	16:3:161:GLU:N	2.37	0.45
1:A:62:HIS:HB2	18:A:1128:CLA:CGA	2.46	0.45
22:A:6007:BCR:H351	22:A:6007:BCR:H15C	1.65	0.45
23:B:5005:LMG:H212	22:F:6016:BCR:H362	1.98	0.45
22:B:6004:BCR:H383	6:G:126:ALA:HB1	1.98	0.45
3:I:24:LEU:O	3:I:28:VAL:HG23	2.16	0.45
4:J:32:LEU:HB3	4:J:33:PHE:CD1	2.52	0.45
6:G:76:ARG:HE	6:G:116:LYS:NZ	2.14	0.45
7:L:130:GLY:C	7:L:132:LEU:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:76:TRP:CD1	13:2:93:GLY:O	2.69	0.45
13:2:140:ALA:O	13:2:143:GLN:HG3	2.17	0.45
13:2:231:ALA:HA	18:2:2003:CLA:HBB1	1.99	0.45
14:4:222:HIS:C	14:4:222:HIS:ND1	2.72	0.45
18:4:4007:CLA:H52	18:4:4007:CLA:H92	1.99	0.45
15:1:192:LEU:HD13	18:1:1004:CLA:HMC3	1.99	0.45
18:1:1001:CLA:CGA	18:1:1001:CLA:C4A	2.95	0.45
16:3:110:MET:HE2	16:3:230:ASN:HB3	1.90	0.45
16:3:263:PRO:CD	16:3:264:VAL:H	2.30	0.45
1:A:222:GLN:NE2	1:A:300:ALA:HA	2.32	0.45
18:A:1130:CLA:C2	18:L:1502:CLA:H93	2.47	0.45
2:B:473:GLY:O	2:B:474:PHE:HB2	2.17	0.45
2:B:548:PRO:HD2	8:C:62:PHE:CZ	2.52	0.45
18:B:1207:CLA:H91	18:B:1207:CLA:H112	1.61	0.45
4:J:32:LEU:HD21	18:J:1302:CLA:C2	2.46	0.45
18:G:1001:CLA:C4	22:G:2011:BCR:C34	2.92	0.45
7:L:121:ARG:HG3	7:L:127:GLY:CA	2.39	0.45
7:L:148:TYR:CE1	7:L:152:SER:OG	2.70	0.45
13:2:129:LEU:CD2	13:2:131:ILE:HG13	2.47	0.45
18:2:2001:CLA:H41	18:2:2002:CLA:HMA2	1.99	0.45
14:4:215:PHE:CE1	27:4:4502:LUT:H12	2.51	0.45
29:4:4505:ZEX:H11	29:4:4505:ZEX:H191	1.79	0.45
16:3:202:TYR:CD1	18:3:3001:CLA:O1D	2.70	0.45
16:3:253:TYR:O	16:3:253:TYR:CD1	2.70	0.45
18:3:3003:CLA:H2	18:3:3003:CLA:H62	1.79	0.45
18:3:3018:CLA:HBA1	18:3:3018:CLA:C4A	2.45	0.45
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.83	0.45
2:B:374:HIS:O	2:B:378:ILE:HG12	2.17	0.45
3:I:9:VAL:HB	3:I:10:PRO:CD	2.47	0.45
4:J:2:ARG:CD	4:J:4:LEU:HB2	2.42	0.45
4:J:9:SER:HA	4:J:13:VAL:HG21	1.99	0.45
4:J:31:ARG:HH22	18:J:1302:CLA:H3A	1.81	0.45
5:F:167:PHE:HB2	22:F:6014:BCR:C40	2.47	0.45
18:F:1302:CLA:H3A	18:F:1302:CLA:HBA1	1.74	0.45
6:G:114:VAL:CG1	18:G:1002:CLA:CBA	2.95	0.45
7:L:145:LEU:CD1	22:L:6019:BCR:H392	2.25	0.45
22:K:2011:BCR:H24C	22:K:2011:BCR:H371	1.73	0.45
13:2:122:ILE:N	13:2:122:ILE:HD12	2.31	0.45
13:2:186:ASN:CB	18:2:2016:CLA:CMA	2.95	0.45
14:4:99:GLY:O	14:4:103:MET:HG2	2.17	0.45
14:4:132:GLU:O	14:4:134:TYR:CE1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:51:LEU:HD12	15:1:60:GLY:HA2	1.99	0.45
15:1:130:THR:HG22	15:1:131:LEU:H	1.80	0.45
18:1:1004:CLA:HMD2	28:1:1009:CHL:CBB	2.47	0.45
16:3:62:LYS:HZ3	16:3:76:TYR:HD2	1.63	0.45
16:3:186:TYR:CD1	16:3:186:TYR:N	2.85	0.45
2:B:172:GLU:HB3	2:B:291:TYR:HB3	1.98	0.45
2:B:226:LEU:HD13	26:B:8002:LMU:H5B	1.99	0.45
2:B:301:ILE:HG21	18:B:1221:CLA:HAC1	1.97	0.45
2:B:477:LEU:C	2:B:479:SER:H	2.25	0.45
18:B:1205:CLA:CGA	18:B:1205:CLA:C1A	2.94	0.45
18:B:1223:CLA:H143	22:B:6009:BCR:C19	2.46	0.45
18:B:1207:CLA:H142	18:B:1207:CLA:H111	1.68	0.45
22:F:6016:BCR:C23	22:F:6016:BCR:C38	2.91	0.45
7:L:55:GLN:O	7:L:56:VAL:HB	2.16	0.45
7:L:98:ARG:NH2	7:L:175:GLN:OE1	2.50	0.45
8:C:5:VAL:HG22	8:C:67:VAL:HG22	1.98	0.45
12:K:136:VAL:O	12:K:140:LEU:HD13	2.17	0.45
13:2:220:LYS:CA	18:2:2007:CLA:CED	2.90	0.45
14:4:60:LEU:CG	14:4:61:ALA:N	2.79	0.45
14:4:167:ASN:OD1	14:4:168:GLN:N	2.49	0.45
18:4:4008:CLA:H3A	18:4:4008:CLA:HBA2	1.59	0.45
15:1:220:ASP:OD2	15:1:223:HIS:CD2	2.70	0.45
16:3:94:GLU:OE2	16:3:95:PRO:N	2.50	0.45
16:3:100:TYR:CD1	16:3:100:TYR:C	2.93	0.45
16:3:229:LYS:HA	16:3:229:LYS:HD2	1.67	0.45
18:3:3001:CLA:CBB	27:3:3501:LUT:H34	2.44	0.45
28:3:3011:CHL:HBC2	28:3:3011:CHL:HHD	1.99	0.45
18:3:3018:CLA:HBC2	18:3:3018:CLA:HMC3	1.98	0.45
1:A:229:ILE:HD11	1:A:245:PRO:HG3	1.99	0.45
1:A:346:LEU:HG	1:A:429:ASN:HD21	1.81	0.45
2:B:358:TYR:CE2	18:B:1225:CLA:HED2	2.52	0.45
2:B:585:ASN:HB2	18:B:1012:CLA:HBC2	1.98	0.45
18:B:1235:CLA:H203	18:B:1235:CLA:H161	1.87	0.45
22:B:6009:BCR:H15C	22:B:6009:BCR:H351	1.71	0.45
5:F:146:PRO:C	5:F:147:HIS:HD2	2.26	0.45
5:F:157:TRP:CH2	18:F:1302:CLA:O1A	2.70	0.45
23:F:5002:LMG:H141	23:F:5002:LMG:H172	1.68	0.45
7:L:164:LEU:N	7:L:164:LEU:HD23	2.31	0.45
10:E:66:ILE:CG2	10:E:93:VAL:HG11	2.45	0.45
13:2:120:ILE:CG2	27:2:2501:LUT:C37	2.86	0.45
13:2:185:ASN:OD1	13:2:186:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:199:GLU:O	14:4:202:GLU:HB2	2.16	0.45
15:1:217:HIS:O	15:1:221:PRO:HA	2.17	0.45
16:3:258:ASP:C	16:3:266:ASN:CG	2.85	0.45
1:A:453:LEU:HD21	18:A:1136:CLA:CAB	2.46	0.44
18:A:1237:CLA:H143	22:I:6020:BCR:H363	1.99	0.44
2:B:6:PRO:HG3	2:B:24:GLY:CA	2.47	0.44
2:B:93:ASP:O	2:B:96:PHE:HB2	2.17	0.44
2:B:603:ARG:HH22	2:B:627:ASN:ND2	2.14	0.44
2:B:645:VAL:HG21	18:B:1205:CLA:HAC1	1.99	0.44
18:B:1202:CLA:HBA2	18:B:1210:CLA:CED	2.47	0.44
18:G:1003:CLA:H3A	18:G:1003:CLA:HBA2	1.57	0.44
11:H:107:GLY:CA	11:H:110:THR:HG22	2.47	0.44
13:2:162:TRP:CD1	13:2:162:TRP:C	2.95	0.44
13:2:194:GLY:O	13:2:195:TYR:CD1	2.70	0.44
14:4:98:ASN:ND2	18:4:4012:CLA:OBD	2.50	0.44
14:4:168:GLN:HE22	14:4:171:ILE:C	2.20	0.44
14:4:169:ASP:HB3	18:4:4016:CLA:C1D	2.47	0.44
14:4:239:ASP:OD1	14:4:242:HIS:CD2	2.70	0.44
18:4:4001:CLA:CGA	18:4:4001:CLA:C3A	2.95	0.44
15:1:105:TRP:H	15:1:105:TRP:HD1	1.62	0.44
16:3:100:TYR:CE1	16:3:104:ILE:HG13	2.52	0.44
16:3:242:PHE:O	16:3:246:LEU:HB2	2.17	0.44
1:A:382:TYR:CE2	18:A:1127:CLA:HED2	2.52	0.44
1:A:614:PHE:HB3	1:A:652:TRP:HZ3	1.82	0.44
1:A:721:GLN:NE2	10:E:109:LYS:HB2	2.32	0.44
18:A:1237:CLA:H92	18:A:1237:CLA:H62	1.86	0.44
18:B:1214:CLA:H61	18:B:1214:CLA:H92	1.74	0.44
18:G:1001:CLA:HMB2	22:G:2011:BCR:C16	2.47	0.44
9:D:113:PHE:N	9:D:113:PHE:CD1	2.85	0.44
10:E:97:PRO:C	10:E:99:THR:H	2.24	0.44
12:K:78:LEU:HD23	12:K:78:LEU:HA	1.75	0.44
18:2:2004:CLA:H41	18:2:2004:CLA:H61	1.67	0.44
28:2:2010:CHL:HBB1	28:2:2013:CHL:CBB	2.41	0.44
14:4:135:PHE:O	14:4:135:PHE:CG	2.71	0.44
28:4:4013:CHL:HHB	27:4:4503:LUT:H191	1.98	0.44
27:4:4502:LUT:H35	27:4:4502:LUT:H401	1.77	0.44
15:1:125:PRO:C	15:1:126:VAL:HG13	2.41	0.44
16:3:134:LEU:HB3	16:3:138:GLN:CD	2.42	0.44
18:3:3003:CLA:HAB	27:3:3501:LUT:C17	2.47	0.44
18:3:3013:CLA:HMA1	22:3:3503:BCR:C35	2.48	0.44
27:3:3502:LUT:C28	27:3:3502:LUT:C37	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1207:CLA:H92	18:B:1207:CLA:H61	1.65	0.44
18:B:1215:CLA:H111	18:B:1215:CLA:H143	1.72	0.44
4:J:2:ARG:O	4:J:2:ARG:HG2	2.16	0.44
6:G:114:VAL:HG11	18:G:1002:CLA:HBA1	1.99	0.44
6:G:132:HIS:CG	22:G:2011:BCR:H19C	2.53	0.44
18:G:1002:CLA:HBA2	18:G:1002:CLA:O2D	2.18	0.44
7:L:204:LEU:O	7:L:207:LEU:HD23	2.17	0.44
9:D:134:ARG:NH2	9:D:136:GLU:CD	2.72	0.44
12:K:128:VAL:CG2	22:K:2011:BCR:H311	2.47	0.44
13:2:79:GLY:N	13:2:84:ASP:OD2	2.50	0.44
13:2:95:ASP:OD1	13:2:98:SER:HB2	2.17	0.44
13:2:129:LEU:HD23	13:2:129:LEU:O	2.17	0.44
13:2:133:LEU:C	13:2:133:LEU:HD12	2.41	0.44
13:2:219:THR:CG2	18:2:2007:CLA:CED	2.86	0.44
13:2:238:GLN:NE2	18:2:2003:CLA:C1A	2.81	0.44
13:2:256:ASP:OD2	13:2:259:HIS:CD2	2.70	0.44
14:4:76:PHE:HB3	18:4:4004:CLA:CAD	2.48	0.44
14:4:219:ILE:CG2	14:4:220:ILE:N	2.81	0.44
18:1:1001:CLA:C1D	27:1:1501:LUT:H383	2.47	0.44
16:3:112:GLY:O	16:3:113:ALA:C	2.59	0.44
16:3:120:GLU:OE2	16:3:253:TYR:HB3	2.16	0.44
16:3:158:PHE:HB2	18:3:3010:CLA:HMC3	2.00	0.44
16:3:263:PRO:CG	18:3:3008:CLA:CMB	2.95	0.44
18:3:3006:CLA:C4	18:3:3018:CLA:C1	2.94	0.44
18:A:1132:CLA:H143	18:A:1132:CLA:H111	1.65	0.44
18:B:1235:CLA:H141	18:B:1235:CLA:H162	1.70	0.44
18:B:1207:CLA:HAC2	27:I:6018:LUT:H181	1.99	0.44
6:G:72:LEU:HD23	6:G:127:TRP:HB2	1.99	0.44
6:G:100:HIS:O	6:G:101:PHE:CG	2.70	0.44
6:G:125:LEU:HD23	6:G:125:LEU:HA	1.77	0.44
9:D:207:GLN:O	9:D:211:LEU:HD13	2.17	0.44
12:K:124:ALA:HA	12:K:127:THR:OG1	2.17	0.44
12:K:126:GLY:O	12:K:130:HIS:CD2	2.70	0.44
13:2:162:TRP:O	13:2:162:TRP:CD1	2.70	0.44
15:1:120:THR:CG2	15:1:125:PRO:HA	2.48	0.44
16:3:65:LEU:C	16:3:68:LEU:HD22	2.43	0.44
21:A:5003:LHG:H371	18:A:1137:CLA:C4D	2.48	0.44
22:A:6003:BCR:H15C	22:A:6003:BCR:H351	1.72	0.44
22:A:6007:BCR:C11	18:A:1119:CLA:H112	2.47	0.44
18:B:1221:CLA:H2	18:B:1210:CLA:H92	1.99	0.44
7:L:102:VAL:CG1	7:L:106:HIS:ND1	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:55:PHE:CD2	11:H:55:PHE:O	2.70	0.44
13:2:146:PHE:CD1	13:2:147:THR:N	2.85	0.44
13:2:188:LEU:O	13:2:189:THR:HG23	2.18	0.44
13:2:220:LYS:HD3	18:2:2002:CLA:HAA2	1.99	0.44
13:2:239:HIS:CE1	13:2:244:THR:O	2.70	0.44
14:4:153:GLU:HG3	14:4:156:ARG:HH11	1.82	0.44
15:1:85:ARG:HH21	18:1:1001:CLA:C1D	2.29	0.44
16:3:135:ALA:CB	16:3:137:PHE:CE2	3.00	0.44
16:3:236:LEU:HD11	18:3:3003:CLA:C15	2.48	0.44
18:3:3005:CLA:OBD	18:3:3012:CLA:HBA2	2.18	0.44
18:A:1105:CLA:HMB3	18:A:1106:CLA:HHB	1.98	0.44
18:A:1110:CLA:H8	18:A:1110:CLA:HBB1	1.99	0.44
18:B:1236:CLA:H52	18:B:1227:CLA:H191	1.99	0.44
5:F:167:PHE:HB2	22:F:6014:BCR:H401	1.99	0.44
23:F:5002:LMG:H292	18:1:1014:CLA:ND	2.32	0.44
27:2:2502:LUT:H31	27:2:2502:LUT:H391	1.88	0.44
18:4:4017:CLA:HED2	28:1:1009:CHL:CMB	2.48	0.44
15:1:98:GLU:N	15:1:102:LEU:CB	2.81	0.44
15:1:116:GLY:O	15:1:118:GLN:HA	2.18	0.44
15:1:180:TYR:CD2	18:1:1001:CLA:O1A	2.71	0.44
1:A:269:PHE:HA	1:A:274:TRP:NE1	2.27	0.44
18:A:1112:CLA:H142	18:A:1112:CLA:H112	1.78	0.44
2:B:166:SER:OG	6:G:95:GLN:NE2	2.51	0.44
20:B:5002:PQN:H292	20:B:5002:PQN:H261	1.71	0.44
18:B:1207:CLA:H51	18:B:1207:CLA:H11	1.77	0.44
18:B:1225:CLA:H202	18:B:1225:CLA:H161	1.76	0.44
7:L:91:THR:CG2	7:L:175:GLN:HE21	2.30	0.44
13:2:105:ALA:O	13:2:109:HIS:HD2	2.00	0.44
14:4:168:GLN:NE2	14:4:171:ILE:O	2.34	0.44
18:4:4001:CLA:H43	18:4:4002:CLA:HMA2	1.98	0.44
15:1:79:SER:CB	18:1:1012:CLA:HED2	2.47	0.44
18:1:1004:CLA:CMD	28:1:1009:CHL:CBB	2.96	0.44
16:3:117:ILE:HG23	16:3:253:TYR:HB2	1.99	0.44
16:3:174:GLN:HB2	16:3:182:MET:CG	2.48	0.44
1:A:375:HIS:ND1	18:A:1116:CLA:OBD	2.50	0.44
1:A:492:ILE:HD11	18:A:1135:CLA:H11	1.99	0.44
27:I:6018:LUT:C28	27:I:6018:LUT:H381	2.45	0.44
7:L:169:ARG:C	7:L:171:LYS:N	2.72	0.44
9:D:176:GLU:CD	9:D:176:GLU:N	2.75	0.44
13:2:111:ARG:HA	13:2:114:MET:HE2	1.99	0.44
15:1:222:TRP:NE1	18:1:1008:CLA:HMA1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:62:LYS:C	16:3:63:GLN:CD	2.86	0.44
16:3:171:ARG:HB3	28:3:3011:CHL:CMC	2.48	0.44
16:3:205:GLY:O	16:3:209:ASN:HB3	2.17	0.44
16:3:241:TYR:CE1	27:3:3501:LUT:C16	2.85	0.44
16:3:268:VAL:HG22	18:3:3003:CLA:C3D	2.48	0.44
18:3:3006:CLA:C2D	18:3:3018:CLA:CAB	2.95	0.44
1:A:374:GLN:HG3	18:A:1124:CLA:HED2	2.00	0.44
22:A:6007:BCR:H371	22:A:6007:BCR:H24C	1.59	0.44
18:B:1229:CLA:H62	18:B:1229:CLA:H2	1.67	0.44
9:D:95:ALA:HA	9:D:99:GLU:O	2.16	0.44
13:2:223:LYS:HZ3	21:2:2801:LHG:P	2.23	0.44
18:2:2016:CLA:CGD	18:2:2016:CLA:CGA	2.96	0.44
15:1:106:VAL:HG21	15:1:208:THR:CG2	2.40	0.44
18:1:1004:CLA:H52	27:1:1502:LUT:H8	2.00	0.44
16:3:78:PHE:O	16:3:78:PHE:CD1	2.70	0.44
18:3:3002:CLA:HBC2	18:3:3002:CLA:HMC3	1.98	0.44
27:I:6018:LUT:H31	27:I:6018:LUT:H391	1.89	0.43
6:G:76:ARG:CG	6:G:116:LYS:HZ1	2.28	0.43
6:G:126:ALA:O	6:G:130:ILE:HG13	2.17	0.43
7:L:122:ASN:HD22	7:L:122:ASN:N	2.16	0.43
14:4:153:GLU:CD	14:4:156:ARG:NH1	2.73	0.43
14:4:221:GLN:HB2	14:4:221:GLN:HE21	1.60	0.43
16:3:122:LEU:C	16:3:124:LYS:N	2.73	0.43
16:3:173:PHE:HB2	18:3:3012:CLA:HMA3	1.99	0.43
16:3:202:TYR:HB3	18:3:3001:CLA:CGD	2.47	0.43
1:A:240:LYS:HB2	1:A:240:LYS:HE3	1.83	0.43
1:A:295:TRP:HB3	1:A:297:THR:HG22	2.00	0.43
18:B:1226:CLA:H141	18:B:1226:CLA:H161	1.70	0.43
9:D:191:SER:C	9:D:192:ILE:CD1	2.87	0.43
13:2:209:ALA:HB3	13:2:214:LEU:CD2	2.48	0.43
14:4:118:ILE:CG2	14:4:120:ILE:H	2.30	0.43
27:4:4503:LUT:H191	27:4:4503:LUT:H11	1.80	0.43
21:1:1801:LHG:H223	21:1:1801:LHG:H382	1.88	0.43
16:3:62:LYS:NZ	16:3:76:TYR:HD2	2.16	0.43
16:3:105:ASN:ND2	18:3:3012:CLA:CMD	2.81	0.43
16:3:183:GLY:HA2	16:3:191:GLU:O	2.18	0.43
16:3:225:LEU:CA	16:3:226:LYS:HZ2	2.31	0.43
1:A:361:ASN:CG	18:A:1123:CLA:HAA1	2.43	0.43
2:B:411:MET:HE1	18:B:1227:CLA:C2D	2.48	0.43
18:B:1204:CLA:H12	18:B:1204:CLA:C4D	2.48	0.43
18:B:1208:CLA:H3A	18:B:1208:CLA:HBA2	1.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4:LEU:HD12	3:I:5:PRO:N	2.34	0.43
5:F:143:ASP:OD1	5:F:144:GLY:N	2.51	0.43
6:G:65:SER:HA	6:G:68:THR:CG2	2.48	0.43
13:2:233:MET:HE3	13:2:233:MET:N	2.33	0.43
14:4:187:GLY:C	14:4:189:PHE:N	2.76	0.43
27:4:4503:LUT:H31	27:4:4503:LUT:H391	1.79	0.43
18:1:1004:CLA:H2	27:1:1502:LUT:C18	2.47	0.43
27:1:1502:LUT:H11	27:1:1502:LUT:H191	1.83	0.43
1:A:55:TRP:HE3	21:A:7001:LHG:H111	1.84	0.43
17:A:1011:CL0:H10	17:A:1011:CL0:H72	1.55	0.43
18:A:1127:CLA:H102	18:A:1127:CLA:H62	1.81	0.43
18:A:1128:CLA:H122	18:A:1128:CLA:H162	1.70	0.43
2:B:195:VAL:HA	2:B:199:ILE:HD12	2.00	0.43
2:B:244:PHE:N	2:B:264:GLN:OE1	2.32	0.43
22:B:6006:BCR:H311	18:B:1212:CLA:HMB2	2.00	0.43
18:B:1218:CLA:H52	18:B:1218:CLA:H8	1.80	0.43
18:B:1232:CLA:H11	18:B:1232:CLA:H52	1.62	0.43
6:G:67:SER:HB2	6:G:135:ALA:HB2	2.00	0.43
6:G:116:LYS:HZ2	18:G:1002:CLA:C1B	2.31	0.43
10:E:79:GLN:HG3	10:E:84:TYR:OH	2.17	0.43
13:2:217:LEU:HD12	13:2:217:LEU:HA	1.77	0.43
13:2:253:HIS:CG	18:2:2003:CLA:HAA2	2.54	0.43
18:2:2005:CLA:H93	18:2:2005:CLA:H61	1.79	0.43
14:4:135:PHE:O	14:4:135:PHE:CD1	2.70	0.43
14:4:168:GLN:C	14:4:168:GLN:CD	2.86	0.43
18:4:4017:CLA:CED	28:1:1009:CHL:HMB2	2.48	0.43
15:1:148:GLN:HA	15:1:148:GLN:HE21	1.83	0.43
16:3:100:TYR:CE1	16:3:104:ILE:CG1	3.01	0.43
16:3:184:LYS:CE	16:3:185:GLN:HE21	2.32	0.43
18:A:1109:CLA:H102	18:A:1101:CLA:HBB2	1.99	0.43
18:B:1220:CLA:H141	22:B:6009:BCR:HC32	1.99	0.43
22:G:2011:BCR:C8	22:G:2011:BCR:H321	2.48	0.43
14:4:144:ILE:CD1	18:1:1008:CLA:HAA2	2.48	0.43
18:4:4008:CLA:HBB1	18:4:4008:CLA:CHC	2.43	0.43
15:1:41:TRP:CD1	15:1:59:PHE:O	2.70	0.43
15:1:158:LYS:HD3	15:1:159:LYS:HZ3	1.83	0.43
15:1:230:VAL:HG13	18:1:1014:CLA:NB	2.33	0.43
16:3:257:LEU:HA	16:3:260:VAL:HB	1.99	0.43
18:3:3006:CLA:CHC	22:3:3503:BCR:HC41	2.48	0.43
1:A:417:PHE:CD1	1:A:421:ASP:HB2	2.54	0.43
2:B:275:HIS:HB3	18:B:1214:CLA:HMB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:ASN:O	2:B:410:ARG:HG2	2.18	0.43
3:I:25:PHE:CE1	7:L:147:ILE:HG22	2.54	0.43
5:F:117:LEU:HA	5:F:117:LEU:HD23	1.77	0.43
6:G:148:PRO:HD2	6:G:148:PRO:O	2.18	0.43
7:L:57:VAL:HG23	7:L:57:VAL:O	2.18	0.43
8:C:14:CYS:O	8:C:15:THR:HG23	2.17	0.43
10:E:84:TYR:CD1	10:E:84:TYR:C	2.95	0.43
13:2:129:LEU:CD2	13:2:131:ILE:HG12	2.49	0.43
18:2:2004:CLA:CMD	18:2:2009:CLA:CBB	2.96	0.43
14:4:105:GLY:CA	18:4:4006:CLA:CBB	2.95	0.43
14:4:136:ALA:HA	15:1:223:HIS:NE2	2.33	0.43
14:4:154:ILE:HD12	14:4:157:TRP:HE3	1.83	0.43
14:4:177:LEU:HD13	18:4:4016:CLA:CMD	2.41	0.43
18:4:4006:CLA:C2B	27:4:4503:LUT:H171	2.48	0.43
15:1:58:ASP:CA	18:1:1004:CLA:CED	2.92	0.43
15:1:85:ARG:NH2	18:1:1001:CLA:C4D	2.72	0.43
15:1:168:LEU:HA	15:1:168:LEU:HD13	1.79	0.43
27:1:1501:LUT:H15	27:1:1501:LUT:H201	1.76	0.43
1:A:103:PHE:HB3	1:A:122:VAL:HG23	2.00	0.43
1:A:445:HIS:O	1:A:449:VAL:HG23	2.19	0.43
18:A:1122:CLA:H143	18:A:1122:CLA:H162	1.86	0.43
18:A:1140:CLA:H62	18:A:1140:CLA:H41	1.63	0.43
2:B:471:SER:C	2:B:473:GLY:H	2.27	0.43
18:B:1231:CLA:H142	18:B:1231:CLA:H112	1.83	0.43
18:B:1222:CLA:H41	18:B:1222:CLA:H61	1.67	0.43
18:B:1222:CLA:H92	18:B:1222:CLA:H62	1.75	0.43
5:F:221:LEU:HB2	5:F:222:LEU:HD23	1.99	0.43
22:F:6016:BCR:H24C	22:F:6016:BCR:H371	1.79	0.43
6:G:68:THR:HG23	6:G:69:GLY:N	2.34	0.43
6:G:116:LYS:HA	18:G:1002:CLA:C2D	2.49	0.43
7:L:181:GLY:O	7:L:184:LYS:HB2	2.18	0.43
13:2:114:MET:HE1	18:2:2001:CLA:HHC	1.98	0.43
13:2:160:ILE:O	13:2:163:ALA:HB3	2.18	0.43
14:4:126:TRP:O	27:4:4502:LUT:O3	2.36	0.43
14:4:141:LEU:HD22	28:4:4013:CHL:C2D	2.49	0.43
14:4:170:PRO:CB	18:4:4016:CLA:CMA	2.85	0.43
18:4:4005:CLA:O1A	18:4:4005:CLA:H2A	2.17	0.43
28:4:4013:CHL:HAC1	28:4:4013:CHL:OMC	2.19	0.43
27:4:4503:LUT:H15	27:4:4503:LUT:H201	1.80	0.43
16:3:67:TYR:CE2	16:3:84:SER:C	2.97	0.43
22:A:6011:BCR:H351	22:A:6011:BCR:H15C	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1205:CLA:H143	18:B:1205:CLA:H161	1.80	0.43
11:H:80:PRO:O	11:H:82:GLN:N	2.47	0.43
13:2:181:PRO:CD	18:2:2016:CLA:CBB	2.95	0.43
14:4:103:MET:CG	18:4:4001:CLA:HMC3	2.49	0.43
14:4:171:ILE:HD13	18:4:4016:CLA:CMA	2.49	0.43
18:4:4007:CLA:HED2	18:4:4007:CLA:HAA1	2.00	0.43
15:1:81:LEU:O	15:1:85:ARG:HG2	2.18	0.43
15:1:85:ARG:HB3	18:1:1011:CLA:HED2	1.98	0.43
15:1:108:ALA:O	15:1:111:TRP:CE3	2.72	0.43
15:1:217:HIS:CE1	15:1:221:PRO:HB2	2.54	0.43
15:1:224:ASN:OD1	15:1:224:ASN:N	2.51	0.43
15:1:230:VAL:CG1	18:1:1014:CLA:NB	2.82	0.43
18:3:3006:CLA:H43	18:3:3018:CLA:C1	2.48	0.43
18:3:3012:CLA:HMB3	18:3:3012:CLA:CBB	2.28	0.43
27:3:3502:LUT:H31	27:3:3502:LUT:H391	1.88	0.43
1:A:434:ARG:HA	1:A:437:ARG:HB2	2.01	0.43
1:A:503:THR:HG21	18:A:1133:CLA:HMD1	2.00	0.43
18:A:1120:CLA:H62	18:A:1120:CLA:H41	1.52	0.43
2:B:17:THR:HA	2:B:696:LYS:HB2	2.01	0.43
18:B:1239:CLA:H62	18:B:1023:CLA:H201	2.00	0.43
18:B:1227:CLA:H62	18:B:1227:CLA:H102	1.74	0.43
5:F:213:TRP:CG	5:F:214:PRO:HD3	2.54	0.43
6:G:116:LYS:HG2	6:G:117:SER:N	2.34	0.43
15:1:85:ARG:HG3	15:1:85:ARG:NH1	2.34	0.43
15:1:158:LYS:HD3	15:1:159:LYS:HZ1	1.81	0.43
28:1:1010:CHL:CMC	28:1:1010:CHL:CBC	2.86	0.43
16:3:148:TYR:O	16:3:150:TYR:CD1	2.72	0.43
16:3:185:GLN:HB2	16:3:186:TYR:HD1	1.77	0.43
1:A:154:ARG:NH2	1:A:233:LEU:HB3	2.34	0.43
1:A:342:GLY:HA3	1:A:431:LEU:HG	2.00	0.43
18:A:1110:CLA:C1	16:3:81:LEU:HD13	2.49	0.43
18:B:1231:CLA:HAB	18:B:1223:CLA:HED1	2.01	0.43
5:F:103:GLU:O	5:F:106:LEU:HB3	2.19	0.43
23:F:5002:LMG:O9	18:1:1014:CLA:HED3	2.19	0.43
12:K:119:LEU:HD12	12:K:119:LEU:HA	1.80	0.43
13:2:104:GLN:NE2	13:2:193:VAL:CB	2.81	0.43
18:4:4005:CLA:C2D	18:4:4012:CLA:C1D	2.97	0.43
27:4:4503:LUT:C36	28:1:1009:CHL:C9	2.85	0.43
2:B:22:TRP:HZ3	20:B:5002:PQN:H302	1.84	0.42
20:B:5002:PQN:H243	20:B:5002:PQN:H262	1.72	0.42
18:B:1224:CLA:H3A	18:B:1224:CLA:HBA2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:7:LEU:HG	11:H:115:SER:HB2	2.00	0.42
4:J:16:THR:HG21	22:J:6013:BCR:H403	1.97	0.42
6:G:141:THR:OG1	23:G:2021:LMG:HC91	2.18	0.42
22:L:6020:BCR:H371	22:L:6020:BCR:H24C	1.79	0.42
10:E:66:ILE:CG2	10:E:95:GLN:NE2	2.72	0.42
13:2:137:TRP:HH2	13:2:236:TRP:CA	2.24	0.42
13:2:160:ILE:CD1	28:2:2013:CHL:HMB2	2.49	0.42
13:2:254:LEU:HD23	13:2:254:LEU:H	1.83	0.42
13:2:262:ILE:HD11	18:2:2003:CLA:C4	2.41	0.42
18:2:2003:CLA:HMA1	18:2:2008:CLA:HBC2	2.00	0.42
14:4:146:PHE:C	14:4:146:PHE:CD1	2.96	0.42
18:4:4001:CLA:HHD	28:4:4011:CHL:O1A	2.18	0.42
15:1:63:PRO:HD2	27:1:1502:LUT:O3	2.19	0.42
15:1:78:GLU:O	15:1:82:ILE:HG12	2.19	0.42
16:3:138:GLN:CB	16:3:145:ALA:CB	2.82	0.42
18:3:3007:CLA:CMC	18:3:3007:CLA:HBC2	2.49	0.42
27:3:3501:LUT:H8	27:3:3501:LUT:C17	2.46	0.42
27:3:3502:LUT:H15	27:3:3502:LUT:H201	1.92	0.42
1:A:205:HIS:HB3	18:A:1111:CLA:HBB1	2.01	0.42
1:A:302:HIS:HB2	18:A:1116:CLA:C1B	2.49	0.42
1:A:455:PHE:HB3	18:A:1132:CLA:HBB2	2.01	0.42
1:A:580:PRO:HB3	1:A:727:ILE:HB	2.01	0.42
18:A:1121:CLA:H61	18:A:1121:CLA:H41	1.59	0.42
18:A:1126:CLA:H192	22:J:6012:BCR:H14C	2.01	0.42
2:B:302:LYS:O	2:B:306:GLU:HG2	2.19	0.42
2:B:658:ALA:O	2:B:661:PHE:HB2	2.19	0.42
18:B:1208:CLA:H62	18:B:1208:CLA:H41	1.56	0.42
18:B:1227:CLA:H162	18:B:1227:CLA:H121	1.78	0.42
4:J:11:ALA:HB1	4:J:12:PRO:HD2	2.01	0.42
22:F:6014:BCR:C23	22:F:6014:BCR:H403	2.48	0.42
6:G:116:LYS:CG	18:G:1002:CLA:ND	2.76	0.42
7:L:176:LEU:CD1	7:L:177:GLN:HG2	2.49	0.42
8:C:30:PRO:HD3	9:D:179:ASN:O	2.18	0.42
11:H:56:ASP:HB2	11:H:59:ASP:OD1	2.18	0.42
12:K:124:ALA:CB	22:K:2011:BCR:C33	2.92	0.42
13:2:123:PRO:CA	13:2:126:LEU:HG	2.49	0.42
13:2:238:GLN:HE21	18:2:2003:CLA:CHA	2.31	0.42
14:4:57:LEU:HD12	14:4:57:LEU:HA	1.72	0.42
14:4:136:ALA:HB1	14:4:140:THR:CG2	2.46	0.42
18:4:4017:CLA:HED1	21:1:1801:LHG:C15	2.37	0.42
15:1:102:LEU:C	15:1:104:ASN:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1001:CLA:HHC	27:1:1501:LUT:C32	2.38	0.42
18:1:1001:CLA:HMC1	27:1:1501:LUT:C32	2.49	0.42
16:3:128:ILE:HG22	16:3:132:THR:HA	2.01	0.42
18:A:1013:CLA:HED2	2:B:532:LEU:HD21	2.01	0.42
18:A:1106:CLA:H11	18:A:1126:CLA:HMD2	2.01	0.42
2:B:590:VAL:HG22	18:B:1234:CLA:HAB	2.01	0.42
18:B:1239:CLA:HED1	18:B:1226:CLA:H102	2.01	0.42
18:B:1204:CLA:H42	3:I:8:PHE:HE2	1.84	0.42
6:G:76:ARG:CD	6:G:116:LYS:NZ	2.82	0.42
7:L:94:ASN:O	7:L:98:ARG:HG3	2.19	0.42
8:C:9:ASP:OD1	9:D:191:SER:N	2.52	0.42
14:4:153:GLU:CG	14:4:156:ARG:NH1	2.82	0.42
18:4:4004:CLA:CBB	27:4:4502:LUT:C32	2.97	0.42
18:4:4007:CLA:H91	18:4:4007:CLA:H112	1.74	0.42
29:4:4505:ZEX:H362	29:4:4505:ZEX:C24	2.49	0.42
29:4:4505:ZEX:H15	29:4:4505:ZEX:H201	1.81	0.42
16:3:81:LEU:HA	16:3:81:LEU:HD23	1.75	0.42
16:3:240:GLY:HA2	18:3:3003:CLA:C3C	2.49	0.42
18:3:3006:CLA:HMB3	27:3:3502:LUT:H182	2.01	0.42
1:A:398:HIS:O	1:A:402:ILE:HG12	2.19	0.42
1:A:740:LEU:HD11	22:A:6011:BCR:HC8	2.02	0.42
18:A:1107:CLA:HAB	18:B:1230:CLA:HMD2	2.01	0.42
2:B:199:ILE:HB	2:B:200:PRO:HD3	2.00	0.42
2:B:221:GLY:O	26:B:8002:LMU:H6D	2.19	0.42
2:B:636:THR:C	2:B:638:LEU:H	2.28	0.42
18:B:1220:CLA:H11	18:B:1220:CLA:H51	1.86	0.42
5:F:157:TRP:CZ2	18:F:1302:CLA:O1A	2.72	0.42
18:G:1003:CLA:C3	23:G:2021:LMG:H332	2.49	0.42
7:L:174:ASP:O	7:L:175:GLN:HB2	2.19	0.42
22:L:6019:BCR:C27	22:L:6019:BCR:C39	2.90	0.42
9:D:192:ILE:HB	9:D:194:LYS:HG3	2.02	0.42
10:E:75:LYS:HB2	10:E:128:VAL:HG21	2.02	0.42
13:2:222:ILE:CD1	13:2:222:ILE:H	2.32	0.42
14:4:184:TYR:C	18:4:4001:CLA:HED2	2.44	0.42
15:1:130:THR:CG2	15:1:132:PRO:CD	2.85	0.42
16:3:169:GLU:HB3	18:3:3012:CLA:C1B	2.50	0.42
16:3:218:LYS:O	16:3:221:LYS:HG3	2.19	0.42
16:3:268:VAL:HG22	18:3:3003:CLA:CAD	2.49	0.42
3:I:25:PHE:CD1	3:I:25:PHE:C	2.98	0.42
7:L:53:THR:O	7:L:53:THR:HG22	2.19	0.42
14:4:223:ASN:C	14:4:225:THR:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:4502:LUT:H162	27:4:4502:LUT:H3	1.84	0.42
15:1:58:ASP:HB2	18:1:1004:CLA:CED	2.48	0.42
15:1:64:LEU:O	15:1:65:ARG:HB2	2.19	0.42
15:1:131:LEU:N	15:1:131:LEU:CD2	2.72	0.42
18:1:1003:CLA:H12	18:1:1008:CLA:C2D	2.49	0.42
27:1:1502:LUT:H35	27:1:1502:LUT:H401	1.80	0.42
1:A:340:GLY:HA2	7:L:55:GLN:OE1	2.20	0.42
22:A:6002:BCR:C33	18:A:1112:CLA:HHB	2.48	0.42
18:A:1102:CLA:H3A	18:A:1102:CLA:HBA1	1.66	0.42
18:A:1106:CLA:H61	18:A:1106:CLA:H93	1.76	0.42
2:B:136:TYR:O	2:B:140:ILE:HG12	2.19	0.42
18:B:1216:CLA:H91	18:B:1216:CLA:H111	1.64	0.42
18:B:1202:CLA:HBD	18:B:1202:CLA:H122	2.02	0.42
18:B:1202:CLA:H142	18:B:1202:CLA:H112	1.80	0.42
18:B:1208:CLA:C4D	26:B:8001:LMU:H32	2.50	0.42
5:F:85:CYS:SG	5:F:138:LEU:O	2.78	0.42
7:L:96:LEU:HB2	7:L:184:LYS:HB3	2.01	0.42
13:2:228:ALA:O	13:2:231:ALA:HB3	2.20	0.42
18:2:2001:CLA:H12	27:2:2501:LUT:H173	1.98	0.42
14:4:108:GLY:HA2	18:4:4006:CLA:C2C	2.50	0.42
14:4:212:MET:HB2	18:4:4004:CLA:CMC	2.49	0.42
15:1:140:LEU:HD23	15:1:140:LEU:C	2.44	0.42
1:A:232:PHE:HD1	1:A:237:VAL:HG11	1.85	0.42
1:A:440:ASP:HB2	9:D:88:THR:CG2	2.43	0.42
21:A:7001:LHG:H202	18:A:1128:CLA:H13	2.02	0.42
18:A:1112:CLA:H112	18:A:1112:CLA:H91	1.82	0.42
18:A:1135:CLA:O1A	18:A:1136:CLA:HBD	2.20	0.42
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.00	0.42
18:B:1207:CLA:C3B	3:I:14:LEU:HD21	2.50	0.42
5:F:156:HIS:HB3	5:F:159:GLU:CD	2.45	0.42
8:C:8:TYR:HB3	9:D:191:SER:CA	2.47	0.42
9:D:77:PRO:O	9:D:77:PRO:CD	2.68	0.42
9:D:139:LEU:HD23	9:D:139:LEU:C	2.43	0.42
13:2:211:PRO:O	13:2:212:GLN:HB2	2.19	0.42
18:2:2008:CLA:O2A	16:3:160:LEU:HD13	2.20	0.42
18:4:4016:CLA:HBC2	18:4:4016:CLA:CMC	2.49	0.42
15:1:66:LEU:HD12	27:1:1502:LUT:H41	2.02	0.42
15:1:121:TYR:CE1	18:1:1006:CLA:H2	2.53	0.42
15:1:126:VAL:HG23	15:1:127:PRO:N	2.31	0.42
18:1:1005:CLA:HBB1	18:1:1005:CLA:CMB	2.30	0.42
16:3:111:LEU:HD21	18:3:3006:CLA:CBB	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TRP:HE1	18:A:1109:CLA:CHB	2.33	0.42
1:A:191:PRO:HB2	1:A:196:PHE:CE2	2.54	0.42
18:A:1112:CLA:H141	18:A:1112:CLA:H162	1.70	0.42
18:B:1207:CLA:H41	7:L:133:ALA:HB2	2.01	0.42
5:F:173:TRP:CD1	5:F:210:GLY:HA3	2.55	0.42
8:C:10:THR:CG2	8:C:64:SER:CB	2.97	0.42
14:4:223:ASN:OD1	14:4:223:ASN:N	2.53	0.42
18:4:4002:CLA:C1D	18:4:4007:CLA:H71	2.50	0.42
18:4:4006:CLA:NB	27:4:4503:LUT:C17	2.80	0.42
15:1:119:ALA:O	15:1:120:THR:HG23	2.19	0.42
15:1:229:ASN:ND2	15:1:229:ASN:O	2.53	0.42
15:1:232:ILE:HD11	18:1:1014:CLA:HMD2	2.02	0.42
27:3:3501:LUT:H35	27:3:3501:LUT:H401	1.80	0.42
18:A:1106:CLA:H3A	18:A:1106:CLA:HBA2	1.48	0.42
18:A:1109:CLA:HHC	18:A:1109:CLA:HBB1	2.01	0.42
18:A:1110:CLA:HBC2	18:A:1111:CLA:HAB	2.00	0.42
18:A:1130:CLA:H11	7:L:83:LEU:HD11	2.01	0.42
2:B:624:LEU:HD22	18:B:1021:CLA:HMD3	2.01	0.42
22:B:6004:BCR:H371	18:B:1218:CLA:HMD1	2.02	0.42
18:B:1215:CLA:H3A	18:B:1215:CLA:HBA2	1.76	0.42
3:I:7:LEU:HA	3:I:7:LEU:HD13	1.65	0.42
6:G:83:GLN:O	6:G:87:VAL:HG23	2.20	0.42
12:K:77:MET:C	12:K:79:PHE:H	2.27	0.42
12:K:79:PHE:CD2	12:K:121:ASP:OD2	2.73	0.42
14:4:156:ARG:O	14:4:160:ILE:HG13	2.20	0.42
15:1:51:LEU:CD1	15:1:60:GLY:HA2	2.50	0.42
15:1:88:MET:CE	18:1:1001:CLA:HAB	2.41	0.42
15:1:200:VAL:HG21	18:1:1003:CLA:HAC1	2.02	0.42
15:1:205:TYR:CE2	18:1:1003:CLA:O1D	2.70	0.42
18:1:1011:CLA:C3	27:1:1501:LUT:C23	2.86	0.42
16:3:102:GLU:OE2	16:3:232:ARG:HD3	2.20	0.42
16:3:182:MET:CA	16:3:182:MET:CE	2.88	0.42
16:3:220:LEU:C	16:3:220:LEU:CD2	2.85	0.42
1:A:112:ASP:OD2	1:A:115:HIS:HB3	2.19	0.42
1:A:315:HIS:NE2	22:K:2011:BCR:H352	2.34	0.42
1:A:437:ARG:HG2	9:D:87:SER:HB2	2.02	0.42
17:A:1011:CL0:H53	17:A:1011:CL0:H61	1.83	0.42
2:B:6:PRO:HD2	2:B:12:ILE:HG23	2.01	0.42
2:B:129:LEU:HD13	2:B:135:LEU:HD23	2.01	0.42
18:B:1226:CLA:H143	18:B:1226:CLA:H111	1.85	0.42
4:J:28:GLU:HG3	18:J:1302:CLA:C1D	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:64:ILE:HD12	18:G:1001:CLA:C2D	2.50	0.42
9:D:190:ARG:H	9:D:190:ARG:HG3	1.62	0.42
10:E:105:VAL:HG12	10:E:106:ARG:N	2.35	0.42
13:2:64:ARG:HE	13:2:79:GLY:HA3	1.85	0.42
13:2:197:GLY:N	18:2:2001:CLA:HED2	2.35	0.42
13:2:207:GLY:CA	18:2:2001:CLA:HAA2	2.49	0.42
13:2:254:LEU:N	13:2:254:LEU:CD2	2.73	0.42
14:4:95:GLU:HG3	18:4:4004:CLA:C1B	2.50	0.42
15:1:166:ASP:O	15:1:169:GLY:N	2.52	0.42
16:3:119:PRO:HB3	16:3:133:ALA:HB2	1.95	0.42
16:3:206:PRO:HD2	16:3:207:PHE:CA	2.49	0.42
16:3:222:GLU:O	16:3:222:GLU:HG2	2.20	0.42
16:3:231:GLY:O	16:3:235:MET:CG	2.68	0.42
1:A:207:LEU:HD11	18:A:1119:CLA:C3B	2.49	0.41
1:A:266:ALA:O	1:A:269:PHE:HB3	2.19	0.41
1:A:650:ASN:HB2	2:B:651:LEU:HD11	2.02	0.41
2:B:487:ASN:HA	2:B:490:ARG:HB2	2.01	0.41
7:L:90:ARG:C	7:L:98:ARG:NH2	2.73	0.41
14:4:73:ASP:HA	18:4:4004:CLA:O1D	2.20	0.41
14:4:126:TRP:C	14:4:128:ASP:N	2.74	0.41
14:4:136:ALA:HB2	15:1:222:TRP:HB3	2.01	0.41
15:1:112:ALA:O	15:1:131:LEU:HD11	2.20	0.41
15:1:130:THR:CG2	15:1:131:LEU:H	2.32	0.41
18:1:1005:CLA:HED1	18:1:1005:CLA:H43	2.02	0.41
16:3:142:ILE:HA	16:3:147:THR:HG23	2.02	0.41
16:3:151:TRP:CE3	16:3:152:ALA:HB2	2.55	0.41
16:3:188:LEU:HD22	16:3:188:LEU:HA	1.88	0.41
1:A:29:THR:HG23	1:A:187:HIS:HD2	1.84	0.41
1:A:694:PHE:HB2	18:A:1013:CLA:HBC2	2.02	0.41
2:B:73:ASN:HD22	2:B:74:PHE:N	2.07	0.41
2:B:519:VAL:HG11	2:B:593:TYR:HB2	2.03	0.41
2:B:569:ASP:HA	2:B:574:ASP:OD2	2.20	0.41
18:B:1201:CLA:H3A	18:B:1201:CLA:HBA2	1.38	0.41
22:J:6012:BCR:H24C	22:J:6012:BCR:H371	1.75	0.41
6:G:100:HIS:O	6:G:101:PHE:CB	2.67	0.41
8:C:14:CYS:O	8:C:15:THR:CB	2.69	0.41
8:C:60:THR:HG1	8:C:64:SER:HG	1.55	0.41
13:2:182:ILE:HD12	18:4:4007:CLA:HAB	1.97	0.41
13:2:219:THR:C	18:2:2007:CLA:CED	2.86	0.41
14:4:113:GLU:OE2	14:4:230:PHE:HB3	2.20	0.41
18:4:4004:CLA:HHC	27:4:4502:LUT:H32	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:4005:CLA:CMD	18:4:4012:CLA:CHD	2.98	0.41
27:4:4501:LUT:H15	27:4:4501:LUT:H201	1.88	0.41
15:1:170:TYR:CE2	27:1:1501:LUT:C37	3.03	0.41
15:1:200:VAL:HG21	18:1:1003:CLA:CAC	2.50	0.41
16:3:93:ILE:O	16:3:93:ILE:HG23	2.21	0.41
16:3:111:LEU:HD23	16:3:111:LEU:C	2.45	0.41
16:3:222:GLU:C	16:3:226:LYS:NZ	2.69	0.41
1:A:395:LEU:HD11	18:A:1127:CLA:HED3	2.02	0.41
1:A:701:GLN:O	1:A:705:GLU:HG3	2.20	0.41
2:B:80:ASP:HB2	2:B:84:VAL:HG23	2.01	0.41
2:B:697:PRO:HB3	18:B:1238:CLA:C2C	2.50	0.41
18:B:1213:CLA:H61	18:B:1213:CLA:H41	1.95	0.41
5:F:188:GLU:HG3	5:F:189:LYS:HG3	2.03	0.41
6:G:65:SER:HA	18:G:1001:CLA:O2A	2.20	0.41
13:2:115:LEU:HD21	18:2:2001:CLA:HBC3	2.02	0.41
27:4:4502:LUT:H15	27:4:4502:LUT:H201	1.84	0.41
15:1:197:GLY:O	15:1:201:GLN:HB2	2.20	0.41
18:1:1004:CLA:HBD	18:1:1004:CLA:HAA1	2.01	0.41
16:3:116:ALA:HA	16:3:136:TRP:HB3	2.03	0.41
16:3:267:ASN:O	18:3:3003:CLA:HED2	2.21	0.41
18:3:3006:CLA:HMD1	18:3:3018:CLA:CAB	2.50	0.41
1:A:201:SER:O	1:A:205:HIS:HD2	2.03	0.41
1:A:209:GLY:HA3	18:A:1111:CLA:CBB	2.50	0.41
1:A:339:THR:OG1	21:A:5003:LHG:O4	2.33	0.41
22:A:6002:BCR:H342	18:A:1112:CLA:CHB	2.51	0.41
18:A:1126:CLA:H143	18:A:1126:CLA:H162	1.68	0.41
2:B:5:LEU:HA	2:B:6:PRO:HA	1.80	0.41
2:B:19:ARG:HD2	8:C:77:MET:HE1	2.01	0.41
22:B:6004:BCR:H371	22:B:6004:BCR:H24C	1.82	0.41
18:B:1222:CLA:HBA2	18:B:1222:CLA:H3A	1.61	0.41
3:I:4:LEU:HD12	3:I:6:SER:N	2.26	0.41
6:G:116:LYS:HB2	18:G:1002:CLA:CHA	2.50	0.41
18:L:1501:CLA:HAA1	18:H:1000:CLA:HMB2	2.02	0.41
12:K:70:MET:HE2	12:K:70:MET:C	2.44	0.41
13:2:157:LEU:HD23	13:2:157:LEU:HA	1.84	0.41
13:2:221:GLU:HB3	13:2:222:ILE:HD12	2.02	0.41
27:2:2501:LUT:H15	27:2:2501:LUT:H201	1.74	0.41
14:4:135:PHE:O	14:4:136:ALA:CB	2.68	0.41
18:4:4012:CLA:HHB	18:4:4017:CLA:HBC2	2.01	0.41
15:1:98:GLU:C	15:1:100:LEU:N	2.76	0.41
15:1:104:ASN:HB2	15:1:107:LYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:153:LYS:HD3	15:1:153:LYS:N	2.31	0.41
15:1:165:PHE:O	27:1:1501:LUT:O23	2.21	0.41
15:1:211:LEU:HD12	15:1:212:GLU:N	2.30	0.41
15:1:232:ILE:CG1	18:1:1014:CLA:HMD2	2.50	0.41
16:3:93:ILE:HD12	16:3:93:ILE:HA	1.85	0.41
16:3:121:TYR:HA	16:3:253:TYR:HD2	1.84	0.41
16:3:129:PRO:O	16:3:132:THR:CB	2.69	0.41
16:3:202:TYR:C	16:3:204:GLY:N	2.79	0.41
23:J:5001:LMG:H453	23:J:5001:LMG:H422	1.81	0.41
9:D:107:SER:OG	9:D:109:LYS:O	2.36	0.41
11:H:125:ILE:O	11:H:127:LYS:N	2.54	0.41
13:2:69:PRO:HB2	16:3:182:MET:HE1	2.02	0.41
13:2:125:PHE:O	13:2:129:LEU:N	2.53	0.41
13:2:135:PRO:HG2	18:2:2006:CLA:HED3	2.01	0.41
13:2:182:ILE:HD13	18:4:4007:CLA:HAB	1.98	0.41
13:2:242:THR:O	13:2:242:THR:CG2	2.68	0.41
18:2:2006:CLA:HMA3	28:2:2013:CHL:CAC	2.50	0.41
14:4:111:LEU:HD12	18:4:4006:CLA:HBC1	2.02	0.41
15:1:58:ASP:OD1	18:1:1004:CLA:HED2	2.19	0.41
15:1:79:SER:OG	18:1:1012:CLA:OBD	2.33	0.41
15:1:85:ARG:CG	15:1:85:ARG:NH1	2.72	0.41
15:1:226:ILE:O	15:1:229:ASN:HB3	2.20	0.41
18:1:1004:CLA:HHD	28:1:1009:CHL:HBB2	2.02	0.41
16:3:100:TYR:HD1	16:3:100:TYR:C	2.29	0.41
16:3:161:GLU:OE2	18:3:3010:CLA:HAB	2.20	0.41
16:3:258:ASP:CB	16:3:266:ASN:ND2	2.73	0.41
18:3:3005:CLA:HMD1	18:3:3012:CLA:C4C	2.50	0.41
1:A:127:VAL:HG22	18:B:1230:CLA:OBD	2.21	0.41
1:A:225:VAL:C	1:A:228:PRO:HD2	2.45	0.41
18:A:1237:CLA:H62	18:B:1238:CLA:H43	2.01	0.41
2:B:158:GLN:HA	2:B:159:PRO:HD3	1.92	0.41
2:B:507:SER:HA	2:B:510:LEU:HD21	2.02	0.41
18:B:1221:CLA:CBA	18:B:1202:CLA:H8	2.51	0.41
18:B:1235:CLA:H111	18:B:1235:CLA:H91	1.88	0.41
18:B:1211:CLA:CBB	18:B:1225:CLA:H162	2.51	0.41
7:L:55:GLN:C	7:L:56:VAL:HG23	2.44	0.41
7:L:176:LEU:CD1	7:L:177:GLN:N	2.71	0.41
9:D:123:MET:HE3	9:D:123:MET:HB2	1.90	0.41
13:2:167:ARG:O	13:2:171:ILE:HG12	2.21	0.41
13:2:188:LEU:HD21	13:2:197:GLY:O	2.20	0.41
18:2:2004:CLA:HMD2	18:2:2009:CLA:CBB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:70:LEU:HD23	14:4:70:LEU:HA	1.85	0.41
18:4:4001:CLA:H71	27:4:4501:LUT:C30	2.51	0.41
18:4:4005:CLA:ND	18:4:4012:CLA:H112	2.36	0.41
15:1:85:ARG:HE	18:1:1001:CLA:CHD	2.33	0.41
18:1:1005:CLA:H3A	18:1:1005:CLA:HBA1	1.76	0.41
16:3:80:PRO:HD2	27:3:3502:LUT:H24	2.02	0.41
16:3:209:ASN:OD1	27:3:3501:LUT:C24	2.69	0.41
16:3:212:GLY:O	16:3:215:LYS:CB	2.68	0.41
16:3:223:LEU:HA	16:3:226:LYS:HG3	1.99	0.41
18:3:3005:CLA:O1D	18:3:3012:CLA:H2	2.21	0.41
1:A:406:LEU:HA	18:A:1128:CLA:HMC2	2.03	0.41
18:A:1116:CLA:NB	18:A:1116:CLA:H43	2.36	0.41
18:A:1117:CLA:HBA2	18:A:1117:CLA:H3A	1.65	0.41
2:B:12:ILE:HD11	2:B:23:PHE:CB	2.47	0.41
6:G:114:VAL:HG12	6:G:115:SER:N	2.36	0.41
7:L:91:THR:CA	7:L:98:ARG:HH21	2.32	0.41
7:L:120:LEU:O	7:L:124:GLU:CB	2.69	0.41
7:L:121:ARG:HG2	7:L:127:GLY:CA	2.48	0.41
7:L:121:ARG:HB3	7:L:122:ASN:H	1.66	0.41
7:L:175:GLN:HB3	7:L:176:LEU:H	1.70	0.41
13:2:186:ASN:ND2	18:2:2016:CLA:H2A	2.35	0.41
13:2:219:THR:HG22	18:2:2007:CLA:HED1	1.99	0.41
13:2:254:LEU:O	13:2:257:PRO:HD3	2.21	0.41
14:4:111:LEU:HD12	18:4:4006:CLA:CBC	2.49	0.41
15:1:118:GLN:O	15:1:119:ALA:CB	2.69	0.41
18:3:3003:CLA:CHA	18:3:3003:CLA:O2A	2.69	0.41
1:A:334:HIS:O	21:A:5003:LHG:O1	2.38	0.41
1:A:714:LEU:HD12	18:A:1138:CLA:HMA2	2.03	0.41
18:A:1112:CLA:HBA1	18:A:1112:CLA:H3A	1.77	0.41
18:A:1124:CLA:CHB	18:A:1137:CLA:HAA2	2.51	0.41
18:B:1204:CLA:H51	18:B:1204:CLA:H11	1.80	0.41
5:F:101:LYS:HE2	5:F:101:LYS:HB3	1.88	0.41
5:F:152:GLY:HA2	5:F:161:ILE:HD11	2.02	0.41
5:F:156:HIS:HB3	5:F:159:GLU:OE1	2.21	0.41
6:G:116:LYS:NZ	18:G:1002:CLA:NB	2.69	0.41
23:G:2021:LMG:C6	15:1:115:PRO:HA	2.44	0.41
9:D:77:PRO:O	9:D:77:PRO:HD2	2.20	0.41
10:E:103:VAL:O	10:E:105:VAL:HG23	2.21	0.41
13:2:131:ILE:CD1	13:2:133:LEU:CD2	2.85	0.41
27:2:2502:LUT:C28	27:2:2502:LUT:C36	2.94	0.41
18:1:1002:CLA:HHC	18:1:1002:CLA:CBB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1004:CLA:H91	18:1:1004:CLA:H112	1.77	0.41
16:3:117:ILE:O	16:3:117:ILE:HG22	2.20	0.41
16:3:120:GLU:CD	16:3:253:TYR:N	2.70	0.41
16:3:141:VAL:HG23	18:3:3010:CLA:CAD	2.51	0.41
16:3:222:GLU:O	16:3:226:LYS:HD2	2.21	0.41
16:3:250:VAL:CG1	16:3:254:GLN:HG2	2.50	0.41
18:3:3006:CLA:HMB1	18:3:3013:CLA:HBB1	2.02	0.41
1:A:206:HIS:ND1	18:A:1123:CLA:OBD	2.49	0.41
1:A:283:PHE:CZ	18:A:1116:CLA:H42	2.56	0.41
1:A:542:HIS:HB2	18:A:1136:CLA:HED2	2.03	0.41
1:A:549:ILE:O	1:A:553:VAL:HG23	2.21	0.41
18:A:1106:CLA:H193	18:A:1106:CLA:H162	1.77	0.41
18:A:1111:CLA:H62	18:A:1111:CLA:H101	1.89	0.41
18:A:1112:CLA:H162	18:A:1112:CLA:H192	1.83	0.41
18:A:1137:CLA:H61	18:A:1137:CLA:H41	1.83	0.41
18:A:1116:CLA:H91	18:A:1116:CLA:H112	1.66	0.41
2:B:268:LEU:HG	2:B:356:PRO:O	2.21	0.41
2:B:292:ARG:NH2	6:G:107:ARG:NH1	2.69	0.41
2:B:352:MET:HE3	18:B:1215:CLA:HBA1	2.02	0.41
18:B:1218:CLA:H202	18:B:1218:CLA:H161	1.75	0.41
18:B:1221:CLA:H142	18:B:1221:CLA:H112	1.69	0.41
18:B:1221:CLA:H61	18:B:1221:CLA:H41	1.77	0.41
18:B:1223:CLA:H92	18:B:1223:CLA:H62	1.86	0.41
5:F:85:CYS:SG	5:F:139:LEU:O	2.78	0.41
6:G:95:GLN:C	6:G:97:GLY:N	2.77	0.41
7:L:104:LEU:O	22:L:6020:BCR:H14C	2.20	0.41
7:L:173:PRO:O	7:L:173:PRO:CD	2.69	0.41
7:L:182:TRP:O	7:L:186:THR:HG23	2.21	0.41
8:C:9:ASP:OD1	9:D:191:SER:CB	2.69	0.41
11:H:113:TYR:C	11:H:115:SER:N	2.78	0.41
22:K:2011:BCR:H351	22:K:2011:BCR:H15C	1.82	0.41
13:2:153:PHE:CD1	28:2:2010:CHL:HAC2	2.55	0.41
14:4:109:MET:HE1	14:4:215:PHE:CD1	2.54	0.41
14:4:209:ARG:NH1	18:4:4004:CLA:C2D	2.83	0.41
15:1:146:GLU:HG2	15:1:149:ARG:HD3	2.02	0.41
15:1:158:LYS:O	15:1:159:LYS:CG	2.69	0.41
15:1:166:ASP:CG	15:1:169:GLY:CA	2.91	0.41
15:1:202:GLN:CD	15:1:208:THR:CB	2.90	0.41
15:1:215:ALA:O	15:1:218:LEU:N	2.54	0.41
18:1:1005:CLA:H12	18:1:1005:CLA:CED	2.43	0.41
18:1:1005:CLA:HMD1	18:1:1012:CLA:C4C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1012:CLA:HBA2	18:1:1012:CLA:H3A	1.76	0.41
16:3:83:LEU:HD23	16:3:83:LEU:HA	1.82	0.41
16:3:127:LEU:C	18:3:3018:CLA:HBC3	2.45	0.41
16:3:134:LEU:HB2	16:3:138:GLN:CG	2.49	0.41
16:3:228:VAL:O	16:3:232:ARG:HG2	2.20	0.41
18:3:3010:CLA:H41	18:3:3010:CLA:H61	1.74	0.41
18:3:3012:CLA:CMB	18:3:3012:CLA:CBB	2.86	0.41
18:3:3012:CLA:C1	18:3:3017:CLA:HBB2	2.50	0.41
18:3:3017:CLA:CBB	18:3:3017:CLA:HHC	2.50	0.41
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.83	0.41
1:A:266:ALA:HB1	1:A:270:PHE:CD1	2.56	0.41
1:A:307:ALA:O	1:A:311:LEU:HG	2.21	0.41
2:B:526:GLY:HA2	2:B:582:TRP:CZ3	2.56	0.41
18:B:1023:CLA:H143	18:B:1023:CLA:H111	1.82	0.41
8:C:25:VAL:O	8:C:43:PRO:HD2	2.22	0.41
10:E:78:ARG:O	10:E:79:GLN:CB	2.69	0.41
10:E:106:ARG:HA	10:E:116:SER:O	2.21	0.41
11:H:111:LEU:HA	11:H:111:LEU:HD12	1.91	0.41
13:2:125:PHE:HB2	13:2:133:LEU:HD21	2.03	0.41
14:4:153:GLU:CD	14:4:156:ARG:HH11	2.29	0.41
15:1:85:ARG:NH2	18:1:1001:CLA:C1D	2.83	0.41
15:1:170:TYR:CE2	27:1:1501:LUT:H372	2.52	0.41
16:3:131:GLU:OE2	18:3:3018:CLA:CMA	2.69	0.41
16:3:161:GLU:OE2	18:3:3010:CLA:CAB	2.69	0.41
18:3:3004:CLA:H2	27:3:3502:LUT:C36	2.49	0.41
1:A:451:ILE:HA	18:B:1023:CLA:CGA	2.51	0.40
1:A:529:LEU:HD12	1:A:529:LEU:HA	1.86	0.40
20:A:5001:PQN:H141	20:A:5001:PQN:H161	1.60	0.40
21:A:7001:LHG:H101	18:A:1128:CLA:H41	2.03	0.40
18:A:1139:CLA:H41	18:A:1139:CLA:H62	1.50	0.40
18:B:1231:CLA:HBA2	18:B:1232:CLA:HMB3	2.02	0.40
18:B:1213:CLA:H11	18:B:1213:CLA:H51	1.71	0.40
22:F:6014:BCR:H15C	22:F:6014:BCR:H351	1.87	0.40
7:L:59:PRO:HD3	9:D:85:GLY:O	2.21	0.40
7:L:116:LYS:HB3	18:L:1503:CLA:HMB2	2.03	0.40
7:L:203:LEU:N	7:L:203:LEU:CD1	2.84	0.40
7:L:207:LEU:O	7:L:208:ASP:CB	2.69	0.40
9:D:77:PRO:O	9:D:77:PRO:CG	2.69	0.40
12:K:77:MET:SD	12:K:77:MET:O	2.79	0.40
13:2:204:LEU:HD12	13:2:206:TRP:CE2	2.56	0.40
13:2:250:LEU:O	13:2:254:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2005:CLA:CBC	18:2:2012:CLA:HBC2	2.51	0.40
14:4:152:VAL:CG1	28:4:4011:CHL:NB	2.81	0.40
14:4:212:MET:HB3	27:4:4502:LUT:C33	2.49	0.40
27:4:4501:LUT:C17	27:4:4501:LUT:H8	2.51	0.40
15:1:94:ILE:O	15:1:102:LEU:CD2	2.69	0.40
15:1:205:TYR:O	15:1:207:GLY:N	2.54	0.40
18:1:1004:CLA:CMD	28:1:1009:CHL:HBB1	2.52	0.40
18:1:1006:CLA:O1A	18:1:1013:CLA:C2D	2.70	0.40
16:3:155:TYR:HA	18:3:3010:CLA:HMC1	2.03	0.40
16:3:161:GLU:OE2	18:3:3010:CLA:HBB2	2.22	0.40
16:3:168:ALA:HB1	28:3:3011:CHL:C1B	2.51	0.40
16:3:248:THR:CG2	16:3:250:VAL:HG23	2.39	0.40
16:3:248:THR:CG2	16:3:255:ASN:ND2	2.73	0.40
18:3:3005:CLA:H61	18:3:3005:CLA:H41	1.80	0.40
18:3:3010:CLA:HAA1	18:3:3010:CLA:CBD	2.50	0.40
18:3:3012:CLA:CBA	18:3:3017:CLA:HBB2	2.51	0.40
18:A:1121:CLA:HAA1	12:K:83:PHE:CE2	2.56	0.40
2:B:330:ILE:HG22	18:B:1202:CLA:HHD	2.02	0.40
2:B:387:PHE:HZ	18:B:1222:CLA:HAB	1.87	0.40
18:B:1216:CLA:C1D	18:B:1220:CLA:H43	2.50	0.40
22:B:6005:BCR:H23C	18:B:1209:CLA:HMC2	2.02	0.40
18:B:1211:CLA:HMC2	18:B:1212:CLA:HAB	2.01	0.40
18:L:1502:CLA:CHD	22:L:6019:BCR:H292	2.50	0.40
8:C:60:THR:CB	8:C:64:SER:HG	2.34	0.40
9:D:174:TYR:HB3	9:D:176:GLU:OE2	2.22	0.40
12:K:75:THR:O	12:K:78:LEU:HB2	2.21	0.40
12:K:128:VAL:HG21	22:K:2011:BCR:C31	2.51	0.40
13:2:114:MET:HE3	18:2:2001:CLA:HMC1	1.94	0.40
13:2:149:THR:HG21	28:2:2010:CHL:CMD	2.52	0.40
13:2:211:PRO:C	13:2:212:GLN:CG	2.87	0.40
18:2:2003:CLA:C1A	18:2:2003:CLA:O2A	2.70	0.40
21:2:2801:LHG:O2	21:2:2801:LHG:P	2.79	0.40
14:4:52:LYS:O	14:4:53:LYS:CB	2.69	0.40
18:4:4009:CLA:HBA2	18:4:4009:CLA:H3A	1.79	0.40
18:4:4004:CLA:CGA	18:4:4004:CLA:C3A	2.99	0.40
18:4:4017:CLA:HED2	28:1:1009:CHL:HMB2	2.02	0.40
15:1:41:TRP:C	15:1:43:PRO:HD2	2.46	0.40
16:3:107:ARG:CZ	16:3:227:GLU:OE1	2.69	0.40
1:A:343:HIS:CE1	1:A:431:LEU:HD11	2.55	0.40
18:B:1207:CLA:CAB	3:I:14:LEU:HD21	2.51	0.40
18:B:1210:CLA:H193	18:B:1210:CLA:H161	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1215:CLA:H41	18:B:1215:CLA:H61	1.66	0.40
5:F:221:LEU:CB	5:F:222:LEU:HD23	2.50	0.40
7:L:122:ASN:O	7:L:123:THR:OG1	2.35	0.40
7:L:166:LEU:C	7:L:166:LEU:CD2	2.85	0.40
10:E:92:THR:OG1	10:E:93:VAL:N	2.53	0.40
11:H:95:LYS:O	11:H:96:ARG:CB	2.69	0.40
13:2:102:ASN:OD1	18:2:2004:CLA:C1	2.70	0.40
13:2:147:THR:O	13:2:148:ASP:CB	2.69	0.40
14:4:153:GLU:OE1	18:4:4012:CLA:C4B	2.70	0.40
14:4:154:ILE:O	28:1:1009:CHL:CED	2.69	0.40
18:4:4009:CLA:HHC	18:4:4009:CLA:CBB	2.20	0.40
18:4:4002:CLA:OBD	18:4:4007:CLA:CGA	2.70	0.40
15:1:78:GLU:CD	15:1:156:GLU:HG3	2.45	0.40
15:1:85:ARG:CZ	15:1:184:GLU:OE1	2.70	0.40
15:1:183:LYS:CE	18:1:1002:CLA:O1A	2.70	0.40
18:1:1013:CLA:H3A	18:1:1013:CLA:HBA1	1.80	0.40
16:3:102:GLU:HB2	18:3:3004:CLA:C1B	2.51	0.40
16:3:114:VAL:HG12	18:3:3006:CLA:HAC1	2.02	0.40
16:3:227:GLU:HB2	18:3:3001:CLA:C2B	2.52	0.40
16:3:266:ASN:O	16:3:267:ASN:CB	2.69	0.40
16:3:272:LEU:HD23	16:3:272:LEU:HA	1.96	0.40
1:A:537:ALA:O	1:A:541:VAL:HG23	2.21	0.40
18:A:1125:CLA:HBB1	18:A:1133:CLA:HAA2	2.04	0.40
18:B:1239:CLA:H172	7:L:144:CYS:SG	2.62	0.40
22:B:6004:BCR:H402	18:B:1218:CLA:C1D	2.50	0.40
7:L:128:GLN:CB	7:L:204:LEU:CG	2.97	0.40
7:L:145:LEU:HB3	7:L:186:THR:HG22	2.04	0.40
12:K:123:LEU:O	12:K:127:THR:HG23	2.21	0.40
14:4:152:VAL:C	14:4:155:ARG:CB	2.84	0.40
29:4:4505:ZEX:H27	29:4:4505:ZEX:H391	1.75	0.40
15:1:40:ASP:N	15:1:40:ASP:OD1	2.54	0.40
15:1:66:LEU:H	15:1:66:LEU:HG	1.73	0.40
15:1:86:TRP:O	15:1:89:LEU:N	2.54	0.40
15:1:218:LEU:HD23	15:1:218:LEU:HA	1.82	0.40
15:1:230:VAL:HG13	18:1:1014:CLA:C2B	2.48	0.40
16:3:131:GLU:O	16:3:132:THR:C	2.64	0.40
16:3:227:GLU:OE2	18:3:3001:CLA:C4A	2.69	0.40
1:A:488:PHE:HB3	18:A:1135:CLA:H2	2.04	0.40
18:A:1136:CLA:H92	18:A:1136:CLA:H61	1.89	0.40
2:B:558:PRO:HB3	2:B:702:ILE:HB	2.03	0.40
2:B:661:PHE:HB3	18:B:1023:CLA:HMC2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1021:CLA:H202	18:B:1021:CLA:H161	1.76	0.40
4:J:26:LEU:HD23	4:J:26:LEU:HA	1.86	0.40
22:J:6012:BCR:H15C	22:J:6012:BCR:H351	1.70	0.40
7:L:122:ASN:O	7:L:123:THR:CB	2.69	0.40
7:L:162:PRO:O	7:L:162:PRO:CG	2.70	0.40
11:H:117:THR:OG1	11:H:118:ALA:N	2.54	0.40
13:2:182:ILE:CG2	13:2:183:PHE:CE1	3.05	0.40
13:2:246:PRO:HG2	13:2:247:ILE:N	2.36	0.40
18:2:2002:CLA:CGA	18:2:2002:CLA:O2D	2.69	0.40
27:4:4501:LUT:H31	27:4:4501:LUT:H391	1.81	0.40
27:4:4502:LUT:H11	27:4:4502:LUT:H191	1.98	0.40
15:1:203:SER:O	15:1:204:ALA:CB	2.69	0.40
15:1:204:ALA:O	15:1:206:PRO:CD	2.70	0.40
15:1:218:LEU:HD22	18:1:1008:CLA:CBB	2.51	0.40
18:1:1011:CLA:C2	27:1:1501:LUT:H23	2.47	0.40
16:3:119:PRO:C	16:3:133:ALA:HB3	2.46	0.40
16:3:210:PRO:HD2	27:3:3501:LUT:O23	2.21	0.40
18:3:3008:CLA:C4A	18:3:3008:CLA:O1A	2.70	0.40

All (3) 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)
5:F:96:LYS:CD	7:L:170:LYS:NZ[3_555]	1.69	0.51
5:F:96:LYS:CE	7:L:170:LYS:NZ[3_555]	1.86	0.34
5:F:96:LYS:CG	7:L:170:LYS:NZ[3_555]	1.99	0.21

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	740/758 (98%)	691 (93%)	45 (6%)	4 (0%)	24 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	730/733 (100%)	695 (95%)	30 (4%)	5 (1%)	18 47
3	I	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	2 9
4	J	39/42 (93%)	34 (87%)	3 (8%)	2 (5%)	1 5
5	F	148/154 (96%)	138 (93%)	8 (5%)	2 (1%)	9 30
6	G	89/97 (92%)	76 (85%)	8 (9%)	5 (6%)	1 4
7	L	158/167 (95%)	133 (84%)	15 (10%)	10 (6%)	1 3
8	C	78/81 (96%)	72 (92%)	6 (8%)	0	100 100
9	D	139/147 (95%)	116 (84%)	14 (10%)	9 (6%)	1 3
10	E	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	7 27
11	H	82/90 (91%)	65 (79%)	10 (12%)	7 (8%)	0 1
12	K	53/129 (41%)	49 (92%)	2 (4%)	2 (4%)	2 9
13	2	205/269 (76%)	184 (90%)	7 (3%)	14 (7%)	1 2
14	4	196/252 (78%)	174 (89%)	15 (8%)	7 (4%)	2 10
15	1	192/202 (95%)	168 (88%)	17 (9%)	7 (4%)	2 10
16	3	213/275 (78%)	189 (89%)	15 (7%)	9 (4%)	2 7
All	All	3153/3492 (90%)	2866 (91%)	202 (6%)	85 (3%)	4 15

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
3	I	6	SER
4	J	11	ALA
6	G	101	PHE
6	G	102	GLU
6	G	104	GLY
7	L	67	GLY
7	L	125	ILE
7	L	152	SER
9	D	77	PRO
9	D	192	ILE
11	H	69	LEU
11	H	97	GLY
11	H	125	ILE
11	H	126	VAL
11	H	133	PRO
11	H	135	LEU

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Mol	Chain	Res	Type
12	K	80	ALA
12	K	86	ALA
13	2	71	SER
13	2	131	ILE
13	2	176	CYS
13	2	178	ASN
13	2	188	LEU
13	2	193	VAL
13	2	212	GLN
14	4	154	ILE
15	1	43	PRO
15	1	155	PRO
16	3	129	PRO
16	3	206	PRO
16	3	250	VAL
16	3	267	ASN
2	B	74	PHE
5	F	112	ASP
7	L	208	ASP
9	D	205	GLY
10	E	102	PRO
13	2	148	ASP
14	4	179	ALA
15	1	219	ALA
16	3	144	PRO
1	A	198	ASP
1	A	581	CYS
2	B	559	CYS
6	G	107	ARG
6	G	148	PRO
7	L	61	ASN
9	D	76	ASP
13	2	174	PRO
13	2	209	ALA
14	4	167	ASN
14	4	199	GLU
15	1	126	VAL
15	1	166	ASP
16	3	179	PRO
16	3	263	PRO
5	F	189	LYS
9	D	160	PRO

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Mol	Chain	Res	Type
9	D	191	SER
9	D	206	LYS
13	2	185	ASN
14	4	170	PRO
14	4	178	PRO
16	3	188	LEU
7	L	158	PRO
7	L	176	LEU
9	D	159	PHE
13	2	165	GLY
16	3	120	GLU
7	L	172	GLN
14	4	127	TYR
15	1	205	TYR
7	L	162	PRO
13	2	203	PRO
2	B	257	ILE
2	B	639	VAL
7	L	56	VAL
15	1	196	VAL
2	B	492	ILE
4	J	10	VAL
13	2	173	ASN
1	A	26	PRO
9	D	172	GLY
11	H	132	PRO

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	603/619 (97%)	590 (98%)	13 (2%)	45 78
2	B	599/600 (100%)	583 (97%)	16 (3%)	39 74
3	I	25/26 (96%)	23 (92%)	2 (8%)	11 34
4	J	33/35 (94%)	28 (85%)	5 (15%)	3 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	123/127 (97%)	114 (93%)	9 (7%)	13 38
6	G	71/76 (93%)	64 (90%)	7 (10%)	7 24
7	L	124/133 (93%)	105 (85%)	19 (15%)	3 10
8	C	69/70 (99%)	64 (93%)	5 (7%)	13 39
9	D	120/125 (96%)	107 (89%)	13 (11%)	6 21
10	E	59/59 (100%)	53 (90%)	6 (10%)	7 23
11	H	69/74 (93%)	63 (91%)	6 (9%)	9 30
12	K	38/99 (38%)	31 (82%)	7 (18%)	1 6
13	2	166/216 (77%)	149 (90%)	17 (10%)	7 23
14	4	161/202 (80%)	145 (90%)	16 (10%)	7 24
15	1	158/167 (95%)	139 (88%)	19 (12%)	5 17
16	3	159/213 (75%)	138 (87%)	21 (13%)	4 14
All	All	2577/2841 (91%)	2396 (93%)	181 (7%)	14 40

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	VAL
1	A	20	ILE
1	A	127	VAL
1	A	204	ASN
1	A	207	LEU
1	A	211	LEU
1	A	339	THR
1	A	348	GLU
1	A	433	ASP
1	A	465	ASP
1	A	485	GLN
1	A	569	ILE
1	A	590	CYS
2	B	73	ASN
2	B	127	ILE
2	B	155	LEU
2	B	172	GLU
2	B	176	ASN
2	B	220	GLN
2	B	280	ILE
2	B	444	LEU

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Mol	Chain	Res	Type
2	B	458	ILE
2	B	476	VAL
2	B	477	LEU
2	B	503	GLU
2	B	552	ASP
2	B	568	CYS
2	B	583	MET
2	B	640	CYS
3	I	4	LEU
3	I	11	LEU
4	J	3	ASP
4	J	10	VAL
4	J	13	VAL
4	J	16	THR
4	J	32	LEU
5	F	82	LEU
5	F	106	LEU
5	F	108	ILE
5	F	113	SER
5	F	139	LEU
5	F	185	ILE
5	F	220	GLU
5	F	222	LEU
5	F	225	GLU
6	G	92	LEU
6	G	99	THR
6	G	111	TYR
6	G	117	SER
6	G	123	ASP
6	G	141	THR
6	G	149	LYS
7	L	54	TYR
7	L	58	GLN
7	L	68	SER
7	L	93	VAL
7	L	121	ARG
7	L	123	THR
7	L	142	SER
7	L	146	THR
7	L	154	ASN
7	L	162	PRO
7	L	163	SER

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Mol	Chain	Res	Type
7	L	165	THR
7	L	169	ARG
7	L	172	GLN
7	L	174	ASP
7	L	176	LEU
7	L	178	THR
7	L	180	ASP
7	L	204	LEU
8	C	26	LEU
8	C	38	GLN
8	C	48	CYS
8	C	53	ARG
8	C	65	VAL
9	D	77	PRO
9	D	79	THR
9	D	91	LEU
9	D	99	GLU
9	D	109	LYS
9	D	112	ILE
9	D	128	ASN
9	D	139	LEU
9	D	163	GLU
9	D	164	VAL
9	D	173	VAL
9	D	190	ARG
9	D	195	ASN
10	E	66	ILE
10	E	79	GLN
10	E	80	GLU
10	E	85	LYS
10	E	110	VAL
10	E	127	GLU
11	H	54	TYR
11	H	59	ASP
11	H	69	LEU
11	H	122	ILE
11	H	123	LEU
11	H	125	ILE
12	K	62	ILE
12	K	68	VAL
12	K	69	ILE
12	K	70	MET

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Mol	Chain	Res	Type
12	K	76	LEU
12	K	88	SER
12	K	140	LEU
13	2	61	GLU
13	2	110	SER
13	2	122	ILE
13	2	133	LEU
13	2	134	THR
13	2	148	ASP
13	2	164	GLU
13	2	173	ASN
13	2	176	CYS
13	2	178	ASN
13	2	188	LEU
13	2	189	THR
13	2	222	ILE
13	2	233	MET
13	2	238	GLN
13	2	250	LEU
13	2	254	LEU
14	4	74	ASN
14	4	103	MET
14	4	116	THR
14	4	118	ILE
14	4	120	ILE
14	4	140	THR
14	4	158	GLN
14	4	162	ASN
14	4	168	GLN
14	4	169	ASP
14	4	171	ILE
14	4	174	GLN
14	4	182	VAL
14	4	221	GLN
14	4	225	THR
14	4	234	LEU
15	1	40	ASP
15	1	42	MET
15	1	43	PRO
15	1	85	ARG
15	1	88	MET
15	1	106	VAL

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Mol	Chain	Res	Type
15	1	120	THR
15	1	124	ASN
15	1	126	VAL
15	1	131	LEU
15	1	135	LEU
15	1	155	PRO
15	1	159	LYS
15	1	175	LYS
15	1	202	GLN
15	1	206	PRO
15	1	211	LEU
15	1	214	LEU
15	1	225	ASN
16	3	68	LEU
16	3	93	ILE
16	3	104	ILE
16	3	131	GLU
16	3	132	THR
16	3	149	ASN
16	3	188	LEU
16	3	190	LEU
16	3	206	PRO
16	3	211	LEU
16	3	218	LYS
16	3	220	LEU
16	3	225	LEU
16	3	226	LYS
16	3	232	ARG
16	3	235	MET
16	3	236	LEU
16	3	238	ILE
16	3	243	ILE
16	3	250	VAL
16	3	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	129	GLN
1	A	187	HIS
1	A	204	ASN

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Mol	Chain	Res	Type
1	A	205	HIS
1	A	222	GLN
1	A	224	HIS
1	A	234	ASN
1	A	303	HIS
1	A	325	HIS
1	A	398	HIS
1	A	543	HIS
1	A	615	HIS
1	A	629	ASN
1	A	631	GLN
1	A	666	GLN
1	A	721	GLN
2	B	14	GLN
2	B	44	GLN
2	B	73	ASN
2	B	176	ASN
2	B	294	ASN
2	B	368	GLN
2	B	627	ASN
5	F	132	ASN
5	F	136	GLN
6	G	59	ASN
6	G	95	GLN
6	G	132	HIS
7	L	122	ASN
7	L	172	GLN
8	C	71	HIS
9	D	96	GLN
9	D	195	ASN
10	E	111	ASN
11	H	82	GLN
12	K	130	HIS
13	2	104	GLN
13	2	109	HIS
13	2	178	ASN
13	2	238	GLN
13	2	259	HIS
14	4	98	ASN
14	4	158	GLN
14	4	162	ASN
14	4	174	GLN

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Mol	Chain	Res	Type
14	4	242	HIS
15	1	83	HIS
15	1	118	GLN
15	1	148	GLN
15	1	201	GLN
15	1	217	HIS
15	1	225	ASN
15	1	229	ASN
16	3	105	ASN
16	3	154	ASN
16	3	185	GLN
16	3	255	ASN
16	3	265	ASN
16	3	266	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 209 ligands modelled in this entry, 1 is monoatomic - leaving 208 for Mogul analysis.

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	$\#\|Z\|>2$
21	LHG	A	7001	-	48,48,48	0.96	2 (4%)	51,54,54	1.15	4 (7%)
27	LUT	3	3502	-	42,43,43	2.48	3 (7%)	51,60,60	2.15	15 (29%)
18	CLA	A	1013	-	69,73,73	2.35	23 (33%)	82,113,113	2.46	25 (30%)
18	CLA	B	1023	-	69,73,73	2.36	22 (31%)	82,113,113	2.45	26 (31%)
18	CLA	F	1302	5	54,58,73	2.61	20 (37%)	64,95,113	2.78	23 (35%)
22	BCR	B	6010	-	41,41,41	2.57	6 (14%)	56,56,56	6.71	23 (41%)
18	CLA	A	1104	-	69,73,73	2.37	23 (33%)	82,113,113	2.49	25 (30%)
18	CLA	A	1137	-	59,63,73	2.56	23 (38%)	70,101,113	2.60	25 (35%)
18	CLA	A	1129	-	54,58,73	2.68	22 (40%)	64,95,113	2.76	25 (39%)
18	CLA	4	4005	14	64,68,73	2.30	19 (29%)	76,107,113	2.70	30 (39%)
18	CLA	4	4008	-	50,54,73	2.61	20 (40%)	59,90,113	3.14	28 (47%)
22	BCR	A	6002	-	41,41,41	2.57	7 (17%)	56,56,56	6.60	23 (41%)
18	CLA	A	1128	-	69,73,73	2.35	21 (30%)	82,113,113	2.36	25 (30%)
23	LMG	B	5005	-	38,38,55	1.08	2 (5%)	46,46,63	1.06	3 (6%)
18	CLA	A	1122	-	69,73,73	2.37	22 (31%)	82,113,113	2.42	24 (29%)
18	CLA	B	1225	-	69,73,73	2.38	21 (30%)	82,113,113	2.40	23 (28%)
18	CLA	1	1003	15	59,63,73	2.42	21 (35%)	70,101,113	2.72	28 (40%)
22	BCR	G	2011	-	41,41,41	2.80	7 (17%)	56,56,56	6.88	29 (51%)
18	CLA	A	1103	-	69,73,73	2.34	22 (31%)	82,113,113	2.49	26 (31%)
18	CLA	B	1206	2	69,73,73	2.37	21 (30%)	82,113,113	2.45	26 (31%)
28	CHL	4	4013	-	41,55,74	2.82	15 (36%)	35,91,114	2.10	10 (28%)
18	CLA	3	3017	-	50,54,73	2.74	18 (36%)	59,90,113	2.70	23 (38%)
18	CLA	J	1302	4	54,58,73	2.70	22 (40%)	64,95,113	2.80	25 (39%)
18	CLA	B	1236	-	59,63,73	2.56	21 (35%)	70,101,113	2.69	24 (34%)
18	CLA	B	1217	-	50,54,73	2.84	22 (44%)	59,90,113	2.71	23 (38%)
18	CLA	A	1118	-	50,54,73	2.82	21 (42%)	59,90,113	2.77	22 (37%)
18	CLA	G	1002	-	50,54,73	2.74	21 (42%)	59,90,113	2.82	24 (40%)
18	CLA	B	1226	-	69,73,73	2.34	21 (30%)	82,113,113	2.39	24 (29%)
18	CLA	B	1238	-	69,73,73	2.38	23 (33%)	82,113,113	2.44	23 (28%)
22	BCR	B	6006	-	41,41,41	2.61	6 (14%)	56,56,56	7.01	27 (48%)
18	CLA	2	2007	-	64,68,73	2.37	21 (32%)	76,107,113	2.55	25 (32%)
22	BCR	L	6020	-	41,41,41	2.64	8 (19%)	56,56,56	6.69	28 (50%)
18	CLA	A	1127	-	69,73,73	2.37	22 (31%)	82,113,113	2.40	23 (28%)
22	BCR	J	6013	-	41,41,41	2.70	8 (19%)	56,56,56	6.69	28 (50%)
18	CLA	B	1222	-	69,73,73	2.34	22 (31%)	82,113,113	2.53	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	1	1001	15	64,68,73	2.32	19 (29%)	76,107,113	2.64	24 (31%)
18	CLA	1	1007	21	50,54,73	2.66	19 (38%)	59,90,113	3.00	25 (42%)
18	CLA	B	1207	-	69,73,73	2.36	22 (31%)	82,113,113	2.48	25 (30%)
18	CLA	3	3019	-	27,35,73	3.45	16 (59%)	32,60,113	3.01	15 (46%)
18	CLA	A	1114	-	50,54,73	2.85	21 (42%)	59,90,113	2.71	23 (38%)
27	LUT	4	4501	-	42,43,43	2.52	2 (4%)	51,60,60	2.00	16 (31%)
18	CLA	A	1132	-	69,73,73	2.37	22 (31%)	82,113,113	2.48	27 (32%)
22	BCR	I	6020	-	41,41,41	2.60	7 (17%)	56,56,56	6.82	19 (33%)
18	CLA	2	2019	-	27,35,73	3.31	16 (59%)	32,60,113	3.03	16 (50%)
22	BCR	A	6008	-	41,41,41	2.64	6 (14%)	56,56,56	6.72	26 (46%)
18	CLA	2	2002	-	50,54,73	2.66	19 (38%)	59,90,113	2.85	25 (42%)
18	CLA	A	1022	-	69,73,73	2.39	20 (28%)	82,113,113	2.41	27 (32%)
18	CLA	A	1115	-	50,54,73	2.85	22 (44%)	59,90,113	2.68	21 (35%)
28	CHL	4	4010	-	41,55,74	3.39	15 (36%)	35,91,114	2.59	14 (40%)
18	CLA	2	2008	-	54,58,73	2.48	19 (35%)	64,95,113	3.11	32 (50%)
18	CLA	A	1133	-	59,63,73	2.56	21 (35%)	70,101,113	2.64	24 (34%)
18	CLA	B	1021	-	69,73,73	2.35	21 (30%)	82,113,113	2.51	25 (30%)
18	CLA	3	3005	-	59,63,73	2.47	19 (32%)	70,101,113	2.75	28 (40%)
18	CLA	B	1231	-	64,68,73	2.49	22 (34%)	76,107,113	2.49	25 (32%)
18	CLA	B	1230	-	62,66,73	2.46	19 (30%)	73,104,113	2.72	24 (32%)
20	PQN	B	5002	-	34,34,34	1.72	2 (5%)	43,45,45	1.10	3 (6%)
18	CLA	3	3007	-	54,58,73	2.57	20 (37%)	64,95,113	2.78	26 (40%)
18	CLA	B	1204	-	59,63,73	2.58	22 (37%)	70,101,113	2.63	24 (34%)
18	CLA	2	2005	-	59,63,73	2.49	20 (33%)	70,101,113	2.60	25 (35%)
22	BCR	J	6012	-	41,41,41	2.72	7 (17%)	56,56,56	6.72	28 (50%)
18	CLA	A	1139	-	69,73,73	2.37	23 (33%)	82,113,113	2.45	26 (31%)
17	CL0	A	1011	-	58,73,73	3.22	17 (29%)	60,113,113	2.91	20 (33%)
23	LMG	J	5001	-	55,55,55	0.89	2 (3%)	63,63,63	1.45	8 (12%)
18	CLA	B	1220	-	69,73,73	2.37	22 (31%)	82,113,113	2.39	25 (30%)
18	CLA	A	1113	-	50,54,73	2.84	22 (44%)	59,90,113	2.72	24 (40%)
18	CLA	B	1235	-	69,73,73	2.36	21 (30%)	82,113,113	2.53	24 (29%)
18	CLA	A	1117	-	69,73,73	2.37	22 (31%)	82,113,113	2.42	24 (29%)
29	ZEX	4	4505	-	43,43,43	1.06	2 (4%)	51,60,60	2.13	19 (37%)
21	LHG	A	5003	18	39,39,48	1.05	2 (5%)	42,45,54	1.20	4 (9%)
18	CLA	G	1003	-	64,68,73	2.37	20 (31%)	76,107,113	2.62	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	B	1210	-	69,73,73	2.35	22 (31%)	82,113,113	2.46	26 (31%)
18	CLA	A	1135	-	55,59,73	2.65	22 (40%)	64,96,113	2.77	24 (37%)
18	CLA	3	3006	-	54,58,73	2.56	20 (37%)	64,95,113	2.86	25 (39%)
28	CHL	3	3011	-	50,64,74	2.84	11 (22%)	46,102,114	1.88	12 (26%)
18	CLA	B	1223	-	69,73,73	2.34	22 (31%)	82,113,113	2.50	27 (32%)
21	LHG	2	2801	-	23,23,48	1.32	2 (8%)	26,29,54	1.15	4 (15%)
22	BCR	B	6005	-	41,41,41	2.55	6 (14%)	56,56,56	6.96	24 (42%)
18	CLA	B	1232	-	59,63,73	2.57	23 (38%)	70,101,113	2.61	23 (32%)
18	CLA	1	1004	15	69,73,73	2.24	19 (27%)	82,113,113	2.55	24 (29%)
18	CLA	2	2004	13	69,73,73	2.39	18 (26%)	82,113,113	2.47	27 (32%)
18	CLA	A	1110	-	59,63,73	2.58	21 (35%)	70,101,113	2.58	24 (34%)
18	CLA	3	3004	16	64,68,73	2.35	19 (29%)	76,107,113	2.56	25 (32%)
22	BCR	B	6004	-	41,41,41	2.60	6 (14%)	56,56,56	6.82	28 (50%)
18	CLA	1	1013	-	50,54,73	2.75	21 (42%)	59,90,113	2.85	21 (35%)
22	BCR	L	6019	-	41,41,41	2.73	8 (19%)	56,56,56	6.70	24 (42%)
18	CLA	A	1124	-	59,63,73	2.57	22 (37%)	70,101,113	2.72	25 (35%)
22	BCR	B	6009	-	41,41,41	2.61	6 (14%)	56,56,56	6.54	22 (39%)
27	LUT	2	2502	-	42,43,43	2.57	4 (9%)	51,60,60	1.95	14 (27%)
18	CLA	B	1203	2	69,73,73	2.33	23 (33%)	82,113,113	2.48	24 (29%)
21	LHG	1	1801	18	48,48,48	0.91	2 (4%)	51,54,54	1.22	5 (9%)
18	CLA	A	1123	-	69,73,73	2.37	22 (31%)	82,113,113	2.48	25 (30%)
18	CLA	B	1239	-	69,73,73	2.37	23 (33%)	82,113,113	2.45	25 (30%)
18	CLA	A	1237	-	64,68,73	2.45	21 (32%)	76,107,113	2.65	25 (32%)
27	LUT	1	1502	-	42,43,43	2.55	4 (9%)	51,60,60	2.25	18 (35%)
18	CLA	B	1240	21	69,73,73	2.36	22 (31%)	82,113,113	2.49	27 (32%)
18	CLA	B	1209	-	50,54,73	2.86	22 (44%)	59,90,113	2.71	20 (33%)
18	CLA	B	1208	-	59,63,73	2.58	22 (37%)	70,101,113	2.67	24 (34%)
19	SF4	C	3003	8	0,12,12	-	-	-		
18	CLA	3	3018	16	54,58,73	2.56	21 (38%)	64,95,113	2.90	27 (42%)
22	BCR	A	6007	-	41,41,41	2.58	7 (17%)	56,56,56	6.67	22 (39%)
18	CLA	B	1228	-	64,68,73	2.46	22 (34%)	76,107,113	2.52	23 (30%)
18	CLA	1	1002	-	50,54,73	2.64	19 (38%)	59,90,113	2.90	24 (40%)
18	CLA	A	1101	-	69,73,73	2.35	22 (31%)	82,113,113	2.52	23 (28%)
27	LUT	1	1501	-	42,43,43	2.60	4 (9%)	51,60,60	2.43	14 (27%)
18	CLA	1	1012	15	54,58,73	2.56	20 (37%)	64,95,113	2.75	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	4	4001	14	64,68,73	2.32	19 (29%)	76,107,113	2.65	28 (36%)
18	CLA	3	3001	16	54,58,73	2.56	20 (37%)	64,95,113	2.85	24 (37%)
18	CLA	A	1102	-	54,58,73	2.66	22 (40%)	64,95,113	2.70	23 (35%)
18	CLA	B	1012	-	69,73,73	2.36	22 (31%)	82,113,113	2.42	25 (30%)
18	CLA	4	4002	-	54,58,73	2.55	18 (33%)	64,95,113	2.79	27 (42%)
20	PQN	A	5001	-	34,34,34	1.65	2 (5%)	43,45,45	1.21	4 (9%)
28	CHL	2	2010	-	41,55,74	2.88	13 (31%)	35,91,114	2.27	12 (34%)
28	CHL	2	2011	-	42,56,74	3.08	13 (30%)	36,92,114	2.07	8 (22%)
18	CLA	3	3008	-	52,56,73	2.51	19 (36%)	61,92,113	3.25	27 (44%)
18	CLA	B	1201	-	54,58,73	2.67	23 (42%)	64,95,113	2.71	26 (40%)
28	CHL	2	2013	-	40,54,74	2.22	10 (25%)	34,90,114	1.94	10 (29%)
18	CLA	1	1011	-	54,58,73	2.54	20 (37%)	64,95,113	2.82	27 (42%)
18	CLA	B	1216	-	69,73,73	2.37	23 (33%)	82,113,113	2.43	25 (30%)
18	CLA	B	1211	-	69,73,73	2.35	21 (30%)	82,113,113	2.54	29 (35%)
21	LHG	B	5004	18	20,20,48	1.37	2 (10%)	23,26,54	1.59	3 (13%)
23	LMG	G	2021	-	41,41,55	0.96	2 (4%)	49,49,63	1.17	5 (10%)
18	CLA	A	1125	-	64,68,73	2.42	22 (34%)	76,107,113	2.56	26 (34%)
28	CHL	1	1009	-	50,64,74	2.16	10 (20%)	46,102,114	1.90	13 (28%)
18	CLA	2	2003	-	59,63,73	2.38	19 (32%)	70,101,113	2.84	24 (34%)
18	CLA	A	1130	-	54,58,73	2.69	23 (42%)	64,95,113	2.74	24 (37%)
18	CLA	A	1131	-	69,73,73	2.37	22 (31%)	82,113,113	2.44	24 (29%)
18	CLA	3	3013	-	50,54,73	2.77	19 (38%)	59,90,113	2.55	22 (37%)
18	CLA	2	2009	13	54,58,73	2.58	20 (37%)	64,95,113	2.78	24 (37%)
18	CLA	4	4007	-	64,68,73	2.28	19 (29%)	76,107,113	2.73	25 (32%)
18	CLA	A	1151	21	54,58,73	2.72	23 (42%)	64,95,113	2.73	22 (34%)
23	LMG	F	5001	-	23,23,55	1.27	3 (13%)	31,31,63	1.75	6 (19%)
22	BCR	A	6017	-	41,41,41	2.52	6 (14%)	56,56,56	7.27	28 (50%)
26	LMU	B	8001	-	36,36,36	0.49	0	47,47,47	1.20	5 (10%)
18	CLA	3	3012	16	54,58,73	2.52	19 (35%)	64,95,113	2.94	27 (42%)
18	CLA	4	4016	-	50,54,73	2.74	20 (40%)	59,90,113	2.80	24 (40%)
18	CLA	A	1140	-	69,73,73	2.39	22 (31%)	82,113,113	2.42	25 (30%)
18	CLA	B	1229	-	69,73,73	2.36	23 (33%)	82,113,113	2.49	26 (31%)
18	CLA	3	3010	-	64,68,73	2.34	19 (29%)	76,107,113	2.61	24 (31%)
18	CLA	B	1218	-	69,73,73	2.37	22 (31%)	82,113,113	2.51	24 (29%)
18	CLA	B	1224	-	69,73,73	2.35	21 (30%)	82,113,113	2.49	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	A	1126	-	69,73,73	2.38	22 (31%)	82,113,113	2.49	27 (32%)
18	CLA	A	1116	-	64,68,73	2.46	21 (32%)	76,107,113	2.62	24 (31%)
18	CLA	B	1205	-	69,73,73	2.35	21 (30%)	82,113,113	2.38	25 (30%)
18	CLA	B	1221	-	69,73,73	2.37	22 (31%)	82,113,113	2.51	27 (32%)
23	LMG	4	4801	-	35,35,55	1.05	3 (8%)	43,43,63	1.64	9 (20%)
18	CLA	2	2012	13	59,63,73	2.41	19 (32%)	70,101,113	2.73	27 (38%)
18	CLA	A	1105	-	55,59,73	2.68	21 (38%)	64,96,113	2.74	28 (43%)
22	BCR	F	6014	-	41,41,41	2.83	7 (17%)	56,56,56	6.85	23 (41%)
22	BCR	A	6003	-	41,41,41	2.60	6 (14%)	56,56,56	6.63	18 (32%)
22	BCR	K	2011	-	41,41,41	2.54	6 (14%)	56,56,56	6.90	29 (51%)
18	CLA	2	2001	13	64,68,73	2.31	20 (31%)	76,107,113	2.68	29 (38%)
18	CLA	A	1138	-	69,73,73	2.39	22 (31%)	82,113,113	2.38	25 (30%)
19	SF4	C	3002	8	0,12,12	-	-	-		
18	CLA	A	1109	-	69,73,73	2.37	21 (30%)	82,113,113	2.45	25 (30%)
22	BCR	A	6011	-	41,41,41	2.68	6 (14%)	56,56,56	6.87	25 (44%)
18	CLA	A	1111	-	64,68,73	2.45	22 (34%)	76,107,113	2.53	26 (34%)
22	BCR	F	6016	-	41,41,41	2.84	8 (19%)	56,56,56	6.86	24 (42%)
18	CLA	A	1120	-	64,68,73	2.45	22 (34%)	76,107,113	2.58	23 (30%)
18	CLA	4	4012	14	69,73,73	2.22	19 (27%)	82,113,113	2.54	30 (36%)
19	SF4	A	3001	1,2	0,12,12	-	-	-		
18	CLA	4	4004	14	64,68,73	2.34	18 (28%)	76,107,113	2.61	27 (35%)
18	CLA	A	1108	-	50,54,73	2.86	22 (44%)	59,90,113	2.71	22 (37%)
18	CLA	B	1219	-	64,68,73	2.47	23 (35%)	76,107,113	2.47	23 (30%)
18	CLA	2	2016	13	54,58,73	2.62	19 (35%)	64,95,113	3.36	30 (46%)
18	CLA	4	4017	-	69,73,73	2.24	19 (27%)	82,113,113	2.50	28 (34%)
18	CLA	4	4009	14	54,58,73	2.50	19 (35%)	64,95,113	2.77	24 (37%)
23	LMG	F	5002	-	37,37,55	1.07	3 (8%)	45,45,63	1.29	5 (11%)
28	CHL	1	1010	15	41,55,74	2.38	13 (31%)	35,91,114	2.00	11 (31%)
18	CLA	4	4006	-	54,58,73	2.50	19 (35%)	64,95,113	2.68	24 (37%)
18	CLA	3	3003	16	64,68,73	2.36	20 (31%)	76,107,113	2.62	27 (35%)
27	LUT	4	4502	-	42,43,43	2.48	3 (7%)	51,60,60	1.81	12 (23%)
18	CLA	A	1106	1	69,73,73	2.37	22 (31%)	82,113,113	2.49	24 (29%)
18	CLA	B	1212	-	59,63,73	2.54	21 (35%)	70,101,113	2.68	26 (37%)
18	CLA	B	1213	-	64,68,73	2.45	21 (32%)	76,107,113	2.53	23 (30%)
18	CLA	B	1234	-	64,68,73	2.47	22 (34%)	76,107,113	2.60	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	A	1134	-	59,63,73	2.57	21 (35%)	70,101,113	2.64	24 (34%)
22	BCR	3	3503	-	41,41,41	2.73	8 (19%)	56,56,56	6.56	30 (53%)
18	CLA	F	1301	-	49,53,73	2.63	19 (38%)	58,89,113	2.76	21 (36%)
18	CLA	B	1215	-	64,68,73	2.48	23 (35%)	76,107,113	2.52	23 (30%)
18	CLA	4	4003	14	69,73,73	2.26	20 (28%)	82,113,113	2.49	25 (30%)
18	CLA	A	1119	-	69,73,73	2.36	22 (31%)	82,113,113	2.42	24 (29%)
27	LUT	I	6018	-	42,43,43	2.56	2 (4%)	51,60,60	2.05	18 (35%)
23	LMG	2	2802	-	35,35,55	1.09	2 (5%)	43,43,63	1.34	7 (16%)
26	LMU	B	8002	-	36,36,36	0.45	0	47,47,47	1.07	3 (6%)
18	CLA	L	1503	-	54,58,73	2.57	19 (35%)	64,95,113	2.78	24 (37%)
18	CLA	1	1014	15	50,54,73	2.70	19 (38%)	59,90,113	2.90	25 (42%)
27	LUT	2	2501	-	42,43,43	2.53	2 (4%)	51,60,60	1.97	14 (27%)
27	LUT	3	3501	-	42,43,43	2.43	1 (2%)	51,60,60	2.28	16 (31%)
28	CHL	4	4011	-	45,59,74	3.05	13 (28%)	40,96,114	1.99	12 (30%)
18	CLA	3	3002	-	50,54,73	2.70	21 (42%)	59,90,113	2.89	26 (44%)
18	CLA	B	1227	-	69,73,73	2.37	23 (33%)	82,113,113	2.48	26 (31%)
18	CLA	B	1202	-	69,73,73	2.35	22 (31%)	82,113,113	2.53	25 (30%)
18	CLA	1	1006	-	54,58,73	2.59	21 (38%)	64,95,113	2.82	26 (40%)
27	LUT	4	4503	-	42,43,43	2.49	3 (7%)	51,60,60	2.45	17 (33%)
18	CLA	1	1008	-	50,54,73	2.67	19 (38%)	59,90,113	2.83	25 (42%)
18	CLA	2	2006	-	59,63,73	2.49	20 (33%)	70,101,113	2.66	25 (35%)
25	DGD	B	7101	-	62,62,67	0.91	1 (1%)	76,76,81	1.32	11 (14%)
18	CLA	L	1502	-	64,68,73	2.36	19 (29%)	76,107,113	2.64	27 (35%)
18	CLA	K	1001	-	50,54,73	2.73	20 (40%)	59,90,113	2.99	23 (38%)
18	CLA	A	1107	1	69,73,73	2.38	23 (33%)	82,113,113	2.47	25 (30%)
18	CLA	B	1214	-	63,67,73	2.48	22 (34%)	74,105,113	2.62	25 (33%)
18	CLA	A	1121	-	59,63,73	2.56	22 (37%)	70,101,113	2.71	26 (37%)
18	CLA	A	1136	-	60,64,73	2.54	22 (36%)	71,102,113	2.65	27 (38%)
18	CLA	G	1001	-	59,63,73	2.44	19 (32%)	70,101,113	2.76	29 (41%)
18	CLA	A	1112	-	69,73,73	2.36	22 (31%)	82,113,113	2.47	25 (30%)
18	CLA	L	1501	7	54,58,73	2.59	18 (33%)	64,95,113	2.79	28 (43%)
18	CLA	H	1000	11	50,54,73	2.84	21 (42%)	59,90,113	2.72	22 (37%)
18	CLA	1	1005	-	59,63,73	2.41	19 (32%)	70,101,113	2.74	28 (40%)

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
21	LHG	A	7001	-	-	30/53/53/53	-
27	LUT	3	3502	-	1/1/12/27	7/29/67/67	0/2/2/2
18	CLA	A	1013	-	1/1/15/20	10/39/115/115	-
18	CLA	B	1023	-	1/1/15/20	10/39/115/115	-
18	CLA	F	1302	5	1/1/12/20	8/21/97/115	-
22	BCR	B	6010	-	-	10/29/63/63	0/2/2/2
18	CLA	A	1104	-	1/1/15/20	18/39/115/115	-
18	CLA	A	1137	-	1/1/13/20	10/27/103/115	-
18	CLA	A	1129	-	1/1/12/20	9/21/97/115	-
18	CLA	4	4005	14	1/1/14/20	14/33/109/115	-
18	CLA	4	4008	-	1/1/11/20	10/17/93/115	-
22	BCR	A	6002	-	-	11/29/63/63	0/2/2/2
18	CLA	A	1128	-	1/1/15/20	13/39/115/115	-
23	LMG	B	5005	-	-	17/33/53/70	0/1/1/1
18	CLA	A	1122	-	1/1/15/20	23/39/115/115	-
18	CLA	B	1225	-	1/1/15/20	16/39/115/115	-
18	CLA	1	1003	15	1/1/13/20	9/27/103/115	-
22	BCR	G	2011	-	-	11/29/63/63	0/2/2/2
18	CLA	A	1103	-	1/1/15/20	20/39/115/115	-
18	CLA	B	1206	2	1/1/15/20	15/39/115/115	-
28	CHL	4	4013	-	3/3/16/26	3/17/115/137	-
18	CLA	3	3017	-	1/1/11/20	5/17/93/115	-
18	CLA	J	1302	4	1/1/12/20	11/21/97/115	-
18	CLA	B	1236	-	1/1/13/20	12/27/103/115	-
18	CLA	B	1217	-	1/1/11/20	9/17/93/115	-
18	CLA	A	1118	-	1/1/11/20	9/17/93/115	-
18	CLA	G	1002	-	1/1/11/20	8/17/93/115	-
18	CLA	B	1226	-	1/1/15/20	16/39/115/115	-
18	CLA	B	1238	-	1/1/15/20	17/39/115/115	-
22	BCR	B	6006	-	-	10/29/63/63	0/2/2/2
18	CLA	2	2007	-	1/1/14/20	14/33/109/115	-
22	BCR	L	6020	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1127	-	1/1/15/20	15/39/115/115	-
22	BCR	J	6013	-	-	12/29/63/63	0/2/2/2
18	CLA	B	1222	-	1/1/15/20	16/39/115/115	-
18	CLA	1	1001	15	1/1/14/20	15/33/109/115	-
18	CLA	1	1007	21	1/1/11/20	10/17/93/115	-
18	CLA	3	3019	-	1/1/5/20	-	-
27	LUT	4	4501	-	1/1/12/27	4/29/67/67	0/2/2/2
18	CLA	A	1114	-	1/1/11/20	7/17/93/115	-
18	CLA	B	1207	-	-	16/39/115/115	-
18	CLA	A	1132	-	1/1/15/20	14/39/115/115	-
22	BCR	I	6020	-	-	10/29/63/63	0/2/2/2
18	CLA	2	2019	-	1/1/5/20	-	-
22	BCR	A	6008	-	-	8/29/63/63	0/2/2/2
18	CLA	2	2002	-	1/1/11/20	6/17/93/115	-
18	CLA	A	1022	-	1/1/15/20	13/39/115/115	-
18	CLA	A	1115	-	1/1/11/20	8/17/93/115	-
28	CHL	4	4010	-	3/3/16/26	3/17/115/137	-
18	CLA	2	2008	-	1/1/12/20	9/21/97/115	-
18	CLA	B	1021	-	1/1/15/20	12/39/115/115	-
18	CLA	A	1133	-	-	11/27/103/115	-
18	CLA	3	3005	-	1/1/13/20	15/27/103/115	-
18	CLA	B	1231	-	1/1/14/20	13/33/109/115	-
18	CLA	B	1230	-	1/1/13/20	18/31/107/115	-
20	PQN	B	5002	-	-	10/23/43/43	0/2/2/2
18	CLA	3	3007	-	1/1/12/20	6/21/97/115	-
18	CLA	B	1204	-	1/1/13/20	12/27/103/115	-
18	CLA	2	2005	-	1/1/13/20	14/27/103/115	-
22	BCR	J	6012	-	-	10/29/63/63	0/2/2/2
18	CLA	A	1139	-	1/1/15/20	14/39/115/115	-
17	CL0	A	1011	-	3/3/20/25	10/37/135/135	-
23	LMG	J	5001	-	-	35/50/70/70	0/1/1/1
18	CLA	B	1220	-	-	16/39/115/115	-
18	CLA	A	1113	-	1/1/11/20	11/17/93/115	-
18	CLA	B	1235	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1117	-	1/1/15/20	13/39/115/115	-
29	ZEX	4	4505	-	-	2/29/67/67	0/2/2/2
21	LHG	A	5003	18	-	20/44/44/53	-
18	CLA	G	1003	-	1/1/14/20	13/33/109/115	-
18	CLA	B	1210	-	1/1/15/20	13/39/115/115	-
18	CLA	A	1135	-	1/1/12/20	5/23/99/115	-
18	CLA	3	3006	-	1/1/12/20	5/21/97/115	-
28	CHL	3	3011	-	4/4/18/26	5/27/125/137	-
18	CLA	B	1223	-	-	15/39/115/115	-
21	LHG	2	2801	-	-	15/28/28/53	-
22	BCR	B	6005	-	-	13/29/63/63	0/2/2/2
18	CLA	B	1232	-	1/1/13/20	7/27/103/115	-
18	CLA	1	1004	15	1/1/15/20	19/39/115/115	-
18	CLA	2	2004	13	1/1/15/20	13/39/115/115	-
18	CLA	A	1110	-	1/1/13/20	10/27/103/115	-
18	CLA	3	3004	16	1/1/14/20	11/33/109/115	-
22	BCR	B	6004	-	-	10/29/63/63	0/2/2/2
18	CLA	1	1013	-	1/1/11/20	8/17/93/115	-
22	BCR	L	6019	-	-	11/29/63/63	0/2/2/2
18	CLA	A	1124	-	1/1/13/20	11/27/103/115	-
27	LUT	2	2502	-	1/1/12/27	4/29/67/67	0/2/2/2
22	BCR	B	6009	-	-	8/29/63/63	0/2/2/2
18	CLA	B	1203	2	1/1/15/20	16/39/115/115	-
21	LHG	1	1801	18	-	22/53/53/53	-
18	CLA	A	1123	-	1/1/15/20	17/39/115/115	-
18	CLA	B	1239	-	1/1/15/20	19/39/115/115	-
18	CLA	A	1237	-	1/1/14/20	15/33/109/115	-
27	LUT	1	1502	-	1/1/12/27	2/29/67/67	0/2/2/2
18	CLA	B	1240	21	1/1/15/20	16/39/115/115	-
18	CLA	B	1209	-	1/1/11/20	5/17/93/115	-
18	CLA	B	1208	-	1/1/13/20	15/27/103/115	-
19	SF4	C	3003	8	-	-	0/6/5/5
18	CLA	3	3018	16	1/1/12/20	7/21/97/115	-
22	BCR	A	6007	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1228	-	1/1/14/20	14/33/109/115	-
18	CLA	1	1002	-	1/1/11/20	6/17/93/115	-
18	CLA	A	1101	-	1/1/15/20	14/39/115/115	-
27	LUT	1	1501	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	1	1012	15	1/1/12/20	10/21/97/115	-
18	CLA	4	4001	14	1/1/14/20	13/33/109/115	-
18	CLA	3	3001	16	1/1/12/20	5/21/97/115	-
18	CLA	A	1102	-	1/1/12/20	5/21/97/115	-
18	CLA	B	1012	-	1/1/15/20	15/39/115/115	-
18	CLA	4	4002	-	1/1/12/20	4/21/97/115	-
28	CHL	2	2010	-	3/3/16/26	1/17/115/137	-
20	PQN	A	5001	-	-	10/23/43/43	0/2/2/2
28	CHL	2	2011	-	3/3/16/26	1/18/116/137	-
18	CLA	3	3008	-	1/1/11/20	10/19/95/115	-
18	CLA	B	1201	-	1/1/12/20	10/21/97/115	-
28	CHL	2	2013	-	3/3/16/26	4/15/113/137	-
18	CLA	1	1011	-	1/1/12/20	10/21/97/115	-
18	CLA	B	1216	-	1/1/15/20	16/39/115/115	-
18	CLA	B	1211	-	1/1/15/20	10/39/115/115	-
21	LHG	B	5004	18	-	15/23/23/53	-
23	LMG	G	2021	-	-	24/36/56/70	0/1/1/1
18	CLA	A	1125	-	1/1/14/20	20/33/109/115	-
28	CHL	1	1009	-	4/4/18/26	5/27/125/137	-
18	CLA	2	2003	-	1/1/13/20	13/27/103/115	-
18	CLA	A	1130	-	-	7/21/97/115	-
18	CLA	A	1131	-	1/1/15/20	12/39/115/115	-
18	CLA	3	3013	-	1/1/11/20	11/17/93/115	-
18	CLA	2	2009	13	1/1/12/20	7/21/97/115	-
18	CLA	4	4007	-	1/1/14/20	14/33/109/115	-
18	CLA	A	1151	21	1/1/12/20	11/21/97/115	-
23	LMG	F	5001	-	-	9/16/36/70	0/1/1/1
22	BCR	A	6017	-	-	10/29/63/63	0/2/2/2
26	LMU	B	8001	-	-	9/21/61/61	0/2/2/2
18	CLA	3	3012	16	1/1/12/20	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	4016	-	1/1/11/20	12/17/93/115	-
18	CLA	A	1140	-	1/1/15/20	18/39/115/115	-
18	CLA	B	1229	-	1/1/15/20	15/39/115/115	-
18	CLA	3	3010	-	1/1/14/20	17/33/109/115	-
18	CLA	B	1218	-	1/1/15/20	15/39/115/115	-
18	CLA	B	1224	-	1/1/15/20	23/39/115/115	-
18	CLA	A	1126	-	1/1/15/20	14/39/115/115	-
18	CLA	A	1116	-	1/1/14/20	17/33/109/115	-
18	CLA	B	1205	-	1/1/15/20	12/39/115/115	-
18	CLA	B	1221	-	1/1/15/20	21/39/115/115	-
23	LMG	4	4801	-	-	17/30/50/70	0/1/1/1
18	CLA	2	2012	13	1/1/13/20	9/27/103/115	-
18	CLA	A	1105	-	1/1/12/20	12/23/99/115	-
22	BCR	F	6014	-	-	12/29/63/63	0/2/2/2
22	BCR	A	6003	-	-	13/29/63/63	0/2/2/2
22	BCR	K	2011	-	-	10/29/63/63	0/2/2/2
18	CLA	2	2001	13	1/1/14/20	17/33/109/115	-
18	CLA	A	1138	-	1/1/15/20	15/39/115/115	-
19	SF4	C	3002	8	-	-	0/6/5/5
18	CLA	A	1109	-	1/1/15/20	11/39/115/115	-
22	BCR	A	6011	-	-	18/29/63/63	0/2/2/2
18	CLA	A	1111	-	1/1/14/20	13/33/109/115	-
22	BCR	F	6016	-	-	8/29/63/63	0/2/2/2
18	CLA	A	1120	-	1/1/14/20	18/33/109/115	-
18	CLA	4	4012	14	1/1/15/20	19/39/115/115	-
19	SF4	A	3001	1,2	-	-	0/6/5/5
18	CLA	4	4004	14	1/1/14/20	13/33/109/115	-
18	CLA	A	1108	-	1/1/11/20	4/17/93/115	-
18	CLA	B	1219	-	1/1/14/20	16/33/109/115	-
18	CLA	2	2016	13	1/1/12/20	9/21/97/115	-
18	CLA	4	4017	-	1/1/15/20	16/39/115/115	-
18	CLA	4	4009	14	1/1/12/20	3/21/97/115	-
28	CHL	1	1010	15	3/3/16/26	6/17/115/137	-
23	LMG	F	5002	-	-	15/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	4006	-	1/1/12/20	4/21/97/115	-
18	CLA	3	3003	16	1/1/14/20	12/33/109/115	-
27	LUT	4	4502	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	A	1106	1	1/1/15/20	15/39/115/115	-
18	CLA	B	1212	-	1/1/13/20	8/27/103/115	-
18	CLA	B	1213	-	-	13/33/109/115	-
18	CLA	B	1234	-	1/1/14/20	12/33/109/115	-
18	CLA	A	1134	-	1/1/13/20	15/27/103/115	-
22	BCR	3	3503	-	-	14/29/63/63	0/2/2/2
18	CLA	F	1301	-	1/1/11/20	2/15/91/115	-
18	CLA	B	1215	-	1/1/14/20	15/33/109/115	-
18	CLA	4	4003	14	1/1/15/20	16/39/115/115	-
18	CLA	A	1119	-	1/1/15/20	23/39/115/115	-
27	LUT	I	6018	-	1/1/12/27	2/29/67/67	0/2/2/2
27	LUT	2	2501	-	1/1/12/27	3/29/67/67	0/2/2/2
27	LUT	3	3501	-	1/1/12/27	5/29/67/67	0/2/2/2
18	CLA	L	1503	-	1/1/12/20	7/21/97/115	-
18	CLA	1	1014	15	1/1/11/20	7/17/93/115	-
23	LMG	2	2802	-	-	13/30/50/70	0/1/1/1
28	CHL	4	4011	-	3/3/17/26	2/21/119/137	-
26	LMU	B	8002	-	-	14/21/61/61	0/2/2/2
18	CLA	3	3002	-	1/1/11/20	6/17/93/115	-
18	CLA	B	1227	-	1/1/15/20	13/39/115/115	-
18	CLA	B	1202	-	1/1/15/20	16/39/115/115	-
18	CLA	1	1006	-	1/1/12/20	8/21/97/115	-
27	LUT	4	4503	-	1/1/12/27	10/29/67/67	0/2/2/2
18	CLA	1	1008	-	1/1/11/20	8/17/93/115	-
18	CLA	2	2006	-	1/1/13/20	11/27/103/115	-
25	DGD	B	7101	-	-	24/50/90/95	0/2/2/2
18	CLA	L	1502	-	1/1/14/20	15/33/109/115	-
18	CLA	K	1001	-	1/1/11/20	8/17/93/115	-
18	CLA	A	1107	1	1/1/15/20	16/39/115/115	-
18	CLA	B	1214	-	1/1/13/20	12/32/108/115	-
18	CLA	A	1121	-	1/1/13/20	17/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1136	-	1/1/13/20	10/29/105/115	-
18	CLA	G	1001	-	1/1/13/20	16/27/103/115	-
18	CLA	A	1112	-	1/1/15/20	16/39/115/115	-
18	CLA	L	1501	7	1/1/12/20	9/21/97/115	-
18	CLA	H	1000	11	1/1/11/20	10/17/93/115	-
18	CLA	1	1005	-	1/1/13/20	8/27/103/115	-

All (3378) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	2502	LUT	C24-C25	15.60	1.51	1.33
27	I	6018	LUT	C24-C25	15.60	1.51	1.33
27	2	2501	LUT	C24-C25	15.52	1.51	1.33
27	1	1501	LUT	C24-C25	15.45	1.51	1.33
27	1	1502	LUT	C24-C25	14.99	1.51	1.33
27	4	4503	LUT	C24-C25	14.98	1.50	1.33
27	4	4501	LUT	C24-C25	14.97	1.50	1.33
27	3	3502	LUT	C24-C25	14.76	1.50	1.33
27	4	4502	LUT	C24-C25	14.75	1.50	1.33
27	3	3501	LUT	C24-C25	14.70	1.50	1.33
28	4	4010	CHL	C3A-C2A	-13.99	1.42	1.54
28	4	4011	CHL	C3A-C2A	-12.37	1.44	1.54
28	3	3011	CHL	C3A-C2A	-11.30	1.44	1.54
28	2	2011	CHL	C3A-C2A	-9.82	1.46	1.54
18	J	1302	CLA	MG-NA	9.71	2.29	2.06
18	A	1022	CLA	MG-NA	9.69	2.29	2.06
18	2	2004	CLA	MG-NA	9.68	2.29	2.06
18	B	1229	CLA	MG-NA	9.66	2.29	2.06
18	A	1105	CLA	MG-NA	9.65	2.29	2.06
18	A	1127	CLA	MG-NA	9.63	2.29	2.06
18	B	1232	CLA	MG-NA	9.62	2.29	2.06
18	A	1102	CLA	MG-NA	9.62	2.29	2.06
18	A	1151	CLA	MG-NA	9.61	2.29	2.06
18	B	1215	CLA	MG-NA	9.61	2.29	2.06
18	A	1114	CLA	MG-NA	9.61	2.29	2.06
18	B	1012	CLA	MG-NA	9.61	2.29	2.06
18	B	1221	CLA	MG-NA	9.60	2.29	2.06
18	B	1206	CLA	MG-NA	9.59	2.29	2.06
18	A	1140	CLA	MG-NA	9.59	2.29	2.06
18	B	1217	CLA	MG-NA	9.58	2.29	2.06
18	A	1126	CLA	MG-NA	9.58	2.29	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1234	CLA	MG-NA	9.57	2.29	2.06
18	B	1236	CLA	MG-NA	9.56	2.29	2.06
18	B	1228	CLA	MG-NA	9.56	2.29	2.06
18	B	1220	CLA	MG-NA	9.56	2.29	2.06
18	B	1238	CLA	MG-NA	9.56	2.29	2.06
18	A	1135	CLA	MG-NA	9.55	2.29	2.06
18	A	1110	CLA	MG-NA	9.55	2.29	2.06
18	A	1129	CLA	MG-NA	9.55	2.28	2.06
18	A	1122	CLA	MG-NA	9.54	2.28	2.06
18	B	1218	CLA	MG-NA	9.54	2.28	2.06
18	A	1130	CLA	MG-NA	9.54	2.28	2.06
18	A	1137	CLA	MG-NA	9.53	2.28	2.06
18	A	1117	CLA	MG-NA	9.53	2.28	2.06
18	A	1107	CLA	MG-NA	9.53	2.28	2.06
18	A	1112	CLA	MG-NA	9.52	2.28	2.06
18	A	1104	CLA	MG-NA	9.52	2.28	2.06
18	A	1119	CLA	MG-NA	9.52	2.28	2.06
18	B	1219	CLA	MG-NA	9.51	2.28	2.06
18	A	1109	CLA	MG-NA	9.51	2.28	2.06
18	A	1134	CLA	MG-NA	9.51	2.28	2.06
18	A	1113	CLA	MG-NA	9.51	2.28	2.06
18	A	1124	CLA	MG-NA	9.51	2.28	2.06
18	B	1222	CLA	MG-NA	9.51	2.28	2.06
18	A	1139	CLA	MG-NA	9.51	2.28	2.06
18	B	1239	CLA	MG-NA	9.50	2.28	2.06
18	A	1133	CLA	MG-NA	9.50	2.28	2.06
18	B	1231	CLA	MG-NA	9.50	2.28	2.06
18	H	1000	CLA	MG-NA	9.50	2.28	2.06
28	2	2010	CHL	C3A-C2A	-9.50	1.46	1.54
18	B	1214	CLA	MG-NA	9.50	2.28	2.06
18	B	1216	CLA	MG-NA	9.49	2.28	2.06
18	B	1225	CLA	MG-NA	9.49	2.28	2.06
18	A	1128	CLA	MG-NA	9.49	2.28	2.06
18	A	1123	CLA	MG-NA	9.49	2.28	2.06
18	B	1240	CLA	MG-NA	9.48	2.28	2.06
18	A	1116	CLA	MG-NA	9.48	2.28	2.06
18	B	1201	CLA	MG-NA	9.48	2.28	2.06
18	B	1209	CLA	MG-NA	9.48	2.28	2.06
18	A	1121	CLA	MG-NA	9.48	2.28	2.06
18	A	1115	CLA	MG-NA	9.48	2.28	2.06
18	B	1208	CLA	MG-NA	9.47	2.28	2.06
18	B	1223	CLA	MG-NA	9.46	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1131	CLA	MG-NA	9.45	2.28	2.06
18	B	1213	CLA	MG-NA	9.45	2.28	2.06
18	A	1125	CLA	MG-NA	9.45	2.28	2.06
18	A	1106	CLA	MG-NA	9.45	2.28	2.06
18	A	1132	CLA	MG-NA	9.45	2.28	2.06
18	A	1120	CLA	MG-NA	9.45	2.28	2.06
18	A	1136	CLA	MG-NA	9.45	2.28	2.06
18	B	1205	CLA	MG-NA	9.44	2.28	2.06
18	B	1023	CLA	MG-NA	9.44	2.28	2.06
18	B	1207	CLA	MG-NA	9.44	2.28	2.06
18	A	1108	CLA	MG-NA	9.44	2.28	2.06
18	B	1226	CLA	MG-NA	9.44	2.28	2.06
18	B	1230	CLA	MG-NA	9.43	2.28	2.06
18	A	1118	CLA	MG-NA	9.43	2.28	2.06
18	A	1111	CLA	MG-NA	9.41	2.28	2.06
18	B	1021	CLA	MG-NA	9.41	2.28	2.06
18	A	1237	CLA	MG-NA	9.40	2.28	2.06
18	B	1224	CLA	MG-NA	9.40	2.28	2.06
18	B	1204	CLA	MG-NA	9.40	2.28	2.06
18	B	1235	CLA	MG-NA	9.39	2.28	2.06
17	A	1011	CL0	C1A-CHA	9.36	1.50	1.40
18	B	1210	CLA	MG-NA	9.35	2.28	2.06
28	2	2011	CHL	C1A-CHA	-9.34	1.29	1.40
18	B	1227	CLA	MG-NA	9.33	2.28	2.06
18	B	1203	CLA	MG-NA	9.32	2.28	2.06
18	B	1212	CLA	MG-NA	9.31	2.28	2.06
18	A	1138	CLA	MG-NA	9.31	2.28	2.06
18	A	1101	CLA	MG-NA	9.29	2.28	2.06
18	A	1013	CLA	MG-NA	9.26	2.28	2.06
18	A	1103	CLA	MG-NA	9.22	2.28	2.06
18	B	1211	CLA	MG-NA	9.15	2.28	2.06
18	3	3019	CLA	MG-NA	9.10	2.27	2.06
18	B	1202	CLA	MG-NA	9.05	2.27	2.06
28	3	3011	CHL	C1A-CHA	-8.94	1.29	1.40
18	F	1301	CLA	MG-NA	8.82	2.27	2.06
18	2	2019	CLA	MG-NA	8.82	2.27	2.06
18	F	1302	CLA	MG-NA	8.80	2.27	2.06
18	3	3003	CLA	MG-NA	8.80	2.27	2.06
17	A	1011	CL0	C3B-C4B	8.78	1.49	1.41
17	A	1011	CL0	C1D-C2D	8.73	1.49	1.39
18	2	2005	CLA	MG-NA	8.71	2.27	2.06
18	1	1013	CLA	MG-NA	8.70	2.26	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2007	CLA	MG-NA	8.70	2.26	2.06
18	G	1003	CLA	MG-NA	8.69	2.26	2.06
18	4	4002	CLA	MG-NA	8.67	2.26	2.06
18	2	2006	CLA	MG-NA	8.67	2.26	2.06
18	3	3013	CLA	MG-NA	8.61	2.26	2.06
22	G	2011	BCR	C11-C10	-8.61	1.16	1.43
18	L	1503	CLA	MG-NA	8.59	2.26	2.06
28	4	4013	CHL	C3A-C2A	-8.58	1.47	1.54
18	3	3018	CLA	MG-NA	8.57	2.26	2.06
18	1	1012	CLA	MG-NA	8.57	2.26	2.06
18	L	1502	CLA	MG-NA	8.56	2.26	2.06
18	2	2009	CLA	MG-NA	8.52	2.26	2.06
18	4	4016	CLA	MG-NA	8.52	2.26	2.06
18	1	1006	CLA	MG-NA	8.51	2.26	2.06
22	A	6011	BCR	C8-C9	-8.51	1.27	1.46
18	3	3001	CLA	MG-NA	8.49	2.26	2.06
17	A	1011	CL0	C1B-C2B	8.46	1.49	1.39
18	3	3005	CLA	MG-NA	8.46	2.26	2.06
18	G	1002	CLA	MG-NA	8.44	2.26	2.06
18	2	2016	CLA	MG-NA	8.43	2.26	2.06
18	4	4003	CLA	MG-NA	8.42	2.26	2.06
22	G	2011	BCR	C8-C9	-8.40	1.28	1.46
22	B	6006	BCR	C8-C9	-8.40	1.28	1.46
18	4	4007	CLA	MG-NA	8.40	2.26	2.06
18	G	1001	CLA	MG-NA	8.38	2.26	2.06
22	F	6016	BCR	C11-C10	-8.37	1.17	1.43
22	A	6003	BCR	C8-C9	-8.37	1.28	1.46
18	4	4017	CLA	MG-NA	8.34	2.26	2.06
22	F	6014	BCR	C8-C9	-8.34	1.28	1.46
18	L	1501	CLA	MG-NA	8.33	2.26	2.06
22	A	6008	BCR	C8-C9	-8.33	1.28	1.46
18	1	1011	CLA	MG-NA	8.31	2.26	2.06
18	K	1001	CLA	MG-NA	8.30	2.26	2.06
18	3	3007	CLA	MG-NA	8.30	2.26	2.06
22	B	6004	BCR	C8-C9	-8.29	1.28	1.46
18	1	1004	CLA	MG-NA	8.29	2.26	2.06
18	1	1001	CLA	MG-NA	8.29	2.26	2.06
22	F	6016	BCR	C8-C9	-8.29	1.28	1.46
18	3	3017	CLA	MG-NA	8.27	2.25	2.06
22	L	6019	BCR	C8-C9	-8.26	1.28	1.46
22	B	6009	BCR	C8-C9	-8.25	1.28	1.46
18	4	4004	CLA	MG-NA	8.24	2.25	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	6010	BCR	C8-C9	-8.23	1.28	1.46
22	F	6014	BCR	C11-C10	-8.21	1.17	1.43
18	4	4001	CLA	MG-NA	8.21	2.25	2.06
18	1	1008	CLA	MG-NA	8.20	2.25	2.06
18	4	4005	CLA	MG-NA	8.17	2.25	2.06
22	A	6011	BCR	C11-C10	-8.16	1.17	1.43
18	3	3006	CLA	MG-NA	8.15	2.25	2.06
22	A	6007	BCR	C8-C9	-8.13	1.28	1.46
22	L	6020	BCR	C8-C9	-8.11	1.28	1.46
22	J	6012	BCR	C8-C9	-8.10	1.28	1.46
22	A	6008	BCR	C11-C10	-8.10	1.18	1.43
22	3	3503	BCR	C8-C9	-8.10	1.28	1.46
18	1	1003	CLA	MG-NA	8.09	2.25	2.06
22	K	2011	BCR	C8-C9	-8.09	1.28	1.46
22	I	6020	BCR	C8-C9	-8.09	1.28	1.46
18	1	1014	CLA	MG-NA	8.09	2.25	2.06
18	1	1005	CLA	MG-NA	8.08	2.25	2.06
20	B	5002	PQN	C3-C2	8.08	1.49	1.35
22	A	6002	BCR	C8-C9	-8.06	1.28	1.46
22	B	6005	BCR	C8-C9	-8.06	1.28	1.46
18	1	1002	CLA	MG-NA	8.05	2.25	2.06
18	4	4009	CLA	MG-NA	8.04	2.25	2.06
22	L	6019	BCR	C11-C10	-8.02	1.18	1.43
22	3	3503	BCR	C11-C10	-7.99	1.18	1.43
22	J	6013	BCR	C8-C9	-7.99	1.28	1.46
22	J	6012	BCR	C11-C10	-7.95	1.18	1.43
18	3	3012	CLA	MG-NA	7.95	2.25	2.06
18	3	3002	CLA	MG-NA	7.95	2.25	2.06
22	J	6013	BCR	C11-C10	-7.93	1.18	1.43
20	A	5001	PQN	C3-C2	7.92	1.49	1.35
22	A	6003	BCR	C11-C10	-7.92	1.18	1.43
22	B	6009	BCR	C11-C10	-7.89	1.18	1.43
22	B	6006	BCR	C11-C10	-7.86	1.18	1.43
22	I	6020	BCR	C11-C10	-7.83	1.18	1.43
18	3	3004	CLA	MG-NA	7.83	2.24	2.06
18	1	1007	CLA	MG-NA	7.82	2.24	2.06
18	4	4006	CLA	MG-NA	7.82	2.24	2.06
18	2	2012	CLA	MG-NA	7.82	2.24	2.06
22	A	6007	BCR	C11-C10	-7.81	1.19	1.43
22	B	6004	BCR	C11-C10	-7.81	1.19	1.43
18	4	4012	CLA	MG-NA	7.81	2.24	2.06
18	2	2001	CLA	MG-NA	7.80	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	6017	BCR	C8-C9	-7.79	1.29	1.46
18	2	2002	CLA	MG-NA	7.78	2.24	2.06
22	A	6002	BCR	C11-C10	-7.77	1.19	1.43
18	3	3008	CLA	MG-NA	7.74	2.24	2.06
18	2	2008	CLA	MG-NA	7.71	2.24	2.06
18	3	3010	CLA	MG-NA	7.71	2.24	2.06
22	B	6005	BCR	C11-C10	-7.71	1.19	1.43
22	B	6010	BCR	C11-C10	-7.71	1.19	1.43
22	F	6016	BCR	C16-C17	-7.70	1.19	1.43
22	A	6017	BCR	C11-C10	-7.69	1.19	1.43
28	4	4011	CHL	C1A-CHA	-7.67	1.31	1.40
18	2	2003	CLA	MG-NA	7.67	2.24	2.06
22	K	2011	BCR	C11-C10	-7.66	1.19	1.43
22	L	6020	BCR	C11-C10	-7.63	1.19	1.43
28	2	2010	CHL	C1A-CHA	-7.61	1.31	1.40
22	G	2011	BCR	C20-C21	-7.49	1.20	1.43
22	J	6012	BCR	C20-C21	-7.47	1.20	1.43
18	4	4008	CLA	MG-NA	7.46	2.24	2.06
22	3	3503	BCR	C16-C17	-7.46	1.20	1.43
22	A	6011	BCR	C20-C21	-7.44	1.20	1.43
22	3	3503	BCR	C20-C21	-7.41	1.20	1.43
22	F	6014	BCR	C16-C17	-7.37	1.20	1.43
22	A	6011	BCR	C16-C17	-7.35	1.20	1.43
22	B	6010	BCR	C20-C21	-7.35	1.20	1.43
22	F	6016	BCR	C20-C21	-7.32	1.20	1.43
22	I	6020	BCR	C20-C21	-7.32	1.20	1.43
22	A	6008	BCR	C16-C17	-7.28	1.20	1.43
22	L	6020	BCR	C20-C21	-7.28	1.20	1.43
22	G	2011	BCR	C16-C17	-7.27	1.20	1.43
22	B	6006	BCR	C20-C21	-7.27	1.20	1.43
22	L	6019	BCR	C20-C21	-7.26	1.20	1.43
22	B	6004	BCR	C20-C21	-7.26	1.20	1.43
22	A	6008	BCR	C20-C21	-7.25	1.20	1.43
22	F	6014	BCR	C20-C21	-7.23	1.20	1.43
22	J	6013	BCR	C16-C17	-7.21	1.20	1.43
22	J	6013	BCR	C20-C21	-7.20	1.20	1.43
22	B	6009	BCR	C16-C17	-7.20	1.20	1.43
22	B	6009	BCR	C20-C21	-7.20	1.20	1.43
22	L	6020	BCR	C16-C17	-7.19	1.20	1.43
22	A	6003	BCR	C20-C21	-7.18	1.20	1.43
22	A	6007	BCR	C20-C21	-7.16	1.21	1.43
22	B	6004	BCR	C16-C17	-7.16	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	6002	BCR	C20-C21	-7.15	1.21	1.43
22	B	6006	BCR	C16-C17	-7.14	1.21	1.43
22	I	6020	BCR	C16-C17	-7.13	1.21	1.43
22	B	6005	BCR	C20-C21	-7.11	1.21	1.43
22	K	2011	BCR	C20-C21	-7.10	1.21	1.43
22	A	6017	BCR	C20-C21	-7.10	1.21	1.43
28	4	4013	CHL	C1A-CHA	-7.09	1.31	1.40
22	A	6003	BCR	C16-C17	-7.08	1.21	1.43
22	L	6019	BCR	C16-C17	-7.08	1.21	1.43
22	K	2011	BCR	C16-C17	-7.07	1.21	1.43
22	A	6007	BCR	C16-C17	-7.06	1.21	1.43
22	J	6012	BCR	C16-C17	-7.06	1.21	1.43
22	A	6017	BCR	C16-C17	-7.06	1.21	1.43
22	A	6002	BCR	C16-C17	-7.04	1.21	1.43
22	B	6005	BCR	C16-C17	-7.01	1.21	1.43
22	B	6010	BCR	C16-C17	-7.00	1.21	1.43
18	1	1014	CLA	O2A-C1	7.00	1.60	1.45
28	4	4010	CHL	C3D-C4D	-6.89	1.31	1.41
28	1	1010	CHL	C3B-C4B	6.88	1.48	1.41
18	G	1002	CLA	O2A-C1	6.87	1.60	1.45
18	A	1114	CLA	O2A-C1	6.87	1.60	1.45
18	A	1118	CLA	O2A-C1	6.86	1.60	1.45
18	B	1209	CLA	O2A-C1	6.84	1.60	1.45
18	A	1113	CLA	O2A-C1	6.84	1.60	1.45
18	4	4016	CLA	O2A-C1	6.83	1.60	1.45
18	3	3013	CLA	O2A-C1	6.83	1.60	1.45
18	A	1115	CLA	O2A-C1	6.83	1.60	1.45
18	H	1000	CLA	O2A-C1	6.82	1.60	1.45
18	2	2002	CLA	O2A-C1	6.81	1.60	1.45
18	A	1108	CLA	O2A-C1	6.80	1.60	1.45
18	K	1001	CLA	O2A-C1	6.78	1.60	1.45
18	3	3017	CLA	O2A-C1	6.78	1.60	1.45
28	4	4011	CHL	C3D-C4D	-6.77	1.31	1.41
18	B	1217	CLA	O2A-C1	6.76	1.60	1.45
18	1	1013	CLA	O2A-C1	6.75	1.60	1.45
18	1	1007	CLA	O2A-C1	6.75	1.60	1.45
18	1	1008	CLA	O2A-C1	6.67	1.60	1.45
18	1	1002	CLA	O2A-C1	6.67	1.60	1.45
28	4	4013	CHL	C3D-C4D	-6.66	1.31	1.41
18	3	3002	CLA	O2A-C1	6.64	1.60	1.45
28	2	2010	CHL	C3D-C4D	-6.61	1.31	1.41
28	2	2011	CHL	C3D-C4D	-6.59	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	3	3011	CHL	C3D-C4D	-6.54	1.31	1.41
28	1	1009	CHL	C3D-C4D	-6.54	1.31	1.41
18	4	4008	CLA	O2A-C1	6.53	1.59	1.45
28	4	4010	CHL	C1A-CHA	-6.51	1.32	1.40
28	1	1010	CHL	C3D-C4D	-6.39	1.31	1.41
28	2	2013	CHL	C3D-C4D	-6.21	1.32	1.41
28	2	2011	CHL	C3B-C4B	6.18	1.47	1.41
28	4	4011	CHL	C3B-C4B	5.85	1.47	1.41
28	2	2013	CHL	C3B-C4B	5.79	1.47	1.41
18	3	3019	CLA	C4D-C3D	-5.78	1.34	1.46
18	2	2016	CLA	O2D-CGD	5.75	1.47	1.33
28	1	1009	CHL	C1A-CHA	-5.73	1.33	1.40
18	A	1107	CLA	O2A-C1	5.69	1.61	1.46
28	1	1009	CHL	C3B-C4B	5.68	1.46	1.41
18	4	4007	CLA	O2A-C1	5.66	1.61	1.46
18	2	2019	CLA	C4D-C3D	-5.59	1.34	1.46
18	2	2016	CLA	O2A-C1	5.58	1.61	1.46
28	2	2010	CHL	C3B-C2B	-5.58	1.32	1.40
17	A	1011	CL0	CHC-C4B	5.58	1.48	1.39
28	4	4013	CHL	C3B-C2B	-5.57	1.32	1.40
18	B	1221	CLA	O2A-C1	5.56	1.61	1.46
18	A	1110	CLA	O2A-C1	5.56	1.61	1.46
18	A	1111	CLA	O2A-C1	5.54	1.61	1.46
18	3	3007	CLA	O2A-C1	5.54	1.61	1.46
18	B	1204	CLA	O2A-C1	5.53	1.61	1.46
18	B	1238	CLA	O2A-C1	5.53	1.61	1.46
18	B	1225	CLA	O2A-C1	5.53	1.61	1.46
18	A	1140	CLA	O2A-C1	5.52	1.61	1.46
18	B	1236	CLA	O2A-C1	5.51	1.60	1.46
18	B	1215	CLA	O2A-C1	5.50	1.60	1.46
18	3	3008	CLA	O2A-C1	5.49	1.60	1.46
18	B	1201	CLA	O2A-C1	5.48	1.60	1.46
18	J	1302	CLA	O2A-C1	5.47	1.60	1.46
18	3	3004	CLA	O2A-C1	5.47	1.60	1.46
18	1	1001	CLA	O2A-C1	5.47	1.60	1.46
18	B	1205	CLA	O2A-C1	5.46	1.60	1.46
18	A	1132	CLA	O2A-C1	5.46	1.60	1.46
18	A	1137	CLA	O2A-C1	5.46	1.60	1.46
18	B	1239	CLA	O2A-C1	5.46	1.60	1.46
18	3	3001	CLA	O2A-C1	5.46	1.60	1.46
18	A	1130	CLA	O2A-C1	5.45	1.60	1.46
18	B	1208	CLA	O2A-C1	5.45	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1211	CLA	O2A-C1	5.45	1.60	1.46
18	B	1207	CLA	O2A-C1	5.45	1.60	1.46
18	A	1128	CLA	O2A-C1	5.45	1.60	1.46
18	B	1206	CLA	O2A-C1	5.44	1.60	1.46
18	A	1102	CLA	O2A-C1	5.44	1.60	1.46
18	A	1120	CLA	O2A-C1	5.43	1.60	1.46
18	A	1105	CLA	O2A-C1	5.43	1.60	1.46
18	B	1212	CLA	O2A-C1	5.43	1.60	1.46
18	A	1129	CLA	O2A-C1	5.42	1.60	1.46
18	A	1101	CLA	O2A-C1	5.42	1.60	1.46
28	4	4010	CHL	C3B-C2B	-5.42	1.33	1.40
18	B	1214	CLA	O2A-C1	5.41	1.60	1.46
18	G	1003	CLA	O2A-C1	5.41	1.60	1.46
18	B	1220	CLA	O2A-C1	5.40	1.60	1.46
18	A	1138	CLA	O2A-C1	5.40	1.60	1.46
18	A	1109	CLA	O2A-C1	5.40	1.60	1.46
18	A	1125	CLA	O2A-C1	5.40	1.60	1.46
28	3	3011	CHL	C3B-C2B	-5.39	1.33	1.40
18	A	1131	CLA	O2A-C1	5.39	1.60	1.46
18	B	1228	CLA	O2A-C1	5.39	1.60	1.46
18	B	1231	CLA	CHC-C1C	5.39	1.49	1.38
18	A	1151	CLA	O2A-C1	5.38	1.60	1.46
18	B	1219	CLA	O2A-C1	5.38	1.60	1.46
18	A	1124	CLA	O2A-C1	5.37	1.60	1.46
18	2	2001	CLA	O2A-C1	5.37	1.60	1.46
18	B	1224	CLA	O2A-C1	5.37	1.60	1.46
18	B	1021	CLA	O2A-C1	5.36	1.60	1.46
18	A	1134	CLA	O2A-C1	5.36	1.60	1.46
18	A	1135	CLA	O2A-C1	5.36	1.60	1.46
18	B	1229	CLA	O2A-C1	5.36	1.60	1.46
18	A	1117	CLA	O2A-C1	5.36	1.60	1.46
18	A	1136	CLA	O2A-C1	5.36	1.60	1.46
20	B	5002	PQN	C10-C5	5.35	1.49	1.40
18	B	1213	CLA	O2A-C1	5.35	1.60	1.46
18	2	2004	CLA	O2A-C1	5.35	1.60	1.46
17	A	1011	CL0	O2A-C1	5.34	1.60	1.46
18	A	1123	CLA	O2A-C1	5.34	1.60	1.46
18	B	1223	CLA	O2A-C1	5.34	1.60	1.46
18	A	1022	CLA	O2A-C1	5.34	1.60	1.46
18	A	1121	CLA	O2A-C1	5.34	1.60	1.46
18	B	1210	CLA	O2A-C1	5.34	1.60	1.46
18	A	1237	CLA	O2A-C1	5.33	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1139	CLA	O2A-C1	5.33	1.60	1.46
18	B	1226	CLA	O2A-C1	5.33	1.60	1.46
18	B	1203	CLA	O2A-C1	5.33	1.60	1.46
18	A	1133	CLA	O2A-C1	5.33	1.60	1.46
18	A	1122	CLA	O2A-C1	5.32	1.60	1.46
18	A	1104	CLA	CHC-C1C	5.32	1.49	1.38
18	A	1106	CLA	O2A-C1	5.32	1.60	1.46
18	3	3012	CLA	O2A-C1	5.32	1.60	1.46
18	B	1023	CLA	O2A-C1	5.32	1.60	1.46
18	A	1104	CLA	O2A-C1	5.32	1.60	1.46
18	B	1227	CLA	O2A-C1	5.32	1.60	1.46
18	3	3010	CLA	O2A-C1	5.32	1.60	1.46
18	4	4001	CLA	O2A-C1	5.31	1.60	1.46
18	L	1501	CLA	O2A-C1	5.31	1.60	1.46
18	A	1119	CLA	O2A-C1	5.31	1.60	1.46
18	B	1218	CLA	O2A-C1	5.31	1.60	1.46
18	4	4002	CLA	O2A-C1	5.31	1.60	1.46
18	L	1501	CLA	C3D-C4D	-5.30	1.32	1.44
18	4	4012	CLA	O2A-C1	5.30	1.60	1.46
18	B	1211	CLA	CHC-C1C	5.30	1.49	1.38
18	L	1503	CLA	O2A-C1	5.30	1.60	1.46
18	F	1302	CLA	O2A-C1	5.30	1.60	1.46
18	A	1112	CLA	O2A-C1	5.29	1.60	1.46
18	B	1232	CLA	O2A-C1	5.29	1.60	1.46
18	B	1235	CLA	O2A-C1	5.28	1.60	1.46
18	B	1202	CLA	O2A-C1	5.28	1.60	1.46
18	A	1127	CLA	O2A-C1	5.28	1.60	1.46
18	2	2005	CLA	O2A-C1	5.28	1.60	1.46
18	B	1230	CLA	O2A-C1	5.28	1.60	1.46
28	4	4010	CHL	C3B-C4B	5.26	1.46	1.41
18	2	2007	CLA	O2A-C1	5.26	1.60	1.46
18	3	3002	CLA	C3D-C4D	-5.26	1.32	1.44
18	4	4005	CLA	O2A-C1	5.26	1.60	1.46
18	B	1234	CLA	CHC-C1C	5.26	1.49	1.38
18	3	3019	CLA	CHC-C1C	5.25	1.48	1.38
18	A	1138	CLA	O2D-CGD	5.25	1.46	1.33
18	4	4002	CLA	C3D-C4D	-5.25	1.32	1.44
18	2	2006	CLA	O2A-C1	5.25	1.60	1.46
18	A	1013	CLA	CHC-C1C	5.24	1.49	1.38
18	A	1103	CLA	O2A-C1	5.24	1.60	1.46
18	2	2008	CLA	C3D-C4D	-5.24	1.32	1.44
18	B	1012	CLA	O2A-C1	5.23	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1231	CLA	O2A-C1	5.23	1.60	1.46
18	H	1000	CLA	O2D-CGD	5.23	1.46	1.33
18	G	1001	CLA	O2A-C1	5.23	1.60	1.46
18	4	4008	CLA	C3D-C4D	-5.23	1.32	1.44
18	A	1133	CLA	O2D-CGD	5.22	1.46	1.33
18	4	4004	CLA	C3D-C4D	-5.21	1.32	1.44
18	B	1240	CLA	O2A-C1	5.21	1.60	1.46
18	3	3006	CLA	C3D-C4D	-5.21	1.32	1.44
18	B	1216	CLA	O2A-C1	5.20	1.60	1.46
18	A	1106	CLA	O2D-CGD	5.20	1.46	1.33
18	A	1022	CLA	O2D-CGD	5.20	1.46	1.33
18	3	3005	CLA	C3D-C4D	-5.19	1.32	1.44
18	A	1120	CLA	O2D-CGD	5.19	1.46	1.33
18	L	1502	CLA	O2A-C1	5.19	1.60	1.46
18	1	1006	CLA	C3D-C4D	-5.18	1.32	1.44
18	1	1005	CLA	O2A-C1	5.18	1.60	1.46
18	A	1113	CLA	O2D-CGD	5.18	1.46	1.33
18	A	1126	CLA	O2A-C1	5.18	1.60	1.46
18	A	1013	CLA	O2A-C1	5.17	1.60	1.46
18	B	1219	CLA	O2D-CGD	5.17	1.45	1.33
18	B	1208	CLA	CHC-C1C	5.17	1.48	1.38
18	B	1234	CLA	O2A-C1	5.17	1.60	1.46
18	A	1116	CLA	O2A-C1	5.16	1.60	1.46
28	2	2011	CHL	C3B-C2B	-5.16	1.33	1.40
18	B	1225	CLA	O2D-CGD	5.16	1.45	1.33
18	B	1204	CLA	O2D-CGD	5.16	1.45	1.33
18	A	1151	CLA	O2D-CGD	5.16	1.45	1.33
18	B	1235	CLA	CHC-C1C	5.16	1.48	1.38
18	B	1238	CLA	O2D-CGD	5.16	1.45	1.33
18	A	1108	CLA	CHC-C1C	5.15	1.48	1.38
18	A	1130	CLA	O2D-CGD	5.15	1.45	1.33
18	B	1230	CLA	O2D-CGD	5.15	1.45	1.33
18	B	1230	CLA	CHC-C1C	5.15	1.48	1.38
18	A	1108	CLA	O2D-CGD	5.15	1.45	1.33
18	3	3003	CLA	O2A-C1	5.15	1.60	1.46
18	A	1119	CLA	O2D-CGD	5.15	1.45	1.33
18	A	1103	CLA	O2D-CGD	5.14	1.45	1.33
28	1	1010	CHL	C3A-C2A	-5.14	1.50	1.54
18	2	2004	CLA	C3D-C4D	-5.14	1.32	1.44
18	B	1021	CLA	O2D-CGD	5.14	1.45	1.33
18	B	1216	CLA	O2D-CGD	5.14	1.45	1.33
18	A	1105	CLA	O2D-CGD	5.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4009	CLA	O2A-C1	5.13	1.59	1.46
18	A	1121	CLA	O2D-CGD	5.13	1.45	1.33
18	A	1124	CLA	CHC-C1C	5.13	1.48	1.38
18	A	1140	CLA	O2D-CGD	5.13	1.45	1.33
18	A	1127	CLA	O2D-CGD	5.13	1.45	1.33
18	A	1111	CLA	O2D-CGD	5.13	1.45	1.33
18	B	1023	CLA	O2D-CGD	5.13	1.45	1.33
18	B	1206	CLA	O2D-CGD	5.12	1.45	1.33
18	A	1114	CLA	O2D-CGD	5.12	1.45	1.33
18	B	1209	CLA	O2D-CGD	5.12	1.45	1.33
18	B	1213	CLA	O2D-CGD	5.12	1.45	1.33
18	A	1115	CLA	O2D-CGD	5.12	1.45	1.33
18	A	1107	CLA	CHC-C1C	5.12	1.48	1.38
18	B	1221	CLA	CHC-C1C	5.12	1.48	1.38
18	B	1222	CLA	O2A-C1	5.12	1.59	1.46
18	B	1234	CLA	O2D-CGD	5.11	1.45	1.33
18	2	2009	CLA	O2A-C1	5.11	1.59	1.46
18	B	1229	CLA	CHC-C1C	5.11	1.48	1.38
18	B	1207	CLA	O2D-CGD	5.11	1.45	1.33
18	2	2004	CLA	CHC-C1C	5.11	1.48	1.38
18	B	1214	CLA	O2D-CGD	5.11	1.45	1.33
18	2	2002	CLA	C3D-C4D	-5.10	1.32	1.44
18	B	1228	CLA	O2D-CGD	5.10	1.45	1.33
18	A	1138	CLA	CHC-C1C	5.10	1.48	1.38
18	A	1128	CLA	O2D-CGD	5.10	1.45	1.33
28	1	1009	CHL	C3A-C2A	-5.10	1.50	1.54
18	B	1227	CLA	O2D-CGD	5.10	1.45	1.33
18	1	1006	CLA	O2A-C1	5.10	1.59	1.46
18	A	1123	CLA	O2D-CGD	5.09	1.45	1.33
18	3	3019	CLA	C3C-C2C	5.09	1.46	1.35
18	B	1217	CLA	O2D-CGD	5.09	1.45	1.33
18	A	1118	CLA	O2D-CGD	5.09	1.45	1.33
18	B	1208	CLA	O2D-CGD	5.09	1.45	1.33
18	A	1013	CLA	O2D-CGD	5.09	1.45	1.33
18	1	1004	CLA	O2A-C1	5.09	1.59	1.46
18	B	1224	CLA	O2D-CGD	5.09	1.45	1.33
17	A	1011	CL0	OBD-CAD	5.08	1.29	1.22
18	B	1238	CLA	CHC-C1C	5.08	1.48	1.38
18	B	1236	CLA	O2D-CGD	5.08	1.45	1.33
18	B	1227	CLA	CHC-C1C	5.08	1.48	1.38
18	A	1110	CLA	CHC-C1C	5.07	1.48	1.38
18	B	1201	CLA	CHC-C1C	5.07	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1140	CLA	CHC-C1C	5.07	1.48	1.38
18	A	1237	CLA	O2D-CGD	5.07	1.45	1.33
18	J	1302	CLA	O2D-CGD	5.07	1.45	1.33
18	A	1116	CLA	O2D-CGD	5.07	1.45	1.33
18	B	1232	CLA	O2D-CGD	5.06	1.45	1.33
18	B	1216	CLA	CHC-C1C	5.06	1.48	1.38
18	A	1022	CLA	CHC-C1C	5.06	1.48	1.38
18	4	4016	CLA	O2D-CGD	5.06	1.45	1.33
18	B	1215	CLA	CHC-C1C	5.06	1.48	1.38
18	B	1239	CLA	O2D-CGD	5.06	1.45	1.33
18	B	1215	CLA	O2D-CGD	5.06	1.45	1.33
18	4	4009	CLA	C3D-C4D	-5.06	1.32	1.44
18	A	1131	CLA	O2D-CGD	5.06	1.45	1.33
18	A	1109	CLA	O2D-CGD	5.06	1.45	1.33
18	B	1231	CLA	O2D-CGD	5.05	1.45	1.33
18	B	1213	CLA	CHC-C1C	5.05	1.48	1.38
18	3	3005	CLA	O2A-C1	5.05	1.59	1.46
18	B	1012	CLA	CHC-C1C	5.05	1.48	1.38
18	B	1012	CLA	O2D-CGD	5.05	1.45	1.33
18	A	1102	CLA	CHC-C1C	5.05	1.48	1.38
17	A	1011	CL0	O2D-CGD	5.05	1.45	1.33
18	A	1132	CLA	CHC-C1C	5.05	1.48	1.38
18	A	1134	CLA	O2D-CGD	5.05	1.45	1.33
18	A	1101	CLA	O2D-CGD	5.05	1.45	1.33
18	A	1117	CLA	O2D-CGD	5.04	1.45	1.33
18	3	3010	CLA	C3D-C4D	-5.04	1.32	1.44
18	B	1236	CLA	CHC-C1C	5.04	1.48	1.38
18	1	1005	CLA	C3D-C4D	-5.04	1.32	1.44
18	A	1151	CLA	C3C-C2C	5.04	1.47	1.36
18	B	1202	CLA	O2D-CGD	5.04	1.45	1.33
18	B	1240	CLA	CHC-C1C	5.04	1.48	1.38
18	A	1131	CLA	CHC-C1C	5.04	1.48	1.38
18	1	1011	CLA	CHC-C1C	5.04	1.48	1.38
18	A	1122	CLA	O2D-CGD	5.04	1.45	1.33
18	A	1112	CLA	CHC-C1C	5.04	1.48	1.38
18	B	1232	CLA	CHC-C1C	5.03	1.48	1.38
18	B	1222	CLA	CHC-C1C	5.03	1.48	1.38
22	G	2011	BCR	C10-C9	-5.03	1.24	1.35
18	A	1136	CLA	CHC-C1C	5.03	1.48	1.38
18	B	1203	CLA	CHC-C1C	5.03	1.48	1.38
18	A	1110	CLA	O2D-CGD	5.02	1.45	1.33
18	A	1135	CLA	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1023	CLA	CHC-C1C	5.02	1.48	1.38
18	B	1235	CLA	O2D-CGD	5.02	1.45	1.33
18	B	1225	CLA	CHC-C1C	5.02	1.48	1.38
18	B	1228	CLA	CHC-C1C	5.02	1.48	1.38
18	4	4012	CLA	C3D-C4D	-5.02	1.32	1.44
18	B	1212	CLA	O2D-CGD	5.01	1.45	1.33
18	B	1203	CLA	O2D-CGD	5.01	1.45	1.33
18	A	1129	CLA	CHC-C1C	5.01	1.48	1.38
18	A	1125	CLA	CHC-C1C	5.01	1.48	1.38
18	B	1204	CLA	CHC-C1C	5.01	1.48	1.38
18	A	1126	CLA	O2D-CGD	5.01	1.45	1.33
18	B	1220	CLA	CHC-C1C	5.01	1.48	1.38
18	2	2003	CLA	O2A-C1	5.01	1.59	1.46
18	1	1007	CLA	C3D-C4D	-5.01	1.32	1.44
18	A	1151	CLA	CHC-C1C	5.01	1.48	1.38
18	A	1137	CLA	O2D-CGD	5.00	1.45	1.33
18	A	1130	CLA	CHC-C1C	5.00	1.48	1.38
18	B	1218	CLA	CHC-C1C	5.00	1.48	1.38
18	B	1220	CLA	O2D-CGD	5.00	1.45	1.33
18	A	1126	CLA	CHC-C1C	5.00	1.48	1.38
18	4	4017	CLA	O2A-C1	4.99	1.59	1.46
18	B	1223	CLA	O2D-CGD	4.99	1.45	1.33
17	A	1011	CL0	CHB-C1B	4.99	1.47	1.39
18	B	1221	CLA	O2D-CGD	4.99	1.45	1.33
18	K	1001	CLA	O2D-CGD	4.99	1.45	1.33
18	A	1115	CLA	CHC-C1C	4.99	1.48	1.38
18	4	4003	CLA	O2A-C1	4.99	1.59	1.46
18	A	1139	CLA	CHC-C1C	4.99	1.48	1.38
18	L	1502	CLA	CHC-C1C	4.99	1.48	1.38
18	B	1211	CLA	O2D-CGD	4.98	1.45	1.33
18	A	1103	CLA	CHC-C1C	4.98	1.48	1.38
18	1	1012	CLA	C3D-C4D	-4.98	1.33	1.44
18	4	4006	CLA	C3D-C4D	-4.98	1.33	1.44
18	A	1120	CLA	CHC-C1C	4.98	1.48	1.38
18	A	1124	CLA	O2D-CGD	4.97	1.45	1.33
18	1	1004	CLA	C3D-C4D	-4.97	1.33	1.44
18	A	1105	CLA	CHC-C1C	4.97	1.48	1.38
18	B	1240	CLA	O2D-CGD	4.97	1.45	1.33
18	B	1201	CLA	O2D-CGD	4.97	1.45	1.33
28	3	3011	CHL	C3B-C4B	4.97	1.46	1.41
18	B	1207	CLA	CHC-C1C	4.97	1.48	1.38
18	A	1125	CLA	O2D-CGD	4.97	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3017	CLA	C3D-C4D	-4.96	1.33	1.44
18	4	4005	CLA	C3D-C4D	-4.96	1.33	1.44
18	A	1129	CLA	O2D-CGD	4.96	1.45	1.33
18	A	1139	CLA	O2D-CGD	4.96	1.45	1.33
18	A	1101	CLA	CHC-C1C	4.95	1.48	1.38
18	1	1008	CLA	C3D-C4D	-4.95	1.33	1.44
18	B	1212	CLA	CHC-C1C	4.95	1.48	1.38
18	B	1229	CLA	O2D-CGD	4.95	1.45	1.33
18	A	1107	CLA	O2D-CGD	4.95	1.45	1.33
18	B	1214	CLA	CHC-C1C	4.95	1.48	1.38
18	B	1205	CLA	CHC-C1C	4.94	1.48	1.38
18	2	2019	CLA	C3C-C2C	4.94	1.46	1.35
18	A	1109	CLA	CHC-C1C	4.94	1.48	1.38
18	L	1503	CLA	CHC-C1C	4.94	1.48	1.38
18	A	1106	CLA	CHC-C1C	4.94	1.48	1.38
18	A	1117	CLA	CHC-C1C	4.94	1.48	1.38
18	2	2003	CLA	C3D-C4D	-4.93	1.33	1.44
18	A	1136	CLA	O2D-CGD	4.93	1.45	1.33
18	G	1001	CLA	C3D-C4D	-4.93	1.33	1.44
18	A	1113	CLA	CHC-C1C	4.93	1.48	1.38
18	A	1102	CLA	O2D-CGD	4.93	1.45	1.33
18	A	1122	CLA	CHC-C1C	4.93	1.48	1.38
18	A	1111	CLA	CHC-C1C	4.92	1.48	1.38
18	B	1218	CLA	O2D-CGD	4.92	1.45	1.33
18	A	1121	CLA	CHC-C1C	4.92	1.48	1.38
18	B	1219	CLA	CHC-C1C	4.92	1.48	1.38
18	3	3018	CLA	O2A-C1	4.92	1.59	1.46
18	A	1137	CLA	CHC-C1C	4.91	1.48	1.38
18	F	1301	CLA	CHC-C1C	4.91	1.48	1.38
18	A	1237	CLA	CHC-C1C	4.91	1.48	1.38
18	B	1217	CLA	CHC-C1C	4.91	1.48	1.38
18	K	1001	CLA	C3D-C4D	-4.91	1.33	1.44
20	A	5001	PQN	C10-C5	4.91	1.48	1.40
18	B	1223	CLA	CHC-C1C	4.91	1.48	1.38
18	4	4004	CLA	CHC-C1C	4.90	1.48	1.38
18	F	1301	CLA	O2D-CGD	4.90	1.45	1.33
18	A	1116	CLA	CHC-C1C	4.89	1.48	1.38
18	3	3003	CLA	O2D-CGD	4.89	1.45	1.33
18	A	1123	CLA	CHC-C1C	4.88	1.48	1.38
18	B	1239	CLA	CHC-C1C	4.88	1.48	1.38
22	F	6014	BCR	C10-C9	-4.87	1.24	1.35
18	A	1132	CLA	O2D-CGD	4.87	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1134	CLA	CHC-C1C	4.87	1.48	1.38
18	A	1119	CLA	CHC-C1C	4.87	1.48	1.38
18	2	2008	CLA	O2A-C1	4.87	1.59	1.46
18	2	2005	CLA	CHC-C1C	4.86	1.48	1.38
18	1	1003	CLA	O2A-C1	4.86	1.59	1.46
18	J	1302	CLA	CHC-C1C	4.86	1.48	1.38
18	B	1209	CLA	CHC-C1C	4.86	1.48	1.38
17	A	1011	CL0	CHD-C1D	4.86	1.47	1.39
18	F	1302	CLA	CHC-C1C	4.86	1.48	1.38
18	4	4007	CLA	C3D-C4D	-4.86	1.33	1.44
18	1	1014	CLA	C3D-C4D	-4.86	1.33	1.44
21	B	5004	LHG	O7-C7	4.85	1.45	1.35
18	B	1021	CLA	CHC-C1C	4.85	1.48	1.38
22	F	6016	BCR	C10-C9	-4.85	1.24	1.35
18	2	2009	CLA	C3D-C4D	-4.85	1.33	1.44
18	B	1224	CLA	CHC-C1C	4.85	1.48	1.38
18	A	1135	CLA	CHC-C1C	4.84	1.48	1.38
18	L	1502	CLA	C3D-C4D	-4.84	1.33	1.44
18	A	1118	CLA	CHC-C1C	4.83	1.48	1.38
18	G	1002	CLA	O2D-CGD	4.83	1.45	1.33
18	4	4003	CLA	CHC-C1C	4.83	1.48	1.38
18	B	1210	CLA	O2D-CGD	4.83	1.45	1.33
18	F	1302	CLA	O2D-CGD	4.82	1.45	1.33
18	2	2006	CLA	O2D-CGD	4.82	1.45	1.33
18	1	1003	CLA	O2D-CGD	4.82	1.45	1.33
18	G	1003	CLA	CHC-C1C	4.82	1.48	1.38
18	3	3004	CLA	C3D-C4D	-4.82	1.33	1.44
18	3	3003	CLA	C3D-C4D	-4.82	1.33	1.44
18	2	2012	CLA	C3D-C4D	-4.82	1.33	1.44
18	3	3006	CLA	O2A-C1	4.81	1.59	1.46
18	H	1000	CLA	CHC-C1C	4.81	1.48	1.38
18	2	2005	CLA	O2D-CGD	4.81	1.45	1.33
18	3	3012	CLA	C3D-C4D	-4.81	1.33	1.44
18	3	3018	CLA	O2D-CGD	4.80	1.45	1.33
18	2	2007	CLA	CHC-C1C	4.80	1.48	1.38
18	A	1127	CLA	CHC-C1C	4.80	1.48	1.38
18	B	1210	CLA	CHC-C1C	4.80	1.48	1.38
18	3	3007	CLA	C3D-C4D	-4.80	1.33	1.44
18	B	1202	CLA	CHC-C1C	4.80	1.48	1.38
18	3	3008	CLA	O2D-CGD	4.80	1.45	1.33
18	4	4017	CLA	C3D-C4D	-4.80	1.33	1.44
18	B	1222	CLA	O2D-CGD	4.79	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1138	CLA	CHD-C1D	4.79	1.47	1.38
18	4	4001	CLA	C3D-C4D	-4.79	1.33	1.44
18	2	2006	CLA	CHC-C1C	4.79	1.48	1.38
18	4	4003	CLA	O2D-CGD	4.78	1.45	1.33
18	A	1133	CLA	CHC-C1C	4.78	1.48	1.38
18	3	3017	CLA	O2D-CGD	4.78	1.45	1.33
18	2	2007	CLA	O2D-CGD	4.78	1.45	1.33
18	3	3013	CLA	C3D-C4D	-4.78	1.33	1.44
18	1	1011	CLA	C3D-C4D	-4.77	1.33	1.44
18	B	1204	CLA	CHD-C1D	4.77	1.47	1.38
18	2	2016	CLA	C3D-C4D	-4.77	1.33	1.44
18	4	4016	CLA	CHC-C1C	4.76	1.48	1.38
18	G	1003	CLA	C3D-C4D	-4.76	1.33	1.44
18	1	1013	CLA	CHD-C1D	4.76	1.47	1.38
18	1	1011	CLA	O2A-C1	4.75	1.58	1.46
18	A	1104	CLA	O2D-CGD	4.75	1.44	1.33
18	3	3001	CLA	CHC-C1C	4.75	1.48	1.38
17	A	1011	CL0	CHC-C1C	4.75	1.48	1.39
18	1	1002	CLA	C3D-C4D	-4.74	1.33	1.44
18	3	3018	CLA	C3D-C4D	-4.74	1.33	1.44
18	A	1128	CLA	CHC-C1C	4.74	1.48	1.38
18	A	1134	CLA	CHD-C1D	4.74	1.47	1.38
18	B	1214	CLA	CHD-C1D	4.74	1.47	1.38
18	3	3001	CLA	C3D-C4D	-4.74	1.33	1.44
18	2	2019	CLA	C2D-C1D	4.74	1.51	1.42
18	3	3017	CLA	CHC-C1C	4.73	1.48	1.38
18	2	2012	CLA	O2A-C1	4.73	1.58	1.46
18	4	4006	CLA	O2A-C1	4.73	1.58	1.46
18	B	1228	CLA	C3C-C2C	4.73	1.47	1.36
18	B	1227	CLA	CHD-C1D	4.72	1.47	1.38
18	B	1216	CLA	CHD-C1D	4.72	1.47	1.38
18	B	1226	CLA	CHD-C1D	4.72	1.47	1.38
18	G	1002	CLA	C3D-C4D	-4.72	1.33	1.44
18	4	4003	CLA	C3D-C4D	-4.72	1.33	1.44
18	A	1114	CLA	CHD-C1D	4.71	1.47	1.38
18	3	3005	CLA	C1D-ND	-4.71	1.31	1.37
18	B	1205	CLA	O2D-CGD	4.71	1.44	1.33
18	B	1234	CLA	C3C-C2C	4.71	1.46	1.36
18	A	1114	CLA	CHC-C1C	4.71	1.47	1.38
22	3	3503	BCR	C10-C9	-4.70	1.24	1.35
18	4	4001	CLA	O2D-CGD	4.70	1.44	1.33
18	4	4016	CLA	C3D-C4D	-4.70	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	1000	CLA	CHD-C1D	4.70	1.47	1.38
18	B	1231	CLA	CHD-C1D	4.70	1.47	1.38
18	A	1105	CLA	CHD-C1D	4.70	1.47	1.38
18	2	2008	CLA	C1D-ND	-4.70	1.31	1.37
18	3	3007	CLA	CHC-C1C	4.69	1.47	1.38
18	2	2019	CLA	CHC-C1C	4.69	1.47	1.38
18	B	1209	CLA	CHD-C1D	4.69	1.47	1.38
18	A	1126	CLA	CHD-C1D	4.69	1.47	1.38
18	4	4002	CLA	O2D-CGD	4.69	1.44	1.33
18	A	1127	CLA	CHD-C1D	4.69	1.47	1.38
18	2	2009	CLA	CHC-C1C	4.69	1.47	1.38
18	1	1012	CLA	O2A-C1	4.69	1.58	1.46
18	A	1151	CLA	CHD-C1D	4.69	1.47	1.38
18	4	4012	CLA	C1B-NB	-4.69	1.31	1.37
18	A	1112	CLA	CHD-C1D	4.68	1.47	1.38
18	A	1022	CLA	CHD-C1D	4.68	1.47	1.38
18	B	1226	CLA	O2D-CGD	4.68	1.44	1.33
18	A	1116	CLA	CHD-C1D	4.67	1.47	1.38
18	G	1002	CLA	CHC-C1C	4.67	1.47	1.38
18	1	1005	CLA	C1D-ND	-4.66	1.31	1.37
18	A	1130	CLA	C3C-C2C	4.66	1.46	1.36
18	4	4004	CLA	O2A-C1	4.66	1.58	1.46
18	J	1302	CLA	CHD-C1D	4.66	1.47	1.38
18	B	1206	CLA	CHD-C1D	4.66	1.47	1.38
18	A	1101	CLA	CHD-C1D	4.66	1.47	1.38
18	3	3013	CLA	CHC-C1C	4.65	1.47	1.38
22	L	6019	BCR	C10-C9	-4.65	1.25	1.35
18	A	1140	CLA	CHD-C1D	4.65	1.47	1.38
18	A	1108	CLA	CHD-C1D	4.65	1.47	1.38
18	A	1135	CLA	CHD-C1D	4.65	1.47	1.38
18	1	1003	CLA	C3D-C4D	-4.65	1.33	1.44
18	L	1503	CLA	C3D-C4D	-4.65	1.33	1.44
18	A	1112	CLA	O2D-CGD	4.65	1.44	1.33
18	3	3005	CLA	CHC-C1C	4.65	1.47	1.38
18	B	1204	CLA	C3C-C2C	4.65	1.46	1.36
18	3	3010	CLA	C1B-NB	-4.65	1.31	1.37
18	A	1122	CLA	CHD-C1D	4.65	1.47	1.38
18	A	1133	CLA	CHD-C1D	4.64	1.47	1.38
18	B	1210	CLA	CHD-C1D	4.64	1.47	1.38
18	A	1124	CLA	CHD-C1D	4.64	1.47	1.38
18	A	1117	CLA	CHD-C1D	4.64	1.47	1.38
18	4	4017	CLA	CHC-C1C	4.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	2010	CHL	C3B-C4B	4.64	1.45	1.41
18	3	3006	CLA	O2D-CGD	4.64	1.44	1.33
18	1	1001	CLA	O2D-CGD	4.64	1.44	1.33
18	A	1128	CLA	C3C-C2C	4.64	1.46	1.36
18	B	1224	CLA	C3C-C2C	4.64	1.46	1.36
18	B	1217	CLA	CHD-C1D	4.64	1.47	1.38
18	1	1005	CLA	CHC-C1C	4.64	1.47	1.38
18	A	1115	CLA	CHD-C1D	4.63	1.47	1.38
18	A	1119	CLA	CHD-C1D	4.63	1.47	1.38
18	G	1001	CLA	O2D-CGD	4.63	1.44	1.33
18	A	1135	CLA	C3C-C2C	4.63	1.46	1.36
18	B	1235	CLA	C3C-C2C	4.63	1.46	1.36
18	A	1108	CLA	C3C-C2C	4.63	1.46	1.36
17	A	1011	CL0	C3D-C2D	4.63	1.47	1.39
18	B	1208	CLA	CHD-C1D	4.63	1.47	1.38
18	A	1110	CLA	C3C-C2C	4.63	1.46	1.36
18	B	1232	CLA	CHD-C1D	4.62	1.47	1.38
18	A	1131	CLA	C3C-C2C	4.62	1.46	1.36
18	B	1219	CLA	C3C-C2C	4.62	1.46	1.36
18	A	1138	CLA	C3C-C2C	4.62	1.46	1.36
18	4	4008	CLA	C4B-NB	-4.62	1.31	1.37
18	A	1124	CLA	C3C-C2C	4.62	1.46	1.36
18	B	1205	CLA	CHD-C1D	4.61	1.47	1.38
18	B	1219	CLA	CHD-C1D	4.61	1.47	1.38
18	3	3010	CLA	C4B-NB	-4.61	1.31	1.37
18	3	3007	CLA	O2D-CGD	4.61	1.44	1.33
28	2	2013	CHL	C1A-CHA	-4.61	1.34	1.40
18	B	1224	CLA	CHD-C1D	4.61	1.47	1.38
18	1	1001	CLA	CHC-C1C	4.61	1.47	1.38
18	B	1232	CLA	C3C-C2C	4.61	1.46	1.36
18	B	1231	CLA	C3C-C2C	4.61	1.46	1.36
18	A	1109	CLA	CHD-C1D	4.60	1.47	1.38
18	3	3008	CLA	C3D-C4D	-4.60	1.33	1.44
18	2	2012	CLA	C1D-ND	-4.60	1.31	1.37
18	L	1501	CLA	CHC-C1C	4.60	1.47	1.38
18	3	3010	CLA	O2D-CGD	4.60	1.44	1.33
18	A	1115	CLA	C3C-C2C	4.60	1.46	1.36
18	B	1208	CLA	C3C-C2C	4.60	1.46	1.36
18	3	3012	CLA	CHC-C1C	4.60	1.47	1.38
18	B	1220	CLA	CHD-C1D	4.60	1.47	1.38
18	B	1212	CLA	C3C-C2C	4.60	1.46	1.36
18	B	1206	CLA	CHC-C1C	4.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2001	CLA	C3D-C4D	-4.60	1.33	1.44
18	B	1240	CLA	CHD-C1D	4.60	1.47	1.38
18	A	1107	CLA	C3C-C2C	4.59	1.46	1.36
18	B	1202	CLA	CHD-C1D	4.59	1.47	1.38
18	B	1239	CLA	CHD-C1D	4.59	1.47	1.38
18	1	1006	CLA	O2D-CGD	4.59	1.44	1.33
18	A	1104	CLA	C3C-C2C	4.59	1.46	1.36
18	A	1110	CLA	CHD-C1D	4.59	1.47	1.38
18	A	1132	CLA	C3C-C2C	4.59	1.46	1.36
18	A	1022	CLA	C3C-C2C	4.59	1.46	1.36
18	A	1131	CLA	CHD-C1D	4.59	1.47	1.38
18	A	1126	CLA	C3C-C2C	4.59	1.46	1.36
18	1	1013	CLA	O2D-CGD	4.58	1.44	1.33
18	B	1235	CLA	CHD-C1D	4.58	1.47	1.38
18	A	1136	CLA	C3C-C2C	4.58	1.46	1.36
18	A	1119	CLA	C3C-C2C	4.58	1.46	1.36
18	B	1225	CLA	C3C-C2C	4.58	1.46	1.36
18	F	1301	CLA	C3D-C4D	-4.58	1.33	1.44
18	A	1121	CLA	C3C-C2C	4.58	1.46	1.36
18	L	1502	CLA	O2D-CGD	4.58	1.44	1.33
18	A	1136	CLA	CHD-C1D	4.58	1.47	1.38
18	B	1221	CLA	CHD-C1D	4.58	1.47	1.38
18	A	1111	CLA	CHD-C1D	4.57	1.47	1.38
18	A	1121	CLA	CHD-C1D	4.57	1.47	1.38
18	A	1130	CLA	CHD-C1D	4.57	1.47	1.38
18	A	1113	CLA	CHD-C1D	4.57	1.47	1.38
18	A	1120	CLA	CHD-C1D	4.57	1.47	1.38
18	B	1239	CLA	C3C-C2C	4.57	1.46	1.36
18	A	1106	CLA	CHD-C1D	4.57	1.47	1.38
18	3	3019	CLA	C2B-C1B	4.57	1.49	1.40
18	B	1218	CLA	C3C-C2C	4.57	1.46	1.36
18	A	1237	CLA	CHD-C1D	4.57	1.47	1.38
18	B	1211	CLA	CHD-C1D	4.56	1.47	1.38
18	B	1238	CLA	CHD-C1D	4.56	1.47	1.38
18	B	1238	CLA	C3C-C2C	4.56	1.46	1.36
18	A	1132	CLA	CHD-C1D	4.56	1.47	1.38
18	A	1118	CLA	C3C-C2C	4.56	1.46	1.36
18	A	1103	CLA	CHD-C1D	4.56	1.47	1.38
18	4	4004	CLA	C4B-NB	-4.56	1.31	1.37
18	A	1106	CLA	C3C-C2C	4.56	1.46	1.36
18	A	1120	CLA	C3C-C2C	4.56	1.46	1.36
18	A	1116	CLA	C3C-C2C	4.56	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1211	CLA	C3C-C2C	4.56	1.46	1.36
18	B	1226	CLA	CHC-C1C	4.56	1.47	1.38
18	4	4005	CLA	C4B-NB	-4.56	1.31	1.37
18	H	1000	CLA	C3C-C2C	4.56	1.46	1.36
18	A	1109	CLA	C3C-C2C	4.55	1.46	1.36
18	A	1129	CLA	C3C-C2C	4.55	1.46	1.36
18	1	1013	CLA	C3D-C4D	-4.55	1.33	1.44
18	A	1139	CLA	CHD-C1D	4.55	1.47	1.38
18	A	1112	CLA	C3C-C2C	4.55	1.46	1.36
18	A	1105	CLA	C3C-C2C	4.55	1.46	1.36
18	B	1209	CLA	C3C-C2C	4.55	1.46	1.36
18	A	1122	CLA	C3C-C2C	4.55	1.46	1.36
18	J	1302	CLA	C3C-C2C	4.55	1.46	1.36
18	B	1205	CLA	C3C-C2C	4.55	1.46	1.36
18	A	1123	CLA	CHD-C1D	4.54	1.47	1.38
18	B	1228	CLA	CHD-C1D	4.54	1.47	1.38
18	B	1213	CLA	CHD-C1D	4.54	1.47	1.38
18	B	1217	CLA	C3C-C2C	4.54	1.46	1.36
18	3	3004	CLA	CHC-C1C	4.54	1.47	1.38
18	B	1222	CLA	C3C-C2C	4.54	1.46	1.36
18	B	1236	CLA	C3C-C2C	4.54	1.46	1.36
18	B	1229	CLA	C3C-C2C	4.54	1.46	1.36
18	4	4008	CLA	C1B-NB	-4.54	1.31	1.37
18	B	1220	CLA	C3C-C2C	4.54	1.46	1.36
18	A	1013	CLA	C3C-C2C	4.53	1.46	1.36
28	1	1010	CHL	C1A-CHA	-4.53	1.34	1.40
18	4	4006	CLA	O2D-CGD	4.53	1.44	1.33
18	3	3017	CLA	C1B-NB	-4.53	1.31	1.37
18	B	1202	CLA	C3C-C2C	4.53	1.46	1.36
18	A	1137	CLA	C3C-C2C	4.53	1.46	1.36
18	B	1023	CLA	C3C-C2C	4.53	1.46	1.36
18	B	1225	CLA	CHD-C1D	4.53	1.47	1.38
18	2	2004	CLA	C4B-NB	-4.53	1.31	1.37
18	B	1218	CLA	CHD-C1D	4.52	1.47	1.38
28	1	1009	CHL	C3B-C2B	-4.52	1.34	1.40
18	G	1003	CLA	CHD-C1D	4.52	1.47	1.38
18	A	1102	CLA	C3C-C2C	4.52	1.46	1.36
18	1	1006	CLA	CHC-C1C	4.52	1.47	1.38
18	F	1302	CLA	C3D-C4D	-4.52	1.34	1.44
18	3	3013	CLA	CHD-C1D	4.52	1.47	1.38
18	3	3012	CLA	O2D-CGD	4.52	1.44	1.33
18	A	1133	CLA	C3C-C2C	4.52	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1129	CLA	CHD-C1D	4.52	1.47	1.38
18	B	1201	CLA	CHD-C1D	4.52	1.47	1.38
18	A	1013	CLA	CHD-C1D	4.51	1.47	1.38
18	B	1215	CLA	CHD-C1D	4.51	1.47	1.38
18	B	1227	CLA	C3C-C2C	4.51	1.46	1.36
18	A	1113	CLA	C3C-C2C	4.51	1.46	1.36
18	A	1123	CLA	C3C-C2C	4.51	1.46	1.36
18	A	1127	CLA	C3C-C2C	4.51	1.46	1.36
18	1	1014	CLA	O2D-CGD	4.51	1.44	1.33
18	1	1008	CLA	CHC-C1C	4.51	1.47	1.38
18	1	1001	CLA	C3D-C4D	-4.50	1.34	1.44
18	B	1012	CLA	C3C-C2C	4.50	1.46	1.36
18	2	2006	CLA	C3D-C4D	-4.50	1.34	1.44
18	B	1212	CLA	CHD-C1D	4.50	1.47	1.38
18	B	1215	CLA	C3C-C2C	4.50	1.46	1.36
18	1	1014	CLA	CHC-C1C	4.50	1.47	1.38
18	1	1014	CLA	C1D-ND	-4.50	1.32	1.37
18	A	1118	CLA	CHD-C1D	4.50	1.47	1.38
18	1	1012	CLA	C1D-ND	-4.50	1.32	1.37
18	B	1240	CLA	C3C-C2C	4.49	1.46	1.36
18	B	1021	CLA	CHD-C1D	4.49	1.47	1.38
18	A	1114	CLA	C3C-C2C	4.49	1.46	1.36
18	A	1101	CLA	C3C-C2C	4.49	1.46	1.36
18	B	1203	CLA	C3C-C2C	4.49	1.46	1.36
18	A	1117	CLA	C3C-C2C	4.49	1.46	1.36
18	A	1107	CLA	CHD-C1D	4.49	1.47	1.38
22	A	6011	BCR	C10-C9	-4.49	1.25	1.35
18	1	1007	CLA	CHC-C1C	4.48	1.47	1.38
18	A	1139	CLA	C3C-C2C	4.48	1.46	1.36
18	2	2009	CLA	O2D-CGD	4.48	1.44	1.33
17	A	1011	CL0	CHD-C4C	4.48	1.48	1.39
18	B	1221	CLA	C3C-C2C	4.48	1.46	1.36
18	4	4009	CLA	CHC-C1C	4.47	1.47	1.38
18	3	3003	CLA	C4B-NB	-4.47	1.32	1.37
18	2	2005	CLA	C3D-C4D	-4.47	1.34	1.44
18	2	2002	CLA	CHC-C1C	4.47	1.47	1.38
18	A	1140	CLA	C3C-C2C	4.47	1.46	1.36
18	A	1134	CLA	C3C-C2C	4.47	1.46	1.36
18	3	3004	CLA	O2D-CGD	4.47	1.44	1.33
18	A	1237	CLA	C3C-C2C	4.47	1.46	1.36
18	B	1216	CLA	C3C-C2C	4.46	1.46	1.36
18	B	1223	CLA	C3C-C2C	4.46	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	4	4013	CHL	C3B-C4B	4.46	1.45	1.41
18	2	2007	CLA	C3D-C4D	-4.46	1.34	1.44
18	4	4006	CLA	C1D-ND	-4.46	1.32	1.37
18	B	1226	CLA	C3D-C4D	-4.46	1.34	1.44
18	A	1125	CLA	C3C-C2C	4.46	1.46	1.36
18	A	1104	CLA	CHD-C1D	4.45	1.47	1.38
18	B	1023	CLA	CHD-C1D	4.45	1.47	1.38
18	B	1207	CLA	CHD-C1D	4.45	1.47	1.38
18	B	1234	CLA	CHD-C1D	4.45	1.47	1.38
18	B	1203	CLA	CHD-C1D	4.44	1.47	1.38
18	A	1137	CLA	CHD-C1D	4.44	1.47	1.38
18	1	1004	CLA	CHC-C1C	4.44	1.47	1.38
18	3	3005	CLA	O2D-CGD	4.44	1.44	1.33
17	A	1011	CL0	C3D-C4D	-4.44	1.34	1.41
18	B	1223	CLA	CHD-C1D	4.44	1.47	1.38
28	2	2013	CHL	O2A-CGA	4.43	1.45	1.30
18	1	1004	CLA	O2D-CGD	4.43	1.44	1.33
18	1	1008	CLA	O2D-CGD	4.43	1.44	1.33
18	3	3018	CLA	CHC-C1C	4.43	1.47	1.38
18	L	1503	CLA	O2D-CGD	4.43	1.44	1.33
18	1	1007	CLA	O2D-CGD	4.42	1.44	1.33
18	B	1206	CLA	C3C-C2C	4.42	1.46	1.36
18	4	4001	CLA	CHC-C1C	4.42	1.47	1.38
18	A	1128	CLA	CHD-C1D	4.42	1.47	1.38
18	B	1214	CLA	C3C-C2C	4.42	1.46	1.36
18	1	1012	CLA	CHC-C1C	4.41	1.47	1.38
18	B	1223	CLA	C3D-C4D	-4.41	1.34	1.44
18	2	2003	CLA	CHC-C1C	4.41	1.47	1.38
22	J	6013	BCR	C10-C9	-4.41	1.25	1.35
18	2	2009	CLA	CHD-C1D	4.41	1.47	1.38
18	2	2012	CLA	C4B-NB	-4.41	1.32	1.37
18	3	3002	CLA	CHC-C1C	4.41	1.47	1.38
18	B	1210	CLA	C3C-C2C	4.41	1.46	1.36
21	A	7001	LHG	O8-C23	4.40	1.46	1.33
18	3	3010	CLA	C1D-ND	-4.40	1.32	1.37
18	2	2016	CLA	OBD-CAD	4.40	1.30	1.22
18	A	1102	CLA	CHD-C1D	4.40	1.47	1.38
18	2	2006	CLA	CHD-C1D	4.40	1.47	1.38
18	B	1213	CLA	C3C-C2C	4.40	1.46	1.36
18	B	1203	CLA	C3D-C4D	-4.40	1.34	1.44
18	A	1111	CLA	C3C-C2C	4.40	1.46	1.36
22	B	6009	BCR	C10-C9	-4.39	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2008	CLA	CHC-C1C	4.39	1.47	1.38
18	A	1125	CLA	C3D-C4D	-4.39	1.34	1.44
18	1	1006	CLA	CHD-C1D	4.39	1.47	1.38
18	B	1201	CLA	C3C-C2C	4.39	1.46	1.36
18	1	1003	CLA	CHC-C1C	4.39	1.47	1.38
18	3	3013	CLA	O2D-CGD	4.38	1.44	1.33
18	K	1001	CLA	C1D-ND	-4.38	1.32	1.37
18	L	1501	CLA	CHD-C1D	4.38	1.47	1.38
18	1	1002	CLA	CHC-C1C	4.38	1.47	1.38
22	L	6020	BCR	C10-C9	-4.37	1.25	1.35
18	B	1231	CLA	CHC-C4B	4.37	1.49	1.39
18	B	1207	CLA	C3C-C2C	4.37	1.46	1.36
18	2	2004	CLA	C1D-ND	-4.37	1.32	1.37
18	3	3002	CLA	O2D-CGD	4.37	1.44	1.33
18	B	1021	CLA	C3C-C2C	4.37	1.46	1.36
18	B	1226	CLA	C3C-C2C	4.37	1.46	1.36
18	L	1501	CLA	O2D-CGD	4.37	1.44	1.33
18	4	4002	CLA	C1D-ND	-4.37	1.32	1.37
28	4	4010	CHL	C2C-C3C	-4.36	1.32	1.36
18	1	1012	CLA	O2D-CGD	4.36	1.43	1.33
18	F	1302	CLA	CHD-C1D	4.35	1.46	1.38
18	4	4012	CLA	C4B-NB	-4.35	1.32	1.37
18	2	2004	CLA	O2D-CGD	4.35	1.43	1.33
18	3	3006	CLA	C4B-NB	-4.35	1.32	1.37
18	B	1012	CLA	CHD-C1D	4.35	1.46	1.38
18	2	2005	CLA	CHD-C1D	4.35	1.46	1.38
18	A	1119	CLA	C3D-C4D	-4.34	1.34	1.44
18	1	1013	CLA	CHC-C1C	4.34	1.47	1.38
18	3	3006	CLA	CHC-C1C	4.34	1.47	1.38
18	4	4005	CLA	O2D-CGD	4.34	1.43	1.33
18	3	3002	CLA	CHD-C1D	4.33	1.46	1.38
18	G	1003	CLA	O2D-CGD	4.33	1.43	1.33
18	B	1236	CLA	CHD-C1D	4.33	1.46	1.38
22	A	6008	BCR	C10-C9	-4.33	1.25	1.35
18	1	1003	CLA	CHD-C1D	4.33	1.46	1.38
18	A	1022	CLA	C3D-C4D	-4.32	1.34	1.44
18	B	1230	CLA	C3C-C2C	4.32	1.46	1.36
18	A	1135	CLA	C3D-C4D	-4.32	1.34	1.44
18	A	1120	CLA	C3D-C4D	-4.32	1.34	1.44
18	B	1238	CLA	C3D-C4D	-4.32	1.34	1.44
18	F	1302	CLA	C3C-C2C	4.31	1.46	1.36
18	2	2006	CLA	C3C-C2C	4.31	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4002	CLA	C4B-NB	-4.31	1.32	1.37
18	A	1107	CLA	C3D-C4D	-4.30	1.34	1.44
18	G	1002	CLA	CHD-C1D	4.30	1.46	1.38
18	3	3019	CLA	C2D-C1D	4.30	1.50	1.42
18	A	1103	CLA	C3C-C2C	4.30	1.46	1.36
18	3	3010	CLA	CHC-C1C	4.30	1.47	1.38
18	2	2012	CLA	C1B-NB	-4.30	1.32	1.37
18	3	3008	CLA	C3C-C2C	4.30	1.46	1.36
18	A	1129	CLA	C3D-C4D	-4.29	1.34	1.44
18	A	1103	CLA	C3D-C4D	-4.29	1.34	1.44
18	2	2009	CLA	C3C-C2C	4.29	1.46	1.36
23	B	5005	LMG	O8-C28	4.29	1.45	1.33
18	B	1222	CLA	CHD-C1D	4.29	1.46	1.38
18	3	3013	CLA	C3C-C2C	4.28	1.46	1.36
18	A	1237	CLA	C3D-C4D	-4.28	1.34	1.44
28	4	4010	CHL	O2A-CGA	4.28	1.46	1.33
18	B	1216	CLA	C3D-C4D	-4.27	1.34	1.44
18	B	1205	CLA	C3D-C4D	-4.27	1.34	1.44
18	B	1218	CLA	C3D-C4D	-4.27	1.34	1.44
18	1	1011	CLA	O2D-CGD	4.27	1.43	1.33
18	B	1213	CLA	C3D-C4D	-4.27	1.34	1.44
18	A	1108	CLA	C3D-C4D	-4.27	1.34	1.44
18	K	1001	CLA	CHC-C1C	4.27	1.47	1.38
18	3	3003	CLA	CHB-C1B	4.26	1.49	1.39
18	A	1117	CLA	C3D-C4D	-4.26	1.34	1.44
18	A	1130	CLA	C3D-C4D	-4.26	1.34	1.44
18	B	1207	CLA	C3D-C4D	-4.26	1.34	1.44
18	4	4004	CLA	C1B-NB	-4.26	1.32	1.37
18	B	1220	CLA	C3D-C4D	-4.26	1.34	1.44
18	A	1134	CLA	C3D-C4D	-4.25	1.34	1.44
22	J	6012	BCR	C10-C9	-4.25	1.26	1.35
18	B	1012	CLA	C3D-C4D	-4.25	1.34	1.44
18	B	1240	CLA	C3D-C4D	-4.25	1.34	1.44
18	3	3013	CLA	C1B-NB	-4.25	1.32	1.37
18	3	3001	CLA	CHD-C1D	4.25	1.46	1.38
21	A	5003	LHG	O8-C23	4.24	1.45	1.33
22	A	6003	BCR	C10-C9	-4.24	1.26	1.35
18	2	2005	CLA	C3C-C2C	4.24	1.45	1.36
18	B	1239	CLA	C3D-C4D	-4.24	1.34	1.44
18	L	1501	CLA	C1B-NB	-4.24	1.32	1.37
18	B	1219	CLA	C3D-C4D	-4.24	1.34	1.44
18	2	2007	CLA	C3C-C2C	4.24	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1227	CLA	C3D-C4D	-4.24	1.34	1.44
18	1	1013	CLA	CHB-C1B	4.24	1.48	1.39
18	4	4016	CLA	CHD-C1D	4.23	1.46	1.38
18	A	1112	CLA	C3D-C4D	-4.23	1.34	1.44
18	H	1000	CLA	C3D-C4D	-4.23	1.34	1.44
18	B	1206	CLA	C3D-C4D	-4.23	1.34	1.44
18	3	3008	CLA	CHB-C1B	4.23	1.48	1.39
28	1	1010	CHL	O2D-CGD	4.23	1.43	1.33
18	B	1211	CLA	CHC-C4B	4.23	1.48	1.39
18	B	1214	CLA	C3D-C4D	-4.23	1.34	1.44
28	3	3011	CHL	O2A-CGA	4.22	1.45	1.33
18	B	1234	CLA	CHC-C4B	4.22	1.48	1.39
18	2	2016	CLA	CHC-C1C	4.22	1.46	1.38
18	A	1123	CLA	C3D-C4D	-4.22	1.34	1.44
18	4	4017	CLA	O2D-CGD	4.22	1.43	1.33
18	A	1114	CLA	C3D-C4D	-4.22	1.34	1.44
18	2	2007	CLA	CHD-C1D	4.22	1.46	1.38
18	4	4002	CLA	CHB-C1B	4.22	1.48	1.39
28	4	4011	CHL	C3B-C2B	-4.22	1.34	1.40
18	3	3018	CLA	CHD-C1D	4.22	1.46	1.38
18	A	1125	CLA	CHD-C1D	4.22	1.46	1.38
18	J	1302	CLA	C3D-C4D	-4.22	1.34	1.44
18	1	1007	CLA	C1D-ND	-4.22	1.32	1.37
18	A	1106	CLA	C3D-C4D	-4.22	1.34	1.44
28	2	2010	CHL	O2A-CGA	4.22	1.46	1.33
18	B	1204	CLA	C3D-C4D	-4.21	1.34	1.44
18	A	1124	CLA	C3D-C4D	-4.21	1.34	1.44
18	A	1113	CLA	C3D-C4D	-4.21	1.34	1.44
18	B	1224	CLA	C3D-C4D	-4.21	1.34	1.44
18	A	1139	CLA	C3D-C4D	-4.21	1.34	1.44
18	B	1210	CLA	C3D-C4D	-4.21	1.34	1.44
18	A	1110	CLA	C3D-C4D	-4.21	1.34	1.44
18	2	2016	CLA	C1D-ND	-4.21	1.32	1.37
18	A	1128	CLA	C3D-C4D	-4.21	1.34	1.44
18	4	4005	CLA	C1D-ND	-4.20	1.32	1.37
18	A	1132	CLA	CHC-C4B	4.20	1.48	1.39
18	B	1202	CLA	C3D-C4D	-4.20	1.34	1.44
18	2	2003	CLA	CHB-C1B	4.20	1.48	1.39
18	A	1104	CLA	CHC-C4B	4.20	1.48	1.39
18	A	1126	CLA	C3D-C4D	-4.20	1.34	1.44
18	B	1211	CLA	C3D-C4D	-4.19	1.34	1.44
18	A	1151	CLA	C3D-C4D	-4.19	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1215	CLA	C3D-C4D	-4.19	1.34	1.44
18	A	1140	CLA	C3D-C4D	-4.19	1.34	1.44
18	G	1003	CLA	C3C-C2C	4.19	1.45	1.36
18	L	1501	CLA	C1D-ND	-4.19	1.32	1.37
18	1	1005	CLA	C4B-NB	-4.19	1.32	1.37
18	A	1104	CLA	C3D-C4D	-4.19	1.34	1.44
18	B	1208	CLA	CHC-C4B	4.19	1.48	1.39
18	A	1132	CLA	C3D-C4D	-4.19	1.34	1.44
18	2	2001	CLA	C1B-NB	-4.19	1.32	1.37
18	B	1229	CLA	CHD-C1D	4.19	1.46	1.38
18	B	1208	CLA	C3D-C4D	-4.19	1.34	1.44
18	B	1235	CLA	C3D-C4D	-4.18	1.34	1.44
18	4	4009	CLA	C1B-NB	-4.18	1.32	1.37
18	3	3004	CLA	C3C-C2C	4.18	1.45	1.36
18	2	2001	CLA	CHD-C1D	4.18	1.46	1.38
18	B	1234	CLA	C3D-C4D	-4.18	1.34	1.44
18	4	4004	CLA	O2D-CGD	4.18	1.43	1.33
18	4	4006	CLA	CHC-C1C	4.18	1.46	1.38
18	B	1221	CLA	C3D-C4D	-4.18	1.34	1.44
18	G	1001	CLA	C1D-ND	-4.18	1.32	1.37
18	1	1007	CLA	C4B-NB	-4.18	1.32	1.37
18	B	1236	CLA	C3D-C4D	-4.18	1.34	1.44
18	B	1232	CLA	CHC-C4B	4.18	1.48	1.39
18	A	1115	CLA	C3D-C4D	-4.18	1.34	1.44
18	A	1138	CLA	C3D-C4D	-4.18	1.34	1.44
18	B	1209	CLA	C3D-C4D	-4.18	1.34	1.44
18	B	1222	CLA	C3D-C4D	-4.18	1.34	1.44
18	A	1131	CLA	C3D-C4D	-4.17	1.34	1.44
18	A	1121	CLA	C3D-C4D	-4.17	1.34	1.44
18	4	4012	CLA	CHD-C1D	4.17	1.46	1.38
18	4	4016	CLA	C3C-C2C	4.17	1.45	1.36
21	2	2801	LHG	O8-C23	4.17	1.45	1.33
18	A	1116	CLA	C3D-C4D	-4.17	1.34	1.44
18	A	1105	CLA	CHC-C4B	4.17	1.48	1.39
18	B	1232	CLA	C3D-C4D	-4.17	1.34	1.44
18	A	1109	CLA	CHC-C4B	4.17	1.48	1.39
18	A	1137	CLA	CHC-C4B	4.17	1.48	1.39
18	A	1013	CLA	CHC-C4B	4.17	1.48	1.39
18	A	1127	CLA	C3D-C4D	-4.17	1.34	1.44
18	3	3012	CLA	C1D-ND	-4.17	1.32	1.37
18	F	1301	CLA	CHB-C1B	4.17	1.48	1.39
18	3	3003	CLA	C3C-C2C	4.17	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	1301	CLA	C3C-C2C	4.17	1.45	1.36
18	F	1301	CLA	CHD-C1D	4.17	1.46	1.38
18	A	1136	CLA	C3D-C4D	-4.16	1.34	1.44
18	B	1225	CLA	C3D-C4D	-4.16	1.34	1.44
18	A	1133	CLA	C3D-C4D	-4.16	1.34	1.44
18	1	1002	CLA	O2D-CGD	4.16	1.43	1.33
18	3	3010	CLA	C3C-C2C	4.16	1.45	1.36
18	A	1110	CLA	CHC-C4B	4.16	1.48	1.39
18	B	1236	CLA	CHC-C4B	4.16	1.48	1.39
18	2	2012	CLA	CHC-C1C	4.16	1.46	1.38
18	A	1118	CLA	C3D-C4D	-4.16	1.34	1.44
18	A	1111	CLA	C3D-C4D	-4.16	1.34	1.44
18	B	1021	CLA	C3D-C4D	-4.16	1.34	1.44
28	2	2013	CHL	O2D-CGD	4.16	1.43	1.33
18	A	1102	CLA	C3D-C4D	-4.15	1.34	1.44
18	G	1001	CLA	C4B-NB	-4.15	1.32	1.37
18	B	1201	CLA	C3D-C4D	-4.15	1.34	1.44
18	4	4006	CLA	C1B-NB	-4.15	1.32	1.37
22	B	6006	BCR	C10-C9	-4.15	1.26	1.35
18	K	1001	CLA	C3C-C2C	4.15	1.45	1.36
18	2	2003	CLA	O2D-CGD	4.15	1.43	1.33
18	A	1122	CLA	C3D-C4D	-4.15	1.34	1.44
18	B	1231	CLA	C3D-C4D	-4.15	1.34	1.44
18	2	2002	CLA	O2D-CGD	4.15	1.43	1.33
18	A	1105	CLA	C3D-C4D	-4.14	1.34	1.44
18	A	1124	CLA	CHC-C4B	4.14	1.48	1.39
18	A	1108	CLA	CHC-C4B	4.14	1.48	1.39
21	A	7001	LHG	O7-C7	4.14	1.46	1.34
17	A	1011	CL0	C3B-C2B	4.14	1.46	1.40
18	3	3001	CLA	C1D-ND	-4.14	1.32	1.37
18	1	1003	CLA	C3C-C2C	4.14	1.45	1.36
18	B	1235	CLA	CHC-C4B	4.14	1.48	1.39
21	A	5003	LHG	O7-C7	4.14	1.46	1.34
18	B	1231	CLA	CHD-C4C	4.14	1.48	1.39
18	A	1137	CLA	C3D-C4D	-4.14	1.34	1.44
18	A	1101	CLA	C3D-C4D	-4.14	1.34	1.44
18	B	1230	CLA	CHD-C1D	4.14	1.46	1.38
18	4	4012	CLA	C1D-ND	-4.14	1.32	1.37
18	B	1212	CLA	C3D-C4D	-4.13	1.34	1.44
18	A	1109	CLA	C3D-C4D	-4.13	1.34	1.44
18	B	1238	CLA	CHC-C4B	4.13	1.48	1.39
18	A	1115	CLA	CHD-C4C	4.13	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	6007	BCR	C10-C9	-4.13	1.26	1.35
18	2	2003	CLA	C1B-NB	-4.13	1.32	1.37
18	4	4004	CLA	C1D-ND	-4.13	1.32	1.37
18	B	1227	CLA	CHC-C4B	4.13	1.48	1.39
23	B	5005	LMG	O7-C10	4.13	1.45	1.34
18	B	1226	CLA	CHD-C4C	4.13	1.48	1.39
18	A	1138	CLA	CHC-C4B	4.12	1.48	1.39
18	A	1140	CLA	CHC-C4B	4.12	1.48	1.39
28	4	4010	CHL	O2D-CGD	4.12	1.43	1.33
18	B	1239	CLA	CHC-C4B	4.12	1.48	1.39
22	B	6004	BCR	C10-C9	-4.12	1.26	1.35
18	A	1120	CLA	CHC-C4B	4.12	1.48	1.39
18	B	1206	CLA	CHB-C1B	4.12	1.48	1.39
18	1	1001	CLA	C1D-ND	-4.12	1.32	1.37
18	B	1012	CLA	CHC-C4B	4.12	1.48	1.39
18	B	1217	CLA	C3D-C4D	-4.11	1.34	1.44
18	4	4009	CLA	C1D-ND	-4.11	1.32	1.37
18	B	1228	CLA	C3D-C4D	-4.11	1.34	1.44
18	2	2016	CLA	C1B-NB	-4.11	1.32	1.37
18	4	4008	CLA	O2D-CGD	4.11	1.43	1.33
18	B	1230	CLA	CHC-C4B	4.11	1.48	1.39
18	4	4006	CLA	C4B-NB	-4.11	1.32	1.37
18	4	4003	CLA	CHD-C1D	4.11	1.46	1.38
18	B	1218	CLA	CHC-C4B	4.11	1.48	1.39
18	B	1229	CLA	CHC-C4B	4.11	1.48	1.39
18	4	4001	CLA	C1B-NB	-4.10	1.32	1.37
18	A	1134	CLA	CHD-C4C	4.10	1.48	1.39
18	2	2004	CLA	C1B-NB	-4.10	1.32	1.37
18	2	2016	CLA	CHB-C1B	4.10	1.48	1.39
18	A	1022	CLA	CHC-C4B	4.10	1.48	1.39
18	3	3008	CLA	CHC-C1C	4.10	1.46	1.38
18	A	1107	CLA	CHC-C4B	4.10	1.48	1.39
22	I	6020	BCR	C10-C9	-4.09	1.26	1.35
18	1	1004	CLA	C3C-C2C	4.09	1.45	1.36
18	A	1138	CLA	CHD-C4C	4.09	1.48	1.39
18	A	1134	CLA	CHC-C4B	4.09	1.48	1.39
18	2	2004	CLA	CHD-C1D	4.09	1.46	1.38
18	A	1116	CLA	CHC-C4B	4.09	1.48	1.39
18	A	1126	CLA	CHC-C4B	4.08	1.48	1.39
18	A	1131	CLA	CHC-C4B	4.08	1.48	1.39
18	B	1221	CLA	CHC-C4B	4.08	1.48	1.39
18	1	1013	CLA	CHD-C4C	4.08	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1022	CLA	CHD-C4C	4.08	1.48	1.39
18	2	2002	CLA	C4B-NB	-4.08	1.32	1.37
18	2	2001	CLA	C1D-ND	-4.08	1.32	1.37
18	3	3004	CLA	C4B-NB	-4.08	1.32	1.37
18	A	1139	CLA	CHC-C4B	4.08	1.48	1.39
18	A	1121	CLA	CHC-C4B	4.08	1.48	1.39
18	A	1117	CLA	CHD-C4C	4.08	1.48	1.39
18	A	1124	CLA	CHD-C4C	4.08	1.48	1.39
18	4	4005	CLA	CHC-C1C	4.07	1.46	1.38
18	B	1204	CLA	CHD-C4C	4.07	1.48	1.39
18	A	1013	CLA	C3D-C4D	-4.07	1.35	1.44
18	B	1229	CLA	C3D-C4D	-4.07	1.35	1.44
18	B	1240	CLA	CHC-C4B	4.07	1.48	1.39
18	H	1000	CLA	CHD-C4C	4.07	1.48	1.39
18	B	1230	CLA	C3D-C4D	-4.07	1.35	1.44
18	2	2006	CLA	CHB-C1B	4.07	1.48	1.39
18	2	2008	CLA	O2D-CGD	4.07	1.43	1.33
18	A	1116	CLA	CHD-C4C	4.06	1.48	1.39
18	4	4007	CLA	O2D-CGD	4.06	1.43	1.33
18	A	1136	CLA	CHC-C4B	4.06	1.48	1.39
18	B	1216	CLA	CHD-C4C	4.06	1.48	1.39
18	4	4012	CLA	O2D-CGD	4.06	1.43	1.33
18	A	1112	CLA	CHD-C4C	4.06	1.48	1.39
18	A	1115	CLA	CHC-C4B	4.06	1.48	1.39
18	A	1112	CLA	CHC-C4B	4.05	1.48	1.39
18	A	1126	CLA	CHD-C4C	4.05	1.48	1.39
18	4	4005	CLA	C1B-NB	-4.05	1.32	1.37
18	B	1023	CLA	CHC-C4B	4.05	1.48	1.39
18	3	3004	CLA	C1D-ND	-4.05	1.32	1.37
18	B	1202	CLA	CHD-C4C	4.05	1.48	1.39
18	1	1012	CLA	CHD-C1D	4.05	1.46	1.38
18	B	1201	CLA	CHC-C4B	4.05	1.48	1.39
18	B	1214	CLA	CHD-C4C	4.05	1.48	1.39
18	B	1204	CLA	CHC-C4B	4.05	1.48	1.39
18	B	1225	CLA	CHB-C1B	4.05	1.48	1.39
23	F	5001	LMG	O7-C10	4.05	1.44	1.35
18	A	1129	CLA	CHC-C4B	4.05	1.48	1.39
18	A	1130	CLA	CHC-C4B	4.05	1.48	1.39
18	2	2007	CLA	CHB-C1B	4.05	1.48	1.39
22	A	6002	BCR	C10-C9	-4.04	1.26	1.35
18	2	2005	CLA	CHB-C1B	4.04	1.48	1.39
18	B	1240	CLA	CHD-C4C	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3012	CLA	C4B-NB	-4.04	1.32	1.37
18	B	1236	CLA	CHB-C1B	4.04	1.48	1.39
18	B	1218	CLA	CHD-C4C	4.04	1.48	1.39
18	B	1208	CLA	CHD-C4C	4.04	1.48	1.39
18	B	1216	CLA	CHC-C4B	4.04	1.48	1.39
18	B	1207	CLA	CHC-C4B	4.04	1.48	1.39
18	A	1113	CLA	CHC-C4B	4.04	1.48	1.39
18	A	1139	CLA	CHD-C4C	4.04	1.48	1.39
18	A	1137	CLA	CHB-C1B	4.04	1.48	1.39
18	B	1228	CLA	CHD-C4C	4.04	1.48	1.39
28	3	3011	CHL	O2D-CGD	4.04	1.43	1.33
18	B	1205	CLA	CHC-C4B	4.04	1.48	1.39
18	B	1213	CLA	CHC-C4B	4.04	1.48	1.39
18	3	3017	CLA	CHD-C1D	4.04	1.46	1.38
18	A	1140	CLA	CHB-C1B	4.04	1.48	1.39
18	A	1109	CLA	CHD-C4C	4.04	1.48	1.39
18	A	1102	CLA	CHC-C4B	4.03	1.48	1.39
18	B	1209	CLA	CHD-C4C	4.03	1.48	1.39
18	3	3003	CLA	C1D-ND	-4.03	1.32	1.37
18	3	3001	CLA	O2D-CGD	4.03	1.43	1.33
18	B	1222	CLA	CHC-C4B	4.03	1.48	1.39
18	A	1118	CLA	CHC-C4B	4.03	1.48	1.39
18	B	1225	CLA	CHC-C4B	4.03	1.48	1.39
18	3	3004	CLA	CHD-C1D	4.03	1.46	1.38
18	A	1107	CLA	CHD-C4C	4.03	1.48	1.39
18	3	3018	CLA	C3C-C2C	4.03	1.45	1.36
18	B	1220	CLA	CHD-C4C	4.03	1.48	1.39
18	1	1008	CLA	CHB-C1B	4.03	1.48	1.39
18	3	3005	CLA	C1B-NB	-4.03	1.32	1.37
18	B	1023	CLA	C3D-C4D	-4.03	1.35	1.44
18	J	1302	CLA	CHD-C4C	4.03	1.48	1.39
18	A	1013	CLA	CHD-C4C	4.02	1.48	1.39
18	A	1103	CLA	CHB-C1B	4.02	1.48	1.39
18	2	2001	CLA	O2D-CGD	4.02	1.43	1.33
18	A	1131	CLA	CHB-C1B	4.02	1.48	1.39
18	3	3006	CLA	CHD-C1D	4.02	1.46	1.38
28	4	4013	CHL	O2A-CGA	4.02	1.45	1.33
18	1	1005	CLA	O2D-CGD	4.02	1.43	1.33
18	1	1011	CLA	CHD-C1D	4.02	1.46	1.38
18	B	1023	CLA	CHD-C4C	4.02	1.48	1.39
18	A	1106	CLA	CHD-C4C	4.02	1.48	1.39
22	G	2011	BCR	C11-C12	-4.02	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1108	CLA	CHD-C4C	4.01	1.48	1.39
18	B	1217	CLA	CHC-C4B	4.01	1.48	1.39
18	A	1237	CLA	CHD-C4C	4.01	1.48	1.39
18	2	2008	CLA	C4B-NB	-4.01	1.32	1.37
18	A	1122	CLA	CHD-C4C	4.01	1.48	1.39
18	A	1130	CLA	CHD-C4C	4.01	1.48	1.39
18	2	2001	CLA	C4B-NB	-4.01	1.32	1.37
18	B	1228	CLA	CHC-C4B	4.01	1.48	1.39
22	K	2011	BCR	C10-C9	-4.01	1.26	1.35
18	K	1001	CLA	C4B-NB	-4.00	1.32	1.37
18	A	1022	CLA	MG-NC	4.00	2.15	2.06
18	B	1215	CLA	CHD-C4C	4.00	1.48	1.39
18	A	1130	CLA	CHB-C1B	4.00	1.48	1.39
28	1	1010	CHL	O2A-CGA	4.00	1.45	1.33
18	A	1114	CLA	CHD-C4C	4.00	1.48	1.39
21	1	1801	LHG	O7-C7	4.00	1.45	1.34
18	B	1219	CLA	CHC-C4B	4.00	1.48	1.39
23	2	2802	LMG	O7-C10	4.00	1.45	1.34
18	B	1230	CLA	CHB-C1B	4.00	1.48	1.39
18	4	4009	CLA	O2D-CGD	4.00	1.43	1.33
23	2	2802	LMG	O8-C28	4.00	1.45	1.33
18	A	1105	CLA	CHD-C4C	4.00	1.48	1.39
18	A	1114	CLA	CHC-C4B	3.99	1.48	1.39
18	2	2003	CLA	C1D-ND	-3.99	1.32	1.37
18	B	1223	CLA	CHC-C4B	3.99	1.48	1.39
18	A	1118	CLA	CHB-C1B	3.99	1.48	1.39
18	B	1234	CLA	CHB-C1B	3.99	1.48	1.39
18	3	3006	CLA	C3C-C2C	3.99	1.45	1.36
18	A	1151	CLA	CHC-C4B	3.99	1.48	1.39
18	A	1132	CLA	CHD-C4C	3.99	1.48	1.39
18	3	3007	CLA	C3C-C2C	3.99	1.45	1.36
18	B	1209	CLA	CHC-C4B	3.99	1.48	1.39
18	A	1121	CLA	CHD-C4C	3.99	1.48	1.39
18	B	1203	CLA	CHC-C4B	3.99	1.48	1.39
18	B	1205	CLA	CHD-C4C	3.99	1.48	1.39
18	J	1302	CLA	CHC-C4B	3.99	1.48	1.39
22	B	6005	BCR	C10-C9	-3.99	1.26	1.35
18	A	1101	CLA	CHD-C4C	3.99	1.48	1.39
18	4	4003	CLA	C3C-C2C	3.99	1.45	1.36
28	1	1009	CHL	O2A-CGA	3.99	1.45	1.33
18	B	1220	CLA	CHC-C4B	3.98	1.48	1.39
18	B	1211	CLA	CHD-C4C	3.98	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1113	CLA	CHD-C4C	3.98	1.48	1.39
18	L	1502	CLA	CHC-C4B	3.98	1.48	1.39
18	B	1210	CLA	CHD-C4C	3.98	1.48	1.39
28	4	4011	CHL	O2A-CGA	3.98	1.45	1.33
18	A	1135	CLA	CHD-C4C	3.98	1.48	1.39
18	1	1002	CLA	CHB-C1B	3.98	1.48	1.39
18	3	3019	CLA	MG-NC	3.98	2.15	2.06
18	B	1227	CLA	CHD-C4C	3.98	1.48	1.39
18	A	1114	CLA	CHB-C1B	3.98	1.48	1.39
18	3	3005	CLA	C4B-NB	-3.98	1.32	1.37
18	A	1134	CLA	CHB-C1B	3.98	1.48	1.39
18	3	3004	CLA	C1B-NB	-3.98	1.32	1.37
18	4	4004	CLA	C3C-C2C	3.97	1.45	1.36
18	A	1237	CLA	CHB-C1B	3.97	1.48	1.39
18	3	3007	CLA	CHD-C1D	3.97	1.46	1.38
23	F	5002	LMG	O8-C28	3.97	1.44	1.33
18	G	1001	CLA	CHC-C1C	3.97	1.46	1.38
22	B	6010	BCR	C10-C9	-3.97	1.26	1.35
18	A	1107	CLA	CHB-C1B	3.97	1.48	1.39
18	A	1122	CLA	CHC-C4B	3.97	1.48	1.39
18	A	1125	CLA	CHC-C4B	3.97	1.48	1.39
18	3	3012	CLA	C3C-C2C	3.97	1.45	1.36
18	3	3018	CLA	C1D-ND	-3.97	1.32	1.37
18	B	1224	CLA	CHD-C4C	3.97	1.48	1.39
18	4	4008	CLA	C1D-ND	-3.97	1.32	1.37
18	B	1021	CLA	CHC-C4B	3.97	1.48	1.39
18	B	1215	CLA	CHC-C4B	3.97	1.48	1.39
18	L	1503	CLA	CHD-C1D	3.97	1.46	1.38
18	B	1217	CLA	CHD-C4C	3.97	1.48	1.39
18	4	4017	CLA	CHD-C1D	3.97	1.46	1.38
18	A	1123	CLA	CHC-C4B	3.97	1.48	1.39
18	A	1151	CLA	CHD-C4C	3.97	1.48	1.39
18	B	1232	CLA	CHD-C4C	3.97	1.48	1.39
18	1	1003	CLA	C1D-ND	-3.97	1.32	1.37
18	B	1212	CLA	CHC-C4B	3.96	1.48	1.39
18	B	1214	CLA	CHC-C4B	3.96	1.48	1.39
18	4	4008	CLA	CHC-C1C	3.96	1.46	1.38
18	A	1127	CLA	CHD-C4C	3.96	1.48	1.39
18	B	1210	CLA	CHC-C4B	3.96	1.48	1.39
28	2	2011	CHL	O2D-CGD	3.96	1.43	1.33
18	L	1502	CLA	C3C-C2C	3.96	1.45	1.36
18	A	1103	CLA	CHC-C4B	3.96	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1008	CLA	CHD-C1D	3.96	1.46	1.38
18	A	1110	CLA	CHD-C4C	3.96	1.48	1.39
18	2	2019	CLA	C2B-C1B	3.96	1.48	1.40
18	4	4007	CLA	CHB-C1B	3.96	1.48	1.39
18	A	1136	CLA	CHD-C4C	3.96	1.48	1.39
18	B	1201	CLA	CHD-C4C	3.96	1.48	1.39
18	A	1119	CLA	CHD-C4C	3.96	1.48	1.39
18	B	1229	CLA	CHB-C1B	3.95	1.48	1.39
18	A	1140	CLA	CHD-C4C	3.95	1.48	1.39
18	B	1217	CLA	CHB-C1B	3.95	1.48	1.39
18	L	1503	CLA	CHC-C4B	3.95	1.48	1.39
18	B	1231	CLA	OBD-CAD	3.95	1.29	1.22
18	B	1235	CLA	CHB-C1B	3.95	1.48	1.39
18	B	1219	CLA	CHD-C4C	3.95	1.48	1.39
18	J	1302	CLA	MG-NC	3.95	2.15	2.06
18	1	1002	CLA	C4B-NB	-3.95	1.32	1.37
18	B	1239	CLA	CHB-C1B	3.95	1.48	1.39
18	A	1120	CLA	CHB-C1B	3.95	1.48	1.39
18	A	1151	CLA	CHB-C1B	3.94	1.48	1.39
18	A	1133	CLA	CHD-C4C	3.94	1.48	1.39
18	A	1129	CLA	CHB-C1B	3.94	1.48	1.39
18	B	1208	CLA	CHB-C1B	3.94	1.48	1.39
18	B	1218	CLA	CHB-C1B	3.94	1.48	1.39
21	2	2801	LHG	O7-C7	3.94	1.45	1.34
18	2	2002	CLA	C1B-NB	-3.94	1.32	1.37
18	4	4016	CLA	CHB-C1B	3.94	1.48	1.39
21	1	1801	LHG	O8-C23	3.94	1.44	1.33
18	B	1238	CLA	CHD-C4C	3.94	1.48	1.39
18	B	1212	CLA	CHB-C1B	3.93	1.48	1.39
18	B	1205	CLA	CHB-C1B	3.93	1.48	1.39
18	B	1213	CLA	CHB-C1B	3.93	1.48	1.39
18	4	4017	CLA	C3C-C2C	3.93	1.45	1.36
18	A	1117	CLA	CHC-C4B	3.93	1.48	1.39
18	G	1001	CLA	C1B-NB	-3.93	1.32	1.37
18	A	1127	CLA	CHB-C1B	3.93	1.48	1.39
18	A	1119	CLA	CHC-C4B	3.93	1.48	1.39
18	4	4001	CLA	C3C-C2C	3.93	1.45	1.36
18	B	1239	CLA	CHD-C4C	3.93	1.48	1.39
18	B	1234	CLA	CHD-C4C	3.93	1.48	1.39
28	2	2011	CHL	O2A-CGA	3.93	1.44	1.33
18	A	1103	CLA	CHD-C4C	3.93	1.48	1.39
18	A	1127	CLA	CHC-C4B	3.93	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1111	CLA	CHD-C4C	3.92	1.48	1.39
18	3	3006	CLA	CHB-C1B	3.92	1.48	1.39
18	B	1206	CLA	CHD-C4C	3.92	1.48	1.39
18	1	1006	CLA	C1D-ND	-3.92	1.32	1.37
18	A	1135	CLA	CHB-C1B	3.92	1.48	1.39
18	3	3001	CLA	C3C-C2C	3.92	1.45	1.36
18	L	1502	CLA	CHD-C1D	3.92	1.46	1.38
28	4	4011	CHL	O2D-CGD	3.92	1.42	1.33
18	A	1135	CLA	CHC-C4B	3.92	1.48	1.39
18	2	2004	CLA	CHC-C4B	3.92	1.48	1.39
18	A	1128	CLA	CHD-C4C	3.92	1.48	1.39
18	1	1011	CLA	C3C-C2C	3.92	1.45	1.36
18	4	4005	CLA	CHB-C1B	3.91	1.48	1.39
18	G	1001	CLA	CHD-C1D	3.91	1.46	1.38
18	B	1203	CLA	CHB-C1B	3.91	1.48	1.39
18	4	4003	CLA	CHB-C1B	3.91	1.48	1.39
18	B	1201	CLA	CHB-C1B	3.91	1.48	1.39
18	A	1131	CLA	CHD-C4C	3.91	1.48	1.39
18	B	1213	CLA	CHD-C4C	3.91	1.48	1.39
18	4	4001	CLA	C1D-ND	-3.91	1.32	1.37
18	B	1202	CLA	CHC-C4B	3.91	1.48	1.39
18	1	1004	CLA	CHD-C1D	3.91	1.46	1.38
18	A	1151	CLA	MG-NC	3.91	2.15	2.06
18	A	1123	CLA	MG-NC	3.91	2.15	2.06
18	A	1120	CLA	CHD-C4C	3.91	1.48	1.39
18	A	1123	CLA	CHD-C4C	3.91	1.48	1.39
18	B	1236	CLA	CHD-C4C	3.91	1.48	1.39
18	3	3008	CLA	C1B-NB	-3.91	1.32	1.37
18	J	1302	CLA	CHB-C1B	3.91	1.48	1.39
18	A	1237	CLA	CHC-C4B	3.91	1.48	1.39
18	2	2002	CLA	CHD-C1D	3.90	1.46	1.38
18	A	1122	CLA	CHB-C1B	3.90	1.48	1.39
18	A	1101	CLA	CHC-C4B	3.90	1.48	1.39
18	G	1002	CLA	C3C-C2C	3.90	1.45	1.36
18	B	1219	CLA	CHB-C1B	3.90	1.48	1.39
18	3	3017	CLA	C1D-ND	-3.90	1.32	1.37
28	2	2010	CHL	O2D-CGD	3.90	1.42	1.33
18	F	1302	CLA	CHB-C1B	3.90	1.48	1.39
18	1	1003	CLA	CHD-C4C	3.90	1.48	1.39
18	A	1125	CLA	CHB-C1B	3.90	1.48	1.39
18	3	3002	CLA	C3C-C2C	3.90	1.45	1.36
18	1	1014	CLA	C1B-NB	-3.90	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1116	CLA	CHB-C1B	3.90	1.48	1.39
18	A	1106	CLA	CHC-C4B	3.89	1.48	1.39
18	A	1115	CLA	CHB-C1B	3.89	1.48	1.39
18	B	1225	CLA	CHD-C4C	3.89	1.48	1.39
18	1	1006	CLA	CHD-C4C	3.89	1.48	1.39
18	A	1105	CLA	CHB-C1B	3.89	1.48	1.39
18	H	1000	CLA	CHB-C1B	3.89	1.48	1.39
18	1	1002	CLA	C1D-ND	-3.89	1.32	1.37
18	A	1118	CLA	CHD-C4C	3.88	1.48	1.39
18	1	1004	CLA	CHB-C1B	3.88	1.48	1.39
18	A	1129	CLA	CHD-C4C	3.88	1.48	1.39
18	B	1206	CLA	MG-NC	3.88	2.15	2.06
18	2	2002	CLA	C1D-ND	-3.88	1.32	1.37
18	2	2004	CLA	C1C-NC	-3.88	1.31	1.37
18	4	4001	CLA	CHD-C1D	3.88	1.46	1.38
18	4	4009	CLA	C4B-NB	-3.88	1.32	1.37
18	3	3002	CLA	CHB-C1B	3.88	1.48	1.39
18	B	1235	CLA	CHD-C4C	3.88	1.48	1.39
18	A	1136	CLA	CHB-C1B	3.88	1.48	1.39
18	A	1133	CLA	CHB-C1B	3.88	1.48	1.39
18	B	1221	CLA	CHD-C4C	3.88	1.48	1.39
18	A	1113	CLA	CHB-C1B	3.87	1.48	1.39
18	A	1134	CLA	MG-NC	3.87	2.15	2.06
18	B	1202	CLA	OBD-CAD	3.87	1.29	1.22
18	A	1106	CLA	OBD-CAD	3.87	1.29	1.22
18	B	1207	CLA	CHB-C1B	3.87	1.48	1.39
18	4	4012	CLA	CHC-C1C	3.87	1.46	1.38
28	4	4013	CHL	O2D-CGD	3.87	1.42	1.33
18	B	1021	CLA	OBD-CAD	3.87	1.29	1.22
18	B	1230	CLA	OBD-CAD	3.87	1.29	1.22
18	2	2001	CLA	CHC-C1C	3.87	1.46	1.38
18	3	3017	CLA	C4B-NB	-3.87	1.32	1.37
18	A	1139	CLA	CHB-C1B	3.87	1.48	1.39
18	B	1238	CLA	CHB-C1B	3.87	1.48	1.39
18	2	2012	CLA	O2D-CGD	3.87	1.42	1.33
18	F	1302	CLA	CHC-C4B	3.87	1.48	1.39
18	B	1204	CLA	CHB-C1B	3.87	1.48	1.39
18	L	1501	CLA	CHC-C4B	3.87	1.48	1.39
18	3	3013	CLA	CHC-C4B	3.87	1.48	1.39
18	B	1229	CLA	MG-NC	3.87	2.15	2.06
18	F	1301	CLA	CHC-C4B	3.87	1.48	1.39
18	B	1202	CLA	CHB-C1B	3.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2019	CLA	C2D-C3D	3.86	1.47	1.36
18	B	1012	CLA	MG-NC	3.86	2.15	2.06
18	A	1126	CLA	MG-NC	3.86	2.15	2.06
18	L	1501	CLA	C4B-NB	-3.86	1.32	1.37
18	B	1215	CLA	CHB-C1B	3.86	1.48	1.39
18	B	1240	CLA	CHB-C1B	3.86	1.48	1.39
18	A	1117	CLA	CHB-C1B	3.85	1.48	1.39
18	A	1128	CLA	CHB-C1B	3.85	1.48	1.39
18	A	1137	CLA	CHD-C4C	3.85	1.48	1.39
18	3	3019	CLA	C2D-C3D	3.85	1.47	1.36
18	A	1139	CLA	MG-NC	3.85	2.15	2.06
18	A	1133	CLA	CHC-C4B	3.85	1.48	1.39
18	2	2016	CLA	C4B-NB	-3.85	1.32	1.37
18	2	2004	CLA	C3C-C2C	3.85	1.45	1.36
18	L	1502	CLA	CHB-C1B	3.85	1.48	1.39
18	4	4007	CLA	C1D-ND	-3.85	1.32	1.37
18	A	1237	CLA	OBD-CAD	3.85	1.29	1.22
23	J	5001	LMG	O7-C10	3.84	1.45	1.34
18	B	1021	CLA	CHB-C1B	3.84	1.48	1.39
18	A	1102	CLA	CHB-C1B	3.84	1.48	1.39
18	G	1001	CLA	CHB-C1B	3.84	1.48	1.39
18	A	1131	CLA	MG-NC	3.84	2.15	2.06
18	B	1215	CLA	OBD-CAD	3.84	1.29	1.22
18	B	1214	CLA	CHB-C1B	3.84	1.48	1.39
18	1	1013	CLA	C3C-C2C	3.84	1.45	1.36
18	H	1000	CLA	CHC-C4B	3.84	1.48	1.39
28	2	2013	CHL	C3A-C2A	-3.84	1.51	1.54
18	A	1111	CLA	CHC-C4B	3.84	1.48	1.39
18	A	1124	CLA	CHB-C1B	3.84	1.48	1.39
18	B	1219	CLA	MG-NC	3.84	2.15	2.06
18	B	1021	CLA	CHD-C4C	3.83	1.47	1.39
18	B	1212	CLA	CHD-C4C	3.83	1.47	1.39
18	B	1012	CLA	CHB-C1B	3.83	1.48	1.39
18	B	1226	CLA	CHB-C1B	3.83	1.48	1.39
18	2	2005	CLA	CHC-C4B	3.83	1.48	1.39
18	B	1221	CLA	OBD-CAD	3.83	1.29	1.22
18	A	1116	CLA	MG-NC	3.83	2.15	2.06
18	2	2008	CLA	C1B-NB	-3.83	1.32	1.37
18	4	4001	CLA	C4B-NB	-3.83	1.32	1.37
18	B	1216	CLA	MG-NC	3.83	2.15	2.06
18	3	3003	CLA	CHD-C1D	3.83	1.45	1.38
18	B	1209	CLA	CHB-C1B	3.83	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1203	CLA	CHD-C4C	3.83	1.47	1.39
18	B	1214	CLA	MG-NC	3.82	2.15	2.06
18	G	1003	CLA	CHC-C4B	3.82	1.48	1.39
18	2	2006	CLA	CHC-C4B	3.82	1.48	1.39
18	A	1123	CLA	CHB-C1B	3.82	1.48	1.39
18	3	3007	CLA	C1B-NB	-3.82	1.32	1.37
22	A	6017	BCR	C10-C9	-3.82	1.27	1.35
18	B	1225	CLA	OBD-CAD	3.82	1.29	1.22
18	2	2006	CLA	CHD-C4C	3.82	1.47	1.39
18	A	1114	CLA	MG-NC	3.82	2.15	2.06
18	A	1104	CLA	CHB-C1B	3.82	1.48	1.39
18	A	1113	CLA	MG-NC	3.82	2.15	2.06
18	A	1123	CLA	OBD-CAD	3.82	1.29	1.22
18	B	1210	CLA	OBD-CAD	3.82	1.29	1.22
18	A	1138	CLA	CHB-C1B	3.82	1.48	1.39
18	B	1220	CLA	CHB-C1B	3.82	1.48	1.39
18	3	3013	CLA	CHD-C4C	3.82	1.47	1.39
18	4	4007	CLA	C4B-NB	-3.82	1.32	1.37
18	B	1208	CLA	OBD-CAD	3.82	1.29	1.22
18	A	1108	CLA	MG-NC	3.82	2.15	2.06
18	2	2007	CLA	CHC-C4B	3.81	1.48	1.39
18	A	1121	CLA	CHB-C1B	3.81	1.48	1.39
28	1	1009	CHL	O2D-CGD	3.81	1.42	1.33
18	B	1207	CLA	CHD-C4C	3.81	1.47	1.39
23	G	2021	LMG	O7-C10	3.81	1.45	1.34
18	F	1302	CLA	CHD-C4C	3.81	1.47	1.39
18	A	1133	CLA	MG-NC	3.81	2.15	2.06
18	2	2012	CLA	CHD-C1D	3.81	1.45	1.38
18	3	3019	CLA	C3B-C4B	3.81	1.48	1.40
18	B	1223	CLA	CHB-C1B	3.81	1.48	1.39
18	4	4007	CLA	CHC-C1C	3.80	1.46	1.38
18	B	1012	CLA	CHD-C4C	3.80	1.47	1.39
18	A	1134	CLA	OBD-CAD	3.80	1.29	1.22
18	A	1137	CLA	MG-NC	3.80	2.15	2.06
18	B	1224	CLA	CHC-C4B	3.80	1.47	1.39
18	2	2012	CLA	C3C-C2C	3.80	1.45	1.36
18	A	1119	CLA	MG-NC	3.80	2.15	2.06
18	A	1101	CLA	OBD-CAD	3.80	1.29	1.22
18	B	1240	CLA	OBD-CAD	3.80	1.29	1.22
18	A	1108	CLA	CHB-C1B	3.80	1.47	1.39
18	A	1127	CLA	MG-NC	3.80	2.15	2.06
18	B	1221	CLA	MG-NC	3.80	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1106	CLA	CHB-C1B	3.80	1.47	1.39
18	2	2002	CLA	CHB-C1B	3.80	1.47	1.39
18	B	1225	CLA	MG-NC	3.80	2.15	2.06
18	H	1000	CLA	MG-NC	3.80	2.15	2.06
18	B	1217	CLA	MG-NC	3.80	2.15	2.06
18	B	1238	CLA	MG-NC	3.80	2.15	2.06
18	1	1012	CLA	C3C-C2C	3.79	1.45	1.36
18	A	1102	CLA	OBD-CAD	3.79	1.29	1.22
18	A	1104	CLA	OBD-CAD	3.79	1.29	1.22
18	A	1118	CLA	OBD-CAD	3.79	1.29	1.22
18	B	1222	CLA	CHB-C1B	3.79	1.47	1.39
18	B	1212	CLA	OBD-CAD	3.79	1.29	1.22
18	J	1302	CLA	OBD-CAD	3.79	1.29	1.22
18	1	1005	CLA	C3C-C2C	3.79	1.44	1.36
18	B	1219	CLA	OBD-CAD	3.79	1.29	1.22
18	B	1229	CLA	CHD-C4C	3.79	1.47	1.39
18	1	1011	CLA	C1D-ND	-3.79	1.32	1.37
18	B	1232	CLA	MG-NC	3.79	2.15	2.06
18	3	3018	CLA	OBD-CAD	3.78	1.29	1.22
18	1	1005	CLA	C1B-NB	-3.78	1.32	1.37
18	A	1124	CLA	MG-NC	3.78	2.15	2.06
18	B	1229	CLA	OBD-CAD	3.78	1.29	1.22
18	A	1127	CLA	OBD-CAD	3.78	1.29	1.22
18	A	1119	CLA	CHB-C1B	3.78	1.47	1.39
18	A	1116	CLA	OBD-CAD	3.78	1.29	1.22
18	B	1223	CLA	CHD-C4C	3.78	1.47	1.39
18	K	1001	CLA	CHD-C1D	3.78	1.45	1.38
18	1	1001	CLA	C1B-NB	-3.78	1.32	1.37
18	4	4004	CLA	CHD-C1D	3.78	1.45	1.38
18	A	1107	CLA	MG-NC	3.78	2.15	2.06
18	B	1236	CLA	MG-NC	3.78	2.15	2.06
18	2	2019	CLA	CHD-C1D	3.78	1.47	1.38
18	2	2005	CLA	CHD-C4C	3.78	1.47	1.39
18	A	1022	CLA	CHB-C1B	3.78	1.47	1.39
18	B	1221	CLA	CHB-C1B	3.78	1.47	1.39
18	A	1135	CLA	MG-NC	3.78	2.15	2.06
18	B	1232	CLA	CHB-C1B	3.78	1.47	1.39
18	A	1138	CLA	OBD-CAD	3.77	1.29	1.22
18	B	1204	CLA	OBD-CAD	3.77	1.29	1.22
18	B	1227	CLA	OBD-CAD	3.77	1.29	1.22
18	A	1121	CLA	OBD-CAD	3.77	1.29	1.22
18	3	3007	CLA	C4B-NB	-3.77	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1231	CLA	CHB-C1B	3.77	1.47	1.39
18	B	1222	CLA	MG-NC	3.77	2.15	2.06
18	B	1206	CLA	OBD-CAD	3.77	1.29	1.22
18	A	1104	CLA	MG-NC	3.77	2.15	2.06
18	G	1003	CLA	CHD-C4C	3.77	1.47	1.39
18	3	3005	CLA	CHC-C4B	3.77	1.47	1.39
18	A	1136	CLA	OBD-CAD	3.77	1.29	1.22
18	A	1124	CLA	OBD-CAD	3.77	1.29	1.22
18	B	1209	CLA	MG-NC	3.77	2.15	2.06
18	B	1215	CLA	MG-NC	3.77	2.15	2.06
18	A	1102	CLA	CHD-C4C	3.77	1.47	1.39
23	F	5002	LMG	O7-C10	3.77	1.44	1.34
18	A	1151	CLA	OBD-CAD	3.77	1.29	1.22
18	A	1112	CLA	MG-NC	3.77	2.15	2.06
18	B	1217	CLA	OBD-CAD	3.77	1.29	1.22
18	B	1208	CLA	MG-NC	3.76	2.15	2.06
18	A	1122	CLA	OBD-CAD	3.76	1.29	1.22
18	B	1227	CLA	CHB-C1B	3.76	1.47	1.39
18	B	1228	CLA	CHB-C1B	3.76	1.47	1.39
18	A	1122	CLA	MG-NC	3.76	2.15	2.06
18	A	1132	CLA	OBD-CAD	3.76	1.29	1.22
18	B	1223	CLA	MG-NC	3.76	2.15	2.06
18	B	1218	CLA	OBD-CAD	3.76	1.29	1.22
18	A	1110	CLA	CHB-C1B	3.76	1.47	1.39
18	1	1005	CLA	CHB-C1B	3.76	1.47	1.39
18	L	1503	CLA	CHB-C1B	3.76	1.47	1.39
18	G	1002	CLA	CHB-C1B	3.76	1.47	1.39
18	B	1234	CLA	OBD-CAD	3.76	1.29	1.22
18	A	1104	CLA	CHD-C4C	3.76	1.47	1.39
18	A	1107	CLA	OBD-CAD	3.76	1.29	1.22
18	B	1209	CLA	OBD-CAD	3.76	1.29	1.22
18	A	1105	CLA	OBD-CAD	3.76	1.28	1.22
18	B	1201	CLA	MG-NC	3.75	2.15	2.06
18	L	1502	CLA	C1D-ND	-3.75	1.32	1.37
18	B	1212	CLA	MG-NC	3.75	2.15	2.06
18	B	1222	CLA	CHD-C4C	3.75	1.47	1.39
18	3	3002	CLA	CHD-C4C	3.75	1.47	1.39
18	1	1006	CLA	CHC-C4B	3.75	1.47	1.39
18	A	1013	CLA	OBD-CAD	3.75	1.28	1.22
18	1	1008	CLA	C3C-C2C	3.75	1.44	1.36
18	B	1234	CLA	MG-NC	3.75	2.15	2.06
18	A	1136	CLA	MG-NC	3.75	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3005	CLA	CHD-C1D	3.75	1.45	1.38
18	1	1004	CLA	C1D-ND	-3.75	1.32	1.37
18	A	1113	CLA	OBD-CAD	3.74	1.28	1.22
18	A	1129	CLA	OBD-CAD	3.74	1.28	1.22
18	H	1000	CLA	OBD-CAD	3.74	1.28	1.22
18	3	3017	CLA	C3C-C2C	3.74	1.44	1.36
18	B	1023	CLA	OBD-CAD	3.74	1.28	1.22
18	B	1232	CLA	OBD-CAD	3.74	1.28	1.22
18	4	4002	CLA	CHC-C1C	3.74	1.46	1.38
18	A	1140	CLA	MG-NC	3.74	2.15	2.06
18	4	4017	CLA	CHC-C4B	3.74	1.47	1.39
18	1	1011	CLA	CHC-C4B	3.74	1.47	1.39
18	4	4017	CLA	C1B-NB	-3.74	1.32	1.37
18	A	1112	CLA	OBD-CAD	3.74	1.28	1.22
18	A	1105	CLA	MG-NC	3.74	2.15	2.06
18	3	3007	CLA	C1D-ND	-3.74	1.32	1.37
18	B	1023	CLA	CHB-C1B	3.74	1.47	1.39
18	A	1022	CLA	OBD-CAD	3.74	1.28	1.22
18	4	4002	CLA	CHD-C1D	3.74	1.45	1.38
18	3	3006	CLA	C1B-NB	-3.74	1.33	1.37
18	3	3017	CLA	CHC-C4B	3.74	1.47	1.39
18	B	1207	CLA	MG-NC	3.74	2.15	2.06
18	4	4009	CLA	CHD-C1D	3.74	1.45	1.38
18	A	1115	CLA	OBD-CAD	3.73	1.28	1.22
18	1	1001	CLA	C4B-NB	-3.73	1.33	1.37
18	B	1216	CLA	OBD-CAD	3.73	1.28	1.22
18	3	3005	CLA	CHB-C1B	3.73	1.47	1.39
18	B	1222	CLA	OBD-CAD	3.73	1.28	1.22
18	A	1117	CLA	OBD-CAD	3.73	1.28	1.22
18	3	3007	CLA	CHC-C4B	3.73	1.47	1.39
18	B	1214	CLA	OBD-CAD	3.73	1.28	1.22
18	A	1101	CLA	CHB-C1B	3.73	1.47	1.39
18	B	1206	CLA	CHC-C4B	3.73	1.47	1.39
18	B	1207	CLA	OBD-CAD	3.73	1.28	1.22
18	A	1109	CLA	CHB-C1B	3.73	1.47	1.39
18	A	1115	CLA	MG-NC	3.72	2.15	2.06
18	A	1111	CLA	MG-NC	3.72	2.15	2.06
18	A	1111	CLA	OBD-CAD	3.72	1.28	1.22
18	L	1503	CLA	C3C-C2C	3.72	1.44	1.36
18	A	1108	CLA	OBD-CAD	3.72	1.28	1.22
18	L	1501	CLA	CHD-C4C	3.72	1.47	1.39
18	B	1235	CLA	MG-NC	3.72	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1109	CLA	MG-NC	3.72	2.15	2.06
18	A	1128	CLA	CHC-C4B	3.72	1.47	1.39
18	4	4006	CLA	C3C-C2C	3.72	1.44	1.36
18	1	1012	CLA	C1B-NB	-3.72	1.33	1.37
18	B	1218	CLA	MG-NC	3.72	2.15	2.06
18	3	3006	CLA	C1D-ND	-3.72	1.33	1.37
18	A	1126	CLA	CHB-C1B	3.71	1.47	1.39
18	B	1220	CLA	MG-NC	3.71	2.15	2.06
18	A	1130	CLA	MG-NC	3.71	2.15	2.06
18	2	2009	CLA	CHD-C4C	3.71	1.47	1.39
18	B	1228	CLA	OBD-CAD	3.71	1.28	1.22
22	F	6016	BCR	C11-C12	-3.71	1.25	1.34
18	A	1117	CLA	MG-NC	3.71	2.15	2.06
18	B	1012	CLA	OBD-CAD	3.71	1.28	1.22
18	B	1213	CLA	OBD-CAD	3.71	1.28	1.22
18	L	1503	CLA	C1D-ND	-3.71	1.33	1.37
18	A	1110	CLA	OBD-CAD	3.71	1.28	1.22
18	2	2007	CLA	CHD-C4C	3.71	1.47	1.39
18	A	1125	CLA	MG-NC	3.70	2.15	2.06
18	2	2009	CLA	C1D-ND	-3.70	1.33	1.37
18	A	1128	CLA	MG-NC	3.70	2.15	2.06
18	4	4016	CLA	CHD-C4C	3.70	1.47	1.39
18	A	1118	CLA	MG-NC	3.70	2.15	2.06
18	1	1007	CLA	C1B-NB	-3.70	1.33	1.37
18	A	1106	CLA	MG-NC	3.70	2.15	2.06
18	1	1006	CLA	C1B-NB	-3.70	1.33	1.37
18	A	1132	CLA	MG-NC	3.70	2.15	2.06
18	3	3001	CLA	CHC-C4B	3.70	1.47	1.39
18	B	1230	CLA	CHD-C4C	3.69	1.47	1.39
18	B	1239	CLA	OBD-CAD	3.69	1.28	1.22
18	4	4004	CLA	CHC-C4B	3.69	1.47	1.39
18	A	1139	CLA	OBD-CAD	3.69	1.28	1.22
18	4	4003	CLA	C1D-ND	-3.69	1.33	1.37
18	2	2001	CLA	C3C-C2C	3.69	1.44	1.36
18	A	1125	CLA	CHD-C4C	3.69	1.47	1.39
18	A	1103	CLA	MG-NC	3.69	2.15	2.06
18	A	1237	CLA	MG-NC	3.69	2.15	2.06
18	A	1129	CLA	MG-NC	3.69	2.15	2.06
18	1	1006	CLA	C3C-C2C	3.69	1.44	1.36
18	A	1140	CLA	OBD-CAD	3.69	1.28	1.22
18	A	1138	CLA	MG-NC	3.68	2.15	2.06
18	2	2012	CLA	C1C-NC	-3.68	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1210	CLA	CHB-C1B	3.68	1.47	1.39
18	A	1132	CLA	CHB-C1B	3.68	1.47	1.39
18	A	1137	CLA	OBD-CAD	3.68	1.28	1.22
18	A	1103	CLA	OBD-CAD	3.68	1.28	1.22
18	B	1203	CLA	MG-NC	3.68	2.15	2.06
18	B	1228	CLA	MG-NC	3.68	2.15	2.06
18	A	1110	CLA	MG-NC	3.68	2.15	2.06
23	G	2021	LMG	O8-C28	3.67	1.44	1.33
18	A	1114	CLA	OBD-CAD	3.67	1.28	1.22
18	2	2009	CLA	CHB-C1B	3.67	1.47	1.39
18	B	1236	CLA	OBD-CAD	3.67	1.28	1.22
28	4	4013	CHL	CHB-C4A	-3.67	1.34	1.38
18	B	1231	CLA	MG-NC	3.67	2.15	2.06
18	A	1131	CLA	OBD-CAD	3.67	1.28	1.22
18	4	4008	CLA	CHB-C1B	3.67	1.47	1.39
18	3	3008	CLA	C4B-NB	-3.67	1.33	1.37
18	A	1120	CLA	MG-NC	3.67	2.15	2.06
18	B	1201	CLA	OBD-CAD	3.67	1.28	1.22
18	G	1002	CLA	CHD-C4C	3.67	1.47	1.39
18	B	1238	CLA	OBD-CAD	3.66	1.28	1.22
18	3	3017	CLA	CHD-C4C	3.66	1.47	1.39
18	B	1204	CLA	MG-NC	3.66	2.15	2.06
18	3	3004	CLA	CHB-C1B	3.66	1.47	1.39
18	A	1126	CLA	OBD-CAD	3.66	1.28	1.22
18	B	1023	CLA	MG-NC	3.66	2.15	2.06
18	B	1205	CLA	MG-NC	3.66	2.15	2.06
18	1	1004	CLA	C4B-NB	-3.66	1.33	1.37
18	B	1226	CLA	MG-NC	3.66	2.15	2.06
18	L	1503	CLA	C1B-NB	-3.66	1.33	1.37
18	2	2009	CLA	CHC-C4B	3.66	1.47	1.39
18	G	1001	CLA	C1C-NC	-3.66	1.32	1.37
18	A	1128	CLA	OBD-CAD	3.66	1.28	1.22
18	2	2009	CLA	C1B-NB	-3.65	1.33	1.37
18	B	1239	CLA	MG-NC	3.65	2.15	2.06
18	G	1003	CLA	CHB-C1B	3.65	1.47	1.39
18	3	3005	CLA	C3C-C2C	3.65	1.44	1.36
18	4	4003	CLA	CHC-C4B	3.65	1.47	1.39
18	B	1224	CLA	OBD-CAD	3.65	1.28	1.22
18	A	1109	CLA	OBD-CAD	3.65	1.28	1.22
18	2	2008	CLA	CHB-C1B	3.65	1.47	1.39
18	B	1240	CLA	MG-NC	3.65	2.14	2.06
18	4	4007	CLA	C3C-C2C	3.65	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2008	CLA	C3C-C2C	3.65	1.44	1.36
18	3	3018	CLA	C4B-NB	-3.65	1.33	1.37
18	3	3006	CLA	CHD-C4C	3.65	1.47	1.39
18	2	2016	CLA	CHD-C1D	3.64	1.45	1.38
18	3	3013	CLA	C1D-ND	-3.64	1.33	1.37
18	A	1135	CLA	OBD-CAD	3.64	1.28	1.22
18	B	1205	CLA	OBD-CAD	3.64	1.28	1.22
18	1	1014	CLA	C3C-C2C	3.63	1.44	1.36
18	B	1227	CLA	MG-NC	3.63	2.14	2.06
18	B	1224	CLA	CHB-C1B	3.63	1.47	1.39
18	3	3002	CLA	C1D-ND	-3.63	1.33	1.37
18	B	1226	CLA	CHC-C4B	3.63	1.47	1.39
18	1	1003	CLA	CHB-C1B	3.63	1.47	1.39
18	3	3001	CLA	C4B-NB	-3.63	1.33	1.37
18	4	4016	CLA	CHC-C4B	3.63	1.47	1.39
18	A	1102	CLA	MG-NC	3.62	2.14	2.06
18	A	1121	CLA	MG-NC	3.62	2.14	2.06
18	A	1130	CLA	OBD-CAD	3.62	1.28	1.22
18	F	1301	CLA	CHD-C4C	3.62	1.47	1.39
18	1	1012	CLA	CHB-C1B	3.62	1.47	1.39
18	A	1013	CLA	CHB-C1B	3.62	1.47	1.39
18	B	1220	CLA	OBD-CAD	3.62	1.28	1.22
18	1	1012	CLA	C4B-NB	-3.61	1.33	1.37
18	1	1008	CLA	MG-NC	3.61	2.14	2.06
18	2	2009	CLA	C4B-NB	-3.61	1.33	1.37
18	4	4017	CLA	C1D-ND	-3.61	1.33	1.37
18	G	1002	CLA	CHC-C4B	3.61	1.47	1.39
18	3	3001	CLA	CHD-C4C	3.61	1.47	1.39
18	A	1112	CLA	CHB-C1B	3.61	1.47	1.39
18	1	1001	CLA	C3C-C2C	3.61	1.44	1.36
18	A	1111	CLA	CHB-C1B	3.60	1.47	1.39
18	3	3001	CLA	OBD-CAD	3.60	1.28	1.22
18	B	1235	CLA	OBD-CAD	3.60	1.28	1.22
28	2	2011	CHL	CHB-C4A	-3.60	1.34	1.38
18	B	1213	CLA	MG-NC	3.60	2.14	2.06
18	3	3018	CLA	CHD-C4C	3.59	1.47	1.39
18	B	1216	CLA	CHB-C1B	3.59	1.47	1.39
18	1	1006	CLA	CHB-C1B	3.59	1.47	1.39
18	B	1021	CLA	MG-NC	3.59	2.14	2.06
18	1	1014	CLA	C4B-NB	-3.59	1.33	1.37
18	B	1230	CLA	MG-NC	3.59	2.14	2.06
18	3	3007	CLA	CHD-C4C	3.59	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4012	CLA	CHB-C1B	3.58	1.47	1.39
18	4	4007	CLA	C1C-NC	-3.58	1.32	1.37
22	F	6014	BCR	C11-C12	-3.58	1.25	1.34
18	2	2004	CLA	CHD-C4C	3.58	1.47	1.39
23	4	4801	LMG	O7-C10	3.58	1.44	1.34
18	1	1002	CLA	C3C-C2C	3.58	1.44	1.36
18	L	1503	CLA	CHD-C4C	3.58	1.47	1.39
18	B	1211	CLA	OBD-CAD	3.58	1.28	1.22
18	B	1226	CLA	OBD-CAD	3.58	1.28	1.22
18	3	3002	CLA	CHC-C4B	3.58	1.47	1.39
18	3	3018	CLA	C1B-NB	-3.58	1.33	1.37
28	4	4011	CHL	C2C-C3C	-3.58	1.32	1.36
18	3	3019	CLA	CHD-C1D	3.57	1.47	1.38
18	1	1001	CLA	CHD-C1D	3.57	1.45	1.38
18	B	1202	CLA	MG-NC	3.57	2.14	2.06
18	3	3018	CLA	CHC-C4B	3.57	1.47	1.39
18	4	4005	CLA	C3C-C2C	3.57	1.44	1.36
18	4	4003	CLA	CHD-C4C	3.57	1.47	1.39
18	1	1011	CLA	CHD-C4C	3.57	1.47	1.39
18	L	1501	CLA	C1C-NC	-3.57	1.32	1.37
18	K	1001	CLA	CHB-C1B	3.57	1.47	1.39
18	1	1007	CLA	CHB-C1B	3.57	1.47	1.39
18	L	1501	CLA	C3C-C2C	3.56	1.44	1.36
22	A	6011	BCR	C11-C12	-3.56	1.25	1.34
18	1	1007	CLA	CHD-C1D	3.56	1.45	1.38
18	B	1210	CLA	MG-NC	3.56	2.14	2.06
18	3	3012	CLA	C1B-NB	-3.56	1.33	1.37
18	4	4004	CLA	C1C-NC	-3.55	1.32	1.37
18	4	4006	CLA	CHD-C1D	3.55	1.45	1.38
18	4	4009	CLA	C3C-C2C	3.55	1.44	1.36
18	4	4017	CLA	C4B-NB	-3.55	1.33	1.37
18	4	4009	CLA	CHC-C4B	3.55	1.47	1.39
18	1	1012	CLA	CHC-C4B	3.54	1.47	1.39
18	B	1211	CLA	CHB-C1B	3.54	1.47	1.39
18	F	1302	CLA	OBD-CAD	3.54	1.28	1.22
18	A	1133	CLA	OBD-CAD	3.54	1.28	1.22
18	2	2003	CLA	C3C-C2C	3.54	1.44	1.36
18	1	1004	CLA	CHC-C4B	3.54	1.47	1.39
18	B	1224	CLA	MG-NC	3.54	2.14	2.06
18	A	1101	CLA	MG-NC	3.53	2.14	2.06
18	3	3012	CLA	CHC-C4B	3.53	1.47	1.39
18	3	3012	CLA	CHB-C1B	3.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	1002	CLA	C1D-ND	-3.53	1.33	1.37
22	J	6012	BCR	C11-C12	-3.53	1.25	1.34
18	3	3002	CLA	C4B-NB	-3.53	1.33	1.37
18	4	4002	CLA	C3C-C2C	3.53	1.44	1.36
18	K	1001	CLA	CHD-C4C	3.53	1.47	1.39
18	4	4002	CLA	C1C-NC	-3.53	1.32	1.37
18	3	3007	CLA	CHB-C1B	3.53	1.47	1.39
18	1	1011	CLA	C4B-NB	-3.53	1.33	1.37
18	4	4012	CLA	CHD-C4C	3.52	1.47	1.39
28	2	2013	CHL	C3B-C2B	-3.52	1.35	1.40
18	2	2003	CLA	CHC-C4B	3.51	1.47	1.39
18	2	2005	CLA	OBD-CAD	3.51	1.28	1.22
28	4	4010	CHL	C3D-C2D	-3.51	1.33	1.39
18	1	1013	CLA	MG-NC	3.51	2.14	2.06
18	1	1001	CLA	CHC-C4B	3.50	1.47	1.39
18	3	3010	CLA	CHD-C1D	3.50	1.45	1.38
18	1	1014	CLA	CHB-C1B	3.50	1.47	1.39
18	1	1002	CLA	OBD-CAD	3.50	1.28	1.22
18	4	4017	CLA	CHB-C1B	3.50	1.47	1.39
18	3	3008	CLA	CHD-C1D	3.50	1.45	1.38
18	1	1014	CLA	CHD-C1D	3.49	1.45	1.38
18	4	4009	CLA	C1C-NC	-3.49	1.32	1.37
18	4	4006	CLA	C1C-NC	-3.49	1.32	1.37
18	1	1011	CLA	CHB-C1B	3.48	1.47	1.39
18	1	1003	CLA	C4B-NB	-3.48	1.33	1.37
18	L	1501	CLA	CHB-C1B	3.48	1.47	1.39
18	F	1301	CLA	MG-NC	3.48	2.14	2.06
18	3	3004	CLA	CHD-C4C	3.48	1.47	1.39
18	2	2006	CLA	OBD-CAD	3.47	1.28	1.22
18	3	3012	CLA	CHD-C1D	3.47	1.45	1.38
28	4	4011	CHL	CHB-C4A	-3.47	1.34	1.38
18	4	4005	CLA	C1C-NC	-3.47	1.32	1.37
22	A	6008	BCR	C11-C12	-3.47	1.25	1.34
18	3	3004	CLA	CHC-C4B	3.47	1.47	1.39
23	J	5001	LMG	O8-C28	3.47	1.43	1.33
18	A	1120	CLA	OBD-CAD	3.46	1.28	1.22
18	3	3006	CLA	CHC-C4B	3.46	1.47	1.39
18	2	2003	CLA	CHD-C1D	3.46	1.45	1.38
18	1	1008	CLA	C1D-ND	-3.46	1.33	1.37
28	3	3011	CHL	CHB-C4A	-3.46	1.34	1.38
18	2	2019	CLA	MG-NC	3.46	2.14	2.06
18	3	3007	CLA	OBD-CAD	3.46	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4001	CLA	CHC-C4B	3.46	1.47	1.39
18	1	1012	CLA	CHD-C4C	3.46	1.47	1.39
18	2	2001	CLA	C1C-NC	-3.46	1.32	1.37
18	1	1007	CLA	C3C-C2C	3.45	1.44	1.36
18	3	3012	CLA	C1C-NC	-3.45	1.32	1.37
18	A	1013	CLA	MG-NC	3.45	2.14	2.06
18	2	2001	CLA	CHD-C4C	3.45	1.47	1.39
18	1	1008	CLA	C4B-NB	-3.45	1.33	1.37
18	4	4012	CLA	C3C-C2C	3.45	1.44	1.36
18	4	4002	CLA	C1B-NB	-3.45	1.33	1.37
18	A	1119	CLA	OBD-CAD	3.45	1.28	1.22
18	4	4007	CLA	CHD-C1D	3.45	1.45	1.38
22	F	6014	BCR	C1-C6	-3.44	1.49	1.53
18	2	2008	CLA	C1C-NC	-3.44	1.32	1.37
18	2	2003	CLA	MG-NC	3.44	2.14	2.06
22	L	6019	BCR	C11-C12	-3.44	1.25	1.34
18	4	4003	CLA	C1B-NB	-3.44	1.33	1.37
18	L	1502	CLA	C4B-NB	-3.43	1.33	1.37
18	2	2007	CLA	OBD-CAD	3.43	1.28	1.22
18	3	3013	CLA	C4B-NB	-3.43	1.33	1.37
18	G	1003	CLA	C4B-NB	-3.43	1.33	1.37
18	4	4003	CLA	C4B-NB	-3.43	1.33	1.37
18	2	2016	CLA	C3C-C2C	3.43	1.44	1.36
18	G	1002	CLA	C1B-NB	-3.43	1.33	1.37
18	1	1006	CLA	C4B-NB	-3.42	1.33	1.37
18	3	3004	CLA	OBD-CAD	3.42	1.28	1.22
18	4	4012	CLA	C1C-NC	-3.42	1.32	1.37
18	3	3003	CLA	CHD-C4C	3.41	1.47	1.39
18	2	2008	CLA	CHC-C4B	3.41	1.47	1.39
18	2	2007	CLA	MG-NC	3.41	2.14	2.06
18	K	1001	CLA	CHC-C4B	3.40	1.47	1.39
18	1	1008	CLA	CHC-C4B	3.40	1.47	1.39
18	1	1012	CLA	OBD-CAD	3.40	1.28	1.22
18	F	1301	CLA	C1D-ND	-3.40	1.33	1.37
18	4	4006	CLA	CHB-C1B	3.40	1.47	1.39
18	3	3019	CLA	CHB-C1B	3.40	1.48	1.39
18	2	2002	CLA	C3C-C2C	3.40	1.44	1.36
18	L	1502	CLA	CHD-C4C	3.40	1.46	1.39
18	B	1211	CLA	MG-NC	3.40	2.14	2.06
18	2	2012	CLA	CHD-C4C	3.40	1.46	1.39
18	1	1001	CLA	C1C-NC	-3.39	1.32	1.37
18	1	1013	CLA	CHC-C4B	3.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1008	CLA	CHD-C4C	3.39	1.46	1.39
18	1	1003	CLA	C1B-NB	-3.39	1.33	1.37
18	G	1002	CLA	MG-NC	3.39	2.14	2.06
18	4	4003	CLA	OBD-CAD	3.39	1.28	1.22
18	3	3003	CLA	C1B-NB	-3.39	1.33	1.37
18	B	1223	CLA	OBD-CAD	3.39	1.28	1.22
18	1	1002	CLA	CHC-C4B	3.39	1.47	1.39
18	2	2002	CLA	CHC-C4B	3.38	1.47	1.39
18	1	1013	CLA	C1B-NB	-3.38	1.33	1.37
18	1	1004	CLA	C1B-NB	-3.38	1.33	1.37
18	4	4017	CLA	CHD-C4C	3.38	1.46	1.39
18	K	1001	CLA	OBD-CAD	3.38	1.28	1.22
18	3	3012	CLA	OBD-CAD	3.37	1.28	1.22
18	4	4008	CLA	CHD-C1D	3.37	1.45	1.38
18	G	1001	CLA	CHD-C4C	3.37	1.46	1.39
18	3	3018	CLA	CHB-C1B	3.37	1.47	1.39
18	4	4016	CLA	OBD-CAD	3.37	1.28	1.22
18	4	4009	CLA	CHB-C1B	3.37	1.47	1.39
18	4	4005	CLA	CHD-C1D	3.37	1.45	1.38
18	1	1003	CLA	CHC-C4B	3.36	1.47	1.39
18	4	4001	CLA	CHB-C1B	3.36	1.47	1.39
18	2	2006	CLA	MG-NC	3.36	2.14	2.06
18	3	3001	CLA	C1B-NB	-3.36	1.33	1.37
18	1	1005	CLA	CHD-C1D	3.36	1.45	1.38
18	1	1003	CLA	OBD-CAD	3.35	1.28	1.22
18	3	3008	CLA	C1D-ND	-3.35	1.33	1.37
18	1	1001	CLA	CHB-C1B	3.35	1.46	1.39
18	4	4007	CLA	OBD-CAD	3.34	1.28	1.22
18	3	3008	CLA	OBD-CAD	3.34	1.28	1.22
18	2	2012	CLA	CHB-C1B	3.34	1.46	1.39
18	G	1003	CLA	C1B-NB	-3.34	1.33	1.37
18	K	1001	CLA	C1B-NB	-3.34	1.33	1.37
18	4	4016	CLA	C4B-NB	-3.34	1.33	1.37
18	1	1005	CLA	C1C-NC	-3.34	1.32	1.37
18	3	3002	CLA	C1B-NB	-3.34	1.33	1.37
18	3	3003	CLA	CHC-C1C	3.33	1.45	1.38
18	F	1301	CLA	OBD-CAD	3.33	1.28	1.22
18	2	2003	CLA	C4B-NB	-3.33	1.33	1.37
18	B	1226	CLA	C1B-NB	-3.33	1.33	1.37
22	J	6013	BCR	C11-C12	-3.32	1.26	1.34
18	F	1302	CLA	MG-NC	3.32	2.14	2.06
18	1	1005	CLA	CHC-C4B	3.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1004	CLA	OBD-CAD	3.32	1.28	1.22
18	3	3001	CLA	CHB-C1B	3.32	1.46	1.39
18	2	2003	CLA	OBD-CAD	3.32	1.28	1.22
29	4	4505	ZEX	C1-C6	-3.32	1.49	1.53
18	2	2001	CLA	CHB-C1B	3.32	1.46	1.39
18	1	1004	CLA	CHD-C4C	3.32	1.46	1.39
22	J	6013	BCR	C30-C25	-3.32	1.49	1.53
18	3	3013	CLA	CHB-C1B	3.31	1.46	1.39
18	G	1001	CLA	C3C-C2C	3.31	1.43	1.36
18	1	1013	CLA	C4B-NB	-3.31	1.33	1.37
18	3	3005	CLA	MG-NC	3.31	2.14	2.06
18	1	1008	CLA	C1B-NB	-3.30	1.33	1.37
17	A	1011	CL0	CHB-C4A	-3.30	1.34	1.38
18	2	2002	CLA	CHD-C4C	3.30	1.46	1.39
18	3	3010	CLA	CHB-C1B	3.30	1.46	1.39
18	L	1502	CLA	C1B-NB	-3.30	1.33	1.37
18	1	1007	CLA	CHC-C4B	3.30	1.46	1.39
18	1	1007	CLA	C1C-NC	-3.29	1.32	1.37
22	A	6003	BCR	C11-C12	-3.28	1.26	1.34
18	G	1002	CLA	OBD-CAD	3.28	1.28	1.22
18	1	1014	CLA	C1C-NC	-3.28	1.32	1.37
18	B	1012	CLA	C3D-C2D	3.28	1.47	1.39
18	A	1125	CLA	OBD-CAD	3.28	1.28	1.22
18	2	2002	CLA	MG-NC	3.27	2.14	2.06
18	B	1203	CLA	OBD-CAD	3.27	1.28	1.22
18	1	1002	CLA	CHD-C1D	3.27	1.44	1.38
18	L	1503	CLA	C4B-NB	-3.27	1.33	1.37
18	3	3010	CLA	CHD-C4C	3.27	1.46	1.39
18	3	3013	CLA	OBD-CAD	3.27	1.28	1.22
18	2	2005	CLA	C1D-ND	-3.26	1.33	1.37
18	4	4017	CLA	OBD-CAD	3.26	1.28	1.22
18	3	3019	CLA	CHC-C4B	3.26	1.48	1.39
18	4	4001	CLA	CHD-C4C	3.26	1.46	1.39
18	1	1004	CLA	C1C-NC	-3.25	1.32	1.37
18	1	1014	CLA	CHC-C4B	3.25	1.46	1.39
18	4	4008	CLA	C1C-NC	-3.25	1.32	1.37
22	3	3503	BCR	C11-C12	-3.24	1.26	1.34
18	A	1128	CLA	C3D-C2D	3.24	1.47	1.39
18	L	1502	CLA	OBD-CAD	3.24	1.28	1.22
18	1	1011	CLA	C1B-NB	-3.24	1.33	1.37
18	G	1002	CLA	C4B-NB	-3.23	1.33	1.37
18	2	2005	CLA	C4B-NB	-3.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4003	CLA	MG-NC	3.23	2.13	2.06
18	3	3012	CLA	CHD-C4C	3.23	1.46	1.39
18	2	2019	CLA	C3B-C4B	3.22	1.47	1.40
18	L	1503	CLA	MG-NC	3.22	2.13	2.06
22	A	6007	BCR	C11-C12	-3.22	1.26	1.34
18	4	4017	CLA	C1C-NC	-3.22	1.32	1.37
18	A	1133	CLA	C3D-C2D	3.22	1.47	1.39
18	2	2005	CLA	MG-NC	3.21	2.13	2.06
18	G	1003	CLA	OBD-CAD	3.21	1.28	1.22
18	1	1007	CLA	CHD-C4C	3.21	1.46	1.39
18	A	1128	CLA	C1B-NB	-3.21	1.33	1.37
22	B	6006	BCR	C11-C12	-3.21	1.26	1.34
18	4	4009	CLA	CHD-C4C	3.21	1.46	1.39
18	3	3003	CLA	MG-NC	3.20	2.13	2.06
28	1	1009	CHL	CHB-C4A	-3.20	1.34	1.38
22	B	6009	BCR	C11-C12	-3.19	1.26	1.34
18	3	3006	CLA	C1C-NC	-3.19	1.32	1.37
18	3	3004	CLA	C1C-NC	-3.19	1.32	1.37
18	1	1007	CLA	OBD-CAD	3.19	1.28	1.22
18	L	1502	CLA	MG-NC	3.18	2.13	2.06
28	4	4010	CHL	CHB-C4A	-3.18	1.34	1.38
18	1	1013	CLA	OBD-CAD	3.18	1.28	1.22
18	L	1503	CLA	OBD-CAD	3.18	1.28	1.22
18	A	1132	CLA	C3D-C2D	3.17	1.47	1.39
18	1	1014	CLA	CHD-C4C	3.17	1.46	1.39
18	2	2006	CLA	C1D-ND	-3.17	1.33	1.37
18	A	1102	CLA	C3D-C2D	3.17	1.47	1.39
18	3	3017	CLA	C1C-NC	-3.17	1.32	1.37
18	1	1012	CLA	C1C-NC	-3.17	1.32	1.37
18	1	1006	CLA	MG-NC	3.17	2.13	2.06
18	4	4016	CLA	MG-NC	3.16	2.13	2.06
18	2	2016	CLA	MG-NC	3.16	2.13	2.06
18	2	2005	CLA	C1B-NB	-3.16	1.33	1.37
18	F	1302	CLA	C4B-NB	-3.16	1.33	1.37
18	1	1002	CLA	CHD-C4C	3.15	1.46	1.39
18	2	2016	CLA	CHC-C4B	3.15	1.46	1.39
22	I	6020	BCR	C11-C12	-3.15	1.26	1.34
18	3	3001	CLA	C1C-NC	-3.15	1.32	1.37
18	A	1022	CLA	C3D-C2D	3.15	1.47	1.39
18	2	2012	CLA	CHC-C4B	3.15	1.46	1.39
18	B	1023	CLA	C3D-C2D	3.15	1.47	1.39
18	G	1001	CLA	CHC-C4B	3.14	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2003	CLA	CHD-C4C	3.14	1.46	1.39
18	1	1014	CLA	OBD-CAD	3.14	1.27	1.22
18	1	1011	CLA	OBD-CAD	3.14	1.27	1.22
18	4	4004	CLA	OBD-CAD	3.14	1.27	1.22
18	2	2008	CLA	CHD-C1D	3.14	1.44	1.38
18	4	4007	CLA	C1B-NB	-3.13	1.33	1.37
18	4	4008	CLA	C3C-C2C	3.13	1.43	1.36
18	4	4006	CLA	CHC-C4B	3.13	1.46	1.39
18	A	1138	CLA	C3D-C2D	3.13	1.47	1.39
18	1	1002	CLA	C1B-NB	-3.13	1.33	1.37
18	4	4007	CLA	CHD-C4C	3.13	1.46	1.39
18	B	1202	CLA	C3D-C2D	3.12	1.47	1.39
22	B	6004	BCR	C11-C12	-3.12	1.26	1.34
22	A	6002	BCR	C11-C12	-3.12	1.26	1.34
18	4	4004	CLA	CHB-C1B	3.12	1.46	1.39
18	2	2006	CLA	C1B-NB	-3.12	1.33	1.37
18	2	2006	CLA	C4B-NB	-3.12	1.33	1.37
28	2	2011	CHL	C3D-C2D	-3.12	1.34	1.39
18	3	3010	CLA	C1C-NC	-3.12	1.33	1.37
18	4	4006	CLA	CHD-C4C	3.12	1.46	1.39
18	B	1206	CLA	C3D-C2D	3.11	1.47	1.39
18	B	1215	CLA	C3D-C2D	3.11	1.47	1.39
18	3	3013	CLA	MG-NC	3.11	2.13	2.06
18	F	1302	CLA	C1B-NB	-3.11	1.33	1.37
18	B	1216	CLA	C3D-C2D	3.11	1.47	1.39
18	F	1301	CLA	C4B-NB	-3.11	1.33	1.37
18	A	1013	CLA	C3D-C2D	3.11	1.47	1.39
18	2	2009	CLA	OBD-CAD	3.11	1.27	1.22
23	4	4801	LMG	O8-C28	3.10	1.42	1.33
28	4	4013	CHL	C2C-C3C	-3.10	1.33	1.36
18	4	4002	CLA	CHD-C4C	3.10	1.46	1.39
22	B	6010	BCR	C11-C12	-3.10	1.26	1.34
18	A	1127	CLA	C3D-C2D	3.10	1.47	1.39
18	A	1140	CLA	C3D-C2D	3.10	1.47	1.39
18	A	1126	CLA	C3D-C2D	3.09	1.47	1.39
18	B	1021	CLA	C3D-C2D	3.09	1.47	1.39
18	3	3008	CLA	CHC-C4B	3.09	1.46	1.39
18	F	1302	CLA	C1D-ND	-3.09	1.33	1.37
18	A	1116	CLA	C3D-C2D	3.09	1.47	1.39
18	B	1224	CLA	C3D-C2D	3.09	1.47	1.39
18	B	1209	CLA	C3D-C2D	3.08	1.47	1.39
18	B	1228	CLA	C3D-C2D	3.08	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2007	CLA	C1D-ND	-3.08	1.33	1.37
18	1	1002	CLA	C1C-NC	-3.08	1.33	1.37
18	1	1003	CLA	C1C-NC	-3.08	1.33	1.37
18	B	1220	CLA	C3D-C2D	3.08	1.47	1.39
18	2	2016	CLA	C1C-NC	-3.08	1.33	1.37
18	3	3005	CLA	C1C-NC	-3.08	1.33	1.37
18	B	1222	CLA	C3D-C2D	3.07	1.47	1.39
18	G	1003	CLA	MG-NC	3.07	2.13	2.06
18	4	4016	CLA	C1D-ND	-3.07	1.33	1.37
18	A	1115	CLA	C3D-C2D	3.07	1.47	1.39
18	B	1235	CLA	C3D-C2D	3.07	1.47	1.39
18	4	4002	CLA	CHC-C4B	3.07	1.46	1.39
18	3	3003	CLA	C1C-NC	-3.07	1.33	1.37
18	A	1112	CLA	C3D-C2D	3.07	1.47	1.39
18	B	1204	CLA	C3D-C2D	3.07	1.47	1.39
28	2	2010	CHL	CHB-C4A	-3.07	1.34	1.38
18	A	1106	CLA	C3D-C2D	3.06	1.47	1.39
28	1	1010	CHL	CHB-C4A	-3.06	1.34	1.38
18	3	3007	CLA	C1C-NC	-3.06	1.33	1.37
18	3	3002	CLA	MG-NC	3.05	2.13	2.06
18	B	1232	CLA	C3D-C2D	3.05	1.47	1.39
18	A	1139	CLA	C3D-C2D	3.05	1.47	1.39
18	A	1110	CLA	C3D-C2D	3.05	1.47	1.39
18	B	1219	CLA	C3D-C2D	3.05	1.47	1.39
22	K	2011	BCR	C11-C12	-3.05	1.26	1.34
18	B	1225	CLA	C3D-C2D	3.05	1.47	1.39
18	A	1151	CLA	C3D-C2D	3.05	1.47	1.39
18	H	1000	CLA	C3D-C2D	3.05	1.47	1.39
18	A	1111	CLA	C3D-C2D	3.05	1.47	1.39
18	A	1131	CLA	C3D-C2D	3.05	1.47	1.39
18	A	1124	CLA	C3D-C2D	3.04	1.47	1.39
18	B	1229	CLA	C3D-C2D	3.04	1.47	1.39
18	B	1236	CLA	C3D-C2D	3.04	1.47	1.39
18	A	1134	CLA	C3D-C2D	3.04	1.47	1.39
18	A	1122	CLA	C3D-C2D	3.04	1.47	1.39
18	A	1117	CLA	C3D-C2D	3.04	1.47	1.39
18	G	1003	CLA	C1D-ND	-3.04	1.33	1.37
28	4	4010	CHL	CBD-CAD	-3.04	1.43	1.53
18	2	2009	CLA	C1C-NC	-3.04	1.33	1.37
18	B	1210	CLA	C3D-C2D	3.04	1.47	1.39
18	B	1208	CLA	C3D-C2D	3.03	1.47	1.39
18	2	2009	CLA	MG-NC	3.03	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1218	CLA	C3D-C2D	3.03	1.47	1.39
18	B	1212	CLA	C3D-C2D	3.03	1.47	1.39
18	K	1001	CLA	C1C-NC	-3.03	1.33	1.37
18	3	3018	CLA	C1C-NC	-3.03	1.33	1.37
18	B	1230	CLA	C3D-C2D	3.03	1.47	1.39
18	B	1223	CLA	C4D-CHA	3.03	1.48	1.38
18	B	1221	CLA	C3D-C2D	3.03	1.47	1.39
18	3	3007	CLA	MG-NC	3.03	2.13	2.06
18	A	1105	CLA	C3D-C2D	3.03	1.47	1.39
22	B	6005	BCR	C11-C12	-3.03	1.26	1.34
18	2	2007	CLA	C4B-NB	-3.02	1.33	1.37
18	A	1123	CLA	C3D-C2D	3.02	1.47	1.39
18	J	1302	CLA	C3D-C2D	3.02	1.47	1.39
18	A	1104	CLA	C3D-C2D	3.02	1.47	1.39
28	1	1010	CHL	C3B-C2B	-3.02	1.36	1.40
18	4	4007	CLA	CHC-C4B	3.02	1.46	1.39
18	3	3013	CLA	C1C-NC	-3.02	1.33	1.37
18	2	2002	CLA	C1C-NC	-3.02	1.33	1.37
18	4	4001	CLA	C1C-NC	-3.01	1.33	1.37
18	1	1001	CLA	OBD-CAD	3.01	1.27	1.22
18	A	1108	CLA	C3D-C2D	3.01	1.47	1.39
18	B	1211	CLA	C3D-C2D	3.01	1.47	1.39
18	A	1113	CLA	C3D-C2D	3.01	1.47	1.39
18	2	2001	CLA	CHC-C4B	3.00	1.46	1.39
18	A	1109	CLA	C3D-C2D	3.00	1.47	1.39
18	B	1239	CLA	C3D-C2D	3.00	1.47	1.39
18	A	1137	CLA	C3D-C2D	3.00	1.47	1.39
18	2	2019	CLA	CHB-C1B	3.00	1.47	1.39
18	A	1119	CLA	C3D-C2D	3.00	1.47	1.39
18	B	1213	CLA	C3D-C2D	3.00	1.47	1.39
18	L	1501	CLA	OBD-CAD	3.00	1.27	1.22
18	B	1231	CLA	C3D-C2D	3.00	1.47	1.39
18	3	3008	CLA	MG-NC	3.00	2.13	2.06
18	B	1226	CLA	C3D-C2D	3.00	1.47	1.39
18	A	1121	CLA	C3D-C2D	2.99	1.47	1.39
18	B	1205	CLA	C3D-C2D	2.99	1.47	1.39
18	1	1008	CLA	OBD-CAD	2.99	1.27	1.22
22	L	6020	BCR	C11-C12	-2.99	1.26	1.34
18	A	1114	CLA	C3D-C2D	2.99	1.47	1.39
18	1	1001	CLA	MG-NC	2.99	2.13	2.06
22	A	6017	BCR	C11-C12	-2.99	1.26	1.34
18	B	1216	CLA	C1B-NB	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1206	CLA	C4D-CHA	2.98	1.48	1.38
18	K	1001	CLA	MG-NC	2.98	2.13	2.06
18	4	4008	CLA	CHC-C4B	2.98	1.46	1.39
18	A	1136	CLA	C3D-C2D	2.98	1.47	1.39
18	B	1221	CLA	C4D-CHA	2.98	1.48	1.38
18	B	1214	CLA	C3D-C2D	2.98	1.47	1.39
18	A	1101	CLA	C3D-C2D	2.98	1.47	1.39
18	1	1006	CLA	OBD-CAD	2.98	1.27	1.22
18	B	1234	CLA	C3D-C2D	2.98	1.47	1.39
18	A	1135	CLA	C3D-C2D	2.97	1.47	1.39
18	B	1217	CLA	C3D-C2D	2.97	1.47	1.39
18	B	1225	CLA	C1B-C2B	2.97	1.50	1.43
17	A	1011	CL0	C3A-C2A	-2.97	1.52	1.54
18	2	2007	CLA	C1B-NB	-2.97	1.34	1.37
18	B	1227	CLA	C3D-C2D	2.96	1.47	1.39
18	B	1201	CLA	C3D-C2D	2.96	1.47	1.39
18	A	1126	CLA	C4D-CHA	2.96	1.48	1.38
18	A	1130	CLA	C3D-C2D	2.96	1.47	1.39
18	A	1103	CLA	C3D-C2D	2.96	1.47	1.39
18	A	1106	CLA	C4D-CHA	2.96	1.48	1.38
18	B	1202	CLA	C1B-C2B	2.96	1.50	1.43
18	3	3010	CLA	OBD-CAD	2.96	1.27	1.22
18	B	1203	CLA	C1B-C2B	2.96	1.50	1.43
18	A	1102	CLA	C4D-CHA	2.96	1.48	1.38
18	A	1118	CLA	C3D-C2D	2.95	1.47	1.39
18	1	1013	CLA	C1D-ND	-2.95	1.34	1.37
18	A	1118	CLA	C4D-CHA	2.95	1.48	1.38
18	G	1001	CLA	OBD-CAD	2.95	1.27	1.22
18	B	1230	CLA	C1B-C2B	2.95	1.50	1.43
18	4	4016	CLA	C1B-NB	-2.95	1.34	1.37
18	A	1129	CLA	C4D-CHA	2.95	1.48	1.38
18	2	2019	CLA	CHC-C4B	2.95	1.47	1.39
18	B	1224	CLA	C4D-CHA	2.94	1.48	1.38
18	B	1225	CLA	C1D-ND	-2.94	1.34	1.37
18	A	1109	CLA	C4D-CHA	2.94	1.48	1.38
18	B	1021	CLA	C4D-CHA	2.94	1.48	1.38
18	B	1240	CLA	C3D-C2D	2.94	1.47	1.39
18	A	1111	CLA	C4D-CHA	2.94	1.48	1.38
18	2	2008	CLA	OBD-CAD	2.94	1.27	1.22
18	B	1216	CLA	C4D-CHA	2.94	1.48	1.38
18	A	1107	CLA	C3D-C2D	2.94	1.47	1.39
18	A	1128	CLA	C1D-ND	-2.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	C4D-CHA	2.93	1.48	1.38
18	B	1012	CLA	C4D-CHA	2.93	1.48	1.38
18	B	1212	CLA	C1B-C2B	2.93	1.50	1.43
18	B	1230	CLA	C1D-ND	-2.93	1.34	1.37
18	B	1226	CLA	C1D-ND	-2.93	1.34	1.37
18	A	1128	CLA	C4D-CHA	2.93	1.48	1.38
18	4	4008	CLA	CHD-C4C	2.93	1.45	1.39
18	F	1301	CLA	C1B-NB	-2.93	1.34	1.37
18	A	1125	CLA	C4D-CHA	2.93	1.48	1.38
18	3	3017	CLA	CHB-C1B	2.93	1.46	1.39
18	B	1201	CLA	C4D-CHA	2.92	1.48	1.38
18	H	1000	CLA	C4D-CHA	2.92	1.48	1.38
18	A	1129	CLA	C3D-C2D	2.92	1.47	1.39
18	A	1133	CLA	C4D-CHA	2.92	1.48	1.38
18	A	1140	CLA	C4D-CHA	2.92	1.48	1.38
18	B	1202	CLA	C1D-ND	-2.92	1.34	1.37
18	2	2016	CLA	CHD-C4C	2.92	1.45	1.39
18	B	1207	CLA	C3D-C2D	2.92	1.47	1.39
18	1	1001	CLA	CHD-C4C	2.92	1.45	1.39
18	1	1005	CLA	CHD-C4C	2.92	1.45	1.39
18	A	1114	CLA	C4D-CHA	2.92	1.48	1.38
18	B	1238	CLA	C3D-C2D	2.92	1.46	1.39
18	A	1103	CLA	C1B-C2B	2.92	1.50	1.43
18	B	1228	CLA	C4D-CHA	2.91	1.48	1.38
18	B	1202	CLA	C4D-CHA	2.91	1.48	1.38
18	B	1229	CLA	C4D-CHA	2.91	1.48	1.38
18	4	4017	CLA	MG-NC	2.91	2.13	2.06
18	J	1302	CLA	C1B-C2B	2.91	1.50	1.43
18	2	2006	CLA	C3D-C2D	2.91	1.46	1.39
18	A	1123	CLA	C1B-C2B	2.91	1.50	1.43
28	3	3011	CHL	C3D-C2D	-2.91	1.34	1.39
18	A	1136	CLA	C1B-C2B	2.91	1.50	1.43
18	A	1122	CLA	C4D-CHA	2.91	1.48	1.38
18	B	1023	CLA	C4D-CHA	2.91	1.48	1.38
18	B	1215	CLA	C4D-CHA	2.90	1.48	1.38
18	B	1214	CLA	C4D-CHA	2.90	1.48	1.38
18	B	1235	CLA	C4D-CHA	2.90	1.48	1.38
18	A	1151	CLA	C4D-CHA	2.90	1.48	1.38
18	B	1209	CLA	C4D-CHA	2.90	1.48	1.38
18	4	4004	CLA	CHD-C4C	2.90	1.45	1.39
18	B	1212	CLA	C1D-ND	-2.90	1.34	1.37
18	1	1006	CLA	C1C-NC	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	1000	CLA	C1B-C2B	2.90	1.49	1.43
18	A	1134	CLA	C4D-CHA	2.90	1.48	1.38
18	1	1011	CLA	C1C-NC	-2.90	1.33	1.37
18	3	3006	CLA	MG-NC	2.90	2.13	2.06
18	B	1227	CLA	C4D-CHA	2.90	1.48	1.38
18	B	1229	CLA	C1B-C2B	2.90	1.49	1.43
18	4	4005	CLA	CHC-C4B	2.89	1.45	1.39
18	B	1235	CLA	C1B-C2B	2.89	1.49	1.43
18	A	1134	CLA	C1B-C2B	2.89	1.49	1.43
18	4	4006	CLA	OBD-CAD	2.89	1.27	1.22
18	A	1123	CLA	C4D-CHA	2.89	1.48	1.38
18	A	1119	CLA	C4D-CHA	2.89	1.48	1.38
18	B	1236	CLA	C4D-CHA	2.89	1.48	1.38
18	A	1115	CLA	C4D-CHA	2.89	1.48	1.38
18	A	1113	CLA	C4D-CHA	2.89	1.48	1.38
18	F	1302	CLA	C3D-C2D	2.89	1.46	1.39
18	A	1120	CLA	C3D-C2D	2.89	1.46	1.39
18	B	1220	CLA	C4D-CHA	2.89	1.48	1.38
18	B	1223	CLA	C3D-C2D	2.89	1.46	1.39
18	A	1140	CLA	C1B-C2B	2.88	1.49	1.43
18	A	1138	CLA	C4D-CHA	2.88	1.48	1.38
18	B	1208	CLA	C4D-CHA	2.88	1.48	1.38
18	1	1001	CLA	C3D-C2D	2.88	1.46	1.39
18	2	2004	CLA	OBD-CAD	2.88	1.27	1.22
18	B	1239	CLA	C4D-CHA	2.88	1.48	1.38
18	B	1219	CLA	C4D-CHA	2.88	1.48	1.38
18	A	1135	CLA	C1B-C2B	2.88	1.49	1.43
18	B	1021	CLA	C1B-C2B	2.88	1.49	1.43
18	A	1105	CLA	C4D-CHA	2.88	1.48	1.38
18	A	1013	CLA	C1D-ND	-2.88	1.34	1.37
18	2	2007	CLA	C3D-C2D	2.88	1.46	1.39
18	2	2005	CLA	C3D-C2D	2.88	1.46	1.39
18	A	1136	CLA	C4D-CHA	2.88	1.48	1.38
18	A	1116	CLA	C4D-CHA	2.88	1.48	1.38
18	B	1222	CLA	C4D-CHA	2.87	1.48	1.38
18	A	1121	CLA	C4D-CHA	2.87	1.48	1.38
18	A	1130	CLA	C4D-CHA	2.87	1.48	1.38
18	A	1129	CLA	C1B-C2B	2.87	1.49	1.43
18	A	1122	CLA	C1B-C2B	2.87	1.49	1.43
18	J	1302	CLA	C4D-CHA	2.87	1.48	1.38
18	A	1135	CLA	C4D-CHA	2.87	1.48	1.38
18	3	3003	CLA	C4D-CHA	2.87	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1120	CLA	C4D-CHA	2.87	1.48	1.38
18	B	1238	CLA	C1D-ND	-2.87	1.34	1.37
18	4	4002	CLA	MG-NC	2.87	2.13	2.06
18	L	1503	CLA	C1C-NC	-2.87	1.33	1.37
18	A	1127	CLA	C4D-CHA	2.87	1.48	1.38
18	B	1232	CLA	C4D-CHA	2.87	1.48	1.38
18	B	1209	CLA	C1B-C2B	2.87	1.49	1.43
18	B	1226	CLA	C4D-CHA	2.87	1.48	1.38
18	A	1117	CLA	C4D-CHA	2.87	1.48	1.38
18	A	1131	CLA	C4D-CHA	2.87	1.48	1.38
18	4	4008	CLA	MG-NC	2.87	2.13	2.06
18	A	1120	CLA	C1B-C2B	2.86	1.49	1.43
18	A	1110	CLA	C4D-CHA	2.86	1.48	1.38
18	B	1225	CLA	C4D-CHA	2.86	1.48	1.38
18	A	1113	CLA	C1B-C2B	2.86	1.49	1.43
18	A	1139	CLA	C1B-C2B	2.86	1.49	1.43
28	2	2013	CHL	CHB-C4A	-2.86	1.35	1.38
18	A	1103	CLA	C4D-CHA	2.86	1.48	1.38
18	B	1021	CLA	C1D-ND	-2.86	1.34	1.37
18	B	1203	CLA	C3D-C2D	2.86	1.46	1.39
18	B	1203	CLA	C4D-CHA	2.86	1.48	1.38
18	3	3002	CLA	C1C-NC	-2.86	1.33	1.37
28	2	2011	CHL	C2C-C3C	-2.86	1.33	1.36
18	L	1502	CLA	C1C-NC	-2.85	1.33	1.37
18	3	3005	CLA	CHD-C4C	2.85	1.45	1.39
18	A	1107	CLA	C1B-C2B	2.85	1.49	1.43
18	1	1012	CLA	MG-NC	2.85	2.13	2.06
18	A	1022	CLA	C4D-CHA	2.85	1.48	1.38
18	A	1131	CLA	C1B-C2B	2.85	1.49	1.43
18	2	2002	CLA	OBD-CAD	2.85	1.27	1.22
18	A	1112	CLA	C4D-CHA	2.85	1.48	1.38
18	B	1230	CLA	C4D-CHA	2.85	1.48	1.38
18	B	1223	CLA	C1D-ND	-2.85	1.34	1.37
18	A	1108	CLA	C4D-CHA	2.85	1.48	1.38
18	B	1212	CLA	C4D-CHA	2.85	1.48	1.38
18	A	1125	CLA	C1B-C2B	2.85	1.49	1.43
18	A	1129	CLA	C1D-ND	-2.84	1.34	1.37
18	B	1220	CLA	C1B-C2B	2.84	1.49	1.43
18	B	1206	CLA	C1B-NB	-2.84	1.34	1.37
18	2	2012	CLA	OBD-CAD	2.84	1.27	1.22
18	B	1206	CLA	C1B-C2B	2.84	1.49	1.43
18	A	1118	CLA	C1B-C2B	2.84	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1207	CLA	C1B-C2B	2.84	1.49	1.43
18	B	1213	CLA	C4D-CHA	2.84	1.48	1.38
18	A	1139	CLA	C4D-CHA	2.84	1.48	1.38
18	G	1003	CLA	C1C-NC	-2.83	1.33	1.37
18	A	1130	CLA	C1B-C2B	2.83	1.49	1.43
18	B	1201	CLA	C1B-C2B	2.83	1.49	1.43
18	B	1217	CLA	C1B-C2B	2.83	1.49	1.43
18	A	1115	CLA	C1B-C2B	2.83	1.49	1.43
18	4	4016	CLA	C1C-NC	-2.83	1.33	1.37
18	B	1204	CLA	C4D-CHA	2.83	1.48	1.38
18	B	1219	CLA	C1D-ND	-2.83	1.34	1.37
18	1	1002	CLA	C3D-C2D	2.83	1.46	1.39
18	B	1231	CLA	C4D-CHA	2.83	1.48	1.38
18	B	1222	CLA	C1B-C2B	2.83	1.49	1.43
18	A	1237	CLA	C1B-C2B	2.83	1.49	1.43
18	1	1003	CLA	C3D-C2D	2.83	1.46	1.39
18	A	1101	CLA	C4D-CHA	2.82	1.48	1.38
18	B	1210	CLA	C4D-CHA	2.82	1.48	1.38
18	A	1151	CLA	C1B-C2B	2.82	1.49	1.43
18	3	3007	CLA	C3D-C2D	2.82	1.46	1.39
18	3	3018	CLA	MG-NC	2.82	2.13	2.06
18	B	1221	CLA	C1B-NB	-2.82	1.34	1.37
18	A	1237	CLA	C3D-C2D	2.82	1.46	1.39
18	A	1013	CLA	C4D-CHA	2.82	1.48	1.38
18	B	1240	CLA	C1B-C2B	2.82	1.49	1.43
18	A	1102	CLA	C1B-C2B	2.82	1.49	1.43
18	A	1125	CLA	C3D-C2D	2.81	1.46	1.39
18	1	1013	CLA	C1B-C2B	2.81	1.49	1.43
18	B	1218	CLA	C1B-C2B	2.81	1.49	1.43
18	A	1106	CLA	C1B-C2B	2.81	1.49	1.43
18	3	3006	CLA	OBD-CAD	2.81	1.27	1.22
18	3	3008	CLA	CHD-C4C	2.81	1.45	1.39
18	B	1208	CLA	C1B-C2B	2.80	1.49	1.43
18	A	1121	CLA	C1B-C2B	2.80	1.49	1.43
22	J	6012	BCR	C30-C25	-2.80	1.50	1.53
18	B	1215	CLA	C1B-NB	-2.80	1.34	1.37
18	A	1133	CLA	C1B-C2B	2.80	1.49	1.43
18	A	1124	CLA	C4D-CHA	2.80	1.48	1.38
18	A	1137	CLA	C1B-C2B	2.80	1.49	1.43
18	A	1116	CLA	C1B-C2B	2.79	1.49	1.43
18	2	2016	CLA	C1B-C2B	2.79	1.49	1.43
18	B	1227	CLA	C1D-C2D	2.79	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	1302	CLA	C4D-CHA	2.79	1.48	1.38
18	F	1301	CLA	C3D-C2D	2.79	1.46	1.39
18	1	1011	CLA	MG-NC	2.79	2.12	2.06
18	A	1137	CLA	C4D-CHA	2.79	1.48	1.38
18	3	3010	CLA	CHC-C4B	2.79	1.45	1.39
18	B	1205	CLA	C1D-ND	-2.79	1.34	1.37
18	A	1127	CLA	C1D-ND	-2.79	1.34	1.37
18	B	1234	CLA	C4D-CHA	2.79	1.47	1.38
18	L	1503	CLA	C3D-C2D	2.79	1.46	1.39
18	4	4005	CLA	CHD-C4C	2.78	1.45	1.39
18	3	3013	CLA	C3D-C2D	2.78	1.46	1.39
18	A	1124	CLA	C1B-C2B	2.78	1.49	1.43
18	A	1104	CLA	C4D-CHA	2.78	1.47	1.38
18	A	1101	CLA	C1B-NB	-2.78	1.34	1.37
18	3	3008	CLA	C4D-CHA	2.78	1.47	1.38
18	1	1005	CLA	OBD-CAD	2.78	1.27	1.22
18	A	1103	CLA	C1D-ND	-2.78	1.34	1.37
18	A	1107	CLA	C4D-CHA	2.78	1.47	1.38
18	4	4005	CLA	MG-NC	2.78	2.12	2.06
18	A	1132	CLA	C4D-CHA	2.78	1.47	1.38
18	B	1209	CLA	C1D-ND	-2.77	1.34	1.37
18	B	1240	CLA	C4D-CHA	2.77	1.47	1.38
18	B	1218	CLA	C4D-CHA	2.77	1.47	1.38
18	A	1127	CLA	C1B-C2B	2.77	1.49	1.43
18	B	1222	CLA	C1D-ND	-2.77	1.34	1.37
18	A	1114	CLA	C1B-C2B	2.77	1.49	1.43
18	B	1204	CLA	C1B-C2B	2.77	1.49	1.43
18	A	1138	CLA	C1B-C2B	2.77	1.49	1.43
18	B	1012	CLA	C1D-ND	-2.77	1.34	1.37
18	4	4001	CLA	OBD-CAD	2.77	1.27	1.22
18	B	1205	CLA	C1B-C2B	2.77	1.49	1.43
18	3	3017	CLA	MG-NC	2.77	2.12	2.06
18	B	1207	CLA	C4D-CHA	2.77	1.47	1.38
18	A	1104	CLA	C1B-C2B	2.77	1.49	1.43
18	B	1218	CLA	C1D-ND	-2.77	1.34	1.37
18	2	2008	CLA	CHD-C4C	2.76	1.45	1.39
18	B	1238	CLA	C4D-CHA	2.76	1.47	1.38
18	B	1206	CLA	C1D-ND	-2.76	1.34	1.37
18	4	4017	CLA	C3D-C2D	2.75	1.46	1.39
18	2	2006	CLA	C4D-CHA	2.75	1.47	1.38
18	1	1003	CLA	MG-NC	2.75	2.12	2.06
18	B	1224	CLA	C1B-C2B	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1004	CLA	MG-NC	2.75	2.12	2.06
18	B	1239	CLA	C1B-C2B	2.75	1.49	1.43
18	A	1111	CLA	C1D-ND	-2.75	1.34	1.37
18	B	1207	CLA	C1D-ND	-2.75	1.34	1.37
18	A	1123	CLA	C1D-ND	-2.75	1.34	1.37
18	4	4001	CLA	C4D-CHA	2.74	1.47	1.38
18	A	1022	CLA	C1B-C2B	2.74	1.49	1.43
18	B	1223	CLA	C1B-C2B	2.74	1.49	1.43
18	B	1231	CLA	C1D-ND	-2.74	1.34	1.37
18	F	1301	CLA	C4D-CHA	2.74	1.47	1.38
18	B	1213	CLA	C1B-C2B	2.74	1.49	1.43
18	B	1214	CLA	C1B-C2B	2.74	1.49	1.43
18	2	2005	CLA	C1C-NC	-2.74	1.33	1.37
18	B	1211	CLA	C4D-CHA	2.74	1.47	1.38
18	A	1109	CLA	C1B-C2B	2.74	1.49	1.43
18	4	4005	CLA	C3D-C2D	2.74	1.46	1.39
18	A	1237	CLA	C4D-CHA	2.74	1.47	1.38
18	4	4007	CLA	C4D-CHA	2.74	1.47	1.38
18	A	1133	CLA	C1D-ND	-2.73	1.34	1.37
18	B	1023	CLA	C1B-C2B	2.73	1.49	1.43
18	1	1007	CLA	MG-NC	2.73	2.12	2.06
18	A	1135	CLA	C1D-ND	-2.73	1.34	1.37
18	4	4006	CLA	C3D-C2D	2.73	1.46	1.39
18	B	1234	CLA	C1B-C2B	2.73	1.49	1.43
18	A	1119	CLA	C1D-ND	-2.73	1.34	1.37
18	2	2007	CLA	C4D-CHA	2.73	1.47	1.38
18	A	1121	CLA	C1D-ND	-2.73	1.34	1.37
18	B	1232	CLA	C1B-C2B	2.73	1.49	1.43
18	B	1229	CLA	C1D-ND	-2.73	1.34	1.37
18	B	1203	CLA	C1D-ND	-2.73	1.34	1.37
18	A	1117	CLA	C1B-C2B	2.73	1.49	1.43
18	B	1216	CLA	C1D-ND	-2.72	1.34	1.37
18	A	1101	CLA	C1B-C2B	2.72	1.49	1.43
18	B	1231	CLA	C1D-C2D	2.72	1.50	1.45
18	B	1012	CLA	C1B-C2B	2.72	1.49	1.43
18	B	1205	CLA	C4D-CHA	2.72	1.47	1.38
18	F	1301	CLA	C1B-C2B	2.72	1.49	1.43
18	1	1014	CLA	MG-NC	2.72	2.12	2.06
18	2	2007	CLA	C1B-C2B	2.72	1.49	1.43
18	B	1224	CLA	C1D-ND	-2.72	1.34	1.37
18	2	2012	CLA	C3D-C2D	2.72	1.46	1.39
18	A	1115	CLA	C1D-ND	-2.72	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1215	CLA	C1D-ND	-2.72	1.34	1.37
18	B	1224	CLA	C1B-NB	-2.72	1.34	1.37
18	B	1211	CLA	C3B-C4B	2.72	1.50	1.42
18	1	1005	CLA	MG-NC	2.71	2.12	2.06
18	3	3003	CLA	CHC-C4B	2.71	1.45	1.39
18	2	2001	CLA	OBD-CAD	2.71	1.27	1.22
18	A	1013	CLA	C1B-NB	-2.71	1.34	1.37
18	B	1202	CLA	C1B-NB	-2.71	1.34	1.37
18	1	1012	CLA	C3D-C2D	2.71	1.46	1.39
18	A	1104	CLA	C1B-NB	-2.71	1.34	1.37
18	B	1236	CLA	C1B-C2B	2.70	1.49	1.43
18	A	1101	CLA	C1D-C2D	2.70	1.50	1.45
18	4	4003	CLA	C3D-C2D	2.70	1.46	1.39
18	A	1108	CLA	C1B-C2B	2.69	1.49	1.43
18	F	1302	CLA	C1C-NC	-2.69	1.33	1.37
18	G	1002	CLA	C3D-C2D	2.69	1.46	1.39
18	B	1023	CLA	C1D-ND	-2.69	1.34	1.37
18	B	1021	CLA	C1B-NB	-2.69	1.34	1.37
18	1	1008	CLA	C1B-C2B	2.69	1.49	1.43
18	4	4009	CLA	OBD-CAD	2.69	1.27	1.22
18	3	3003	CLA	C1B-C2B	2.69	1.49	1.43
18	3	3003	CLA	OBD-CAD	2.68	1.27	1.22
18	B	1215	CLA	C1B-C2B	2.68	1.49	1.43
18	4	4001	CLA	MG-NC	2.68	2.12	2.06
29	4	4505	ZEX	C21-C26	-2.68	1.50	1.53
18	1	1013	CLA	C1C-NC	-2.68	1.33	1.37
18	2	2001	CLA	C3D-C2D	2.68	1.46	1.39
18	4	4017	CLA	C4D-CHA	2.68	1.47	1.38
18	A	1112	CLA	C1D-ND	-2.68	1.34	1.37
18	B	1219	CLA	C1B-C2B	2.68	1.49	1.43
18	4	4012	CLA	OBD-CAD	2.67	1.27	1.22
18	B	1213	CLA	C1B-NB	-2.67	1.34	1.37
18	A	1105	CLA	C1B-C2B	2.67	1.49	1.43
28	2	2013	CHL	C1B-C2B	2.67	1.42	1.39
18	A	1110	CLA	C1B-NB	-2.67	1.34	1.37
18	B	1220	CLA	C1D-ND	-2.67	1.34	1.37
18	A	1112	CLA	C1B-C2B	2.67	1.49	1.43
18	B	1227	CLA	C1D-ND	-2.67	1.34	1.37
18	1	1008	CLA	C4D-CHA	2.67	1.47	1.38
18	L	1501	CLA	MG-NC	2.67	2.12	2.06
18	2	2004	CLA	CHB-C1B	2.66	1.45	1.39
18	A	1127	CLA	C1B-NB	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3004	CLA	C3D-C2D	2.66	1.46	1.39
18	A	1110	CLA	C1D-ND	-2.66	1.34	1.37
18	B	1221	CLA	C1B-C2B	2.66	1.49	1.43
18	A	1130	CLA	C1D-ND	-2.66	1.34	1.37
18	1	1013	CLA	C4D-CHA	2.65	1.47	1.38
18	A	1237	CLA	C1D-ND	-2.65	1.34	1.37
18	F	1301	CLA	C1C-NC	-2.65	1.33	1.37
18	G	1002	CLA	C4D-CHA	2.65	1.47	1.38
18	A	1132	CLA	C1D-ND	-2.65	1.34	1.37
18	A	1119	CLA	C1B-NB	-2.65	1.34	1.37
18	4	4016	CLA	C1B-C2B	2.65	1.49	1.43
18	3	3018	CLA	C4D-CHA	2.65	1.47	1.38
18	A	1136	CLA	C1D-ND	-2.65	1.34	1.37
18	A	1117	CLA	C1D-ND	-2.65	1.34	1.37
18	B	1239	CLA	C1B-NB	-2.65	1.34	1.37
18	A	1111	CLA	C1B-C2B	2.65	1.49	1.43
18	A	1126	CLA	C1B-C2B	2.64	1.49	1.43
28	1	1010	CHL	C3D-C2D	-2.64	1.35	1.39
18	A	1237	CLA	C1D-C2D	2.64	1.50	1.45
18	B	1204	CLA	C1D-C2D	2.64	1.50	1.45
18	B	1210	CLA	C1B-NB	-2.64	1.34	1.37
18	A	1137	CLA	C1D-ND	-2.64	1.34	1.37
18	A	1112	CLA	C1D-C2D	2.64	1.50	1.45
18	3	3008	CLA	C1B-C2B	2.63	1.49	1.43
22	G	2011	BCR	C1-C6	-2.63	1.50	1.53
18	B	1219	CLA	C1B-NB	-2.63	1.34	1.37
18	2	2005	CLA	C4D-CHA	2.63	1.47	1.38
18	B	1214	CLA	C1D-C2D	2.62	1.50	1.45
18	B	1231	CLA	C1B-C2B	2.62	1.49	1.43
18	1	1011	CLA	C3D-C2D	2.62	1.46	1.39
18	3	3004	CLA	MG-NC	2.62	2.12	2.06
18	A	1118	CLA	C1D-ND	-2.62	1.34	1.37
18	A	1108	CLA	C1D-ND	-2.62	1.34	1.37
18	A	1022	CLA	C1D-ND	-2.62	1.34	1.37
18	A	1118	CLA	C1B-NB	-2.62	1.34	1.37
18	2	2016	CLA	C4D-CHA	2.62	1.47	1.38
18	A	1138	CLA	C1D-ND	-2.62	1.34	1.37
18	4	4016	CLA	C4D-CHA	2.62	1.47	1.38
18	4	4002	CLA	C4D-CHA	2.61	1.47	1.38
18	3	3005	CLA	OBD-CAD	2.61	1.27	1.22
18	4	4012	CLA	CHC-C4B	2.61	1.45	1.39
18	B	1238	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1134	CLA	C1D-C2D	2.61	1.50	1.45
18	H	1000	CLA	C1D-ND	-2.61	1.34	1.37
18	J	1302	CLA	C1D-ND	-2.61	1.34	1.37
18	A	1107	CLA	C1D-ND	-2.61	1.34	1.37
18	A	1125	CLA	C1D-ND	-2.61	1.34	1.37
18	A	1108	CLA	C1D-C2D	2.60	1.50	1.45
18	A	1133	CLA	C1B-NB	-2.60	1.34	1.37
18	4	4012	CLA	C3D-C2D	2.60	1.46	1.39
18	A	1120	CLA	C1D-ND	-2.60	1.34	1.37
18	B	1210	CLA	C1B-C2B	2.60	1.49	1.43
18	A	1138	CLA	C1B-NB	-2.60	1.34	1.37
18	4	4006	CLA	MG-NC	2.60	2.12	2.06
18	2	2006	CLA	C1B-C2B	2.60	1.49	1.43
18	A	1132	CLA	C1D-C2D	2.60	1.50	1.45
18	B	1209	CLA	C1B-NB	-2.60	1.34	1.37
18	A	1119	CLA	C1B-C2B	2.59	1.49	1.43
18	G	1001	CLA	MG-NC	2.59	2.12	2.06
18	1	1013	CLA	C1D-C2D	2.59	1.50	1.45
18	4	4003	CLA	C4D-CHA	2.59	1.47	1.38
18	B	1227	CLA	C1B-C2B	2.59	1.49	1.43
18	G	1001	CLA	C3D-C2D	2.59	1.46	1.39
18	B	1210	CLA	C1D-C2D	2.59	1.50	1.45
18	1	1014	CLA	C3D-C2D	2.59	1.46	1.39
18	A	1110	CLA	C1B-C2B	2.58	1.49	1.43
18	A	1140	CLA	C1D-ND	-2.58	1.34	1.37
18	A	1132	CLA	C1B-C2B	2.58	1.49	1.43
18	A	1117	CLA	C1D-C2D	2.58	1.50	1.45
28	4	4013	CHL	CBD-CAD	-2.58	1.44	1.53
18	2	2004	CLA	C3D-C2D	2.58	1.46	1.39
18	B	1228	CLA	C1D-ND	-2.58	1.34	1.37
28	4	4011	CHL	C3D-C2D	-2.58	1.35	1.39
21	B	5004	LHG	O8-C23	2.58	1.45	1.33
18	A	1111	CLA	C1B-NB	-2.58	1.34	1.37
18	4	4009	CLA	MG-NC	2.58	2.12	2.06
18	B	1240	CLA	C1D-ND	-2.58	1.34	1.37
18	B	1228	CLA	C1B-C2B	2.57	1.49	1.43
18	B	1210	CLA	C1C-NC	-2.57	1.33	1.37
18	4	4003	CLA	C1C-NC	-2.57	1.33	1.37
18	2	2001	CLA	C2A-C1A	-2.57	1.46	1.52
18	A	1105	CLA	C1D-ND	-2.57	1.34	1.37
18	G	1001	CLA	C4D-CHA	2.57	1.47	1.38
23	F	5001	LMG	O7-C8	-2.57	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1213	CLA	C1D-ND	-2.57	1.34	1.37
18	1	1004	CLA	C3D-C2D	2.57	1.46	1.39
18	A	1113	CLA	C1D-ND	-2.57	1.34	1.37
18	B	1227	CLA	C1B-NB	-2.57	1.34	1.37
18	2	2003	CLA	C1C-NC	-2.57	1.33	1.37
18	A	1130	CLA	C1B-NB	-2.57	1.34	1.37
18	B	1211	CLA	C1D-ND	-2.57	1.34	1.37
18	B	1204	CLA	C1D-ND	-2.57	1.34	1.37
18	B	1214	CLA	C1D-ND	-2.57	1.34	1.37
22	F	6016	BCR	C1-C6	-2.57	1.50	1.53
18	B	1217	CLA	C1D-ND	-2.56	1.34	1.37
18	B	1231	CLA	C1B-NB	-2.56	1.34	1.37
18	B	1228	CLA	C1B-NB	-2.56	1.34	1.37
18	2	2006	CLA	C1C-NC	-2.56	1.33	1.37
18	A	1116	CLA	C1D-ND	-2.56	1.34	1.37
18	1	1001	CLA	C4D-CHA	2.56	1.47	1.38
18	L	1503	CLA	C4D-CHA	2.56	1.47	1.38
18	4	4007	CLA	MG-NC	2.56	2.12	2.06
18	A	1114	CLA	C1D-ND	-2.56	1.34	1.37
18	B	1223	CLA	C1B-NB	-2.56	1.34	1.37
22	L	6019	BCR	C1-C6	-2.56	1.50	1.53
18	G	1002	CLA	C1C-NC	-2.56	1.33	1.37
28	4	4011	CHL	CBD-CAD	-2.56	1.44	1.53
18	3	3017	CLA	C3D-C2D	2.55	1.46	1.39
18	A	1129	CLA	C1B-NB	-2.55	1.34	1.37
28	4	4011	CHL	C1B-C2B	2.55	1.42	1.39
18	A	1121	CLA	C1B-NB	-2.55	1.34	1.37
27	3	3502	LUT	C1-C6	-2.55	1.50	1.53
18	4	4008	CLA	OBD-CAD	2.55	1.26	1.22
18	A	1126	CLA	C1D-ND	-2.55	1.34	1.37
18	K	1001	CLA	C1B-C2B	2.55	1.49	1.43
18	A	1116	CLA	C1D-C2D	2.55	1.50	1.45
25	B	7101	DGD	O2G-C2G	-2.55	1.40	1.46
18	A	1117	CLA	C1B-NB	-2.55	1.34	1.37
18	2	2009	CLA	C3D-C2D	2.55	1.45	1.39
18	3	3003	CLA	C3D-C2D	2.55	1.45	1.39
18	A	1122	CLA	C1D-ND	-2.55	1.34	1.37
18	B	1211	CLA	C1C-NC	-2.55	1.33	1.37
18	A	1131	CLA	C1D-ND	-2.55	1.34	1.37
18	4	4016	CLA	C3D-C2D	2.55	1.45	1.39
18	B	1240	CLA	C1D-C2D	2.55	1.50	1.45
18	4	4008	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1224	CLA	C4C-C3C	2.55	1.49	1.45
18	B	1211	CLA	C1B-NB	-2.54	1.34	1.37
18	A	1126	CLA	C4C-C3C	2.54	1.49	1.45
18	B	1216	CLA	C1D-C2D	2.54	1.50	1.45
18	B	1208	CLA	C1D-C2D	2.54	1.50	1.45
18	A	1101	CLA	C1D-ND	-2.54	1.34	1.37
18	B	1023	CLA	C1B-NB	-2.54	1.34	1.37
18	B	1201	CLA	C1D-C2D	2.54	1.50	1.45
18	A	1114	CLA	C1D-C2D	2.54	1.50	1.45
18	G	1003	CLA	C4D-CHA	2.54	1.47	1.38
27	1	1501	LUT	C1-C6	-2.54	1.50	1.53
18	B	1023	CLA	C4C-C3C	2.54	1.49	1.45
18	A	1151	CLA	C1D-C2D	2.54	1.50	1.45
18	B	1225	CLA	C1B-NB	-2.54	1.34	1.37
18	B	1239	CLA	C1D-ND	-2.54	1.34	1.37
18	G	1002	CLA	C1D-C2D	2.53	1.50	1.45
22	3	3503	BCR	C1-C6	-2.53	1.50	1.53
18	B	1236	CLA	C1D-ND	-2.53	1.34	1.37
18	B	1234	CLA	C1D-ND	-2.53	1.34	1.37
18	2	2005	CLA	C1B-C2B	2.53	1.49	1.43
18	1	1002	CLA	MG-NC	2.53	2.12	2.06
18	B	1211	CLA	C1B-C2B	2.53	1.49	1.43
18	A	1131	CLA	C1D-C2D	2.53	1.50	1.45
18	B	1215	CLA	C1D-C2D	2.53	1.50	1.45
18	B	1232	CLA	C1D-ND	-2.53	1.34	1.37
18	A	1115	CLA	C1D-C2D	2.53	1.50	1.45
18	B	1234	CLA	C1B-NB	-2.52	1.34	1.37
18	A	1125	CLA	C1B-NB	-2.52	1.34	1.37
18	3	3017	CLA	OBD-CAD	2.52	1.26	1.22
18	A	1114	CLA	C1B-NB	-2.52	1.34	1.37
18	B	1210	CLA	C1D-ND	-2.52	1.34	1.37
18	1	1004	CLA	C1B-C2B	2.52	1.49	1.43
18	A	1105	CLA	C1D-C2D	2.52	1.50	1.45
18	B	1201	CLA	C1D-ND	-2.52	1.34	1.37
18	3	3017	CLA	C4D-CHA	2.52	1.47	1.38
18	A	1109	CLA	C1D-ND	-2.52	1.34	1.37
18	A	1132	CLA	C1B-NB	-2.52	1.34	1.37
18	A	1151	CLA	C4C-C3C	2.52	1.49	1.45
18	4	4007	CLA	C1B-C2B	2.52	1.49	1.43
18	A	1102	CLA	C1D-ND	-2.51	1.34	1.37
18	K	1001	CLA	C4D-CHA	2.51	1.47	1.38
18	A	1105	CLA	C3B-C4B	2.51	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1008	CLA	C3D-C2D	2.51	1.45	1.39
18	A	1123	CLA	C1B-NB	-2.51	1.34	1.37
18	A	1105	CLA	C1B-NB	-2.51	1.34	1.37
18	A	1139	CLA	C1D-ND	-2.51	1.34	1.37
18	B	1208	CLA	C1D-ND	-2.51	1.34	1.37
18	A	1121	CLA	C1D-C2D	2.51	1.50	1.45
18	H	1000	CLA	C1B-NB	-2.50	1.34	1.37
18	B	1236	CLA	C1D-C2D	2.50	1.50	1.45
18	A	1122	CLA	C1D-C2D	2.50	1.50	1.45
18	1	1008	CLA	C1C-NC	-2.50	1.34	1.37
18	4	4005	CLA	C4D-CHA	2.50	1.47	1.38
22	J	6013	BCR	C1-C6	-2.50	1.50	1.53
18	A	1138	CLA	C1D-C2D	2.50	1.50	1.45
18	A	1122	CLA	C1B-NB	-2.50	1.34	1.37
18	B	1012	CLA	C1B-NB	-2.50	1.34	1.37
27	1	1502	LUT	C26-C27	-2.50	1.47	1.50
18	A	1135	CLA	C1B-NB	-2.50	1.34	1.37
18	B	1209	CLA	C4B-NB	-2.50	1.34	1.37
18	A	1139	CLA	C1D-C2D	2.50	1.50	1.45
18	3	3012	CLA	C3D-C2D	2.50	1.45	1.39
18	A	1111	CLA	C4B-NB	-2.50	1.34	1.37
18	A	1151	CLA	C1D-ND	-2.50	1.34	1.37
18	A	1133	CLA	C4B-NB	-2.49	1.34	1.37
18	3	3005	CLA	C4D-CHA	2.49	1.47	1.38
18	2	2007	CLA	C1C-NC	-2.49	1.34	1.37
18	B	1228	CLA	C1D-C2D	2.49	1.50	1.45
18	G	1003	CLA	C3D-C2D	2.49	1.45	1.39
18	4	4002	CLA	C1B-C2B	2.49	1.49	1.43
18	H	1000	CLA	C1D-C2D	2.49	1.50	1.45
18	A	1137	CLA	C1C-NC	-2.49	1.34	1.37
18	A	1013	CLA	C1B-C2B	2.49	1.49	1.43
18	2	2003	CLA	C3D-C2D	2.49	1.45	1.39
18	B	1214	CLA	C1B-NB	-2.49	1.34	1.37
18	L	1502	CLA	C4D-CHA	2.49	1.46	1.38
18	A	1109	CLA	C1D-C2D	2.49	1.50	1.45
18	3	3010	CLA	C3D-C2D	2.48	1.45	1.39
18	B	1217	CLA	C1B-NB	-2.48	1.34	1.37
18	2	2001	CLA	MG-NC	2.48	2.12	2.06
27	4	4503	LUT	C1-C6	-2.48	1.50	1.53
18	1	1007	CLA	C4D-CHA	2.48	1.46	1.38
27	1	1501	LUT	C26-C27	-2.48	1.47	1.50
18	B	1232	CLA	C1D-C2D	2.48	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1022	CLA	C1B-NB	-2.48	1.34	1.37
18	4	4003	CLA	C1B-C2B	2.48	1.48	1.43
18	A	1106	CLA	C1D-ND	-2.47	1.34	1.37
18	A	1134	CLA	C1D-ND	-2.47	1.34	1.37
18	3	3002	CLA	C1B-C2B	2.47	1.48	1.43
18	B	1235	CLA	C1D-C2D	2.47	1.50	1.45
18	2	2003	CLA	C4D-CHA	2.47	1.46	1.38
18	B	1210	CLA	C3B-C4B	2.47	1.49	1.42
18	A	1136	CLA	C1B-NB	-2.47	1.34	1.37
18	A	1140	CLA	C1D-C2D	2.47	1.50	1.45
18	A	1113	CLA	C4C-C3C	2.47	1.49	1.45
18	B	1235	CLA	C1D-ND	-2.47	1.34	1.37
18	A	1109	CLA	C1B-NB	-2.47	1.34	1.37
18	A	1114	CLA	C4C-C3C	2.47	1.49	1.45
18	A	1120	CLA	C1D-C2D	2.46	1.50	1.45
18	3	3006	CLA	C1B-C2B	2.46	1.48	1.43
18	F	1302	CLA	C1B-C2B	2.46	1.48	1.43
18	A	1151	CLA	C1B-NB	-2.46	1.34	1.37
18	3	3001	CLA	C1B-C2B	2.46	1.48	1.43
18	A	1126	CLA	C1B-NB	-2.46	1.34	1.37
18	B	1207	CLA	C1B-NB	-2.46	1.34	1.37
18	A	1130	CLA	C1D-C2D	2.46	1.50	1.45
18	A	1102	CLA	C1B-NB	-2.46	1.34	1.37
28	1	1009	CHL	C1D-C2D	2.46	1.42	1.39
18	B	1209	CLA	C1D-C2D	2.46	1.50	1.45
18	B	1234	CLA	C4B-NB	-2.46	1.34	1.37
18	B	1204	CLA	C1B-NB	-2.46	1.34	1.37
18	A	1112	CLA	C1B-NB	-2.45	1.34	1.37
18	B	1207	CLA	C4B-NB	-2.45	1.34	1.37
18	B	1220	CLA	C1B-NB	-2.45	1.34	1.37
18	A	1111	CLA	C1D-C2D	2.45	1.50	1.45
18	A	1110	CLA	C1D-C2D	2.45	1.50	1.45
28	2	2013	CHL	C1D-C2D	2.45	1.42	1.39
18	A	1237	CLA	C1B-NB	-2.45	1.34	1.37
18	B	1238	CLA	C1B-NB	-2.45	1.34	1.37
18	L	1502	CLA	C3D-C2D	2.45	1.45	1.39
18	A	1124	CLA	C1D-ND	-2.45	1.34	1.37
18	1	1005	CLA	C4D-CHA	2.44	1.46	1.38
18	A	1106	CLA	C1B-NB	-2.44	1.34	1.37
18	J	1302	CLA	C1D-C2D	2.44	1.50	1.45
18	A	1112	CLA	C4B-NB	-2.44	1.34	1.37
18	B	1223	CLA	C1C-NC	-2.44	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1115	CLA	C4C-C3C	2.44	1.49	1.45
27	4	4503	LUT	C26-C27	-2.44	1.47	1.50
18	A	1132	CLA	C4B-NB	-2.44	1.34	1.37
18	J	1302	CLA	C1B-NB	-2.44	1.34	1.37
18	A	1104	CLA	C1D-C2D	2.44	1.50	1.45
18	A	1108	CLA	C1B-NB	-2.44	1.34	1.37
18	A	1124	CLA	C1B-NB	-2.44	1.34	1.37
18	A	1106	CLA	C1D-C2D	2.44	1.50	1.45
18	A	1113	CLA	C1D-C2D	2.44	1.50	1.45
18	2	2012	CLA	MG-NC	2.44	2.12	2.06
18	1	1003	CLA	C1B-C2B	2.43	1.48	1.43
18	B	1210	CLA	C4C-C3C	2.43	1.49	1.45
18	4	4002	CLA	C3D-C2D	2.43	1.45	1.39
18	B	1224	CLA	C1D-C2D	2.43	1.50	1.45
18	B	1209	CLA	C4C-C3C	2.43	1.49	1.45
18	1	1006	CLA	C4D-CHA	2.43	1.46	1.38
18	B	1240	CLA	C1B-NB	-2.43	1.34	1.37
28	2	2010	CHL	C2C-C3C	-2.42	1.34	1.36
18	A	1107	CLA	C1D-C2D	2.42	1.50	1.45
18	A	1103	CLA	C1D-C2D	2.42	1.50	1.45
18	B	1239	CLA	C1D-C2D	2.42	1.50	1.45
18	B	1236	CLA	C1B-NB	-2.42	1.34	1.37
18	4	4005	CLA	OBD-CAD	2.42	1.26	1.22
18	B	1218	CLA	C1D-C2D	2.42	1.50	1.45
18	L	1502	CLA	C1B-C2B	2.42	1.48	1.43
27	1	1502	LUT	C1-C6	-2.42	1.50	1.53
18	A	1119	CLA	C1D-C2D	2.42	1.50	1.45
18	A	1124	CLA	C1D-C2D	2.42	1.50	1.45
18	B	1212	CLA	C1B-NB	-2.42	1.34	1.37
18	A	1101	CLA	C4C-C3C	2.42	1.49	1.45
18	A	1125	CLA	C1C-NC	-2.42	1.34	1.37
18	G	1003	CLA	C1D-C2D	2.42	1.50	1.45
18	3	3001	CLA	MG-NC	2.42	2.12	2.06
18	B	1238	CLA	C1D-C2D	2.41	1.50	1.45
18	A	1139	CLA	C1B-NB	-2.41	1.34	1.37
18	A	1126	CLA	C1D-C2D	2.41	1.50	1.45
18	3	3010	CLA	MG-NC	2.41	2.12	2.06
18	A	1114	CLA	C3B-C4B	2.41	1.49	1.42
18	A	1135	CLA	C1D-C2D	2.41	1.50	1.45
18	B	1211	CLA	C1D-C2D	2.41	1.50	1.45
18	A	1137	CLA	C1D-C2D	2.41	1.50	1.45
18	1	1003	CLA	C4D-CHA	2.41	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	C1D-C2D	2.41	1.50	1.45
18	A	1022	CLA	C4C-C3C	2.41	1.49	1.45
18	B	1221	CLA	C1D-ND	-2.41	1.34	1.37
18	4	4016	CLA	C1D-C2D	2.41	1.50	1.45
18	3	3019	CLA	C3C-C4C	2.41	1.48	1.43
18	A	1110	CLA	C3B-C4B	2.40	1.49	1.42
18	3	3018	CLA	C1B-C2B	2.40	1.48	1.43
18	4	4009	CLA	C4D-CHA	2.40	1.46	1.38
18	B	1213	CLA	C1D-C2D	2.40	1.50	1.45
18	B	1218	CLA	C1B-NB	-2.40	1.34	1.37
28	2	2011	CHL	C1D-C2D	2.40	1.42	1.39
18	2	2009	CLA	C4D-CHA	2.40	1.46	1.38
18	1	1012	CLA	C4D-CHA	2.40	1.46	1.38
18	A	1107	CLA	C1B-NB	-2.40	1.34	1.37
18	A	1151	CLA	C1C-NC	-2.40	1.34	1.37
18	A	1111	CLA	C1C-NC	-2.40	1.34	1.37
18	A	1109	CLA	C3B-C4B	2.40	1.49	1.42
18	A	1113	CLA	C1B-NB	-2.39	1.34	1.37
18	B	1220	CLA	C1C-NC	-2.39	1.34	1.37
18	1	1011	CLA	C1B-C2B	2.39	1.48	1.43
18	3	3002	CLA	OBD-CAD	2.39	1.26	1.22
18	3	3012	CLA	MG-NC	2.39	2.12	2.06
18	A	1126	CLA	C4B-NB	-2.39	1.34	1.37
18	A	1135	CLA	C4C-C3C	2.39	1.49	1.45
18	A	1136	CLA	C1D-C2D	2.39	1.50	1.45
18	2	2001	CLA	C4D-CHA	2.39	1.46	1.38
28	1	1010	CHL	C1B-C2B	2.39	1.42	1.39
18	B	1208	CLA	C1B-NB	-2.39	1.34	1.37
18	1	1004	CLA	C4D-CHA	2.39	1.46	1.38
18	B	1021	CLA	C4B-NB	-2.38	1.34	1.37
18	B	1229	CLA	C1C-NC	-2.38	1.34	1.37
18	A	1115	CLA	C1B-NB	-2.38	1.34	1.37
18	1	1013	CLA	C3D-C2D	2.38	1.45	1.39
18	B	1224	CLA	C4B-NB	-2.38	1.34	1.37
18	A	1013	CLA	C3B-C4B	2.38	1.49	1.42
18	B	1234	CLA	C4C-C3C	2.38	1.49	1.45
18	B	1207	CLA	C1C-NC	-2.38	1.34	1.37
18	B	1204	CLA	C4C-C3C	2.38	1.49	1.45
18	A	1116	CLA	C1B-NB	-2.38	1.34	1.37
18	A	1132	CLA	C1C-NC	-2.38	1.34	1.37
22	F	6016	BCR	C30-C25	-2.38	1.50	1.53
18	3	3002	CLA	C1D-C2D	2.37	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1226	CLA	C1D-C2D	2.37	1.50	1.45
22	3	3503	BCR	C30-C25	-2.37	1.50	1.53
18	1	1014	CLA	C4D-CHA	2.37	1.46	1.38
18	J	1302	CLA	C4C-C3C	2.37	1.49	1.45
18	B	1208	CLA	C3B-C4B	2.37	1.49	1.42
18	A	1120	CLA	C1B-NB	-2.37	1.34	1.37
18	A	1104	CLA	C3B-C4B	2.37	1.49	1.42
18	A	1133	CLA	C1C-NC	-2.37	1.34	1.37
18	B	1205	CLA	C1C-NC	-2.37	1.34	1.37
18	B	1236	CLA	C4B-NB	-2.37	1.34	1.37
18	A	1134	CLA	C4C-C3C	2.37	1.49	1.45
18	4	4012	CLA	MG-NC	2.37	2.11	2.06
18	B	1207	CLA	C1D-C2D	2.37	1.50	1.45
18	A	1112	CLA	C4C-C3C	2.37	1.49	1.45
18	B	1230	CLA	C1B-NB	-2.37	1.34	1.37
18	H	1000	CLA	C4C-C3C	2.37	1.49	1.45
18	B	1204	CLA	C1C-NC	-2.37	1.34	1.37
18	A	1122	CLA	C4C-C3C	2.36	1.49	1.45
18	3	3019	CLA	C2C-C1C	2.36	1.48	1.43
18	A	1134	CLA	C1B-NB	-2.36	1.34	1.37
18	A	1123	CLA	C4C-C3C	2.36	1.49	1.45
18	L	1501	CLA	C3D-C2D	2.36	1.45	1.39
18	A	1101	CLA	C1C-NC	-2.36	1.34	1.37
18	3	3010	CLA	C4D-CHA	2.36	1.46	1.38
18	B	1219	CLA	C1D-C2D	2.36	1.50	1.45
18	3	3019	CLA	C3B-C2B	2.36	1.47	1.39
18	4	4004	CLA	C3D-C2D	2.36	1.45	1.39
18	G	1002	CLA	C1B-C2B	2.36	1.48	1.43
18	2	2008	CLA	C1B-C2B	2.36	1.48	1.43
18	B	1202	CLA	C1D-C2D	2.35	1.50	1.45
18	3	3008	CLA	C3D-C2D	2.35	1.45	1.39
18	2	2019	CLA	CHD-C4C	2.35	1.48	1.40
18	3	3001	CLA	C4D-CHA	2.35	1.46	1.38
18	B	1205	CLA	C1B-NB	-2.35	1.34	1.37
18	A	1110	CLA	C1C-NC	-2.35	1.34	1.37
18	B	1203	CLA	C1B-NB	-2.35	1.34	1.37
18	A	1237	CLA	C1C-NC	-2.35	1.34	1.37
18	A	1136	CLA	C4C-C3C	2.35	1.49	1.45
18	B	1221	CLA	C4B-NB	-2.35	1.34	1.37
28	1	1009	CHL	C1B-C2B	2.34	1.42	1.39
18	A	1131	CLA	C1B-NB	-2.34	1.34	1.37
18	3	3007	CLA	C4D-CHA	2.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1133	CLA	C4C-C3C	2.34	1.49	1.45
18	B	1234	CLA	C1D-C2D	2.34	1.50	1.45
18	4	4006	CLA	C4D-CHA	2.34	1.46	1.38
18	3	3008	CLA	C1C-NC	-2.34	1.34	1.37
18	A	1138	CLA	C4C-C3C	2.34	1.49	1.45
18	A	1123	CLA	C1D-C2D	2.34	1.50	1.45
18	A	1137	CLA	C1B-NB	-2.34	1.34	1.37
18	A	1118	CLA	C1D-C2D	2.34	1.50	1.45
18	B	1202	CLA	C4B-NB	-2.34	1.34	1.37
18	B	1232	CLA	C3B-C4B	2.34	1.49	1.42
18	A	1140	CLA	C1B-NB	-2.34	1.34	1.37
18	3	3012	CLA	C4D-CHA	2.34	1.46	1.38
18	B	1235	CLA	C1B-NB	-2.33	1.34	1.37
18	B	1231	CLA	C3B-C4B	2.33	1.49	1.42
18	B	1212	CLA	C1D-C2D	2.33	1.50	1.45
18	A	1119	CLA	C4C-C3C	2.33	1.49	1.45
18	A	1103	CLA	C1B-NB	-2.33	1.34	1.37
18	A	1013	CLA	C1D-C2D	2.33	1.49	1.45
18	K	1001	CLA	C3D-C2D	2.33	1.45	1.39
18	B	1232	CLA	C1B-NB	-2.33	1.34	1.37
18	A	1114	CLA	C1C-NC	-2.33	1.34	1.37
18	B	1220	CLA	C4B-NB	-2.32	1.34	1.37
18	B	1232	CLA	C4C-C3C	2.32	1.49	1.45
18	A	1119	CLA	C1C-NC	-2.32	1.34	1.37
18	A	1101	CLA	C4B-NB	-2.32	1.34	1.37
28	2	2010	CHL	C1B-C2B	2.32	1.42	1.39
18	A	1105	CLA	C4C-C3C	2.32	1.49	1.45
18	A	1108	CLA	C4C-C3C	2.32	1.49	1.45
22	I	6020	BCR	C30-C25	-2.32	1.50	1.53
18	B	1236	CLA	C1C-NC	-2.32	1.34	1.37
18	B	1226	CLA	C4C-C3C	2.32	1.49	1.45
18	B	1213	CLA	C1C-NC	-2.32	1.34	1.37
18	A	1121	CLA	C1C-NC	-2.32	1.34	1.37
18	B	1201	CLA	C1B-NB	-2.32	1.34	1.37
18	3	3002	CLA	C3D-C2D	2.32	1.45	1.39
18	B	1217	CLA	C1C-NC	-2.32	1.34	1.37
18	4	4009	CLA	C3D-C2D	2.32	1.45	1.39
18	B	1023	CLA	C1C-NC	-2.32	1.34	1.37
18	A	1116	CLA	C3B-C4B	2.31	1.49	1.42
18	H	1000	CLA	C1C-NC	-2.31	1.34	1.37
27	4	4501	LUT	C1-C6	-2.31	1.50	1.53
18	B	1205	CLA	C4C-C3C	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	2010	CHL	CHD-C1D	-2.31	1.35	1.39
18	1	1002	CLA	C4D-CHA	2.31	1.46	1.38
18	A	1105	CLA	C1C-NC	-2.31	1.34	1.37
18	A	1113	CLA	C1C-NC	-2.31	1.34	1.37
18	3	3018	CLA	C3D-C2D	2.31	1.45	1.39
18	4	4008	CLA	C1B-C2B	2.31	1.48	1.43
18	B	1228	CLA	C1C-NC	-2.31	1.34	1.37
18	3	3006	CLA	C3D-C2D	2.31	1.45	1.39
18	A	1104	CLA	C1D-ND	-2.31	1.34	1.37
18	B	1232	CLA	C1C-NC	-2.31	1.34	1.37
18	B	1202	CLA	C4C-C3C	2.31	1.49	1.45
18	A	1128	CLA	C1C-NC	-2.30	1.34	1.37
18	F	1302	CLA	C1D-C2D	2.30	1.49	1.45
18	3	3019	CLA	CHD-C4C	2.30	1.48	1.40
18	B	1205	CLA	C4B-NB	-2.30	1.34	1.37
18	2	2009	CLA	C1B-C2B	2.30	1.48	1.43
18	4	4001	CLA	C3D-C2D	2.30	1.45	1.39
18	B	1214	CLA	C4C-C3C	2.30	1.48	1.45
18	A	1109	CLA	C1C-NC	-2.30	1.34	1.37
18	3	3013	CLA	C4D-CHA	2.30	1.46	1.38
18	2	2005	CLA	C1D-C2D	2.30	1.49	1.45
18	A	1120	CLA	C1C-NC	-2.30	1.34	1.37
18	A	1124	CLA	C4C-C3C	2.30	1.48	1.45
18	A	1106	CLA	C1C-NC	-2.30	1.34	1.37
18	B	1209	CLA	C1C-NC	-2.30	1.34	1.37
18	A	1139	CLA	C4C-C3C	2.30	1.48	1.45
18	B	1222	CLA	C1B-NB	-2.30	1.34	1.37
18	B	1023	CLA	C4B-NB	-2.30	1.34	1.37
18	A	1112	CLA	C1C-NC	-2.29	1.34	1.37
28	3	3011	CHL	C1B-C2B	2.29	1.42	1.39
18	B	1220	CLA	C1D-C2D	2.29	1.49	1.45
18	A	1139	CLA	C3B-C4B	2.29	1.49	1.42
18	A	1135	CLA	C4B-NB	-2.29	1.34	1.37
18	L	1503	CLA	C1B-C2B	2.29	1.48	1.43
18	1	1002	CLA	C1B-C2B	2.29	1.48	1.43
18	B	1202	CLA	C1C-NC	-2.29	1.34	1.37
18	B	1214	CLA	C1C-NC	-2.29	1.34	1.37
18	A	1127	CLA	C4C-C3C	2.29	1.48	1.45
18	A	1103	CLA	C1C-NC	-2.29	1.34	1.37
18	A	1138	CLA	C1C-NC	-2.29	1.34	1.37
18	A	1110	CLA	C4C-C3C	2.29	1.48	1.45
18	B	1238	CLA	C1C-NC	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	1003	CLA	C1B-C2B	2.29	1.48	1.43
18	A	1109	CLA	C4C-C3C	2.29	1.48	1.45
18	4	4006	CLA	C1B-C2B	2.28	1.48	1.43
18	A	1113	CLA	C4B-NB	-2.28	1.34	1.37
18	B	1229	CLA	C1B-NB	-2.28	1.34	1.37
18	B	1239	CLA	C1C-NC	-2.28	1.34	1.37
18	B	1231	CLA	C4C-C3C	2.28	1.48	1.45
18	A	1108	CLA	C1C-NC	-2.28	1.34	1.37
18	B	1205	CLA	C1D-C2D	2.28	1.49	1.45
18	1	1012	CLA	C1B-C2B	2.27	1.48	1.43
18	A	1140	CLA	C1C-NC	-2.27	1.34	1.37
28	1	1010	CHL	C1D-C2D	2.27	1.42	1.39
18	B	1229	CLA	C1D-C2D	2.27	1.49	1.45
18	B	1201	CLA	C4C-C3C	2.27	1.48	1.45
18	1	1005	CLA	C3D-C2D	2.27	1.45	1.39
18	B	1230	CLA	C1C-NC	-2.27	1.34	1.37
18	2	2003	CLA	C1B-C2B	2.27	1.48	1.43
28	4	4013	CHL	C1B-C2B	2.27	1.42	1.39
18	B	1203	CLA	C1C-NC	-2.27	1.34	1.37
28	4	4010	CHL	C1B-C2B	2.27	1.42	1.39
18	A	1022	CLA	C1D-C2D	2.27	1.49	1.45
27	1	1501	LUT	C23-C24	2.27	1.53	1.50
18	B	1222	CLA	C1C-NC	-2.27	1.34	1.37
18	B	1214	CLA	C4B-NB	-2.27	1.34	1.37
18	B	1221	CLA	C1D-C2D	2.27	1.49	1.45
18	B	1212	CLA	C1C-NC	-2.27	1.34	1.37
18	B	1204	CLA	C4B-NB	-2.27	1.34	1.37
18	1	1007	CLA	C1B-C2B	2.27	1.48	1.43
18	B	1203	CLA	C1D-C2D	2.26	1.49	1.45
18	B	1219	CLA	C4C-C3C	2.26	1.48	1.45
18	2	2002	CLA	C4D-CHA	2.26	1.46	1.38
18	4	4012	CLA	C4D-CHA	2.26	1.46	1.38
18	A	1106	CLA	C4B-NB	-2.26	1.34	1.37
18	A	1107	CLA	C4C-C3C	2.26	1.48	1.45
18	A	1130	CLA	C4B-NB	-2.26	1.34	1.37
28	4	4011	CHL	C1D-C2D	2.26	1.42	1.39
18	B	1021	CLA	C1D-C2D	2.26	1.49	1.45
18	B	1220	CLA	C4C-C3C	2.26	1.48	1.45
18	2	2002	CLA	C3D-C2D	2.26	1.45	1.39
18	A	1104	CLA	C4C-C3C	2.26	1.48	1.45
18	2	2007	CLA	C1D-C2D	2.26	1.49	1.45
18	B	1206	CLA	C1D-C2D	2.26	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1240	CLA	C1C-NC	-2.26	1.34	1.37
18	A	1108	CLA	C4B-NB	-2.26	1.34	1.37
18	3	3005	CLA	C3D-C2D	2.26	1.45	1.39
18	A	1133	CLA	C1D-C2D	2.25	1.49	1.45
18	B	1206	CLA	C4C-C3C	2.25	1.48	1.45
18	B	1228	CLA	C4B-NB	-2.25	1.34	1.37
18	A	1102	CLA	C1D-C2D	2.25	1.49	1.45
18	4	4005	CLA	C1B-C2B	2.25	1.48	1.43
18	1	1013	CLA	C4C-C3C	2.25	1.48	1.45
18	A	1121	CLA	C3B-C4B	2.25	1.49	1.42
18	A	1118	CLA	C1C-NC	-2.25	1.34	1.37
18	B	1216	CLA	C4B-NB	-2.25	1.34	1.37
18	2	2008	CLA	C4D-CHA	2.25	1.46	1.38
18	A	1121	CLA	C4C-C3C	2.25	1.48	1.45
18	A	1126	CLA	C1C-NC	-2.25	1.34	1.37
18	B	1218	CLA	C3B-C4B	2.25	1.49	1.42
18	A	1138	CLA	C4B-NB	-2.25	1.34	1.37
18	A	1013	CLA	C1C-NC	-2.25	1.34	1.37
18	3	3004	CLA	C4D-CHA	2.25	1.46	1.38
18	A	1125	CLA	C4B-NB	-2.25	1.34	1.37
18	2	2006	CLA	C1D-C2D	2.25	1.49	1.45
18	A	1137	CLA	C4B-NB	-2.25	1.34	1.37
18	1	1014	CLA	C1B-C2B	2.25	1.48	1.43
18	A	1116	CLA	C4C-C3C	2.25	1.48	1.45
28	4	4013	CHL	C1D-C2D	2.24	1.42	1.39
18	A	1117	CLA	C4C-C3C	2.24	1.48	1.45
18	A	1130	CLA	C1C-NC	-2.24	1.34	1.37
18	A	1116	CLA	C1C-NC	-2.24	1.34	1.37
18	A	1136	CLA	C1C-NC	-2.24	1.34	1.37
18	B	1226	CLA	C1C-NC	-2.24	1.34	1.37
18	A	1111	CLA	C4C-C3C	2.24	1.48	1.45
18	2	2004	CLA	C4D-CHA	2.24	1.46	1.38
18	3	3005	CLA	C1B-C2B	2.24	1.48	1.43
18	F	1301	CLA	C1D-C2D	2.24	1.49	1.45
18	A	1123	CLA	C1C-NC	-2.24	1.34	1.37
18	A	1102	CLA	C1C-NC	-2.23	1.34	1.37
18	B	1221	CLA	C4C-C3C	2.23	1.48	1.45
18	B	1213	CLA	C4B-NB	-2.23	1.34	1.37
18	B	1012	CLA	C1C-NC	-2.23	1.34	1.37
18	A	1129	CLA	C4C-C3C	2.23	1.48	1.45
18	B	1207	CLA	C4C-C3C	2.23	1.48	1.45
18	A	1139	CLA	C1C-NC	-2.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1127	CLA	C1C-NC	-2.23	1.34	1.37
28	3	3011	CHL	C1D-C2D	2.23	1.42	1.39
18	1	1006	CLA	C3D-C2D	2.23	1.45	1.39
18	3	3012	CLA	C1B-C2B	2.23	1.48	1.43
18	B	1239	CLA	C4C-C3C	2.23	1.48	1.45
27	2	2502	LUT	C1-C6	-2.23	1.50	1.53
18	B	1012	CLA	C4B-NB	-2.23	1.34	1.37
28	2	2010	CHL	CBD-CAD	-2.23	1.45	1.53
18	3	3003	CLA	C4C-C3C	2.23	1.48	1.45
18	A	1117	CLA	C1C-NC	-2.23	1.34	1.37
18	J	1302	CLA	C4B-NB	-2.23	1.34	1.37
18	A	1132	CLA	C4C-C3C	2.23	1.48	1.45
18	B	1235	CLA	C1C-NC	-2.22	1.34	1.37
18	B	1212	CLA	C4B-NB	-2.22	1.34	1.37
18	B	1023	CLA	C1D-C2D	2.22	1.49	1.45
18	A	1103	CLA	C4B-NB	-2.22	1.34	1.37
18	A	1127	CLA	C1D-C2D	2.22	1.49	1.45
18	B	1217	CLA	C4C-C3C	2.22	1.48	1.45
18	B	1219	CLA	C1C-NC	-2.22	1.34	1.37
18	B	1227	CLA	C4B-NB	-2.22	1.34	1.37
18	3	3006	CLA	C4D-CHA	2.22	1.46	1.38
18	A	1128	CLA	C1B-C2B	2.22	1.48	1.43
18	A	1104	CLA	C1C-C2C	2.22	1.49	1.44
18	B	1208	CLA	C1C-NC	-2.22	1.34	1.37
18	B	1218	CLA	C4C-C3C	2.22	1.48	1.45
18	A	1140	CLA	C3B-C4B	2.22	1.49	1.42
18	2	2012	CLA	C4D-CHA	2.21	1.46	1.38
18	A	1237	CLA	C4B-NB	-2.21	1.35	1.37
18	A	1151	CLA	C4B-NB	-2.21	1.35	1.37
18	2	2009	CLA	C1D-C2D	2.21	1.49	1.45
18	A	1121	CLA	C4B-NB	-2.21	1.35	1.37
18	A	1119	CLA	C4B-NB	-2.21	1.35	1.37
18	1	1007	CLA	C3D-C2D	2.21	1.45	1.39
18	4	4017	CLA	C1B-C2B	2.21	1.48	1.43
28	1	1010	CHL	C2C-C3C	-2.21	1.34	1.36
18	A	1237	CLA	C4C-C3C	2.21	1.48	1.45
18	A	1104	CLA	C4B-NB	-2.21	1.35	1.37
18	B	1216	CLA	C1C-NC	-2.21	1.34	1.37
18	A	1122	CLA	C1C-NC	-2.21	1.34	1.37
18	A	1128	CLA	C4C-C3C	2.21	1.48	1.45
18	A	1103	CLA	C4C-C3C	2.21	1.48	1.45
18	B	1217	CLA	C3B-C4B	2.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1135	CLA	C1C-NC	-2.21	1.34	1.37
18	B	1223	CLA	C4B-NB	-2.20	1.35	1.37
18	1	1001	CLA	C1B-C2B	2.20	1.48	1.43
18	A	1134	CLA	C1C-NC	-2.20	1.34	1.37
18	4	4008	CLA	C3D-C2D	2.20	1.45	1.39
18	G	1001	CLA	C1B-C2B	2.20	1.48	1.43
18	B	1201	CLA	C4B-NB	-2.20	1.35	1.37
18	4	4009	CLA	C1B-C2B	2.20	1.48	1.43
18	B	1216	CLA	C4C-C3C	2.20	1.48	1.45
18	H	1000	CLA	C4B-NB	-2.20	1.35	1.37
18	B	1208	CLA	C4C-C3C	2.20	1.48	1.45
18	B	1222	CLA	C3B-C4B	2.20	1.49	1.42
18	A	1104	CLA	C1C-NC	-2.20	1.34	1.37
18	J	1302	CLA	C1C-NC	-2.20	1.34	1.37
18	B	1240	CLA	C3B-C4B	2.19	1.49	1.42
28	2	2010	CHL	C1D-C2D	2.19	1.42	1.39
18	4	4004	CLA	C4D-CHA	2.19	1.45	1.38
18	B	1222	CLA	C1D-C2D	2.19	1.49	1.45
18	A	1129	CLA	C1D-C2D	2.19	1.49	1.45
18	3	3001	CLA	C3D-C2D	2.19	1.45	1.39
18	2	2002	CLA	C1B-C2B	2.19	1.48	1.43
18	B	1213	CLA	C3B-C4B	2.19	1.49	1.42
18	A	1123	CLA	C4B-NB	-2.19	1.35	1.37
18	B	1215	CLA	C4C-C3C	2.19	1.48	1.45
18	A	1129	CLA	C4B-NB	-2.18	1.35	1.37
27	2	2502	LUT	C26-C27	-2.18	1.47	1.50
22	A	6007	BCR	C30-C25	-2.18	1.51	1.53
18	B	1201	CLA	C1C-NC	-2.18	1.34	1.37
18	A	1124	CLA	C3B-C4B	2.18	1.49	1.42
18	B	1218	CLA	C1C-NC	-2.18	1.34	1.37
18	B	1206	CLA	C1C-NC	-2.18	1.34	1.37
18	2	2019	CLA	C1C-NC	-2.18	1.33	1.38
18	B	1215	CLA	C1C-NC	-2.18	1.34	1.37
18	B	1227	CLA	C4C-C3C	2.18	1.48	1.45
18	B	1228	CLA	C3B-C4B	2.18	1.49	1.42
28	2	2011	CHL	C1B-C2B	2.18	1.42	1.39
18	2	2008	CLA	MG-NC	2.18	2.11	2.06
18	B	1238	CLA	C3B-C4B	2.18	1.49	1.42
18	4	4007	CLA	C3D-C2D	2.18	1.44	1.39
18	1	1005	CLA	C1B-C2B	2.18	1.48	1.43
18	A	1124	CLA	C1C-NC	-2.18	1.34	1.37
28	4	4013	CHL	CHB-C1B	-2.18	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1222	CLA	C4B-NB	-2.17	1.35	1.37
18	A	1130	CLA	C4C-C3C	2.17	1.48	1.45
18	B	1240	CLA	C4B-NB	-2.17	1.35	1.37
27	4	4502	LUT	C1-C6	-2.17	1.51	1.53
18	B	1227	CLA	C1C-NC	-2.17	1.34	1.37
18	B	1206	CLA	C4B-NB	-2.17	1.35	1.37
18	B	1212	CLA	C4C-C3C	2.17	1.48	1.45
18	A	1120	CLA	C4B-NB	-2.17	1.35	1.37
18	A	1118	CLA	C4B-NB	-2.17	1.35	1.37
18	B	1021	CLA	C1C-NC	-2.17	1.34	1.37
18	A	1102	CLA	C3B-C4B	2.16	1.49	1.42
18	A	1107	CLA	C4B-NB	-2.16	1.35	1.37
22	L	6020	BCR	C1-C6	-2.16	1.51	1.53
18	3	3004	CLA	C1B-C2B	2.16	1.48	1.43
18	A	1131	CLA	C1C-NC	-2.16	1.34	1.37
18	A	1106	CLA	C4C-C3C	2.16	1.48	1.45
18	2	2019	CLA	C3B-C2B	2.16	1.46	1.39
18	B	1239	CLA	C3B-C4B	2.16	1.49	1.42
18	A	1101	CLA	C3B-C4B	2.16	1.49	1.42
18	4	4012	CLA	C1B-C2B	2.16	1.48	1.43
18	B	1215	CLA	C3B-C4B	2.16	1.49	1.42
18	A	1115	CLA	C4B-NB	-2.16	1.35	1.37
18	3	3018	CLA	C1D-C2D	2.15	1.49	1.45
22	L	6019	BCR	C30-C25	-2.15	1.51	1.53
18	A	1137	CLA	C3B-C4B	2.15	1.49	1.42
18	1	1011	CLA	C4D-CHA	2.15	1.45	1.38
18	A	1115	CLA	C1C-NC	-2.15	1.34	1.37
18	3	3007	CLA	C1B-C2B	2.15	1.48	1.43
18	B	1216	CLA	C1B-C2B	2.15	1.48	1.43
28	4	4013	CHL	CHC-C4B	-2.15	1.36	1.39
18	4	4008	CLA	MG-NB	-2.15	2.01	2.05
18	B	1235	CLA	C3B-C4B	2.14	1.49	1.42
18	B	1219	CLA	C4B-NB	-2.14	1.35	1.37
18	A	1137	CLA	C4C-C3C	2.14	1.48	1.45
27	2	2501	LUT	C1-C6	-2.14	1.51	1.53
18	B	1229	CLA	C4B-NB	-2.14	1.35	1.37
18	A	1108	CLA	C3B-C4B	2.14	1.49	1.42
18	A	1129	CLA	C1C-NC	-2.14	1.34	1.37
18	3	3007	CLA	C1D-C2D	2.14	1.49	1.45
22	A	6002	BCR	C30-C25	-2.14	1.51	1.53
18	A	1127	CLA	C4B-NB	-2.14	1.35	1.37
18	2	2004	CLA	CHB-C4A	-2.14	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1120	CLA	C3B-C4B	2.14	1.49	1.42
18	A	1136	CLA	C3B-C4B	2.14	1.49	1.42
18	B	1203	CLA	C4B-NB	-2.14	1.35	1.37
18	4	4004	CLA	MG-NC	2.14	2.11	2.06
18	1	1006	CLA	C4C-C3C	2.13	1.48	1.45
18	B	1225	CLA	C1D-C2D	2.13	1.49	1.45
18	B	1211	CLA	C4C-C3C	2.13	1.48	1.45
18	B	1225	CLA	C1C-NC	-2.13	1.34	1.37
18	A	1013	CLA	C4B-NB	-2.13	1.35	1.37
18	1	1006	CLA	C1B-C2B	2.13	1.48	1.43
18	A	1140	CLA	C4C-C3C	2.13	1.48	1.45
18	B	1224	CLA	C1C-NC	-2.13	1.34	1.37
18	B	1226	CLA	C4B-NB	-2.13	1.35	1.37
18	B	1227	CLA	C3B-C4B	2.13	1.48	1.42
18	4	4001	CLA	C1B-C2B	2.13	1.48	1.43
18	B	1225	CLA	C3B-C4B	2.13	1.48	1.42
23	F	5001	LMG	O8-C28	2.13	1.43	1.33
18	B	1216	CLA	C3B-C4B	2.13	1.48	1.42
27	4	4502	LUT	C22-C21	-2.12	1.52	1.54
18	A	1138	CLA	C3B-C4B	2.12	1.48	1.42
18	A	1131	CLA	C4B-NB	-2.12	1.35	1.37
18	B	1222	CLA	C1C-C2C	2.12	1.48	1.44
18	A	1117	CLA	C4B-NB	-2.12	1.35	1.37
18	B	1231	CLA	C1C-NC	-2.12	1.34	1.37
18	1	1003	CLA	C4C-C3C	2.12	1.48	1.45
18	B	1023	CLA	C3B-C4B	2.12	1.48	1.42
18	A	1125	CLA	C1D-C2D	2.12	1.49	1.45
18	2	2019	CLA	C4C-NC	-2.12	1.33	1.37
18	A	1128	CLA	C1D-C2D	2.12	1.49	1.45
18	A	1134	CLA	C3B-C4B	2.11	1.48	1.42
18	1	1011	CLA	C3B-C4B	2.11	1.48	1.42
18	G	1002	CLA	C4C-C3C	2.11	1.48	1.45
18	B	1234	CLA	C1C-NC	-2.11	1.34	1.37
18	A	1128	CLA	C4B-NB	-2.11	1.35	1.37
18	B	1232	CLA	C1C-C2C	2.11	1.48	1.44
18	A	1124	CLA	C4B-NB	-2.11	1.35	1.37
28	4	4010	CHL	C1D-C2D	2.11	1.41	1.39
18	3	3002	CLA	C4D-CHA	2.11	1.45	1.38
18	A	1131	CLA	C4C-C3C	2.11	1.48	1.45
18	3	3001	CLA	C1D-C2D	2.11	1.49	1.45
18	A	1129	CLA	C3B-C4B	2.11	1.48	1.42
18	B	1234	CLA	C3B-C4B	2.11	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1225	CLA	C4C-C3C	2.11	1.48	1.45
18	B	1228	CLA	C4C-C3C	2.11	1.48	1.45
18	2	2012	CLA	C1B-C2B	2.11	1.48	1.43
27	3	3502	LUT	C21-C26	-2.10	1.50	1.56
18	A	1132	CLA	C3B-C4B	2.10	1.48	1.42
18	B	1215	CLA	C4B-NB	-2.10	1.35	1.37
18	B	1229	CLA	C4C-C3C	2.10	1.48	1.45
18	3	3006	CLA	C1D-C2D	2.10	1.49	1.45
18	A	1107	CLA	C3B-C4B	2.10	1.48	1.42
18	A	1115	CLA	C3B-C4B	2.10	1.48	1.42
18	2	2008	CLA	C3D-C2D	2.10	1.44	1.39
28	4	4013	CHL	C3D-C2D	-2.10	1.36	1.39
18	B	1221	CLA	C3B-C4B	2.10	1.48	1.42
18	B	1021	CLA	C3B-C4B	2.09	1.48	1.42
18	B	1229	CLA	C3B-C4B	2.09	1.48	1.42
18	B	1221	CLA	C1C-NC	-2.09	1.34	1.37
18	A	1013	CLA	C1C-C2C	2.09	1.48	1.44
18	A	1123	CLA	C3B-C4B	2.09	1.48	1.42
18	B	1203	CLA	C3B-C4B	2.09	1.48	1.42
18	B	1208	CLA	C1C-C2C	2.09	1.48	1.44
18	B	1210	CLA	C4B-NB	-2.09	1.35	1.37
18	B	1202	CLA	C3B-C4B	2.09	1.48	1.42
18	B	1201	CLA	C3B-C4B	2.09	1.48	1.42
18	B	1220	CLA	C3B-C4B	2.09	1.48	1.42
18	B	1238	CLA	C4B-NB	-2.09	1.35	1.37
18	A	1136	CLA	C4B-NB	-2.09	1.35	1.37
18	B	1012	CLA	C1D-C2D	2.08	1.49	1.45
18	A	1126	CLA	C3B-C4B	2.08	1.48	1.42
18	A	1122	CLA	C4B-NB	-2.08	1.35	1.37
18	B	1204	CLA	C3B-C4B	2.08	1.48	1.42
28	2	2011	CHL	CBD-CAD	-2.08	1.46	1.53
18	1	1006	CLA	C1D-C2D	2.08	1.49	1.45
18	3	3018	CLA	C4C-C3C	2.08	1.48	1.45
18	B	1239	CLA	C4B-NB	-2.08	1.35	1.37
23	F	5002	LMG	O7-C8	-2.08	1.41	1.46
27	2	2502	LUT	C21-C26	-2.08	1.50	1.56
18	A	1013	CLA	C4C-C3C	2.08	1.48	1.45
18	B	1231	CLA	C1C-C2C	2.08	1.48	1.44
18	A	1113	CLA	C3B-C4B	2.08	1.48	1.42
18	B	1240	CLA	C4C-C3C	2.08	1.48	1.45
18	B	1223	CLA	C1D-C2D	2.08	1.49	1.45
18	A	1103	CLA	C3B-C4B	2.07	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1235	CLA	C1C-C2C	2.07	1.48	1.44
18	J	1302	CLA	C3B-C4B	2.07	1.48	1.42
18	2	2016	CLA	C1A-CHA	2.07	1.51	1.43
18	A	1118	CLA	C3B-C4B	2.06	1.48	1.42
18	B	1226	CLA	C1B-C2B	2.06	1.48	1.43
18	B	1012	CLA	C3B-C4B	2.06	1.48	1.42
18	B	1201	CLA	C1C-C2C	2.06	1.48	1.44
18	A	1117	CLA	C3B-C4B	2.06	1.48	1.42
22	L	6020	BCR	C30-C25	-2.06	1.51	1.53
18	A	1125	CLA	C3B-C4B	2.06	1.48	1.42
18	B	1207	CLA	C1C-C2C	2.06	1.48	1.44
18	B	1238	CLA	C4C-C3C	2.06	1.48	1.45
18	A	1102	CLA	C1C-C2C	2.06	1.48	1.44
18	4	4003	CLA	C1D-C2D	2.05	1.49	1.45
18	A	1130	CLA	C3B-C4B	2.05	1.48	1.42
18	B	1227	CLA	C1C-C2C	2.05	1.48	1.44
27	I	6018	LUT	C26-C27	-2.05	1.47	1.50
18	A	1139	CLA	C1C-C2C	2.05	1.48	1.44
18	A	1106	CLA	C3B-C4B	2.05	1.48	1.42
18	A	1139	CLA	C4B-NB	-2.05	1.35	1.37
18	A	1107	CLA	C1C-NC	-2.05	1.34	1.37
28	4	4010	CHL	MG-ND	-2.05	2.01	2.05
18	3	3010	CLA	MG-NB	-2.05	2.01	2.05
18	B	1229	CLA	C1C-C2C	2.05	1.48	1.44
18	A	1119	CLA	C3B-C4B	2.05	1.48	1.42
18	A	1111	CLA	C3B-C4B	2.05	1.48	1.42
18	3	3002	CLA	C4C-C3C	2.04	1.48	1.45
23	4	4801	LMG	O7-C8	-2.04	1.41	1.46
18	A	1107	CLA	C1C-C2C	2.04	1.48	1.44
18	B	1223	CLA	C4C-C3C	2.04	1.48	1.45
18	1	1003	CLA	C1D-C2D	2.04	1.49	1.45
18	2	2007	CLA	C4C-C3C	2.04	1.48	1.45
18	A	1122	CLA	C3B-C4B	2.04	1.48	1.42
18	B	1203	CLA	C1C-C2C	2.04	1.48	1.44
18	3	3013	CLA	C1D-C2D	2.04	1.49	1.45
28	1	1010	CHL	CHA-CBD	2.04	1.54	1.51
18	A	1131	CLA	C1C-C2C	2.03	1.48	1.44
18	A	1120	CLA	C4C-C3C	2.03	1.48	1.45
18	A	1137	CLA	C1C-C2C	2.03	1.48	1.44
18	1	1012	CLA	C1D-C2D	2.03	1.49	1.45
18	K	1001	CLA	C1D-C2D	2.03	1.49	1.45
18	A	1151	CLA	C1C-C2C	2.03	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2001	CLA	C1B-C2B	2.03	1.47	1.43
18	A	1127	CLA	C3B-C4B	2.03	1.48	1.42
18	A	1125	CLA	C1C-C2C	2.02	1.48	1.44
18	B	1236	CLA	C1C-C2C	2.02	1.48	1.44
18	B	1209	CLA	C3B-C4B	2.02	1.48	1.42
18	B	1214	CLA	C3B-C4B	2.02	1.48	1.42
18	B	1012	CLA	C4C-C3C	2.02	1.48	1.45
18	B	1230	CLA	C3B-C4B	2.02	1.48	1.42
18	B	1215	CLA	C1C-C2C	2.02	1.48	1.44
18	B	1219	CLA	C3B-C4B	2.02	1.48	1.42
18	A	1130	CLA	C1C-C2C	2.02	1.48	1.44
18	B	1232	CLA	C4B-NB	-2.02	1.35	1.37
18	B	1216	CLA	C1C-C2C	2.02	1.48	1.44
18	L	1501	CLA	C4D-CHA	2.02	1.45	1.38
18	B	1203	CLA	C4C-C3C	2.01	1.48	1.45
27	1	1502	LUT	C22-C21	-2.01	1.52	1.54
18	B	1238	CLA	C1C-C2C	2.01	1.48	1.44
18	A	1140	CLA	C4B-NB	-2.01	1.35	1.37
18	A	1022	CLA	C3B-C4B	2.01	1.48	1.42
18	A	1151	CLA	C3B-C4B	2.01	1.48	1.42
18	A	1112	CLA	C3B-C4B	2.01	1.48	1.42
18	B	1219	CLA	C1C-C2C	2.01	1.48	1.44
18	A	1102	CLA	C4B-NB	-2.01	1.35	1.37
28	4	4010	CHL	CHD-C1D	-2.01	1.36	1.39
18	A	1135	CLA	C3B-C4B	2.00	1.48	1.42
18	B	1217	CLA	C4B-NB	-2.00	1.35	1.37
18	B	1223	CLA	C3B-C4B	2.00	1.48	1.42
18	B	1239	CLA	C1C-C2C	2.00	1.48	1.44
18	B	1218	CLA	C1C-C2C	2.00	1.48	1.44

All (4561) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	6017	BCR	C16-C17-C18	30.40	169.91	127.28
22	G	2011	BCR	C16-C17-C18	28.47	167.20	127.28
22	B	6005	BCR	C16-C17-C18	28.22	166.86	127.28
22	K	2011	BCR	C16-C17-C18	28.11	166.70	127.28
22	I	6020	BCR	C16-C17-C18	27.65	166.06	127.28
22	B	6004	BCR	C16-C17-C18	27.48	165.82	127.28
22	B	6006	BCR	C20-C21-C22	25.46	162.98	127.28
22	F	6016	BCR	C16-C17-C18	24.15	161.15	127.28
22	A	6011	BCR	C16-C17-C18	23.95	160.87	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	6010	BCR	C20-C21-C22	23.38	160.06	127.28
22	F	6014	BCR	C16-C17-C18	22.75	159.18	127.28
22	F	6016	BCR	C20-C21-C22	22.38	158.67	127.28
22	A	6011	BCR	C20-C21-C22	22.03	158.17	127.28
22	K	2011	BCR	C20-C21-C22	21.72	157.73	127.28
22	J	6013	BCR	C15-C16-C17	21.48	167.46	123.52
22	L	6019	BCR	C20-C21-C22	21.31	157.16	127.28
22	A	6008	BCR	C20-C21-C22	21.23	157.06	127.28
22	F	6014	BCR	C20-C21-C22	21.16	156.95	127.28
22	A	6002	BCR	C15-C16-C17	21.14	166.77	123.52
22	A	6003	BCR	C20-C21-C22	21.07	156.82	127.28
22	B	6005	BCR	C20-C21-C22	20.79	156.43	127.28
22	F	6014	BCR	C15-C16-C17	20.74	165.97	123.52
22	L	6020	BCR	C20-C21-C22	20.74	156.36	127.28
22	B	6009	BCR	C20-C21-C22	20.71	156.32	127.28
22	A	6003	BCR	C15-C16-C17	20.59	165.65	123.52
22	3	3503	BCR	C20-C21-C22	20.53	156.07	127.28
22	A	6008	BCR	C16-C17-C18	20.46	155.97	127.28
22	A	6007	BCR	C16-C17-C18	20.45	155.96	127.28
22	B	6009	BCR	C15-C16-C17	20.35	165.16	123.52
22	B	6010	BCR	C16-C17-C18	20.32	155.77	127.28
22	L	6019	BCR	C16-C17-C18	20.28	155.72	127.28
22	J	6012	BCR	C15-C16-C17	20.26	164.97	123.52
22	B	6010	BCR	C15-C16-C17	20.21	164.87	123.52
22	B	6006	BCR	C16-C17-C18	20.21	155.62	127.28
22	J	6012	BCR	C20-C21-C22	20.20	155.61	127.28
22	B	6006	BCR	C15-C16-C17	20.10	164.64	123.52
22	A	6007	BCR	C15-C16-C17	20.09	164.63	123.52
22	B	6009	BCR	C16-C17-C18	20.08	155.43	127.28
22	B	6004	BCR	C20-C21-C22	19.98	155.30	127.28
22	A	6003	BCR	C16-C17-C18	19.97	155.29	127.28
22	J	6012	BCR	C16-C17-C18	19.97	155.28	127.28
22	A	6007	BCR	C20-C21-C22	19.90	155.18	127.28
22	G	2011	BCR	C20-C21-C22	19.88	155.16	127.28
22	L	6019	BCR	C15-C16-C17	19.78	164.00	123.52
22	L	6020	BCR	C16-C17-C18	19.73	154.95	127.28
22	A	6002	BCR	C20-C21-C22	19.72	154.94	127.28
22	L	6020	BCR	C15-C16-C17	19.70	163.82	123.52
22	K	2011	BCR	C10-C11-C12	19.59	179.97	123.20
22	G	2011	BCR	C10-C11-C12	19.58	179.94	123.20
22	J	6013	BCR	C20-C21-C22	19.53	154.66	127.28
22	3	3503	BCR	C16-C17-C18	19.35	154.41	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	6020	BCR	C10-C11-C12	19.22	178.90	123.20
22	L	6019	BCR	C10-C11-C12	18.85	177.82	123.20
22	F	6016	BCR	C10-C11-C12	18.82	177.72	123.20
22	A	6007	BCR	C10-C11-C12	18.73	177.47	123.20
22	3	3503	BCR	C15-C16-C17	18.71	161.80	123.52
22	J	6013	BCR	C10-C11-C12	18.64	177.20	123.20
22	A	6003	BCR	C10-C11-C12	18.61	177.14	123.20
22	I	6020	BCR	C20-C21-C22	18.57	153.32	127.28
22	F	6016	BCR	C15-C16-C17	18.54	161.46	123.52
22	F	6014	BCR	C10-C11-C12	18.44	176.62	123.20
22	A	6008	BCR	C15-C16-C17	18.40	161.17	123.52
22	J	6012	BCR	C10-C11-C12	18.39	176.49	123.20
22	B	6005	BCR	C10-C11-C12	18.38	176.46	123.20
22	3	3503	BCR	C10-C11-C12	18.36	176.40	123.20
22	A	6002	BCR	C10-C11-C12	18.29	176.19	123.20
22	A	6008	BCR	C10-C11-C12	18.29	176.19	123.20
22	A	6002	BCR	C16-C17-C18	18.17	152.76	127.28
22	I	6020	BCR	C10-C11-C12	18.09	175.61	123.20
22	A	6011	BCR	C15-C16-C17	18.07	160.50	123.52
22	B	6009	BCR	C10-C11-C12	18.00	175.35	123.20
22	A	6017	BCR	C20-C21-C22	17.96	152.47	127.28
22	B	6010	BCR	C10-C11-C12	17.96	175.24	123.20
22	A	6017	BCR	C10-C11-C12	17.93	175.16	123.20
22	A	6017	BCR	C16-C15-C14	17.86	160.05	123.52
22	J	6013	BCR	C16-C17-C18	17.73	152.14	127.28
22	B	6006	BCR	C10-C11-C12	17.22	173.10	123.20
22	B	6004	BCR	C10-C11-C12	16.96	172.34	123.20
22	A	6011	BCR	C10-C11-C12	16.84	172.00	123.20
22	B	6006	BCR	C11-C10-C9	16.44	150.33	127.28
22	B	6004	BCR	C15-C16-C17	16.09	156.44	123.52
22	A	6017	BCR	C21-C20-C19	15.78	168.93	123.20
22	G	2011	BCR	C15-C16-C17	15.74	155.72	123.52
22	A	6011	BCR	C11-C10-C9	15.64	149.22	127.28
22	B	6004	BCR	C21-C20-C19	15.52	168.18	123.20
22	I	6020	BCR	C15-C16-C17	15.51	155.26	123.52
22	B	6005	BCR	C15-C16-C17	15.49	155.21	123.52
22	K	2011	BCR	C15-C16-C17	15.42	155.08	123.52
22	I	6020	BCR	C21-C20-C19	15.22	167.30	123.20
22	A	6008	BCR	C16-C15-C14	15.18	154.59	123.52
22	J	6012	BCR	C11-C10-C9	15.09	148.44	127.28
22	B	6005	BCR	C21-C20-C19	14.95	166.53	123.20
22	A	6007	BCR	C21-C20-C19	14.89	166.34	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	I	6020	BCR	C11-C10-C9	14.86	148.12	127.28
22	A	6002	BCR	C21-C20-C19	14.58	165.45	123.20
22	3	3503	BCR	C16-C15-C14	14.54	153.26	123.52
22	L	6020	BCR	C16-C15-C14	14.51	153.22	123.52
22	F	6014	BCR	C11-C10-C9	14.47	147.57	127.28
22	B	6010	BCR	C21-C20-C19	14.44	165.04	123.20
22	A	6002	BCR	C11-C10-C9	14.32	147.36	127.28
22	G	2011	BCR	C21-C20-C19	14.30	164.64	123.20
22	3	3503	BCR	C21-C20-C19	14.20	164.34	123.20
22	A	6003	BCR	C21-C20-C19	14.14	164.18	123.20
22	F	6014	BCR	C21-C20-C19	14.12	164.10	123.20
22	A	6017	BCR	C15-C16-C17	14.09	152.35	123.52
22	J	6012	BCR	C21-C20-C19	14.06	163.94	123.20
22	A	6008	BCR	C21-C20-C19	13.95	163.62	123.20
17	A	1011	CL0	C1B-CHB-C4A	13.94	130.29	121.32
22	J	6013	BCR	C21-C20-C19	13.94	163.58	123.20
22	L	6019	BCR	C21-C20-C19	13.89	163.46	123.20
22	B	6004	BCR	C16-C15-C14	13.73	151.61	123.52
22	L	6020	BCR	C21-C20-C19	13.72	162.95	123.20
22	A	6017	BCR	C11-C10-C9	13.70	146.49	127.28
22	F	6016	BCR	C11-C10-C9	13.59	146.34	127.28
22	A	6007	BCR	C11-C10-C9	13.55	146.28	127.28
22	B	6009	BCR	C21-C20-C19	13.51	162.34	123.20
22	B	6005	BCR	C11-C10-C9	13.38	146.05	127.28
22	L	6019	BCR	C16-C15-C14	13.34	150.81	123.52
22	G	2011	BCR	C16-C15-C14	13.32	150.78	123.52
22	J	6013	BCR	C11-C10-C9	13.16	145.73	127.28
22	A	6007	BCR	C16-C15-C14	13.13	150.38	123.52
22	I	6020	BCR	C16-C15-C14	13.05	150.22	123.52
22	A	6008	BCR	C11-C10-C9	12.98	145.48	127.28
22	K	2011	BCR	C16-C15-C14	12.97	150.05	123.52
22	F	6016	BCR	C21-C20-C19	12.95	160.73	123.20
22	B	6005	BCR	C16-C15-C14	12.94	149.99	123.52
22	A	6011	BCR	C21-C20-C19	12.89	160.56	123.20
22	A	6003	BCR	C11-C10-C9	12.85	145.30	127.28
22	J	6013	BCR	C16-C15-C14	12.83	149.78	123.52
22	B	6010	BCR	C16-C15-C14	12.83	149.76	123.52
22	A	6011	BCR	C16-C15-C14	12.71	149.53	123.52
22	A	6011	BCR	C11-C12-C13	12.59	160.88	126.36
22	A	6003	BCR	C16-C15-C14	12.57	149.24	123.52
22	B	6006	BCR	C16-C15-C14	12.57	149.23	123.52
22	F	6016	BCR	C16-C15-C14	12.53	149.15	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	6009	BCR	C16-C15-C14	12.42	148.92	123.52
22	B	6006	BCR	C11-C12-C13	12.29	160.07	126.36
22	A	6002	BCR	C16-C15-C14	12.20	148.49	123.52
22	J	6012	BCR	C16-C15-C14	12.20	148.49	123.52
22	L	6020	BCR	C11-C10-C9	11.88	143.94	127.28
22	B	6006	BCR	C21-C20-C19	11.78	157.33	123.20
22	F	6014	BCR	C16-C15-C14	11.78	147.62	123.52
22	B	6010	BCR	C11-C10-C9	11.68	143.66	127.28
18	3	3008	CLA	C4A-NA-C1A	11.66	112.00	106.68
22	K	2011	BCR	C21-C20-C19	11.60	156.81	123.20
22	L	6019	BCR	C11-C10-C9	11.58	143.51	127.28
22	B	6005	BCR	C11-C12-C13	11.38	157.56	126.36
27	1	1501	LUT	C21-C26-C27	11.30	125.81	112.83
18	2	2016	CLA	C4A-NA-C1A	11.29	111.83	106.68
22	A	6002	BCR	C11-C12-C13	11.28	157.30	126.36
22	K	2011	BCR	C11-C10-C9	11.24	143.04	127.28
22	L	6019	BCR	C11-C12-C13	11.23	157.16	126.36
22	I	6020	BCR	C11-C12-C13	11.11	156.83	126.36
22	B	6009	BCR	C11-C12-C13	11.09	156.78	126.36
22	J	6013	BCR	C11-C12-C13	11.06	156.68	126.36
22	B	6009	BCR	C11-C10-C9	10.99	142.70	127.28
22	A	6003	BCR	C11-C12-C13	10.90	156.26	126.36
22	F	6014	BCR	C11-C12-C13	10.74	155.81	126.36
22	F	6016	BCR	C11-C12-C13	10.70	155.71	126.36
22	A	6017	BCR	C11-C12-C13	10.35	154.75	126.36
22	B	6010	BCR	C11-C12-C13	10.35	154.74	126.36
22	A	6008	BCR	C11-C12-C13	10.34	154.72	126.36
22	K	2011	BCR	C11-C12-C13	10.30	154.59	126.36
22	J	6012	BCR	C11-C12-C13	10.29	154.59	126.36
22	3	3503	BCR	C11-C12-C13	10.25	154.46	126.36
22	B	6004	BCR	C11-C10-C9	10.20	141.58	127.28
18	4	4008	CLA	C4A-NA-C1A	10.03	111.25	106.68
22	A	6007	BCR	C11-C12-C13	9.91	153.53	126.36
22	B	6004	BCR	C11-C12-C13	9.90	153.52	126.36
18	3	3001	CLA	CMD-C2D-C1D	9.78	141.95	124.73
18	2	2003	CLA	C4A-NA-C1A	9.75	111.13	106.68
22	3	3503	BCR	C11-C10-C9	9.75	140.95	127.28
28	4	4010	CHL	C1B-CHB-C4A	9.69	127.56	121.32
22	L	6020	BCR	C11-C12-C13	9.60	152.69	126.36
22	G	2011	BCR	C11-C12-C13	9.32	151.91	126.36
18	2	2008	CLA	C4A-NA-C1A	9.28	110.91	106.68
18	1	1007	CLA	CMD-C2D-C1D	9.17	140.87	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1007	CLA	C4A-NA-C1A	9.17	110.86	106.68
18	3	3002	CLA	CMD-C2D-C1D	9.11	140.78	124.73
18	4	4016	CLA	CMD-C2D-C1D	9.10	140.75	124.73
18	4	4007	CLA	CMD-C2D-C1D	9.05	140.67	124.73
18	4	4001	CLA	CMD-C2D-C1D	8.99	140.56	124.73
18	K	1001	CLA	CMD-C2D-C1D	8.97	140.53	124.73
18	4	4007	CLA	C4A-NA-C1A	8.96	110.77	106.68
18	3	3006	CLA	CMD-C2D-C1D	8.94	140.47	124.73
18	3	3018	CLA	CMD-C2D-C1D	8.93	140.46	124.73
18	2	2016	CLA	CMD-C2D-C1D	8.93	140.45	124.73
18	G	1003	CLA	CMD-C2D-C1D	8.91	140.43	124.73
18	1	1006	CLA	CMD-C2D-C1D	8.86	140.34	124.73
22	G	2011	BCR	C11-C10-C9	8.86	139.70	127.28
18	1	1002	CLA	C4A-NA-C1A	8.84	110.71	106.68
18	1	1013	CLA	CMD-C2D-C1D	8.82	140.26	124.73
18	A	1237	CLA	CMD-C2D-C1D	8.82	140.25	124.73
18	1	1008	CLA	C4A-NA-C1A	8.75	110.67	106.68
18	K	1001	CLA	C4A-NA-C1A	8.72	110.66	106.68
18	2	2002	CLA	CMD-C2D-C1D	8.64	139.95	124.73
18	2	2009	CLA	CMD-C2D-C1D	8.62	139.90	124.73
18	L	1502	CLA	CMD-C2D-C1D	8.61	139.89	124.73
18	4	4008	CLA	CMD-C2D-C1D	8.58	139.84	124.73
18	3	3008	CLA	CMD-C2D-C1D	8.58	139.83	124.73
18	3	3010	CLA	CMD-C2D-C1D	8.55	139.79	124.73
22	F	6016	BCR	C20-C19-C18	8.54	149.79	126.36
18	B	1214	CLA	CMD-C2D-C1D	8.51	139.72	124.73
18	A	1120	CLA	CMD-C2D-C1D	8.50	139.69	124.73
18	G	1002	CLA	CMD-C2D-C1D	8.50	139.69	124.73
27	3	3501	LUT	C21-C26-C27	8.46	122.55	112.83
18	1	1014	CLA	CMD-C2D-C1D	8.40	139.53	124.73
17	A	1011	CL0	O2D-CGD-CBD	8.40	120.18	110.95
18	2	2008	CLA	CMD-C2D-C1D	8.37	139.47	124.73
18	B	1240	CLA	CMD-C2D-C1D	8.34	139.41	124.73
18	1	1012	CLA	CMD-C2D-C1D	8.32	139.38	124.73
18	B	1226	CLA	CMD-C2D-C1D	8.30	139.35	124.73
18	2	2002	CLA	C4A-NA-C1A	8.28	110.46	106.68
18	B	1227	CLA	CMD-C2D-C1D	8.28	139.30	124.73
18	1	1004	CLA	CMD-C2D-C1D	8.27	139.29	124.73
18	A	1108	CLA	CMD-C2D-C1D	8.26	139.27	124.73
18	B	1204	CLA	CMD-C2D-C1D	8.25	139.26	124.73
18	B	1231	CLA	CMD-C2D-C1D	8.24	139.25	124.73
18	B	1238	CLA	CMD-C2D-C1D	8.23	139.22	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1134	CLA	CMD-C2D-C1D	8.23	139.22	124.73
18	A	1101	CLA	CMD-C2D-C1D	8.21	139.19	124.73
18	B	1203	CLA	CMD-C2D-C1D	8.20	139.18	124.73
18	A	1122	CLA	CMD-C2D-C1D	8.19	139.15	124.73
18	4	4009	CLA	CMD-C2D-C1D	8.19	139.15	124.73
18	4	4005	CLA	C4A-NA-C1A	8.19	110.42	106.68
18	3	3007	CLA	CMD-C2D-C1D	8.18	139.14	124.73
18	3	3003	CLA	CMD-C2D-C1D	8.18	139.13	124.73
18	A	1119	CLA	CMD-C2D-C1D	8.17	139.12	124.73
18	B	1210	CLA	CMD-C2D-C1D	8.16	139.10	124.73
18	B	1232	CLA	CMD-C2D-C1D	8.16	139.09	124.73
18	3	3012	CLA	CMD-C2D-C1D	8.16	139.09	124.73
18	L	1501	CLA	CMD-C2D-C1D	8.15	139.08	124.73
18	A	1116	CLA	CMD-C2D-C1D	8.15	139.08	124.73
18	A	1130	CLA	CMD-C2D-C1D	8.14	139.07	124.73
18	B	1239	CLA	CMD-C2D-C1D	8.14	139.07	124.73
18	A	1125	CLA	CMD-C2D-C1D	8.14	139.06	124.73
18	3	3003	CLA	C4A-NA-C1A	8.13	110.39	106.68
18	A	1114	CLA	CMD-C2D-C1D	8.13	139.04	124.73
18	F	1302	CLA	CMD-C2D-C1D	8.12	139.03	124.73
18	4	4002	CLA	CMD-C2D-C1D	8.12	139.03	124.73
18	B	1218	CLA	CMD-C2D-C1D	8.12	139.03	124.73
18	A	1136	CLA	CMD-C2D-C1D	8.11	139.01	124.73
18	4	4003	CLA	CMD-C2D-C1D	8.11	139.00	124.73
18	B	1208	CLA	CMD-C2D-C1D	8.11	139.00	124.73
18	A	1117	CLA	CMD-C2D-C1D	8.10	138.99	124.73
18	A	1112	CLA	CMD-C2D-C1D	8.10	138.99	124.73
18	A	1103	CLA	CMD-C2D-C1D	8.10	138.99	124.73
18	B	1213	CLA	CMD-C2D-C1D	8.09	138.98	124.73
18	2	2005	CLA	CMD-C2D-C1D	8.09	138.98	124.73
18	B	1235	CLA	CMD-C2D-C1D	8.09	138.98	124.73
18	A	1107	CLA	CMD-C2D-C1D	8.09	138.97	124.73
18	A	1135	CLA	CMD-C2D-C1D	8.09	138.97	124.73
18	F	1301	CLA	CMD-C2D-C1D	8.09	138.97	124.73
18	A	1109	CLA	CMD-C2D-C1D	8.09	138.97	124.73
18	A	1104	CLA	CMD-C2D-C1D	8.08	138.96	124.73
18	A	1105	CLA	CMD-C2D-C1D	8.08	138.96	124.73
18	A	1151	CLA	CMD-C2D-C1D	8.08	138.95	124.73
18	H	1000	CLA	CMD-C2D-C1D	8.07	138.94	124.73
18	A	1113	CLA	CMD-C2D-C1D	8.07	138.94	124.73
22	L	6019	BCR	C20-C19-C18	8.06	148.48	126.36
18	4	4017	CLA	CMD-C2D-C1D	8.06	138.92	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1011	CLA	CMD-C2D-C1D	8.05	138.91	124.73
18	1	1014	CLA	C4A-NA-C1A	8.05	110.35	106.68
18	B	1207	CLA	CMD-C2D-C1D	8.05	138.90	124.73
18	1	1008	CLA	CMD-C2D-C1D	8.05	138.90	124.73
18	B	1201	CLA	CMD-C2D-C1D	8.05	138.90	124.73
18	4	4012	CLA	CMD-C2D-C1D	8.04	138.89	124.73
18	B	1228	CLA	CMD-C2D-C1D	8.04	138.88	124.73
18	B	1217	CLA	CMD-C2D-C1D	8.02	138.85	124.73
18	3	3017	CLA	CMD-C2D-C1D	8.01	138.83	124.73
18	A	1129	CLA	CMD-C2D-C1D	8.01	138.83	124.73
18	A	1126	CLA	CMD-C2D-C1D	8.00	138.82	124.73
18	B	1223	CLA	CMD-C2D-C1D	8.00	138.81	124.73
18	B	1236	CLA	CMD-C2D-C1D	8.00	138.81	124.73
18	3	3012	CLA	C4A-NA-C1A	7.99	110.32	106.68
18	A	1118	CLA	CMD-C2D-C1D	7.99	138.79	124.73
18	2	2006	CLA	CMD-C2D-C1D	7.98	138.79	124.73
18	2	2007	CLA	CMD-C2D-C1D	7.98	138.78	124.73
18	A	1137	CLA	CMD-C2D-C1D	7.97	138.77	124.73
18	A	1131	CLA	CMD-C2D-C1D	7.97	138.76	124.73
18	A	1121	CLA	CMD-C2D-C1D	7.97	138.76	124.73
22	A	6017	BCR	C15-C14-C13	-7.97	116.11	127.28
18	A	1124	CLA	CMD-C2D-C1D	7.96	138.75	124.73
18	A	1139	CLA	CMD-C2D-C1D	7.96	138.75	124.73
18	B	1211	CLA	CMD-C2D-C1D	7.96	138.74	124.73
18	A	1115	CLA	CMD-C2D-C1D	7.96	138.74	124.73
18	B	1205	CLA	CMD-C2D-C1D	7.96	138.74	124.73
18	A	1140	CLA	CMD-C2D-C1D	7.95	138.74	124.73
18	J	1302	CLA	CMD-C2D-C1D	7.95	138.73	124.73
18	A	1110	CLA	CMD-C2D-C1D	7.95	138.73	124.73
18	A	1111	CLA	CMD-C2D-C1D	7.94	138.71	124.73
18	B	1215	CLA	CMD-C2D-C1D	7.94	138.71	124.73
18	B	1216	CLA	CMD-C2D-C1D	7.93	138.69	124.73
18	3	3004	CLA	CMD-C2D-C1D	7.92	138.68	124.73
18	A	1123	CLA	CMD-C2D-C1D	7.92	138.68	124.73
18	1	1013	CLA	C4A-NA-C1A	7.92	110.29	106.68
18	B	1222	CLA	CMD-C2D-C1D	7.91	138.65	124.73
18	B	1224	CLA	CMD-C2D-C1D	7.90	138.64	124.73
18	4	4004	CLA	CMD-C2D-C1D	7.84	138.53	124.73
18	1	1002	CLA	CMD-C2D-C1D	7.83	138.51	124.73
18	B	1202	CLA	CMD-C2D-C1D	7.81	138.48	124.73
18	B	1229	CLA	CMD-C2D-C1D	7.81	138.48	124.73
18	A	1106	CLA	CMD-C2D-C1D	7.80	138.47	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2004	CLA	CMD-C2D-C1D	7.80	138.47	124.73
18	A	1132	CLA	CMD-C2D-C1D	7.80	138.46	124.73
18	B	1234	CLA	CMD-C2D-C1D	7.79	138.45	124.73
18	1	1001	CLA	C4A-NA-C1A	7.79	110.23	106.68
18	B	1219	CLA	CMD-C2D-C1D	7.78	138.43	124.73
18	2	2003	CLA	CMD-C2D-C1D	7.78	138.43	124.73
18	B	1209	CLA	CMD-C2D-C1D	7.77	138.41	124.73
18	G	1001	CLA	CMD-C2D-C1D	7.76	138.40	124.73
18	1	1005	CLA	CMD-C2D-C1D	7.76	138.38	124.73
18	B	1220	CLA	CMD-C2D-C1D	7.73	138.35	124.73
18	1	1003	CLA	CMD-C2D-C1D	7.73	138.34	124.73
18	A	1138	CLA	CMD-C2D-C1D	7.73	138.34	124.73
18	B	1221	CLA	CMD-C2D-C1D	7.72	138.32	124.73
22	B	6009	BCR	C20-C19-C18	7.72	147.52	126.36
18	3	3005	CLA	C4A-NA-C1A	7.71	110.19	106.68
18	3	3005	CLA	CMD-C2D-C1D	7.68	138.25	124.73
18	A	1022	CLA	CMD-C2D-C1D	7.68	138.25	124.73
18	B	1212	CLA	CMD-C2D-C1D	7.68	138.25	124.73
22	A	6011	BCR	C20-C19-C18	7.67	147.41	126.36
22	F	6014	BCR	C20-C19-C18	7.62	147.27	126.36
18	A	1102	CLA	CMD-C2D-C1D	7.60	138.11	124.73
18	2	2012	CLA	CMD-C2D-C1D	7.59	138.09	124.73
28	2	2010	CHL	C1B-CHB-C4A	7.58	126.20	121.32
18	3	3013	CLA	CMD-C2D-C1D	7.56	138.04	124.73
18	B	1206	CLA	CMD-C2D-C1D	7.55	138.03	124.73
18	4	4001	CLA	C4A-NA-C1A	7.51	110.10	106.68
18	4	4006	CLA	CMD-C2D-C1D	7.44	137.83	124.73
18	B	1023	CLA	CMD-C2D-C1D	7.44	137.83	124.73
18	B	1021	CLA	CMD-C2D-C1D	7.43	137.82	124.73
18	A	1013	CLA	CMD-C2D-C1D	7.42	137.80	124.73
22	B	6006	BCR	C20-C19-C18	7.42	146.71	126.36
22	J	6012	BCR	C20-C19-C18	7.35	146.53	126.36
18	2	2012	CLA	C4A-NA-C1A	7.35	110.03	106.68
18	3	3003	CLA	C2C-C1C-NC	7.35	117.70	109.98
18	2	2016	CLA	O2D-CGD-CBD	7.34	124.06	111.23
18	L	1503	CLA	CMD-C2D-C1D	7.33	137.64	124.73
18	4	4012	CLA	C4A-NA-C1A	7.33	110.02	106.68
18	2	2001	CLA	CMD-C2D-C1D	7.32	137.63	124.73
18	1	1001	CLA	CMD-C2D-C1D	7.30	137.59	124.73
18	B	1202	CLA	C4A-NA-C1A	7.29	110.01	106.68
22	J	6013	BCR	C20-C19-C18	7.29	146.34	126.36
18	A	1127	CLA	CMD-C2D-C1D	7.25	137.49	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1133	CLA	CMD-C2D-C1D	7.22	137.44	124.73
18	2	2007	CLA	C4A-NA-C1A	7.21	109.97	106.68
18	B	1230	CLA	CMD-C2D-C1D	7.19	137.39	124.73
22	A	6008	BCR	C20-C19-C18	7.17	146.01	126.36
18	4	4005	CLA	CMD-C2D-C1D	7.16	137.34	124.73
18	1	1005	CLA	C4A-NA-C1A	7.14	109.94	106.68
18	4	4009	CLA	C4A-NA-C1A	7.14	109.94	106.68
18	B	1225	CLA	CMD-C2D-C1D	7.13	137.28	124.73
18	4	4003	CLA	C4A-NA-C1A	7.11	109.92	106.68
18	3	3008	CLA	C2C-C1C-NC	7.08	117.42	109.98
27	4	4503	LUT	C7-C8-C9	-7.06	115.80	126.23
18	B	1230	CLA	O2D-CGD-CBD	7.06	123.56	111.23
22	A	6003	BCR	C20-C19-C18	7.04	145.68	126.36
18	G	1001	CLA	C4A-NA-C1A	7.03	109.89	106.68
18	A	1128	CLA	CMD-C2D-C1D	7.02	137.09	124.73
22	K	2011	BCR	C20-C19-C18	7.01	145.58	126.36
18	2	2001	CLA	C4A-NA-C1A	6.98	109.86	106.68
18	3	3018	CLA	C4A-NA-C1A	6.97	109.86	106.68
27	3	3502	LUT	C7-C8-C9	-6.97	115.93	126.23
22	L	6020	BCR	C20-C19-C18	6.94	145.39	126.36
18	4	4002	CLA	C4A-NA-C1A	6.91	109.83	106.68
18	B	1012	CLA	CMD-C2D-C1D	6.87	136.82	124.73
18	2	2006	CLA	C4A-NA-C1A	6.85	109.81	106.68
18	1	1004	CLA	C4A-NA-C1A	6.84	109.80	106.68
18	2	2004	CLA	O2D-CGD-CBD	6.83	123.17	111.23
18	3	3019	CLA	C4A-NA-C1A	6.81	109.79	106.68
18	2	2019	CLA	C4A-NA-C1A	6.81	109.78	106.68
18	B	1211	CLA	O2D-CGD-CBD	6.76	123.05	111.23
18	4	4016	CLA	C4A-NA-C1A	6.73	109.75	106.68
27	1	1502	LUT	C26-C27-C28	-6.72	114.11	124.58
18	B	1221	CLA	O2D-CGD-CBD	6.72	122.98	111.23
22	A	6002	BCR	C20-C19-C18	6.72	144.78	126.36
18	L	1503	CLA	C4A-NA-C1A	6.70	109.73	106.68
18	1	1012	CLA	C4A-NA-C1A	6.68	109.73	106.68
18	4	4008	CLA	C2C-C1C-NC	6.64	116.96	109.98
18	4	4006	CLA	C4A-NA-C1A	6.60	109.69	106.68
18	3	3008	CLA	C1C-C2C-C3C	-6.60	100.04	106.98
18	3	3010	CLA	C4A-NA-C1A	6.60	109.69	106.68
18	1	1003	CLA	C4A-NA-C1A	6.57	109.68	106.68
18	F	1301	CLA	C4A-NA-C1A	6.56	109.67	106.68
22	B	6010	BCR	C20-C19-C18	6.56	144.35	126.36
18	4	4001	CLA	C1C-C2C-C3C	-6.54	100.10	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3004	CLA	C4A-NA-C1A	6.48	109.64	106.68
22	A	6007	BCR	C20-C19-C18	6.48	144.13	126.36
18	A	1128	CLA	O2D-CGD-CBD	6.47	122.55	111.23
18	G	1002	CLA	C4A-NA-C1A	6.46	109.63	106.68
18	F	1302	CLA	C4A-NA-C1A	6.46	109.63	106.68
18	L	1501	CLA	O2D-CGD-CBD	6.46	122.52	111.23
18	2	2005	CLA	C4A-NA-C1A	6.46	109.62	106.68
18	4	4017	CLA	C4A-NA-C1A	6.46	109.62	106.68
18	3	3002	CLA	C4A-NA-C1A	6.40	109.60	106.68
18	2	2003	CLA	C1D-ND-C4D	-6.40	101.83	106.31
22	3	3503	BCR	C20-C19-C18	6.38	143.85	126.36
18	2	2001	CLA	C2C-C1C-NC	6.34	116.64	109.98
18	B	1230	CLA	C4A-NA-C1A	6.34	109.57	106.68
18	3	3007	CLA	C4A-NA-C1A	6.34	109.57	106.68
18	4	4002	CLA	C2C-C1C-NC	6.34	116.64	109.98
22	A	6007	BCR	C24-C23-C22	-6.34	116.86	126.23
22	A	6008	BCR	C15-C14-C13	-6.30	118.44	127.28
18	B	1235	CLA	C4A-NA-C1A	6.30	109.55	106.68
18	B	1206	CLA	C2C-C1C-NC	6.28	116.57	109.98
22	B	6005	BCR	C20-C19-C18	6.27	143.55	126.36
18	B	1021	CLA	C4A-NA-C1A	6.26	109.53	106.68
18	1	1013	CLA	C2C-C1C-NC	6.26	116.56	109.98
18	2	2019	CLA	C3B-C2B-C1B	-6.25	99.86	106.81
18	3	3019	CLA	C3B-C2B-C1B	-6.25	99.86	106.81
18	2	2009	CLA	C4A-NA-C1A	6.23	109.52	106.68
18	1	1011	CLA	C4A-NA-C1A	6.19	109.50	106.68
18	B	1206	CLA	C4A-NA-C1A	6.18	109.50	106.68
18	4	4007	CLA	O2A-CGA-O1A	-6.17	108.20	123.63
18	2	2016	CLA	C2C-C1C-NC	6.16	116.46	109.98
18	A	1104	CLA	C1D-ND-C4D	-6.16	101.99	106.31
18	4	4005	CLA	C2C-C1C-NC	6.16	116.45	109.98
18	B	1023	CLA	C4A-NA-C1A	6.15	109.48	106.68
18	G	1002	CLA	O2D-CGD-CBD	6.15	121.98	111.23
18	1	1008	CLA	C2C-C1C-NC	6.14	116.43	109.98
22	J	6012	BCR	C24-C23-C22	-6.14	117.15	126.23
28	1	1009	CHL	C1B-CHB-C4A	6.14	125.27	121.32
18	A	1106	CLA	O2D-CGD-CBD	6.12	121.93	111.23
28	2	2011	CHL	C1B-CHB-C4A	6.11	125.25	121.32
18	A	1114	CLA	C2C-C1C-NC	6.10	116.39	109.98
18	A	1132	CLA	O2D-CGD-CBD	6.09	121.88	111.23
18	4	4004	CLA	O2D-CGD-CBD	6.09	121.87	111.23
18	3	3006	CLA	C3B-C2B-C1B	-6.08	100.00	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2001	CLA	C1C-C2C-C3C	-6.08	100.58	106.98
18	B	1226	CLA	C2C-C1C-NC	6.07	116.36	109.98
18	G	1003	CLA	C4A-NA-C1A	6.07	109.45	106.68
18	A	1123	CLA	O2D-CGD-CBD	6.06	121.83	111.23
18	A	1129	CLA	C4A-NA-C1A	6.05	109.44	106.68
18	A	1116	CLA	C1-C2-C3	-6.05	116.29	126.20
18	A	1112	CLA	O2D-CGD-CBD	6.04	121.80	111.23
18	A	1151	CLA	C2C-C1C-NC	6.04	116.33	109.98
18	3	3008	CLA	C1D-ND-C4D	-6.04	102.08	106.31
18	H	1000	CLA	C2C-C1C-NC	6.03	116.32	109.98
18	B	1230	CLA	C1D-ND-C4D	-6.03	102.08	106.31
18	4	4001	CLA	C2C-C1C-NC	6.03	116.31	109.98
18	K	1001	CLA	C1C-C2C-C3C	-6.02	100.64	106.98
18	B	1230	CLA	C2D-C1D-ND	6.02	116.09	110.13
18	2	2016	CLA	C2D-C1D-ND	6.02	116.08	110.13
18	4	4007	CLA	C2C-C1C-NC	6.01	116.30	109.98
22	J	6013	BCR	C24-C23-C22	-6.00	117.35	126.23
18	G	1001	CLA	C2C-C1C-NC	5.99	116.28	109.98
18	A	1102	CLA	C4A-NA-C1A	5.99	109.41	106.68
18	K	1001	CLA	C2C-C1C-NC	5.97	116.26	109.98
22	G	2011	BCR	C20-C19-C18	5.97	142.74	126.36
18	2	2009	CLA	C1C-C2C-C3C	-5.97	100.70	106.98
18	3	3010	CLA	C1C-C2C-C3C	-5.97	100.70	106.98
18	1	1002	CLA	C2D-C1D-ND	5.96	116.03	110.13
18	3	3001	CLA	C1C-C2C-C3C	-5.96	100.71	106.98
18	2	2016	CLA	C1C-C2C-C3C	-5.95	100.72	106.98
18	A	1123	CLA	C4A-NA-C1A	5.95	109.39	106.68
18	3	3005	CLA	C2C-C1C-NC	5.94	116.22	109.98
18	2	2008	CLA	C2D-C1D-ND	5.93	116.00	110.13
18	B	1224	CLA	C2C-C1C-NC	5.93	116.21	109.98
18	B	1223	CLA	O2D-CGD-CBD	5.93	121.59	111.23
18	B	1212	CLA	C4A-NA-C1A	5.92	109.38	106.68
18	A	1135	CLA	C2C-C1C-NC	5.92	116.20	109.98
18	A	1123	CLA	C2C-C1C-NC	5.92	116.20	109.98
18	4	4004	CLA	C4A-NA-C1A	5.91	109.38	106.68
18	2	2008	CLA	C1D-ND-C4D	-5.91	102.17	106.31
18	3	3002	CLA	C2C-C1C-NC	5.91	116.19	109.98
18	3	3003	CLA	C1C-C2C-C3C	-5.91	100.77	106.98
18	4	4002	CLA	C1C-C2C-C3C	-5.91	100.77	106.98
18	1	1003	CLA	O2A-CGA-O1A	-5.90	108.87	123.63
18	B	1218	CLA	O2D-CGD-CBD	5.89	121.53	111.23
18	4	4012	CLA	C2C-C1C-NC	5.89	116.17	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3010	CLA	C2C-C1C-NC	5.88	116.16	109.98
18	A	1118	CLA	C4A-NA-C1A	5.88	109.36	106.68
18	B	1208	CLA	O2D-CGD-CBD	5.88	121.50	111.23
18	A	1128	CLA	C2C-C1C-NC	5.87	116.15	109.98
18	J	1302	CLA	C2C-C1C-NC	5.87	116.15	109.98
18	A	1133	CLA	C2C-C1C-NC	5.87	116.14	109.98
18	1	1004	CLA	O2A-CGA-O1A	-5.87	108.95	123.63
18	A	1103	CLA	C4A-NA-C1A	5.87	109.36	106.68
18	2	2012	CLA	C2D-C1D-ND	5.86	115.93	110.13
18	A	1119	CLA	C2C-C1C-NC	5.86	116.14	109.98
18	A	1134	CLA	C2C-C1C-NC	5.86	116.14	109.98
18	A	1124	CLA	C1D-ND-C4D	-5.86	102.20	106.31
18	1	1003	CLA	C2C-C1C-NC	5.85	116.12	109.98
18	B	1202	CLA	C2C-C1C-NC	5.85	116.12	109.98
18	B	1221	CLA	C4A-NA-C1A	5.85	109.35	106.68
18	B	1211	CLA	C1D-ND-C4D	-5.84	102.21	106.31
18	A	1118	CLA	O2D-CGD-CBD	5.84	121.44	111.23
18	B	1209	CLA	C2C-C1C-NC	5.83	116.10	109.98
18	2	2003	CLA	C2D-C1D-ND	5.83	115.89	110.13
18	A	1127	CLA	C2C-C1C-NC	5.83	116.10	109.98
27	4	4503	LUT	C21-C26-C27	5.81	119.51	112.83
18	A	1013	CLA	C1D-ND-C4D	-5.81	102.24	106.31
18	B	1224	CLA	C4A-NA-C1A	5.81	109.33	106.68
18	B	1227	CLA	O2D-CGD-CBD	5.80	121.38	111.23
18	2	2019	CLA	C3C-C2C-C1C	-5.80	99.90	107.24
18	L	1502	CLA	C4A-NA-C1A	5.80	109.33	106.68
18	A	1139	CLA	C2C-C1C-NC	5.80	116.07	109.98
18	3	3017	CLA	C4A-NA-C1A	5.79	109.32	106.68
18	A	1118	CLA	C2C-C1C-NC	5.78	116.06	109.98
18	B	1234	CLA	C1-C2-C3	-5.78	116.72	126.20
18	3	3012	CLA	C2D-C1D-ND	5.78	115.84	110.13
18	A	1122	CLA	C4A-NA-C1A	5.78	109.31	106.68
18	2	2001	CLA	O2A-CGA-O1A	-5.77	109.20	123.63
18	1	1013	CLA	C1C-C2C-C3C	-5.77	100.91	106.98
18	B	1217	CLA	C2C-C1C-NC	5.76	116.03	109.98
18	3	3004	CLA	C2C-C1C-NC	5.76	116.03	109.98
18	G	1002	CLA	C2C-C1C-NC	5.76	116.03	109.98
18	2	2003	CLA	C2C-C1C-NC	5.76	116.03	109.98
18	B	1225	CLA	C4A-NA-C1A	5.76	109.31	106.68
18	1	1002	CLA	C1D-ND-C4D	-5.75	102.28	106.31
18	2	2008	CLA	C1C-C2C-C3C	-5.75	100.94	106.98
18	1	1014	CLA	C2D-C1D-ND	5.75	115.81	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1113	CLA	C2C-C1C-NC	5.74	116.01	109.98
18	K	1001	CLA	C3B-C2B-C1B	-5.73	100.41	107.17
18	3	3001	CLA	C3B-C2B-C1B	-5.73	100.41	107.17
18	2	2004	CLA	C3B-C2B-C1B	-5.72	100.42	107.17
18	A	1116	CLA	C2C-C1C-NC	5.72	115.99	109.98
18	3	3006	CLA	C4A-NA-C1A	5.72	109.29	106.68
18	3	3018	CLA	C2C-C1C-NC	5.72	115.99	109.98
18	3	3004	CLA	C1C-C2C-C3C	-5.71	100.97	106.98
18	B	1234	CLA	C1D-ND-C4D	-5.71	102.31	106.31
18	A	1101	CLA	O2D-CGD-CBD	5.71	121.21	111.23
18	B	1239	CLA	C2C-C1C-NC	5.71	115.98	109.98
18	A	1117	CLA	C2C-C1C-NC	5.71	115.98	109.98
18	A	1137	CLA	C2C-C1C-NC	5.71	115.97	109.98
18	A	1120	CLA	C4A-NA-C1A	5.70	109.28	106.68
18	2	2016	CLA	C1D-ND-C4D	-5.70	102.31	106.31
18	3	3008	CLA	C2D-C1D-ND	5.70	115.77	110.13
22	L	6020	BCR	C24-C23-C22	-5.70	117.80	126.23
18	1	1004	CLA	O2D-CGD-CBD	5.70	121.19	111.23
18	B	1205	CLA	O2A-CGA-O1A	-5.70	109.38	123.63
18	A	1104	CLA	C2D-C1D-ND	5.69	115.76	110.13
18	2	2009	CLA	C2C-C1C-NC	5.69	115.96	109.98
18	3	3005	CLA	C1C-C2C-C3C	-5.69	101.00	106.98
18	A	1022	CLA	C2C-C1C-NC	5.68	115.95	109.98
18	4	4007	CLA	C1C-C2C-C3C	-5.68	101.00	106.98
18	B	1229	CLA	C2D-C1D-ND	5.68	115.75	110.13
18	4	4005	CLA	C2D-C1D-ND	5.68	115.75	110.13
18	A	1125	CLA	C4A-NA-C1A	5.67	109.27	106.68
18	B	1226	CLA	O2A-CGA-O1A	-5.67	109.44	123.63
23	F	5001	LMG	O7-C10-C11	5.67	121.20	111.09
18	B	1222	CLA	C2D-C1D-ND	5.67	115.73	110.13
18	4	4005	CLA	C3D-C2D-C1D	-5.67	98.10	105.83
18	B	1214	CLA	C2C-C1C-NC	5.66	115.92	109.98
18	B	1206	CLA	C1C-C2C-C3C	-5.66	101.03	106.98
18	G	1001	CLA	O2A-CGA-O1A	-5.65	109.48	123.63
18	A	1101	CLA	C2C-C1C-NC	5.65	115.92	109.98
27	1	1502	LUT	C7-C8-C9	-5.65	117.88	126.23
18	B	1211	CLA	C4A-NA-C1A	5.65	109.26	106.68
18	2	2008	CLA	C3D-C2D-C1D	-5.65	98.13	105.83
18	A	1112	CLA	C2C-C1C-NC	5.64	115.91	109.98
18	2	2007	CLA	C2C-C1C-NC	5.64	115.91	109.98
18	A	1237	CLA	C1D-ND-C4D	-5.64	102.35	106.31
18	B	1219	CLA	C2C-C1C-NC	5.64	115.91	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1201	CLA	C4A-NA-C1A	5.64	109.25	106.68
18	A	1125	CLA	C3D-C2D-C1D	-5.64	98.14	105.83
18	B	1235	CLA	O2A-CGA-O1A	-5.64	109.53	123.63
18	A	1118	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
18	A	1106	CLA	C2C-C1C-NC	5.64	115.90	109.98
18	4	4008	CLA	C3D-C2D-C1D	-5.63	98.14	105.83
18	2	2008	CLA	O2A-CGA-O1A	-5.63	109.55	123.63
18	B	1212	CLA	O2D-CGD-CBD	5.63	121.06	111.23
18	B	1226	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
18	A	1140	CLA	C4A-NA-C1A	5.62	109.25	106.68
18	B	1207	CLA	C1D-ND-C4D	-5.62	102.37	106.31
18	B	1228	CLA	C4A-NA-C1A	5.62	109.24	106.68
18	A	1126	CLA	C2C-C1C-NC	5.62	115.88	109.98
18	4	4004	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
18	B	1215	CLA	C2C-C1C-NC	5.61	115.88	109.98
18	B	1223	CLA	C2C-C1C-NC	5.61	115.88	109.98
18	B	1229	CLA	C4A-NA-C1A	5.61	109.24	106.68
18	A	1124	CLA	C2C-C1C-NC	5.61	115.87	109.98
18	A	1129	CLA	C2C-C1C-NC	5.60	115.86	109.98
18	A	1105	CLA	C2C-C1C-NC	5.60	115.86	109.98
18	A	1109	CLA	C2C-C1C-NC	5.59	115.86	109.98
18	B	1240	CLA	C2C-C1C-NC	5.59	115.86	109.98
18	2	2016	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
18	B	1229	CLA	O2A-CGA-O1A	-5.59	109.65	123.63
18	A	1112	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
18	1	1007	CLA	C3D-C2D-C1D	-5.59	98.21	105.83
18	1	1007	CLA	C2C-C1C-NC	5.58	115.85	109.98
18	4	4017	CLA	O2A-CGA-O1A	-5.58	109.67	123.63
18	4	4012	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
18	L	1502	CLA	O2A-CGA-O1A	-5.58	109.68	123.63
18	A	1122	CLA	C2C-C1C-NC	5.57	115.84	109.98
18	A	1115	CLA	C2C-C1C-NC	5.57	115.84	109.98
18	B	1210	CLA	C2C-C1C-NC	5.57	115.83	109.98
18	A	1126	CLA	C3B-C2B-C1B	-5.57	100.60	107.17
18	4	4008	CLA	C2D-C1D-ND	5.57	115.64	110.13
18	A	1114	CLA	O2D-CGD-CBD	5.57	120.96	111.23
18	A	1237	CLA	C2C-C1C-NC	5.57	115.83	109.98
22	B	6009	BCR	C24-C23-C22	-5.57	118.00	126.23
18	B	1212	CLA	C2C-C1C-NC	5.56	115.83	109.98
18	B	1225	CLA	C2C-C1C-NC	5.56	115.83	109.98
18	1	1012	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
18	A	1111	CLA	C2C-C1C-NC	5.56	115.82	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4005	CLA	O2D-CGD-CBD	5.56	120.95	111.23
18	2	2012	CLA	C3D-C2D-C1D	-5.56	98.25	105.83
18	A	1135	CLA	O2D-CGD-CBD	5.56	120.94	111.23
18	F	1301	CLA	C2C-C1C-NC	5.55	115.81	109.98
18	A	1121	CLA	O2D-CGD-CBD	5.55	120.93	111.23
18	3	3012	CLA	C3B-C2B-C1B	-5.55	100.63	107.17
18	A	1136	CLA	C2C-C1C-NC	5.55	115.81	109.98
18	B	1216	CLA	C2C-C1C-NC	5.55	115.81	109.98
18	1	1012	CLA	C2C-C1C-NC	5.55	115.81	109.98
18	A	1139	CLA	C1C-C2C-C3C	-5.55	101.15	106.98
18	1	1002	CLA	C3D-C2D-C1D	-5.55	98.26	105.83
18	A	1130	CLA	C1D-ND-C4D	-5.54	102.42	106.31
18	B	1204	CLA	C2C-C1C-NC	5.54	115.81	109.98
18	4	4005	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
18	A	1126	CLA	C4A-NA-C1A	5.54	109.21	106.68
18	A	1101	CLA	O2A-CGA-O1A	-5.54	109.77	123.63
18	B	1209	CLA	O2D-CGD-CBD	5.54	120.92	111.23
18	4	4017	CLA	O2D-CGD-CBD	5.54	120.92	111.23
18	3	3001	CLA	C4A-NA-C1A	5.54	109.21	106.68
18	A	1130	CLA	C2C-C1C-NC	5.54	115.80	109.98
18	B	1218	CLA	C2C-C1C-NC	5.54	115.80	109.98
18	A	1013	CLA	C2D-C1D-ND	5.54	115.61	110.13
18	A	1121	CLA	C2C-C1C-NC	5.54	115.80	109.98
18	1	1005	CLA	C2D-C1D-ND	5.53	115.60	110.13
18	B	1236	CLA	C2D-C1D-ND	5.53	115.60	110.13
18	B	1012	CLA	C2C-C1C-NC	5.53	115.79	109.98
18	4	4004	CLA	C3B-C2B-C1B	-5.53	100.65	107.17
18	1	1006	CLA	C2C-C1C-NC	5.53	115.79	109.98
18	4	4006	CLA	C2C-C1C-NC	5.53	115.79	109.98
22	A	6017	BCR	C19-C18-C17	5.53	127.70	119.01
18	1	1003	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
18	B	1234	CLA	O2D-CGD-CBD	5.52	120.89	111.23
18	3	3018	CLA	C3B-C2B-C1B	-5.52	100.67	107.17
18	3	3012	CLA	C1D-ND-C4D	-5.52	102.44	106.31
18	B	1229	CLA	O2D-CGD-CBD	5.51	120.87	111.23
18	A	1132	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
18	L	1503	CLA	O2A-CGA-O1A	-5.51	109.84	123.63
18	B	1240	CLA	C4A-NA-C1A	5.51	109.19	106.68
18	A	1104	CLA	C2C-C1C-NC	5.50	115.76	109.98
18	1	1005	CLA	C2C-C1C-NC	5.50	115.76	109.98
18	A	1109	CLA	C4A-NA-C1A	5.50	109.19	106.68
18	A	1132	CLA	C2C-C1C-NC	5.50	115.76	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1208	CLA	C1D-ND-C4D	-5.50	102.45	106.31
18	3	3018	CLA	C1C-C2C-C3C	-5.50	101.20	106.98
18	B	1236	CLA	C1D-ND-C4D	-5.50	102.45	106.31
18	A	1013	CLA	C4A-NA-C1A	5.50	109.19	106.68
18	A	1127	CLA	C4A-NA-C1A	5.50	109.19	106.68
18	2	2008	CLA	O2D-CGD-CBD	5.50	120.84	111.23
18	3	3002	CLA	O2D-CGD-CBD	5.49	120.84	111.23
18	4	4016	CLA	C2C-C1C-NC	5.49	115.75	109.98
18	4	4009	CLA	C1C-C2C-C3C	-5.49	101.20	106.98
18	A	1103	CLA	C2C-C1C-NC	5.49	115.75	109.98
18	1	1014	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
18	B	1222	CLA	C2C-C1C-NC	5.48	115.74	109.98
18	A	1124	CLA	C2D-C1D-ND	5.48	115.55	110.13
18	B	1221	CLA	C2C-C1C-NC	5.48	115.74	109.98
18	A	1125	CLA	C2D-C1D-ND	5.48	115.55	110.13
18	1	1005	CLA	O2A-CGA-O1A	-5.48	109.92	123.63
29	4	4505	ZEX	C7-C8-C9	-5.48	118.13	126.23
18	2	2004	CLA	O2A-CGA-O1A	-5.47	109.94	123.63
18	B	1240	CLA	C1D-ND-C4D	-5.47	102.47	106.31
18	B	1236	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
18	B	1232	CLA	C2C-C1C-NC	5.47	115.73	109.98
18	F	1302	CLA	O2D-CGD-CBD	5.47	120.79	111.23
18	A	1108	CLA	C2C-C1C-NC	5.46	115.72	109.98
18	L	1503	CLA	C2D-C1D-ND	5.46	115.53	110.13
18	B	1229	CLA	C2C-C1C-NC	5.46	115.72	109.98
18	A	1113	CLA	C4A-NA-C1A	5.46	109.17	106.68
17	A	1011	CL0	O2A-CGA-O1A	-5.46	109.97	123.63
18	J	1302	CLA	O2A-CGA-O1A	-5.46	109.97	123.63
18	B	1217	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
18	3	3012	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
18	A	1128	CLA	O2A-CGA-O1A	-5.45	109.98	123.63
18	B	1212	CLA	C2D-C1D-ND	5.45	115.52	110.13
18	3	3005	CLA	O2D-CGD-CBD	5.45	120.76	111.23
18	A	1136	CLA	C4A-NA-C1A	5.45	109.17	106.68
18	B	1223	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
18	A	1120	CLA	C2C-C1C-NC	5.45	115.70	109.98
18	B	1205	CLA	C2C-C1C-NC	5.44	115.70	109.98
18	B	1239	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
18	B	1235	CLA	O2D-CGD-CBD	5.44	120.74	111.23
18	B	1207	CLA	C2D-C1D-ND	5.44	115.51	110.13
18	4	4009	CLA	C2C-C1C-NC	5.44	115.70	109.98
18	A	1131	CLA	C4A-NA-C1A	5.44	109.16	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2006	CLA	C2C-C1C-NC	5.44	115.69	109.98
23	J	5001	LMG	O7-C10-C11	5.44	123.24	111.48
18	1	1006	CLA	C1C-C2C-C3C	-5.43	101.26	106.98
18	B	1218	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
18	3	3006	CLA	O2A-CGA-O1A	-5.43	110.04	123.63
18	A	1103	CLA	O2D-CGD-CBD	5.43	120.72	111.23
18	B	1235	CLA	C1D-ND-C4D	-5.43	102.50	106.31
18	B	1229	CLA	C1D-ND-C4D	-5.43	102.50	106.31
18	4	4008	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
18	2	2008	CLA	C2C-C1C-NC	5.43	115.68	109.98
18	A	1111	CLA	O2D-CGD-CBD	5.43	120.72	111.23
18	B	1213	CLA	C1D-ND-C4D	-5.43	102.50	106.31
18	B	1207	CLA	C2C-C1C-NC	5.43	115.68	109.98
18	A	1138	CLA	C1D-ND-C4D	-5.42	102.51	106.31
18	H	1000	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
18	1	1008	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
18	B	1203	CLA	C2C-C1C-NC	5.42	115.68	109.98
18	4	4017	CLA	C2C-C1C-NC	5.42	115.67	109.98
18	3	3010	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
18	A	1107	CLA	C2C-C1C-NC	5.42	115.67	109.98
18	B	1218	CLA	C1D-ND-C4D	-5.42	102.51	106.31
18	B	1021	CLA	C2D-C1D-ND	5.42	115.49	110.13
18	1	1014	CLA	C1D-ND-C4D	-5.42	102.51	106.31
18	G	1001	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
18	B	1222	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
18	B	1220	CLA	C2C-C1C-NC	5.41	115.67	109.98
18	1	1001	CLA	C2D-C1D-ND	5.41	115.48	110.13
18	B	1224	CLA	O2A-CGA-O1A	-5.41	110.10	123.63
23	4	4801	LMG	O7-C10-C11	5.41	123.17	111.48
18	B	1229	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
18	3	3007	CLA	C2C-C1C-NC	5.40	115.66	109.98
18	G	1003	CLA	C2C-C1C-NC	5.40	115.66	109.98
18	B	1021	CLA	C1D-ND-C4D	-5.40	102.52	106.31
18	B	1204	CLA	C1D-ND-C4D	-5.40	102.52	106.31
22	B	6004	BCR	C20-C19-C18	5.40	141.17	126.36
21	B	5004	LHG	O7-C7-C8	5.40	120.72	111.09
18	A	1131	CLA	C2C-C1C-NC	5.40	115.65	109.98
18	B	1238	CLA	O2D-CGD-CBD	5.40	120.67	111.23
18	3	3012	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
18	3	3002	CLA	C3D-C2D-C1D	-5.40	98.47	105.83
18	A	1111	CLA	C4A-NA-C1A	5.39	109.14	106.68
18	B	1209	CLA	C3B-C2B-C1B	-5.39	100.81	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1120	CLA	C1D-ND-C4D	-5.39	102.53	106.31
18	A	1139	CLA	C1D-ND-C4D	-5.39	102.53	106.31
18	B	1217	CLA	O2D-CGD-CBD	5.39	120.65	111.23
18	B	1203	CLA	C4A-NA-C1A	5.39	109.14	106.68
18	B	1222	CLA	C4A-NA-C1A	5.39	109.14	106.68
18	H	1000	CLA	C4A-NA-C1A	5.39	109.14	106.68
18	B	1212	CLA	C1D-ND-C4D	-5.38	102.53	106.31
18	B	1238	CLA	C2C-C1C-NC	5.38	115.64	109.98
18	B	1223	CLA	C4A-NA-C1A	5.38	109.14	106.68
18	G	1003	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
18	2	2005	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
18	B	1234	CLA	C2D-C1D-ND	5.38	115.45	110.13
22	B	6004	BCR	C24-C23-C22	-5.38	118.28	126.23
18	1	1011	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
18	L	1503	CLA	C2C-C1C-NC	5.38	115.63	109.98
18	3	3008	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
18	2	2012	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
18	B	1208	CLA	C2C-C1C-NC	5.37	115.63	109.98
18	B	1228	CLA	C2D-C1D-ND	5.37	115.44	110.13
18	A	1125	CLA	C2C-C1C-NC	5.37	115.62	109.98
18	A	1104	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
29	4	4505	ZEX	C28-C27-C26	-5.37	118.30	126.94
18	B	1222	CLA	C1D-ND-C4D	-5.37	102.55	106.31
18	B	1021	CLA	C2C-C1C-NC	5.37	115.62	109.98
18	A	1151	CLA	C1C-C2C-C3C	-5.37	101.34	106.98
18	A	1121	CLA	C1D-ND-C4D	-5.36	102.55	106.31
18	L	1501	CLA	C1D-ND-C4D	-5.36	102.55	106.31
18	A	1123	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
18	A	1135	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
18	A	1114	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
18	2	2005	CLA	C2C-C1C-NC	5.36	115.61	109.98
18	4	4008	CLA	C1D-ND-C4D	-5.36	102.55	106.31
18	A	1130	CLA	C2D-C1D-ND	5.36	115.43	110.13
18	1	1007	CLA	C2D-C1D-ND	5.36	115.43	110.13
18	B	1240	CLA	O2D-CGD-CBD	5.36	120.60	111.23
18	A	1116	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
18	A	1102	CLA	C2C-C1C-NC	5.36	115.61	109.98
18	F	1302	CLA	C2C-C1C-NC	5.36	115.61	109.98
18	3	3006	CLA	C2C-C1C-NC	5.36	115.61	109.98
18	3	3007	CLA	C3B-C2B-C1B	-5.36	100.86	107.17
18	A	1134	CLA	C4A-NA-C1A	5.35	109.12	106.68
18	A	1106	CLA	C1C-C2C-C3C	-5.35	101.35	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1225	CLA	C1D-ND-C4D	-5.35	102.56	106.31
18	A	1132	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
18	B	1012	CLA	C4A-NA-C1A	5.35	109.12	106.68
18	B	1203	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
18	1	1001	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
18	B	1235	CLA	C2C-C1C-NC	5.35	115.60	109.98
18	1	1005	CLA	C1D-ND-C4D	-5.35	102.56	106.31
22	A	6017	BCR	C20-C19-C18	5.35	141.02	126.36
18	B	1236	CLA	C2C-C1C-NC	5.34	115.59	109.98
18	A	1140	CLA	C1D-ND-C4D	-5.34	102.56	106.31
18	A	1130	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
18	B	1224	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
18	A	1105	CLA	C1D-ND-C4D	-5.34	102.56	106.31
18	A	1116	CLA	O2A-CGA-O1A	-5.34	110.27	123.63
18	A	1117	CLA	O2D-CGD-CBD	5.34	120.56	111.23
18	B	1225	CLA	O2D-CGD-CBD	5.34	120.56	111.23
18	A	1134	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
18	4	4012	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
18	A	1101	CLA	C1D-ND-C4D	-5.34	102.57	106.31
18	1	1008	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
18	B	1224	CLA	O2D-CGD-CBD	5.33	120.56	111.23
18	A	1133	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
18	A	1119	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
18	A	1125	CLA	O2D-CGD-CBD	5.33	120.55	111.23
18	B	1218	CLA	O2A-CGA-O1A	-5.33	110.29	123.63
18	A	1101	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
18	A	1124	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
18	G	1002	CLA	C1C-C2C-C3C	-5.33	101.38	106.98
18	A	1131	CLA	C1D-ND-C4D	-5.33	102.57	106.31
18	4	4001	CLA	O2A-CGA-O1A	-5.33	110.31	123.63
18	4	4008	CLA	O2D-CGD-CBD	5.32	120.54	111.23
18	B	1238	CLA	C1D-ND-C4D	-5.32	102.58	106.31
18	B	1228	CLA	C2C-C1C-NC	5.32	115.57	109.98
18	4	4005	CLA	O2A-CGA-O1A	-5.32	110.31	123.63
18	4	4008	CLA	C3B-C2B-C1B	-5.32	100.89	107.17
18	B	1214	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
18	1	1004	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
18	A	1130	CLA	C4A-NA-C1A	5.32	109.11	106.68
18	B	1209	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
18	J	1302	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
18	A	1124	CLA	O2A-CGA-O1A	-5.32	110.32	123.63
18	A	1136	CLA	C1D-ND-C4D	-5.32	102.58	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1215	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
18	4	4004	CLA	O2A-CGA-O1A	-5.31	110.34	123.63
18	A	1121	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
22	3	3503	BCR	C33-C5-C6	-5.31	118.69	124.48
18	B	1223	CLA	C2D-C1D-ND	5.31	115.38	110.13
18	A	1109	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
18	2	2002	CLA	C2C-C1C-NC	5.31	115.56	109.98
18	B	1228	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
18	B	1021	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
18	B	1203	CLA	C2D-C1D-ND	5.30	115.38	110.13
18	B	1203	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
18	A	1107	CLA	C1D-ND-C4D	-5.30	102.59	106.31
18	A	1136	CLA	C2D-C1D-ND	5.30	115.37	110.13
18	1	1014	CLA	C2C-C1C-NC	5.30	115.55	109.98
18	3	3013	CLA	C2C-C1C-NC	5.30	115.55	109.98
18	1	1004	CLA	C2C-C1C-NC	5.30	115.55	109.98
18	3	3012	CLA	O2A-CGA-O1A	-5.30	110.37	123.63
18	B	1215	CLA	O2D-CGD-CBD	5.30	120.49	111.23
18	B	1225	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
18	B	1023	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
18	B	1221	CLA	C1D-ND-C4D	-5.30	102.60	106.31
18	L	1502	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
18	A	1122	CLA	O2A-CGA-O1A	-5.30	110.38	123.63
18	A	1109	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
18	3	3002	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
18	A	1137	CLA	C2D-C1D-ND	5.29	115.36	110.13
18	B	1203	CLA	C1D-ND-C4D	-5.29	102.60	106.31
18	A	1124	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
18	B	1228	CLA	C1D-ND-C4D	-5.29	102.60	106.31
18	A	1121	CLA	C2D-C1D-ND	5.29	115.36	110.13
18	L	1503	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
18	A	1140	CLA	O2D-CGD-CBD	5.29	120.48	111.23
18	A	1115	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
18	B	1220	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
18	B	1234	CLA	C4A-NA-C1A	5.28	109.09	106.68
18	3	3001	CLA	C2C-C1C-NC	5.28	115.53	109.98
18	B	1202	CLA	O2D-CGD-CBD	5.28	120.47	111.23
18	A	1137	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
18	G	1001	CLA	O2D-CGD-CBD	5.28	120.46	111.23
18	2	2004	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
18	1	1007	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
18	A	1110	CLA	C2C-C1C-NC	5.28	115.52	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1235	CLA	C2D-C1D-ND	5.27	115.35	110.13
18	B	1229	CLA	C3B-C2B-C1B	-5.27	100.95	107.17
22	I	6020	BCR	C20-C19-C18	5.27	140.82	126.36
18	A	1136	CLA	O2A-CGA-O1A	-5.27	110.44	123.63
18	2	2007	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
18	2	2006	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
18	B	1239	CLA	O2D-CGD-CBD	5.27	120.44	111.23
18	A	1237	CLA	C1-C2-C3	-5.27	117.57	126.20
18	4	4003	CLA	C2C-C1C-NC	5.27	115.51	109.98
18	1	1005	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
18	A	1140	CLA	C2D-C1D-ND	5.27	115.34	110.13
18	B	1227	CLA	C2C-C1C-NC	5.26	115.51	109.98
18	2	2006	CLA	O2A-CGA-O1A	-5.26	110.46	123.63
18	A	1136	CLA	O2D-CGD-CBD	5.26	120.43	111.23
18	A	1137	CLA	C1D-ND-C4D	-5.26	102.62	106.31
18	B	1202	CLA	C1-C2-C3	-5.26	117.58	126.20
18	B	1230	CLA	O2A-CGA-O1A	-5.26	110.47	123.63
18	A	1121	CLA	O2A-CGA-O1A	-5.26	110.47	123.63
18	B	1216	CLA	O2D-CGD-CBD	5.26	120.42	111.23
18	1	1011	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
18	A	1107	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
18	2	2012	CLA	C1D-ND-C4D	-5.26	102.62	106.31
18	1	1001	CLA	O2A-CGA-O1A	-5.26	110.48	123.63
18	B	1215	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
18	A	1130	CLA	O2D-CGD-CBD	5.26	120.42	111.23
18	B	1202	CLA	C1C-C2C-C3C	-5.25	101.45	106.98
18	B	1224	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
18	4	4009	CLA	O2A-CGA-O1A	-5.25	110.49	123.63
18	A	1128	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
18	B	1211	CLA	C2D-C1D-ND	5.25	115.32	110.13
18	A	1109	CLA	C2D-C1D-ND	5.25	115.32	110.13
18	B	1234	CLA	C2C-C1C-NC	5.25	115.50	109.98
18	B	1219	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
18	A	1134	CLA	O2A-CGA-O1A	-5.25	110.50	123.63
18	4	4017	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
18	B	1227	CLA	C1D-ND-C4D	-5.25	102.63	106.31
18	A	1121	CLA	C4A-NA-C1A	5.25	109.07	106.68
18	B	1207	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
18	B	1220	CLA	C1D-ND-C4D	-5.25	102.63	106.31
18	A	1124	CLA	C3D-C2D-C1D	-5.24	98.67	105.83
18	A	1113	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
18	2	2001	CLA	CAA-C2A-C1A	-5.24	94.79	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1137	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
18	B	1213	CLA	C2D-C1D-ND	5.24	115.31	110.13
18	3	3007	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
18	2	2002	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
18	A	1120	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
18	F	1302	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
18	A	1130	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
18	4	4002	CLA	O2A-CGA-O1A	-5.24	110.52	123.63
18	A	1102	CLA	O2D-CGD-CBD	5.24	120.39	111.23
18	J	1302	CLA	C4A-NA-C1A	5.24	109.07	106.68
18	B	1232	CLA	O2A-CGA-O1A	-5.24	110.53	123.63
18	B	1222	CLA	C1C-C2C-C3C	-5.23	101.47	106.98
18	B	1227	CLA	C1C-C2C-C3C	-5.23	101.47	106.98
18	A	1131	CLA	C2D-C1D-ND	5.23	115.31	110.13
18	A	1118	CLA	C2D-C1D-ND	5.23	115.31	110.13
18	A	1131	CLA	O2A-CGA-O1A	-5.23	110.54	123.63
18	B	1236	CLA	O2D-CGD-CBD	5.23	120.38	111.23
18	B	1208	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
18	A	1117	CLA	C4A-NA-C1A	5.23	109.07	106.68
18	1	1013	CLA	O2D-CGD-CBD	5.23	120.38	111.23
18	B	1236	CLA	O2A-CGA-O1A	-5.23	110.54	123.63
18	B	1023	CLA	C2D-C1D-ND	5.23	115.30	110.13
18	B	1210	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
18	A	1111	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
18	1	1011	CLA	C1D-ND-C4D	-5.23	102.64	106.31
18	L	1502	CLA	O2D-CGD-CBD	5.23	120.37	111.23
18	B	1240	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
18	A	1107	CLA	O2D-CGD-CBD	5.23	120.36	111.23
18	3	3012	CLA	C2C-C1C-NC	5.23	115.47	109.98
18	1	1002	CLA	C1C-C2C-C3C	-5.22	101.48	106.98
18	A	1133	CLA	O2A-CGA-O1A	-5.22	110.56	123.63
18	A	1138	CLA	C2C-C1C-NC	5.22	115.47	109.98
18	A	1131	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
18	B	1012	CLA	C3B-C2B-C1B	-5.22	101.01	107.17
18	A	1129	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
18	A	1140	CLA	C2C-C1C-NC	5.22	115.47	109.98
18	A	1127	CLA	O2A-CGA-O1A	-5.22	110.57	123.63
18	A	1110	CLA	O2D-CGD-CBD	5.22	120.36	111.23
18	1	1014	CLA	O2D-CGD-CBD	5.22	120.35	111.23
18	A	1117	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
18	B	1221	CLA	C2D-C1D-ND	5.22	115.29	110.13
18	A	1127	CLA	C1C-C2C-C3C	-5.22	101.49	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1235	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
18	4	4006	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
18	A	1139	CLA	C4A-NA-C1A	5.21	109.06	106.68
18	B	1214	CLA	O2A-CGA-O1A	-5.21	110.59	123.63
18	3	3017	CLA	C2C-C1C-NC	5.21	115.45	109.98
18	B	1240	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
18	B	1012	CLA	C2D-C1D-ND	5.21	115.28	110.13
18	1	1001	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
18	A	1108	CLA	C1D-ND-C4D	-5.21	102.66	106.31
18	3	3017	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
18	B	1238	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
18	L	1503	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
18	A	1105	CLA	C2D-C1D-ND	5.21	115.28	110.13
18	B	1023	CLA	C2C-C1C-NC	5.21	115.45	109.98
22	A	6008	BCR	C24-C23-C22	-5.20	118.54	126.23
18	B	1201	CLA	C2C-C1C-NC	5.20	115.45	109.98
18	A	1120	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
18	4	4003	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
18	1	1003	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
18	B	1240	CLA	C2D-C1D-ND	5.20	115.27	110.13
18	B	1215	CLA	C2D-C1D-ND	5.20	115.27	110.13
18	B	1213	CLA	C4A-NA-C1A	5.20	109.05	106.68
18	A	1237	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
18	A	1013	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
18	B	1230	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
18	B	1205	CLA	C4A-NA-C1A	5.20	109.05	106.68
18	B	1212	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
18	A	1115	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
18	3	3019	CLA	C1C-NC-C4C	-5.20	104.31	106.68
18	A	1105	CLA	C1C-C2C-C3C	-5.20	101.52	106.98
18	B	1218	CLA	C2D-C1D-ND	5.19	115.27	110.13
18	A	1237	CLA	C4A-NA-C1A	5.19	109.05	106.68
18	G	1003	CLA	C1D-ND-C4D	-5.19	102.67	106.31
18	4	4003	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
18	A	1138	CLA	C4A-NA-C1A	5.19	109.05	106.68
18	A	1121	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
18	B	1235	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
18	B	1212	CLA	C1C-C2C-C3C	-5.19	101.53	106.98
18	B	1208	CLA	C2D-C1D-ND	5.19	115.26	110.13
18	B	1219	CLA	C4A-NA-C1A	5.19	109.05	106.68
18	A	1136	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
18	A	1140	CLA	C3D-C2D-C1D	-5.19	98.76	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1104	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
18	A	1108	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
18	B	1012	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
22	K	2011	BCR	C24-C23-C22	-5.18	118.57	126.23
18	B	1232	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
27	4	4503	LUT	C1-C6-C5	-5.18	115.56	122.64
18	A	1109	CLA	O2A-CGA-O1A	-5.18	110.68	123.63
18	B	1012	CLA	O2A-CGA-O1A	-5.18	110.68	123.63
18	F	1301	CLA	C1C-C2C-C3C	-5.18	101.54	106.98
18	B	1201	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
18	A	1119	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
18	A	1129	CLA	C2D-C1D-ND	5.17	115.25	110.13
18	1	1012	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
18	B	1206	CLA	O2A-CGA-O1A	-5.17	110.69	123.63
18	B	1239	CLA	C1D-ND-C4D	-5.17	102.68	106.31
18	L	1503	CLA	C1D-ND-C4D	-5.17	102.68	106.31
22	F	6014	BCR	C24-C23-C22	-5.17	118.59	126.23
18	B	1239	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
18	L	1502	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
18	B	1213	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
18	A	1132	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
18	L	1502	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
18	A	1126	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
18	A	1108	CLA	C3B-C2B-C1B	-5.16	101.08	107.17
18	1	1001	CLA	C2C-C1C-NC	5.16	115.41	109.98
18	B	1239	CLA	C4A-NA-C1A	5.16	109.03	106.68
18	A	1131	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
18	A	1118	CLA	C1D-ND-C4D	-5.16	102.69	106.31
18	A	1120	CLA	C2D-C1D-ND	5.16	115.24	110.13
18	B	1204	CLA	C4A-NA-C1A	5.16	109.03	106.68
18	A	1112	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
18	A	1134	CLA	O2D-CGD-CBD	5.16	120.25	111.23
18	A	1119	CLA	O2A-CGA-O1A	-5.16	110.72	123.63
18	A	1118	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
18	B	1213	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
18	2	2002	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
18	B	1220	CLA	C2D-C1D-ND	5.16	115.23	110.13
18	4	4004	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
18	4	4012	CLA	C2D-C1D-ND	5.16	115.23	110.13
18	B	1238	CLA	O2A-CGA-O1A	-5.15	110.73	123.63
18	3	3004	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
18	B	1204	CLA	C1C-C2C-C3C	-5.15	101.56	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1232	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
18	B	1236	CLA	C4A-NA-C1A	5.15	109.03	106.68
18	B	1236	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
18	2	2012	CLA	C2C-C1C-NC	5.15	115.39	109.98
18	A	1122	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
18	B	1225	CLA	C2D-C1D-ND	5.15	115.22	110.13
18	1	1006	CLA	O2A-CGA-O1A	-5.15	110.75	123.63
18	B	1223	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
18	2	2005	CLA	C1D-ND-C4D	-5.15	102.70	106.31
18	4	4003	CLA	O2A-CGA-O1A	-5.14	110.76	123.63
18	A	1022	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
18	A	1131	CLA	O2D-CGD-CBD	5.14	120.22	111.23
18	A	1114	CLA	C4A-NA-C1A	5.14	109.02	106.68
18	B	1216	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
18	F	1302	CLA	O2A-CGA-O1A	-5.14	110.77	123.63
18	B	1214	CLA	C4A-NA-C1A	5.14	109.02	106.68
18	G	1001	CLA	C3B-C2B-C1B	-5.14	101.12	107.17
18	4	4004	CLA	C1D-ND-C4D	-5.13	102.71	106.31
18	A	1102	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
18	A	1106	CLA	C4A-NA-C1A	5.13	109.02	106.68
18	A	1113	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
18	A	1102	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
18	A	1132	CLA	O2A-CGA-O1A	-5.13	110.79	123.63
18	B	1205	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
18	2	2009	CLA	O2A-CGA-O1A	-5.13	110.80	123.63
18	A	1105	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
18	A	1151	CLA	O2A-CGA-O1A	-5.13	110.80	123.63
18	4	4002	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
18	A	1116	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
18	3	3004	CLA	C1D-ND-C4D	-5.13	102.71	106.31
18	A	1123	CLA	O2A-CGA-O1A	-5.13	110.80	123.63
18	L	1502	CLA	C1D-ND-C4D	-5.13	102.72	106.31
18	A	1129	CLA	O2D-CGD-CBD	5.13	120.19	111.23
18	A	1132	CLA	C1D-ND-C4D	-5.12	102.72	106.31
18	A	1106	CLA	O2A-CGA-O1A	-5.12	110.81	123.63
18	B	1239	CLA	C2D-C1D-ND	5.12	115.20	110.13
18	J	1302	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
18	2	2003	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
18	B	1221	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
18	A	1115	CLA	C1D-ND-C4D	-5.12	102.72	106.31
18	B	1234	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
18	2	2008	CLA	C3B-C2B-C1B	-5.12	101.14	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1123	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
18	A	1102	CLA	C2D-C1D-ND	5.12	115.19	110.13
18	A	1134	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
18	A	1103	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
18	A	1122	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
18	A	1133	CLA	O2D-CGD-CBD	5.11	120.17	111.23
18	B	1236	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
18	B	1021	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
18	B	1204	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
18	2	2002	CLA	C1D-ND-C4D	-5.11	102.72	106.31
18	A	1109	CLA	C1D-ND-C4D	-5.11	102.72	106.31
18	B	1217	CLA	C1D-ND-C4D	-5.11	102.72	106.31
18	A	1139	CLA	C2D-C1D-ND	5.11	115.18	110.13
18	3	3019	CLA	C3C-C2C-C1C	-5.11	100.78	107.24
18	B	1216	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
18	B	1231	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
18	B	1217	CLA	C4A-NA-C1A	5.11	109.01	106.68
18	2	2002	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
18	B	1222	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
18	B	1213	CLA	C2C-C1C-NC	5.10	115.34	109.98
18	G	1003	CLA	O2D-CGD-CBD	5.10	120.15	111.23
18	A	1110	CLA	C4A-NA-C1A	5.10	109.01	106.68
18	B	1232	CLA	C1D-ND-C4D	-5.10	102.73	106.31
18	A	1117	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
18	4	4012	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
18	A	1237	CLA	O2A-CGA-O1A	-5.10	110.87	123.63
18	A	1138	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
18	A	1132	CLA	C2D-C1D-ND	5.10	115.17	110.13
18	L	1501	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
18	B	1224	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
18	A	1151	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
18	B	1212	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
18	1	1007	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
18	B	1210	CLA	C1D-ND-C4D	-5.10	102.74	106.31
18	B	1211	CLA	O2A-CGA-O1A	-5.09	110.88	123.63
18	A	1120	CLA	C3B-C2B-C1B	-5.09	101.16	107.17
18	A	1136	CLA	C1C-C2C-C3C	-5.09	101.62	106.98
18	A	1151	CLA	C4A-NA-C1A	5.09	109.00	106.68
22	G	2011	BCR	C19-C18-C17	5.09	127.02	119.01
18	B	1201	CLA	C1D-ND-C4D	-5.09	102.74	106.31
18	A	1133	CLA	C2D-C1D-ND	5.09	115.17	110.13
18	B	1208	CLA	C3D-C2D-C1D	-5.09	98.88	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1130	CLA	O2A-CGA-O1A	-5.09	110.89	123.63
18	A	1133	CLA	C4A-NA-C1A	5.09	109.00	106.68
18	A	1101	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
18	B	1218	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
18	B	1232	CLA	C2D-C1D-ND	5.09	115.16	110.13
18	3	3018	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
18	L	1502	CLA	C2C-C1C-NC	5.09	115.32	109.98
18	B	1223	CLA	O2A-CGA-O1A	-5.09	110.91	123.63
18	B	1021	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
18	B	1220	CLA	C1C-C2C-C3C	-5.08	101.63	106.98
18	A	1103	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
18	A	1112	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
18	B	1228	CLA	C1C-C2C-C3C	-5.08	101.63	106.98
18	B	1207	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
18	4	4001	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
27	3	3502	LUT	C18-C5-C6	-5.08	118.94	124.48
18	4	4004	CLA	C2D-C1D-ND	5.08	115.15	110.13
18	4	4007	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
18	A	1103	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
18	A	1111	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
18	B	1201	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
18	A	1124	CLA	O2D-CGD-CBD	5.08	120.10	111.23
18	B	1214	CLA	C3B-C2B-C1B	-5.08	101.19	107.17
18	A	1135	CLA	O2A-CGA-O1A	-5.08	110.93	123.63
18	A	1237	CLA	C2D-C1D-ND	5.08	115.15	110.13
18	L	1502	CLA	C2D-C1D-ND	5.08	115.15	110.13
18	A	1102	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
18	H	1000	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
18	B	1202	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
18	A	1237	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
18	B	1211	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
18	A	1135	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
18	B	1210	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
18	B	1217	CLA	C2D-C1D-ND	5.07	115.14	110.13
18	B	1227	CLA	C4A-NA-C1A	5.07	108.99	106.68
18	A	1114	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
18	A	1110	CLA	C1D-ND-C4D	-5.07	102.75	106.31
18	B	1218	CLA	C4A-NA-C1A	5.07	108.99	106.68
18	3	3013	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
18	A	1101	CLA	C2D-C1D-ND	5.07	115.14	110.13
18	B	1230	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
22	L	6019	BCR	C24-C23-C22	-5.06	118.74	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1136	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
18	A	1126	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
18	A	1138	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
27	4	4501	LUT	C21-C26-C27	5.06	118.64	112.83
18	B	1203	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
18	B	1220	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
18	B	1215	CLA	C1D-ND-C4D	-5.06	102.76	106.31
18	A	1108	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
18	B	1221	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
18	G	1003	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
18	4	4017	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
18	B	1208	CLA	O2A-CGA-O1A	-5.06	110.98	123.63
18	B	1234	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
18	2	2003	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
18	A	1110	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
18	A	1106	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
18	B	1023	CLA	O2A-CGA-O1A	-5.05	110.99	123.63
18	B	1222	CLA	O2A-CGA-O1A	-5.05	110.99	123.63
18	B	1202	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
18	A	1123	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
18	A	1151	CLA	C1D-ND-C4D	-5.05	102.77	106.31
18	A	1115	CLA	C2D-C1D-ND	5.05	115.12	110.13
18	B	1227	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
18	B	1238	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
27	2	2501	LUT	C21-C26-C27	5.05	118.63	112.83
18	B	1240	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
18	1	1004	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
18	1	1006	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
18	B	1204	CLA	C2D-C1D-ND	5.05	115.12	110.13
18	A	1107	CLA	C4A-NA-C1A	5.05	108.98	106.68
18	A	1129	CLA	C1C-C2C-C3C	-5.04	101.67	106.98
18	A	1115	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
18	A	1110	CLA	C2D-C1D-ND	5.04	115.12	110.13
18	2	2007	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
18	2	2007	CLA	O2A-CGA-O1A	-5.04	111.01	123.63
18	B	1228	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
18	G	1003	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
18	A	1114	CLA	C1D-ND-C4D	-5.04	102.78	106.31
18	A	1126	CLA	C1-C2-C3	-5.04	117.94	126.20
18	B	1023	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
18	1	1007	CLA	C1D-ND-C4D	-5.04	102.78	106.31
18	A	1139	CLA	C3D-C2D-C1D	-5.04	98.96	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1209	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
18	B	1214	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
18	A	1107	CLA	C3B-C2B-C1B	-5.03	101.23	107.17
18	A	1125	CLA	C1D-ND-C4D	-5.03	102.78	106.31
18	3	3006	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
18	1	1002	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
18	B	1217	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
18	1	1002	CLA	C2C-C1C-NC	5.03	115.27	109.98
18	B	1215	CLA	C4A-NA-C1A	5.03	108.97	106.68
18	J	1302	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
18	B	1213	CLA	O2A-CGA-O1A	-5.03	111.05	123.63
18	1	1004	CLA	C1D-ND-C4D	-5.03	102.78	106.31
18	2	2006	CLA	O2D-CGD-CBD	5.03	120.02	111.23
18	2	2012	CLA	O2A-CGA-O1A	-5.03	111.05	123.63
18	A	1128	CLA	C4A-NA-C1A	5.03	108.97	106.68
18	3	3003	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
18	B	1235	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
18	A	1135	CLA	C4A-NA-C1A	5.03	108.97	106.68
18	B	1209	CLA	C4A-NA-C1A	5.03	108.97	106.68
18	A	1139	CLA	C3B-C2B-C1B	-5.03	101.25	107.17
18	A	1122	CLA	C2D-C1D-ND	5.02	115.10	110.13
18	A	1137	CLA	O2D-CGD-CBD	5.02	120.01	111.23
18	A	1106	CLA	C1D-ND-C4D	-5.02	102.79	106.31
18	A	1022	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
18	1	1004	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
18	B	1207	CLA	O2D-CGD-CBD	5.02	120.01	111.23
18	1	1014	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
18	A	1013	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
18	A	1111	CLA	C2D-C1D-ND	5.02	115.10	110.13
18	B	1205	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
18	4	4016	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
18	B	1201	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
18	3	3004	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
18	A	1127	CLA	C2D-C1D-ND	5.01	115.09	110.13
18	B	1204	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
18	A	1116	CLA	C2D-C1D-ND	5.01	115.09	110.13
22	A	6002	BCR	C24-C23-C22	-5.01	118.82	126.23
18	A	1101	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
18	J	1302	CLA	O2D-CGD-CBD	5.01	119.99	111.23
18	B	1201	CLA	C2D-C1D-ND	5.01	115.08	110.13
18	A	1106	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
28	4	4013	CHL	C1B-CHB-C4A	5.01	124.54	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1234	CLA	O2A-CGA-O1A	-5.01	111.11	123.63
18	2	2007	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
18	3	3017	CLA	C1C-C2C-C3C	-5.01	101.72	106.98
18	B	1227	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
18	A	1138	CLA	C2D-C1D-ND	5.00	115.08	110.13
18	A	1137	CLA	C4A-NA-C1A	5.00	108.96	106.68
18	2	2009	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
18	4	4009	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
18	A	1111	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
18	A	1113	CLA	O2D-CGD-CBD	5.00	119.97	111.23
18	B	1204	CLA	O2D-CGD-CBD	5.00	119.97	111.23
18	B	1209	CLA	C2D-C1D-ND	5.00	115.08	110.13
18	B	1202	CLA	C2D-C1D-ND	5.00	115.08	110.13
18	A	1013	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
18	A	1101	CLA	C4A-NA-C1A	5.00	108.96	106.68
18	4	4016	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
18	A	1127	CLA	O2D-CGD-CBD	5.00	119.97	111.23
18	A	1151	CLA	C2D-C1D-ND	5.00	115.07	110.13
18	B	1238	CLA	C2D-C1D-ND	5.00	115.07	110.13
18	B	1232	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
27	4	4503	LUT	C35-C34-C33	-5.00	120.27	127.28
18	4	4006	CLA	C1D-ND-C4D	-5.00	102.81	106.31
18	A	1121	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
18	A	1127	CLA	C1D-ND-C4D	-5.00	102.81	106.31
18	A	1116	CLA	C1D-ND-C4D	-5.00	102.81	106.31
18	1	1005	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
18	B	1221	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
18	A	1130	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
18	B	1207	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
18	4	4002	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
18	3	3005	CLA	O2A-CGA-O1A	-4.99	111.15	123.63
18	A	1107	CLA	O2A-CGA-O1A	-4.99	111.15	123.63
18	L	1501	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
18	3	3008	CLA	O2A-CGA-O1A	-4.99	111.15	123.63
18	A	1135	CLA	C1D-ND-C4D	-4.99	102.81	106.31
18	A	1151	CLA	O2D-CGD-CBD	4.99	119.95	111.23
18	B	1226	CLA	O2D-CGD-CBD	4.99	119.95	111.23
18	B	1207	CLA	C4A-NA-C1A	4.99	108.95	106.68
18	H	1000	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
18	4	4005	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
18	A	1133	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
18	A	1110	CLA	O2A-CGA-O1A	-4.98	111.16	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	F	1301	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
18	B	1210	CLA	O2D-CGD-CBD	4.98	119.94	111.23
18	A	1133	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
18	F	1302	CLA	C1D-ND-C4D	-4.98	102.82	106.31
18	2	2009	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
18	A	1151	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
18	B	1231	CLA	C2C-C1C-NC	4.98	115.21	109.98
18	A	1123	CLA	C2D-C1D-ND	4.98	115.05	110.13
18	2	2019	CLA	C2C-C1C-NC	4.98	116.96	109.48
18	A	1129	CLA	O2A-CGA-O1A	-4.98	111.18	123.63
18	F	1301	CLA	C1D-ND-C4D	-4.98	102.82	106.31
18	A	1129	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
18	A	1022	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
18	A	1116	CLA	O2D-CGD-CBD	4.97	119.93	111.23
18	4	4007	CLA	O2D-CGD-CBD	4.97	119.93	111.23
18	A	1113	CLA	C2D-C1D-ND	4.97	115.05	110.13
18	3	3003	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
18	4	4009	CLA	C1D-ND-C4D	-4.97	102.82	106.31
18	3	3018	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
18	4	4006	CLA	C2D-C1D-ND	4.97	115.05	110.13
18	B	1012	CLA	C1C-C2C-C3C	-4.97	101.75	106.98
18	A	1112	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
18	A	1107	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
27	1	1502	LUT	C21-C26-C27	4.97	118.54	112.83
18	B	1231	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
18	4	4016	CLA	C1D-ND-C4D	-4.97	102.83	106.31
18	A	1108	CLA	C2D-C1D-ND	4.97	115.04	110.13
18	A	1110	CLA	C1C-C2C-C3C	-4.96	101.76	106.98
18	4	4017	CLA	C2D-C1D-ND	4.96	115.04	110.13
18	B	1238	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
18	2	2001	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
18	4	4003	CLA	O2D-CGD-CBD	4.96	119.90	111.23
18	1	1011	CLA	O2D-CGD-CBD	4.96	119.90	111.23
18	4	4004	CLA	C2C-C1C-NC	4.96	115.19	109.98
18	3	3001	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
18	A	1111	CLA	O2A-CGA-O1A	-4.96	111.22	123.63
18	A	1116	CLA	C4A-NA-C1A	4.96	108.94	106.68
18	3	3002	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
18	F	1301	CLA	O2A-CGA-O1A	-4.96	110.58	123.33
18	B	1206	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
18	A	1119	CLA	C2D-C1D-ND	4.96	115.03	110.13
18	A	1120	CLA	O2A-CGA-O1A	-4.96	111.23	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1116	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
18	2	2005	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
18	A	1106	CLA	C2D-C1D-ND	4.95	115.03	110.13
18	B	1023	CLA	C1D-ND-C4D	-4.95	102.84	106.31
18	F	1302	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
18	H	1000	CLA	O2D-CGD-CBD	4.95	119.89	111.23
18	H	1000	CLA	C2D-C1D-ND	4.95	115.03	110.13
18	A	1115	CLA	C4A-NA-C1A	4.95	108.94	106.68
18	A	1122	CLA	C1D-ND-C4D	-4.95	102.84	106.31
18	A	1134	CLA	C1D-ND-C4D	-4.95	102.84	106.31
18	4	4003	CLA	C1D-ND-C4D	-4.95	102.84	106.31
18	G	1002	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
18	A	1138	CLA	O2A-CGA-O1A	-4.95	111.25	123.63
18	B	1231	CLA	C1C-C2C-C3C	-4.95	101.77	106.98
18	4	4017	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
18	B	1214	CLA	C1-C2-C3	-4.95	118.09	126.20
18	2	2006	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
18	A	1125	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
18	4	4009	CLA	C2D-C1D-ND	4.94	115.02	110.13
18	B	1231	CLA	C1D-ND-C4D	-4.94	102.84	106.31
18	A	1126	CLA	C2D-C1D-ND	4.94	115.02	110.13
18	A	1013	CLA	C2C-C1C-NC	4.94	115.17	109.98
18	A	1114	CLA	C2D-C1D-ND	4.94	115.02	110.13
18	A	1135	CLA	C2D-C1D-ND	4.94	115.02	110.13
18	A	1107	CLA	C2D-C1D-ND	4.94	115.02	110.13
18	B	1223	CLA	C1C-C2C-C3C	-4.94	101.78	106.98
18	B	1203	CLA	O2A-CGA-O1A	-4.94	111.28	123.63
18	B	1231	CLA	C2D-C1D-ND	4.94	115.01	110.13
18	2	2005	CLA	C2D-C1D-ND	4.94	115.01	110.13
18	A	1108	CLA	O2D-CGD-CBD	4.94	119.86	111.23
18	A	1135	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
18	B	1211	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
18	H	1000	CLA	C1D-ND-C4D	-4.93	102.85	106.31
18	A	1118	CLA	C3B-C2B-C1B	-4.93	101.35	107.17
18	1	1007	CLA	O2D-CGD-CBD	4.93	119.85	111.23
18	3	3005	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
18	F	1302	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
18	B	1210	CLA	C2D-C1D-ND	4.93	115.01	110.13
18	A	1133	CLA	C1D-ND-C4D	-4.93	102.85	106.31
18	A	1117	CLA	C1D-ND-C4D	-4.93	102.85	106.31
18	A	1113	CLA	C1C-C2C-C3C	-4.93	101.80	106.98
18	1	1011	CLA	C3D-C2D-C1D	-4.93	99.10	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1011	CLA	C2D-C1D-ND	4.93	115.00	110.13
18	B	1209	CLA	C1D-ND-C4D	-4.93	102.85	106.31
18	A	1134	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
18	4	4009	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
18	B	1206	CLA	C2D-C1D-ND	4.93	115.00	110.13
18	A	1102	CLA	C1D-ND-C4D	-4.92	102.86	106.31
18	B	1234	CLA	C1C-C2C-C3C	-4.92	101.80	106.98
18	A	1137	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
18	2	2019	CLA	C1B-NB-C4B	4.92	109.76	106.31
18	J	1302	CLA	C2D-C1D-ND	4.92	114.99	110.13
18	B	1219	CLA	O2A-CGA-O1A	-4.92	111.33	123.63
18	K	1001	CLA	C1D-ND-C4D	-4.92	102.86	106.31
18	A	1125	CLA	C1C-C2C-C3C	-4.92	101.81	106.98
18	B	1225	CLA	O2A-CGA-O1A	-4.92	111.33	123.63
18	A	1113	CLA	C1D-ND-C4D	-4.91	102.86	106.31
18	B	1229	CLA	C1C-C2C-C3C	-4.91	101.81	106.98
18	2	2006	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
18	2	2003	CLA	O2A-CGA-O1A	-4.91	111.35	123.63
18	A	1139	CLA	O2D-CGD-CBD	4.91	119.81	111.23
18	A	1131	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
18	B	1226	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
18	A	1103	CLA	C2D-C1D-ND	4.91	114.98	110.13
18	K	1001	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
18	1	1006	CLA	O2A-CGA-CBA	4.90	126.79	111.83
18	B	1021	CLA	O2A-CGA-O1A	-4.90	111.36	123.63
18	B	1216	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
18	4	4016	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
18	2	2016	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
18	A	1104	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
18	A	1128	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
18	A	1102	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
18	A	1013	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
18	3	3010	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
18	B	1212	CLA	O2A-CGA-O1A	-4.89	111.40	123.63
18	2	2006	CLA	C1D-ND-C4D	-4.89	102.88	106.31
18	A	1117	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
18	A	1117	CLA	C2D-C1D-ND	4.89	114.96	110.13
18	J	1302	CLA	C1D-ND-C4D	-4.89	102.88	106.31
18	B	1228	CLA	O2A-CGA-O1A	-4.88	111.42	123.63
18	F	1301	CLA	C2D-C1D-ND	4.88	114.96	110.13
18	3	3013	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
18	A	1134	CLA	C2D-C1D-ND	4.88	114.95	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1216	CLA	C2D-C1D-ND	4.88	114.95	110.13
18	F	1301	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
18	B	1023	CLA	O2D-CGD-CBD	4.88	119.76	111.23
18	2	2007	CLA	C1D-ND-C4D	-4.88	102.89	106.31
18	A	1237	CLA	O2D-CGD-CBD	4.87	119.75	111.23
18	1	1005	CLA	C1C-C2C-C3C	-4.87	101.85	106.98
18	B	1227	CLA	C2D-C1D-ND	4.87	114.95	110.13
18	A	1119	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
18	B	1214	CLA	O2D-CGD-CBD	4.87	119.75	111.23
18	3	3005	CLA	C2D-C1D-ND	4.87	114.95	110.13
18	B	1219	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
18	A	1140	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
18	B	1220	CLA	O2A-CGA-O1A	-4.87	111.44	123.63
18	A	1128	CLA	C2D-C1D-ND	4.87	114.95	110.13
18	2	2002	CLA	C2D-C1D-ND	4.87	114.95	110.13
18	3	3006	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
18	1	1006	CLA	C4A-NA-C1A	4.87	108.90	106.68
18	1	1008	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
18	A	1103	CLA	C1D-ND-C4D	-4.87	102.90	106.31
18	3	3017	CLA	C2D-C1D-ND	4.87	114.94	110.13
18	3	3008	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
18	A	1111	CLA	C1D-ND-C4D	-4.86	102.90	106.31
18	2	2003	CLA	O2D-CGD-CBD	4.86	119.73	111.23
18	2	2007	CLA	C2D-C1D-ND	4.86	114.94	110.13
18	4	4006	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
18	4	4001	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
18	A	1127	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
18	1	1014	CLA	C1C-C2C-C3C	-4.86	101.87	106.98
18	3	3018	CLA	O2D-CGD-CBD	4.85	119.72	111.23
18	3	3004	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
18	B	1219	CLA	C1D-ND-C4D	-4.85	102.91	106.31
18	A	1108	CLA	C4A-NA-C1A	4.85	108.89	106.68
18	A	1119	CLA	C1D-ND-C4D	-4.85	102.91	106.31
18	B	1205	CLA	C1D-ND-C4D	-4.85	102.91	106.31
18	B	1021	CLA	O2D-CGD-CBD	4.84	119.70	111.23
18	A	1022	CLA	O2A-CGA-O1A	-4.84	111.52	123.63
18	B	1219	CLA	C2D-C1D-ND	4.84	114.92	110.13
18	A	1123	CLA	C1D-ND-C4D	-4.84	102.92	106.31
22	B	6004	BCR	C19-C18-C17	4.84	126.62	119.01
18	2	2016	CLA	C4D-C3D-CAD	4.84	113.36	108.11
18	A	1126	CLA	O2D-CGD-CBD	4.84	119.69	111.23
18	1	1001	CLA	C1C-C2C-C3C	-4.83	101.90	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	2	2013	CHL	C1C-CHC-C4B	4.83	133.37	116.07
18	B	1217	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
28	4	4011	CHL	C1B-CHB-C4A	4.83	124.43	121.32
18	B	1213	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
18	A	1105	CLA	C4A-NA-C1A	4.83	108.88	106.68
17	A	1011	CL0	CMA-C3A-C4A	-4.83	104.21	114.61
18	3	3017	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
18	A	1237	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
18	B	1202	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
18	4	4007	CLA	C2D-C1D-ND	4.83	114.90	110.13
18	1	1008	CLA	C2D-C1D-ND	4.83	114.90	110.13
22	A	6002	BCR	C7-C8-C9	-4.83	119.09	126.23
18	B	1224	CLA	C2D-C1D-ND	4.83	114.90	110.13
27	1	1501	LUT	C27-C28-C29	-4.83	115.94	126.32
18	B	1225	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
18	3	3004	CLA	C2D-C1D-ND	4.82	114.90	110.13
18	B	1230	CLA	C2C-C1C-NC	4.82	115.04	109.98
18	A	1112	CLA	C2D-C1D-ND	4.82	114.89	110.13
22	A	6011	BCR	C3-C4-C5	-4.82	105.47	114.06
18	A	1129	CLA	C1D-ND-C4D	-4.81	102.93	106.31
18	1	1003	CLA	O2A-CGA-CBA	4.81	126.51	111.83
18	F	1302	CLA	C2D-C1D-ND	4.81	114.89	110.13
18	2	2006	CLA	C2D-C1D-ND	4.81	114.89	110.13
18	A	1109	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
18	L	1501	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
18	1	1004	CLA	C2D-C1D-ND	4.81	114.89	110.13
18	B	1012	CLA	O2D-CGD-CBD	4.81	119.63	111.23
18	A	1140	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
18	B	1219	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
27	2	2501	LUT	C15-C14-C13	-4.80	120.54	127.28
18	B	1205	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
18	A	1138	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
18	1	1003	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
18	A	1112	CLA	C1D-ND-C4D	-4.80	102.94	106.31
18	1	1003	CLA	C1D-ND-C4D	-4.80	102.94	106.31
18	B	1201	CLA	O2A-CGA-O1A	-4.80	111.63	123.63
27	3	3501	LUT	C18-C5-C6	-4.79	119.25	124.48
18	1	1011	CLA	C2C-C1C-NC	4.79	115.02	109.98
18	A	1122	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
18	4	4012	CLA	C1D-ND-C4D	-4.79	102.95	106.31
18	4	4003	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
27	4	4503	LUT	C26-C27-C28	-4.79	117.13	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	1002	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
18	3	3005	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
18	A	1125	CLA	O2A-CGA-O1A	-4.78	111.66	123.63
18	A	1120	CLA	O2D-CGD-CBD	4.78	119.59	111.23
18	B	1232	CLA	C4A-NA-C1A	4.78	108.86	106.68
18	A	1104	CLA	O2A-CGA-O1A	-4.78	111.67	123.63
28	4	4011	CHL	C1C-CHC-C4B	4.78	133.18	116.07
18	B	1223	CLA	C1D-ND-C4D	-4.78	102.96	106.31
18	1	1003	CLA	C2D-C1D-ND	4.78	114.85	110.13
18	3	3010	CLA	C2D-C1D-ND	4.78	114.85	110.13
18	A	1115	CLA	O2D-CGD-CBD	4.77	119.57	111.23
18	F	1301	CLA	O2D-CGD-CBD	4.77	119.57	111.23
18	B	1218	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
18	B	1215	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
27	3	3502	LUT	C21-C26-C27	4.77	118.30	112.83
18	B	1203	CLA	O2D-CGD-CBD	4.76	119.56	111.23
18	1	1004	CLA	O2A-CGA-CBA	4.76	126.36	111.83
18	B	1206	CLA	O2D-CGD-CBD	4.76	119.55	111.23
18	A	1124	CLA	O2A-CGA-CBA	4.76	126.34	111.83
18	3	3003	CLA	C2D-C1D-ND	4.75	114.83	110.13
18	B	1210	CLA	C1C-C2C-C3C	-4.75	101.98	106.98
18	B	1231	CLA	O2D-CGD-CBD	4.75	119.54	111.23
18	A	1127	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
18	B	1220	CLA	C4A-NA-C1A	4.75	108.85	106.68
18	4	4003	CLA	C2D-C1D-ND	4.75	114.83	110.13
18	3	3018	CLA	C2D-C1D-ND	4.75	114.83	110.13
18	B	1226	CLA	C4A-NA-C1A	4.75	108.84	106.68
18	3	3013	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
18	A	1119	CLA	C4A-NA-C1A	4.74	108.84	106.68
18	1	1012	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
18	B	1012	CLA	C1D-ND-C4D	-4.74	102.99	106.31
18	B	1205	CLA	C2D-C1D-ND	4.73	114.81	110.13
18	2	2005	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
18	2	2009	CLA	C1D-ND-C4D	-4.73	102.99	106.31
22	B	6006	BCR	C7-C8-C9	-4.73	119.24	126.23
18	A	1022	CLA	C4A-NA-C1A	4.73	108.84	106.68
18	A	1110	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
18	3	3006	CLA	C1D-ND-C4D	-4.72	103.00	106.31
18	B	1225	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
18	3	3006	CLA	OBD-CAD-C3D	-4.72	117.38	128.42
18	L	1503	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
28	3	3011	CHL	C1A-CHA-C4D	4.72	126.85	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1208	CLA	C4A-NA-C1A	4.71	108.83	106.68
18	B	1214	CLA	C2D-C1D-ND	4.71	114.79	110.13
18	K	1001	CLA	C2D-C1D-ND	4.71	114.79	110.13
18	A	1105	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
18	1	1011	CLA	O2A-CGA-O1A	-4.71	111.84	123.63
22	L	6020	BCR	C19-C18-C17	4.71	126.41	119.01
18	A	1104	CLA	C4A-NA-C1A	4.71	108.83	106.68
18	A	1119	CLA	O2D-CGD-CBD	4.70	119.45	111.23
18	1	1013	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
18	J	1302	CLA	O2A-CGA-CBA	4.70	126.17	111.83
18	B	1239	CLA	O2A-CGA-O1A	-4.70	111.87	123.63
18	B	1206	CLA	C1D-ND-C4D	-4.70	103.02	106.31
22	B	6006	BCR	C39-C30-C25	4.70	117.61	110.24
18	B	1204	CLA	O2A-CGA-O1A	-4.69	111.89	123.63
18	A	1126	CLA	O2A-CGA-O1A	-4.69	111.89	123.63
18	4	4006	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
18	3	3019	CLA	C2C-C1C-NC	4.69	116.53	109.48
18	3	3007	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
22	B	6010	BCR	C38-C26-C25	-4.69	119.37	124.48
18	A	1022	CLA	C2D-C1D-ND	4.68	114.76	110.13
18	B	1239	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
18	G	1001	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
18	B	1231	CLA	C4A-NA-C1A	4.68	108.81	106.68
18	B	1216	CLA	C1D-ND-C4D	-4.68	103.03	106.31
18	3	3018	CLA	C1D-ND-C4D	-4.68	103.03	106.31
18	B	1230	CLA	C1C-C2C-C3C	-4.67	102.06	106.98
21	1	1801	LHG	O7-C7-C8	4.67	121.59	111.48
22	3	3503	BCR	C24-C23-C22	-4.67	119.32	126.23
18	2	2012	CLA	C1C-C2C-C3C	-4.67	102.06	106.98
27	I	6018	LUT	C15-C35-C34	-4.67	113.96	123.52
22	B	6010	BCR	C33-C5-C6	-4.67	119.39	124.48
18	B	1208	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
18	3	3001	CLA	C1D-ND-C4D	-4.67	103.04	106.31
18	B	1210	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
18	1	1006	CLA	C1D-ND-C4D	-4.66	103.04	106.31
18	A	1022	CLA	O2D-CGD-CBD	4.66	119.38	111.23
18	B	1214	CLA	C1D-ND-C4D	-4.66	103.04	106.31
28	1	1010	CHL	C1C-CHC-C4B	4.66	132.75	116.07
18	B	1224	CLA	O2A-CGA-CBA	4.66	126.03	111.83
18	A	1137	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
18	G	1003	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
18	A	1139	CLA	O2A-CGA-O1A	-4.66	111.98	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3005	CLA	C1D-ND-C4D	-4.65	103.05	106.31
18	1	1005	CLA	O2D-CGD-CBD	4.65	119.36	111.23
22	A	6008	BCR	C7-C8-C9	-4.65	119.36	126.23
18	4	4006	CLA	O2A-CGA-O1A	-4.65	112.01	123.63
18	2	2001	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
18	3	3007	CLA	C1D-ND-C4D	-4.64	103.05	106.31
28	4	4011	CHL	C1A-CHA-C4D	4.64	126.73	118.98
18	B	1222	CLA	C1-C2-C3	-4.64	118.59	126.20
18	B	1215	CLA	O2A-CGA-O1A	-4.64	112.02	123.63
22	B	6006	BCR	C33-C5-C6	-4.64	119.42	124.48
28	2	2011	CHL	C1C-CHC-C4B	4.64	132.66	116.07
28	3	3011	CHL	C1C-CHC-C4B	4.64	132.66	116.07
18	A	1105	CLA	O2D-CGD-CBD	4.64	119.33	111.23
18	4	4005	CLA	C1D-ND-C4D	-4.63	103.06	106.31
18	A	1138	CLA	O2D-CGD-CBD	4.63	119.33	111.23
18	2	2005	CLA	O2A-CGA-O1A	-4.63	112.05	123.63
18	G	1001	CLA	O2A-CGA-CBA	4.63	125.95	111.83
18	L	1501	CLA	C2D-C1D-ND	4.62	114.70	110.13
18	3	3002	CLA	C1D-ND-C4D	-4.62	103.07	106.31
18	B	1211	CLA	C2C-C1C-NC	4.62	114.84	109.98
18	B	1202	CLA	C1D-ND-C4D	-4.61	103.08	106.31
18	3	3007	CLA	O2A-CGA-O1A	-4.61	112.10	123.63
18	3	3004	CLA	O2D-CGD-CBD	4.61	119.29	111.23
18	2	2019	CLA	C4D-ND-C1D	-4.61	103.08	106.31
18	1	1012	CLA	C1D-ND-C4D	-4.61	103.08	106.31
18	G	1003	CLA	C2D-C1D-ND	4.61	114.69	110.13
18	B	1210	CLA	C4A-NA-C1A	4.61	108.78	106.68
18	A	1122	CLA	O2D-CGD-CBD	4.60	119.28	111.23
18	A	1105	CLA	O2A-CGA-O1A	-4.60	112.12	123.63
18	1	1001	CLA	C1D-ND-C4D	-4.60	103.08	106.31
18	2	2004	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
18	B	1227	CLA	O2A-CGA-O1A	-4.59	112.14	123.63
18	A	1126	CLA	C1D-ND-C4D	-4.59	103.09	106.31
18	2	2009	CLA	C2D-C1D-ND	4.59	114.67	110.13
18	A	1104	CLA	O2D-CGD-CBD	4.59	119.25	111.23
18	L	1501	CLA	O2A-CGA-O1A	-4.59	112.16	123.63
18	2	2001	CLA	C2D-C1D-ND	4.59	114.67	110.13
23	F	5002	LMG	O7-C10-C11	4.58	121.40	111.48
18	B	1240	CLA	O2A-CGA-O1A	-4.58	112.17	123.63
22	A	6003	BCR	C7-C8-C9	-4.57	119.47	126.23
18	A	1133	CLA	O2A-CGA-CBA	4.57	125.77	111.83
18	3	3001	CLA	C2D-C1D-ND	4.56	114.64	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1012	CLA	C2D-C1D-ND	4.56	114.64	110.13
22	A	6017	BCR	C7-C8-C9	-4.56	119.49	126.23
18	L	1501	CLA	C2C-C1C-NC	4.55	114.76	109.98
18	B	1219	CLA	O2D-CGD-CBD	4.55	119.18	111.23
18	1	1006	CLA	O2D-CGD-CBD	4.55	119.18	111.23
18	L	1501	CLA	C4A-NA-C1A	4.54	108.75	106.68
18	2	2001	CLA	O2A-CGA-CBA	4.54	125.68	111.83
18	3	3013	CLA	C2D-C1D-ND	4.54	114.62	110.13
18	A	1103	CLA	O2A-CGA-O1A	-4.54	112.28	123.63
18	B	1207	CLA	O2A-CGA-O1A	-4.54	112.28	123.63
18	B	1229	CLA	O2A-CGA-CBA	4.54	125.67	111.83
22	A	6007	BCR	C38-C26-C25	-4.54	119.53	124.48
28	4	4013	CHL	C1C-CHC-C4B	4.53	132.28	116.07
18	A	1132	CLA	C4A-NA-C1A	4.53	108.75	106.68
18	3	3001	CLA	O2A-CGA-O1A	-4.53	112.30	123.63
18	2	2007	CLA	O2D-CGD-CBD	4.53	119.15	111.23
22	A	6003	BCR	C38-C26-C25	-4.53	119.55	124.48
22	B	6004	BCR	C33-C5-C6	-4.52	119.55	124.48
18	2	2012	CLA	O2D-CGD-CBD	4.52	119.14	111.23
27	3	3501	LUT	C11-C10-C9	-4.52	120.93	127.28
18	B	1216	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
18	4	4017	CLA	C1D-ND-C4D	-4.52	103.14	106.31
18	B	1228	CLA	O2D-CGD-CBD	4.52	119.13	111.23
18	B	1214	CLA	O2A-CGA-CBA	4.52	125.61	111.83
18	3	3013	CLA	C1D-ND-C4D	-4.52	103.14	106.31
18	B	1231	CLA	O2A-CGA-O1A	-4.51	112.34	123.63
18	3	3013	CLA	C4A-NA-C1A	4.51	108.73	106.68
18	3	3004	CLA	O2A-CGA-CBA	4.51	125.57	111.83
22	A	6011	BCR	C7-C8-C9	-4.50	119.58	126.23
18	B	1218	CLA	O2A-CGA-CBA	4.50	125.55	111.83
22	A	6003	BCR	C33-C5-C6	-4.50	119.58	124.48
22	A	6007	BCR	C7-C8-C9	-4.50	119.58	126.23
18	B	1215	CLA	O2A-CGA-CBA	4.49	125.53	111.83
18	G	1001	CLA	C2D-C1D-ND	4.49	114.57	110.13
29	4	4505	ZEX	C27-C28-C29	-4.49	119.59	126.23
18	2	2001	CLA	C1D-ND-C4D	-4.49	103.16	106.31
18	1	1006	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
18	B	1226	CLA	C2D-C1D-ND	4.49	114.57	110.13
18	3	3019	CLA	C1B-NB-C4B	4.49	109.46	106.31
18	3	3010	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
22	3	3503	BCR	C34-C9-C10	-4.48	115.56	122.82
18	1	1013	CLA	C1D-ND-C4D	-4.47	103.17	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	1011	CL0	O2A-CGA-CBA	4.47	125.47	111.83
27	4	4503	LUT	C31-C30-C29	-4.47	121.01	127.28
18	4	4007	CLA	C1D-ND-C4D	-4.47	103.18	106.31
28	2	2011	CHL	C1A-CHA-C4D	4.46	126.42	118.98
18	A	1124	CLA	C4A-NA-C1A	4.46	108.71	106.68
18	A	1140	CLA	O2A-CGA-O1A	-4.45	112.48	123.63
18	B	1213	CLA	O2D-CGD-CBD	4.45	119.02	111.23
18	3	3006	CLA	O2D-CGD-CBD	4.45	119.02	111.23
18	3	3017	CLA	O2A-CGA-O1A	-4.45	109.92	123.20
18	A	1117	CLA	O2A-CGA-O1A	-4.45	112.50	123.63
18	B	1224	CLA	C1D-ND-C4D	-4.45	103.19	106.31
18	3	3017	CLA	C1D-ND-C4D	-4.45	103.19	106.31
18	1	1002	CLA	O2D-CGD-CBD	4.44	118.99	111.23
18	A	1122	CLA	O2A-CGA-CBA	4.44	125.36	111.83
18	4	4016	CLA	C2D-C1D-ND	4.43	114.52	110.13
18	3	3007	CLA	O2D-CGD-CBD	4.43	118.98	111.23
18	2	2004	CLA	C2D-C1D-ND	4.43	114.51	110.13
18	4	4002	CLA	C2D-C1D-ND	4.43	114.51	110.13
18	G	1002	CLA	C1D-ND-C4D	-4.43	103.21	106.31
18	2	2004	CLA	C1D-ND-C4D	-4.43	103.21	106.31
18	2	2004	CLA	O2A-CGA-CBA	4.42	125.32	111.83
18	B	1211	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
18	B	1226	CLA	O2A-CGA-CBA	4.42	125.31	111.83
18	A	1237	CLA	O2A-C1-C2	4.42	125.11	108.11
18	4	4012	CLA	O2A-CGA-O1A	-4.41	112.59	123.63
18	A	1107	CLA	O2A-CGA-CBA	4.41	125.28	111.83
18	B	1235	CLA	O2A-CGA-CBA	4.41	125.27	111.83
27	4	4501	LUT	C18-C5-C6	-4.41	119.68	124.48
18	A	1022	CLA	C1D-ND-C4D	-4.40	103.23	106.31
18	1	1001	CLA	C1-C2-C3	-4.40	118.99	126.20
18	3	3010	CLA	O2A-CGA-CBA	4.40	125.24	111.83
21	A	5003	LHG	O7-C7-C8	4.40	120.99	111.48
18	3	3019	CLA	C4D-ND-C1D	-4.39	103.23	106.31
28	2	2013	CHL	C1A-CHA-C4D	4.39	126.31	118.98
18	B	1023	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
18	3	3006	CLA	C1-C2-C3	-4.39	119.66	126.76
18	4	4007	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
18	B	1222	CLA	O2D-CGD-CBD	4.39	118.90	111.23
18	A	1112	CLA	C4A-NA-C1A	4.39	108.68	106.68
22	B	6009	BCR	C33-C5-C6	-4.39	119.70	124.48
18	3	3008	CLA	O2A-CGA-CBA	4.39	125.21	111.83
18	3	3007	CLA	C2D-C1D-ND	4.39	114.47	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3010	CLA	O2D-CGD-CBD	4.38	118.89	111.23
18	A	1134	CLA	O2A-CGA-CBA	4.38	125.20	111.83
28	4	4011	CHL	CHA-C1A-C2A	-4.38	123.03	133.31
18	1	1008	CLA	O2A-CGA-O1A	-4.37	110.14	123.20
18	4	4009	CLA	O2A-CGA-CBA	4.37	125.16	111.83
28	1	1009	CHL	C1C-CHC-C4B	4.37	131.71	116.07
18	3	3002	CLA	C2D-C1D-ND	4.36	114.45	110.13
18	A	1127	CLA	O2A-CGA-CBA	4.36	125.12	111.83
18	A	1109	CLA	O2D-CGD-CBD	4.35	118.84	111.23
18	F	1302	CLA	O2A-CGA-CBA	4.35	125.11	111.83
18	4	4009	CLA	O2D-CGD-CBD	4.35	118.84	111.23
18	G	1001	CLA	CAA-C2A-C3A	-4.35	101.25	113.00
27	I	6018	LUT	C21-C26-C27	4.35	117.82	112.83
18	1	1001	CLA	O2A-CGA-CBA	4.34	125.08	111.83
18	A	1128	CLA	C1D-ND-C4D	-4.34	103.26	106.31
28	4	4013	CHL	C1A-CHA-C4D	4.34	126.22	118.98
18	1	1013	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
18	A	1116	CLA	O2A-CGA-CBA	4.33	125.04	111.83
18	1	1003	CLA	O2D-CGD-CBD	4.33	118.80	111.23
18	B	1238	CLA	C4A-NA-C1A	4.33	108.65	106.68
18	A	1121	CLA	C1-C2-C3	-4.32	119.11	126.20
18	B	1201	CLA	O2D-CGD-CBD	4.32	118.79	111.23
22	J	6013	BCR	C1-C6-C5	-4.32	116.73	122.64
18	2	2019	CLA	CHD-C1D-ND	-4.32	118.75	124.84
18	B	1230	CLA	O2A-CGA-CBA	4.32	124.99	111.83
18	4	4001	CLA	C2D-C1D-ND	4.31	114.39	110.13
18	2	2007	CLA	O2A-CGA-CBA	4.31	124.97	111.83
18	B	1211	CLA	O2A-CGA-CBA	4.30	124.95	111.83
18	L	1503	CLA	O2D-CGD-CBD	4.30	118.75	111.23
18	2	2003	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
18	A	1121	CLA	O2A-CGA-CBA	4.30	124.94	111.83
18	4	4017	CLA	O2A-CGA-CBA	4.30	124.93	111.83
22	A	6007	BCR	C33-C5-C6	-4.29	119.80	124.48
18	A	1114	CLA	C3B-C2B-C1B	-4.29	102.12	107.17
22	3	3503	BCR	C7-C8-C9	-4.28	119.90	126.23
18	B	1213	CLA	C1-C2-C3	-4.28	119.18	126.20
18	B	1216	CLA	C4A-NA-C1A	4.28	108.63	106.68
18	A	1136	CLA	O2A-CGA-CBA	4.28	124.88	111.83
17	A	1011	CL0	CHA-C1A-C2A	-4.27	123.28	133.31
18	1	1008	CLA	C1D-ND-C4D	-4.27	103.32	106.31
22	A	6008	BCR	C38-C26-C25	-4.27	119.83	124.48
18	B	1222	CLA	O2A-CGA-CBA	4.27	124.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1238	CLA	O2A-CGA-CBA	4.26	124.84	111.83
27	4	4503	LUT	C15-C14-C13	-4.26	121.30	127.28
18	A	1132	CLA	O2A-CGA-CBA	4.26	124.83	111.83
18	L	1503	CLA	O2A-CGA-CBA	4.26	124.83	111.83
18	B	1226	CLA	C1D-ND-C4D	-4.26	103.32	106.31
18	G	1001	CLA	C1D-ND-C4D	-4.26	103.33	106.31
18	B	1204	CLA	O2A-C1-C2	4.26	124.48	108.11
18	G	1002	CLA	C2D-C1D-ND	4.25	114.34	110.13
28	1	1010	CHL	CHA-C1A-C2A	-4.25	123.32	133.31
18	B	1207	CLA	O2A-C1-C2	4.25	124.47	108.11
18	B	1236	CLA	C1-C2-C3	-4.25	119.23	126.20
18	2	2009	CLA	O2A-CGA-CBA	4.25	124.80	111.83
18	4	4005	CLA	O2A-CGA-CBA	4.25	124.80	111.83
18	B	1232	CLA	O2D-CGD-CBD	4.25	118.66	111.23
22	B	6005	BCR	C19-C18-C17	4.25	125.69	119.01
18	4	4002	CLA	O2A-C1-C2	4.24	124.44	108.11
22	I	6020	BCR	C19-C18-C17	4.24	125.68	119.01
18	A	1140	CLA	O2A-C1-C2	4.24	124.42	108.11
27	3	3501	LUT	C22-C23-C24	-4.24	104.89	111.18
18	J	1302	CLA	C1-C2-C3	-4.23	119.92	126.76
18	A	1116	CLA	O2A-C1-C2	4.23	124.39	108.11
18	2	2008	CLA	C1-C2-C3	-4.23	119.92	126.76
18	2	2003	CLA	O2A-CGA-CBA	4.22	124.70	111.83
22	B	6004	BCR	C7-C8-C9	-4.22	119.99	126.23
18	3	3007	CLA	C1-C2-C3	-4.22	119.94	126.76
18	B	1210	CLA	O2A-CGA-CBA	4.22	124.69	111.83
17	A	1011	CL0	C1C-CHC-C4B	4.21	131.15	116.07
18	B	1223	CLA	O2A-CGA-CBA	4.21	124.68	111.83
28	1	1010	CHL	C1B-CHB-C4A	4.21	124.03	121.32
22	J	6013	BCR	C7-C8-C9	-4.21	120.01	126.23
18	2	2004	CLA	O2A-C1-C2	4.21	124.30	108.11
18	B	1206	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
18	B	1225	CLA	O2A-CGA-CBA	4.20	124.64	111.83
22	J	6013	BCR	C19-C18-C17	4.20	125.61	119.01
18	B	1216	CLA	C1-C2-C3	-4.20	119.32	126.20
22	A	6002	BCR	C38-C26-C25	-4.20	119.90	124.48
18	1	1012	CLA	C1-C2-C3	-4.20	119.97	126.76
28	2	2010	CHL	C1C-CHC-C4B	4.20	131.08	116.07
18	G	1003	CLA	O2A-CGA-CBA	4.19	124.62	111.83
17	A	1011	CL0	C1-C2-C3	-4.19	119.33	126.20
18	A	1118	CLA	O2A-CGA-O1A	-4.19	110.69	123.20
18	B	1220	CLA	O2D-CGD-CBD	4.19	118.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	2502	LUT	C15-C14-C13	-4.19	121.40	127.28
18	2	2006	CLA	O2A-CGA-CBA	4.19	124.61	111.83
18	4	4016	CLA	O2A-CGA-O1A	-4.19	110.70	123.20
18	A	1106	CLA	O2A-CGA-CBA	4.19	124.60	111.83
18	B	1205	CLA	O2A-CGA-CBA	4.18	124.59	111.83
18	B	1230	CLA	C4-C3-C5	4.18	122.49	115.23
18	A	1107	CLA	O2A-C1-C2	4.18	124.20	108.11
18	3	3006	CLA	C2D-C1D-ND	4.17	114.26	110.13
18	H	1000	CLA	O2A-CGA-O1A	-4.17	110.75	123.20
18	B	1012	CLA	O2A-CGA-CBA	4.17	124.55	111.83
27	4	4503	LUT	C11-C10-C9	-4.17	121.43	127.28
22	B	6010	BCR	C7-C8-C9	-4.17	120.07	126.23
18	A	1110	CLA	O2A-CGA-CBA	4.17	124.54	111.83
22	A	6017	BCR	C38-C26-C25	-4.16	119.94	124.48
22	B	6005	BCR	C38-C26-C25	-4.16	119.94	124.48
18	A	1119	CLA	O2A-CGA-CBA	4.16	124.53	111.83
18	4	4012	CLA	CHD-C1D-ND	-4.16	118.95	124.80
18	A	1131	CLA	O2A-CGA-CBA	4.16	124.52	111.83
23	B	5005	LMG	O7-C10-C11	4.16	120.48	111.48
18	A	1108	CLA	O2A-CGA-O1A	-4.16	110.78	123.20
18	A	1013	CLA	O2D-CGD-CBD	4.16	118.50	111.23
18	B	1236	CLA	O2A-CGA-CBA	4.16	124.51	111.83
22	F	6016	BCR	C24-C23-C22	-4.16	120.09	126.23
18	3	3001	CLA	O2A-CGA-CBA	4.15	124.50	111.83
18	A	1140	CLA	O2A-CGA-CBA	4.15	124.50	111.83
18	K	1001	CLA	O2D-CGD-CBD	4.15	118.49	111.23
22	G	2011	BCR	C37-C22-C21	-4.15	116.09	122.82
22	G	2011	BCR	C33-C5-C6	-4.15	119.96	124.48
22	A	6011	BCR	C28-C27-C26	-4.15	106.66	114.06
18	1	1001	CLA	CAA-C2A-C3A	-4.14	101.80	113.00
18	A	1101	CLA	O2A-CGA-CBA	4.14	124.47	111.83
22	J	6013	BCR	C34-C9-C10	-4.14	116.11	122.82
18	B	1219	CLA	O2A-CGA-CBA	4.14	124.45	111.83
29	4	4505	ZEX	C18-C5-C6	-4.14	119.97	124.48
18	A	1151	CLA	O2A-CGA-CBA	4.13	124.44	111.83
18	B	1221	CLA	O2A-CGA-O1A	-4.13	113.29	123.63
18	4	4007	CLA	O2A-CGA-CBA	4.13	124.43	111.83
22	F	6014	BCR	C2-C1-C6	4.13	116.44	110.44
18	B	1206	CLA	O2A-CGA-CBA	4.13	124.43	111.83
26	B	8001	LMU	C1B-O1B-C4'	-4.13	108.19	117.98
18	A	1237	CLA	O2A-CGA-CBA	4.13	124.42	111.83
18	B	1203	CLA	C1-C2-C3	-4.13	119.43	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1208	CLA	O2A-CGA-CBA	4.13	124.42	111.83
18	A	1126	CLA	O2A-CGA-CBA	4.13	124.42	111.83
18	3	3019	CLA	C3C-C4C-NC	4.12	113.53	109.92
18	A	1123	CLA	O2A-CGA-CBA	4.12	124.41	111.83
18	3	3005	CLA	O2A-CGA-CBA	4.12	124.40	111.83
18	B	1217	CLA	O2A-CGA-O1A	-4.12	110.91	123.20
18	B	1208	CLA	C1-C2-C3	-4.12	119.45	126.20
18	A	1137	CLA	O2A-CGA-CBA	4.12	124.39	111.83
18	B	1232	CLA	O2A-CGA-CBA	4.12	124.39	111.83
18	A	1120	CLA	O2A-CGA-CBA	4.12	124.38	111.83
18	B	1021	CLA	O2A-CGA-CBA	4.11	124.38	111.83
18	A	1104	CLA	O2A-CGA-CBA	4.11	124.38	111.83
18	1	1011	CLA	C1-C2-C3	-4.11	120.11	126.76
18	2	2016	CLA	CMB-C2B-C1B	4.11	131.68	125.42
18	3	3001	CLA	C4D-C3D-CAD	4.10	112.56	108.11
18	1	1006	CLA	CMC-C2C-C1C	4.10	131.44	125.03
18	3	3008	CLA	O2D-CGD-CBD	4.10	118.39	111.23
27	1	1502	LUT	C15-C14-C13	-4.10	121.53	127.28
18	B	1220	CLA	O2A-CGA-CBA	4.10	124.32	111.83
18	3	3018	CLA	O2A-CGA-CBA	4.10	124.32	111.83
18	3	3007	CLA	O2A-CGA-CBA	4.09	124.32	111.83
28	3	3011	CHL	CHA-C1A-C2A	-4.09	123.69	133.31
18	A	1129	CLA	O2A-CGA-CBA	4.09	124.31	111.83
18	A	1130	CLA	O2A-CGA-CBA	4.08	124.29	111.83
18	3	3003	CLA	C1D-ND-C4D	-4.08	103.45	106.31
18	A	1112	CLA	O2A-CGA-CBA	4.08	124.28	111.83
18	2	2009	CLA	O2D-CGD-CBD	4.08	118.36	111.23
18	1	1005	CLA	O2A-CGA-CBA	4.08	124.26	111.83
18	B	1208	CLA	O2A-C1-C2	4.08	123.79	108.11
18	4	4006	CLA	C1-C2-C3	-4.07	120.17	126.76
18	2	2012	CLA	O2A-CGA-CBA	4.07	124.24	111.83
18	A	1115	CLA	O2A-CGA-O1A	-4.07	111.06	123.20
18	2	2016	CLA	O2A-CGA-O1A	-4.07	113.46	123.63
18	A	1109	CLA	O2A-CGA-CBA	4.07	124.23	111.83
18	B	1023	CLA	O2A-CGA-CBA	4.06	124.22	111.83
18	2	2016	CLA	O2A-CGA-CBA	4.06	124.22	111.83
18	A	1109	CLA	C1-C2-C3	-4.06	119.54	126.20
18	B	1228	CLA	O2A-CGA-CBA	4.06	124.22	111.83
18	1	1012	CLA	CHD-C1D-ND	-4.06	119.09	124.80
18	4	4002	CLA	O2A-CGA-CBA	4.06	124.20	111.83
18	J	1302	CLA	O2A-C1-C2	4.06	123.72	108.11
18	2	2001	CLA	C1-C2-C3	-4.05	119.56	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2005	CLA	O2D-CGD-CBD	4.05	118.31	111.23
28	1	1009	CHL	C3D-C4D-CHA	4.05	114.70	108.54
22	3	3503	BCR	C19-C18-C17	4.05	125.38	119.01
28	4	4013	CHL	CHA-C1A-C2A	-4.05	123.80	133.31
18	1	1001	CLA	O2D-CGD-CBD	4.05	118.31	111.23
27	2	2502	LUT	C22-C23-C24	-4.05	105.17	111.18
18	2	2016	CLA	CMC-C2C-C1C	4.04	131.35	125.03
18	B	1202	CLA	O2A-CGA-CBA	4.04	124.16	111.83
28	2	2013	CHL	CHA-C1A-C2A	-4.04	123.82	133.31
27	4	4502	LUT	C31-C30-C29	-4.04	121.61	127.28
18	A	1135	CLA	O2A-CGA-CBA	4.04	124.14	111.83
18	A	1113	CLA	O2A-CGA-O1A	-4.04	111.15	123.20
22	A	6007	BCR	C15-C14-C13	-4.03	121.62	127.28
22	A	6003	BCR	C24-C23-C22	-4.03	120.27	126.23
18	1	1012	CLA	O2D-CGD-CBD	4.03	118.27	111.23
18	4	4001	CLA	O2A-CGA-CBA	4.03	124.11	111.83
18	A	1133	CLA	C1-C2-C3	-4.03	119.60	126.20
18	3	3013	CLA	O2D-CGD-CBD	4.02	118.26	111.23
18	B	1236	CLA	O2A-C1-C2	4.02	123.58	108.11
22	G	2011	BCR	C34-C9-C10	-4.02	116.30	122.82
18	A	1111	CLA	O2A-CGA-CBA	4.02	124.08	111.83
18	B	1239	CLA	O2A-CGA-CBA	4.02	124.08	111.83
18	K	1001	CLA	CHD-C1D-ND	-4.01	119.15	124.80
18	A	1101	CLA	O2A-C1-C2	4.01	123.56	108.11
28	2	2011	CHL	CHA-C1A-C2A	-4.01	123.89	133.31
18	3	3018	CLA	CAA-C2A-C3A	-4.01	102.17	113.00
18	A	1103	CLA	O2A-C1-C2	4.01	123.53	108.11
18	L	1503	CLA	C1-C2-C3	-4.01	120.28	126.76
18	4	4012	CLA	O2D-CGD-CBD	4.01	118.23	111.23
18	3	3003	CLA	CMB-C2B-C1B	4.00	131.51	125.42
18	3	3013	CLA	O2A-CGA-O1A	-4.00	111.27	123.20
18	3	3012	CLA	O2A-CGA-CBA	3.99	124.02	111.83
18	A	1110	CLA	O2A-C1-C2	3.99	123.47	108.11
18	A	1114	CLA	O2A-CGA-O1A	-3.99	111.29	123.20
18	4	4008	CLA	O2A-CGA-O1A	-3.98	111.33	123.20
27	4	4502	LUT	C21-C26-C27	3.98	117.40	112.83
18	A	1237	CLA	CHD-C1D-ND	-3.97	119.21	124.80
18	B	1224	CLA	C1-C2-C3	-3.97	119.69	126.20
18	B	1209	CLA	O2A-CGA-O1A	-3.97	111.34	123.20
18	3	3010	CLA	C1D-ND-C4D	-3.97	103.53	106.31
18	2	2009	CLA	C1-C2-C3	-3.97	120.34	126.76
18	F	1302	CLA	C1-C2-C3	-3.96	120.35	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3012	CLA	O2D-CGD-CBD	3.96	118.16	111.23
18	A	1105	CLA	O2A-CGA-CBA	3.96	123.91	111.83
22	J	6012	BCR	C2-C1-C6	3.96	116.19	110.44
27	1	1501	LUT	C31-C30-C29	-3.96	121.73	127.28
18	B	1211	CLA	C2B-C1B-NB	3.96	114.43	110.33
27	2	2502	LUT	C31-C30-C29	-3.96	121.73	127.28
18	4	4007	CLA	O2A-C1-C2	3.95	123.33	108.11
22	A	6008	BCR	C33-C5-C6	-3.95	120.17	124.48
22	A	6002	BCR	C19-C18-C17	3.95	125.23	119.01
18	G	1003	CLA	CHD-C1D-ND	-3.95	119.24	124.80
18	A	1128	CLA	O2A-CGA-CBA	3.95	123.87	111.83
18	B	1201	CLA	O2A-CGA-CBA	3.94	123.86	111.83
18	K	1001	CLA	O2A-CGA-O1A	-3.94	111.44	123.20
18	B	1021	CLA	C1-C2-C3	-3.94	119.74	126.20
18	3	3001	CLA	CHD-C1D-ND	-3.94	119.26	124.80
18	2	2002	CLA	O2D-CGD-CBD	3.94	118.11	111.23
18	A	1125	CLA	O2A-CGA-CBA	3.94	123.84	111.83
18	A	1106	CLA	C1-C2-C3	-3.94	119.75	126.20
20	A	5001	PQN	C14-C13-C15	3.93	122.05	115.23
27	3	3501	LUT	C35-C34-C33	-3.93	121.76	127.28
27	2	2501	LUT	C18-C5-C6	-3.93	120.19	124.48
28	4	4010	CHL	C1C-CHC-C4B	3.93	130.13	116.07
22	J	6013	BCR	C23-C22-C21	3.93	125.19	119.01
18	2	2008	CLA	O2A-CGA-CBA	3.93	123.81	111.83
28	1	1010	CHL	C3D-C4D-CHA	3.92	114.50	108.54
18	1	1006	CLA	C2D-C1D-ND	3.92	114.00	110.13
18	2	2004	CLA	C2C-C1C-NC	3.91	114.09	109.98
18	2	2016	CLA	C1-C2-C3	-3.91	120.43	126.76
18	A	1103	CLA	C1-C2-C3	-3.91	119.80	126.20
18	A	1022	CLA	O2A-CGA-CBA	3.90	123.74	111.83
18	3	3001	CLA	O2A-C1-C2	3.90	123.13	108.11
18	B	1202	CLA	O2A-C1-C2	3.90	123.13	108.11
18	B	1234	CLA	O2A-CGA-CBA	3.90	123.73	111.83
18	2	2016	CLA	O2A-C1-C2	3.90	123.11	108.11
18	3	3007	CLA	O2A-C1-C2	3.90	123.11	108.11
18	B	1203	CLA	O2A-CGA-CBA	3.90	123.72	111.83
18	2	2002	CLA	O2A-CGA-O1A	-3.90	111.56	123.20
18	3	3006	CLA	O2A-CGA-CBA	3.90	123.71	111.83
27	I	6018	LUT	C10-C11-C12	-3.89	111.92	123.20
21	A	7001	LHG	O7-C7-C8	3.89	119.90	111.48
18	A	1128	CLA	C3B-C2B-C1B	-3.89	102.58	107.17
22	L	6020	BCR	C34-C9-C10	-3.89	116.51	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1023	CLA	O2A-C1-C2	3.89	123.08	108.11
28	2	2013	CHL	C3D-C4D-CHA	3.89	114.45	108.54
27	2	2501	LUT	C7-C8-C9	-3.89	120.48	126.23
18	1	1007	CLA	CHD-C1D-ND	-3.89	119.33	124.80
18	B	1212	CLA	O2A-C1-C2	3.89	123.06	108.11
18	A	1013	CLA	O2A-C1-C2	3.89	123.06	108.11
22	J	6012	BCR	C7-C8-C9	-3.88	120.49	126.23
18	B	1212	CLA	O2A-CGA-CBA	3.88	123.67	111.83
28	3	3011	CHL	C1B-CHB-C4A	3.88	123.82	121.32
22	J	6012	BCR	C4-C5-C6	-3.88	117.46	122.70
18	4	4001	CLA	C1D-ND-C4D	-3.88	103.59	106.31
18	B	1234	CLA	O2A-C1-C2	3.88	123.04	108.11
18	4	4004	CLA	O2A-CGA-CBA	3.88	123.66	111.83
18	3	3017	CLA	O2D-CGD-CBD	3.88	118.01	111.23
18	G	1002	CLA	O2A-CGA-O1A	-3.88	111.63	123.20
18	4	4006	CLA	O2D-CGD-CBD	3.87	117.99	111.23
22	B	6009	BCR	C38-C26-C25	-3.87	120.27	124.48
18	L	1501	CLA	O2A-C1-C2	3.86	122.96	108.11
18	A	1121	CLA	O2A-C1-C2	3.86	122.96	108.11
18	2	2012	CLA	CMB-C2B-C1B	3.86	131.29	125.42
18	L	1501	CLA	CHD-C1D-ND	-3.85	119.38	124.80
18	3	3012	CLA	CHD-C1D-ND	-3.85	119.39	124.80
27	4	4501	LUT	C22-C23-C24	-3.85	105.47	111.18
18	3	3008	CLA	O2A-C1-C2	3.85	122.31	109.44
18	4	4016	CLA	O2D-CGD-CBD	3.84	117.95	111.23
28	4	4013	CHL	C3C-C4C-NC	-3.84	105.27	114.65
22	G	2011	BCR	C23-C22-C21	3.83	125.04	119.01
18	1	1007	CLA	O2A-CGA-O1A	-3.83	111.76	123.20
22	B	6005	BCR	C7-C8-C9	-3.83	120.57	126.23
22	B	6009	BCR	C7-C8-C9	-3.83	120.57	126.23
18	B	1240	CLA	CHD-C1D-ND	-3.83	119.42	124.80
18	B	1239	CLA	O2A-C1-C2	3.83	122.84	108.11
18	B	1213	CLA	O2A-CGA-CBA	3.83	123.50	111.83
18	1	1006	CLA	CHD-C1D-ND	-3.82	119.42	124.80
18	A	1105	CLA	O2A-C1-C2	3.82	122.82	108.11
18	1	1006	CLA	CAC-C3C-C4C	3.82	129.76	124.79
18	A	1139	CLA	O2A-CGA-CBA	3.82	123.49	111.83
18	B	1221	CLA	O2A-C1-C2	3.82	122.80	108.11
18	A	1135	CLA	O2A-C1-C2	3.82	122.80	108.11
18	3	3017	CLA	CHD-C1D-ND	-3.82	119.43	124.80
18	1	1003	CLA	CHD-C1D-ND	-3.81	119.44	124.80
18	2	2005	CLA	O2A-CGA-CBA	3.81	123.46	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	1501	CLA	C1-C2-C3	-3.81	120.60	126.76
18	B	1216	CLA	O2A-CGA-CBA	3.81	123.45	111.83
18	B	1213	CLA	O2A-C1-C2	3.81	122.76	108.11
18	4	4003	CLA	O2A-CGA-CBA	3.81	123.44	111.83
18	B	1204	CLA	O2A-CGA-CBA	3.80	123.44	111.83
22	B	6009	BCR	C3-C4-C5	-3.80	107.27	114.06
28	3	3011	CHL	C3D-C4D-CHA	3.80	114.32	108.54
18	A	1109	CLA	O2A-C1-C2	3.80	122.73	108.11
18	A	1013	CLA	CHD-C1D-ND	-3.80	119.46	124.80
18	3	3002	CLA	CHD-C1D-ND	-3.80	119.46	124.80
18	3	3001	CLA	CMD-C2D-C3D	-3.80	118.98	127.69
18	A	1106	CLA	O2A-C1-C2	3.80	122.72	108.11
22	L	6019	BCR	C33-C5-C6	-3.80	120.34	124.48
18	L	1502	CLA	O2A-CGA-CBA	3.79	123.40	111.83
18	3	3003	CLA	O2D-CGD-CBD	3.79	117.86	111.23
27	1	1501	LUT	C15-C14-C13	-3.79	121.96	127.28
18	1	1014	CLA	CHD-C1D-ND	-3.79	119.47	124.80
28	4	4010	CHL	CGD-CBD-CAD	-3.79	98.58	110.85
18	A	1104	CLA	C1-C2-C3	-3.79	119.99	126.20
18	2	2019	CLA	C1C-NC-C4C	-3.79	104.95	106.68
28	2	2010	CHL	C3D-C4D-CHA	3.78	114.29	108.54
22	J	6013	BCR	C37-C22-C21	-3.78	116.69	122.82
18	B	1231	CLA	O2A-CGA-CBA	3.78	123.35	111.83
18	B	1201	CLA	O2A-C1-C2	3.77	122.63	108.11
18	1	1014	CLA	O2A-CGA-CBA	3.77	126.39	112.14
18	B	1218	CLA	CHD-C1D-ND	-3.77	119.49	124.80
18	3	3005	CLA	O2A-C1-C2	3.77	122.61	108.11
18	1	1008	CLA	O2D-CGD-CBD	3.77	117.81	111.23
18	A	1127	CLA	C1-C2-C3	-3.76	120.03	126.20
18	K	1001	CLA	C4D-C3D-CAD	3.76	112.19	108.11
18	B	1215	CLA	O2A-C1-C2	3.76	122.58	108.11
18	1	1011	CLA	O2A-CGA-CBA	3.76	123.30	111.83
18	1	1013	CLA	C2D-C1D-ND	3.76	113.85	110.13
18	A	1121	CLA	CHD-C1D-ND	-3.75	119.52	124.80
22	K	2011	BCR	C7-C8-C9	-3.75	120.68	126.23
18	B	1227	CLA	CHD-C1D-ND	-3.75	119.52	124.80
18	4	4012	CLA	O2A-C1-C2	3.75	122.54	108.11
18	B	1205	CLA	O2D-CGD-CBD	3.75	117.78	111.23
18	A	1102	CLA	O2A-CGA-CBA	3.75	123.26	111.83
18	B	1227	CLA	C1-C2-C3	-3.75	120.06	126.20
18	A	1124	CLA	CHD-C1D-ND	-3.75	119.53	124.80
18	4	4012	CLA	O2A-CGA-CBA	3.74	123.24	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1002	CLA	CHD-C1D-ND	-3.74	119.54	124.80
18	3	3007	CLA	CHD-C1D-ND	-3.74	119.55	124.80
18	B	1227	CLA	O2A-C1-C2	3.73	122.48	108.11
22	J	6013	BCR	C39-C30-C25	-3.73	104.39	110.24
18	A	1108	CLA	CHD-C1D-ND	-3.73	119.55	124.80
23	2	2802	LMG	O7-C10-C11	3.73	119.54	111.48
18	A	1138	CLA	O2A-CGA-CBA	3.73	123.19	111.83
18	3	3003	CLA	O2A-CGA-O1A	-3.72	114.31	123.63
18	4	4017	CLA	C1-C2-C3	-3.72	120.09	126.20
22	J	6012	BCR	C29-C30-C25	3.72	115.85	110.44
18	A	1129	CLA	C1-C2-C3	-3.72	120.74	126.76
18	A	1132	CLA	CHD-C1D-ND	-3.72	119.56	124.80
20	B	5002	PQN	C14-C13-C15	3.72	121.69	115.23
18	1	1013	CLA	O2A-CGA-O1A	-3.72	112.09	123.20
21	A	7001	LHG	O8-C23-C24	3.72	123.17	111.83
22	K	2011	BCR	C19-C18-C17	3.72	124.86	119.01
18	1	1014	CLA	O2A-CGA-O1A	-3.71	112.11	123.20
18	A	1013	CLA	C2B-C1B-NB	3.71	114.18	110.33
18	1	1005	CLA	O2A-C1-C2	3.71	122.40	108.11
22	A	6017	BCR	C3-C4-C5	-3.71	107.44	114.06
23	F	5001	LMG	C8-O7-C10	-3.71	111.29	117.85
18	3	3008	CLA	C4D-C3D-CAD	3.71	112.14	108.11
22	L	6019	BCR	C30-C25-C26	-3.71	117.57	122.64
27	4	4501	LUT	C10-C11-C12	-3.71	112.46	123.20
22	A	6017	BCR	C23-C22-C21	3.71	124.84	119.01
22	K	2011	BCR	C3-C4-C5	-3.70	107.45	114.06
27	I	6018	LUT	C18-C5-C4	3.70	121.23	114.42
18	1	1001	CLA	O2A-C1-C2	3.70	122.36	108.11
18	B	1223	CLA	C1-C2-C3	-3.70	120.13	126.20
28	4	4010	CHL	C3D-C4D-CHA	3.70	114.17	108.54
22	3	3503	BCR	C15-C14-C13	-3.70	122.09	127.28
22	F	6014	BCR	C31-C1-C6	-3.70	104.44	110.24
22	I	6020	BCR	C33-C5-C6	-3.70	120.45	124.48
18	L	1501	CLA	O2A-CGA-CBA	3.70	123.11	111.83
18	B	1210	CLA	O2A-C1-C2	3.70	122.34	108.11
18	B	1210	CLA	C1-C2-C3	-3.70	120.14	126.20
18	3	3018	CLA	CHD-C1D-ND	-3.69	119.61	124.80
18	A	1125	CLA	O2A-C1-C2	3.69	122.31	108.11
18	1	1013	CLA	C4D-C3D-CAD	3.69	112.11	108.11
18	4	4016	CLA	CHD-C1D-ND	-3.69	119.61	124.80
22	A	6002	BCR	C36-C18-C17	-3.69	116.84	122.82
22	3	3503	BCR	C36-C18-C17	-3.68	116.85	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3019	CLA	C2D-C1D-ND	3.68	114.53	109.50
18	B	1211	CLA	O2A-C1-C2	3.68	122.28	108.11
18	A	1112	CLA	CHD-C1D-ND	-3.68	119.62	124.80
18	B	1223	CLA	O2A-C1-C2	3.68	122.27	108.11
27	2	2502	LUT	C27-C28-C29	-3.68	118.41	126.32
18	B	1206	CLA	O2A-C1-C2	3.68	122.27	108.11
18	B	1221	CLA	C1-O2A-CGA	3.68	125.56	116.65
18	2	2009	CLA	CHD-C1D-ND	-3.68	119.62	124.80
18	A	1013	CLA	O2A-CGA-CBA	3.68	123.05	111.83
18	3	3010	CLA	CAC-C3C-C4C	3.68	129.57	124.79
18	B	1221	CLA	O2A-CGA-CBA	3.67	123.04	111.83
18	3	3004	CLA	CHD-C1D-ND	-3.67	119.63	124.80
18	A	1117	CLA	C1-C2-C3	-3.67	120.18	126.20
18	4	4002	CLA	C1D-ND-C4D	-3.67	103.74	106.31
18	K	1001	CLA	CMB-C2B-C1B	3.67	131.01	125.42
18	B	1204	CLA	CHD-C1D-ND	-3.67	119.64	124.80
18	2	2002	CLA	CHD-C1D-ND	-3.67	119.64	124.80
22	A	6011	BCR	C35-C13-C12	3.67	123.69	118.09
27	4	4501	LUT	C15-C14-C13	-3.66	122.14	127.28
18	B	1235	CLA	CHD-C1D-ND	-3.66	119.65	124.80
18	B	1215	CLA	CHD-C1D-ND	-3.66	119.65	124.80
18	A	1101	CLA	CHD-C1D-ND	-3.66	119.65	124.80
18	A	1151	CLA	C1-C2-C3	-3.66	120.84	126.76
18	B	1216	CLA	CHD-C1D-ND	-3.65	119.66	124.80
22	L	6019	BCR	C34-C9-C10	-3.65	116.90	122.82
18	B	1232	CLA	O2A-C1-C2	3.65	122.17	108.11
18	B	1216	CLA	O2A-C1-C2	3.65	122.16	108.11
18	1	1012	CLA	CAA-CBA-CGA	-3.65	102.84	113.21
18	2	2008	CLA	C4D-C3D-CAD	3.65	112.07	108.11
18	B	1231	CLA	CHD-C1D-ND	-3.65	119.67	124.80
18	A	1133	CLA	O2A-C1-C2	3.65	122.16	108.11
18	B	1232	CLA	C1-C2-C3	-3.65	120.22	126.20
22	J	6013	BCR	C36-C18-C17	-3.65	116.91	122.82
18	A	1109	CLA	CHD-C1D-ND	-3.64	119.67	124.80
28	2	2011	CHL	C3C-C4C-NC	-3.64	105.74	114.65
18	A	1135	CLA	C1-C2-C3	-3.64	120.23	126.20
18	2	2019	CLA	C2D-C1D-ND	3.64	114.48	109.50
18	A	1130	CLA	CHD-C1D-ND	-3.64	119.68	124.80
27	2	2502	LUT	C18-C5-C6	-3.64	120.51	124.48
18	A	1117	CLA	O2A-CGA-CBA	3.64	122.93	111.83
18	2	2012	CLA	CHD-C1D-ND	-3.64	119.68	124.80
18	A	1134	CLA	CHD-C1D-ND	-3.64	119.68	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	4	4011	CHL	C3C-C4C-NC	-3.64	105.76	114.65
22	3	3503	BCR	C33-C5-C4	3.64	121.35	113.60
22	L	6019	BCR	C39-C30-C25	-3.63	104.54	110.24
22	B	6006	BCR	C29-C30-C25	-3.63	105.16	110.44
18	B	1238	CLA	CHD-C1D-ND	-3.63	119.69	124.80
18	A	1103	CLA	O2A-CGA-CBA	3.63	122.91	111.83
22	G	2011	BCR	C8-C9-C10	3.63	124.72	119.01
18	A	1116	CLA	CHD-C1D-ND	-3.63	119.69	124.80
22	A	6017	BCR	C33-C5-C6	-3.63	120.52	124.48
22	3	3503	BCR	C8-C9-C10	3.63	124.72	119.01
18	F	1302	CLA	CHD-C1D-ND	-3.63	119.69	124.80
18	4	4008	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
22	L	6020	BCR	C37-C22-C21	-3.63	116.94	122.82
18	3	3010	CLA	CHD-C1D-ND	-3.63	119.70	124.80
18	A	1119	CLA	CHD-C1D-ND	-3.63	119.70	124.80
27	4	4502	LUT	C35-C34-C33	-3.62	122.20	127.28
22	B	6004	BCR	C28-C27-C26	-3.62	107.59	114.06
28	1	1009	CHL	CHA-C1A-C2A	-3.62	124.80	133.31
22	I	6020	BCR	C38-C26-C25	-3.62	120.53	124.48
18	B	1208	CLA	CHD-C1D-ND	-3.62	119.71	124.80
22	A	6017	BCR	C36-C18-C17	-3.62	116.96	122.82
18	B	1210	CLA	CHD-C1D-ND	-3.61	119.72	124.80
27	2	2501	LUT	C15-C35-C34	-3.61	116.13	123.52
18	3	3002	CLA	O2A-CGA-O1A	-3.61	112.42	123.20
18	B	1228	CLA	CHD-C1D-ND	-3.61	119.72	124.80
18	A	1119	CLA	C1-C2-C3	-3.61	120.28	126.20
21	B	5004	LHG	C5-O7-C7	-3.61	111.48	117.85
23	F	5002	LMG	O8-C28-C29	3.61	122.83	111.83
18	2	2005	CLA	CHD-C1D-ND	-3.60	119.73	124.80
18	B	1207	CLA	O2A-CGA-CBA	3.60	122.82	111.83
18	A	1124	CLA	C1-C2-C3	-3.60	120.30	126.20
18	A	1115	CLA	CHD-C1D-ND	-3.60	119.73	124.80
18	A	1117	CLA	O2A-C1-C2	3.60	121.96	108.11
18	B	1226	CLA	CHD-C1D-ND	-3.60	119.74	124.80
22	B	6006	BCR	C8-C9-C10	3.60	124.67	119.01
18	3	3012	CLA	CMB-C2B-C1B	3.60	130.90	125.42
18	B	1023	CLA	CAC-C3C-C4C	3.60	129.47	124.79
18	A	1129	CLA	O2A-C1-C2	3.60	121.94	108.11
18	B	1213	CLA	CHD-C1D-ND	-3.59	119.75	124.80
22	B	6006	BCR	C3-C4-C5	-3.59	107.65	114.06
18	B	1238	CLA	O2A-C1-C2	3.59	121.92	108.11
18	B	1236	CLA	CHD-C1D-ND	-3.59	119.75	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1107	CLA	CHD-C1D-ND	-3.59	119.76	124.80
18	B	1228	CLA	C1-C2-C3	-3.58	120.33	126.20
18	A	1120	CLA	CHD-C1D-ND	-3.58	119.76	124.80
18	A	1136	CLA	CHD-C1D-ND	-3.58	119.76	124.80
18	A	1124	CLA	O2A-C1-C2	3.58	121.88	108.11
18	B	1227	CLA	O2A-CGA-CBA	3.58	122.75	111.83
22	L	6020	BCR	C7-C8-C9	-3.58	120.94	126.23
27	I	6018	LUT	C22-C23-C24	-3.58	105.87	111.18
28	1	1010	CHL	C1A-CHA-C4D	3.58	124.95	118.98
18	A	1111	CLA	CHD-C1D-ND	-3.58	119.77	124.80
18	1	1011	CLA	CAA-CBA-CGA	-3.58	103.05	113.21
18	4	4005	CLA	CMB-C2B-C1B	3.58	130.86	125.42
18	A	1117	CLA	CHD-C1D-ND	-3.58	119.77	124.80
18	B	1212	CLA	C1-C2-C3	-3.57	120.34	126.20
18	A	1138	CLA	CHD-C1D-ND	-3.57	119.78	124.80
18	4	4003	CLA	C1-C2-C3	-3.57	120.35	126.20
28	4	4010	CHL	C4D-CHA-CBD	-3.57	105.37	108.97
18	4	4012	CLA	CAC-C3C-C4C	3.57	129.43	124.79
22	B	6010	BCR	C1-C6-C7	3.57	125.32	115.65
23	G	2021	LMG	O7-C10-C11	3.57	119.19	111.48
18	1	1013	CLA	CHD-C1D-ND	-3.56	119.79	124.80
18	A	1126	CLA	C2B-C1B-NB	3.56	114.02	110.33
22	L	6019	BCR	C36-C18-C17	-3.56	117.04	122.82
18	2	2012	CLA	C4-C3-C5	3.56	121.41	115.23
18	B	1202	CLA	CHD-C1D-ND	-3.56	119.79	124.80
18	3	3013	CLA	CHD-C1D-ND	-3.56	119.79	124.80
23	J	5001	LMG	O8-C28-C29	3.56	122.69	111.83
18	3	3005	CLA	CMC-C2C-C1C	3.56	130.59	125.03
22	L	6020	BCR	C33-C5-C6	-3.56	120.60	124.48
18	B	1211	CLA	CHD-C1D-ND	-3.55	119.80	124.80
18	A	1139	CLA	O2A-C1-C2	3.55	121.78	108.11
18	B	1209	CLA	C2B-C1B-NB	3.55	114.01	110.33
22	L	6020	BCR	C15-C14-C13	-3.55	122.30	127.28
28	1	1009	CHL	C1A-CHA-C4D	3.55	124.90	118.98
18	4	4001	CLA	CAA-C2A-C3A	-3.55	103.42	113.00
18	B	1021	CLA	O2A-C1-C2	3.55	121.76	108.11
18	F	1302	CLA	O2A-C1-C2	3.55	121.76	108.11
18	1	1012	CLA	O2A-CGA-O1A	-3.55	114.76	123.63
18	A	1132	CLA	C2B-C1B-NB	3.55	114.00	110.33
18	G	1002	CLA	CHD-C1D-ND	-3.55	119.81	124.80
18	A	1112	CLA	C2B-C1B-NB	3.54	114.00	110.33
18	3	3001	CLA	CMB-C2B-C1B	3.54	130.82	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1105	CLA	C4-C3-C5	3.54	120.30	116.13
28	4	4010	CHL	C3C-C4C-NC	-3.54	105.99	114.65
28	3	3011	CHL	C3C-C4C-NC	-3.54	105.99	114.65
28	4	4011	CHL	C3D-C4D-CHA	3.54	113.92	108.54
18	L	1503	CLA	O2A-C1-C2	3.54	121.73	108.11
18	B	1203	CLA	CHD-C1D-ND	-3.54	119.82	124.80
18	1	1013	CLA	CMB-C2B-C1B	3.54	130.81	125.42
22	B	6004	BCR	C15-C14-C13	-3.54	122.32	127.28
18	B	1219	CLA	O2A-C1-C2	3.54	121.72	108.11
18	B	1231	CLA	C2B-C1B-NB	3.54	113.99	110.33
18	A	1103	CLA	CHD-C1D-ND	-3.54	119.83	124.80
18	2	2008	CLA	O2A-C1-C2	3.53	121.71	108.11
28	4	4013	CHL	C3D-C4D-CHA	3.53	113.91	108.54
18	B	1232	CLA	CHD-C1D-ND	-3.53	119.83	124.80
18	A	1151	CLA	CHD-C1D-ND	-3.53	119.83	124.80
18	A	1134	CLA	O2A-C1-C2	3.53	121.70	108.11
22	B	6010	BCR	C1-C6-C5	-3.53	117.81	122.64
18	A	1122	CLA	CHD-C1D-ND	-3.53	119.84	124.80
18	A	1139	CLA	CHD-C1D-ND	-3.53	119.84	124.80
18	3	3006	CLA	CHD-C1D-ND	-3.53	119.84	124.80
18	B	1214	CLA	O2A-C1-C2	3.53	121.67	108.11
22	B	6004	BCR	C3-C4-C5	-3.52	107.77	114.06
18	B	1211	CLA	C1-C2-C3	-3.52	120.42	126.20
18	A	1104	CLA	CHD-C1D-ND	-3.52	119.84	124.80
18	L	1503	CLA	CMC-C2C-C1C	3.52	130.53	125.03
18	B	1209	CLA	CHD-C1D-ND	-3.52	119.85	124.80
22	A	6017	BCR	C28-C27-C26	-3.52	107.78	114.06
22	L	6019	BCR	C19-C18-C17	3.52	124.54	119.01
18	3	3001	CLA	CAA-C2A-C3A	-3.52	103.49	113.00
18	2	2008	CLA	CHD-C1D-ND	-3.52	119.85	124.80
26	B	8002	LMU	C1B-O1B-C4'	-3.52	109.64	117.98
18	B	1210	CLA	C2B-C1B-NB	3.51	113.97	110.33
18	G	1001	CLA	C4-C3-C5	3.51	121.32	115.23
18	4	4003	CLA	CHD-C1D-ND	-3.50	119.87	124.80
22	F	6016	BCR	C34-C9-C10	-3.50	117.14	122.82
18	2	2006	CLA	C1-C2-C3	-3.50	120.46	126.20
18	2	2006	CLA	CHD-C1D-ND	-3.50	119.88	124.80
18	A	1122	CLA	C4-C3-C5	3.50	121.30	115.23
18	B	1204	CLA	C1-O2A-CGA	3.50	125.12	116.65
18	A	1105	CLA	CHD-C1D-ND	-3.50	119.88	124.80
18	3	3004	CLA	CMB-C2B-C1B	3.50	130.75	125.42
22	A	6008	BCR	C3-C4-C5	-3.50	107.82	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	1003	CLA	O2A-C1-C2	3.50	121.56	108.11
18	L	1501	CLA	C3D-C4D-ND	3.50	115.67	109.99
18	2	2005	CLA	O2A-C1-C2	3.50	121.56	108.11
22	3	3503	BCR	C37-C22-C21	-3.49	117.15	122.82
18	B	1214	CLA	CHD-C1D-ND	-3.49	119.88	124.80
18	3	3017	CLA	O2A-CGA-CBA	3.49	125.34	112.14
18	L	1503	CLA	CHD-C1D-ND	-3.49	119.89	124.80
18	H	1000	CLA	CHD-C1D-ND	-3.49	119.89	124.80
18	A	1131	CLA	CHD-C1D-ND	-3.49	119.89	124.80
18	A	1102	CLA	O2A-C1-C2	3.49	121.55	108.11
17	A	1011	CL0	O2A-C1-C2	3.49	121.55	108.11
18	B	1021	CLA	CHD-C1D-ND	-3.49	119.89	124.80
18	A	1104	CLA	O2A-C1-C2	3.49	121.53	108.11
22	F	6014	BCR	C23-C22-C21	3.49	124.49	119.01
27	2	2501	LUT	C22-C23-C24	-3.49	106.01	111.18
18	B	1222	CLA	CHD-C1D-ND	-3.49	119.90	124.80
18	4	4006	CLA	O2A-CGA-CBA	3.49	122.46	111.83
18	3	3002	CLA	CAC-C3C-C4C	3.49	129.32	124.79
27	I	6018	LUT	C18-C5-C6	-3.48	120.68	124.48
18	B	1212	CLA	CHD-C1D-ND	-3.48	119.90	124.80
18	4	4017	CLA	O2A-C1-C2	3.48	121.51	108.11
27	3	3501	LUT	C15-C14-C13	-3.48	122.40	127.28
18	A	1135	CLA	CHD-C1D-ND	-3.48	119.90	124.80
18	B	1229	CLA	CHD-C1D-ND	-3.48	119.91	124.80
18	B	1239	CLA	CHD-C1D-ND	-3.48	119.91	124.80
18	B	1224	CLA	CHD-C1D-ND	-3.48	119.91	124.80
18	2	2007	CLA	C1-C2-C3	-3.48	120.50	126.20
18	A	1130	CLA	O2A-C1-C2	3.48	121.49	108.11
18	4	4001	CLA	O2A-C1-C2	3.48	121.49	108.11
18	A	1111	CLA	C2B-C1B-NB	3.48	113.93	110.33
28	2	2010	CHL	C3C-C4C-NC	-3.47	106.16	114.65
18	A	1110	CLA	CHD-C1D-ND	-3.47	119.92	124.80
18	B	1201	CLA	C1-C2-C3	-3.47	121.15	126.76
18	4	4007	CLA	CMB-C2B-C1B	3.47	130.70	125.42
18	2	2006	CLA	O2A-C1-C2	3.47	121.46	108.11
18	A	1120	CLA	O2A-C1-C2	3.47	121.46	108.11
18	3	3006	CLA	C4D-C3D-CAD	3.47	111.87	108.11
18	A	1112	CLA	C1-C2-C3	-3.47	120.52	126.20
27	2	2502	LUT	C21-C26-C27	3.47	116.81	112.83
18	A	1140	CLA	CHD-C1D-ND	-3.47	119.92	124.80
22	J	6013	BCR	C29-C30-C25	3.47	115.47	110.44
28	2	2010	CHL	C1C-C2C-CMC	3.47	133.05	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1113	CLA	CHD-C1D-ND	-3.46	119.93	124.80
18	L	1502	CLA	CHD-C1D-ND	-3.46	119.93	124.80
18	B	1220	CLA	CHD-C1D-ND	-3.46	119.93	124.80
18	F	1301	CLA	CHD-C1D-ND	-3.46	119.93	124.80
18	B	1218	CLA	C4-C3-C5	3.46	121.23	115.23
18	1	1011	CLA	CHD-C1D-ND	-3.46	119.94	124.80
18	A	1151	CLA	O2A-C1-C2	3.46	121.41	108.11
28	4	4010	CHL	CMA-C3A-C4A	-3.45	107.17	114.61
18	2	2004	CLA	O1D-CGD-CBD	-3.45	117.71	124.52
18	2	2001	CLA	CHD-C1D-ND	-3.45	119.94	124.80
18	B	1023	CLA	C2B-C1B-NB	3.45	113.90	110.33
18	2	2001	CLA	O2D-CGD-CBD	3.45	117.26	111.23
18	2	2007	CLA	CHD-C1D-ND	-3.44	119.96	124.80
18	B	1203	CLA	O2A-C1-C2	3.44	121.34	108.11
18	3	3019	CLA	CHD-C1D-ND	-3.44	119.99	124.84
22	G	2011	BCR	C33-C5-C4	3.44	120.92	113.60
18	B	1215	CLA	C1-C2-C3	-3.44	120.57	126.20
18	F	1301	CLA	O2A-CGA-CBA	3.43	124.85	114.00
18	A	1022	CLA	O2A-C1-C2	3.43	121.32	108.11
18	A	1137	CLA	O2A-C1-C2	3.43	121.32	108.11
18	G	1001	CLA	CAC-C3C-C4C	3.43	129.26	124.79
18	B	1228	CLA	O2A-C1-C2	3.43	121.31	108.11
18	1	1013	CLA	CMD-C2D-C3D	-3.43	119.82	127.69
18	4	4005	CLA	O2A-C1-C2	3.43	121.31	108.11
18	A	1124	CLA	C2B-C1B-NB	3.43	113.88	110.33
18	1	1006	CLA	C1-C2-C3	-3.43	121.22	126.76
22	J	6012	BCR	C19-C18-C17	3.43	124.40	119.01
18	2	2004	CLA	C2B-C1B-NB	3.43	113.88	110.33
27	4	4502	LUT	C15-C14-C13	-3.42	122.48	127.28
18	B	1231	CLA	C1-C2-C3	-3.42	120.59	126.20
18	B	1238	CLA	C2B-C1B-NB	3.42	113.88	110.33
27	1	1501	LUT	C18-C5-C6	-3.42	120.75	124.48
18	3	3004	CLA	C3D-C4D-ND	3.42	115.54	109.99
18	L	1502	CLA	O2A-C1-C2	3.42	121.26	108.11
27	1	1502	LUT	C22-C23-C24	-3.42	106.11	111.18
22	G	2011	BCR	C36-C18-C17	-3.41	117.28	122.82
18	3	3010	CLA	O2A-C1-C2	3.41	121.24	108.11
18	A	1114	CLA	CHD-C1D-ND	-3.41	120.00	124.80
18	H	1000	CLA	O2A-CGA-CBA	3.41	125.03	112.14
28	1	1009	CHL	C3C-C4C-NC	-3.41	106.31	114.65
18	A	1131	CLA	O2A-C1-C2	3.41	121.23	108.11
18	1	1004	CLA	CHD-C1D-ND	-3.41	120.00	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1228	CLA	C2B-C1B-NB	3.41	113.86	110.33
18	A	1126	CLA	CHD-C1D-ND	-3.41	120.01	124.80
28	1	1010	CHL	C1C-C2C-CMC	3.41	132.94	126.80
22	A	6017	BCR	C34-C9-C10	-3.41	117.30	122.82
18	A	1105	CLA	C2B-C1B-NB	3.40	113.86	110.33
18	A	1118	CLA	CHD-C1D-ND	-3.40	120.02	124.80
18	2	2004	CLA	C1-C2-C3	-3.40	120.62	126.20
18	1	1007	CLA	CMB-C2B-C1B	3.40	130.60	125.42
18	1	1004	CLA	C1-C2-C3	-3.40	120.62	126.20
22	I	6020	BCR	C7-C8-C9	-3.40	121.20	126.23
18	3	3018	CLA	C4D-C3D-CAD	3.40	111.80	108.11
18	2	2001	CLA	O2A-C1-C2	3.40	121.18	108.11
27	1	1501	LUT	C31-C32-C33	-3.40	117.05	126.36
18	A	1109	CLA	C2B-C1B-NB	3.40	113.85	110.33
18	B	1230	CLA	CHD-C1D-ND	-3.39	120.03	124.80
18	4	4009	CLA	CHD-C1D-ND	-3.39	120.03	124.80
18	A	1134	CLA	C1-C2-C3	-3.39	120.64	126.20
27	1	1502	LUT	C11-C10-C9	-3.39	122.53	127.28
22	J	6013	BCR	C33-C5-C4	3.39	120.82	113.60
18	A	1101	CLA	C2B-C1B-NB	3.39	113.84	110.33
18	4	4001	CLA	C4D-C3D-CAD	3.39	111.79	108.11
29	4	4505	ZEX	C15-C14-C13	-3.39	122.53	127.28
18	3	3010	CLA	C4-C3-C5	3.38	121.10	115.23
18	B	1211	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
27	I	6018	LUT	C31-C30-C29	-3.38	122.54	127.28
18	A	1120	CLA	C1-C2-C3	-3.38	120.66	126.20
18	B	1232	CLA	C2B-C1B-NB	3.38	113.83	110.33
18	B	1201	CLA	CHD-C1D-ND	-3.37	120.06	124.80
18	1	1006	CLA	CMD-C2D-C3D	-3.37	119.95	127.69
18	A	1123	CLA	C2B-C1B-NB	3.37	113.82	110.33
27	4	4501	LUT	C31-C30-C29	-3.37	122.56	127.28
22	G	2011	BCR	C24-C23-C22	-3.37	121.25	126.23
18	4	4004	CLA	O2A-C1-C2	3.36	121.06	108.11
18	B	1202	CLA	C2B-C1B-NB	3.36	113.81	110.33
22	F	6014	BCR	C33-C5-C6	-3.36	120.81	124.48
18	B	1219	CLA	CHD-C1D-ND	-3.36	120.07	124.80
18	B	1217	CLA	CHD-C1D-ND	-3.36	120.07	124.80
18	A	1115	CLA	C2B-C1B-NB	3.36	113.81	110.33
18	B	1213	CLA	C2B-C1B-NB	3.36	113.81	110.33
18	2	2004	CLA	CHD-C1D-ND	-3.36	120.08	124.80
18	A	1137	CLA	CHD-C1D-ND	-3.36	120.08	124.80
18	A	1105	CLA	C1-C2-C3	-3.36	120.70	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3004	CLA	C4D-C3D-CAD	3.36	111.75	108.11
18	4	4001	CLA	C1-O2A-CGA	3.35	124.77	116.65
18	G	1003	CLA	C1-C2-C3	-3.35	120.70	126.20
18	1	1008	CLA	O2A-CGA-CBA	3.35	124.80	112.14
27	1	1501	LUT	C22-C23-C24	-3.35	106.21	111.18
18	A	1101	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
18	J	1302	CLA	CHD-C1D-ND	-3.35	120.09	124.80
22	J	6012	BCR	C34-C9-C10	-3.35	117.40	122.82
18	A	1121	CLA	C2B-C1B-NB	3.35	113.80	110.33
18	4	4003	CLA	O2A-C1-C2	3.35	120.98	108.11
18	3	3013	CLA	O2A-CGA-CBA	3.34	124.77	112.14
18	B	1225	CLA	O2A-C1-C2	3.34	120.97	108.11
18	1	1003	CLA	C1-C2-C3	-3.34	120.72	126.20
18	A	1136	CLA	O2A-C1-C2	3.34	120.97	108.11
18	A	1013	CLA	C1-C2-C3	-3.34	120.72	126.20
18	A	1022	CLA	CHD-C1D-ND	-3.34	120.10	124.80
18	B	1207	CLA	CHD-C1D-ND	-3.34	120.10	124.80
18	1	1011	CLA	CMC-C2C-C1C	3.34	130.26	125.03
18	1	1002	CLA	O2A-CGA-O1A	-3.34	113.23	123.20
18	B	1235	CLA	O2A-C1-C2	3.34	120.96	108.11
18	B	1201	CLA	C2B-C1B-NB	3.34	113.79	110.33
18	A	1106	CLA	CHD-C1D-ND	-3.34	120.11	124.80
18	4	4001	CLA	CHD-C1D-ND	-3.34	120.11	124.80
22	J	6013	BCR	C28-C27-C26	-3.34	108.11	114.06
18	3	3007	CLA	C3D-C4D-ND	3.34	115.41	109.99
27	4	4503	LUT	C17-C1-C6	-3.33	105.01	110.24
18	A	1123	CLA	CHD-C1D-ND	-3.33	120.11	124.80
18	B	1240	CLA	O2A-CGA-CBA	3.33	121.99	111.83
18	A	1101	CLA	C1-C2-C3	-3.33	120.74	126.20
18	2	2003	CLA	O2A-C1-C2	3.33	120.91	108.11
18	4	4007	CLA	C4D-C3D-CAD	3.33	111.72	108.11
22	B	6005	BCR	C36-C18-C17	-3.33	117.43	122.82
28	2	2011	CHL	C3D-C4D-CHA	3.33	113.59	108.54
28	2	2013	CHL	C1B-CHB-C4A	3.33	123.46	121.32
18	A	1022	CLA	CMB-C2B-C1B	3.33	130.48	125.42
23	G	2021	LMG	O8-C28-C29	3.32	121.97	111.83
22	J	6013	BCR	C4-C5-C6	-3.32	118.21	122.70
18	A	1127	CLA	O2A-C1-C2	3.32	120.90	108.11
18	B	1224	CLA	C2B-C1B-NB	3.32	113.77	110.33
18	A	1116	CLA	C2B-C1B-NB	3.32	113.77	110.33
18	A	1135	CLA	C4-C3-C5	3.32	120.04	116.13
18	A	1111	CLA	O2A-C1-C2	3.32	120.88	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	I	6018	LUT	C26-C27-C28	-3.32	119.42	124.58
18	B	1230	CLA	O2A-C1-C2	3.32	120.87	108.11
18	4	4016	CLA	C4D-C3D-CAD	3.31	111.71	108.11
18	B	1239	CLA	C1-C2-C3	-3.31	120.77	126.20
18	B	1207	CLA	CMC-C2C-C1C	3.31	130.21	125.03
18	B	1226	CLA	C3B-C2B-C1B	-3.31	103.26	107.17
18	4	4005	CLA	CHD-C1D-ND	-3.31	120.14	124.80
22	J	6012	BCR	C1-C6-C5	-3.31	118.11	122.64
18	1	1005	CLA	CHD-C1D-ND	-3.31	120.14	124.80
18	B	1227	CLA	C2B-C1B-NB	3.31	113.76	110.33
18	4	4016	CLA	CMD-C2D-C3D	-3.31	120.10	127.69
18	A	1102	CLA	C2B-C1B-NB	3.31	113.76	110.33
18	B	1021	CLA	C2B-C1B-NB	3.31	113.76	110.33
18	B	1225	CLA	C4-C3-C5	3.31	120.97	115.23
18	3	3018	CLA	CMB-C2B-C1B	3.30	130.45	125.42
18	4	4006	CLA	CHD-C1D-ND	-3.30	120.15	124.80
22	B	6006	BCR	C30-C25-C26	-3.30	118.12	122.64
22	A	6007	BCR	C19-C18-C17	3.30	124.20	119.01
18	3	3001	CLA	C2B-C1B-NB	3.30	113.75	110.33
27	3	3502	LUT	C1-C6-C5	-3.30	118.13	122.64
18	A	1102	CLA	CHD-C1D-ND	-3.30	120.16	124.80
18	B	1023	CLA	C1-C2-C3	-3.30	120.79	126.20
18	2	2003	CLA	CHD-C1D-ND	-3.30	120.16	124.80
18	4	4017	CLA	CHD-C1D-ND	-3.30	120.16	124.80
18	4	4009	CLA	C1-C2-C3	-3.30	121.43	126.76
18	3	3004	CLA	O2A-C1-C2	3.30	120.79	108.11
18	B	1221	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
22	J	6013	BCR	C8-C9-C10	3.29	124.19	119.01
27	2	2502	LUT	C35-C34-C33	-3.29	122.66	127.28
18	B	1235	CLA	C1-C2-C3	-3.29	120.80	126.20
18	4	4007	CLA	CHD-C1D-ND	-3.29	120.17	124.80
22	F	6016	BCR	C34-C9-C8	3.29	123.12	118.09
28	2	2013	CHL	C3C-C4C-NC	-3.29	106.61	114.65
18	2	2016	CLA	C3C-C4C-NC	3.29	114.64	110.43
18	2	2003	CLA	C1-C2-C3	-3.29	120.81	126.20
18	2	2007	CLA	O2A-C1-C2	3.29	120.77	108.11
18	A	1113	CLA	O2A-CGA-CBA	3.29	124.56	112.14
18	B	1012	CLA	C1-C2-C3	-3.29	120.81	126.20
18	1	1013	CLA	CAC-C3C-C4C	3.29	129.06	124.79
18	B	1240	CLA	C2B-C1B-NB	3.29	113.73	110.33
18	4	4002	CLA	C1-C2-C3	-3.28	121.45	126.76
18	2	2003	CLA	CMC-C2C-C1C	3.28	130.16	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	6011	BCR	C12-C13-C14	-3.28	113.85	119.01
18	1	1011	CLA	C3D-C4D-ND	3.28	115.32	109.99
18	A	1129	CLA	CHD-C1D-ND	-3.28	120.19	124.80
18	L	1502	CLA	C4D-C3D-CAD	3.28	111.67	108.11
18	B	1214	CLA	C2B-C1B-NB	3.28	113.72	110.33
18	1	1001	CLA	C6-C5-C3	-3.28	105.49	113.47
18	2	2003	CLA	C3D-C4D-ND	3.28	115.31	109.99
18	L	1501	CLA	C1-O2A-CGA	3.28	124.58	116.65
18	A	1118	CLA	O2A-CGA-CBA	3.28	124.51	112.14
18	L	1502	CLA	C1-C2-C3	-3.27	120.83	126.20
18	1	1001	CLA	CMB-C2B-C1B	3.27	130.40	125.42
22	K	2011	BCR	C36-C18-C17	-3.27	117.52	122.82
18	B	1217	CLA	O2A-CGA-CBA	3.27	124.49	112.14
18	1	1012	CLA	C3D-C4D-ND	3.27	115.30	109.99
18	2	2008	CLA	OBD-CAD-C3D	-3.27	120.78	128.42
18	B	1216	CLA	C2B-C1B-NB	3.27	113.71	110.33
18	B	1211	CLA	C3D-C4D-ND	3.27	115.30	109.99
18	A	1119	CLA	O2A-C1-C2	3.27	120.68	108.11
18	3	3012	CLA	C4D-C3D-CAD	3.26	111.65	108.11
18	4	4004	CLA	CMB-C2B-C1B	3.26	130.39	125.42
18	A	1132	CLA	O2A-C1-C2	3.26	120.66	108.11
18	A	1108	CLA	C2B-C1B-NB	3.26	113.71	110.33
22	A	6011	BCR	C33-C5-C6	-3.26	120.93	124.48
18	A	1136	CLA	C1-C2-C3	-3.26	120.86	126.20
18	4	4002	CLA	O2D-CGD-CBD	3.26	116.93	111.23
18	A	1126	CLA	O2A-C1-C2	3.26	120.65	108.11
18	A	1110	CLA	C2B-C1B-NB	3.26	113.70	110.33
18	1	1002	CLA	O2A-CGA-CBA	3.26	124.45	112.14
18	A	1133	CLA	CHD-C1D-ND	-3.26	120.22	124.80
18	B	1209	CLA	O2A-CGA-CBA	3.26	124.44	112.14
27	4	4501	LUT	C8-C7-C6	-3.26	118.30	127.00
18	4	4016	CLA	O2A-CGA-CBA	3.25	124.43	112.14
28	1	1010	CHL	C3C-C4C-NC	-3.25	106.70	114.65
18	1	1003	CLA	C3D-C4D-ND	3.25	115.27	109.99
22	J	6013	BCR	C33-C5-C6	-3.25	120.94	124.48
18	B	1220	CLA	C2B-C1B-NB	3.25	113.70	110.33
18	4	4001	CLA	CMD-C2D-C3D	-3.25	120.24	127.69
18	B	1224	CLA	O2A-C1-C2	3.25	120.61	108.11
18	B	1205	CLA	CHD-C1D-ND	-3.25	120.23	124.80
28	2	2010	CHL	CHA-C1A-C2A	-3.25	125.68	133.31
18	B	1231	CLA	O2A-C1-C2	3.25	120.60	108.11
18	G	1002	CLA	CAC-C3C-C4C	3.24	129.01	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1219	CLA	C1-C2-C3	-3.24	120.88	126.20
18	4	4009	CLA	CMC-C2C-C1C	3.24	130.10	125.03
18	3	3017	CLA	CMC-C2C-C1C	3.24	130.10	125.03
18	3	3012	CLA	C1-C2-C3	-3.24	121.52	126.76
18	G	1001	CLA	CHD-C1D-ND	-3.24	120.24	124.80
18	B	1230	CLA	C1-C2-C3	-3.24	120.89	126.20
18	A	1127	CLA	CHD-C1D-ND	-3.24	120.24	124.80
18	A	1108	CLA	O2A-CGA-CBA	3.24	124.37	112.14
22	F	6016	BCR	C23-C24-C25	-3.24	118.35	127.00
18	B	1222	CLA	C2B-C1B-NB	3.24	113.68	110.33
22	B	6004	BCR	C36-C18-C17	-3.23	117.58	122.82
18	4	4008	CLA	CMC-C2C-C1C	3.23	130.09	125.03
18	B	1201	CLA	CMC-C2C-C1C	3.23	130.08	125.03
27	4	4502	LUT	C18-C5-C6	-3.23	120.96	124.48
22	B	6004	BCR	C30-C25-C26	-3.23	118.22	122.64
18	1	1007	CLA	O2A-CGA-CBA	3.23	124.33	112.14
22	A	6017	BCR	C35-C13-C14	-3.23	117.59	122.82
18	3	3017	CLA	C2B-C1B-NB	3.22	113.67	110.33
18	K	1001	CLA	O2A-CGA-CBA	3.22	124.32	112.14
18	A	1106	CLA	C2B-C1B-NB	3.22	113.67	110.33
18	1	1012	CLA	O2A-CGA-CBA	3.22	121.65	111.83
18	A	1113	CLA	C2B-C1B-NB	3.22	113.67	110.33
18	A	1139	CLA	C2B-C1B-NB	3.22	113.67	110.33
18	A	1114	CLA	O2A-CGA-CBA	3.22	124.29	112.14
18	2	2001	CLA	CBA-CAA-C2A	3.22	123.36	113.79
23	J	5001	LMG	O8-C28-O10	-3.21	115.60	123.63
18	B	1225	CLA	CHD-C1D-ND	-3.21	120.29	124.80
18	A	1013	CLA	C3D-C4D-ND	3.21	115.20	109.99
18	K	1001	CLA	CMD-C2D-C3D	-3.21	120.33	127.69
18	B	1206	CLA	CHD-C1D-ND	-3.21	120.29	124.80
18	3	3006	CLA	CMD-C2D-C3D	-3.21	120.34	127.69
18	B	1229	CLA	C2B-C1B-NB	3.20	113.65	110.33
23	4	4801	LMG	C8-O7-C10	-3.20	110.13	117.80
18	A	1119	CLA	C2B-C1B-NB	3.20	113.65	110.33
18	H	1000	CLA	CMB-C2B-C1B	3.20	130.29	125.42
18	L	1502	CLA	CMB-C2B-C1B	3.20	130.29	125.42
22	3	3503	BCR	C38-C26-C25	-3.20	120.99	124.48
18	4	4002	CLA	OBD-CAD-C3D	-3.20	120.94	128.42
27	4	4503	LUT	C18-C5-C6	-3.20	121.00	124.48
18	1	1008	CLA	CAC-C3C-C4C	3.20	128.95	124.79
18	B	1023	CLA	CHD-C1D-ND	-3.20	120.30	124.80
18	3	3018	CLA	C1-C2-C3	-3.20	121.59	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1006	CLA	C3D-C4D-ND	3.19	115.18	109.99
18	B	1235	CLA	C2B-C1B-NB	3.19	113.64	110.33
18	A	1112	CLA	O2A-C1-C2	3.19	120.39	108.11
18	A	1123	CLA	O2A-C1-C2	3.19	120.39	108.11
22	I	6020	BCR	C24-C23-C22	-3.19	121.52	126.23
27	1	1502	LUT	C10-C11-C12	-3.19	113.96	123.20
18	4	4006	CLA	C3D-C4D-ND	3.19	115.17	109.99
18	1	1002	CLA	CMC-C2C-C1C	3.19	130.02	125.03
18	2	2016	CLA	O1D-CGD-CBD	-3.19	118.23	124.52
18	3	3005	CLA	C1-C2-C3	-3.19	120.97	126.20
18	A	1117	CLA	C2B-C1B-NB	3.19	113.63	110.33
18	2	2009	CLA	O2A-C1-C2	3.19	120.37	108.11
22	A	6002	BCR	C33-C5-C6	-3.19	121.01	124.48
22	A	6003	BCR	C19-C18-C17	3.19	124.02	119.01
18	2	2016	CLA	CAA-C2A-C3A	-3.19	104.39	113.00
18	L	1502	CLA	CMC-C2C-C1C	3.19	130.01	125.03
27	3	3501	LUT	C8-C7-C6	-3.18	118.49	127.00
18	A	1237	CLA	C3D-C4D-ND	3.18	115.16	109.99
18	A	1115	CLA	O2A-CGA-CBA	3.18	124.16	112.14
22	F	6014	BCR	C7-C8-C9	-3.18	121.53	126.23
18	3	3002	CLA	O2A-CGA-CBA	3.18	124.14	112.14
18	K	1001	CLA	C3D-C4D-ND	3.18	115.15	109.99
18	A	1136	CLA	C2B-C1B-NB	3.17	113.62	110.33
18	4	4002	CLA	CHD-C1D-ND	-3.17	120.33	124.80
22	J	6012	BCR	C38-C26-C25	-3.17	121.02	124.48
25	B	7101	DGD	O6D-C1D-O3G	-3.17	102.55	110.04
18	4	4008	CLA	O2A-CGA-CBA	3.17	124.12	112.14
22	J	6013	BCR	C3-C4-C5	-3.17	108.40	114.06
18	1	1006	CLA	O2A-C1-C2	3.17	120.31	108.11
18	A	1022	CLA	C2B-C1B-NB	3.17	113.61	110.33
18	4	4007	CLA	CMD-C2D-C3D	-3.17	120.43	127.69
18	1	1006	CLA	CAA-C2A-C3A	-3.17	104.44	113.00
18	1	1005	CLA	CMB-C2B-C1B	3.17	130.24	125.42
18	A	1138	CLA	C3D-C4D-ND	3.16	115.13	109.99
22	L	6020	BCR	C36-C18-C17	-3.16	117.69	122.82
18	L	1502	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
18	4	4008	CLA	C3C-C4C-NC	3.16	114.48	110.43
18	1	1013	CLA	O2A-CGA-CBA	3.16	124.09	112.14
18	B	1223	CLA	C2B-C1B-NB	3.16	113.61	110.33
18	G	1002	CLA	O2A-CGA-CBA	3.16	124.08	112.14
18	L	1502	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
18	4	4008	CLA	CHD-C1D-ND	-3.16	120.36	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1021	CLA	CMC-C2C-C1C	3.16	129.97	125.03
23	J	5001	LMG	C12-C11-C10	-3.16	102.13	113.69
18	B	1227	CLA	CMC-C2C-C1C	3.16	129.97	125.03
18	A	1140	CLA	C4-C3-C5	3.15	120.70	115.23
18	2	2016	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
18	A	1138	CLA	C2B-C1B-NB	3.15	113.60	110.33
18	B	1217	CLA	C2B-C1B-NB	3.15	113.60	110.33
29	4	4505	ZEX	C31-C30-C29	-3.15	122.86	127.28
18	1	1011	CLA	CMB-C2B-C1B	3.15	130.22	125.42
18	B	1215	CLA	C2B-C1B-NB	3.15	113.59	110.33
22	K	2011	BCR	C33-C5-C6	-3.15	121.05	124.48
18	2	2005	CLA	C3D-C4D-ND	3.15	115.10	109.99
18	A	1107	CLA	C2B-C1B-NB	3.15	113.59	110.33
18	J	1302	CLA	C2B-C1B-NB	3.15	113.59	110.33
18	A	1102	CLA	C1-C2-C3	-3.15	121.67	126.76
18	3	3008	CLA	CHD-C1D-ND	-3.15	120.37	124.80
22	L	6020	BCR	C23-C22-C21	3.14	123.95	119.01
18	A	1104	CLA	C3D-C4D-ND	3.14	115.09	109.99
18	1	1002	CLA	C3D-C4D-ND	3.14	115.09	109.99
18	A	1128	CLA	CHD-C1D-ND	-3.14	120.38	124.80
27	I	6018	LUT	C7-C8-C9	-3.14	121.59	126.23
18	B	1207	CLA	C1-C2-C3	-3.14	121.06	126.20
18	A	1124	CLA	C3D-C4D-ND	3.14	115.09	109.99
28	3	3011	CHL	CMA-C3A-C4A	-3.14	107.85	114.61
18	A	1139	CLA	CMC-C2C-C1C	3.14	129.94	125.03
27	2	2501	LUT	C26-C27-C28	-3.13	119.70	124.58
18	B	1230	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
18	3	3006	CLA	C3D-C4D-ND	3.13	115.08	109.99
18	1	1004	CLA	O2A-C1-C2	3.13	120.16	108.11
18	A	1125	CLA	C1-C2-C3	-3.13	121.07	126.20
18	A	1112	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
18	L	1501	CLA	CMC-C2C-C1C	3.13	129.92	125.03
18	B	1207	CLA	C1-O2A-CGA	3.13	124.22	116.65
18	1	1007	CLA	C4D-C3D-CAD	3.13	111.50	108.11
18	2	2002	CLA	O2A-CGA-CBA	3.13	123.94	112.14
18	2	2001	CLA	C3D-C4D-ND	3.12	115.06	109.99
18	3	3008	CLA	OBD-CAD-C3D	-3.12	121.11	128.42
18	4	4017	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
18	F	1301	CLA	CMB-C2B-C1B	3.12	130.18	125.42
22	J	6013	BCR	C38-C26-C25	-3.12	121.08	124.48
18	A	1122	CLA	O2A-C1-C2	3.12	120.12	108.11
27	4	4501	LUT	C18-C5-C4	3.12	120.16	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1128	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
18	B	1223	CLA	CHD-C1D-ND	-3.12	120.42	124.80
18	B	1238	CLA	C3D-C4D-ND	3.12	115.05	109.99
22	F	6014	BCR	C37-C22-C21	-3.12	117.77	122.82
18	4	4006	CLA	CAA-C2A-C3A	-3.11	104.58	113.00
18	B	1226	CLA	O2A-C1-C2	3.11	120.09	108.11
18	4	4001	CLA	CBC-CAC-C3C	-3.11	103.98	112.42
18	B	1205	CLA	O2A-C1-C2	3.11	120.08	108.11
18	A	1132	CLA	C1-C2-C3	-3.11	121.10	126.20
18	B	1213	CLA	C4-C3-C5	3.11	120.63	115.23
22	J	6012	BCR	C37-C22-C21	-3.11	117.78	122.82
18	A	1129	CLA	C2B-C1B-NB	3.11	113.55	110.33
18	B	1218	CLA	C1-C2-C3	-3.11	121.10	126.20
18	A	1131	CLA	C1-C2-C3	-3.11	121.10	126.20
18	1	1001	CLA	CHD-C1D-ND	-3.11	120.43	124.80
18	G	1002	CLA	CMB-C2B-C1B	3.11	130.15	125.42
25	B	7101	DGD	O3G-C3G-C2G	-3.10	103.27	110.82
18	A	1103	CLA	C2B-C1B-NB	3.10	113.54	110.33
18	4	4012	CLA	C1-C2-C3	-3.10	121.11	126.20
18	3	3002	CLA	C4D-C3D-CAD	3.10	111.48	108.11
18	3	3003	CLA	C4D-C3D-CAD	3.10	111.48	108.11
18	1	1005	CLA	C1-C2-C3	-3.10	121.12	126.20
18	B	1204	CLA	C3D-C4D-ND	3.10	115.03	109.99
27	1	1502	LUT	C35-C34-C33	-3.10	122.93	127.28
18	B	1211	CLA	C4D-C3D-CAD	3.10	111.47	108.11
22	B	6006	BCR	C34-C9-C10	-3.10	117.80	122.82
18	B	1236	CLA	CMC-C2C-C1C	3.10	129.88	125.03
18	B	1218	CLA	C3D-C4D-ND	3.10	115.02	109.99
28	4	4010	CHL	C1C-C2C-CMC	3.10	132.38	126.80
18	4	4016	CLA	C3D-C4D-ND	3.10	115.02	109.99
18	B	1222	CLA	O2A-C1-C2	3.10	120.02	108.11
18	A	1112	CLA	CMB-C2B-C1B	3.09	130.13	125.42
29	4	4505	ZEX	C11-C10-C9	-3.09	122.94	127.28
18	B	1221	CLA	CHD-C1D-ND	-3.09	120.45	124.80
18	1	1004	CLA	C3D-C4D-ND	3.09	115.01	109.99
18	B	1012	CLA	C2B-C1B-NB	3.09	113.53	110.33
28	3	3011	CHL	C1-O2A-CGA	3.09	124.13	116.65
18	A	1132	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
18	B	1231	CLA	C4-C3-C5	3.09	120.59	115.23
28	3	3011	CHL	C1-C2-C3	-3.09	121.14	126.20
18	B	1227	CLA	C3D-C4D-ND	3.09	115.01	109.99
18	B	1235	CLA	CMC-C2C-C1C	3.09	129.86	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	3501	LUT	C35-C15-C14	-3.09	117.20	123.52
18	B	1218	CLA	O2A-C1-C2	3.08	119.98	108.11
18	G	1003	CLA	C3D-C4D-ND	3.08	115.00	109.99
22	B	6010	BCR	C19-C18-C17	3.08	123.85	119.01
18	A	1120	CLA	C2B-C1B-NB	3.08	113.52	110.33
29	4	4505	ZEX	C15-C35-C34	-3.08	117.22	123.52
18	3	3005	CLA	C4-C3-C5	3.08	120.57	115.23
18	A	1130	CLA	C2B-C1B-NB	3.08	113.52	110.33
18	2	2001	CLA	C4D-C3D-CAD	3.07	111.44	108.11
18	A	1107	CLA	C3D-C4D-ND	3.07	114.98	109.99
18	G	1003	CLA	CMD-C2D-C3D	-3.07	120.65	127.69
18	B	1223	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
18	4	4009	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
22	B	6005	BCR	C1-C6-C5	-3.07	118.44	122.64
28	4	4013	CHL	CMA-C3A-C4A	-3.07	108.00	114.61
18	B	1204	CLA	C2B-C1B-NB	3.07	113.51	110.33
18	3	3018	CLA	CMD-C2D-C3D	-3.07	120.66	127.69
18	4	4003	CLA	C3D-C4D-ND	3.06	114.97	109.99
22	B	6005	BCR	C38-C26-C27	3.06	120.12	113.60
18	4	4001	CLA	C2B-C1B-NB	3.06	113.50	110.33
27	3	3502	LUT	C35-C34-C33	-3.06	122.99	127.28
18	2	2002	CLA	CMC-C2C-C1C	3.06	129.81	125.03
18	3	3013	CLA	C3D-C4D-ND	3.06	114.96	109.99
18	A	1132	CLA	C3D-C4D-ND	3.05	114.95	109.99
18	A	1125	CLA	CHD-C1D-ND	-3.05	120.51	124.80
18	B	1208	CLA	C3D-C4D-ND	3.05	114.95	109.99
18	1	1011	CLA	C2B-C1B-NB	3.05	113.49	110.33
18	3	3001	CLA	C3D-C4D-ND	3.05	114.94	109.99
18	B	1240	CLA	C3D-C4D-ND	3.05	114.94	109.99
18	4	4004	CLA	CHD-C1D-ND	-3.05	120.51	124.80
23	J	5001	LMG	O6-C5-C4	-3.05	104.21	109.70
18	3	3010	CLA	C1-C2-C3	-3.05	121.20	126.20
18	B	1222	CLA	C4-C3-C5	3.05	120.52	115.23
22	A	6002	BCR	C3-C4-C5	-3.04	108.63	114.06
18	B	1225	CLA	C3D-C4D-ND	3.04	114.93	109.99
18	G	1003	CLA	C4D-C3D-CAD	3.04	111.41	108.11
18	B	1210	CLA	CAC-C3C-C4C	3.04	128.75	124.79
18	1	1013	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
18	B	1220	CLA	O2A-C1-C2	3.04	119.81	108.11
18	3	3018	CLA	CAC-C3C-C4C	3.04	128.75	124.79
18	1	1005	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
18	4	4006	CLA	C4D-C3D-CAD	3.04	111.41	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3007	CLA	C4D-C3D-CAD	3.04	111.40	108.11
18	B	1226	CLA	C1-C2-C3	-3.04	121.22	126.20
18	A	1128	CLA	O2A-C1-C2	3.04	119.79	108.11
18	A	1134	CLA	C2B-C1B-NB	3.04	113.47	110.33
18	1	1006	CLA	C4D-C3D-CAD	3.03	111.40	108.11
18	L	1501	CLA	O1D-CGD-CBD	-3.03	118.53	124.52
18	B	1221	CLA	C2B-C1B-NB	3.03	113.47	110.33
18	B	1234	CLA	C3D-C4D-ND	3.03	114.92	109.99
22	K	2011	BCR	C38-C26-C25	-3.03	121.18	124.48
18	A	1022	CLA	OBD-CAD-C3D	-3.03	121.33	128.42
18	2	2019	CLA	C3C-C4C-NC	3.03	112.57	109.92
18	2	2012	CLA	CMA-C3A-C4A	-3.03	103.63	111.77
18	3	3003	CLA	O2A-CGA-CBA	3.03	121.06	111.83
18	A	1104	CLA	CAA-C2A-C3A	-3.03	104.82	113.00
18	4	4001	CLA	CMA-C3A-C4A	-3.03	103.64	111.77
18	2	2004	CLA	C3D-C4D-ND	3.03	114.90	109.99
18	1	1001	CLA	C3C-C4C-NC	3.02	114.30	110.43
18	3	3002	CLA	CMD-C2D-C3D	-3.02	120.75	127.69
18	A	1118	CLA	C2B-C1B-NB	3.02	113.46	110.33
18	2	2012	CLA	C3D-C4D-ND	3.02	114.89	109.99
18	B	1205	CLA	C2B-C1B-NB	3.02	113.46	110.33
18	3	3002	CLA	C3D-C4D-ND	3.02	114.89	109.99
18	A	1121	CLA	C4-C3-C5	3.02	120.47	115.23
18	B	1203	CLA	C2B-C1B-NB	3.02	113.46	110.33
18	A	1135	CLA	C2B-C1B-NB	3.02	113.45	110.33
18	4	4004	CLA	C3D-C4D-ND	3.02	114.89	109.99
18	G	1001	CLA	C4D-C3D-CAD	3.01	111.38	108.11
18	4	4007	CLA	C1-O2A-CGA	3.01	123.94	116.65
18	A	1108	CLA	C3D-C4D-ND	3.01	114.88	109.99
21	1	1801	LHG	C6-C5-C4	-3.01	104.77	111.78
22	J	6012	BCR	C33-C5-C4	3.01	120.01	113.60
18	H	1000	CLA	C2B-C1B-NB	3.01	113.45	110.33
18	B	1208	CLA	C2B-C1B-NB	3.01	113.44	110.33
18	A	1103	CLA	CMC-C2C-C1C	3.01	129.73	125.03
18	B	1240	CLA	O2A-C1-C2	3.01	119.68	108.11
18	A	1139	CLA	C3D-C4D-ND	3.01	114.87	109.99
18	B	1219	CLA	C2B-C1B-NB	3.01	113.44	110.33
22	A	6003	BCR	C36-C18-C17	-3.01	117.95	122.82
18	1	1008	CLA	CHD-C1D-ND	-3.00	120.57	124.80
18	3	3012	CLA	CAA-C2A-C3A	-3.00	104.88	113.00
18	B	1220	CLA	CMB-C2B-C1B	3.00	129.99	125.42
18	3	3008	CLA	CHC-C1C-C2C	-3.00	118.42	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1218	CLA	C2B-C1B-NB	3.00	113.44	110.33
18	B	1012	CLA	CHD-C1D-ND	-3.00	120.58	124.80
18	F	1301	CLA	C3D-C4D-ND	3.00	114.87	109.99
18	B	1240	CLA	CMC-C2C-C1C	3.00	129.72	125.03
18	2	2009	CLA	C4D-C3D-CAD	3.00	111.36	108.11
22	L	6020	BCR	C38-C26-C25	-3.00	121.21	124.48
18	A	1101	CLA	C3D-C4D-ND	3.00	114.86	109.99
18	A	1122	CLA	CMB-C2B-C1B	3.00	129.99	125.42
18	G	1001	CLA	CAA-C2A-C1A	-3.00	102.15	111.97
18	2	2002	CLA	C3D-C4D-ND	3.00	114.86	109.99
18	K	1001	CLA	OBD-CAD-C3D	-3.00	121.41	128.42
18	4	4008	CLA	CAC-C3C-C4C	3.00	128.69	124.79
27	1	1502	LUT	C15-C35-C34	-3.00	117.39	123.52
18	3	3005	CLA	C4D-C3D-CAD	3.00	111.36	108.11
27	1	1502	LUT	C18-C5-C6	-2.99	121.22	124.48
18	A	1107	CLA	CMC-C2C-C1C	2.99	129.71	125.03
18	A	1120	CLA	C4-C3-C5	2.99	120.42	115.23
18	A	1123	CLA	CMC-C2C-C1C	2.99	129.70	125.03
28	2	2011	CHL	CMA-C3A-C4A	-2.99	108.17	114.61
22	L	6020	BCR	C8-C9-C10	2.99	123.71	119.01
22	A	6002	BCR	C38-C26-C27	2.99	119.97	113.60
18	A	1237	CLA	CMD-C2D-C3D	-2.99	120.84	127.69
18	A	1133	CLA	CMB-C2B-C1B	2.99	129.97	125.42
18	B	1210	CLA	C3D-C4D-ND	2.99	114.84	109.99
18	2	2004	CLA	C4B-CHC-C1C	2.99	133.27	126.25
18	1	1005	CLA	C3C-C4C-NC	2.99	114.25	110.43
18	A	1151	CLA	C2B-C1B-NB	2.99	113.42	110.33
18	A	1139	CLA	C1-C2-C3	-2.99	121.31	126.20
18	2	2005	CLA	C4-C3-C5	2.98	120.41	115.23
18	B	1234	CLA	CHD-C1D-ND	-2.98	120.60	124.80
18	B	1207	CLA	CAC-C3C-C4C	2.98	128.67	124.79
18	B	1216	CLA	CMC-C2C-C1C	2.98	129.69	125.03
27	I	6018	LUT	C8-C7-C6	-2.98	119.04	127.00
18	2	2008	CLA	C3D-C4D-ND	2.98	114.83	109.99
18	A	1140	CLA	C1-C2-C3	-2.98	121.32	126.20
18	B	1205	CLA	C3D-C4D-ND	2.98	114.83	109.99
18	A	1123	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
22	L	6019	BCR	C8-C9-C10	2.98	123.69	119.01
18	A	1140	CLA	C2B-C1B-NB	2.98	113.41	110.33
18	A	1112	CLA	C4-C3-C5	2.98	120.39	115.23
18	A	1123	CLA	C1-C2-C3	-2.97	121.32	126.20
18	3	3003	CLA	C1-C2-C3	-2.97	121.32	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	3502	LUT	C11-C10-C9	-2.97	123.11	127.28
18	B	1214	CLA	C4D-C3D-CAD	2.97	111.34	108.11
18	F	1302	CLA	C3D-C4D-ND	2.97	114.82	109.99
18	2	2002	CLA	CMB-C2B-C1B	2.97	129.94	125.42
18	A	1237	CLA	C4D-C3D-CAD	2.97	111.33	108.11
18	B	1231	CLA	C4D-C3D-CAD	2.97	111.33	108.11
18	G	1002	CLA	O1D-CGD-CBD	-2.97	118.66	124.52
18	G	1002	CLA	C3D-C4D-ND	2.97	114.82	109.99
18	1	1012	CLA	C4D-C3D-CAD	2.97	111.33	108.11
18	2	2009	CLA	C3D-C4D-ND	2.97	114.82	109.99
18	A	1115	CLA	C3D-C4D-ND	2.97	114.81	109.99
18	B	1220	CLA	C3D-C4D-ND	2.97	114.81	109.99
18	3	3012	CLA	C3D-C4D-ND	2.97	114.81	109.99
18	4	4008	CLA	CMB-C2B-C1B	2.97	129.94	125.42
18	4	4012	CLA	CMB-C2B-C1B	2.97	129.94	125.42
18	A	1105	CLA	C1-O2A-CGA	2.97	123.83	116.65
18	1	1014	CLA	C3D-C4D-ND	2.97	114.81	109.99
18	3	3012	CLA	O2A-C1-C2	2.97	119.52	108.11
18	2	2006	CLA	C3D-C4D-ND	2.96	114.80	109.99
22	L	6019	BCR	C37-C22-C21	-2.96	118.02	122.82
18	A	1131	CLA	C3D-C4D-ND	2.96	114.80	109.99
18	3	3002	CLA	CMB-C2B-C1B	2.96	129.93	125.42
18	A	1137	CLA	C2B-C1B-NB	2.96	113.39	110.33
18	B	1230	CLA	O1D-CGD-CBD	-2.96	118.69	124.52
22	F	6014	BCR	C34-C9-C10	-2.96	118.03	122.82
18	B	1202	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
18	B	1207	CLA	C3D-C4D-ND	2.96	114.79	109.99
18	A	1127	CLA	C2B-C1B-NB	2.96	113.39	110.33
18	A	1138	CLA	CED-O2D-CGD	2.95	122.62	115.92
18	A	1140	CLA	C3D-C4D-ND	2.95	114.79	109.99
18	1	1007	CLA	CMD-C2D-C3D	-2.95	120.92	127.69
18	G	1002	CLA	CMC-C2C-C1C	2.95	129.65	125.03
18	B	1212	CLA	C3D-C4D-ND	2.95	114.78	109.99
18	A	1114	CLA	C2B-C1B-NB	2.95	113.39	110.33
18	B	1231	CLA	CMC-C2C-C1C	2.95	129.65	125.03
23	F	5001	LMG	O7-C10-O9	-2.95	117.30	122.99
18	4	4009	CLA	O2A-C1-C2	2.95	119.46	108.11
18	B	1235	CLA	C3D-C4D-ND	2.95	114.78	109.99
18	3	3018	CLA	C2B-C1B-NB	2.95	113.38	110.33
18	4	4004	CLA	C1-C2-C3	-2.95	121.37	126.20
27	1	1501	LUT	C10-C11-C12	-2.95	114.66	123.20
18	B	1012	CLA	C4-C3-C5	2.95	120.34	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1205	CLA	C4D-C3D-CAD	2.95	111.31	108.11
18	L	1503	CLA	C3D-C4D-ND	2.94	114.77	109.99
18	B	1212	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
18	3	3001	CLA	C1-C2-C3	-2.94	122.00	126.76
18	L	1501	CLA	C4D-C3D-CAD	2.94	111.30	108.11
18	B	1213	CLA	C3D-C4D-ND	2.94	114.77	109.99
18	B	1230	CLA	C3D-C4D-ND	2.94	114.77	109.99
22	A	6002	BCR	C23-C22-C21	2.94	123.63	119.01
18	A	1105	CLA	C3D-C4D-ND	2.94	114.77	109.99
18	A	1125	CLA	C2B-C1B-NB	2.94	113.37	110.33
22	3	3503	BCR	C3-C4-C5	-2.94	108.81	114.06
28	2	2010	CHL	C1A-CHA-C4D	2.94	123.89	118.98
18	A	1117	CLA	C3D-C4D-ND	2.94	114.76	109.99
18	1	1003	CLA	CMB-C2B-C1B	2.93	129.89	125.42
18	2	2006	CLA	CAA-C2A-C3A	-2.93	105.07	113.00
18	B	1229	CLA	O2A-C1-C2	2.93	119.39	108.11
18	A	1137	CLA	CMC-C2C-C1C	2.93	129.62	125.03
18	A	1112	CLA	C3D-C4D-ND	2.93	114.75	109.99
18	B	1021	CLA	C3D-C4D-ND	2.93	114.75	109.99
18	A	1130	CLA	C3D-C4D-ND	2.93	114.75	109.99
22	B	6004	BCR	C37-C22-C21	-2.93	118.07	122.82
18	A	1022	CLA	C4-C3-C5	2.92	120.30	115.23
18	1	1003	CLA	C4D-C3D-CAD	2.92	111.28	108.11
18	1	1008	CLA	CMC-C2C-C1C	2.92	129.60	125.03
18	A	1121	CLA	C3D-C4D-ND	2.92	114.74	109.99
18	1	1014	CLA	C4D-C3D-CAD	2.92	111.28	108.11
18	B	1213	CLA	CMC-C2C-C1C	2.92	129.60	125.03
17	A	1011	CL0	CBC-CAC-C3C	-2.92	108.69	112.87
28	1	1009	CHL	C1-C2-C3	-2.92	121.41	126.20
18	B	1219	CLA	C3D-C4D-ND	2.92	114.73	109.99
20	A	5001	PQN	C11-C12-C13	-2.92	121.81	126.83
18	2	2012	CLA	CAA-C2A-C3A	-2.92	105.12	113.00
18	A	1120	CLA	C3D-C4D-ND	2.92	114.73	109.99
18	B	1231	CLA	C3D-C4D-ND	2.91	114.72	109.99
18	3	3002	CLA	OBD-CAD-C3D	-2.91	121.61	128.42
18	B	1216	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
18	G	1002	CLA	CMD-C2D-C3D	-2.91	121.01	127.69
18	4	4003	CLA	C4D-C3D-CAD	2.91	111.27	108.11
18	A	1127	CLA	C3D-C4D-ND	2.91	114.72	109.99
18	B	1230	CLA	CMC-C2C-C1C	2.91	129.58	125.03
18	A	1103	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
18	2	2016	CLA	CHD-C1D-ND	-2.91	120.71	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	3501	LUT	C17-C1-C6	-2.91	105.68	110.24
18	B	1240	CLA	C1-C2-C3	-2.91	121.43	126.20
22	B	6005	BCR	C23-C24-C25	-2.91	119.23	127.00
18	2	2007	CLA	C3D-C4D-ND	2.91	114.72	109.99
18	B	1216	CLA	C4-C3-C5	2.91	120.28	115.23
18	B	1212	CLA	C2B-C1B-NB	2.91	113.34	110.33
27	3	3502	LUT	C10-C11-C12	-2.91	114.77	123.20
18	3	3003	CLA	CHD-C1D-ND	-2.91	120.71	124.80
27	4	4502	LUT	C1-C2-C3	-2.91	107.22	113.59
18	1	1014	CLA	O1D-CGD-CBD	-2.91	118.78	124.52
18	G	1001	CLA	CMC-C2C-C1C	2.91	129.57	125.03
18	L	1502	CLA	C3D-C4D-ND	2.91	114.71	109.99
18	1	1005	CLA	C3D-C4D-ND	2.91	114.71	109.99
18	A	1137	CLA	C3D-C4D-ND	2.90	114.71	109.99
18	B	1209	CLA	C3D-C4D-ND	2.90	114.71	109.99
27	4	4501	LUT	C27-C28-C29	-2.90	120.08	126.32
22	I	6020	BCR	C3-C4-C5	-2.90	108.88	114.06
18	B	1021	CLA	CMA-C3A-C4A	-2.90	103.97	111.77
18	2	2002	CLA	CAC-C3C-C4C	2.90	128.57	124.79
18	B	1209	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
18	4	4006	CLA	CMC-C2C-C1C	2.90	129.57	125.03
18	A	1133	CLA	C3D-C4D-ND	2.90	114.70	109.99
18	3	3008	CLA	C3D-C4D-ND	2.90	114.70	109.99
18	B	1222	CLA	CAA-C2A-C3A	-2.90	105.16	113.00
18	A	1130	CLA	C1-C2-C3	-2.90	122.07	126.76
18	1	1011	CLA	C4D-C3D-CAD	2.90	111.26	108.11
22	F	6016	BCR	C38-C26-C25	-2.90	121.32	124.48
18	B	1226	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
18	B	1232	CLA	C3D-C4D-ND	2.90	114.70	109.99
18	3	3005	CLA	CHD-C1D-ND	-2.90	120.72	124.80
28	4	4010	CHL	C1A-CHA-C4D	2.90	123.82	118.98
18	A	1116	CLA	C3D-C4D-ND	2.90	114.69	109.99
18	F	1301	CLA	C4D-C3D-CAD	2.90	111.25	108.11
29	4	4505	ZEX	C38-C24-C25	-2.90	105.83	110.76
18	B	1227	CLA	C4-C3-C5	2.89	120.25	115.23
22	F	6016	BCR	C36-C18-C17	-2.89	118.13	122.82
18	4	4004	CLA	C2B-C1B-NB	2.89	113.32	110.33
18	B	1206	CLA	C1-C2-C3	-2.89	121.46	126.20
18	A	1133	CLA	C2B-C1B-NB	2.89	113.32	110.33
18	2	2009	CLA	CMD-C2D-C3D	-2.89	121.06	127.69
18	B	1221	CLA	CMC-C2C-C1C	2.89	129.55	125.03
18	A	1106	CLA	O2D-CGD-O1D	-2.89	118.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4017	CLA	C2B-C1B-NB	2.89	113.32	110.33
22	A	6007	BCR	C36-C18-C17	-2.89	118.14	122.82
18	A	1237	CLA	CMC-C2C-C1C	2.89	129.54	125.03
18	A	1135	CLA	C3D-C4D-ND	2.89	114.68	109.99
18	A	1107	CLA	C1-O2A-CGA	2.89	123.64	116.65
22	3	3503	BCR	C23-C24-C25	-2.88	119.29	127.00
18	A	1104	CLA	C2B-C1B-NB	2.88	113.32	110.33
18	B	1236	CLA	C3D-C4D-ND	2.88	114.67	109.99
18	B	1207	CLA	C2B-C1B-NB	2.88	113.31	110.33
18	A	1102	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
21	A	5003	LHG	O8-C23-C24	2.88	120.62	111.83
18	1	1013	CLA	C3D-C4D-ND	2.88	114.67	109.99
18	A	1124	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
18	B	1222	CLA	CMC-C2C-C1C	2.88	129.53	125.03
18	B	1215	CLA	C3D-C4D-ND	2.88	114.67	109.99
18	B	1218	CLA	CMC-C2C-C1C	2.88	129.53	125.03
18	A	1110	CLA	C3D-C4D-ND	2.88	114.66	109.99
18	B	1228	CLA	C3D-C4D-ND	2.88	114.66	109.99
18	2	2019	CLA	C3A-C4A-CHB	-2.88	120.39	123.91
18	B	1230	CLA	C2B-C1B-NB	2.88	113.31	110.33
18	1	1005	CLA	C4D-C3D-CAD	2.88	111.23	108.11
29	4	4505	ZEX	C17-C1-C6	-2.88	105.73	110.24
23	B	5005	LMG	O8-C28-C29	2.87	120.60	111.83
18	B	1218	CLA	C4D-C3D-CAD	2.87	111.23	108.11
18	A	1139	CLA	C4D-C3D-CAD	2.87	111.22	108.11
18	3	3012	CLA	CMA-C3A-C4A	-2.87	104.07	111.77
18	4	4006	CLA	O2A-C1-C2	2.87	119.14	108.11
18	A	1114	CLA	C3D-C4D-ND	2.87	114.64	109.99
18	B	1227	CLA	C4D-C3D-CAD	2.87	111.22	108.11
18	A	1237	CLA	C2B-C1B-NB	2.86	113.30	110.33
18	B	1236	CLA	C2B-C1B-NB	2.86	113.30	110.33
18	4	4012	CLA	C3D-C4D-ND	2.86	114.64	109.99
18	A	1134	CLA	C3D-C4D-ND	2.86	114.64	109.99
27	1	1502	LUT	C40-C33-C32	2.86	122.46	118.09
18	G	1002	CLA	C4D-C3D-CAD	2.86	111.21	108.11
21	1	1801	LHG	O8-C23-C24	2.86	120.56	111.83
18	B	1234	CLA	C4D-C3D-CAD	2.86	111.21	108.11
18	A	1109	CLA	C4-C3-C5	2.86	120.19	115.23
22	B	6004	BCR	C33-C5-C4	2.86	119.69	113.60
18	1	1011	CLA	CAC-C3C-C4C	2.86	128.51	124.79
18	2	2001	CLA	CMA-C3A-C4A	-2.86	104.09	111.77
18	1	1002	CLA	C4D-C3D-CAD	2.86	111.21	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1007	CLA	CMC-C2C-C1C	2.86	129.50	125.03
18	2	2003	CLA	CAC-C3C-C4C	2.86	128.51	124.79
18	B	1238	CLA	CMC-C2C-C1C	2.86	129.50	125.03
18	A	1104	CLA	C4-C3-C5	2.86	120.19	115.23
28	4	4010	CHL	CAA-CBA-CGA	2.86	121.32	113.21
18	2	2007	CLA	CMB-C2B-C1B	2.86	129.77	125.42
18	A	1103	CLA	C3D-C4D-ND	2.85	114.62	109.99
18	4	4016	CLA	CAC-C3C-C4C	2.85	128.50	124.79
18	1	1014	CLA	CMB-C2B-C1B	2.85	129.76	125.42
18	B	1210	CLA	C4D-C3D-CAD	2.85	111.20	108.11
18	A	1120	CLA	CMC-C2C-C1C	2.85	129.49	125.03
18	G	1003	CLA	CMC-C2C-C1C	2.85	129.49	125.03
18	B	1224	CLA	C4-C3-C5	2.85	120.17	115.23
18	3	3007	CLA	CAC-C3C-C4C	2.85	128.50	124.79
22	J	6013	BCR	C1-C6-C7	2.85	123.37	115.65
18	3	3003	CLA	O2A-C1-C2	2.84	119.05	108.11
22	F	6014	BCR	C34-C9-C8	2.84	122.43	118.09
18	A	1151	CLA	C3D-C4D-ND	2.84	114.61	109.99
27	3	3502	LUT	C22-C23-C24	-2.84	106.96	111.18
18	3	3013	CLA	CMC-C2C-C1C	2.84	129.48	125.03
22	A	6002	BCR	C37-C22-C21	-2.84	118.21	122.82
18	A	1136	CLA	C3D-C4D-ND	2.84	114.61	109.99
18	B	1239	CLA	C3D-C4D-ND	2.84	114.61	109.99
18	B	1208	CLA	CMC-C2C-C1C	2.84	129.47	125.03
18	2	2004	CLA	CMC-C2C-C1C	2.84	129.47	125.03
22	A	6017	BCR	C37-C22-C21	-2.84	118.22	122.82
22	B	6009	BCR	C36-C18-C17	-2.84	118.22	122.82
18	B	1239	CLA	CMC-C2C-C1C	2.84	129.47	125.03
18	A	1120	CLA	C4D-C3D-CAD	2.84	111.19	108.11
18	J	1302	CLA	C4D-C3D-CAD	2.84	111.19	108.11
18	A	1107	CLA	C4D-C3D-CAD	2.84	111.19	108.11
18	A	1102	CLA	CMC-C2C-C1C	2.84	129.47	125.03
18	J	1302	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
18	B	1215	CLA	CMC-C2C-C1C	2.83	129.46	125.03
22	A	6008	BCR	C36-C18-C17	-2.83	118.22	122.82
18	3	3005	CLA	CMB-C2B-C1B	2.83	129.73	125.42
18	1	1004	CLA	CMB-C2B-C1B	2.83	129.73	125.42
22	J	6012	BCR	C35-C13-C12	2.83	122.42	118.09
22	A	6011	BCR	C34-C9-C10	-2.83	118.23	122.82
18	4	4005	CLA	OBD-CAD-C3D	-2.83	121.80	128.42
18	3	3018	CLA	O2A-C1-C2	2.83	119.00	108.11
23	2	2802	LMG	O6-C1-C2	-2.83	104.55	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	3501	LUT	C18-C5-C4	2.83	119.62	114.42
18	4	4001	CLA	O2D-CGD-CBD	2.83	116.18	111.23
18	A	1133	CLA	CMC-C2C-C1C	2.83	129.46	125.03
22	J	6012	BCR	C31-C1-C6	-2.83	105.81	110.24
18	B	1212	CLA	CMB-C2B-C1B	2.83	129.73	125.42
18	4	4004	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
18	B	1012	CLA	O2A-C1-C2	2.83	118.99	108.11
27	4	4502	LUT	C8-C7-C6	-2.83	119.44	127.00
18	B	1217	CLA	C4D-C3D-CAD	2.83	111.18	108.11
18	4	4008	CLA	C4D-C3D-CAD	2.83	111.18	108.11
18	A	1106	CLA	CMC-C2C-C1C	2.83	129.45	125.03
22	3	3503	BCR	C23-C22-C21	2.83	123.45	119.01
18	B	1229	CLA	C3C-C4C-NC	2.83	114.05	110.43
18	4	4002	CLA	CMB-C2B-C1B	2.83	129.72	125.42
18	3	3006	CLA	O2A-C1-C2	2.83	118.98	108.11
18	A	1113	CLA	C3D-C4D-ND	2.83	114.58	109.99
22	A	6011	BCR	C23-C24-C25	-2.82	119.45	127.00
18	2	2008	CLA	CMC-C2C-C1C	2.82	129.45	125.03
18	G	1001	CLA	C3D-C4D-ND	2.82	114.58	109.99
18	A	1106	CLA	C3D-C4D-ND	2.82	114.58	109.99
18	B	1201	CLA	C3D-C4D-ND	2.82	114.58	109.99
18	H	1000	CLA	C3D-C4D-ND	2.82	114.57	109.99
22	3	3503	BCR	C31-C1-C6	-2.82	105.82	110.24
18	1	1012	CLA	CMB-C2B-C1B	2.82	129.72	125.42
18	4	4002	CLA	CBC-CAC-C3C	-2.82	104.77	112.42
27	4	4503	LUT	C27-C28-C29	-2.82	120.26	126.32
18	4	4012	CLA	C4D-C3D-CAD	2.82	111.17	108.11
22	F	6014	BCR	C36-C18-C17	-2.82	118.25	122.82
18	J	1302	CLA	CMB-C2B-C1B	2.82	129.71	125.42
18	B	1232	CLA	C4-C3-C5	2.82	120.12	115.23
27	2	2502	LUT	C8-C7-C6	-2.82	119.47	127.00
18	3	3019	CLA	C2D-C3D-C4D	2.82	108.48	106.08
18	B	1217	CLA	C3D-C4D-ND	2.82	114.56	109.99
18	B	1207	CLA	C4D-C3D-CAD	2.82	111.16	108.11
18	4	4009	CLA	CMB-C2B-C1B	2.81	129.70	125.42
22	L	6020	BCR	C38-C26-C27	2.81	119.59	113.60
18	A	1111	CLA	C1-C2-C3	-2.81	121.59	126.20
18	A	1125	CLA	C3C-C4C-NC	2.81	114.03	110.43
18	A	1113	CLA	CMB-C2B-C1B	2.81	129.70	125.42
22	A	6017	BCR	C12-C13-C14	2.81	123.43	119.01
18	1	1012	CLA	CMD-C2D-C3D	-2.81	121.26	127.69
18	B	1012	CLA	CMB-C2B-C1B	2.80	129.69	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1225	CLA	CMC-C2C-C1C	2.80	129.41	125.03
18	1	1003	CLA	C2B-C1B-NB	2.80	113.23	110.33
18	A	1104	CLA	CMC-C2C-C1C	2.80	129.41	125.03
18	3	3006	CLA	CMC-C2C-C1C	2.80	129.41	125.03
18	B	1230	CLA	C4D-C3D-CAD	2.80	111.15	108.11
18	1	1003	CLA	O2A-C1-C2	2.80	118.89	108.11
22	K	2011	BCR	C37-C22-C21	-2.80	118.28	122.82
18	2	2004	CLA	C4D-C3D-CAD	2.80	111.15	108.11
18	A	1131	CLA	CMC-C2C-C1C	2.80	129.41	125.03
22	A	6017	BCR	C8-C9-C10	2.80	123.41	119.01
22	J	6012	BCR	C36-C18-C17	-2.80	118.28	122.82
18	B	1239	CLA	C2B-C1B-NB	2.80	113.23	110.33
18	B	1208	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
21	A	5003	LHG	C5-O7-C7	-2.80	111.10	117.80
18	A	1108	CLA	CMC-C2C-C1C	2.80	129.41	125.03
28	2	2010	CHL	C1-O2A-CGA	2.80	125.02	116.07
18	A	1140	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
18	B	1238	CLA	C4D-C3D-CAD	2.79	111.14	108.11
18	A	1111	CLA	C3D-C4D-ND	2.79	114.53	109.99
18	A	1119	CLA	C3D-C4D-ND	2.79	114.53	109.99
22	F	6014	BCR	C19-C18-C17	2.79	123.40	119.01
18	3	3006	CLA	C2B-C1B-NB	2.79	113.22	110.33
27	I	6018	LUT	C30-C31-C32	-2.79	115.11	123.20
18	A	1136	CLA	C4D-C3D-CAD	2.79	111.14	108.11
18	A	1130	CLA	CMC-C2C-C1C	2.79	129.40	125.03
18	B	1216	CLA	C3D-C4D-ND	2.79	114.52	109.99
18	J	1302	CLA	C3D-C4D-ND	2.79	114.52	109.99
18	A	1104	CLA	C4D-C3D-CAD	2.79	111.13	108.11
18	B	1226	CLA	C4D-C3D-CAD	2.79	111.13	108.11
18	A	1129	CLA	CMC-C2C-C1C	2.79	129.39	125.03
18	B	1203	CLA	CMC-C2C-C1C	2.79	129.39	125.03
23	2	2802	LMG	C9-C8-C7	-2.79	105.29	111.78
18	B	1225	CLA	C2B-C1B-NB	2.79	113.22	110.33
18	B	1234	CLA	C2B-C1B-NB	2.79	113.22	110.33
28	3	3011	CHL	C4D-CHA-CBD	-2.79	106.16	108.97
18	A	1121	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
18	A	1123	CLA	C3D-C4D-ND	2.78	114.51	109.99
18	F	1302	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
18	3	3001	CLA	CMC-C2C-C1C	2.78	129.38	125.03
18	3	3018	CLA	C3D-C4D-ND	2.78	114.51	109.99
18	B	1230	CLA	CMB-C2B-C1B	2.78	129.66	125.42
18	B	1229	CLA	C3D-C4D-ND	2.78	114.51	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1235	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
27	3	3502	LUT	C18-C5-C4	2.78	119.53	114.42
18	A	1122	CLA	C3D-C4D-ND	2.78	114.51	109.99
18	3	3005	CLA	C3D-C4D-ND	2.78	114.51	109.99
18	B	1203	CLA	C3D-C4D-ND	2.78	114.50	109.99
18	B	1214	CLA	CMD-C2D-C3D	-2.78	121.32	127.69
28	1	1009	CHL	CMA-C3A-C4A	-2.78	108.63	114.61
18	B	1203	CLA	C4-C3-C5	2.77	120.04	115.23
18	A	1101	CLA	C4D-C3D-CAD	2.77	111.12	108.11
22	F	6016	BCR	C33-C5-C6	-2.77	121.46	124.48
18	L	1502	CLA	CMD-C2D-C3D	-2.77	121.33	127.69
18	3	3003	CLA	C1-O2A-CGA	2.77	123.36	116.65
29	4	4505	ZEX	O23-C23-C22	-2.77	103.52	109.97
23	F	5001	LMG	O6-C5-C4	-2.77	104.70	109.70
18	A	1013	CLA	CAA-C2A-C3A	-2.77	105.51	113.00
18	A	1131	CLA	C4-C3-C5	2.77	120.04	115.23
18	B	1023	CLA	C3D-C4D-ND	2.77	114.49	109.99
18	2	2006	CLA	C4D-C3D-CAD	2.77	111.11	108.11
22	L	6020	BCR	C39-C30-C25	-2.77	105.90	110.24
18	A	1135	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
18	2	2016	CLA	CMD-C2D-C3D	-2.77	121.34	127.69
22	F	6016	BCR	C2-C1-C6	2.77	114.46	110.44
18	F	1301	CLA	CMC-C2C-C1C	2.76	129.35	125.03
22	3	3503	BCR	C1-C6-C7	2.76	123.15	115.65
18	B	1218	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
22	L	6019	BCR	C29-C28-C27	2.76	117.35	111.28
18	A	1124	CLA	CMB-C2B-C1B	2.76	129.62	125.42
18	2	2009	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
18	B	1204	CLA	C4D-C3D-CAD	2.76	111.11	108.11
18	A	1138	CLA	C4D-C3D-CAD	2.76	111.10	108.11
18	2	2004	CLA	CMB-C2B-C1B	2.76	129.62	125.42
28	1	1009	CHL	C4D-CHA-CBD	-2.76	106.19	108.97
18	B	1012	CLA	C3C-C4C-NC	2.76	113.96	110.43
18	A	1102	CLA	C3D-C4D-ND	2.76	114.47	109.99
18	4	4003	CLA	CMC-C2C-C1C	2.76	129.34	125.03
18	2	2002	CLA	CMD-C2D-C3D	-2.76	121.37	127.69
18	A	1123	CLA	C4D-C3D-CAD	2.76	111.10	108.11
18	1	1001	CLA	C3D-C4D-ND	2.76	114.47	109.99
18	A	1105	CLA	C4D-C3D-CAD	2.76	111.10	108.11
18	B	1208	CLA	C4D-C3D-CAD	2.76	111.10	108.11
18	B	1223	CLA	CMB-C2B-C1B	2.76	129.62	125.42
18	B	1215	CLA	C4-C3-C5	2.75	120.01	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4009	CLA	C3D-C4D-ND	2.75	114.46	109.99
18	B	1012	CLA	C3D-C4D-ND	2.75	114.46	109.99
22	B	6006	BCR	C38-C26-C25	-2.75	121.48	124.48
18	A	1134	CLA	CMB-C2B-C1B	2.75	129.61	125.42
18	B	1225	CLA	C4D-C3D-CAD	2.75	111.09	108.11
22	B	6005	BCR	C33-C5-C6	-2.75	121.48	124.48
18	B	1238	CLA	C4-C3-C5	2.75	120.00	115.23
18	B	1203	CLA	CMB-C2B-C1B	2.75	129.60	125.42
18	B	1232	CLA	C4D-C3D-CAD	2.75	111.09	108.11
22	G	2011	BCR	C15-C14-C13	-2.75	123.42	127.28
18	A	1116	CLA	C4-C3-C5	2.75	120.00	115.23
18	4	4001	CLA	C4-C3-C5	2.75	120.00	115.23
18	B	1213	CLA	C4D-C3D-CAD	2.75	111.09	108.11
18	1	1006	CLA	CMB-C2B-C1B	2.75	129.60	125.42
18	3	3008	CLA	C3C-C4C-NC	2.75	113.95	110.43
18	A	1128	CLA	C4-C3-C5	2.75	119.99	115.23
18	3	3012	CLA	C2B-C1B-NB	2.75	113.17	110.33
18	G	1001	CLA	C1-C2-C3	-2.74	121.70	126.20
18	A	1132	CLA	CMC-C2C-C1C	2.74	129.32	125.03
18	J	1302	CLA	CMC-C2C-C1C	2.74	129.32	125.03
18	2	2003	CLA	C4-C3-C5	2.74	119.99	115.23
18	A	1013	CLA	C4-C3-C5	2.74	119.99	115.23
18	3	3005	CLA	C3C-C4C-NC	2.74	113.94	110.43
18	4	4007	CLA	CMC-C2C-C1C	2.74	129.32	125.03
18	A	1138	CLA	C1-C2-C3	-2.74	121.70	126.20
18	A	1122	CLA	C2B-C1B-NB	2.74	113.17	110.33
18	B	1221	CLA	C3D-C4D-ND	2.74	114.44	109.99
18	4	4012	CLA	CMC-C2C-C1C	2.74	129.32	125.03
17	A	1011	CL0	CMC-C2C-C1C	2.74	129.67	124.73
18	A	1116	CLA	CMC-C2C-C1C	2.74	129.32	125.03
18	F	1302	CLA	CMC-C2C-C1C	2.74	129.32	125.03
27	3	3502	LUT	C1-C6-C7	2.74	123.08	115.65
18	B	1240	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
18	B	1205	CLA	CMB-C2B-C1B	2.74	129.59	125.42
18	2	2016	CLA	C1-O2A-CGA	2.74	123.28	116.65
18	B	1222	CLA	C3D-C4D-ND	2.74	114.44	109.99
18	3	3018	CLA	CMC-C2C-C1C	2.74	129.31	125.03
18	A	1101	CLA	C4-C3-C5	2.74	119.98	115.23
28	4	4011	CHL	CMA-C3A-C4A	-2.74	108.72	114.61
18	2	2002	CLA	C4D-C3D-CAD	2.73	111.08	108.11
18	4	4006	CLA	CAC-C3C-C4C	2.73	128.35	124.79
18	B	1012	CLA	CMC-C2C-C1C	2.73	129.31	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2007	CLA	C4-C3-C5	2.73	119.97	115.23
18	3	3007	CLA	CMD-C2D-C3D	-2.73	121.43	127.69
18	A	1121	CLA	CMC-C2C-C1C	2.73	129.29	125.03
27	2	2501	LUT	C31-C30-C29	-2.73	123.45	127.28
22	B	6006	BCR	C35-C13-C12	2.73	122.25	118.09
18	A	1118	CLA	C3D-C4D-ND	2.72	114.42	109.99
18	A	1124	CLA	CMC-C2C-C1C	2.72	129.29	125.03
22	B	6006	BCR	C7-C6-C5	-2.72	115.28	121.56
18	4	4004	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
18	1	1012	CLA	CBC-CAC-C3C	-2.72	105.04	112.42
18	A	1107	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
18	B	1206	CLA	C3D-C4D-ND	2.72	114.41	109.99
18	A	1109	CLA	C3D-C4D-ND	2.72	114.41	109.99
18	B	1214	CLA	C3D-C4D-ND	2.72	114.41	109.99
18	B	1012	CLA	OBD-CAD-C3D	-2.72	122.06	128.42
18	4	4012	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
18	A	1114	CLA	C4D-C3D-CAD	2.72	111.06	108.11
18	B	1219	CLA	C4D-C3D-CAD	2.72	111.06	108.11
18	3	3007	CLA	CMB-C2B-C1B	2.72	129.56	125.42
23	4	4801	LMG	O7-C10-O9	-2.72	117.35	123.70
18	A	1112	CLA	C4D-C3D-CAD	2.72	111.06	108.11
22	B	6009	BCR	C37-C22-C21	-2.72	118.42	122.82
18	A	1127	CLA	C4-C3-C5	2.72	119.94	115.23
18	A	1131	CLA	C2B-C1B-NB	2.71	113.14	110.33
18	1	1005	CLA	OBD-CAD-C3D	-2.71	122.08	128.42
18	A	1136	CLA	C1-O2A-CGA	2.71	123.22	116.65
18	2	2003	CLA	C4D-C3D-CAD	2.71	111.05	108.11
18	2	2005	CLA	CMC-C2C-C1C	2.71	129.27	125.03
18	B	1223	CLA	C3C-C4C-NC	2.71	113.90	110.43
27	4	4502	LUT	C22-C23-C24	-2.71	107.16	111.18
18	A	1118	CLA	C4D-C3D-CAD	2.71	111.05	108.11
18	4	4017	CLA	CMB-C2B-C1B	2.71	129.55	125.42
22	G	2011	BCR	C29-C28-C27	2.71	117.23	111.28
28	4	4011	CHL	C4D-CHA-CBD	-2.71	106.24	108.97
27	3	3502	LUT	C27-C28-C29	-2.71	120.50	126.32
18	B	1219	CLA	CMC-C2C-C1C	2.71	129.27	125.03
18	B	1232	CLA	CMB-C2B-C1B	2.71	129.54	125.42
18	1	1011	CLA	O2A-C1-C2	2.71	118.53	108.11
18	1	1011	CLA	C5-C3-C4	2.71	120.82	114.59
27	2	2502	LUT	C10-C11-C12	-2.71	115.36	123.20
18	B	1023	CLA	C4-C3-C5	2.71	119.93	115.23
18	3	3013	CLA	C4D-C3D-CAD	2.71	111.04	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4008	CLA	CAA-C2A-C1A	-2.70	103.11	111.97
18	B	1202	CLA	C3D-C4D-ND	2.70	114.38	109.99
18	A	1120	CLA	CMB-C2B-C1B	2.70	129.53	125.42
18	A	1137	CLA	C4-C3-C5	2.70	119.92	115.23
18	B	1220	CLA	C1-C2-C3	-2.70	121.77	126.20
18	3	3010	CLA	C3D-C4D-ND	2.70	114.38	109.99
18	A	1111	CLA	CMC-C2C-C1C	2.70	129.25	125.03
18	1	1005	CLA	CAC-C3C-C4C	2.70	128.30	124.79
18	3	3017	CLA	C3D-C4D-ND	2.70	114.38	109.99
18	1	1013	CLA	CMC-C2C-C1C	2.70	129.25	125.03
18	A	1103	CLA	C4-C3-C5	2.70	119.91	115.23
18	4	4005	CLA	C3C-C4C-NC	2.70	113.89	110.43
18	A	1125	CLA	C4-C3-C5	2.70	119.91	115.23
18	1	1002	CLA	CBA-CAA-C2A	-2.70	105.77	113.79
18	4	4012	CLA	C2B-C1B-NB	2.70	113.12	110.33
18	4	4001	CLA	CMB-C2B-C1B	2.70	129.53	125.42
18	B	1206	CLA	C4-C3-C5	2.70	119.91	115.23
18	1	1008	CLA	CMB-C2B-C1B	2.70	129.52	125.42
18	B	1239	CLA	C4D-C3D-CAD	2.70	111.03	108.11
18	A	1113	CLA	CAA-C2A-C3A	-2.70	105.72	113.00
18	1	1005	CLA	CMC-C2C-C1C	2.70	129.25	125.03
18	3	3007	CLA	C2B-C1B-NB	2.70	113.12	110.33
18	B	1206	CLA	CMC-C2C-C1C	2.69	129.24	125.03
18	A	1110	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
27	2	2502	LUT	C37-C21-C36	2.69	111.79	107.87
18	A	1022	CLA	C3D-C4D-ND	2.69	114.36	109.99
18	A	1105	CLA	CMC-C2C-C1C	2.69	129.24	125.03
18	B	1210	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
18	A	1125	CLA	CMC-C2C-C1C	2.69	129.24	125.03
18	G	1003	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
18	B	1226	CLA	CMD-C2D-C3D	-2.69	121.52	127.69
18	4	4016	CLA	CMB-C2B-C1B	2.69	129.52	125.42
18	4	4002	CLA	CHA-C4D-ND	2.69	138.10	132.55
18	3	3003	CLA	CHC-C4B-NB	2.69	128.09	124.05
18	A	1139	CLA	CMB-C2B-C1B	2.69	129.51	125.42
28	2	2013	CHL	CMA-C3A-C4A	-2.69	108.82	114.61
18	B	1021	CLA	CMA-C3A-C2A	-2.69	103.60	113.98
22	A	6007	BCR	C38-C26-C27	2.69	119.32	113.60
18	A	1126	CLA	CMC-C2C-C1C	2.68	129.23	125.03
18	A	1135	CLA	CMC-C2C-C1C	2.68	129.23	125.03
18	3	3004	CLA	OBD-CAD-C3D	-2.68	122.14	128.42
23	4	4801	LMG	O8-C28-O10	-2.68	116.91	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1212	CLA	CMC-C2C-C1C	2.68	129.23	125.03
18	A	1133	CLA	C4-C3-C5	2.68	119.89	115.23
18	2	2008	CLA	CMA-C3A-C4A	-2.68	104.57	111.77
18	B	1226	CLA	C3D-C4D-ND	2.68	114.34	109.99
18	A	1118	CLA	CMC-C2C-C1C	2.68	129.22	125.03
18	B	1217	CLA	CMC-C2C-C1C	2.68	129.22	125.03
17	A	1011	CL0	CAA-C2A-C3A	-2.68	105.76	113.00
18	A	1135	CLA	C4D-C3D-CAD	2.68	111.02	108.11
18	B	1206	CLA	C4D-C3D-CAD	2.68	111.02	108.11
18	4	4002	CLA	C4D-C3D-CAD	2.68	111.02	108.11
18	2	2005	CLA	C4D-C3D-CAD	2.68	111.02	108.11
22	L	6020	BCR	C31-C1-C6	-2.68	106.04	110.24
18	A	1137	CLA	CMB-C2B-C1B	2.68	129.49	125.42
18	B	1209	CLA	C4D-C3D-CAD	2.67	111.01	108.11
18	A	1116	CLA	C4-C3-C2	-2.67	116.76	123.63
18	A	1121	CLA	C4D-C3D-CAD	2.67	111.01	108.11
18	1	1002	CLA	CMB-C2B-C1B	2.67	129.49	125.42
18	1	1007	CLA	C3D-C4D-ND	2.67	114.33	109.99
17	A	1011	CL0	O2D-CGD-O1D	-2.67	118.65	123.85
18	3	3007	CLA	CMC-C2C-C1C	2.67	129.21	125.03
18	A	1103	CLA	CAA-C2A-C3A	-2.67	105.78	113.00
18	2	2009	CLA	CMB-C2B-C1B	2.67	129.49	125.42
18	A	1237	CLA	CMB-C2B-C1B	2.67	129.48	125.42
18	4	4017	CLA	C3D-C4D-ND	2.67	114.33	109.99
18	A	1115	CLA	CMC-C2C-C1C	2.67	129.20	125.03
18	A	1013	CLA	CMC-C2C-C1C	2.67	129.20	125.03
18	A	1120	CLA	CMD-C2D-C3D	-2.67	121.57	127.69
23	G	2021	LMG	O8-C28-O10	-2.67	116.96	123.63
18	A	1117	CLA	C4-C3-C5	2.67	119.86	115.23
18	A	1022	CLA	C1-C2-C3	-2.67	121.83	126.20
18	2	2004	CLA	C1-O2A-CGA	2.66	123.10	116.65
18	2	2012	CLA	C1-C2-C3	-2.66	121.83	126.20
18	B	1201	CLA	C1-O2A-CGA	2.66	123.10	116.65
18	3	3017	CLA	CAC-C3C-C4C	2.66	128.25	124.79
27	1	1501	LUT	C7-C8-C9	-2.66	122.30	126.23
18	2	2009	CLA	CMC-C2C-C1C	2.66	129.19	125.03
18	4	4004	CLA	C4D-C3D-CAD	2.66	111.00	108.11
18	3	3017	CLA	CED-O2D-CGD	2.66	121.95	115.92
22	A	6007	BCR	C23-C22-C21	2.66	123.19	119.01
18	2	2001	CLA	C4-C3-C5	2.66	119.85	115.23
18	4	4016	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
18	B	1227	CLA	O2D-CGD-O1D	-2.66	118.67	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2004	CLA	CBC-CAC-C3C	-2.66	105.21	112.42
22	A	6007	BCR	C37-C22-C21	-2.66	118.51	122.82
18	4	4003	CLA	C4-C3-C5	2.66	119.84	115.23
18	2	2003	CLA	CMA-C3A-C4A	-2.66	104.64	111.77
18	1	1003	CLA	CAC-C3C-C4C	2.65	128.24	124.79
22	G	2011	BCR	C4-C5-C6	-2.65	119.12	122.70
18	B	1205	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
22	F	6016	BCR	C19-C18-C17	2.65	123.18	119.01
22	A	6017	BCR	C24-C23-C22	-2.65	122.32	126.23
18	A	1136	CLA	CMB-C2B-C1B	2.65	129.45	125.42
18	B	1235	CLA	C4-C3-C5	2.65	119.83	115.23
18	H	1000	CLA	C4D-C3D-CAD	2.65	110.98	108.11
18	A	1111	CLA	CAC-C3C-C4C	2.65	128.24	124.79
18	A	1113	CLA	CAC-C3C-C4C	2.65	128.23	124.79
18	1	1014	CLA	C3C-C4C-NC	2.65	113.82	110.43
18	2	2007	CLA	CMC-C2C-C1C	2.65	129.17	125.03
18	A	1128	CLA	C3D-C4D-ND	2.65	114.29	109.99
18	B	1224	CLA	C3D-C4D-ND	2.65	114.29	109.99
22	A	6007	BCR	C3-C4-C5	-2.65	109.34	114.06
18	A	1107	CLA	CMB-C2B-C1B	2.65	129.45	125.42
18	A	1127	CLA	C4D-C3D-CAD	2.65	110.98	108.11
18	B	1201	CLA	C4D-C3D-CAD	2.65	110.98	108.11
22	L	6020	BCR	C29-C28-C27	2.65	117.09	111.28
18	A	1117	CLA	C4D-C3D-CAD	2.65	110.98	108.11
22	A	6008	BCR	C38-C26-C27	2.65	119.24	113.60
27	2	2502	LUT	C15-C35-C34	-2.64	118.11	123.52
18	3	3004	CLA	CAA-C2A-C3A	-2.64	105.85	113.00
18	A	1117	CLA	CMC-C2C-C1C	2.64	129.17	125.03
18	A	1151	CLA	C4D-C3D-CAD	2.64	110.98	108.11
23	F	5002	LMG	O7-C10-O9	-2.64	117.53	123.70
25	B	7101	DGD	O5D-C6D-C5D	-2.64	103.47	109.42
17	A	1011	CL0	C4D-ND-C1D	-2.64	103.22	105.22
18	A	1125	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
18	B	1236	CLA	CMB-C2B-C1B	2.64	129.44	125.42
18	3	3010	CLA	C4D-C3D-CAD	2.64	110.97	108.11
18	F	1302	CLA	C4D-C3D-CAD	2.64	110.97	108.11
18	3	3012	CLA	OBD-CAD-C3D	-2.63	122.26	128.42
18	A	1118	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
18	L	1501	CLA	CMD-C2D-C3D	-2.63	121.65	127.69
18	1	1003	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
18	A	1122	CLA	C4D-C3D-CAD	2.63	110.96	108.11
18	B	1229	CLA	CMC-C2C-C1C	2.63	129.15	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1235	CLA	CMB-C2B-C1B	2.63	129.42	125.42
18	A	1134	CLA	CMC-C2C-C1C	2.63	129.14	125.03
18	B	1212	CLA	C4D-C3D-CAD	2.63	110.96	108.11
22	B	6010	BCR	C24-C23-C22	-2.63	122.35	126.23
18	A	1151	CLA	C3C-C4C-NC	2.63	113.79	110.43
18	4	4003	CLA	CMB-C2B-C1B	2.63	129.42	125.42
18	4	4008	CLA	CMA-C3A-C4A	-2.63	104.72	111.77
18	A	1131	CLA	CMB-C2B-C1B	2.63	129.42	125.42
18	F	1302	CLA	CMB-C2B-C1B	2.63	129.42	125.42
26	B	8002	LMU	C1'-O5'-C5'	2.62	118.85	113.72
23	F	5002	LMG	O8-C28-O10	-2.62	117.06	123.63
18	3	3008	CLA	CMD-C2D-C3D	-2.62	121.67	127.69
18	3	3003	CLA	CHC-C1C-C2C	-2.62	119.49	126.95
18	A	1115	CLA	CMB-C2B-C1B	2.62	129.41	125.42
18	B	1214	CLA	CMC-C2C-C1C	2.62	129.13	125.03
18	4	4017	CLA	CMC-C2C-C1C	2.62	129.13	125.03
18	B	1215	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
18	2	2005	CLA	C1-C2-C3	-2.62	121.90	126.20
18	B	1236	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
18	A	1109	CLA	CMC-C2C-C1C	2.62	129.13	125.03
18	A	1108	CLA	C4D-C3D-CAD	2.62	110.95	108.11
18	3	3010	CLA	C1-O2A-CGA	2.62	122.99	116.65
21	2	2801	LHG	O7-C7-C8	2.62	120.55	110.93
18	A	1013	CLA	C4D-C3D-CAD	2.62	110.95	108.11
22	B	6010	BCR	C36-C18-C17	-2.61	118.58	122.82
18	B	1227	CLA	CMD-C2D-C3D	-2.61	121.70	127.69
18	A	1103	CLA	CMB-C2B-C1B	2.61	129.40	125.42
18	4	4003	CLA	CMD-C2D-C3D	-2.61	121.70	127.69
18	1	1001	CLA	C2B-C1B-NB	2.61	113.03	110.33
18	G	1001	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
18	A	1139	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
27	2	2502	LUT	C37-C21-C26	-2.61	105.59	109.55
22	K	2011	BCR	C1-C6-C7	2.61	122.73	115.65
18	B	1229	CLA	CMB-C2B-C1B	2.61	129.39	125.42
18	4	4004	CLA	C4-C3-C5	2.61	119.75	115.23
23	4	4801	LMG	O2-C2-C3	-2.61	104.23	110.38
18	A	1114	CLA	CMB-C2B-C1B	2.61	129.39	125.42
18	G	1003	CLA	CMB-C2B-C1B	2.61	129.39	125.42
18	2	2012	CLA	O2A-C1-C2	2.61	118.14	108.11
18	2	2006	CLA	C4-C3-C5	2.61	119.75	115.23
18	B	1214	CLA	CMB-C2B-C1B	2.61	129.39	125.42
22	A	6011	BCR	C33-C5-C4	2.61	119.15	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1219	CLA	C4-C3-C5	2.61	119.75	115.23
18	4	4003	CLA	C2B-C1B-NB	2.61	113.03	110.33
18	B	1021	CLA	CAA-C2A-C3A	-2.60	105.96	113.00
18	2	2006	CLA	CMC-C2C-C1C	2.60	129.10	125.03
18	A	1022	CLA	C4D-C3D-CAD	2.60	110.93	108.11
18	B	1238	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
18	B	1229	CLA	C4-C3-C5	2.60	119.75	115.23
18	L	1501	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
28	2	2010	CHL	C4C-CHD-C1D	2.60	125.38	116.07
18	A	1119	CLA	CMC-C2C-C1C	2.60	129.10	125.03
18	B	1226	CLA	C4-C3-C5	2.60	119.74	115.23
18	3	3013	CLA	CMB-C2B-C1B	2.60	129.38	125.42
18	2	2002	CLA	CBC-CAC-C3C	-2.60	105.37	112.42
18	A	1126	CLA	CMB-C2B-C1B	2.60	129.38	125.42
18	1	1004	CLA	C4D-C3D-CAD	2.60	110.93	108.11
22	L	6020	BCR	C27-C26-C25	-2.60	119.19	122.70
18	2	2003	CLA	C3C-C4C-NC	2.60	113.76	110.43
18	B	1209	CLA	CMC-C2C-C1C	2.60	129.09	125.03
18	B	1227	CLA	CAA-C2A-C3A	-2.60	105.98	113.00
18	1	1004	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
18	B	1240	CLA	CMB-C2B-C1B	2.60	129.37	125.42
18	2	2016	CLA	CGD-CBD-CAD	-2.59	102.45	110.85
18	A	1130	CLA	C4D-C3D-CAD	2.59	110.92	108.11
18	B	1232	CLA	CMC-C2C-C1C	2.59	129.09	125.03
18	A	1138	CLA	C4-C3-C5	2.59	119.73	115.23
18	L	1502	CLA	C1-O2A-CGA	2.59	122.92	116.65
28	2	2010	CHL	CMA-C3A-C4A	-2.59	109.03	114.61
18	A	1124	CLA	C4-C3-C5	2.59	119.72	115.23
18	3	3003	CLA	C4-C3-C5	2.59	119.72	115.23
18	B	1204	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
18	L	1503	CLA	CAC-C3C-C4C	2.59	128.16	124.79
18	A	1138	CLA	CMC-C2C-C1C	2.59	129.08	125.03
22	B	6004	BCR	C38-C26-C27	2.59	119.11	113.60
18	1	1003	CLA	C4-C3-C5	2.59	119.72	115.23
22	B	6004	BCR	C38-C26-C25	-2.59	121.66	124.48
22	G	2011	BCR	C8-C7-C6	-2.59	120.08	127.00
18	B	1240	CLA	C4D-C3D-CAD	2.59	110.92	108.11
18	A	1114	CLA	CMC-C2C-C1C	2.59	129.08	125.03
18	B	1235	CLA	C4D-C3D-CAD	2.59	110.92	108.11
18	1	1011	CLA	O1D-CGD-CBD	-2.59	119.42	124.52
18	B	1216	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
28	4	4013	CHL	C4D-CHA-CBD	-2.58	106.36	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	1010	CHL	C4D-CHA-CBD	-2.58	106.36	108.97
26	B	8002	LMU	C1-O1'-C1'	-2.58	109.27	113.68
18	A	1124	CLA	C4D-C3D-CAD	2.58	110.91	108.11
18	B	1225	CLA	CMB-C2B-C1B	2.58	129.35	125.42
22	K	2011	BCR	C34-C9-C10	-2.58	118.63	122.82
18	A	1125	CLA	CMB-C2B-C1B	2.58	129.35	125.42
18	B	1221	CLA	C4D-C3D-CAD	2.58	110.91	108.11
18	L	1501	CLA	C2B-C1B-NB	2.58	113.00	110.33
18	3	3010	CLA	CMD-C2D-C3D	-2.58	121.77	127.69
18	A	1140	CLA	CMC-C2C-C1C	2.58	129.06	125.03
18	B	1021	CLA	C4D-C3D-CAD	2.58	110.91	108.11
18	B	1211	CLA	C4-C3-C5	2.58	119.70	115.23
22	B	6004	BCR	C27-C26-C25	-2.58	119.22	122.70
28	4	4010	CHL	C1-O2A-CGA	2.58	124.32	116.07
18	A	1126	CLA	C3D-C4D-ND	2.58	114.17	109.99
25	B	7101	DGD	CDB-CCB-CBB	-2.57	101.35	114.37
18	A	1101	CLA	CMC-C2C-C1C	2.57	129.06	125.03
18	A	1116	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
18	4	4002	CLA	C1-O2A-CGA	2.57	122.88	116.65
18	B	1207	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
18	A	1129	CLA	C3C-C4C-NC	2.57	113.72	110.43
18	B	1226	CLA	CAC-C3C-C4C	2.57	128.13	124.79
18	3	3005	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
18	A	1129	CLA	C4D-C3D-CAD	2.57	110.90	108.11
18	A	1110	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
18	A	1121	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
18	B	1221	CLA	C1-C2-C3	-2.57	121.99	126.20
29	4	4505	ZEX	C16-C1-C6	-2.57	106.21	110.24
18	3	3008	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
18	A	1109	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
18	A	1112	CLA	CMC-C2C-C1C	2.57	129.05	125.03
18	B	1210	CLA	CMB-C2B-C1B	2.57	129.33	125.42
18	B	1211	CLA	CMB-C2B-C1B	2.57	129.33	125.42
18	B	1222	CLA	C3C-C4C-NC	2.57	113.72	110.43
22	I	6020	BCR	C38-C26-C27	2.57	119.07	113.60
18	A	1129	CLA	CMB-C2B-C1B	2.57	129.33	125.42
18	B	1218	CLA	CMB-C2B-C1B	2.57	129.33	125.42
28	2	2010	CHL	C4D-CHA-CBD	-2.57	106.38	108.97
18	4	4008	CLA	C3D-C4D-ND	2.57	114.16	109.99
18	A	1114	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
18	A	1108	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
18	A	1127	CLA	O2D-CGD-O1D	-2.57	118.85	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3001	CLA	C1-O2A-CGA	2.56	122.86	116.65
18	A	1123	CLA	CAC-C3C-C4C	2.56	128.13	124.79
18	B	1023	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
18	B	1225	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
18	B	1234	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
28	4	4010	CHL	C4C-CHD-C1D	2.56	125.24	116.07
28	1	1009	CHL	C1C-C2C-CMC	2.56	131.42	126.80
18	A	1022	CLA	CMC-C2C-C1C	2.56	129.04	125.03
18	A	1106	CLA	C4D-C3D-CAD	2.56	110.88	108.11
18	A	1128	CLA	C2B-C1B-NB	2.56	112.98	110.33
18	B	1204	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
27	1	1501	LUT	C35-C34-C33	-2.55	123.70	127.28
22	A	6008	BCR	C19-C18-C17	2.55	123.03	119.01
18	B	1236	CLA	C1-O2A-CGA	2.55	122.83	116.65
18	B	1217	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
18	4	4005	CLA	CMC-C2C-C1C	2.55	129.02	125.03
18	2	2012	CLA	CAC-C3C-C4C	2.55	128.11	124.79
18	B	1212	CLA	C4-C3-C5	2.55	119.66	115.23
18	A	1140	CLA	C1-O2A-CGA	2.55	122.83	116.65
22	I	6020	BCR	C36-C18-C17	-2.55	118.68	122.82
18	B	1203	CLA	C4D-C3D-CAD	2.55	110.88	108.11
18	1	1008	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
18	B	1023	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
18	2	2005	CLA	CMB-C2B-C1B	2.55	129.30	125.42
18	4	4009	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
18	A	1102	CLA	C3C-C4C-NC	2.55	113.69	110.43
18	1	1004	CLA	CMC-C2C-C1C	2.55	129.01	125.03
18	A	1121	CLA	CMB-C2B-C1B	2.55	129.30	125.42
18	A	1131	CLA	C4D-C3D-CAD	2.55	110.87	108.11
18	B	1023	CLA	C4D-C3D-CAD	2.55	110.87	108.11
18	2	2006	CLA	CMB-C2B-C1B	2.55	129.29	125.42
18	A	1118	CLA	CMB-C2B-C1B	2.54	129.29	125.42
18	B	1201	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
22	3	3503	BCR	C30-C25-C26	-2.54	119.16	122.64
18	1	1012	CLA	O2A-C1-C2	2.54	117.89	108.11
18	B	1206	CLA	C2B-C1B-NB	2.54	112.96	110.33
18	B	1228	CLA	C4D-C3D-CAD	2.54	110.87	108.11
18	B	1021	CLA	C4-C3-C5	2.54	119.64	115.23
27	1	1501	LUT	O23-C23-C22	2.54	114.56	110.06
18	A	1137	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
18	A	1116	CLA	CMB-C2B-C1B	2.54	129.29	125.42
18	A	1022	CLA	C3C-C4C-NC	2.54	113.69	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	1000	CLA	CMC-C2C-C1C	2.54	129.00	125.03
18	3	3002	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
18	B	1239	CLA	CMB-C2B-C1B	2.54	129.28	125.42
18	F	1302	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
18	1	1001	CLA	CMC-C2C-C1C	2.54	129.00	125.03
18	A	1113	CLA	C4D-C3D-CAD	2.54	110.86	108.11
27	4	4501	LUT	C19-C9-C8	2.54	121.97	118.09
18	B	1240	CLA	C4-C3-C5	2.54	119.63	115.23
18	B	1208	CLA	CMB-C2B-C1B	2.54	129.28	125.42
18	A	1123	CLA	C4-C3-C5	2.54	119.63	115.23
18	1	1004	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
18	A	1101	CLA	CAC-C3C-C4C	2.54	128.09	124.79
18	B	1239	CLA	C4-C3-C5	2.53	119.63	115.23
18	A	1116	CLA	C4D-C3D-CAD	2.53	110.86	108.11
27	2	2502	LUT	C36-C21-C26	-2.53	105.71	109.55
18	A	1129	CLA	C3D-C4D-ND	2.53	114.11	109.99
18	A	1122	CLA	CMC-C2C-C1C	2.53	128.99	125.03
18	3	3010	CLA	CMC-C2C-C1C	2.53	128.99	125.03
18	A	1013	CLA	CAA-C2A-C1A	-2.53	103.67	111.97
18	2	2007	CLA	C4D-C3D-CAD	2.53	110.86	108.11
18	3	3002	CLA	CAA-CBA-CGA	-2.53	106.02	113.21
29	4	4505	ZEX	C18-C5-C4	2.53	119.08	114.42
18	A	1111	CLA	C4-C3-C5	2.53	119.62	115.23
18	L	1501	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
18	F	1302	CLA	C2B-C1B-NB	2.53	112.95	110.33
18	B	1240	CLA	CMD-C2D-C3D	-2.53	121.89	127.69
27	2	2501	LUT	C11-C10-C9	-2.53	123.73	127.28
22	B	6004	BCR	C23-C22-C21	2.53	122.99	119.01
18	B	1234	CLA	C4-C3-C5	2.53	119.61	115.23
18	A	1138	CLA	C1-O2A-CGA	2.53	122.77	116.65
22	L	6019	BCR	C40-C30-C25	2.53	114.20	110.24
18	B	1231	CLA	CMD-C2D-C3D	-2.53	121.90	127.69
18	B	1204	CLA	CMB-C2B-C1B	2.53	129.26	125.42
18	3	3003	CLA	CMD-C2D-C3D	-2.53	121.90	127.69
18	B	1215	CLA	C4D-C3D-CAD	2.53	110.85	108.11
18	B	1023	CLA	CED-O2D-CGD	2.52	121.64	115.92
18	B	1201	CLA	CAC-C3C-C4C	2.52	128.07	124.79
22	I	6020	BCR	C23-C24-C25	-2.52	120.25	127.00
18	4	4005	CLA	C4-C3-C5	2.52	119.61	115.23
22	3	3503	BCR	C1-C6-C5	-2.52	119.19	122.64
18	2	2008	CLA	C3C-C4C-NC	2.52	113.66	110.43
18	B	1224	CLA	C4D-C3D-CAD	2.52	110.85	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1126	CLA	CAC-C3C-C4C	2.52	128.07	124.79
23	4	4801	LMG	O6-C1-C2	-2.52	105.19	110.37
18	K	1001	CLA	C2B-C1B-NB	2.52	112.94	110.33
18	A	1237	CLA	C4-C3-C5	2.52	119.61	115.23
18	A	1132	CLA	C4-C3-C5	2.52	119.61	115.23
18	A	1136	CLA	CMC-C2C-C1C	2.52	128.97	125.03
18	A	1119	CLA	C4-C3-C5	2.52	119.61	115.23
18	B	1228	CLA	C4-C3-C5	2.52	119.61	115.23
22	K	2011	BCR	C38-C26-C27	2.52	118.97	113.60
27	I	6018	LUT	C20-C13-C12	2.52	121.94	118.09
18	4	4003	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
18	A	1122	CLA	C4-C3-C2	-2.51	117.17	123.63
18	2	2012	CLA	C4D-C3D-CAD	2.51	110.84	108.11
18	A	1101	CLA	CMD-C2D-C3D	-2.51	121.92	127.69
18	A	1124	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
18	A	1102	CLA	C4D-C3D-CAD	2.51	110.84	108.11
18	A	1125	CLA	C4D-C3D-CAD	2.51	110.83	108.11
18	A	1134	CLA	C4-C3-C5	2.51	119.59	115.23
18	A	1136	CLA	C4-C3-C5	2.51	119.59	115.23
18	A	1110	CLA	C4D-C3D-CAD	2.51	110.83	108.11
18	4	4009	CLA	C4D-C3D-CAD	2.51	110.83	108.11
18	A	1138	CLA	O2A-C1-C2	2.51	117.77	108.11
18	A	1134	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
18	B	1206	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
21	2	2801	LHG	O8-C23-C24	2.51	119.49	111.83
18	B	1205	CLA	CMC-C2C-C1C	2.51	128.95	125.03
18	A	1114	CLA	CAC-C3C-C4C	2.51	128.05	124.79
22	B	6009	BCR	C34-C9-C10	-2.51	118.75	122.82
18	4	4003	CLA	CAC-C3C-C4C	2.51	128.05	124.79
18	A	1117	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
18	B	1221	CLA	O1D-CGD-CBD	-2.51	119.58	124.52
18	2	2001	CLA	CBC-CAC-C3C	-2.51	105.63	112.42
18	1	1003	CLA	C1-O2A-CGA	2.50	122.71	116.65
18	4	4016	CLA	C2B-C1B-NB	2.50	112.92	110.33
18	K	1001	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
18	3	3002	CLA	CMC-C2C-C1C	2.50	128.95	125.03
18	2	2005	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
18	A	1111	CLA	C4D-C3D-CAD	2.50	110.82	108.11
18	4	4002	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
18	B	1230	CLA	CAA-CBA-CGA	-2.50	106.10	113.21
18	B	1220	CLA	CMC-C2C-C1C	2.50	128.94	125.03
22	3	3503	BCR	C29-C28-C27	2.50	116.78	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	6006	BCR	C24-C23-C22	-2.50	122.54	126.23
18	A	1132	CLA	CMB-C2B-C1B	2.50	129.23	125.42
18	A	1104	CLA	C3C-C4C-NC	2.50	113.63	110.43
18	3	3010	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
18	G	1003	CLA	C1-O2A-CGA	2.50	122.70	116.65
18	A	1140	CLA	CMB-C2B-C1B	2.50	129.22	125.42
18	B	1222	CLA	C4D-C3D-CAD	2.50	110.82	108.11
18	2	2004	CLA	CMD-C2D-C3D	-2.50	121.97	127.69
18	4	4012	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
22	K	2011	BCR	C23-C22-C21	2.49	122.93	119.01
18	4	4005	CLA	C4-C3-C2	-2.49	117.22	123.63
18	1	1008	CLA	C4D-C3D-CAD	2.49	110.81	108.11
18	2	2009	CLA	CMA-C3A-C4A	-2.49	105.07	111.77
18	2	2004	CLA	C4-C3-C5	2.49	119.55	115.23
18	A	1115	CLA	C4D-C3D-CAD	2.49	110.81	108.11
18	B	1209	CLA	CAC-C3C-C4C	2.49	128.03	124.79
18	A	1108	CLA	CED-O2D-CGD	2.49	121.56	115.92
18	B	1205	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
18	B	1204	CLA	CMC-C2C-C1C	2.49	128.92	125.03
18	A	1107	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
18	B	1207	CLA	C4-C3-C5	2.49	119.55	115.23
18	1	1011	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
22	L	6019	BCR	C38-C26-C25	-2.49	121.77	124.48
18	1	1007	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
18	B	1210	CLA	CMD-C2D-C3D	-2.49	121.99	127.69
18	A	1133	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
29	4	4505	ZEX	C20-C13-C12	2.48	121.88	118.09
18	A	1122	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
18	3	3018	CLA	CGD-CBD-CAD	-2.48	102.81	110.85
27	4	4501	LUT	C37-C21-C26	-2.48	105.78	109.55
22	B	6005	BCR	C30-C25-C26	-2.48	119.24	122.64
18	A	1132	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
18	A	1127	CLA	CMC-C2C-C1C	2.48	128.91	125.03
18	F	1301	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
27	2	2501	LUT	C38-C25-C24	-2.48	117.49	123.36
18	2	2019	CLA	C2D-C3D-C4D	2.48	108.19	106.08
18	1	1008	CLA	CHC-C1C-C2C	-2.48	119.90	126.95
27	2	2501	LUT	C35-C34-C33	-2.48	123.80	127.28
18	3	3007	CLA	C1-O2A-CGA	2.48	122.65	116.65
18	4	4007	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
18	B	1230	CLA	C3C-C4C-NC	2.48	113.60	110.43
18	K	1001	CLA	CMC-C2C-C1C	2.48	128.90	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	6016	BCR	C8-C7-C6	-2.47	120.39	127.00
29	4	4505	ZEX	C19-C9-C10	-2.47	118.81	122.82
18	2	2001	CLA	C2B-C1B-NB	2.47	112.89	110.33
18	3	3008	CLA	C1D-CHD-C4C	-2.47	120.76	126.02
18	A	1140	CLA	C4D-C3D-CAD	2.47	110.79	108.11
28	1	1009	CHL	C4C-CHD-C1D	2.47	124.92	116.07
18	4	4008	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
18	3	3003	CLA	OBD-CAD-C3D	-2.47	122.64	128.42
18	3	3008	CLA	C1-O2A-CGA	2.47	122.63	116.65
18	3	3012	CLA	CMC-C2C-C1C	2.47	128.90	125.03
27	I	6018	LUT	C12-C13-C14	-2.47	115.12	119.01
18	2	2008	CLA	CMB-C2B-C1B	2.47	129.18	125.42
18	A	1126	CLA	C4D-C3D-CAD	2.47	110.79	108.11
18	B	1012	CLA	C4D-C3D-CAD	2.47	110.79	108.11
18	B	1231	CLA	CMB-C2B-C1B	2.47	129.18	125.42
18	A	1107	CLA	C1-C2-C3	-2.47	122.16	126.20
18	1	1012	CLA	C2B-C1B-NB	2.47	112.88	110.33
27	3	3502	LUT	C19-C9-C10	-2.46	118.82	122.82
18	1	1001	CLA	C4D-C3D-CAD	2.46	110.78	108.11
18	A	1114	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
18	A	1105	CLA	CMB-C2B-C1B	2.46	129.16	125.42
22	B	6009	BCR	C33-C5-C4	2.46	118.84	113.60
18	A	1128	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
22	B	6005	BCR	C37-C22-C21	-2.46	118.83	122.82
18	B	1228	CLA	CED-O2D-CGD	2.46	121.49	115.92
21	A	7001	LHG	C5-O7-C7	-2.46	111.92	117.80
18	A	1134	CLA	C4D-C3D-CAD	2.46	110.77	108.11
18	4	4005	CLA	CHC-C1C-C2C	-2.46	119.97	126.95
18	A	1151	CLA	CMB-C2B-C1B	2.46	129.16	125.42
18	3	3006	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
18	1	1013	CLA	CHC-C1C-C2C	-2.45	119.97	126.95
18	G	1003	CLA	C2B-C1B-NB	2.45	112.87	110.33
18	4	4009	CLA	C2B-C1B-NB	2.45	112.87	110.33
18	B	1216	CLA	C3C-C4C-NC	2.45	113.57	110.43
18	B	1211	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
18	A	1110	CLA	CMC-C2C-C1C	2.45	128.87	125.03
18	B	1214	CLA	C4-C3-C5	2.45	119.48	115.23
18	L	1502	CLA	C2B-C1B-NB	2.45	112.87	110.33
17	A	1011	CL0	C4-C3-C5	2.45	119.48	115.23
18	B	1212	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
22	F	6014	BCR	C29-C28-C27	2.45	116.66	111.28
18	A	1129	CLA	O2D-CGD-O1D	-2.45	119.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1111	CLA	CMB-C2B-C1B	2.45	129.15	125.42
18	A	1125	CLA	C1-O2A-CGA	2.45	122.58	116.65
18	A	1106	CLA	C4-C3-C5	2.45	119.48	115.23
18	B	1210	CLA	C4-C3-C5	2.45	119.47	115.23
18	2	2006	CLA	CMD-C2D-C3D	-2.44	122.08	127.69
18	B	1236	CLA	C3C-C4C-NC	2.44	113.56	110.43
18	G	1001	CLA	CHC-C1C-C2C	-2.44	120.00	126.95
27	4	4501	LUT	C35-C15-C14	-2.44	118.52	123.52
18	B	1238	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
18	A	1123	CLA	C3C-C4C-NC	2.44	113.56	110.43
18	B	1218	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
18	B	1217	CLA	CMB-C2B-C1B	2.44	129.14	125.42
18	4	4006	CLA	CMB-C2B-C1B	2.44	129.14	125.42
18	3	3013	CLA	OBD-CAD-C3D	-2.44	122.71	128.42
18	4	4005	CLA	C6-C5-C3	-2.44	107.52	113.47
18	B	1212	CLA	C3C-C4C-NC	2.44	113.56	110.43
18	B	1224	CLA	CMB-C2B-C1B	2.44	129.14	125.42
18	A	1116	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
18	B	1223	CLA	CMC-C2C-C1C	2.44	128.85	125.03
18	A	1013	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
18	B	1023	CLA	CMB-C2B-C1B	2.44	129.14	125.42
18	B	1221	CLA	C6-C5-C3	-2.44	107.52	113.47
18	4	4002	CLA	C3C-C4C-NC	2.44	113.56	110.43
18	2	2016	CLA	C5-C3-C4	2.44	120.21	114.59
18	G	1001	CLA	C2B-C1B-NB	2.44	112.86	110.33
18	A	1126	CLA	C4-C3-C5	2.44	119.46	115.23
22	B	6009	BCR	C38-C26-C27	2.44	118.80	113.60
18	4	4005	CLA	C3D-C4D-ND	2.44	113.95	109.99
18	A	1022	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
18	A	1130	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
18	A	1119	CLA	C4D-C3D-CAD	2.44	110.75	108.11
18	B	1210	CLA	CMC-C2C-C1C	2.44	128.84	125.03
22	J	6012	BCR	C8-C9-C10	2.44	122.84	119.01
18	G	1003	CLA	OBD-CAD-C3D	-2.44	122.72	128.42
18	2	2009	CLA	C2B-C1B-NB	2.44	112.85	110.33
23	J	5001	LMG	O4-C4-C5	-2.44	103.33	109.32
18	B	1202	CLA	C4D-C3D-CAD	2.44	110.75	108.11
18	B	1221	CLA	CMB-C2B-C1B	2.44	129.13	125.42
18	B	1232	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
18	L	1502	CLA	C3C-C4C-NC	2.43	113.55	110.43
18	B	1219	CLA	C3C-C4C-NC	2.43	113.55	110.43
18	A	1103	CLA	CMD-C2D-C3D	-2.43	122.11	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4005	CLA	CAC-C3C-C4C	2.43	127.95	124.79
18	A	1119	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
18	B	1208	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
18	3	3004	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
18	4	4005	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
18	1	1014	CLA	CAA-CBA-CGA	-2.43	106.31	113.21
18	B	1239	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
18	B	1229	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
18	4	4002	CLA	CMC-C2C-C1C	2.43	128.83	125.03
18	A	1112	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
27	3	3501	LUT	C26-C27-C28	-2.43	120.80	124.58
18	A	1113	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
18	2	2004	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
18	A	1134	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
18	A	1135	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
18	A	1126	CLA	CAA-CBA-CGA	-2.43	106.32	113.21
18	4	4008	CLA	CHC-C1C-C2C	-2.43	120.05	126.95
18	B	1225	CLA	C3C-C4C-NC	2.43	113.54	110.43
18	4	4017	CLA	C4D-C3D-CAD	2.43	110.74	108.11
22	B	6004	BCR	C30-C25-C24	2.43	122.23	115.65
18	4	4016	CLA	CMC-C2C-C1C	2.43	128.82	125.03
18	B	1229	CLA	C4D-C3D-CAD	2.43	110.74	108.11
18	1	1014	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
22	A	6008	BCR	C30-C25-C26	-2.42	119.32	122.64
18	3	3012	CLA	C5-C3-C4	2.42	120.17	114.59
27	4	4502	LUT	C10-C11-C12	-2.42	116.18	123.20
18	H	1000	CLA	CAC-C3C-C4C	2.42	127.94	124.79
18	B	1223	CLA	C4D-C3D-CAD	2.42	110.74	108.11
18	4	4008	CLA	OBD-CAD-C3D	-2.42	122.75	128.42
18	B	1222	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
18	3	3003	CLA	C3C-C4C-NC	2.42	113.53	110.43
21	A	7001	LHG	O8-C23-O10	-2.42	117.57	123.63
18	J	1302	CLA	CBA-CAA-C2A	-2.42	106.59	113.79
18	4	4002	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
18	A	1117	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
18	A	1133	CLA	C4D-C3D-CAD	2.42	110.73	108.11
18	2	2006	CLA	C2B-C1B-NB	2.42	112.83	110.33
18	A	1137	CLA	C4D-C3D-CAD	2.42	110.73	108.11
18	2	2001	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
22	A	6002	BCR	C30-C25-C26	-2.42	119.33	122.64
22	B	6004	BCR	C1-C6-C7	2.42	122.20	115.65
18	4	4012	CLA	C1-O2A-CGA	2.42	122.50	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1137	CLA	C3C-C4C-NC	2.42	113.53	110.43
18	H	1000	CLA	CMD-C2D-C3D	-2.42	122.15	127.69
22	A	6008	BCR	C34-C9-C10	-2.42	118.90	122.82
18	B	1239	CLA	CMD-C2D-C3D	-2.41	122.15	127.69
18	A	1104	CLA	CMB-C2B-C1B	2.41	129.10	125.42
18	B	1222	CLA	CED-O2D-CGD	2.41	121.39	115.92
18	1	1006	CLA	C1-O2A-CGA	2.41	122.50	116.65
18	A	1138	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
18	B	1226	CLA	CMC-C2C-C1C	2.41	128.81	125.03
18	1	1012	CLA	CMC-C2C-C1C	2.41	128.81	125.03
18	3	3002	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
18	B	1235	CLA	C3C-C4C-NC	2.41	113.52	110.43
18	G	1001	CLA	CMB-C2B-C1B	2.41	129.09	125.42
18	3	3003	CLA	CHA-C4D-ND	2.41	137.52	132.55
18	A	1118	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
27	I	6018	LUT	C27-C28-C29	-2.41	121.14	126.32
22	A	6008	BCR	C37-C22-C21	-2.41	118.91	122.82
18	B	1211	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
27	I	6018	LUT	C40-C33-C32	2.41	121.77	118.09
18	A	1128	CLA	CAA-C2A-C3A	-2.41	106.49	113.00
18	G	1001	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
28	1	1010	CHL	CMA-C3A-C4A	-2.41	109.42	114.61
18	B	1202	CLA	CMC-C2C-C1C	2.41	128.80	125.03
18	B	1207	CLA	CMB-C2B-C1B	2.41	129.08	125.42
18	A	1151	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
18	L	1501	CLA	CMB-C2B-C1B	2.41	129.08	125.42
22	B	6005	BCR	C24-C23-C22	-2.40	122.68	126.23
18	A	1107	CLA	C4-C3-C5	2.40	119.40	115.23
22	J	6012	BCR	C39-C30-C25	-2.40	106.47	110.24
18	2	2008	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
18	B	1217	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
18	B	1216	CLA	C4D-C3D-CAD	2.40	110.71	108.11
18	4	4004	CLA	C4B-CHC-C1C	2.40	131.89	126.25
18	4	4004	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
18	A	1103	CLA	C4D-C3D-CAD	2.40	110.71	108.11
18	A	1136	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
18	2	2008	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
18	B	1220	CLA	C4D-C3D-CAD	2.40	110.71	108.11
18	1	1006	CLA	C5-C3-C4	2.40	120.11	114.59
18	A	1103	CLA	CAC-C3C-C4C	2.40	127.91	124.79
22	B	6006	BCR	C36-C18-C17	-2.40	118.94	122.82
22	A	6008	BCR	C28-C27-C26	-2.40	109.78	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1223	CLA	C3D-C4D-ND	2.40	113.88	109.99
18	3	3013	CLA	C2B-C1B-NB	2.39	112.81	110.33
18	3	3008	CLA	CBC-CAC-C3C	-2.39	105.93	112.42
22	G	2011	BCR	C30-C25-C24	2.39	122.14	115.65
18	B	1201	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
18	A	1109	CLA	C4D-C3D-CAD	2.39	110.70	108.11
18	B	1021	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
18	A	1105	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
27	1	1502	LUT	C3-C4-C5	-2.39	106.23	112.18
22	J	6013	BCR	C31-C1-C6	-2.39	106.50	110.24
18	1	1003	CLA	CMC-C2C-C1C	2.39	128.77	125.03
18	B	1205	CLA	C4-C3-C5	2.39	119.37	115.23
18	A	1237	CLA	CAC-C3C-C4C	2.39	127.90	124.79
22	B	6010	BCR	C33-C5-C4	2.39	118.69	113.60
18	4	4009	CLA	C5-C3-C4	2.39	120.08	114.59
22	B	6006	BCR	C1-C6-C7	2.39	122.12	115.65
27	3	3502	LUT	C30-C31-C32	-2.39	116.28	123.20
22	K	2011	BCR	C35-C13-C12	2.39	121.73	118.09
18	B	1224	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
18	B	1206	CLA	C3C-C4C-NC	2.39	113.49	110.43
18	3	3019	CLA	C3A-C2A-C1A	-2.39	101.31	104.67
27	I	6018	LUT	C1-C6-C7	2.38	122.12	115.65
22	A	6011	BCR	C8-C9-C10	2.38	122.76	119.01
18	2	2007	CLA	CMD-C2D-C3D	-2.38	122.22	127.69
18	B	1207	CLA	C3C-C4C-NC	2.38	113.48	110.43
18	4	4005	CLA	CHA-C1A-NA	-2.38	121.00	126.39
18	1	1007	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
18	B	1220	CLA	CED-O2D-CGD	2.38	121.32	115.92
18	B	1220	CLA	CAC-C3C-C4C	2.38	127.89	124.79
18	A	1104	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
18	A	1113	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
18	A	1125	CLA	C3D-C4D-ND	2.38	113.85	109.99
18	2	2019	CLA	C2A-C3A-C4A	-2.38	100.86	103.58
18	B	1213	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
18	A	1136	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
18	4	4001	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
27	4	4501	LUT	C38-C25-C24	-2.38	117.74	123.36
18	A	1118	CLA	O1D-CGD-CBD	-2.37	119.83	124.52
18	B	1203	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
18	A	1117	CLA	CAC-C3C-C4C	2.37	127.88	124.79
18	A	1130	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
18	4	4012	CLA	CMA-C3A-C4A	-2.37	105.40	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3018	CLA	C5-C3-C4	2.37	120.05	114.59
18	2	2001	CLA	CAA-CBA-CGA	2.37	119.94	113.21
18	A	1119	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
18	A	1106	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
22	A	6017	BCR	C2-C1-C6	2.37	113.88	110.44
18	2	2002	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
27	4	4503	LUT	C36-C21-C26	-2.37	105.96	109.55
18	A	1140	CLA	C3C-C4C-NC	2.37	113.46	110.43
18	B	1235	CLA	CMD-C2D-C3D	-2.37	122.27	127.69
18	A	1151	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
18	A	1131	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
22	G	2011	BCR	C1-C6-C7	2.36	122.06	115.65
22	A	6017	BCR	C38-C26-C27	2.36	118.63	113.60
18	3	3017	CLA	CHA-C1A-NA	-2.36	121.04	126.39
18	3	3003	CLA	C3D-C4D-ND	2.36	113.82	109.99
28	4	4011	CHL	C1-C2-C3	-2.36	122.94	126.76
18	A	1133	CLA	CAC-C3C-C4C	2.36	127.86	124.79
23	G	2021	LMG	O4-C4-C3	-2.36	104.81	110.38
18	1	1003	CLA	C6-C5-C3	-2.36	107.72	113.47
22	B	6010	BCR	C28-C27-C26	-2.36	109.85	114.06
18	3	3006	CLA	C5-C3-C4	2.36	120.02	114.59
18	G	1003	CLA	C4-C3-C5	2.36	119.32	115.23
18	4	4007	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
22	A	6011	BCR	C8-C7-C6	-2.36	120.71	127.00
18	B	1240	CLA	C3C-C4C-NC	2.36	113.45	110.43
22	L	6020	BCR	C35-C13-C14	-2.35	119.00	122.82
18	A	1127	CLA	C3C-C4C-NC	2.35	113.44	110.43
18	B	1023	CLA	C3C-C4C-NC	2.35	113.44	110.43
18	A	1139	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
18	4	4001	CLA	C3D-C4D-ND	2.35	113.81	109.99
18	4	4017	CLA	CAC-C3C-C4C	2.35	127.85	124.79
18	B	1203	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
22	G	2011	BCR	C27-C26-C25	-2.35	119.53	122.70
18	B	1223	CLA	C4-C3-C5	2.35	119.31	115.23
22	B	6006	BCR	C28-C27-C26	-2.35	109.86	114.06
18	J	1302	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
18	B	1224	CLA	CAC-C3C-C4C	2.35	127.85	124.79
23	4	4801	LMG	O8-C28-C29	2.35	119.00	111.83
18	L	1503	CLA	C4D-C3D-CAD	2.35	110.66	108.11
18	B	1221	CLA	CAC-C3C-C4C	2.35	127.84	124.79
18	3	3004	CLA	CMC-C2C-C1C	2.35	128.70	125.03
18	A	1105	CLA	C3C-C4C-NC	2.35	113.44	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1115	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
18	B	1215	CLA	C3C-C4C-NC	2.34	113.43	110.43
18	1	1004	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
18	A	1111	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
18	1	1011	CLA	CMA-C3A-C4A	-2.34	105.47	111.77
18	B	1023	CLA	CMC-C2C-C1C	2.34	128.70	125.03
27	2	2501	LUT	C8-C7-C6	-2.34	120.74	127.00
18	A	1136	CLA	C3C-C4C-NC	2.34	113.43	110.43
18	A	1120	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
18	B	1012	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
18	1	1014	CLA	C1-O2A-CGA	2.34	123.57	116.07
28	1	1009	CHL	C1-O2A-CGA	2.34	122.32	116.65
17	A	1011	CL0	O1D-CGD-CBD	-2.34	121.17	124.72
22	B	6010	BCR	C23-C24-C25	-2.34	120.75	127.00
18	B	1235	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
18	A	1237	CLA	C4-C3-C2	-2.34	117.62	123.63
21	1	1801	LHG	O7-C7-O9	-2.34	118.23	123.70
23	4	4801	LMG	O4-C4-C5	-2.34	103.56	109.32
22	A	6011	BCR	C24-C23-C22	-2.34	122.77	126.23
18	B	1219	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
18	B	1211	CLA	CMC-C2C-C1C	2.34	128.69	125.03
18	A	1138	CLA	CAC-C3C-C4C	2.34	127.83	124.79
18	A	1135	CLA	C3C-C4C-NC	2.34	113.42	110.43
27	4	4502	LUT	C27-C28-C29	-2.34	121.30	126.32
18	2	2008	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
18	A	1139	CLA	C4-C3-C5	2.34	119.28	115.23
18	B	1202	CLA	CAC-C3C-C4C	2.34	127.83	124.79
22	F	6014	BCR	C30-C25-C26	-2.34	119.44	122.64
18	4	4006	CLA	C3C-C4C-NC	2.33	113.42	110.43
18	A	1109	CLA	CMB-C2B-C1B	2.33	128.97	125.42
18	L	1503	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
18	L	1501	CLA	CBC-CAC-C3C	-2.33	106.09	112.42
18	A	1110	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
18	4	4008	CLA	CHA-C4D-ND	2.33	137.36	132.55
27	3	3501	LUT	C31-C30-C29	-2.33	124.01	127.28
23	2	2802	LMG	O1-C7-C8	-2.33	105.15	110.82
18	A	1133	CLA	C3C-C4C-NC	2.33	113.41	110.43
23	2	2802	LMG	O8-C28-C29	2.33	118.94	111.83
18	B	1240	CLA	CAA-CBA-CGA	-2.33	106.60	113.21
18	L	1503	CLA	C3C-C4C-NC	2.33	113.41	110.43
22	F	6016	BCR	C37-C22-C21	-2.33	119.04	122.82
18	2	2001	CLA	CMB-C2B-C1B	2.33	128.96	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1220	CLA	CAA-CBA-CGA	-2.32	106.61	113.21
18	A	1108	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
18	4	4005	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
18	2	2007	CLA	C2B-C1B-NB	2.32	112.73	110.33
22	A	6008	BCR	C30-C25-C24	2.32	121.95	115.65
18	B	1206	CLA	C1-O2A-CGA	2.32	122.27	116.65
18	2	2008	CLA	CGD-CBD-CAD	-2.32	103.33	110.85
18	A	1115	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
18	2	2016	CLA	CAA-CBA-CGA	-2.32	106.62	113.21
18	A	1120	CLA	C3C-C4C-NC	2.32	113.40	110.43
18	G	1001	CLA	O2A-C1-C2	2.32	117.03	108.11
18	J	1302	CLA	CAC-C3C-C4C	2.32	127.81	124.79
18	J	1302	CLA	C3C-C4C-NC	2.32	113.40	110.43
18	A	1108	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
27	3	3502	LUT	C31-C30-C29	-2.31	124.03	127.28
18	B	1227	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
18	B	1236	CLA	C4D-C3D-CAD	2.31	110.62	108.11
22	L	6019	BCR	C2-C1-C6	2.31	113.80	110.44
18	A	1119	CLA	C3C-C4C-NC	2.31	113.39	110.43
18	A	1135	CLA	CAC-C3C-C4C	2.31	127.80	124.79
18	A	1111	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
18	A	1123	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
18	1	1003	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
18	1	1008	CLA	C3D-C4D-ND	2.31	113.75	109.99
18	A	1138	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
22	A	6011	BCR	C27-C26-C25	-2.31	119.58	122.70
18	B	1232	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
18	B	1203	CLA	C3C-C4C-NC	2.31	113.39	110.43
18	A	1122	CLA	CAC-C3C-C4C	2.31	127.80	124.79
18	B	1219	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
18	B	1238	CLA	C3C-C4C-NC	2.31	113.39	110.43
18	A	1126	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
18	B	1206	CLA	CAC-C3C-C4C	2.31	127.79	124.79
18	4	4007	CLA	C3D-C4D-ND	2.31	113.74	109.99
18	2	2016	CLA	CHA-C4D-ND	2.31	137.31	132.55
18	1	1006	CLA	C2B-C1B-NB	2.31	112.72	110.33
27	4	4503	LUT	C15-C35-C34	-2.31	118.80	123.52
18	G	1002	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
18	2	2008	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
18	B	1228	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
18	4	4009	CLA	C3C-C4C-NC	2.30	113.38	110.43
20	B	5002	PQN	C12-C11-C3	-2.30	106.41	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	3501	LUT	C38-C25-C24	-2.30	117.92	123.36
18	1	1002	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
18	4	4017	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
18	B	1232	CLA	C3C-C4C-NC	2.30	113.38	110.43
18	4	4006	CLA	C5-C3-C4	2.30	119.88	114.59
22	L	6019	BCR	C33-C5-C4	2.30	118.50	113.60
18	B	1214	CLA	C6-C5-C3	-2.30	107.87	113.47
18	A	1118	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
18	A	1129	CLA	CAC-C3C-C4C	2.30	127.78	124.79
18	4	4007	CLA	C1-C2-C3	-2.30	122.43	126.20
18	2	2012	CLA	C2B-C1B-NB	2.30	112.71	110.33
26	B	8001	LMU	O1B-C4'-C3'	2.30	113.07	107.23
18	A	1137	CLA	C1-C2-C3	-2.30	122.43	126.20
18	A	1114	CLA	C3C-C4C-NC	2.30	113.37	110.43
18	B	1228	CLA	CMC-C2C-C1C	2.30	128.62	125.03
18	2	2007	CLA	CAC-C3C-C4C	2.30	127.78	124.79
20	A	5001	PQN	C2M-C2-C3	-2.30	120.68	124.45
18	B	1207	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
18	2	2001	CLA	CAC-C3C-C4C	2.29	127.78	124.79
18	4	4017	CLA	C3C-C4C-NC	2.29	113.37	110.43
18	A	1109	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
18	4	4017	CLA	C4-C3-C5	2.29	119.21	115.23
27	4	4503	LUT	C22-C23-C24	-2.29	107.78	111.18
18	A	1134	CLA	CAC-C3C-C4C	2.29	127.77	124.79
18	4	4005	CLA	C4D-C3D-CAD	2.29	110.60	108.11
18	A	1111	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
18	3	3004	CLA	C2B-C1B-NB	2.29	112.70	110.33
18	B	1218	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
18	A	1111	CLA	C1-O2A-CGA	2.29	122.20	116.65
18	B	1202	CLA	C3C-C4C-NC	2.29	113.36	110.43
18	2	2008	CLA	C2B-C1B-NB	2.29	112.70	110.33
18	1	1003	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
18	A	1115	CLA	CAC-C3C-C4C	2.29	127.77	124.79
18	B	1234	CLA	CMC-C2C-C1C	2.29	128.61	125.03
18	3	3012	CLA	CBB-CAB-C3B	-2.29	116.09	127.53
18	3	3017	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
18	B	1229	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
18	1	1002	CLA	C3C-C4C-NC	2.29	113.36	110.43
18	L	1503	CLA	C2B-C1B-NB	2.29	112.70	110.33
22	K	2011	BCR	C29-C28-C27	2.28	116.30	111.28
18	3	3003	CLA	CAC-C3C-C4C	2.28	127.76	124.79
18	4	4002	CLA	C3D-C4D-ND	2.28	113.70	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2012	CLA	CBB-CAB-C3B	-2.28	116.11	127.53
18	A	1136	CLA	CAC-C3C-C4C	2.28	127.76	124.79
22	B	6004	BCR	C34-C9-C10	-2.28	119.12	122.82
21	A	5003	LHG	O8-C23-O10	-2.28	117.92	123.63
18	B	1213	CLA	CAC-C3C-C4C	2.28	127.76	124.79
27	1	1502	LUT	C38-C25-C24	-2.28	117.96	123.36
22	K	2011	BCR	C33-C5-C4	2.28	118.46	113.60
18	A	1131	CLA	C3C-C4C-NC	2.28	113.35	110.43
18	A	1013	CLA	C6-C5-C3	-2.28	107.91	113.47
18	H	1000	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
18	B	1216	CLA	CAC-C3C-C4C	2.28	127.76	124.79
18	B	1224	CLA	CMC-C2C-C1C	2.28	128.60	125.03
18	A	1126	CLA	C3C-C4C-NC	2.28	113.35	110.43
18	1	1008	CLA	CHA-C4D-ND	2.28	137.25	132.55
18	2	2006	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
22	L	6019	BCR	C23-C22-C21	2.28	122.59	119.01
22	F	6016	BCR	C31-C1-C6	-2.28	106.67	110.24
17	A	1011	CL0	C4C-C3C-C2C	-2.28	104.38	113.37
18	A	1137	CLA	CAC-C3C-C4C	2.28	127.75	124.79
18	A	1129	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
27	4	4502	LUT	C28-C29-C30	2.28	122.59	119.01
18	A	1127	CLA	CAC-C3C-C4C	2.27	127.75	124.79
18	3	3010	CLA	CMB-C2B-C3B	2.27	131.90	126.55
18	B	1202	CLA	C4-C3-C5	2.27	119.17	115.23
18	F	1302	CLA	C5-C3-C4	2.27	119.82	114.59
18	4	4003	CLA	C6-C5-C3	-2.27	107.93	113.47
18	B	1211	CLA	CAC-C3C-C4C	2.27	127.75	124.79
27	I	6018	LUT	C7-C6-C5	-2.27	116.32	121.56
18	A	1112	CLA	C3C-C4C-NC	2.27	113.34	110.43
18	A	1121	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
18	B	1224	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
18	2	2012	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
18	B	1221	CLA	C4-C3-C5	2.27	119.17	115.23
18	2	2002	CLA	C1-O2A-CGA	2.27	123.33	116.07
18	1	1002	CLA	CHD-C4C-C3C	-2.27	121.47	124.77
21	2	2801	LHG	C5-O7-C7	-2.27	112.37	117.80
18	A	1124	CLA	CAC-C3C-C4C	2.27	127.74	124.79
22	A	6017	BCR	C33-C5-C4	2.27	118.43	113.60
18	A	1105	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
22	L	6020	BCR	C2-C1-C6	2.27	113.73	110.44
18	A	1140	CLA	CAC-C3C-C4C	2.27	127.74	124.79
22	B	6006	BCR	C19-C18-C17	2.27	122.57	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1216	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
18	A	1111	CLA	C3C-C4C-NC	2.26	113.33	110.43
18	B	1226	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
18	3	3012	CLA	C3C-C4C-NC	2.26	113.33	110.43
18	4	4001	CLA	CHA-C4D-ND	2.26	137.22	132.55
18	2	2012	CLA	C3C-C4C-NC	2.26	113.33	110.43
28	2	2011	CHL	C1A-CHA-CBD	-2.26	126.57	132.36
18	3	3010	CLA	C4D-CHA-C1A	2.26	123.94	121.24
18	A	1140	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
18	B	1234	CLA	CMB-C2B-C1B	2.26	128.86	125.42
27	2	2501	LUT	C10-C11-C12	-2.26	116.66	123.20
18	1	1005	CLA	CAA-CBA-CGA	-2.26	106.80	113.21
18	L	1501	CLA	C5-C3-C4	2.26	119.78	114.59
18	B	1214	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
18	A	1108	CLA	CAC-C3C-C4C	2.25	127.72	124.79
18	1	1007	CLA	CAC-C3C-C4C	2.25	127.72	124.79
18	B	1240	CLA	C4-C3-C2	-2.25	117.84	123.63
29	4	4505	ZEX	C21-C26-C27	2.25	121.76	115.65
18	A	1151	CLA	C5-C3-C4	2.25	119.77	114.59
18	4	4007	CLA	CHA-C4D-ND	2.25	137.20	132.55
18	B	1234	CLA	C3C-C4C-NC	2.25	113.32	110.43
18	2	2016	CLA	C3D-C4D-ND	2.25	113.65	109.99
18	3	3012	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
18	1	1011	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
18	1	1005	CLA	C2B-C1B-NB	2.25	112.66	110.33
18	B	1228	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
18	A	1135	CLA	CMB-C2B-C1B	2.25	128.85	125.42
18	B	1201	CLA	CMB-C2B-C1B	2.25	128.85	125.42
18	1	1004	CLA	C2B-C1B-NB	2.25	112.66	110.33
18	2	2003	CLA	CHC-C1C-C2C	-2.25	120.55	126.95
18	B	1222	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
18	A	1110	CLA	C1-C2-C3	-2.25	122.51	126.20
18	H	1000	CLA	C3C-C4C-NC	2.25	113.31	110.43
18	G	1003	CLA	CAA-C2A-C1A	-2.25	104.61	111.97
18	A	1104	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
18	2	2003	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
18	3	3018	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
18	A	1106	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
18	A	1131	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
18	4	4001	CLA	CMC-C2C-C1C	2.25	128.54	125.03
22	B	6005	BCR	C23-C22-C21	2.25	122.54	119.01
22	A	6008	BCR	C31-C1-C6	-2.25	106.72	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	4	4010	CHL	CHA-C1A-C2A	-2.25	128.03	133.31
18	B	1021	CLA	C3C-C4C-NC	2.25	113.31	110.43
22	B	6010	BCR	C38-C26-C27	2.24	118.38	113.60
18	3	3008	CLA	CHD-C4C-C3C	-2.24	121.50	124.77
18	2	2009	CLA	C5-C3-C4	2.24	119.75	114.59
18	B	1228	CLA	C3C-C4C-NC	2.24	113.30	110.43
22	K	2011	BCR	C15-C14-C13	-2.24	124.13	127.28
18	B	1208	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
18	1	1008	CLA	C3C-C4C-NC	2.24	113.30	110.43
18	B	1231	CLA	CAC-C3C-C4C	2.24	127.71	124.79
18	1	1002	CLA	C4D-CHA-C1A	2.24	123.92	121.24
18	1	1008	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
18	A	1137	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
18	A	1113	CLA	C3C-C4C-NC	2.24	113.30	110.43
27	1	1502	LUT	C17-C1-C6	-2.24	106.73	110.24
18	4	4002	CLA	CHA-C1A-NA	-2.24	121.32	126.39
18	3	3005	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
18	3	3017	CLA	C4D-C3D-CAD	2.24	110.54	108.11
18	A	1105	CLA	CAC-C3C-C4C	2.24	127.70	124.79
22	F	6014	BCR	C30-C25-C24	2.24	121.72	115.65
18	2	2001	CLA	CMC-C2C-C1C	2.24	128.53	125.03
18	1	1003	CLA	CAA-CBA-CGA	-2.24	106.86	113.21
18	B	1204	CLA	CAC-C3C-C4C	2.24	127.70	124.79
18	A	1103	CLA	CAA-C2A-C1A	-2.23	104.65	111.97
18	4	4012	CLA	CMD-C2D-C3D	-2.23	122.56	127.69
22	F	6016	BCR	C35-C13-C12	2.23	121.50	118.09
18	B	1205	CLA	CAC-C3C-C4C	2.23	127.69	124.79
18	A	1123	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
18	A	1117	CLA	C3C-C4C-NC	2.23	113.29	110.43
18	A	1124	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
27	1	1502	LUT	C30-C31-C32	-2.23	116.74	123.20
18	4	4004	CLA	CMC-C2C-C1C	2.23	128.52	125.03
18	A	1130	CLA	C3C-C4C-NC	2.23	113.28	110.43
18	A	1126	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
18	2	2005	CLA	C1-O2A-CGA	2.23	122.04	116.65
27	1	1501	LUT	C15-C35-C34	-2.23	118.97	123.52
18	B	1213	CLA	C3C-C4C-NC	2.22	113.28	110.43
18	B	1205	CLA	C1-C2-C3	-2.22	122.55	126.20
18	B	1220	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
18	A	1022	CLA	CAC-C3C-C4C	2.22	127.68	124.79
18	3	3001	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
18	A	1116	CLA	C3C-C4C-NC	2.22	113.27	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2002	CLA	C2B-C1B-NB	2.22	112.63	110.33
18	4	4016	CLA	CED-O2D-CGD	2.22	120.95	115.92
18	1	1007	CLA	C2B-C1B-NB	2.22	112.63	110.33
18	1	1014	CLA	C2B-C1B-NB	2.22	112.63	110.33
18	4	4016	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
18	B	1227	CLA	CAC-C3C-C4C	2.22	127.67	124.79
22	G	2011	BCR	C38-C26-C27	2.22	118.32	113.60
18	A	1130	CLA	C5-C3-C4	2.22	119.69	114.59
18	1	1005	CLA	C4C-C3C-C2C	-2.22	103.67	106.89
22	A	6003	BCR	C37-C22-C21	-2.22	119.23	122.82
18	A	1139	CLA	C3C-C4C-NC	2.21	113.27	110.43
18	B	1205	CLA	CAA-C2A-C3A	-2.21	107.02	113.00
18	B	1202	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
18	A	1129	CLA	C5-C3-C4	2.21	119.68	114.59
18	B	1210	CLA	C4B-CHC-C1C	2.21	131.45	126.25
18	B	1201	CLA	C5-C3-C4	2.21	119.68	114.59
27	3	3501	LUT	C30-C31-C32	-2.21	116.79	123.20
18	A	1105	CLA	CAA-CBA-CGA	-2.21	106.93	113.21
18	A	1107	CLA	CAC-C3C-C4C	2.21	127.66	124.79
18	B	1221	CLA	C3C-C4C-NC	2.21	113.26	110.43
18	B	1210	CLA	C3C-C4C-NC	2.21	113.26	110.43
18	2	2012	CLA	CMC-C2C-C1C	2.21	128.49	125.03
22	3	3503	BCR	C39-C30-C25	-2.21	106.78	110.24
18	B	1215	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
18	2	2007	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
20	A	5001	PQN	C11-C3-C2	-2.21	121.11	124.89
18	B	1209	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
22	A	6008	BCR	C35-C13-C14	-2.21	119.24	122.82
18	B	1208	CLA	C3C-C4C-NC	2.21	113.25	110.43
18	2	2008	CLA	CAA-C2A-C1A	-2.21	104.75	111.97
18	B	1239	CLA	C1-O2A-CGA	2.20	121.99	116.65
18	4	4004	CLA	CMA-C3A-C4A	-2.20	105.85	111.77
18	3	3006	CLA	CAC-C3C-C4C	2.20	127.66	124.79
25	B	7101	DGD	CFB-CEB-CDB	-2.20	103.24	114.37
18	A	1134	CLA	C3C-C4C-NC	2.20	113.25	110.43
18	1	1007	CLA	C3C-C4C-NC	2.20	113.25	110.43
18	A	1106	CLA	C3C-C4C-NC	2.20	113.25	110.43
18	A	1103	CLA	C3C-C4C-NC	2.20	113.25	110.43
18	A	1114	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
18	F	1301	CLA	C3C-C4C-NC	2.20	113.25	110.43
18	3	3004	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
22	B	6005	BCR	C30-C25-C24	2.20	121.61	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	3502	LUT	C15-C14-C13	-2.20	124.20	127.28
18	A	1124	CLA	C3C-C4C-NC	2.20	113.24	110.43
27	3	3501	LUT	C39-C29-C28	2.19	121.44	118.09
18	3	3006	CLA	CMB-C2B-C1B	2.19	128.76	125.42
27	2	2501	LUT	C27-C28-C29	-2.19	121.61	126.32
18	A	1132	CLA	C1-O2A-CGA	2.19	121.96	116.65
27	4	4502	LUT	C7-C8-C9	-2.19	122.99	126.23
27	1	1502	LUT	C1-C6-C5	-2.19	119.64	122.64
18	4	4016	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
18	F	1301	CLA	CAC-C3C-C4C	2.19	127.64	124.79
18	4	4001	CLA	CED-O2D-CGD	2.19	120.89	115.92
18	A	1237	CLA	C3C-C4C-NC	2.19	113.24	110.43
18	A	1122	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
18	L	1503	CLA	CMB-C2B-C1B	2.19	128.75	125.42
18	A	1104	CLA	C4B-CHC-C1C	2.19	131.40	126.25
18	4	4005	CLA	C4D-CHA-C1A	2.19	123.86	121.24
22	B	6006	BCR	C30-C25-C24	2.19	121.59	115.65
18	B	1202	CLA	CMB-C2B-C1B	2.19	128.75	125.42
18	1	1002	CLA	OBD-CAD-C3D	-2.19	123.30	128.42
18	B	1209	CLA	C3C-C4C-NC	2.19	113.23	110.43
18	B	1227	CLA	CMB-C2B-C1B	2.19	128.75	125.42
18	1	1004	CLA	C4-C3-C5	2.19	119.03	115.23
18	G	1002	CLA	CBB-CAB-C3B	-2.19	116.59	127.53
27	I	6018	LUT	C38-C25-C24	-2.19	118.18	123.36
18	4	4004	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
18	A	1110	CLA	C3C-C4C-NC	2.19	113.23	110.43
22	J	6012	BCR	C35-C13-C14	-2.19	119.27	122.82
18	A	1133	CLA	C1-O2A-CGA	2.19	121.94	116.65
18	J	1302	CLA	C5-C3-C4	2.19	119.62	114.59
18	A	1118	CLA	C3C-C4C-NC	2.19	113.23	110.43
18	L	1503	CLA	C5-C3-C4	2.18	119.62	114.59
22	I	6020	BCR	C15-C14-C13	-2.18	124.22	127.28
18	A	1237	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
18	A	1119	CLA	CAC-C3C-C4C	2.18	127.63	124.79
22	F	6016	BCR	C38-C26-C27	2.18	118.25	113.60
22	A	6003	BCR	C3-C4-C5	-2.18	110.17	114.06
18	A	1106	CLA	C6-C5-C3	-2.18	108.16	113.47
18	2	2002	CLA	CBA-CAA-C2A	-2.18	107.31	113.79
18	3	3003	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
18	B	1229	CLA	C6-C7-C8	-2.18	108.72	115.97
18	A	1108	CLA	C3C-C4C-NC	2.18	113.22	110.43
18	2	2016	CLA	CHD-C4C-C3C	-2.18	121.60	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1121	CLA	C3C-C4C-NC	2.18	113.22	110.43
18	A	1121	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
18	B	1224	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
28	2	2010	CHL	CMD-C2D-C3D	2.18	129.03	124.68
18	3	3017	CLA	C4D-CHA-C1A	2.18	123.84	121.24
18	3	3004	CLA	CBB-CAB-C3B	-2.18	116.66	127.53
27	4	4503	LUT	C35-C15-C14	-2.17	119.07	123.52
18	A	1128	CLA	C3C-C4C-NC	2.17	113.22	110.43
18	B	1239	CLA	C3C-C4C-NC	2.17	113.22	110.43
18	G	1002	CLA	C2B-C1B-NB	2.17	112.58	110.33
18	A	1105	CLA	CED-O2D-CGD	2.17	120.85	115.92
23	B	5005	LMG	O7-C10-O9	-2.17	118.62	123.70
22	B	6010	BCR	C39-C30-C25	-2.17	106.83	110.24
18	B	1234	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
18	A	1022	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
18	2	2005	CLA	C2B-C1B-NB	2.17	112.58	110.33
18	3	3004	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
18	A	1013	CLA	C3C-C4C-NC	2.17	113.21	110.43
22	B	6004	BCR	C1-C6-C5	-2.17	119.67	122.64
18	G	1001	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
18	A	1112	CLA	CAC-C3C-C4C	2.17	127.61	124.79
27	1	1501	LUT	C11-C10-C9	-2.17	124.24	127.28
18	B	1238	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
21	2	2801	LHG	O7-C7-O9	-2.17	118.64	123.70
18	3	3002	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
18	A	1122	CLA	C3C-C4C-NC	2.17	113.20	110.43
18	B	1203	CLA	C1-O2A-CGA	2.17	121.89	116.65
26	B	8001	LMU	C1B-C2B-C3B	2.16	114.56	110.01
18	B	1220	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
22	A	6008	BCR	C33-C5-C4	2.16	118.21	113.60
22	G	2011	BCR	C39-C30-C25	-2.16	106.85	110.24
18	A	1128	CLA	CHC-C1C-C2C	-2.16	120.80	126.95
18	2	2003	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
18	B	1234	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
18	H	1000	CLA	CED-O2D-CGD	2.16	120.82	115.92
28	2	2013	CHL	C1A-CHA-CBD	-2.16	126.83	132.36
18	B	1223	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
18	4	4006	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
22	J	6012	BCR	C23-C22-C21	2.16	122.40	119.01
25	B	7101	DGD	C3G-C2G-C1G	-2.16	106.75	111.78
18	4	4002	CLA	CED-O2D-CGD	2.16	120.81	115.92
18	B	1201	CLA	C3C-C4C-NC	2.16	113.19	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1220	CLA	C3C-C4C-NC	2.16	113.19	110.43
27	4	4501	LUT	C39-C29-C30	-2.16	119.32	122.82
18	B	1214	CLA	CAC-C3C-C4C	2.15	127.59	124.79
18	B	1221	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
21	B	5004	LHG	O7-C7-O9	-2.15	118.83	122.99
18	B	1217	CLA	C3C-C4C-NC	2.15	113.19	110.43
18	A	1126	CLA	C6-C5-C3	-2.15	108.22	113.47
18	B	1210	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
22	K	2011	BCR	C7-C6-C5	-2.15	116.60	121.56
18	3	3005	CLA	CAC-C3C-C4C	2.15	127.59	124.79
18	A	1128	CLA	CAC-C3C-C4C	2.15	127.59	124.79
18	1	1012	CLA	C1-O2A-CGA	2.15	121.86	116.65
18	K	1001	CLA	CBB-CAB-C3B	-2.15	116.78	127.53
25	B	7101	DGD	O2D-C2D-C1D	-2.15	104.95	110.08
18	A	1132	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
22	F	6016	BCR	C23-C22-C21	2.15	122.39	119.01
18	2	2008	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
18	A	1132	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
18	L	1503	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
18	B	1204	CLA	C1-C2-C3	-2.15	122.68	126.20
18	2	2019	CLA	C3A-C2A-C1A	-2.15	101.64	104.67
18	L	1501	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
18	1	1008	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
18	3	3013	CLA	CMA-C3A-C4A	-2.14	106.01	111.77
22	G	2011	BCR	C38-C26-C25	-2.14	122.15	124.48
18	1	1014	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
25	B	7101	DGD	O6E-C1E-O5D	-2.14	104.98	110.04
28	1	1009	CHL	CMD-C2D-C3D	2.14	128.96	124.68
18	A	1139	CLA	CAC-C3C-C4C	2.14	127.57	124.79
18	B	1211	CLA	C4B-CHC-C1C	2.14	131.28	126.25
17	A	1011	CL0	C1-O2A-CGA	2.14	121.83	116.65
18	B	1208	CLA	C4-C3-C5	2.14	118.94	115.23
18	3	3013	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
18	A	1129	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
18	B	1240	CLA	C1-O2A-CGA	2.14	121.83	116.65
22	A	6002	BCR	C30-C25-C24	2.14	121.45	115.65
18	A	1107	CLA	C3C-C4C-NC	2.14	113.17	110.43
18	3	3002	CLA	CHA-C4D-ND	2.14	136.96	132.55
27	1	1502	LUT	C37-C21-C26	-2.14	106.31	109.55
22	J	6012	BCR	C40-C30-C25	-2.14	106.89	110.24
18	G	1001	CLA	CHA-C4D-ND	2.14	136.96	132.55
18	B	1223	CLA	CMD-C2D-C3D	-2.14	122.79	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2	2802	LMG	C3-C4-C5	2.14	114.10	110.23
18	3	3002	CLA	CBA-CAA-C2A	-2.14	107.44	113.79
18	2	2019	CLA	C2C-C1C-CHC	-2.14	120.25	125.84
18	G	1002	CLA	CHC-C1C-C2C	-2.14	120.88	126.95
18	A	1136	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
18	A	1138	CLA	CMB-C2B-C1B	2.13	128.67	125.42
18	4	4005	CLA	CHA-C4D-ND	2.13	136.95	132.55
18	G	1003	CLA	CAC-C3C-C4C	2.13	127.56	124.79
18	1	1012	CLA	CBB-CAB-C3B	-2.13	116.87	127.53
18	G	1002	CLA	CHA-C4D-ND	2.13	136.95	132.55
18	A	1022	CLA	C6-C5-C3	-2.13	108.28	113.47
18	1	1011	CLA	C4B-CHC-C1C	2.13	131.26	126.25
18	3	3013	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
18	B	1023	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
28	2	2013	CHL	C4D-CHA-CBD	-2.13	106.82	108.97
18	A	1125	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
18	B	1212	CLA	CAC-C3C-C4C	2.13	127.56	124.79
18	L	1502	CLA	C4-C3-C5	2.13	118.92	115.23
18	3	3017	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
18	3	3005	CLA	CHA-C4D-ND	2.13	136.94	132.55
18	B	1204	CLA	C3C-C4C-NC	2.13	113.15	110.43
18	A	1102	CLA	C5-C3-C4	2.13	119.48	114.59
18	A	1110	CLA	CAC-C3C-C4C	2.13	127.56	124.79
27	4	4503	LUT	C11-C12-C13	-2.13	120.54	126.36
23	2	2802	LMG	O1-C1-C2	2.12	111.50	108.27
18	3	3013	CLA	C3C-C4C-NC	2.12	113.15	110.43
22	L	6020	BCR	C12-C13-C14	2.12	122.35	119.01
25	B	7101	DGD	O3E-C3E-C2E	-2.12	105.37	110.38
18	4	4005	CLA	CBB-CAB-C3B	-2.12	116.91	127.53
18	K	1001	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
18	1	1014	CLA	CMC-C2C-C1C	2.12	128.35	125.03
18	A	1139	CLA	C6-C5-C3	-2.12	108.30	113.47
23	G	2021	LMG	C7-O1-C1	-2.12	109.25	113.80
25	B	7101	DGD	CBB-CAB-C9B	-2.12	103.65	114.37
29	4	4505	ZEX	C10-C11-C12	-2.12	117.06	123.20
18	B	1236	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
18	1	1013	CLA	CHA-C4D-ND	2.12	136.92	132.55
18	4	4012	CLA	C6-C5-C3	-2.12	108.31	113.47
18	F	1301	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
18	4	4008	CLA	CHA-C1A-NA	-2.12	121.60	126.39
18	A	1121	CLA	CAC-C3C-C4C	2.12	127.54	124.79
18	1	1004	CLA	CBC-CAC-C3C	-2.12	106.69	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	2502	LUT	C19-C9-C8	2.11	121.32	118.09
18	A	1125	CLA	OBD-CAD-C3D	-2.11	123.47	128.42
18	A	1128	CLA	C4D-C3D-CAD	2.11	110.40	108.11
18	B	1238	CLA	C1-C2-C3	-2.11	122.73	126.20
18	B	1227	CLA	C3C-C4C-NC	2.11	113.14	110.43
18	3	3007	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
18	1	1008	CLA	CHA-C1A-NA	-2.11	121.61	126.39
22	A	6007	BCR	C31-C1-C6	-2.11	106.93	110.24
18	L	1502	CLA	CHA-C4D-ND	2.11	136.91	132.55
18	3	3006	CLA	CHA-C4D-ND	2.11	136.91	132.55
18	4	4008	CLA	C2B-C1B-NB	2.11	112.52	110.33
18	A	1128	CLA	C1-C2-C3	-2.11	122.74	126.20
22	K	2011	BCR	C27-C26-C25	-2.11	119.85	122.70
18	A	1123	CLA	CMB-C2B-C1B	2.11	128.63	125.42
18	2	2004	CLA	CHA-C4D-ND	2.11	136.90	132.55
18	4	4017	CLA	CHA-C4D-ND	2.11	136.90	132.55
17	A	1011	CL0	CMA-C3A-C2A	-2.11	105.99	114.13
22	B	6009	BCR	C15-C14-C13	-2.11	124.32	127.28
18	2	2001	CLA	CGD-CBD-CAD	2.11	117.67	110.85
28	3	3011	CHL	C1A-CHA-CBD	-2.11	126.97	132.36
18	2	2016	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
18	A	1119	CLA	CED-O2D-CGD	2.10	120.68	115.92
18	2	2007	CLA	C3C-C4C-NC	2.10	113.12	110.43
27	3	3501	LUT	C37-C21-C26	-2.10	106.36	109.55
18	2	2001	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
18	4	4017	CLA	CHA-C1A-NA	-2.10	121.64	126.39
18	A	1109	CLA	C3C-C4C-NC	2.10	113.12	110.43
28	1	1010	CHL	C1-O2A-CGA	2.10	122.78	116.07
18	B	1223	CLA	CAC-C3C-C4C	2.10	127.52	124.79
18	B	1224	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
18	A	1136	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
18	4	4012	CLA	CBC-CAC-C3C	-2.10	106.74	112.42
22	B	6006	BCR	C33-C5-C4	2.10	118.06	113.60
18	B	1216	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
18	2	2019	CLA	CBD-CAD-C3D	2.10	108.58	105.94
18	B	1240	CLA	CAC-C3C-C4C	2.09	127.52	124.79
29	4	4505	ZEX	C30-C31-C32	-2.09	117.13	123.20
18	3	3007	CLA	OBD-CAD-C3D	-2.09	123.52	128.42
18	B	1206	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
18	B	1206	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
18	4	4008	CLA	C1D-CHD-C4C	-2.09	121.58	126.02
23	J	5001	LMG	C8-O7-C10	2.09	122.80	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	6002	BCR	C34-C9-C10	-2.09	119.43	122.82
18	3	3005	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
22	B	6005	BCR	C1-C6-C7	2.09	121.32	115.65
18	B	1211	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
18	A	1139	CLA	C1-O2A-CGA	2.09	121.71	116.65
22	K	2011	BCR	C31-C1-C6	-2.09	106.97	110.24
18	B	1231	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
18	2	2012	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
18	L	1501	CLA	C4B-CHC-C1C	2.09	131.16	126.25
18	B	1222	CLA	CAA-CBA-CGA	-2.09	107.28	113.21
18	B	1234	CLA	CAC-C3C-C4C	2.09	127.51	124.79
18	F	1301	CLA	C2B-C1B-NB	2.09	112.49	110.33
18	K	1001	CLA	C4D-CHA-C1A	2.09	123.73	121.24
18	B	1217	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
18	1	1007	CLA	CHC-C1C-C2C	-2.09	121.02	126.95
18	B	1222	CLA	CMD-C2D-C3D	-2.09	122.91	127.69
18	B	1212	CLA	C1-O2A-CGA	2.09	121.70	116.65
28	4	4011	CHL	C1A-CHA-CBD	-2.08	127.02	132.36
26	B	8001	LMU	C3'-C4'-C5'	-2.08	106.31	110.93
18	4	4009	CLA	CHA-C4D-ND	2.08	136.85	132.55
18	A	1022	CLA	C1-O2A-CGA	2.08	121.69	116.65
18	3	3008	CLA	CMC-C2C-C1C	2.08	128.29	125.03
23	F	5002	LMG	O6-C1-C2	-2.08	106.09	110.37
23	4	4801	LMG	O1-C1-C2	2.08	111.44	108.27
18	B	1224	CLA	C3C-C4C-NC	2.08	113.10	110.43
28	2	2013	CHL	CMD-C2D-C3D	2.08	128.84	124.68
18	B	1226	CLA	C2B-C1B-NB	2.08	112.48	110.33
18	A	1132	CLA	C4D-C3D-CAD	2.08	110.37	108.11
18	B	1215	CLA	CAC-C3C-C4C	2.08	127.50	124.79
18	4	4012	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
18	4	4012	CLA	CHA-C4D-ND	2.08	136.84	132.55
18	A	1109	CLA	CAC-C3C-C4C	2.08	127.50	124.79
18	A	1113	CLA	CAA-CBA-CGA	-2.08	107.31	113.21
28	1	1010	CHL	CMD-C2D-C3D	2.08	128.84	124.68
22	A	6011	BCR	C29-C30-C25	2.08	113.45	110.44
22	K	2011	BCR	C30-C25-C26	-2.08	119.80	122.64
18	A	1109	CLA	CAA-C2A-C3A	-2.07	107.39	113.00
18	1	1002	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
22	A	6011	BCR	C37-C22-C21	-2.07	119.46	122.82
18	B	1217	CLA	CAC-C3C-C4C	2.07	127.49	124.79
17	A	1011	CL0	C4C-CHD-C1D	2.07	123.48	116.07
18	4	4007	CLA	C1D-CHD-C4C	-2.07	121.61	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3019	CLA	CBD-CAD-C3D	2.07	108.55	105.94
29	4	4505	ZEX	C21-C26-C25	-2.07	121.24	122.84
18	B	1012	CLA	C6-C5-C3	-2.07	108.42	113.47
18	3	3018	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
28	4	4013	CHL	C1-O2A-CGA	2.07	122.70	116.07
22	A	6003	BCR	C33-C5-C4	2.07	118.01	113.60
18	B	1239	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
28	3	3011	CHL	CMD-C2D-C3D	2.07	128.82	124.68
18	A	1112	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
18	A	1132	CLA	CBB-CAB-C3B	-2.07	117.19	127.53
18	L	1502	CLA	C4B-CHC-C1C	2.07	131.11	126.25
18	B	1211	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
18	1	1012	CLA	C5-C3-C4	2.07	119.34	114.59
22	G	2011	BCR	C3-C4-C5	-2.07	110.37	114.06
18	B	1231	CLA	CED-O2D-CGD	2.07	120.60	115.92
27	4	4501	LUT	C40-C33-C32	2.07	121.24	118.09
18	B	1205	CLA	C3C-C4C-NC	2.07	113.08	110.43
18	A	1115	CLA	C3C-C4C-NC	2.06	113.08	110.43
25	B	7101	DGD	C5B-C4B-C3B	-2.06	103.93	114.37
18	A	1128	CLA	C1-O2A-CGA	2.06	121.65	116.65
18	B	1206	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
18	1	1005	CLA	CHC-C1C-C2C	-2.06	121.08	126.95
20	B	5002	PQN	C11-C3-C2	-2.06	121.35	124.89
18	A	1132	CLA	C3C-C4C-NC	2.06	113.07	110.43
18	3	3007	CLA	C4D-CHA-C1A	2.06	123.70	121.24
18	B	1229	CLA	CAC-C3C-C4C	2.06	127.47	124.79
18	A	1102	CLA	CMB-C2B-C1B	2.06	128.56	125.42
18	1	1005	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
18	3	3005	CLA	CBB-CAB-C3B	-2.06	117.23	127.53
21	1	1801	LHG	O8-C23-O10	-2.06	118.48	123.63
22	A	6011	BCR	C4-C5-C6	-2.06	119.92	122.70
18	4	4006	CLA	CBC-CAC-C3C	-2.06	106.84	112.42
18	A	1114	CLA	C4B-CHC-C1C	2.06	131.09	126.25
18	A	1105	CLA	C4B-CHC-C1C	2.06	131.08	126.25
18	A	1130	CLA	C1-O2A-CGA	2.06	121.63	116.65
27	1	1501	LUT	C8-C7-C6	-2.06	121.50	127.00
18	B	1222	CLA	CMB-C2B-C1B	2.06	128.55	125.42
27	1	1502	LUT	C40-C33-C34	-2.06	119.49	122.82
18	B	1231	CLA	C3C-C4C-NC	2.05	113.06	110.43
28	4	4011	CHL	C1C-C2C-CMC	2.05	130.50	126.80
18	B	1236	CLA	C4-C3-C5	2.05	118.79	115.23
18	A	1117	CLA	O1D-CGD-CBD	-2.05	120.47	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1012	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
26	B	8001	LMU	O5'-C1'-C2'	2.05	114.59	110.37
18	B	1217	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
18	2	2002	CLA	CHA-C4D-ND	2.05	136.78	132.55
22	B	6009	BCR	C19-C18-C17	2.05	122.24	119.01
18	A	1127	CLA	CED-O2D-CGD	2.05	120.57	115.92
22	B	6005	BCR	C27-C26-C25	-2.05	119.93	122.70
18	B	1229	CLA	C4C-C3C-C2C	-2.05	103.91	106.89
18	A	1102	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
18	A	1130	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
18	1	1001	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
22	A	6007	BCR	C33-C5-C4	2.05	117.97	113.60
18	B	1218	CLA	C3C-C4C-NC	2.05	113.06	110.43
18	1	1006	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
18	B	1223	CLA	CHA-C4D-ND	2.05	136.78	132.55
18	B	1214	CLA	C3C-C4C-NC	2.05	113.05	110.43
18	A	1110	CLA	CBA-CAA-C2A	2.05	119.89	113.79
18	G	1001	CLA	C4-C3-C2	-2.05	118.37	123.63
18	2	2008	CLA	CHC-C1C-C2C	-2.05	121.13	126.95
18	B	1012	CLA	C6-C7-C8	-2.05	109.16	115.97
18	1	1003	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
18	B	1211	CLA	C1-O2A-CGA	2.05	121.61	116.65
18	4	4004	CLA	C3C-C4C-NC	2.05	113.05	110.43
18	3	3005	CLA	CHA-C1A-NA	-2.05	121.76	126.39
27	4	4503	LUT	C10-C11-C12	-2.05	117.27	123.20
18	2	2005	CLA	O2D-CGD-O1D	-2.05	119.87	123.85
18	2	2009	CLA	CHA-C4D-ND	2.04	136.77	132.55
18	F	1302	CLA	C3C-C4C-NC	2.04	113.05	110.43
18	1	1008	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
18	B	1021	CLA	C6-C5-C3	-2.04	108.49	113.47
28	4	4013	CHL	CMD-C2D-C3D	2.04	128.76	124.68
18	G	1003	CLA	C4B-CHC-C1C	2.04	131.05	126.25
18	3	3005	CLA	C4B-CHC-C1C	2.04	131.05	126.25
28	4	4010	CHL	CMD-C2D-C3D	2.04	128.76	124.68
23	F	5001	LMG	O8-C28-C29	2.04	121.04	112.38
28	4	4011	CHL	CMD-C2D-C3D	2.04	128.76	124.68
22	B	6010	BCR	C7-C6-C5	-2.04	116.86	121.56
18	3	3008	CLA	CMC-C2C-C3C	2.04	131.66	126.15
18	1	1007	CLA	OBD-CAD-C3D	-2.04	123.65	128.42
18	1	1005	CLA	CHA-C1A-NA	-2.04	121.78	126.39
18	2	2008	CLA	C5-C3-C4	2.04	119.28	114.59
18	1	1006	CLA	O1D-CGD-CBD	-2.04	120.50	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1202	CLA	CHB-C4A-NA	2.04	127.34	124.40
18	B	1212	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
18	3	3002	CLA	C2B-C1B-NB	2.03	112.44	110.33
18	4	4017	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
18	4	4003	CLA	CBC-CAC-C3C	-2.03	106.91	112.42
18	A	1113	CLA	CMC-C2C-C1C	2.03	128.21	125.03
18	2	2005	CLA	CED-O2D-CGD	2.03	120.52	115.92
18	2	2008	CLA	CHD-C4C-C3C	-2.03	121.81	124.77
18	A	1126	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
18	4	4001	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	F	5001	LMG	C3-C4-C5	-2.03	106.55	110.23
18	2	2002	CLA	CHC-C1C-C2C	-2.03	121.18	126.95
18	B	1234	CLA	C4-C3-C2	-2.03	118.42	123.63
22	3	3503	BCR	C4-C5-C6	-2.03	119.96	122.70
27	4	4501	LUT	C7-C8-C9	-2.03	123.23	126.23
18	3	3007	CLA	C5-C3-C4	2.03	119.25	114.59
18	4	4012	CLA	CBB-CAB-C3B	-2.03	117.40	127.53
18	2	2005	CLA	CAA-C2A-C1A	-2.03	105.33	111.97
23	J	5001	LMG	O6-C1-O1	-2.03	105.25	110.04
18	1	1002	CLA	C1D-CHD-C4C	-2.03	121.71	126.02
18	B	1213	CLA	CED-O2D-CGD	2.03	120.51	115.92
18	B	1226	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
18	B	1223	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
22	B	6009	BCR	C23-C22-C21	2.02	122.19	119.01
18	3	3012	CLA	C4B-CHC-C1C	2.02	131.01	126.25
18	B	1219	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
18	3	3019	CLA	C2A-C3A-C4A	-2.02	101.27	103.58
22	A	6017	BCR	C30-C25-C24	2.02	121.13	115.65
18	A	1131	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
18	3	3018	CLA	CHA-C4D-ND	2.02	136.72	132.55
18	B	1201	CLA	CED-O2D-CGD	2.02	120.50	115.92
18	A	1101	CLA	C1-O2A-CGA	2.02	121.54	116.65
18	1	1001	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
22	A	6002	BCR	C31-C1-C6	-2.02	107.08	110.24
18	1	1014	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
18	2	2004	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
18	B	1225	CLA	CAC-C3C-C4C	2.02	127.41	124.79
18	B	1229	CLA	CMD-C2D-C3D	-2.02	123.07	127.69
18	4	4016	CLA	CHA-C4D-ND	2.02	136.71	132.55
18	2	2007	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
18	3	3001	CLA	CED-O2D-CGD	2.01	120.48	115.92
18	3	3019	CLA	C3A-C4A-CHB	-2.01	121.44	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2006	CLA	C3C-C4C-NC	2.01	113.01	110.43
18	B	1211	CLA	CHB-C4A-NA	2.01	127.30	124.40
18	4	4017	CLA	C4B-CHC-C1C	2.01	130.97	126.25
18	3	3008	CLA	CHA-C4D-ND	2.01	136.70	132.55
18	B	1225	CLA	CED-O2D-CGD	2.01	120.48	115.92
18	1	1014	CLA	CBB-CAB-C3B	-2.01	117.48	127.53
18	3	3004	CLA	CAC-C3C-C4C	2.01	127.40	124.79
18	3	3017	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
18	A	1125	CLA	CHA-C4D-ND	2.01	136.69	132.55
18	4	4007	CLA	C3C-C4C-NC	2.01	113.00	110.43
18	3	3001	CLA	CBB-CAB-C3B	-2.00	117.51	127.53
18	A	1137	CLA	C4B-CHC-C1C	2.00	130.96	126.25
18	2	2006	CLA	O1D-CGD-CBD	-2.00	120.56	124.52
18	1	1007	CLA	CHA-C4D-ND	2.00	136.68	132.55
18	A	1013	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
18	A	1113	CLA	CHC-C1C-C2C	-2.00	121.26	126.95

All (182) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	1011	CL0	ND
17	A	1011	CL0	NA
17	A	1011	CL0	NC
18	A	1013	CLA	ND
18	A	1151	CLA	ND
18	A	1237	CLA	ND
18	A	1022	CLA	ND
18	A	1102	CLA	ND
18	A	1103	CLA	ND
18	A	1104	CLA	ND
18	A	1105	CLA	ND
18	A	1106	CLA	ND
18	A	1107	CLA	ND
18	A	1108	CLA	ND
18	A	1109	CLA	ND
18	A	1110	CLA	ND
18	A	1111	CLA	ND
18	A	1112	CLA	ND
18	A	1113	CLA	ND
18	A	1114	CLA	ND
18	A	1120	CLA	ND
18	A	1121	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	1122	CLA	ND
18	A	1123	CLA	ND
18	A	1124	CLA	ND
18	A	1125	CLA	ND
18	A	1126	CLA	ND
18	A	1127	CLA	ND
18	A	1128	CLA	ND
18	A	1131	CLA	ND
18	A	1132	CLA	ND
18	A	1134	CLA	ND
18	A	1135	CLA	ND
18	A	1136	CLA	ND
18	A	1137	CLA	ND
18	A	1139	CLA	ND
18	A	1140	CLA	ND
18	A	1115	CLA	ND
18	A	1116	CLA	ND
18	A	1117	CLA	ND
18	A	1118	CLA	ND
18	A	1119	CLA	ND
18	A	1129	CLA	ND
18	A	1138	CLA	ND
18	A	1101	CLA	ND
18	B	1012	CLA	ND
18	B	1216	CLA	ND
18	B	1231	CLA	ND
18	B	1236	CLA	ND
18	B	1238	CLA	ND
18	B	1239	CLA	ND
18	B	1240	CLA	ND
18	B	1021	CLA	ND
18	B	1023	CLA	ND
18	B	1203	CLA	ND
18	B	1204	CLA	ND
18	B	1205	CLA	ND
18	B	1206	CLA	ND
18	B	1217	CLA	ND
18	B	1218	CLA	ND
18	B	1219	CLA	ND
18	B	1221	CLA	ND
18	B	1222	CLA	ND
18	B	1235	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	1201	CLA	ND
18	B	1202	CLA	ND
18	B	1208	CLA	ND
18	B	1209	CLA	ND
18	B	1210	CLA	ND
18	B	1211	CLA	ND
18	B	1212	CLA	ND
18	B	1214	CLA	ND
18	B	1215	CLA	ND
18	B	1224	CLA	ND
18	B	1225	CLA	ND
18	B	1226	CLA	ND
18	B	1227	CLA	ND
18	B	1228	CLA	ND
18	B	1229	CLA	ND
18	B	1230	CLA	ND
18	B	1232	CLA	ND
18	B	1234	CLA	ND
18	J	1302	CLA	ND
18	F	1301	CLA	ND
18	F	1302	CLA	ND
18	G	1001	CLA	ND
18	G	1002	CLA	ND
18	G	1003	CLA	ND
18	L	1501	CLA	ND
18	L	1502	CLA	ND
18	L	1503	CLA	ND
18	H	1000	CLA	ND
18	K	1001	CLA	ND
18	2	2001	CLA	ND
18	2	2002	CLA	ND
18	2	2003	CLA	ND
18	2	2004	CLA	ND
18	2	2005	CLA	ND
18	2	2006	CLA	ND
18	2	2007	CLA	ND
18	2	2008	CLA	ND
18	2	2012	CLA	ND
18	2	2016	CLA	ND
18	2	2019	CLA	ND
18	2	2009	CLA	ND
18	4	4009	CLA	ND

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Mol	Chain	Res	Type	Atom
18	4	4001	CLA	ND
18	4	4002	CLA	ND
18	4	4003	CLA	ND
18	4	4004	CLA	ND
18	4	4005	CLA	ND
18	4	4006	CLA	ND
18	4	4007	CLA	ND
18	4	4008	CLA	ND
18	4	4012	CLA	ND
18	4	4016	CLA	ND
18	4	4017	CLA	ND
18	1	1001	CLA	ND
18	1	1002	CLA	ND
18	1	1003	CLA	ND
18	1	1004	CLA	ND
18	1	1005	CLA	ND
18	1	1006	CLA	ND
18	1	1007	CLA	ND
18	1	1008	CLA	ND
18	1	1011	CLA	ND
18	1	1012	CLA	ND
18	1	1013	CLA	ND
18	1	1014	CLA	ND
18	3	3001	CLA	ND
18	3	3002	CLA	ND
18	3	3003	CLA	ND
18	3	3004	CLA	ND
18	3	3005	CLA	ND
18	3	3006	CLA	ND
18	3	3007	CLA	ND
18	3	3008	CLA	ND
18	3	3010	CLA	ND
18	3	3012	CLA	ND
18	3	3013	CLA	ND
18	3	3017	CLA	ND
18	3	3018	CLA	ND
18	3	3019	CLA	ND
27	I	6018	LUT	C26
27	2	2501	LUT	C26
27	2	2502	LUT	C26
27	4	4501	LUT	C26
27	4	4502	LUT	C26

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Mol	Chain	Res	Type	Atom
27	4	4503	LUT	C26
27	1	1501	LUT	C26
27	1	1502	LUT	C26
27	3	3501	LUT	C26
27	3	3502	LUT	C26
28	2	2010	CHL	ND
28	2	2010	CHL	NA
28	2	2010	CHL	NC
28	2	2011	CHL	ND
28	2	2011	CHL	NA
28	2	2011	CHL	NC
28	2	2013	CHL	ND
28	2	2013	CHL	NA
28	2	2013	CHL	NC
28	4	4010	CHL	ND
28	4	4010	CHL	NA
28	4	4010	CHL	NC
28	4	4011	CHL	ND
28	4	4011	CHL	NA
28	4	4011	CHL	NC
28	4	4013	CHL	ND
28	4	4013	CHL	NA
28	4	4013	CHL	NC
28	1	1009	CHL	ND
28	1	1009	CHL	NA
28	1	1009	CHL	C8
28	1	1009	CHL	NC
28	1	1010	CHL	ND
28	1	1010	CHL	NA
28	1	1010	CHL	NC
28	3	3011	CHL	ND
28	3	3011	CHL	NA
28	3	3011	CHL	C8
28	3	3011	CHL	NC

All (2376) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1151	CLA	C2B-C3B-CAB-CBB
18	A	1151	CLA	C4B-C3B-CAB-CBB
18	A	1151	CLA	CBD-CGD-O2D-CED
18	A	1237	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	A	1237	CLA	C4B-C3B-CAB-CBB
18	A	1022	CLA	C4B-C3B-CAB-CBB
18	A	1022	CLA	CBD-CGD-O2D-CED
18	A	1103	CLA	C1A-C2A-CAA-CBA
18	A	1103	CLA	CAD-CBD-CGD-O1D
18	A	1103	CLA	CAD-CBD-CGD-O2D
18	A	1104	CLA	CBD-CGD-O2D-CED
18	A	1105	CLA	C1A-C2A-CAA-CBA
18	A	1105	CLA	C3A-C2A-CAA-CBA
18	A	1105	CLA	C2-C1-O2A-CGA
18	A	1105	CLA	CBD-CGD-O2D-CED
18	A	1105	CLA	C2-C3-C5-C6
18	A	1105	CLA	C4-C3-C5-C6
18	A	1106	CLA	C3A-C2A-CAA-CBA
18	A	1106	CLA	CHA-CBD-CGD-O1D
18	A	1106	CLA	CHA-CBD-CGD-O2D
18	A	1107	CLA	C1A-C2A-CAA-CBA
18	A	1107	CLA	C2B-C3B-CAB-CBB
18	A	1107	CLA	C4B-C3B-CAB-CBB
18	A	1107	CLA	CBD-CGD-O2D-CED
18	A	1109	CLA	C1A-C2A-CAA-CBA
18	A	1109	CLA	C3A-C2A-CAA-CBA
18	A	1109	CLA	C2-C3-C5-C6
18	A	1109	CLA	C4-C3-C5-C6
18	A	1110	CLA	C1A-C2A-CAA-CBA
18	A	1110	CLA	C3A-C2A-CAA-CBA
18	A	1111	CLA	C2B-C3B-CAB-CBB
18	A	1111	CLA	C4B-C3B-CAB-CBB
18	A	1112	CLA	C1A-C2A-CAA-CBA
18	A	1112	CLA	C3A-C2A-CAA-CBA
18	A	1112	CLA	C2B-C3B-CAB-CBB
18	A	1112	CLA	C4B-C3B-CAB-CBB
18	A	1113	CLA	C4B-C3B-CAB-CBB
18	A	1114	CLA	CBA-CGA-O2A-C1
18	A	1114	CLA	O1A-CGA-O2A-C1
18	A	1114	CLA	CBD-CGD-O2D-CED
18	A	1121	CLA	CHA-CBD-CGD-O1D
18	A	1121	CLA	CHA-CBD-CGD-O2D
18	A	1122	CLA	C1A-C2A-CAA-CBA
18	A	1123	CLA	C2-C1-O2A-CGA
18	A	1123	CLA	C11-C12-C13-C14
18	A	1124	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	A	1126	CLA	C2B-C3B-CAB-CBB
18	A	1126	CLA	C4B-C3B-CAB-CBB
18	A	1128	CLA	CHA-CBD-CGD-O1D
18	A	1128	CLA	CHA-CBD-CGD-O2D
18	A	1131	CLA	C2B-C3B-CAB-CBB
18	A	1131	CLA	C4B-C3B-CAB-CBB
18	A	1131	CLA	CBD-CGD-O2D-CED
18	A	1132	CLA	C2B-C3B-CAB-CBB
18	A	1132	CLA	C4B-C3B-CAB-CBB
18	A	1133	CLA	C2B-C3B-CAB-CBB
18	A	1133	CLA	C4B-C3B-CAB-CBB
18	A	1133	CLA	CBD-CGD-O2D-CED
18	A	1135	CLA	C4-C3-C5-C6
18	A	1137	CLA	CBD-CGD-O2D-CED
18	A	1139	CLA	CBD-CGD-O2D-CED
18	A	1139	CLA	C4-C3-C5-C6
18	A	1140	CLA	C1A-C2A-CAA-CBA
18	A	1115	CLA	C2B-C3B-CAB-CBB
18	A	1115	CLA	C4B-C3B-CAB-CBB
18	A	1116	CLA	C3A-C2A-CAA-CBA
18	A	1116	CLA	CBD-CGD-O2D-CED
18	A	1117	CLA	C1A-C2A-CAA-CBA
18	A	1117	CLA	C3A-C2A-CAA-CBA
18	A	1119	CLA	C1A-C2A-CAA-CBA
18	A	1119	CLA	C2B-C3B-CAB-CBB
18	A	1119	CLA	C4B-C3B-CAB-CBB
18	A	1129	CLA	C2B-C3B-CAB-CBB
18	A	1129	CLA	C4B-C3B-CAB-CBB
18	A	1101	CLA	C2-C1-O2A-CGA
18	A	1130	CLA	CBD-CGD-O2D-CED
18	B	1012	CLA	CBD-CGD-O2D-CED
18	B	1216	CLA	C4B-C3B-CAB-CBB
18	B	1236	CLA	C4B-C3B-CAB-CBB
18	B	1238	CLA	C2-C1-O2A-CGA
18	B	1238	CLA	C4B-C3B-CAB-CBB
18	B	1239	CLA	C1A-C2A-CAA-CBA
18	B	1239	CLA	C3A-C2A-CAA-CBA
18	B	1239	CLA	CBD-CGD-O2D-CED
18	B	1240	CLA	CBD-CGD-O2D-CED
18	B	1203	CLA	C6-C7-C8-C9
18	B	1205	CLA	CBD-CGD-O2D-CED
18	B	1206	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	B	1218	CLA	C2-C1-O2A-CGA
18	B	1218	CLA	C2-C3-C5-C6
18	B	1218	CLA	C4-C3-C5-C6
18	B	1220	CLA	C2B-C3B-CAB-CBB
18	B	1220	CLA	C4B-C3B-CAB-CBB
18	B	1221	CLA	C2-C1-O2A-CGA
18	B	1221	CLA	C2B-C3B-CAB-CBB
18	B	1221	CLA	C4B-C3B-CAB-CBB
18	B	1221	CLA	CHA-CBD-CGD-O1D
18	B	1221	CLA	CHA-CBD-CGD-O2D
18	B	1222	CLA	C1A-C2A-CAA-CBA
18	B	1223	CLA	C1A-C2A-CAA-CBA
18	B	1223	CLA	C4B-C3B-CAB-CBB
18	B	1201	CLA	C1A-C2A-CAA-CBA
18	B	1201	CLA	C3A-C2A-CAA-CBA
18	B	1201	CLA	CBD-CGD-O2D-CED
18	B	1202	CLA	C3A-C2A-CAA-CBA
18	B	1202	CLA	CAD-CBD-CGD-O1D
18	B	1202	CLA	CAD-CBD-CGD-O2D
18	B	1207	CLA	C2-C1-O2A-CGA
18	B	1208	CLA	C1A-C2A-CAA-CBA
18	B	1208	CLA	C3A-C2A-CAA-CBA
18	B	1208	CLA	CHA-CBD-CGD-O1D
18	B	1208	CLA	CHA-CBD-CGD-O2D
18	B	1209	CLA	CBA-CGA-O2A-C1
18	B	1210	CLA	CBD-CGD-O2D-CED
18	B	1212	CLA	C2B-C3B-CAB-CBB
18	B	1212	CLA	C4B-C3B-CAB-CBB
18	B	1213	CLA	CBD-CGD-O2D-CED
18	B	1214	CLA	CBD-CGD-O2D-CED
18	B	1215	CLA	C3A-C2A-CAA-CBA
18	B	1215	CLA	CBD-CGD-O2D-CED
18	B	1224	CLA	C1A-C2A-CAA-CBA
18	B	1224	CLA	C3A-C2A-CAA-CBA
18	B	1224	CLA	C2B-C3B-CAB-CBB
18	B	1224	CLA	C4B-C3B-CAB-CBB
18	B	1224	CLA	CBD-CGD-O2D-CED
18	B	1225	CLA	C1A-C2A-CAA-CBA
18	B	1225	CLA	C3A-C2A-CAA-CBA
18	B	1226	CLA	C11-C12-C13-C14
18	B	1227	CLA	C2B-C3B-CAB-CBB
18	B	1227	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	B	1228	CLA	C1A-C2A-CAA-CBA
18	B	1228	CLA	C3A-C2A-CAA-CBA
18	B	1228	CLA	CBD-CGD-O2D-CED
18	B	1229	CLA	C2-C1-O2A-CGA
18	B	1230	CLA	C1A-C2A-CAA-CBA
18	B	1230	CLA	C3A-C2A-CAA-CBA
18	B	1230	CLA	C2B-C3B-CAB-CBB
18	B	1230	CLA	C4B-C3B-CAB-CBB
18	B	1230	CLA	CHA-CBD-CGD-O1D
18	B	1230	CLA	CHA-CBD-CGD-O2D
18	B	1232	CLA	CBD-CGD-O2D-CED
18	J	1302	CLA	CAD-CBD-CGD-O1D
18	J	1302	CLA	CAD-CBD-CGD-O2D
18	J	1302	CLA	CBD-CGD-O2D-CED
18	F	1302	CLA	CBD-CGD-O2D-CED
18	G	1001	CLA	C2-C1-O2A-CGA
18	G	1001	CLA	CBD-CGD-O2D-CED
18	G	1001	CLA	O1D-CGD-O2D-CED
18	G	1003	CLA	C3A-C2A-CAA-CBA
18	L	1501	CLA	C1A-C2A-CAA-CBA
18	L	1501	CLA	C2B-C3B-CAB-CBB
18	L	1501	CLA	C4B-C3B-CAB-CBB
18	L	1502	CLA	C1A-C2A-CAA-CBA
18	L	1502	CLA	C3A-C2A-CAA-CBA
18	L	1502	CLA	C2B-C3B-CAB-CBB
18	L	1502	CLA	C4B-C3B-CAB-CBB
18	L	1503	CLA	C4B-C3B-CAB-CBB
18	L	1503	CLA	CBD-CGD-O2D-CED
18	H	1000	CLA	C3A-C2A-CAA-CBA
18	H	1000	CLA	C2B-C3B-CAB-CBB
18	H	1000	CLA	C4B-C3B-CAB-CBB
18	K	1001	CLA	CBA-CGA-O2A-C1
18	2	2001	CLA	C1A-C2A-CAA-CBA
18	2	2001	CLA	C3A-C2A-CAA-CBA
18	2	2001	CLA	CBD-CGD-O2D-CED
18	2	2002	CLA	CBD-CGD-O2D-CED
18	2	2003	CLA	C4B-C3B-CAB-CBB
18	2	2003	CLA	CBD-CGD-O2D-CED
18	2	2004	CLA	C3A-C2A-CAA-CBA
18	2	2004	CLA	CHA-CBD-CGD-O1D
18	2	2004	CLA	CHA-CBD-CGD-O2D
18	2	2004	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	2	2005	CLA	C2-C1-O2A-CGA
18	2	2005	CLA	C2B-C3B-CAB-CBB
18	2	2005	CLA	C4B-C3B-CAB-CBB
18	2	2005	CLA	CBD-CGD-O2D-CED
18	2	2006	CLA	O1A-CGA-O2A-C1
18	2	2006	CLA	C2-C1-O2A-CGA
18	2	2006	CLA	CBD-CGD-O2D-CED
18	2	2007	CLA	CBD-CGD-O2D-CED
18	2	2008	CLA	C2-C1-O2A-CGA
18	2	2008	CLA	CBD-CGD-O2D-CED
18	2	2012	CLA	C2-C1-O2A-CGA
18	2	2016	CLA	C2-C1-O2A-CGA
18	2	2016	CLA	CAD-CBD-CGD-O1D
18	2	2016	CLA	CAD-CBD-CGD-O2D
18	2	2016	CLA	CBD-CGD-O2D-CED
18	2	2009	CLA	C1A-C2A-CAA-CBA
18	2	2009	CLA	C3A-C2A-CAA-CBA
18	2	2009	CLA	CBD-CGD-O2D-CED
18	4	4001	CLA	C2B-C3B-CAB-CBB
18	4	4001	CLA	C4B-C3B-CAB-CBB
18	4	4004	CLA	CHA-CBD-CGD-O1D
18	4	4004	CLA	CHA-CBD-CGD-O2D
18	4	4005	CLA	C3A-C2A-CAA-CBA
18	4	4005	CLA	C4B-C3B-CAB-CBB
18	4	4005	CLA	CHA-CBD-CGD-O2D
18	4	4006	CLA	CBD-CGD-O2D-CED
18	4	4007	CLA	CHA-CBD-CGD-O1D
18	4	4007	CLA	CHA-CBD-CGD-O2D
18	4	4008	CLA	C1A-C2A-CAA-CBA
18	4	4008	CLA	C3A-C2A-CAA-CBA
18	4	4008	CLA	CBA-CGA-O2A-C1
18	4	4016	CLA	C1A-C2A-CAA-CBA
18	4	4016	CLA	CBA-CGA-O2A-C1
18	4	4016	CLA	CBD-CGD-O2D-CED
18	4	4017	CLA	C2-C1-O2A-CGA
18	1	1001	CLA	C2B-C3B-CAB-CBB
18	1	1001	CLA	C4B-C3B-CAB-CBB
18	1	1001	CLA	CBD-CGD-O2D-CED
18	1	1002	CLA	CHA-CBD-CGD-O1D
18	1	1002	CLA	CHA-CBD-CGD-O2D
18	1	1003	CLA	CBA-CGA-O2A-C1
18	1	1003	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	1	1003	CLA	C2B-C3B-CAB-CBB
18	1	1003	CLA	C4B-C3B-CAB-CBB
18	1	1003	CLA	CBD-CGD-O2D-CED
18	1	1004	CLA	C2B-C3B-CAB-CBB
18	1	1004	CLA	C4B-C3B-CAB-CBB
18	1	1004	CLA	C11-C12-C13-C14
18	1	1006	CLA	C4B-C3B-CAB-CBB
18	1	1006	CLA	CBD-CGD-O2D-CED
18	1	1007	CLA	C4B-C3B-CAB-CBB
18	1	1007	CLA	CBD-CGD-O2D-CED
18	1	1008	CLA	CBD-CGD-O2D-CED
18	1	1011	CLA	C1A-C2A-CAA-CBA
18	1	1012	CLA	C3A-C2A-CAA-CBA
18	1	1013	CLA	CBD-CGD-O2D-CED
18	1	1014	CLA	CBA-CGA-O2A-C1
18	1	1014	CLA	CBD-CGD-O2D-CED
18	3	3002	CLA	CBD-CGD-O2D-CED
18	3	3003	CLA	C2B-C3B-CAB-CBB
18	3	3003	CLA	C4B-C3B-CAB-CBB
18	3	3003	CLA	CBD-CGD-O2D-CED
18	3	3006	CLA	CBD-CGD-O2D-CED
18	3	3007	CLA	C2B-C3B-CAB-CBB
18	3	3007	CLA	C4B-C3B-CAB-CBB
18	3	3008	CLA	C1A-C2A-CAA-CBA
18	3	3008	CLA	C3A-C2A-CAA-CBA
18	3	3008	CLA	CBD-CGD-O2D-CED
18	3	3010	CLA	CBA-CGA-O2A-C1
18	3	3010	CLA	O1A-CGA-O2A-C1
18	3	3010	CLA	CHA-CBD-CGD-O1D
18	3	3010	CLA	CHA-CBD-CGD-O2D
18	3	3012	CLA	C2-C1-O2A-CGA
18	3	3012	CLA	CBD-CGD-O2D-CED
18	3	3013	CLA	C3A-C2A-CAA-CBA
18	3	3017	CLA	CBD-CGD-O2D-CED
18	3	3018	CLA	C2-C1-O2A-CGA
21	A	5003	LHG	O2-C2-C3-O3
21	A	5003	LHG	C3-O3-P-O5
21	A	5003	LHG	C3-O3-P-O6
21	A	7001	LHG	C3-O3-P-O5
21	A	7001	LHG	C3-O3-P-O6
21	A	7001	LHG	C4-O6-P-O3
21	A	7001	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
21	A	7001	LHG	C4-O6-P-O5
21	B	5004	LHG	C3-O3-P-O4
21	B	5004	LHG	C3-O3-P-O6
21	B	5004	LHG	C4-O6-P-O3
21	B	5004	LHG	C4-O6-P-O4
21	B	5004	LHG	C8-C7-O7-C5
21	2	2801	LHG	O1-C1-C2-C3
21	2	2801	LHG	C4-O6-P-O3
21	2	2801	LHG	C4-O6-P-O4
21	2	2801	LHG	C4-O6-P-O5
21	1	1801	LHG	C3-O3-P-O4
21	1	1801	LHG	C3-O3-P-O5
21	1	1801	LHG	C3-O3-P-O6
21	1	1801	LHG	C4-O6-P-O5
21	1	1801	LHG	O9-C7-O7-C5
21	1	1801	LHG	C8-C7-O7-C5
22	A	6002	BCR	C7-C8-C9-C10
22	A	6002	BCR	C7-C8-C9-C34
22	A	6002	BCR	C11-C10-C9-C8
22	A	6002	BCR	C11-C10-C9-C34
22	A	6002	BCR	C10-C11-C12-C13
22	A	6002	BCR	C21-C22-C23-C24
22	A	6002	BCR	C37-C22-C23-C24
22	A	6003	BCR	C11-C10-C9-C8
22	A	6003	BCR	C11-C10-C9-C34
22	A	6003	BCR	C17-C18-C19-C20
22	A	6003	BCR	C36-C18-C19-C20
22	A	6003	BCR	C21-C22-C23-C24
22	A	6003	BCR	C37-C22-C23-C24
22	A	6007	BCR	C11-C10-C9-C8
22	A	6007	BCR	C11-C10-C9-C34
22	A	6007	BCR	C10-C11-C12-C13
22	A	6008	BCR	C11-C10-C9-C8
22	A	6008	BCR	C11-C10-C9-C34
22	A	6008	BCR	C10-C11-C12-C13
22	A	6011	BCR	C11-C12-C13-C14
22	A	6011	BCR	C11-C12-C13-C35
22	A	6011	BCR	C21-C22-C23-C24
22	A	6011	BCR	C37-C22-C23-C24
22	A	6017	BCR	C11-C10-C9-C8
22	A	6017	BCR	C11-C10-C9-C34
22	A	6017	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	6017	BCR	C21-C22-C23-C24
22	A	6017	BCR	C37-C22-C23-C24
22	A	6017	BCR	C23-C24-C25-C26
22	A	6017	BCR	C23-C24-C25-C30
22	B	6004	BCR	C7-C8-C9-C10
22	B	6004	BCR	C7-C8-C9-C34
22	B	6005	BCR	C11-C10-C9-C8
22	B	6005	BCR	C11-C10-C9-C34
22	B	6006	BCR	C1-C6-C7-C8
22	B	6006	BCR	C5-C6-C7-C8
22	B	6006	BCR	C21-C22-C23-C24
22	B	6009	BCR	C1-C6-C7-C8
22	B	6009	BCR	C5-C6-C7-C8
22	B	6009	BCR	C7-C8-C9-C10
22	B	6009	BCR	C7-C8-C9-C34
22	B	6010	BCR	C11-C10-C9-C8
22	B	6010	BCR	C11-C10-C9-C34
22	B	6010	BCR	C17-C18-C19-C20
22	B	6010	BCR	C36-C18-C19-C20
22	I	6020	BCR	C11-C10-C9-C8
22	I	6020	BCR	C11-C10-C9-C34
22	I	6020	BCR	C10-C11-C12-C13
22	J	6012	BCR	C7-C8-C9-C10
22	J	6012	BCR	C7-C8-C9-C34
22	J	6012	BCR	C11-C10-C9-C8
22	J	6012	BCR	C11-C10-C9-C34
22	J	6012	BCR	C10-C11-C12-C13
22	J	6012	BCR	C11-C12-C13-C14
22	J	6012	BCR	C11-C12-C13-C35
22	J	6013	BCR	C7-C8-C9-C10
22	J	6013	BCR	C7-C8-C9-C34
22	J	6013	BCR	C11-C10-C9-C8
22	J	6013	BCR	C11-C10-C9-C34
22	J	6013	BCR	C10-C11-C12-C13
22	J	6013	BCR	C21-C22-C23-C24
22	J	6013	BCR	C37-C22-C23-C24
22	F	6014	BCR	C7-C8-C9-C10
22	F	6014	BCR	C11-C10-C9-C8
22	F	6014	BCR	C11-C10-C9-C34
22	F	6014	BCR	C23-C24-C25-C30
22	F	6016	BCR	C11-C10-C9-C8
22	F	6016	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
22	F	6016	BCR	C10-C11-C12-C13
22	G	2011	BCR	C1-C6-C7-C8
22	G	2011	BCR	C5-C6-C7-C8
22	G	2011	BCR	C10-C11-C12-C13
22	L	6020	BCR	C7-C8-C9-C10
22	L	6020	BCR	C7-C8-C9-C34
22	L	6020	BCR	C11-C10-C9-C8
22	L	6020	BCR	C11-C10-C9-C34
22	L	6020	BCR	C9-C10-C11-C12
22	L	6020	BCR	C10-C11-C12-C13
22	L	6019	BCR	C5-C6-C7-C8
22	L	6019	BCR	C11-C10-C9-C8
22	L	6019	BCR	C11-C10-C9-C34
22	L	6019	BCR	C10-C11-C12-C13
22	K	2011	BCR	C7-C8-C9-C10
22	K	2011	BCR	C7-C8-C9-C34
22	3	3503	BCR	C1-C6-C7-C8
22	3	3503	BCR	C5-C6-C7-C8
22	3	3503	BCR	C7-C8-C9-C10
22	3	3503	BCR	C7-C8-C9-C34
22	3	3503	BCR	C11-C10-C9-C8
22	3	3503	BCR	C11-C10-C9-C34
22	3	3503	BCR	C10-C11-C12-C13
22	3	3503	BCR	C15-C16-C17-C18
22	3	3503	BCR	C23-C24-C25-C26
22	3	3503	BCR	C23-C24-C25-C30
23	B	5005	LMG	C11-C10-O7-C8
23	J	5001	LMG	O9-C10-O7-C8
23	4	4801	LMG	O6-C1-O1-C7
25	B	7101	DGD	C2B-C1B-O2G-C2G
25	B	7101	DGD	O1B-C1B-O2G-C2G
26	B	8002	LMU	C2'-C1'-O1'-C1
26	B	8002	LMU	C2-C1-O1'-C1'
27	I	6018	LUT	C25-C26-C27-C28
27	2	2501	LUT	C21-C26-C27-C28
27	2	2502	LUT	C21-C26-C27-C28
27	2	2502	LUT	C27-C28-C29-C30
27	2	2502	LUT	C27-C28-C29-C39
27	4	4501	LUT	C5-C6-C7-C8
27	4	4501	LUT	C21-C26-C27-C28
27	4	4502	LUT	C1-C6-C7-C8
27	4	4502	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	4	4502	LUT	C21-C26-C27-C28
27	4	4502	LUT	C25-C26-C27-C28
27	4	4503	LUT	C21-C26-C27-C28
27	4	4503	LUT	C27-C28-C29-C39
27	4	4503	LUT	C31-C32-C33-C34
27	4	4503	LUT	C31-C32-C33-C40
27	1	1501	LUT	C7-C8-C9-C10
27	1	1501	LUT	C7-C8-C9-C19
27	1	1501	LUT	C21-C26-C27-C28
27	1	1501	LUT	C27-C28-C29-C30
27	1	1501	LUT	C31-C32-C33-C34
27	1	1501	LUT	C31-C32-C33-C40
27	1	1502	LUT	C21-C26-C27-C28
27	3	3501	LUT	C21-C26-C27-C28
27	3	3501	LUT	C27-C28-C29-C30
27	3	3501	LUT	C27-C28-C29-C39
27	3	3502	LUT	C21-C26-C27-C28
27	3	3502	LUT	C25-C26-C27-C28
28	2	2013	CHL	C4C-C3C-CAC-CBC
28	4	4010	CHL	C4C-C3C-CAC-CBC
28	4	4011	CHL	C4C-C3C-CAC-CBC
28	4	4013	CHL	C2C-C3C-CAC-CBC
28	4	4013	CHL	C4C-C3C-CAC-CBC
28	1	1010	CHL	C4C-C3C-CAC-CBC
28	1	1010	CHL	CHA-CBD-CGD-O1D
28	3	3011	CHL	C2-C1-O2A-CGA
29	4	4505	ZEX	C25-C26-C27-C28
28	4	4011	CHL	C2C-C3C-CAC-CBC
18	A	1151	CLA	O1D-CGD-O2D-CED
18	A	1113	CLA	O1D-CGD-O2D-CED
18	B	1023	CLA	O1D-CGD-O2D-CED
18	B	1203	CLA	O1D-CGD-O2D-CED
18	B	1219	CLA	O1D-CGD-O2D-CED
18	B	1201	CLA	O1D-CGD-O2D-CED
18	B	1232	CLA	O1D-CGD-O2D-CED
18	L	1503	CLA	O1D-CGD-O2D-CED
18	2	2001	CLA	O1D-CGD-O2D-CED
18	2	2002	CLA	O1D-CGD-O2D-CED
18	4	4002	CLA	O1D-CGD-O2D-CED
18	4	4003	CLA	O1D-CGD-O2D-CED
18	4	4006	CLA	O1D-CGD-O2D-CED
18	1	1008	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	1	1011	CLA	O1D-CGD-O2D-CED
18	1	1012	CLA	O1D-CGD-O2D-CED
18	3	3018	CLA	O1D-CGD-O2D-CED
23	F	5001	LMG	C11-C10-O7-C8
28	4	4010	CHL	C2C-C3C-CAC-CBC
18	A	1151	CLA	C4C-C3C-CAC-CBC
18	2	2002	CLA	C4C-C3C-CAC-CBC
18	A	1104	CLA	O1D-CGD-O2D-CED
18	A	1126	CLA	O1D-CGD-O2D-CED
18	A	1115	CLA	O1D-CGD-O2D-CED
18	B	1240	CLA	O1D-CGD-O2D-CED
18	B	1210	CLA	O1D-CGD-O2D-CED
18	B	1213	CLA	O1D-CGD-O2D-CED
18	B	1226	CLA	O1D-CGD-O2D-CED
18	F	1301	CLA	O1D-CGD-O2D-CED
18	H	1000	CLA	O1D-CGD-O2D-CED
18	K	1001	CLA	O1D-CGD-O2D-CED
18	2	2007	CLA	O1D-CGD-O2D-CED
18	2	2016	CLA	O1D-CGD-O2D-CED
18	2	2009	CLA	O1D-CGD-O2D-CED
18	4	4007	CLA	O1D-CGD-O2D-CED
18	4	4016	CLA	O1D-CGD-O2D-CED
18	1	1003	CLA	O1D-CGD-O2D-CED
18	1	1007	CLA	O1D-CGD-O2D-CED
18	1	1013	CLA	O1D-CGD-O2D-CED
18	3	3003	CLA	O1D-CGD-O2D-CED
18	3	3006	CLA	O1D-CGD-O2D-CED
18	3	3012	CLA	O1D-CGD-O2D-CED
21	B	5004	LHG	O9-C7-O7-C5
23	F	5001	LMG	C29-C28-O8-C9
18	A	1013	CLA	CBD-CGD-O2D-CED
18	A	1237	CLA	CBD-CGD-O2D-CED
18	A	1106	CLA	CBD-CGD-O2D-CED
18	A	1108	CLA	CBD-CGD-O2D-CED
18	A	1109	CLA	CBD-CGD-O2D-CED
18	A	1112	CLA	CBD-CGD-O2D-CED
18	A	1113	CLA	CBD-CGD-O2D-CED
18	A	1120	CLA	CBD-CGD-O2D-CED
18	A	1121	CLA	CBD-CGD-O2D-CED
18	A	1124	CLA	CBD-CGD-O2D-CED
18	A	1126	CLA	CBD-CGD-O2D-CED
18	A	1127	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	1128	CLA	CBD-CGD-O2D-CED
18	A	1135	CLA	CBD-CGD-O2D-CED
18	A	1140	CLA	CBD-CGD-O2D-CED
18	A	1115	CLA	CBD-CGD-O2D-CED
18	A	1117	CLA	CBD-CGD-O2D-CED
18	A	1118	CLA	CBD-CGD-O2D-CED
18	A	1119	CLA	CBD-CGD-O2D-CED
18	A	1129	CLA	CBD-CGD-O2D-CED
18	A	1138	CLA	CBD-CGD-O2D-CED
18	B	1231	CLA	CBD-CGD-O2D-CED
18	B	1021	CLA	CBD-CGD-O2D-CED
18	B	1023	CLA	CBD-CGD-O2D-CED
18	B	1203	CLA	CBD-CGD-O2D-CED
18	B	1204	CLA	CBD-CGD-O2D-CED
18	B	1206	CLA	CBD-CGD-O2D-CED
18	B	1217	CLA	CBD-CGD-O2D-CED
18	B	1219	CLA	CBD-CGD-O2D-CED
18	B	1222	CLA	CBD-CGD-O2D-CED
18	B	1202	CLA	CBD-CGD-O2D-CED
18	B	1207	CLA	CBD-CGD-O2D-CED
18	B	1208	CLA	CBD-CGD-O2D-CED
18	B	1209	CLA	CBD-CGD-O2D-CED
18	B	1212	CLA	CBD-CGD-O2D-CED
18	B	1226	CLA	CBD-CGD-O2D-CED
18	B	1230	CLA	CBD-CGD-O2D-CED
18	B	1234	CLA	CBD-CGD-O2D-CED
18	F	1301	CLA	CBD-CGD-O2D-CED
18	G	1002	CLA	CBD-CGD-O2D-CED
18	L	1502	CLA	CBD-CGD-O2D-CED
18	H	1000	CLA	CBD-CGD-O2D-CED
18	K	1001	CLA	CBD-CGD-O2D-CED
18	2	2012	CLA	CBD-CGD-O2D-CED
18	4	4002	CLA	CBD-CGD-O2D-CED
18	4	4003	CLA	CBD-CGD-O2D-CED
18	4	4005	CLA	CBD-CGD-O2D-CED
18	4	4007	CLA	CBD-CGD-O2D-CED
18	1	1004	CLA	CBD-CGD-O2D-CED
18	1	1011	CLA	CBD-CGD-O2D-CED
18	1	1012	CLA	CBD-CGD-O2D-CED
18	3	3001	CLA	CBD-CGD-O2D-CED
18	3	3004	CLA	CBD-CGD-O2D-CED
18	3	3005	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	3	3018	CLA	CBD-CGD-O2D-CED
18	A	1237	CLA	O1A-CGA-O2A-C1
18	A	1133	CLA	O1A-CGA-O2A-C1
18	B	1222	CLA	O1A-CGA-O2A-C1
18	B	1234	CLA	O1A-CGA-O2A-C1
18	4	4008	CLA	O1A-CGA-O2A-C1
18	4	4016	CLA	O1A-CGA-O2A-C1
18	1	1014	CLA	O1A-CGA-O2A-C1
18	3	3013	CLA	O1A-CGA-O2A-C1
18	2	2007	CLA	C4C-C3C-CAC-CBC
18	F	1302	CLA	C2C-C3C-CAC-CBC
18	2	2002	CLA	C2C-C3C-CAC-CBC
18	B	1205	CLA	O1D-CGD-O2D-CED
18	3	3017	CLA	O1D-CGD-O2D-CED
18	A	1118	CLA	CBA-CGA-O2A-C1
18	G	1002	CLA	CBA-CGA-O2A-C1
18	1	1002	CLA	CBA-CGA-O2A-C1
18	3	3013	CLA	CBA-CGA-O2A-C1
18	A	1237	CLA	O1D-CGD-O2D-CED
18	A	1109	CLA	O1D-CGD-O2D-CED
18	A	1120	CLA	O1D-CGD-O2D-CED
18	B	1231	CLA	O1D-CGD-O2D-CED
18	B	1021	CLA	O1D-CGD-O2D-CED
18	B	1206	CLA	O1D-CGD-O2D-CED
18	3	3005	CLA	O1D-CGD-O2D-CED
18	A	1237	CLA	CBA-CGA-O2A-C1
18	A	1120	CLA	CBA-CGA-O2A-C1
18	A	1133	CLA	CBA-CGA-O2A-C1
18	B	1222	CLA	CBA-CGA-O2A-C1
18	B	1232	CLA	CBA-CGA-O2A-C1
18	A	1122	CLA	CBD-CGD-O2D-CED
18	A	1125	CLA	CBD-CGD-O2D-CED
18	B	1235	CLA	CBD-CGD-O2D-CED
18	B	1229	CLA	CBD-CGD-O2D-CED
18	A	1102	CLA	O1A-CGA-O2A-C1
18	A	1120	CLA	O1A-CGA-O2A-C1
18	B	1232	CLA	O1A-CGA-O2A-C1
18	F	1302	CLA	O1A-CGA-O2A-C1
18	2	2009	CLA	O1A-CGA-O2A-C1
18	4	4002	CLA	O1A-CGA-O2A-C1
18	4	4003	CLA	O1A-CGA-O2A-C1
18	4	4007	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	4	4012	CLA	O1A-CGA-O2A-C1
18	3	3018	CLA	O1A-CGA-O2A-C1
18	A	1126	CLA	C10-C11-C12-C13
18	A	1115	CLA	O1A-CGA-O2A-C1
18	B	1209	CLA	O1A-CGA-O2A-C1
18	G	1002	CLA	O1A-CGA-O2A-C1
18	K	1001	CLA	O1A-CGA-O2A-C1
18	1	1013	CLA	O1A-CGA-O2A-C1
18	F	1302	CLA	C4C-C3C-CAC-CBC
18	A	1151	CLA	C2C-C3C-CAC-CBC
18	A	1105	CLA	O1D-CGD-O2D-CED
18	A	1131	CLA	O1D-CGD-O2D-CED
18	A	1137	CLA	O1D-CGD-O2D-CED
18	A	1116	CLA	O1D-CGD-O2D-CED
18	B	1012	CLA	O1D-CGD-O2D-CED
18	B	1207	CLA	O1D-CGD-O2D-CED
18	B	1214	CLA	O1D-CGD-O2D-CED
18	B	1228	CLA	O1D-CGD-O2D-CED
18	F	1302	CLA	O1D-CGD-O2D-CED
18	2	2005	CLA	O1D-CGD-O2D-CED
18	2	2006	CLA	O1D-CGD-O2D-CED
18	2	2012	CLA	O1D-CGD-O2D-CED
18	1	1001	CLA	O1D-CGD-O2D-CED
18	1	1006	CLA	O1D-CGD-O2D-CED
18	3	3018	CLA	C4C-C3C-CAC-CBC
18	2	2007	CLA	C2C-C3C-CAC-CBC
18	4	4007	CLA	C2C-C3C-CAC-CBC
18	A	1107	CLA	O1D-CGD-O2D-CED
18	A	1114	CLA	O1D-CGD-O2D-CED
18	A	1133	CLA	O1D-CGD-O2D-CED
18	A	1139	CLA	O1D-CGD-O2D-CED
18	B	1215	CLA	O1D-CGD-O2D-CED
18	B	1224	CLA	O1D-CGD-O2D-CED
18	2	2003	CLA	O1D-CGD-O2D-CED
18	2	2008	CLA	O1D-CGD-O2D-CED
18	1	1014	CLA	O1D-CGD-O2D-CED
18	3	3002	CLA	O1D-CGD-O2D-CED
18	3	3008	CLA	O1D-CGD-O2D-CED
18	A	1124	CLA	O1A-CGA-O2A-C1
18	A	1135	CLA	O1A-CGA-O2A-C1
18	3	3005	CLA	O1A-CGA-O2A-C1
18	3	3018	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	B	5005	LMG	O9-C10-O7-C8
18	A	1108	CLA	CBA-CGA-O2A-C1
18	A	1115	CLA	CBA-CGA-O2A-C1
18	B	1217	CLA	CBA-CGA-O2A-C1
18	1	1013	CLA	CBA-CGA-O2A-C1
18	A	1108	CLA	O1A-CGA-O2A-C1
23	J	5001	LMG	C4-C5-C6-O5
18	A	1013	CLA	C3-C5-C6-C7
18	A	1103	CLA	C3-C5-C6-C7
18	A	1107	CLA	C3-C5-C6-C7
18	A	1131	CLA	C3-C5-C6-C7
18	B	1203	CLA	C3-C5-C6-C7
18	B	1226	CLA	C3-C5-C6-C7
18	G	1001	CLA	C3-C5-C6-C7
18	G	1003	CLA	C3-C5-C6-C7
18	L	1502	CLA	C3-C5-C6-C7
18	2	2001	CLA	C3-C5-C6-C7
18	4	4003	CLA	C3-C5-C6-C7
18	4	4007	CLA	C4C-C3C-CAC-CBC
18	A	1022	CLA	O1D-CGD-O2D-CED
18	B	1204	CLA	O1D-CGD-O2D-CED
18	A	1102	CLA	CBA-CGA-O2A-C1
18	A	1116	CLA	CBA-CGA-O2A-C1
18	B	1204	CLA	CBA-CGA-O2A-C1
18	B	1234	CLA	CBA-CGA-O2A-C1
18	F	1302	CLA	CBA-CGA-O2A-C1
18	2	2006	CLA	CBA-CGA-O2A-C1
18	2	2009	CLA	CBA-CGA-O2A-C1
18	4	4001	CLA	CBA-CGA-O2A-C1
18	4	4003	CLA	CBA-CGA-O2A-C1
18	4	4007	CLA	CBA-CGA-O2A-C1
18	3	3018	CLA	CBA-CGA-O2A-C1
23	F	5001	LMG	O10-C28-O8-C9
18	A	1103	CLA	CBD-CGD-O2D-CED
18	B	1216	CLA	CBD-CGD-O2D-CED
18	B	1238	CLA	CBD-CGD-O2D-CED
18	B	1225	CLA	CBD-CGD-O2D-CED
18	G	1003	CLA	CBD-CGD-O2D-CED
18	L	1501	CLA	CBD-CGD-O2D-CED
18	4	4008	CLA	CBD-CGD-O2D-CED
18	4	4012	CLA	CBD-CGD-O2D-CED
18	4	4017	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	3	3013	CLA	CBD-CGD-O2D-CED
23	J	5001	LMG	C11-C10-O7-C8
18	3	3002	CLA	C2C-C3C-CAC-CBC
18	A	1013	CLA	O1D-CGD-O2D-CED
18	A	1140	CLA	O1D-CGD-O2D-CED
18	A	1130	CLA	O1D-CGD-O2D-CED
18	J	1302	CLA	O1D-CGD-O2D-CED
18	2	2012	CLA	O1A-CGA-O2A-C1
18	1	1006	CLA	O1A-CGA-O2A-C1
18	A	1113	CLA	O1A-CGA-O2A-C1
18	A	1118	CLA	O1A-CGA-O2A-C1
18	B	1217	CLA	O1A-CGA-O2A-C1
18	1	1002	CLA	O1A-CGA-O2A-C1
18	4	4016	CLA	C2C-C3C-CAC-CBC
18	B	1239	CLA	O1D-CGD-O2D-CED
18	B	1212	CLA	O1D-CGD-O2D-CED
18	A	1120	CLA	C4-C3-C5-C6
18	A	1122	CLA	C4-C3-C5-C6
18	A	1137	CLA	C4-C3-C5-C6
18	A	1140	CLA	C4-C3-C5-C6
18	A	1116	CLA	C4-C3-C5-C6
18	A	1101	CLA	C4-C3-C5-C6
18	B	1207	CLA	C4-C3-C5-C6
18	B	1208	CLA	C4-C3-C5-C6
18	B	1213	CLA	C4-C3-C5-C6
18	B	1215	CLA	C4-C3-C5-C6
18	B	1230	CLA	C4-C3-C5-C6
18	2	2001	CLA	C4-C3-C5-C6
18	2	2005	CLA	C4-C3-C5-C6
18	2	2006	CLA	C4-C3-C5-C6
18	2	2007	CLA	C4-C3-C5-C6
18	3	3010	CLA	C4-C3-C5-C6
20	B	5002	PQN	C14-C13-C15-C16
18	A	1120	CLA	C2-C3-C5-C6
18	A	1122	CLA	C2-C3-C5-C6
18	A	1137	CLA	C2-C3-C5-C6
18	A	1139	CLA	C2-C3-C5-C6
18	B	1207	CLA	C2-C3-C5-C6
18	B	1208	CLA	C2-C3-C5-C6
18	B	1213	CLA	C2-C3-C5-C6
18	B	1215	CLA	C2-C3-C5-C6
18	B	1230	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	2	2001	CLA	C2-C3-C5-C6
18	2	2004	CLA	C2-C3-C5-C6
18	2	2005	CLA	C2-C3-C5-C6
18	2	2007	CLA	C2-C3-C5-C6
20	B	5002	PQN	C12-C13-C15-C16
18	A	1113	CLA	CBA-CGA-O2A-C1
18	1	1007	CLA	CBA-CGA-O2A-C1
18	A	1121	CLA	O1D-CGD-O2D-CED
18	A	1124	CLA	O1D-CGD-O2D-CED
18	B	1214	CLA	C2A-CAA-CBA-CGA
18	4	4008	CLA	C2A-CAA-CBA-CGA
28	4	4010	CHL	C2A-CAA-CBA-CGA
18	A	1104	CLA	O1A-CGA-O2A-C1
18	A	1106	CLA	C3-C5-C6-C7
18	A	1120	CLA	C3-C5-C6-C7
18	A	1134	CLA	C3-C5-C6-C7
18	B	1204	CLA	C3-C5-C6-C7
18	B	1220	CLA	C3-C5-C6-C7
18	2	2004	CLA	C3-C5-C6-C7
18	1	1003	CLA	C3-C5-C6-C7
28	1	1010	CHL	C2C-C3C-CAC-CBC
18	2	2008	CLA	C2C-C3C-CAC-CBC
18	A	1104	CLA	CBA-CGA-O2A-C1
18	A	1112	CLA	CBA-CGA-O2A-C1
18	A	1124	CLA	CBA-CGA-O2A-C1
18	A	1135	CLA	CBA-CGA-O2A-C1
18	A	1130	CLA	CBA-CGA-O2A-C1
18	B	1211	CLA	CBA-CGA-O2A-C1
18	B	1230	CLA	CBA-CGA-O2A-C1
18	4	4002	CLA	CBA-CGA-O2A-C1
18	4	4012	CLA	CBA-CGA-O2A-C1
18	3	3005	CLA	CBA-CGA-O2A-C1
18	3	3012	CLA	CBA-CGA-O2A-C1
21	1	1801	LHG	C24-C23-O8-C6
23	F	5001	LMG	O9-C10-O7-C8
18	1	1007	CLA	O1A-CGA-O2A-C1
23	J	5001	LMG	O6-C5-C6-O5
23	F	5001	LMG	O6-C5-C6-O5
26	B	8001	LMU	O5B-C5B-C6B-O6B
22	A	6003	BCR	C9-C10-C11-C12
22	L	6020	BCR	C19-C20-C21-C22
22	3	3503	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	A	1112	CLA	O1A-CGA-O2A-C1
18	B	1204	CLA	O1A-CGA-O2A-C1
18	B	1211	CLA	O1A-CGA-O2A-C1
18	B	1227	CLA	O1A-CGA-O2A-C1
18	B	1230	CLA	O1A-CGA-O2A-C1
18	4	4009	CLA	O1A-CGA-O2A-C1
18	3	3007	CLA	C2C-C3C-CAC-CBC
18	A	1108	CLA	O1D-CGD-O2D-CED
18	B	1222	CLA	O1D-CGD-O2D-CED
18	B	1234	CLA	O1D-CGD-O2D-CED
26	B	8002	LMU	O5B-C5B-C6B-O6B
18	A	1106	CLA	O1D-CGD-O2D-CED
18	A	1117	CLA	O1D-CGD-O2D-CED
18	A	1129	CLA	O1D-CGD-O2D-CED
18	B	1202	CLA	O1D-CGD-O2D-CED
18	A	1124	CLA	C3-C5-C6-C7
18	A	1138	CLA	C3-C5-C6-C7
18	B	1205	CLA	C3-C5-C6-C7
18	B	1218	CLA	C3-C5-C6-C7
18	A	1102	CLA	CBD-CGD-O2D-CED
18	A	1110	CLA	CBD-CGD-O2D-CED
18	4	4016	CLA	C4C-C3C-CAC-CBC
21	B	5004	LHG	O2-C2-C3-O3
21	2	2801	LHG	O2-C2-C3-O3
18	A	1127	CLA	O1D-CGD-O2D-CED
18	B	1217	CLA	O1D-CGD-O2D-CED
18	B	1209	CLA	O1D-CGD-O2D-CED
18	G	1002	CLA	O1D-CGD-O2D-CED
18	L	1502	CLA	O1D-CGD-O2D-CED
18	4	4005	CLA	O1D-CGD-O2D-CED
18	3	3001	CLA	O1D-CGD-O2D-CED
18	A	1101	CLA	CBA-CGA-O2A-C1
18	B	1227	CLA	CBA-CGA-O2A-C1
18	2	2005	CLA	CBA-CGA-O2A-C1
18	2	2012	CLA	CBA-CGA-O2A-C1
18	4	4009	CLA	CBA-CGA-O2A-C1
18	4	4006	CLA	CBA-CGA-O2A-C1
23	B	5005	LMG	C29-C28-O8-C9
18	A	1116	CLA	O1A-CGA-O2A-C1
18	4	4001	CLA	O1A-CGA-O2A-C1
23	F	5001	LMG	C4-C5-C6-O5
18	3	3002	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
18	4	4008	CLA	C2C-C3C-CAC-CBC
18	1	1002	CLA	C2C-C3C-CAC-CBC
18	3	3008	CLA	C2C-C3C-CAC-CBC
18	A	1135	CLA	O1D-CGD-O2D-CED
18	A	1138	CLA	O1D-CGD-O2D-CED
18	B	1208	CLA	O1D-CGD-O2D-CED
18	1	1004	CLA	O1D-CGD-O2D-CED
18	A	1111	CLA	CBD-CGD-O2D-CED
18	B	1236	CLA	CBD-CGD-O2D-CED
18	1	1008	CLA	CBA-CGA-O2A-C1
18	B	1230	CLA	O1D-CGD-O2D-CED
18	1	1007	CLA	C2C-C3C-CAC-CBC
18	A	1119	CLA	O1D-CGD-O2D-CED
18	B	1219	CLA	C3-C5-C6-C7
18	B	1234	CLA	C3-C5-C6-C7
18	A	1128	CLA	O1D-CGD-O2D-CED
18	A	1118	CLA	O1D-CGD-O2D-CED
18	3	3004	CLA	O1D-CGD-O2D-CED
18	2	2007	CLA	CBA-CGA-O2A-C1
18	1	1006	CLA	CBA-CGA-O2A-C1
23	J	5001	LMG	C29-C28-O8-C9
18	A	1121	CLA	C4-C3-C5-C6
18	B	1222	CLA	C4-C3-C5-C6
18	B	1225	CLA	C4-C3-C5-C6
18	4	4001	CLA	C4-C3-C5-C6
18	A	1121	CLA	C2-C3-C5-C6
18	A	1140	CLA	C2-C3-C5-C6
18	B	1222	CLA	C2-C3-C5-C6
18	B	1225	CLA	C2-C3-C5-C6
18	2	2006	CLA	C2-C3-C5-C6
18	4	4001	CLA	C2-C3-C5-C6
20	A	5001	PQN	C12-C13-C15-C16
21	B	5004	LHG	C24-C23-O8-C6
18	A	1130	CLA	O1A-CGA-O2A-C1
18	2	2005	CLA	O1A-CGA-O2A-C1
21	1	1801	LHG	O10-C23-O8-C6
21	2	2801	LHG	C2-C3-O3-P
23	F	5002	LMG	O6-C5-C6-O5
18	A	1105	CLA	C2A-CAA-CBA-CGA
18	B	1208	CLA	C2A-CAA-CBA-CGA
18	K	1001	CLA	C2C-C3C-CAC-CBC
18	A	1112	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	1101	CLA	O1A-CGA-O2A-C1
18	L	1503	CLA	O1A-CGA-O2A-C1
18	2	2007	CLA	O1A-CGA-O2A-C1
18	4	4006	CLA	O1A-CGA-O2A-C1
18	3	3012	CLA	O1A-CGA-O2A-C1
23	B	5005	LMG	O10-C28-O8-C9
23	J	5001	LMG	O10-C28-O8-C9
23	B	5005	LMG	O6-C1-O1-C7
18	2	2008	CLA	C4C-C3C-CAC-CBC
18	A	1136	CLA	CBA-CGA-O2A-C1
18	A	1137	CLA	CBA-CGA-O2A-C1
18	B	1235	CLA	CBA-CGA-O2A-C1
18	B	1226	CLA	CBA-CGA-O2A-C1
18	L	1503	CLA	CBA-CGA-O2A-C1
18	1	1001	CLA	C2C-C3C-CAC-CBC
18	3	3002	CLA	CBA-CGA-O2A-C1
23	B	5005	LMG	O6-C5-C6-O5
18	A	1122	CLA	O1D-CGD-O2D-CED
18	A	1125	CLA	O1D-CGD-O2D-CED
23	F	5002	LMG	C4-C5-C6-O5
18	B	1207	CLA	C3-C5-C6-C7
26	B	8002	LMU	C4B-C5B-C6B-O6B
22	A	6008	BCR	C15-C16-C17-C18
22	K	2011	BCR	C19-C20-C21-C22
18	A	1137	CLA	O1A-CGA-O2A-C1
18	B	1226	CLA	O1A-CGA-O2A-C1
18	3	3008	CLA	O1A-CGA-O2A-C1
18	3	3012	CLA	C2C-C3C-CAC-CBC
21	B	5004	LHG	C1-C2-C3-O3
18	A	1123	CLA	CBA-CGA-O2A-C1
18	A	1125	CLA	CBA-CGA-O2A-C1
18	A	1128	CLA	CBA-CGA-O2A-C1
18	A	1132	CLA	CBA-CGA-O2A-C1
18	A	1117	CLA	CBA-CGA-O2A-C1
18	A	1129	CLA	CBA-CGA-O2A-C1
18	B	1231	CLA	CBA-CGA-O2A-C1
18	B	1240	CLA	CBA-CGA-O2A-C1
18	B	1219	CLA	CBA-CGA-O2A-C1
18	B	1202	CLA	CBA-CGA-O2A-C1
18	B	1210	CLA	CBA-CGA-O2A-C1
18	B	1215	CLA	CBA-CGA-O2A-C1
18	J	1302	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	G	1001	CLA	CBA-CGA-O2A-C1
18	2	2004	CLA	CBA-CGA-O2A-C1
18	2	2008	CLA	CBA-CGA-O2A-C1
18	4	4017	CLA	CBA-CGA-O2A-C1
18	1	1004	CLA	CBA-CGA-O2A-C1
18	1	1005	CLA	CBA-CGA-O2A-C1
18	3	3006	CLA	CBA-CGA-O2A-C1
18	3	3008	CLA	CBA-CGA-O2A-C1
23	G	2021	LMG	C29-C28-O8-C9
23	4	4801	LMG	C29-C28-O8-C9
23	G	2021	LMG	O6-C5-C6-O5
18	B	1220	CLA	CBD-CGD-O2D-CED
18	B	1235	CLA	O1D-CGD-O2D-CED
18	B	1229	CLA	O1D-CGD-O2D-CED
18	3	3005	CLA	C4-C3-C5-C6
20	A	5001	PQN	C14-C13-C15-C16
18	A	1116	CLA	C2-C3-C5-C6
18	A	1101	CLA	C2-C3-C5-C6
18	3	3005	CLA	C2-C3-C5-C6
18	3	3010	CLA	C2-C3-C5-C6
18	4	4001	CLA	C3-C5-C6-C7
18	A	1237	CLA	C11-C10-C8-C9
18	A	1103	CLA	C14-C13-C15-C16
18	A	1112	CLA	C11-C10-C8-C9
18	A	1120	CLA	C11-C10-C8-C9
18	A	1122	CLA	C11-C12-C13-C14
18	A	1139	CLA	C11-C12-C13-C14
18	A	1140	CLA	C11-C10-C8-C9
18	A	1119	CLA	C11-C12-C13-C14
18	B	1220	CLA	C14-C13-C15-C16
18	B	1221	CLA	C11-C12-C13-C14
18	B	1222	CLA	C6-C7-C8-C9
18	B	1207	CLA	C6-C7-C8-C9
18	B	1226	CLA	C14-C13-C15-C16
18	2	2001	CLA	C6-C7-C8-C9
18	4	4001	CLA	C6-C7-C8-C9
18	4	4003	CLA	C6-C7-C8-C9
18	1	1001	CLA	C11-C10-C8-C9
23	B	5005	LMG	C4-C5-C6-O5
26	B	8001	LMU	C4B-C5B-C6B-O6B
18	B	1225	CLA	O1D-CGD-O2D-CED
18	3	3013	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	5005	LMG	C2-C1-O1-C7
26	B	8001	LMU	C2'-C1'-O1'-C1
21	A	5003	LHG	C23-C24-C25-C26
18	A	1129	CLA	O1A-CGA-O2A-C1
18	3	3006	CLA	O1A-CGA-O2A-C1
18	4	4012	CLA	O1D-CGD-O2D-CED
22	A	6003	BCR	C7-C8-C9-C34
22	A	6011	BCR	C7-C8-C9-C34
22	B	6006	BCR	C7-C8-C9-C34
22	B	6006	BCR	C37-C22-C23-C24
22	B	6010	BCR	C7-C8-C9-C34
22	F	6014	BCR	C7-C8-C9-C34
22	F	6014	BCR	C37-C22-C23-C24
22	G	2011	BCR	C37-C22-C23-C24
22	L	6019	BCR	C7-C8-C9-C34
27	4	4502	LUT	C27-C28-C29-C39
27	4	4503	LUT	C7-C8-C9-C19
27	1	1501	LUT	C27-C28-C29-C39
27	3	3501	LUT	C7-C8-C9-C19
27	3	3502	LUT	C7-C8-C9-C19
22	A	6003	BCR	C7-C8-C9-C10
22	A	6011	BCR	C7-C8-C9-C10
22	B	6006	BCR	C7-C8-C9-C10
22	B	6010	BCR	C7-C8-C9-C10
22	F	6014	BCR	C21-C22-C23-C24
22	G	2011	BCR	C21-C22-C23-C24
22	L	6019	BCR	C7-C8-C9-C10
27	4	4502	LUT	C27-C28-C29-C30
27	4	4503	LUT	C7-C8-C9-C10
27	4	4503	LUT	C27-C28-C29-C30
27	3	3501	LUT	C7-C8-C9-C10
27	3	3502	LUT	C7-C8-C9-C10
18	A	1115	CLA	C2A-CAA-CBA-CGA
18	3	3013	CLA	C2A-CAA-CBA-CGA
18	3	3013	CLA	C2C-C3C-CAC-CBC
21	A	7001	LHG	C23-C24-C25-C26
21	1	1801	LHG	C23-C24-C25-C26
18	1	1008	CLA	O1A-CGA-O2A-C1
18	A	1128	CLA	O1A-CGA-O2A-C1
18	B	1219	CLA	O1A-CGA-O2A-C1
18	B	1202	CLA	O1A-CGA-O2A-C1
18	B	1210	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	J	1302	CLA	O1A-CGA-O2A-C1
18	2	2008	CLA	O1A-CGA-O2A-C1
18	1	1004	CLA	O1A-CGA-O2A-C1
18	G	1002	CLA	C2C-C3C-CAC-CBC
18	B	1216	CLA	O1D-CGD-O2D-CED
18	A	1119	CLA	CBA-CGA-O2A-C1
18	B	1201	CLA	CBA-CGA-O2A-C1
18	B	1207	CLA	CBA-CGA-O2A-C1
18	1	1011	CLA	CBA-CGA-O2A-C1
18	A	1107	CLA	C13-C15-C16-C17
18	B	1203	CLA	C8-C10-C11-C12
18	A	1022	CLA	C2-C1-O2A-CGA
18	A	1103	CLA	C2-C1-O2A-CGA
18	A	1104	CLA	C2-C1-O2A-CGA
18	A	1112	CLA	C2-C1-O2A-CGA
18	A	1120	CLA	C2-C1-O2A-CGA
18	A	1137	CLA	C2-C1-O2A-CGA
18	A	1139	CLA	C2-C1-O2A-CGA
18	A	1140	CLA	C2-C1-O2A-CGA
18	A	1119	CLA	C2-C1-O2A-CGA
18	B	1012	CLA	C2-C1-O2A-CGA
18	B	1203	CLA	C2-C1-O2A-CGA
18	B	1230	CLA	C2-C1-O2A-CGA
18	J	1302	CLA	C2-C1-O2A-CGA
18	1	1011	CLA	C2-C1-O2A-CGA
18	B	1240	CLA	O1A-CGA-O2A-C1
18	4	4008	CLA	O1D-CGD-O2D-CED
18	3	3007	CLA	C4C-C3C-CAC-CBC
18	A	1123	CLA	C10-C11-C12-C13
18	A	1132	CLA	C13-C15-C16-C17
18	B	1240	CLA	C15-C16-C17-C18
18	B	1220	CLA	C8-C10-C11-C12
18	B	1220	CLA	C10-C11-C12-C13
18	B	1229	CLA	C13-C15-C16-C17
21	A	5003	LHG	O1-C1-C2-O2
21	B	5004	LHG	O1-C1-C2-O2
18	B	1012	CLA	C3-C5-C6-C7
18	B	1206	CLA	C3-C5-C6-C7
18	2	2012	CLA	C3-C5-C6-C7
18	2	2016	CLA	C2C-C3C-CAC-CBC
18	B	1238	CLA	O1D-CGD-O2D-CED
18	A	1117	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	4	4801	LMG	O10-C28-O8-C9
18	B	1216	CLA	C8-C10-C11-C12
18	3	3010	CLA	CBD-CGD-O2D-CED
23	G	2021	LMG	C4-C5-C6-O5
18	A	1104	CLA	C12-C13-C15-C16
18	A	1122	CLA	C11-C10-C8-C7
18	B	1223	CLA	C11-C10-C8-C7
18	A	1139	CLA	C15-C16-C17-C18
21	B	5004	LHG	O10-C23-O8-C6
22	A	6017	BCR	C9-C10-C11-C12
27	I	6018	LUT	C13-C14-C15-C35
27	1	1501	LUT	C29-C30-C31-C32
27	1	1502	LUT	C13-C14-C15-C35
18	3	3008	CLA	C4C-C3C-CAC-CBC
18	A	1120	CLA	C8-C10-C11-C12
18	A	1127	CLA	C5-C6-C7-C8
18	B	1221	CLA	C15-C16-C17-C18
18	B	1214	CLA	C5-C6-C7-C8
18	B	1227	CLA	C13-C15-C16-C17
18	B	1232	CLA	C5-C6-C7-C8
18	3	3010	CLA	C10-C11-C12-C13
20	B	5002	PQN	C25-C26-C27-C28
18	1	1011	CLA	C2C-C3C-CAC-CBC
23	G	2021	LMG	C28-C29-C30-C31
18	A	1123	CLA	O1A-CGA-O2A-C1
18	A	1136	CLA	O1A-CGA-O2A-C1
18	B	1231	CLA	O1A-CGA-O2A-C1
18	B	1235	CLA	O1A-CGA-O2A-C1
18	B	1201	CLA	O1A-CGA-O2A-C1
18	1	1005	CLA	O1A-CGA-O2A-C1
18	1	1011	CLA	O1A-CGA-O2A-C1
18	A	1103	CLA	O1D-CGD-O2D-CED
18	L	1501	CLA	O1D-CGD-O2D-CED
18	4	4017	CLA	O1D-CGD-O2D-CED
18	A	1151	CLA	CBA-CGA-O2A-C1
18	A	1022	CLA	C10-C11-C12-C13
18	A	1106	CLA	C13-C15-C16-C17
18	A	1112	CLA	C13-C15-C16-C17
18	A	1123	CLA	C13-C15-C16-C17
18	A	1131	CLA	C8-C10-C11-C12
18	B	1203	CLA	C13-C15-C16-C17
18	B	1224	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	B	1225	CLA	C15-C16-C17-C18
18	B	1228	CLA	C10-C11-C12-C13
18	4	4003	CLA	C15-C16-C17-C18
20	B	5002	PQN	C23-C25-C26-C27
18	A	1109	CLA	C2A-CAA-CBA-CGA
18	A	1129	CLA	C2A-CAA-CBA-CGA
18	B	1239	CLA	C2A-CAA-CBA-CGA
18	G	1001	CLA	C2A-CAA-CBA-CGA
18	G	1003	CLA	C2A-CAA-CBA-CGA
18	L	1502	CLA	C2A-CAA-CBA-CGA
18	H	1000	CLA	C2A-CAA-CBA-CGA
18	1	1011	CLA	C2A-CAA-CBA-CGA
18	1	1014	CLA	C2A-CAA-CBA-CGA
28	3	3011	CHL	C2A-CAA-CBA-CGA
22	A	6011	BCR	C10-C11-C12-C13
22	F	6014	BCR	C10-C11-C12-C13
18	A	1104	CLA	C15-C16-C17-C18
18	A	1128	CLA	C5-C6-C7-C8
18	A	1132	CLA	C8-C10-C11-C12
18	A	1119	CLA	C10-C11-C12-C13
18	A	1119	CLA	C13-C15-C16-C17
18	B	1021	CLA	C15-C16-C17-C18
18	B	1203	CLA	C5-C6-C7-C8
18	B	1204	CLA	C5-C6-C7-C8
18	B	1221	CLA	C10-C11-C12-C13
18	B	1223	CLA	C15-C16-C17-C18
18	B	1225	CLA	C5-C6-C7-C8
18	B	1226	CLA	C8-C10-C11-C12
18	B	1230	CLA	C5-C6-C7-C8
18	L	1502	CLA	C10-C11-C12-C13
18	2	2004	CLA	C15-C16-C17-C18
18	2	2007	CLA	C10-C11-C12-C13
18	2	2012	CLA	C5-C6-C7-C8
18	4	4012	CLA	C8-C10-C11-C12
21	A	7001	LHG	C7-C8-C9-C10
21	1	1801	LHG	C7-C8-C9-C10
18	G	1003	CLA	O1D-CGD-O2D-CED
18	A	1125	CLA	O1A-CGA-O2A-C1
18	2	2004	CLA	O1A-CGA-O2A-C1
18	4	4017	CLA	O1A-CGA-O2A-C1
26	B	8001	LMU	O5'-C1'-O1'-C1
18	A	1112	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	A	1122	CLA	C13-C15-C16-C17
18	A	1132	CLA	C10-C11-C12-C13
18	B	1012	CLA	C13-C15-C16-C17
18	B	1021	CLA	C13-C15-C16-C17
18	B	1205	CLA	C10-C11-C12-C13
18	B	1218	CLA	C8-C10-C11-C12
18	B	1221	CLA	C8-C10-C11-C12
18	B	1207	CLA	C8-C10-C11-C12
18	B	1210	CLA	C15-C16-C17-C18
18	2	2001	CLA	C10-C11-C12-C13
18	4	4004	CLA	C8-C10-C11-C12
18	4	4005	CLA	C8-C10-C11-C12
18	1	1004	CLA	C13-C15-C16-C17
18	4	4008	CLA	C4C-C3C-CAC-CBC
18	4	4003	CLA	C2C-C3C-CAC-CBC
18	L	1502	CLA	CBA-CGA-O2A-C1
23	F	5002	LMG	C29-C28-O8-C9
18	A	1132	CLA	O1A-CGA-O2A-C1
18	B	1207	CLA	O1A-CGA-O2A-C1
18	B	1215	CLA	O1A-CGA-O2A-C1
18	G	1001	CLA	O1A-CGA-O2A-C1
18	A	1104	CLA	C5-C6-C7-C8
18	A	1107	CLA	C15-C16-C17-C18
18	B	1215	CLA	C10-C11-C12-C13
23	2	2802	LMG	C4-C5-C6-O5
18	1	1005	CLA	C3-C5-C6-C7
18	B	1235	CLA	C13-C15-C16-C17
18	B	1207	CLA	C5-C6-C7-C8
18	B	1234	CLA	C8-C10-C11-C12
20	B	5002	PQN	C15-C16-C17-C18
18	A	1110	CLA	O1D-CGD-O2D-CED
18	3	3005	CLA	C2C-C3C-CAC-CBC
18	A	1124	CLA	C5-C6-C7-C8
18	A	1126	CLA	C15-C16-C17-C18
18	A	1119	CLA	C8-C10-C11-C12
18	G	1001	CLA	C5-C6-C7-C8
18	G	1003	CLA	C5-C6-C7-C8
18	1	1004	CLA	C5-C6-C7-C8
20	A	5001	PQN	C23-C25-C26-C27
18	B	1216	CLA	CBA-CGA-O2A-C1
18	B	1218	CLA	CBA-CGA-O2A-C1
18	B	1208	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	4	4801	LMG	C11-C10-O7-C8
18	A	1105	CLA	O1A-CGA-O2A-C1
23	G	2021	LMG	O10-C28-O8-C9
18	3	3017	CLA	CBA-CGA-O2A-C1
18	A	1139	CLA	C3-C5-C6-C7
18	A	1117	CLA	C15-C16-C17-C18
18	B	1216	CLA	C13-C15-C16-C17
18	B	1222	CLA	C5-C6-C7-C8
18	A	1119	CLA	O1A-CGA-O2A-C1
23	4	4801	LMG	O9-C10-O7-C8
21	A	5003	LHG	C1-C2-C3-O3
21	2	2801	LHG	C1-C2-C3-O3
18	A	1151	CLA	C2A-CAA-CBA-CGA
18	B	1225	CLA	C2A-CAA-CBA-CGA
18	B	1228	CLA	C2A-CAA-CBA-CGA
18	A	1105	CLA	CBA-CGA-O2A-C1
18	B	1229	CLA	CBA-CGA-O2A-C1
18	3	3004	CLA	CBA-CGA-O2A-C1
18	1	1007	CLA	C4C-C3C-CAC-CBC
18	A	1122	CLA	C5-C6-C7-C8
18	B	1238	CLA	C5-C6-C7-C8
18	B	1219	CLA	C5-C6-C7-C8
18	B	1202	CLA	C15-C16-C17-C18
18	1	1001	CLA	C5-C6-C7-C8
18	A	1022	CLA	C3-C5-C6-C7
18	A	1123	CLA	C15-C16-C17-C18
18	A	1140	CLA	C5-C6-C7-C8
18	A	1138	CLA	C8-C10-C11-C12
18	B	1210	CLA	C8-C10-C11-C12
18	3	3005	CLA	C5-C6-C7-C8
18	A	1102	CLA	O1D-CGD-O2D-CED
18	A	1134	CLA	CBD-CGD-O2D-CED
18	1	1002	CLA	C4C-C3C-CAC-CBC
18	A	1107	CLA	C8-C10-C11-C12
18	A	1109	CLA	C13-C15-C16-C17
18	A	1126	CLA	C13-C15-C16-C17
18	B	1012	CLA	C5-C6-C7-C8
18	B	1222	CLA	C15-C16-C17-C18
18	B	1207	CLA	C13-C15-C16-C17
18	B	1224	CLA	C15-C16-C17-C18
18	4	4004	CLA	C10-C11-C12-C13
17	A	1011	CL0	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	1218	CLA	C13-C15-C16-C17
18	A	1125	CLA	C6-C7-C8-C9
18	A	1111	CLA	O1D-CGD-O2D-CED
18	B	1236	CLA	O1D-CGD-O2D-CED
18	4	4012	CLA	C2C-C3C-CAC-CBC
18	4	4001	CLA	C8-C10-C11-C12
18	3	3010	CLA	C5-C6-C7-C8
18	A	1107	CLA	CBA-CGA-O2A-C1
18	B	1206	CLA	CBA-CGA-O2A-C1
18	B	1219	CLA	C11-C12-C13-C15
18	B	1229	CLA	C16-C17-C18-C19
18	2	2003	CLA	C6-C7-C8-C9
18	K	1001	CLA	C4C-C3C-CAC-CBC
18	B	1208	CLA	C5-C6-C7-C8
22	G	2011	BCR	C11-C10-C9-C34
22	K	2011	BCR	C11-C10-C9-C34
22	B	6005	BCR	C7-C8-C9-C34
22	B	6005	BCR	C37-C22-C23-C24
22	F	6014	BCR	C36-C18-C19-C20
22	F	6016	BCR	C11-C12-C13-C35
22	3	3503	BCR	C36-C18-C19-C20
22	B	6005	BCR	C7-C8-C9-C10
22	B	6005	BCR	C21-C22-C23-C24
18	B	1216	CLA	O1A-CGA-O2A-C1
18	B	1218	CLA	O1A-CGA-O2A-C1
18	B	1229	CLA	O1A-CGA-O2A-C1
18	A	1106	CLA	C2A-CAA-CBA-CGA
18	A	1127	CLA	C2A-CAA-CBA-CGA
18	A	1116	CLA	C2A-CAA-CBA-CGA
18	L	1501	CLA	C2A-CAA-CBA-CGA
18	A	1132	CLA	C15-C16-C17-C18
20	A	5001	PQN	C18-C20-C21-C22
21	A	5003	LHG	C28-C29-C30-C31
21	A	5003	LHG	O1-C1-C2-C3
21	B	5004	LHG	O1-C1-C2-C3
23	J	5001	LMG	C9-C8-O7-C10
18	A	1122	CLA	C16-C17-C18-C19
18	A	1133	CLA	C6-C7-C8-C9
18	A	1137	CLA	C6-C7-C8-C10
18	B	1223	CLA	C16-C17-C18-C19
18	B	1211	CLA	C16-C17-C18-C19
18	2	2012	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	4	4012	CLA	C16-C17-C18-C19
26	B	8002	LMU	O1'-C1-C2-C3
18	A	1151	CLA	O1A-CGA-O2A-C1
23	F	5002	LMG	O10-C28-O8-C9
18	A	1123	CLA	C3-C5-C6-C7
18	A	1137	CLA	C3-C5-C6-C7
18	B	1223	CLA	C3-C5-C6-C7
18	B	1229	CLA	C3-C5-C6-C7
18	4	4007	CLA	C3-C5-C6-C7
18	3	3003	CLA	C3-C5-C6-C7
28	3	3011	CHL	C3-C5-C6-C7
18	A	1109	CLA	C10-C11-C12-C13
18	B	1226	CLA	C10-C11-C12-C13
22	K	2011	BCR	C11-C10-C9-C8
23	J	5001	LMG	O6-C1-O1-C7
26	B	8002	LMU	O5'-C1'-O1'-C1
18	B	1213	CLA	CBA-CGA-O2A-C1
18	2	2001	CLA	CBA-CGA-O2A-C1
18	4	4004	CLA	CBA-CGA-O2A-C1
18	1	1001	CLA	C4C-C3C-CAC-CBC
18	1	1004	CLA	C15-C16-C17-C18
18	A	1151	CLA	C2-C1-O2A-CGA
18	A	1107	CLA	C2-C1-O2A-CGA
18	A	1125	CLA	C2-C1-O2A-CGA
18	A	1126	CLA	C2-C1-O2A-CGA
18	A	1127	CLA	C2-C1-O2A-CGA
18	A	1130	CLA	C2-C1-O2A-CGA
18	B	1239	CLA	C2-C1-O2A-CGA
18	B	1201	CLA	C2-C1-O2A-CGA
18	B	1212	CLA	C2-C1-O2A-CGA
18	B	1215	CLA	C2-C1-O2A-CGA
18	B	1232	CLA	C2-C1-O2A-CGA
18	G	1003	CLA	C2-C1-O2A-CGA
18	2	2001	CLA	C2-C1-O2A-CGA
18	4	4009	CLA	C2-C1-O2A-CGA
18	3	3005	CLA	C2-C1-O2A-CGA
17	A	1011	CL0	C16-C17-C18-C19
18	A	1111	CLA	C11-C12-C13-C14
18	A	1127	CLA	C16-C17-C18-C20
18	A	1133	CLA	C6-C7-C8-C10
18	B	1219	CLA	C11-C12-C13-C14
18	B	1208	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	1117	CLA	C5-C6-C7-C8
18	B	1238	CLA	C8-C10-C11-C12
23	J	5001	LMG	C40-C41-C42-C43
23	4	4801	LMG	C11-C12-C13-C14
23	4	4801	LMG	C32-C33-C34-C35
21	A	7001	LHG	C13-C14-C15-C16
23	J	5001	LMG	C16-C17-C18-C19
23	J	5001	LMG	C29-C30-C31-C32
23	G	2021	LMG	C13-C14-C15-C16
18	B	1221	CLA	C5-C6-C7-C8
21	A	5003	LHG	C31-C32-C33-C34
18	3	3004	CLA	O1A-CGA-O2A-C1
23	2	2802	LMG	C31-C32-C33-C34
25	B	7101	DGD	C5A-C6A-C7A-C8A
25	B	7101	DGD	CAB-CBB-CCB-CDB
21	1	1801	LHG	C10-C11-C12-C13
23	J	5001	LMG	C41-C42-C43-C44
18	A	1122	CLA	C4B-C3B-CAB-CBB
18	A	1124	CLA	C4B-C3B-CAB-CBB
18	A	1136	CLA	C4B-C3B-CAB-CBB
18	A	1140	CLA	C4B-C3B-CAB-CBB
18	B	1012	CLA	C4B-C3B-CAB-CBB
18	B	1240	CLA	C4B-C3B-CAB-CBB
18	B	1203	CLA	C4B-C3B-CAB-CBB
18	B	1205	CLA	C4B-C3B-CAB-CBB
18	B	1235	CLA	C4B-C3B-CAB-CBB
18	B	1225	CLA	C4B-C3B-CAB-CBB
18	J	1302	CLA	C4B-C3B-CAB-CBB
18	4	4012	CLA	C4B-C3B-CAB-CBB
18	1	1012	CLA	C4B-C3B-CAB-CBB
18	3	3013	CLA	C4B-C3B-CAB-CBB
23	F	5002	LMG	C19-C20-C21-C22
18	A	1122	CLA	C16-C17-C18-C20
18	A	1127	CLA	C16-C17-C18-C19
18	A	1137	CLA	C6-C7-C8-C9
18	B	1223	CLA	C16-C17-C18-C20
18	2	2003	CLA	C6-C7-C8-C10
18	2	2012	CLA	C6-C7-C8-C10
18	3	3002	CLA	O1A-CGA-O2A-C1
25	B	7101	DGD	C8A-C9A-CAA-CBA
18	B	1239	CLA	C15-C16-C17-C18
23	F	5002	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
23	2	2802	LMG	O6-C5-C6-O5
21	A	7001	LHG	C28-C29-C30-C31
18	B	1227	CLA	C6-C7-C8-C10
20	B	5002	PQN	C17-C18-C20-C21
23	J	5001	LMG	C28-C29-C30-C31
21	1	1801	LHG	C26-C27-C28-C29
17	A	1011	CL0	O1A-CGA-O2A-C1
18	B	1206	CLA	O1A-CGA-O2A-C1
18	A	1121	CLA	C3-C5-C6-C7
18	A	1103	CLA	C3A-C2A-CAA-CBA
18	A	1104	CLA	C3A-C2A-CAA-CBA
18	A	1107	CLA	C3A-C2A-CAA-CBA
18	A	1113	CLA	C3A-C2A-CAA-CBA
18	A	1140	CLA	C3A-C2A-CAA-CBA
18	A	1119	CLA	C3A-C2A-CAA-CBA
18	A	1101	CLA	C3A-C2A-CAA-CBA
18	B	1221	CLA	C3A-C2A-CAA-CBA
18	B	1223	CLA	C3A-C2A-CAA-CBA
18	B	1210	CLA	C3A-C2A-CAA-CBA
18	J	1302	CLA	C3A-C2A-CAA-CBA
18	G	1002	CLA	C3A-C2A-CAA-CBA
18	L	1501	CLA	C3A-C2A-CAA-CBA
18	4	4016	CLA	C3A-C2A-CAA-CBA
18	1	1011	CLA	C3A-C2A-CAA-CBA
18	1	1014	CLA	C3A-C2A-CAA-CBA
18	3	3005	CLA	C3A-C2A-CAA-CBA
28	1	1009	CHL	C3A-C2A-CAA-CBA
23	G	2021	LMG	C29-C30-C31-C32
18	A	1111	CLA	C8-C10-C11-C12
18	B	1240	CLA	C13-C15-C16-C17
18	B	1220	CLA	O1D-CGD-O2D-CED
22	B	6005	BCR	C19-C20-C21-C22
18	A	1111	CLA	C11-C12-C13-C15
18	A	1123	CLA	C16-C17-C18-C20
18	B	1211	CLA	C16-C17-C18-C20
18	L	1502	CLA	C11-C12-C13-C14
26	B	8002	LMU	C1-C2-C3-C4
18	A	1107	CLA	O1A-CGA-O2A-C1
18	L	1502	CLA	O1A-CGA-O2A-C1
21	1	1801	LHG	C34-C35-C36-C37
18	3	3012	CLA	C4C-C3C-CAC-CBC
18	1	1006	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
21	A	5003	LHG	C26-C27-C28-C29
18	A	1106	CLA	CBA-CGA-O2A-C1
18	A	1127	CLA	CBA-CGA-O2A-C1
18	B	1238	CLA	CBA-CGA-O2A-C1
18	4	4005	CLA	CBA-CGA-O2A-C1
21	A	5003	LHG	C33-C34-C35-C36
23	J	5001	LMG	C18-C19-C20-C21
23	J	5001	LMG	C21-C22-C23-C24
18	3	3010	CLA	C3-C5-C6-C7
20	A	5001	PQN	C13-C15-C16-C17
21	A	5003	LHG	C24-C25-C26-C27
21	A	7001	LHG	C31-C32-C33-C34
25	B	7101	DGD	CCB-CDB-CEB-CFB
18	B	1213	CLA	O1A-CGA-O2A-C1
18	4	4004	CLA	O1A-CGA-O2A-C1
26	B	8001	LMU	C5-C6-C7-C8
18	B	1213	CLA	C11-C12-C13-C15
18	A	1022	CLA	C2B-C3B-CAB-CBB
18	A	1113	CLA	C2B-C3B-CAB-CBB
18	A	1122	CLA	C2B-C3B-CAB-CBB
18	A	1136	CLA	C2B-C3B-CAB-CBB
18	A	1140	CLA	C2B-C3B-CAB-CBB
18	B	1216	CLA	C2B-C3B-CAB-CBB
18	B	1236	CLA	C2B-C3B-CAB-CBB
18	B	1238	CLA	C2B-C3B-CAB-CBB
18	B	1240	CLA	C2B-C3B-CAB-CBB
18	B	1204	CLA	C2B-C3B-CAB-CBB
18	B	1205	CLA	C2B-C3B-CAB-CBB
18	B	1223	CLA	C2B-C3B-CAB-CBB
18	B	1235	CLA	C2B-C3B-CAB-CBB
18	B	1214	CLA	C2B-C3B-CAB-CBB
18	B	1225	CLA	C2B-C3B-CAB-CBB
18	J	1302	CLA	C2B-C3B-CAB-CBB
18	L	1503	CLA	C2B-C3B-CAB-CBB
18	2	2003	CLA	C2B-C3B-CAB-CBB
18	4	4005	CLA	C2B-C3B-CAB-CBB
18	4	4012	CLA	C2B-C3B-CAB-CBB
18	1	1006	CLA	C2B-C3B-CAB-CBB
18	1	1007	CLA	C2B-C3B-CAB-CBB
18	1	1012	CLA	C2B-C3B-CAB-CBB
18	3	3013	CLA	C2B-C3B-CAB-CBB
22	A	6003	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	6003	BCR	C5-C6-C7-C8
22	A	6008	BCR	C23-C24-C25-C26
22	A	6008	BCR	C23-C24-C25-C30
22	A	6011	BCR	C1-C6-C7-C8
22	A	6011	BCR	C5-C6-C7-C8
22	B	6004	BCR	C1-C6-C7-C8
22	B	6004	BCR	C5-C6-C7-C8
22	B	6004	BCR	C23-C24-C25-C26
22	B	6004	BCR	C23-C24-C25-C30
22	B	6010	BCR	C23-C24-C25-C26
22	B	6010	BCR	C23-C24-C25-C30
22	J	6012	BCR	C23-C24-C25-C26
22	J	6012	BCR	C23-C24-C25-C30
22	F	6014	BCR	C23-C24-C25-C26
22	L	6019	BCR	C1-C6-C7-C8
22	L	6019	BCR	C23-C24-C25-C26
27	4	4501	LUT	C1-C6-C7-C8
18	A	1237	CLA	C3-C5-C6-C7
18	A	1116	CLA	C3-C5-C6-C7
18	B	1201	CLA	C2A-CAA-CBA-CGA
28	1	1010	CHL	C2A-CAA-CBA-CGA
23	J	5001	LMG	C10-C11-C12-C13
18	2	2001	CLA	O1A-CGA-O2A-C1
18	B	1214	CLA	C10-C11-C12-C13
23	B	5005	LMG	C14-C15-C16-C17
23	F	5002	LMG	C13-C14-C15-C16
23	F	5002	LMG	O9-C10-O7-C8
18	4	4017	CLA	C4-C3-C5-C6
25	B	7101	DGD	C2B-C3B-C4B-C5B
22	K	2011	BCR	C10-C11-C12-C13
18	3	3010	CLA	C11-C12-C13-C14
18	G	1002	CLA	C4C-C3C-CAC-CBC
18	B	1021	CLA	CBA-CGA-O2A-C1
18	2	2003	CLA	CBA-CGA-O2A-C1
18	1	1001	CLA	CBA-CGA-O2A-C1
23	2	2802	LMG	C29-C28-O8-C9
18	A	1123	CLA	C11-C10-C8-C9
18	L	1502	CLA	C6-C7-C8-C9
23	F	5002	LMG	C14-C15-C16-C17
23	G	2021	LMG	C11-C12-C13-C14
18	A	1103	CLA	C8-C10-C11-C12
18	3	3013	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	G	2021	LMG	C33-C34-C35-C36
25	B	7101	DGD	C5B-C6B-C7B-C8B
18	B	1219	CLA	C8-C10-C11-C12
23	B	5005	LMG	C11-C12-C13-C14
22	B	6004	BCR	C19-C20-C21-C22
22	J	6012	BCR	C9-C10-C11-C12
22	F	6016	BCR	C9-C10-C11-C12
18	B	1236	CLA	C6-C7-C8-C9
21	A	5003	LHG	C8-C7-O7-C5
21	A	7001	LHG	C8-C7-O7-C5
21	2	2801	LHG	C8-C7-O7-C5
18	A	1127	CLA	O1A-CGA-O2A-C1
18	2	2016	CLA	C4C-C3C-CAC-CBC
25	B	7101	DGD	C4B-C5B-C6B-C7B
18	4	4012	CLA	C10-C11-C12-C13
21	A	7001	LHG	O9-C7-O7-C5
21	2	2801	LHG	O9-C7-O7-C5
26	B	8002	LMU	C9-C10-C11-C12
23	G	2021	LMG	C31-C32-C33-C34
17	A	1011	CL0	C16-C17-C18-C20
18	A	1237	CLA	C11-C12-C13-C14
18	A	1237	CLA	C11-C12-C13-C15
18	A	1110	CLA	C6-C7-C8-C9
18	A	1123	CLA	C16-C17-C18-C19
18	B	1236	CLA	C6-C7-C8-C10
18	B	1213	CLA	C11-C12-C13-C14
18	B	1229	CLA	C16-C17-C18-C20
18	4	4012	CLA	C16-C17-C18-C20
18	3	3010	CLA	C11-C12-C13-C15
18	A	1119	CLA	C4-C3-C5-C6
18	3	3003	CLA	C4-C3-C5-C6
28	3	3011	CHL	C2C-C3C-CAC-CBC
18	A	1134	CLA	C5-C6-C7-C8
18	A	1101	CLA	C10-C11-C12-C13
23	J	5001	LMG	C15-C16-C17-C18
26	B	8001	LMU	C1-C2-C3-C4
18	2	2002	CLA	CBA-CGA-O2A-C1
18	2	2003	CLA	O1A-CGA-O2A-C1
18	4	4005	CLA	O1A-CGA-O2A-C1
18	1	1004	CLA	C3-C5-C6-C7
18	B	1223	CLA	C8-C10-C11-C12
18	B	1225	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	1	1003	CLA	C5-C6-C7-C8
23	2	2802	LMG	C28-C29-C30-C31
18	A	1116	CLA	C5-C6-C7-C8
18	B	1206	CLA	C15-C16-C17-C18
18	B	1222	CLA	C13-C15-C16-C17
18	B	1230	CLA	C8-C10-C11-C12
18	L	1502	CLA	C11-C12-C13-C15
18	A	1106	CLA	O1A-CGA-O2A-C1
18	B	1021	CLA	O1A-CGA-O2A-C1
18	B	1021	CLA	C8-C10-C11-C12
18	B	1023	CLA	C10-C11-C12-C13
18	B	1234	CLA	C10-C11-C12-C13
26	B	8002	LMU	O5'-C5'-C6'-O6'
23	F	5001	LMG	O1-C7-C8-O7
23	4	4801	LMG	O7-C8-C9-O8
18	A	1134	CLA	CBA-CGA-O2A-C1
23	J	5001	LMG	C39-C40-C41-C42
23	B	5005	LMG	C15-C16-C17-C18
23	B	5005	LMG	C29-C30-C31-C32
18	B	1225	CLA	C13-C15-C16-C17
23	F	5002	LMG	C17-C18-C19-C20
18	A	1111	CLA	C3-C5-C6-C7
18	A	1127	CLA	C3-C5-C6-C7
18	A	1119	CLA	C2-C3-C5-C6
18	3	3003	CLA	C2-C3-C5-C6
21	A	7001	LHG	C26-C27-C28-C29
25	B	7101	DGD	C3A-C4A-C5A-C6A
18	4	4003	CLA	C2A-CAA-CBA-CGA
18	1	1012	CLA	C2A-CAA-CBA-CGA
28	1	1009	CHL	CBD-CGD-O2D-CED
25	B	7101	DGD	C2A-C3A-C4A-C5A
23	J	5001	LMG	C8-C9-O8-C28
18	A	1123	CLA	C5-C6-C7-C8
18	B	1240	CLA	C10-C11-C12-C13
18	B	1218	CLA	C15-C16-C17-C18
23	G	2021	LMG	C30-C31-C32-C33
18	A	1134	CLA	C6-C7-C8-C10
18	4	4017	CLA	C16-C17-C18-C19
21	2	2801	LHG	O1-C1-C2-O2
18	B	1238	CLA	O1A-CGA-O2A-C1
23	2	2802	LMG	O10-C28-O8-C9
18	B	1208	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	7001	LHG	C10-C11-C12-C13
21	A	7001	LHG	C33-C34-C35-C36
26	B	8001	LMU	O1'-C1-C2-C3
18	A	1104	CLA	C1A-C2A-CAA-CBA
18	A	1106	CLA	C1A-C2A-CAA-CBA
18	A	1113	CLA	C1A-C2A-CAA-CBA
18	A	1121	CLA	C1A-C2A-CAA-CBA
18	A	1128	CLA	C1A-C2A-CAA-CBA
18	A	1115	CLA	C1A-C2A-CAA-CBA
18	A	1116	CLA	C1A-C2A-CAA-CBA
18	A	1101	CLA	C1A-C2A-CAA-CBA
18	B	1216	CLA	C1A-C2A-CAA-CBA
18	B	1219	CLA	C1A-C2A-CAA-CBA
18	B	1220	CLA	C1A-C2A-CAA-CBA
18	B	1221	CLA	C1A-C2A-CAA-CBA
18	B	1202	CLA	C1A-C2A-CAA-CBA
18	B	1210	CLA	C1A-C2A-CAA-CBA
18	B	1214	CLA	C1A-C2A-CAA-CBA
18	B	1215	CLA	C1A-C2A-CAA-CBA
18	B	1229	CLA	C1A-C2A-CAA-CBA
18	J	1302	CLA	C1A-C2A-CAA-CBA
18	G	1002	CLA	C1A-C2A-CAA-CBA
18	G	1003	CLA	C1A-C2A-CAA-CBA
18	H	1000	CLA	C1A-C2A-CAA-CBA
18	2	2004	CLA	C1A-C2A-CAA-CBA
18	4	4005	CLA	C1A-C2A-CAA-CBA
18	1	1012	CLA	C1A-C2A-CAA-CBA
18	1	1014	CLA	C1A-C2A-CAA-CBA
18	3	3001	CLA	C1A-C2A-CAA-CBA
18	3	3005	CLA	C1A-C2A-CAA-CBA
18	3	3013	CLA	C1A-C2A-CAA-CBA
21	A	7001	LHG	C25-C26-C27-C28
25	B	7101	DGD	C8B-C9B-CAB-CBB
23	4	4801	LMG	C30-C31-C32-C33
21	1	1801	LHG	C28-C29-C30-C31
21	B	5004	LHG	O6-C4-C5-C6
21	1	1801	LHG	C25-C26-C27-C28
18	A	1140	CLA	C3-C5-C6-C7
18	A	1107	CLA	C11-C12-C13-C15
18	A	1125	CLA	C11-C10-C8-C7
18	A	1127	CLA	C12-C13-C15-C16
18	A	1128	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	A	1138	CLA	C11-C10-C8-C7
18	A	1101	CLA	C11-C10-C8-C7
18	B	1216	CLA	C6-C7-C8-C10
18	B	1231	CLA	C6-C7-C8-C10
18	B	1239	CLA	C11-C12-C13-C15
18	B	1239	CLA	C12-C13-C15-C16
18	B	1218	CLA	C12-C13-C15-C16
18	B	1220	CLA	C12-C13-C15-C16
18	B	1202	CLA	C12-C13-C15-C16
18	B	1213	CLA	C6-C7-C8-C10
18	B	1224	CLA	C11-C10-C8-C7
18	B	1229	CLA	C12-C13-C15-C16
18	4	4017	CLA	C6-C7-C8-C10
18	4	4017	CLA	C11-C12-C13-C15
18	A	1119	CLA	C16-C17-C18-C19
18	A	1103	CLA	C5-C6-C7-C8
18	B	1211	CLA	CBD-CGD-O2D-CED
20	B	5002	PQN	C20-C21-C22-C23
18	A	1120	CLA	C10-C11-C12-C13
18	B	1224	CLA	C13-C15-C16-C17
18	A	1126	CLA	C2A-CAA-CBA-CGA
18	A	1103	CLA	C11-C12-C13-C14
18	A	1104	CLA	C11-C12-C13-C14
18	A	1107	CLA	C11-C12-C13-C14
18	A	1126	CLA	C11-C10-C8-C9
18	A	1139	CLA	C14-C13-C15-C16
18	A	1138	CLA	C11-C10-C8-C9
18	A	1101	CLA	C11-C10-C8-C9
18	B	1231	CLA	C6-C7-C8-C9
18	B	1219	CLA	C6-C7-C8-C9
18	4	4004	CLA	C6-C7-C8-C9
18	4	4012	CLA	C6-C7-C8-C9
18	4	4017	CLA	C6-C7-C8-C9
18	4	4017	CLA	C11-C12-C13-C14
18	3	3010	CLA	C6-C7-C8-C9
22	F	6014	BCR	C19-C20-C21-C22
18	A	1121	CLA	CBA-CGA-O2A-C1
18	A	1101	CLA	CBD-CGD-O2D-CED
23	4	4801	LMG	C7-C8-C9-O8
28	2	2013	CHL	C2C-C3C-CAC-CBC
23	G	2021	LMG	C14-C15-C16-C17
18	A	1134	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	2	2802	LMG	C11-C12-C13-C14
18	3	3017	CLA	O1A-CGA-O2A-C1
28	1	1010	CHL	CHA-CBD-CGD-O2D
18	A	1133	CLA	C5-C6-C7-C8
18	1	1001	CLA	O1A-CGA-O2A-C1
18	4	4017	CLA	C2-C3-C5-C6
18	A	1122	CLA	C10-C11-C12-C13
18	B	1219	CLA	C10-C11-C12-C13
18	B	1202	CLA	C13-C15-C16-C17
22	A	6008	BCR	C36-C18-C19-C20
22	G	2011	BCR	C7-C8-C9-C34
18	A	1110	CLA	C6-C7-C8-C10
18	1	1005	CLA	C6-C7-C8-C9
18	A	1134	CLA	O1A-CGA-O2A-C1
18	A	1133	CLA	C2A-CAA-CBA-CGA
18	A	1130	CLA	C2A-CAA-CBA-CGA
18	F	1302	CLA	C2A-CAA-CBA-CGA
23	J	5001	LMG	C31-C32-C33-C34
22	B	6010	BCR	C10-C11-C12-C13
23	J	5001	LMG	C14-C15-C16-C17
22	L	6020	BCR	C13-C14-C15-C16
27	4	4503	LUT	C33-C34-C35-C15
18	4	4017	CLA	C16-C17-C18-C20
18	3	3005	CLA	C4C-C3C-CAC-CBC
23	2	2802	LMG	C29-C30-C31-C32
18	B	1212	CLA	CBA-CGA-O2A-C1
18	G	1001	CLA	C2C-C3C-CAC-CBC
21	1	1801	LHG	C30-C31-C32-C33
18	A	1138	CLA	C2-C3-C5-C6
21	A	7001	LHG	C11-C10-C9-C8
25	B	7101	DGD	CEB-CFB-CGB-CHB
25	B	7101	DGD	C4A-C5A-C6A-C7A
18	2	2004	CLA	C2C-C3C-CAC-CBC
21	A	7001	LHG	O7-C5-C6-O8
23	F	5002	LMG	O7-C8-C9-O8
18	1	1011	CLA	C4C-C3C-CAC-CBC
18	1	1003	CLA	C2A-CAA-CBA-CGA
18	B	1231	CLA	C3-C5-C6-C7
18	4	4005	CLA	C3-C5-C6-C7
18	B	1212	CLA	C5-C6-C7-C8
23	J	5001	LMG	C36-C37-C38-C39
18	A	1103	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	A	1121	CLA	O1A-CGA-O2A-C1
23	2	2802	LMG	C10-C11-C12-C13
18	A	1125	CLA	C5-C6-C7-C8
18	B	1213	CLA	C8-C10-C11-C12
18	B	1226	CLA	C13-C15-C16-C17
18	B	1239	CLA	C16-C17-C18-C20
18	1	1005	CLA	C6-C7-C8-C10
18	A	1128	CLA	C4-C3-C5-C6
18	A	1138	CLA	C4-C3-C5-C6
18	A	1237	CLA	C10-C11-C12-C13
23	4	4801	LMG	C29-C30-C31-C32
18	A	1125	CLA	C11-C10-C8-C9
18	A	1126	CLA	C14-C13-C15-C16
18	A	1127	CLA	C14-C13-C15-C16
18	A	1132	CLA	C11-C12-C13-C14
18	A	1117	CLA	C14-C13-C15-C16
18	A	1119	CLA	C11-C10-C8-C9
18	B	1216	CLA	C6-C7-C8-C9
18	B	1216	CLA	C11-C10-C8-C9
18	B	1239	CLA	C11-C12-C13-C14
18	B	1239	CLA	C14-C13-C15-C16
18	B	1240	CLA	C11-C12-C13-C14
18	B	1205	CLA	C11-C10-C8-C9
18	B	1206	CLA	C6-C7-C8-C9
18	B	1218	CLA	C14-C13-C15-C16
18	B	1235	CLA	C6-C7-C8-C9
18	B	1235	CLA	C14-C13-C15-C16
18	B	1202	CLA	C14-C13-C15-C16
18	B	1213	CLA	C6-C7-C8-C9
18	B	1225	CLA	C14-C13-C15-C16
18	B	1229	CLA	C14-C13-C15-C16
18	4	4012	CLA	C14-C13-C15-C16
18	1	1004	CLA	C14-C13-C15-C16
18	A	1127	CLA	C15-C16-C17-C18
18	A	1103	CLA	C4B-C3B-CAB-CBB
18	A	1118	CLA	C4B-C3B-CAB-CBB
18	B	1023	CLA	C4B-C3B-CAB-CBB
18	B	1204	CLA	C4B-C3B-CAB-CBB
18	B	1214	CLA	C4B-C3B-CAB-CBB
18	B	1229	CLA	C4B-C3B-CAB-CBB
18	4	4016	CLA	C4B-C3B-CAB-CBB
21	1	1801	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
18	4	4012	CLA	C4C-C3C-CAC-CBC
18	A	1134	CLA	CAA-CBA-CGA-O2A
18	1	1004	CLA	C10-C11-C12-C13
18	A	1119	CLA	C16-C17-C18-C20
18	A	1134	CLA	O1D-CGD-O2D-CED
18	B	1223	CLA	CBA-CGA-O2A-C1
21	A	7001	LHG	C24-C25-C26-C27
23	J	5001	LMG	C2-C1-O1-C7
23	4	4801	LMG	C2-C1-O1-C7
18	4	4003	CLA	C4C-C3C-CAC-CBC
18	B	1236	CLA	C5-C6-C7-C8
18	B	1223	CLA	C5-C6-C7-C8
18	B	1230	CLA	C3-C5-C6-C7
21	A	5003	LHG	C9-C10-C11-C12
18	A	1103	CLA	C11-C12-C13-C15
18	A	1104	CLA	C11-C12-C13-C15
18	A	1123	CLA	C11-C12-C13-C15
18	A	1126	CLA	C11-C10-C8-C7
18	A	1139	CLA	C12-C13-C15-C16
18	A	1116	CLA	C6-C7-C8-C10
18	A	1117	CLA	C12-C13-C15-C16
18	A	1119	CLA	C11-C10-C8-C7
18	B	1240	CLA	C11-C12-C13-C15
18	B	1203	CLA	C6-C7-C8-C10
18	B	1205	CLA	C11-C10-C8-C7
18	B	1206	CLA	C6-C7-C8-C10
18	B	1219	CLA	C6-C7-C8-C10
18	B	1235	CLA	C6-C7-C8-C10
18	B	1211	CLA	C12-C13-C15-C16
18	B	1214	CLA	C11-C10-C8-C7
18	B	1224	CLA	C11-C12-C13-C15
18	B	1225	CLA	C12-C13-C15-C16
18	B	1226	CLA	C11-C12-C13-C15
18	4	4004	CLA	C6-C7-C8-C10
18	4	4012	CLA	C6-C7-C8-C10
18	1	1004	CLA	C11-C12-C13-C15
18	1	1004	CLA	C12-C13-C15-C16
18	3	3010	CLA	C6-C7-C8-C10
21	A	5003	LHG	O9-C7-O7-C5
21	1	1801	LHG	C35-C36-C37-C38
23	2	2802	LMG	C33-C34-C35-C36
18	A	1120	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	1123	CLA	C4-C3-C5-C6
18	B	1222	CLA	C3A-C2A-CAA-CBA
18	B	1214	CLA	C3A-C2A-CAA-CBA
28	2	2011	CHL	C3A-C2A-CAA-CBA
28	1	1010	CHL	C3A-C2A-CAA-CBA
18	B	1231	CLA	C10-C11-C12-C13
18	B	1023	CLA	C2C-C3C-CAC-CBC
22	J	6013	BCR	C9-C10-C11-C12
22	J	6013	BCR	C19-C20-C21-C22
29	4	4505	ZEX	C29-C30-C31-C32
18	B	1240	CLA	CAA-CBA-CGA-O2A
21	1	1801	LHG	C16-C17-C18-C19
18	A	1128	CLA	C13-C15-C16-C17
18	4	4012	CLA	C15-C16-C17-C18
26	B	8002	LMU	C2-C3-C4-C5
18	A	1119	CLA	C2A-CAA-CBA-CGA
23	B	5005	LMG	C7-C8-C9-O8
23	J	5001	LMG	C7-C8-C9-O8
23	G	2021	LMG	O1-C7-C8-C9
25	B	7101	DGD	O1G-C1G-C2G-C3G
23	J	5001	LMG	C34-C35-C36-C37
18	3	3010	CLA	O1D-CGD-O2D-CED
18	A	1106	CLA	C15-C16-C17-C18
18	B	1240	CLA	C4-C3-C5-C6
18	B	1205	CLA	C4-C3-C5-C6
18	B	1220	CLA	C4-C3-C5-C6
18	B	1202	CLA	C4-C3-C5-C6
18	4	4003	CLA	C4-C3-C5-C6
25	B	7101	DGD	CBB-CCB-CDB-CEB
21	A	7001	LHG	O6-C4-C5-O7
21	B	5004	LHG	O6-C4-C5-O7
18	4	4016	CLA	C2B-C3B-CAB-CBB
22	B	6005	BCR	C1-C6-C7-C8
22	J	6013	BCR	C23-C24-C25-C26
27	4	4503	LUT	C5-C6-C7-C8
18	B	1229	CLA	C15-C16-C17-C18
25	B	7101	DGD	C6A-C7A-C8A-C9A
18	2	2016	CLA	CAA-CBA-CGA-O2A
18	A	1237	CLA	C8-C10-C11-C12
23	B	5005	LMG	O7-C8-C9-O8
25	B	7101	DGD	O2G-C2G-C3G-O3G
18	1	1005	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	A	1101	CLA	C8-C10-C11-C12
18	A	1123	CLA	C2-C3-C5-C6
18	1	1005	CLA	C2-C3-C5-C6
18	B	1238	CLA	C16-C17-C18-C20
18	A	1013	CLA	CBA-CGA-O2A-C1
18	B	1227	CLA	C3-C5-C6-C7
18	A	1132	CLA	C14-C13-C15-C16
18	B	1012	CLA	C14-C13-C15-C16
18	B	1224	CLA	C11-C10-C8-C9
21	A	7001	LHG	C11-C12-C13-C14
18	A	1101	CLA	C3-C5-C6-C7
23	4	4801	LMG	C33-C34-C35-C36
18	B	1210	CLA	C10-C11-C12-C13
21	A	7001	LHG	O1-C1-C2-O2
18	B	1210	CLA	C3-C5-C6-C7
18	3	3005	CLA	C3-C5-C6-C7
18	B	1239	CLA	C16-C17-C18-C19
18	G	1001	CLA	C6-C7-C8-C10
18	4	4007	CLA	C11-C12-C13-C14
18	B	1215	CLA	C5-C6-C7-C8
18	4	4005	CLA	C5-C6-C7-C8
18	B	1212	CLA	O1A-CGA-O2A-C1
18	B	1236	CLA	CBA-CGA-O2A-C1
21	A	5003	LHG	O6-C4-C5-C6
18	A	1132	CLA	C16-C17-C18-C19
18	B	1021	CLA	C16-C17-C18-C20
18	A	1013	CLA	C15-C16-C17-C18
18	B	1222	CLA	C8-C10-C11-C12
18	B	1227	CLA	C5-C6-C7-C8
18	A	1022	CLA	C6-C7-C8-C10
18	A	1022	CLA	C11-C10-C8-C7
18	A	1120	CLA	C11-C10-C8-C7
18	A	1126	CLA	C11-C12-C13-C15
18	A	1140	CLA	C6-C7-C8-C10
18	B	1012	CLA	C12-C13-C15-C16
18	B	1239	CLA	C11-C10-C8-C7
18	B	1218	CLA	C11-C12-C13-C15
18	B	1222	CLA	C11-C10-C8-C7
18	B	1213	CLA	C11-C10-C8-C7
18	B	1224	CLA	C6-C7-C8-C10
18	4	4012	CLA	C11-C12-C13-C15
20	A	5001	PQN	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
20	A	5001	PQN	C21-C22-C23-C25
22	F	6016	BCR	C11-C12-C13-C14
22	G	2011	BCR	C7-C8-C9-C10
18	A	1122	CLA	CBA-CGA-O2A-C1
18	B	1012	CLA	CBA-CGA-O2A-C1
18	A	1140	CLA	C10-C11-C12-C13
18	B	1224	CLA	C8-C10-C11-C12
18	A	1013	CLA	O1A-CGA-O2A-C1
18	B	1012	CLA	O1A-CGA-O2A-C1
18	B	1205	CLA	C2-C3-C5-C6
18	B	1202	CLA	C2-C3-C5-C6
21	1	1801	LHG	O1-C1-C2-C3
18	B	1236	CLA	O1A-CGA-O2A-C1
18	B	1223	CLA	O1A-CGA-O2A-C1
18	A	1110	CLA	C5-C6-C7-C8
22	G	2011	BCR	C11-C10-C9-C8
21	A	5003	LHG	O6-C4-C5-O7
21	A	7001	LHG	C4-C5-C6-O8
23	F	5002	LMG	C7-C8-C9-O8
18	A	1120	CLA	C5-C6-C7-C8
18	4	4001	CLA	C10-C11-C12-C13
18	1	1001	CLA	C3-C5-C6-C7
18	1	1006	CLA	C4C-C3C-CAC-CBC
23	J	5001	LMG	O7-C8-C9-O8
23	G	2021	LMG	O1-C7-C8-O7
25	B	7101	DGD	O1G-C1G-C2G-O2G
18	B	1205	CLA	C8-C10-C11-C12
18	B	1234	CLA	C5-C6-C7-C8
18	1	1005	CLA	C5-C6-C7-C8
18	A	1022	CLA	C6-C7-C8-C9
18	A	1140	CLA	C6-C7-C8-C9
18	B	1213	CLA	C11-C10-C8-C9
18	B	1224	CLA	C6-C7-C8-C9
18	G	1003	CLA	C6-C7-C8-C9
20	A	5001	PQN	C21-C22-C23-C24
20	B	5002	PQN	C24-C23-C25-C26
21	A	7001	LHG	C14-C15-C16-C17
18	B	1220	CLA	C5-C6-C7-C8
18	A	1122	CLA	O1A-CGA-O2A-C1
23	J	5001	LMG	C23-C24-C25-C26
18	A	1131	CLA	C2-C1-O2A-CGA
18	A	1116	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	B	1225	CLA	C2-C1-O2A-CGA
18	3	3008	CLA	C2-C1-O2A-CGA
18	3	3005	CLA	C6-C7-C8-C10
18	A	1139	CLA	C13-C15-C16-C17
18	B	1012	CLA	C10-C11-C12-C13
18	2	2005	CLA	C5-C6-C7-C8
18	B	1204	CLA	C4-C3-C5-C6
18	B	1204	CLA	C2A-CAA-CBA-CGA
18	A	1138	CLA	C16-C17-C18-C19
18	B	1238	CLA	C16-C17-C18-C19
18	4	4004	CLA	C11-C12-C13-C14
18	A	1013	CLA	C8-C10-C11-C12
18	G	1001	CLA	C6-C7-C8-C9
18	3	3005	CLA	C6-C7-C8-C9
18	B	1214	CLA	C3-C5-C6-C7
23	J	5001	LMG	C13-C14-C15-C16
18	A	1120	CLA	C1A-C2A-CAA-CBA
18	A	1120	CLA	C4B-C3B-CAB-CBB
18	A	1121	CLA	C4B-C3B-CAB-CBB
18	A	1134	CLA	C4B-C3B-CAB-CBB
18	B	1231	CLA	C4B-C3B-CAB-CBB
18	B	1239	CLA	C4B-C3B-CAB-CBB
18	B	1217	CLA	C4B-C3B-CAB-CBB
18	2	2006	CLA	C4B-C3B-CAB-CBB
18	4	4004	CLA	C4B-C3B-CAB-CBB
18	3	3001	CLA	C4B-C3B-CAB-CBB
18	3	3007	CLA	C1A-C2A-CAA-CBA
18	A	1101	CLA	O1D-CGD-O2D-CED
22	F	6014	BCR	C17-C18-C19-C20
22	3	3503	BCR	C17-C18-C19-C20
18	1	1008	CLA	C2A-CAA-CBA-CGA
18	B	1228	CLA	C5-C6-C7-C8
21	A	7001	LHG	O6-C4-C5-C6
25	B	7101	DGD	C9A-CAA-CBA-CCA
23	G	2021	LMG	C12-C13-C14-C15
18	A	1112	CLA	C11-C10-C8-C7
18	A	1122	CLA	C6-C7-C8-C10
18	A	1138	CLA	C11-C12-C13-C15
18	B	1231	CLA	C11-C10-C8-C7
18	B	1221	CLA	C6-C7-C8-C10
18	B	1221	CLA	C11-C12-C13-C15
18	B	1222	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	B	1235	CLA	C11-C12-C13-C15
18	B	1226	CLA	C11-C10-C8-C7
18	2	2001	CLA	C6-C7-C8-C10
18	4	4003	CLA	C11-C10-C8-C7
18	4	4007	CLA	C6-C7-C8-C10
23	B	5005	LMG	C13-C14-C15-C16
18	B	1215	CLA	C11-C12-C13-C14
18	A	1102	CLA	C3A-C2A-CAA-CBA
18	A	1122	CLA	C3A-C2A-CAA-CBA
18	A	1125	CLA	C3A-C2A-CAA-CBA
18	A	1130	CLA	C3A-C2A-CAA-CBA
18	G	1001	CLA	C3A-C2A-CAA-CBA
18	2	2003	CLA	C4-C3-C5-C6
18	A	1022	CLA	C11-C10-C8-C9
18	A	1104	CLA	C14-C13-C15-C16
18	B	1218	CLA	C11-C12-C13-C14
18	B	1222	CLA	C11-C10-C8-C9
18	B	1223	CLA	C11-C10-C8-C9
18	4	4012	CLA	C11-C12-C13-C14
20	A	5001	PQN	C16-C17-C18-C19
18	4	4017	CLA	C15-C16-C17-C18
22	B	6009	BCR	C19-C20-C21-C22
27	4	4501	LUT	C33-C34-C35-C15
27	3	3502	LUT	C9-C10-C11-C12
18	H	1000	CLA	CBA-CGA-O2A-C1
18	B	1207	CLA	C10-C11-C12-C13
23	G	2021	LMG	C15-C16-C17-C18
18	3	3008	CLA	O2A-C1-C2-C3
18	A	1112	CLA	C8-C10-C11-C12
18	B	1238	CLA	C15-C16-C17-C18
23	J	5001	LMG	C33-C34-C35-C36
18	4	4007	CLA	C11-C12-C13-C15
18	A	1103	CLA	C4-C3-C5-C6
18	B	1216	CLA	C15-C16-C17-C18
18	A	1111	CLA	CAD-CBD-CGD-O2D
18	A	1125	CLA	CAD-CBD-CGD-O2D
18	B	1217	CLA	CAD-CBD-CGD-O2D
18	2	2006	CLA	CAD-CBD-CGD-O2D
18	2	2007	CLA	CAD-CBD-CGD-O2D
18	1	1008	CLA	CAD-CBD-CGD-O2D
18	A	1119	CLA	C5-C6-C7-C8
18	B	1211	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	1224	CLA	CBA-CGA-O2A-C1
18	1	1001	CLA	C11-C12-C13-C14
18	A	1121	CLA	C2A-CAA-CBA-CGA
18	A	1111	CLA	O1A-CGA-O2A-C1
18	A	1139	CLA	O1A-CGA-O2A-C1
17	A	1011	CL0	CHA-CBD-CGD-O1D
17	A	1011	CL0	CHA-CBD-CGD-O2D
18	A	1111	CLA	CAD-CBD-CGD-O1D
18	A	1114	CLA	CHA-CBD-CGD-O1D
18	A	1114	CLA	CHA-CBD-CGD-O2D
18	A	1123	CLA	CHA-CBD-CGD-O1D
18	A	1123	CLA	CHA-CBD-CGD-O2D
18	A	1125	CLA	CAD-CBD-CGD-O1D
18	B	1217	CLA	CAD-CBD-CGD-O1D
18	B	1211	CLA	CAD-CBD-CGD-O1D
18	2	2006	CLA	CAD-CBD-CGD-O1D
18	2	2007	CLA	CAD-CBD-CGD-O1D
18	4	4005	CLA	CHA-CBD-CGD-O1D
18	1	1008	CLA	CAD-CBD-CGD-O1D
18	3	3004	CLA	CHA-CBD-CGD-O1D
18	3	3004	CLA	CHA-CBD-CGD-O2D
21	A	5003	LHG	C4-O6-P-O5
21	B	5004	LHG	C4-O6-P-O5
21	2	2801	LHG	C3-O3-P-O5
22	A	6002	BCR	C9-C10-C11-C12
22	A	6002	BCR	C19-C20-C21-C22
22	B	6006	BCR	C19-C20-C21-C22
22	B	6009	BCR	C11-C10-C9-C34
22	B	6010	BCR	C19-C20-C21-C22
22	I	6020	BCR	C19-C20-C21-C22
22	L	6019	BCR	C9-C10-C11-C12
22	K	2011	BCR	C13-C14-C15-C16
18	A	1122	CLA	C3-C5-C6-C7
25	B	7101	DGD	C1B-C2B-C3B-C4B
23	G	2021	LMG	C34-C35-C36-C37
18	A	1120	CLA	C2B-C3B-CAB-CBB
18	A	1124	CLA	C2B-C3B-CAB-CBB
18	A	1134	CLA	C2B-C3B-CAB-CBB
18	A	1118	CLA	C2B-C3B-CAB-CBB
18	B	1012	CLA	C2B-C3B-CAB-CBB
18	B	1203	CLA	C2B-C3B-CAB-CBB
18	4	4004	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	L	6019	BCR	C23-C24-C25-C30
18	A	1237	CLA	C5-C6-C7-C8
21	A	5003	LHG	C2-C3-O3-P
22	A	6011	BCR	C36-C18-C19-C20
27	4	4502	LUT	C11-C12-C13-C20
27	3	3502	LUT	C11-C12-C13-C20
18	4	4007	CLA	C10-C11-C12-C13
18	B	1218	CLA	C16-C17-C18-C20
23	F	5002	LMG	C15-C16-C17-C18
23	G	2021	LMG	C9-C8-O7-C10
23	2	2802	LMG	C9-C8-O7-C10
22	B	6006	BCR	C18-C19-C20-C21
22	K	2011	BCR	C18-C19-C20-C21
18	B	1240	CLA	C5-C6-C7-C8
18	A	1128	CLA	C2-C3-C5-C6
23	B	5005	LMG	C10-C11-C12-C13
23	J	5001	LMG	C17-C18-C19-C20
18	A	1117	CLA	C16-C17-C18-C20
18	B	1215	CLA	C11-C12-C13-C15
18	4	4003	CLA	C16-C17-C18-C20
18	2	2002	CLA	O1A-CGA-O2A-C1
18	A	1111	CLA	CBA-CGA-O2A-C1
18	4	4003	CLA	C8-C10-C11-C12
18	A	1109	CLA	C6-C7-C8-C9
18	A	1126	CLA	C11-C12-C13-C14
18	A	1128	CLA	C6-C7-C8-C9
18	A	1131	CLA	C11-C12-C13-C14
18	A	1116	CLA	C6-C7-C8-C9
18	A	1138	CLA	C6-C7-C8-C9
18	A	1138	CLA	C11-C12-C13-C14
18	B	1207	CLA	C11-C10-C8-C9
18	B	1211	CLA	C14-C13-C15-C16
18	B	1224	CLA	C11-C12-C13-C14
18	4	4012	CLA	C11-C10-C8-C9
18	A	1237	CLA	C11-C10-C8-C7
18	A	1109	CLA	C6-C7-C8-C10
18	A	1122	CLA	C11-C12-C13-C15
18	B	1206	CLA	C11-C12-C13-C15
18	4	4005	CLA	C6-C7-C8-C10
18	3	3004	CLA	C6-C7-C8-C10
22	A	6017	BCR	C16-C17-C18-C19
23	B	5005	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
18	2	2001	CLA	C2A-CAA-CBA-CGA
18	A	1104	CLA	C16-C17-C18-C19
18	A	1138	CLA	C16-C17-C18-C20
18	2	2005	CLA	C6-C7-C8-C9
18	A	1132	CLA	C16-C17-C18-C20
23	F	5002	LMG	C11-C12-C13-C14
23	F	5002	LMG	C28-C29-C30-C31
18	A	1139	CLA	CBA-CGA-O2A-C1
18	A	1104	CLA	C16-C17-C18-C20
18	A	1129	CLA	C2-C1-O2A-CGA
18	1	1012	CLA	C2-C1-O2A-CGA
23	F	5001	LMG	O1-C7-C8-C9
18	G	1001	CLA	C4C-C3C-CAC-CBC
23	4	4801	LMG	C13-C14-C15-C16
18	A	1127	CLA	CAA-CBA-CGA-O2A
26	B	8001	LMU	C4'-C5'-C6'-O6'
22	3	3503	BCR	C13-C14-C15-C16
18	A	1121	CLA	C6-C7-C8-C10
18	B	1224	CLA	O1A-CGA-O2A-C1
18	1	1004	CLA	C8-C10-C11-C12
18	B	1227	CLA	O1D-CGD-O2D-CED
17	A	1011	CL0	CAA-CBA-CGA-O2A
21	A	7001	LHG	O8-C23-C24-C25
18	A	1122	CLA	C6-C7-C8-C9
18	B	1231	CLA	C11-C10-C8-C9
18	B	1221	CLA	C6-C7-C8-C9
18	B	1226	CLA	C11-C10-C8-C9
18	A	1104	CLA	C4B-C3B-CAB-CBB
18	B	1234	CLA	C4B-C3B-CAB-CBB
18	A	1125	CLA	C11-C12-C13-C15
18	A	1116	CLA	C8-C10-C11-C12
22	L	6019	BCR	C15-C16-C17-C18
18	B	1203	CLA	C16-C17-C18-C19
18	B	1230	CLA	C11-C10-C8-C7
18	4	4001	CLA	C6-C7-C8-C10
18	A	1132	CLA	C5-C6-C7-C8
18	A	1151	CLA	CAA-CBA-CGA-O2A
18	2	2005	CLA	C6-C7-C8-C10
18	A	1110	CLA	O1A-CGA-O2A-C1
18	1	1013	CLA	C2C-C3C-CAC-CBC
17	A	1011	CL0	C3A-C2A-CAA-CBA
18	A	1127	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	1133	CLA	C3A-C2A-CAA-CBA
18	B	1224	CLA	C4-C3-C5-C6
28	4	4013	CHL	C3A-C2A-CAA-CBA
18	2	2003	CLA	C2-C3-C5-C6
22	A	6011	BCR	C16-C17-C18-C36
22	A	6017	BCR	C16-C17-C18-C36
22	B	6004	BCR	C16-C17-C18-C36
22	B	6005	BCR	C16-C17-C18-C36
22	B	6006	BCR	C11-C10-C9-C34
22	I	6020	BCR	C16-C17-C18-C36
22	I	6020	BCR	C20-C21-C22-C37
22	F	6016	BCR	C16-C17-C18-C36
22	G	2011	BCR	C16-C17-C18-C36
22	K	2011	BCR	C16-C17-C18-C36
26	B	8002	LMU	C3-C4-C5-C6
18	B	1220	CLA	C13-C15-C16-C17
18	B	1206	CLA	C8-C10-C11-C12
18	B	1231	CLA	C2-C1-O2A-CGA
18	3	3004	CLA	C2-C1-O2A-CGA
18	3	3006	CLA	C2-C1-O2A-CGA
22	A	6011	BCR	C19-C20-C21-C22
22	I	6020	BCR	C9-C10-C11-C12
27	2	2502	LUT	C29-C30-C31-C32
18	A	1112	CLA	C5-C6-C7-C8
18	3	3003	CLA	C8-C10-C11-C12
28	1	1009	CHL	C4-C3-C5-C6
18	B	1235	CLA	C3-C5-C6-C7
18	4	4001	CLA	C2C-C3C-CAC-CBC
18	A	1103	CLA	C2-C3-C5-C6
18	B	1012	CLA	C16-C17-C18-C20
26	B	8002	LMU	C5-C6-C7-C8
18	B	1223	CLA	C2A-CAA-CBA-CGA
18	A	1107	CLA	C6-C7-C8-C9
18	A	1112	CLA	C14-C13-C15-C16
18	B	1230	CLA	C11-C10-C8-C9
18	B	1234	CLA	C6-C7-C8-C9
18	L	1502	CLA	C11-C10-C8-C9
18	3	3004	CLA	C11-C10-C8-C9
20	B	5002	PQN	C19-C18-C20-C21
18	B	1227	CLA	CBD-CGD-O2D-CED
28	1	1009	CHL	C1A-C2A-CAA-CBA
28	3	3011	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	5001	PQN	C15-C16-C17-C18
26	B	8002	LMU	C7-C8-C9-C10
28	2	2013	CHL	CAA-CBA-CGA-O1A
18	A	1106	CLA	C5-C6-C7-C8
18	B	1214	CLA	CAA-CBA-CGA-O2A
18	H	1000	CLA	CAA-CBA-CGA-O2A
18	4	4008	CLA	CAA-CBA-CGA-O2A
28	1	1009	CHL	C2-C3-C5-C6
18	B	1221	CLA	C3-C5-C6-C7
18	B	1209	CLA	C2A-CAA-CBA-CGA
18	2	2005	CLA	C2A-CAA-CBA-CGA
26	B	8002	LMU	C6-C7-C8-C9
18	A	1114	CLA	C1A-C2A-CAA-CBA
18	A	1125	CLA	C1A-C2A-CAA-CBA
18	2	2005	CLA	C1A-C2A-CAA-CBA
18	4	4001	CLA	C1A-C2A-CAA-CBA
18	4	4017	CLA	C1A-C2A-CAA-CBA
22	A	6011	BCR	C16-C17-C18-C19
22	B	6004	BCR	C16-C17-C18-C19
22	B	6005	BCR	C16-C17-C18-C19
22	B	6006	BCR	C11-C10-C9-C8
22	I	6020	BCR	C16-C17-C18-C19
22	I	6020	BCR	C20-C21-C22-C23
22	F	6016	BCR	C16-C17-C18-C19
22	G	2011	BCR	C16-C17-C18-C19
22	K	2011	BCR	C16-C17-C18-C19
18	A	1103	CLA	C2B-C3B-CAB-CBB
18	A	1121	CLA	C2B-C3B-CAB-CBB
18	A	1125	CLA	C2B-C3B-CAB-CBB
18	B	1231	CLA	C2B-C3B-CAB-CBB
18	B	1239	CLA	C2B-C3B-CAB-CBB
18	B	1023	CLA	C2B-C3B-CAB-CBB
18	B	1217	CLA	C2B-C3B-CAB-CBB
18	B	1229	CLA	C2B-C3B-CAB-CBB
18	B	1234	CLA	C2B-C3B-CAB-CBB
18	G	1003	CLA	C2B-C3B-CAB-CBB
18	2	2006	CLA	C2B-C3B-CAB-CBB
18	3	3001	CLA	C2B-C3B-CAB-CBB
22	A	6003	BCR	C23-C24-C25-C30
22	A	6007	BCR	C23-C24-C25-C30
22	A	6011	BCR	C23-C24-C25-C30
22	B	6005	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	6005	BCR	C23-C24-C25-C30
22	J	6013	BCR	C23-C24-C25-C30
27	2	2501	LUT	C1-C6-C7-C8
18	B	1021	CLA	C16-C17-C18-C19
18	A	1119	CLA	C3-C5-C6-C7
18	A	1131	CLA	C4-C3-C5-C6
18	A	1134	CLA	C4-C3-C5-C6
18	B	1206	CLA	C4-C3-C5-C6
22	A	6007	BCR	C19-C20-C21-C22
18	A	1140	CLA	C11-C10-C8-C7
18	B	1021	CLA	C12-C13-C15-C16
18	B	1203	CLA	C11-C12-C13-C15
18	B	1202	CLA	C11-C10-C8-C7
18	B	1228	CLA	C6-C7-C8-C10
18	A	1121	CLA	C6-C7-C8-C9
21	2	2801	LHG	O7-C5-C6-O8
18	A	1110	CLA	CBA-CGA-O2A-C1
18	A	1117	CLA	C16-C17-C18-C19
18	A	1136	CLA	C11-C10-C8-C7
18	A	1104	CLA	C4-C3-C5-C6
23	J	5001	LMG	C32-C33-C34-C35
18	A	1134	CLA	C2-C3-C5-C6
18	B	1240	CLA	C2-C3-C5-C6
18	B	1224	CLA	C2-C3-C5-C6
18	A	1110	CLA	C2-C1-O2A-CGA
18	2	2001	CLA	C5-C6-C7-C8
18	B	1023	CLA	C16-C17-C18-C19
18	A	1134	CLA	CAA-CBA-CGA-O1A
18	B	1238	CLA	C11-C12-C13-C14
18	B	1210	CLA	C13-C15-C16-C17
28	2	2013	CHL	CAA-CBA-CGA-O2A
18	B	1216	CLA	C4-C3-C5-C6
18	3	3003	CLA	C10-C11-C12-C13
18	B	1204	CLA	C2-C3-C5-C6
18	B	1220	CLA	C2-C3-C5-C6
18	4	4003	CLA	C2-C3-C5-C6
18	4	4003	CLA	C16-C17-C18-C19
18	B	1203	CLA	O1A-CGA-O2A-C1
18	B	1221	CLA	O1A-CGA-O2A-C1
18	A	1237	CLA	C2A-CAA-CBA-CGA
18	B	1224	CLA	C2A-CAA-CBA-CGA
23	J	5001	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
18	B	1023	CLA	C13-C15-C16-C17
18	A	1013	CLA	C4-C3-C5-C6
18	B	1236	CLA	C4-C3-C5-C6
18	B	1235	CLA	C8-C10-C11-C12
23	J	5001	LMG	C38-C39-C40-C41
18	A	1125	CLA	C4B-C3B-CAB-CBB
18	L	1501	CLA	O1A-CGA-O2A-C1
18	A	1117	CLA	C8-C10-C11-C12
18	B	1228	CLA	O1A-CGA-O2A-C1
18	A	1125	CLA	C11-C12-C13-C14
18	A	1131	CLA	C5-C6-C7-C8
22	A	6011	BCR	C11-C10-C9-C34
28	2	2010	CHL	CHA-CBD-CGD-O2D
18	A	1120	CLA	CAA-CBA-CGA-O2A
21	1	1801	LHG	O6-C4-C5-C6
23	F	5001	LMG	O7-C8-C9-O8
18	A	1013	CLA	C2-C3-C5-C6
18	A	1103	CLA	C12-C13-C15-C16
18	B	1234	CLA	C6-C7-C8-C10
21	1	1801	LHG	C11-C12-C13-C14
25	B	7101	DGD	C9B-CAB-CBB-CCB
18	A	1131	CLA	C14-C13-C15-C16
18	B	1215	CLA	C6-C7-C8-C9
18	B	1226	CLA	C6-C7-C8-C9
18	A	1118	CLA	C2C-C3C-CAC-CBC
18	B	1207	CLA	C2A-CAA-CBA-CGA
18	A	1136	CLA	C2-C1-O2A-CGA
18	L	1501	CLA	C2-C1-O2A-CGA
18	4	4004	CLA	C2-C1-O2A-CGA
18	3	3003	CLA	C2-C1-O2A-CGA
18	A	1136	CLA	C11-C10-C8-C9
18	1	1004	CLA	C16-C17-C18-C19
18	B	1021	CLA	CAA-CBA-CGA-O2A
18	1	1013	CLA	C4C-C3C-CAC-CBC
18	3	3004	CLA	C3-C5-C6-C7
21	A	7001	LHG	C19-C20-C21-C22
18	A	1022	CLA	C16-C17-C18-C20
18	B	1203	CLA	CBA-CGA-O2A-C1
18	A	1140	CLA	CAA-CBA-CGA-O2A
21	A	7001	LHG	C27-C28-C29-C30
18	B	1224	CLA	CAA-CBA-CGA-O2A
18	4	4017	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	B	1238	CLA	C2A-CAA-CBA-CGA
23	4	4801	LMG	C31-C32-C33-C34
18	G	1001	CLA	C4-C3-C5-C6
18	B	1221	CLA	CBA-CGA-O2A-C1
22	A	6011	BCR	C11-C10-C9-C8
18	B	1023	CLA	C15-C16-C17-C18
25	B	7101	DGD	C1G-C2G-C3G-O3G
18	B	1240	CLA	CAA-CBA-CGA-O1A
18	B	1227	CLA	C4-C3-C5-C6
18	A	1113	CLA	C2A-CAA-CBA-CGA
18	A	1118	CLA	C2A-CAA-CBA-CGA
18	B	1221	CLA	C2A-CAA-CBA-CGA
18	2	2004	CLA	C4C-C3C-CAC-CBC
23	J	5001	LMG	C11-C12-C13-C14
18	2	2004	CLA	C13-C15-C16-C17
18	1	1007	CLA	CAA-CBA-CGA-O2A
21	A	5003	LHG	C35-C36-C37-C38
18	2	2007	CLA	C5-C6-C7-C8
18	B	1239	CLA	C11-C10-C8-C9
18	B	1206	CLA	C11-C12-C13-C14
18	B	1207	CLA	C11-C12-C13-C14
18	4	4007	CLA	C6-C7-C8-C9
18	1	1004	CLA	C11-C10-C8-C9
18	A	1138	CLA	O1A-CGA-O2A-C1
22	I	6020	BCR	C21-C22-C23-C24
18	A	1131	CLA	C12-C13-C15-C16
18	A	1140	CLA	C12-C13-C15-C16
18	A	1119	CLA	C11-C12-C13-C15
18	B	1238	CLA	C11-C12-C13-C15
18	B	1215	CLA	C6-C7-C8-C10
18	B	1226	CLA	C6-C7-C8-C10
18	1	1001	CLA	C11-C10-C8-C7
18	2	2016	CLA	CAA-CBA-CGA-O1A
18	A	1104	CLA	C2B-C3B-CAB-CBB
18	1	1013	CLA	C2B-C3B-CAB-CBB
18	3	3012	CLA	C2B-C3B-CAB-CBB
22	A	6002	BCR	C23-C24-C25-C26
22	A	6002	BCR	C23-C24-C25-C30
22	A	6003	BCR	C23-C24-C25-C26
22	A	6007	BCR	C23-C24-C25-C26
22	A	6011	BCR	C23-C24-C25-C26
22	B	6005	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	J	6013	BCR	C5-C6-C7-C8
27	2	2501	LUT	C5-C6-C7-C8
27	4	4503	LUT	C1-C6-C7-C8
27	3	3502	LUT	C5-C6-C7-C8
18	A	1113	CLA	CAA-CBA-CGA-O2A
18	B	1220	CLA	CAA-CBA-CGA-O2A
21	2	2801	LHG	O8-C23-C24-C25
18	B	1224	CLA	C2-C1-O2A-CGA
18	B	1216	CLA	C16-C17-C18-C19
18	A	1105	CLA	CAA-CBA-CGA-O2A
18	B	1201	CLA	CAA-CBA-CGA-O2A
18	B	1228	CLA	CAA-CBA-CGA-O2A
18	2	2001	CLA	CAA-CBA-CGA-O2A
21	A	7001	LHG	C30-C31-C32-C33
23	G	2021	LMG	C10-C11-C12-C13
18	A	1122	CLA	CAA-CBA-CGA-O2A
18	B	1236	CLA	CAA-CBA-CGA-O2A
23	G	2021	LMG	O8-C28-C29-C30
18	B	1217	CLA	C2A-CAA-CBA-CGA
18	B	1023	CLA	C8-C10-C11-C12
18	A	1125	CLA	CAA-CBA-CGA-O2A
18	2	2008	CLA	CAA-CBA-CGA-O2A
18	1	1012	CLA	CAA-CBA-CGA-O2A
18	A	1138	CLA	C5-C6-C7-C8
18	2	2007	CLA	CAA-CBA-CGA-O2A
18	2	2003	CLA	CAA-CBA-CGA-O2A
23	G	2021	LMG	O7-C10-C11-C12
18	B	1235	CLA	CAA-CBA-CGA-O2A
18	B	1208	CLA	CAA-CBA-CGA-O2A
18	B	1210	CLA	CAA-CBA-CGA-O2A
18	K	1001	CLA	CAA-CBA-CGA-O2A
18	A	1103	CLA	O1A-CGA-O2A-C1
18	B	1021	CLA	C14-C13-C15-C16
18	B	1203	CLA	C11-C12-C13-C14
18	B	1235	CLA	C11-C12-C13-C14
18	B	1202	CLA	C11-C10-C8-C9
18	B	1228	CLA	C6-C7-C8-C9
18	B	1238	CLA	CAA-CBA-CGA-O2A
18	4	4016	CLA	CAA-CBA-CGA-O2A
18	3	3010	CLA	CAA-CBA-CGA-O2A
18	A	1116	CLA	C4B-C3B-CAB-CBB
18	B	1206	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	1218	CLA	C4B-C3B-CAB-CBB
18	B	1219	CLA	C4B-C3B-CAB-CBB
18	B	1232	CLA	C4B-C3B-CAB-CBB
18	F	1302	CLA	C1A-C2A-CAA-CBA
18	G	1003	CLA	C4B-C3B-CAB-CBB
18	H	1000	CLA	O1A-CGA-O2A-C1
18	1	1001	CLA	C1A-C2A-CAA-CBA
18	1	1013	CLA	C4B-C3B-CAB-CBB
18	3	3017	CLA	C1A-C2A-CAA-CBA
18	B	1211	CLA	C4-C3-C5-C6
18	A	1136	CLA	CAA-CBA-CGA-O2A
18	B	1239	CLA	CAA-CBA-CGA-O2A
18	3	3003	CLA	CAA-CBA-CGA-O2A
22	A	6008	BCR	C17-C18-C19-C20
22	A	6011	BCR	C17-C18-C19-C20
22	B	6004	BCR	C21-C22-C23-C24
27	4	4502	LUT	C11-C12-C13-C14
18	B	1205	CLA	CAA-CBA-CGA-O2A
18	G	1001	CLA	CAA-CBA-CGA-O2A
23	G	2021	LMG	C17-C18-C19-C20
18	B	1204	CLA	C6-C7-C8-C10
18	B	1219	CLA	CAA-CBA-CGA-O2A
23	J	5001	LMG	C19-C20-C21-C22
18	A	1111	CLA	C2-C1-O2A-CGA
18	B	1226	CLA	C2-C1-O2A-CGA
18	B	1228	CLA	C2-C1-O2A-CGA
18	2	2003	CLA	C2-C1-O2A-CGA
18	2	2009	CLA	C2-C1-O2A-CGA
18	B	1221	CLA	C11-C10-C8-C7
18	B	1227	CLA	C11-C10-C8-C7
18	B	1227	CLA	C12-C13-C15-C16
18	A	1013	CLA	C16-C17-C18-C20
23	2	2802	LMG	C7-C8-O7-C10
18	B	1228	CLA	CBA-CGA-O2A-C1
18	B	1220	CLA	CAA-CBA-CGA-O1A
18	A	1124	CLA	C2A-CAA-CBA-CGA
20	B	5002	PQN	C26-C27-C28-C29
18	1	1007	CLA	CAA-CBA-CGA-O1A
18	A	1022	CLA	C3A-C2A-CAA-CBA
18	B	1206	CLA	C3A-C2A-CAA-CBA
18	B	1235	CLA	C5-C6-C7-C8
22	B	6009	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	A	1122	CLA	CAA-CBA-CGA-O1A
18	A	1125	CLA	CAA-CBA-CGA-O1A
18	G	1001	CLA	CAA-CBA-CGA-O1A
18	A	1113	CLA	CAA-CBA-CGA-O1A
18	B	1228	CLA	CAA-CBA-CGA-O1A
18	A	1136	CLA	C5-C6-C7-C8
21	2	2801	LHG	C23-C24-C25-C26
18	1	1001	CLA	C6-C7-C8-C9
18	3	3004	CLA	C6-C7-C8-C9
18	K	1001	CLA	CAA-CBA-CGA-O1A
18	2	2007	CLA	CAA-CBA-CGA-O1A
21	2	2801	LHG	O10-C23-C24-C25
18	B	1012	CLA	C16-C17-C18-C19
18	A	1125	CLA	C4-C3-C5-C6
18	B	1221	CLA	C4-C3-C5-C6
23	G	2021	LMG	O9-C10-C11-C12
18	A	1106	CLA	CAA-CBA-CGA-O2A
18	3	3007	CLA	O1A-CGA-O2A-C1
18	B	1239	CLA	CAA-CBA-CGA-O1A
18	B	1201	CLA	CAA-CBA-CGA-O1A
18	2	2008	CLA	CAA-CBA-CGA-O1A
23	4	4801	LMG	O8-C28-C29-C30
18	4	4004	CLA	C11-C12-C13-C15
18	A	1139	CLA	C8-C10-C11-C12
22	B	6009	BCR	C21-C22-C23-C24
17	A	1011	CL0	C5-C6-C7-C8
23	2	2802	LMG	C8-C7-O1-C1
23	4	4801	LMG	O1-C7-C8-O7
18	A	1105	CLA	CAA-CBA-CGA-O1A
18	A	1136	CLA	CAA-CBA-CGA-O1A
18	B	1238	CLA	CAA-CBA-CGA-O1A
18	B	1208	CLA	CAA-CBA-CGA-O1A
18	2	2001	CLA	CAA-CBA-CGA-O1A
18	4	4016	CLA	CAA-CBA-CGA-O1A
23	G	2021	LMG	O10-C28-C29-C30
18	3	3010	CLA	CAA-CBA-CGA-O1A
18	G	1003	CLA	C10-C11-C12-C13
18	B	1216	CLA	C2-C3-C5-C6
18	B	1236	CLA	CAA-CBA-CGA-O1A
18	B	1210	CLA	CAA-CBA-CGA-O1A
18	3	3003	CLA	CAA-CBA-CGA-O1A
18	1	1012	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	G	1003	CLA	O1A-CGA-O2A-C1
25	B	7101	DGD	C7A-C8A-C9A-CAA
18	A	1118	CLA	C4C-C3C-CAC-CBC
18	A	1132	CLA	C2-C1-O2A-CGA
18	A	1134	CLA	C2-C1-O2A-CGA
18	1	1004	CLA	C2-C1-O2A-CGA
18	B	1235	CLA	CAA-CBA-CGA-O1A
18	2	2003	CLA	CAA-CBA-CGA-O1A
18	A	1121	CLA	CAA-CBA-CGA-O2A
18	1	1008	CLA	CAA-CBA-CGA-O2A
17	A	1011	CL0	C1A-C2A-CAA-CBA
26	B	8001	LMU	O5'-C5'-C6'-O6'
18	A	1124	CLA	CAA-CBA-CGA-O2A
18	L	1503	CLA	CAA-CBA-CGA-O2A
18	A	1121	CLA	CAA-CBA-CGA-O1A
18	A	1116	CLA	CAA-CBA-CGA-O2A
18	A	1129	CLA	CAA-CBA-CGA-O2A
21	A	7001	LHG	C18-C19-C20-C21
18	A	1106	CLA	CAA-CBA-CGA-O1A
18	B	1219	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

204 monomers are involved in 1868 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	7001	LHG	6	0
27	3	3502	LUT	23	0
18	A	1013	CLA	7	0
18	B	1023	CLA	7	0
18	F	1302	CLA	11	0
22	B	6010	BCR	1	0
18	A	1104	CLA	3	0
18	A	1137	CLA	3	0
18	4	4005	CLA	13	0
18	4	4008	CLA	15	0
22	A	6002	BCR	4	0
18	A	1128	CLA	11	0
23	B	5005	LMG	3	0
18	A	1122	CLA	7	0
18	B	1225	CLA	3	0
18	1	1003	CLA	32	0
22	G	2011	BCR	28	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1103	CLA	5	0
18	B	1206	CLA	4	0
28	4	4013	CHL	19	0
18	3	3017	CLA	11	0
18	J	1302	CLA	7	0
18	B	1236	CLA	6	0
18	B	1217	CLA	1	0
18	A	1118	CLA	3	0
18	G	1002	CLA	23	0
18	B	1226	CLA	7	0
18	B	1238	CLA	7	0
22	B	6006	BCR	6	0
18	2	2007	CLA	24	0
22	L	6020	BCR	5	0
18	A	1127	CLA	5	0
22	J	6013	BCR	8	0
18	B	1222	CLA	8	0
18	1	1001	CLA	48	0
18	1	1007	CLA	7	0
18	B	1207	CLA	11	0
18	3	3019	CLA	1	0
18	A	1114	CLA	1	0
27	4	4501	LUT	21	0
18	A	1132	CLA	6	0
22	I	6020	BCR	3	0
22	A	6008	BCR	2	0
18	2	2002	CLA	34	0
18	A	1022	CLA	5	0
18	A	1115	CLA	1	0
28	4	4010	CHL	7	0
18	2	2008	CLA	14	0
18	A	1133	CLA	3	0
18	B	1021	CLA	7	0
18	3	3005	CLA	14	0
18	B	1231	CLA	3	0
18	B	1230	CLA	8	0
20	B	5002	PQN	5	0
18	3	3007	CLA	4	0
18	B	1204	CLA	9	0
18	2	2005	CLA	21	0
22	J	6012	BCR	7	0
18	A	1139	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	1011	CL0	5	0
23	J	5001	LMG	10	0
18	B	1220	CLA	10	0
18	A	1113	CLA	3	0
18	B	1235	CLA	6	0
18	A	1117	CLA	4	0
29	4	4505	ZEX	12	0
21	A	5003	LHG	6	0
18	G	1003	CLA	30	0
18	B	1210	CLA	7	0
18	A	1135	CLA	3	0
18	3	3006	CLA	37	0
28	3	3011	CHL	22	0
18	B	1223	CLA	4	0
21	2	2801	LHG	6	0
22	B	6005	BCR	3	0
18	B	1232	CLA	3	0
18	1	1004	CLA	26	0
18	2	2004	CLA	24	0
18	A	1110	CLA	10	0
18	3	3004	CLA	16	0
22	B	6004	BCR	9	0
18	1	1013	CLA	13	0
22	L	6019	BCR	22	0
18	A	1124	CLA	4	0
22	B	6009	BCR	6	0
27	2	2502	LUT	32	0
18	B	1203	CLA	2	0
21	1	1801	LHG	15	0
18	A	1123	CLA	6	0
18	B	1239	CLA	5	0
18	A	1237	CLA	4	0
27	1	1502	LUT	17	0
18	B	1240	CLA	6	0
18	B	1209	CLA	3	0
18	B	1208	CLA	6	0
18	3	3018	CLA	20	0
22	A	6007	BCR	3	0
18	B	1228	CLA	3	0
18	1	1002	CLA	17	0
18	A	1101	CLA	4	0
27	1	1501	LUT	32	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	1012	CLA	16	0
18	4	4001	CLA	24	0
18	3	3001	CLA	21	0
18	A	1102	CLA	3	0
18	B	1012	CLA	5	0
18	4	4002	CLA	11	0
20	A	5001	PQN	3	0
28	2	2010	CHL	18	0
28	2	2011	CHL	5	0
18	3	3008	CLA	17	0
18	B	1201	CLA	1	0
28	2	2013	CHL	17	0
18	1	1011	CLA	15	0
18	B	1216	CLA	4	0
18	B	1211	CLA	8	0
21	B	5004	LHG	1	0
23	G	2021	LMG	20	0
18	A	1125	CLA	4	0
28	1	1009	CHL	28	0
18	2	2003	CLA	29	0
18	A	1130	CLA	2	0
18	A	1131	CLA	1	0
18	3	3013	CLA	24	0
18	2	2009	CLA	16	0
18	4	4007	CLA	20	0
18	A	1151	CLA	3	0
23	F	5001	LMG	7	0
22	A	6017	BCR	8	0
26	B	8001	LMU	1	0
18	3	3012	CLA	31	0
18	4	4016	CLA	26	0
18	A	1140	CLA	3	0
18	B	1229	CLA	5	0
18	3	3010	CLA	35	0
18	B	1218	CLA	9	0
18	B	1224	CLA	6	0
18	A	1126	CLA	9	0
18	A	1116	CLA	7	0
18	B	1205	CLA	7	0
18	B	1221	CLA	10	0
23	4	4801	LMG	6	0
18	2	2012	CLA	22	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1105	CLA	4	0
22	F	6014	BCR	8	0
22	A	6003	BCR	2	0
22	K	2011	BCR	17	0
18	2	2001	CLA	36	0
18	A	1138	CLA	7	0
18	A	1109	CLA	6	0
22	A	6011	BCR	4	0
18	A	1111	CLA	7	0
22	F	6016	BCR	9	0
18	A	1120	CLA	2	0
18	4	4012	CLA	24	0
19	A	3001	SF4	1	0
18	4	4004	CLA	17	0
18	A	1108	CLA	2	0
18	B	1219	CLA	2	0
18	2	2016	CLA	37	0
18	4	4017	CLA	11	0
18	4	4009	CLA	9	0
23	F	5002	LMG	6	0
28	1	1010	CHL	8	0
18	4	4006	CLA	21	0
18	3	3003	CLA	49	0
27	4	4502	LUT	28	0
18	A	1106	CLA	11	0
18	B	1212	CLA	5	0
18	B	1213	CLA	5	0
18	B	1234	CLA	6	0
18	A	1134	CLA	2	0
22	3	3503	BCR	20	0
18	F	1301	CLA	5	0
18	B	1215	CLA	5	0
18	4	4003	CLA	13	0
18	A	1119	CLA	6	0
27	I	6018	LUT	12	0
23	2	2802	LMG	9	0
26	B	8002	LMU	3	0
18	L	1503	CLA	11	0
18	1	1014	CLA	14	0
27	2	2501	LUT	21	0
27	3	3501	LUT	39	0
28	4	4011	CHL	20	0

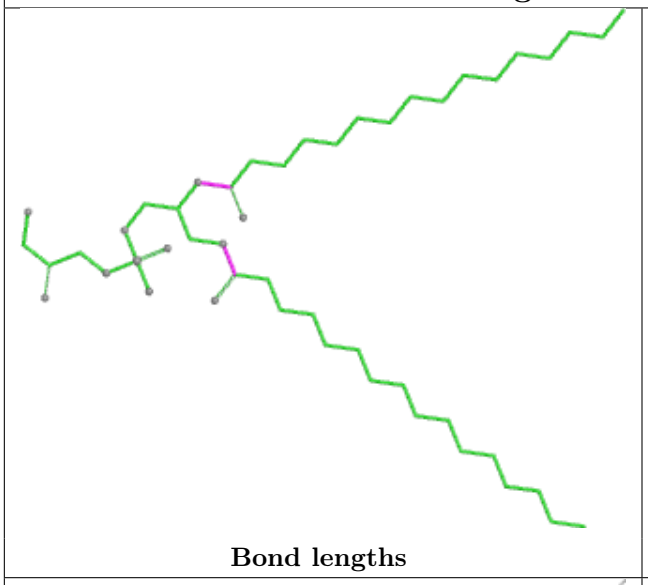
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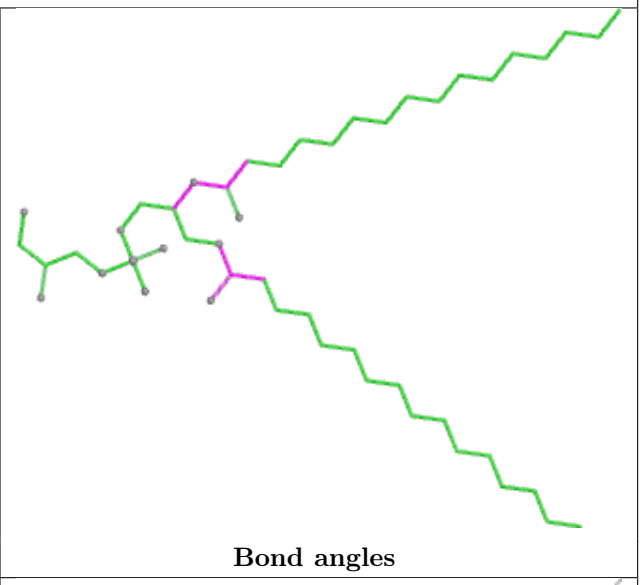
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	3002	CLA	8	0
18	B	1227	CLA	7	0
18	B	1202	CLA	7	0
18	1	1006	CLA	7	0
27	4	4503	LUT	32	0
18	1	1008	CLA	33	0
18	2	2006	CLA	22	0
25	B	7101	DGD	4	0
18	L	1502	CLA	13	0
18	K	1001	CLA	12	0
18	A	1107	CLA	2	0
18	B	1214	CLA	4	0
18	A	1121	CLA	4	0
18	A	1136	CLA	6	0
18	G	1001	CLA	34	0
18	A	1112	CLA	10	0
18	L	1501	CLA	13	0
18	H	1000	CLA	5	0
18	1	1005	CLA	16	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.

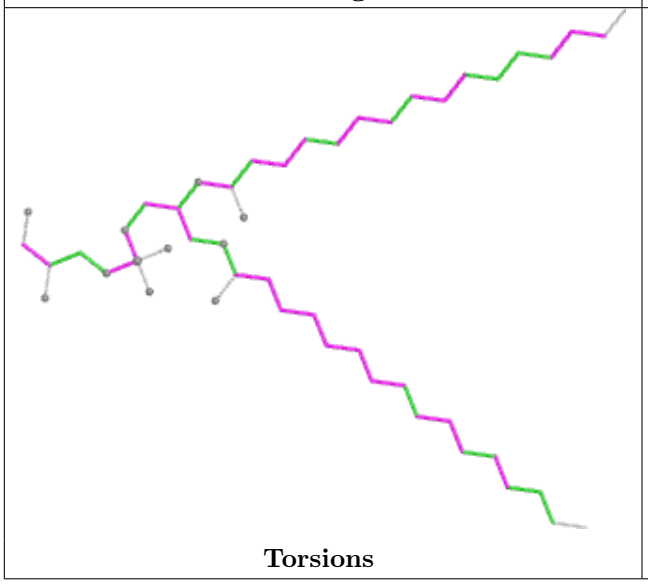
Ligand LHG A 7001



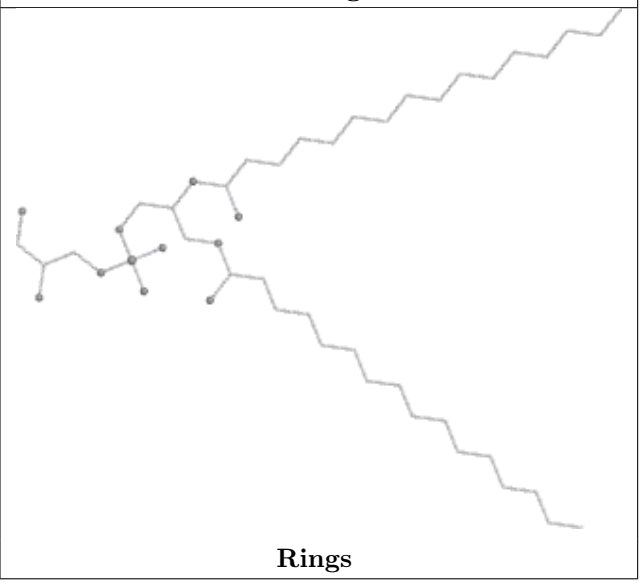
Bond lengths



Bond angles

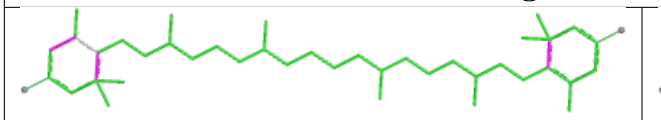


Torsions



Rings

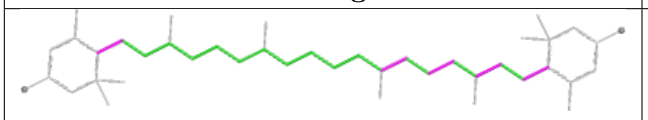
Ligand LUT 3 3502



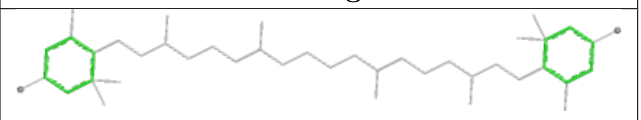
Bond lengths



Bond angles

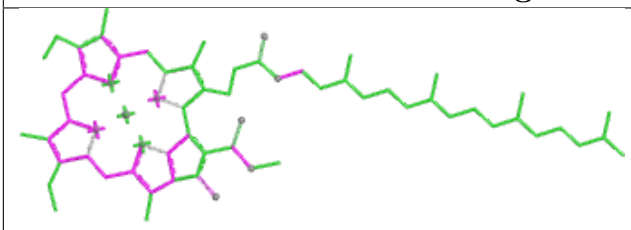


Torsions

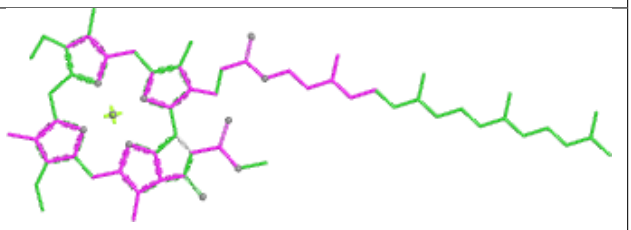


Rings

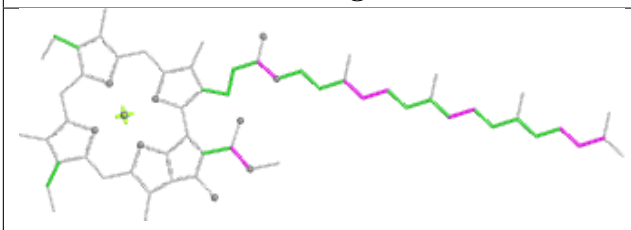
Ligand CLA A 1013



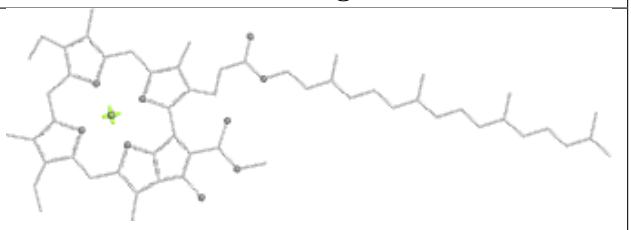
Bond lengths



Bond angles

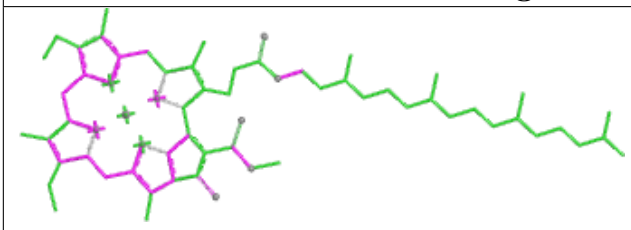


Torsions

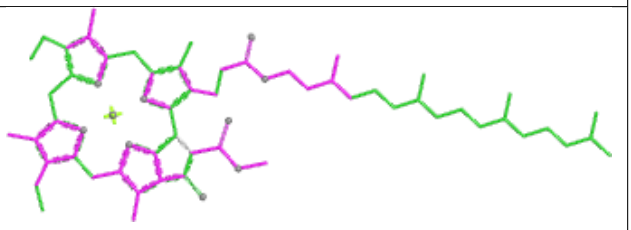


Rings

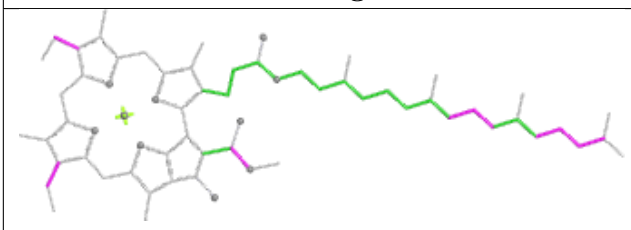
Ligand CLA B 1023



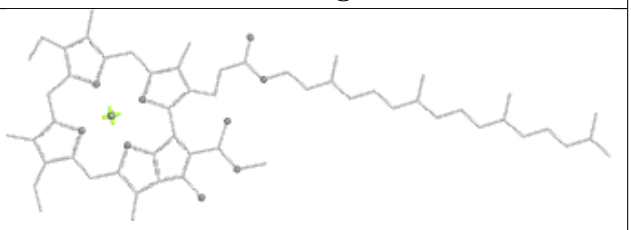
Bond lengths



Bond angles

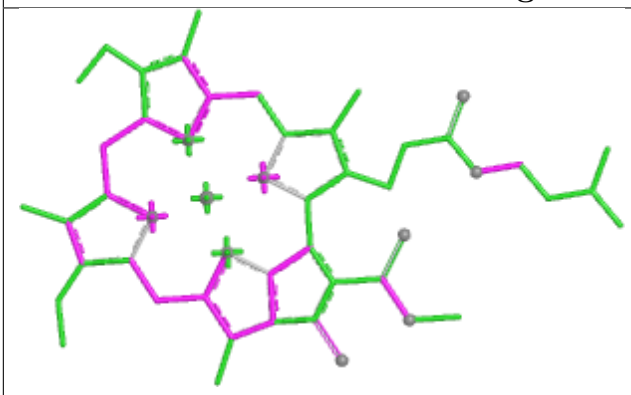


Torsions

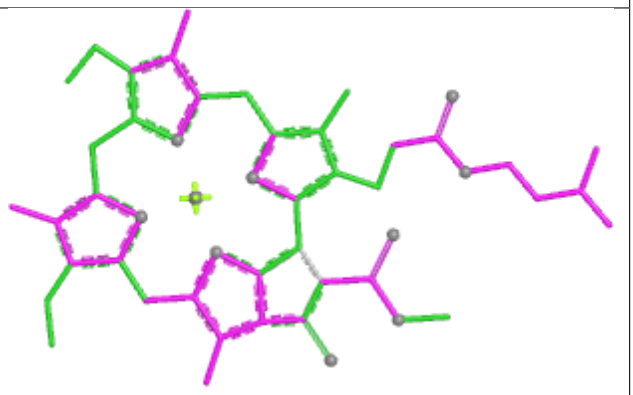


Rings

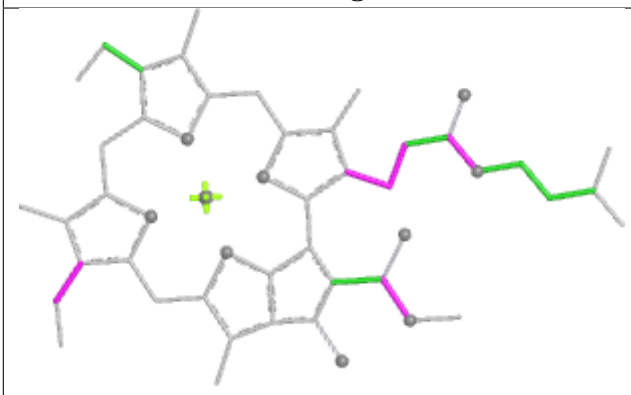
Ligand CLA F 1302



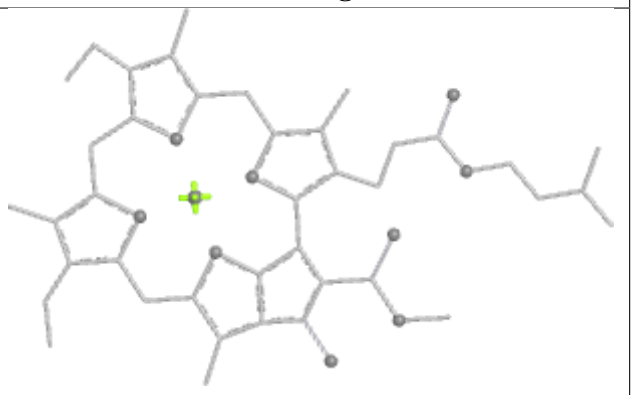
Bond lengths



Bond angles

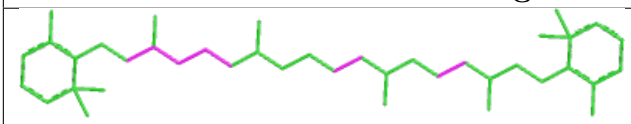


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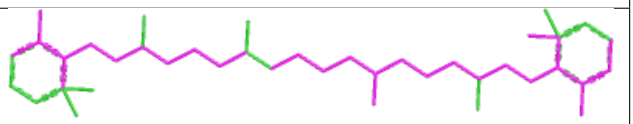


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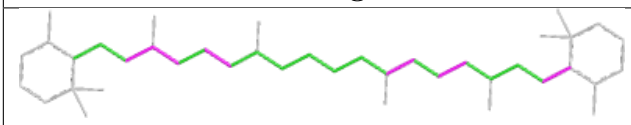
Ligand BCR B 6010



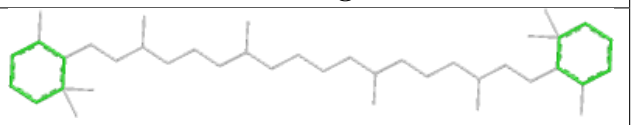
Bond lengths



Bond angles

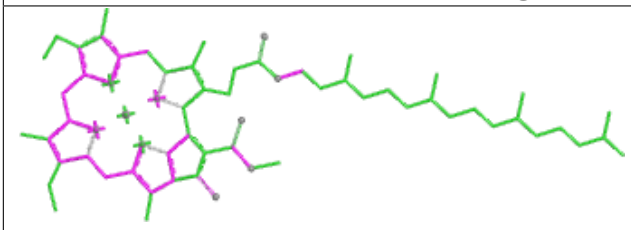


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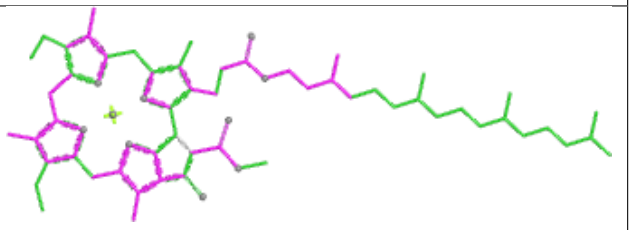


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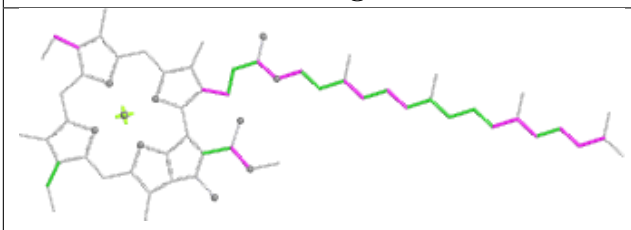
Ligand CLA A 1104



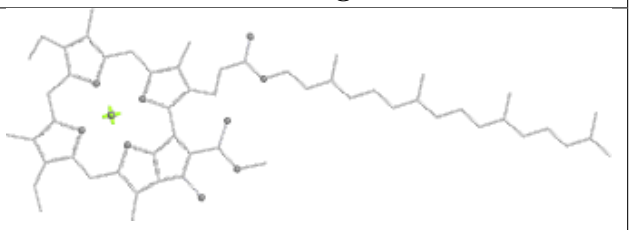
Bond lengths



Bond angles

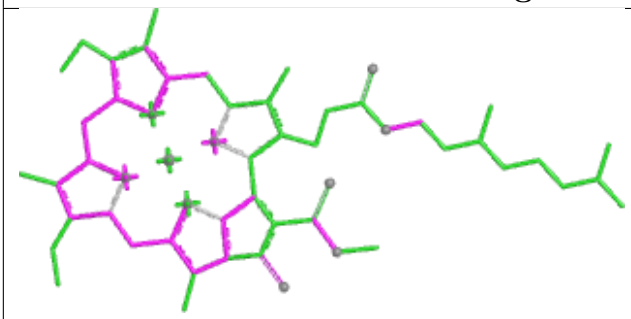


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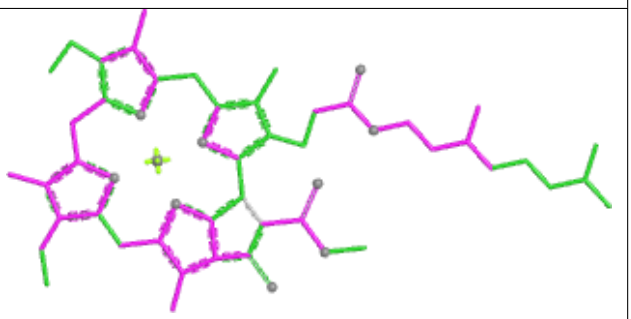


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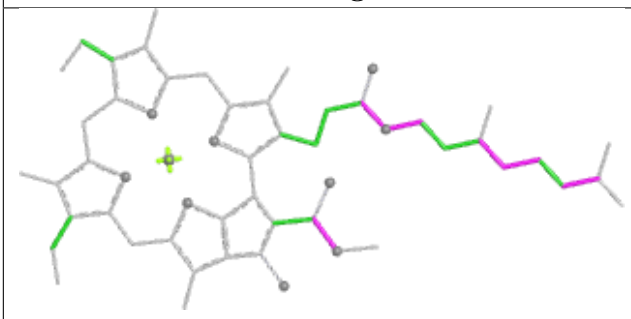
Ligand CLA A 1137



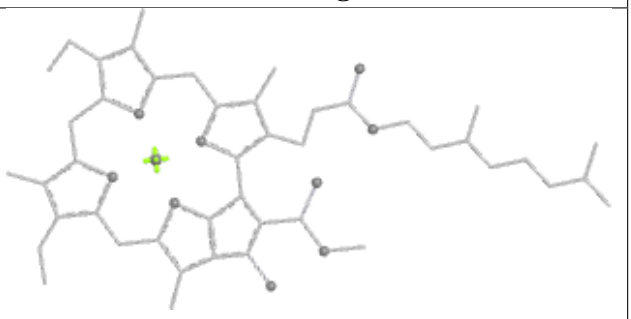
Bond lengths



Bond angles

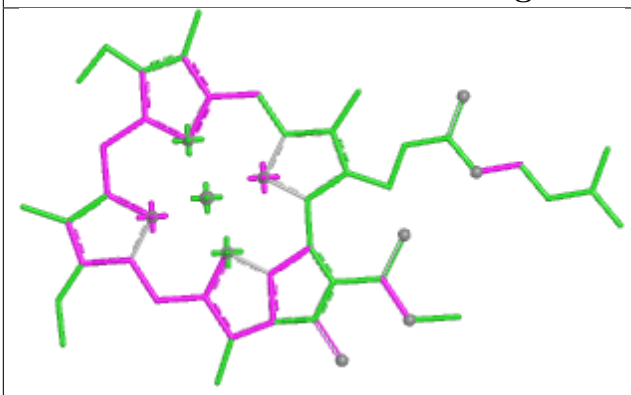


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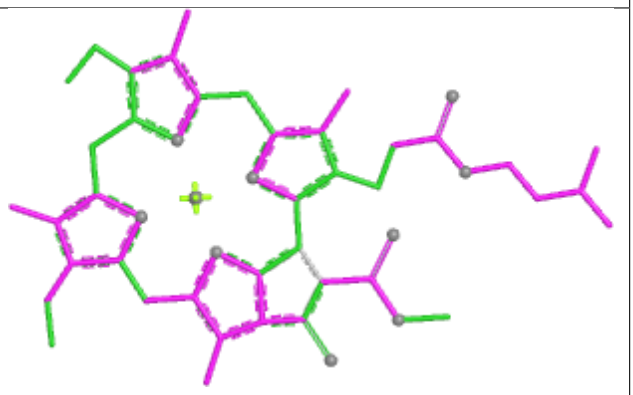


Rings

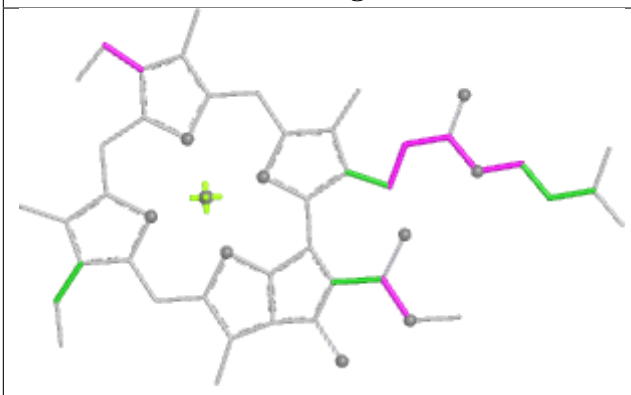
Ligand CLA A 1129



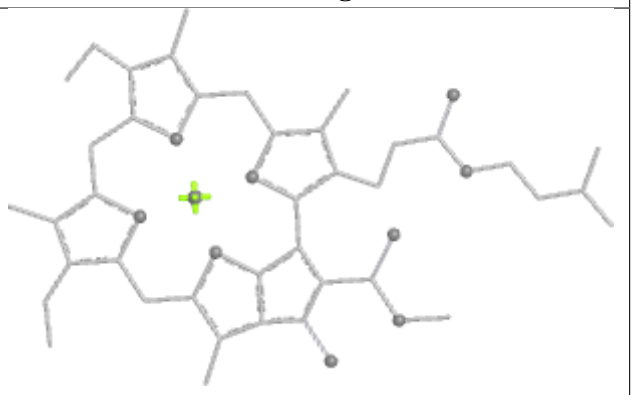
Bond lengths



Bond angles

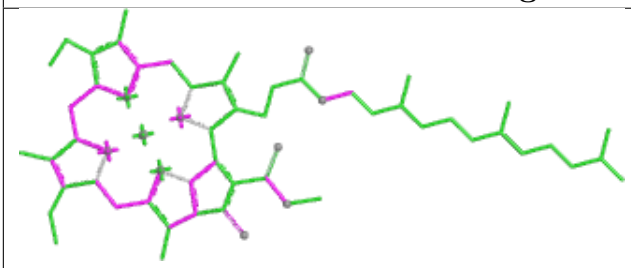


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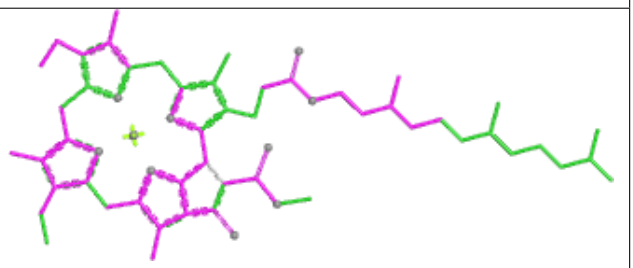


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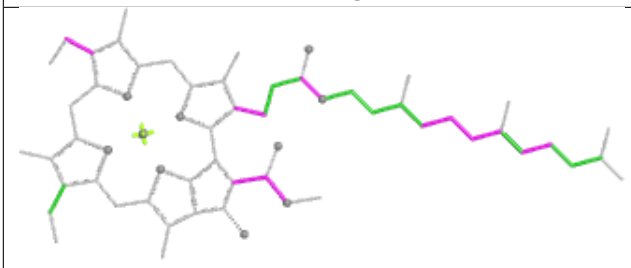
Ligand CLA 4 4005



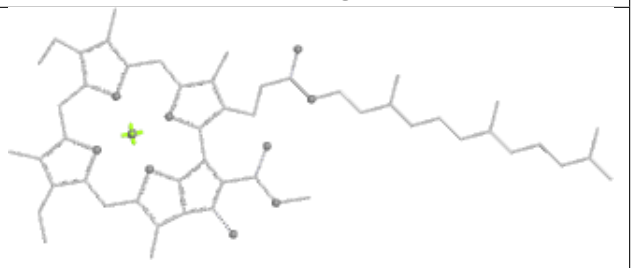
Bond lengths



Bond angles

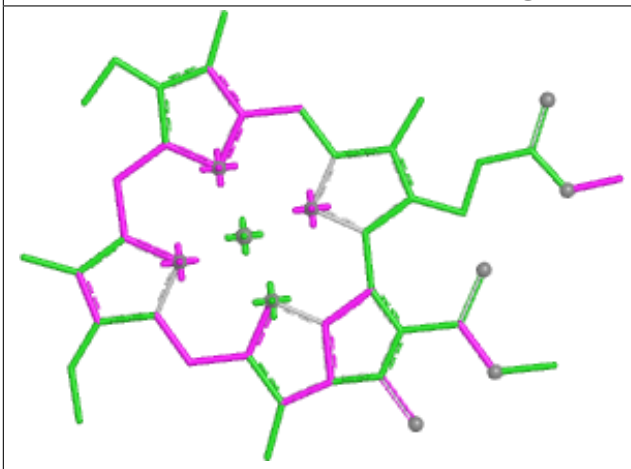


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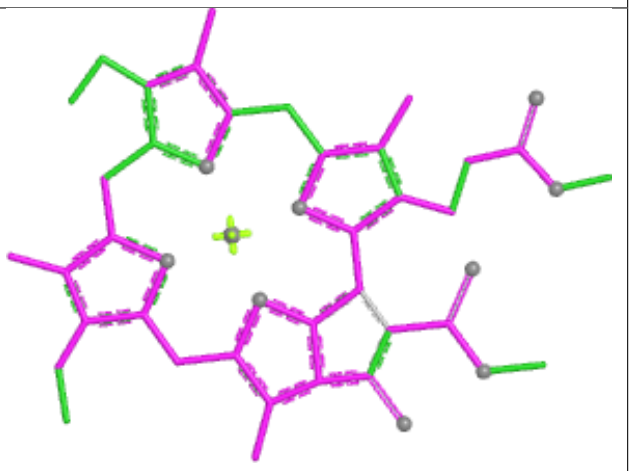


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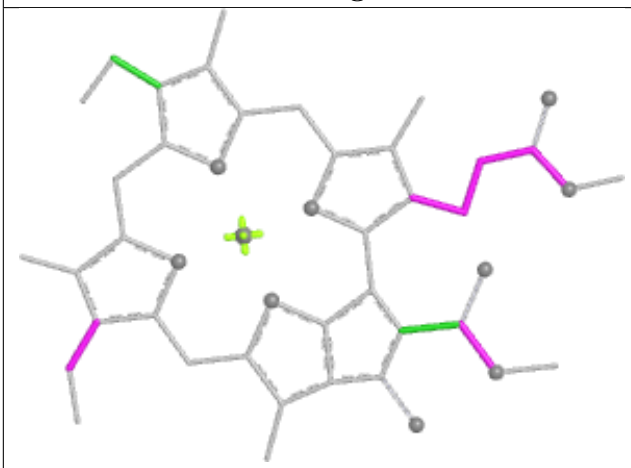
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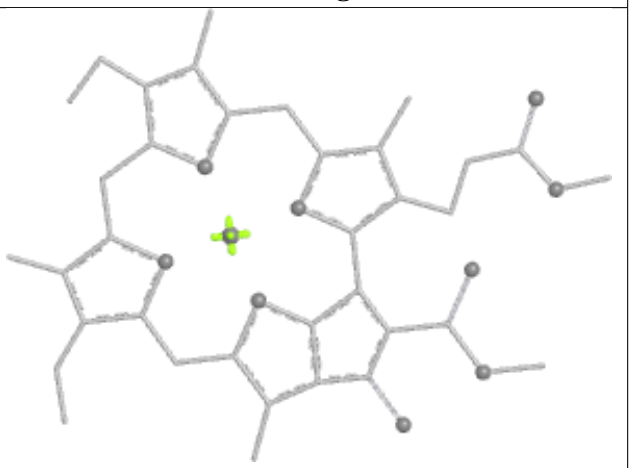
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Bond angles

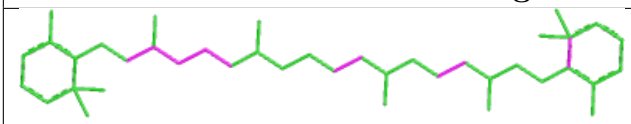


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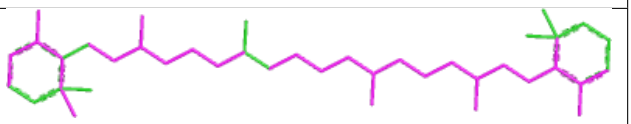


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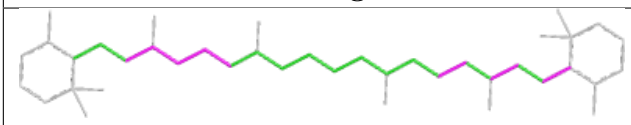
Ligand BCR A 6002



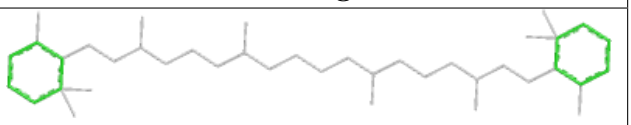
Bond lengths



Bond angles

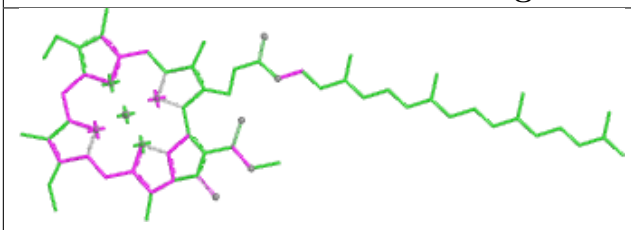


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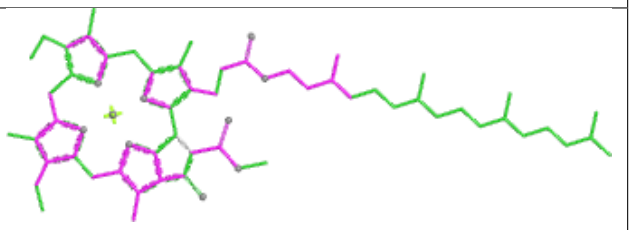


Rings

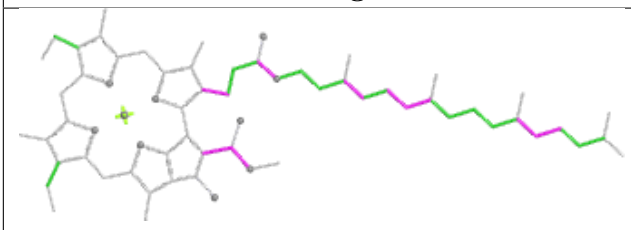
Ligand CLA A 1128



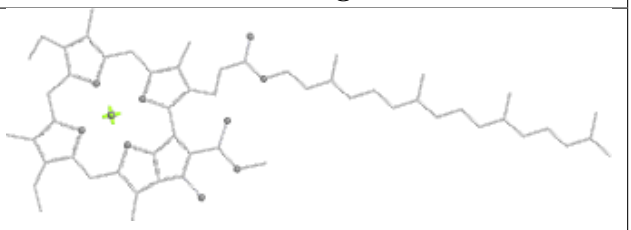
Bond lengths



Bond angles

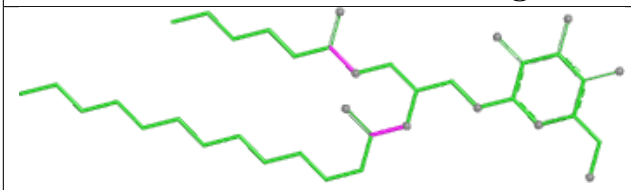


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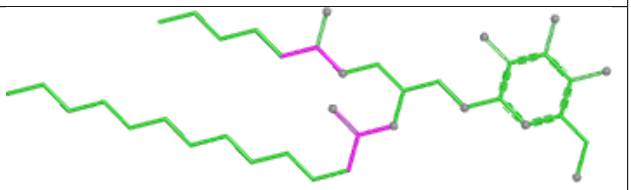


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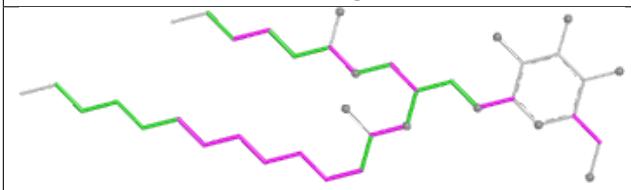
Ligand LMG B 5005



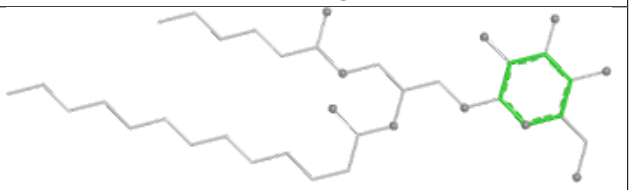
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Bond angles

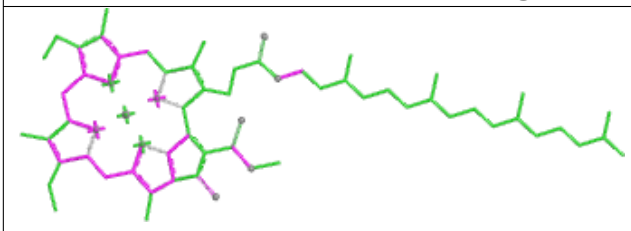


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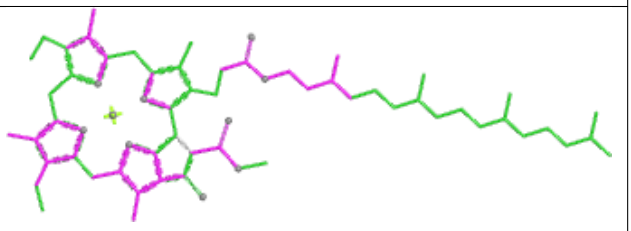


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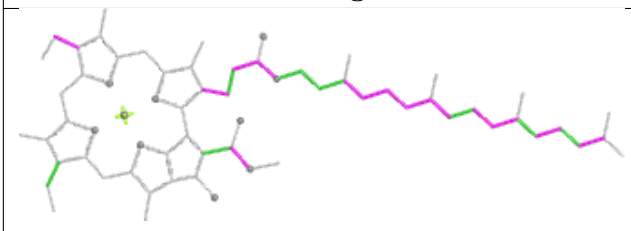
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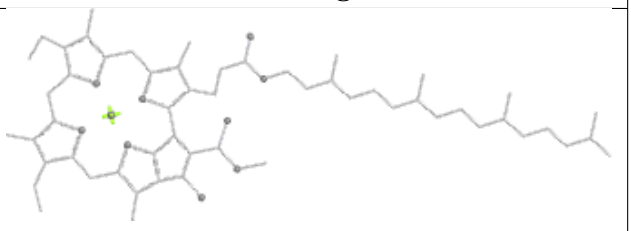
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Bond angles

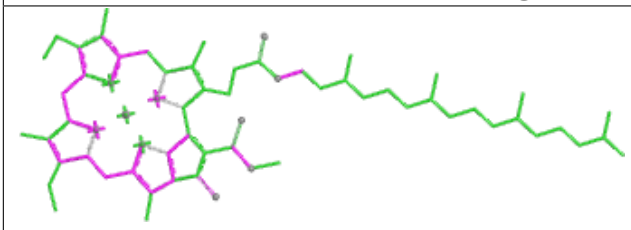


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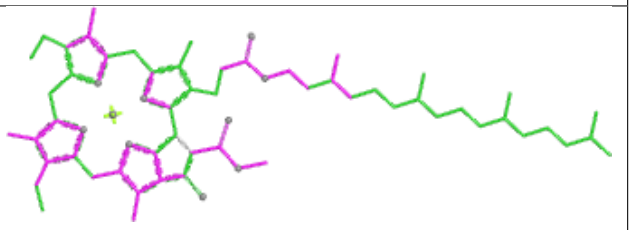


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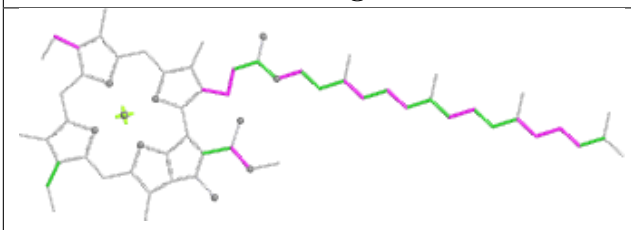
Ligand CLA B 1225



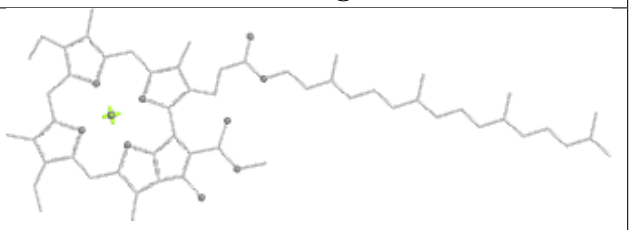
Bond lengths



Bond angles

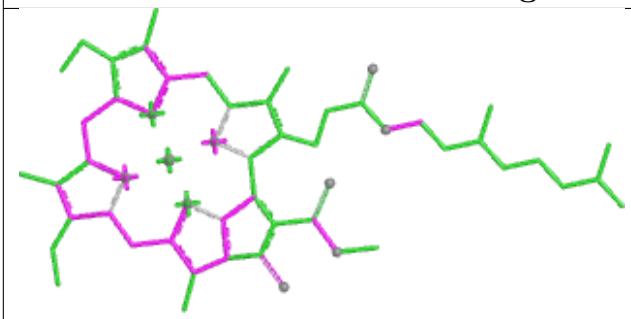


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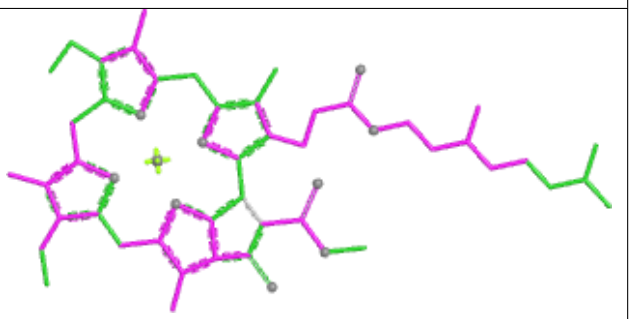


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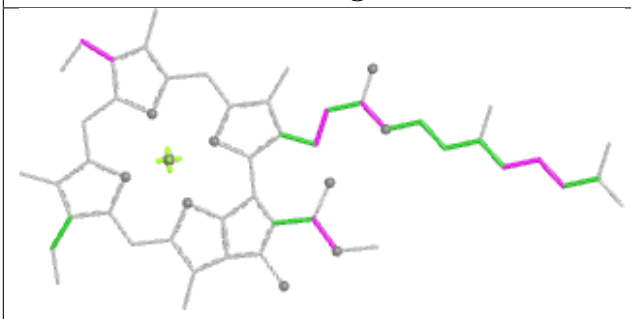
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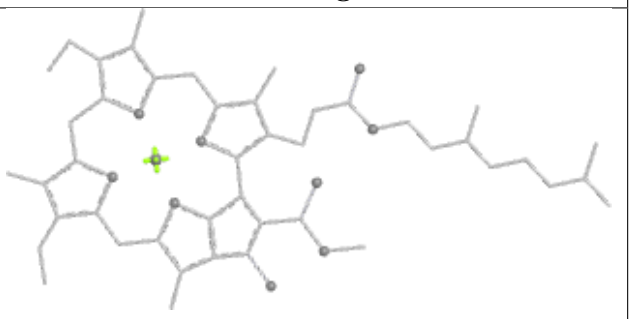
Bond lengths



Bond angles

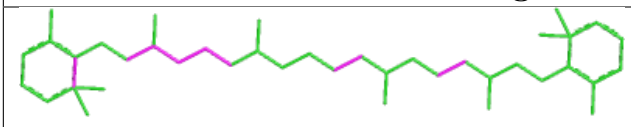


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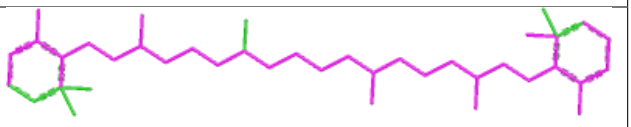


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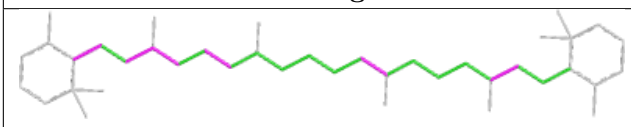
Ligand BCR G 2011



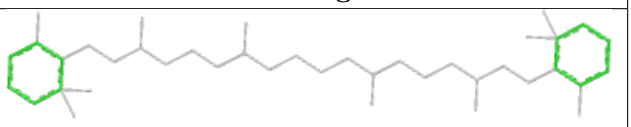
Bond lengths



Bond angles

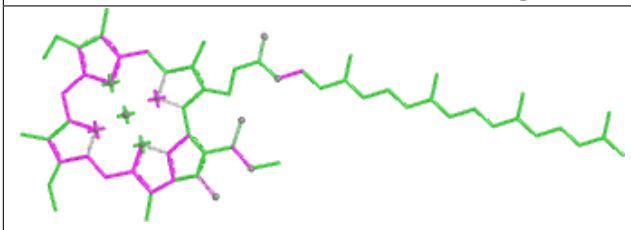


Torsions

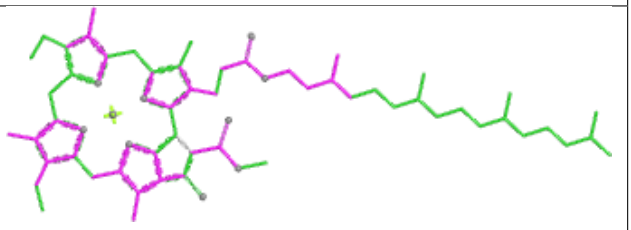


Rings

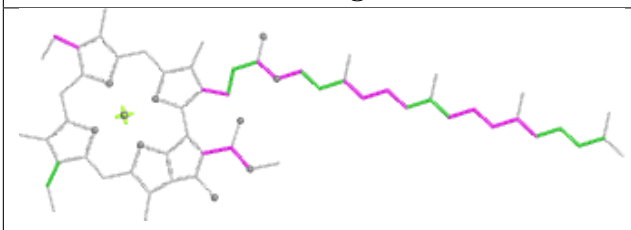
Ligand CLA A 1103



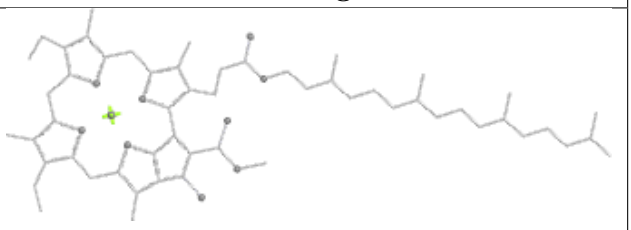
Bond lengths



Bond angles

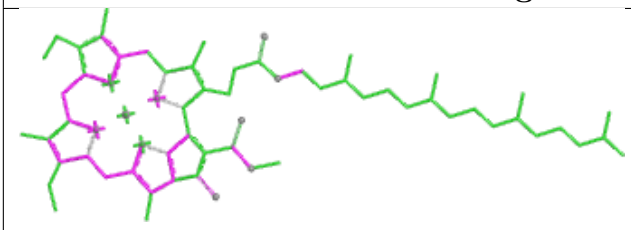


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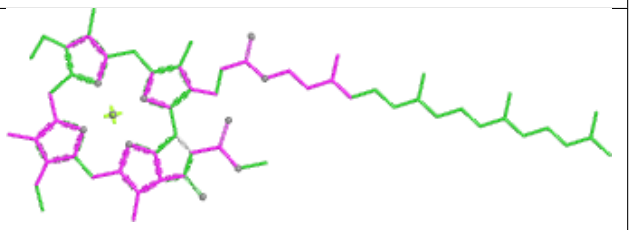


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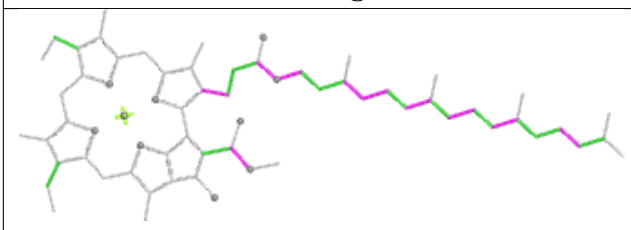
Ligand CLA B 1206



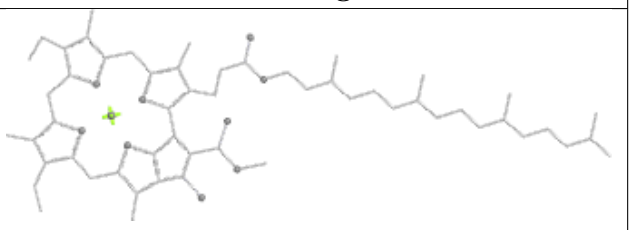
Bond lengths



Bond angles

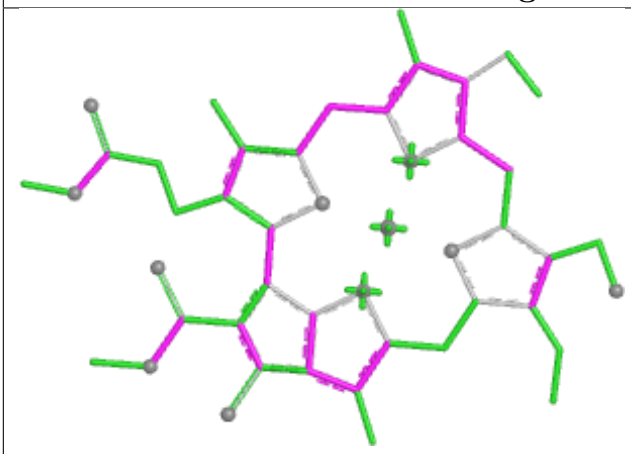


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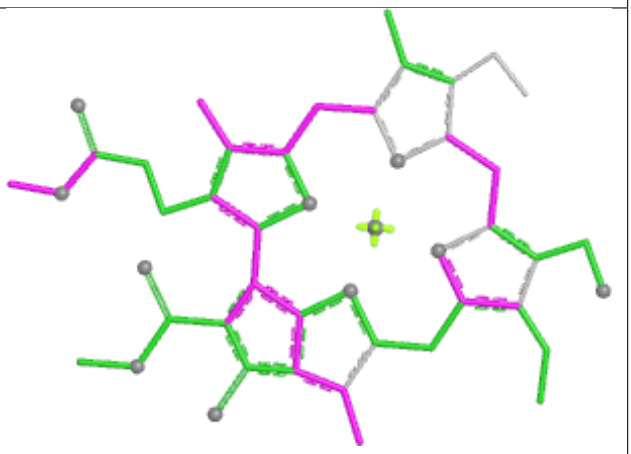


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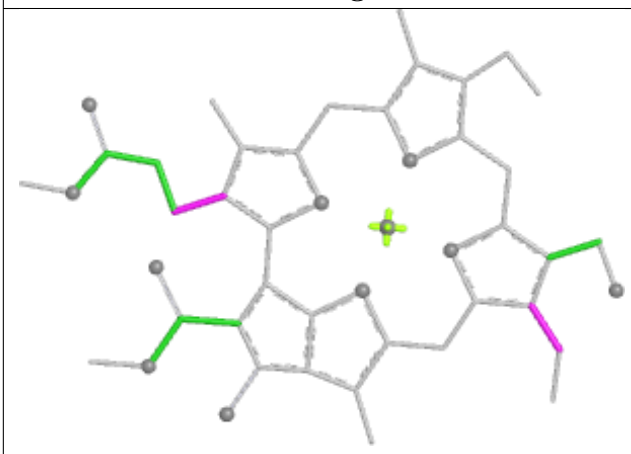
Ligand CHL 4 4013



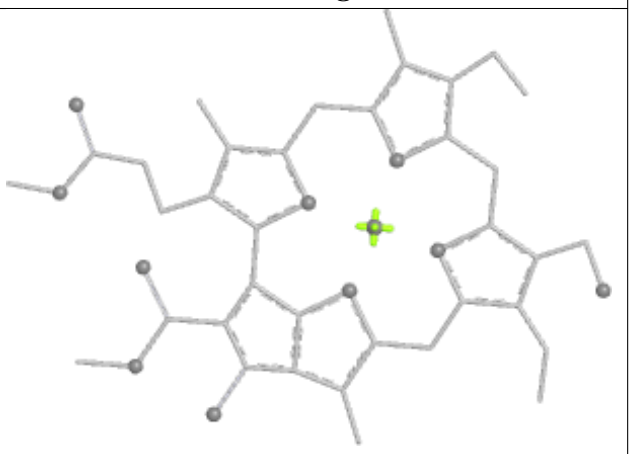
Bond lengths



Bond angles

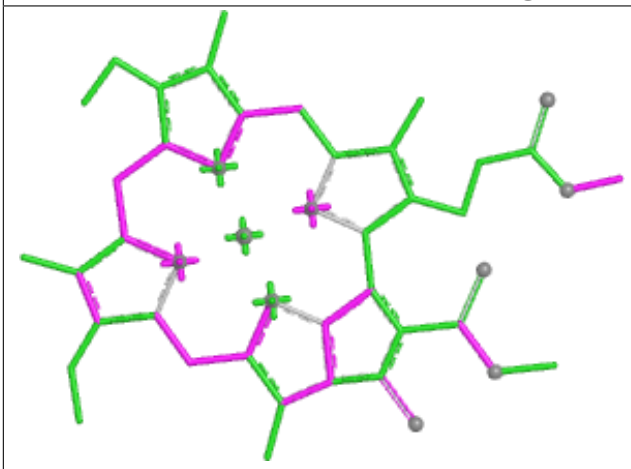


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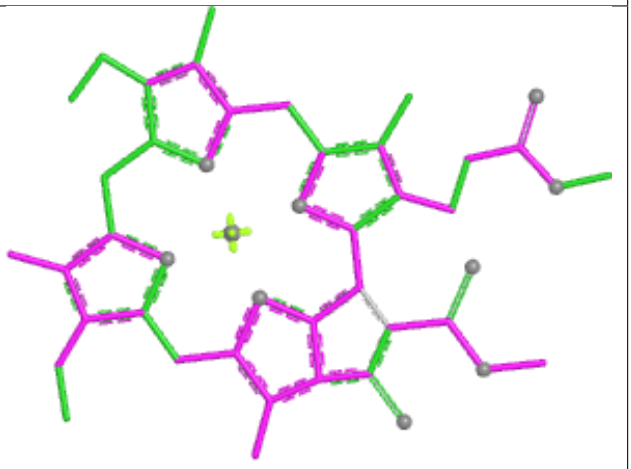


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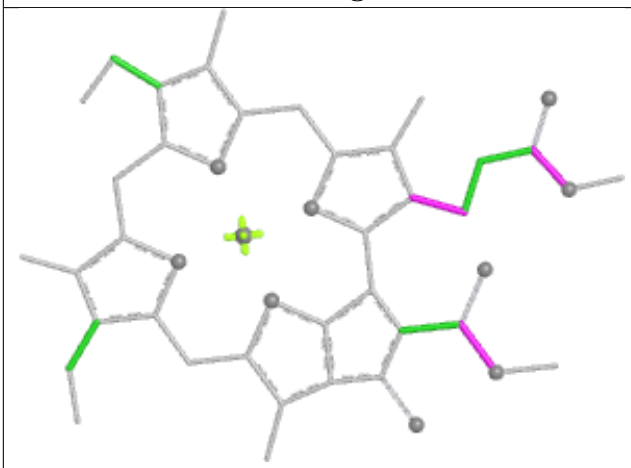
Ligand CLA 3 3017



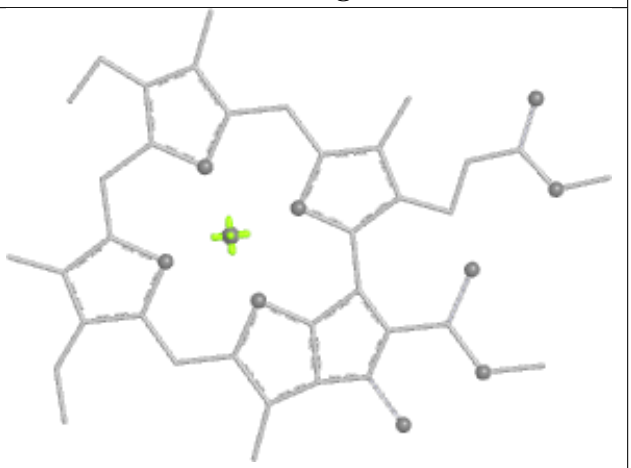
Bond lengths



Bond angles

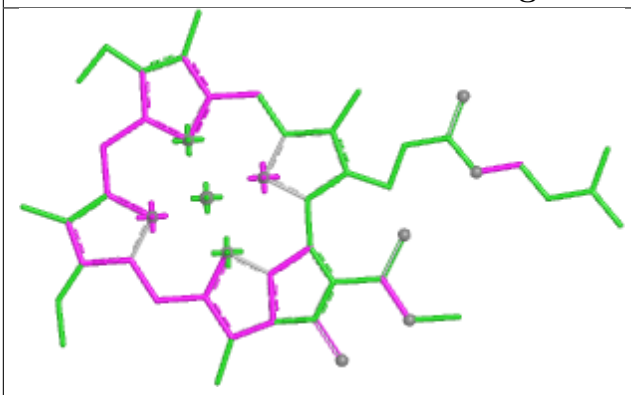


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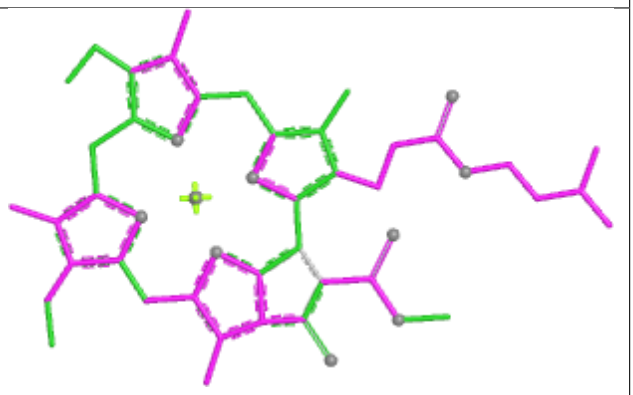


Rings

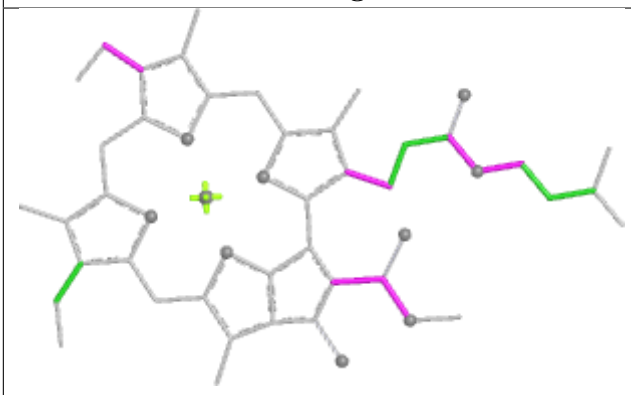
Ligand CLA J 1302



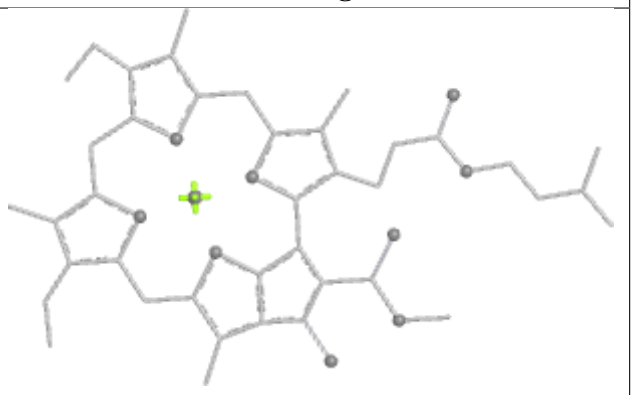
Bond lengths



Bond angles

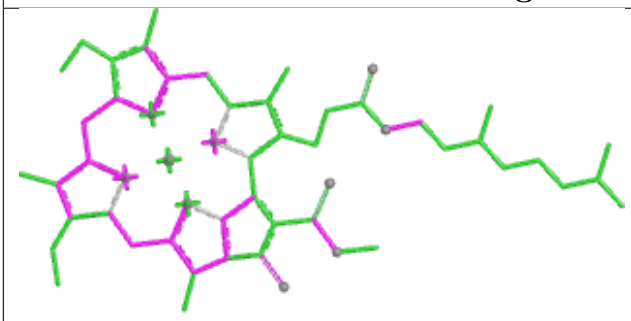


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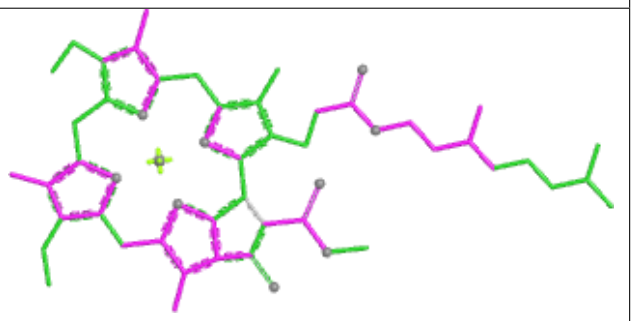


Rings

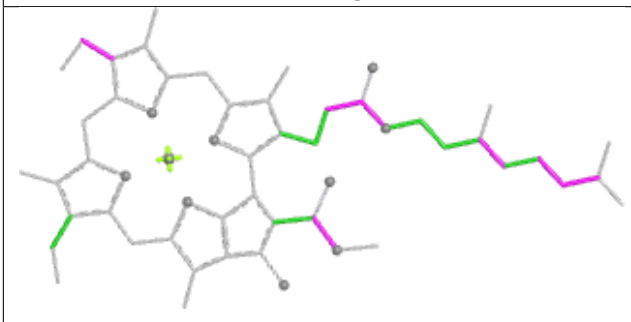
Ligand CLA B 1236



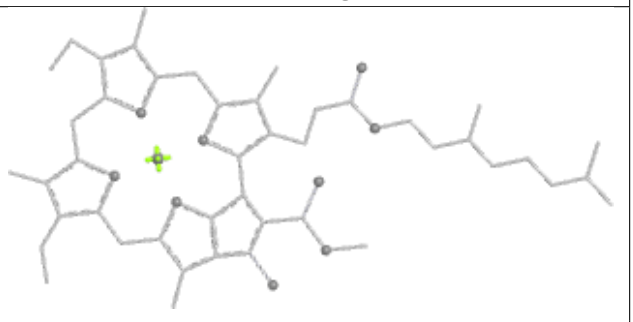
Bond lengths



Bond angles

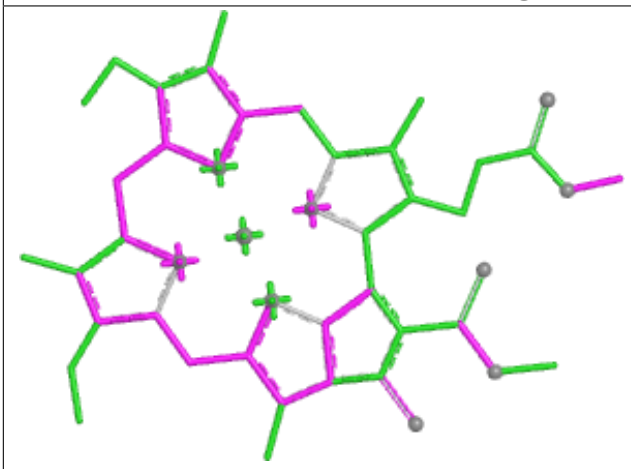


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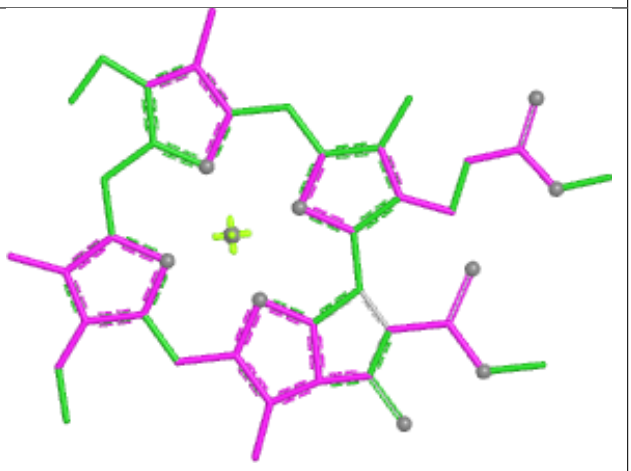


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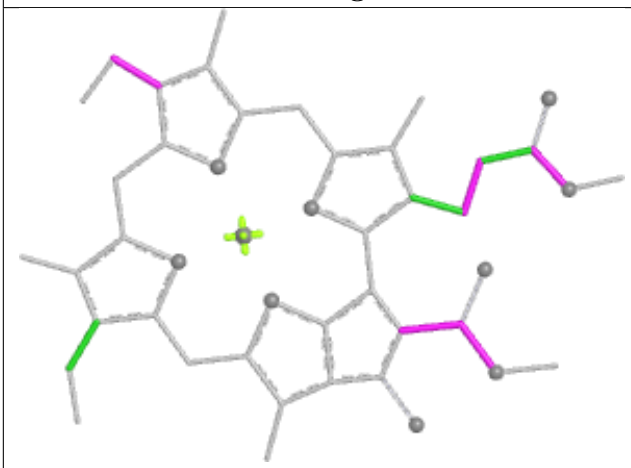
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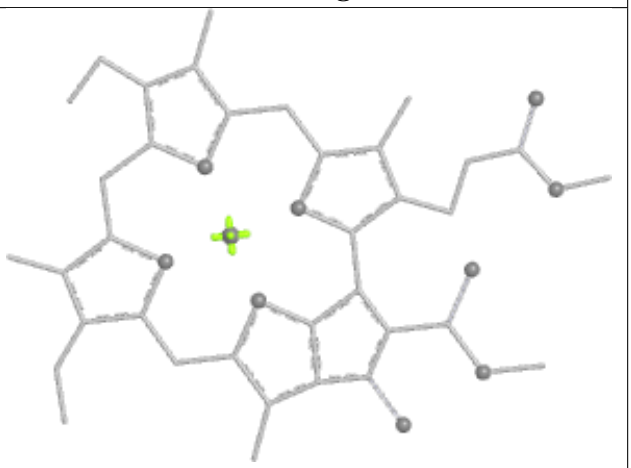
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Bond angles

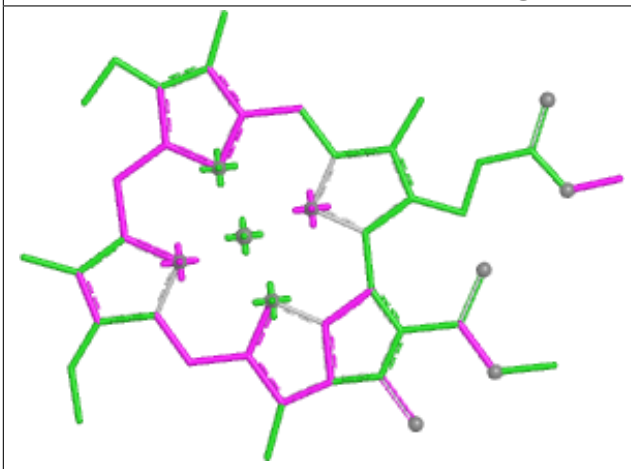


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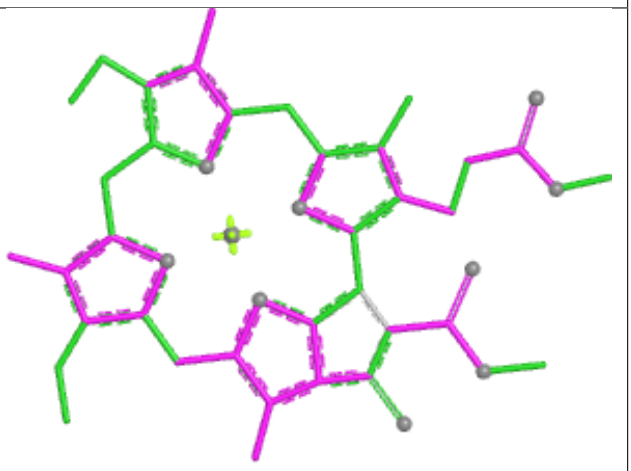


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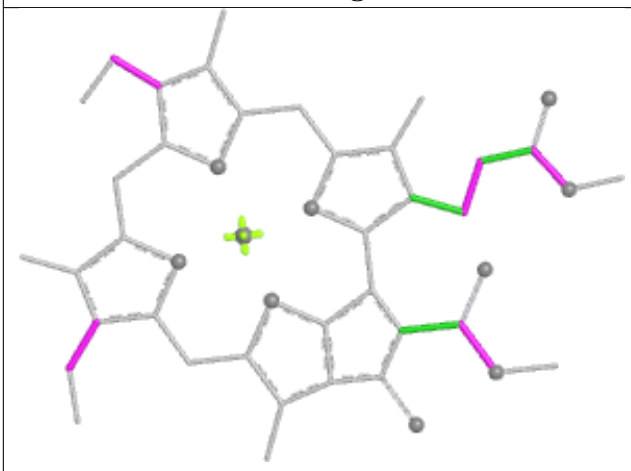
Ligand CLA A 1118



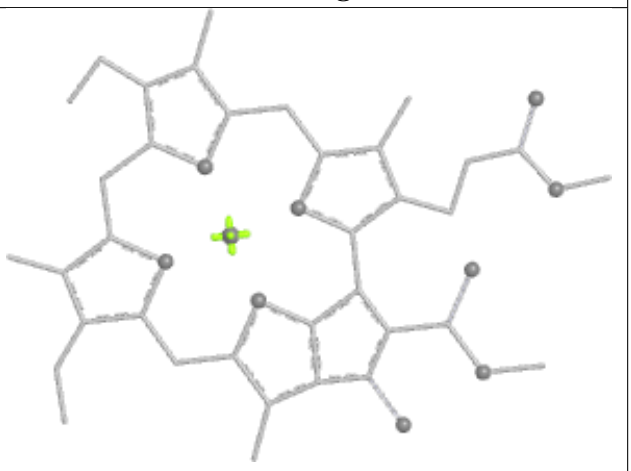
Bond lengths



Bond angles

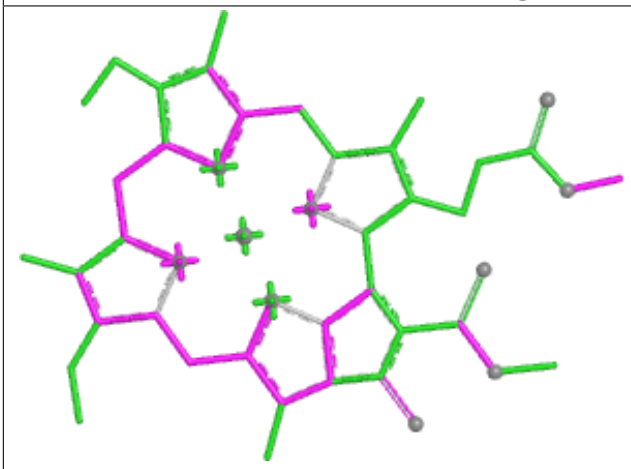


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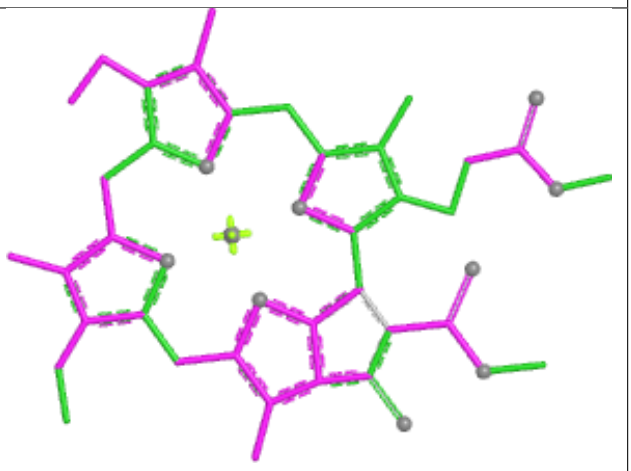


Rings

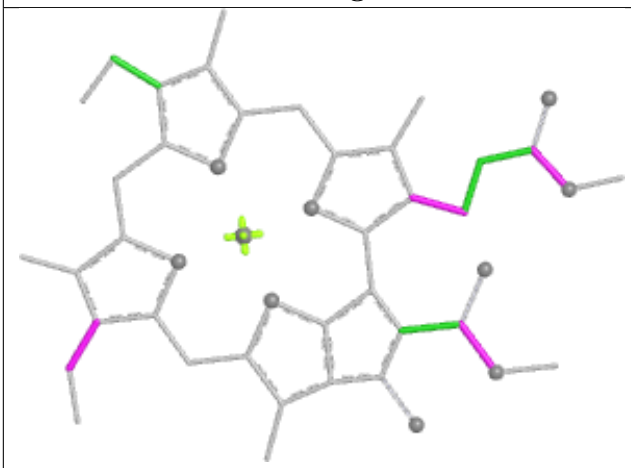
Ligand CLA G 1002



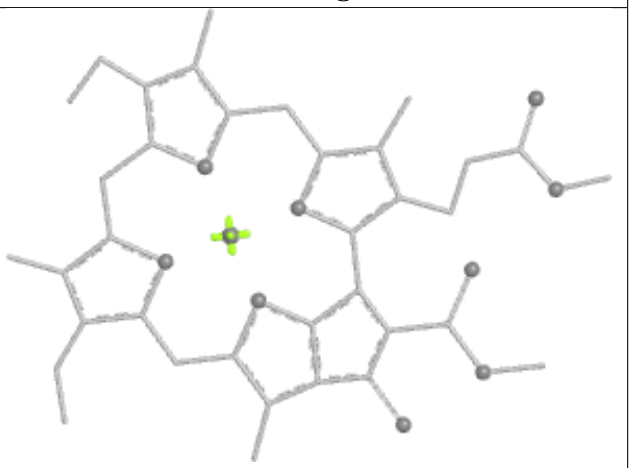
Bond lengths



Bond angles

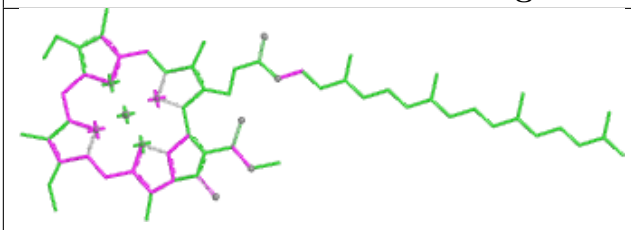


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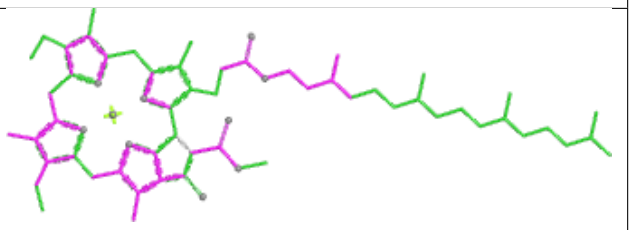


Rings

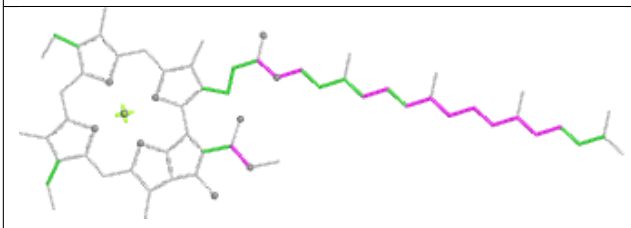
Ligand CLA B 1226



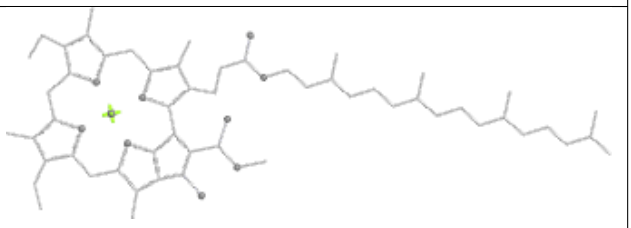
Bond lengths



Bond angles

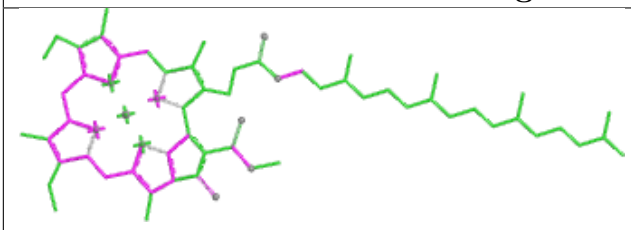


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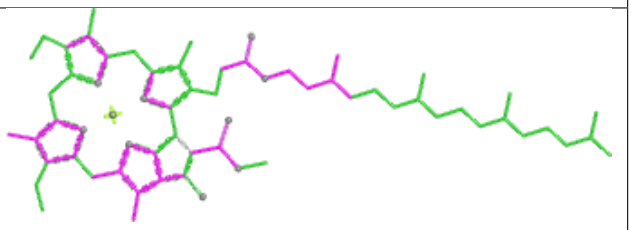


Rings

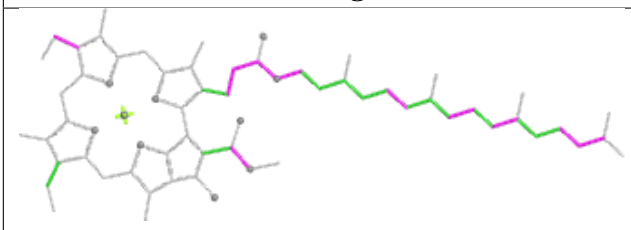
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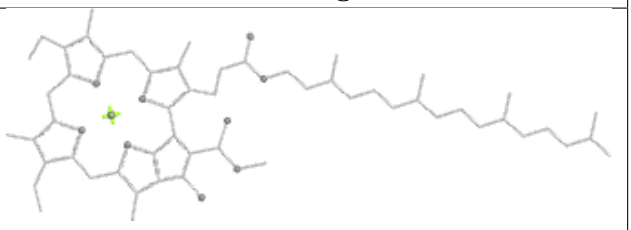
Bond lengths



Bond angles

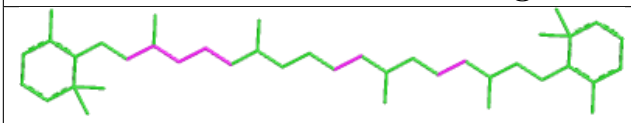


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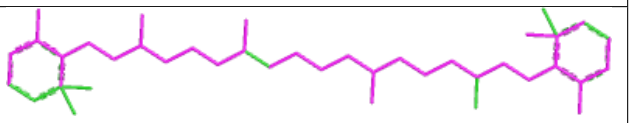


Rings

Ligand BCR B 6006



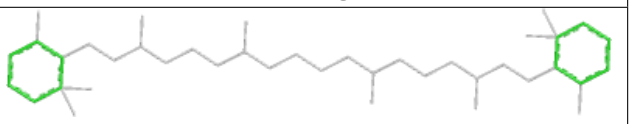
Bond lengths



Bond angles

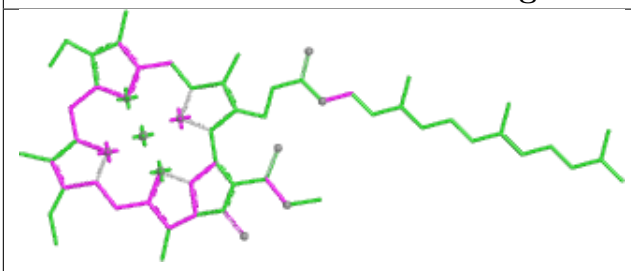


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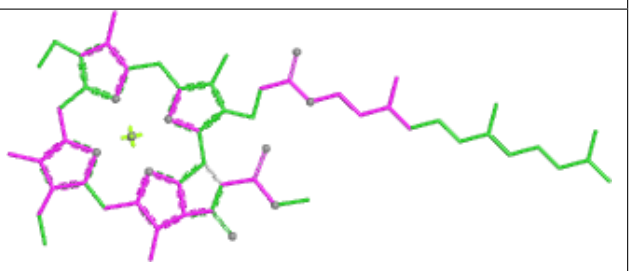


Rings

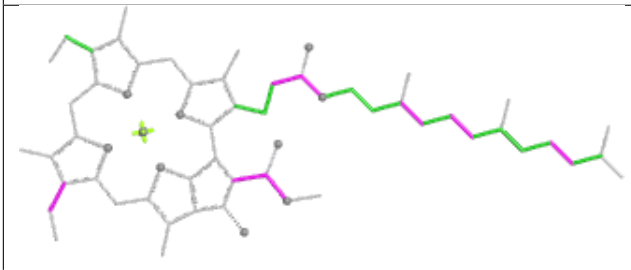
Ligand CLA 2 2007



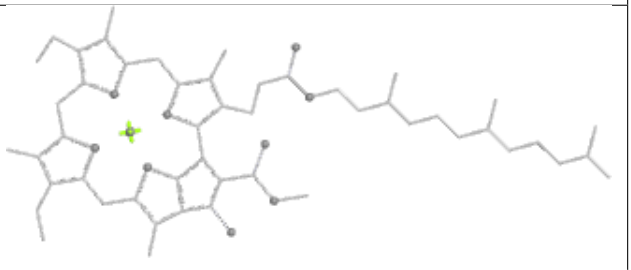
Bond lengths



Bond angles

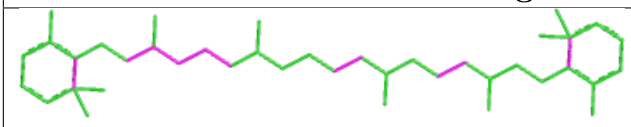


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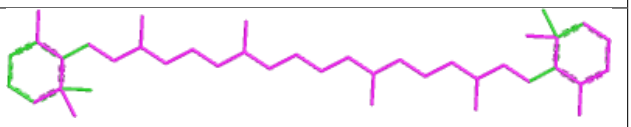


Rings

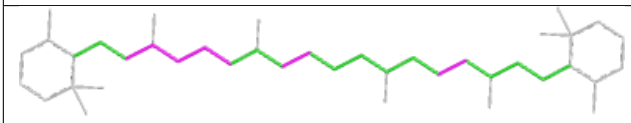
Ligand BCR L 6020



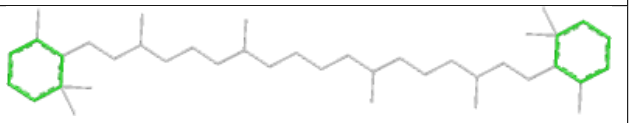
Bond lengths



Bond angles

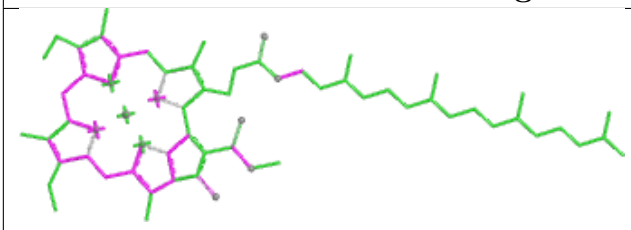


Torsions

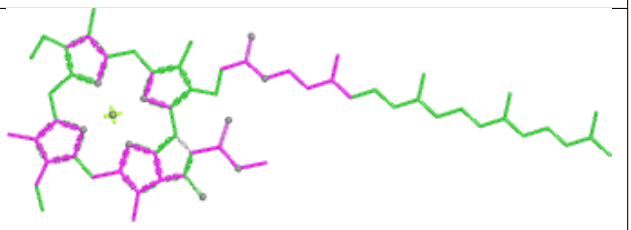


Rings

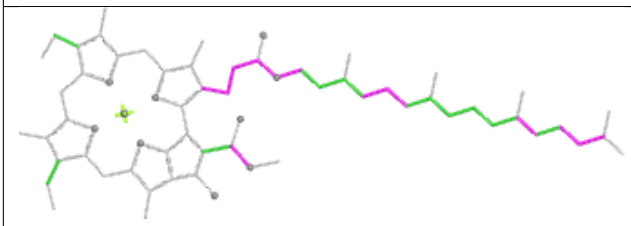
Ligand CLA A 1127



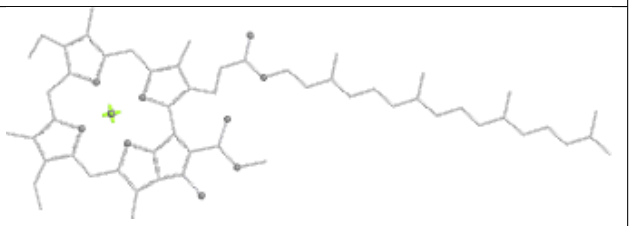
Bond lengths



Bond angles

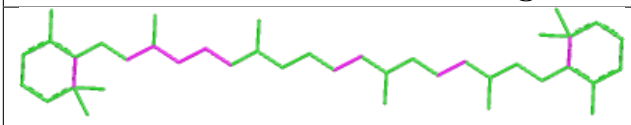


Torsions

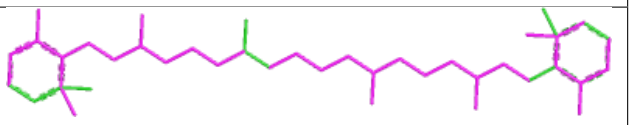


Rings

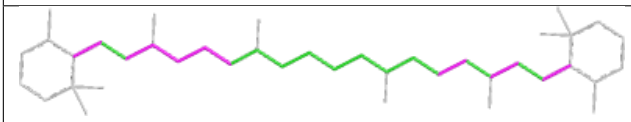
Ligand BCR J 6013



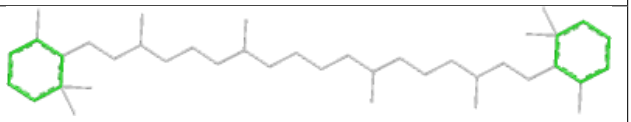
Bond lengths



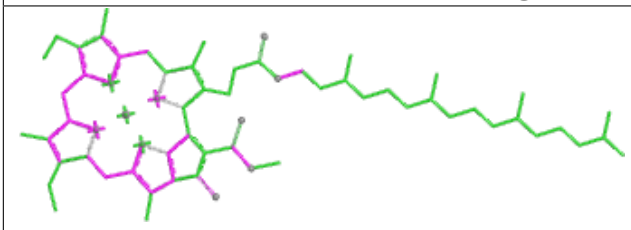
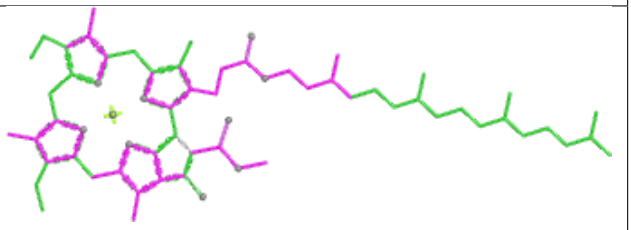
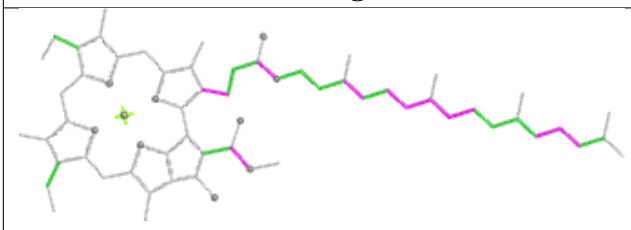
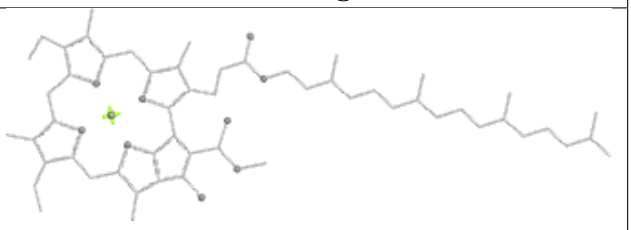
Bond angles

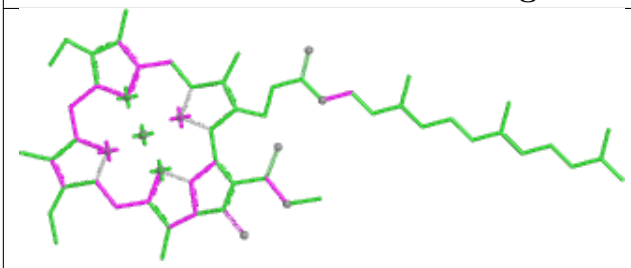
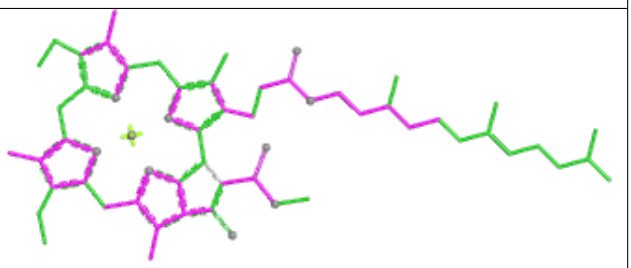
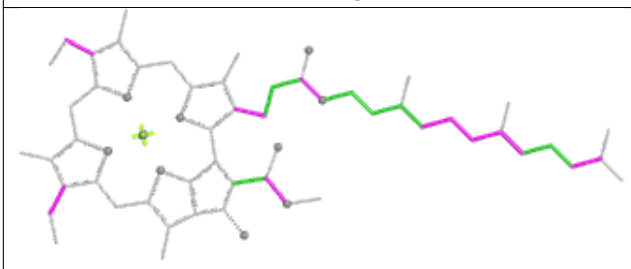
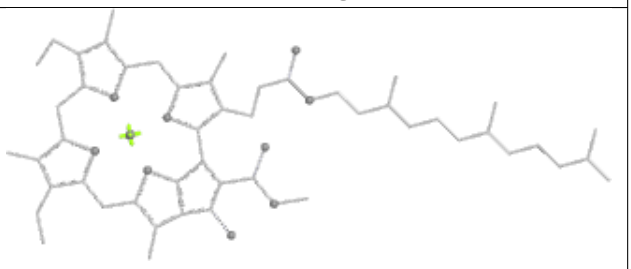


Torsions

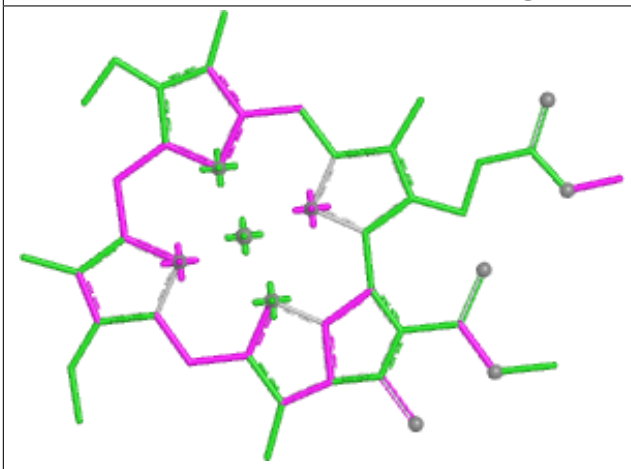


Rings

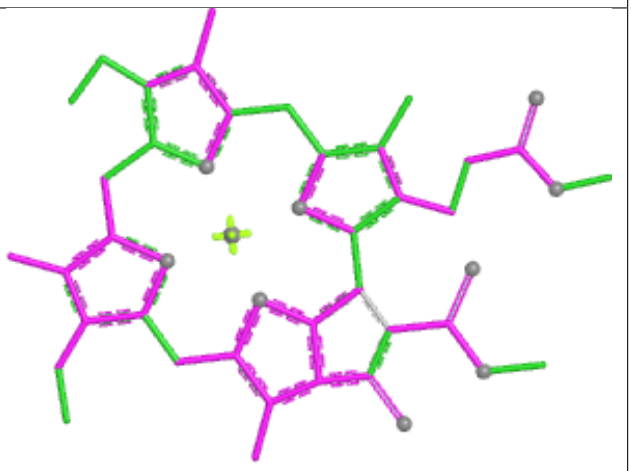
Ligand CLA B 1222	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

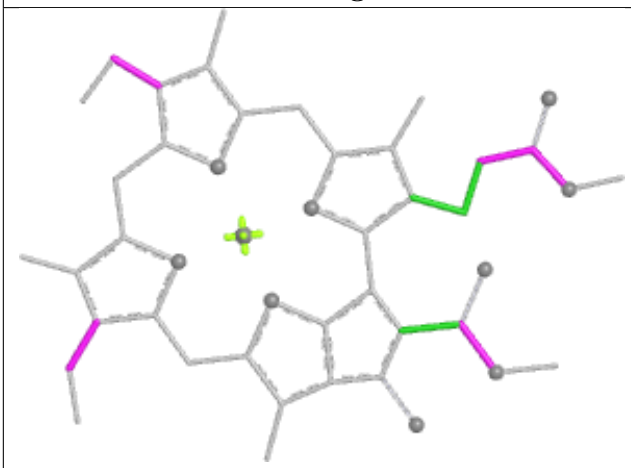
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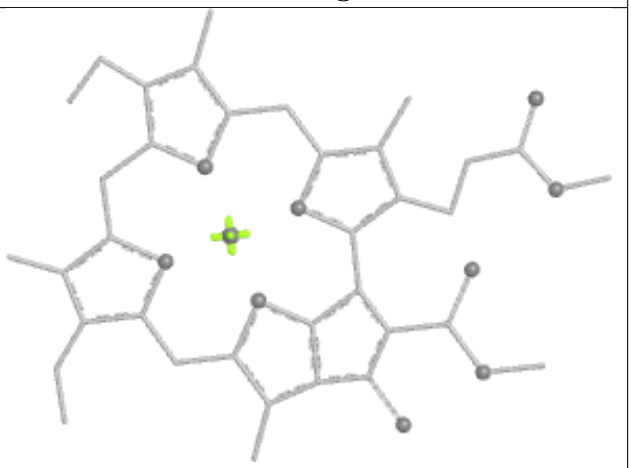
Bond lengths



Bond angles

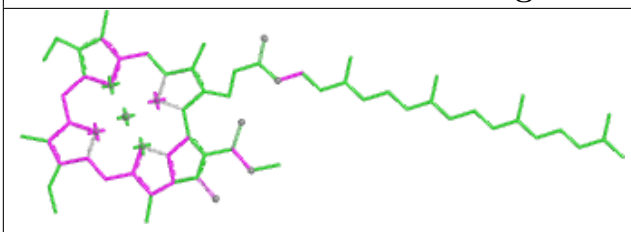


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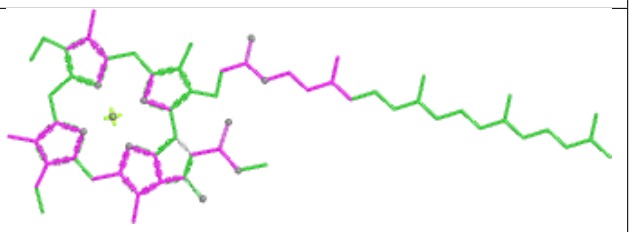


Rings

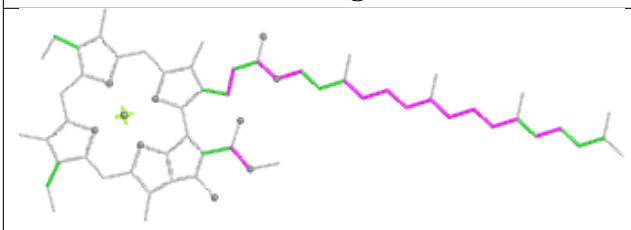
Ligand CLA B 1207



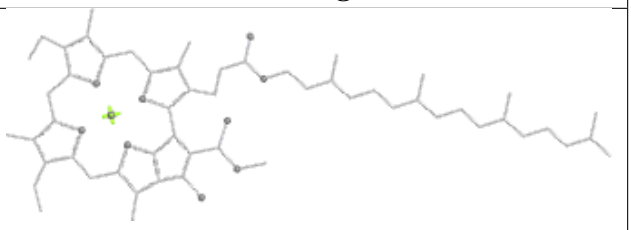
Bond lengths



Bond angles

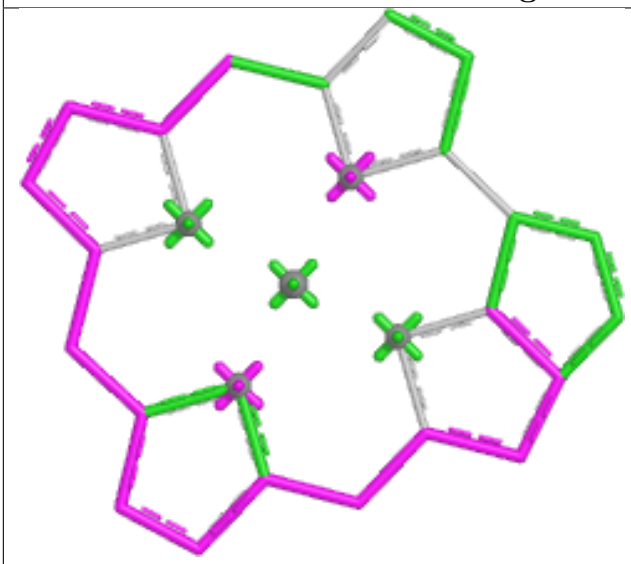


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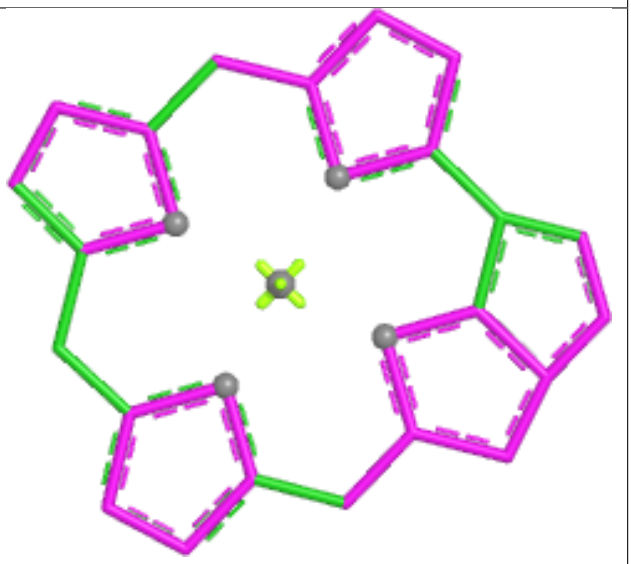


Rings

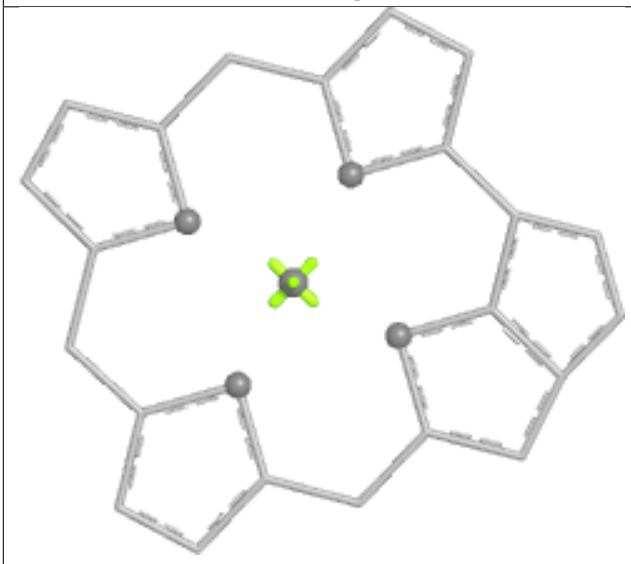
Ligand CLA 3 3019



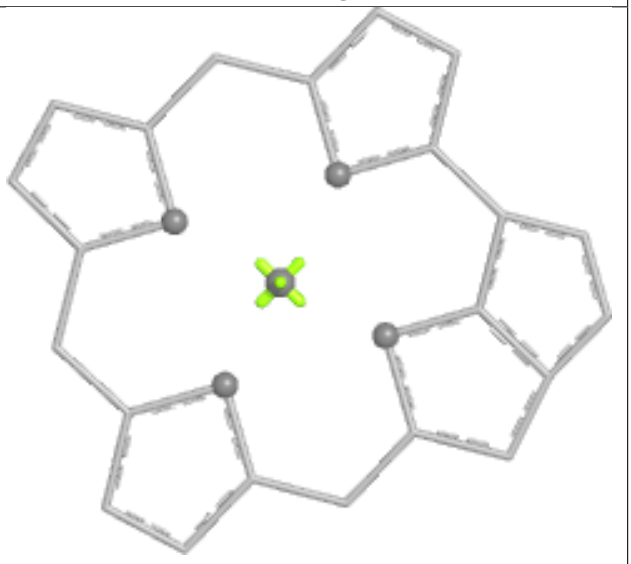
Bond lengths



Bond angles

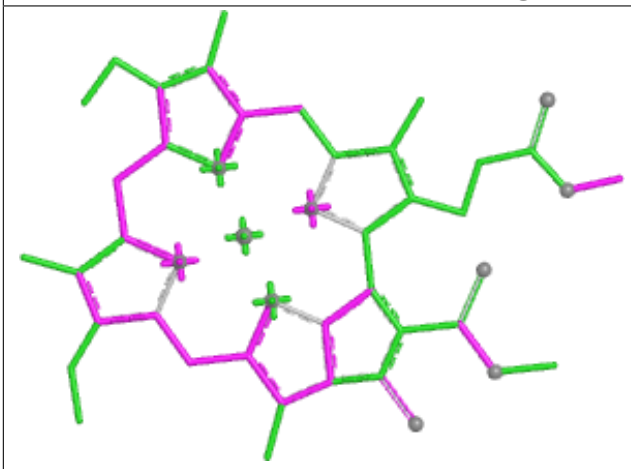


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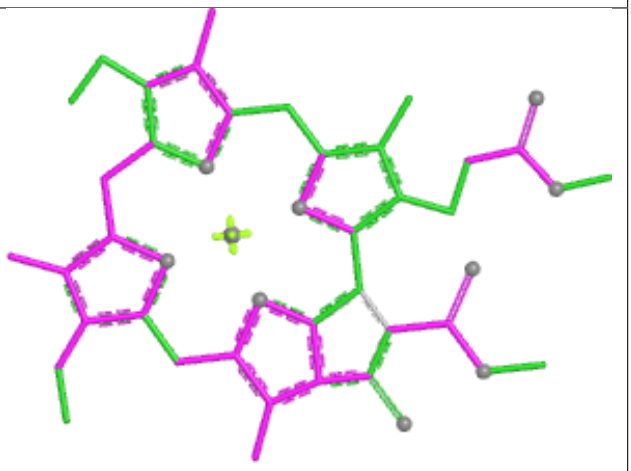


Rings

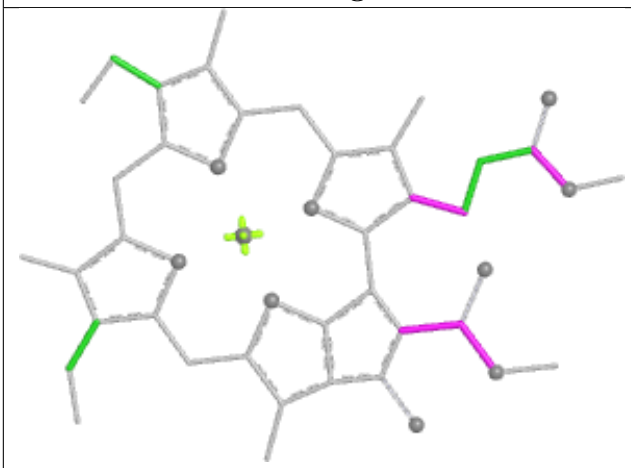
Ligand CLA A 1114



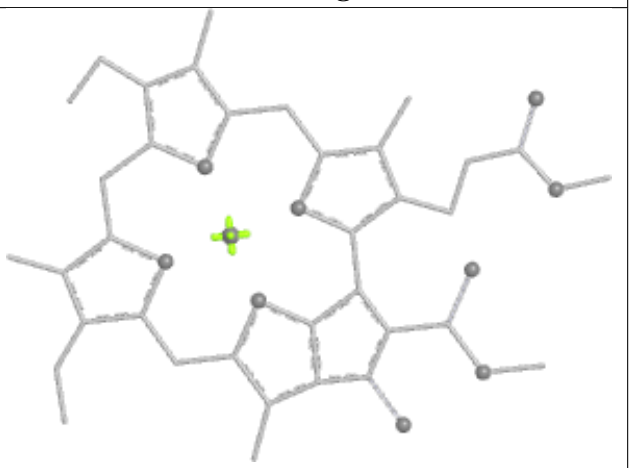
Bond lengths



Bond angles



Torsions

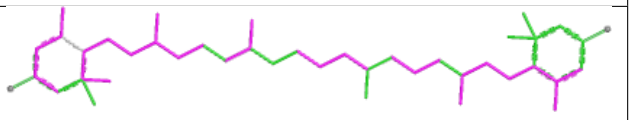


Rings

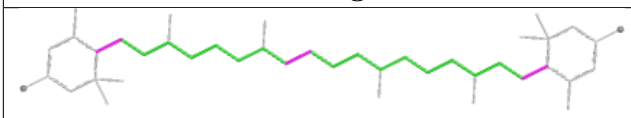
Ligand LUT 4 4501



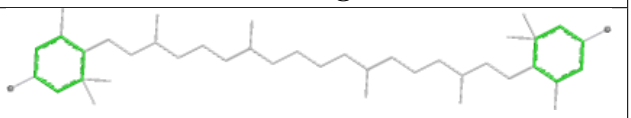
Bond lengths



Bond angles

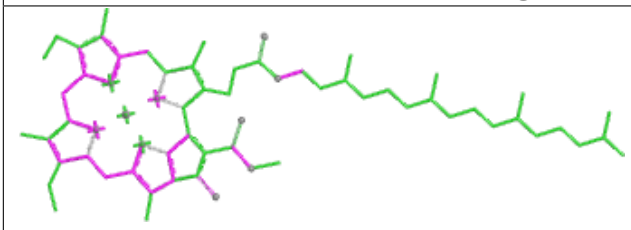


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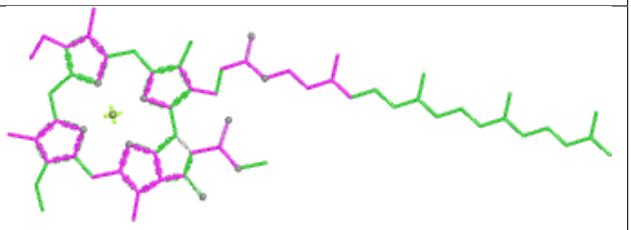


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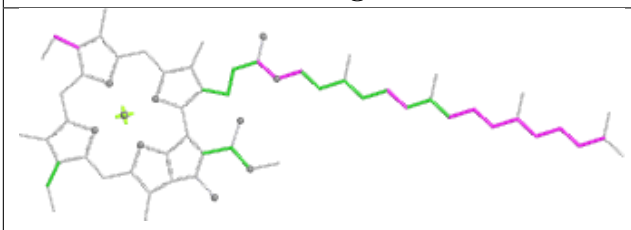
Ligand CLA A 1132



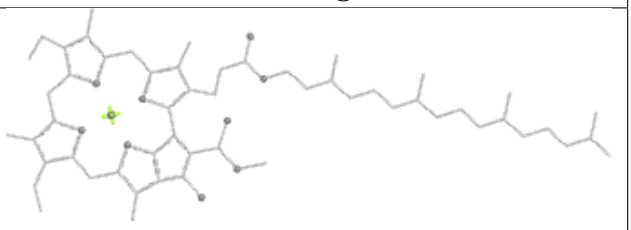
Bond lengths



Bond angles

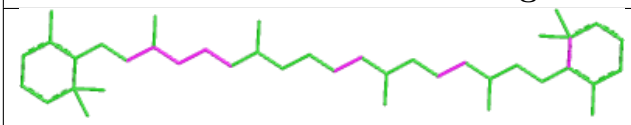


Torsions



Rings

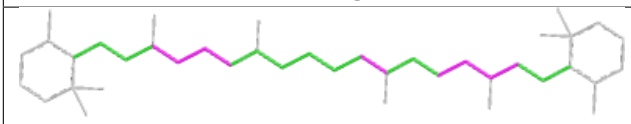
Ligand BCR I 6020



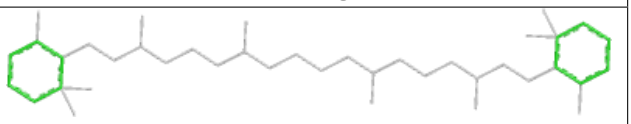
Bond lengths



Bond angles

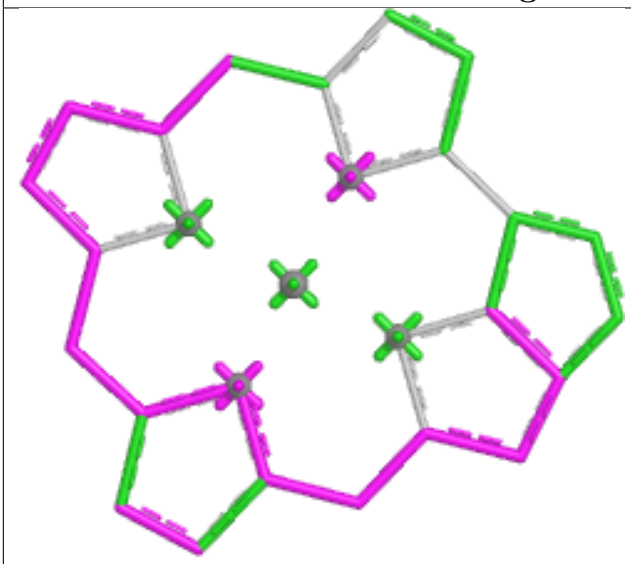


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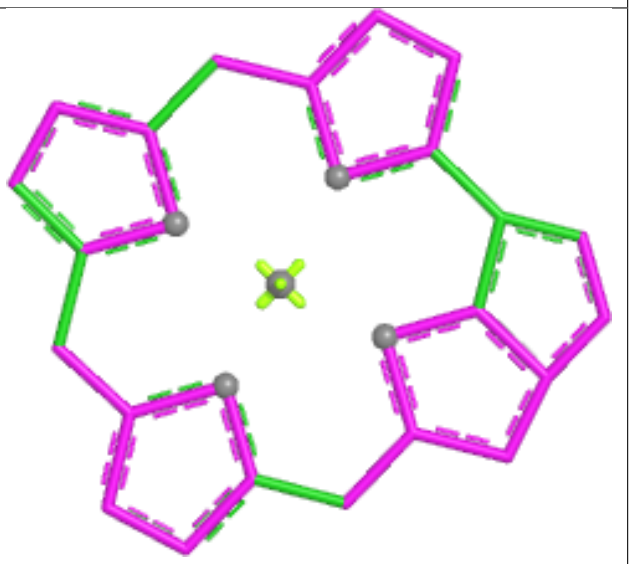


Rings

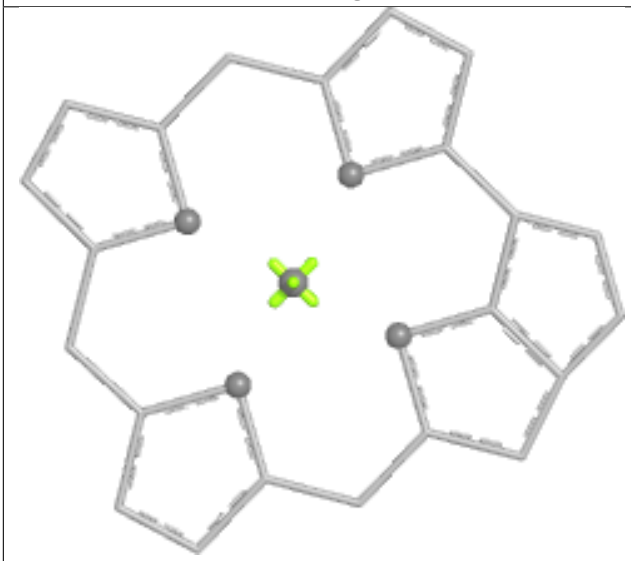
Ligand CLA 2 2019



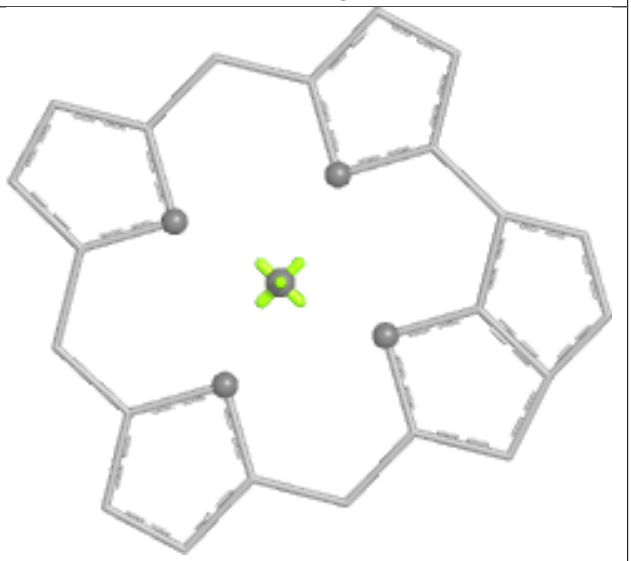
Bond lengths



Bond angles

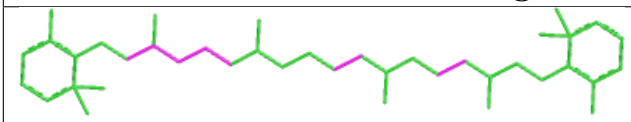


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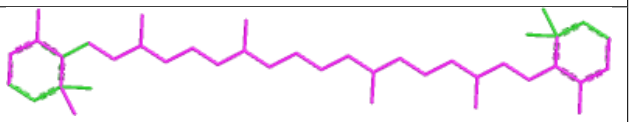


Rings

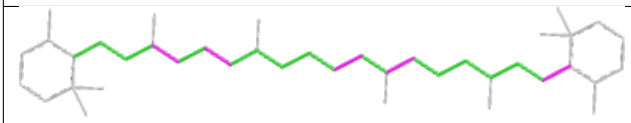
Ligand BCR A 6008



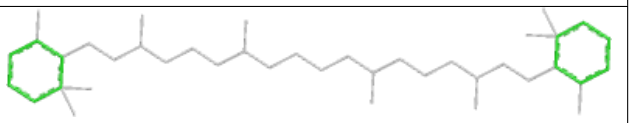
Bond lengths



Bond angles

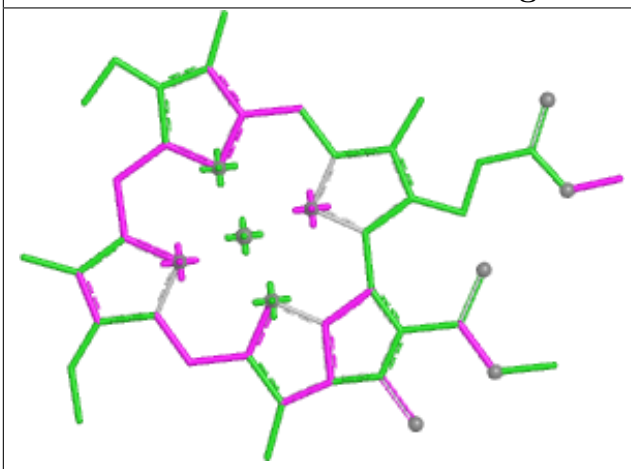


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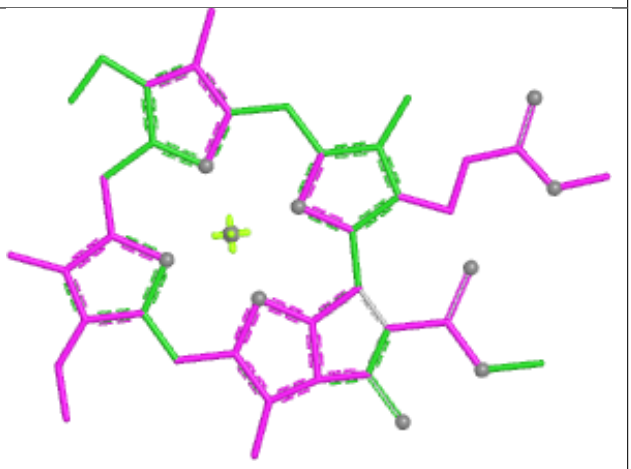


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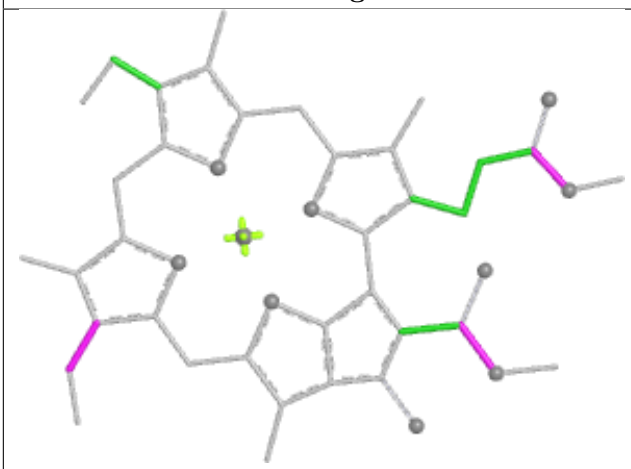
Ligand CLA 2 2002



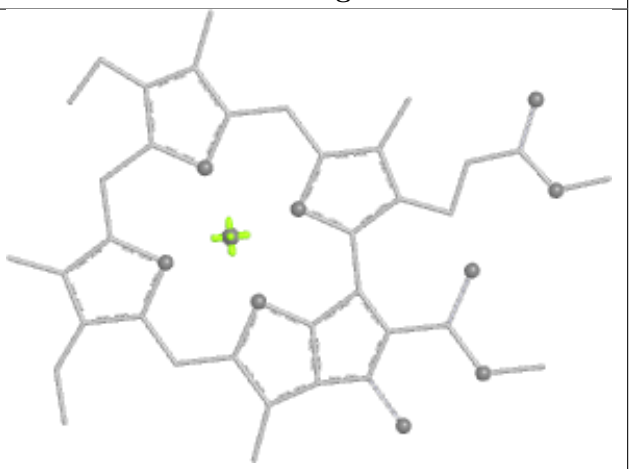
Bond lengths



Bond angles

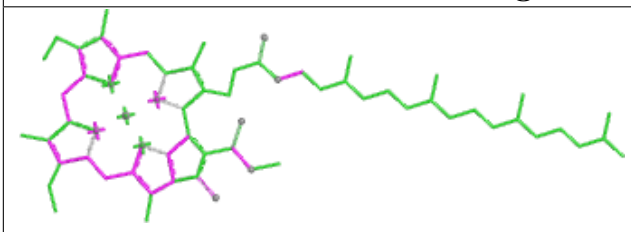


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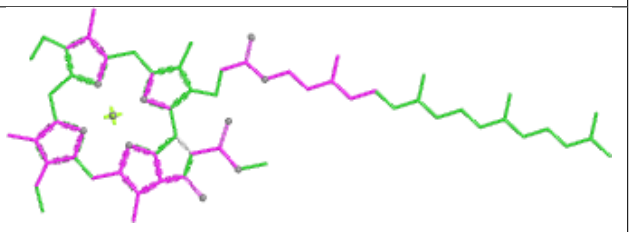


Rings

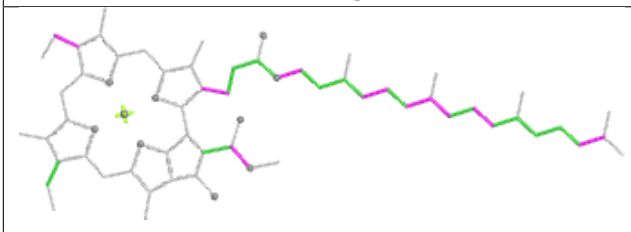
Ligand CLA A 1022



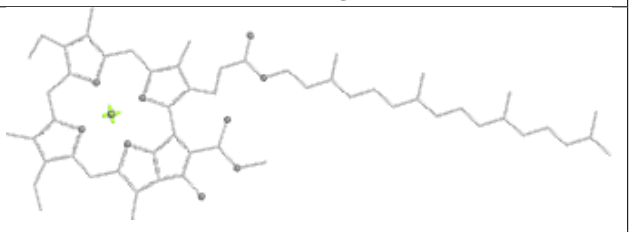
Bond lengths



Bond angles

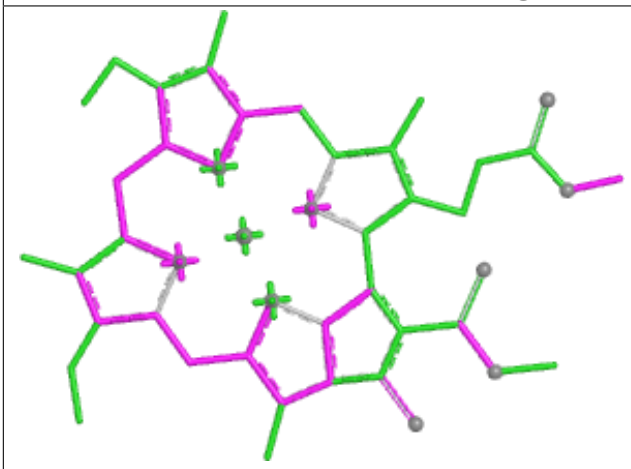


Torsions

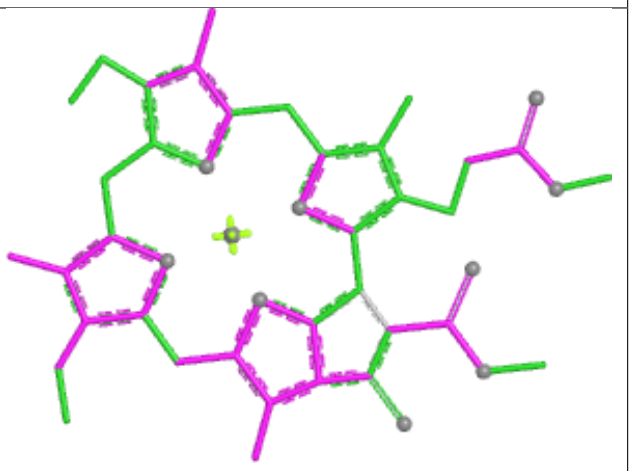


Rings

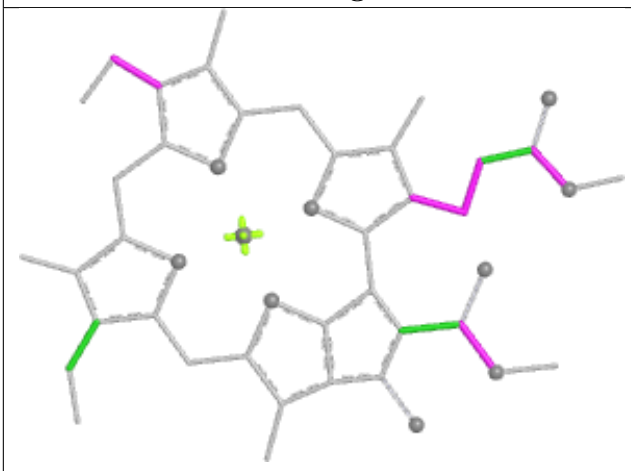
Ligand CLA A 1115



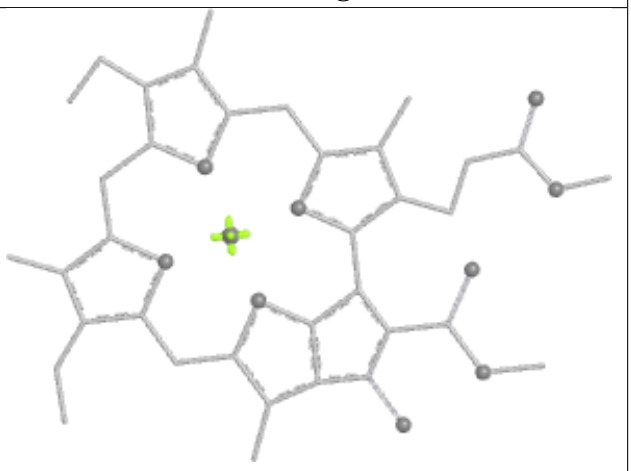
Bond lengths



Bond angles

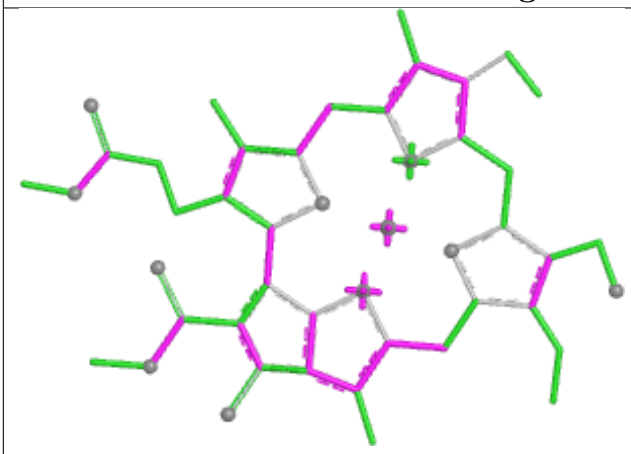


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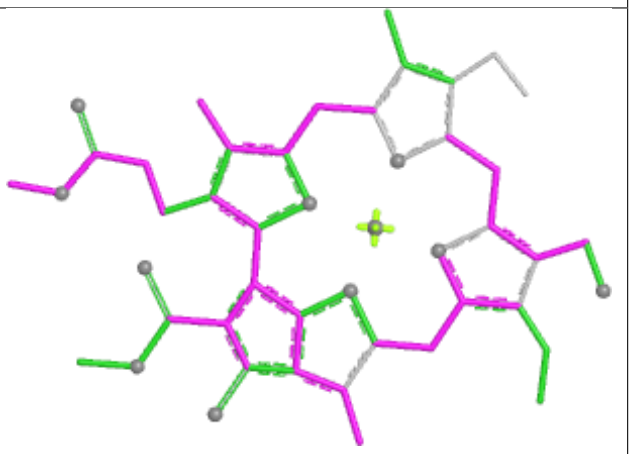


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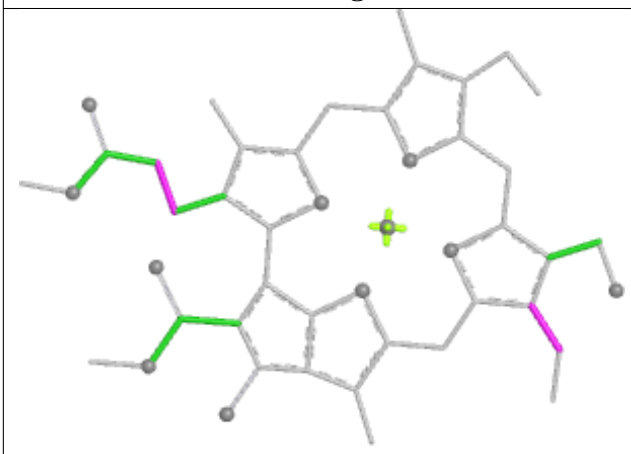
Ligand CHL 4 4010



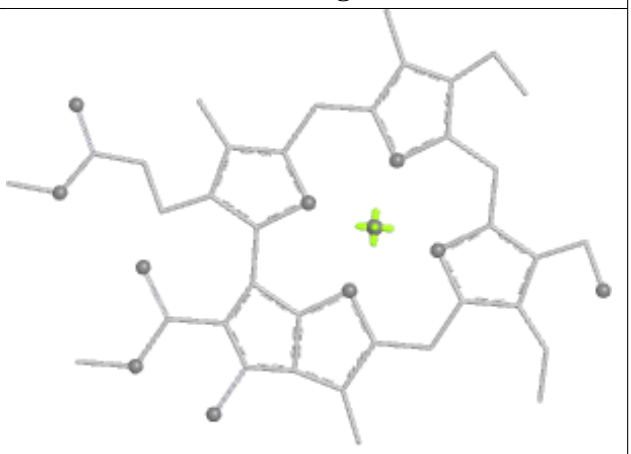
Bond lengths



Bond angles

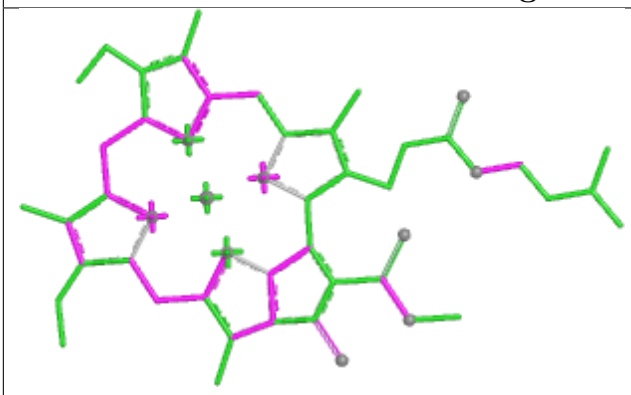


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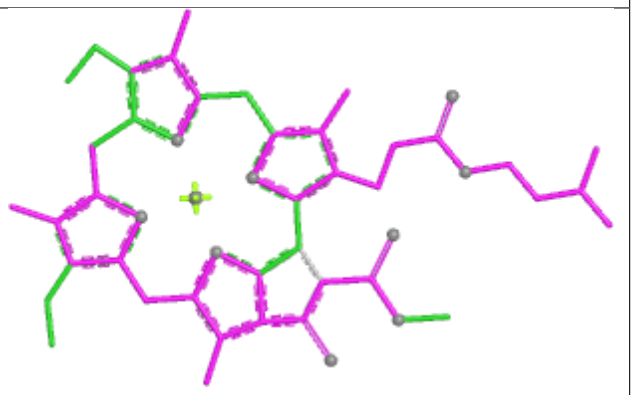


Rings

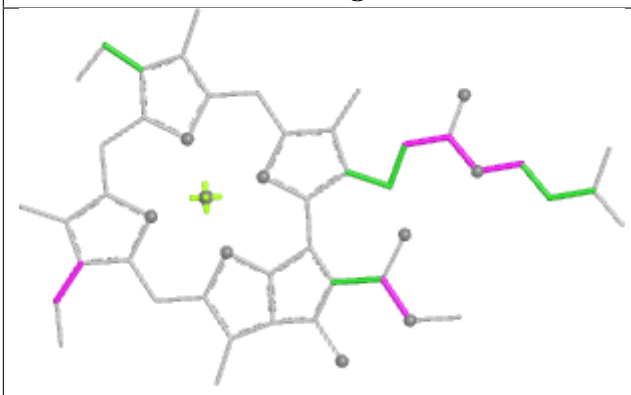
Ligand CLA 2 2008



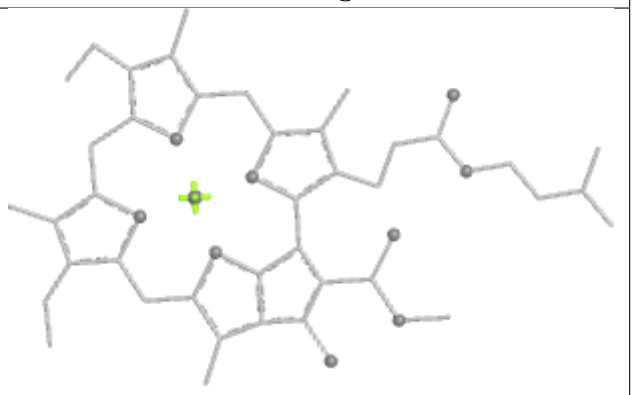
Bond lengths



Bond angles

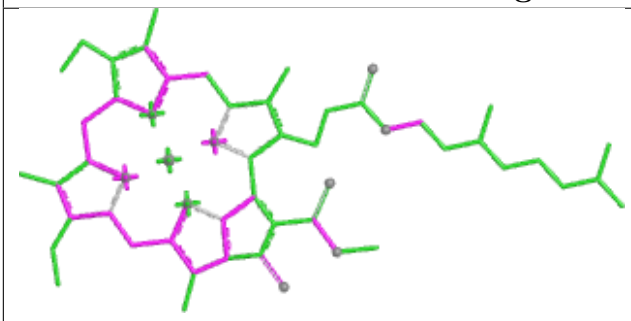


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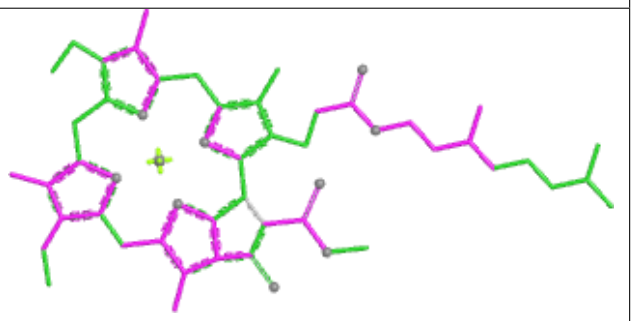


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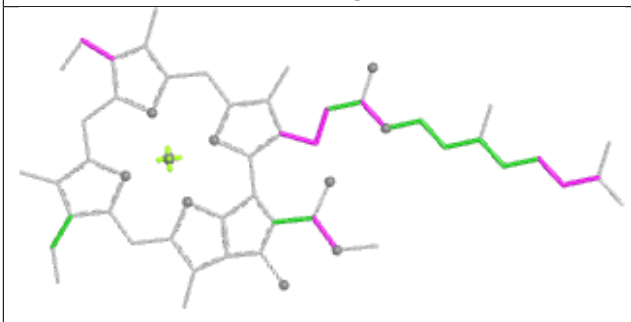
Ligand CLA A 1133



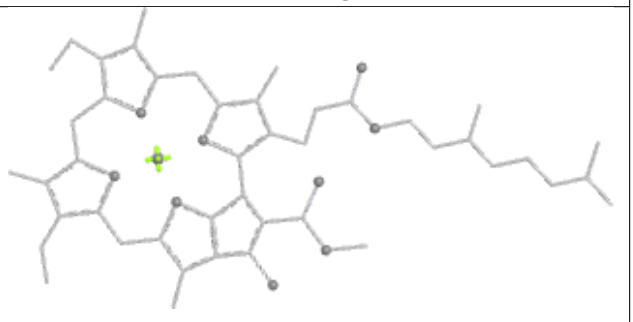
Bond lengths



Bond angles

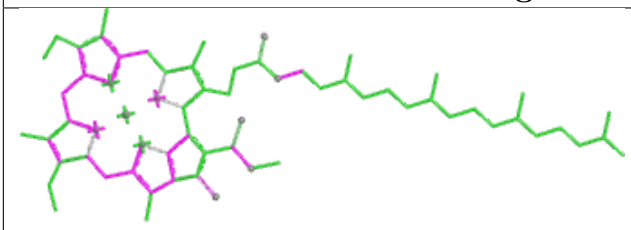


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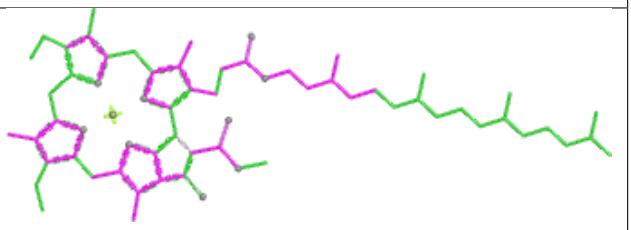


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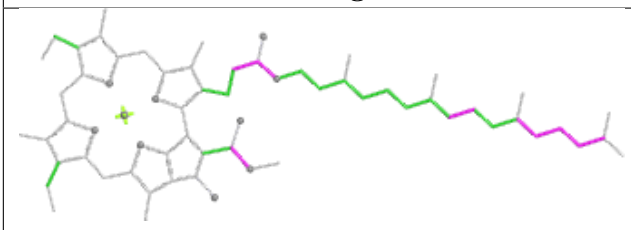
Ligand CLA B 1021



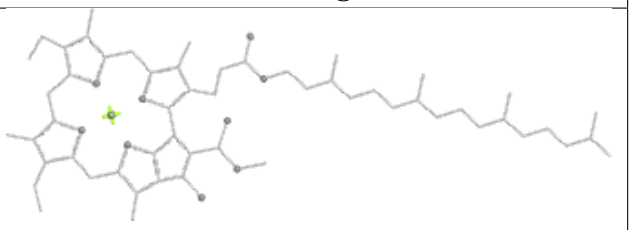
Bond lengths



Bond angles

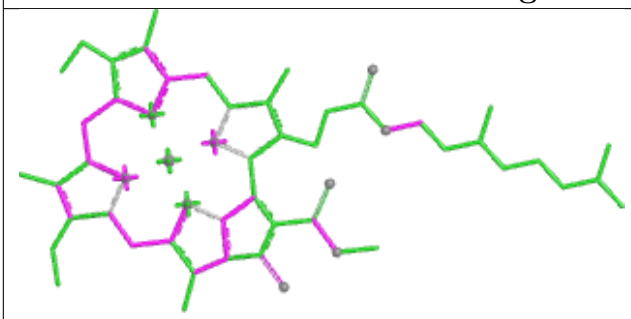


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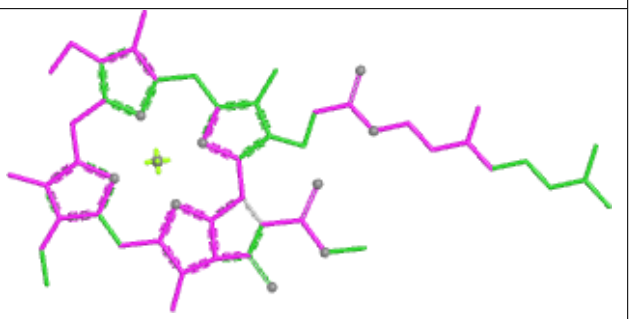


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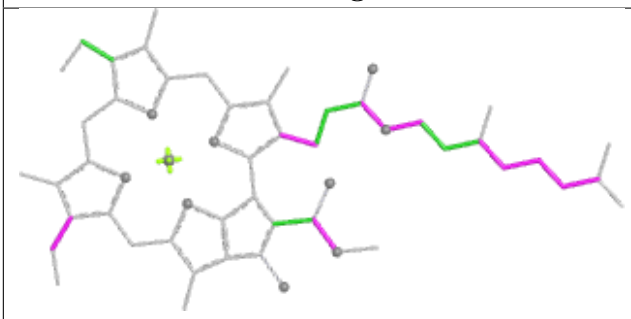
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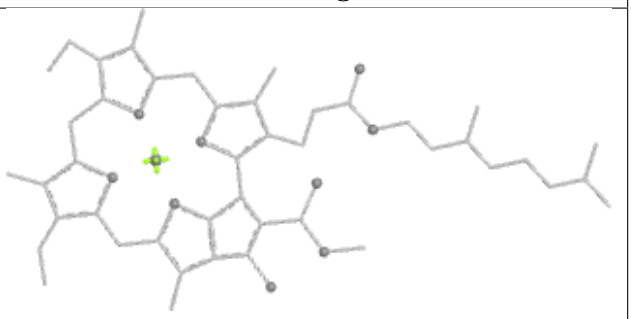
Bond lengths



Bond angles

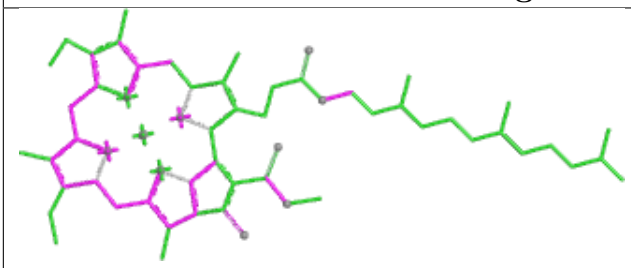


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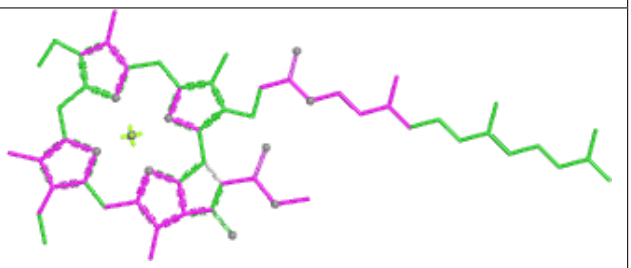


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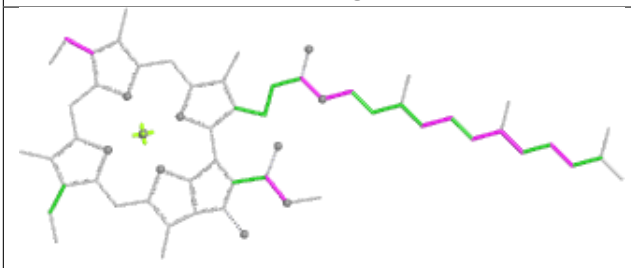
Ligand CLA B 1231



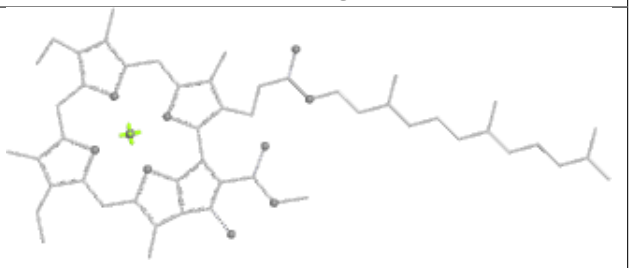
Bond lengths



Bond angles

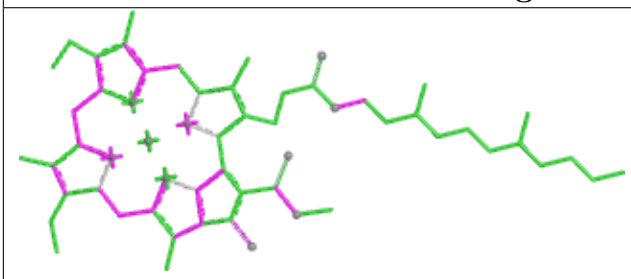


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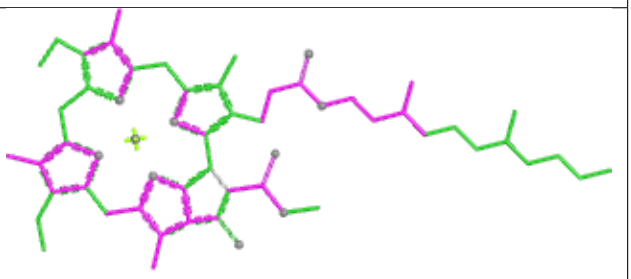


Rings

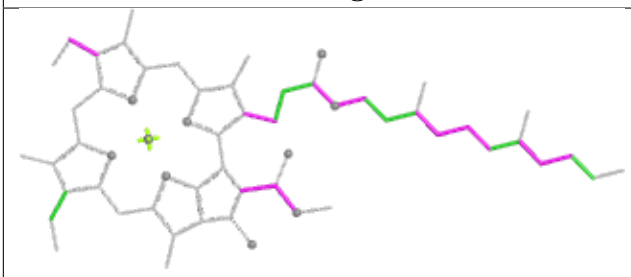
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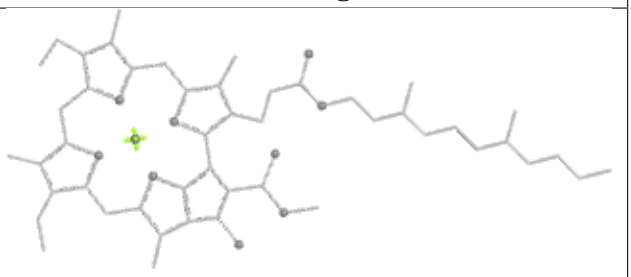
Bond lengths



Bond angles

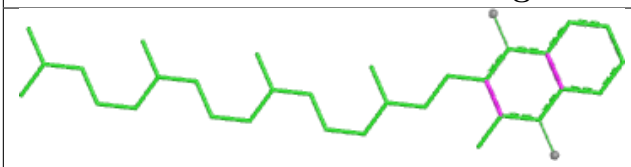


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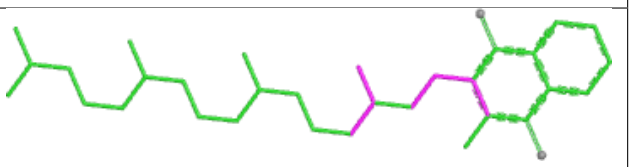


Rings

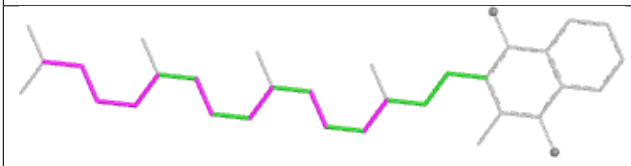
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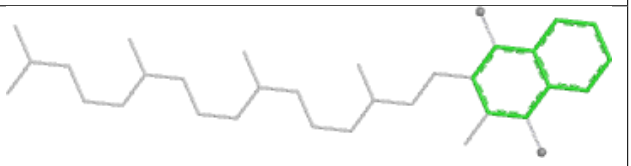
Bond lengths



Bond angles

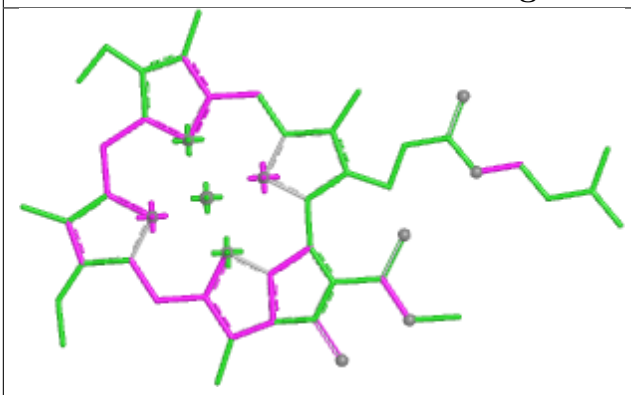


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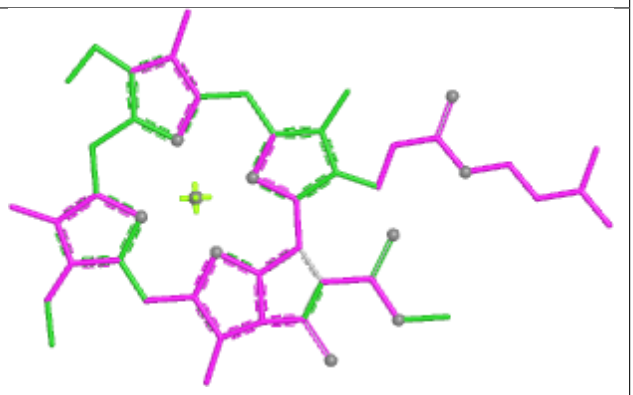


Rings

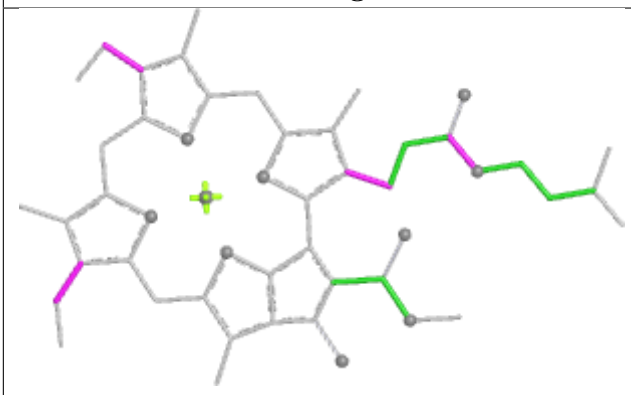
Ligand CLA 3 3007



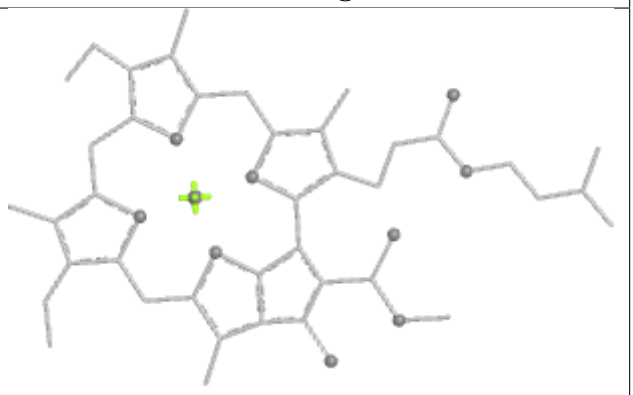
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Bond angles

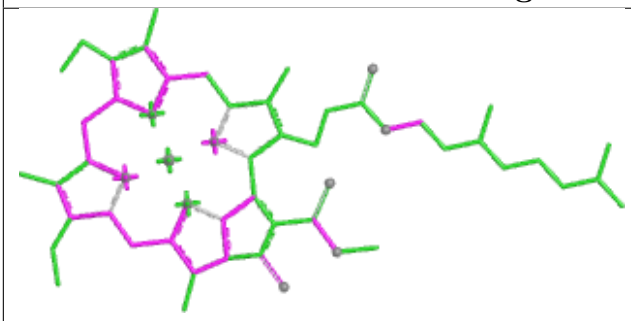


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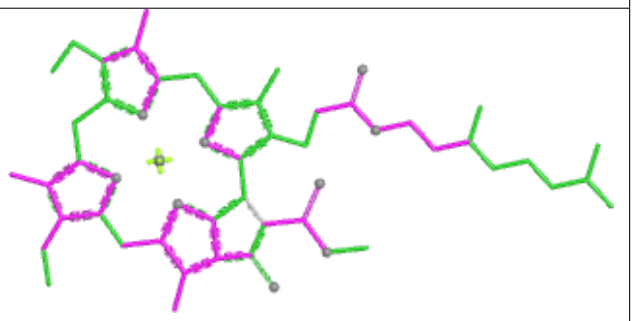


Rings

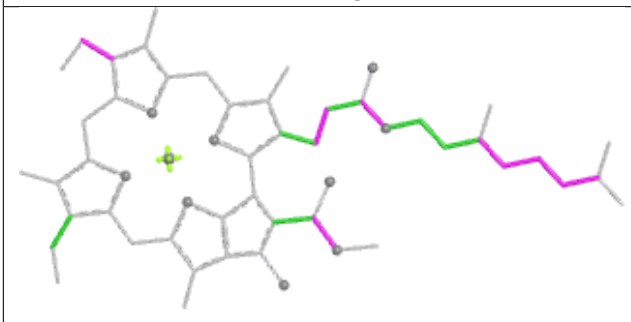
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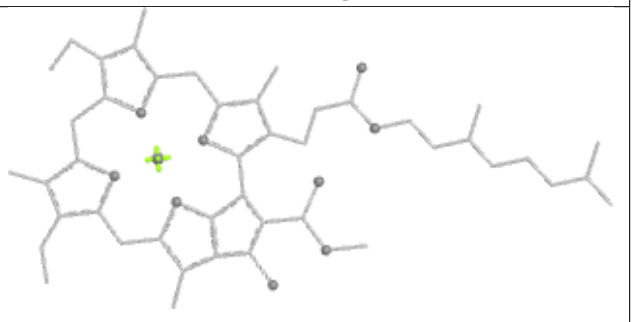
Bond lengths



Bond angles

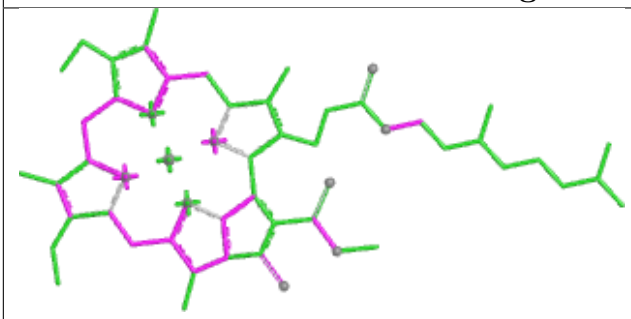


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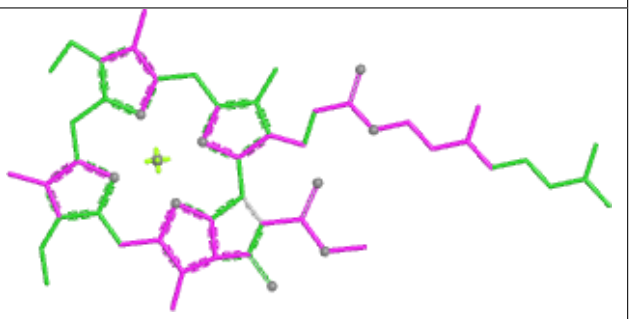


Rings

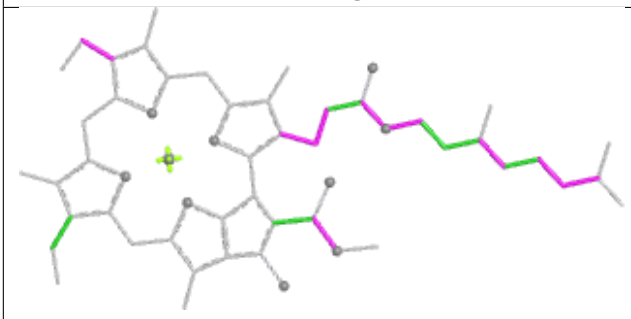
Ligand CLA 2 2005



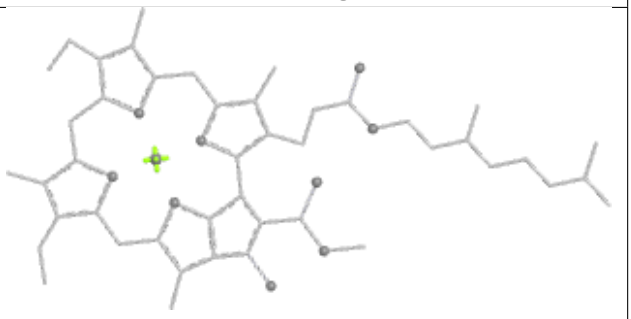
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Bond angles

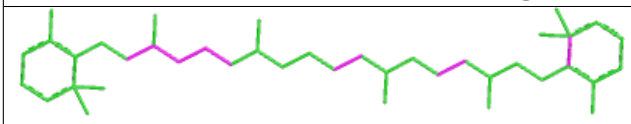


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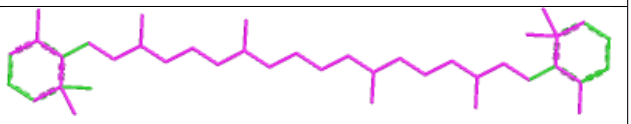


Rings

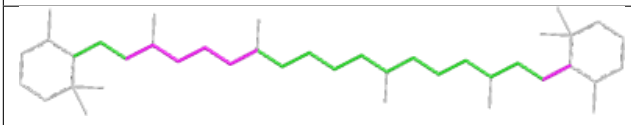
Ligand BCR J 6012



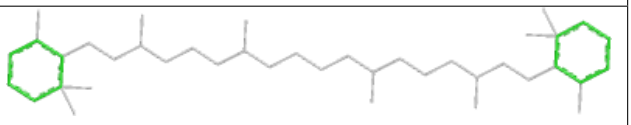
Bond lengths



Bond angles

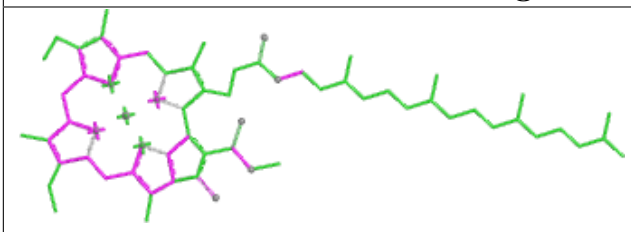


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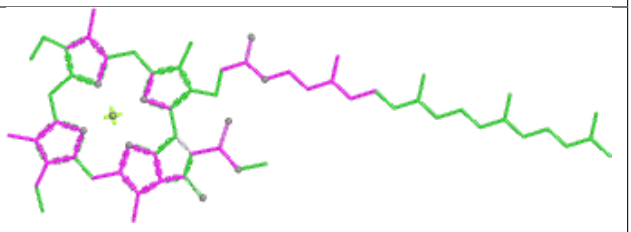


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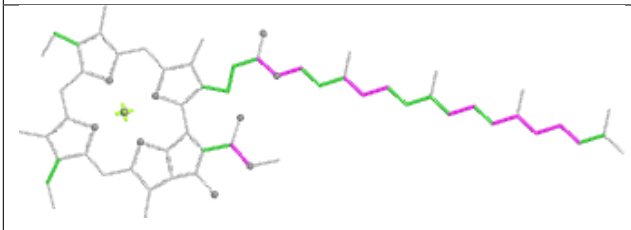
Ligand CLA A 1139



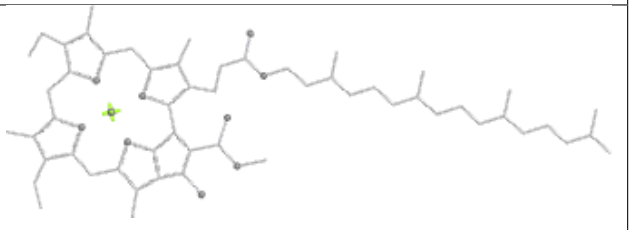
Bond lengths



Bond angles

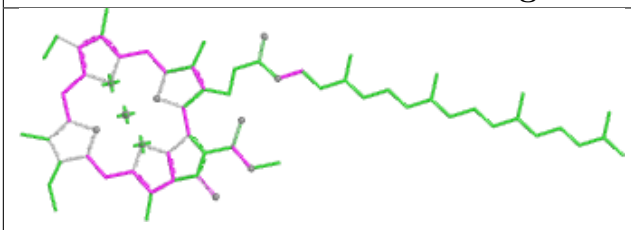


Torsions

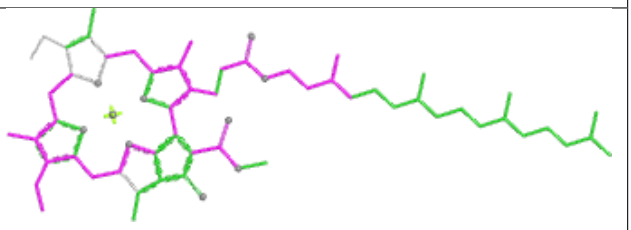


Rings

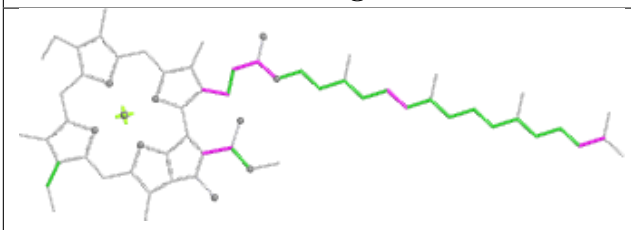
Ligand CL0 A 1011



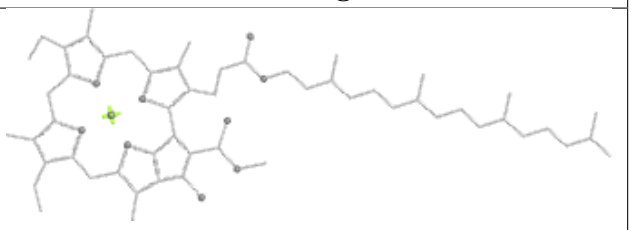
Bond lengths



Bond angles

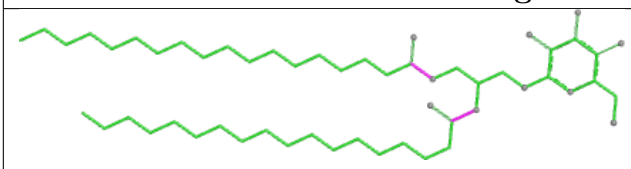


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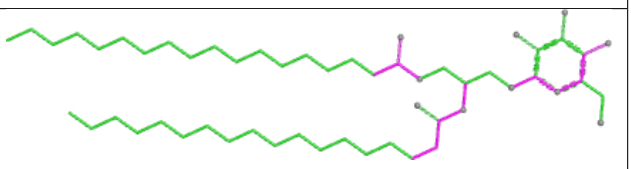


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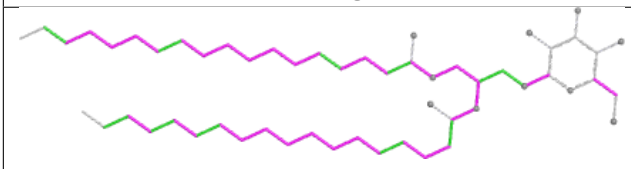
Ligand LMG J 5001



Bond lengths



Bond angles

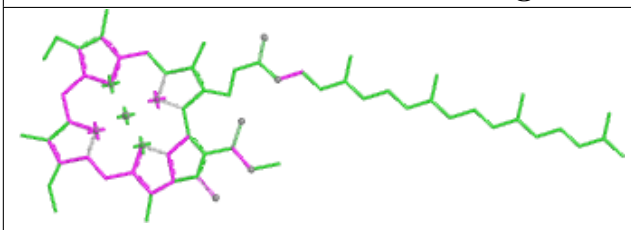


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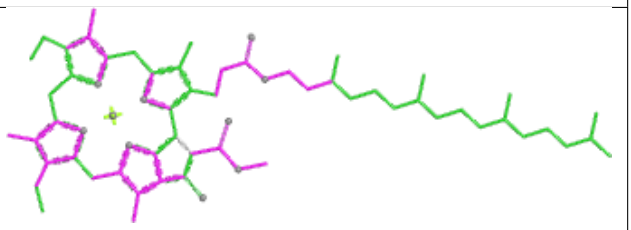


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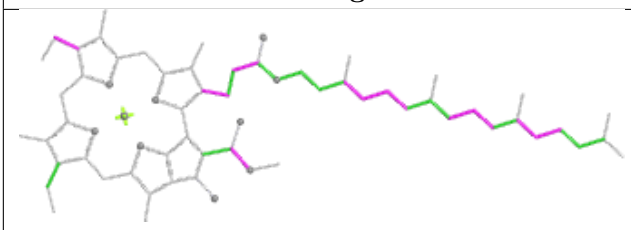
Ligand CLA B 1220



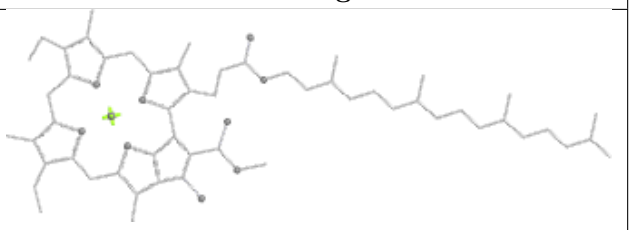
Bond lengths



Bond angles

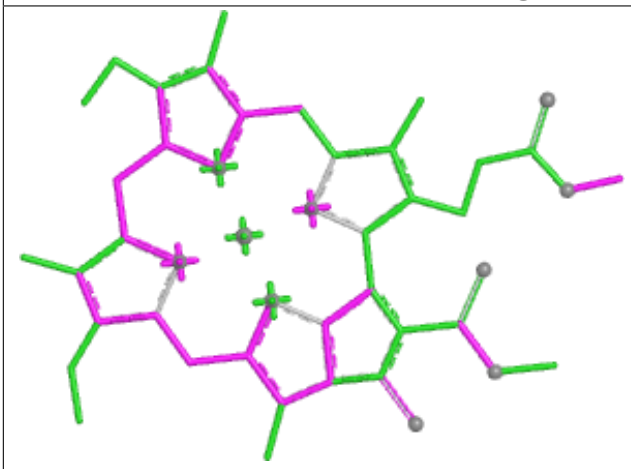


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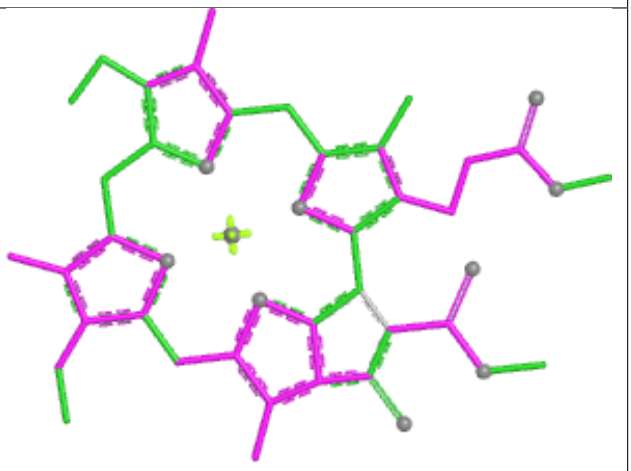


Rings

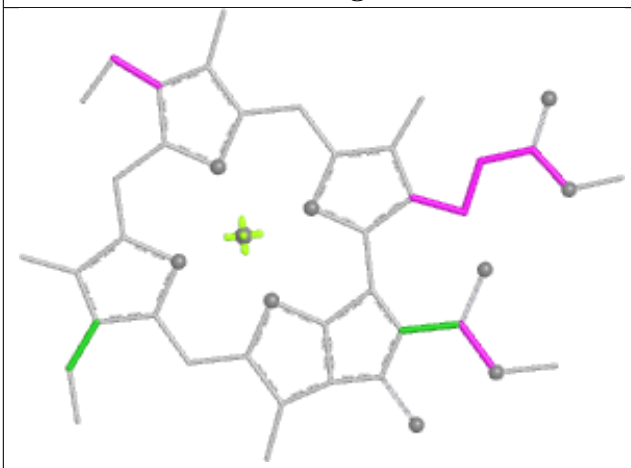
Ligand CLA A 1113



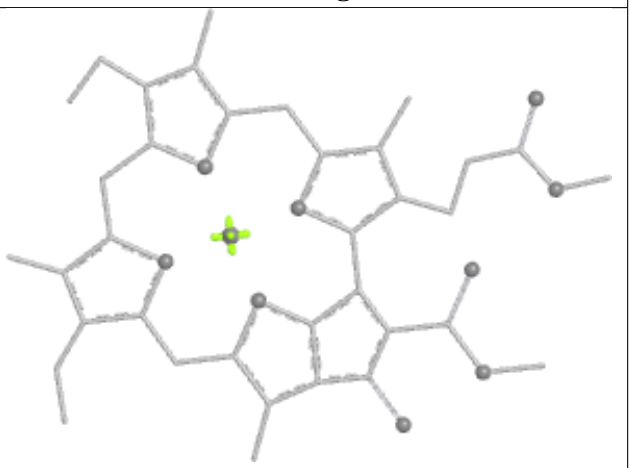
Bond lengths



Bond angles

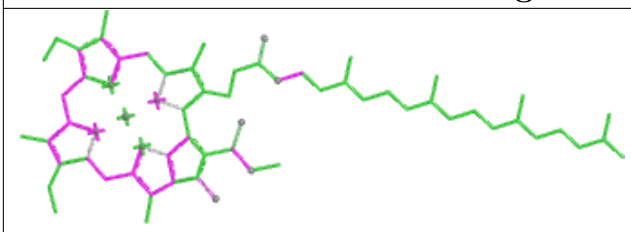


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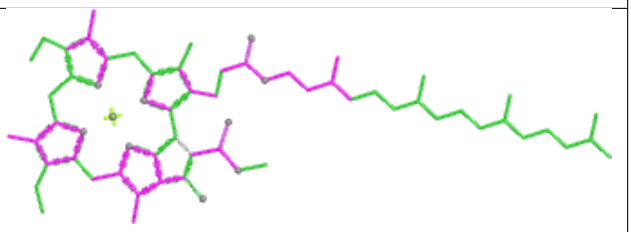


Rings

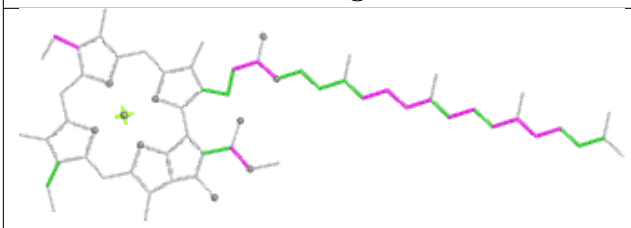
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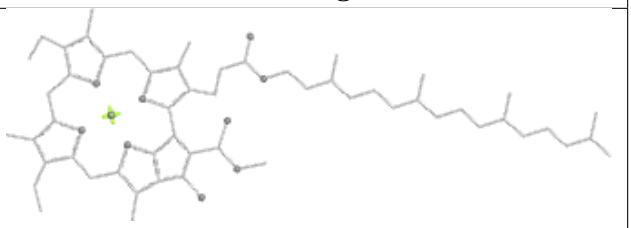
Bond lengths



Bond angles

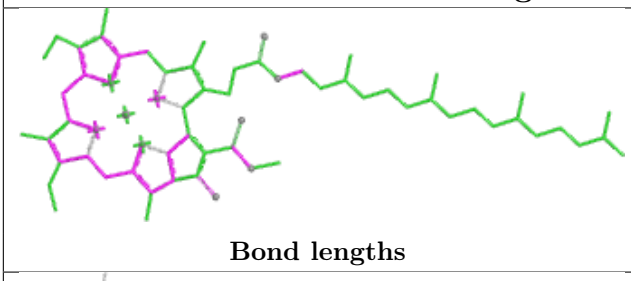


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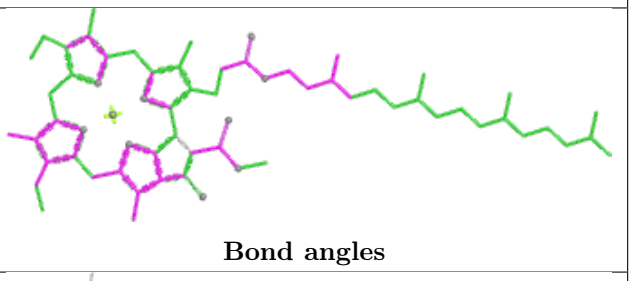


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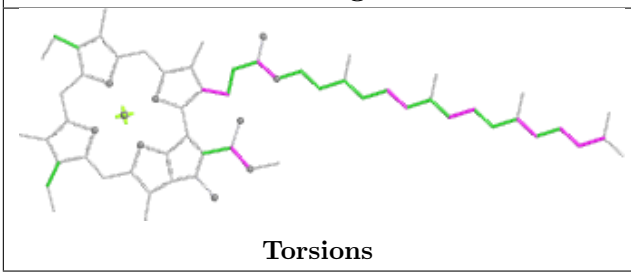
Ligand CLA A 1117



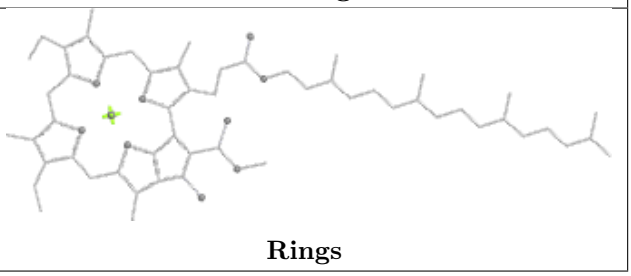
Bond lengths



Bond angles

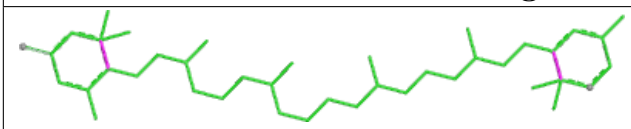


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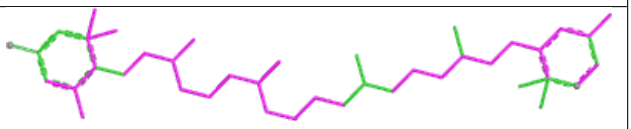


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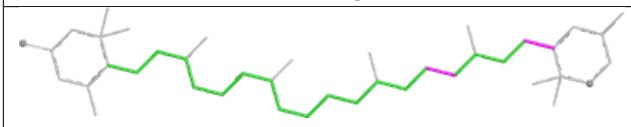
Ligand ZEX 4 4505



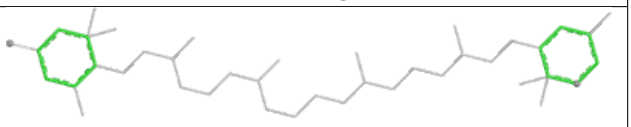
Bond lengths



Bond angles

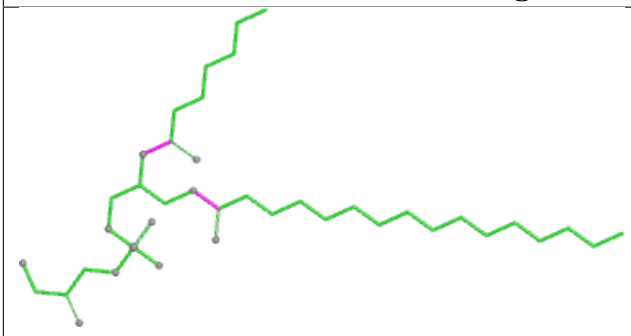


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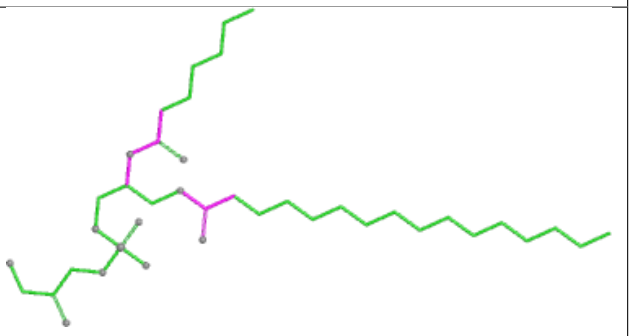


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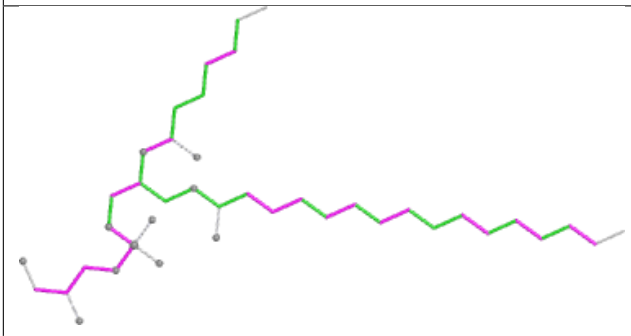
Ligand LHG A 5003



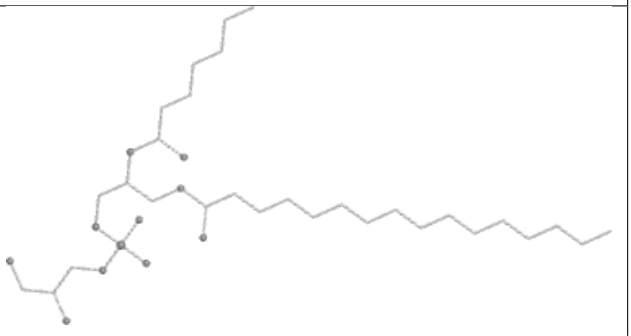
Bond lengths



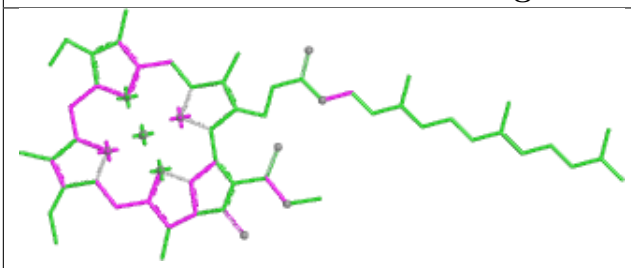
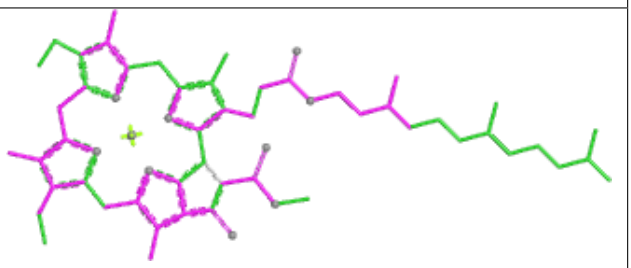
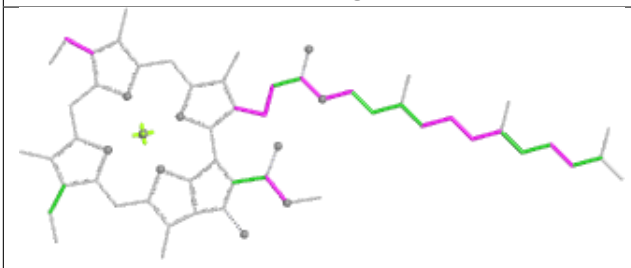
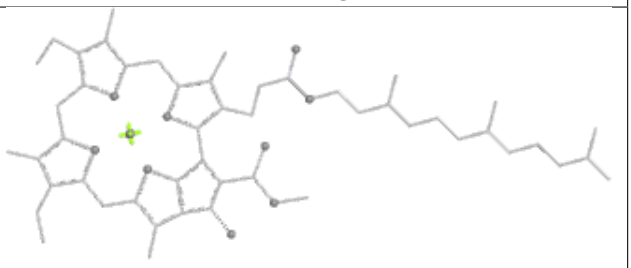
Bond angles

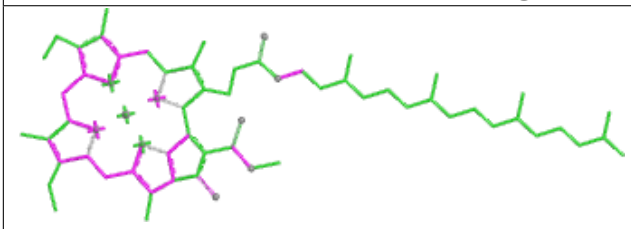
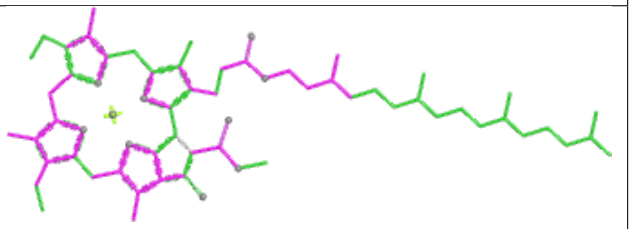
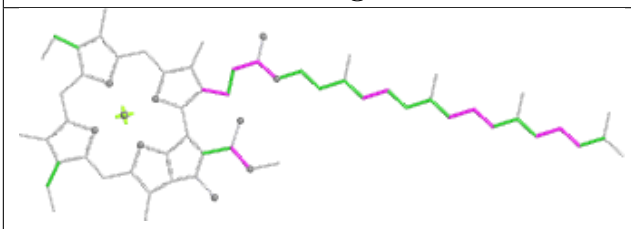
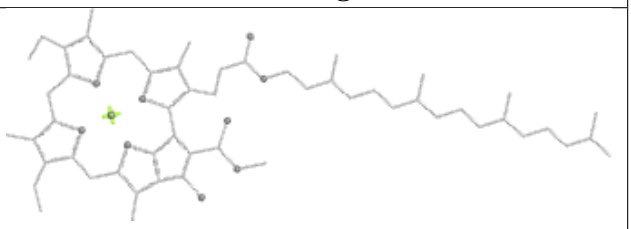


Torsions

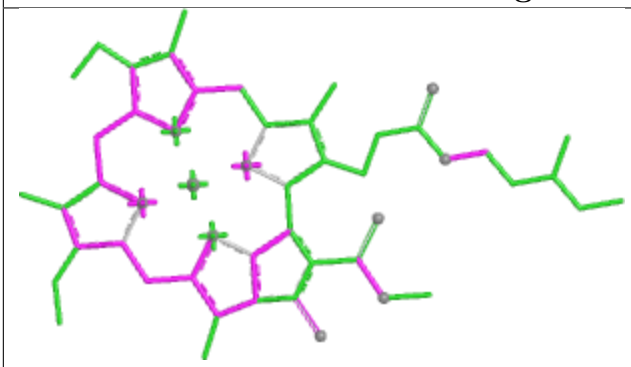


Rings

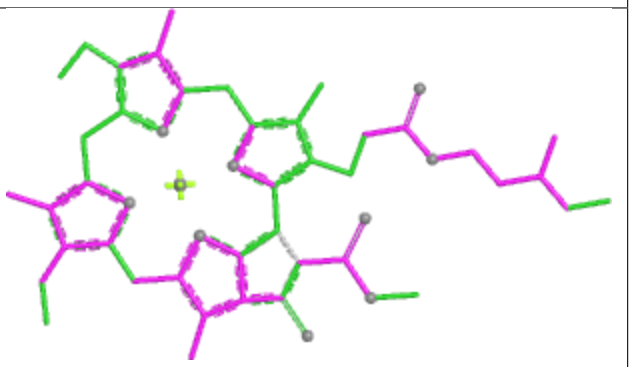
Ligand CLA G 1003	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1210	
	
Bond lengths	Bond angles
	
Torsions	Rings

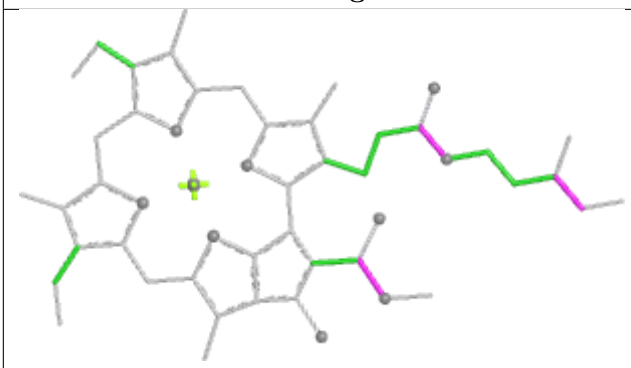
Ligand CLA A 1135



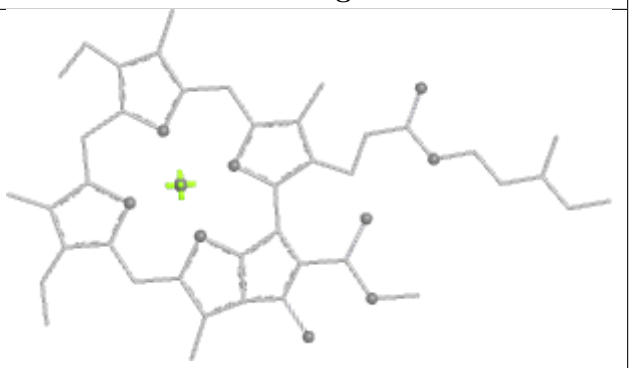
Bond lengths



Bond angles

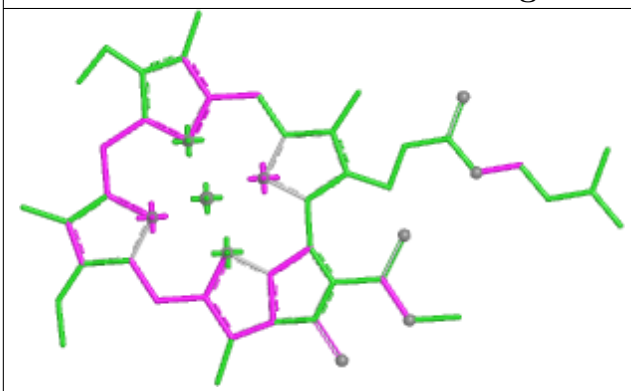


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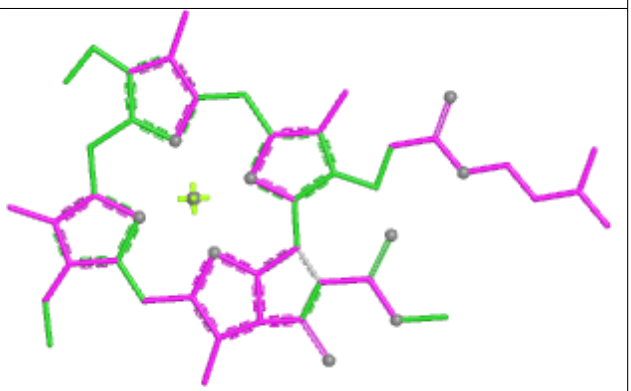


Rings

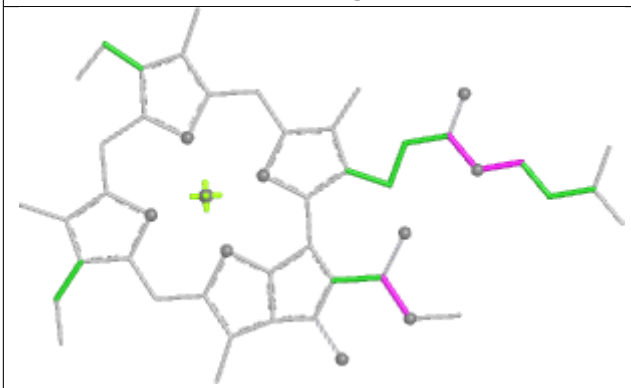
Ligand CLA 3 3006



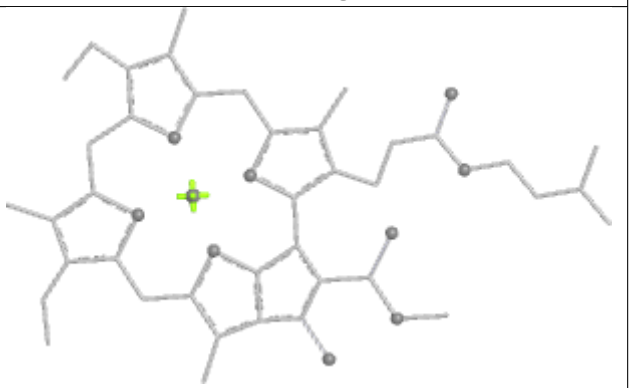
Bond lengths



Bond angles

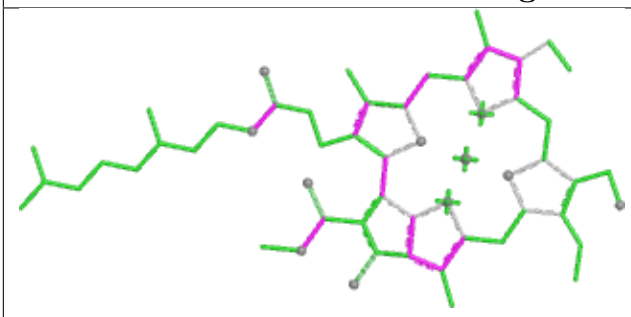


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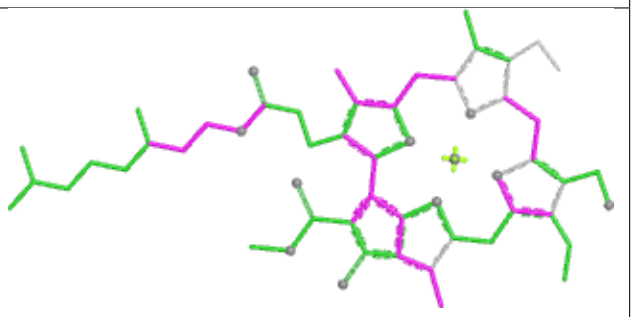


Rings

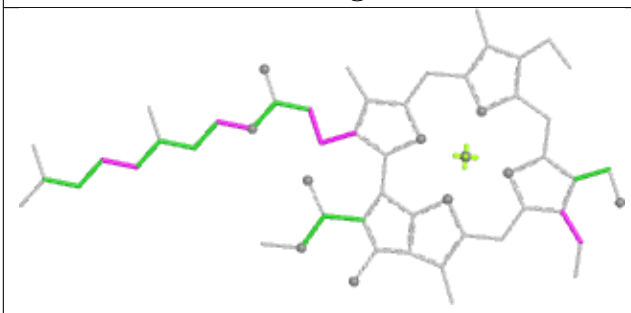
Ligand CHL 3 3011



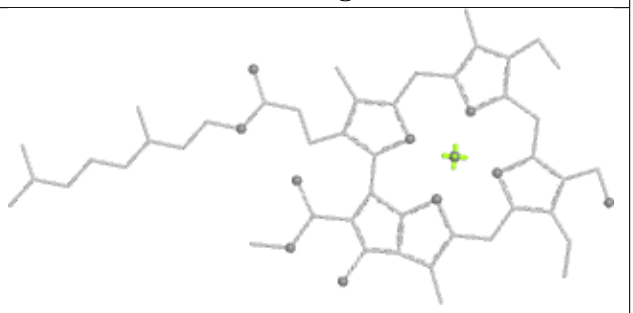
Bond lengths



Bond angles

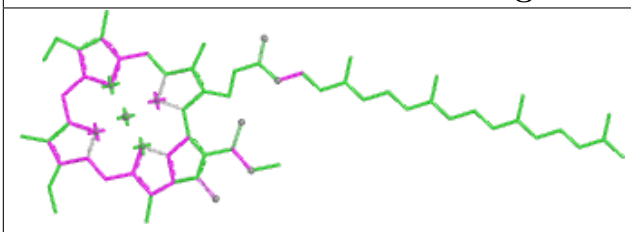


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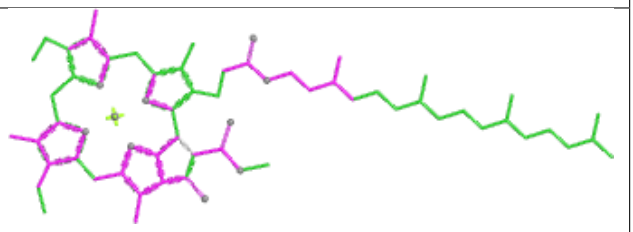


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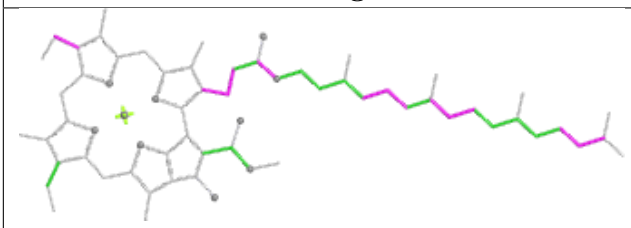
Ligand CLA B 1223



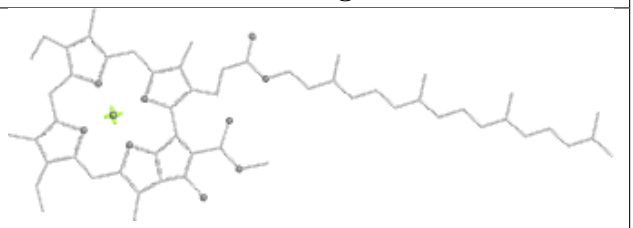
Bond lengths



Bond angles

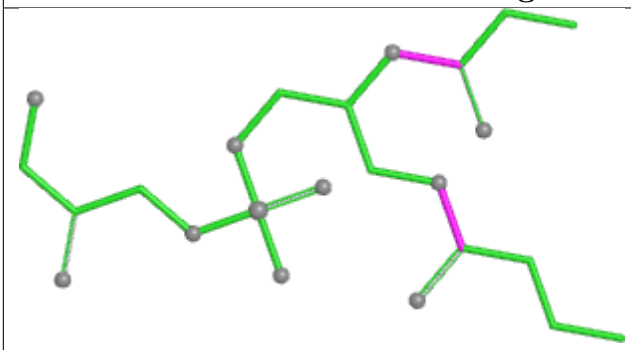


Torsions

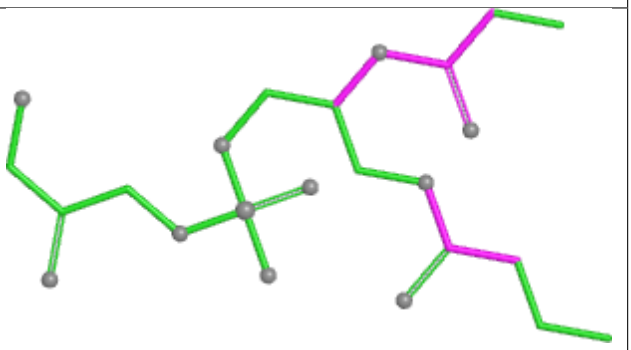


Rings

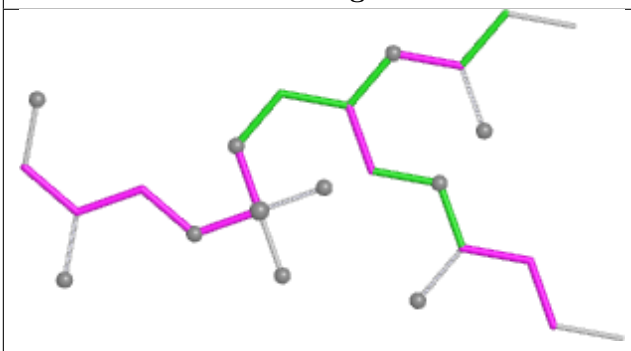
Ligand LHG 2 2801



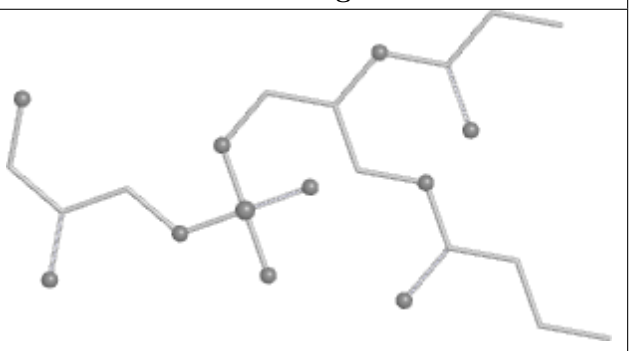
Bond lengths



Bond angles

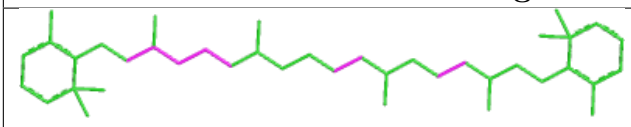


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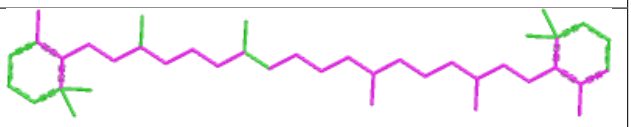


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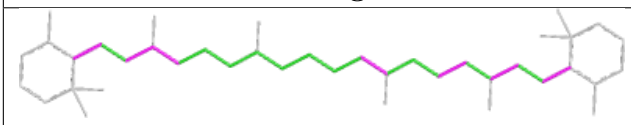
Ligand BCR B 6005



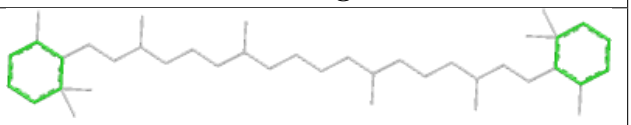
Bond lengths



Bond angles

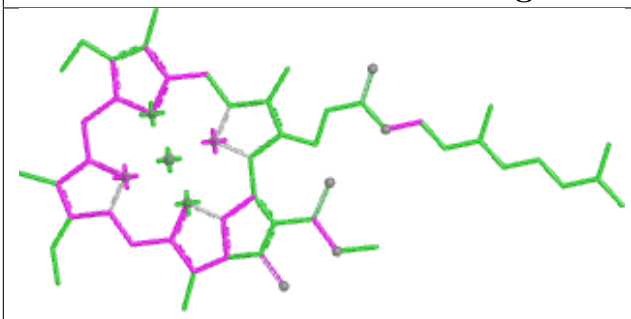


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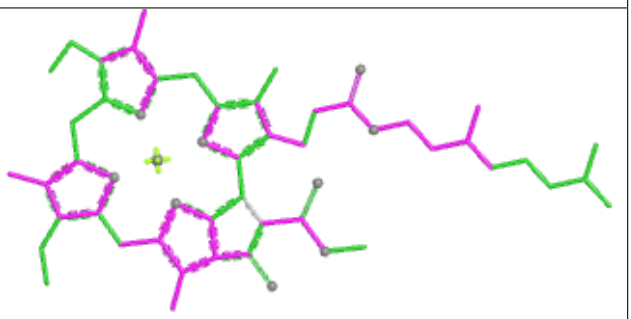


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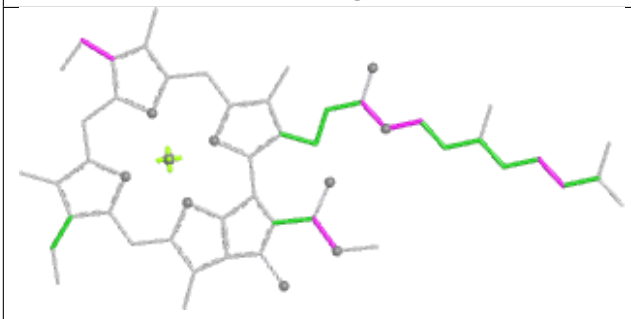
Ligand CLA B 1232



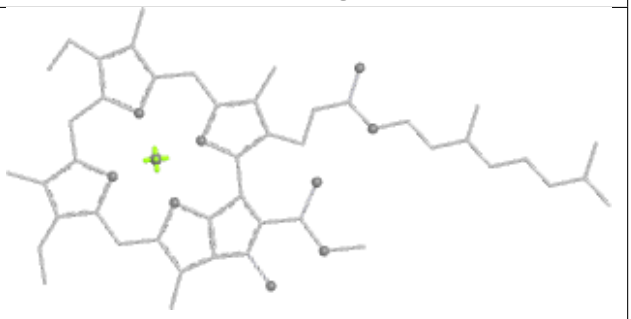
Bond lengths



Bond angles

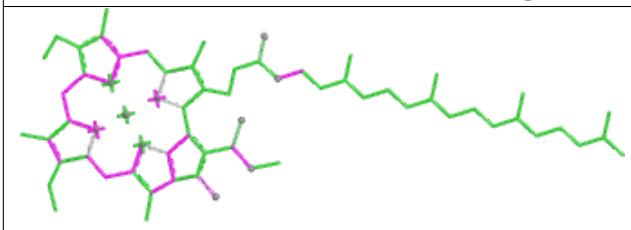


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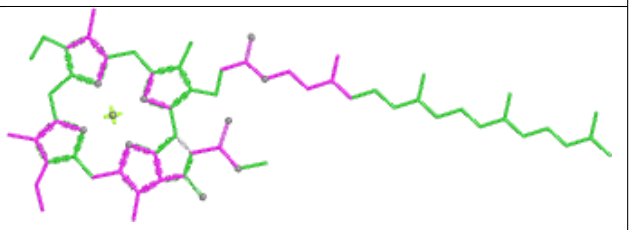


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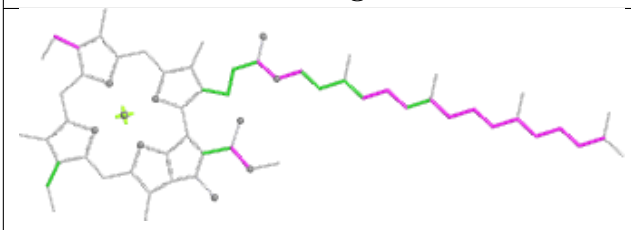
Ligand CLA 1 1004



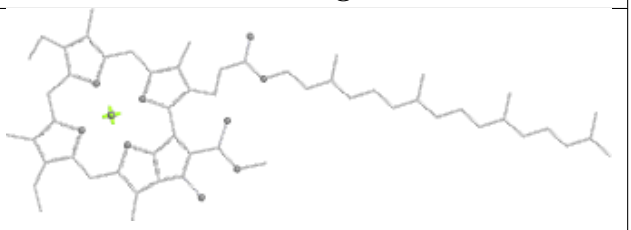
Bond lengths



Bond angles

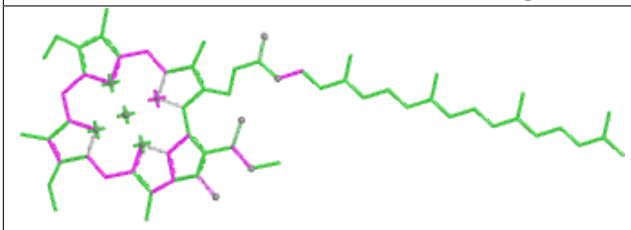


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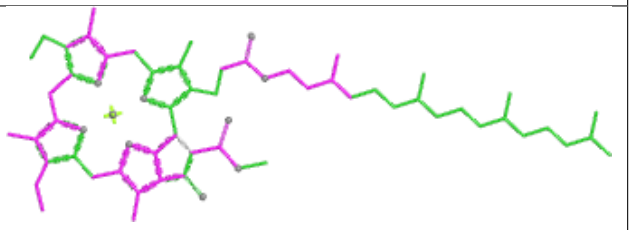


Rings

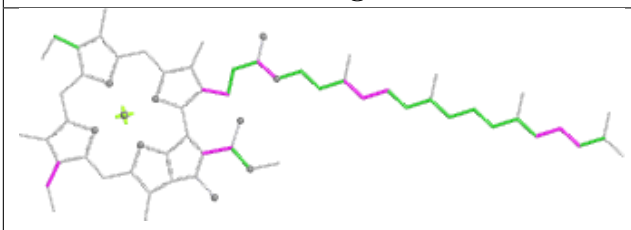
Ligand CLA 2 2004



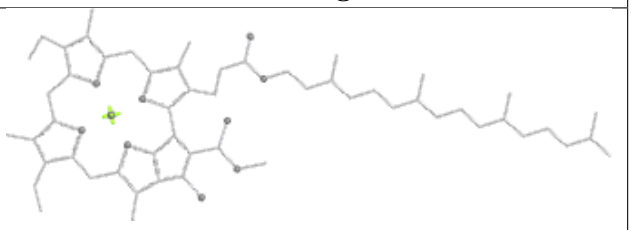
Bond lengths



Bond angles

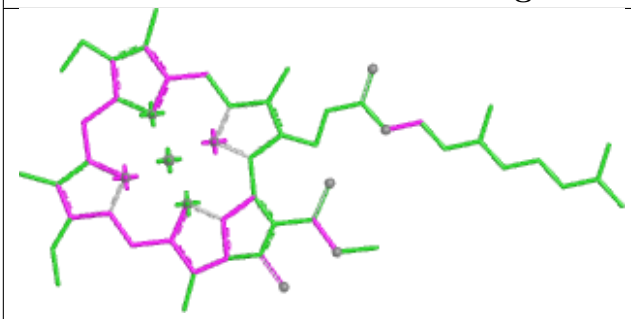


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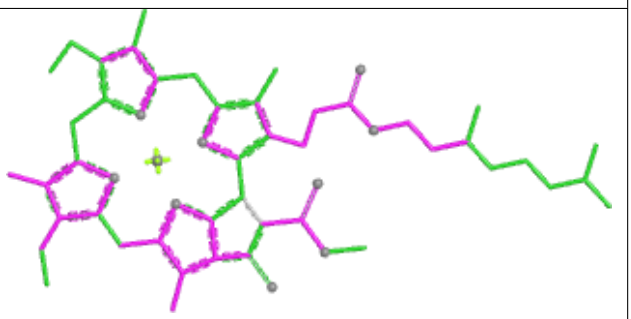


Rings

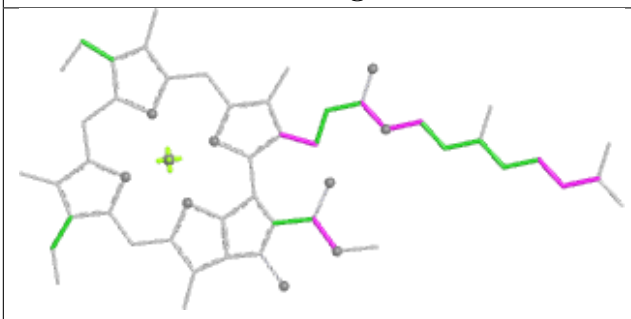
Ligand CLA A 1110



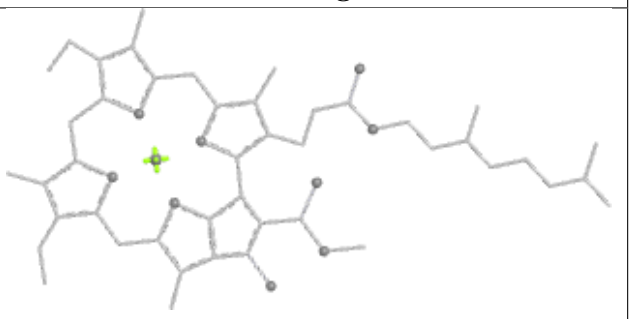
Bond lengths



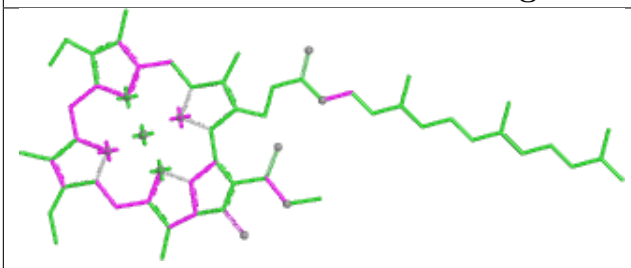
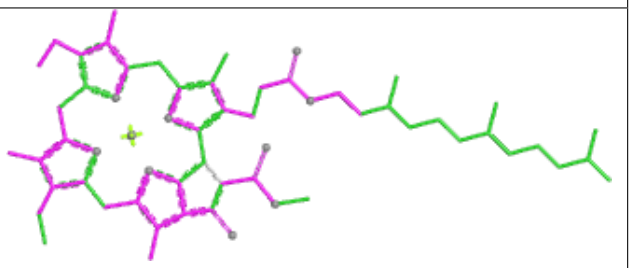
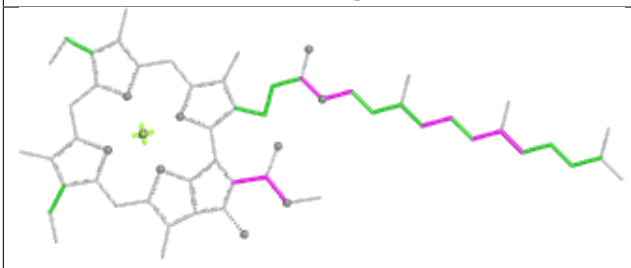
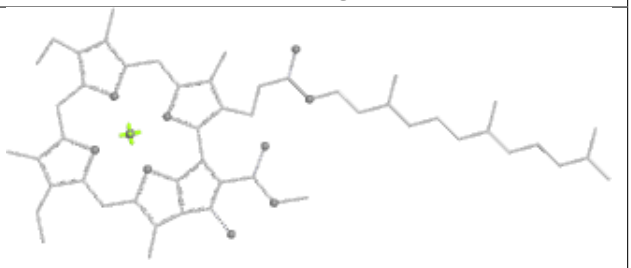
Bond angles

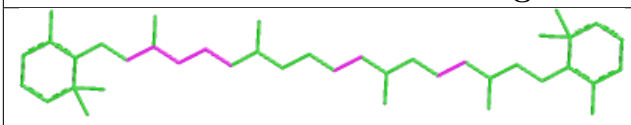
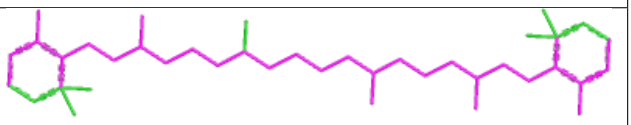
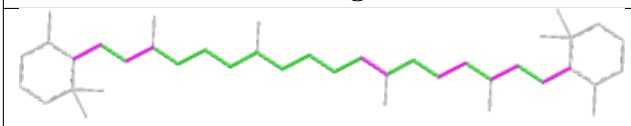
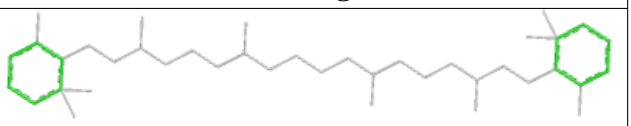


Torsions

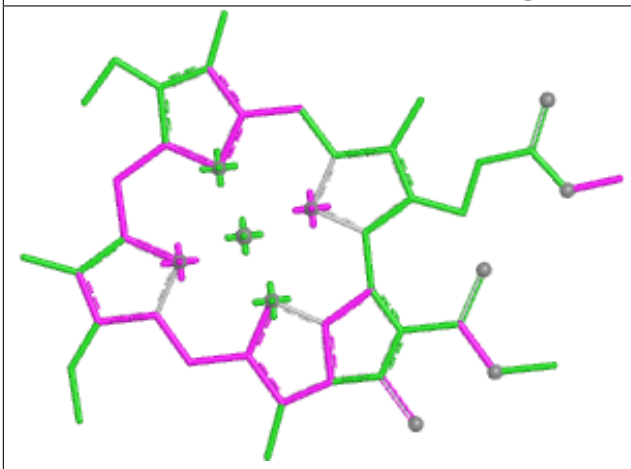


Rings

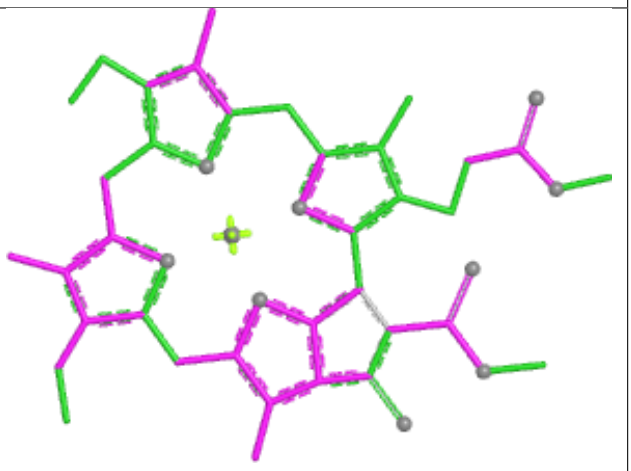
Ligand CLA 3 3004	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand BCR B 6004	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

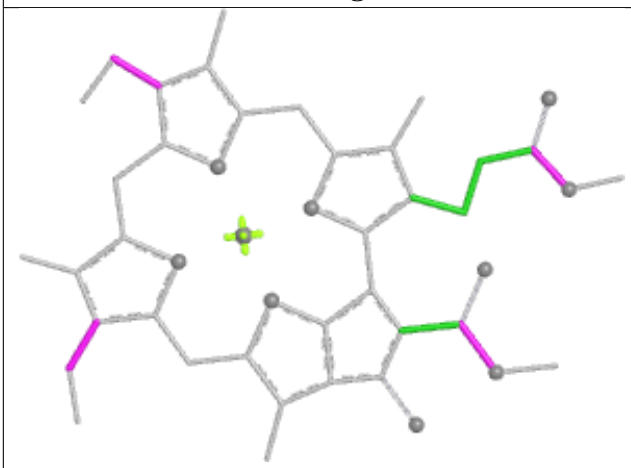
Ligand CLA 1 1013



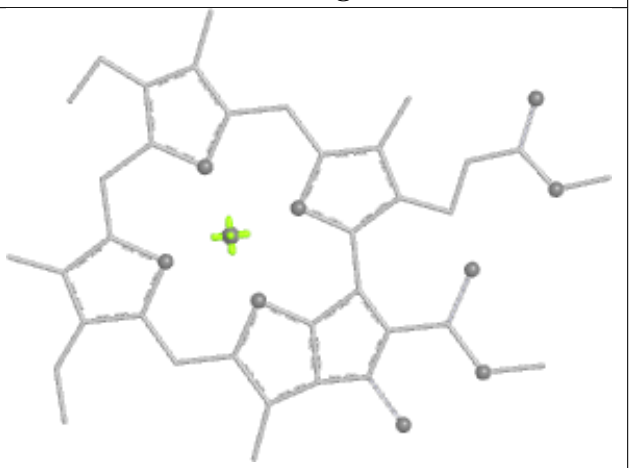
Bond lengths



Bond angles

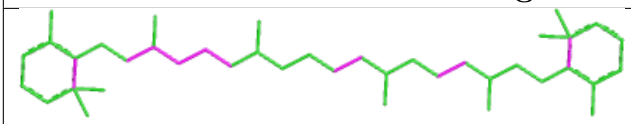


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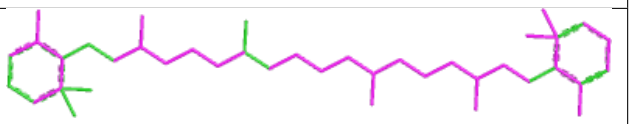


Rings

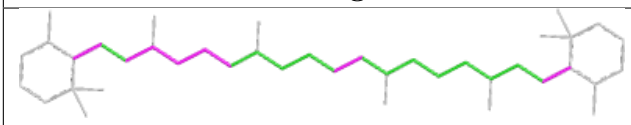
Ligand BCR L 6019



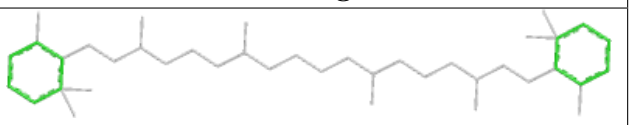
Bond lengths



Bond angles

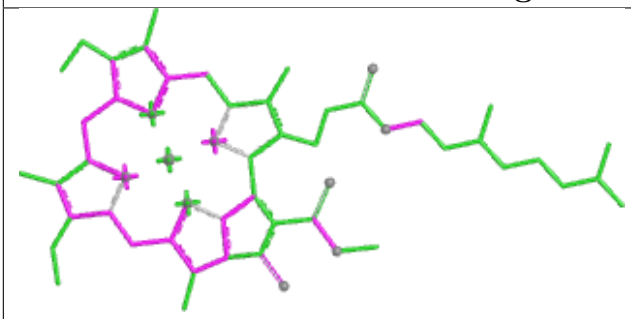


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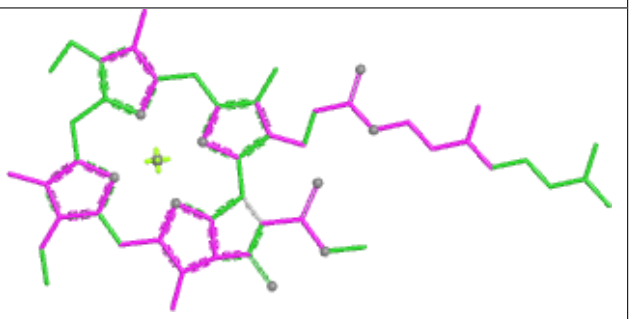


Rings

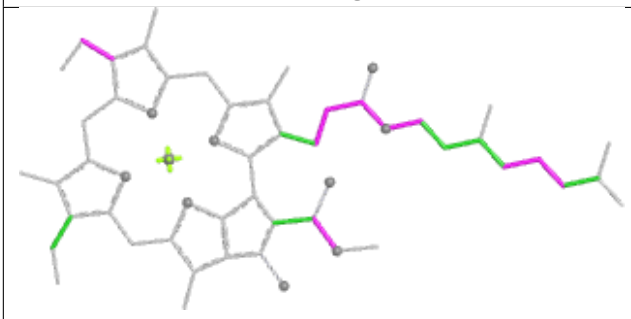
Ligand CLA A 1124



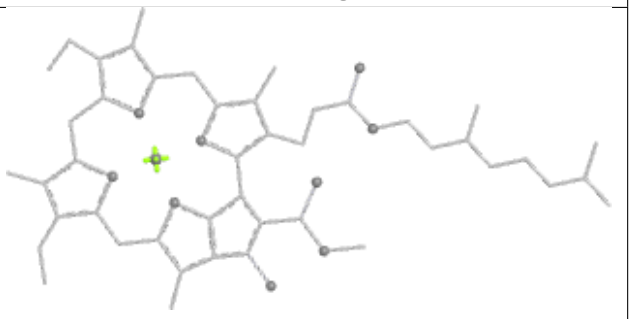
Bond lengths



Bond angles

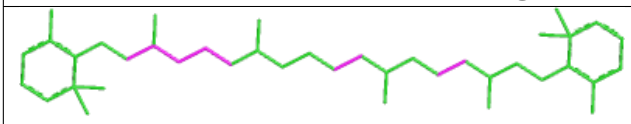


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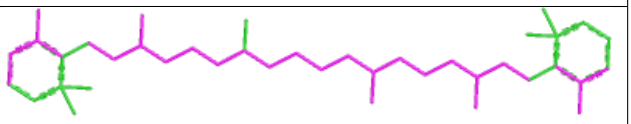


Rings

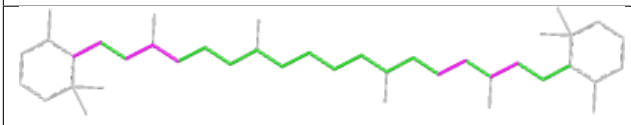
Ligand BCR B 6009



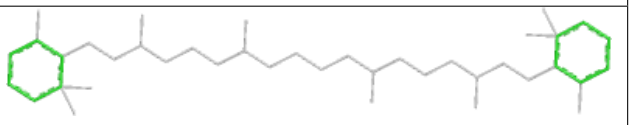
Bond lengths



Bond angles

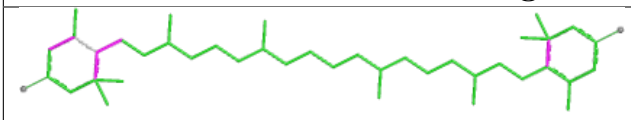


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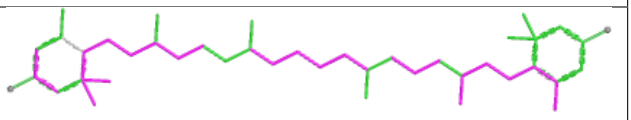


Rings

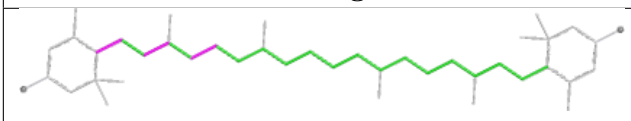
Ligand LUT 2 2502



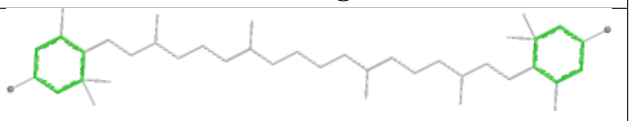
Bond lengths



Bond angles

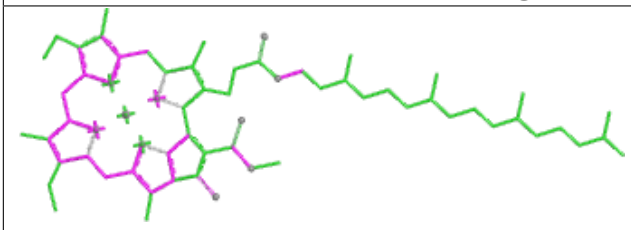


Torsions

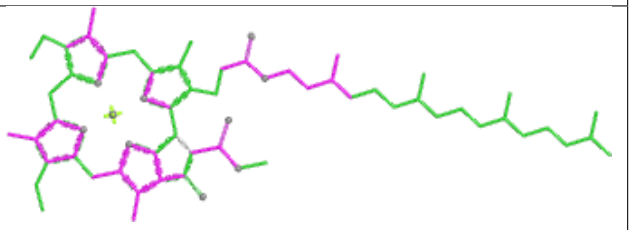


Rings

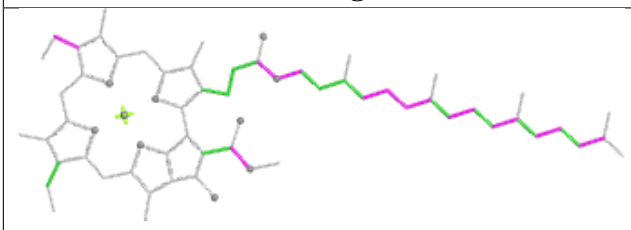
Ligand CLA B 1203



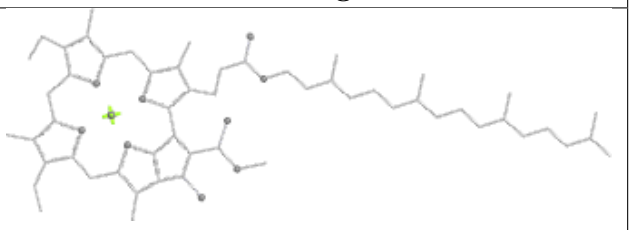
Bond lengths



Bond angles

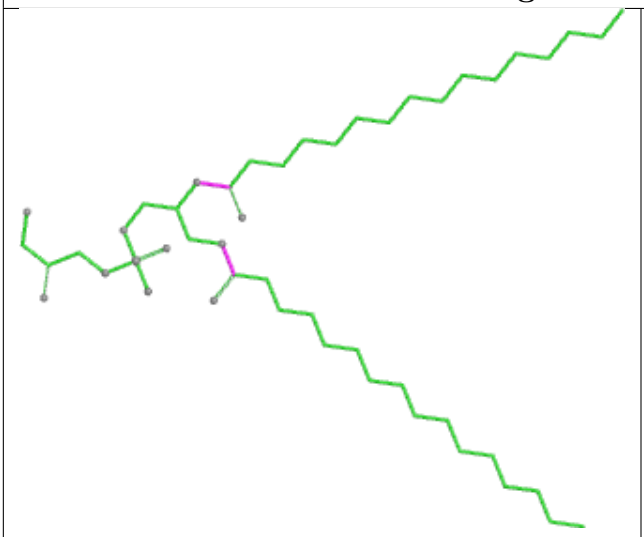


Torsions

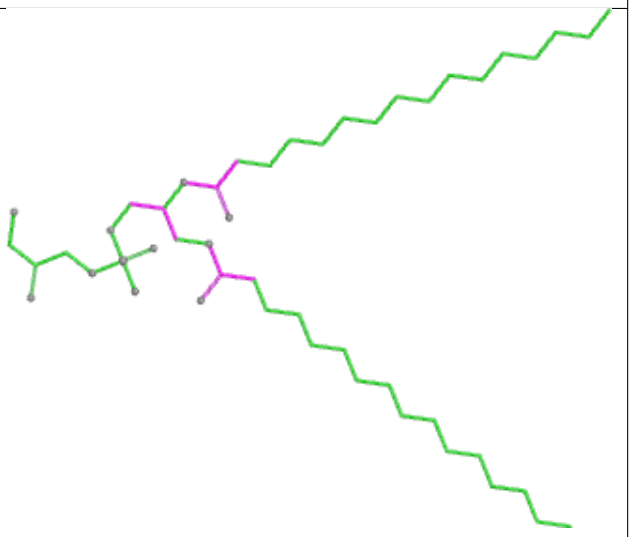


Rings

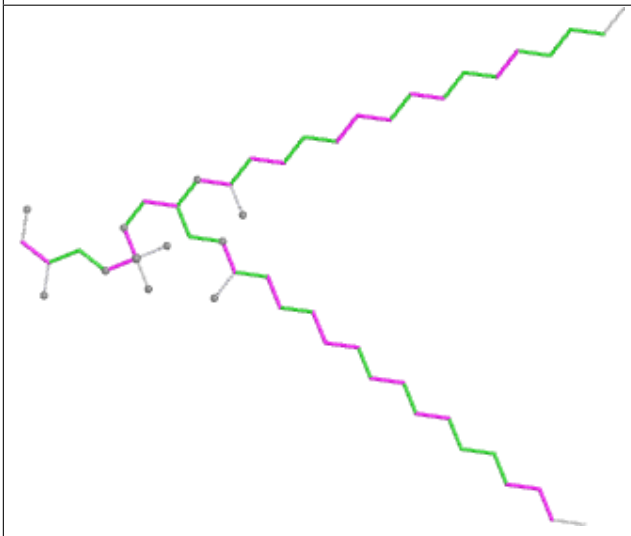
Ligand LHG 1 1801



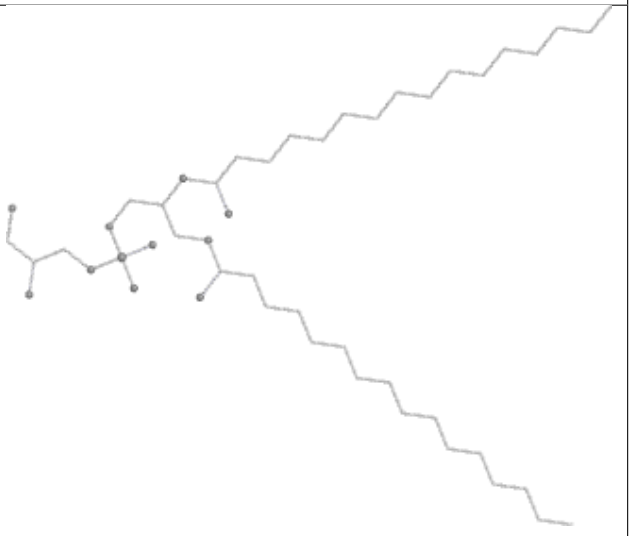
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Bond angles

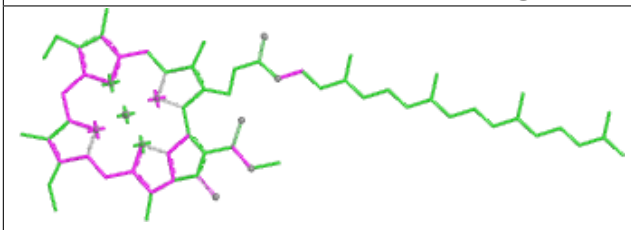


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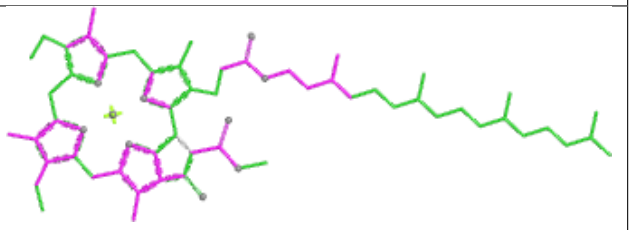


Rings

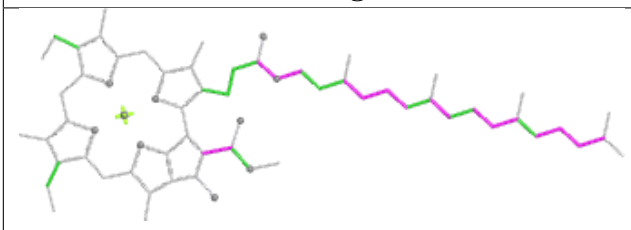
Ligand CLA A 1123



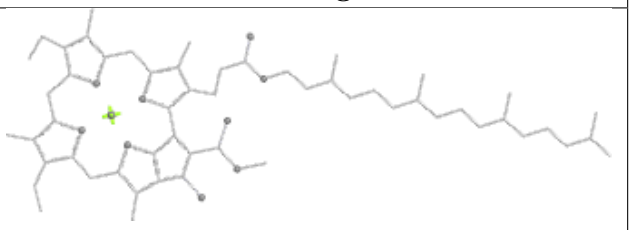
Bond lengths



Bond angles

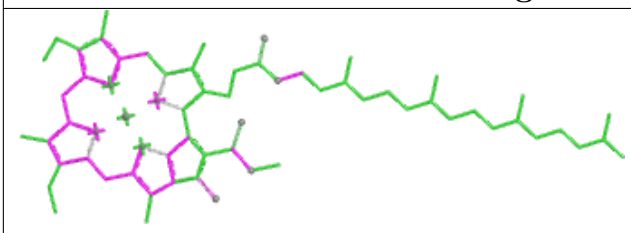


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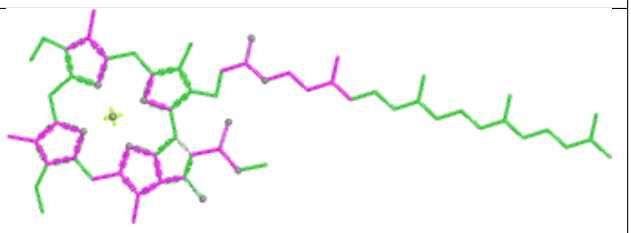


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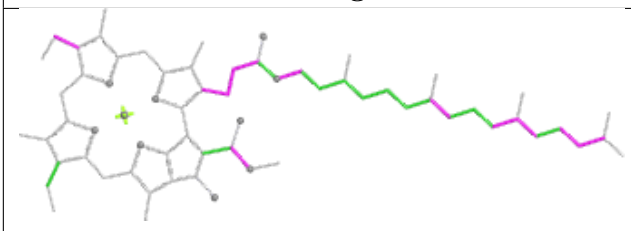
Ligand CLA B 1239



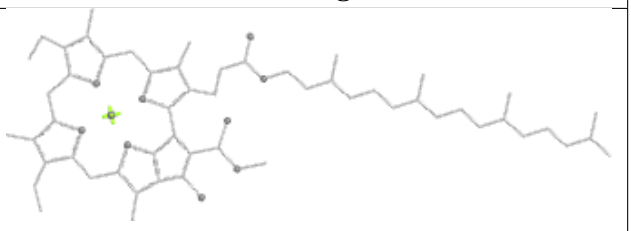
Bond lengths



Bond angles

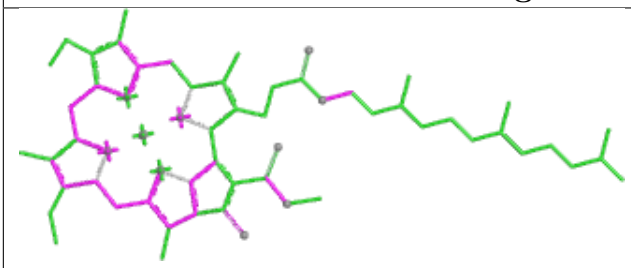


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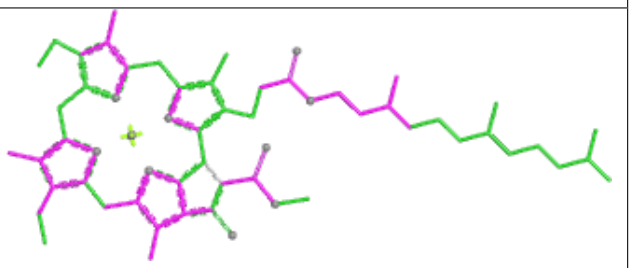


Rings

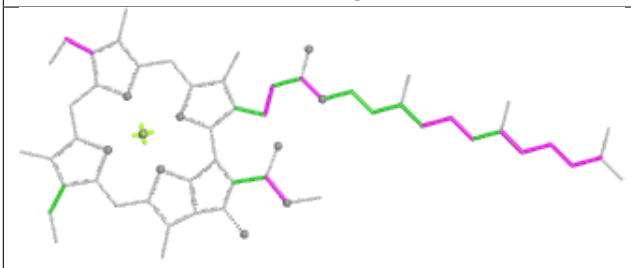
Ligand CLA A 1237



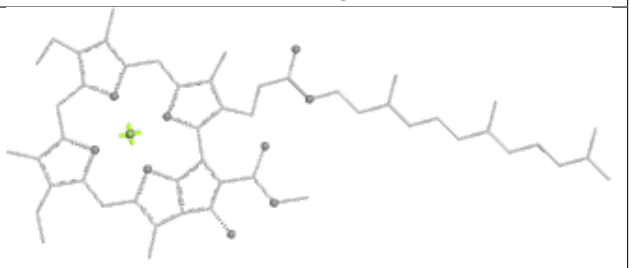
Bond lengths



Bond angles

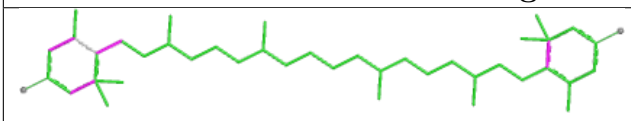


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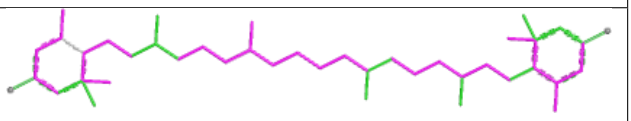


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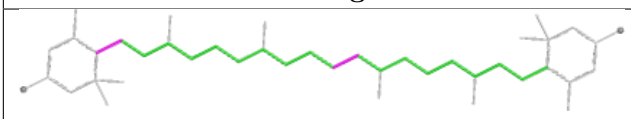
Ligand LUT 1 1502



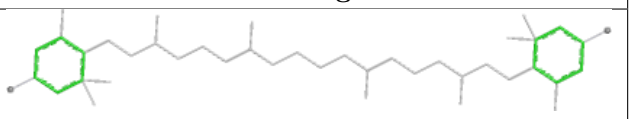
Bond lengths



Bond angles

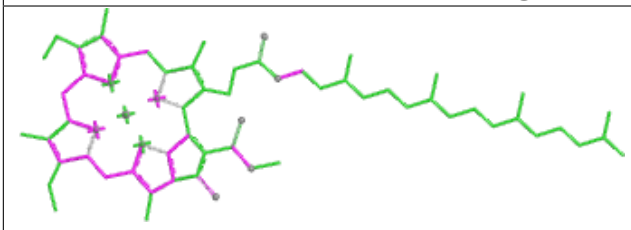


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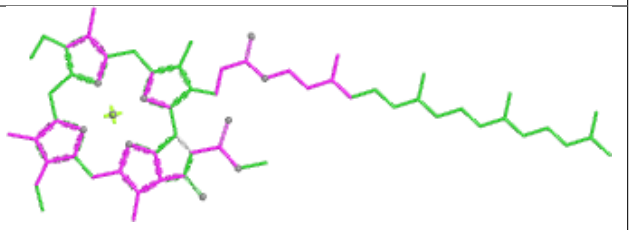


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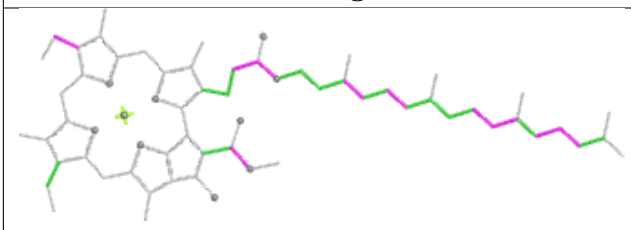
Ligand CLA B 1240



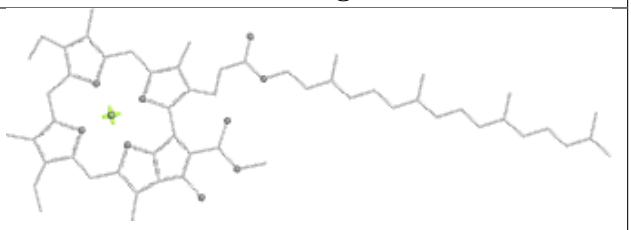
Bond lengths



Bond angles

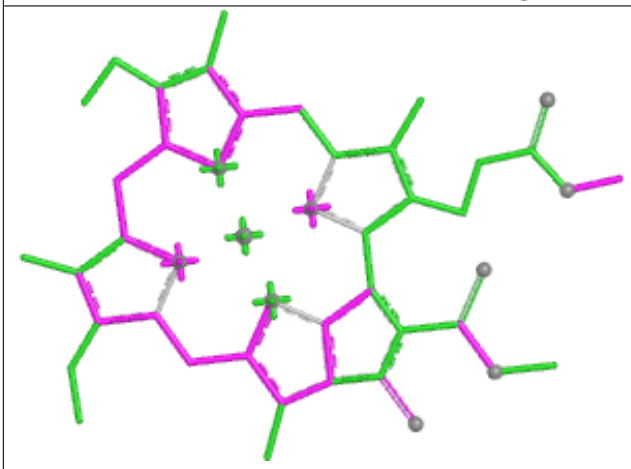


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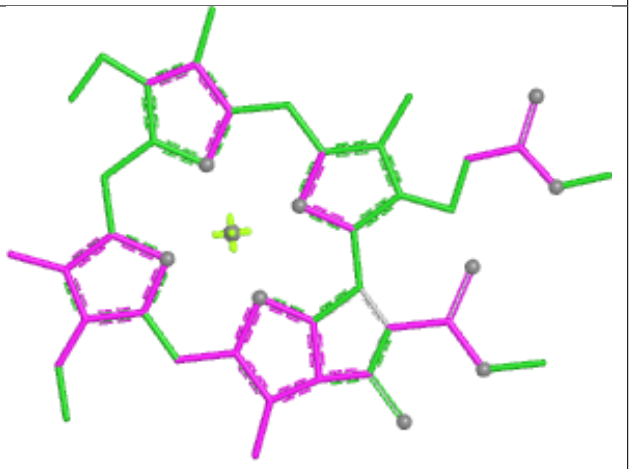


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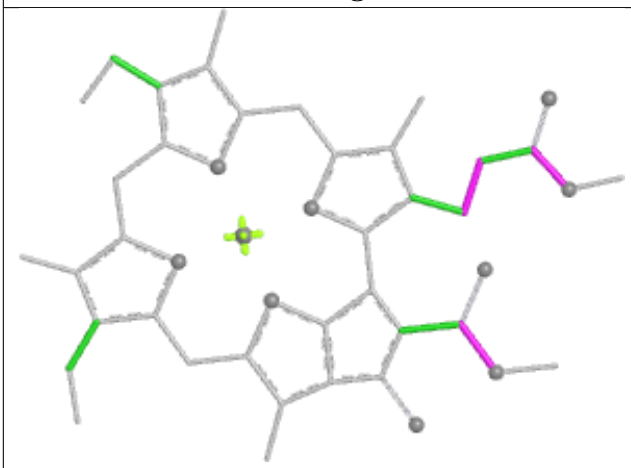
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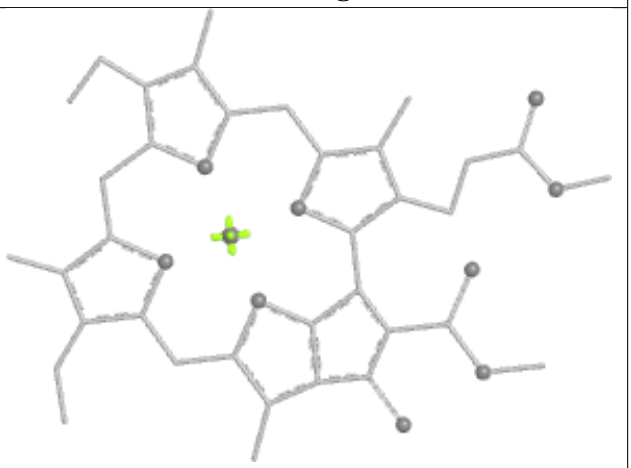
Bond lengths



Bond angles

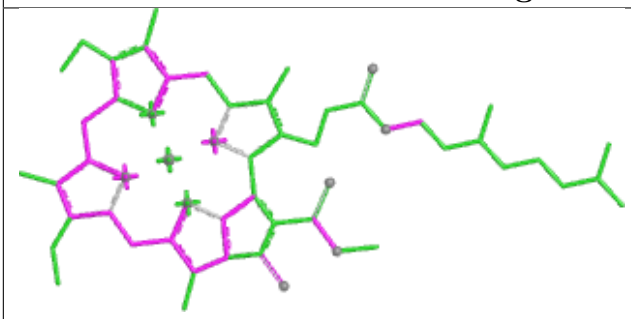


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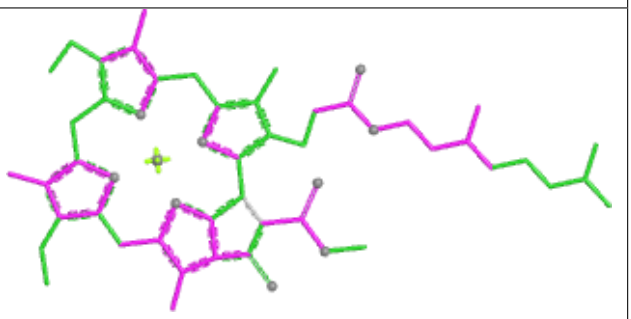


Rings

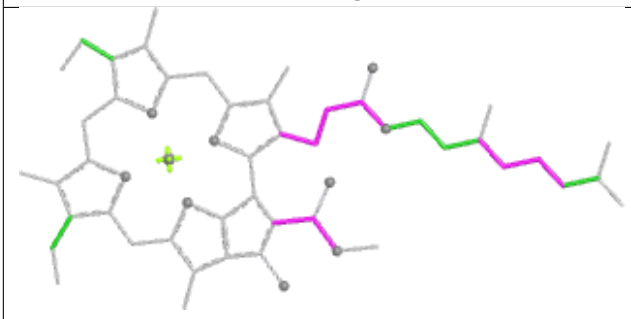
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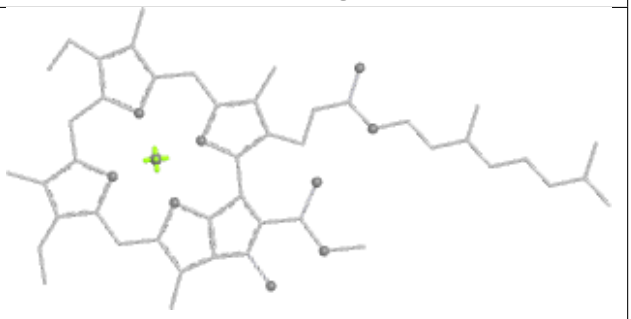
Bond lengths



Bond angles

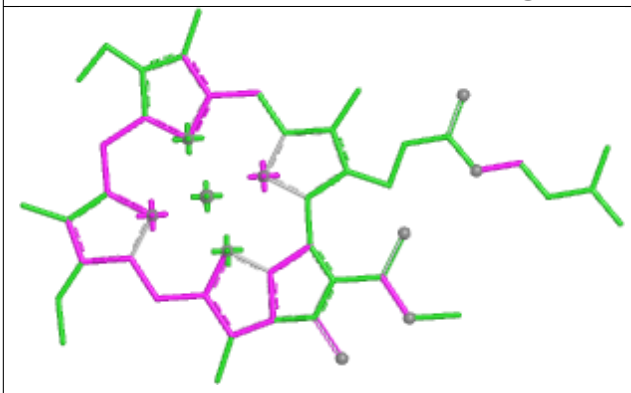


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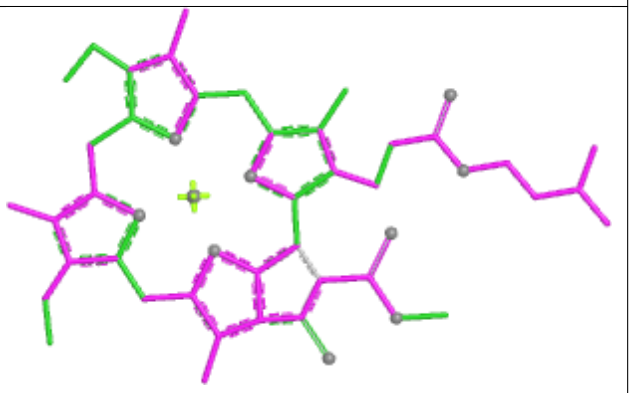


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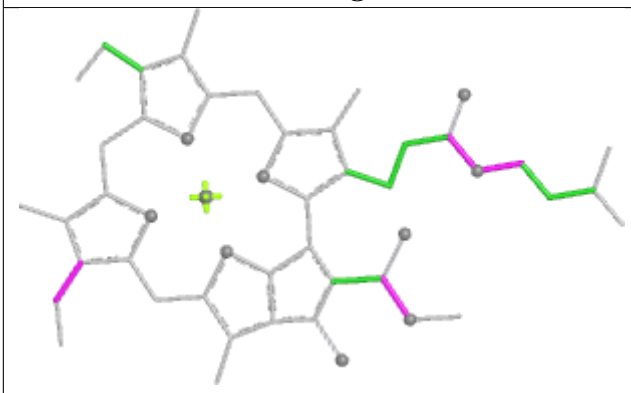
Ligand CLA 3 3018



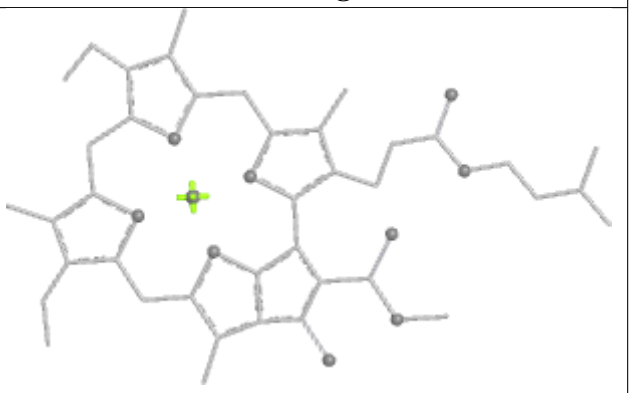
Bond lengths



Bond angles

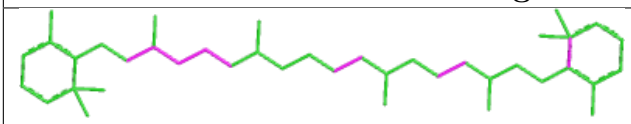


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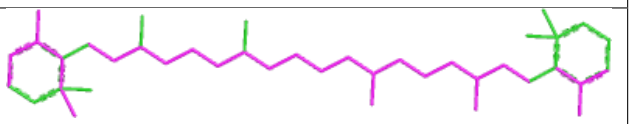


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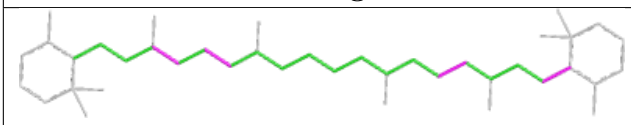
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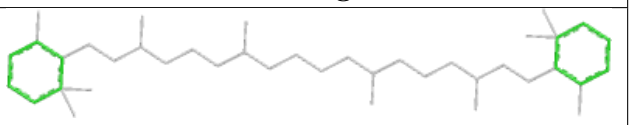
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Bond angles

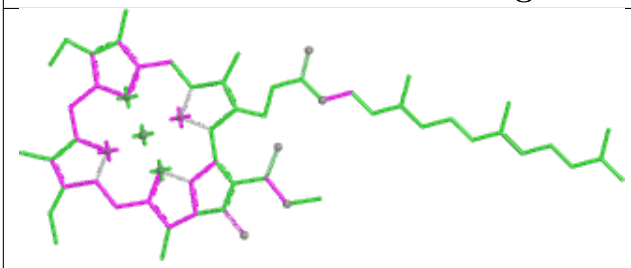


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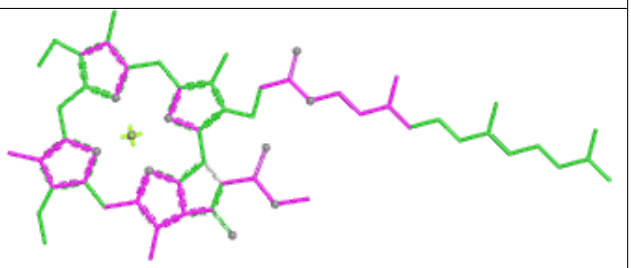


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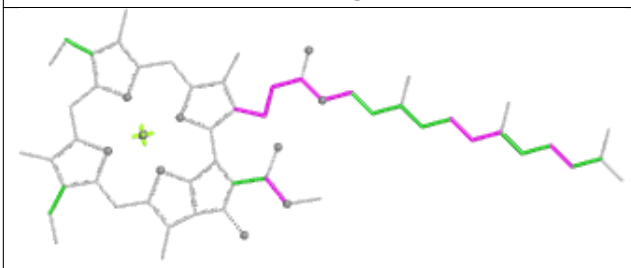
Ligand CLA B 1228



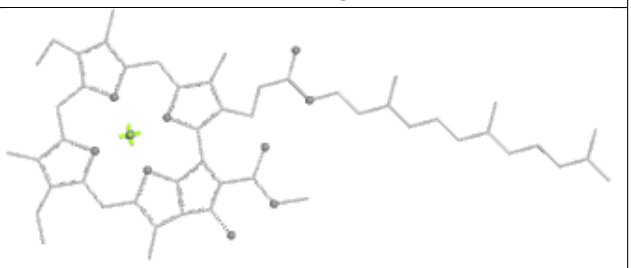
Bond lengths



Bond angles

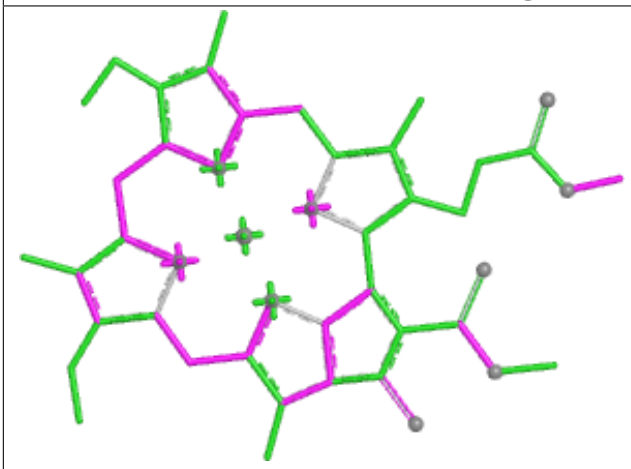


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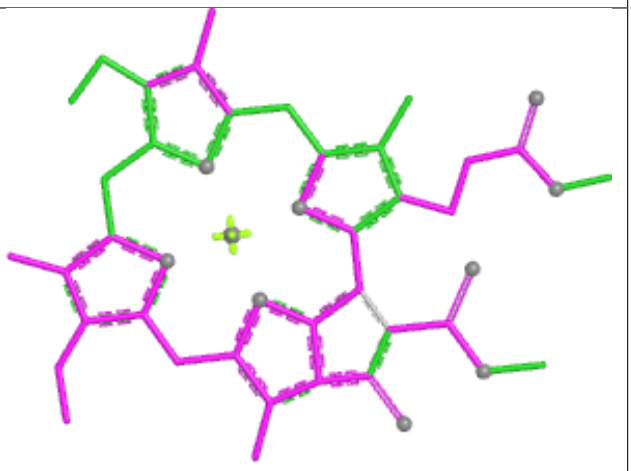


Rings

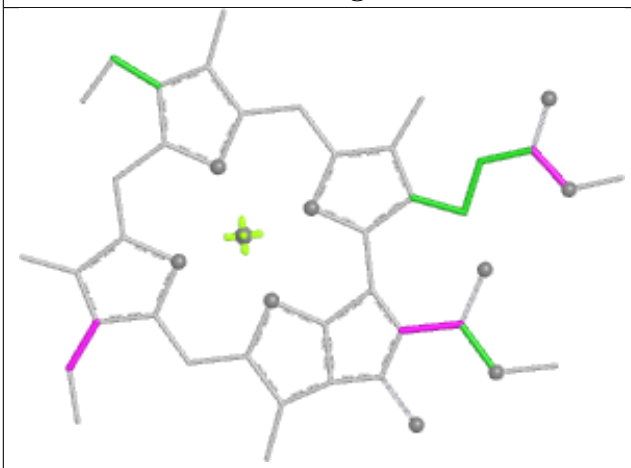
Ligand CLA 1 1002



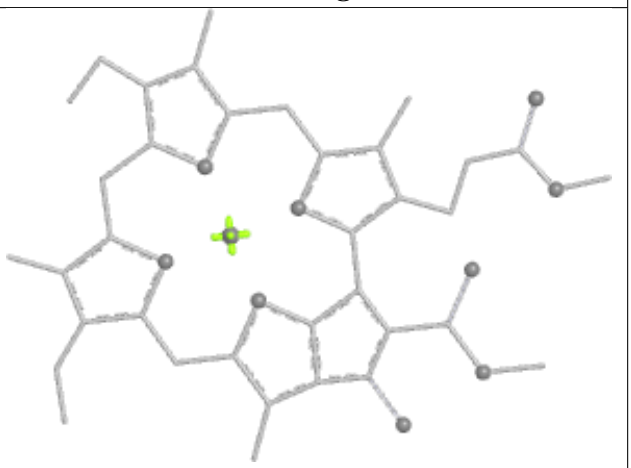
Bond lengths



Bond angles

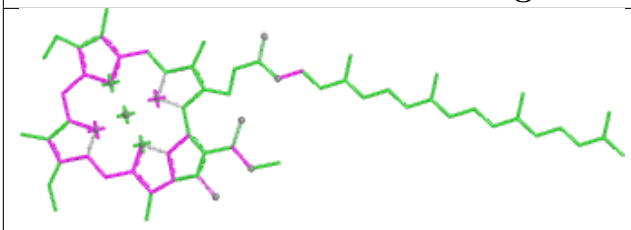


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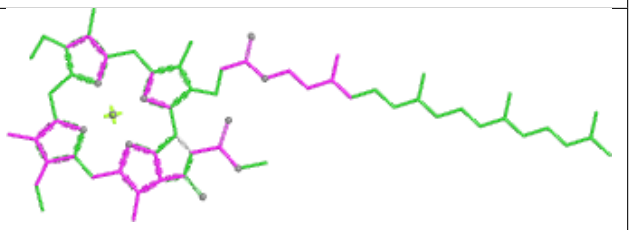


Rings

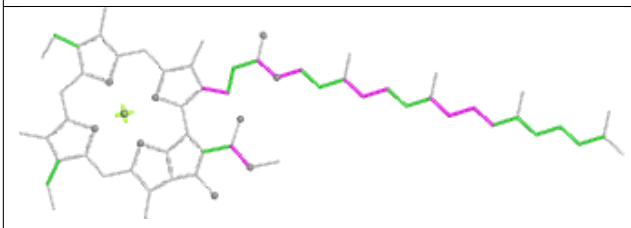
Ligand CLA A 1101



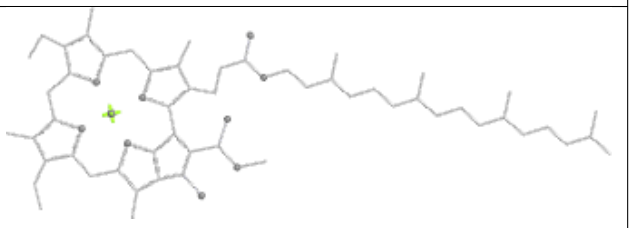
Bond lengths



Bond angles

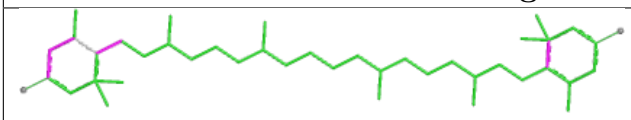


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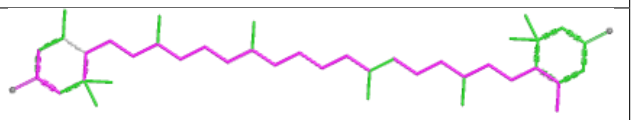


Rings

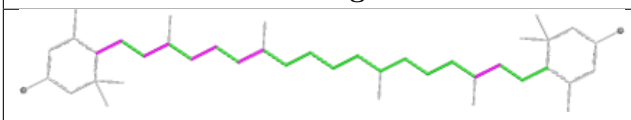
Ligand LUT 1 1501



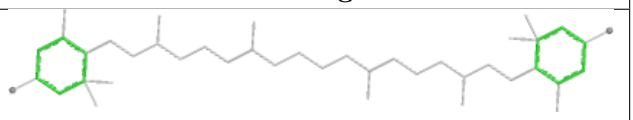
Bond lengths



Bond angles

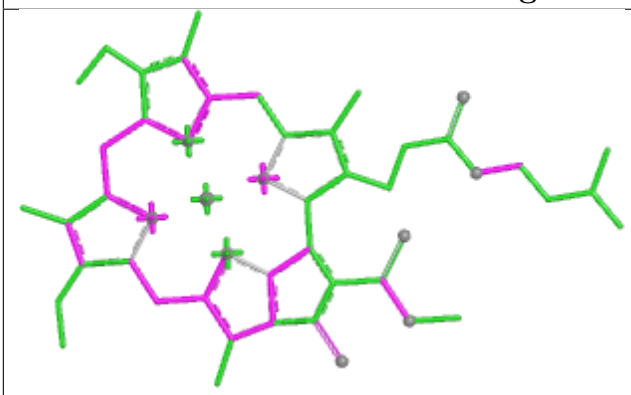


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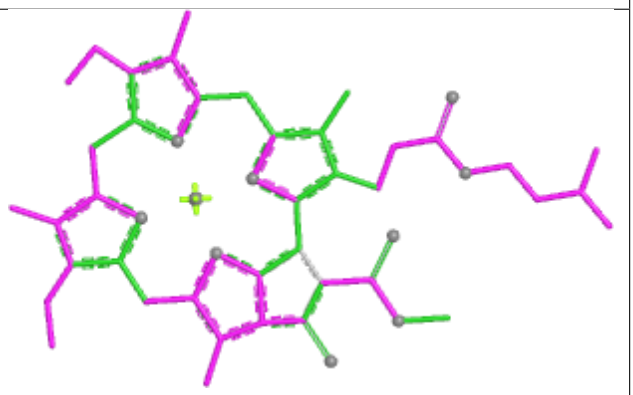


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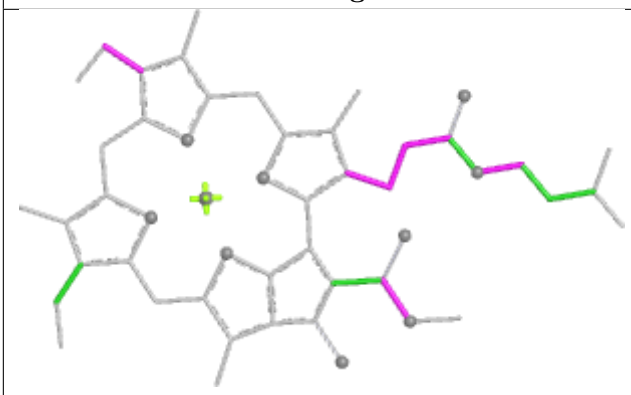
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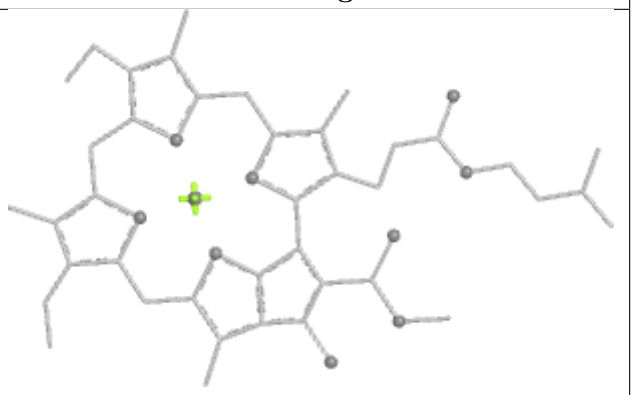
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Bond angles

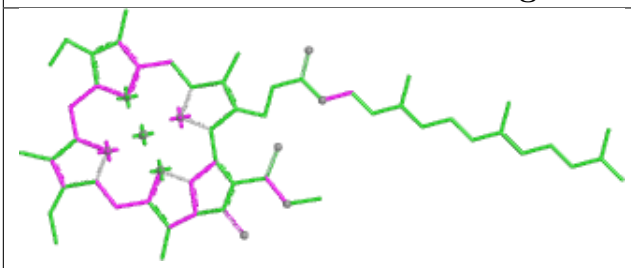


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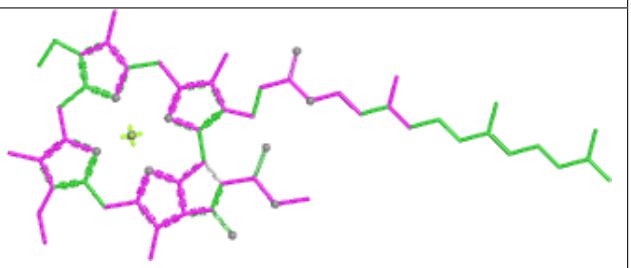


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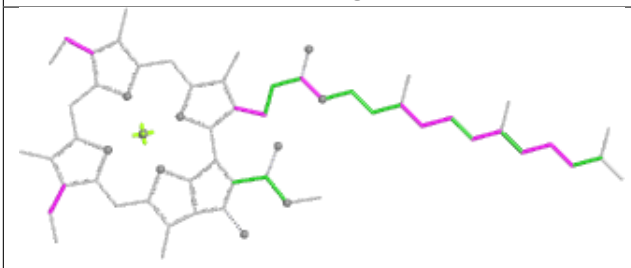
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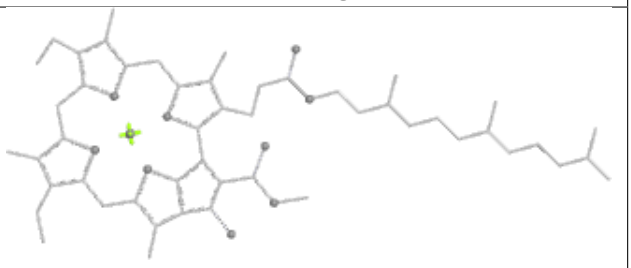
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Bond angles

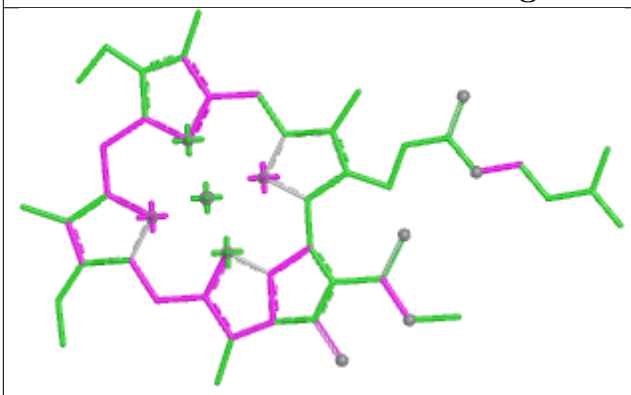


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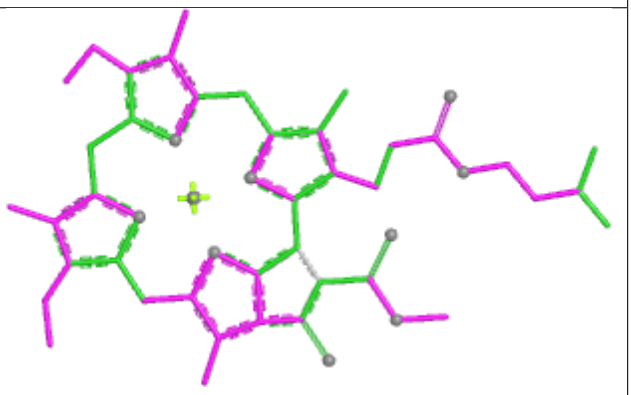


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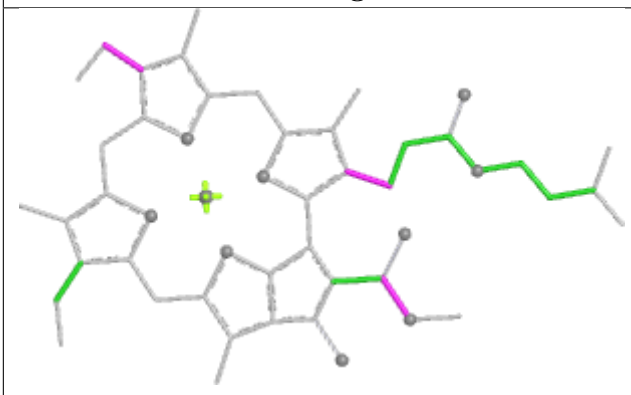
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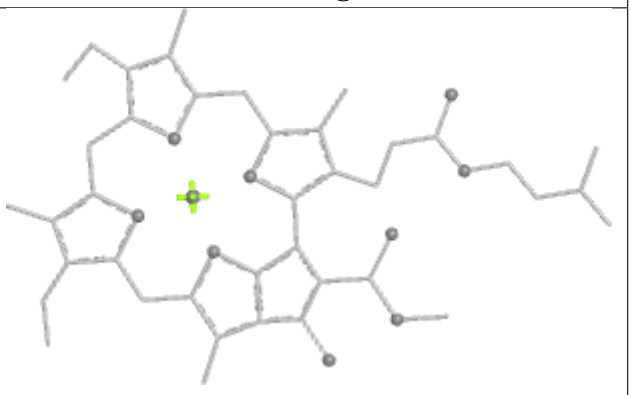
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Bond angles

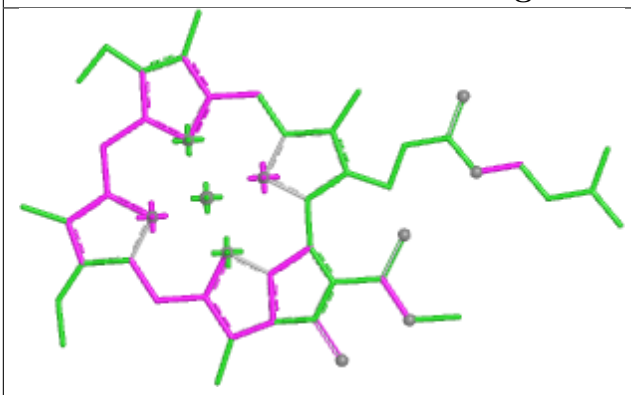


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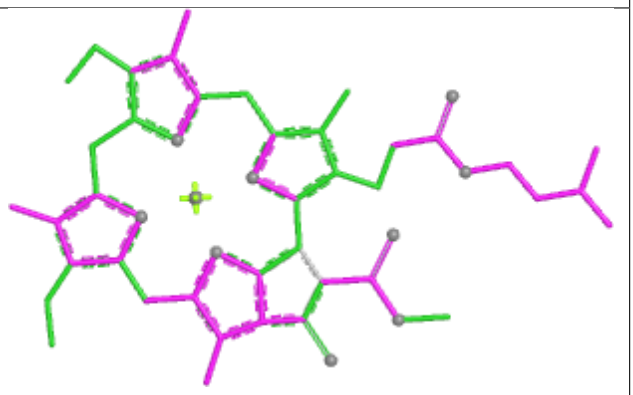


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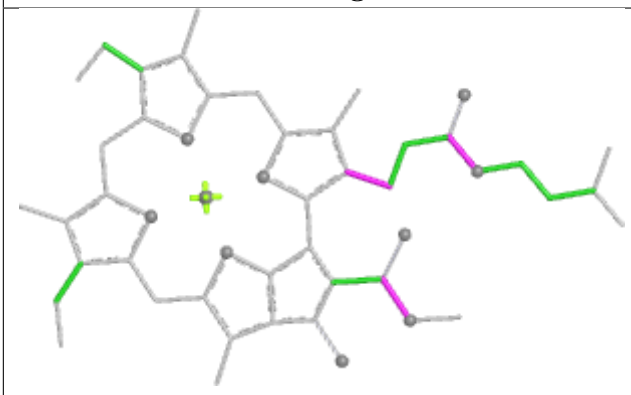
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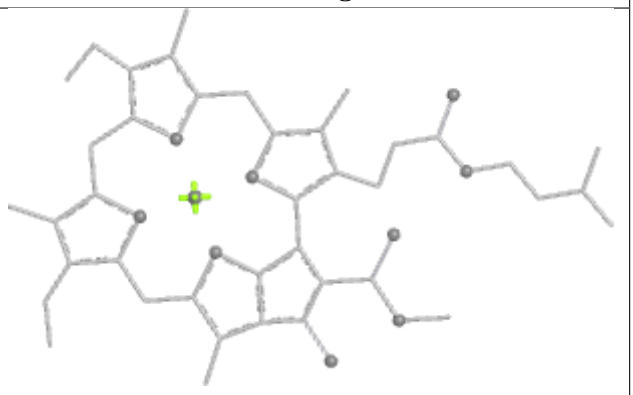
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Bond angles

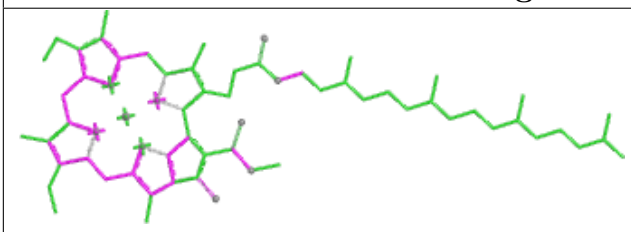


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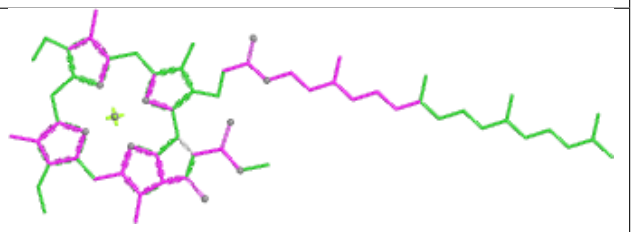


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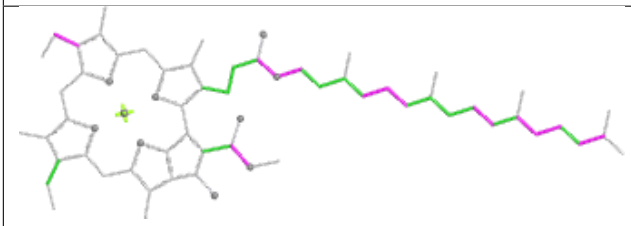
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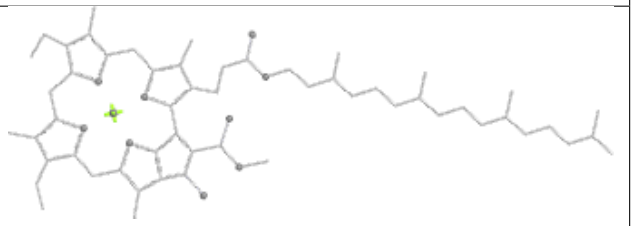
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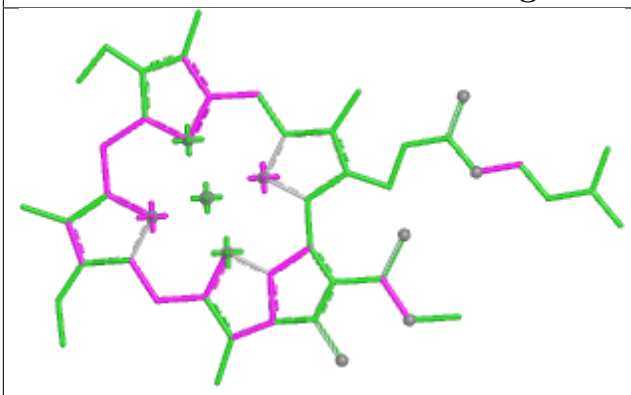


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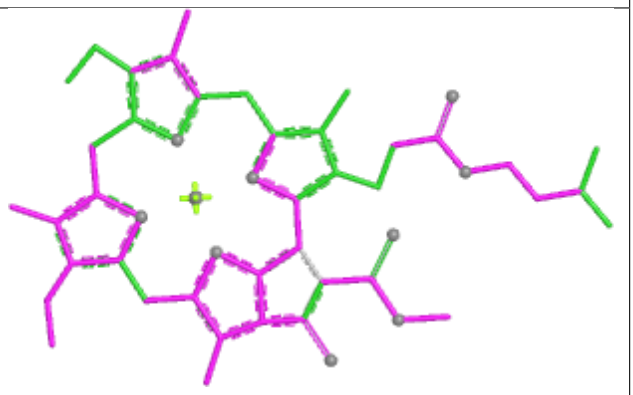


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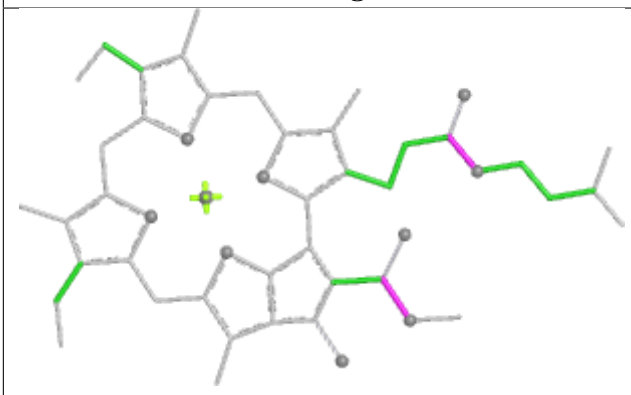
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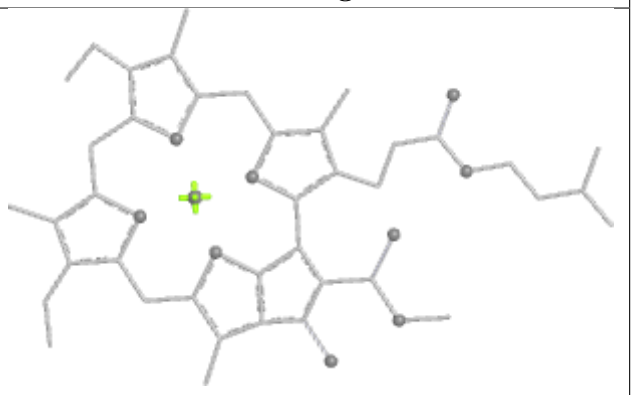
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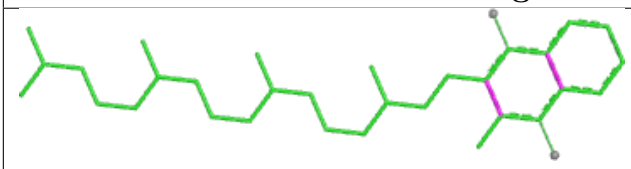


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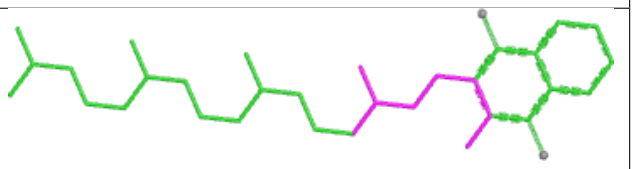


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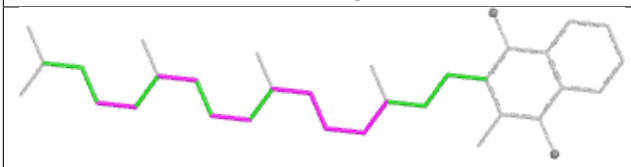
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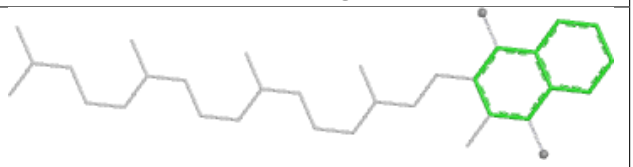
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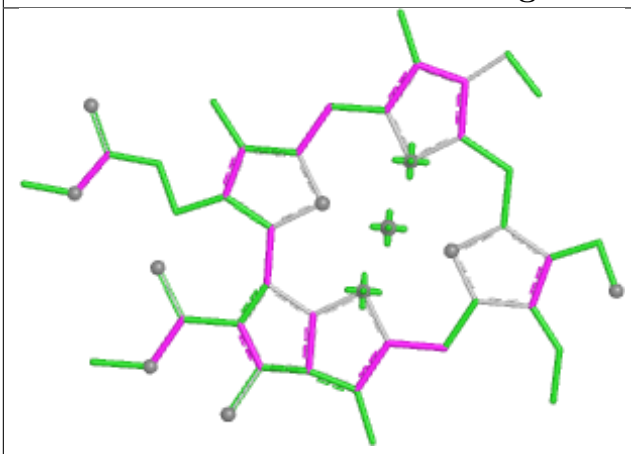


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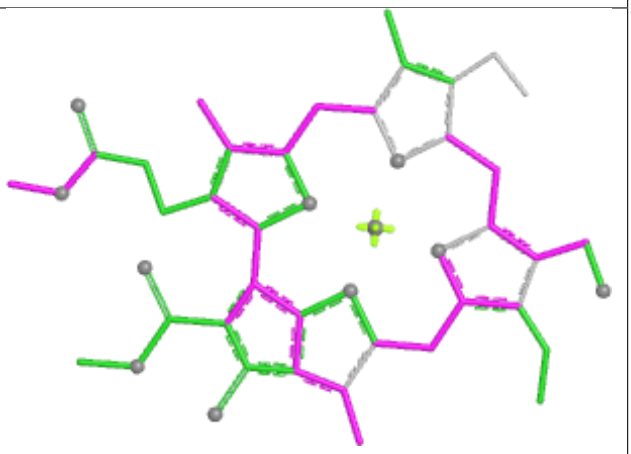


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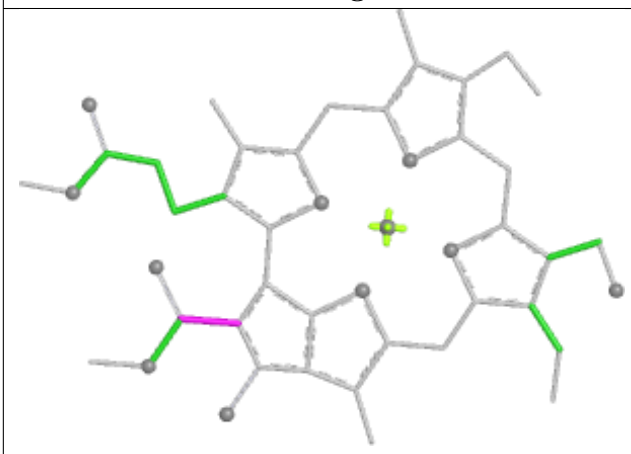
Ligand CHL 2 2010



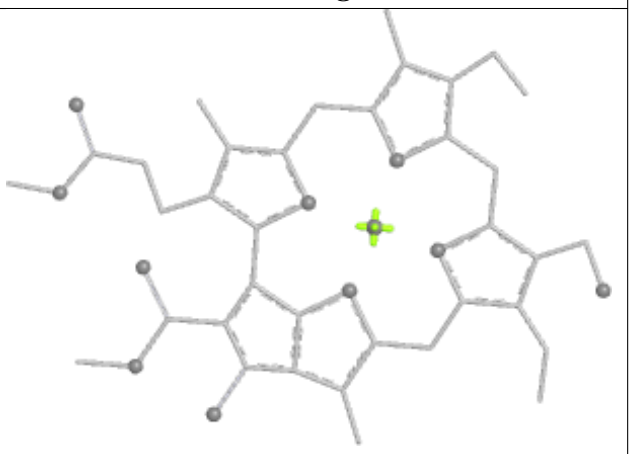
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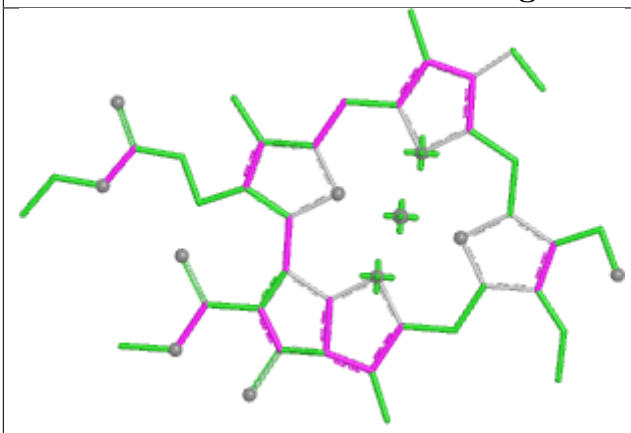


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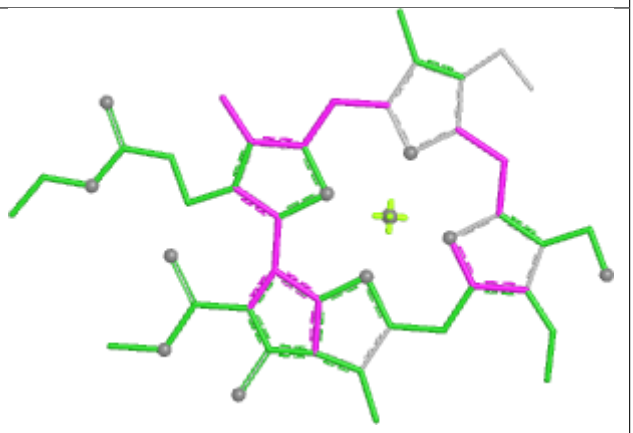


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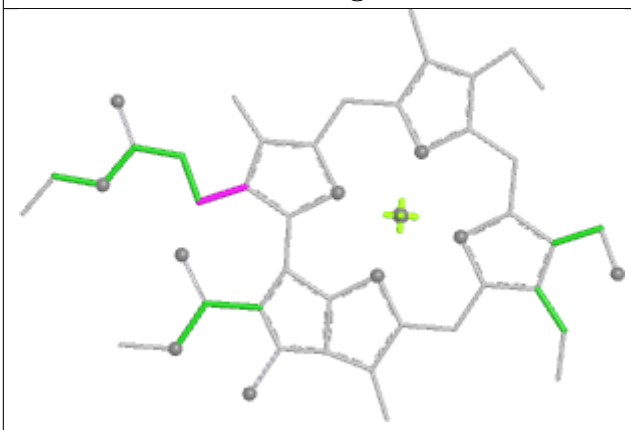
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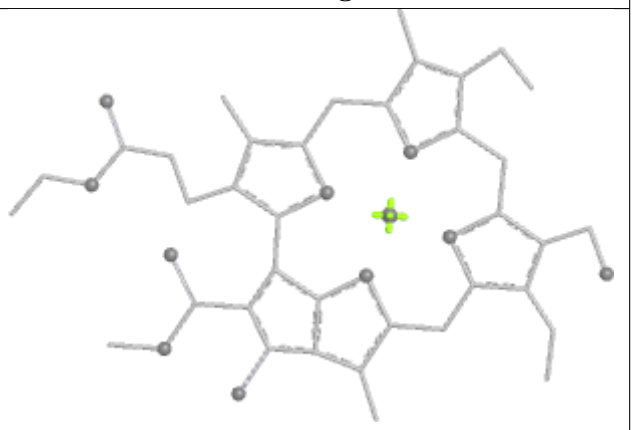
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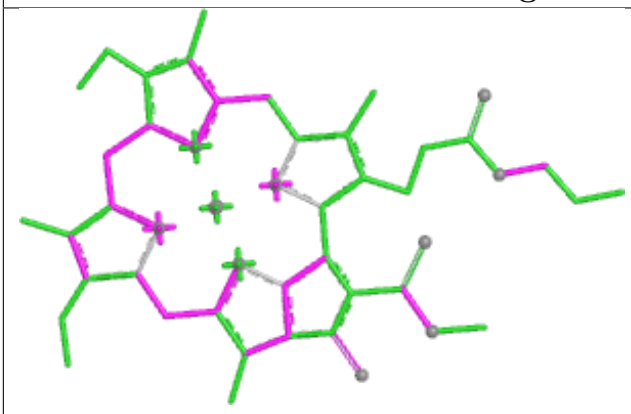


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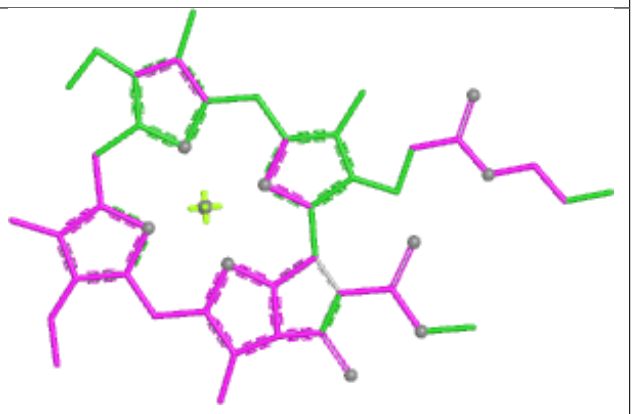


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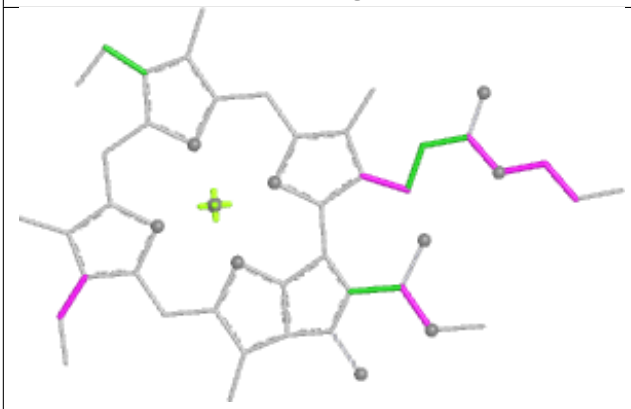
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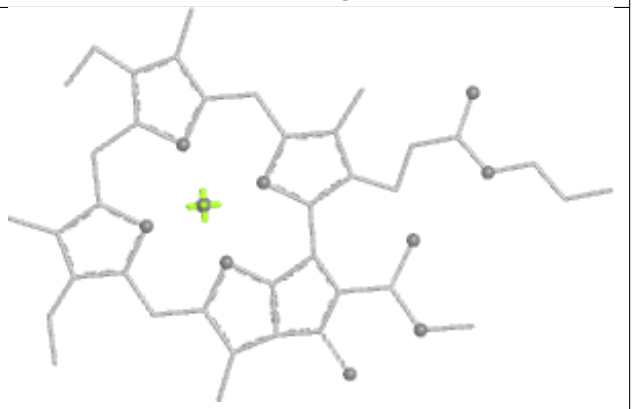
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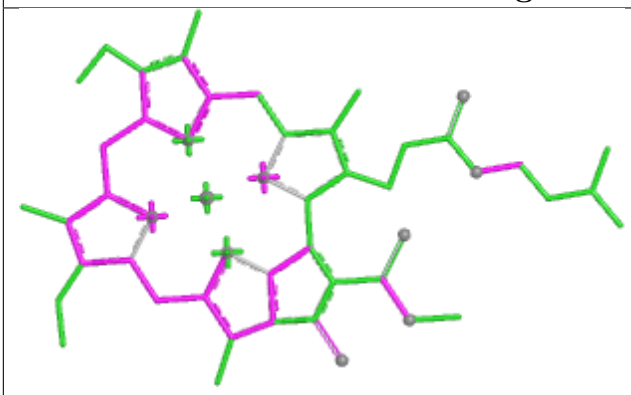


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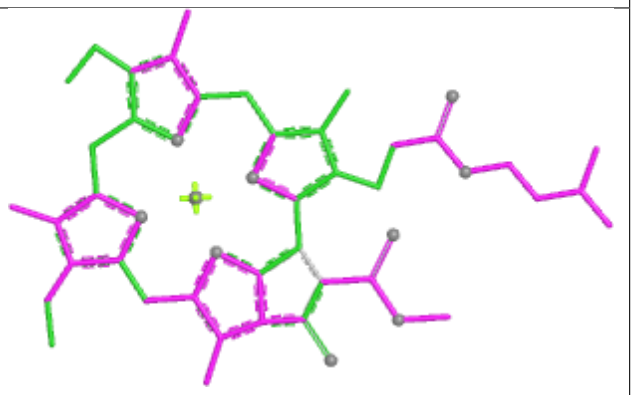


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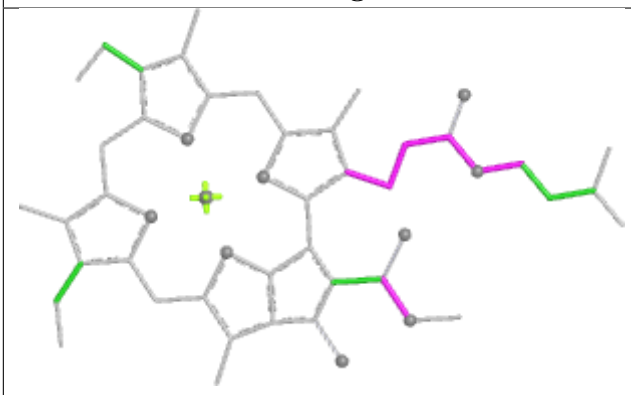
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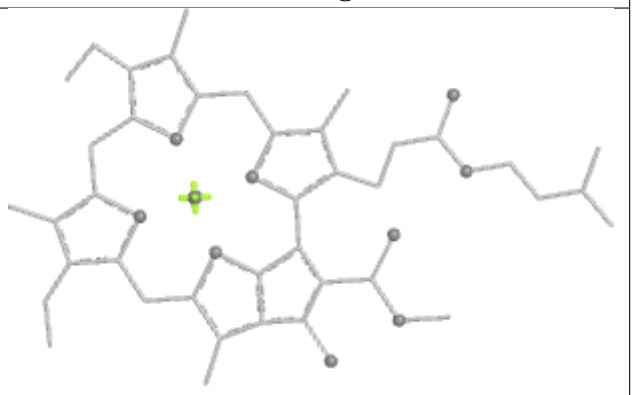
Bond lengths



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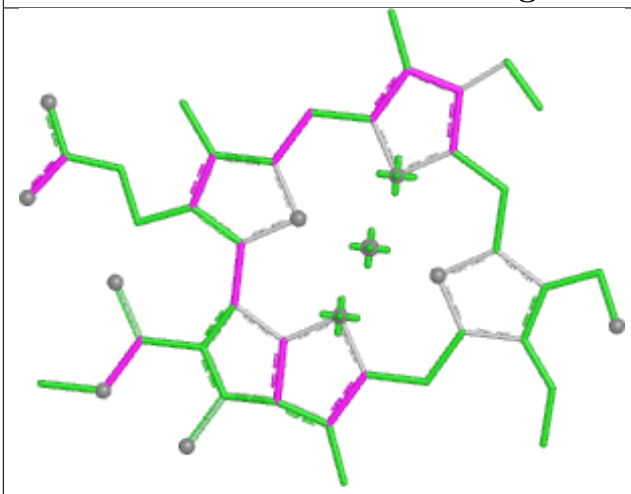


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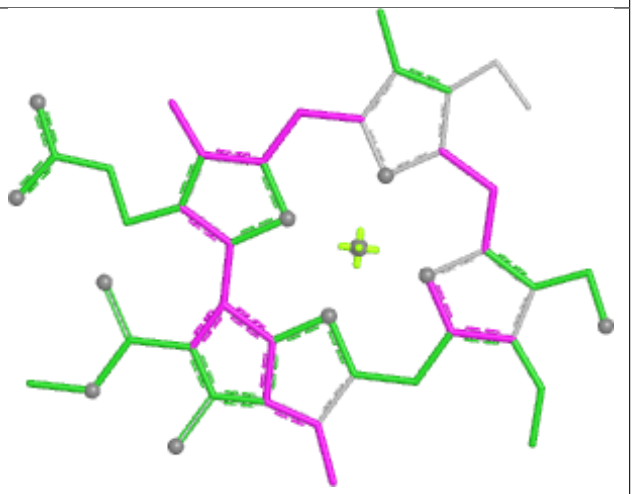


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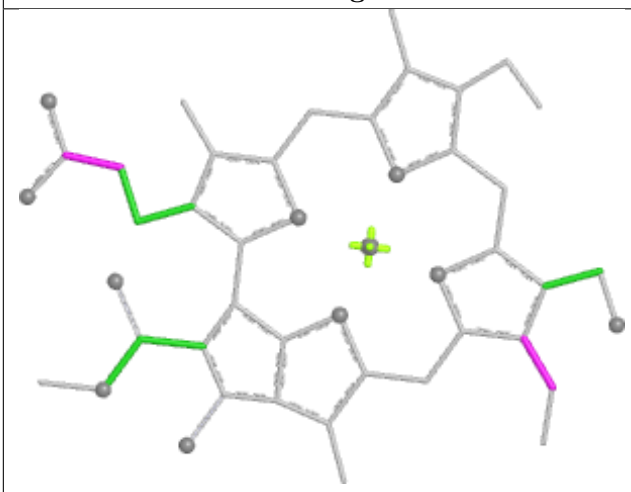
Ligand CHL 2 2013



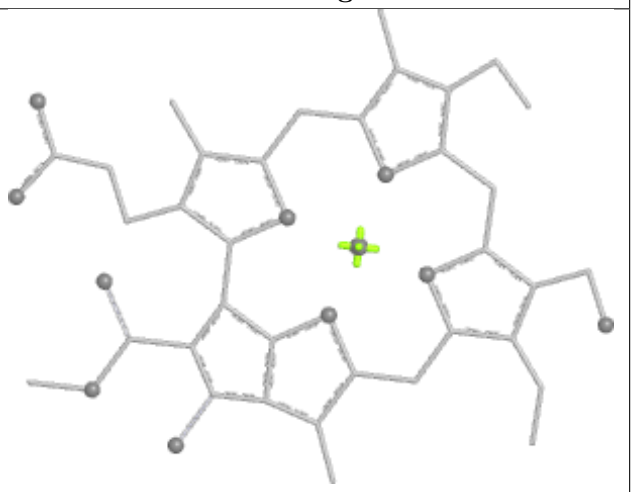
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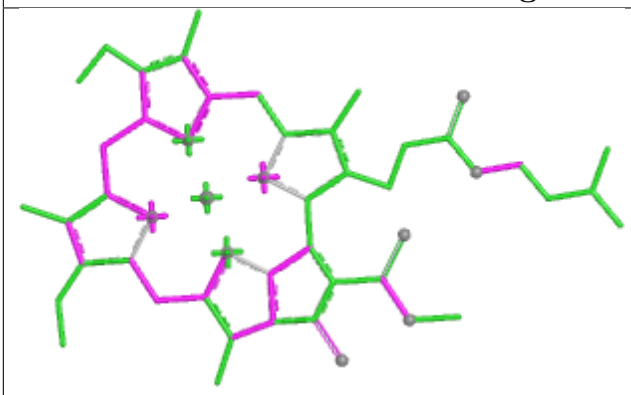


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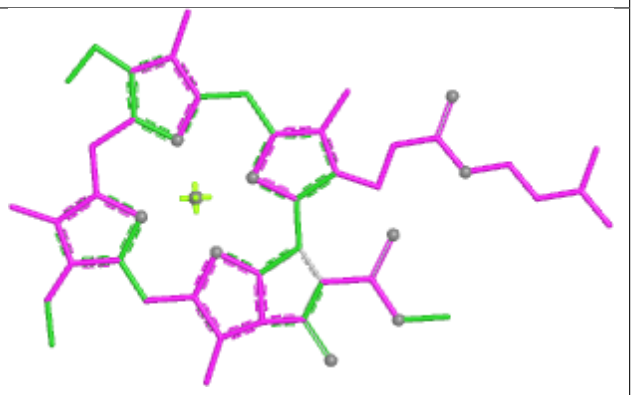


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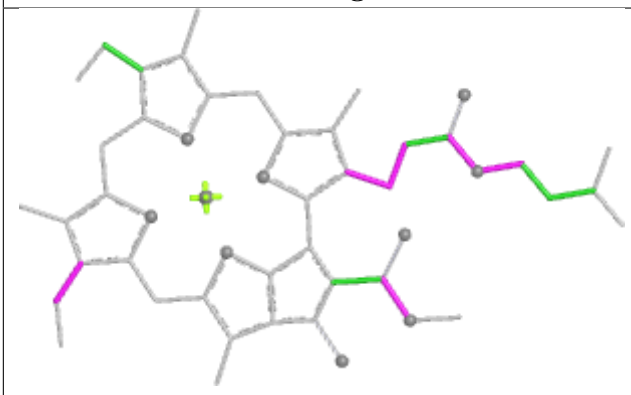
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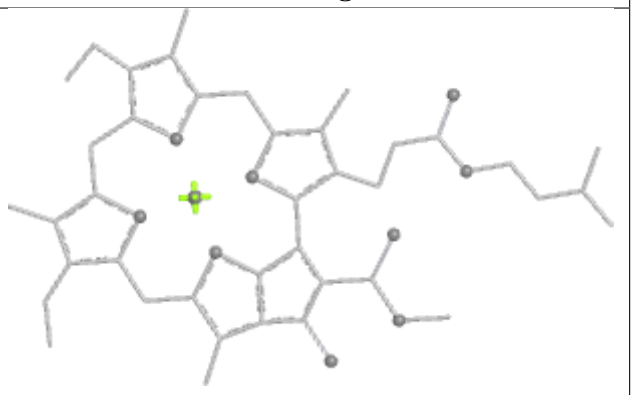
Bond lengths



Bond angles

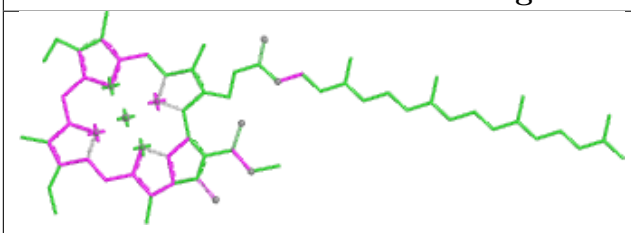


Torsions

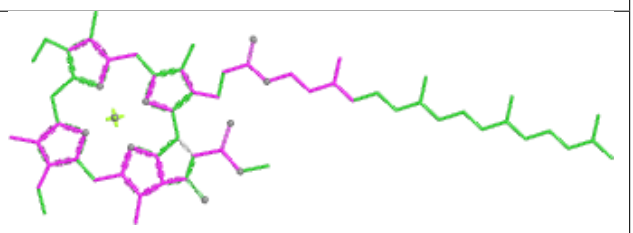


Rings

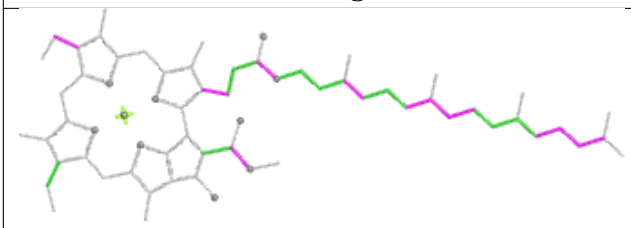
Ligand CLA B 1216



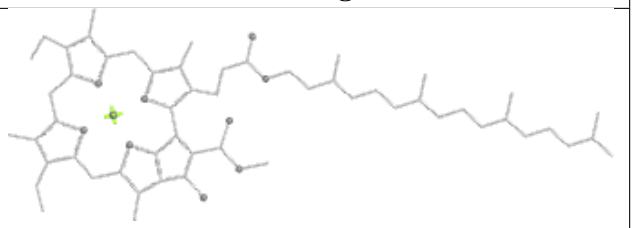
Bond lengths



Bond angles

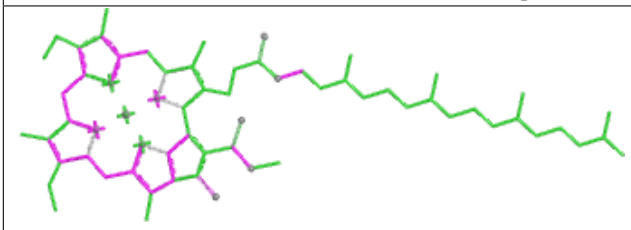


Torsions

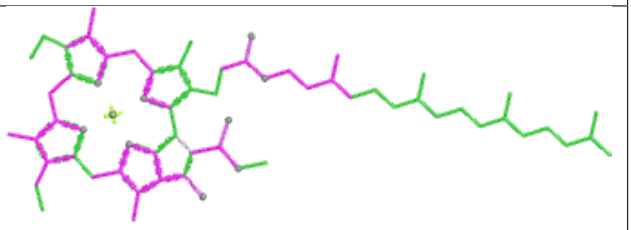


Rings

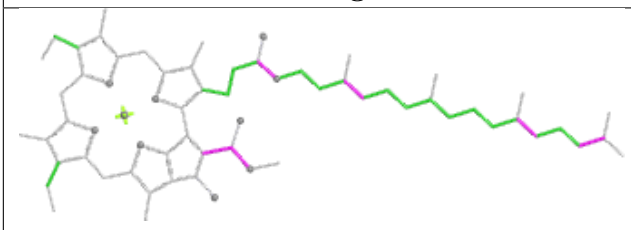
Ligand CLA B 1211



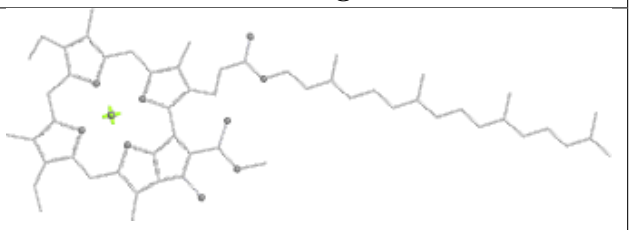
Bond lengths



Bond angles

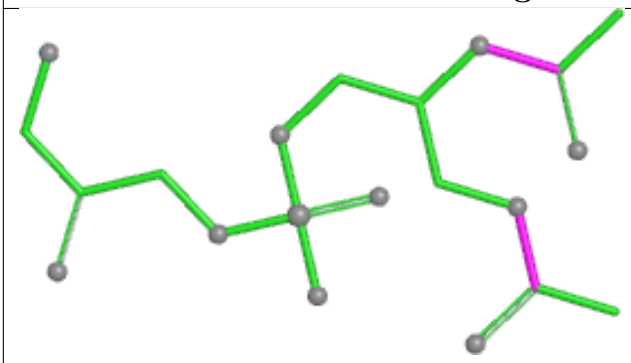


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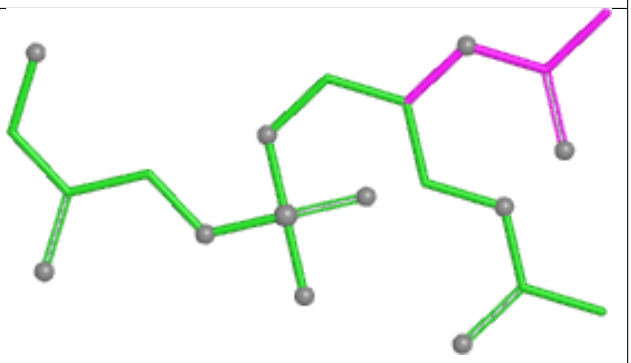


Rings

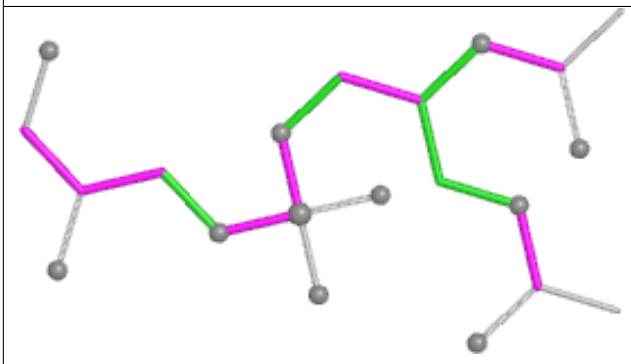
Ligand LHG B 5004



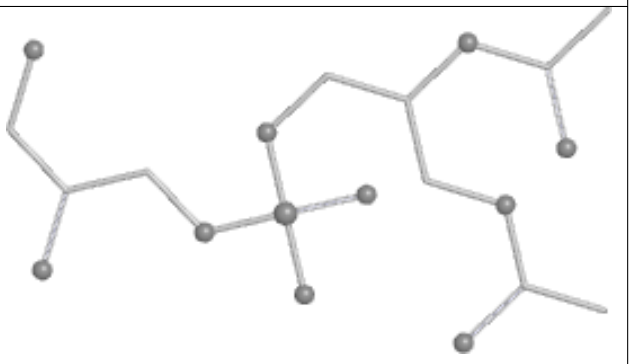
Bond lengths



Bond angles

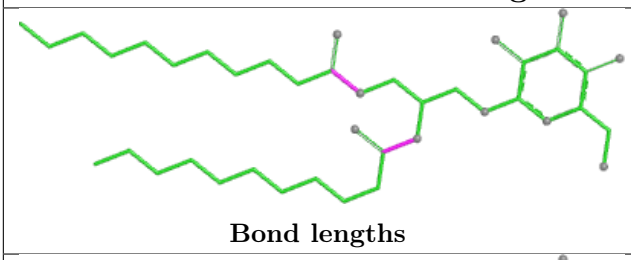


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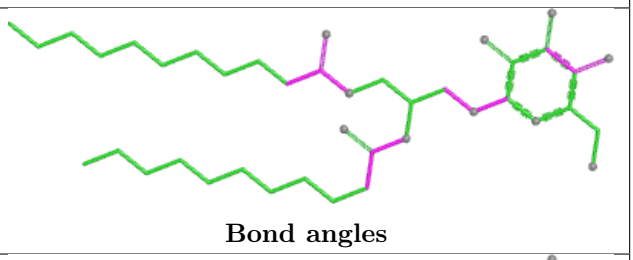


Rings

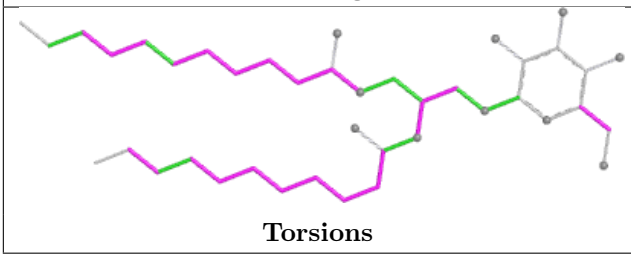
Ligand LMG G 2021



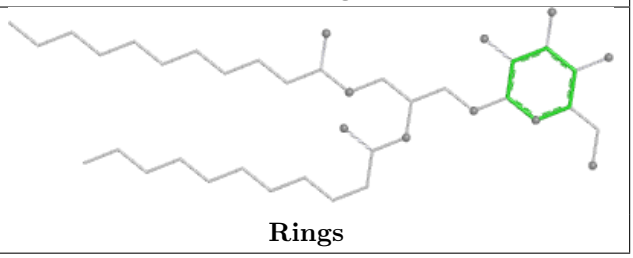
Bond lengths



Bond angles

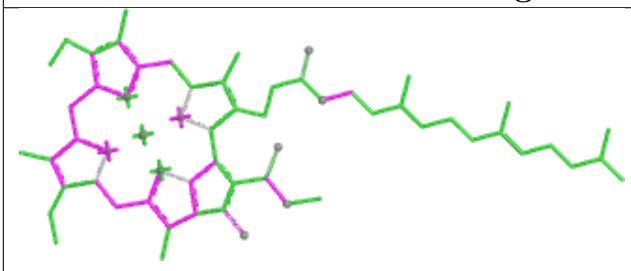


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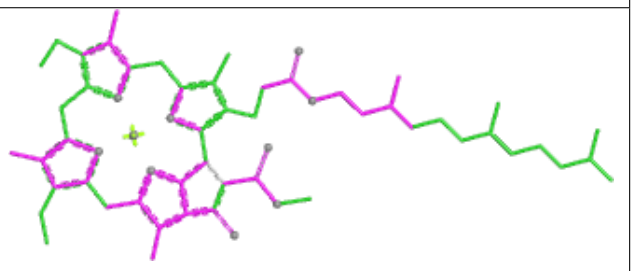


Rings

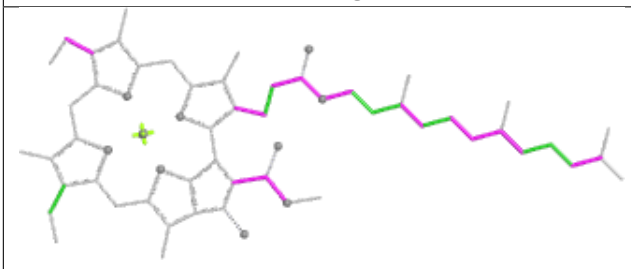
Ligand CLA A 1125



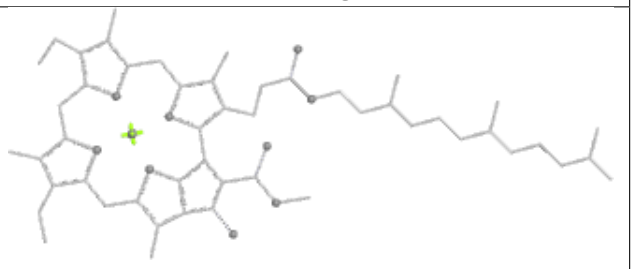
Bond lengths



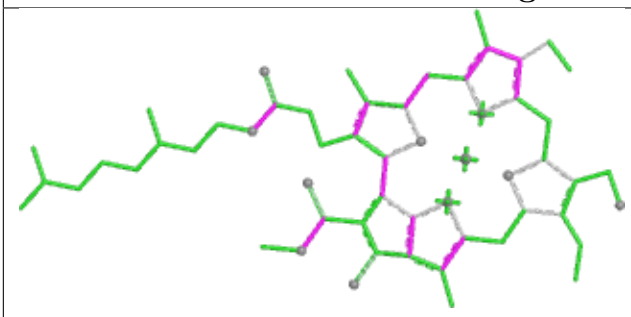
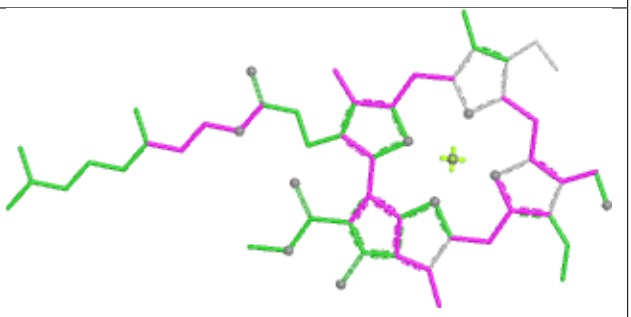
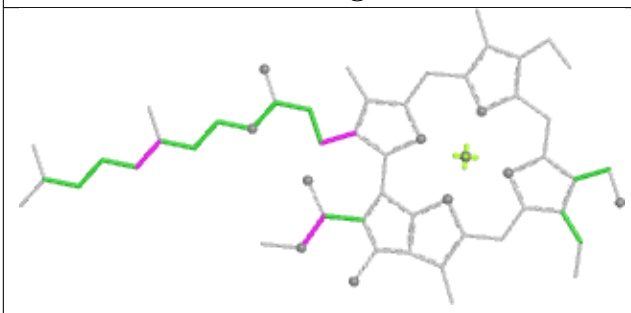
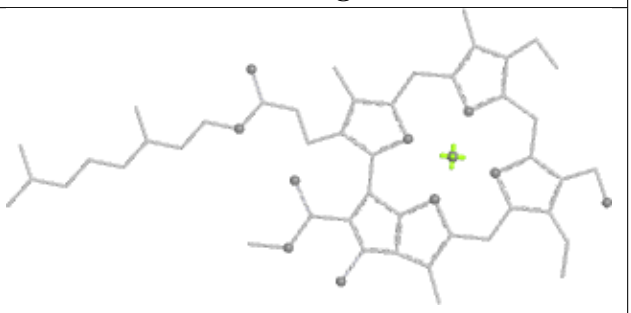
Bond angles

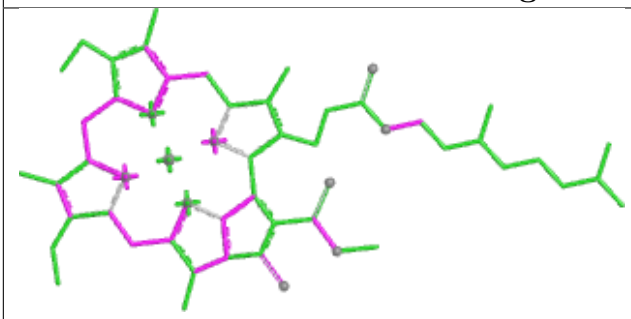
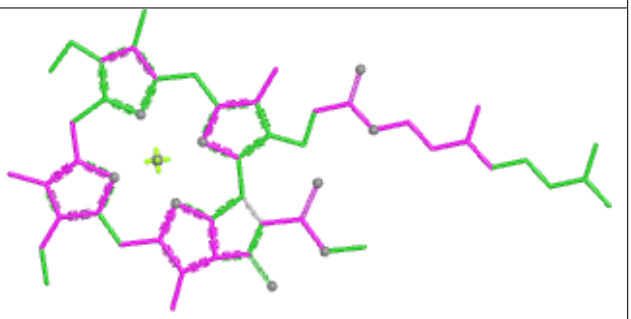
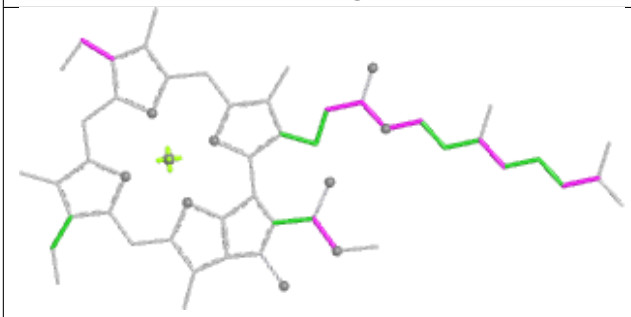
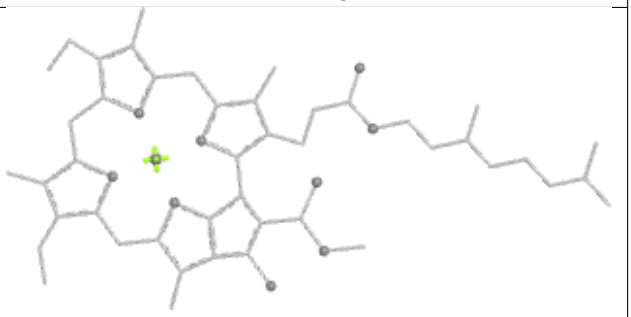


Torsions

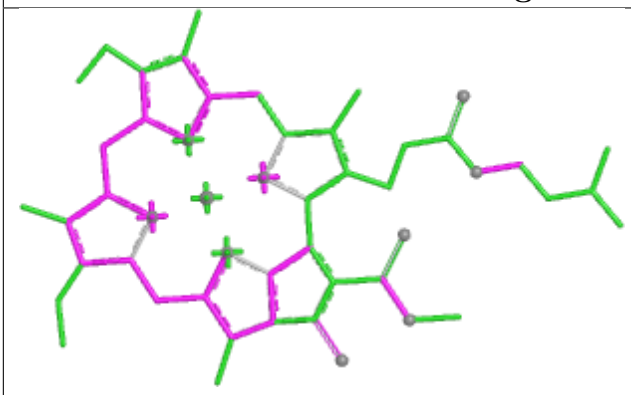


Rings

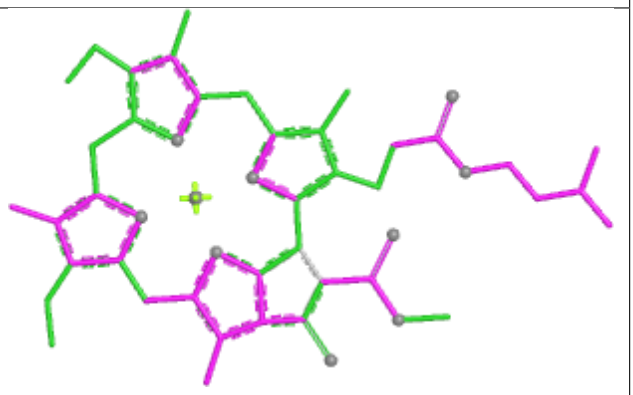
Ligand CHL 1 1009	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 2003	
 Bond lengths	 Bond angles
 Torsions	 Rings

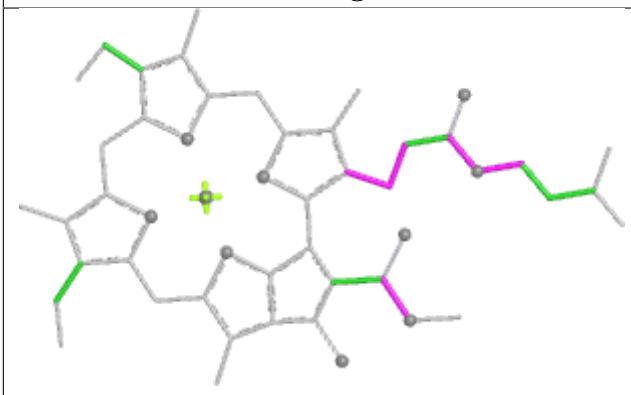
Ligand CLA A 1130



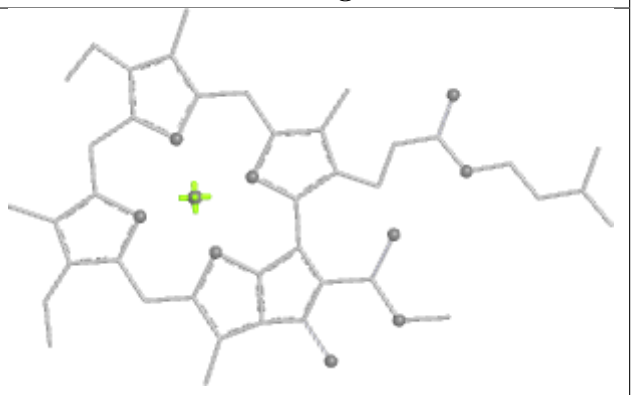
Bond lengths



Bond angles

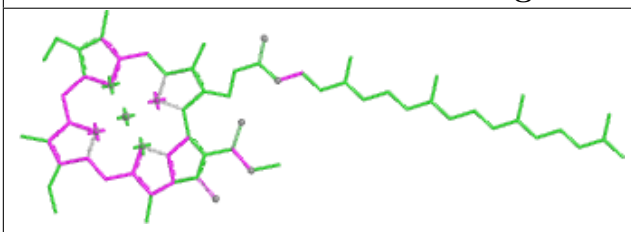


Torsions

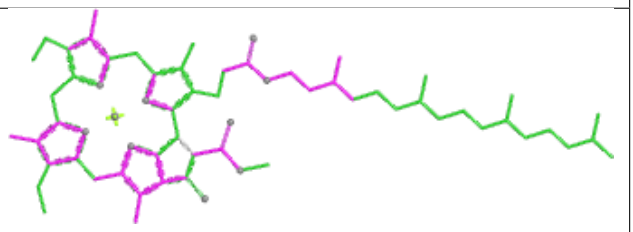


Rings

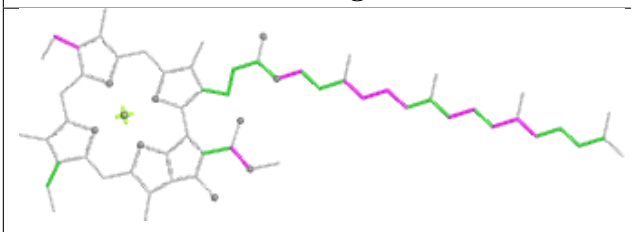
Ligand CLA A 1131



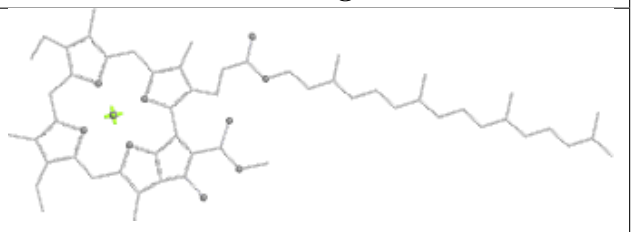
Bond lengths



Bond angles

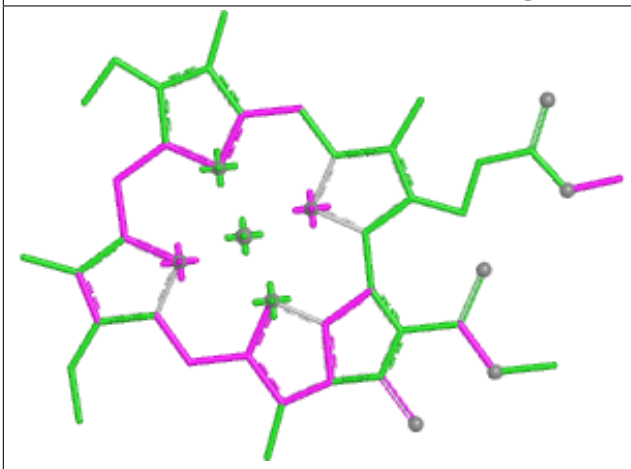


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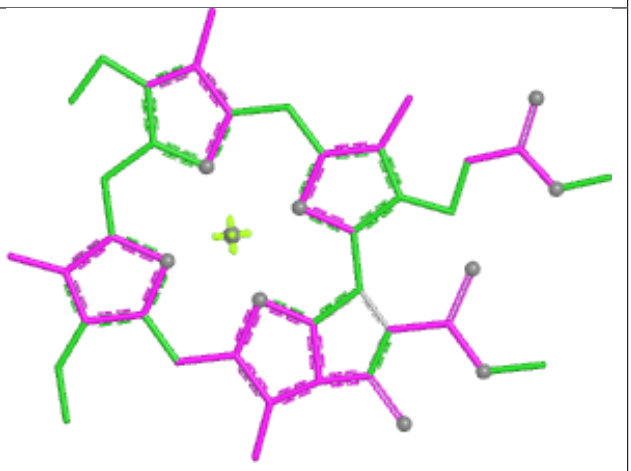


Rings

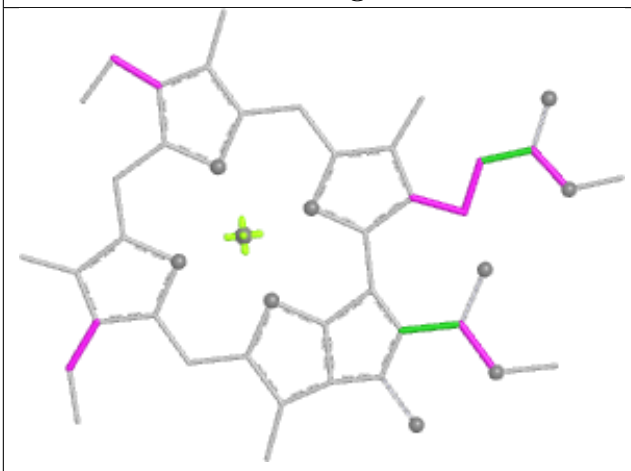
Ligand CLA 3 3013



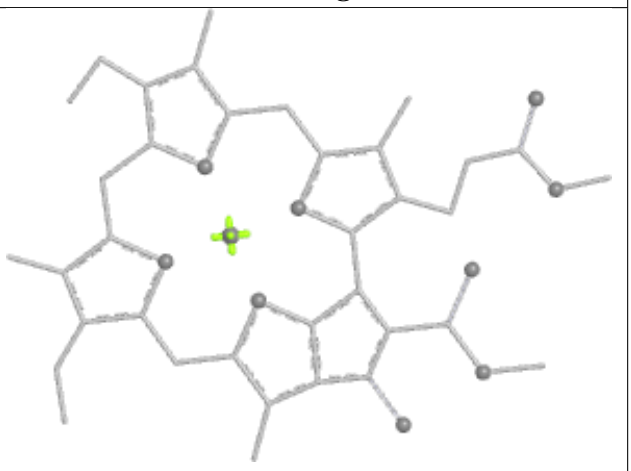
Bond lengths



Bond angles

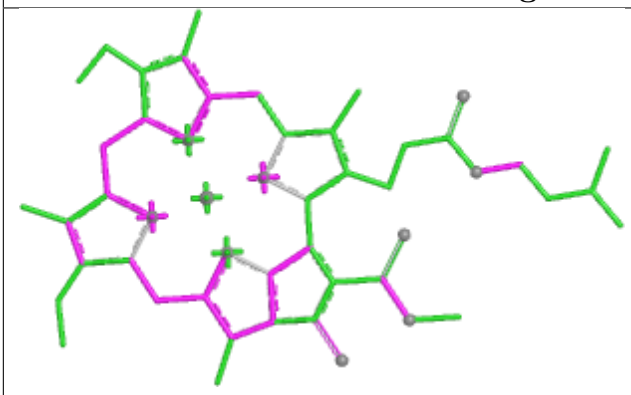


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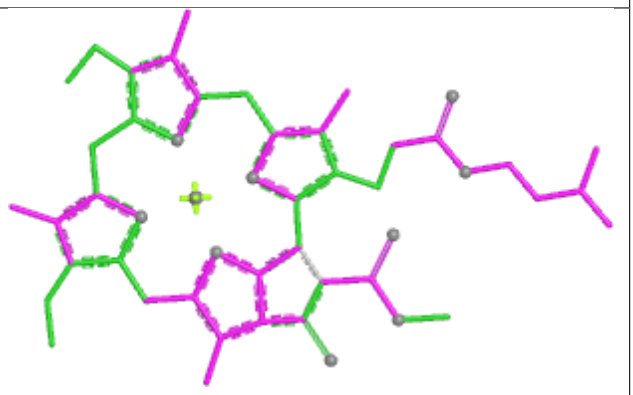


Rings

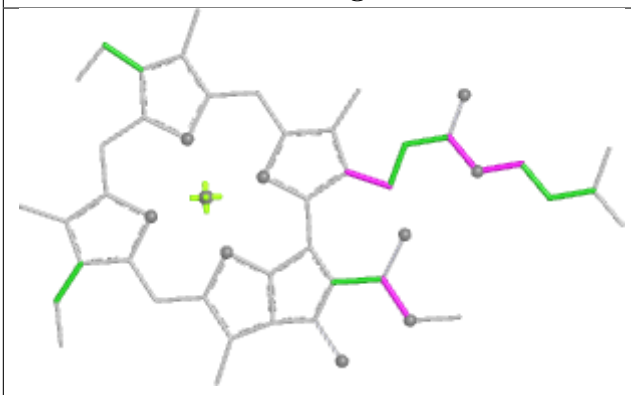
Ligand CLA 2 2009



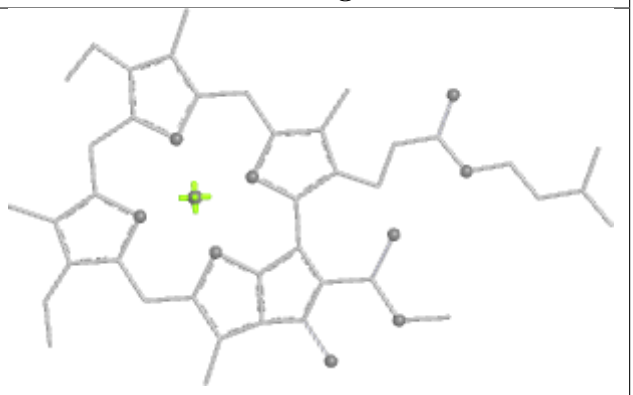
Bond lengths



Bond angles

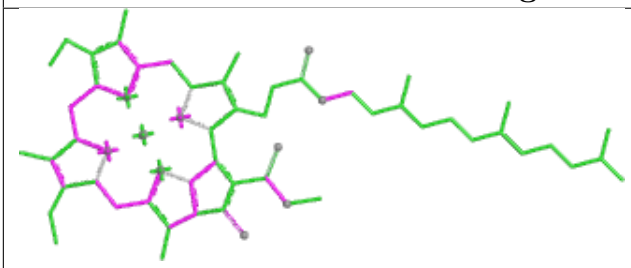


Torsions

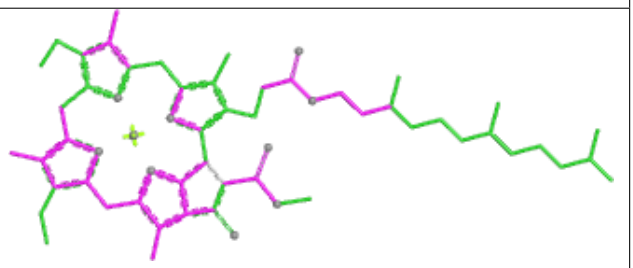


Rings

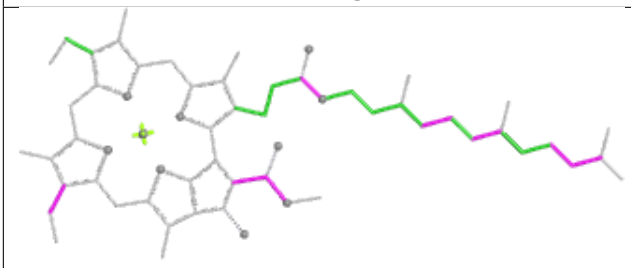
Ligand CLA 4 4007



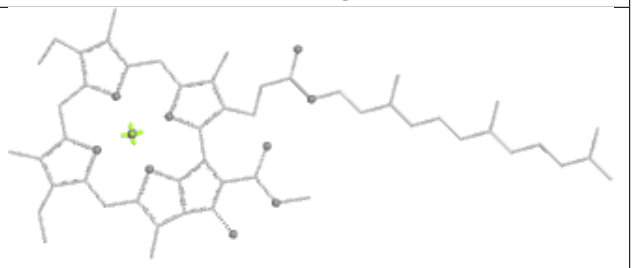
Bond lengths



Bond angles

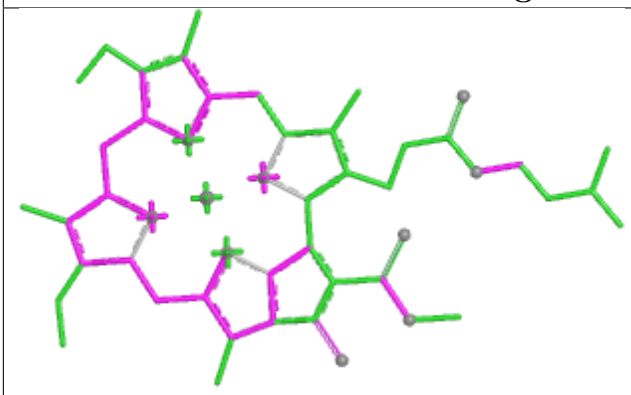


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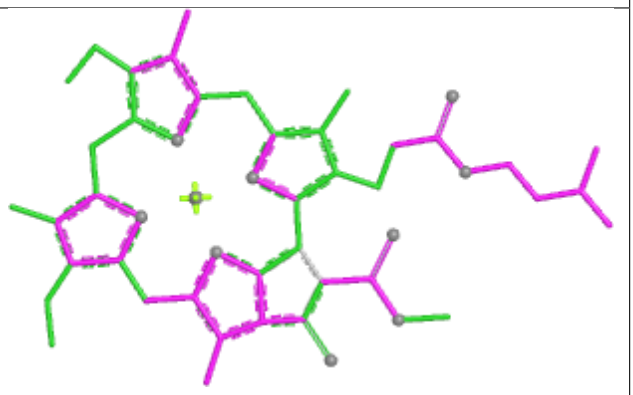


Rings

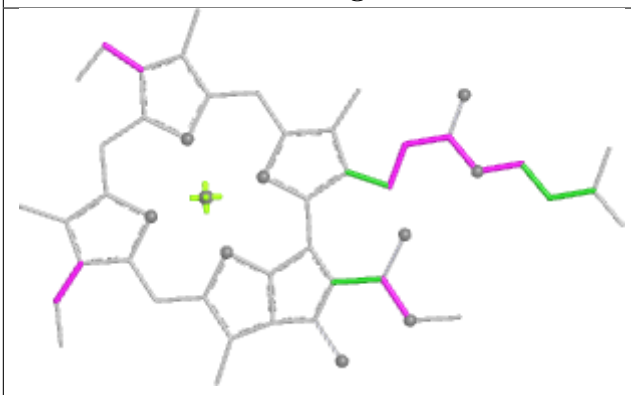
Ligand CLA A 1151



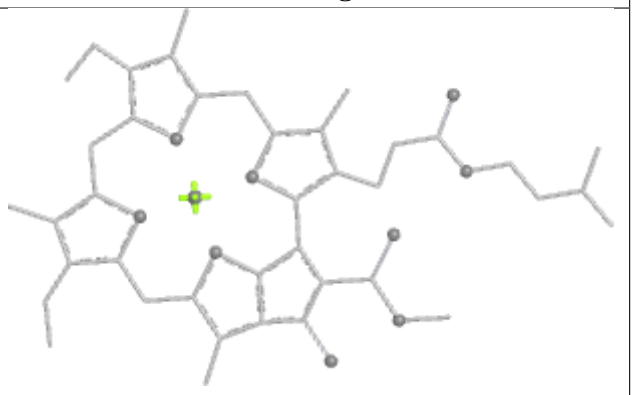
Bond lengths



Bond angles

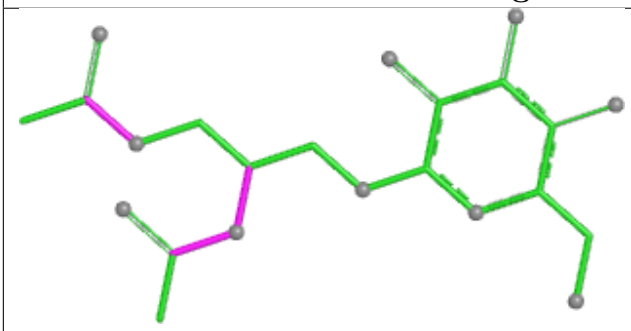


Torsions

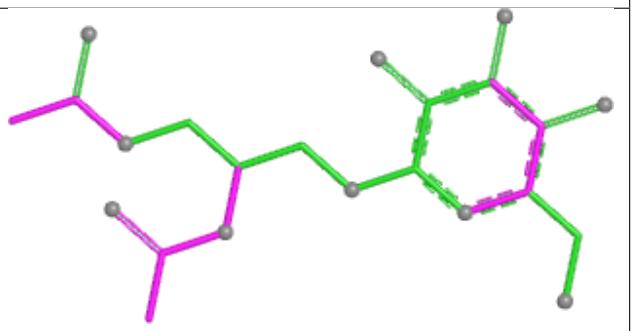


Rings

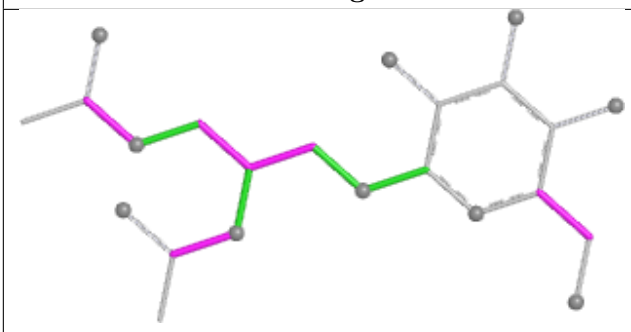
Ligand LMG F 5001



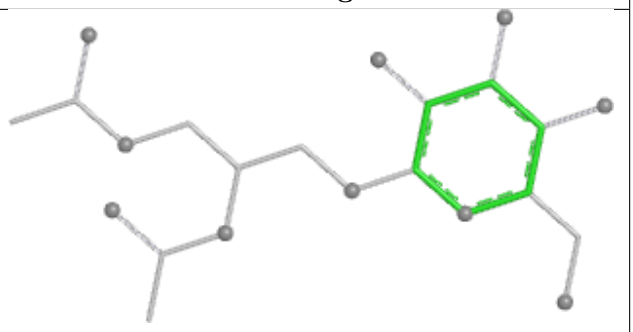
Bond lengths



Bond angles

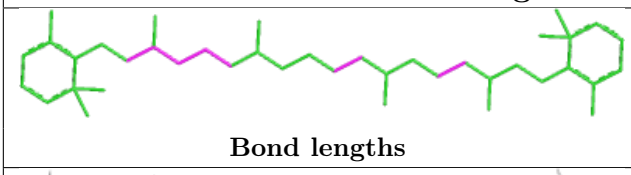


Torsions

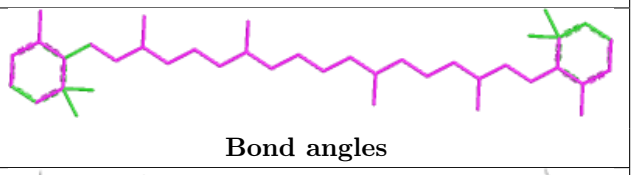


Rings

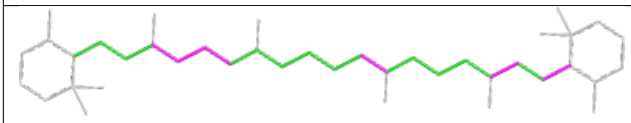
Ligand BCR A 6017



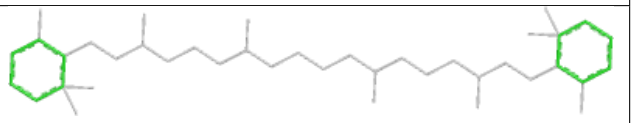
Bond lengths



Bond angles

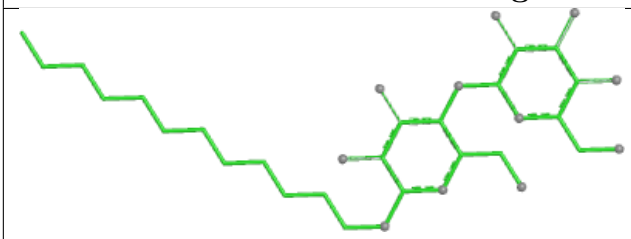


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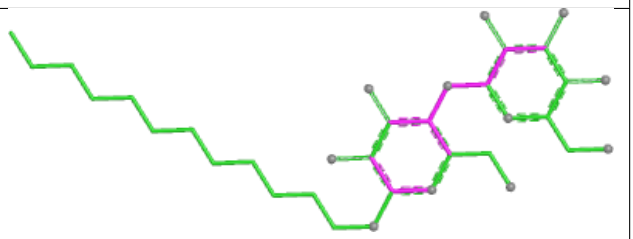


Rings

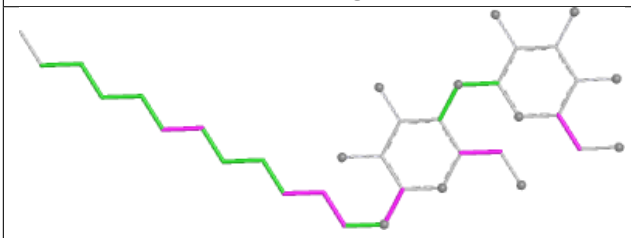
Ligand LMU B 8001



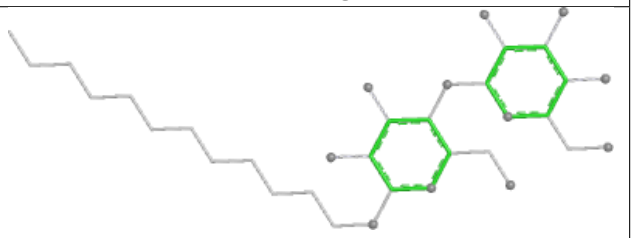
Bond lengths



Bond angles

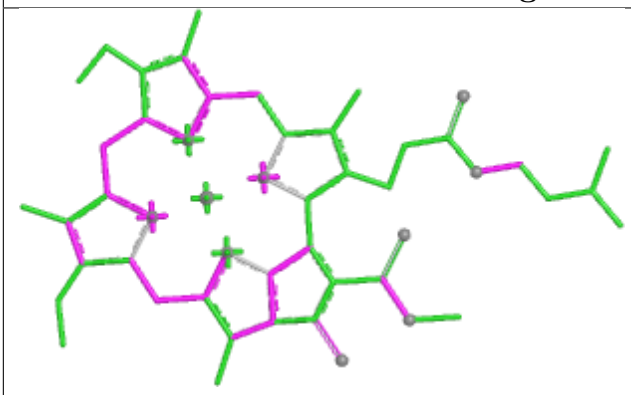


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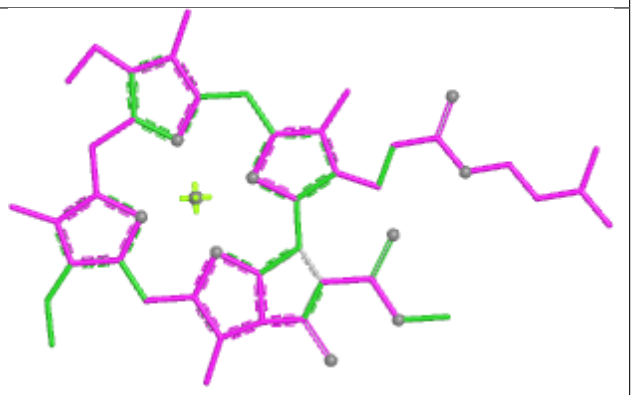


Rings

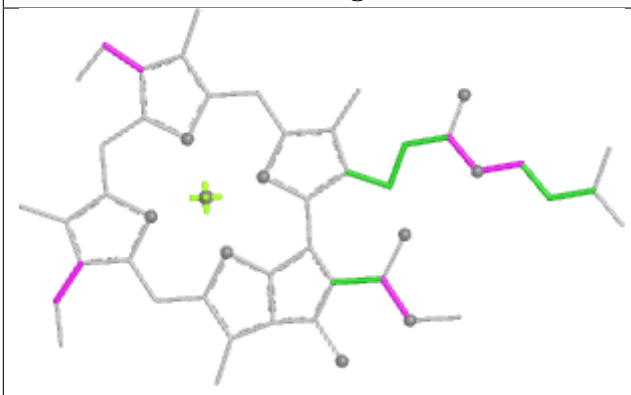
Ligand CLA 3 3012



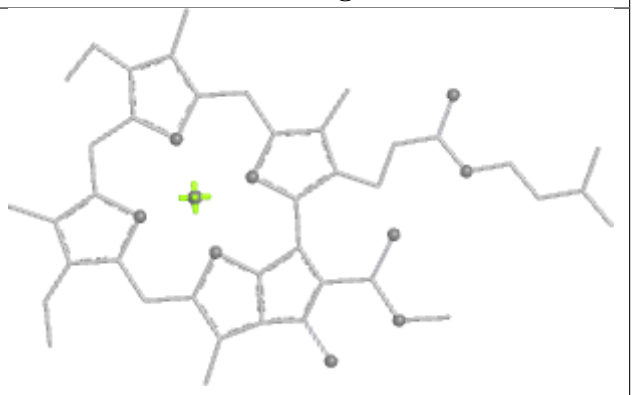
Bond lengths



Bond angles

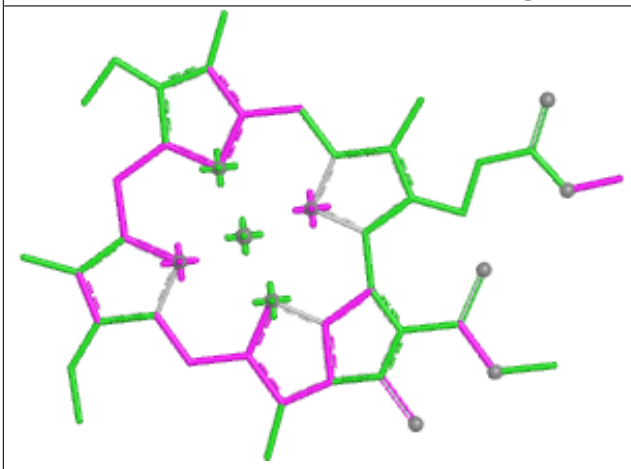


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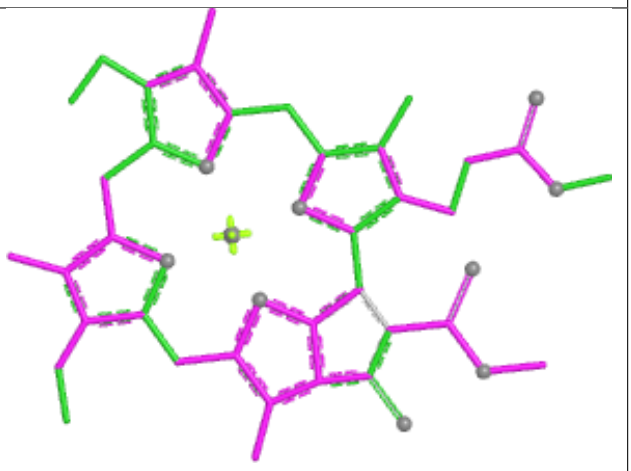


Rings

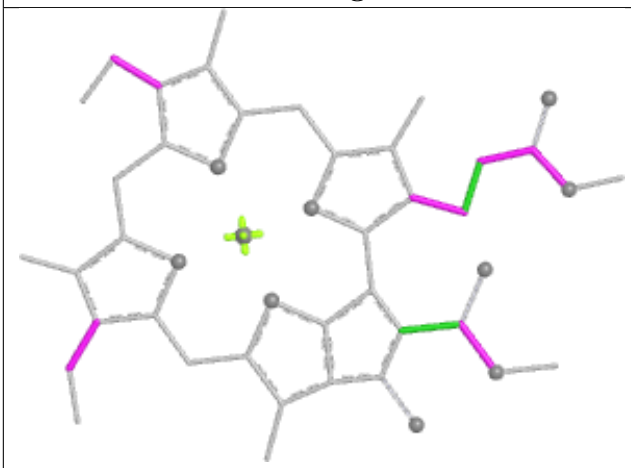
Ligand CLA 4 4016



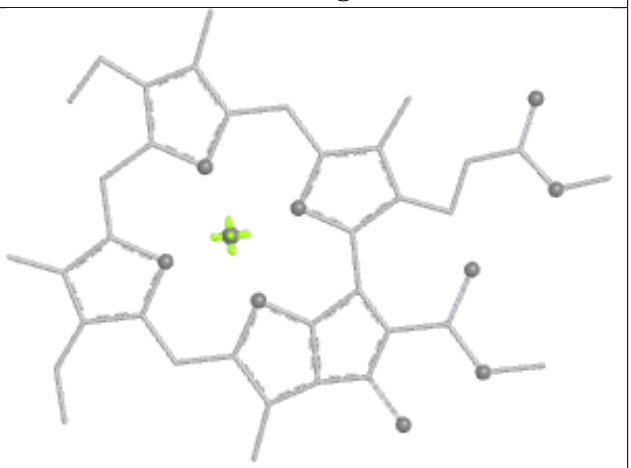
Bond lengths



Bond angles

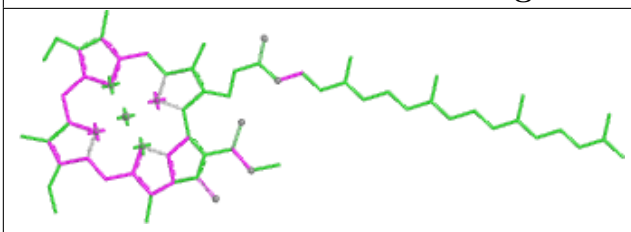


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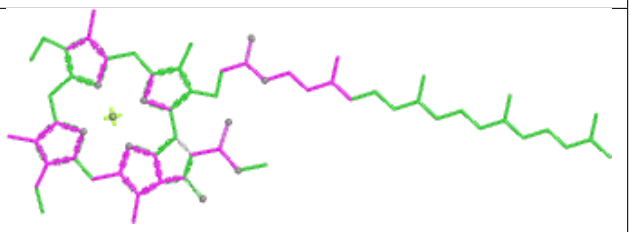


Rings

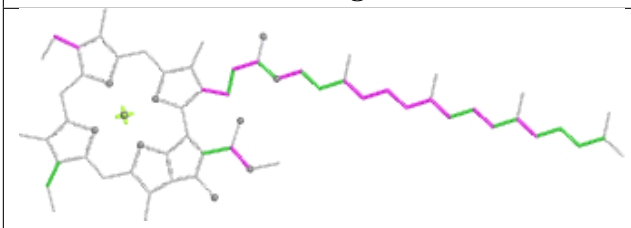
Ligand CLA A 1140



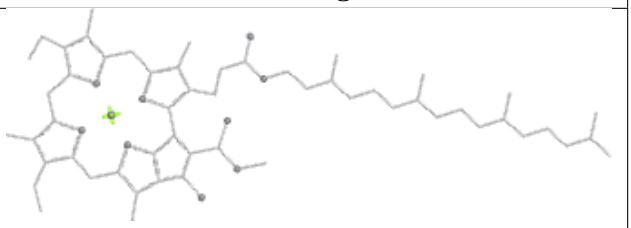
Bond lengths



Bond angles

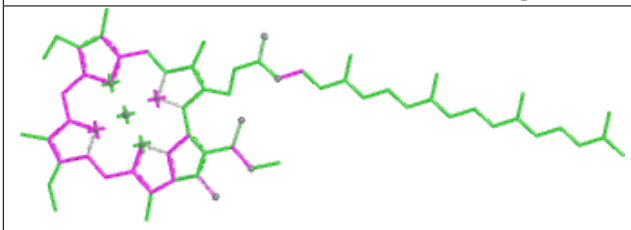


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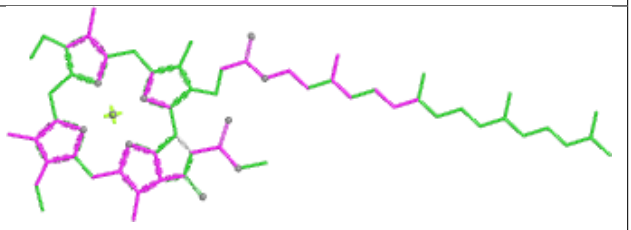


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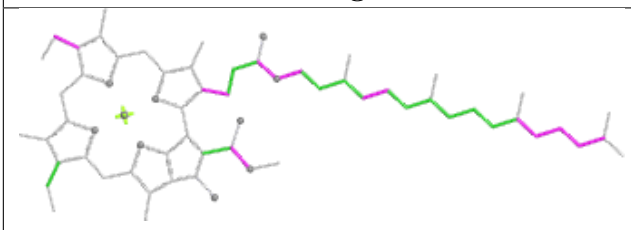
Ligand CLA B 1229



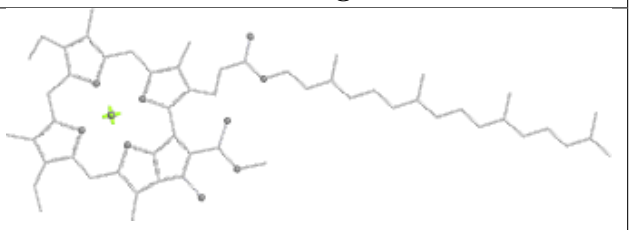
Bond lengths



Bond angles

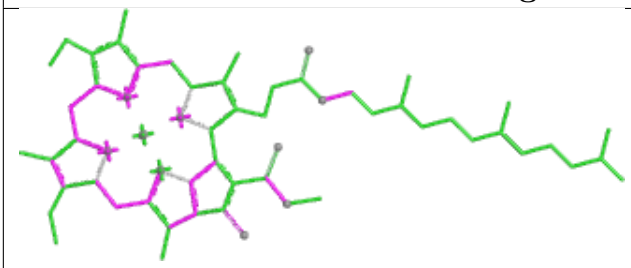


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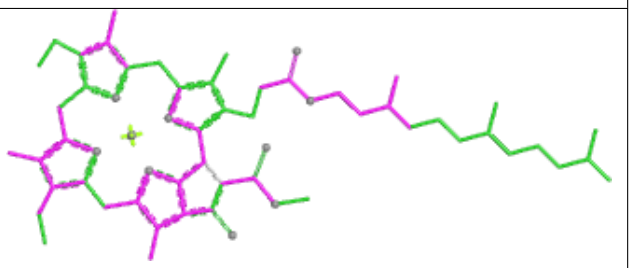


Rings

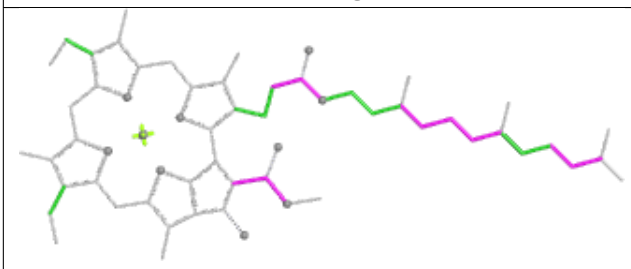
Ligand CLA 3 3010



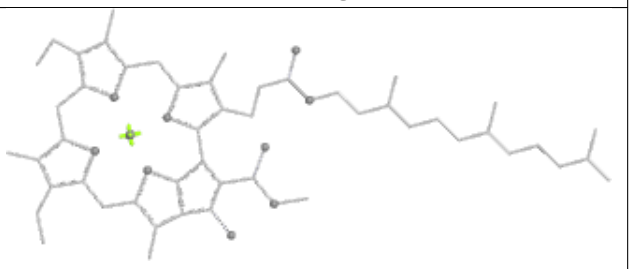
Bond lengths



Bond angles

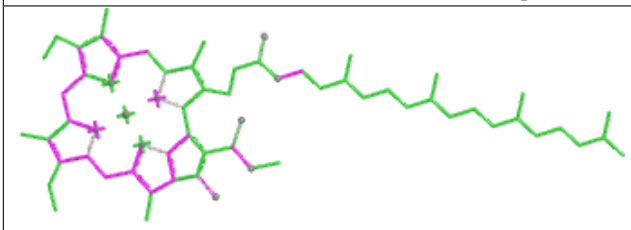


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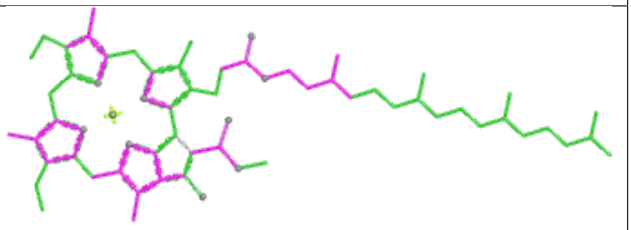


Rings

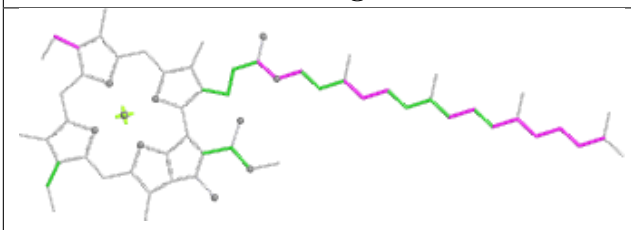
Ligand CLA B 1218



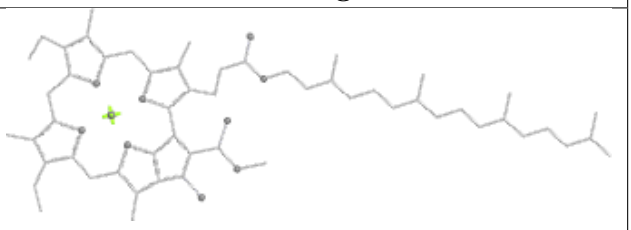
Bond lengths



Bond angles

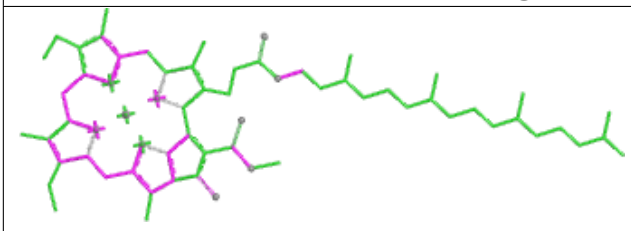


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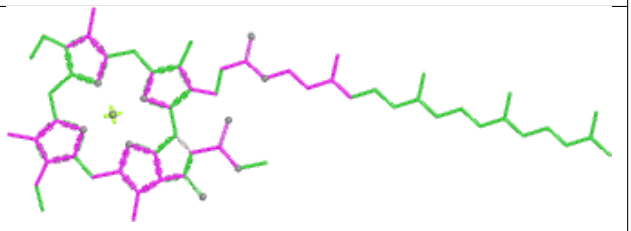


Rings

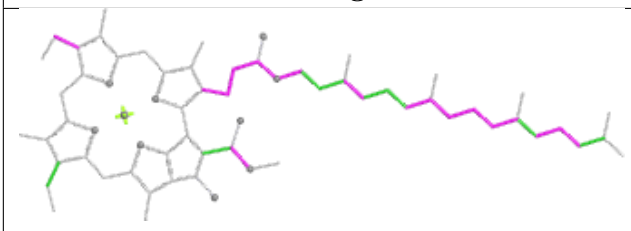
Ligand CLA B 1224



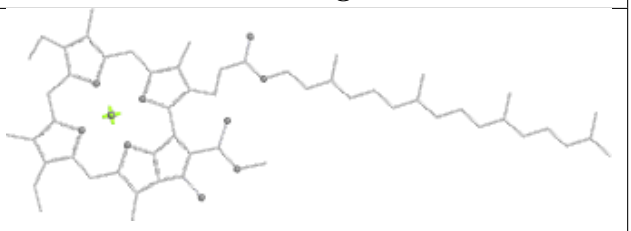
Bond lengths



Bond angles

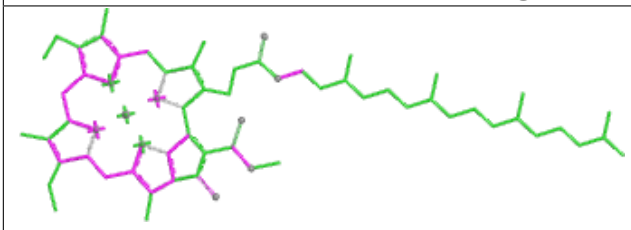


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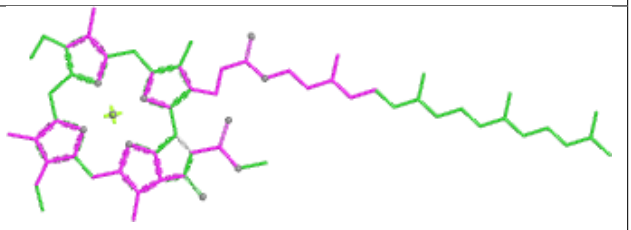


Rings

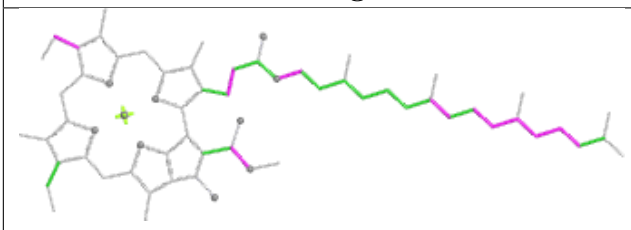
Ligand CLA A 1126



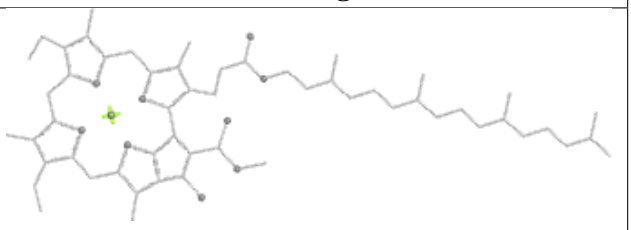
Bond lengths



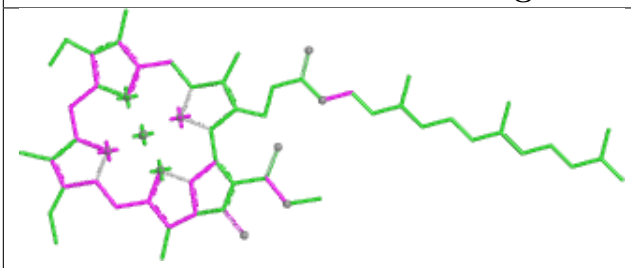
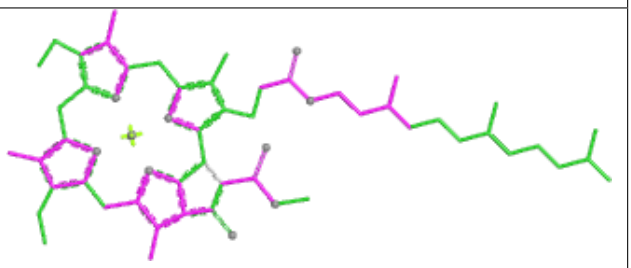
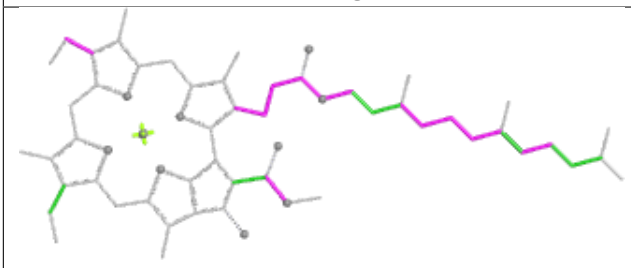
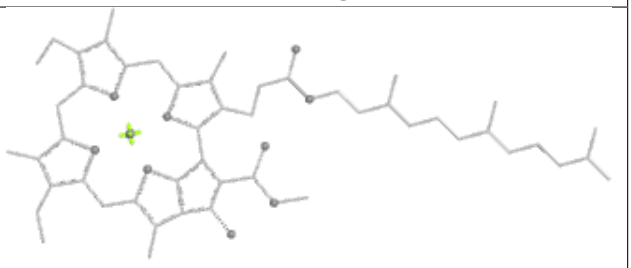
Bond angles

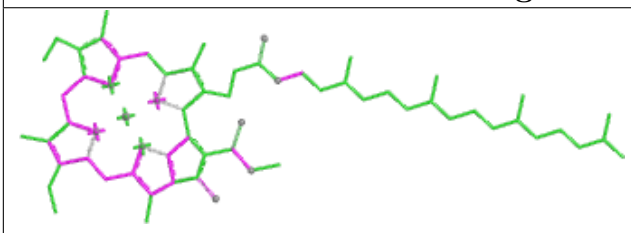
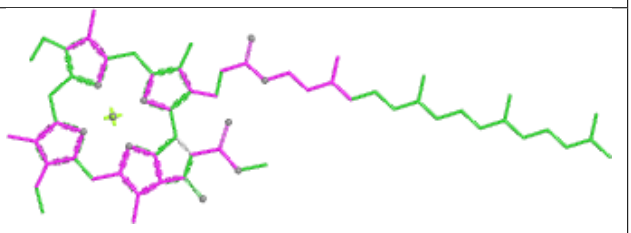
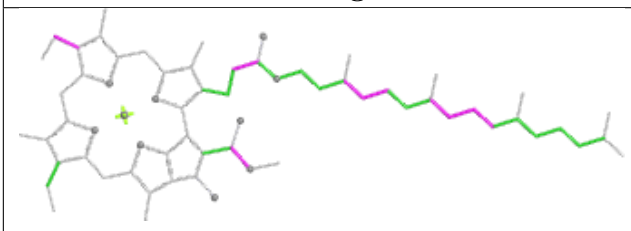
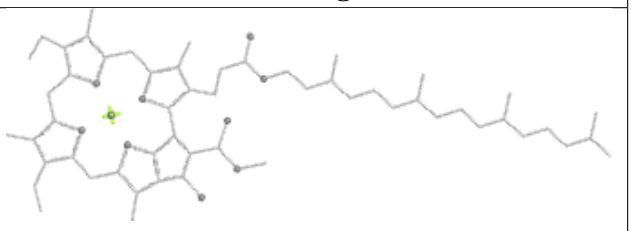


Torsions

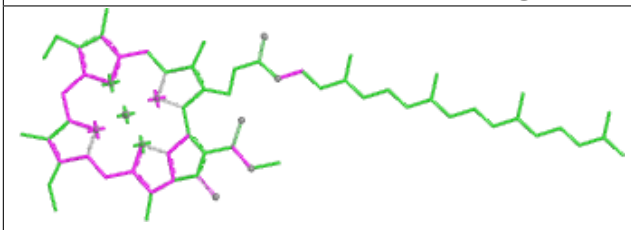


Rings

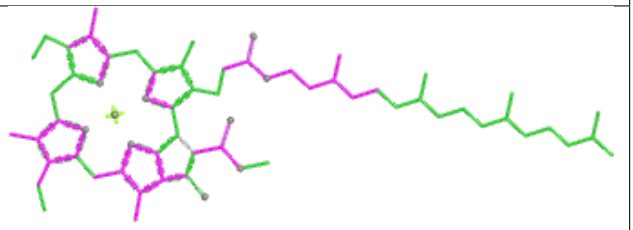
Ligand CLA A 1116	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 1205	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

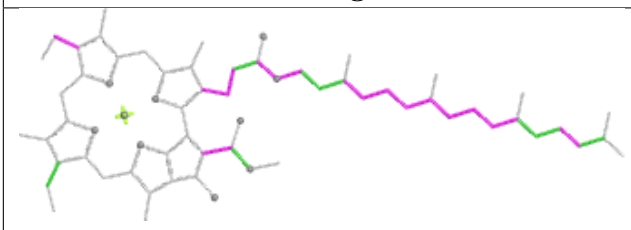
Ligand CLA B 1221



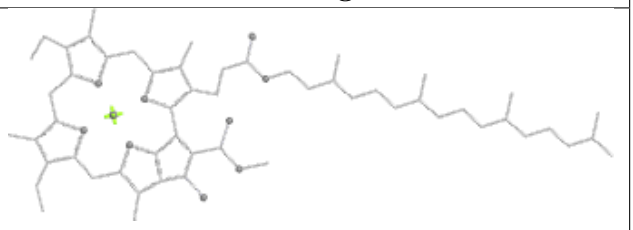
Bond lengths



Bond angles

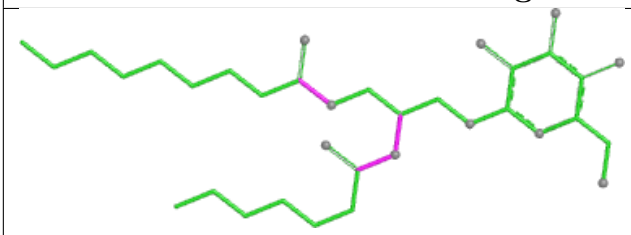


Torsions

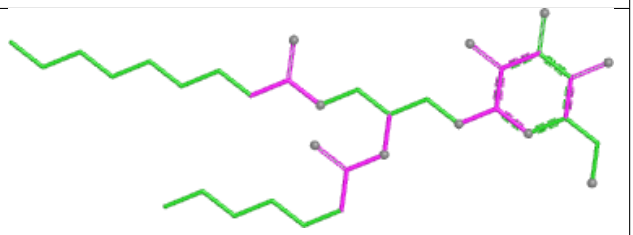


Rings

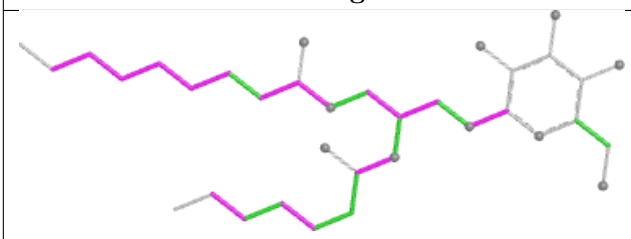
Ligand LMG 4 4801



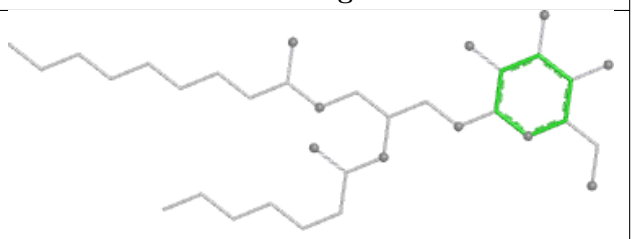
Bond lengths



Bond angles

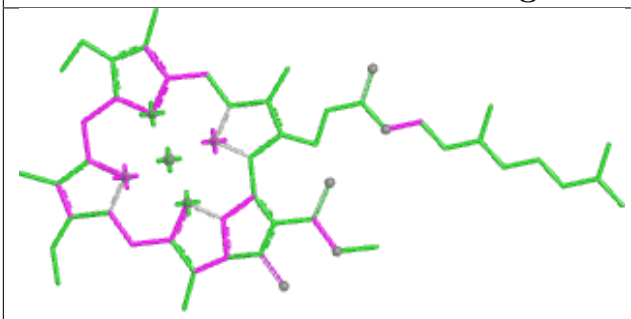


Torsions

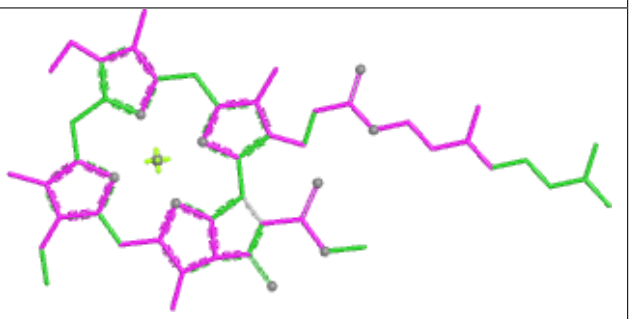


Rings

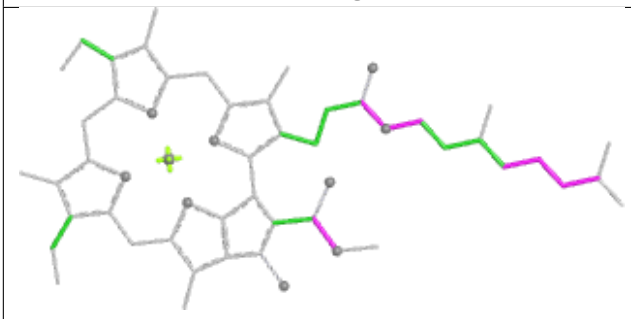
Ligand CLA 2 2012



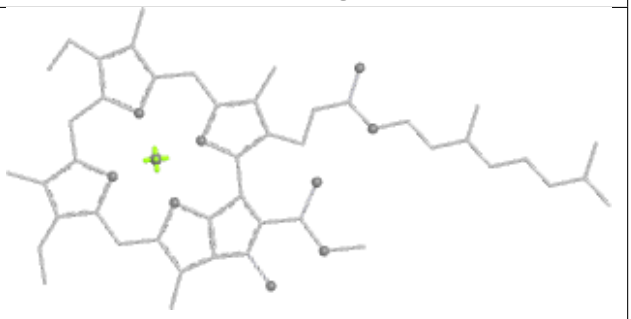
Bond lengths



Bond angles

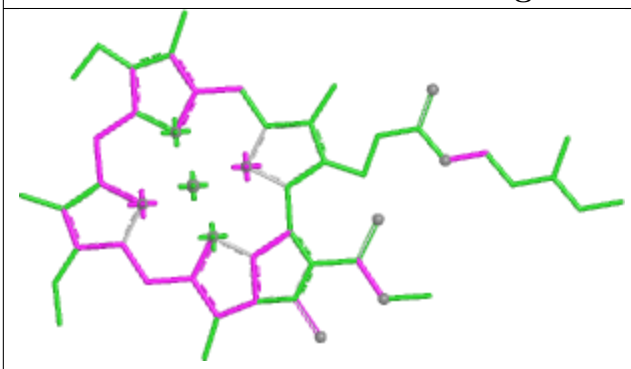


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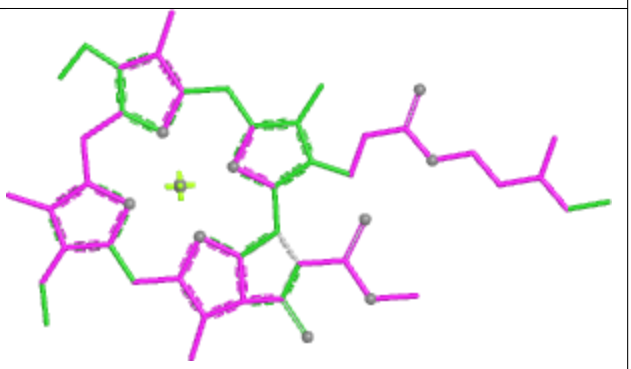


Rings

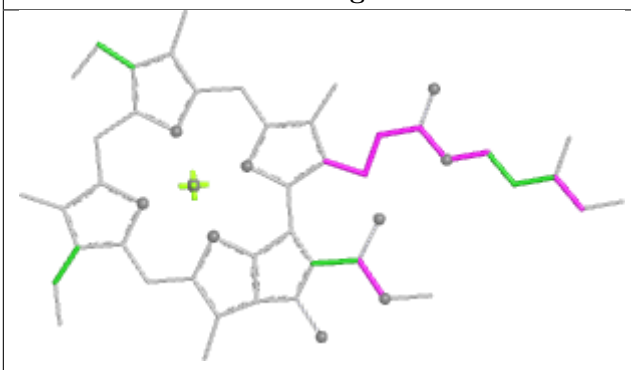
Ligand CLA A 1105



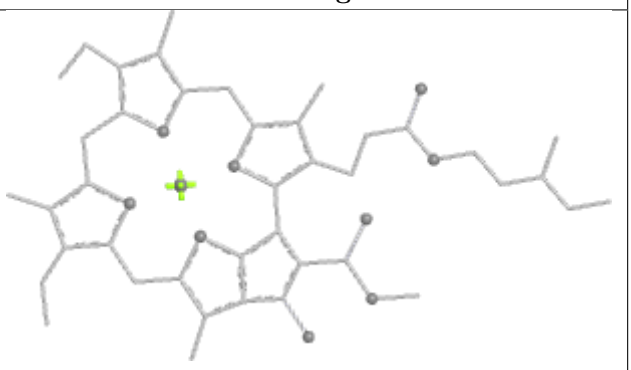
Bond lengths



Bond angles

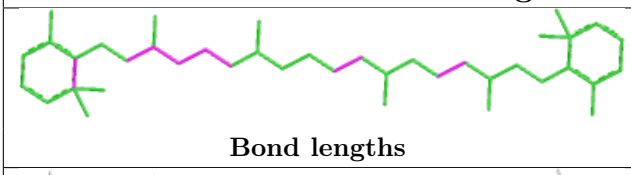


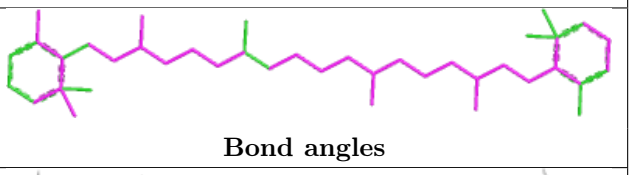
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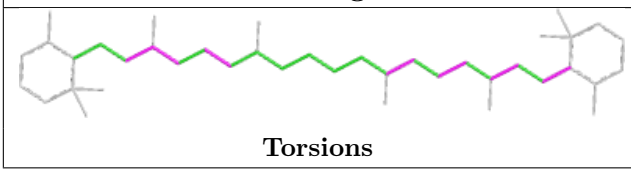


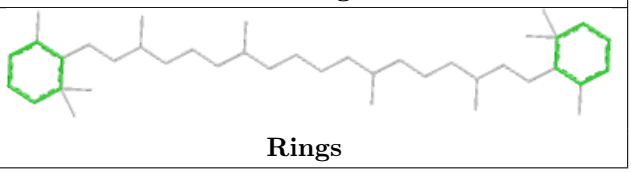
Rings

Ligand BCR F 6014

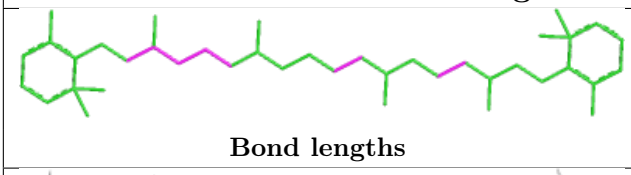

Bond lengths

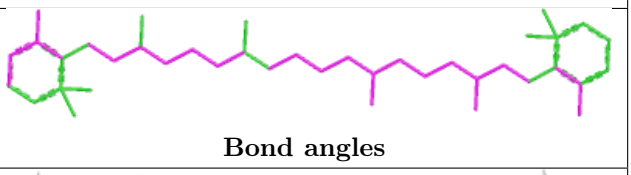

Bond angles

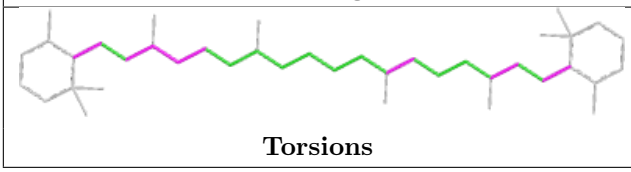

Torsions

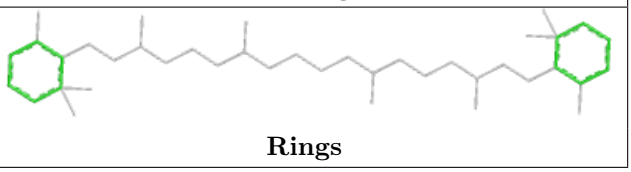

Rings

Ligand BCR A 6003

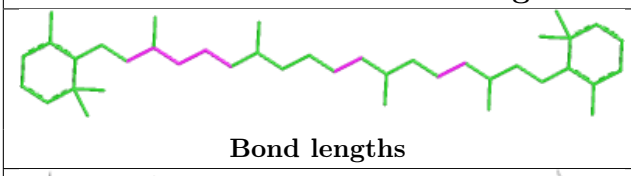

Bond lengths

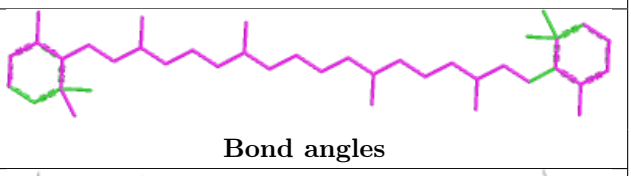

Bond angles

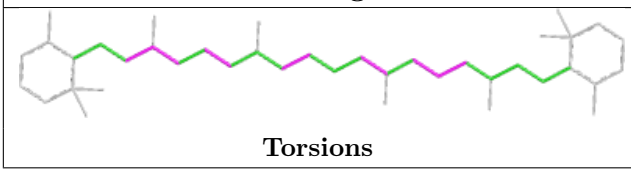

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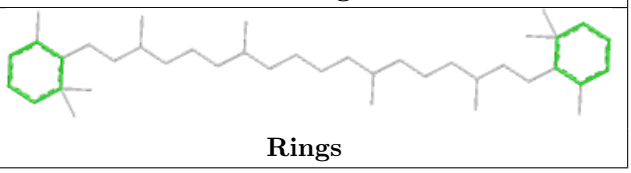

Rings

Ligand BCR K 2011

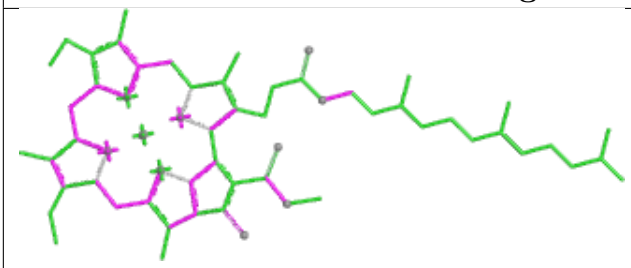

Bond lengths

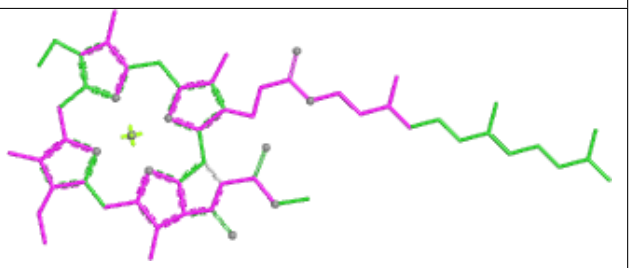

Bond angles

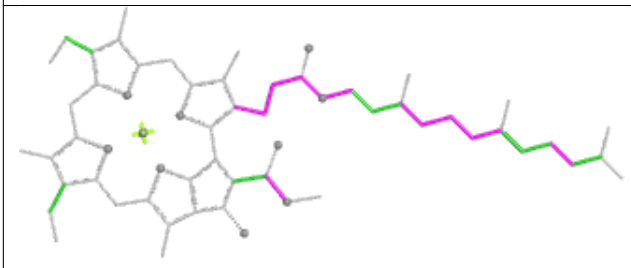

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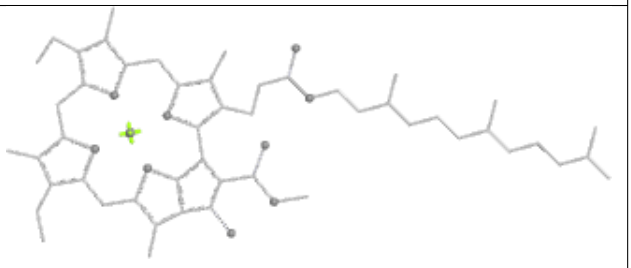

Rings

Ligand CLA 2 2001

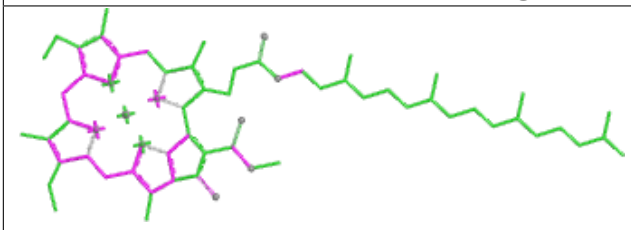

Bond lengths


Bond angles

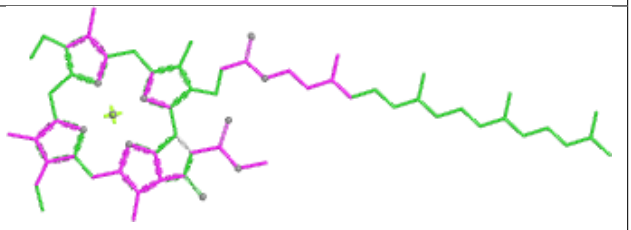

Torsions


Rings

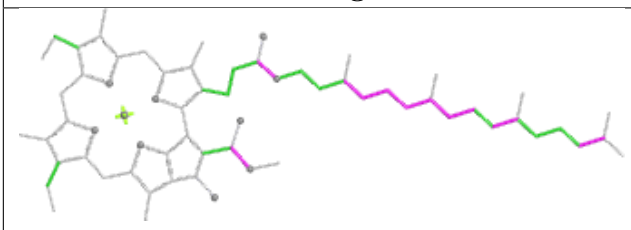
Ligand CLA A 1138



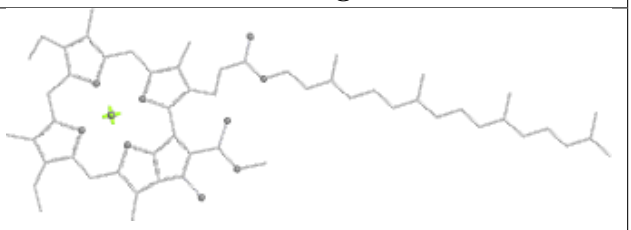
Bond lengths



Bond angles

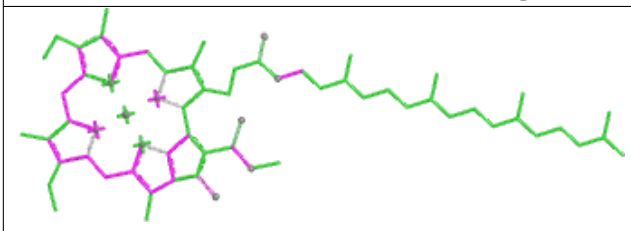


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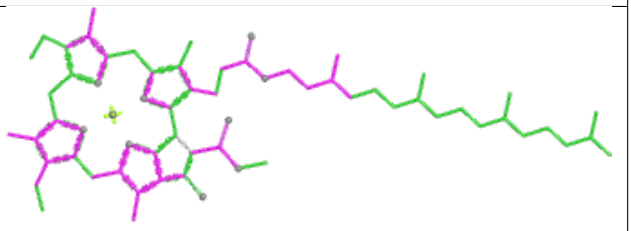


Rings

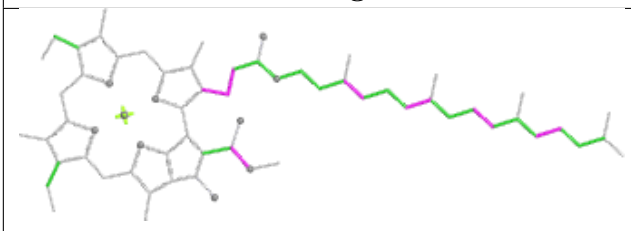
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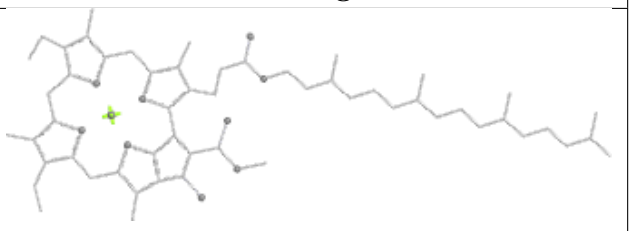
Bond lengths



Bond angles

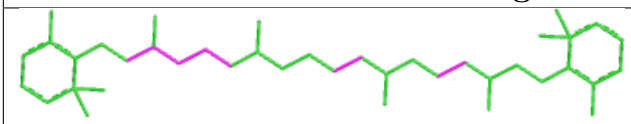


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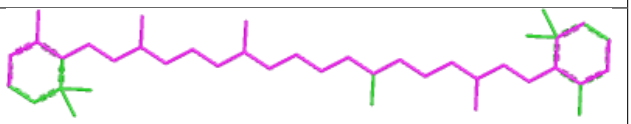


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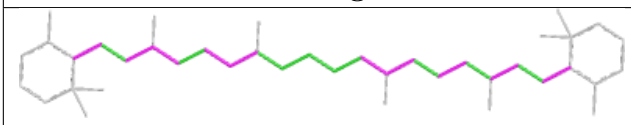
Ligand BCR A 6011



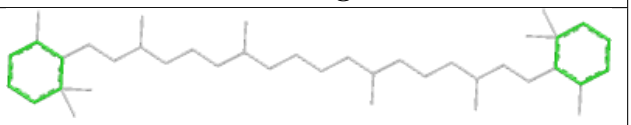
Bond lengths



Bond angles

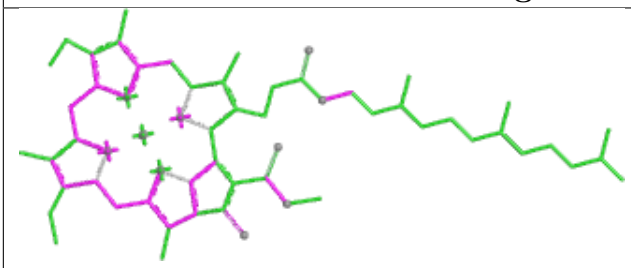


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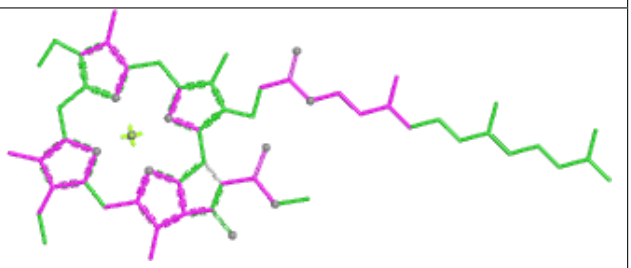


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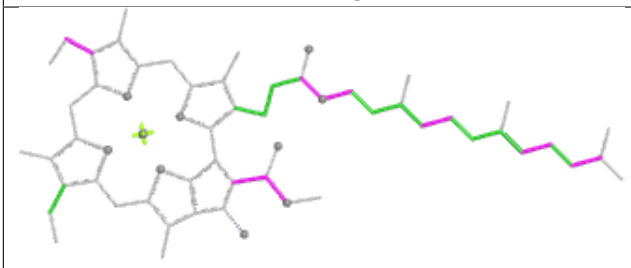
Ligand CLA A 1111



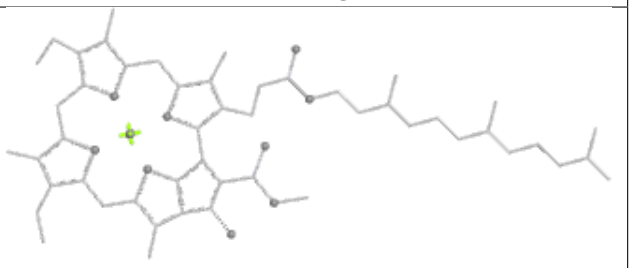
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Bond angles

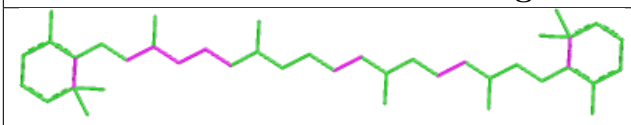


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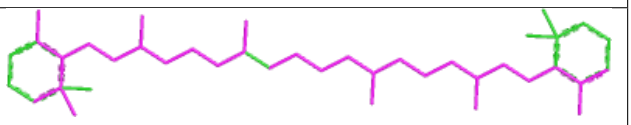


Rings

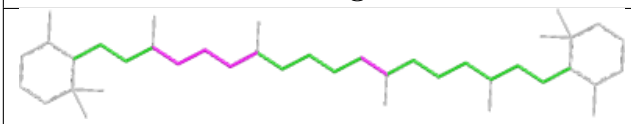
Ligand BCR F 6016



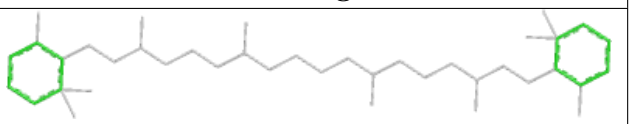
Bond lengths



Bond angles

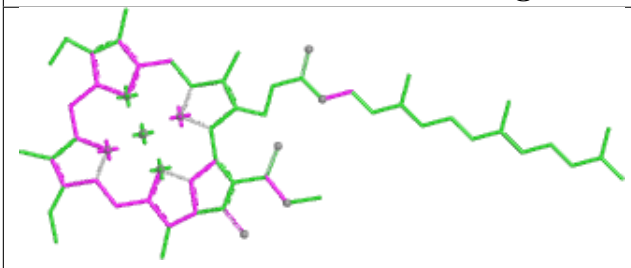


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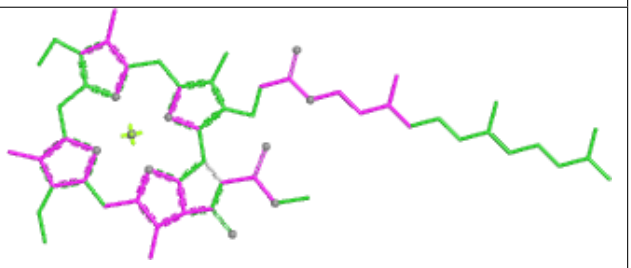


Rings

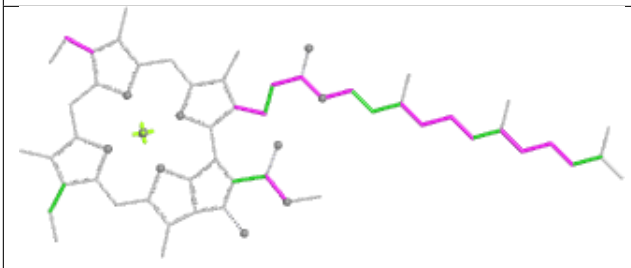
Ligand CLA A 1120



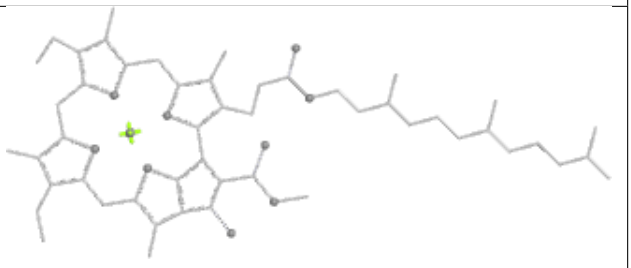
Bond lengths



Bond angles

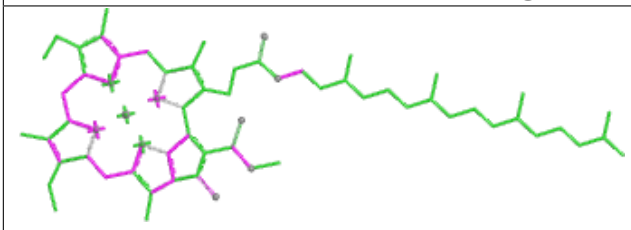


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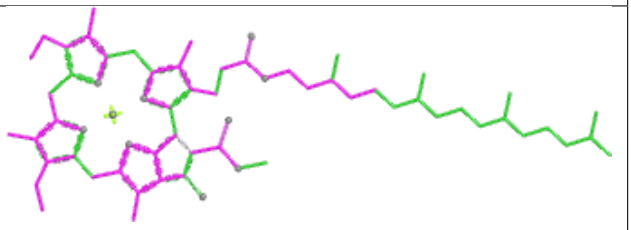


Rings

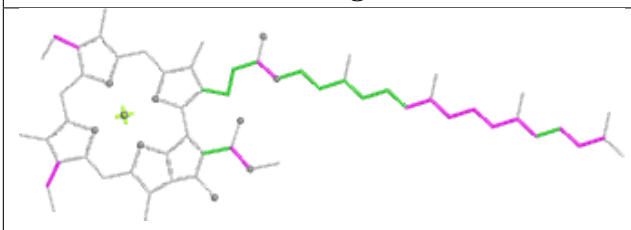
Ligand CLA 4 4012



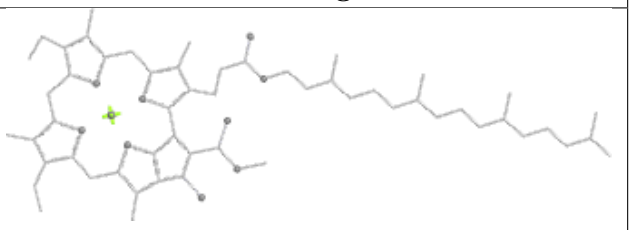
Bond lengths



Bond angles

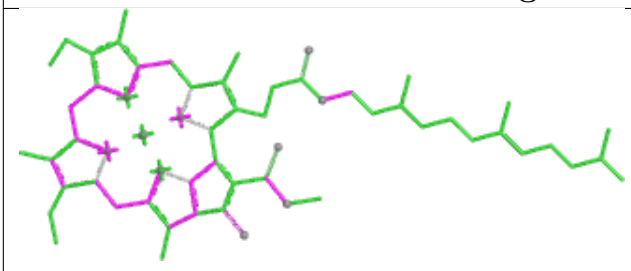


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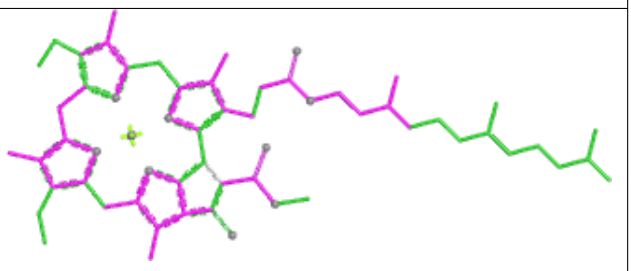


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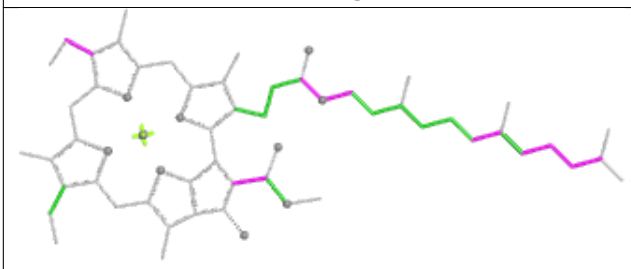
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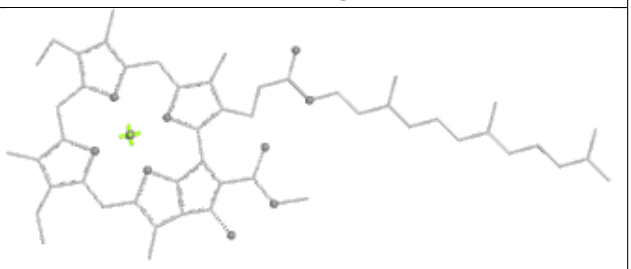
Bond lengths



Bond angles

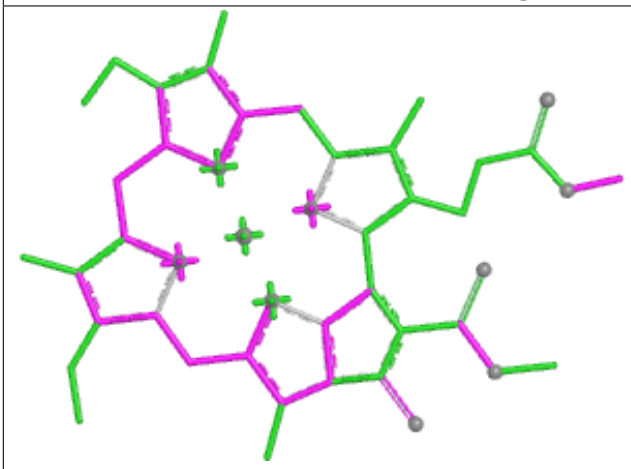


Torsions

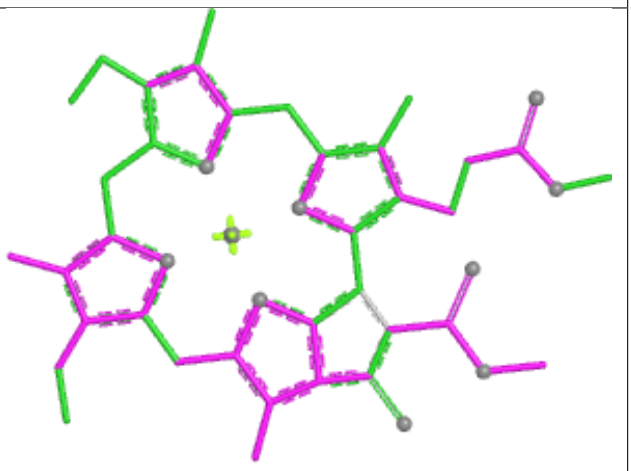


Rings

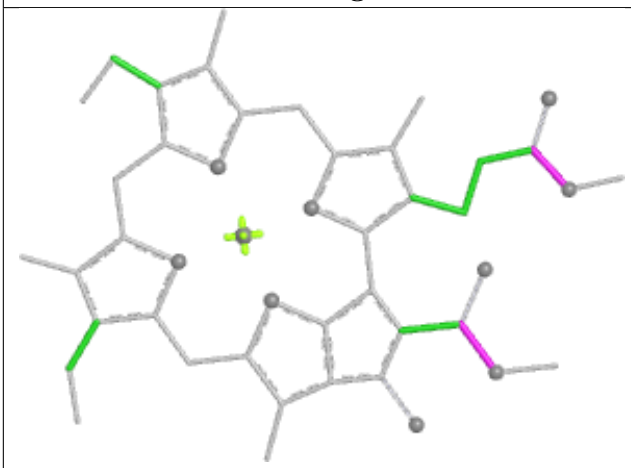
Ligand CLA A 1108



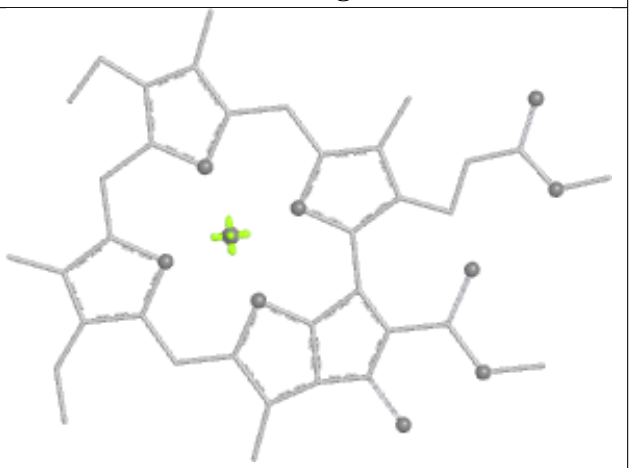
Bond lengths



Bond angles

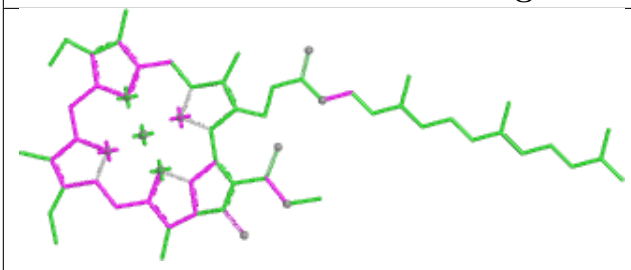


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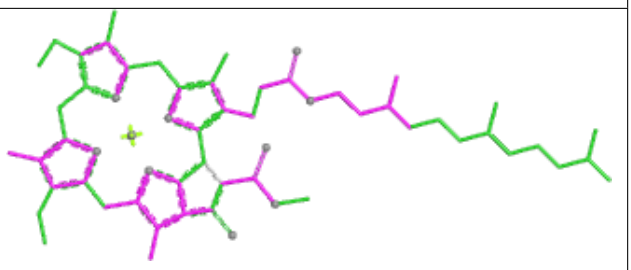


Rings

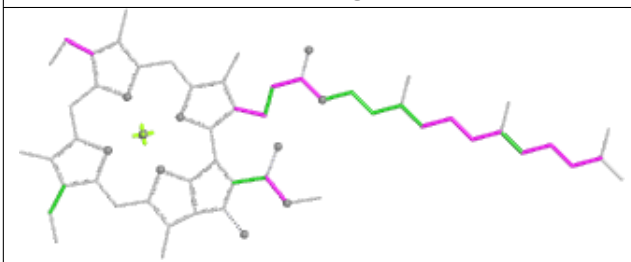
Ligand CLA B 1219



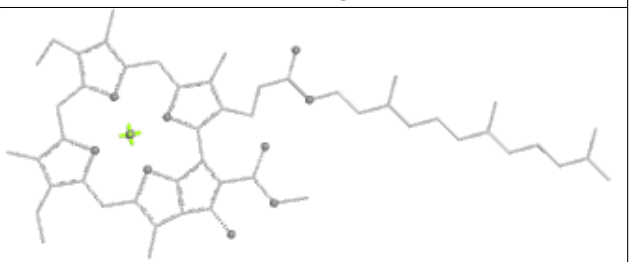
Bond lengths



Bond angles

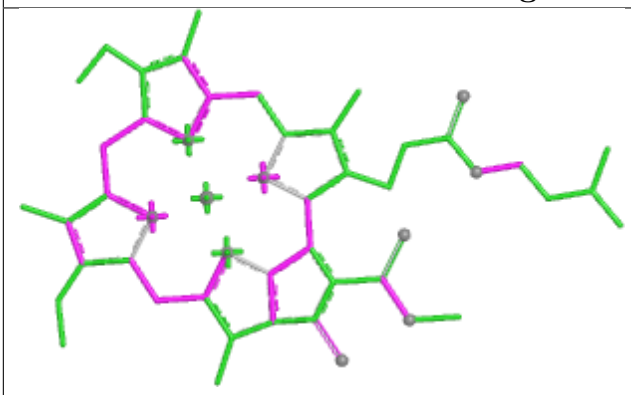


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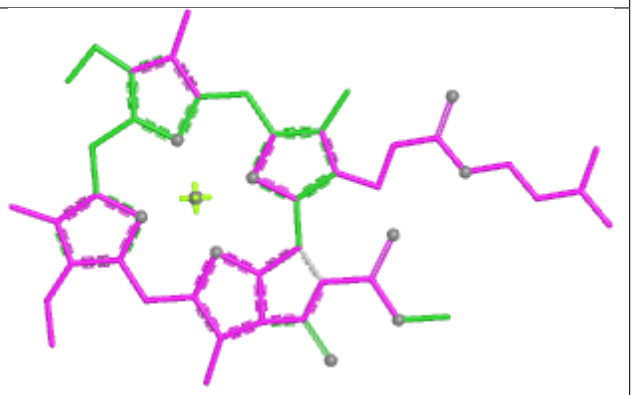


Rings

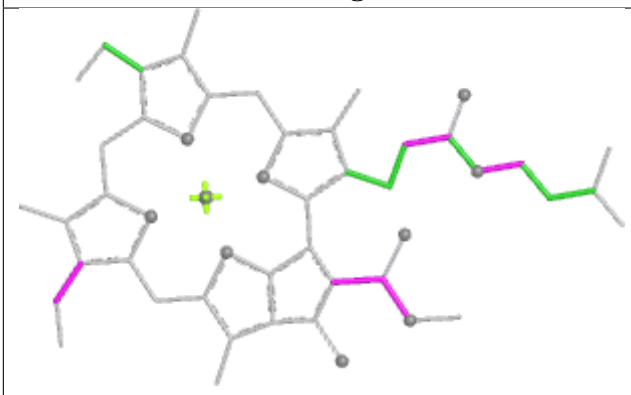
Ligand CLA 2 2016



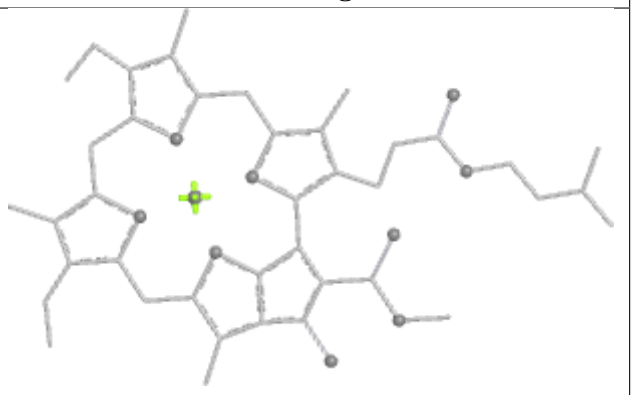
Bond lengths



Bond angles

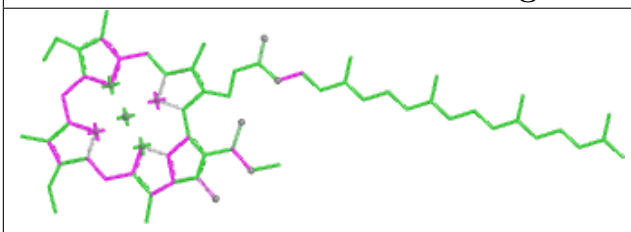


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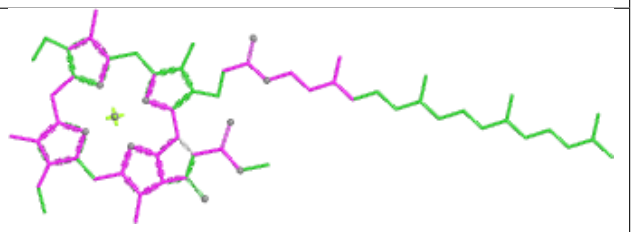


Rings

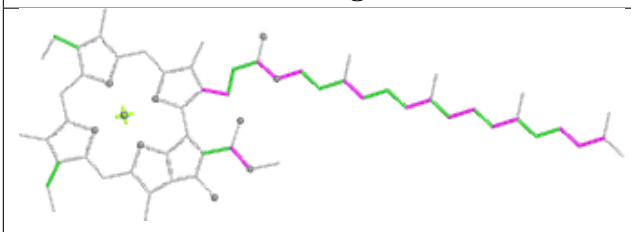
Ligand CLA 4 4017



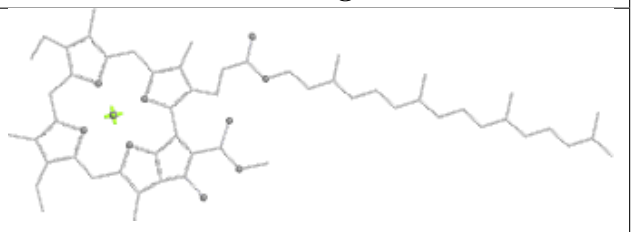
Bond lengths



Bond angles

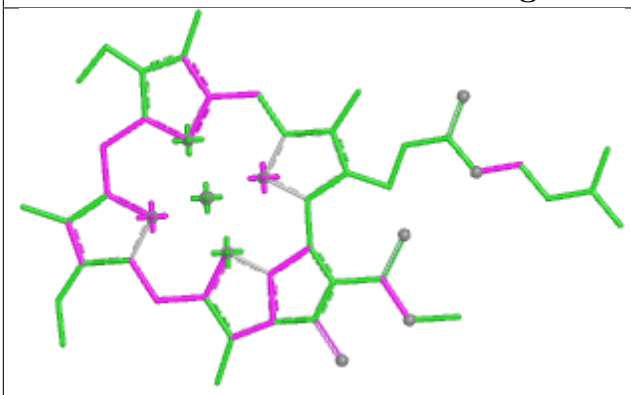


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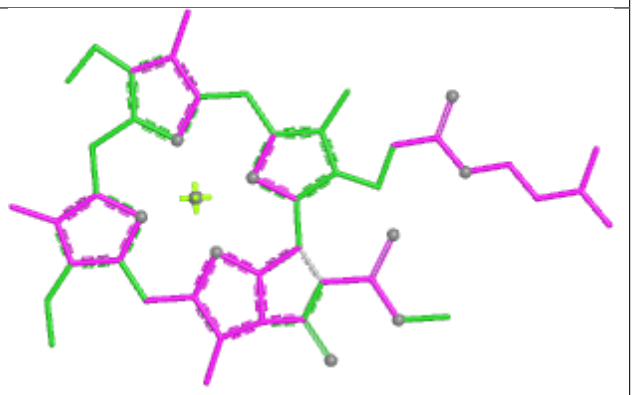


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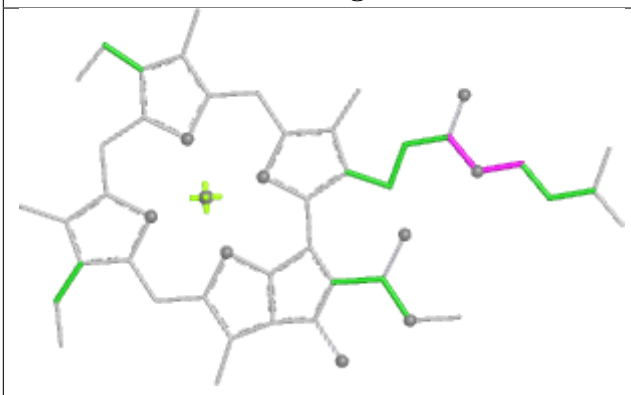
Ligand CLA 4 4009



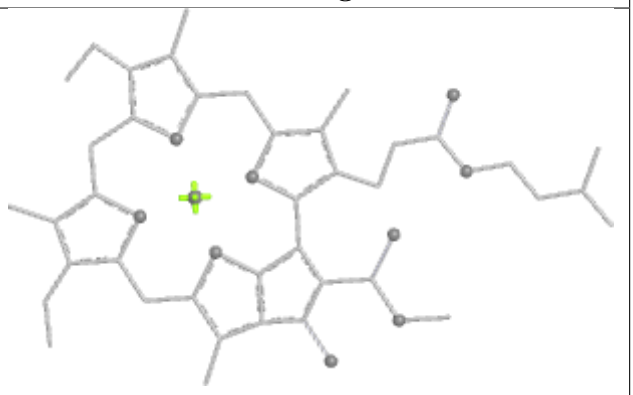
Bond lengths



Bond angles

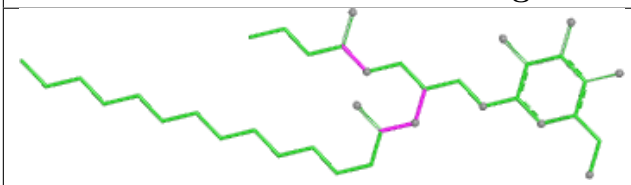


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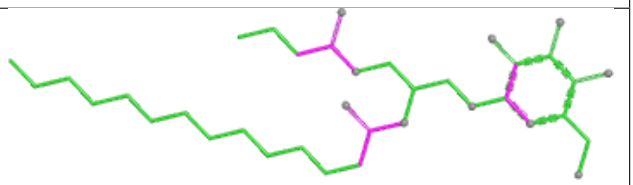


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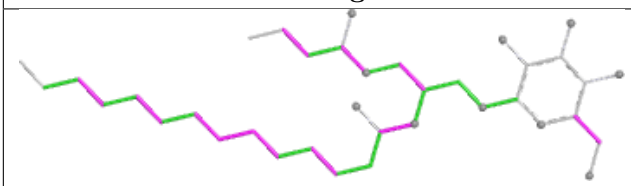
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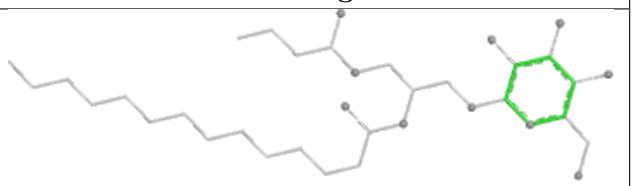
Bond lengths



Bond angles

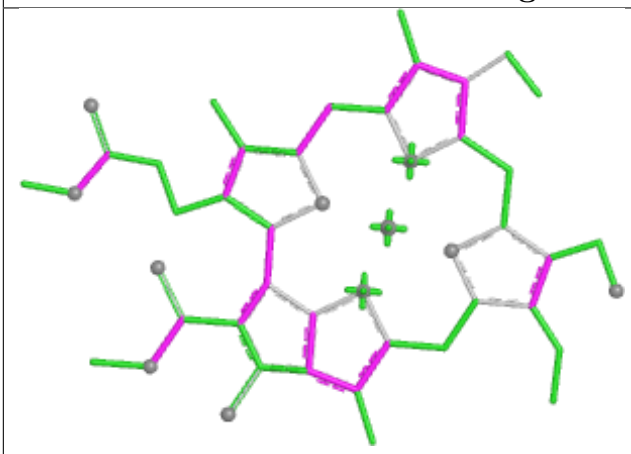


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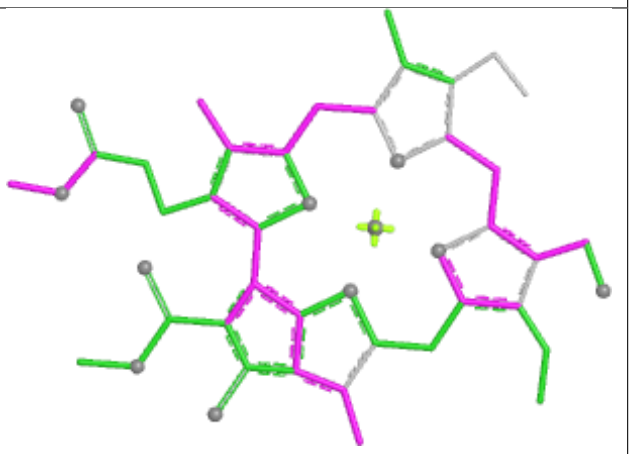


Rings

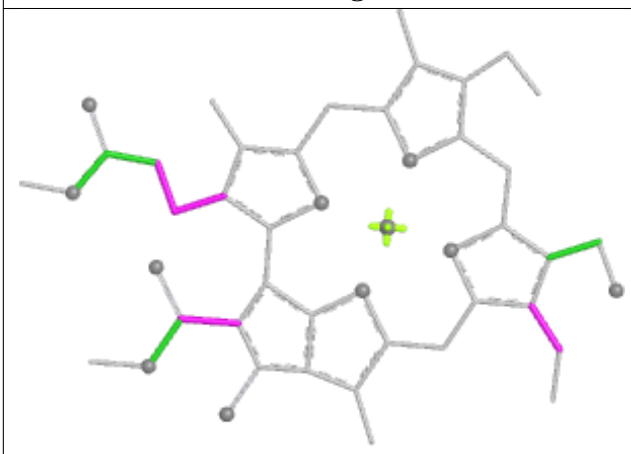
Ligand CHL 1 1010



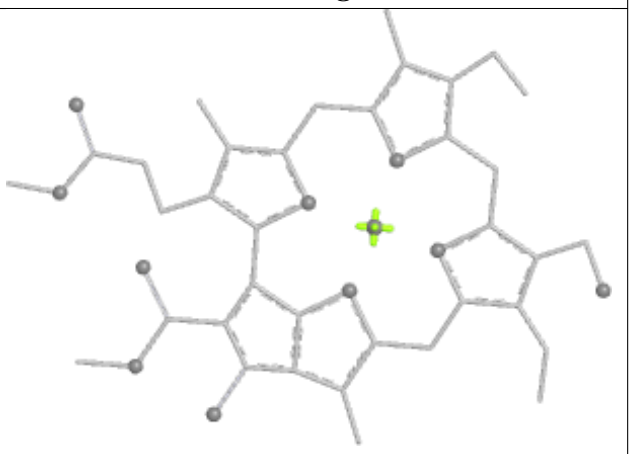
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Bond angles

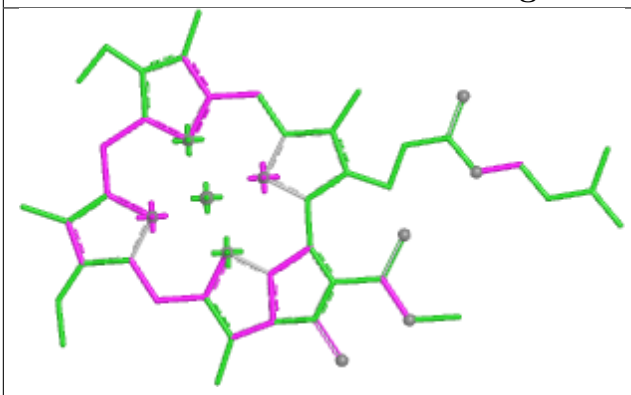


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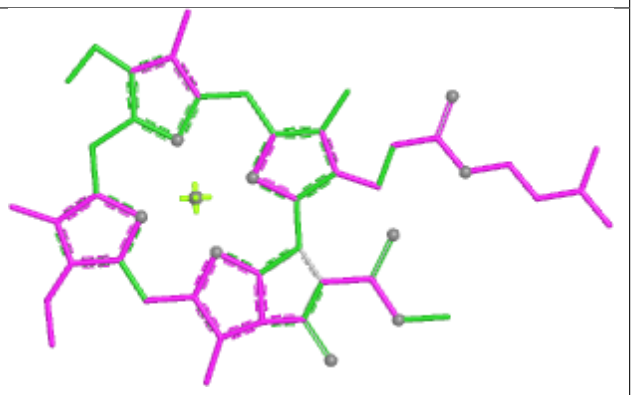


Rings

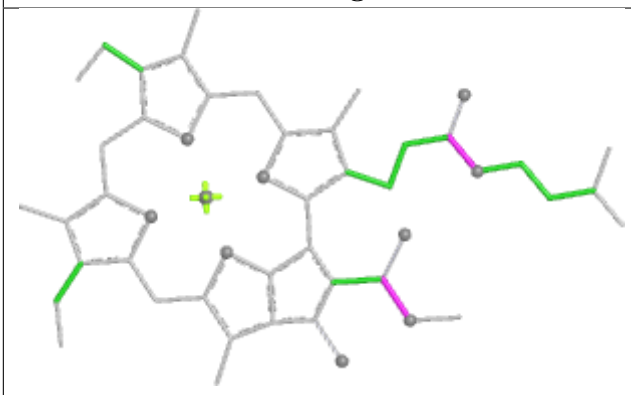
Ligand CLA 4 4006



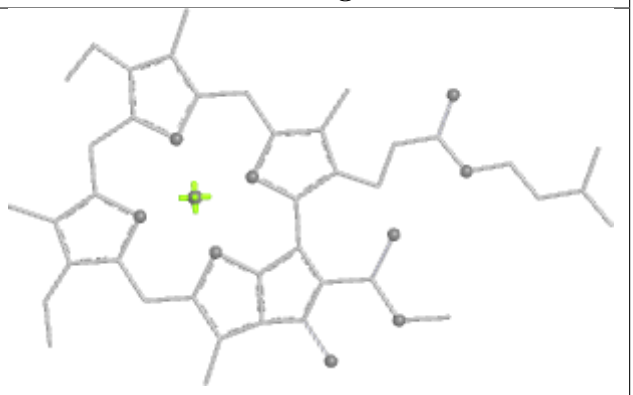
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Bond angles

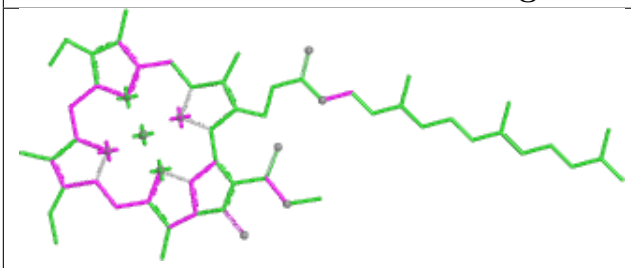


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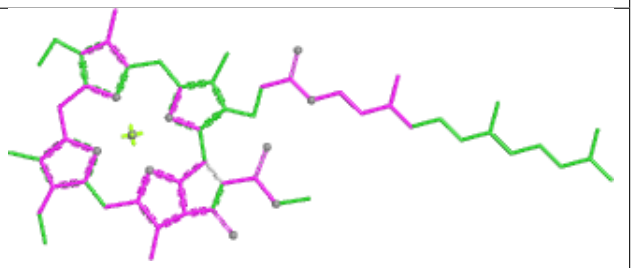


Rings

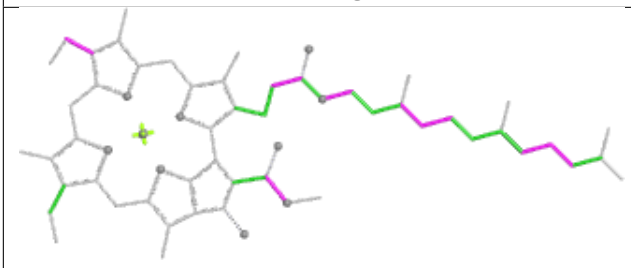
Ligand CLA 3 3003



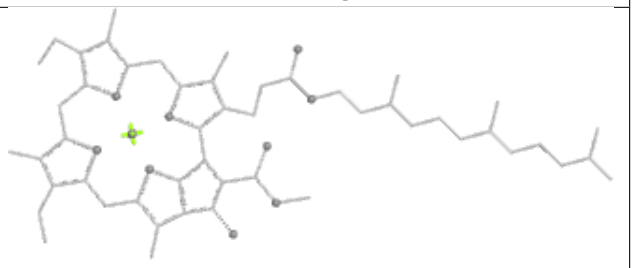
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Bond angles

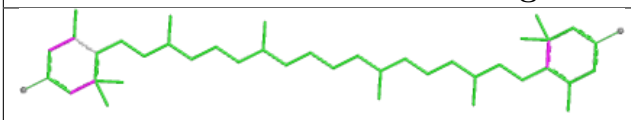


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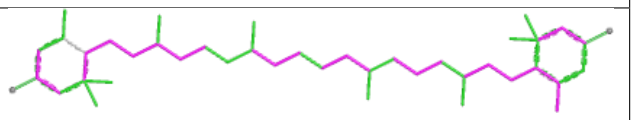


Rings

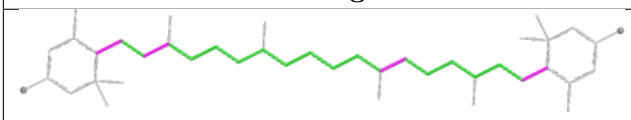
Ligand LUT 4 4502



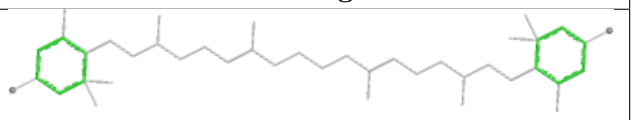
Bond lengths



Bond angles

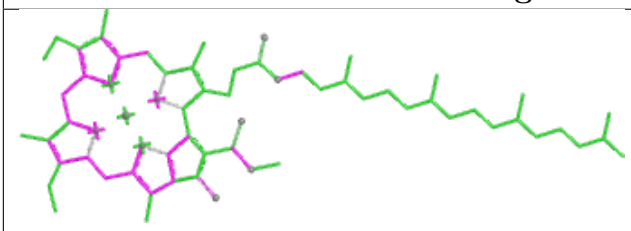


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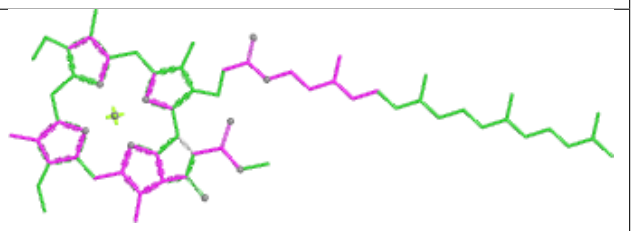


Rings

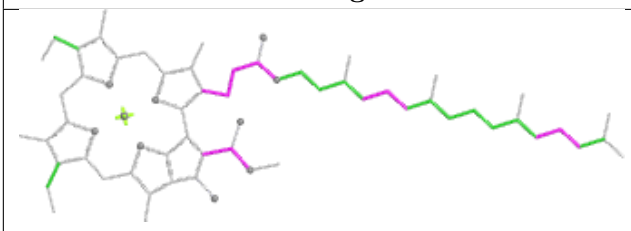
Ligand CLA A 1106



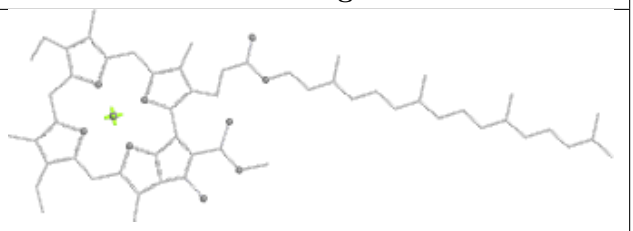
Bond lengths



Bond angles

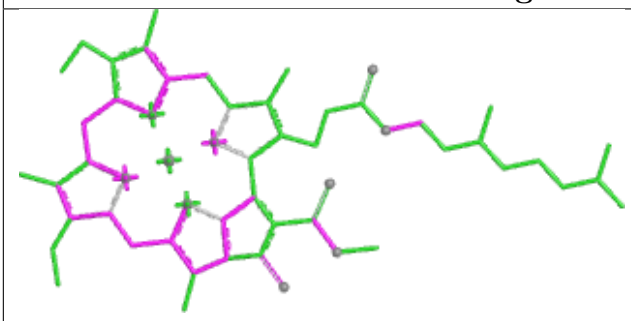


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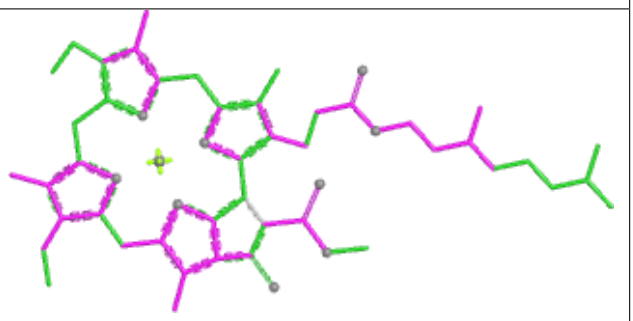


Rings

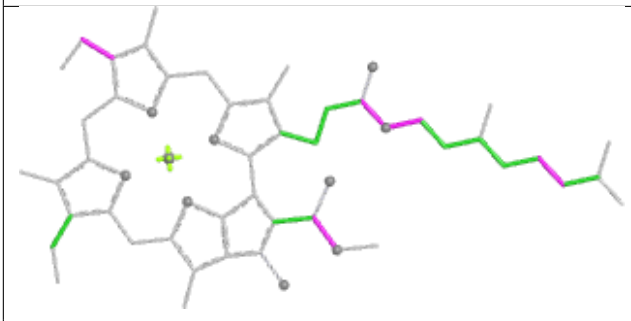
Ligand CLA B 1212



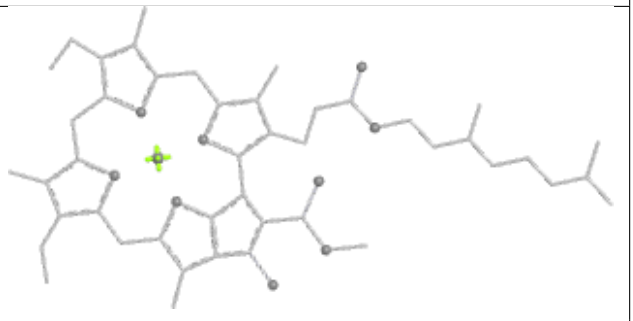
Bond lengths



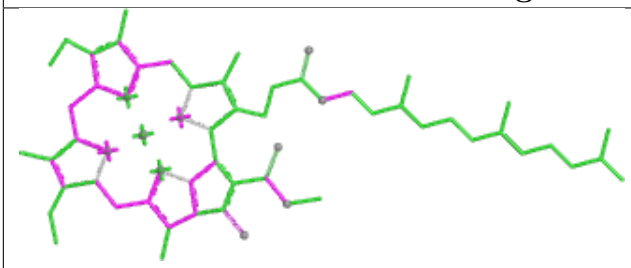
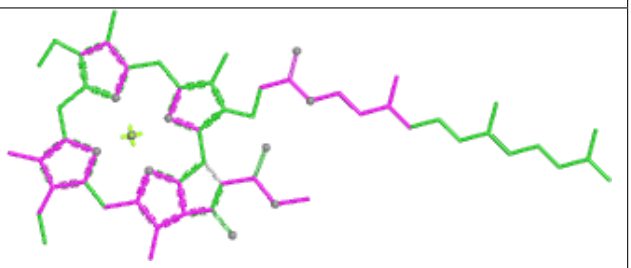
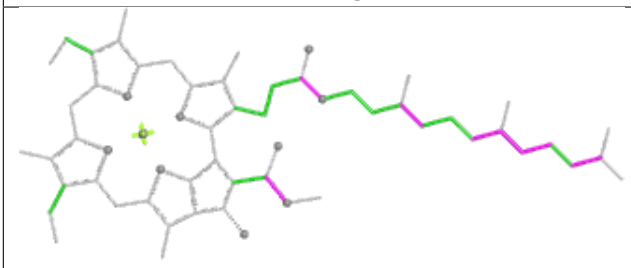
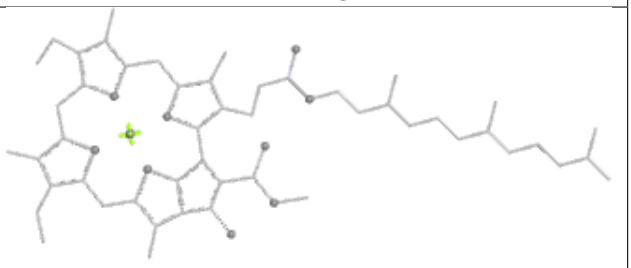
Bond angles

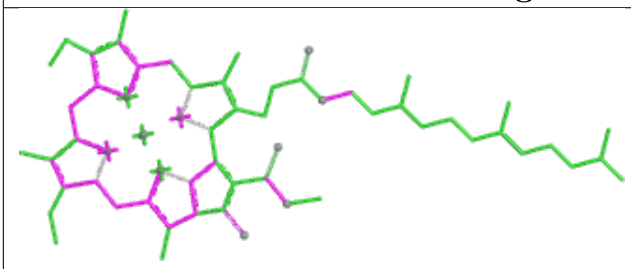
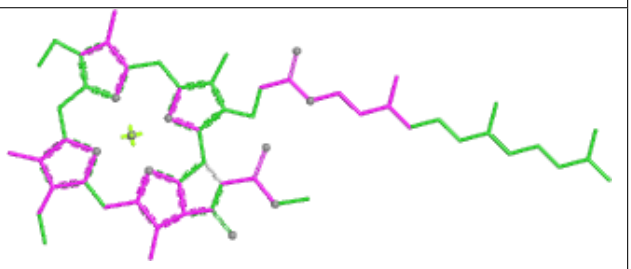
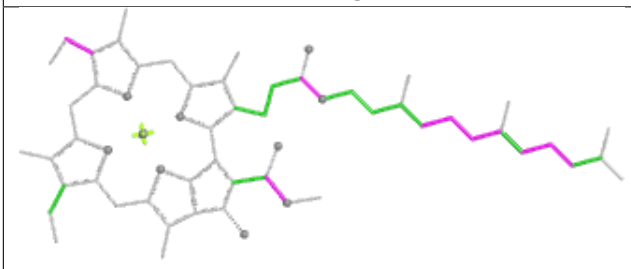
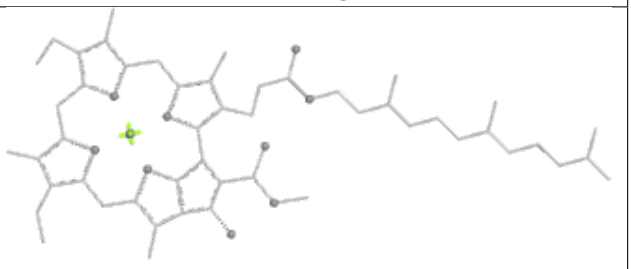


Torsions

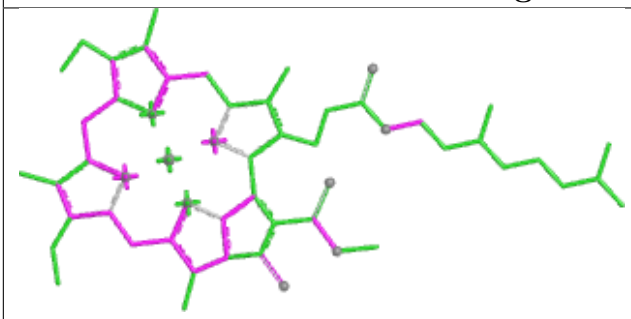


Rings

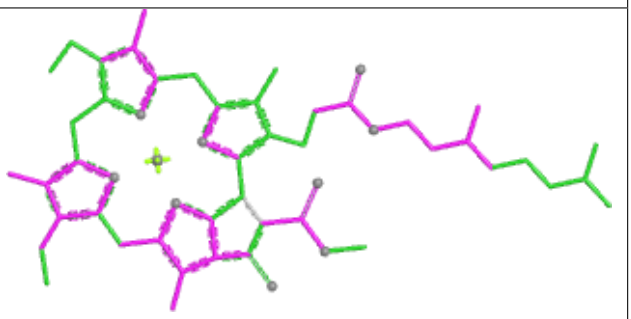
Ligand CLA B 1213	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1234	
 Bond lengths	 Bond angles
 Torsions	 Rings

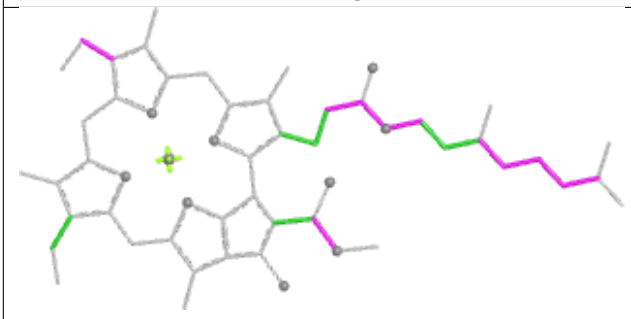
Ligand CLA A 1134



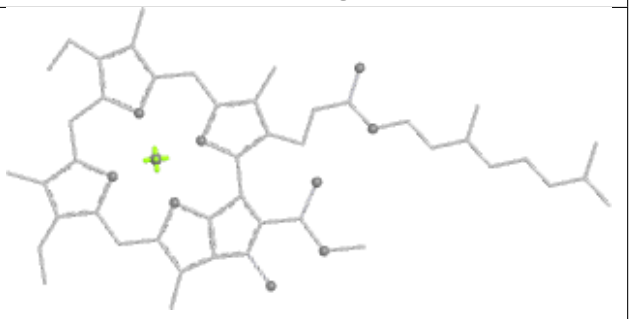
Bond lengths



Bond angles

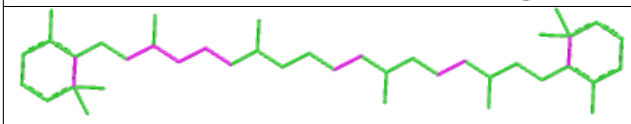


Torsions

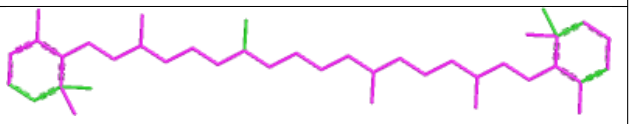


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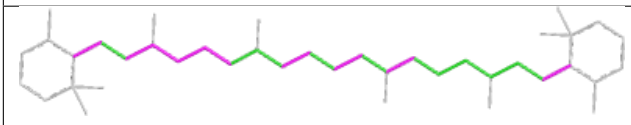
Ligand BCR 3 3503



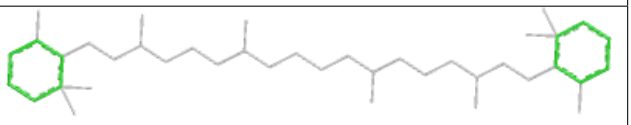
Bond lengths



Bond angles

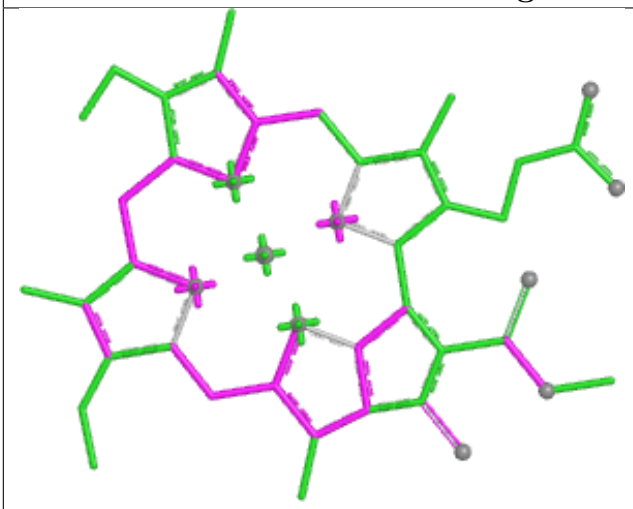


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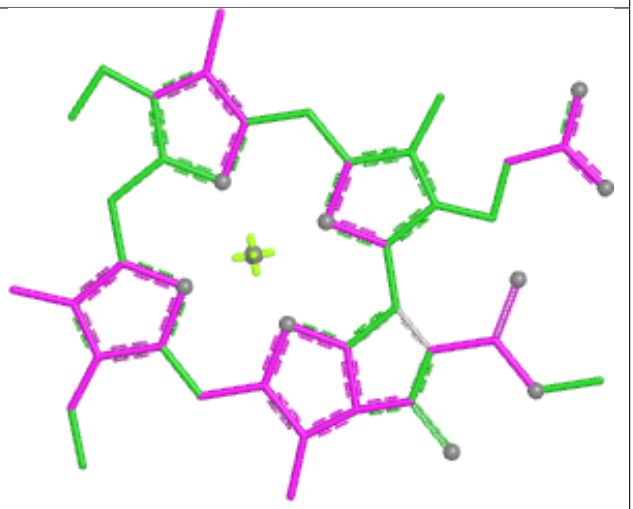


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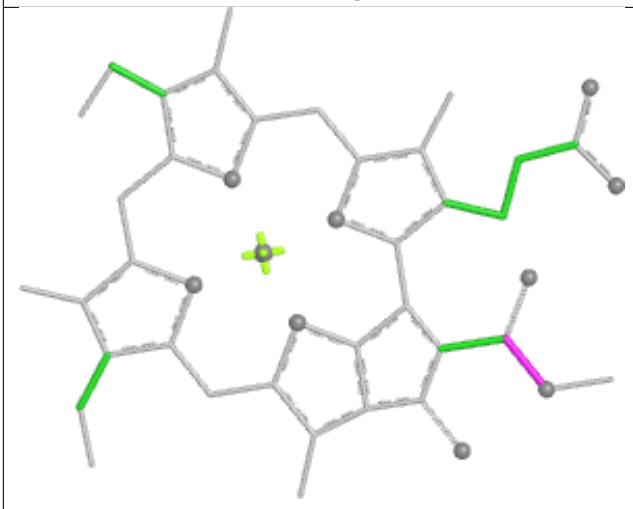
Ligand CLA F 1301



Bond lengths



Bond angles

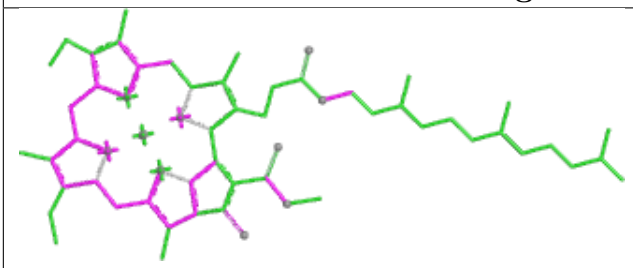


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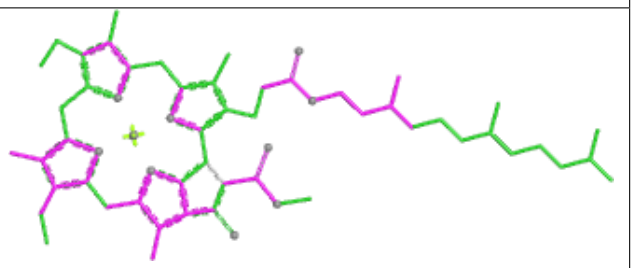


Rings

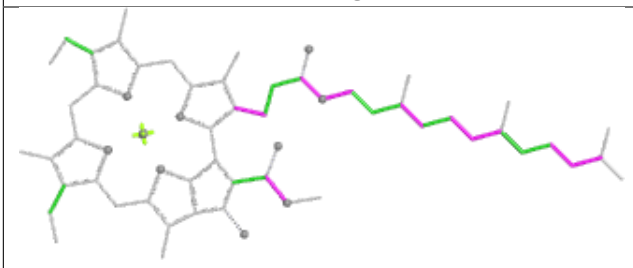
Ligand CLA B 1215



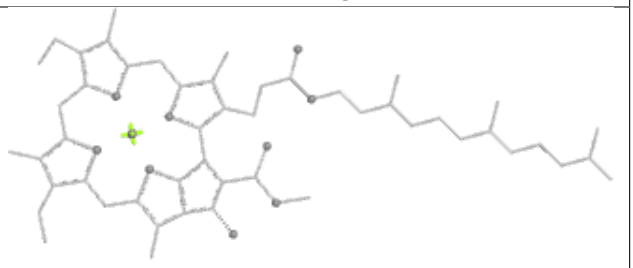
Bond lengths



Bond angles

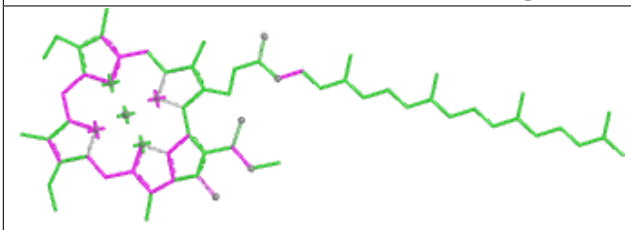


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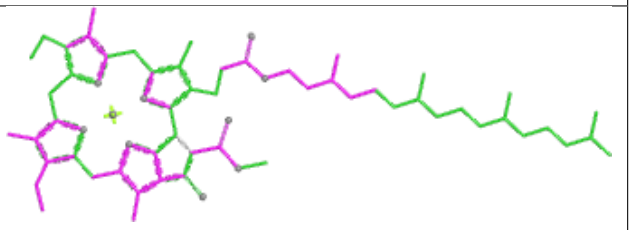


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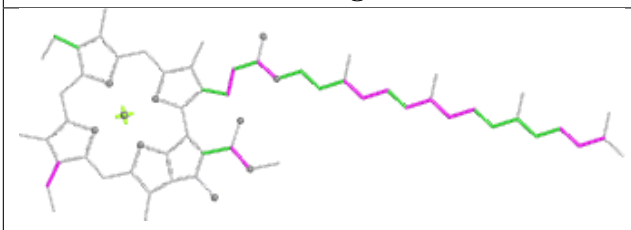
Ligand CLA 4 4003



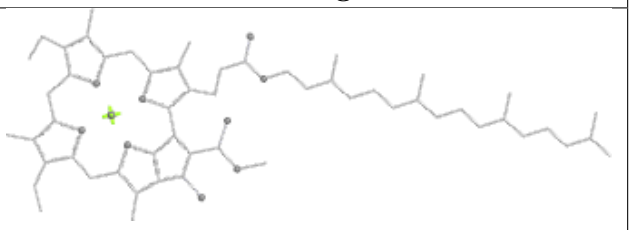
Bond lengths



Bond angles

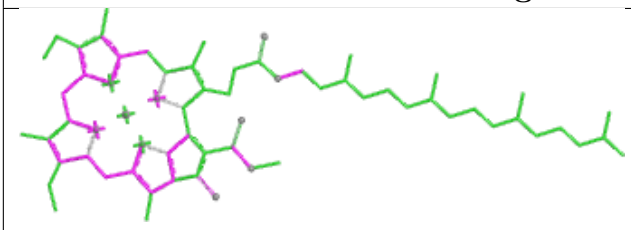


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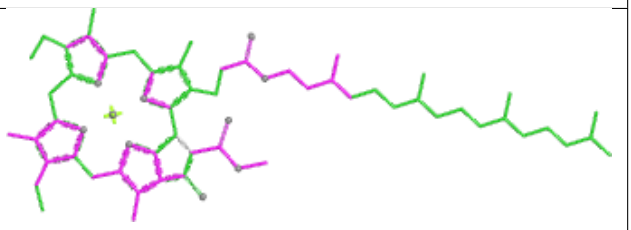


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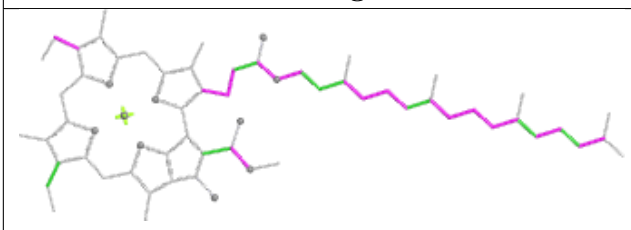
Ligand CLA A 1119



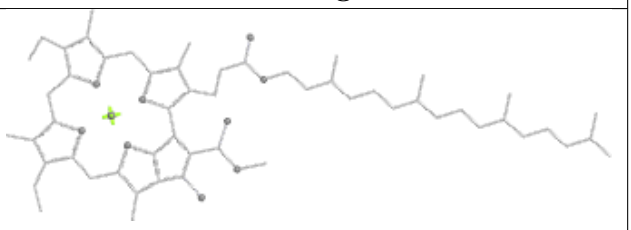
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Bond angles

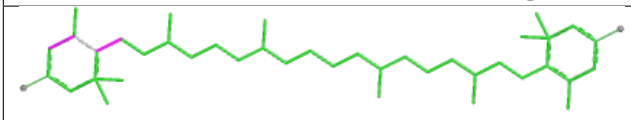


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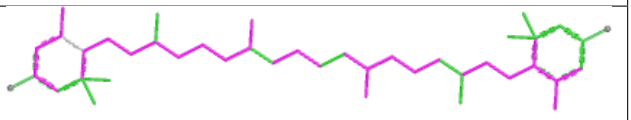


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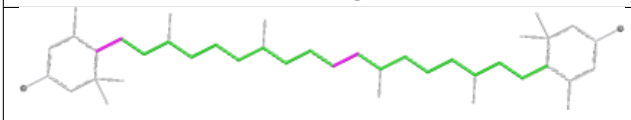
Ligand LUT I 6018



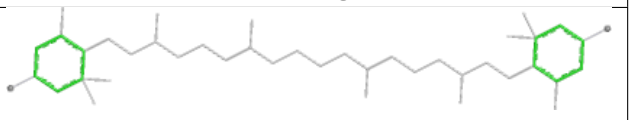
Bond lengths



Bond angles

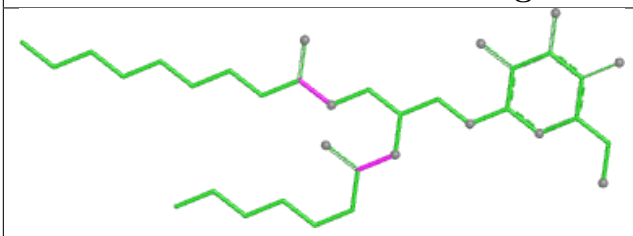


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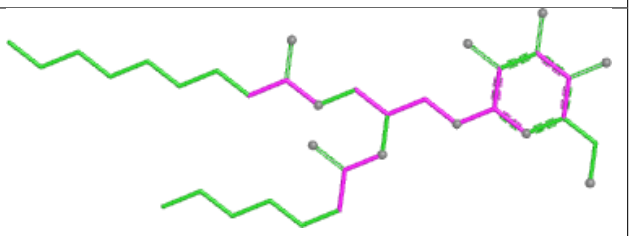


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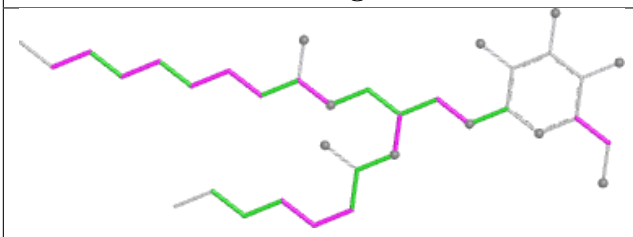
Ligand LMG 2 2802



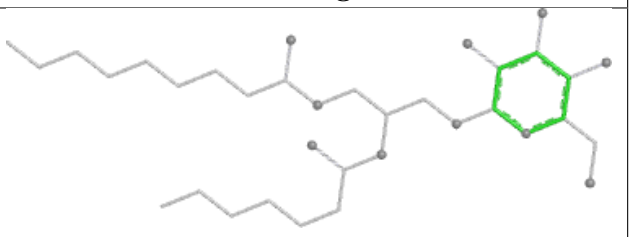
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Bond angles

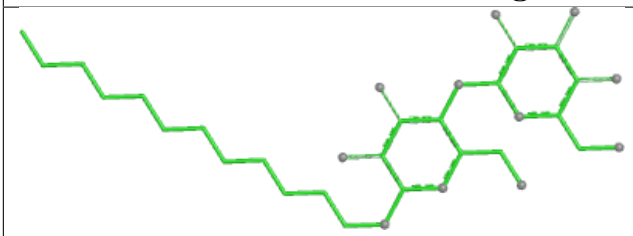


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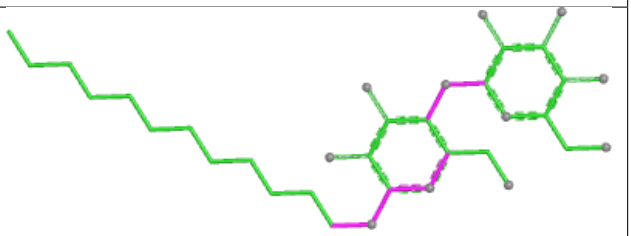


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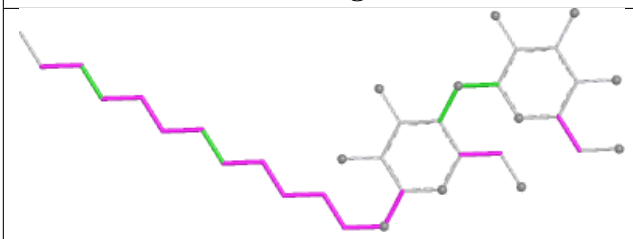
Ligand LMU B 8002



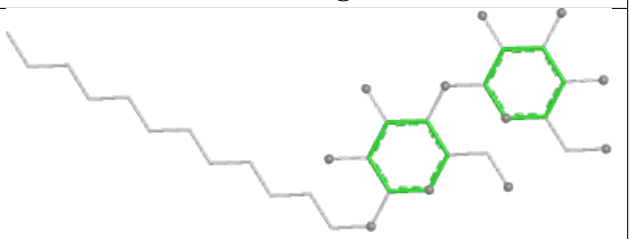
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Bond angles

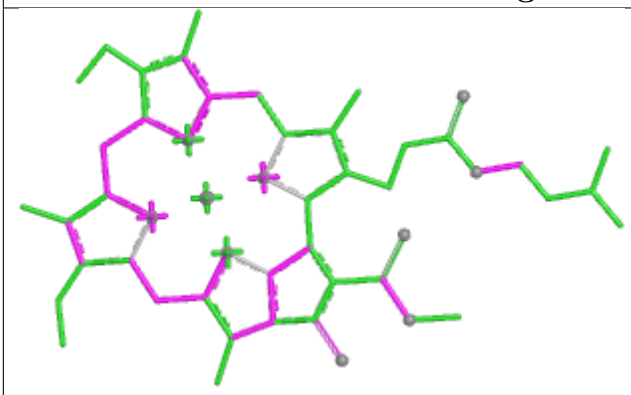


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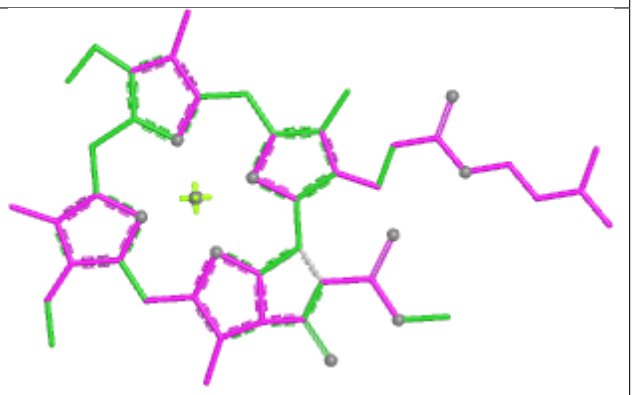


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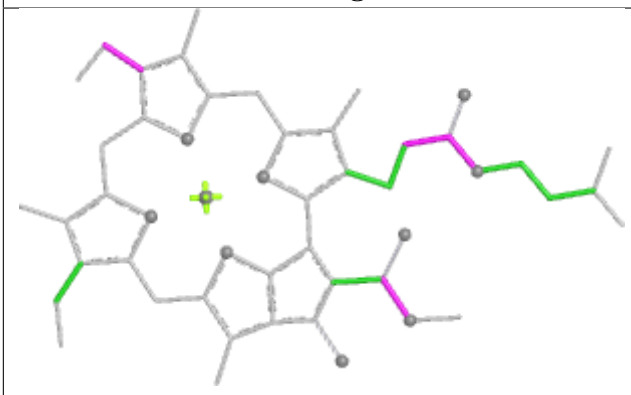
Ligand CLA L 1503



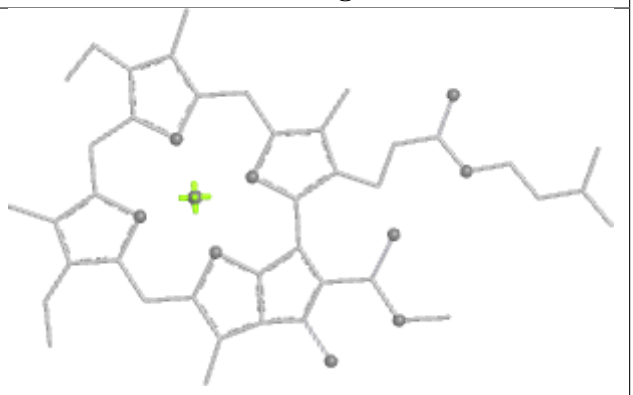
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Bond angles

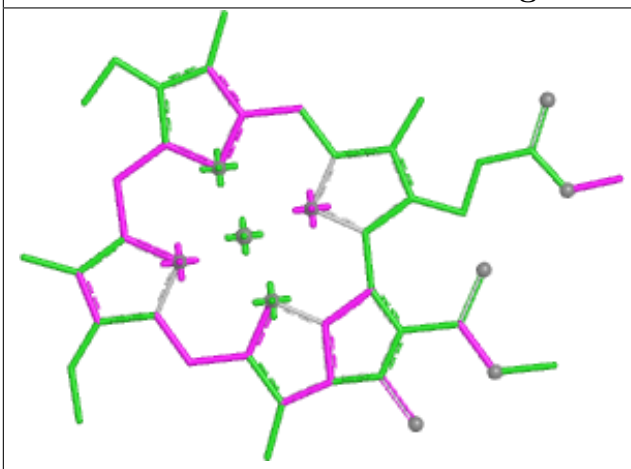


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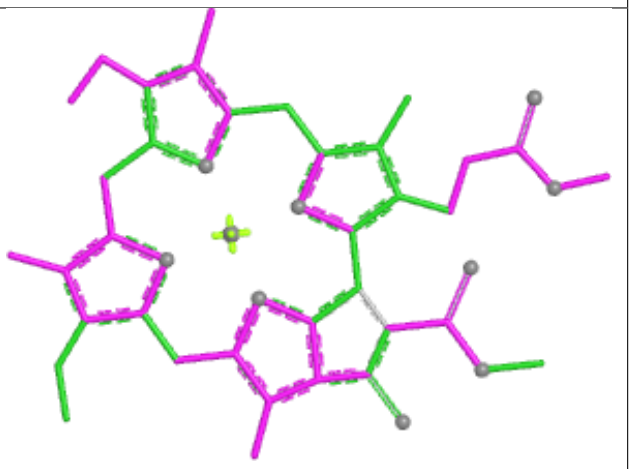


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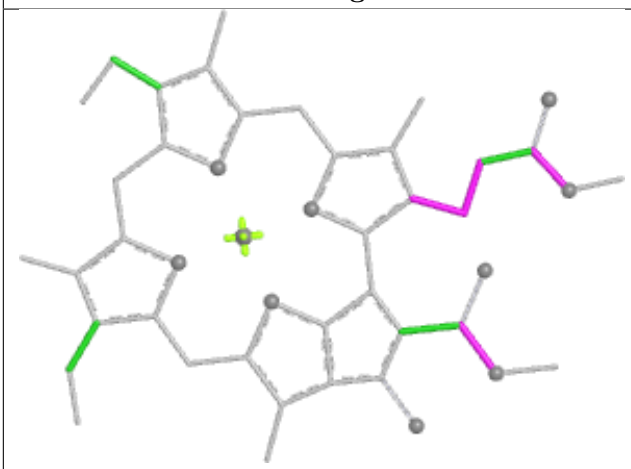
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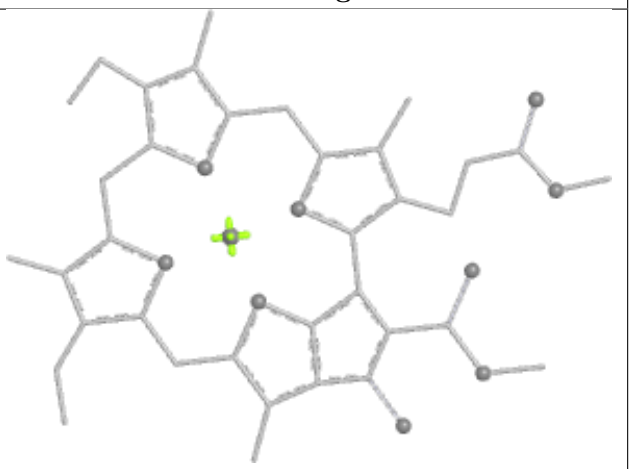
Bond lengths



Bond angles

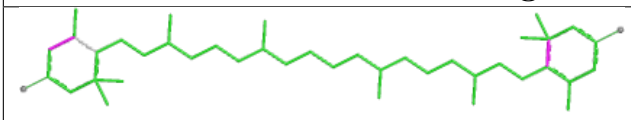


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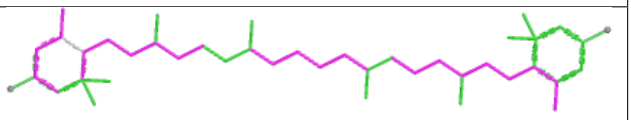


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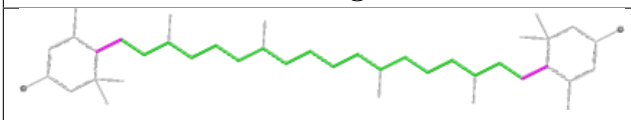
Ligand LUT 2 2501



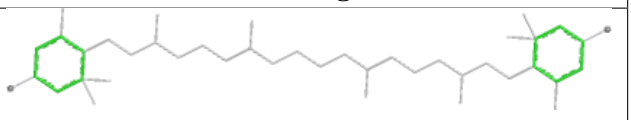
Bond lengths



Bond angles

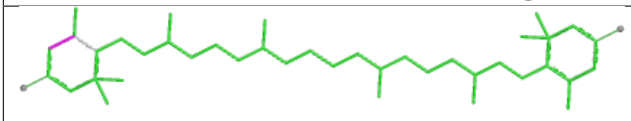


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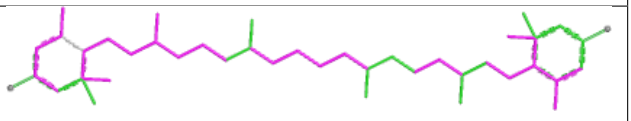


Rings

Ligand LUT 3 3501



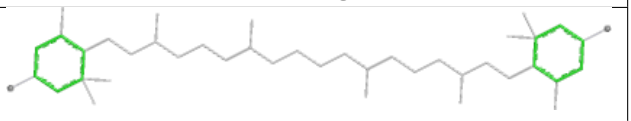
Bond lengths



Bond angles

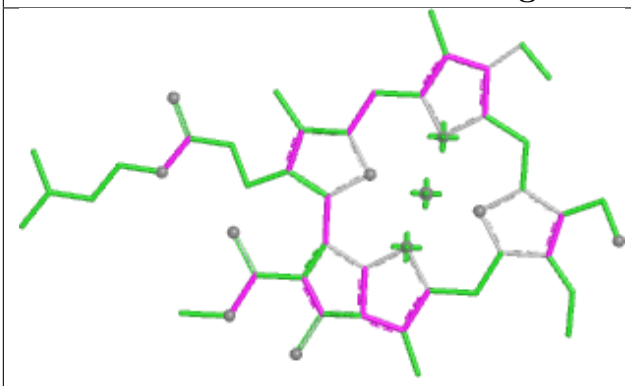


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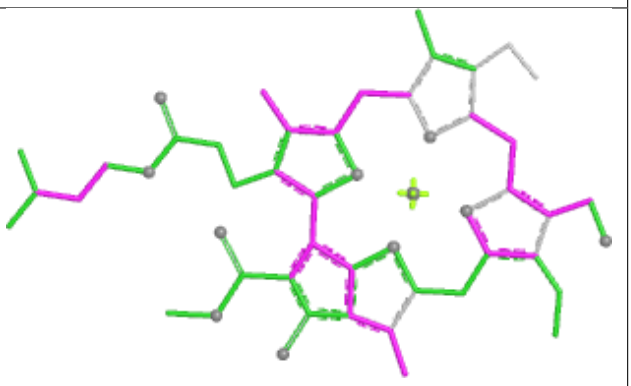


Rings

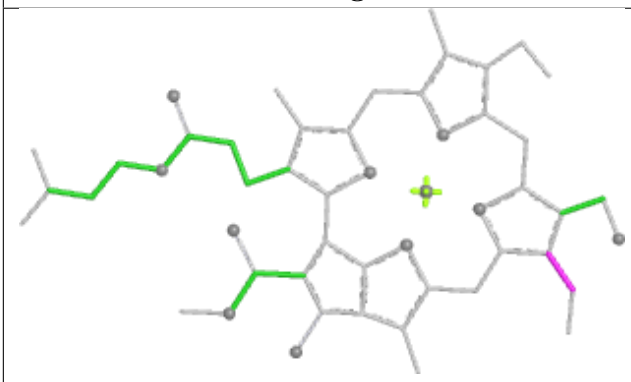
Ligand CHL 4 4011



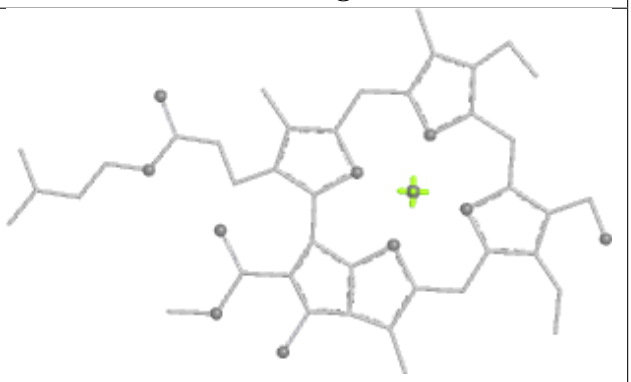
Bond lengths



Bond angles

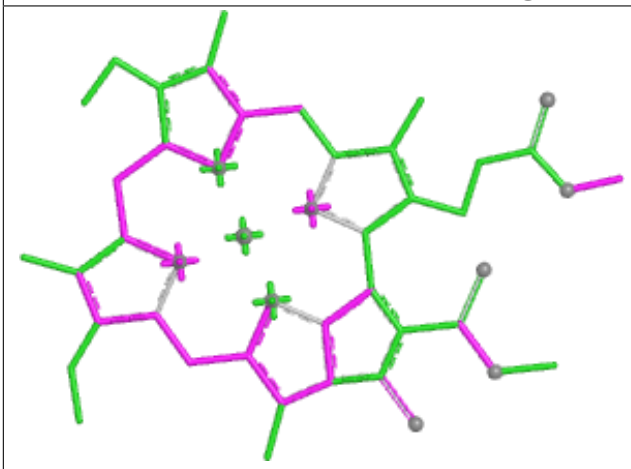


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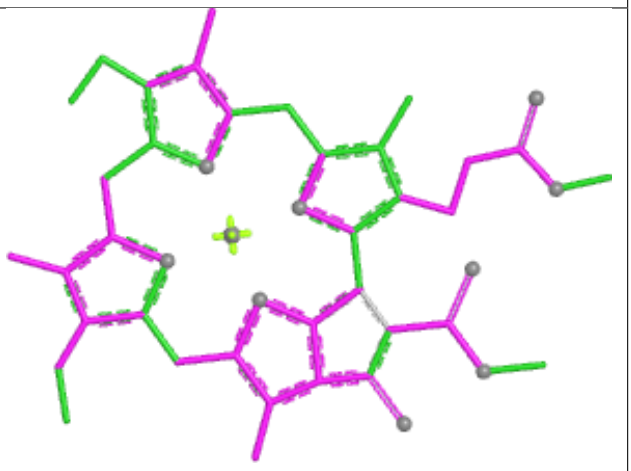


Rings

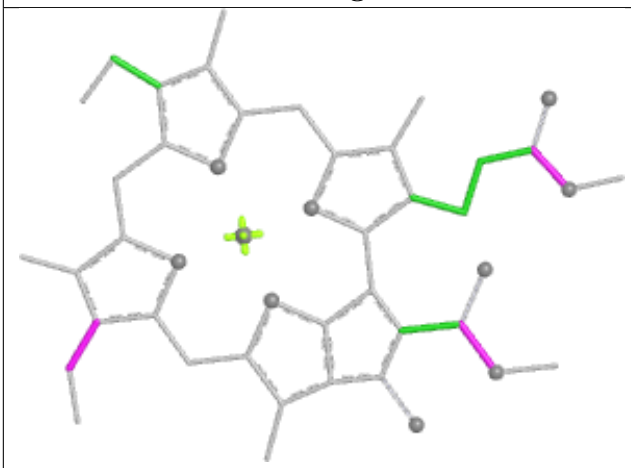
Ligand CLA 3 3002



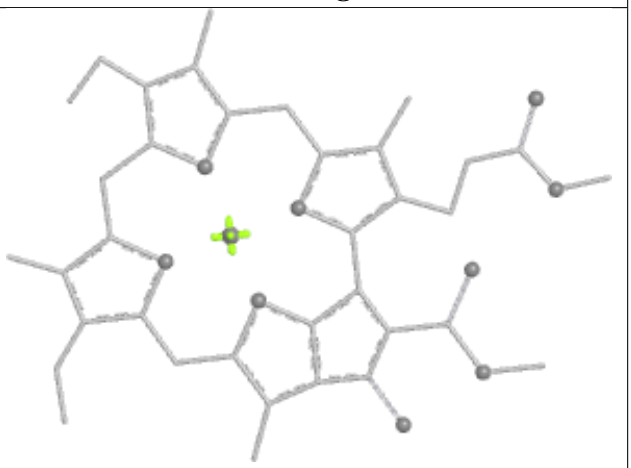
Bond lengths



Bond angles

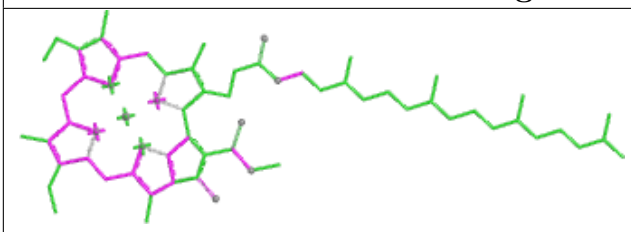


Torsions

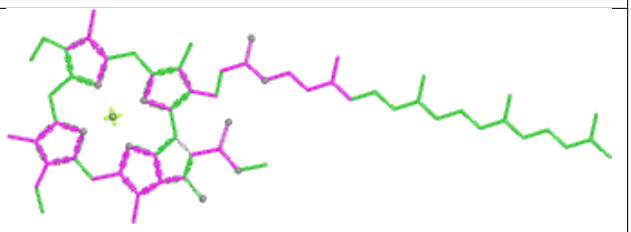


Rings

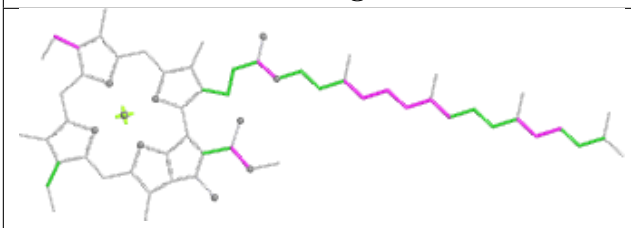
Ligand CLA B 1227



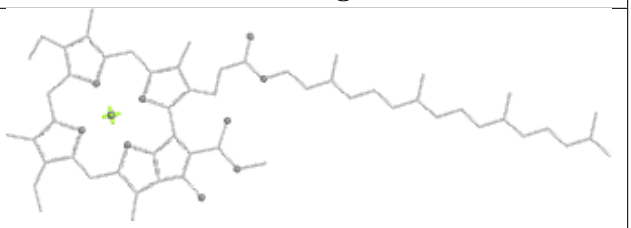
Bond lengths



Bond angles

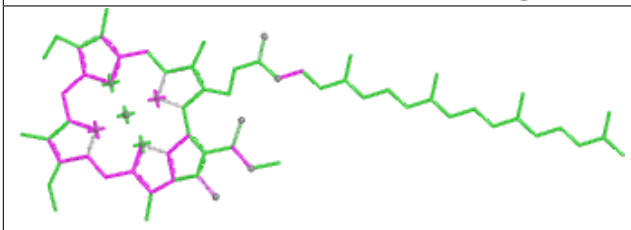


Torsions

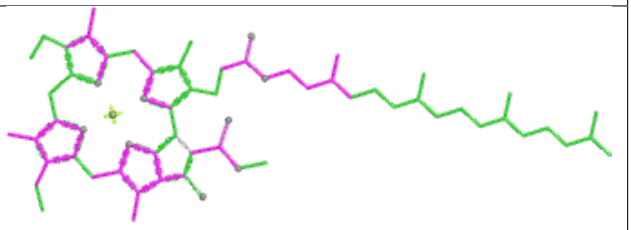


Rings

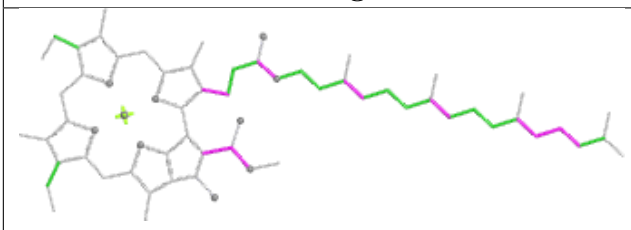
Ligand CLA B 1202



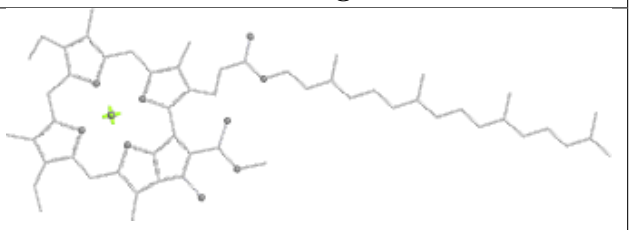
Bond lengths



Bond angles

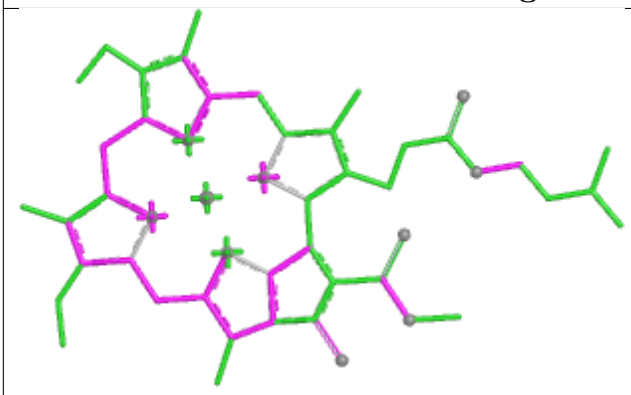


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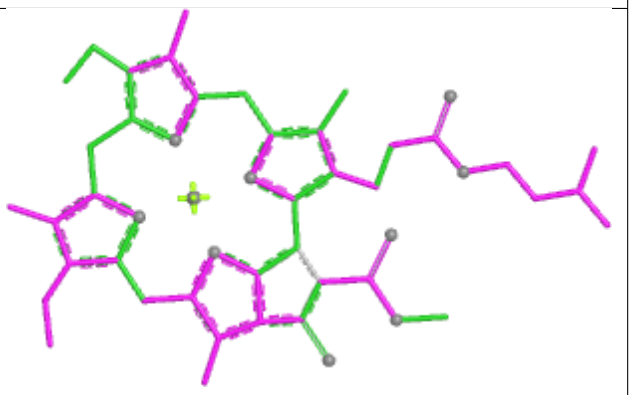


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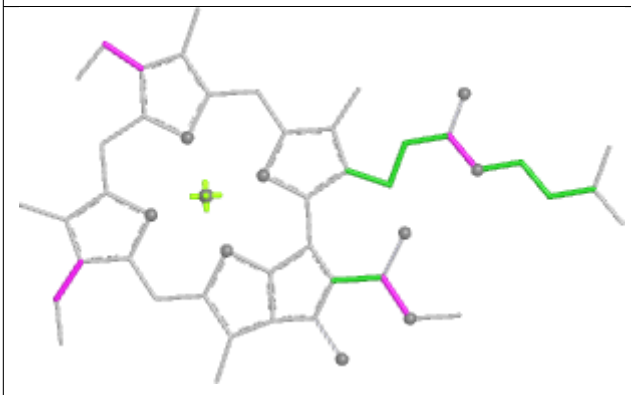
Ligand CLA 1 1006



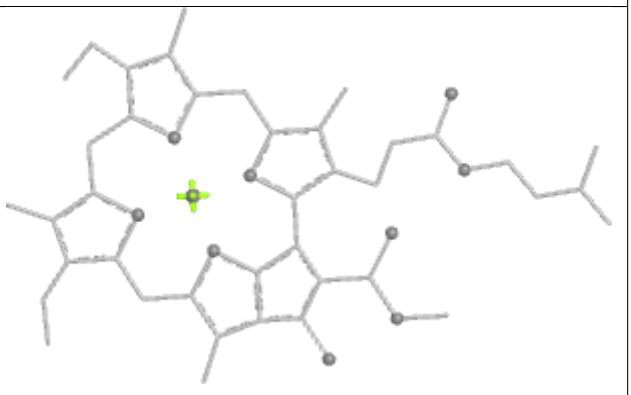
Bond lengths



Bond angles

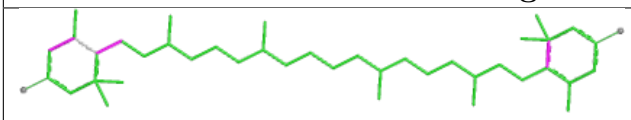


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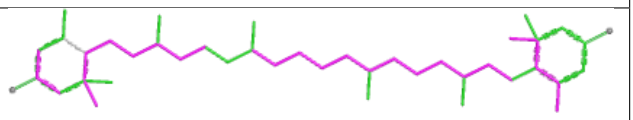


Rings

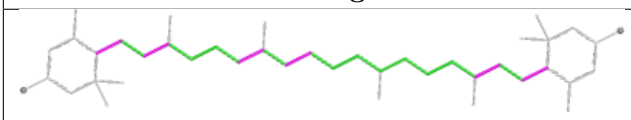
Ligand LUT 4 4503



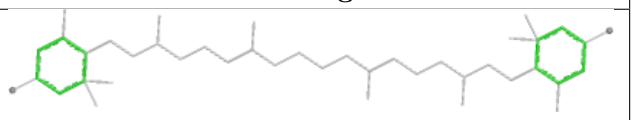
Bond lengths



Bond angles

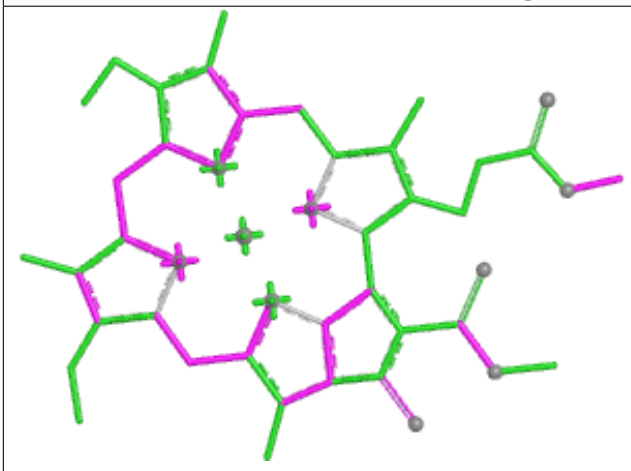


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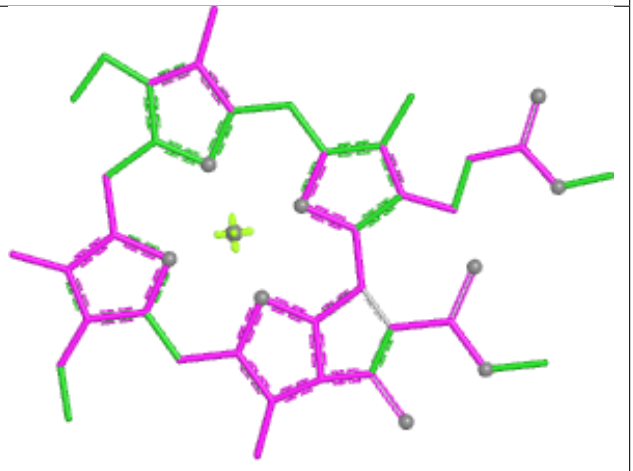


Rings

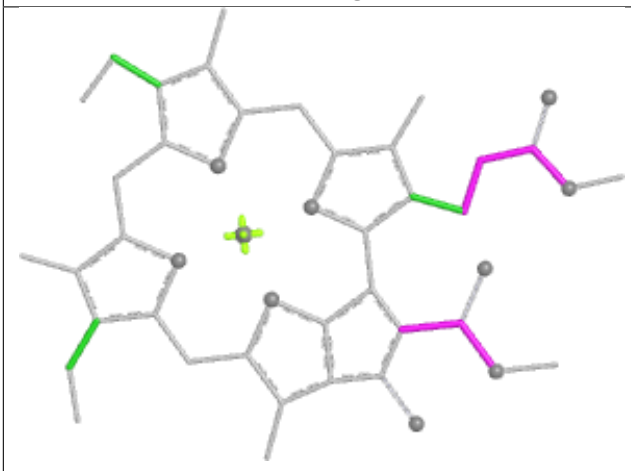
Ligand CLA 1 1008



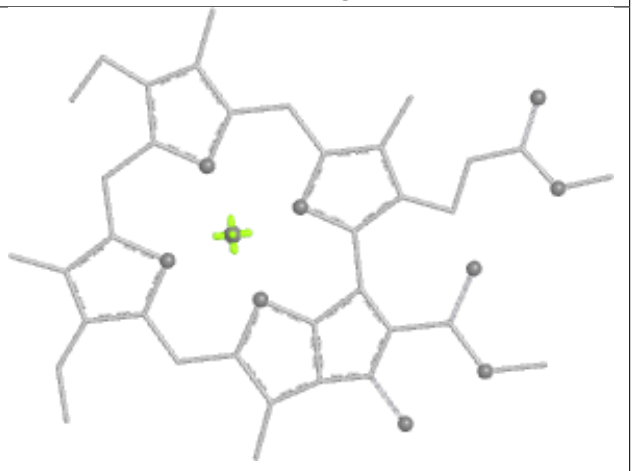
Bond lengths



Bond angles

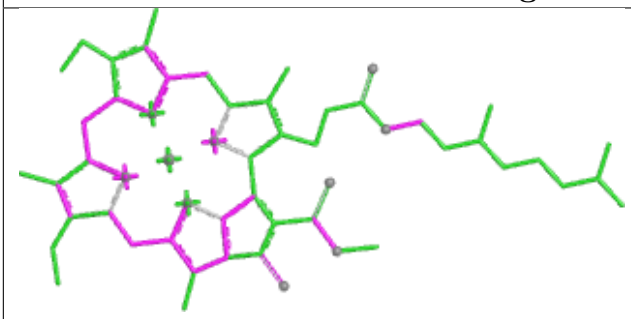


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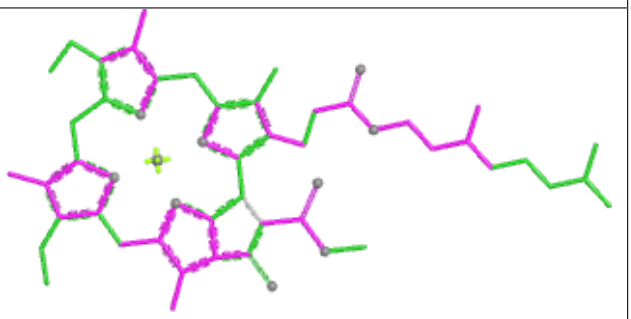


Rings

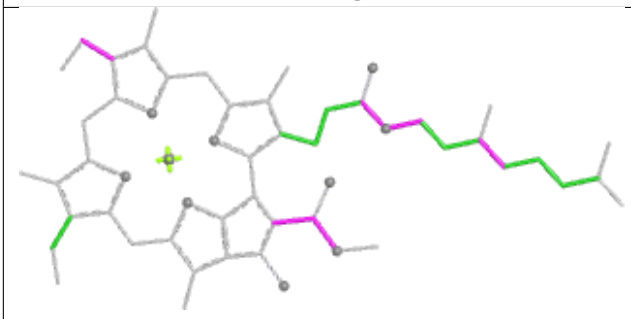
Ligand CLA 2 2006



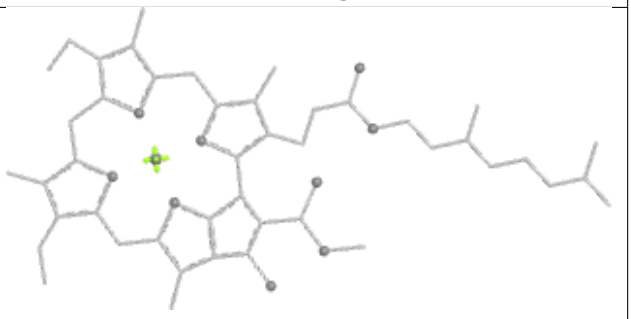
Bond lengths



Bond angles

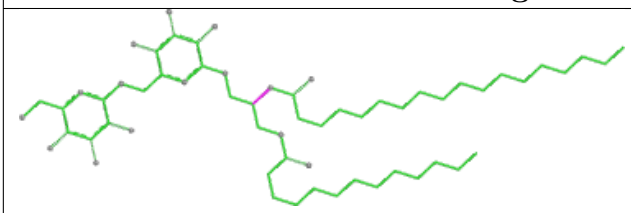


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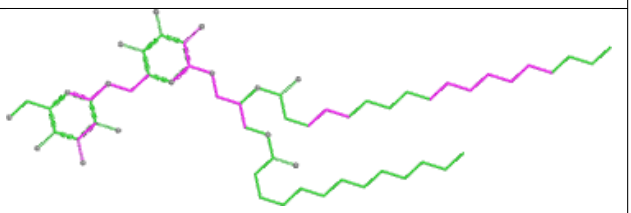


Rings

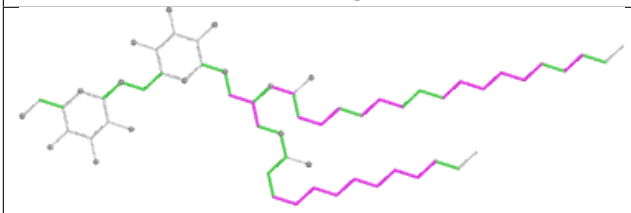
Ligand DGD B 7101



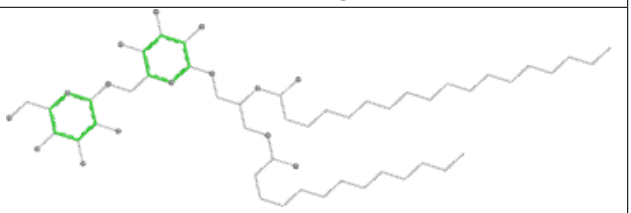
Bond lengths



Bond angles

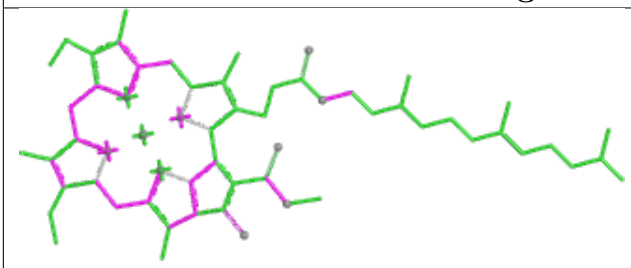


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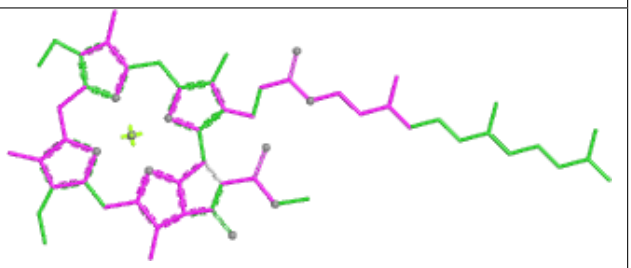


Rings

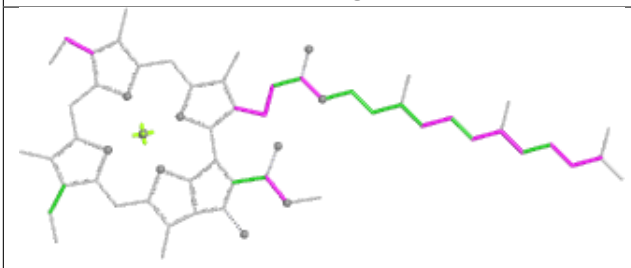
Ligand CLA L 1502



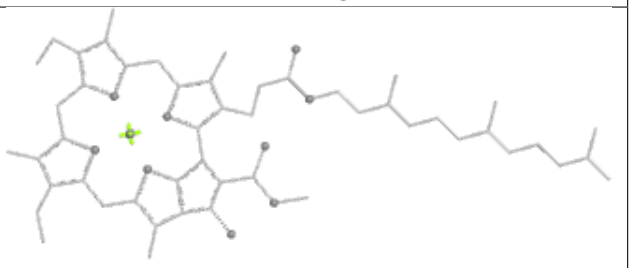
Bond lengths



Bond angles

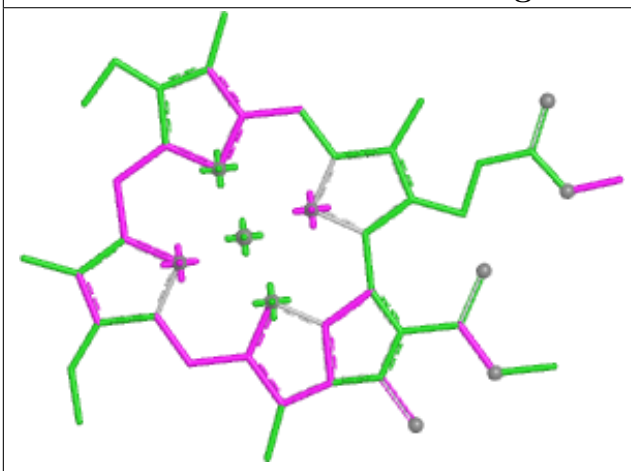


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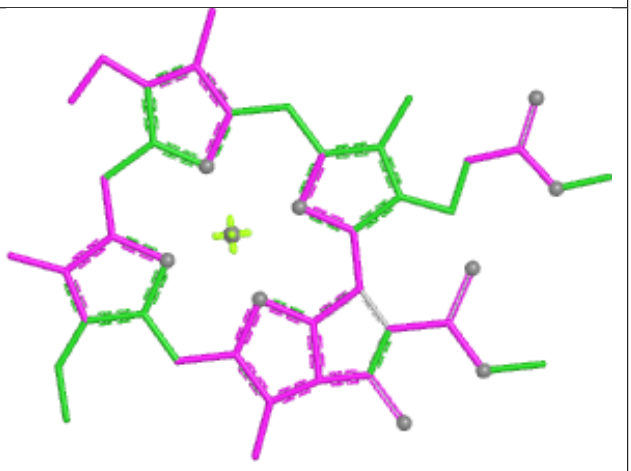


Rings

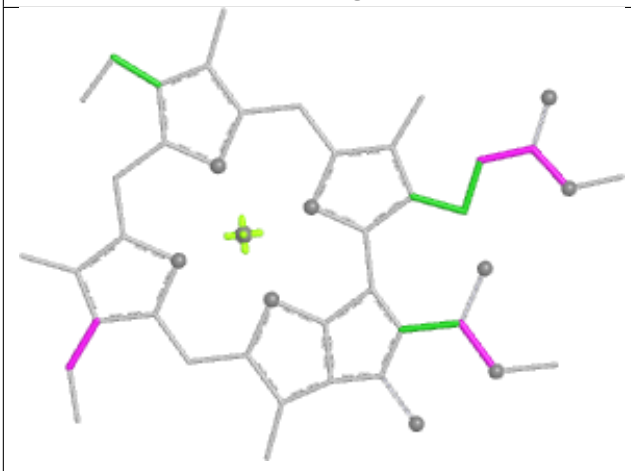
Ligand CLA K 1001



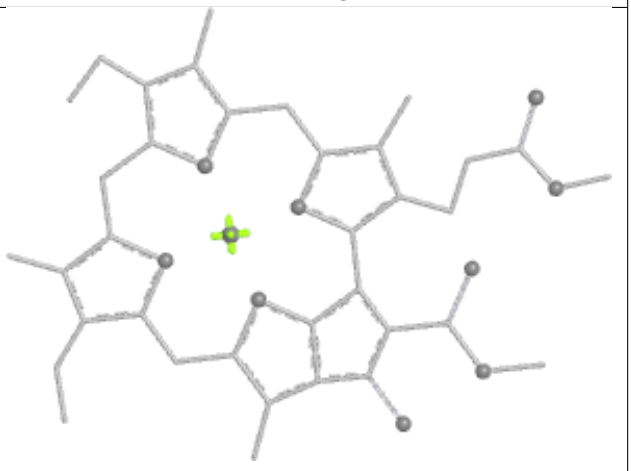
Bond lengths



Bond angles

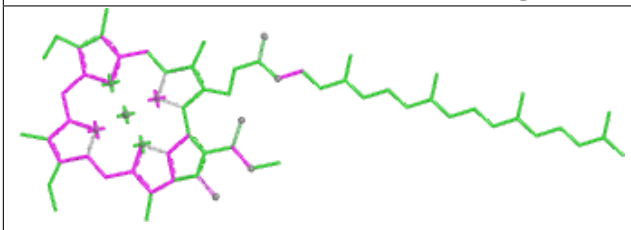


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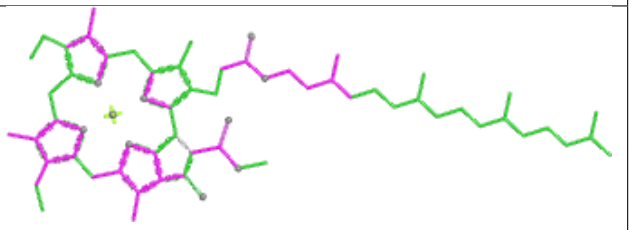


Rings

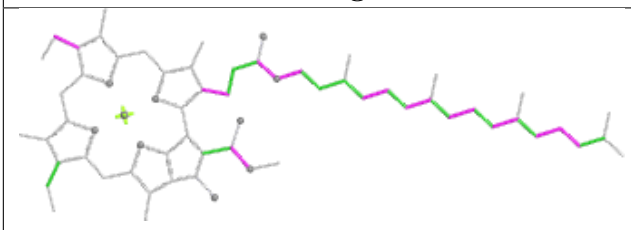
Ligand CLA A 1107



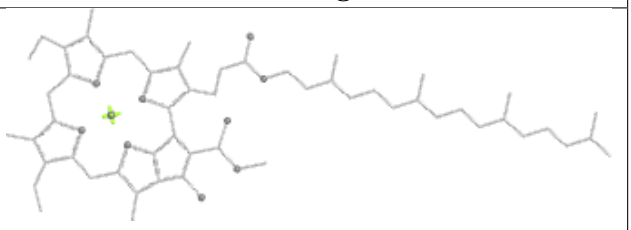
Bond lengths



Bond angles

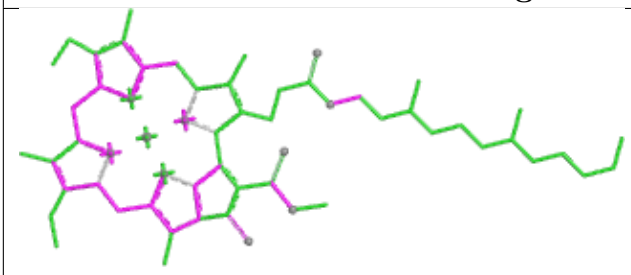


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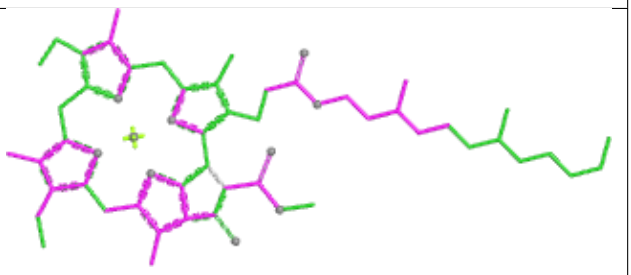


Rings

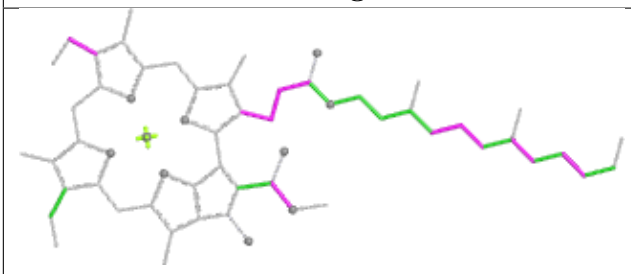
Ligand CLA B 1214



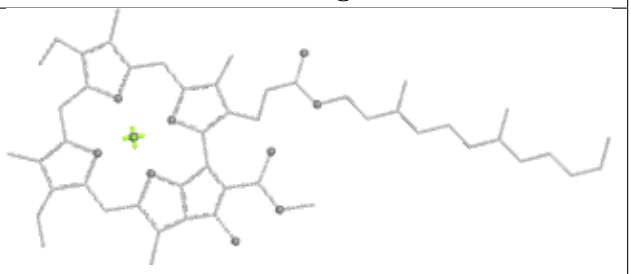
Bond lengths



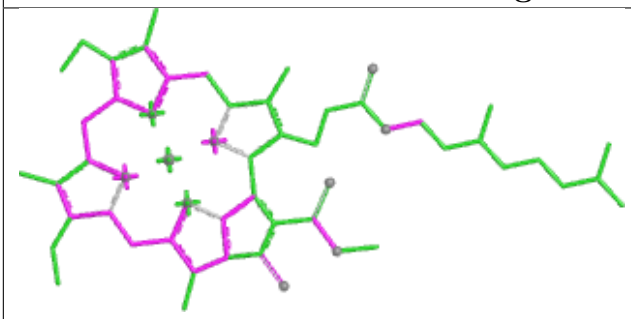
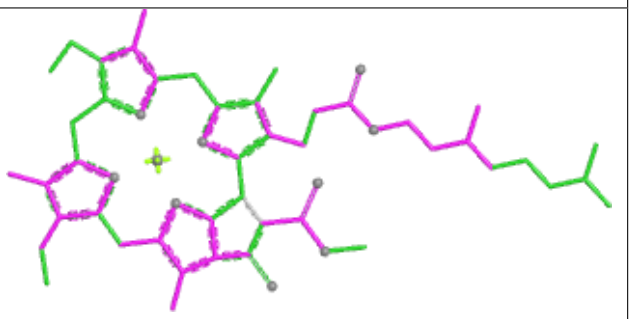
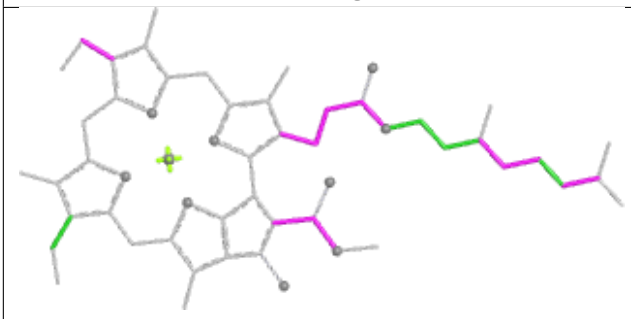
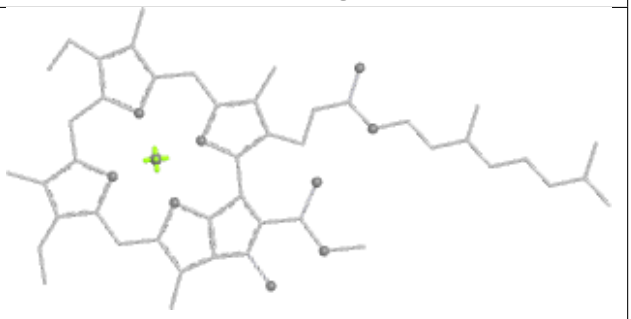
Bond angles

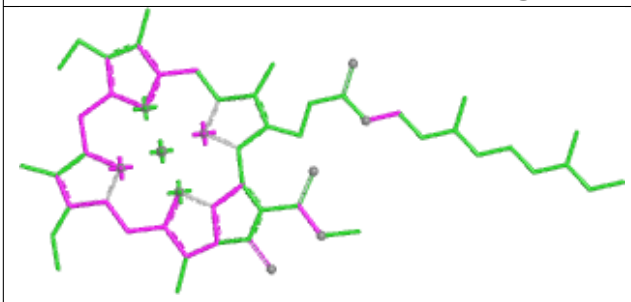
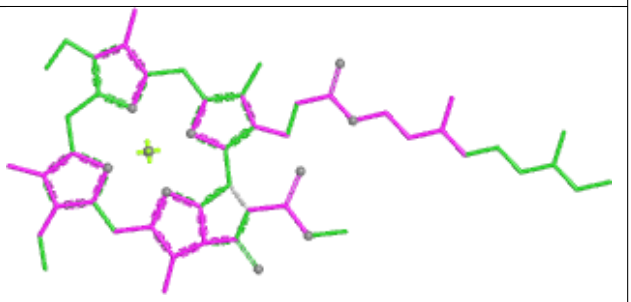
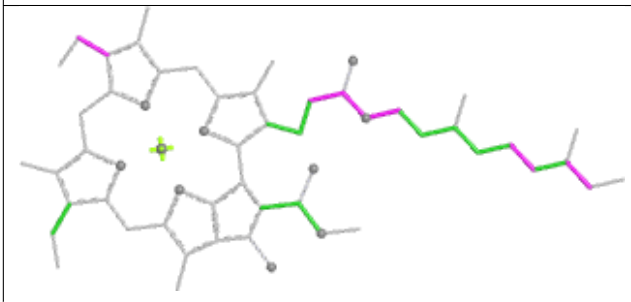
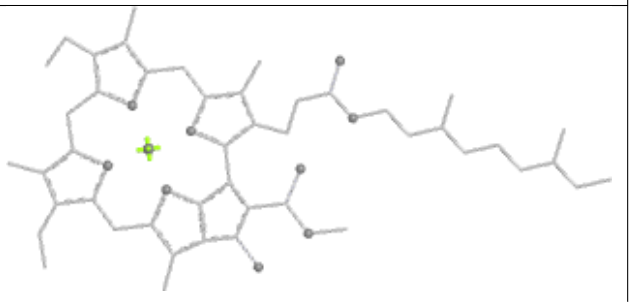


Torsions

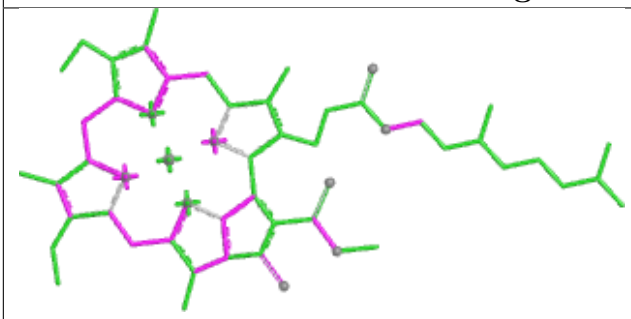


Rings

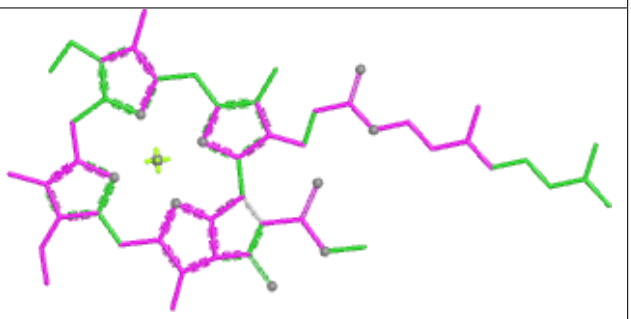
Ligand CLA A 1121	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1136	
 Bond lengths	 Bond angles
 Torsions	 Rings

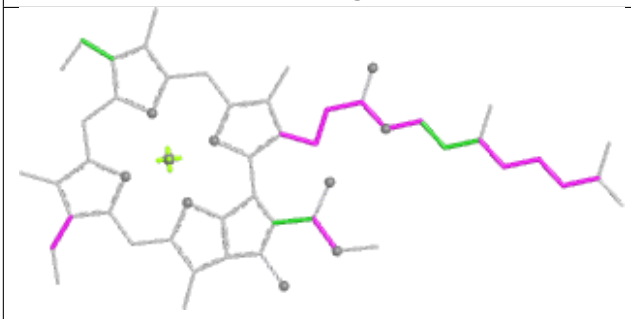
Ligand CLA G 1001



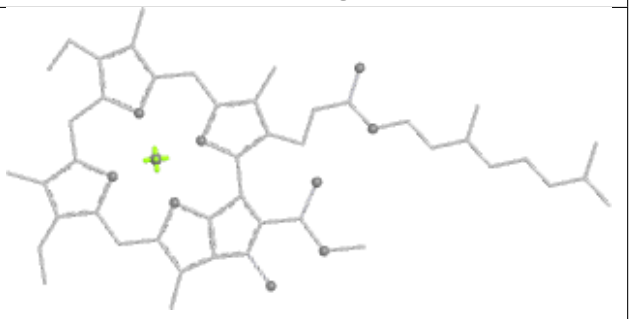
Bond lengths



Bond angles

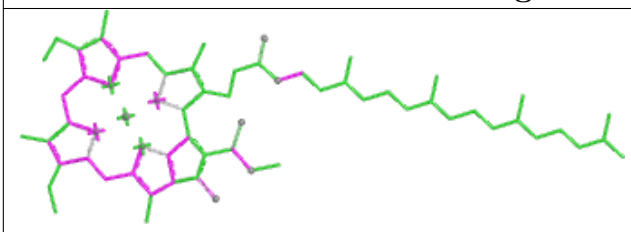


Torsions

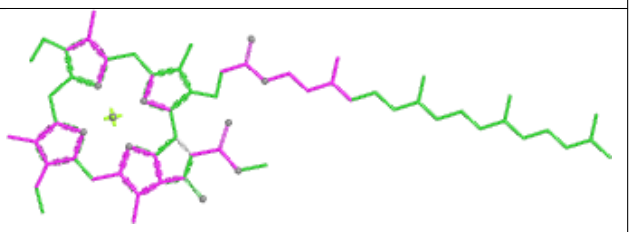


Rings

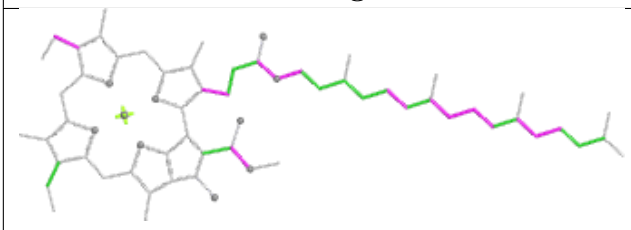
Ligand CLA A 1112



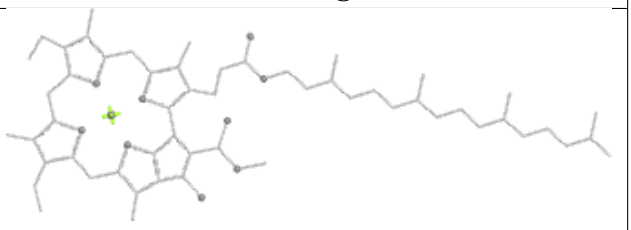
Bond lengths



Bond angles

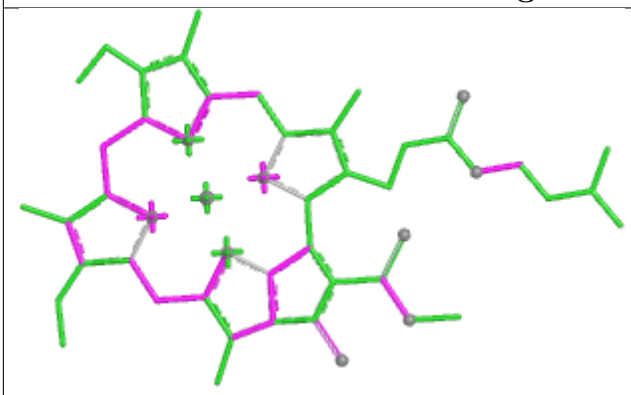


Torsions

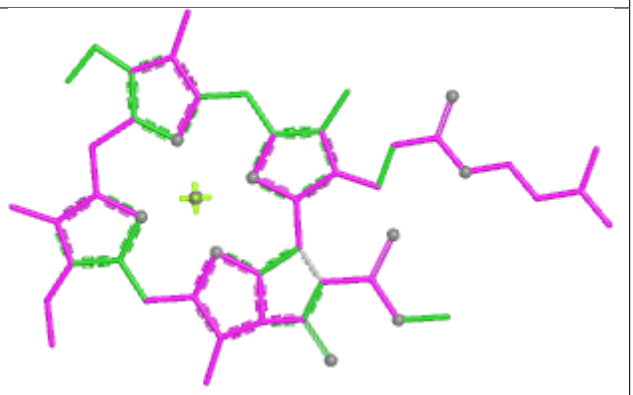


Rings

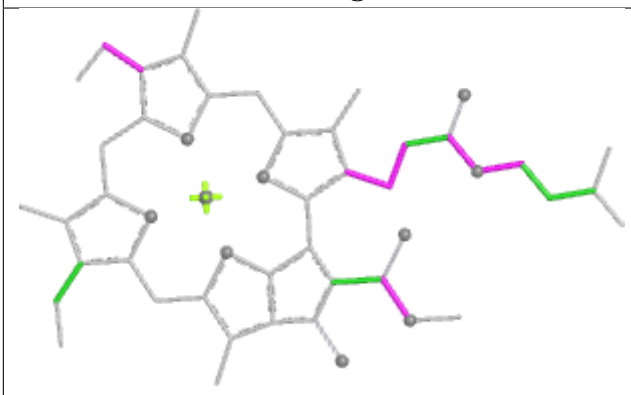
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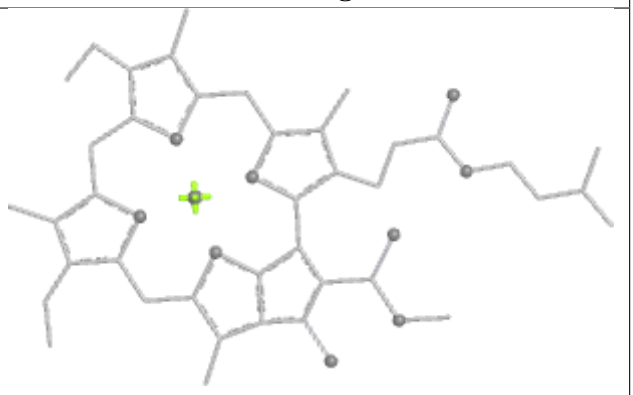
Bond lengths



Bond angles

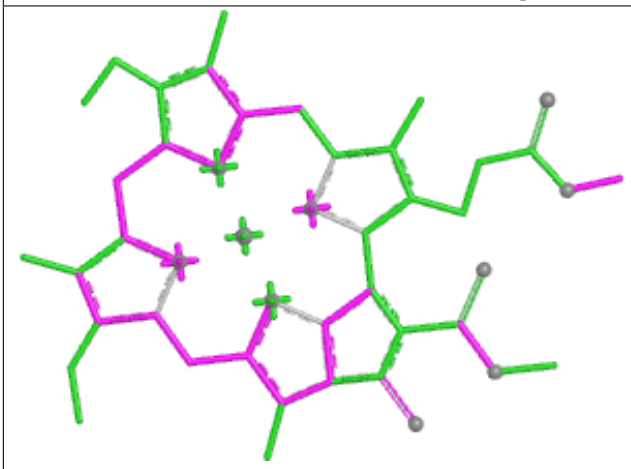


Torsions

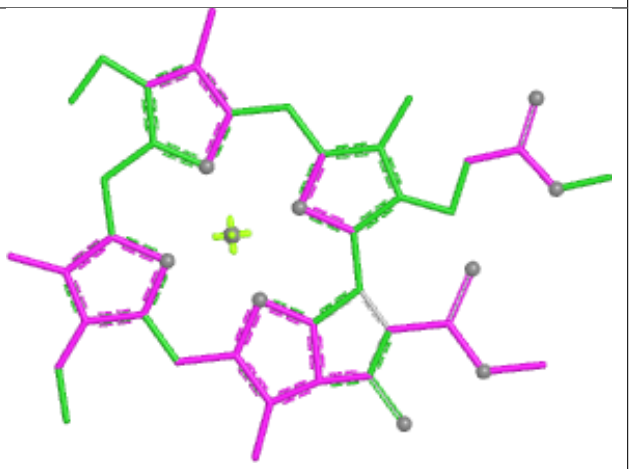


Rings

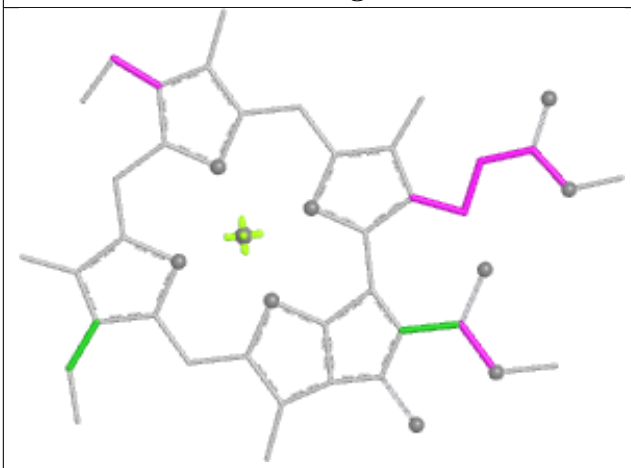
Ligand CLA H 1000



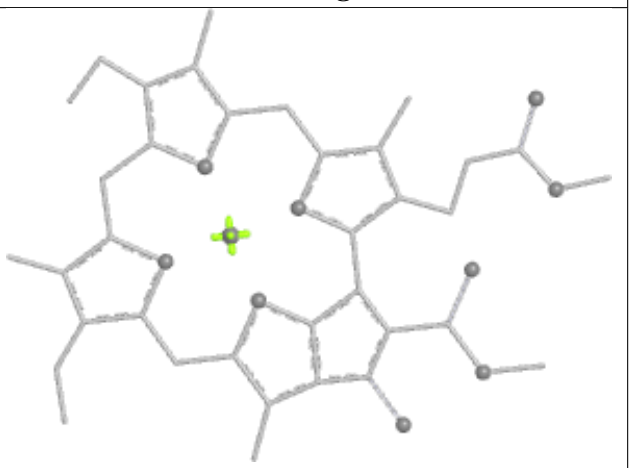
Bond lengths



Bond angles

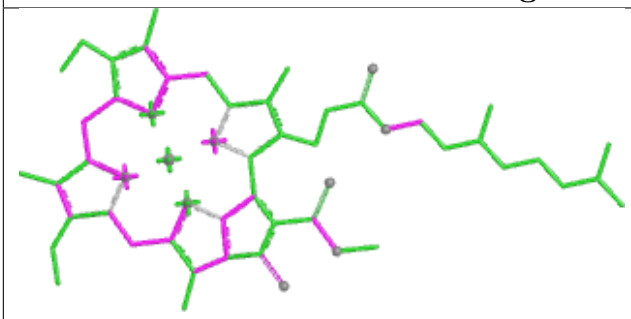


Torsions

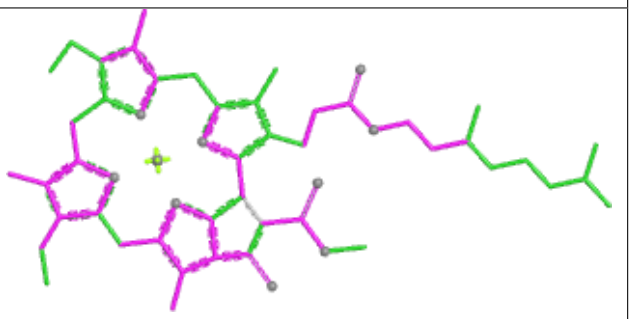


Rings

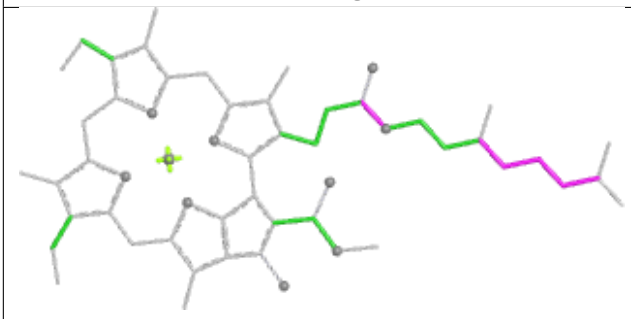
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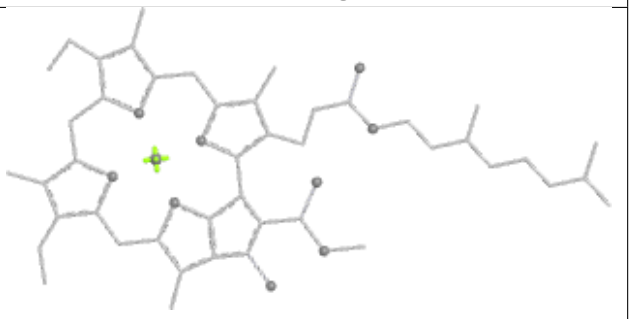
Bond lengths



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	742/758 (97%)	0.64	67 (9%) 15 11	56, 92, 150, 244	0
2	B	732/733 (99%)	0.66	63 (8%) 16 12	61, 89, 126, 157	0
3	I	29/30 (96%)	0.81	5 (17%) 4 3	89, 114, 148, 153	0
4	J	41/42 (97%)	0.78	6 (14%) 6 4	70, 80, 116, 164	0
5	F	150/154 (97%)	0.60	17 (11%) 10 7	66, 90, 122, 157	0
6	G	91/97 (93%)	1.43	24 (26%) 1 1	98, 129, 174, 184	0
7	L	160/167 (95%)	1.21	35 (21%) 2 2	86, 123, 172, 197	0
8	C	80/81 (98%)	0.63	7 (8%) 15 11	66, 81, 96, 106	0
9	D	141/147 (95%)	1.34	35 (24%) 2 1	77, 97, 120, 139	0
10	E	66/66 (100%)	0.55	5 (7%) 20 14	65, 91, 136, 183	0
11	H	84/90 (93%)	1.35	23 (27%) 1 1	103, 138, 178, 234	0
12	K	57/129 (44%)	1.48	18 (31%) 1 1	147, 215, 286, 324	0
13	2	207/269 (76%)	1.00	33 (15%) 5 4	85, 130, 180, 270	0
14	4	198/252 (78%)	0.72	22 (11%) 10 7	84, 121, 193, 274	0
15	1	194/202 (96%)	1.50	51 (26%) 1 1	95, 147, 225, 289	0
16	3	215/275 (78%)	1.46	64 (29%) 1 1	111, 179, 317, 368	0
All	All	3187/3492 (91%)	0.90	475 (14%) 5 4	56, 106, 205, 368	0

All (475) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	D	196	VAL	12.0
2	B	82	PHE	11.4
9	D	200	GLU	9.9
2	B	552	ASP	9.5
9	D	206	LYS	8.6

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Mol	Chain	Res	Type	RSRZ
15	1	103	GLY	8.5
6	G	107	ARG	8.3
15	1	171	SER	8.0
5	F	225	GLU	7.9
16	3	87	GLU	7.4
15	1	162	GLY	7.3
2	B	295	PHE	7.2
11	H	126	VAL	6.9
2	B	157	LEU	6.9
16	3	140	GLY	6.7
2	B	159	PRO	6.6
9	D	197	SER	6.6
7	L	171	LYS	6.6
16	3	272	LEU	6.6
15	1	100	LEU	6.5
1	A	263	ALA	6.3
9	D	208	PRO	6.3
16	3	96	ARG	6.3
15	1	172	LYS	6.2
13	2	132	LEU	6.2
6	G	103	ALA	6.1
7	L	173	PRO	5.8
9	D	207	GLN	5.8
9	D	195	ASN	5.8
15	1	99	ALA	5.7
15	1	174	PRO	5.6
2	B	491	ASN	5.6
9	D	210	ASP	5.5
1	A	139	GLY	5.5
12	K	62	ILE	5.5
2	B	296	GLY	5.5
6	G	147	ASP	5.4
6	G	108	ALA	5.3
16	3	190	LEU	5.3
11	H	117	THR	5.3
13	2	59	VAL	5.2
6	G	109	LYS	5.2
13	2	175	GLY	5.1
15	1	161	PRO	5.1
9	D	211	LEU	5.1
16	3	132	THR	5.0
6	G	88	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
10	E	64	PRO	5.0
4	J	7	TYR	5.0
2	B	88	ALA	4.9
13	2	78	ASP	4.9
13	2	80	SER	4.9
2	B	294	ASN	4.9
15	1	96	VAL	4.8
1	A	250	LEU	4.7
2	B	161	TRP	4.7
7	L	211	TYR	4.7
15	1	160	TYR	4.7
9	D	201	VAL	4.7
1	A	261	SER	4.7
16	3	127	LEU	4.7
5	F	215	ILE	4.7
2	B	282	PHE	4.7
10	E	91	VAL	4.7
15	1	159	LYS	4.6
1	A	517	GLY	4.6
16	3	177	ALA	4.6
2	B	575	ASP	4.6
2	B	639	VAL	4.6
2	B	550	LYS	4.6
1	A	23	ASP	4.5
1	A	277	TYR	4.5
11	H	73	ASP	4.4
13	2	193	VAL	4.4
16	3	77	GLY	4.4
2	B	551	LYS	4.4
2	B	549	ASP	4.3
13	2	157	LEU	4.3
15	1	157	LYS	4.3
15	1	41	TRP	4.2
2	B	554	GLY	4.2
16	3	61	SER	4.2
7	L	53	THR	4.2
16	3	62	LYS	4.2
6	G	144	ASN	4.1
15	1	101	GLY	4.1
11	H	76	SER	4.1
6	G	104	GLY	4.1
14	4	198	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
15	1	102	LEU	4.0
16	3	268	VAL	4.0
7	L	116	LYS	4.0
7	L	111	VAL	4.0
1	A	19	LYS	4.0
11	H	132	PRO	4.0
8	C	32	GLY	4.0
1	A	240	LYS	4.0
15	1	131	LEU	3.9
15	1	158	LYS	3.9
7	L	172	GLN	3.9
7	L	163	SER	3.9
9	D	198	PRO	3.9
1	A	502	THR	3.9
15	1	173	ASP	3.9
1	A	107	GLU	3.9
7	L	115	VAL	3.9
12	K	88	SER	3.9
1	A	614	PHE	3.8
16	3	92	PHE	3.8
16	3	253	TYR	3.8
1	A	354	TRP	3.8
2	B	70	TRP	3.8
2	B	158	GLN	3.8
16	3	144	PRO	3.8
5	F	226	LEU	3.8
12	K	64	SER	3.8
9	D	76	ASP	3.8
1	A	652	TRP	3.8
7	L	170	LYS	3.8
15	1	228	ILE	3.8
10	E	98	ASN	3.8
7	L	131	SER	3.7
9	D	199	ILE	3.7
7	L	176	LEU	3.7
15	1	54	SER	3.7
5	F	229	LYS	3.7
7	L	205	TYR	3.7
13	2	60	ALA	3.7
15	1	168	LEU	3.7
1	A	276	LYS	3.7
1	A	115	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
6	G	105	ASP	3.6
2	B	604	GLY	3.6
9	D	77	PRO	3.6
16	3	143	PRO	3.6
5	F	227	VAL	3.6
13	2	209	ALA	3.6
16	3	60	ALA	3.6
9	D	159	PHE	3.6
2	B	154	TRP	3.6
7	L	212	TYR	3.6
11	H	54	TYR	3.6
16	3	121	TYR	3.6
13	2	184	PRO	3.6
15	1	107	LYS	3.5
2	B	542	ARG	3.5
15	1	204	ALA	3.5
9	D	192	ILE	3.5
2	B	2	ALA	3.5
15	1	59	PHE	3.5
14	4	186	GLY	3.5
6	G	110	GLU	3.5
16	3	122	LEU	3.5
5	F	80	SER	3.5
11	H	121	ASP	3.5
6	G	119	ALA	3.5
15	1	219	ALA	3.5
11	H	53	VAL	3.4
16	3	125	VAL	3.4
1	A	17	GLU	3.4
5	F	143	ASP	3.4
13	2	189	THR	3.4
1	A	758	GLY	3.4
9	D	193	GLY	3.4
16	3	123	GLY	3.4
9	D	204	THR	3.4
15	1	42	MET	3.4
15	1	148	GLN	3.4
16	3	186	TYR	3.4
11	H	81	LEU	3.3
13	2	176	CYS	3.3
6	G	106	SER	3.3
11	H	89	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	555	TYR	3.3
1	A	264	GLU	3.3
1	A	108	ALA	3.3
13	2	208	SER	3.3
14	4	59	GLY	3.3
15	1	60	GLY	3.3
13	2	123	PRO	3.3
7	L	174	ASP	3.3
16	3	178	LYS	3.3
7	L	125	ILE	3.3
4	J	11	ALA	3.3
14	4	164	GLY	3.3
11	H	78	TYR	3.2
15	1	178	HIS	3.2
13	2	86	GLY	3.2
9	D	190	ARG	3.2
2	B	565	GLY	3.2
15	1	227	GLY	3.2
4	J	12	PRO	3.2
16	3	173	PHE	3.2
6	G	102	GLU	3.2
1	A	260	PRO	3.2
16	3	93	ILE	3.2
14	4	74	ASN	3.1
15	1	225	ASN	3.1
2	B	66	PHE	3.1
16	3	130	GLN	3.1
7	L	120	LEU	3.1
9	D	209	TYR	3.1
5	F	228	ALA	3.1
7	L	135	ALA	3.1
9	D	194	LYS	3.1
14	4	139	SER	3.1
1	A	257	GLN	3.1
1	A	649	ILE	3.1
16	3	94	GLU	3.1
1	A	387	THR	3.1
2	B	92	TRP	3.1
1	A	456	HIS	3.1
7	L	208	ASP	3.1
5	F	187	ASP	3.0
2	B	638	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
16	3	95	PRO	3.0
16	3	188	LEU	3.0
7	L	186	THR	3.0
2	B	71	GLN	3.0
9	D	78	ASN	3.0
14	4	52	LYS	3.0
2	B	584	LEU	3.0
2	B	688	ALA	3.0
16	3	118	ALA	3.0
16	3	250	VAL	3.0
15	1	205	TYR	3.0
14	4	149	SER	3.0
16	3	63	GLN	3.0
14	4	178	PRO	3.0
1	A	259	TYR	3.0
1	A	265	GLY	3.0
2	B	5	LEU	3.0
7	L	166	LEU	3.0
16	3	103	VAL	3.0
11	H	125	ILE	2.9
6	G	62	LEU	2.9
6	G	91	GLY	2.9
16	3	134	LEU	2.9
16	3	174	GLN	2.9
14	4	143	VAL	2.9
14	4	172	PHE	2.9
13	2	120	ILE	2.9
8	C	63	LEU	2.9
16	3	269	LEU	2.9
1	A	230	ASN	2.9
13	2	188	LEU	2.9
5	F	216	ALA	2.9
16	3	252	PRO	2.9
16	3	124	LYS	2.9
13	2	121	PHE	2.9
8	C	34	CYS	2.9
1	A	201	SER	2.8
1	A	610	SER	2.8
11	H	123	LEU	2.8
16	3	117	ILE	2.8
9	D	202	LYS	2.8
13	2	226	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	20	ILE	2.8
15	1	117	GLY	2.8
2	B	220	GLN	2.8
7	L	65	PHE	2.8
8	C	4	SER	2.8
11	H	136	GLY	2.8
9	D	73	PRO	2.8
4	J	2	ARG	2.8
16	3	201	ALA	2.8
15	1	232	ILE	2.8
6	G	61	SER	2.8
12	K	87	PRO	2.8
2	B	297	ILE	2.7
5	F	109	TYR	2.7
2	B	229	GLN	2.7
13	2	212	GLN	2.7
5	F	118	ALA	2.7
16	3	257	LEU	2.7
3	I	5	PRO	2.7
7	L	121	ARG	2.7
13	2	165	GLY	2.7
16	3	88	GLY	2.7
7	L	159	SER	2.7
12	K	134	VAL	2.7
13	2	119	GLY	2.7
14	4	226	GLY	2.7
5	F	154	GLN	2.7
3	I	32	LEU	2.7
9	D	184	GLY	2.6
11	H	77	PRO	2.6
1	A	279	ASP	2.6
4	J	10	VAL	2.6
7	L	96	LEU	2.6
15	1	231	LEU	2.6
2	B	395	ILE	2.6
12	K	131	ILE	2.6
7	L	126	ALA	2.6
8	C	35	LYS	2.6
2	B	143	LEU	2.6
2	B	165	VAL	2.6
15	1	218	LEU	2.6
2	B	87	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
13	2	137	TRP	2.6
9	D	116	PRO	2.6
12	K	135	GLY	2.6
16	3	89	THR	2.6
1	A	613	ILE	2.6
2	B	127	ILE	2.6
2	B	98	GLN	2.6
1	A	455	PHE	2.6
12	K	83	PHE	2.6
2	B	180	SER	2.6
13	2	126	LEU	2.6
13	2	127	THR	2.6
14	4	120	ILE	2.6
15	1	151	MET	2.6
9	D	163	GLU	2.6
1	A	549	ILE	2.5
1	A	278	ALA	2.5
1	A	504	ALA	2.5
2	B	360	PHE	2.5
2	B	490	ARG	2.5
11	H	65	GLY	2.5
12	K	138	LEU	2.5
15	1	95	LEU	2.5
15	1	210	PRO	2.5
5	F	81	GLY	2.5
16	3	128	ILE	2.5
12	K	89	ALA	2.5
4	J	8	LEU	2.5
7	L	110	LEU	2.5
15	1	116	GLY	2.5
2	B	487	ASN	2.5
12	K	121	ASP	2.5
11	H	133	PRO	2.5
16	3	228	VAL	2.5
6	G	101	PHE	2.5
1	A	35	ALA	2.5
5	F	189	LYS	2.5
16	3	229	LYS	2.5
16	3	256	LEU	2.4
16	3	65	LEU	2.4
16	3	260	VAL	2.4
1	A	42	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	616	PHE	2.4
6	G	118	ALA	2.4
12	K	86	ALA	2.4
15	1	128	TRP	2.4
15	1	164	ALA	2.4
1	A	271	THR	2.4
9	D	117	THR	2.4
1	A	304	LEU	2.4
1	A	112	ASP	2.4
2	B	101	VAL	2.4
6	G	98	VAL	2.4
10	E	71	GLY	2.4
16	3	114	VAL	2.4
16	3	99	ALA	2.4
1	A	357	GLN	2.4
16	3	141	VAL	2.4
1	A	155	ALA	2.4
16	3	145	ALA	2.4
3	I	15	LEU	2.4
2	B	570	ILE	2.4
6	G	97	GLY	2.3
1	A	513	LEU	2.3
7	L	146	THR	2.3
15	1	155	PRO	2.3
16	3	218	LYS	2.3
1	A	18	VAL	2.3
1	A	122	VAL	2.3
2	B	603	ARG	2.3
1	A	138	GLY	2.3
13	2	178	ASN	2.3
16	3	194	PHE	2.3
14	4	73	ASP	2.3
7	L	207	LEU	2.3
11	H	83	SER	2.3
15	1	176	LYS	2.3
12	K	91	ARG	2.3
2	B	605	ASN	2.3
1	A	460	LEU	2.3
1	A	657	LEU	2.3
11	H	69	LEU	2.3
1	A	27	ILE	2.3
8	C	2	SER	2.3

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Mol	Chain	Res	Type	RSRZ
15	1	150	SER	2.3
6	G	99	THR	2.3
2	B	283	LEU	2.3
7	L	158	PRO	2.3
13	2	181	PRO	2.3
15	1	165	PHE	2.2
16	3	78	PHE	2.2
9	D	133	ALA	2.2
16	3	217	GLU	2.2
16	3	192	LYS	2.2
2	B	136	TYR	2.2
2	B	240	SER	2.2
12	K	68	VAL	2.2
9	D	205	GLY	2.2
16	3	189	GLY	2.2
1	A	103	PHE	2.2
1	A	520	LEU	2.2
1	A	650	ASN	2.2
2	B	232	LEU	2.2
3	I	4	LEU	2.2
14	4	188	ILE	2.2
2	B	391	PRO	2.2
9	D	71	THR	2.2
2	B	505	SER	2.2
14	4	184	TYR	2.2
2	B	557	PHE	2.2
2	B	663	PHE	2.2
2	B	488	ALA	2.2
11	H	135	LEU	2.2
13	2	228	ALA	2.2
16	3	211	LEU	2.2
6	G	59	ASN	2.2
14	4	118	ILE	2.2
11	H	88	THR	2.2
13	2	138	TYR	2.2
13	2	89	PRO	2.2
2	B	226	LEU	2.2
15	1	110	GLU	2.2
1	A	550	HIS	2.1
12	K	122	THR	2.1
15	1	111	TRP	2.1
12	K	85	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
16	3	213	PHE	2.1
2	B	292	ARG	2.1
7	L	138	VAL	2.1
10	E	129	LYS	2.1
2	B	214	ASP	2.1
14	4	119	GLY	2.1
1	A	140	PHE	2.1
7	L	114	PHE	2.1
13	2	77	LEU	2.1
15	1	144	PHE	2.1
5	F	220	GLU	2.1
9	D	161	SER	2.1
1	A	408	VAL	2.1
1	A	487	VAL	2.1
14	4	191	PRO	2.1
6	G	92	LEU	2.1
7	L	97	LEU	2.1
13	2	190	GLY	2.1
7	L	169	ARG	2.1
1	A	386	ALA	2.1
2	B	166	SER	2.1
3	I	6	SER	2.1
5	F	113	SER	2.1
6	G	96	ASN	2.1
9	D	100	PHE	2.1
8	C	61	ASP	2.1
11	H	96	ARG	2.1
9	D	98	GLU	2.1
13	2	195	TYR	2.1
16	3	181	SER	2.0
1	A	644	GLN	2.0
14	4	192	LEU	2.0
1	A	750	PHE	2.0
2	B	119	GLY	2.0
1	A	291	THR	2.0
1	A	639	THR	2.0
7	L	123	THR	2.0
12	K	142	THR	2.0
15	1	170	TYR	2.0
1	A	543	HIS	2.0
14	4	98	ASN	2.0
16	3	149	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
15	1	177	PHE	2.0
1	A	323	ILE	2.0
11	H	122	ILE	2.0
14	4	219	ILE	2.0
16	3	216	ASP	2.0
12	K	92	LYS	2.0
9	D	156	TYR	2.0
1	A	449	VAL	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
18	CLA	3	3019	27/65	0.45	0.27	158,174,188,189	1
23	LMG	B	5005	38/55	0.63	0.20	76,120,141,143	0
18	CLA	J	1302	50/65	0.66	0.20	137,152,189,196	0
18	CLA	4	4016	46/65	0.68	0.18	126,166,177,183	0
18	CLA	3	3008	48/65	0.69	0.17	180,199,214,217	0
18	CLA	2	2019	27/65	0.71	0.17	148,159,174,174	1
18	CLA	3	3010	60/65	0.73	0.26	122,158,181,196	0
18	CLA	2	2016	50/65	0.75	0.19	114,164,207,211	0
26	LMU	B	8002	35/35	0.76	0.18	162,173,189,191	0
18	CLA	3	3018	50/65	0.78	0.16	173,190,207,213	0
23	LMG	F	5002	37/55	0.78	0.13	84,107,120,126	0
26	LMU	B	8001	35/35	0.78	0.14	104,158,168,172	0
18	CLA	K	1001	46/65	0.78	0.16	147,173,200,209	0
18	CLA	3	3007	50/65	0.79	0.18	175,193,239,246	0
18	CLA	1	1013	46/65	0.80	0.17	127,154,181,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	3	3013	46/65	0.80	0.16	127,157,166,176	0
18	CLA	G	1003	60/65	0.81	0.16	97,121,149,153	0
18	CLA	H	1000	46/65	0.82	0.14	119,150,170,176	0
22	BCR	G	2011	40/40	0.82	0.20	112,132,172,174	0
28	CHL	2	2010	47/66	0.82	0.12	111,134,142,143	0
22	BCR	J	6013	40/40	0.83	0.18	74,94,112,116	0
23	LMG	F	5001	23/55	0.83	0.10	86,94,106,109	0
18	CLA	1	1001	60/65	0.83	0.17	122,151,165,171	0
22	BCR	K	2011	40/40	0.84	0.22	125,136,144,147	0
18	CLA	3	3006	50/65	0.84	0.12	125,157,167,170	0
23	LMG	G	2021	41/55	0.84	0.19	138,156,175,176	0
28	CHL	3	3011	56/66	0.84	0.18	144,156,197,200	0
18	CLA	A	1151	50/65	0.85	0.13	99,113,187,189	0
18	CLA	A	1113	46/65	0.85	0.16	119,135,172,187	0
27	LUT	3	3501	42/42	0.85	0.26	202,209,216,218	0
18	CLA	L	1501	50/65	0.85	0.15	106,129,153,159	0
28	CHL	4	4010	47/66	0.85	0.16	105,125,180,187	0
23	LMG	2	2802	35/55	0.85	0.17	108,127,149,152	0
18	CLA	A	1134	55/65	0.86	0.16	112,124,168,172	0
22	BCR	L	6020	40/40	0.86	0.19	98,131,157,164	0
18	CLA	1	1006	50/65	0.86	0.14	125,138,144,148	0
18	CLA	1	1008	46/65	0.86	0.17	112,129,142,150	0
18	CLA	A	1114	46/65	0.86	0.12	107,117,124,136	0
18	CLA	4	4006	50/65	0.86	0.16	110,127,148,156	0
18	CLA	2	2006	55/65	0.86	0.15	105,132,173,174	0
22	BCR	A	6007	40/40	0.87	0.17	77,90,147,151	0
18	CLA	A	1115	46/65	0.87	0.15	107,141,170,178	0
28	CHL	2	2013	46/66	0.87	0.14	110,125,130,135	0
18	CLA	3	3002	46/65	0.87	0.15	173,188,195,222	0
18	CLA	G	1001	55/65	0.87	0.14	119,145,181,184	0
18	CLA	B	1218	65/65	0.88	0.17	86,100,155,160	0
18	CLA	1	1014	46/65	0.88	0.12	83,110,123,143	0
18	CLA	4	4008	46/65	0.88	0.14	93,112,129,137	0
28	CHL	1	1010	47/66	0.88	0.14	125,137,152,155	0
22	BCR	3	3503	40/40	0.88	0.21	119,136,175,177	0
27	LUT	1	1501	42/42	0.89	0.23	115,142,189,197	0
18	CLA	1	1011	50/65	0.89	0.17	126,153,175,185	0
23	LMG	4	4801	35/55	0.89	0.18	104,117,128,132	0
18	CLA	G	1002	46/65	0.89	0.11	142,160,173,181	0
22	BCR	B	6004	40/40	0.89	0.22	105,112,138,144	0
27	LUT	2	2502	42/42	0.89	0.22	102,115,124,131	0
27	LUT	4	4503	42/42	0.89	0.22	110,135,158,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	LMG	J	5001	55/55	0.90	0.17	62,96,110,122	0
18	CLA	L	1503	50/65	0.90	0.12	106,114,143,149	0
18	CLA	B	1232	55/65	0.90	0.12	80,97,118,122	0
27	LUT	1	1502	42/42	0.90	0.19	85,116,128,129	0
18	CLA	3	3001	50/65	0.90	0.11	147,169,201,206	0
27	LUT	3	3502	42/42	0.90	0.21	133,142,164,166	0
18	CLA	4	4001	60/65	0.90	0.17	113,129,158,160	0
18	CLA	A	1121	55/65	0.90	0.13	104,123,209,211	0
21	LHG	B	5004	21/49	0.90	0.11	86,102,116,119	0
28	CHL	4	4013	47/66	0.90	0.12	98,118,130,134	0
18	CLA	B	1213	60/65	0.90	0.15	85,105,118,126	0
27	LUT	2	2501	42/42	0.90	0.20	121,137,141,143	0
29	ZEX	4	4505	42/42	0.90	0.13	85,96,107,114	0
22	BCR	A	6008	40/40	0.91	0.20	76,97,137,139	0
18	CLA	1	1002	46/65	0.91	0.15	120,155,171,194	0
22	BCR	B	6009	40/40	0.91	0.17	63,78,94,95	0
18	CLA	1	1005	55/65	0.91	0.13	84,113,122,124	0
18	CLA	B	1201	50/65	0.91	0.14	80,93,131,134	0
18	CLA	B	1208	55/65	0.91	0.13	82,114,133,137	0
18	CLA	B	1238	65/65	0.91	0.15	70,85,96,116	0
18	CLA	3	3017	46/65	0.91	0.14	101,119,134,145	0
18	CLA	B	1228	60/65	0.91	0.15	63,73,111,114	0
18	CLA	B	1217	46/65	0.91	0.14	96,109,124,127	0
21	LHG	A	5003	40/49	0.91	0.16	101,117,132,134	0
18	CLA	A	1120	60/65	0.91	0.14	95,118,178,182	0
21	LHG	2	2801	24/49	0.91	0.14	109,123,148,152	0
22	BCR	A	6003	40/40	0.91	0.21	79,94,139,140	0
18	CLA	B	1219	60/65	0.91	0.16	82,97,134,135	0
25	DGD	B	7101	61/66	0.91	0.15	62,79,104,113	0
18	CLA	A	1105	51/65	0.92	0.12	66,88,97,100	0
18	CLA	2	2002	46/65	0.92	0.12	137,154,171,183	0
18	CLA	2	2004	65/65	0.92	0.14	84,105,117,125	0
18	CLA	2	2005	55/65	0.92	0.13	93,103,129,135	0
18	CLA	3	3003	60/65	0.92	0.14	137,170,188,190	0
18	CLA	3	3004	60/65	0.92	0.15	125,139,154,155	0
18	CLA	B	1209	46/65	0.92	0.13	100,109,118,145	0
18	CLA	B	1212	55/65	0.92	0.16	109,129,146,154	0
18	CLA	B	1231	60/65	0.92	0.12	65,81,101,104	0
18	CLA	A	1108	46/65	0.92	0.12	85,101,121,126	0
18	CLA	3	3012	50/65	0.92	0.13	117,135,142,144	0
18	CLA	4	4002	50/65	0.92	0.15	107,141,171,211	0
18	CLA	B	1240	65/65	0.92	0.12	66,84,103,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	4	4007	60/65	0.92	0.17	110,130,179,183	0
18	CLA	B	1021	65/65	0.92	0.15	61,72,80,83	0
18	CLA	F	1301	45/65	0.92	0.12	61,73,86,101	0
18	CLA	4	4017	65/65	0.92	0.16	93,103,120,121	0
18	CLA	B	1204	55/65	0.92	0.12	80,103,118,124	0
21	LHG	1	1801	49/49	0.92	0.17	94,113,164,170	0
22	BCR	A	6002	40/40	0.92	0.21	82,115,168,169	0
18	CLA	A	1112	65/65	0.92	0.15	101,118,138,140	0
18	CLA	A	1124	55/65	0.92	0.14	59,77,104,116	0
18	CLA	A	1022	65/65	0.92	0.14	58,76,88,99	0
18	CLA	1	1007	46/65	0.92	0.12	112,131,162,181	0
22	BCR	B	6005	40/40	0.92	0.21	87,103,182,184	0
18	CLA	B	1220	65/65	0.92	0.15	61,76,114,118	0
22	BCR	J	6012	40/40	0.92	0.15	67,80,89,91	0
18	CLA	A	1139	65/65	0.92	0.14	56,70,98,104	0
18	CLA	A	1133	55/65	0.93	0.14	83,109,120,126	0
18	CLA	2	2003	55/65	0.93	0.12	103,127,135,158	0
22	BCR	F	6016	40/40	0.93	0.12	66,75,91,94	0
18	CLA	B	1211	65/65	0.93	0.13	93,107,131,136	0
18	CLA	A	1109	65/65	0.93	0.12	71,85,94,101	0
22	BCR	L	6019	40/40	0.93	0.24	88,105,132,135	0
18	CLA	B	1239	65/65	0.93	0.14	69,82,111,116	0
18	CLA	2	2007	60/65	0.93	0.15	116,142,189,195	0
18	CLA	2	2012	55/65	0.93	0.13	86,104,149,153	0
18	CLA	B	1214	59/65	0.93	0.16	71,91,100,108	0
18	CLA	B	1227	65/65	0.93	0.13	60,74,99,105	0
18	CLA	2	2009	50/65	0.93	0.12	100,117,138,139	0
18	CLA	A	1135	51/65	0.93	0.14	72,92,114,117	0
18	CLA	A	1137	55/65	0.93	0.13	71,85,125,126	0
18	CLA	4	4003	65/65	0.93	0.13	84,106,135,143	0
18	CLA	4	4004	60/65	0.93	0.14	76,99,112,118	0
18	CLA	B	1234	60/65	0.93	0.15	64,77,106,108	0
18	CLA	A	1126	65/65	0.93	0.15	65,79,87,97	0
27	LUT	I	6018	42/42	0.93	0.15	101,109,116,121	0
18	CLA	A	1131	65/65	0.93	0.16	79,93,103,112	0
18	CLA	4	4012	65/65	0.93	0.14	92,104,117,120	0
27	LUT	4	4501	42/42	0.93	0.15	107,121,142,149	0
27	LUT	4	4502	42/42	0.93	0.16	88,106,117,121	0
18	CLA	A	1118	46/65	0.93	0.13	99,108,127,131	0
18	CLA	A	1129	50/65	0.93	0.11	71,93,115,126	0
18	CLA	A	1101	65/65	0.93	0.12	58,72,90,113	0
18	CLA	B	1222	65/65	0.93	0.15	58,74,103,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	1	1004	65/65	0.93	0.14	98,114,122,125	0
18	CLA	L	1502	60/65	0.93	0.13	86,116,125,130	0
28	CHL	2	2011	48/66	0.93	0.14	108,124,129,136	0
18	CLA	B	1012	65/65	0.93	0.15	51,69,85,92	0
18	CLA	B	1207	65/65	0.93	0.14	78,102,122,129	0
22	BCR	B	6006	40/40	0.93	0.19	94,115,164,164	0
28	CHL	1	1009	56/66	0.93	0.12	92,105,113,130	0
18	CLA	B	1216	65/65	0.93	0.14	73,86,105,108	0
22	BCR	B	6010	40/40	0.93	0.15	64,73,96,100	0
22	BCR	I	6020	40/40	0.93	0.16	85,97,110,111	0
18	CLA	A	1123	65/65	0.94	0.16	70,88,93,96	0
18	CLA	B	1221	65/65	0.94	0.14	66,78,115,122	0
18	CLA	A	1119	65/65	0.94	0.14	78,95,107,115	0
18	CLA	B	1223	65/65	0.94	0.14	59,78,90,96	0
18	CLA	A	1102	50/65	0.94	0.11	58,69,95,104	0
18	CLA	A	1110	55/65	0.94	0.15	97,114,138,143	0
24	CA	B	6000	1/1	0.94	0.09	100,100,100,100	0
18	CLA	A	1127	65/65	0.94	0.15	69,83,95,99	0
18	CLA	1	1003	55/65	0.94	0.14	100,122,134,142	0
18	CLA	2	2001	60/65	0.94	0.16	114,134,167,169	0
18	CLA	A	1111	60/65	0.94	0.13	75,91,112,118	0
18	CLA	A	1132	65/65	0.94	0.14	79,94,120,129	0
18	CLA	B	1236	55/65	0.94	0.14	56,69,117,124	0
18	CLA	A	1104	65/65	0.94	0.13	55,73,81,85	0
18	CLA	A	1237	60/65	0.94	0.14	75,94,113,116	0
18	CLA	1	1012	50/65	0.94	0.11	103,125,130,132	0
18	CLA	B	1224	65/65	0.94	0.15	65,83,100,107	0
18	CLA	B	1226	65/65	0.94	0.14	65,76,97,103	0
18	CLA	A	1106	65/65	0.94	0.13	59,74,90,106	0
18	CLA	A	1136	56/65	0.94	0.12	84,98,115,119	0
18	CLA	B	1023	65/65	0.94	0.12	57,70,94,105	0
22	BCR	F	6014	40/40	0.94	0.12	54,64,73,74	0
18	CLA	A	1107	65/65	0.94	0.13	60,77,94,105	0
18	CLA	3	3005	55/65	0.94	0.14	107,131,144,157	0
17	CL0	A	1011	65/65	0.94	0.13	52,70,82,84	0
18	CLA	A	1122	65/65	0.94	0.15	76,96,122,139	0
18	CLA	F	1302	50/65	0.94	0.09	67,84,114,124	0
18	CLA	4	4005	60/65	0.94	0.13	84,97,106,120	0
18	CLA	A	1116	60/65	0.94	0.14	89,119,137,142	0
21	LHG	A	7001	49/49	0.95	0.13	56,72,84,92	0
18	CLA	A	1130	50/65	0.95	0.13	83,100,123,127	0
18	CLA	A	1013	65/65	0.95	0.12	49,62,74,90	0

Continued on next page...

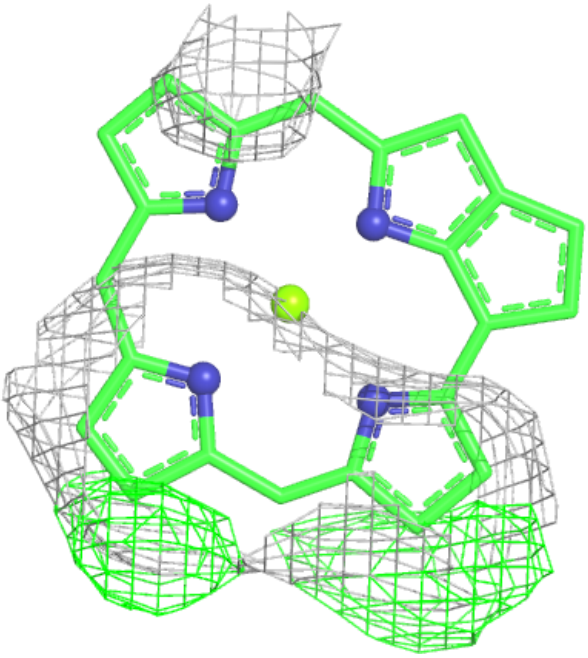
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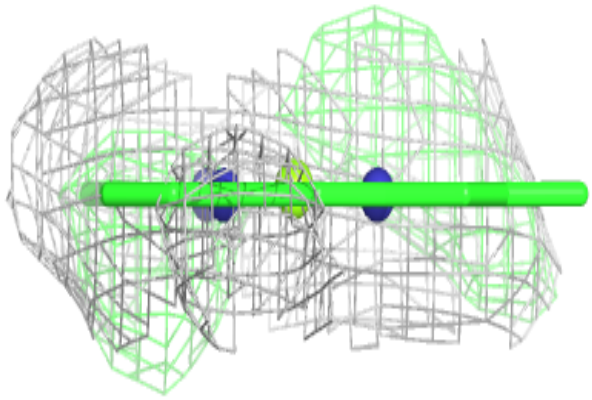
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	2	2008	50/65	0.95	0.13	109,138,148,156	0
18	CLA	A	1117	65/65	0.95	0.16	85,98,110,114	0
18	CLA	B	1215	60/65	0.95	0.13	82,91,102,109	0
18	CLA	A	1103	65/65	0.95	0.12	66,83,104,107	0
18	CLA	B	1225	65/65	0.95	0.14	66,81,98,105	0
22	BCR	A	6017	40/40	0.95	0.16	71,86,105,122	0
18	CLA	B	1235	65/65	0.95	0.09	54,68,78,92	0
18	CLA	B	1205	65/65	0.95	0.15	90,103,116,152	0
18	CLA	B	1202	65/65	0.95	0.14	71,82,91,104	0
18	CLA	B	1230	58/65	0.95	0.10	58,74,83,86	0
28	CHL	4	4011	51/66	0.95	0.13	117,131,149,154	0
18	CLA	B	1206	65/65	0.95	0.12	86,104,112,127	0
18	CLA	A	1128	65/65	0.95	0.12	56,66,74,85	0
18	CLA	A	1140	65/65	0.95	0.12	58,66,78,106	0
20	PQN	A	5001	33/33	0.95	0.12	53,63,76,85	0
18	CLA	A	1125	60/65	0.95	0.12	79,94,102,114	0
18	CLA	A	1138	65/65	0.96	0.11	55,65,75,82	0
22	BCR	A	6011	40/40	0.96	0.13	61,73,88,96	0
18	CLA	B	1229	65/65	0.96	0.11	60,72,82,84	0
18	CLA	B	1203	65/65	0.96	0.11	68,82,97,104	0
20	PQN	B	5002	33/33	0.96	0.11	54,72,91,93	0
18	CLA	B	1210	65/65	0.96	0.14	81,94,107,113	0
18	CLA	4	4009	50/65	0.96	0.11	85,94,116,131	0
19	SF4	C	3003	8/8	0.97	0.05	89,106,119,126	0
19	SF4	C	3002	8/8	0.97	0.05	73,103,107,107	0
19	SF4	A	3001	8/8	0.98	0.04	69,95,97,99	0

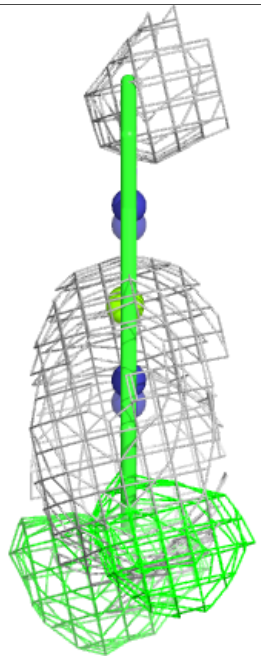
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA 3 3019:

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

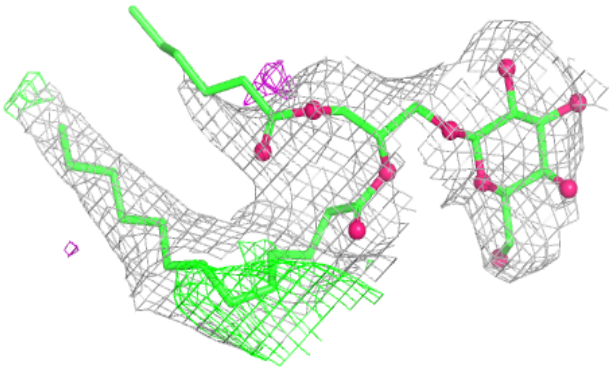


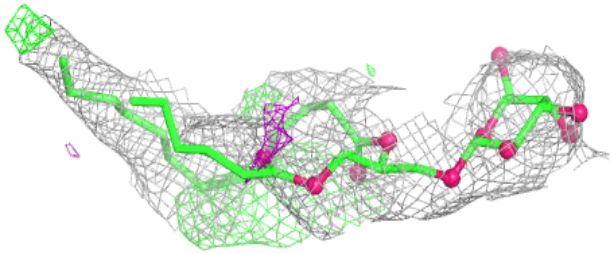


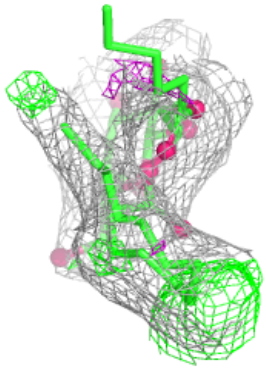


Electron density around LMG B 5005:

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

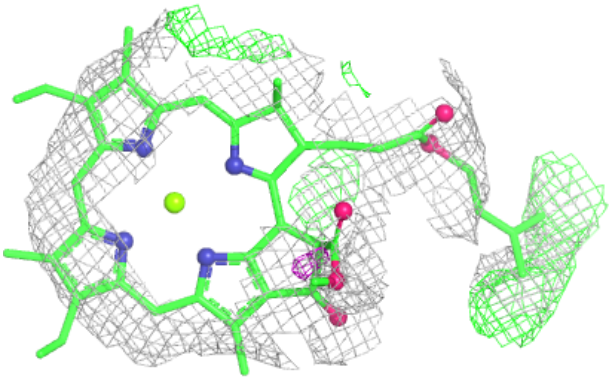


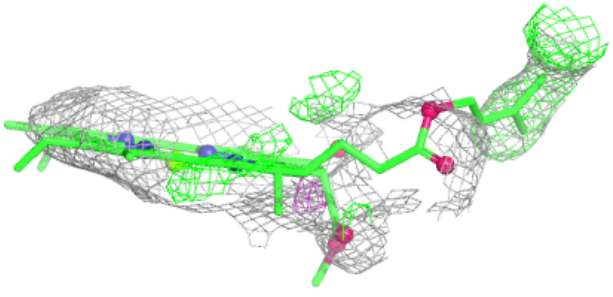


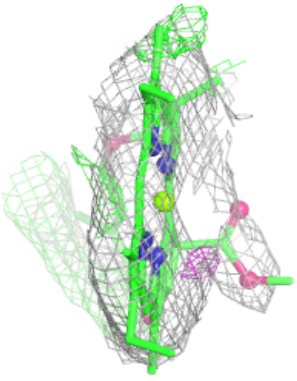


Electron density around CLA J 1302:

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

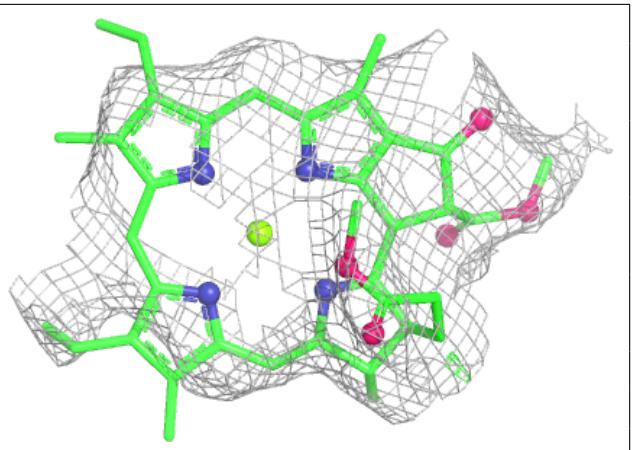


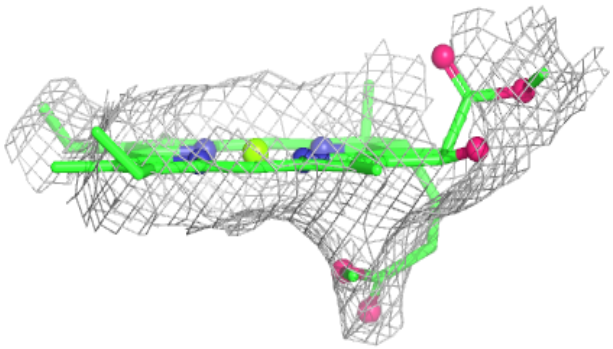


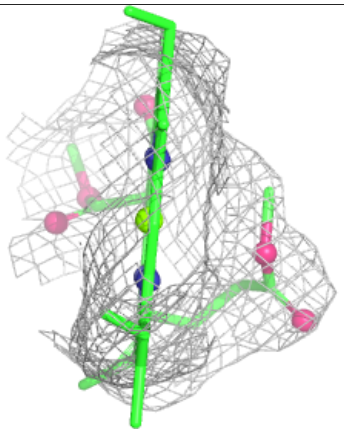


Electron density around CLA 4 4016:

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

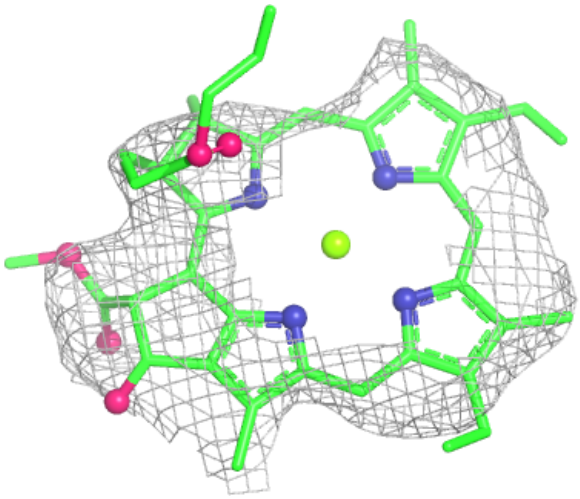


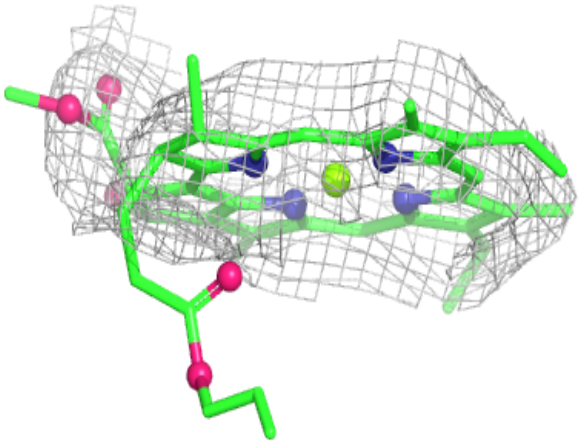




Electron density around CLA 3 3008:

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

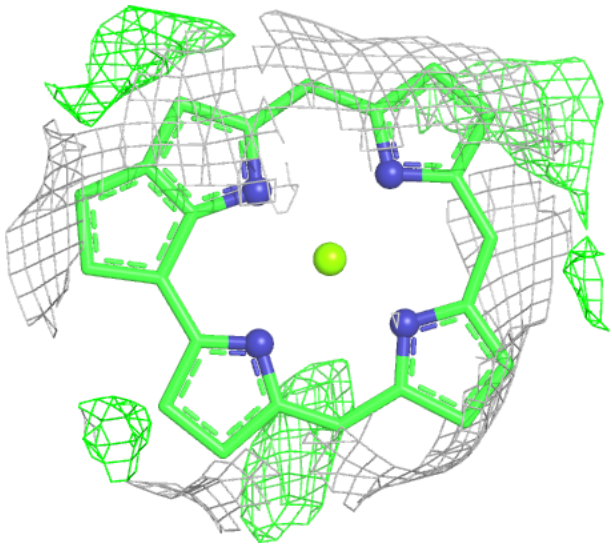


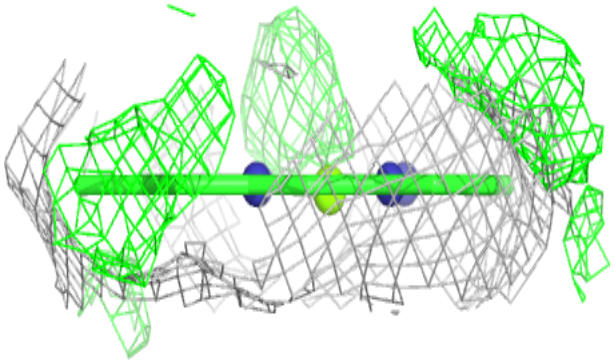


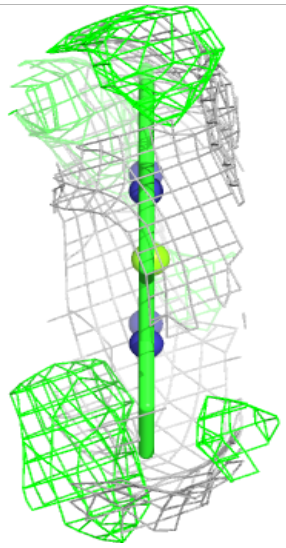


Electron density around CLA 2 2019:

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

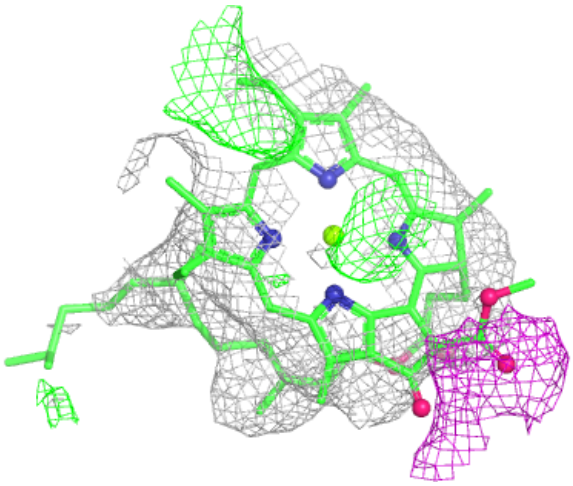


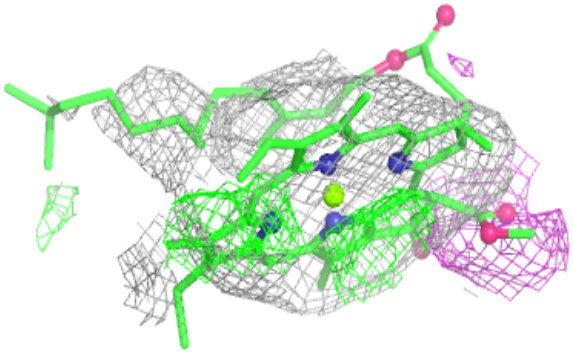


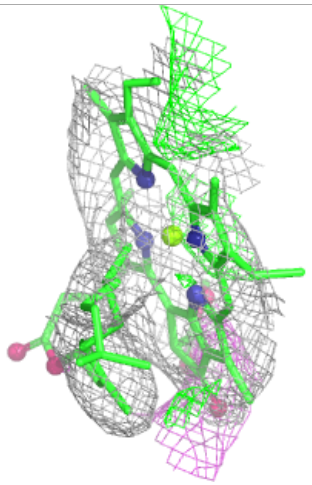


Electron density around CLA 3 3010:

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

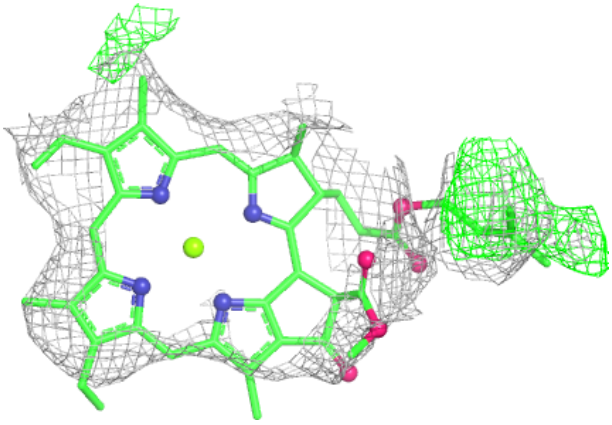


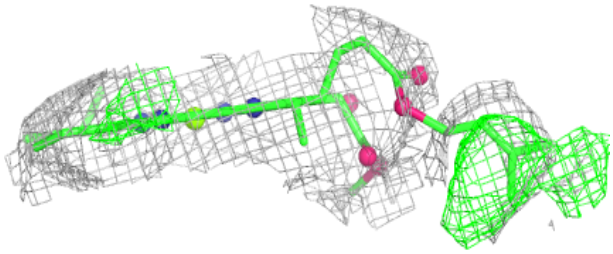


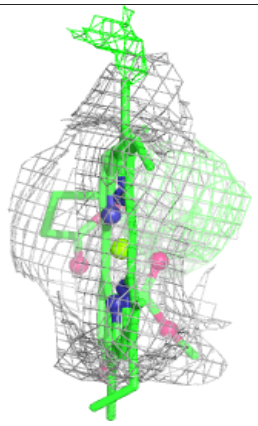


Electron density around CLA 2 2016:

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

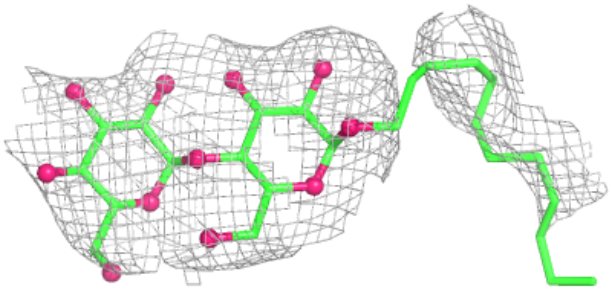


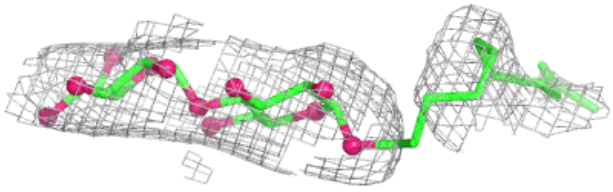


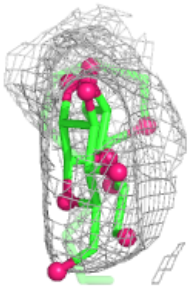


Electron density around LMU B 8002:

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

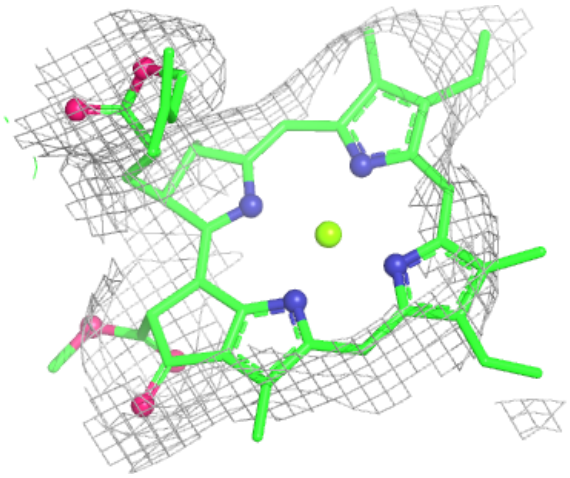


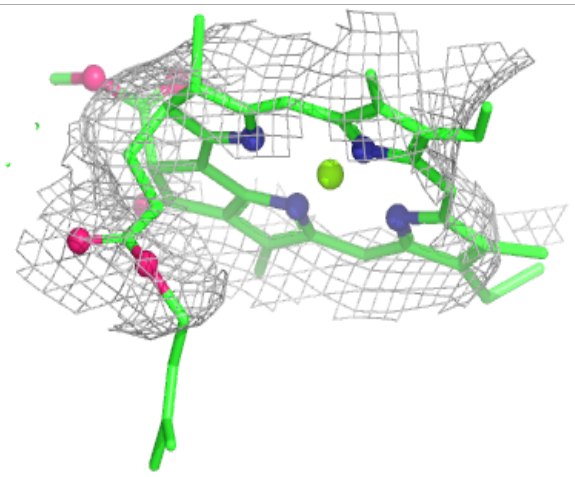


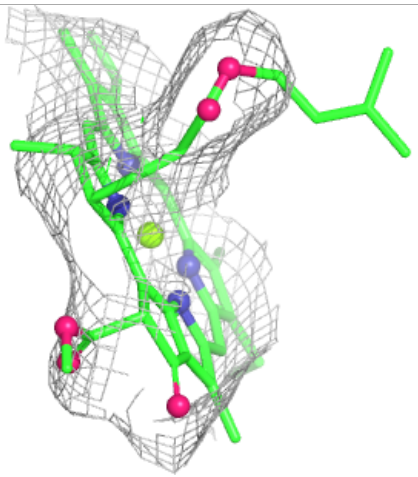


Electron density around CLA 3 3018:

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

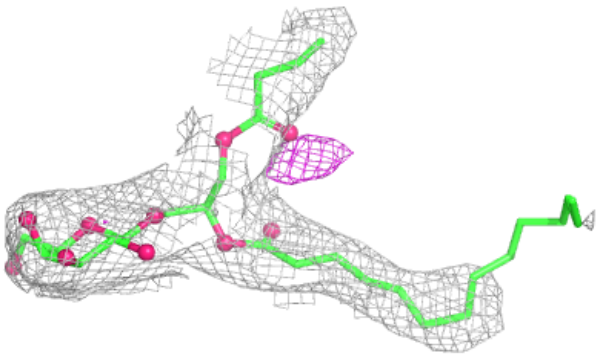


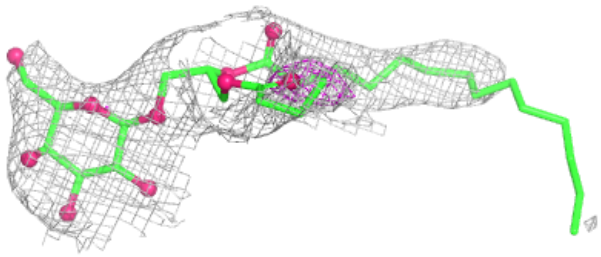


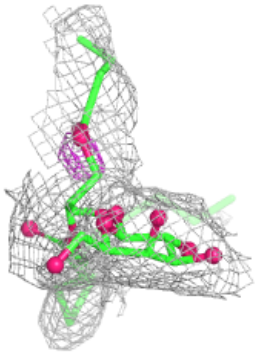


Electron density around LMG F 5002:

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

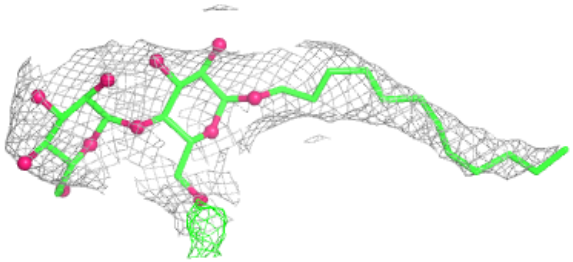


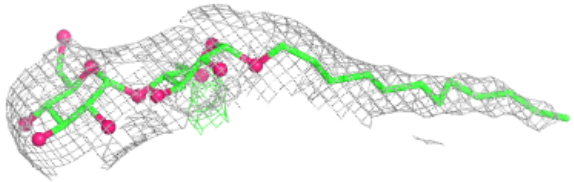


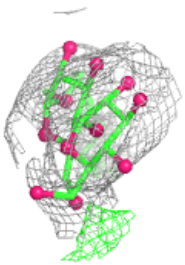


Electron density around LMU B 8001:

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

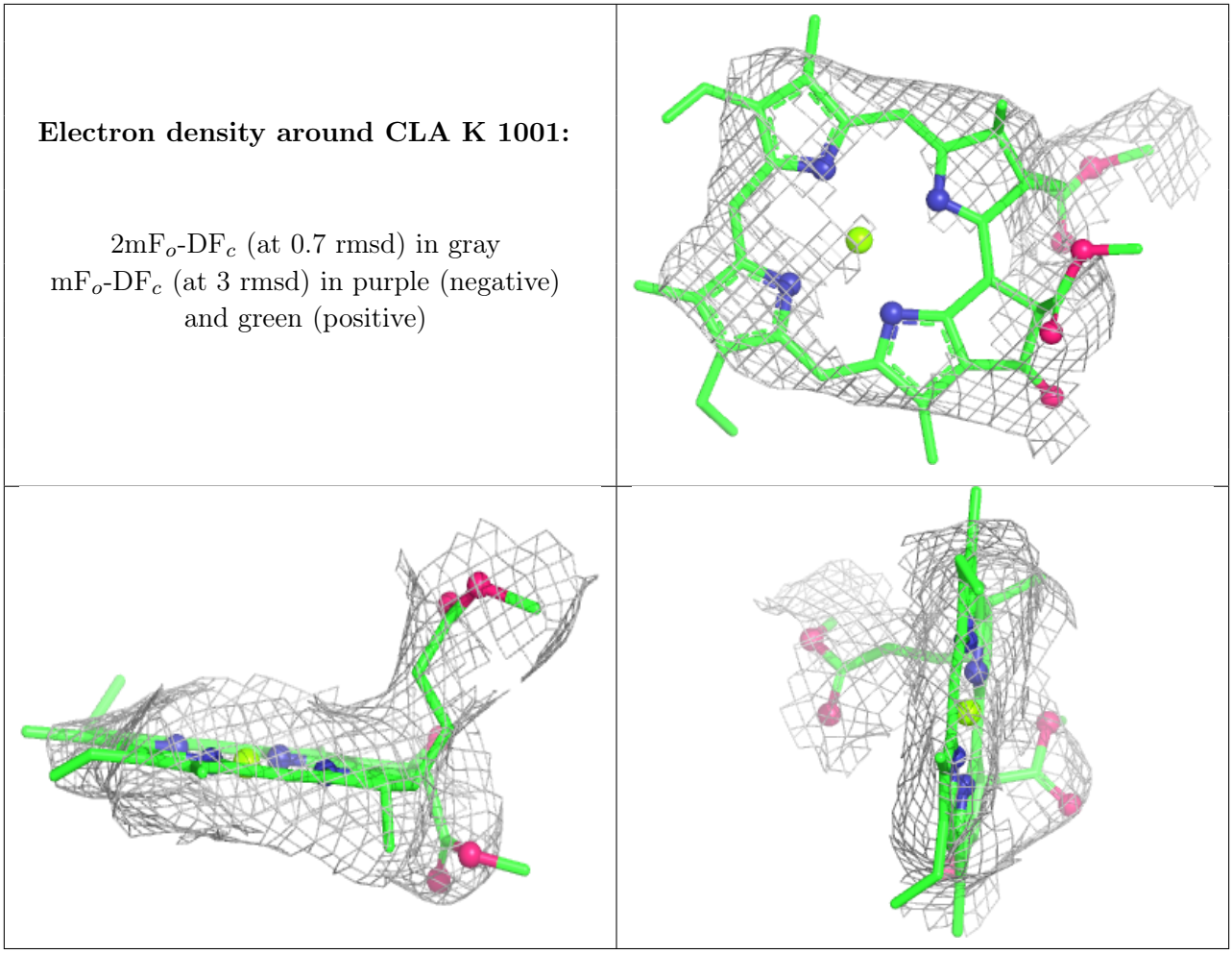






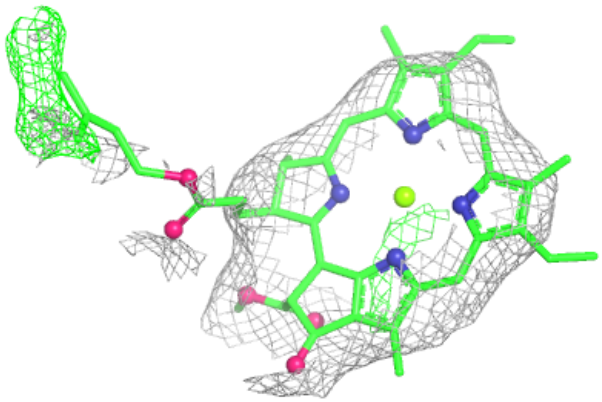
Electron density around CLA K 1001:

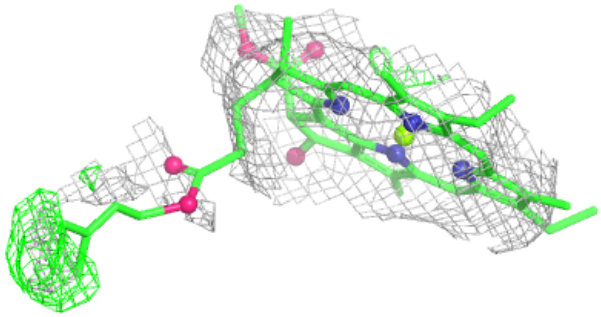
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

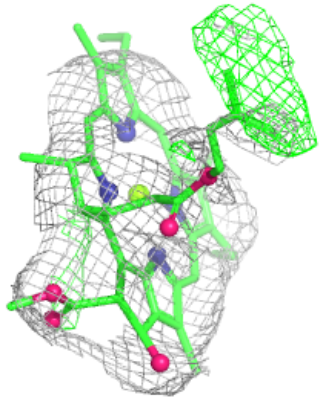


Electron density around CLA 3 3007:

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

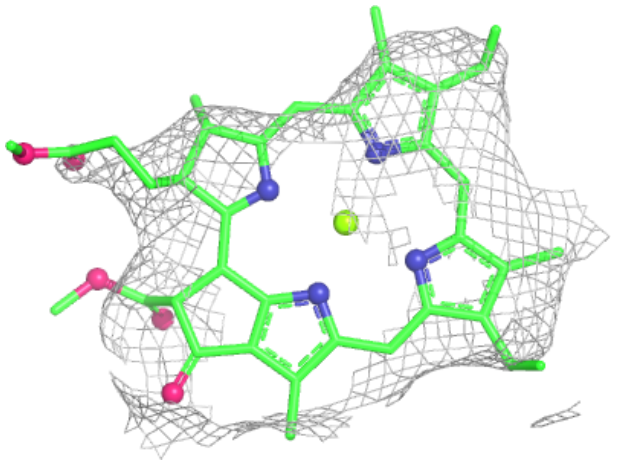


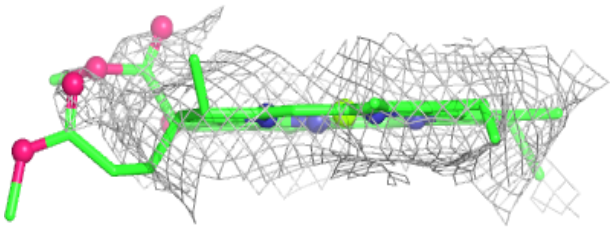


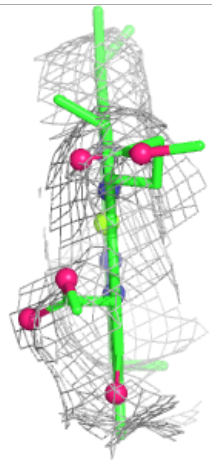


Electron density around CLA 1 1013:

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

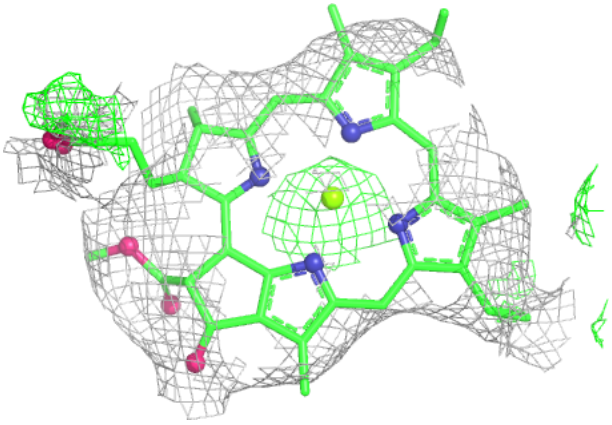


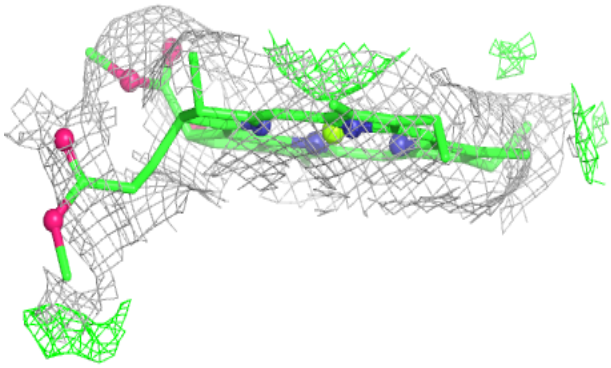


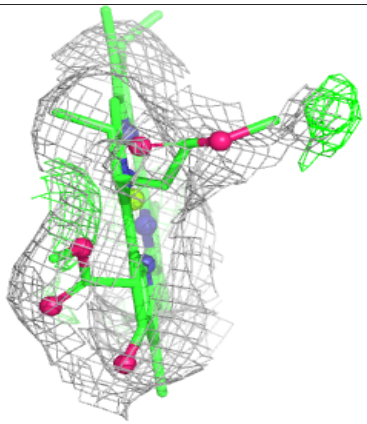


Electron density around CLA 3 3013:

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

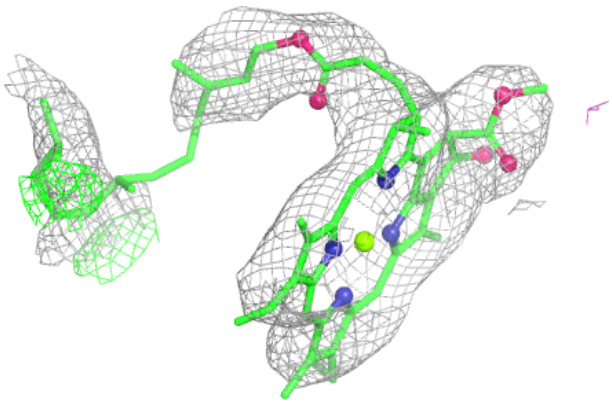


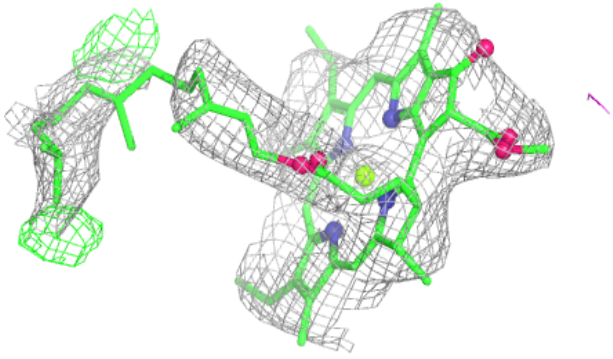


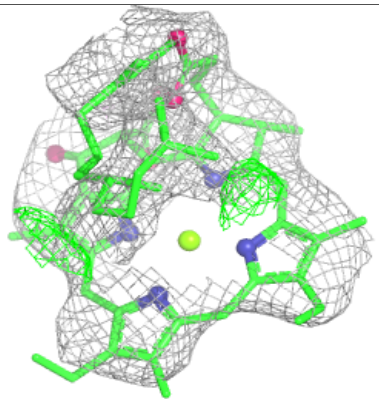


Electron density around CLA G 1003:

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

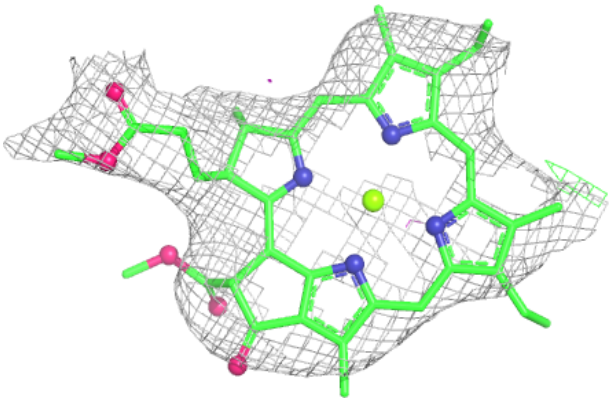


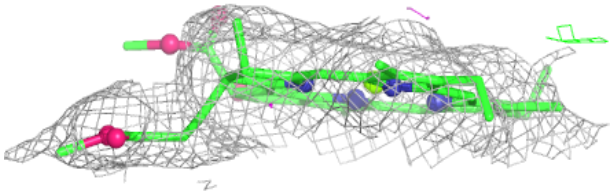


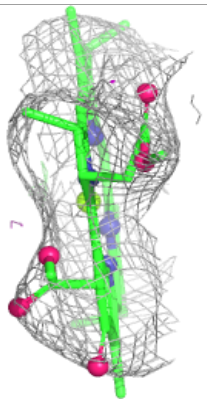


Electron density around CLA H 1000:

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

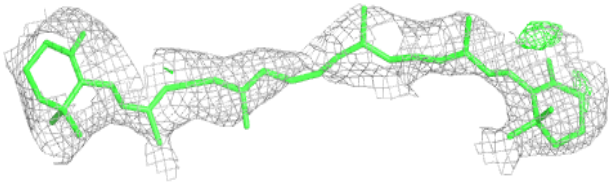


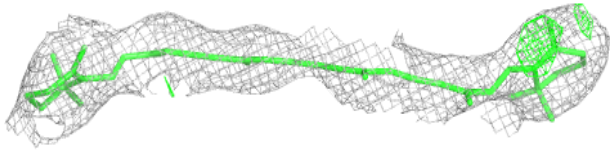


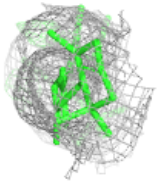


Electron density around BCR G 2011:

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

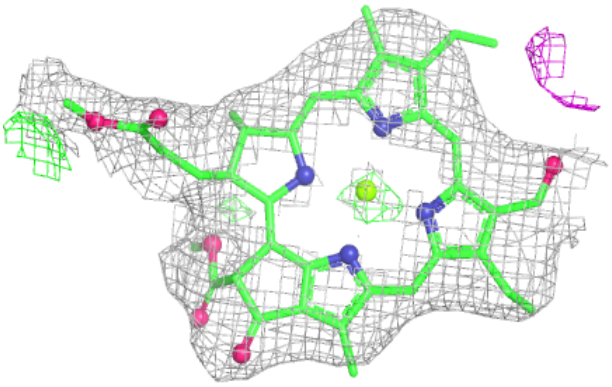


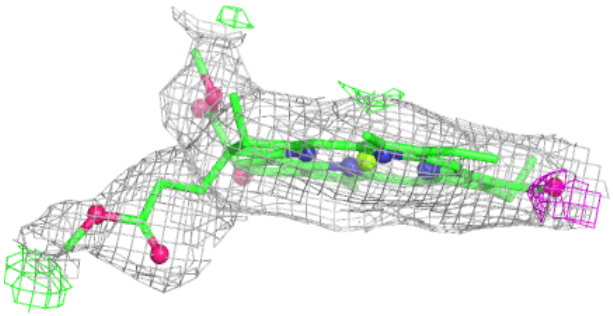




Electron density around CHL 2 2010:

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

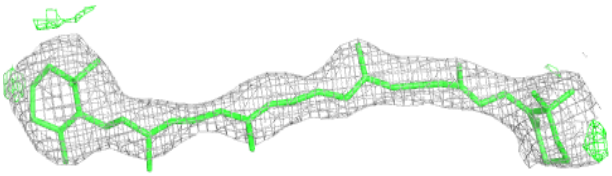


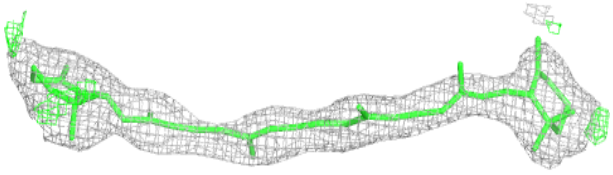


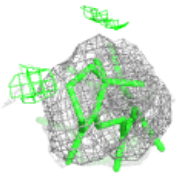


Electron density around BCR J 6013:

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



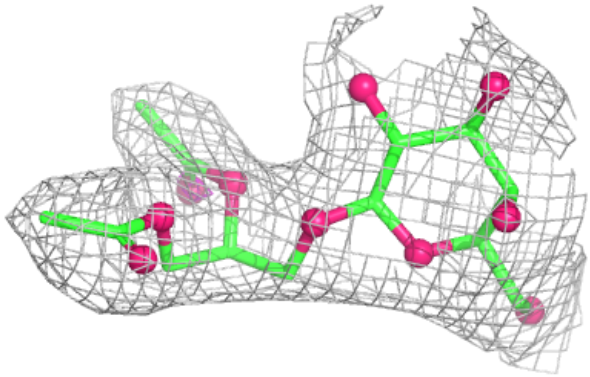


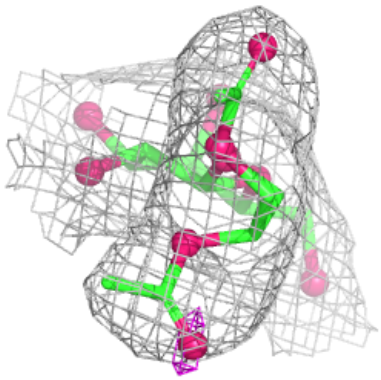


Electron density around LMG F 5001:

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

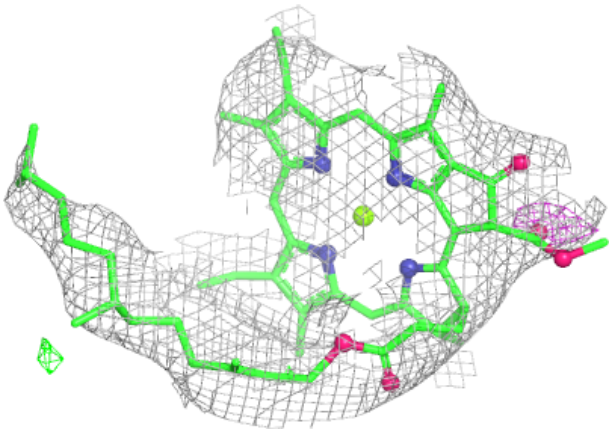


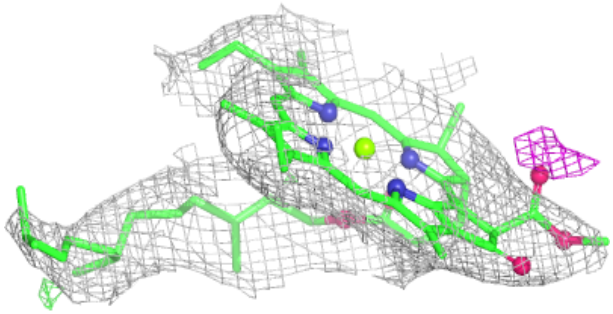


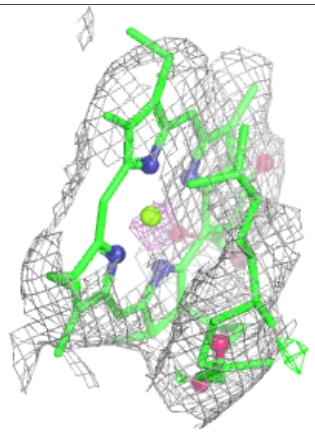


Electron density around CLA 1 1001:

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

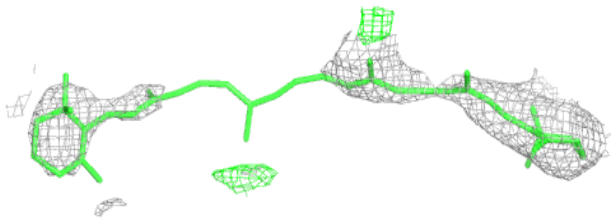


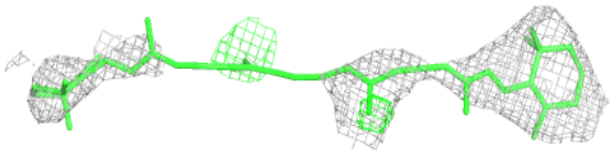


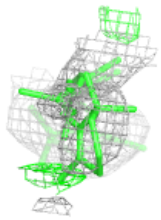


Electron density around BCR K 2011:

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

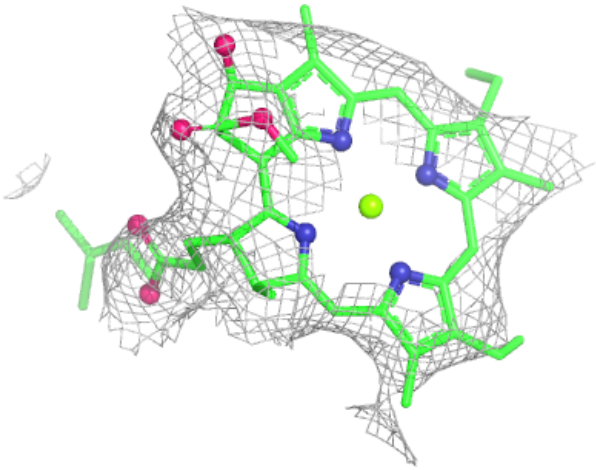


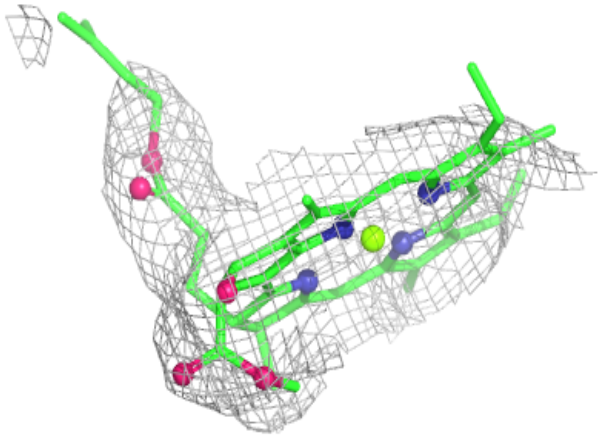


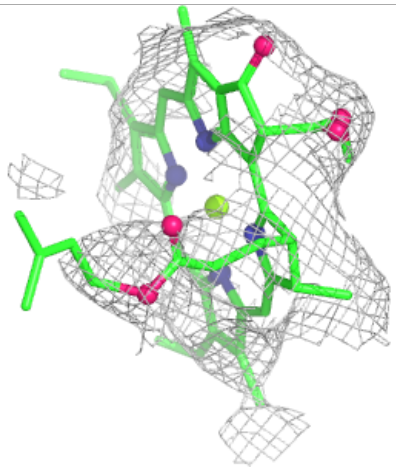


Electron density around CLA 3 3006:

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



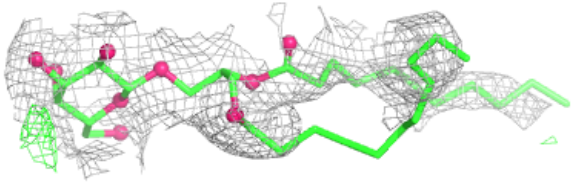


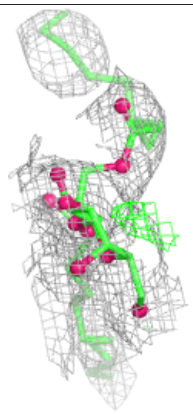


Electron density around LMG G 2021:

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

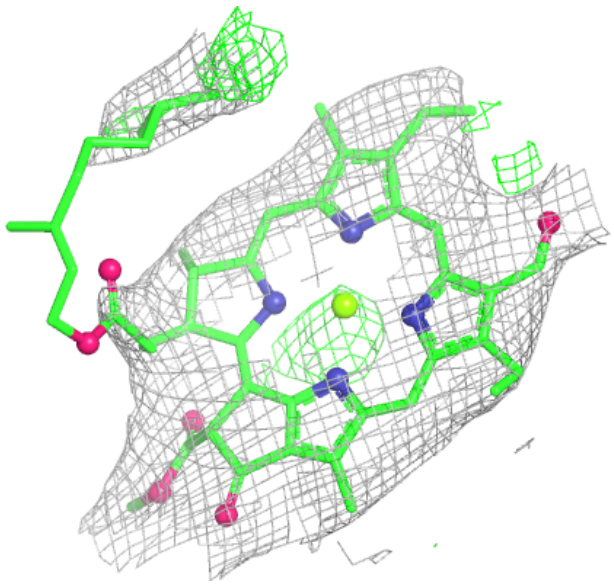


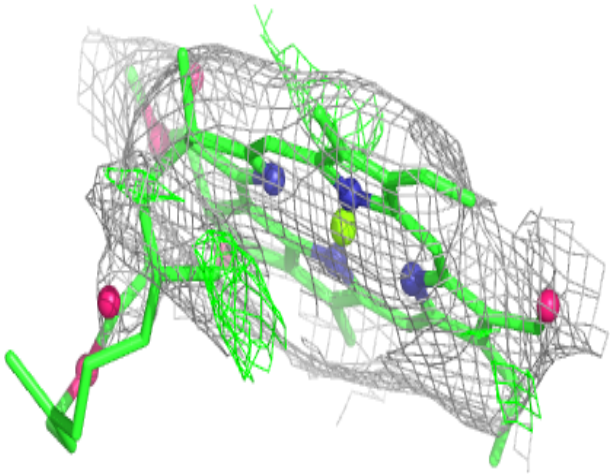


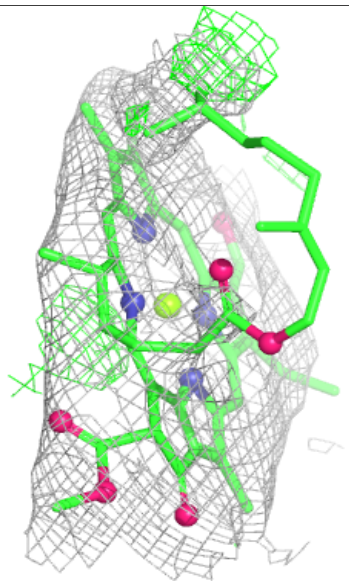


Electron density around CHL 3 3011:

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

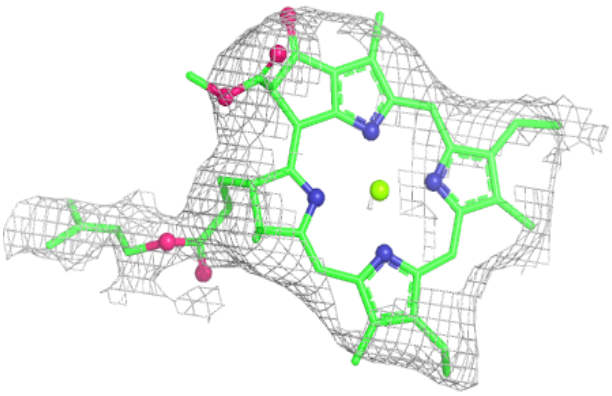


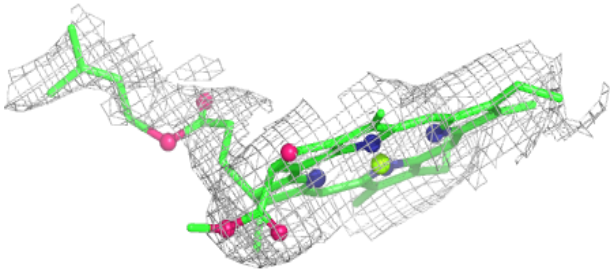


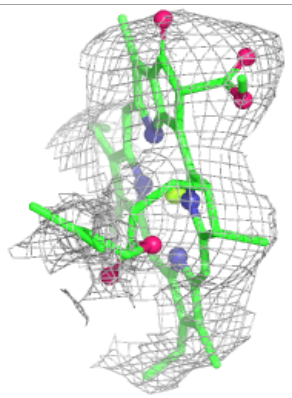


Electron density around CLA A 1151:

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

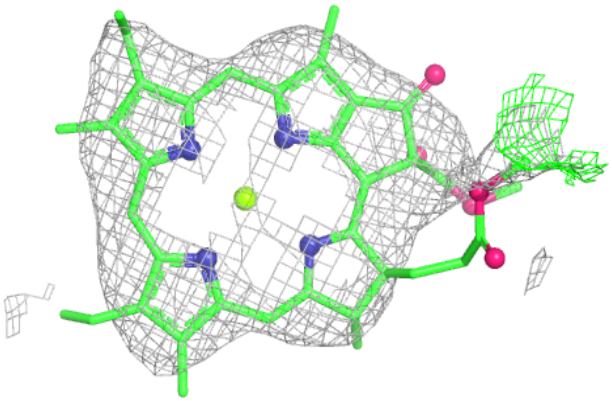


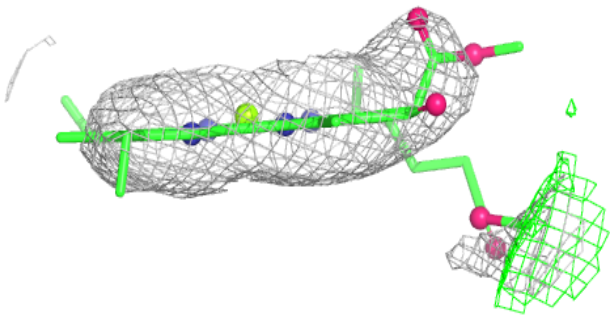


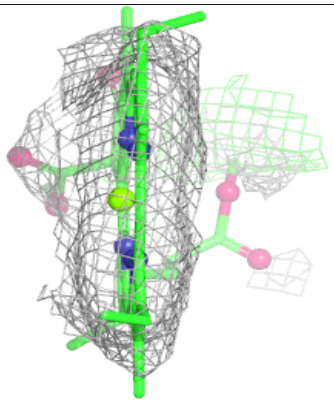


Electron density around CLA A 1113:

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

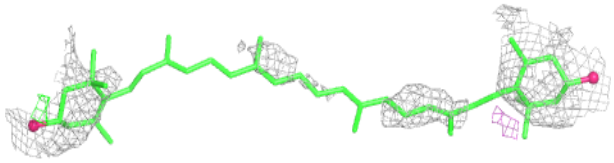


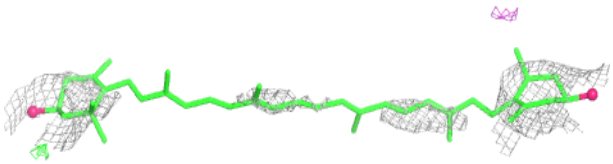


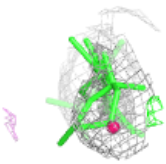


Electron density around LUT 3 3501:

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

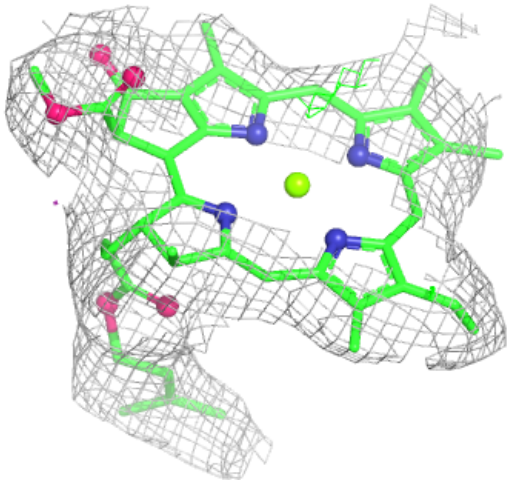


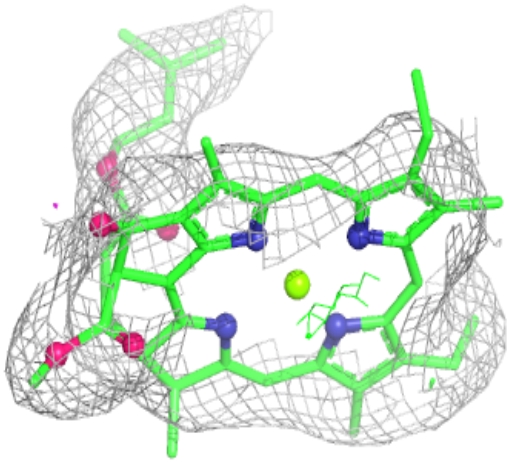


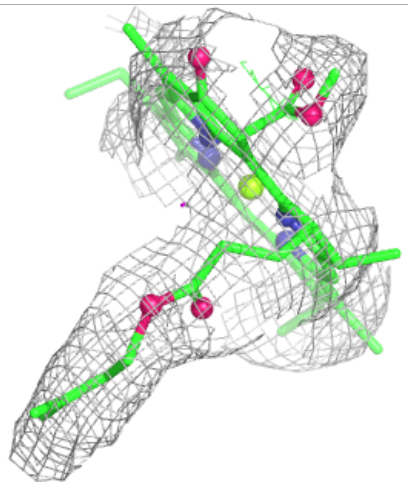


Electron density around CLA L 1501:

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

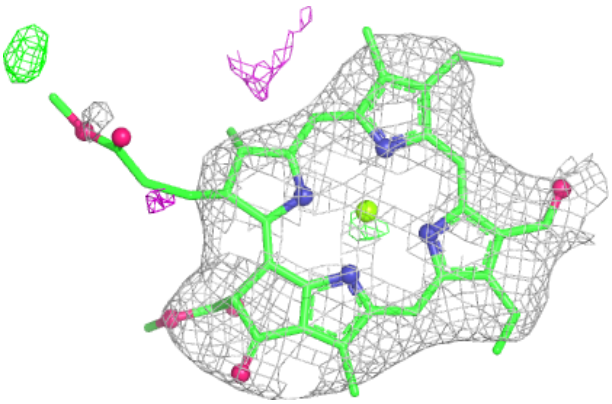


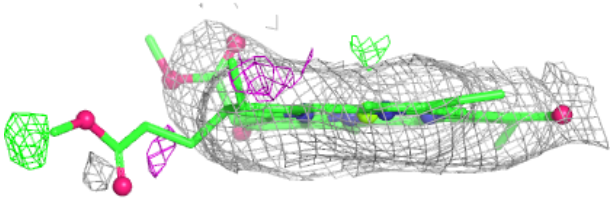


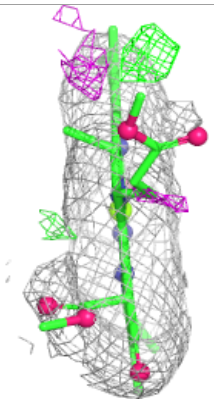


Electron density around CHL 4 4010:

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

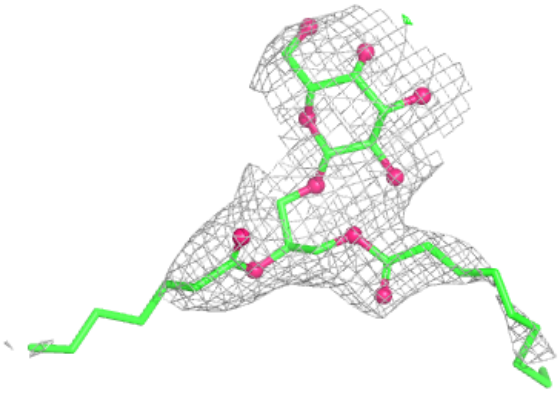


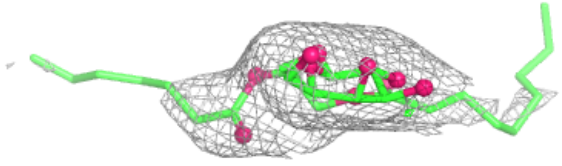


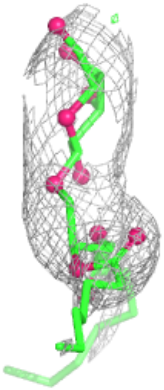


Electron density around LMG 2 2802:

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

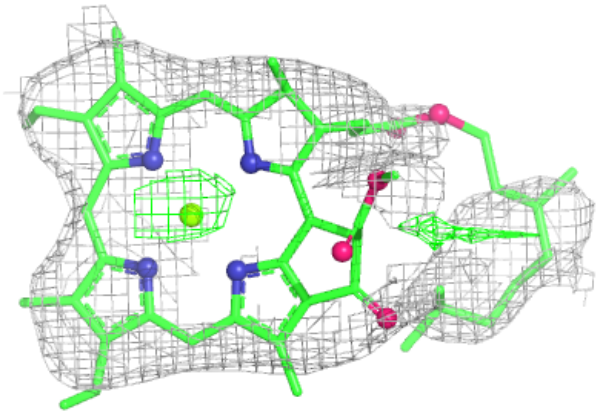


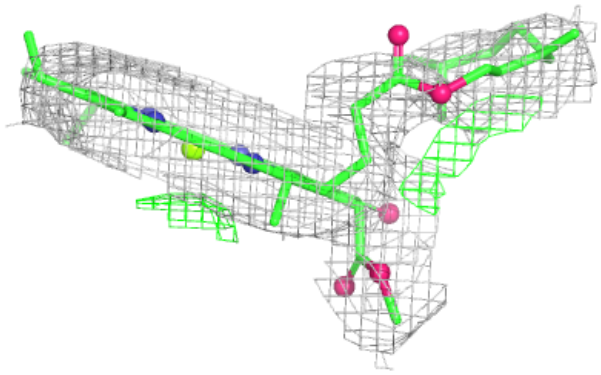


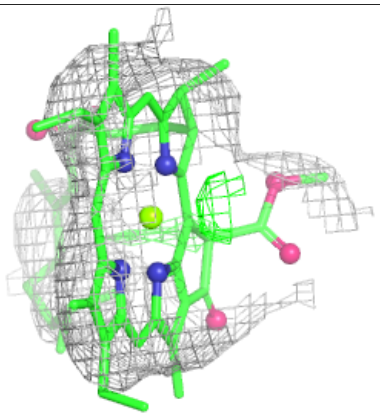


Electron density around CLA A 1134:

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

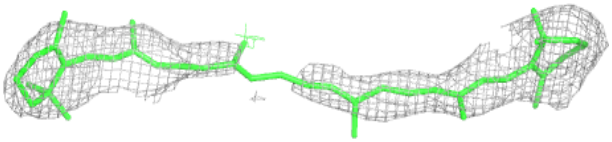


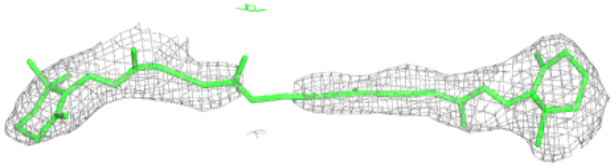


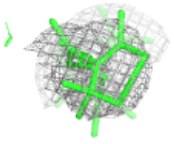


Electron density around BCR L 6020:

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

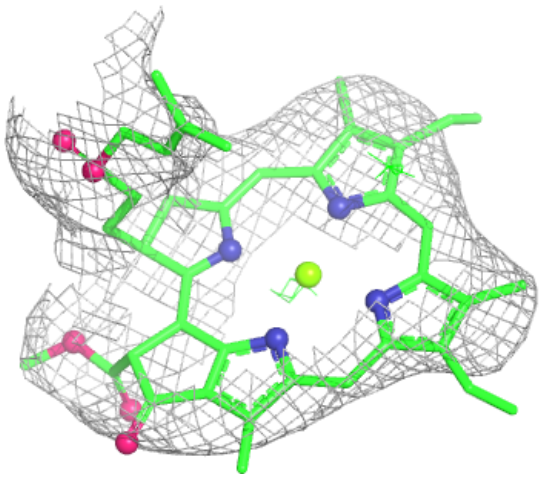


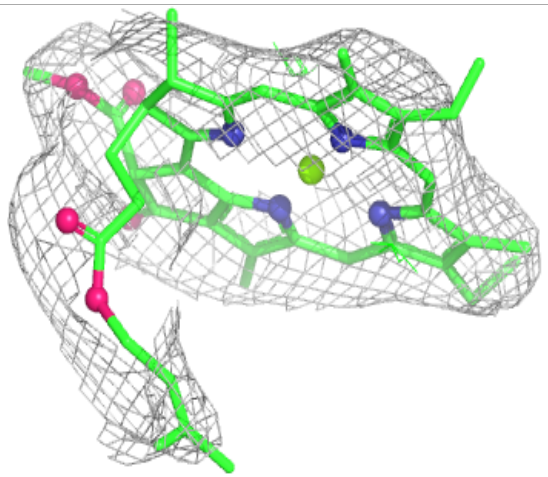


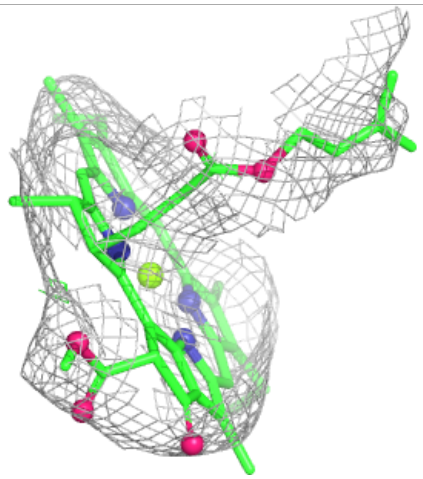


Electron density around CLA 1 1006:

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

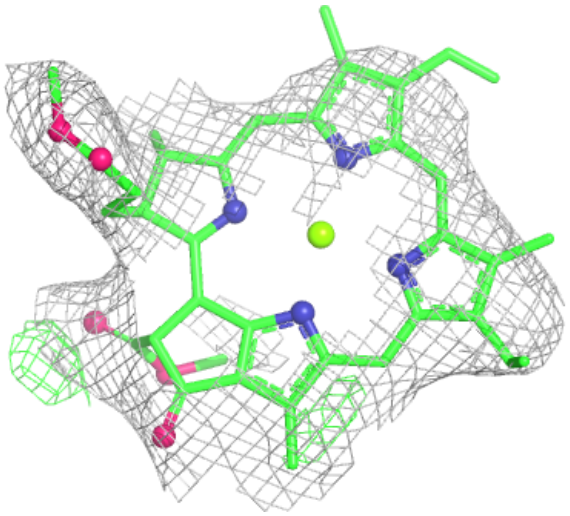


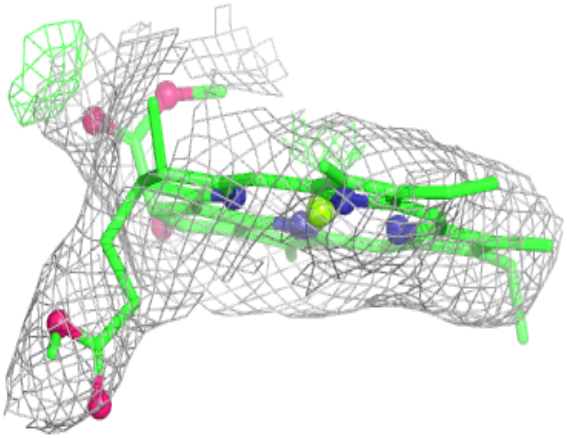




Electron density around CLA 1 1008:

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

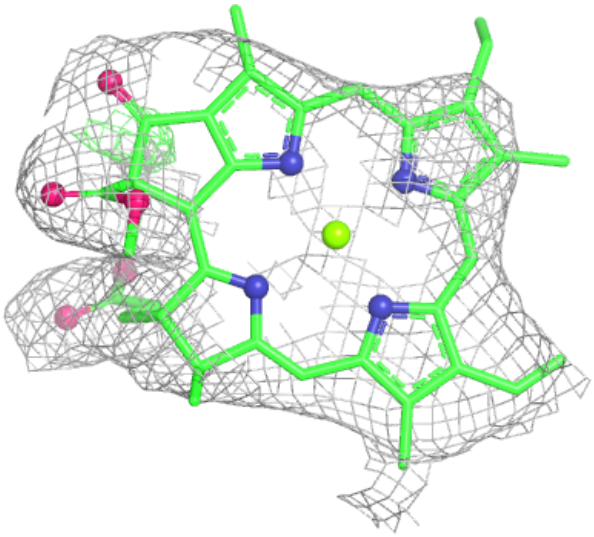


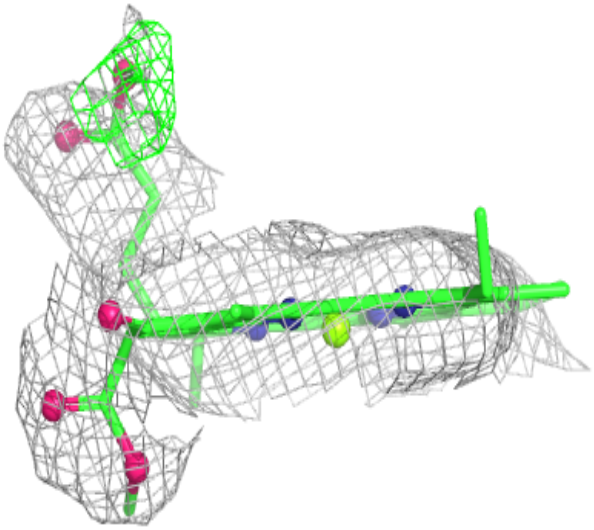


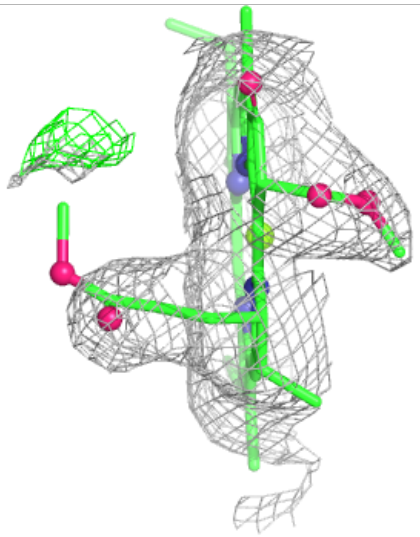


Electron density around CLA A 1114:

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

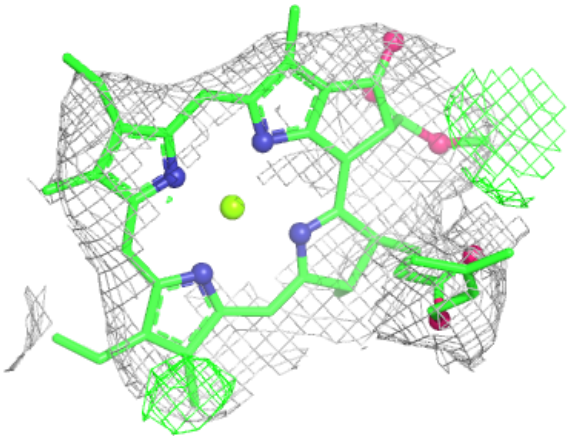


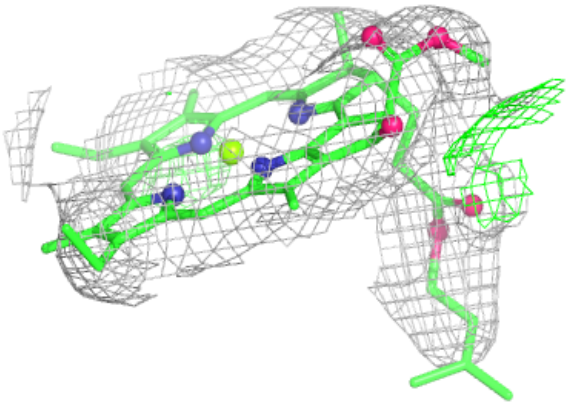


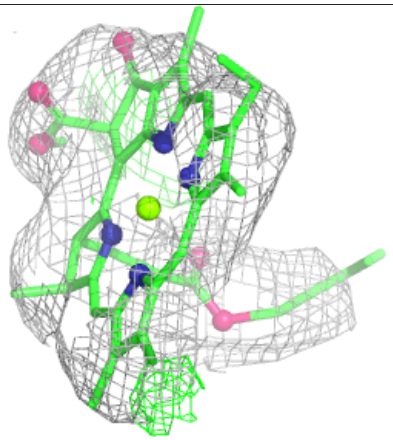


Electron density around CLA 4 4006:

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

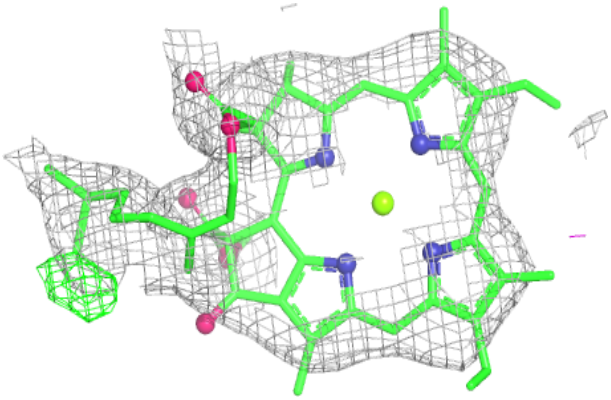


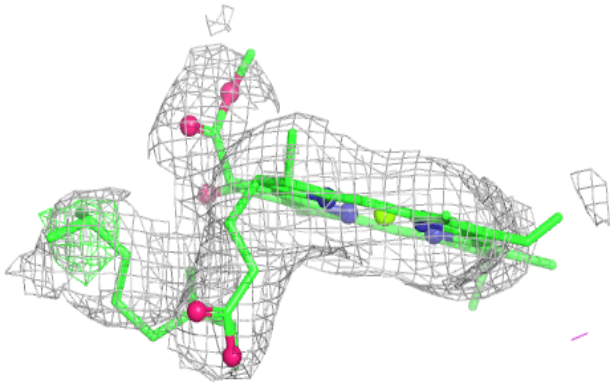


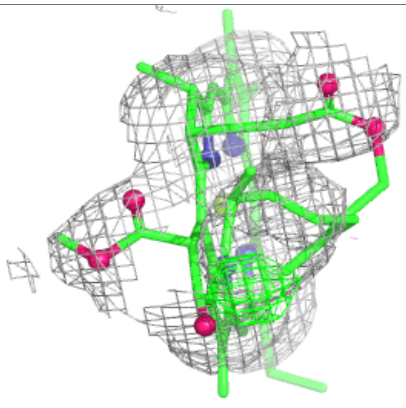


Electron density around CLA 2 2006:

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

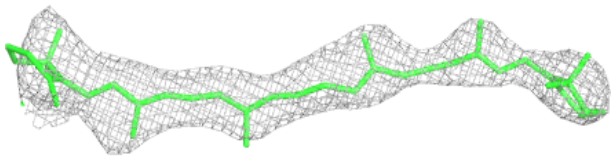


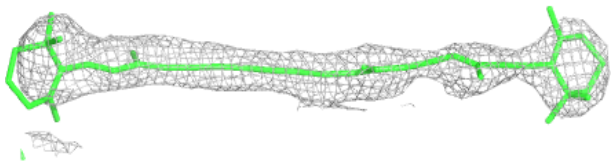


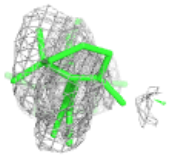


Electron density around BCR A 6007:

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

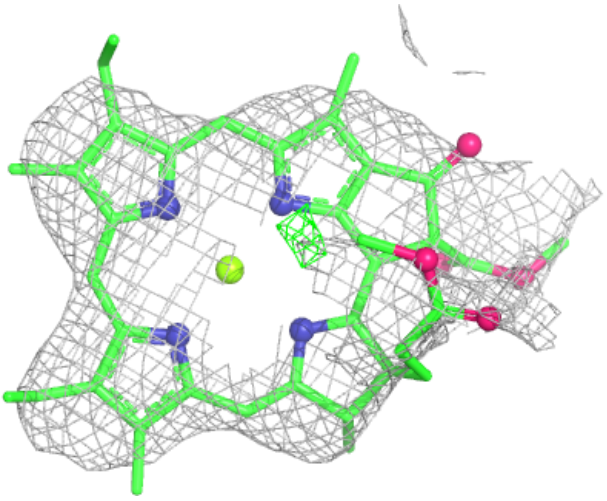


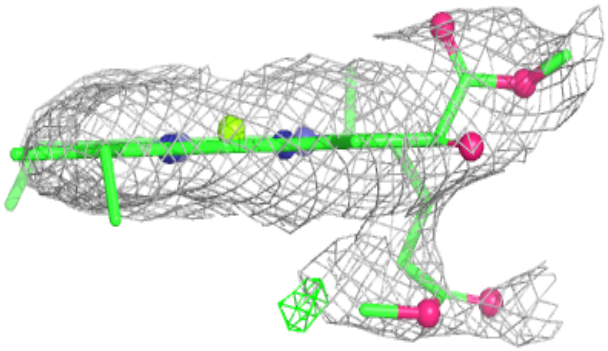


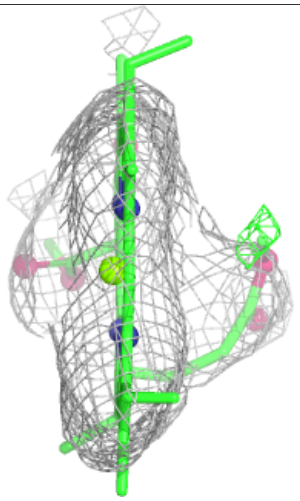


Electron density around CLA A 1115:

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

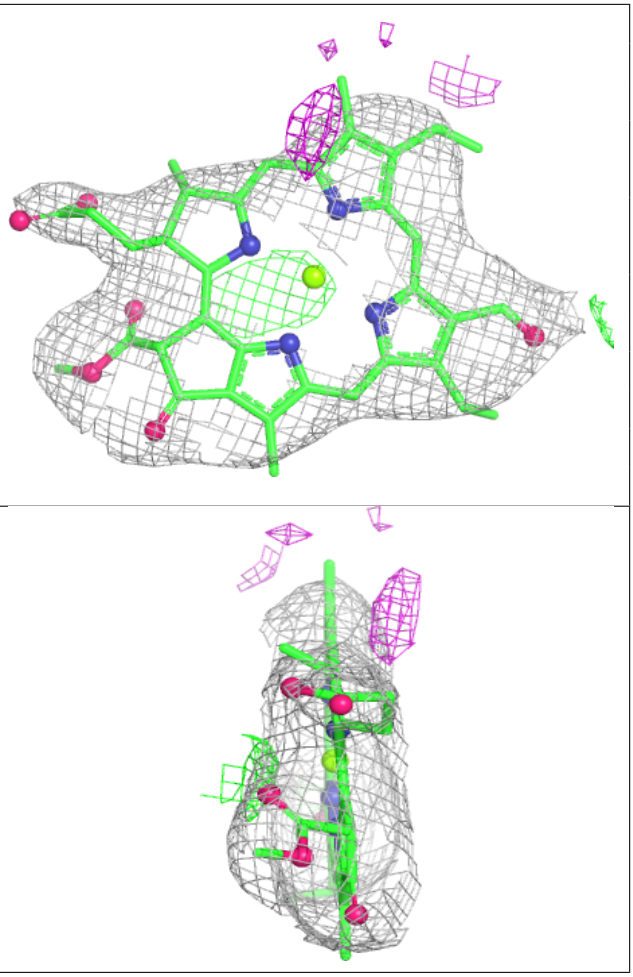






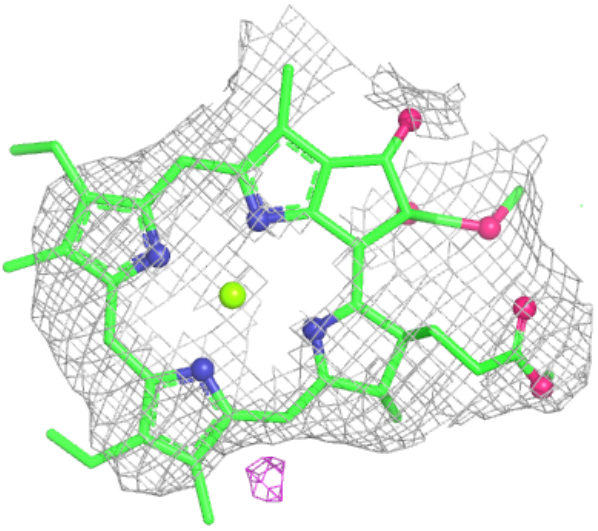
Electron density around CHL 2 2013:

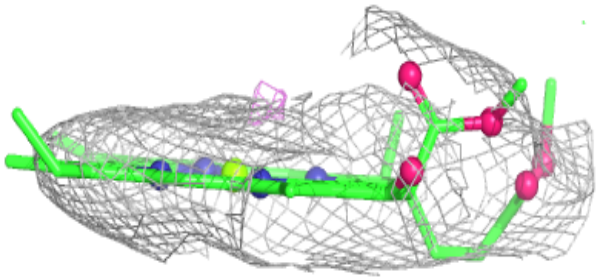
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

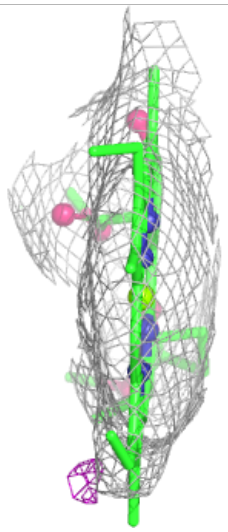


Electron density around CLA 3 3002:

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

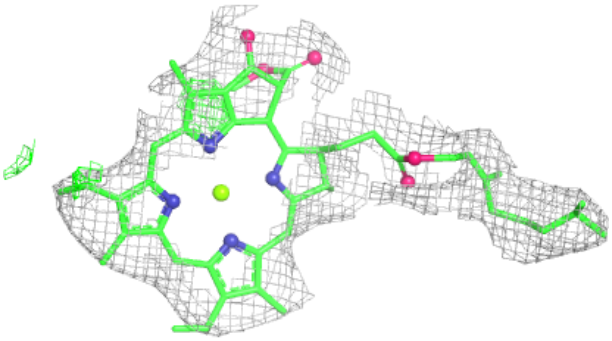


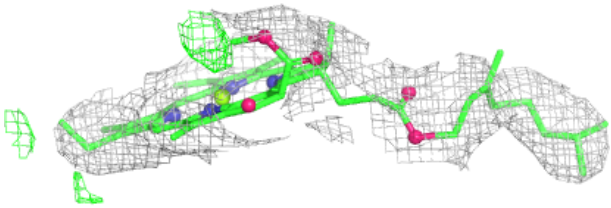


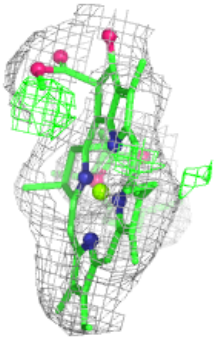


Electron density around CLA G 1001:

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

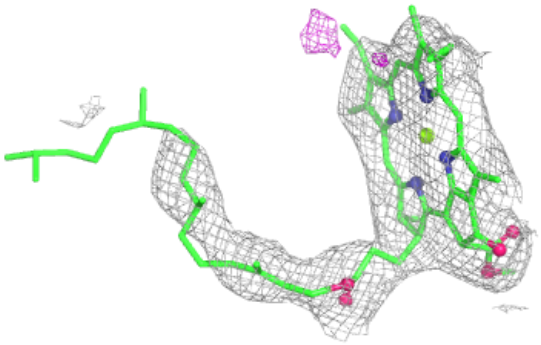


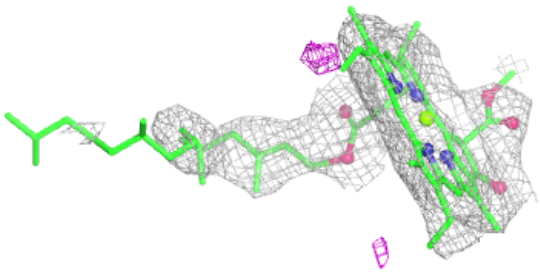


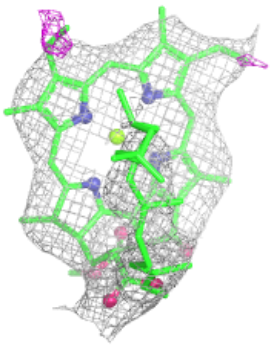


Electron density around CLA B 1218:

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

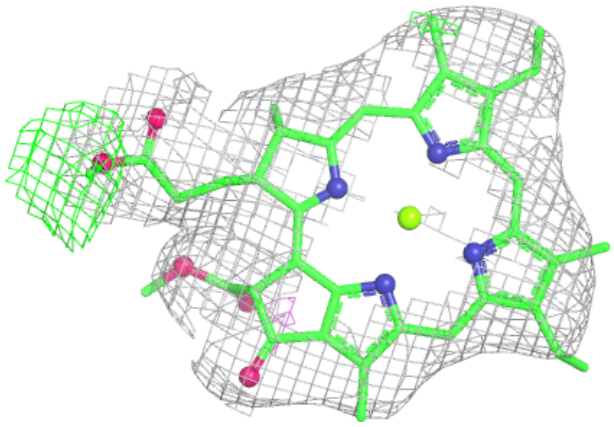


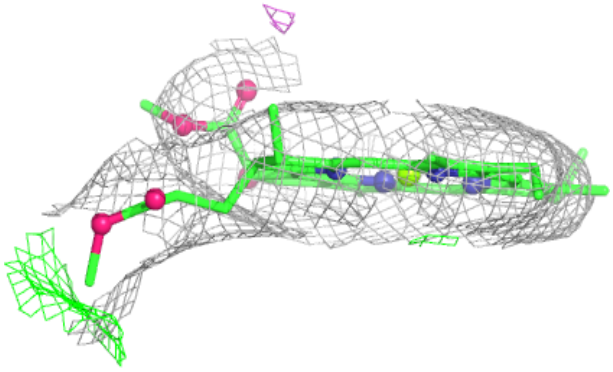


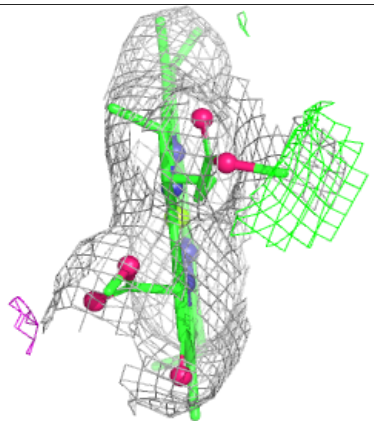


Electron density around CLA 1 1014:

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

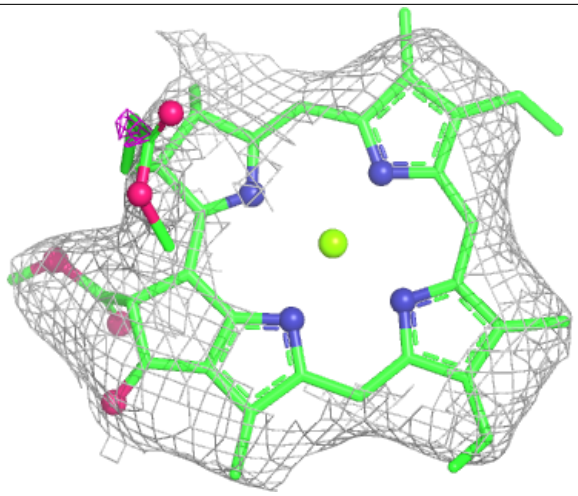


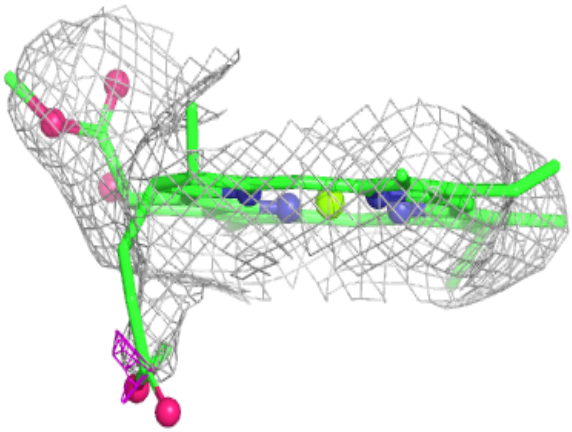


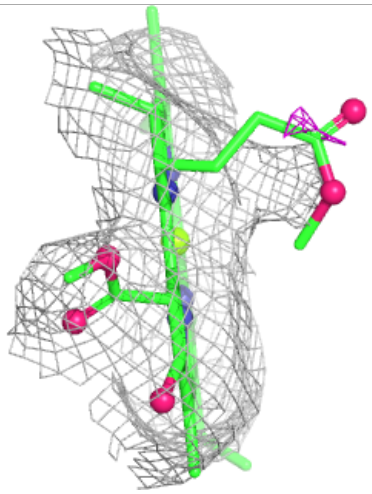


Electron density around CLA 4 4008:

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

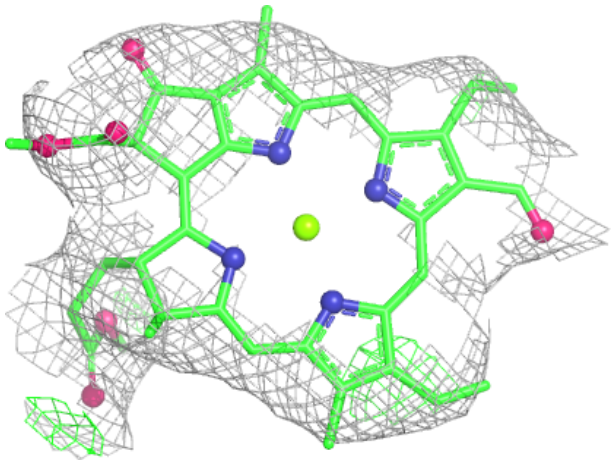


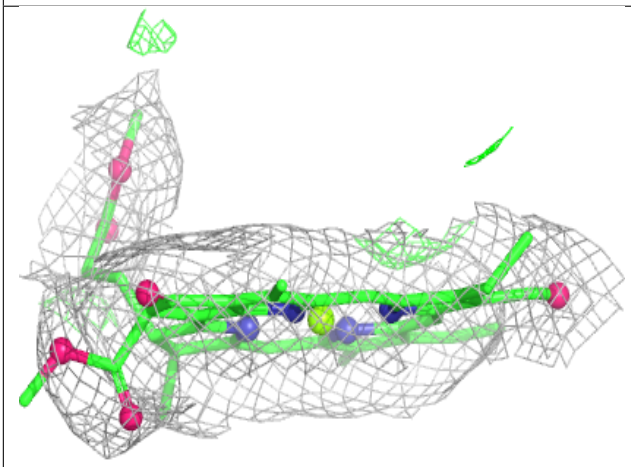


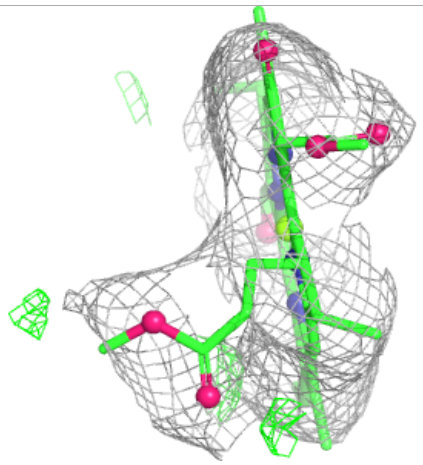


Electron density around CHL 1 1010:

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

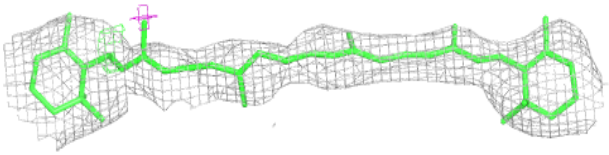


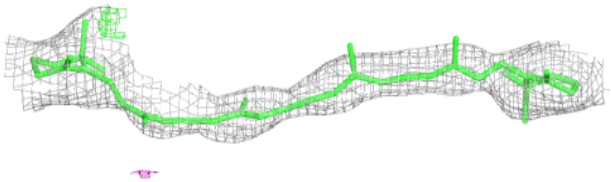


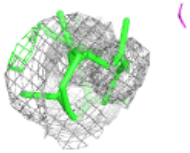


Electron density around BCR 3 3503:

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

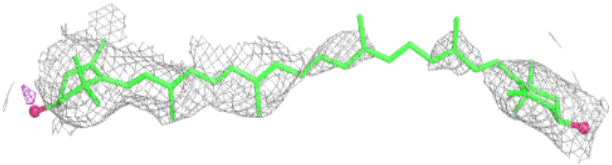


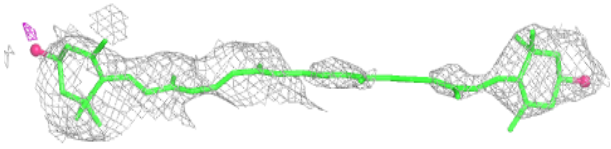


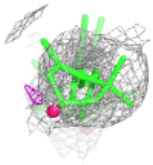


Electron density around LUT 1 1501:

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

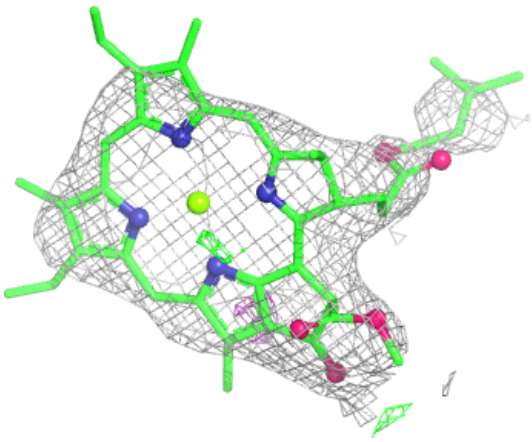


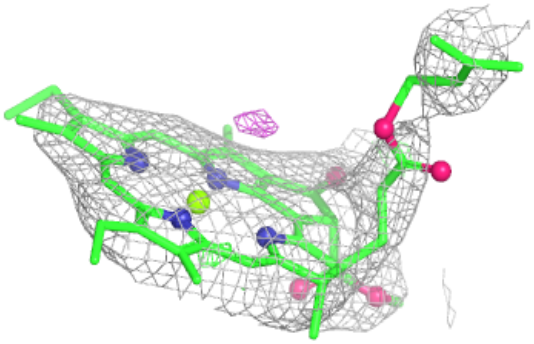


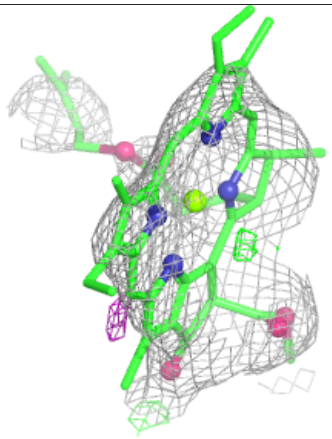


Electron density around CLA 1 1011:

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

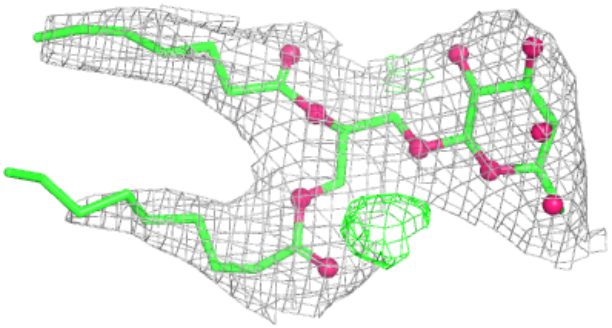


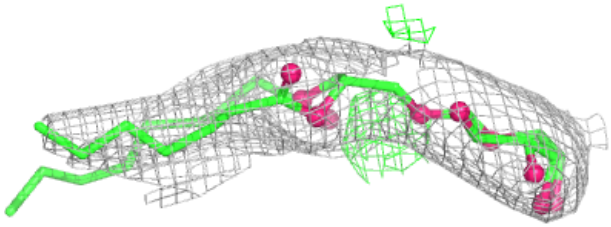


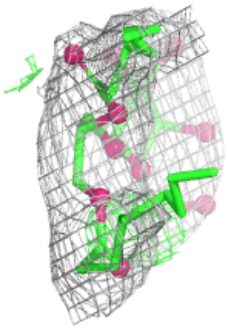


Electron density around LMG 4 4801:

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

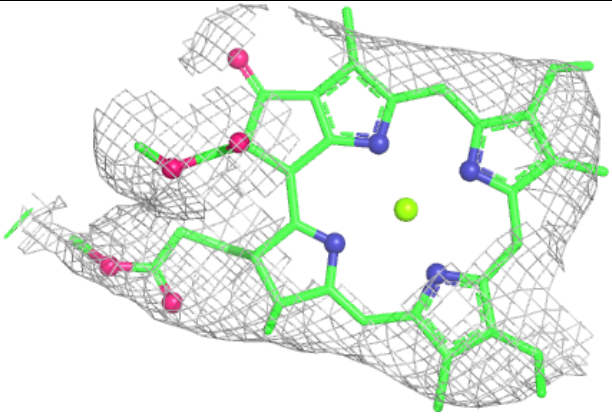


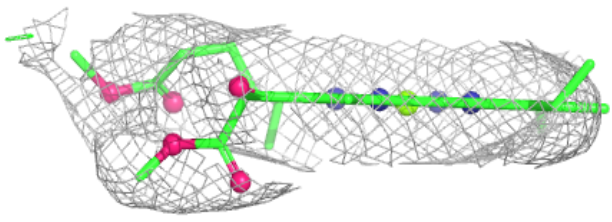


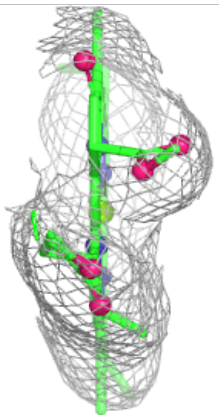


Electron density around CLA G 1002:

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

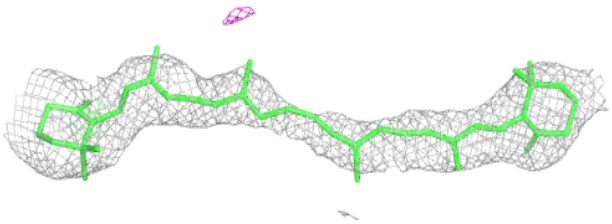


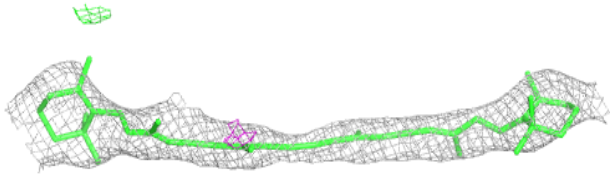


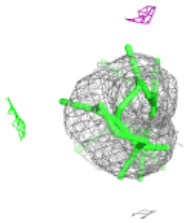


Electron density around BCR B 6004:

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

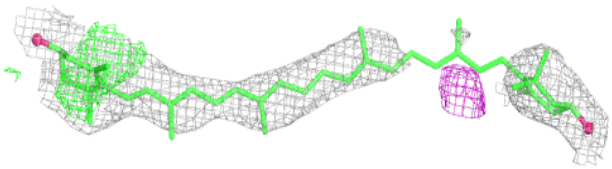


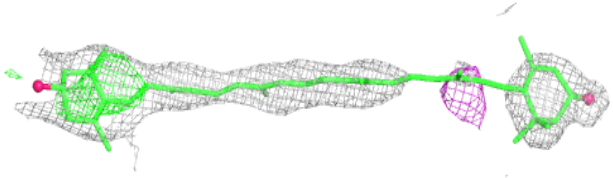


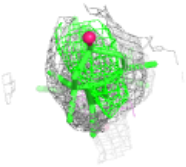


Electron density around LUT 2 2502:

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

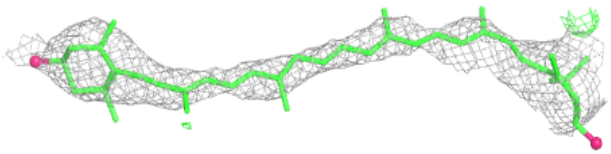


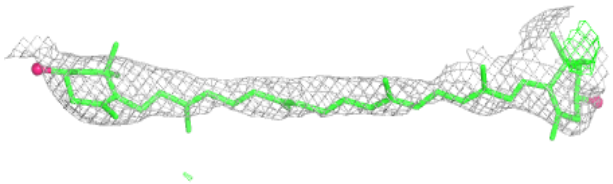


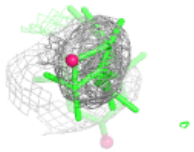


Electron density around LUT 4 4503:

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

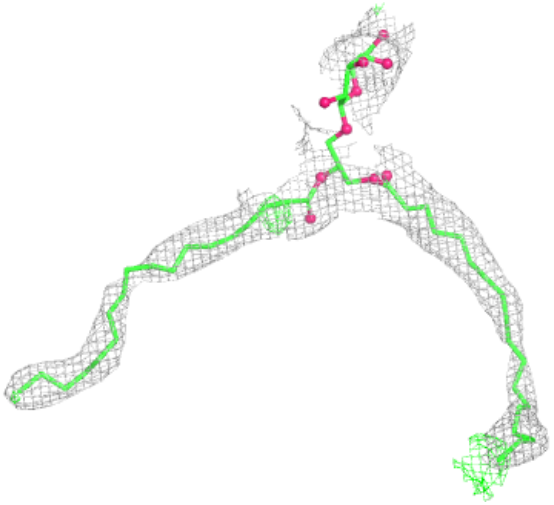


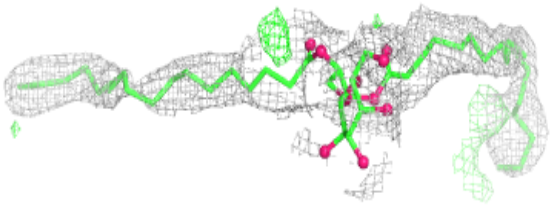


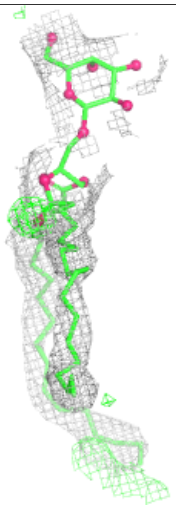


Electron density around LMG J 5001:

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

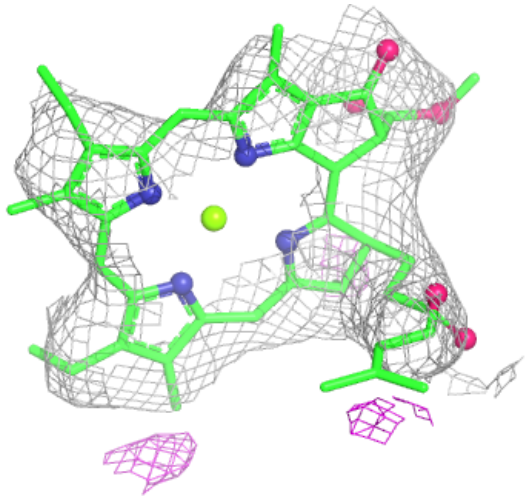


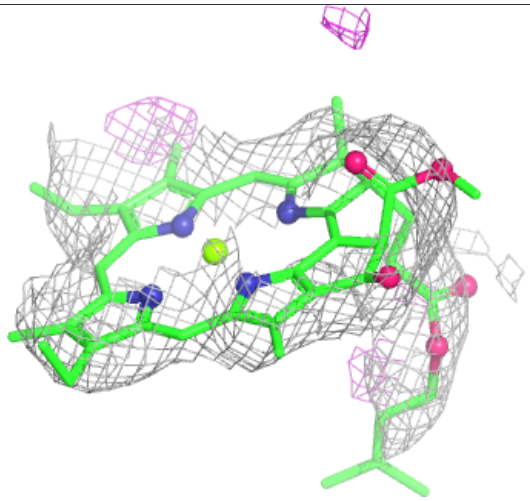


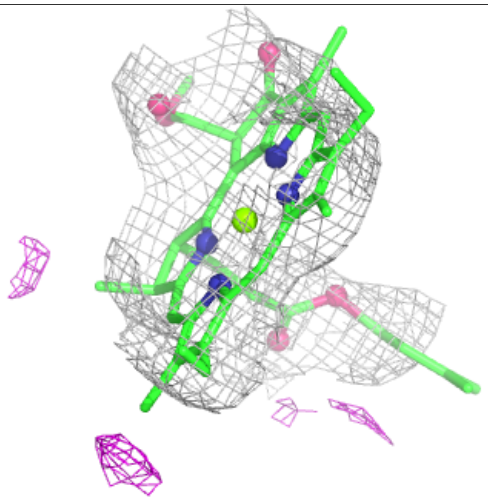


Electron density around CLA L 1503:

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

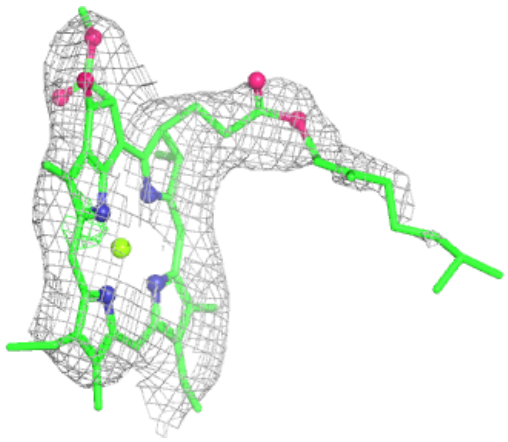


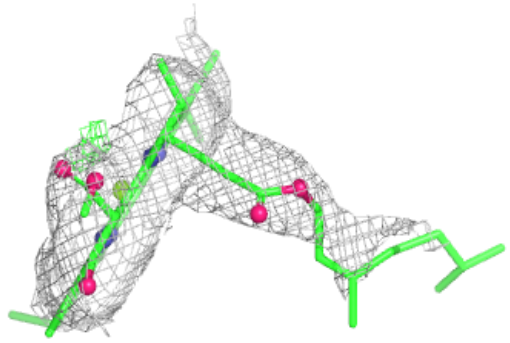


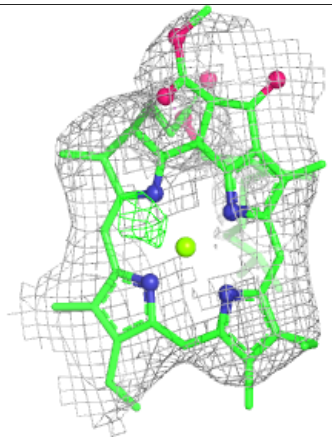


Electron density around CLA B 1232:

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

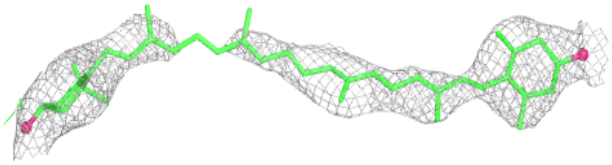


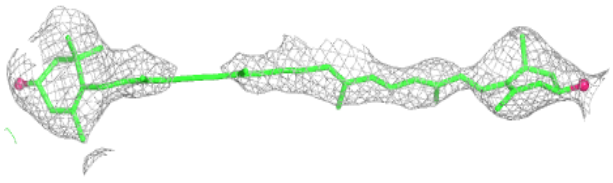


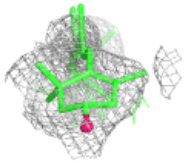


Electron density around LUT 1 1502:

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

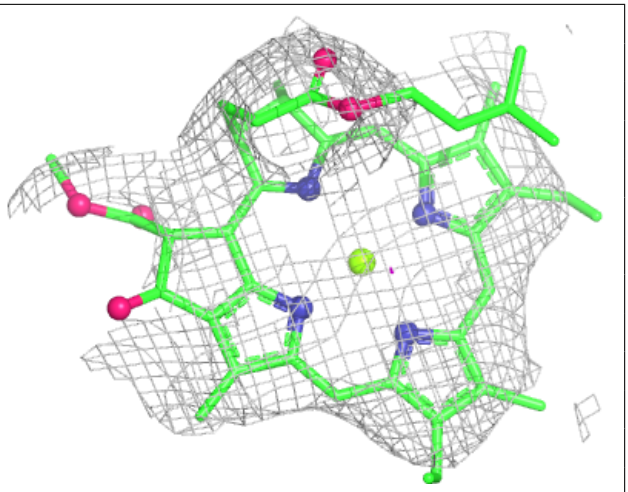


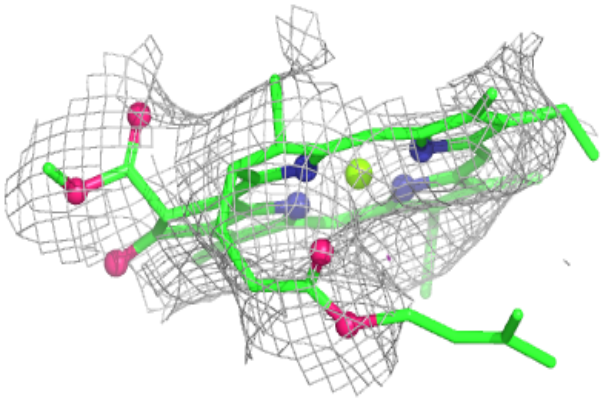


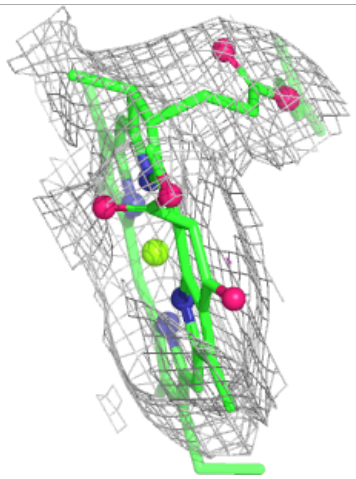


Electron density around CLA 3 3001:

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

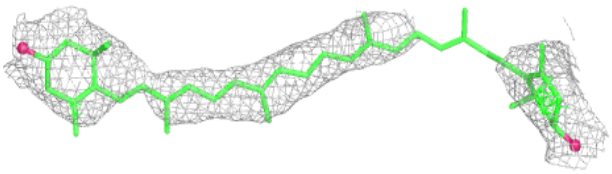


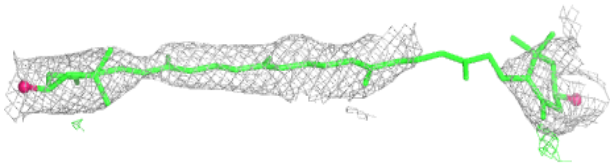


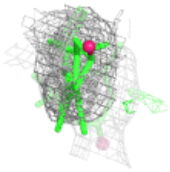


Electron density around LUT 3 3502:

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

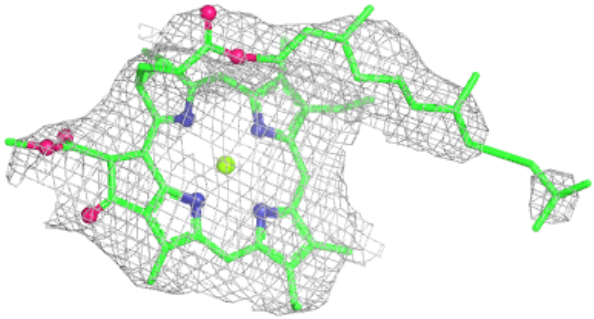


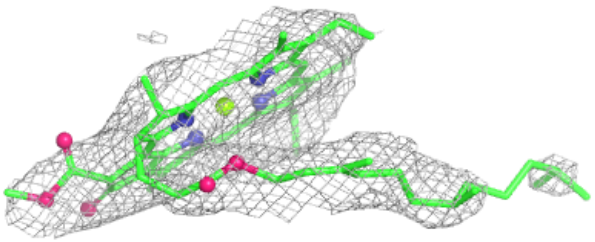


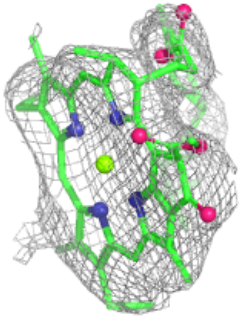


Electron density around CLA 4 4001:

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

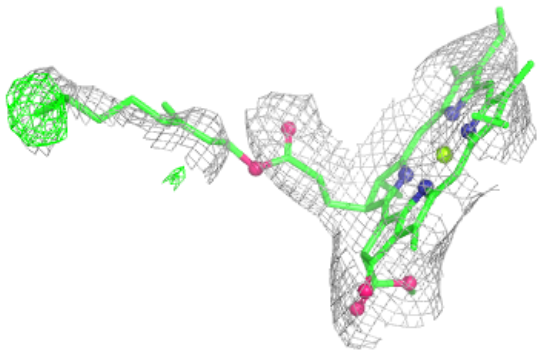


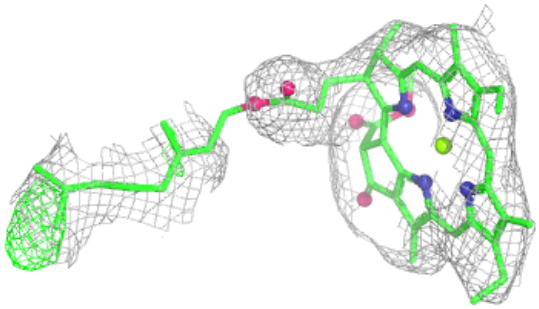


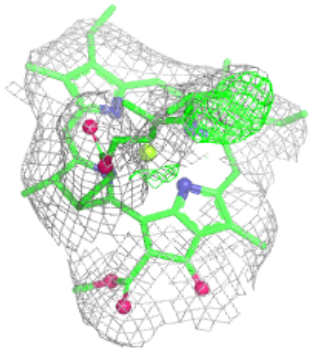


Electron density around CLA A 1121:

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

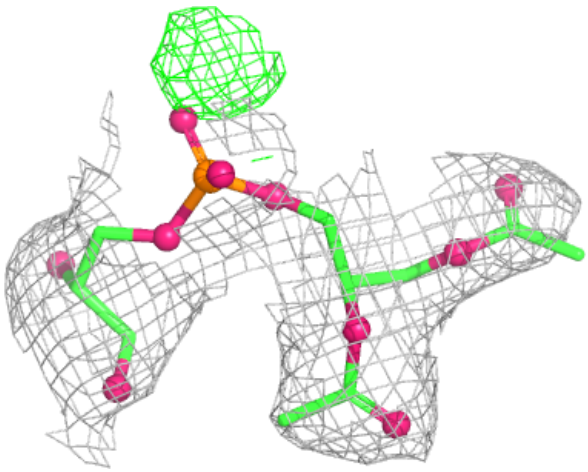


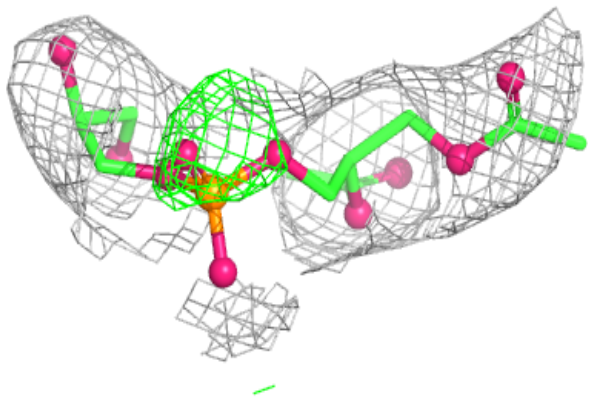


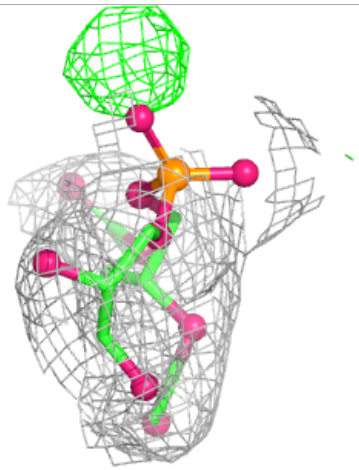


Electron density around LHG B 5004:

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

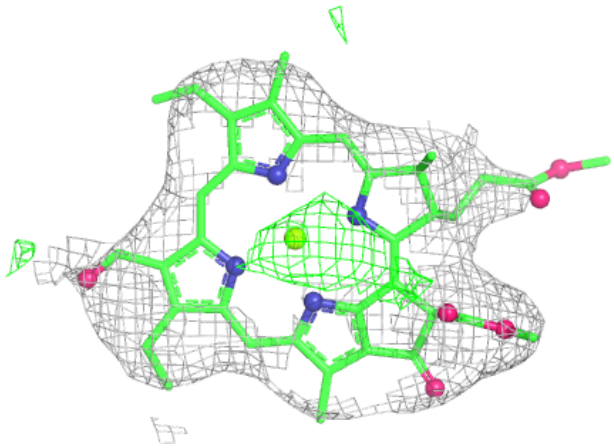


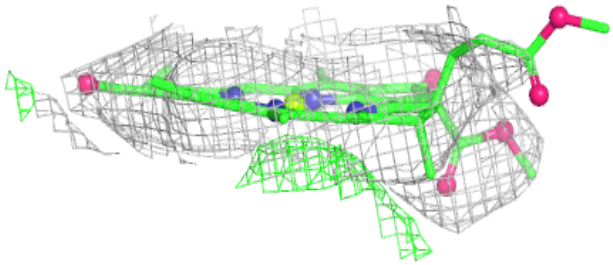


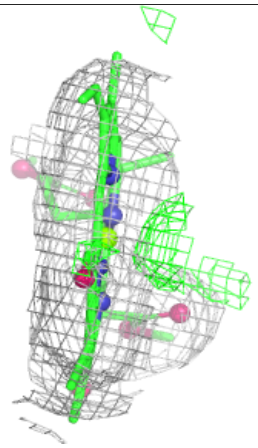


Electron density around CHL 4 4013:

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

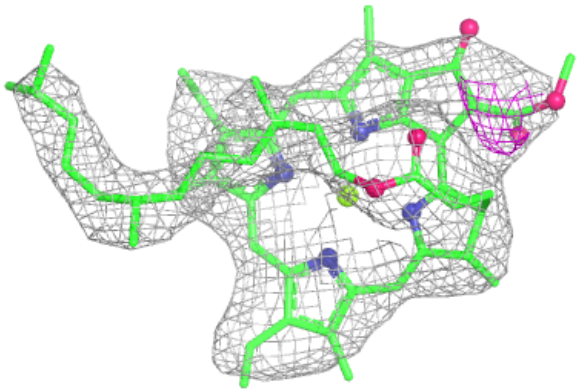


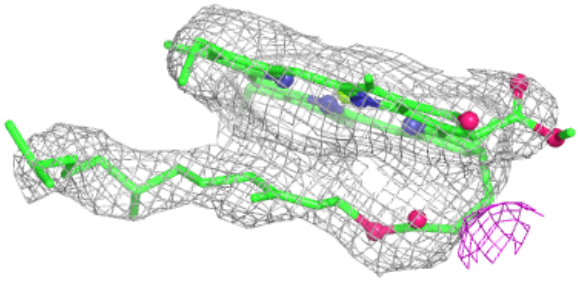


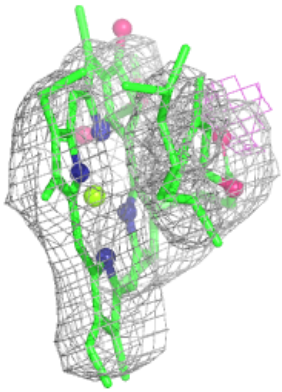


Electron density around CLA B 1213:

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

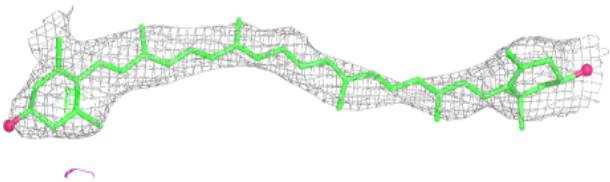


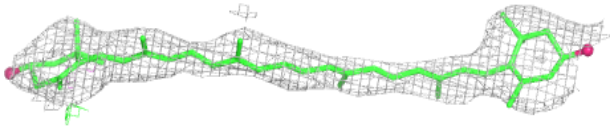




Electron density around LUT 2 2501:

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

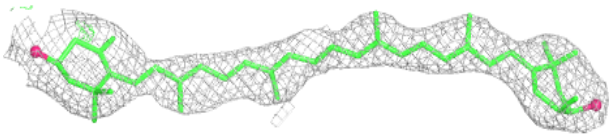


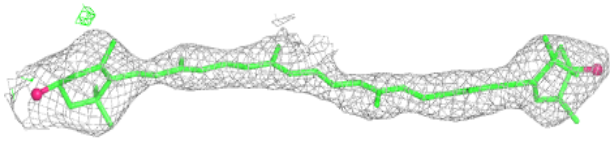


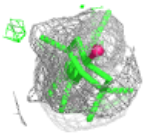


Electron density around ZEX 4 4505:

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

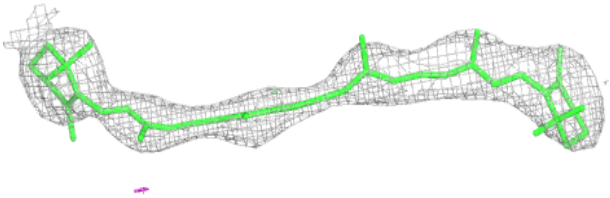


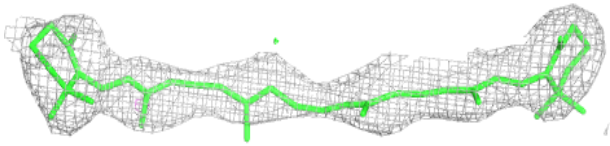


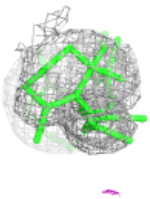


Electron density around BCR A 6008:

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

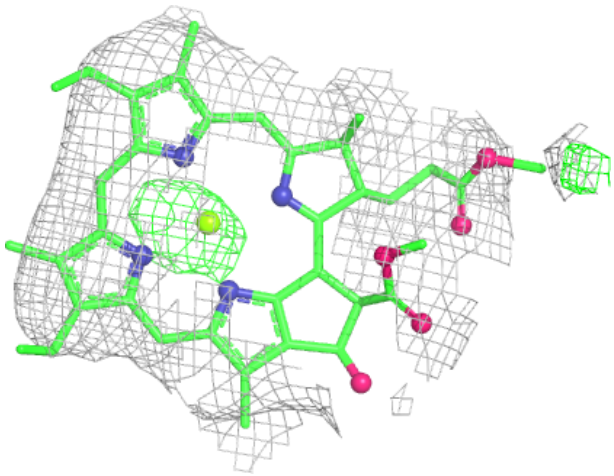


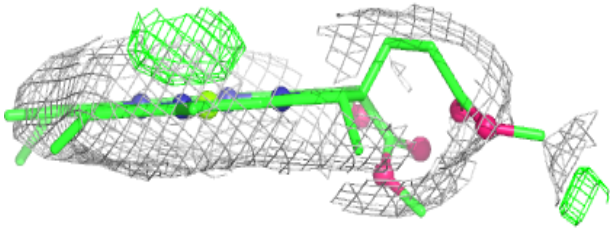


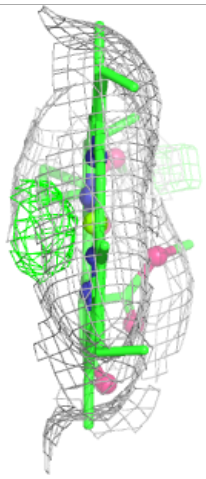


Electron density around CLA 1 1002:

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

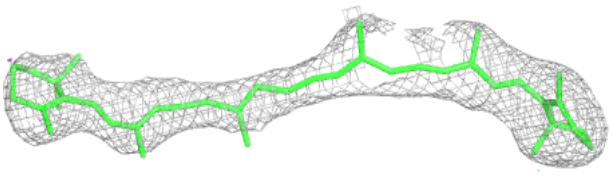


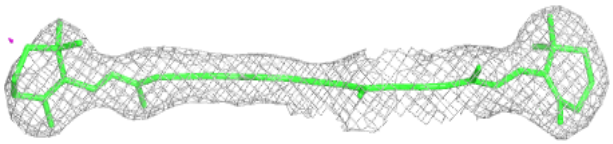


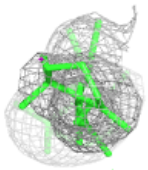


Electron density around BCR B 6009:

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

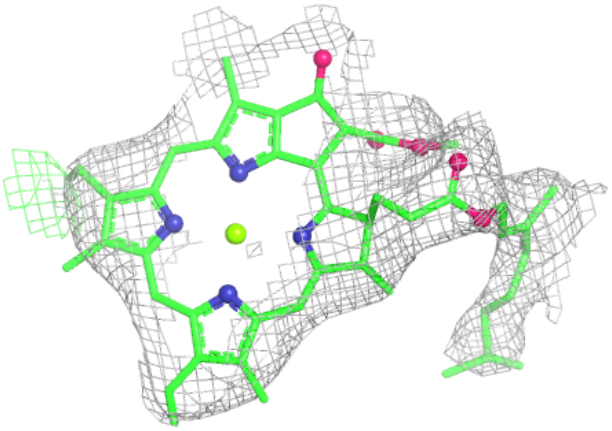


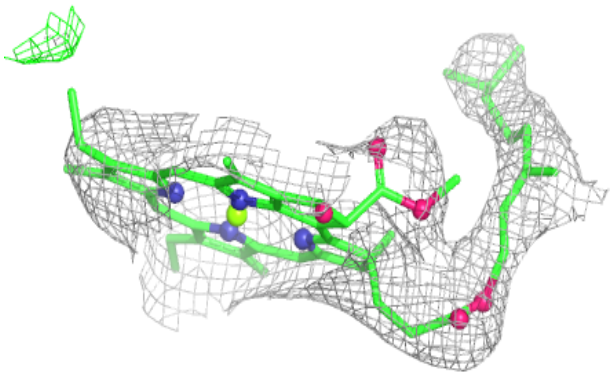


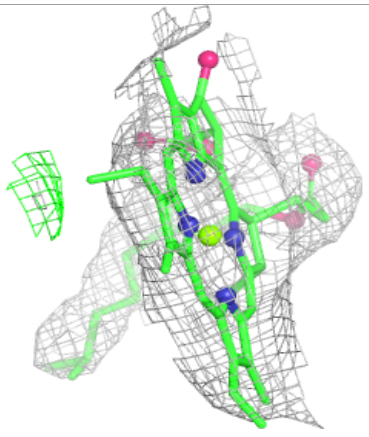


Electron density around CLA 1 1005:

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

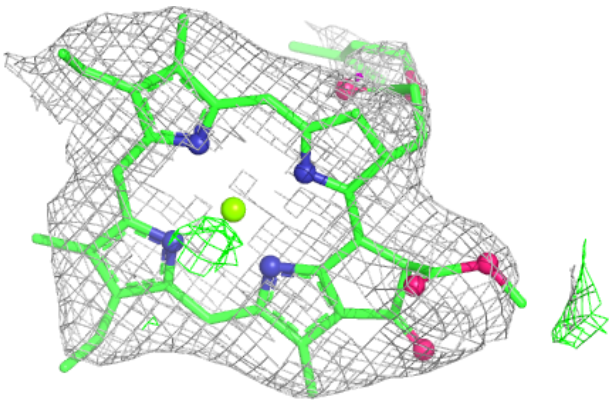


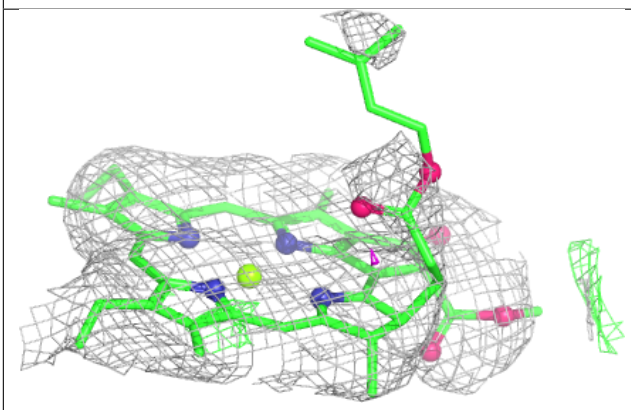


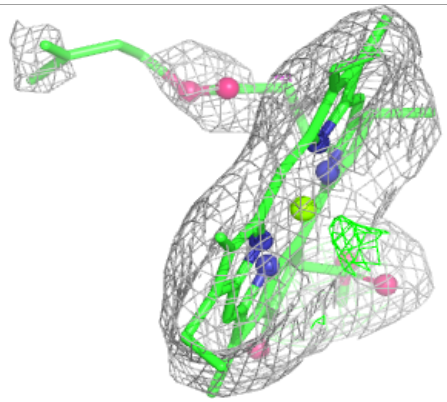


Electron density around CLA B 1201:

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

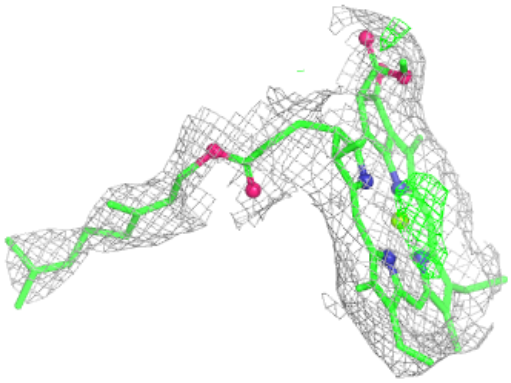


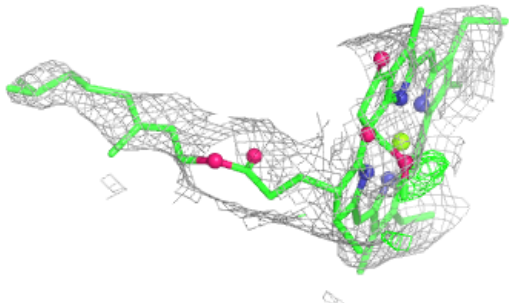


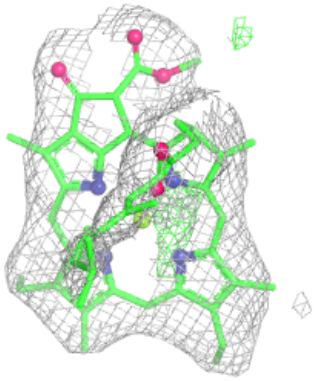


Electron density around CLA B 1208:

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

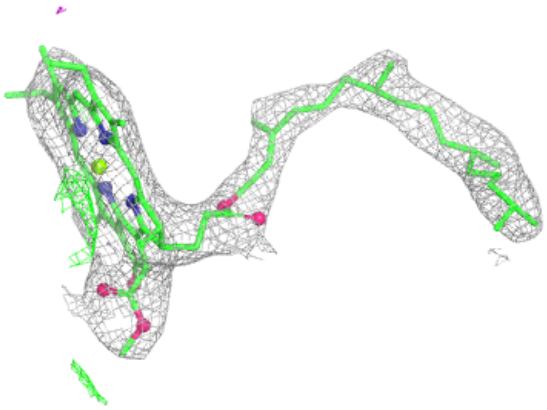


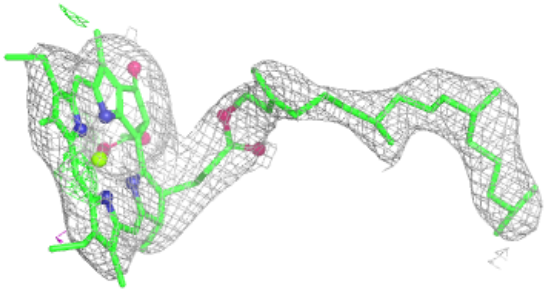


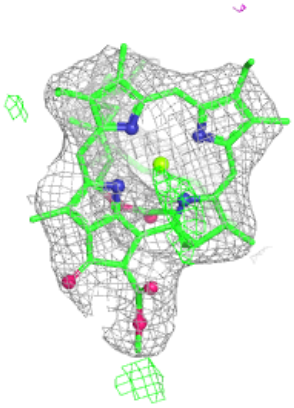


Electron density around CLA B 1238:

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

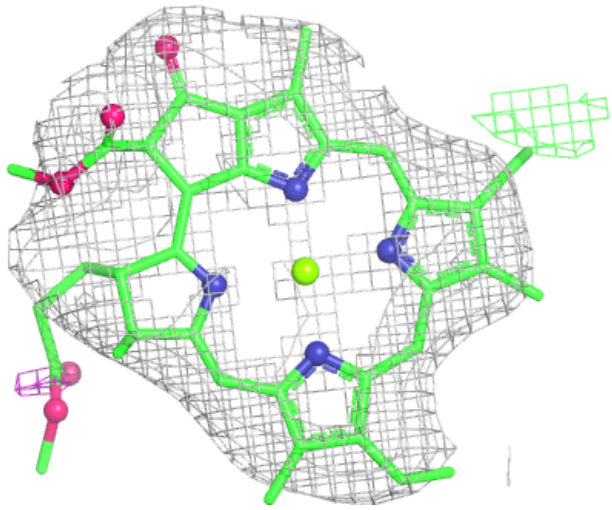


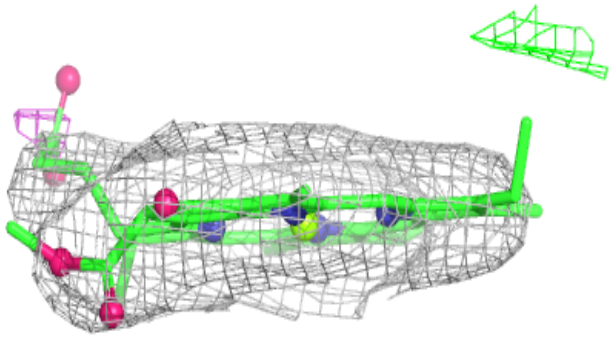


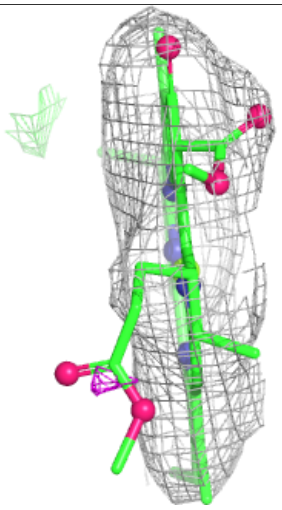


Electron density around CLA 3 3017:

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

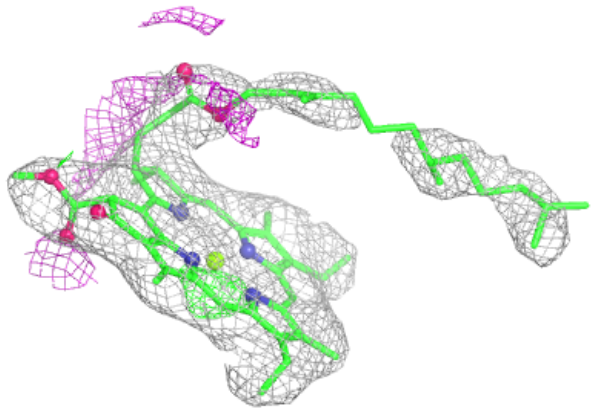


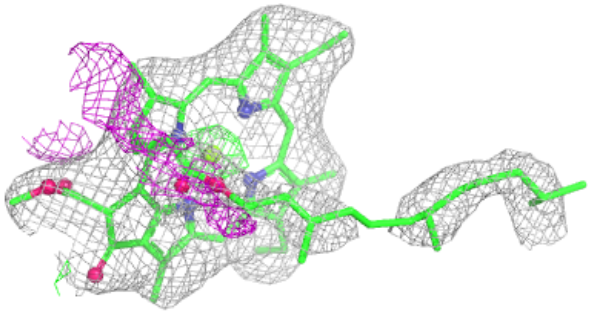


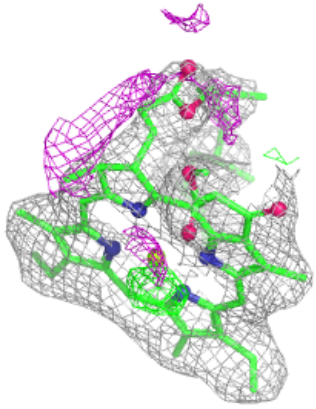


Electron density around CLA B 1228:

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

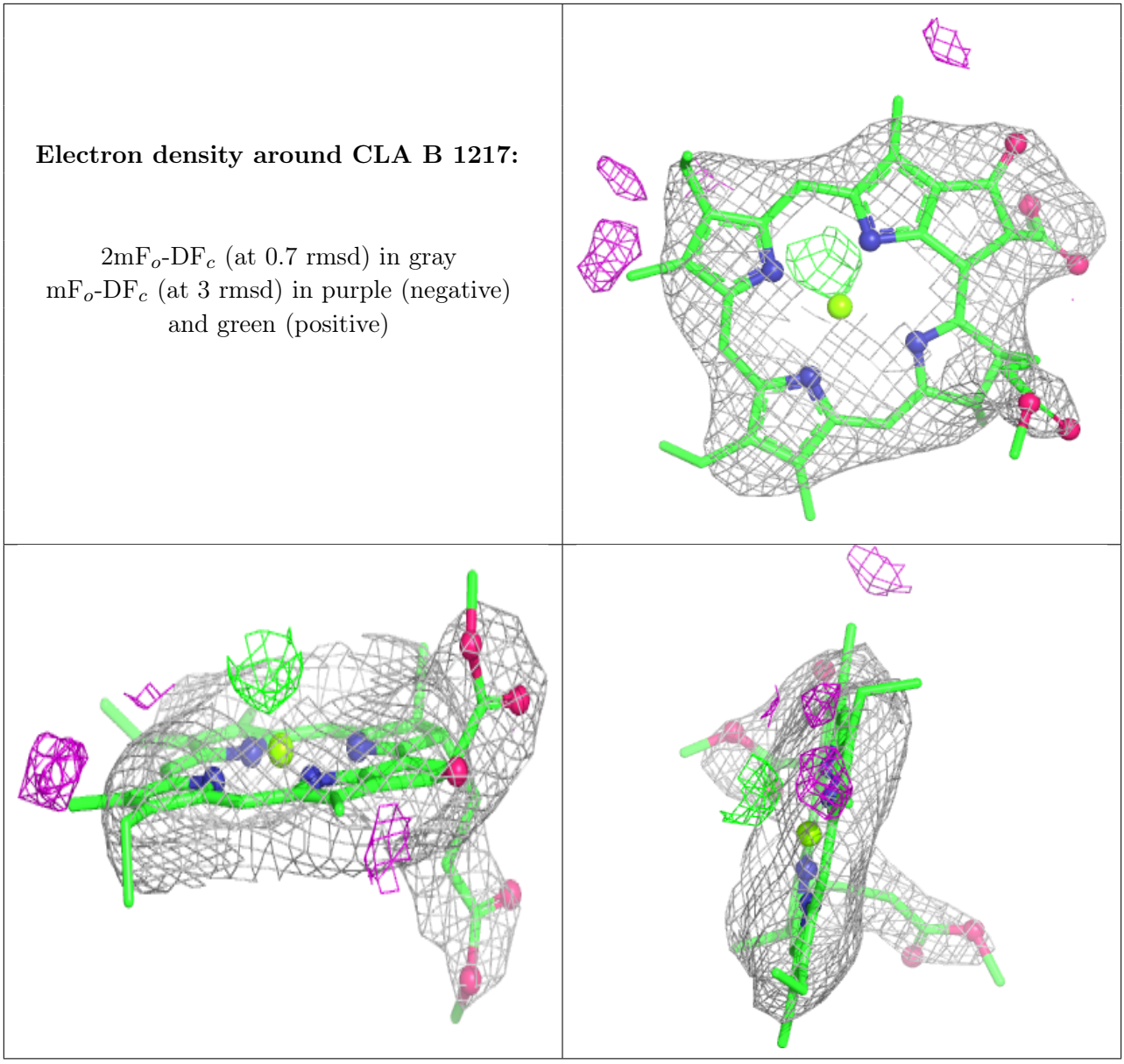






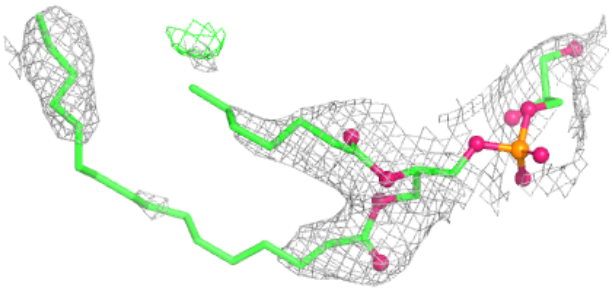
Electron density around CLA B 1217:

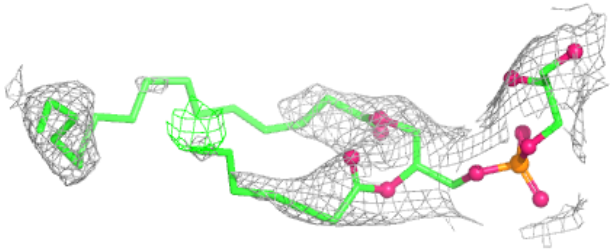
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

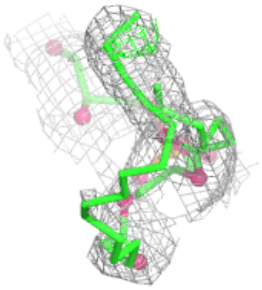


Electron density around LHG A 5003:

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

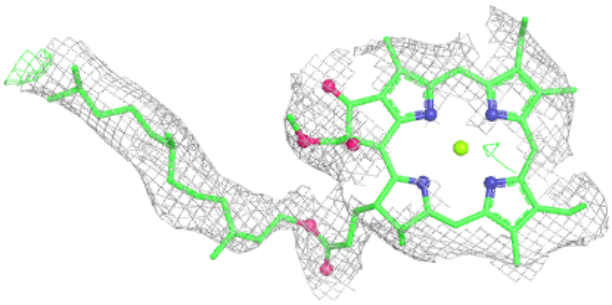


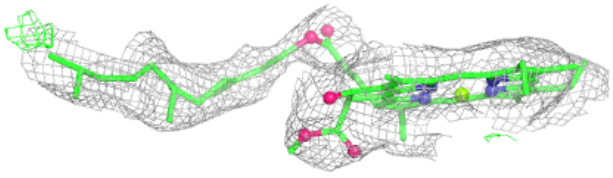




Electron density around CLA A 1120:

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

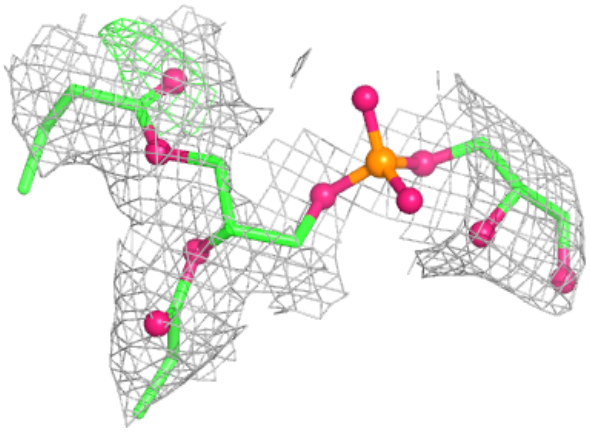


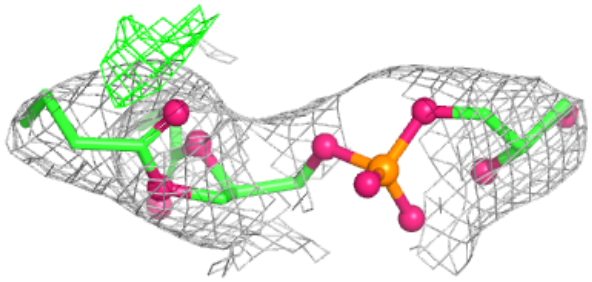


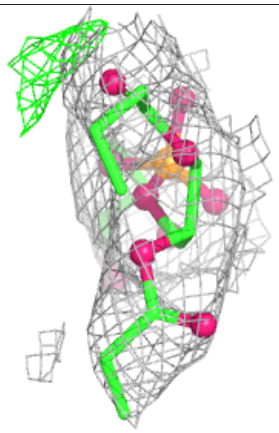


Electron density around LHG 2 2801:

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

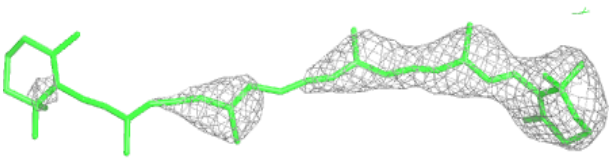


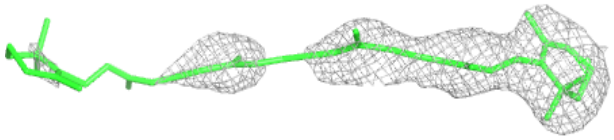


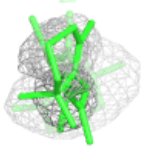


Electron density around BCR A 6003:

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

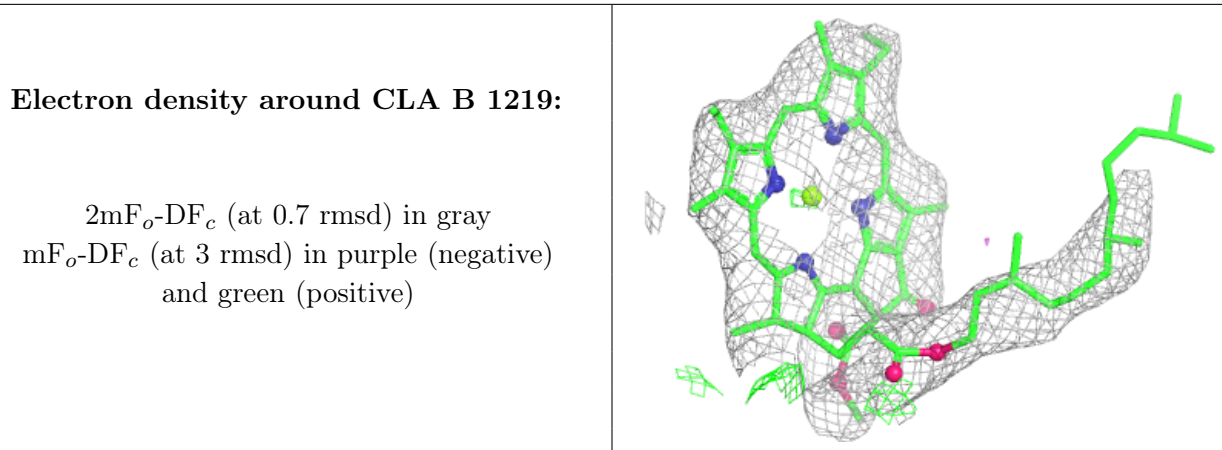






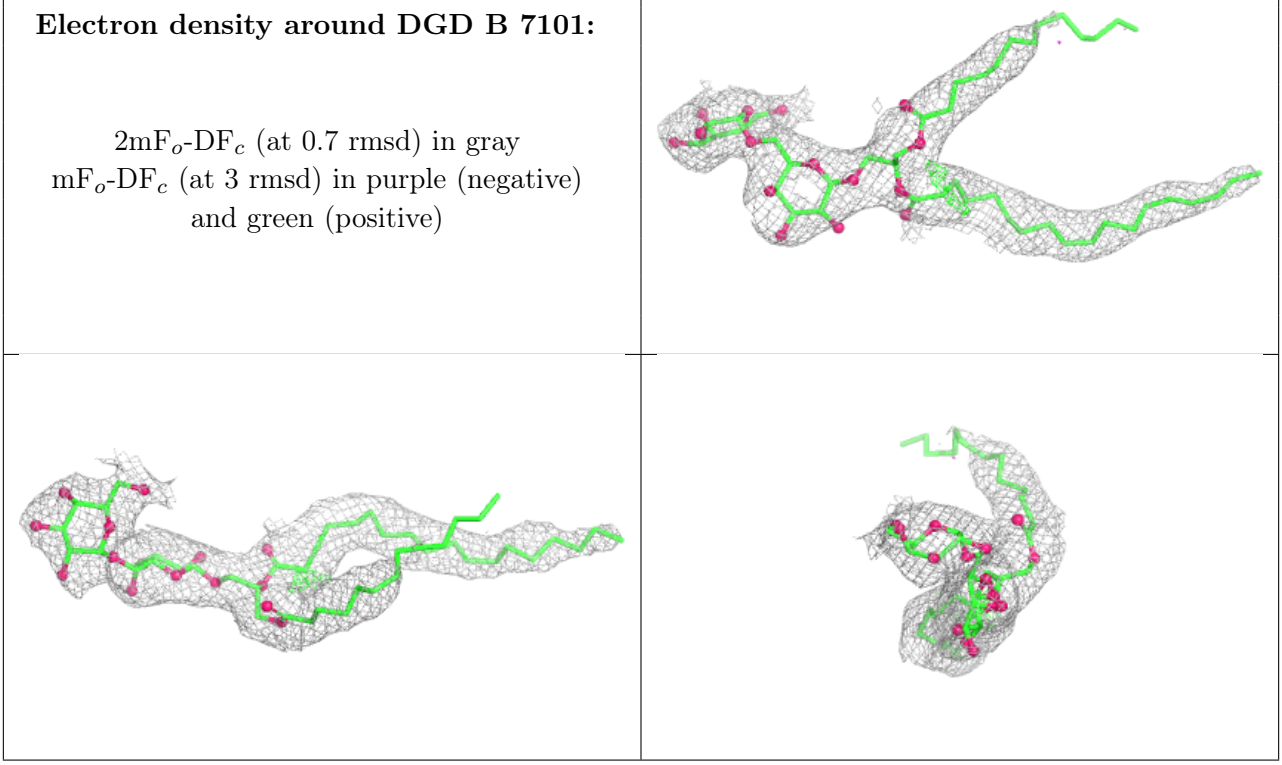
Electron density around CLA B 1219:

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



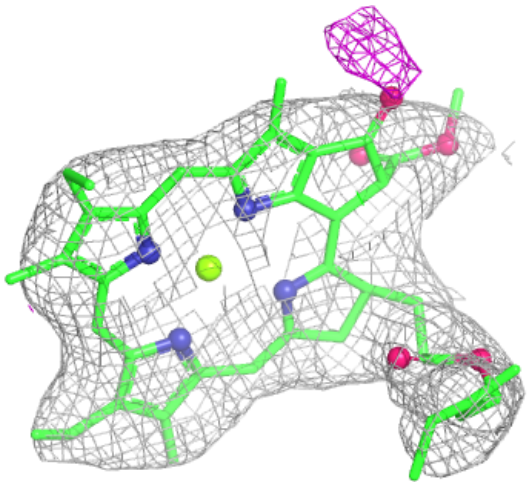
Electron density around DGD B 7101:

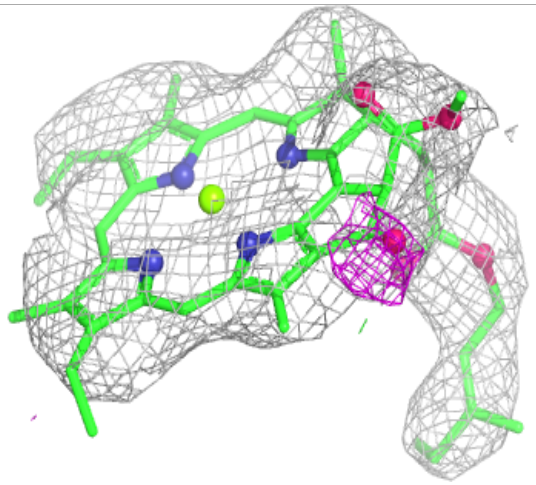
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

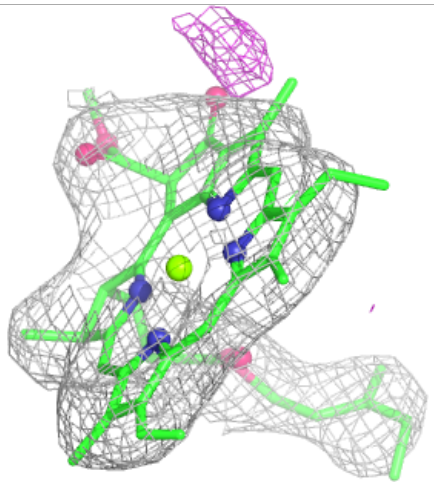


Electron density around CLA A 1105:

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

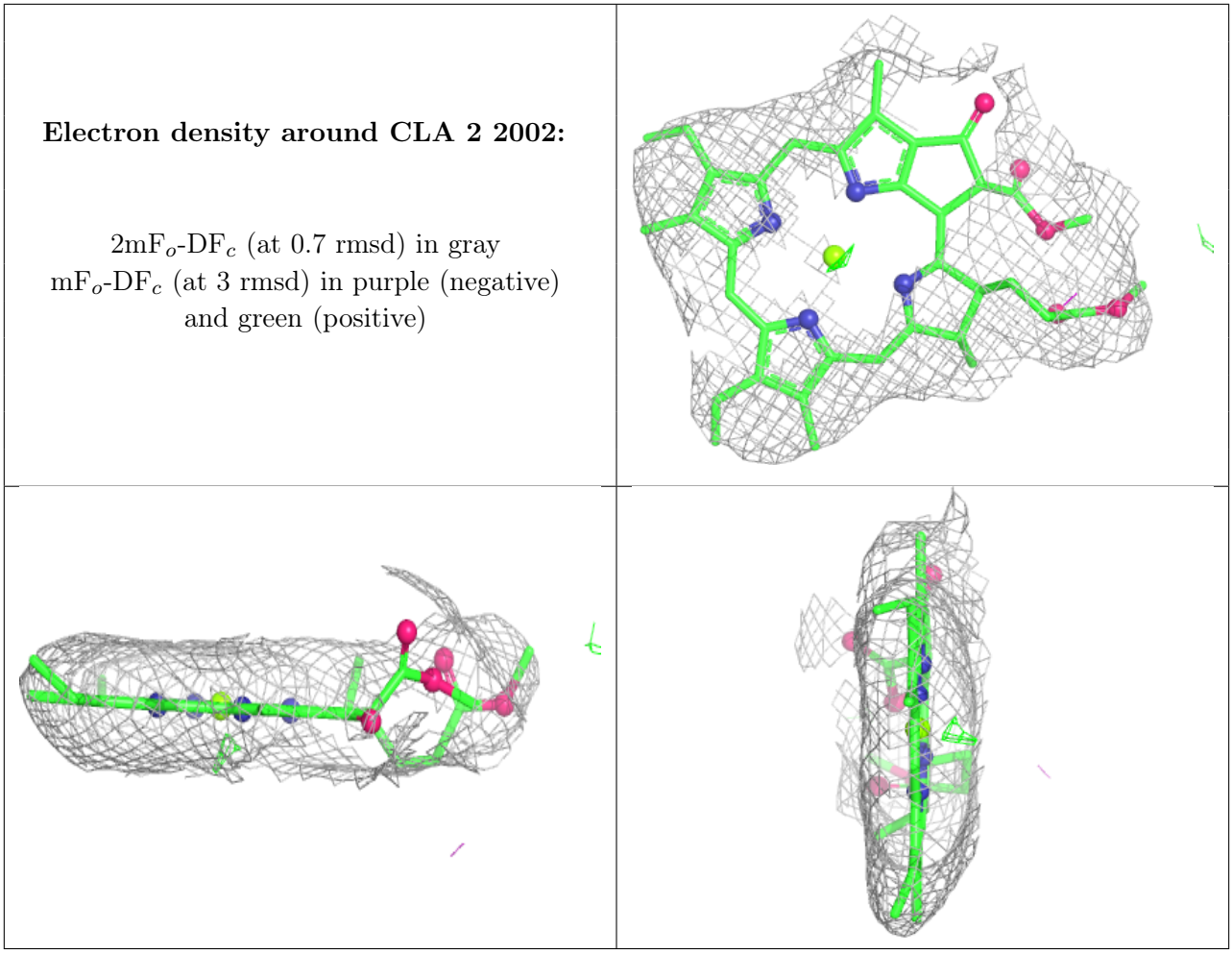






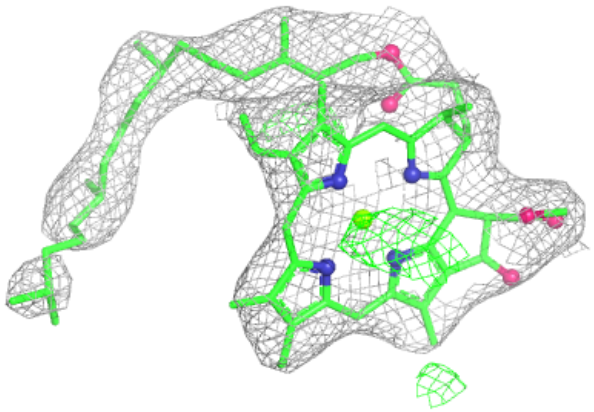
Electron density around CLA 2 2002:

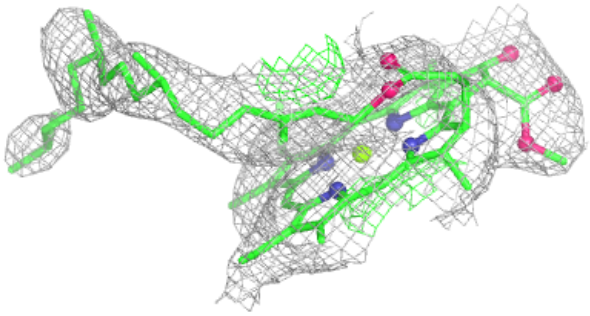
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 2 2004:

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

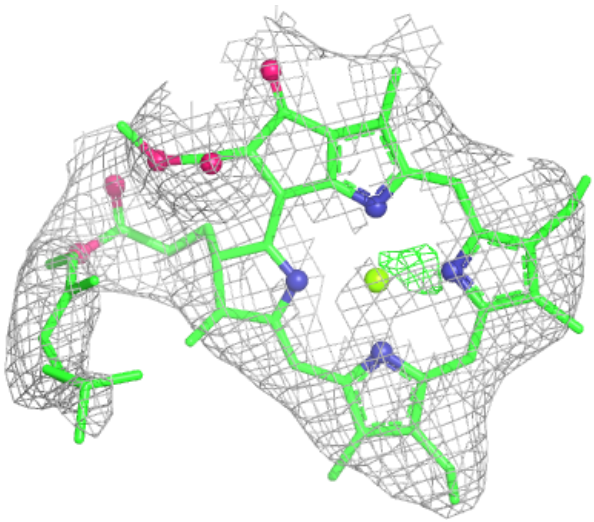


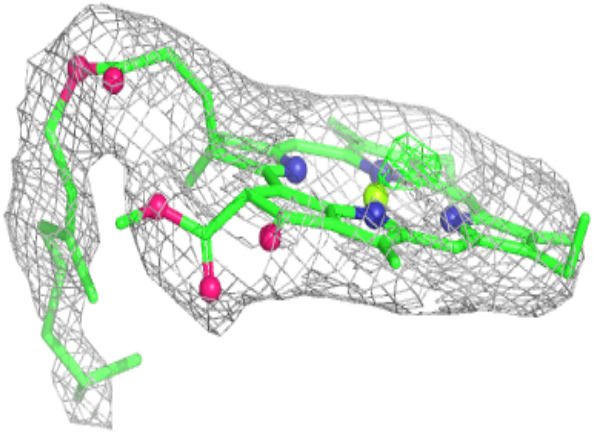


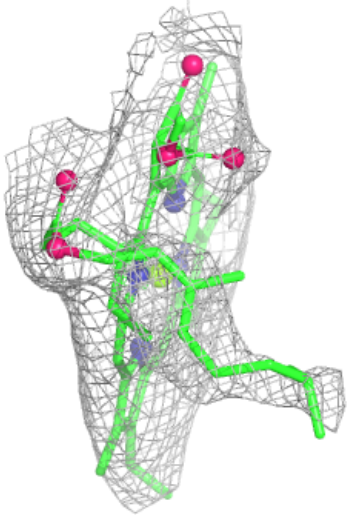


Electron density around CLA 2 2005:

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

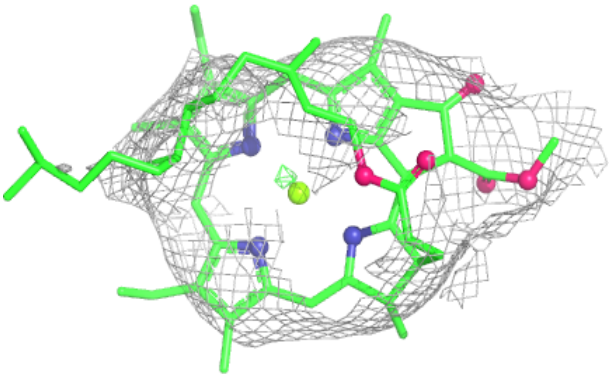


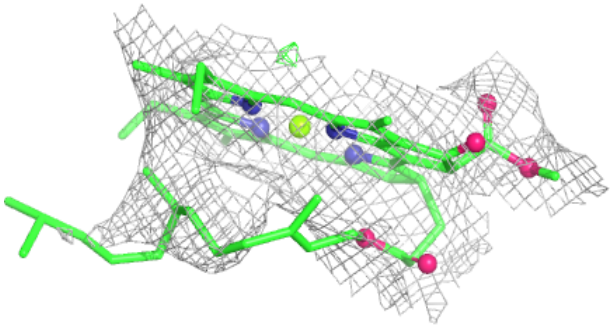


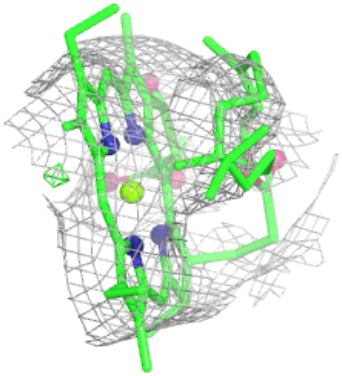


Electron density around CLA 3 3003:

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

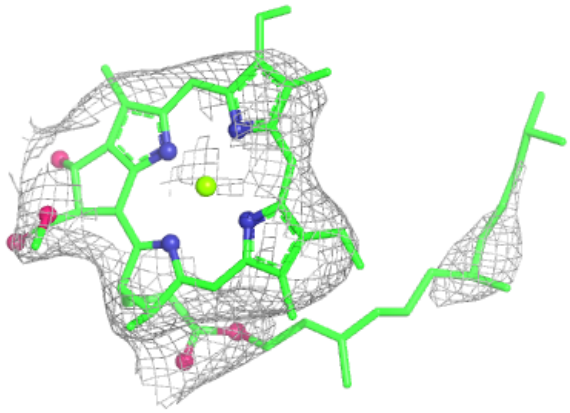


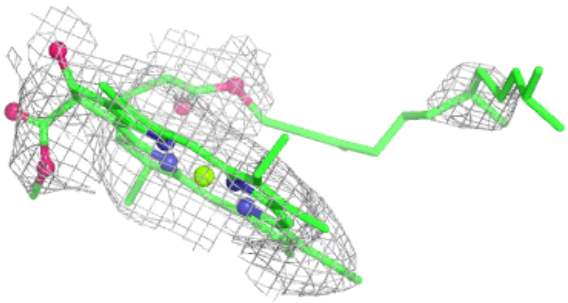


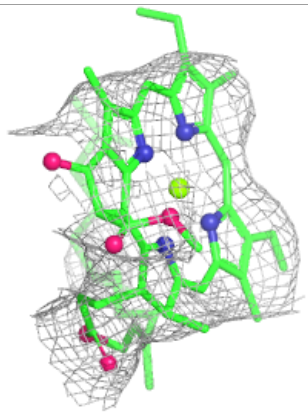


Electron density around CLA 3 3004:

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

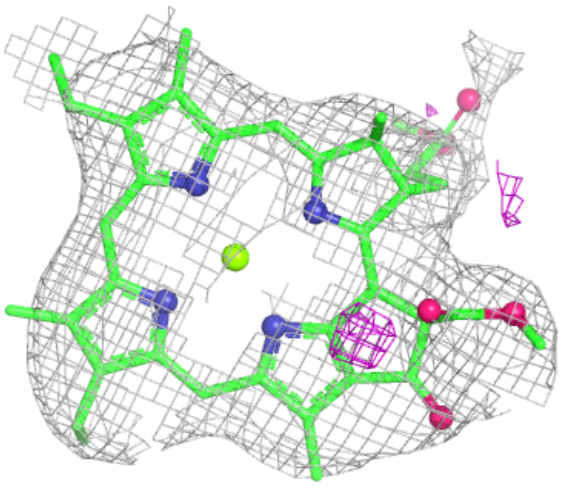


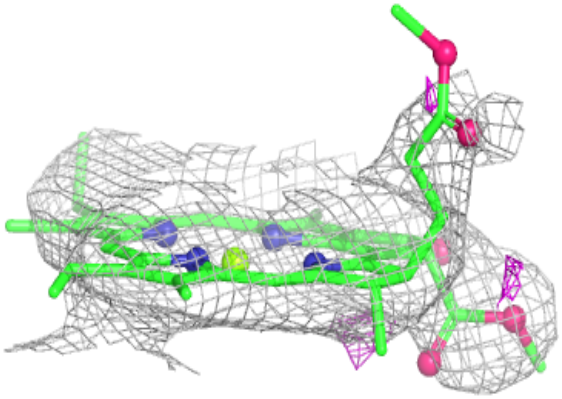


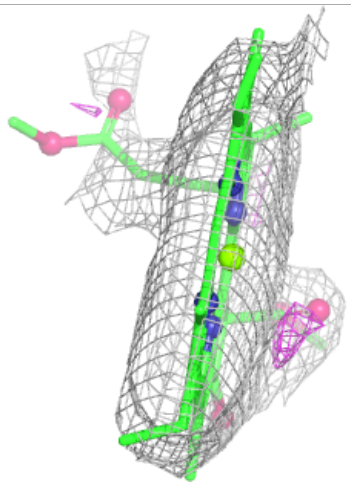


Electron density around CLA B 1209:

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

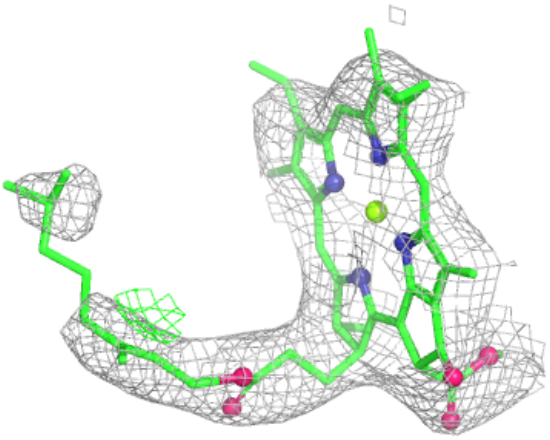


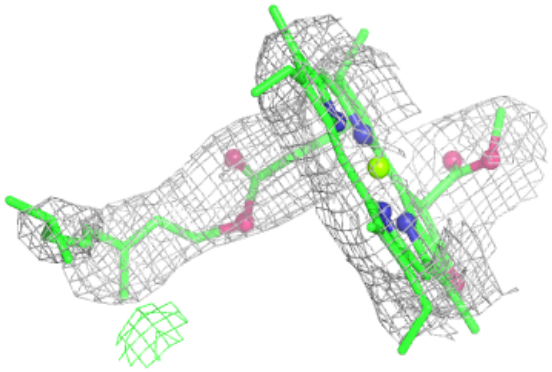


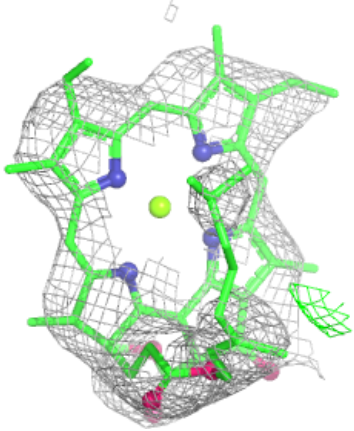


Electron density around CLA B 1212:

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

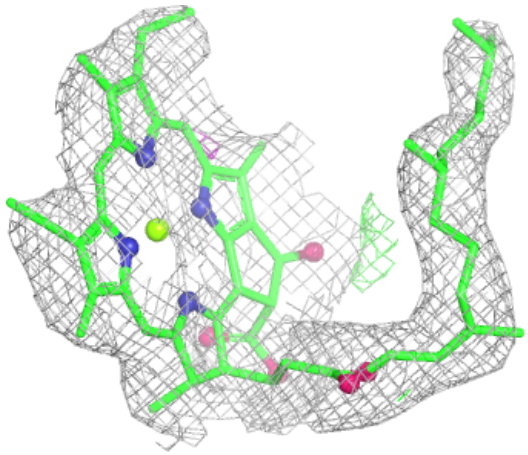


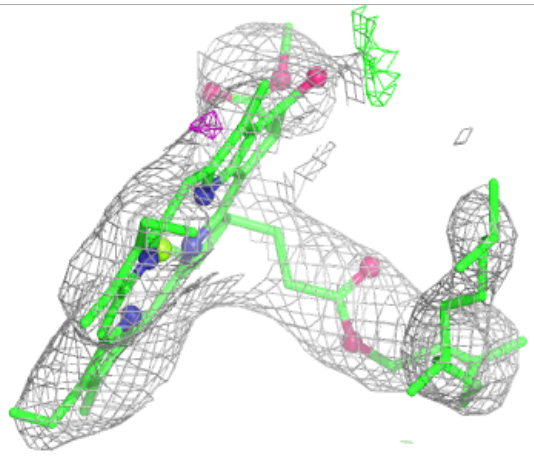


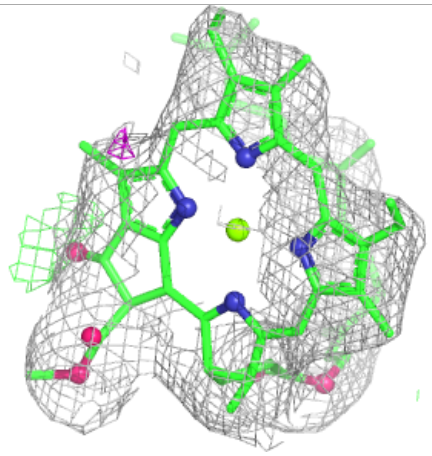


Electron density around CLA B 1231:

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

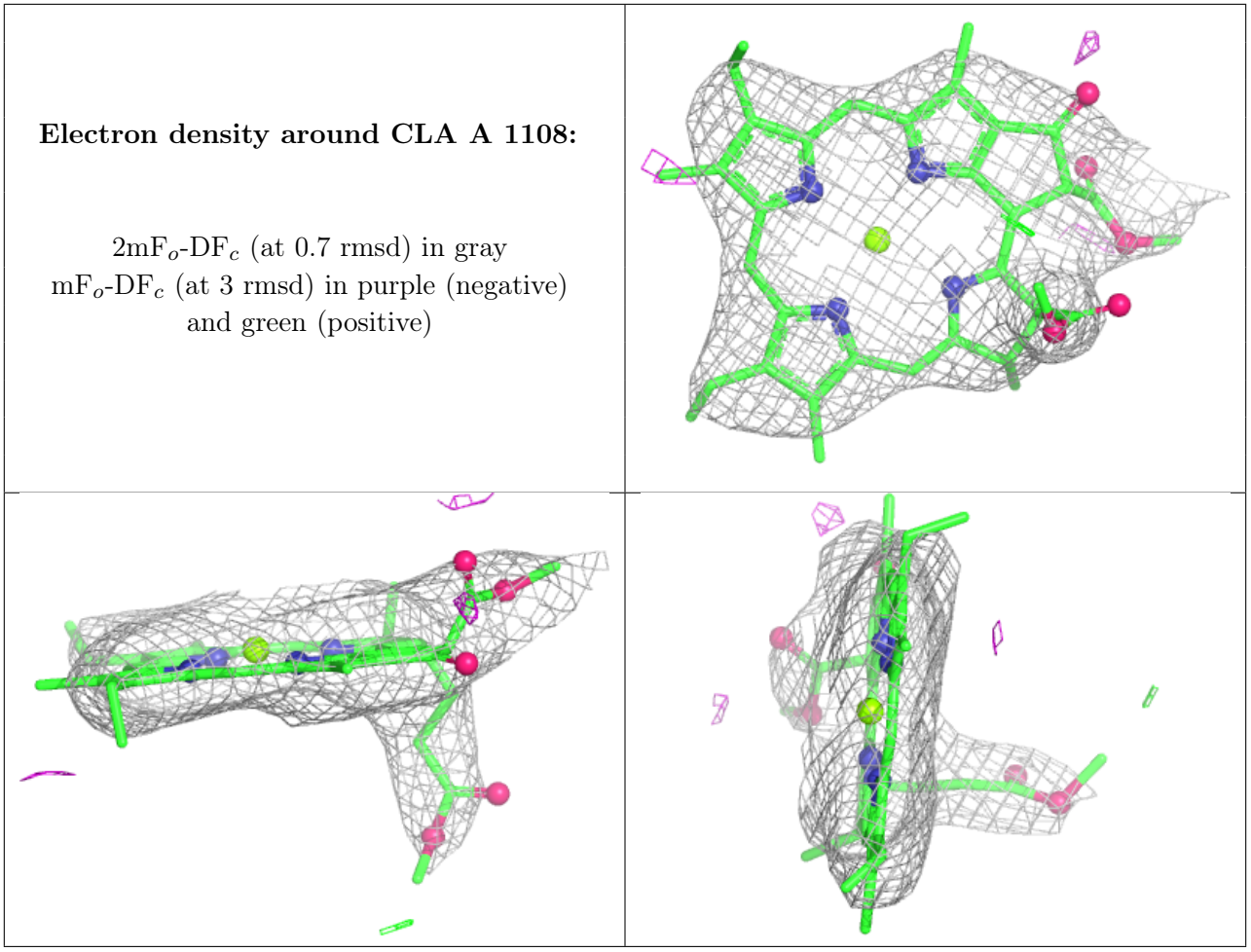






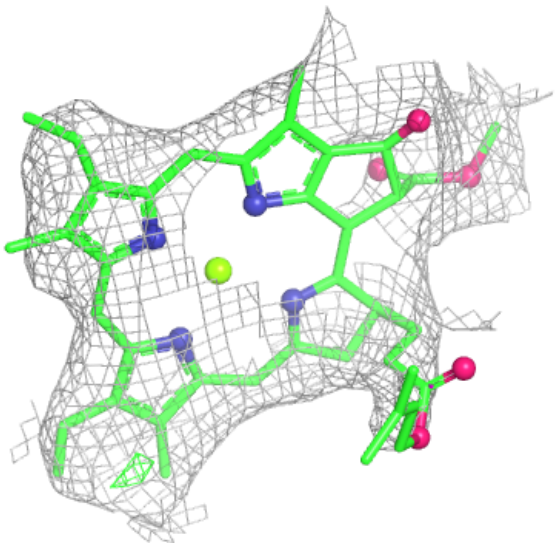
Electron density around CLA A 1108:

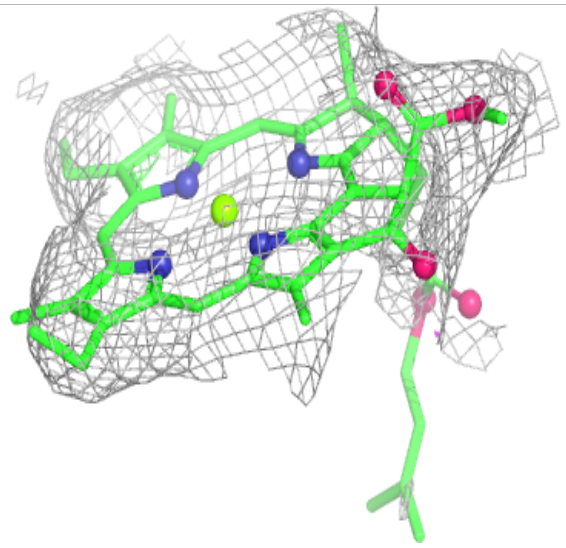
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 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)

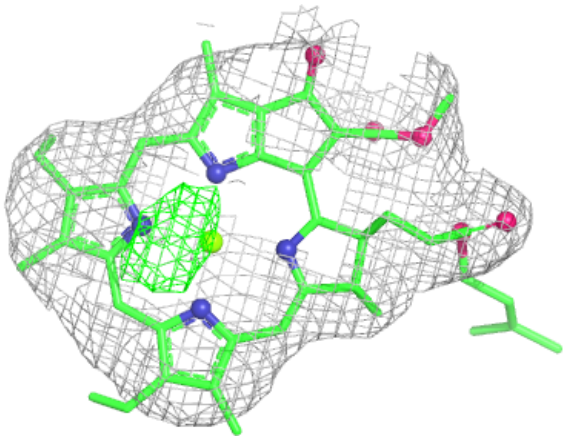


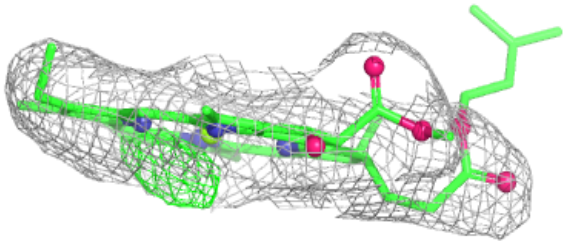


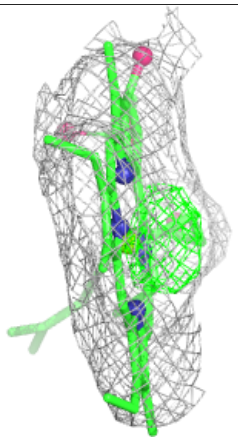


Electron density around CLA 4 4002:

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

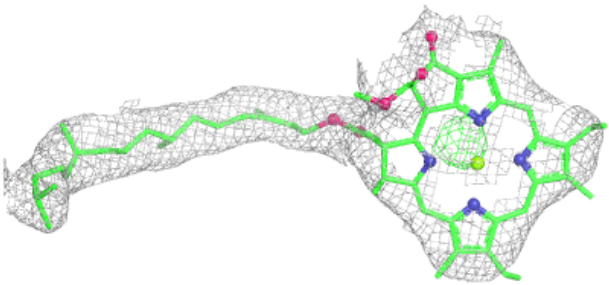


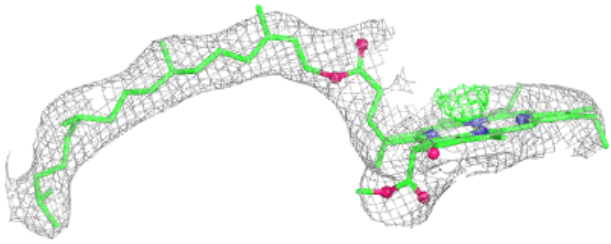




Electron density around CLA B 1240:

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

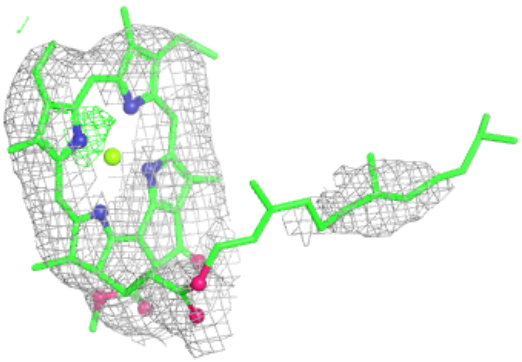


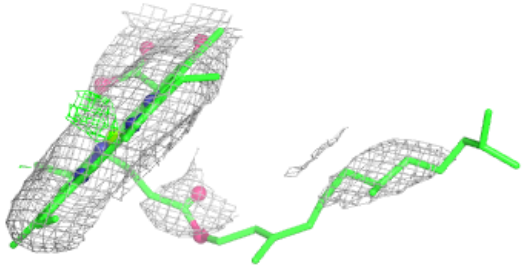


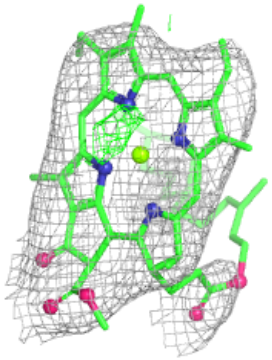


Electron density around CLA 4 4007:

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

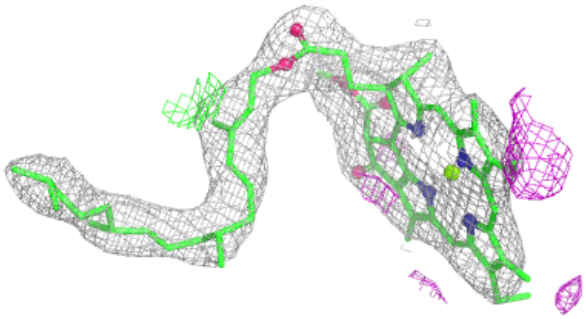


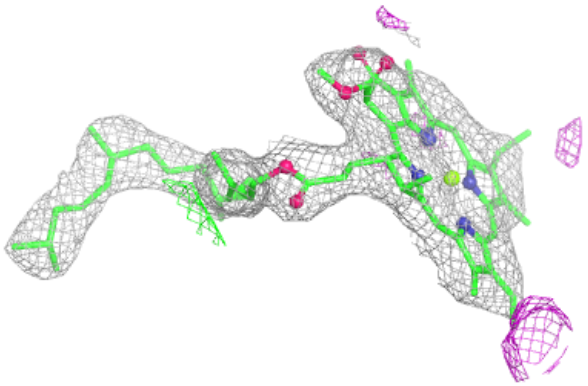


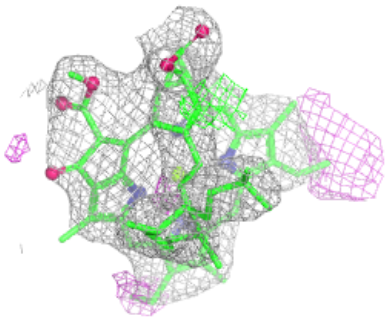


Electron density around CLA B 1021:

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

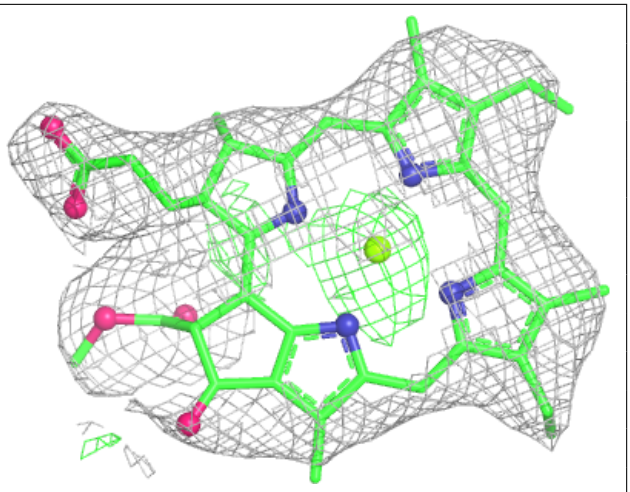


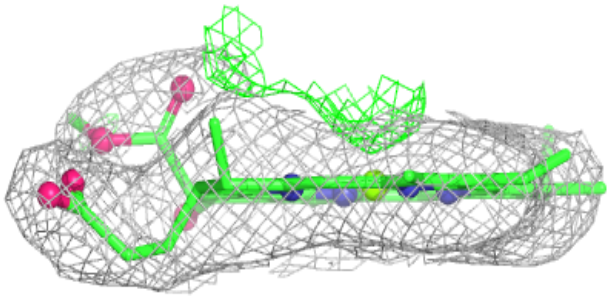


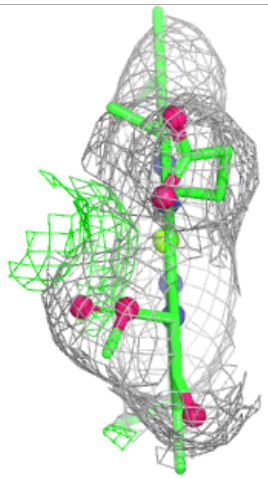


Electron density around CLA F 1301:

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

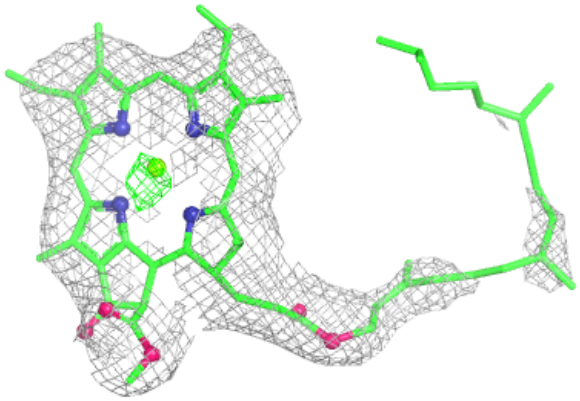


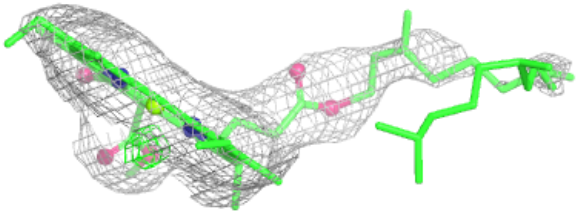


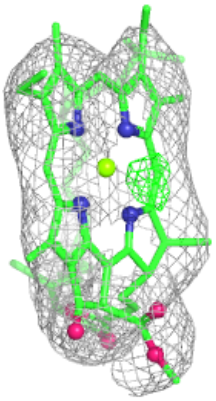


Electron density around CLA 4 4017:

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

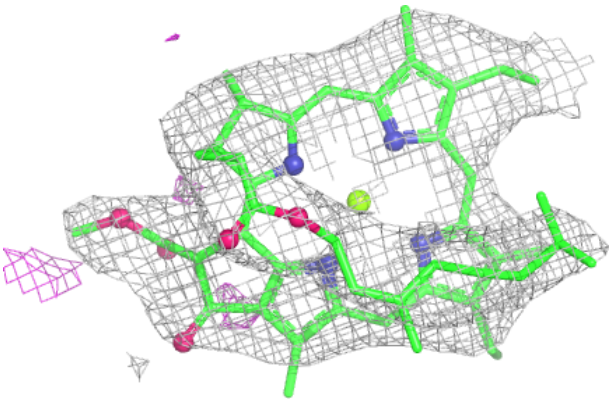


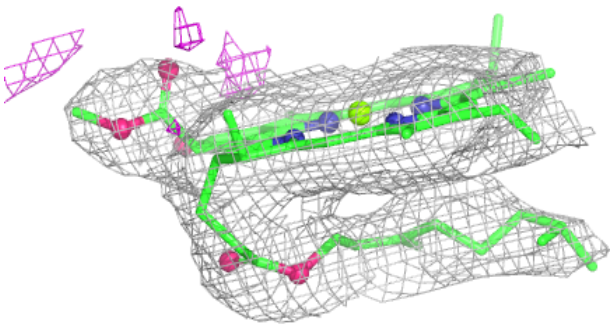


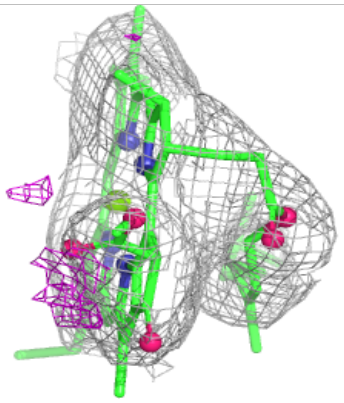


Electron density around CLA B 1204:

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

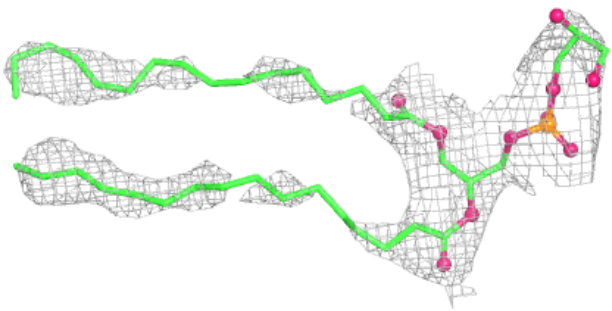


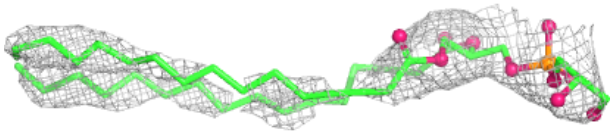


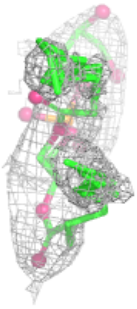


Electron density around LHG 1 1801:

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

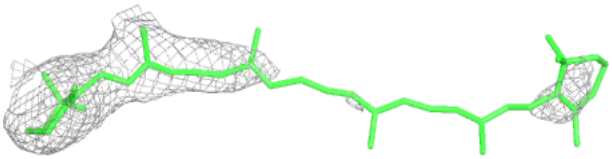


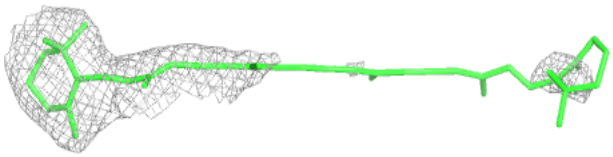


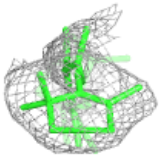


Electron density around BCR A 6002:

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

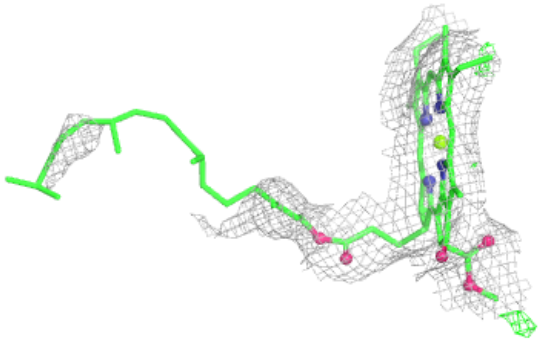


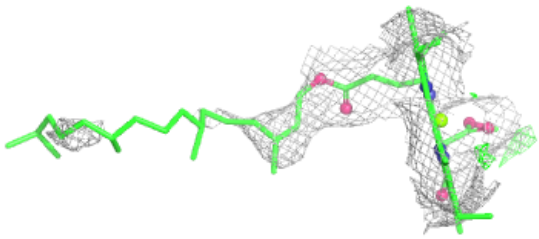


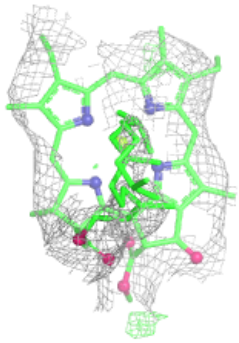


Electron density around CLA A 1112:

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

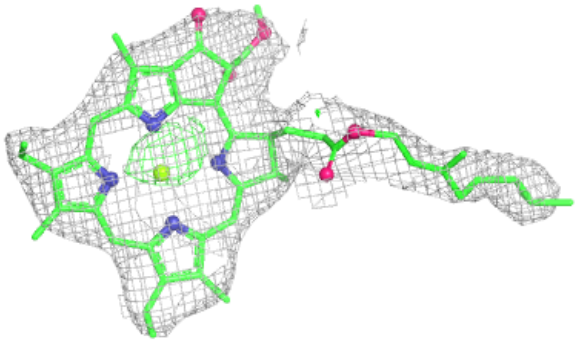


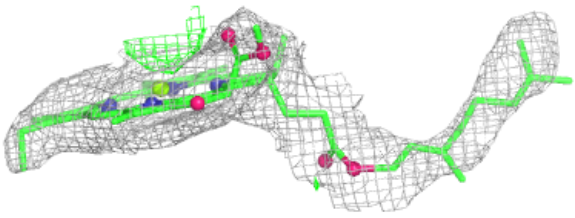


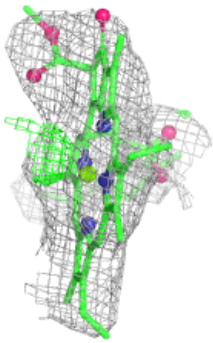


Electron density around CLA A 1124:

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

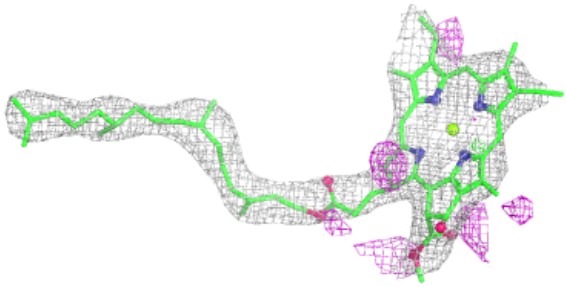


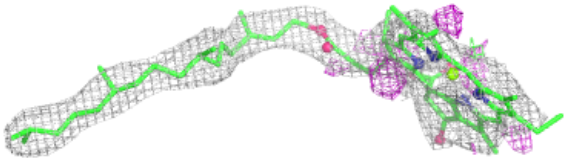


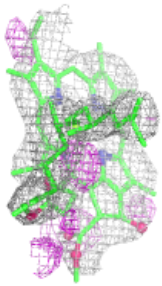


Electron density around CLA A 1022:

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

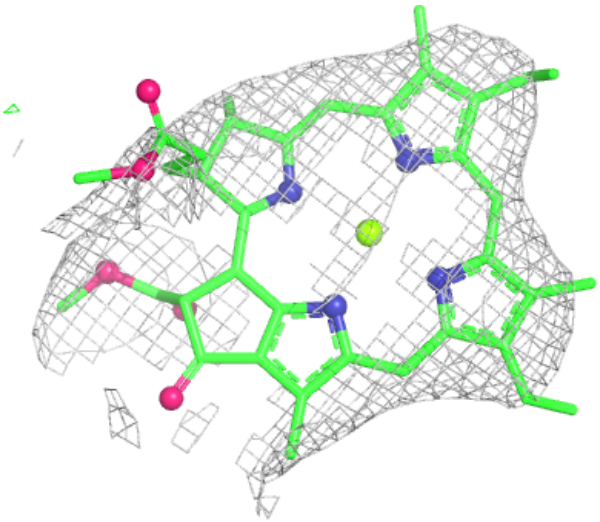


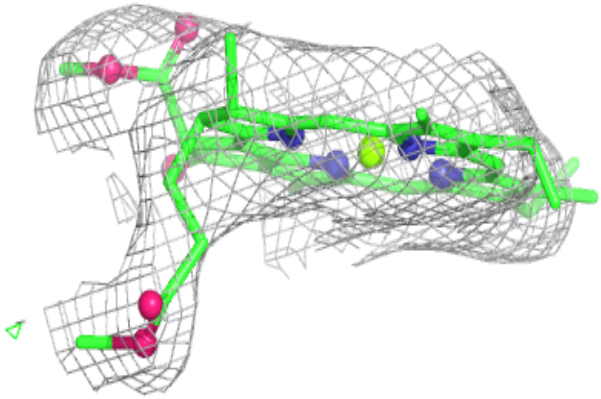


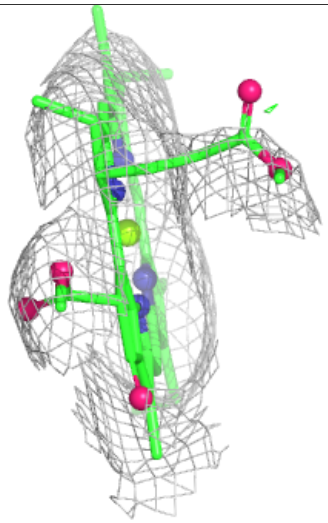


Electron density around CLA 1 1007:

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

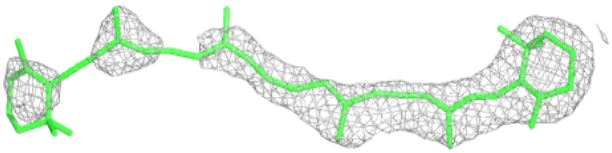


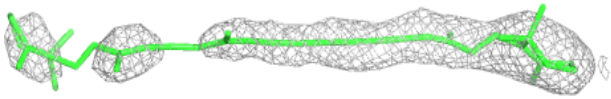


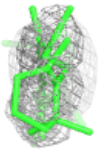


Electron density around BCR B 6005:

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

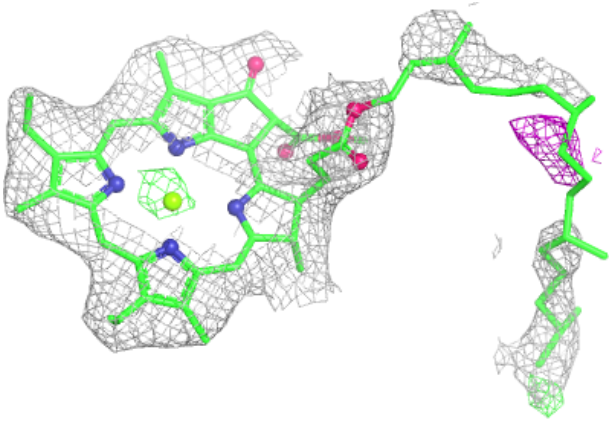


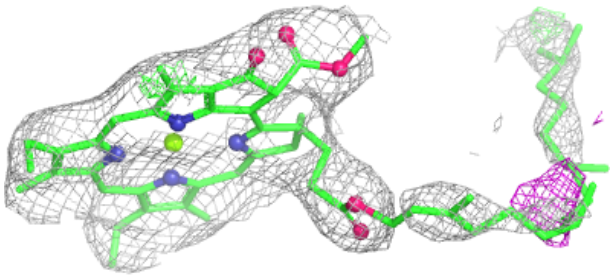


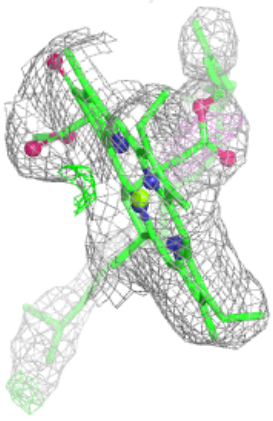


Electron density around CLA B 1220:

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

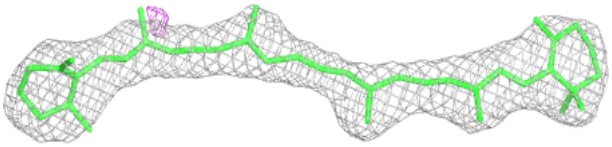


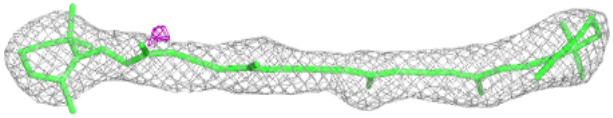


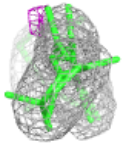


Electron density around BCR J 6012:

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

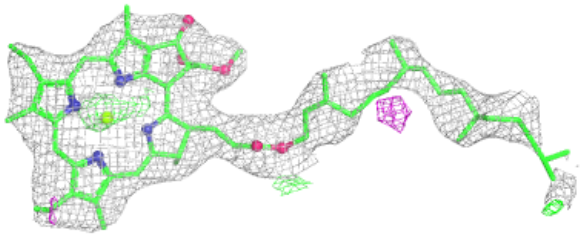


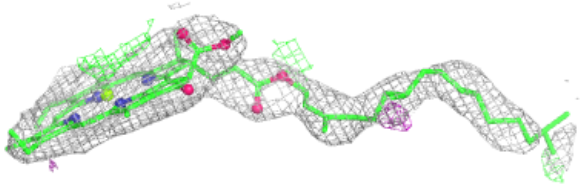


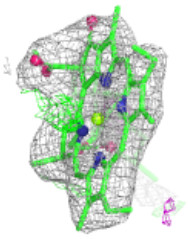


Electron density around CLA A 1139:

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

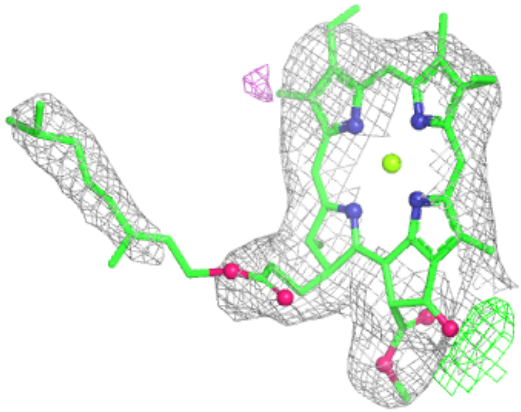


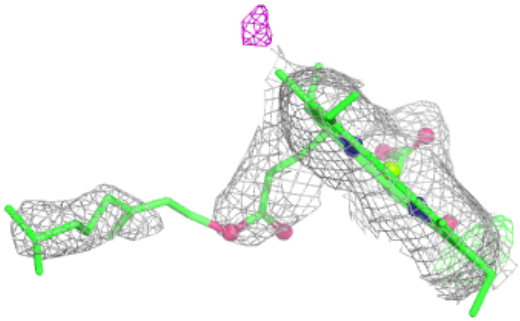


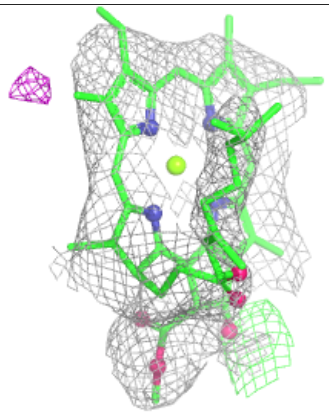


Electron density around CLA A 1133:

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

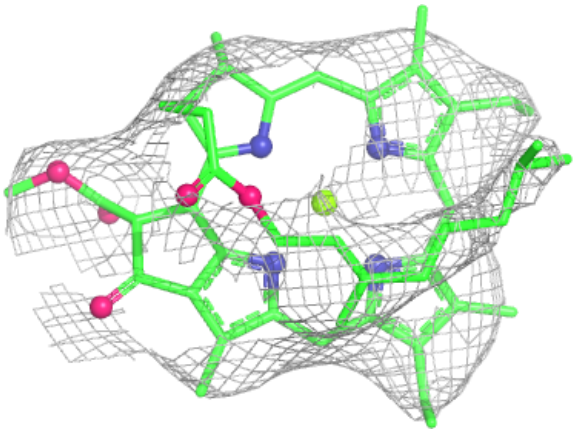


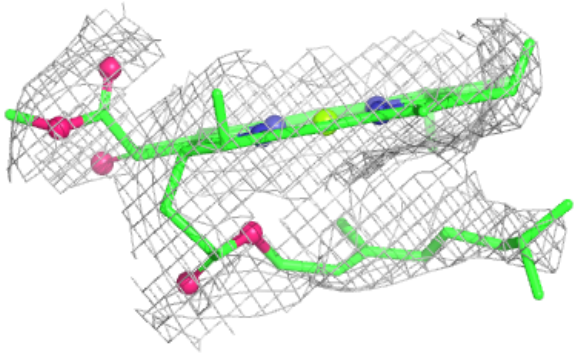


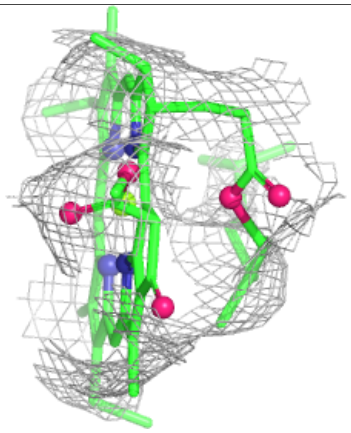


Electron density around CLA 2 2003:

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

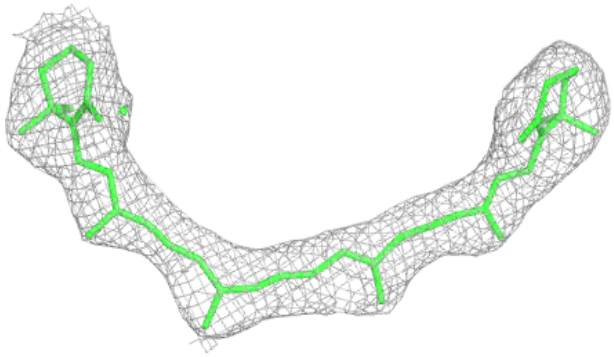


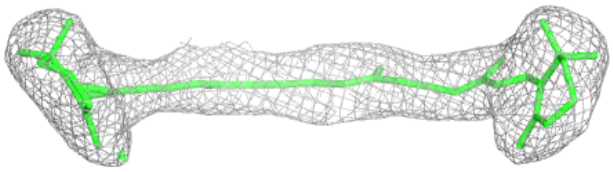


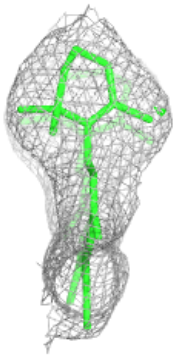


Electron density around BCR F 6016:

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

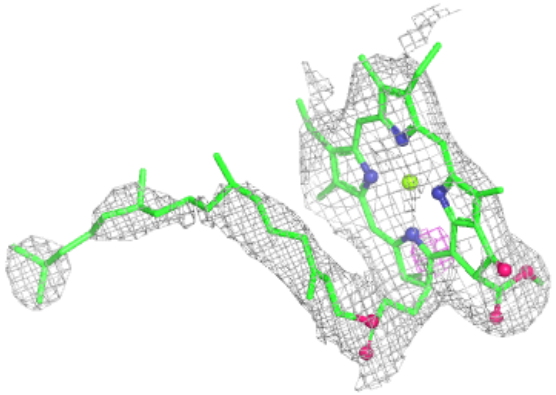


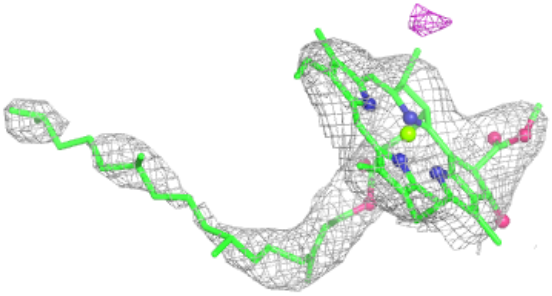


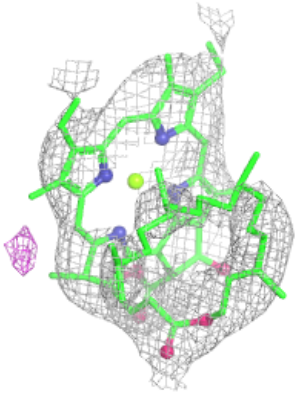


Electron density around CLA B 1211:

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

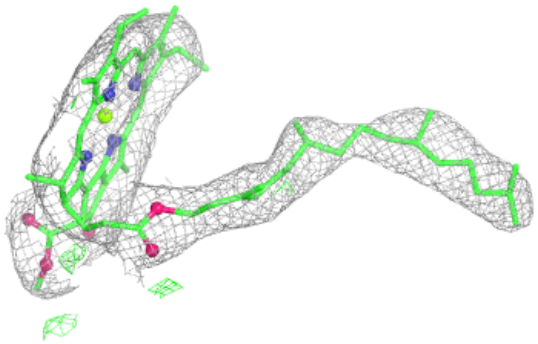


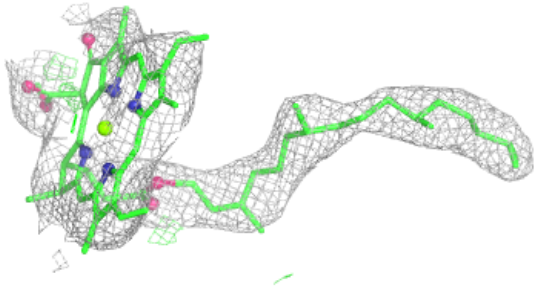


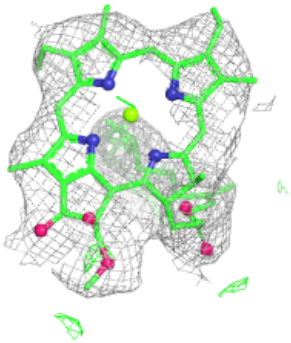


Electron density around CLA A 1109:

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

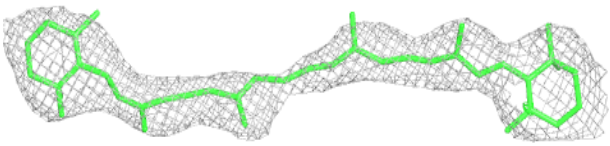


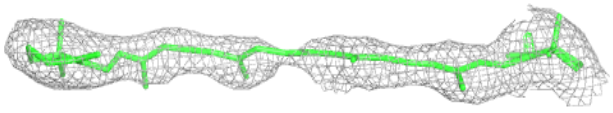


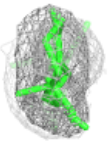


Electron density around BCR L 6019:

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

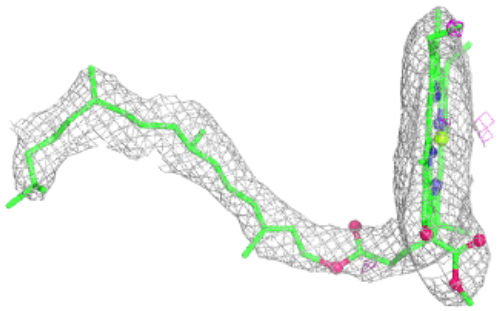


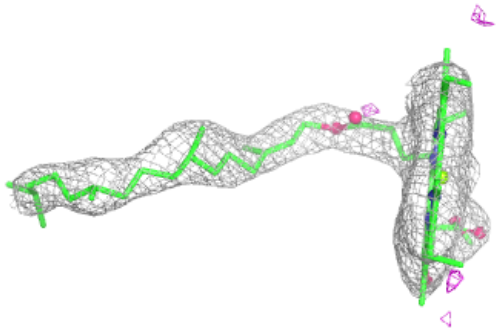


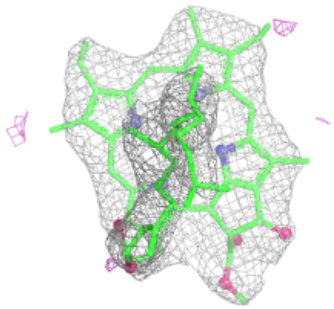


Electron density around CLA B 1239:

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

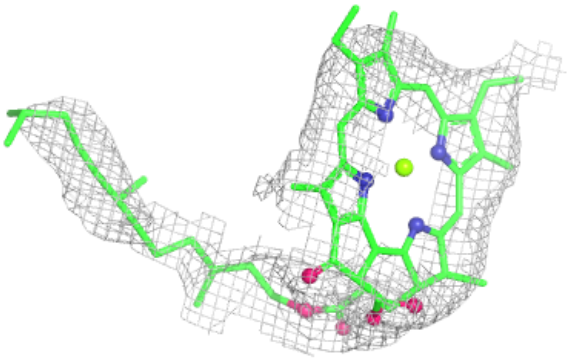


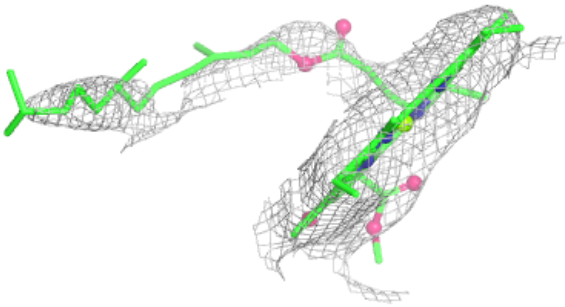


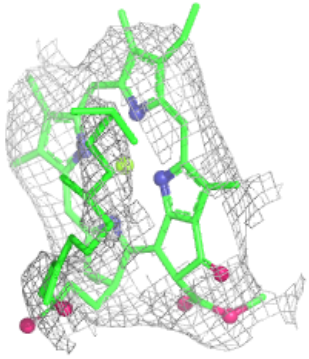


Electron density around CLA 2 2007:

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

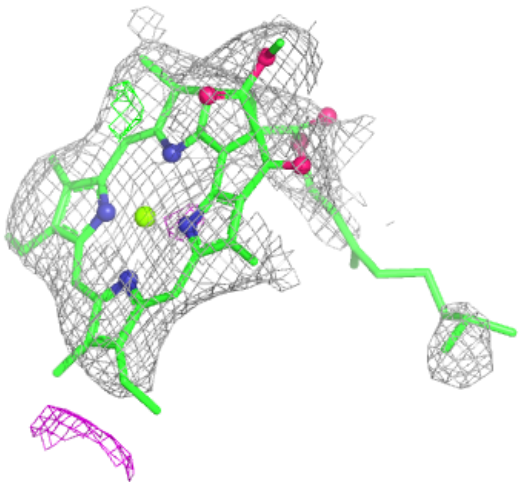


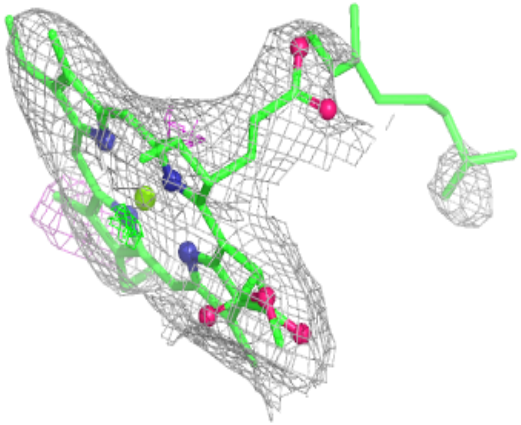


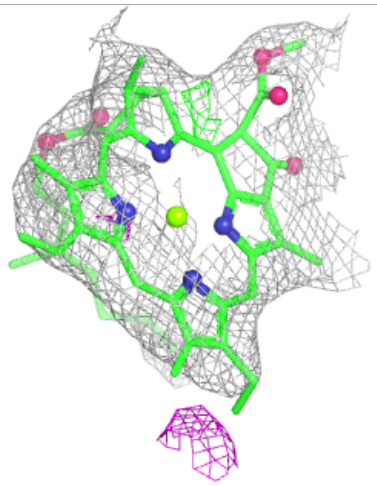


Electron density around CLA 2 2012:

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

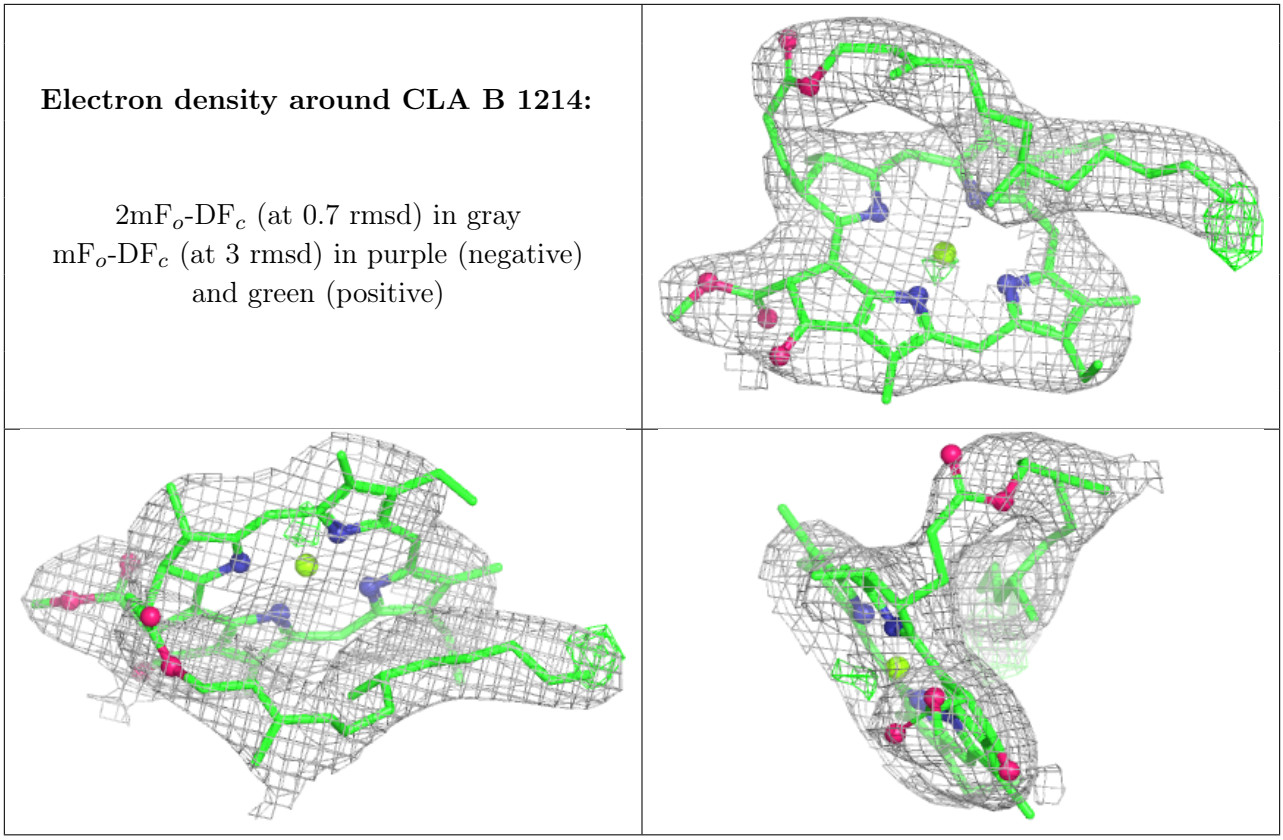






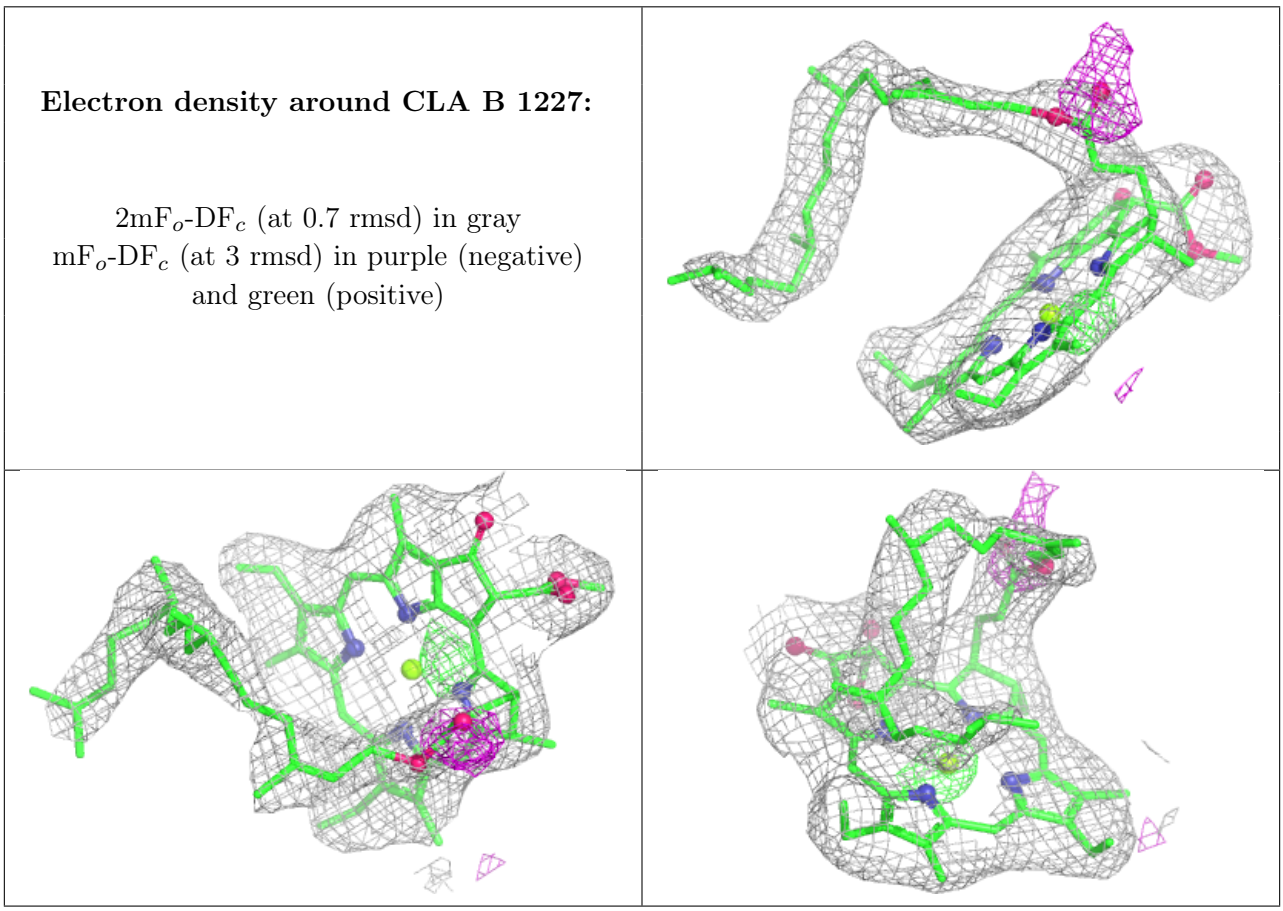
Electron density around CLA B 1214:

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



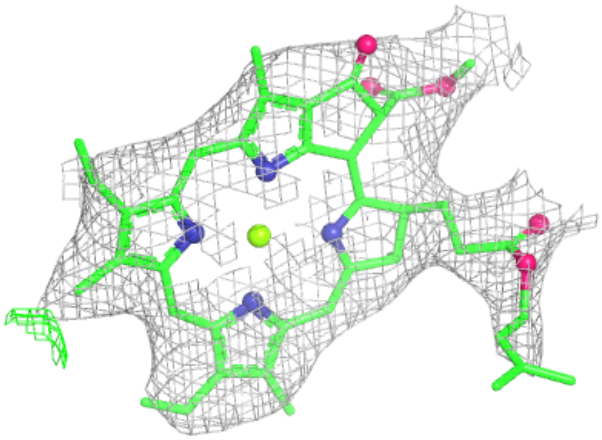
Electron density around CLA B 1227:

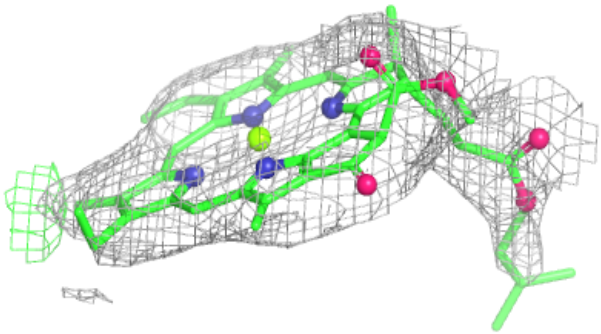
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

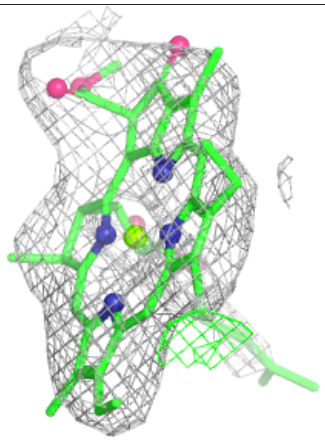


Electron density around CLA 2 2009:

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

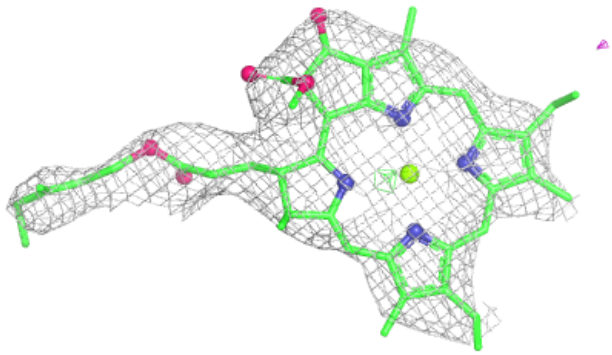


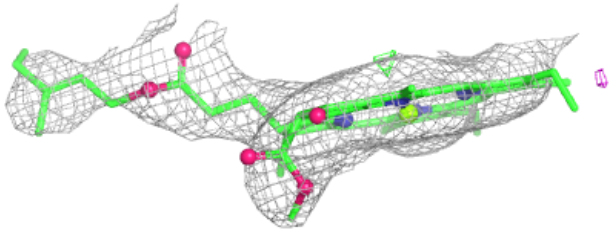


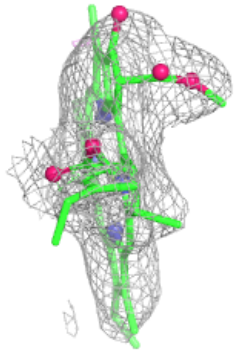


Electron density around CLA A 1135:

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

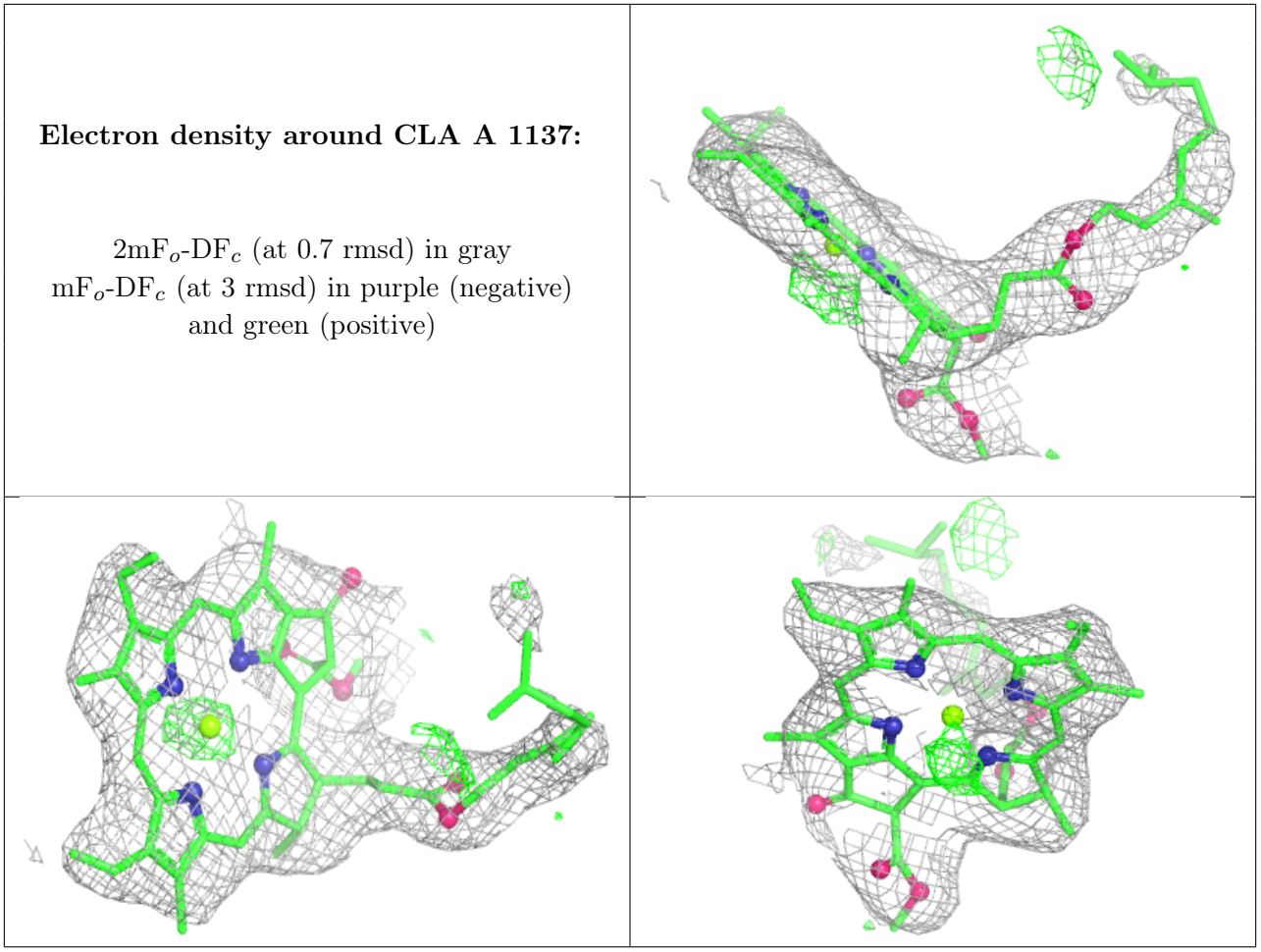






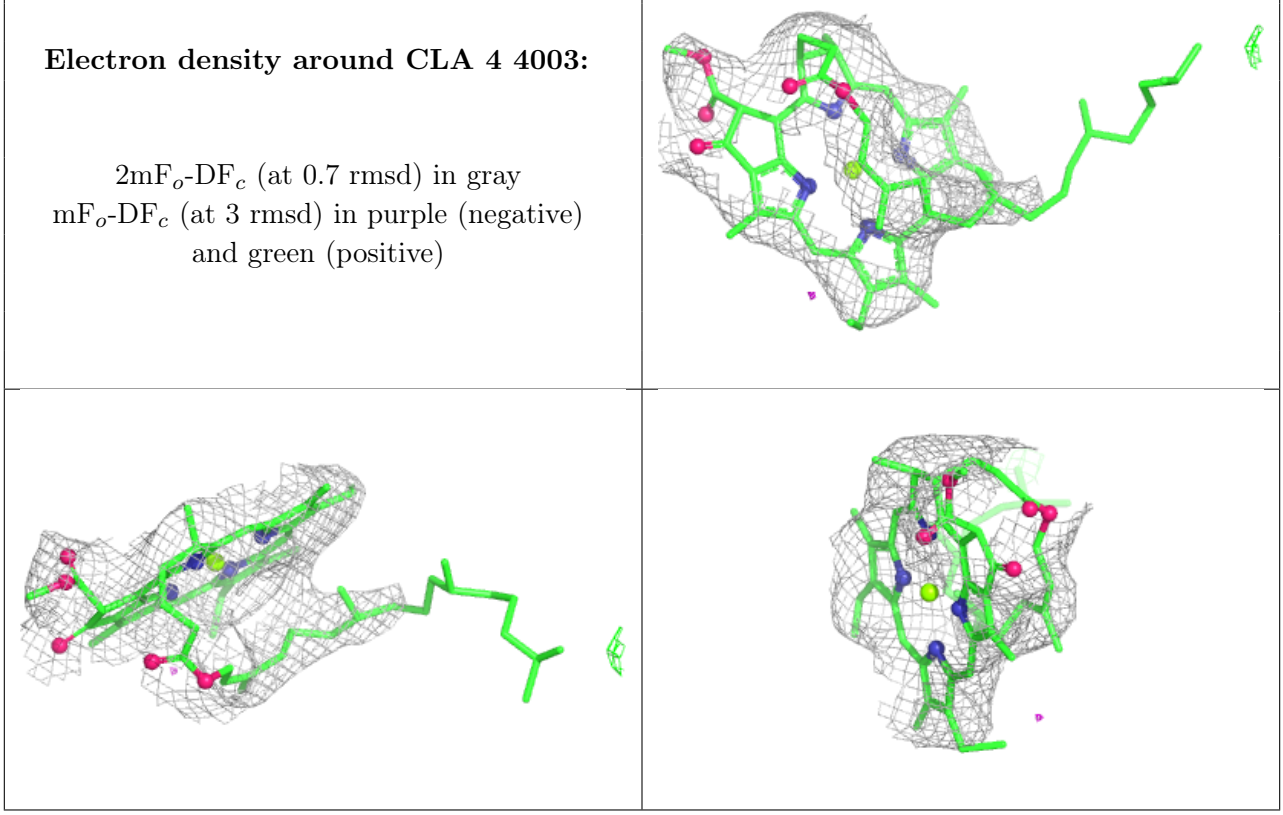
Electron density around CLA A 1137:

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



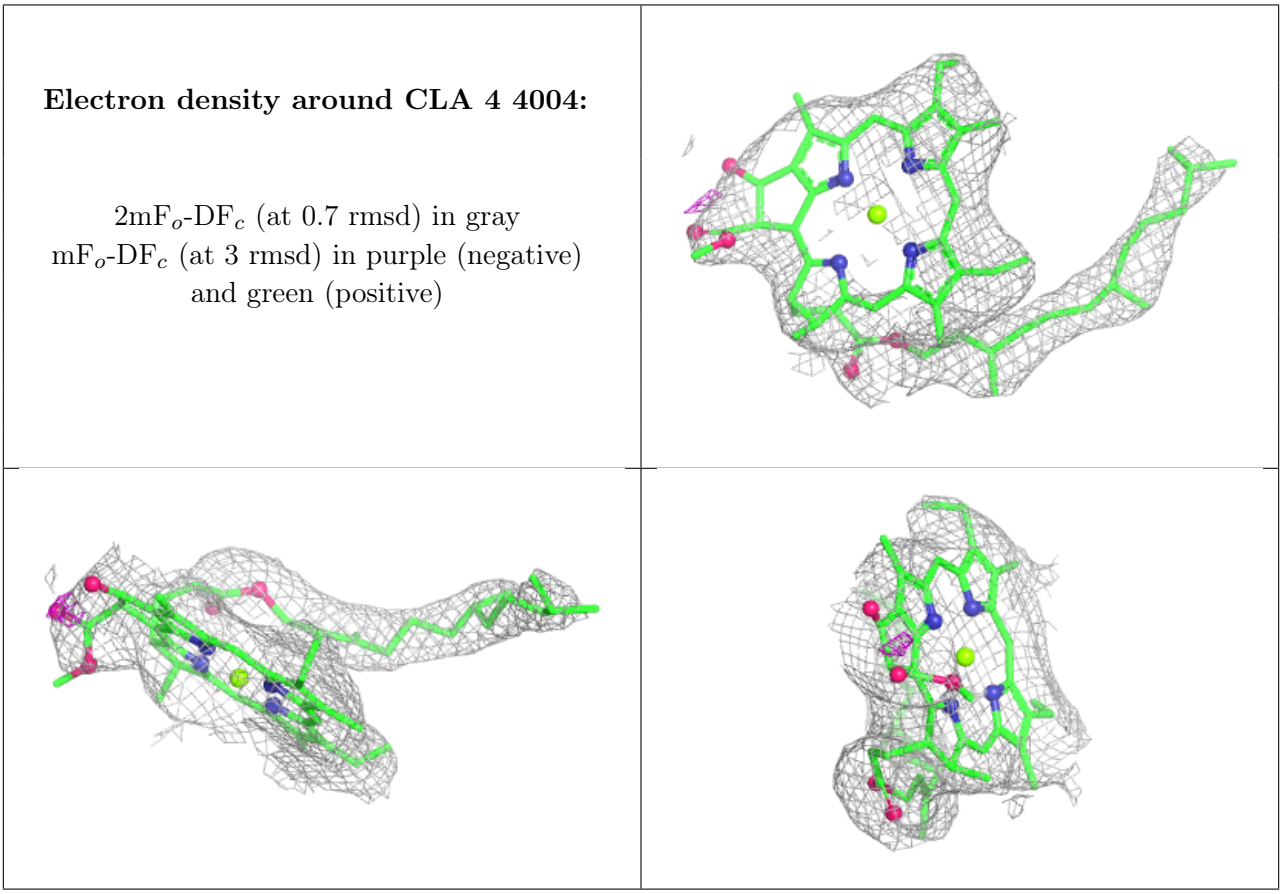
Electron density around CLA 4 4003:

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



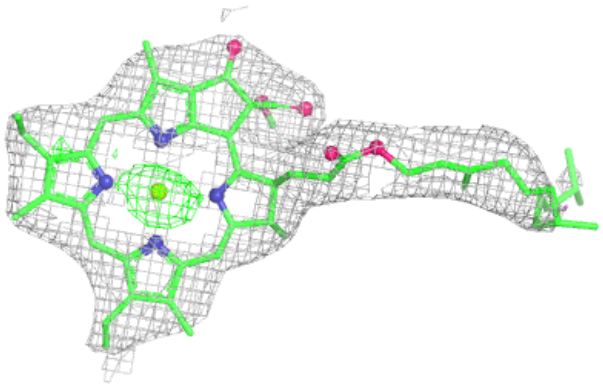
Electron density around CLA 4 4004:

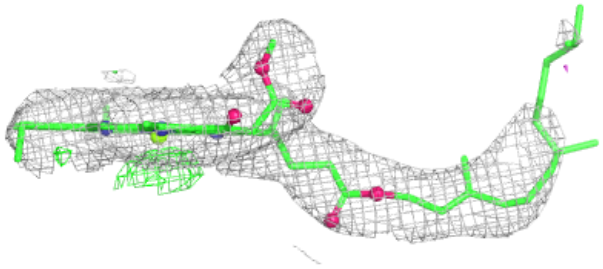
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 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)

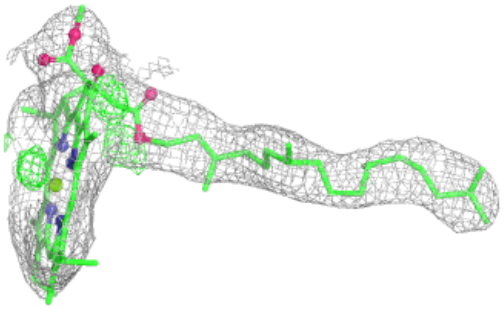


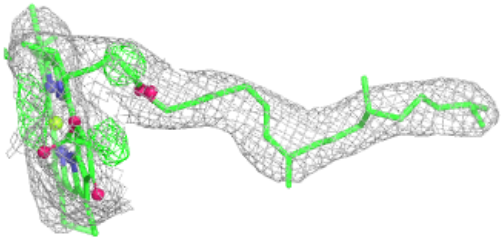


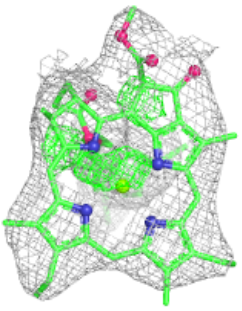


Electron density around CLA A 1126:

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

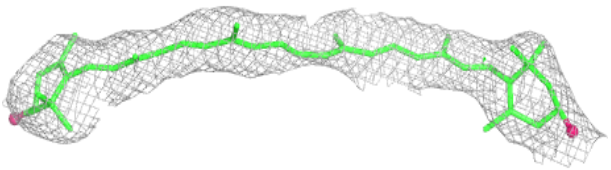


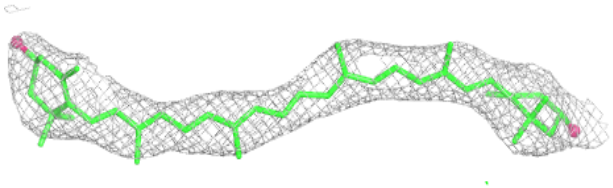


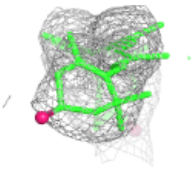


Electron density around LUT I 6018:

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

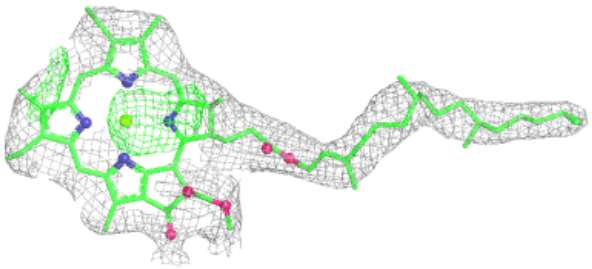


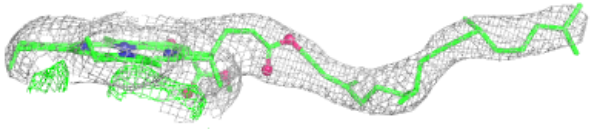


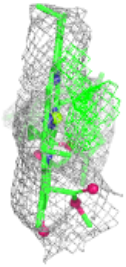


Electron density around CLA A 1131:

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

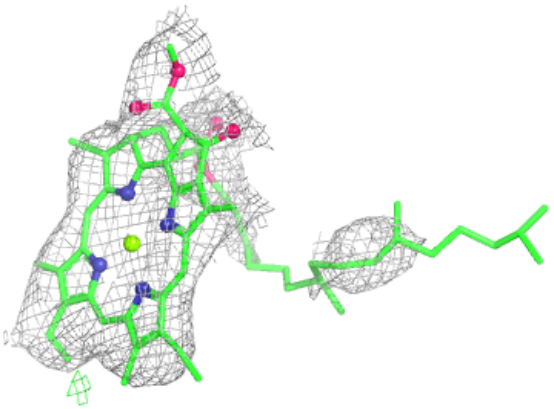


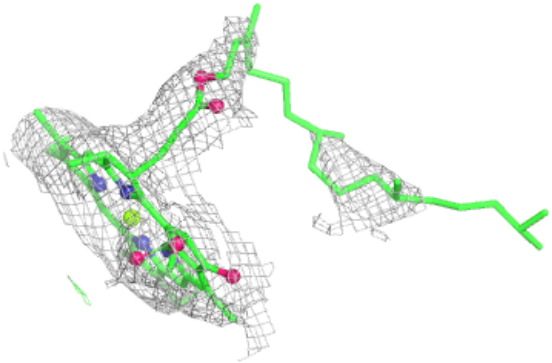


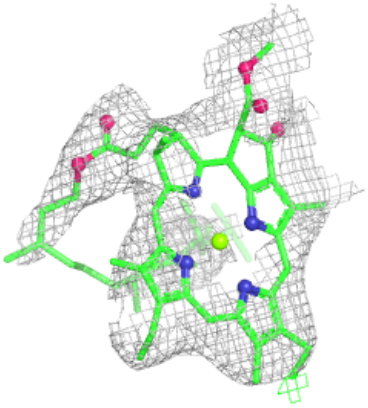


Electron density around CLA 4 4012:

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

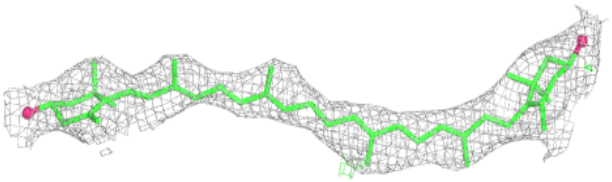


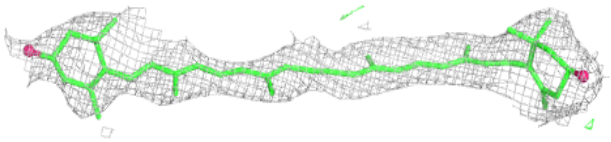


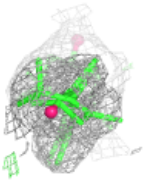


Electron density around LUT 4 4501:

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

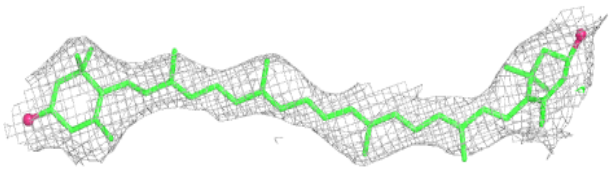


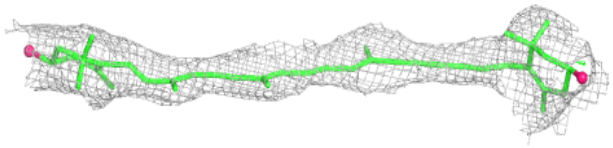


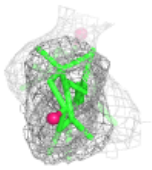


Electron density around LUT 4 4502:

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

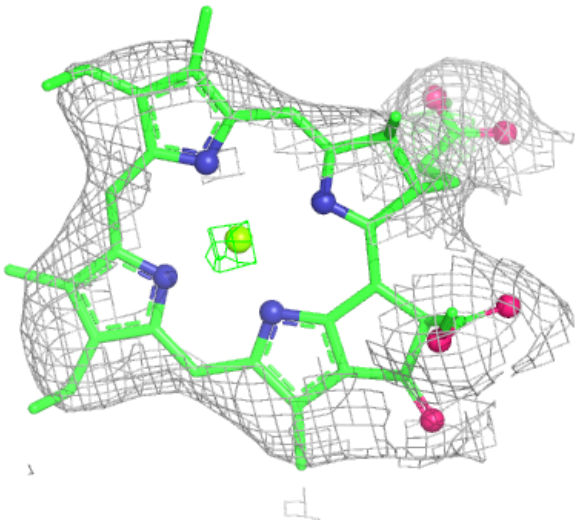


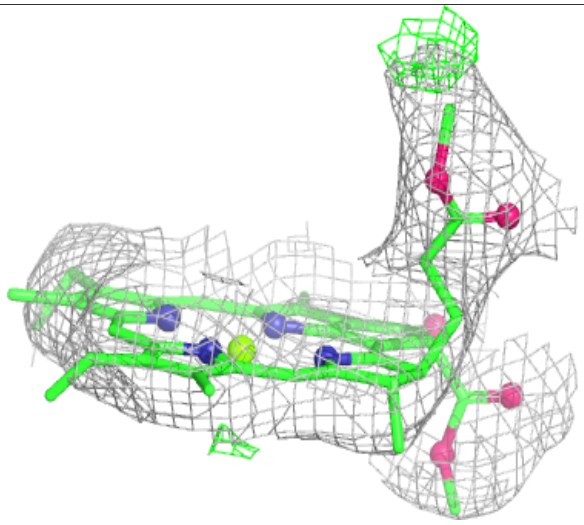


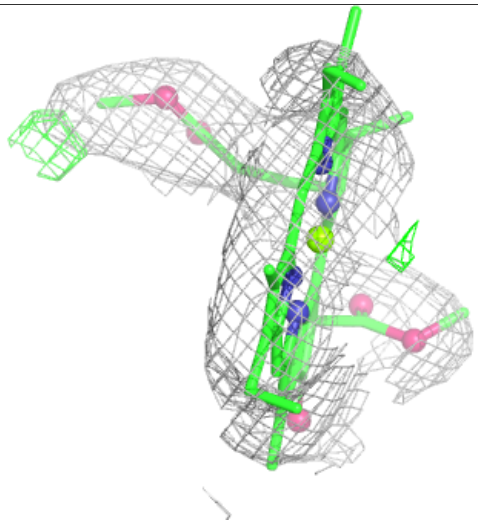


Electron density around CLA A 1118:

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

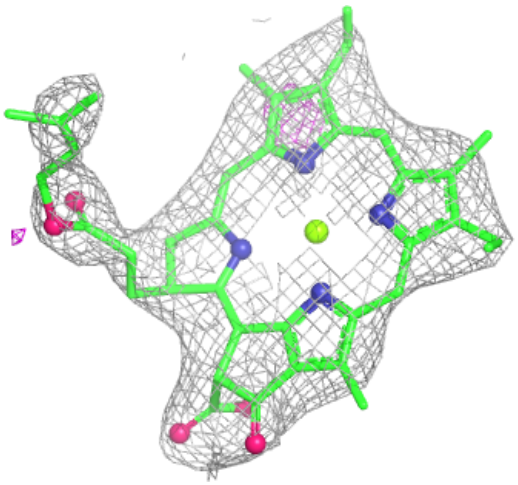


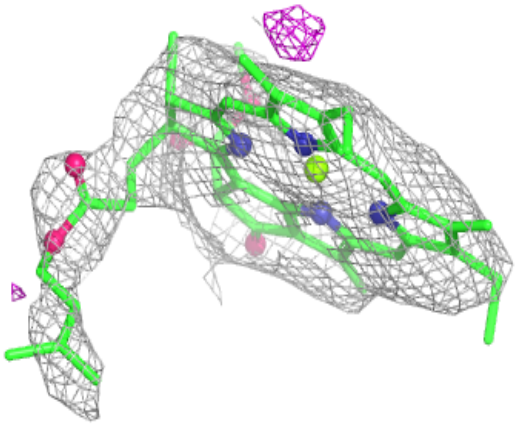


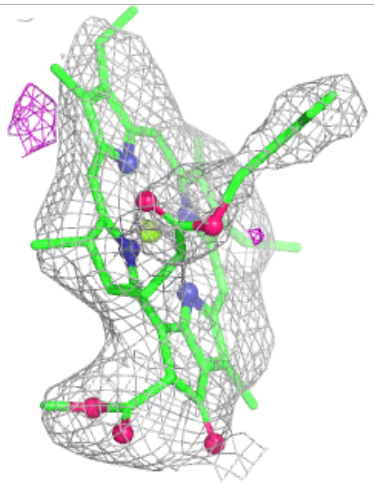


Electron density around CLA A 1129:

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

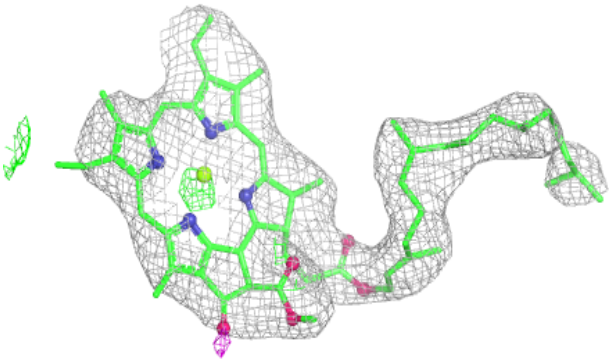


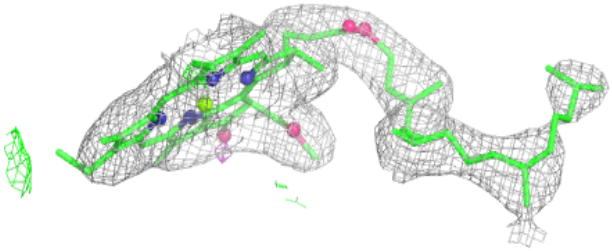


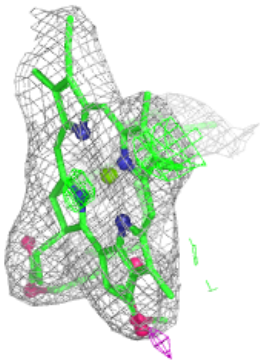


Electron density around CLA A 1101:

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

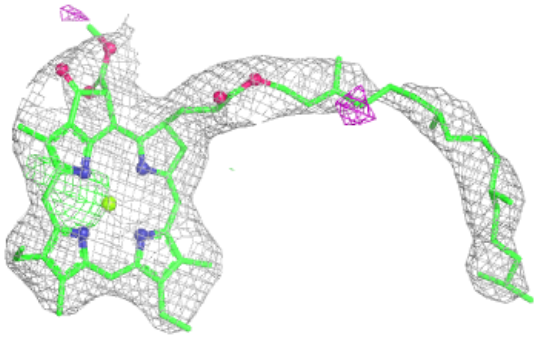


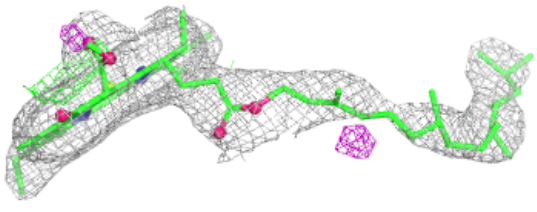


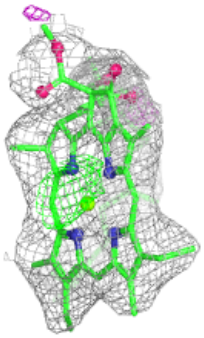


Electron density around CLA B 1222:

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

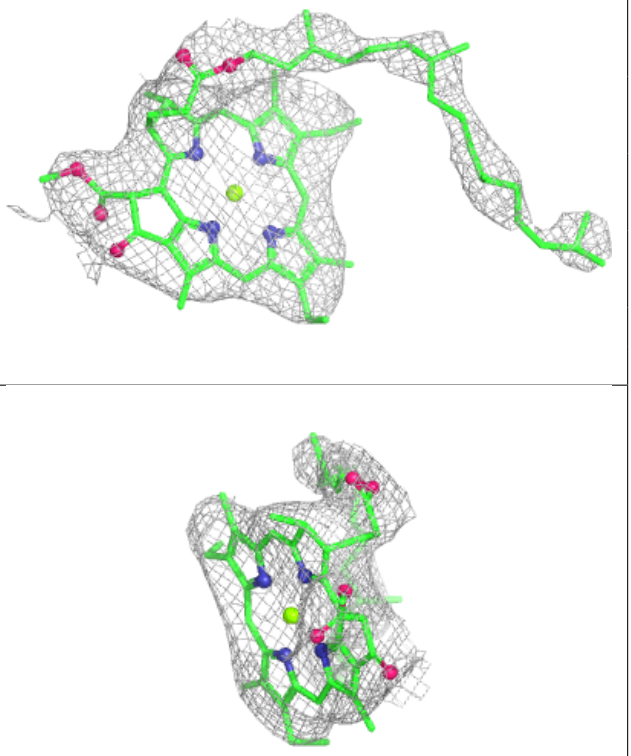






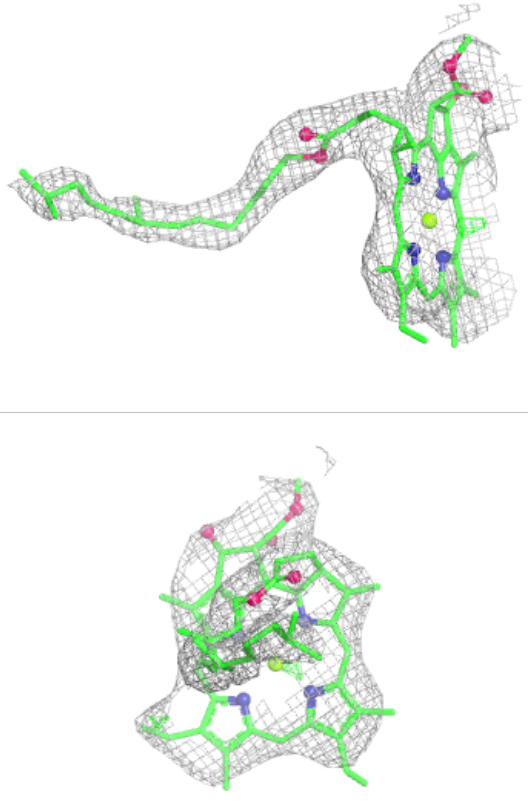
Electron density around CLA 1 1004:

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



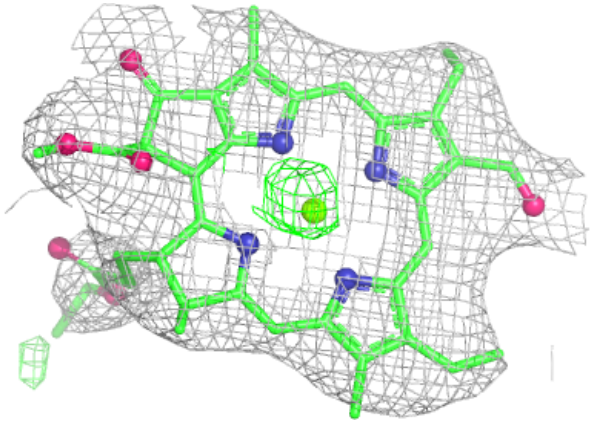
Electron density around CLA L 1502:

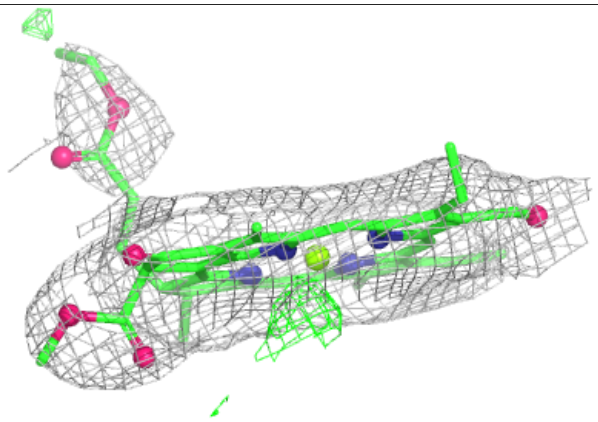
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

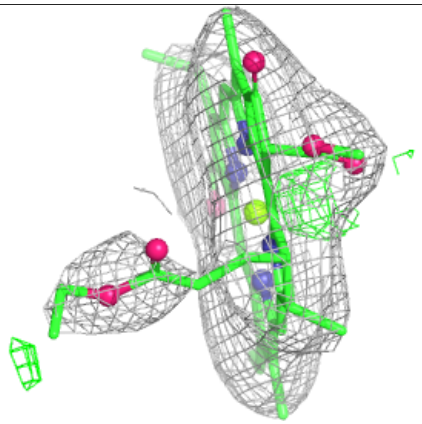


Electron density around CHL 2 2011:

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

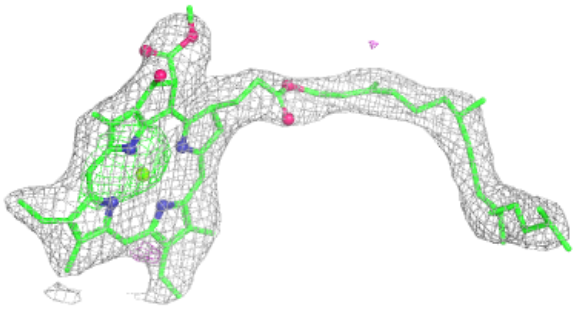


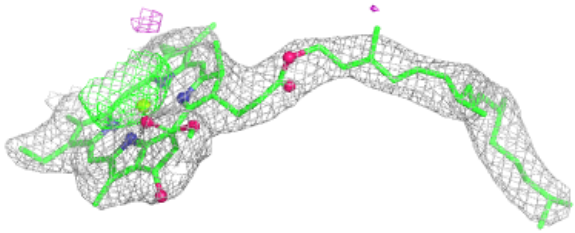


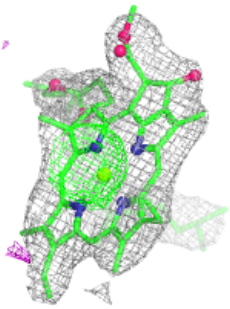


Electron density around CLA B 1012:

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

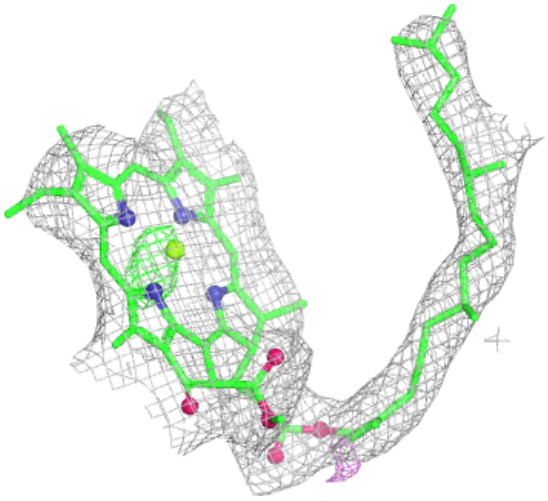


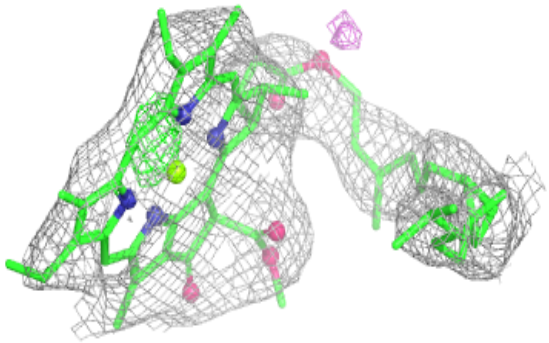


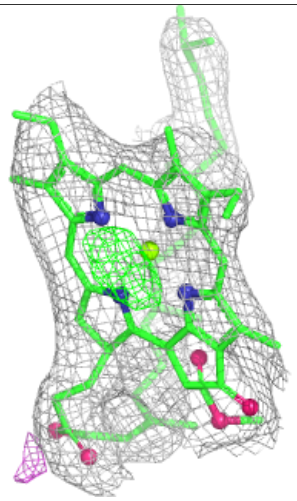


Electron density around CLA B 1207:

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

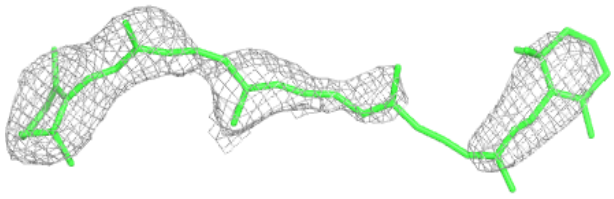


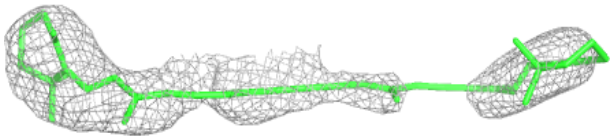


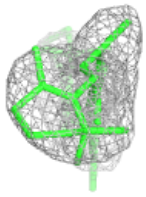


Electron density around BCR B 6006:

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

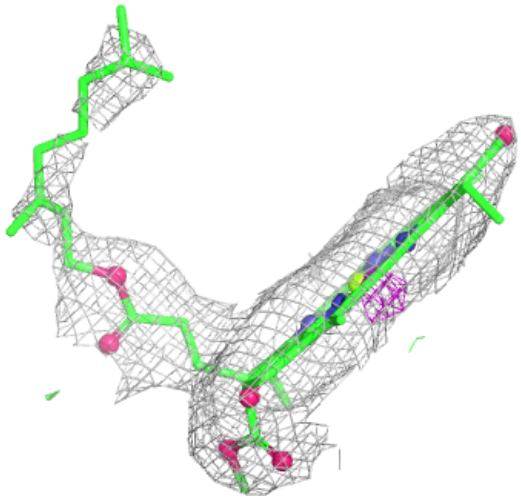


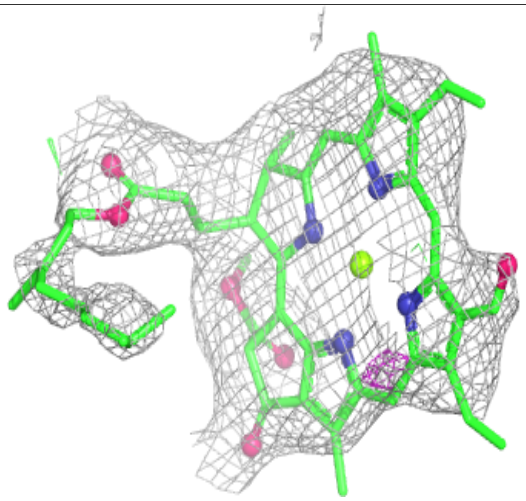


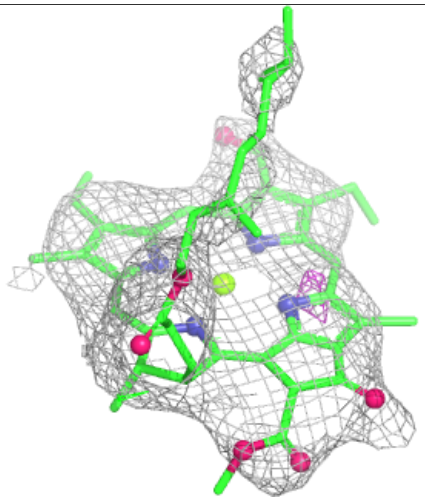


Electron density around CHL 1 1009:

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

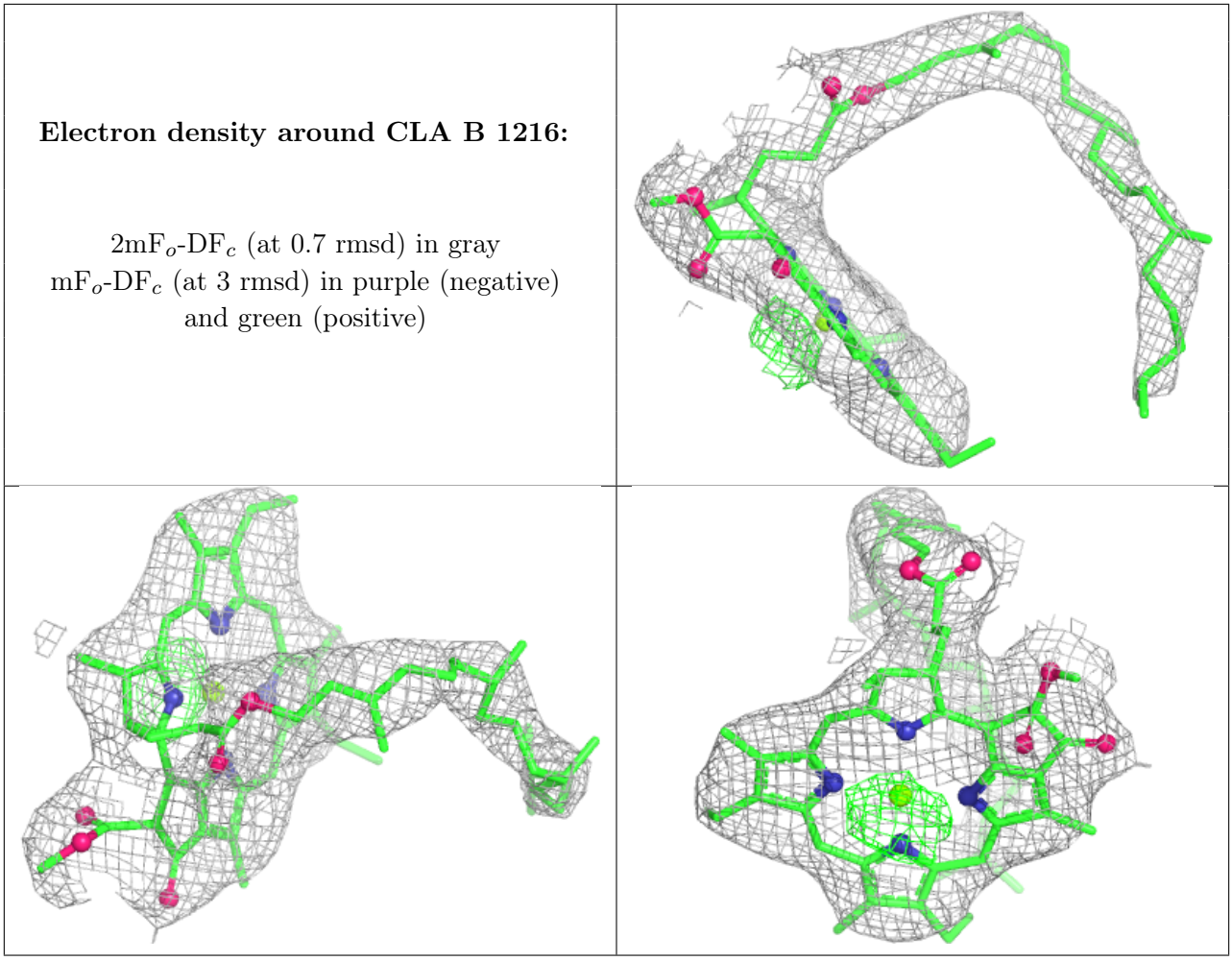






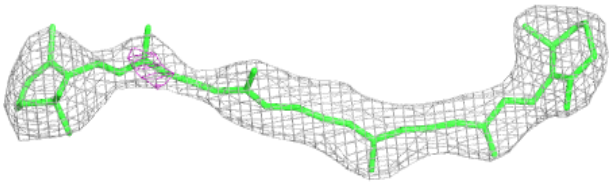
Electron density around CLA B 1216:

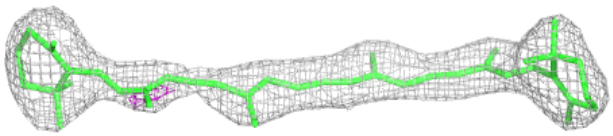
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

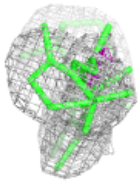


Electron density around BCR B 6010:

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

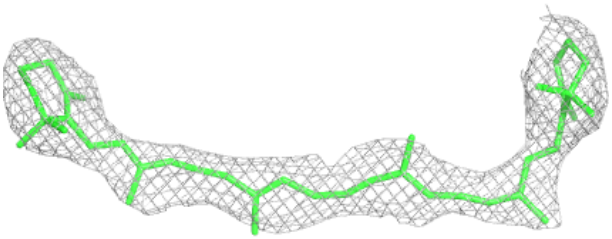


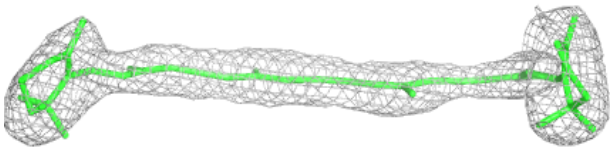


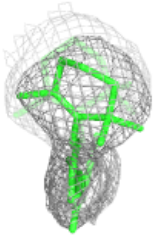


Electron density around BCR I 6020:

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

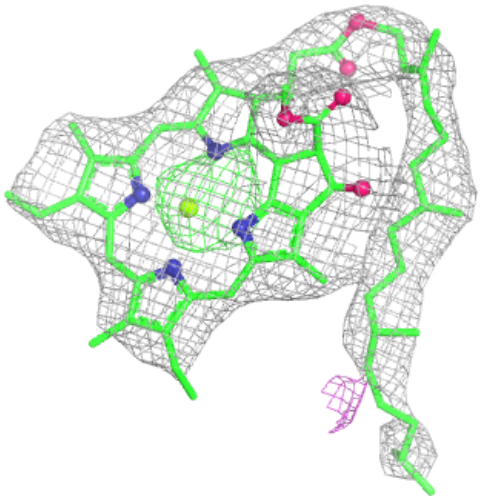


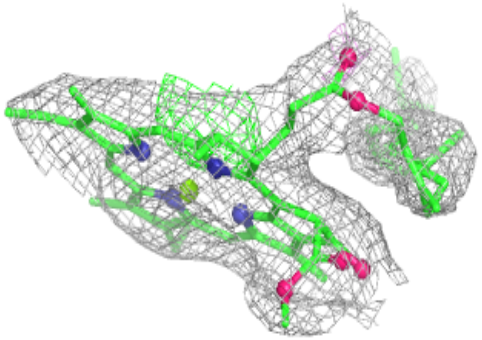


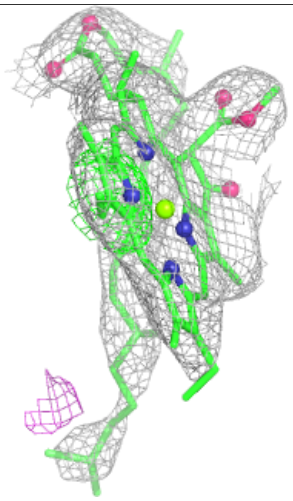


Electron density around CLA A 1123:

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

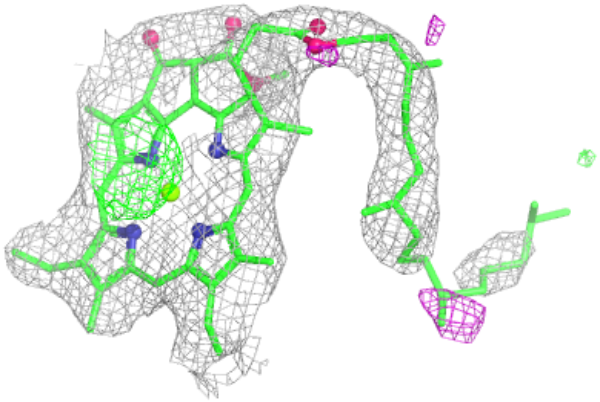


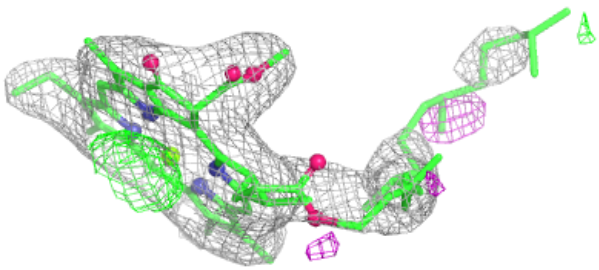


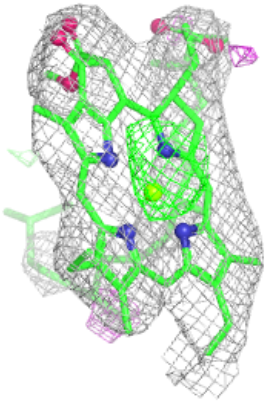


Electron density around CLA B 1221:

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

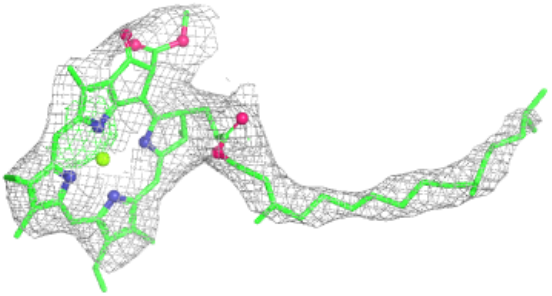


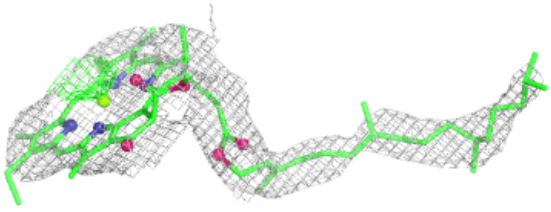


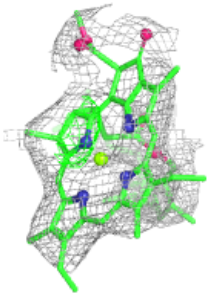


Electron density around CLA A 1119:

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

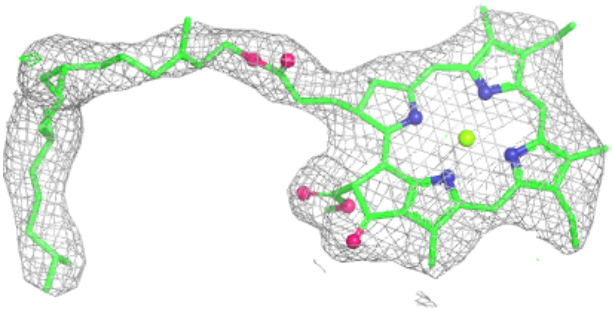


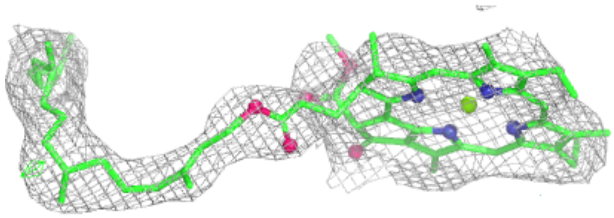


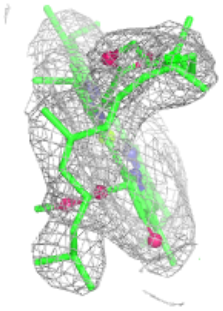


Electron density around CLA B 1223:

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

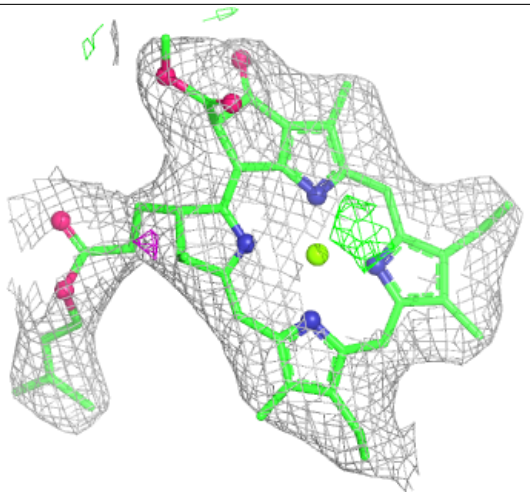


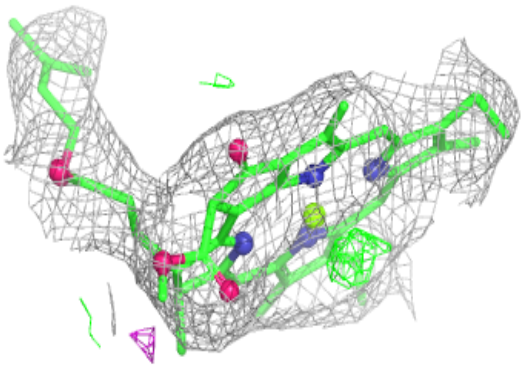


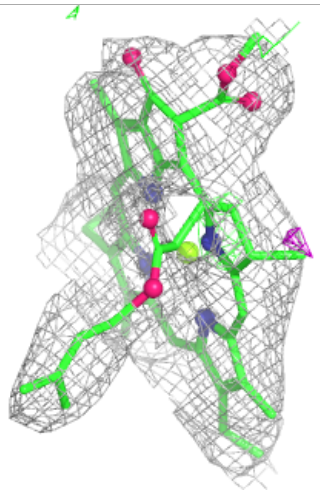


Electron density around CLA A 1102:

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

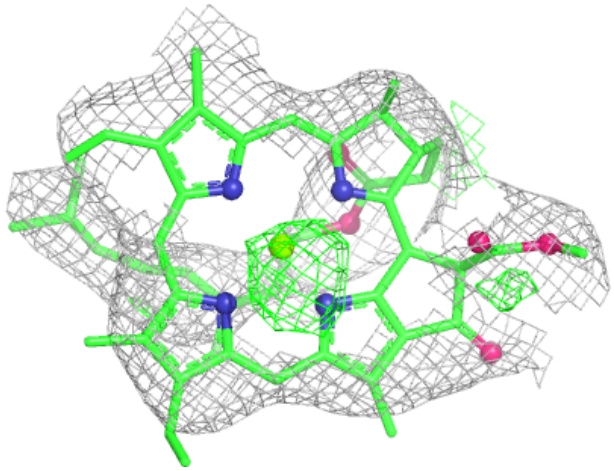


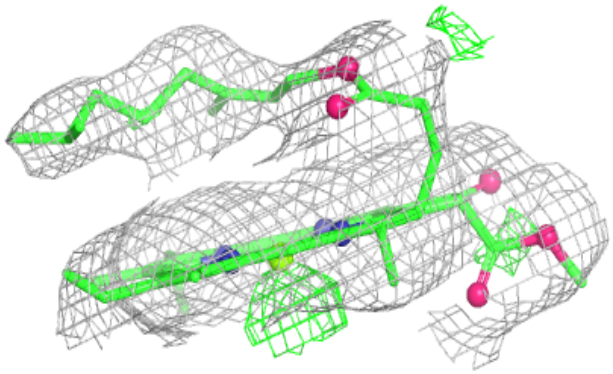


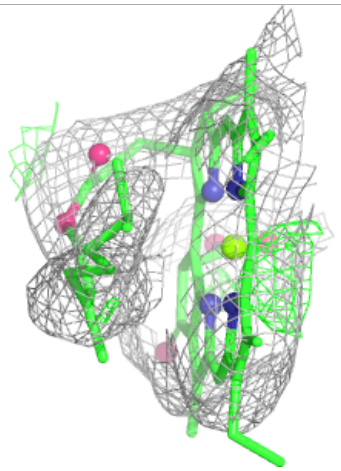


Electron density around CLA A 1110:

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

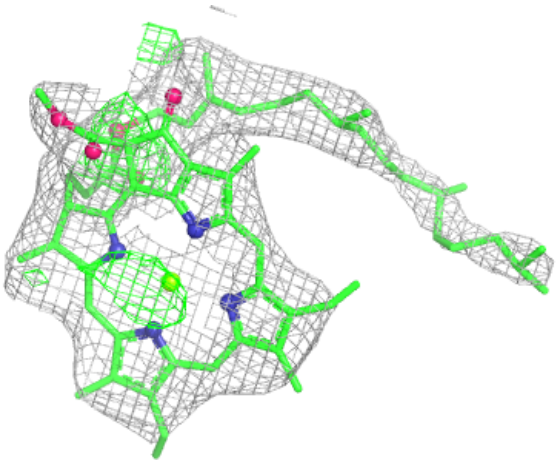


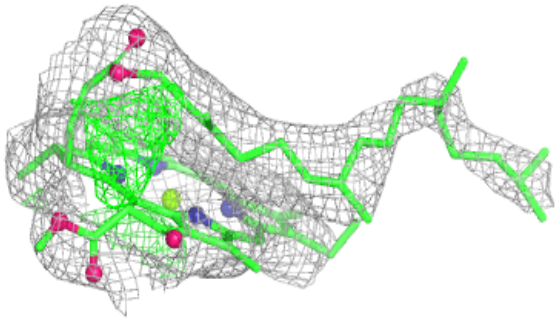


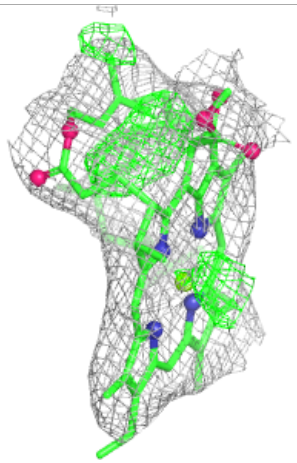


Electron density around CLA A 1127:

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

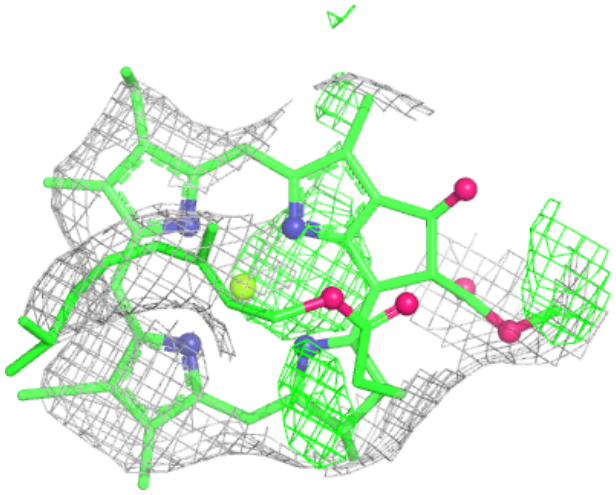


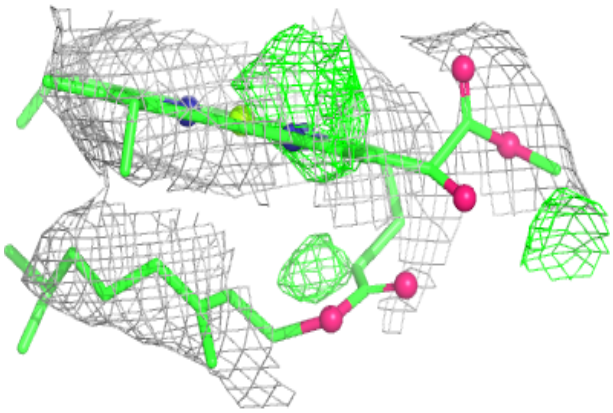


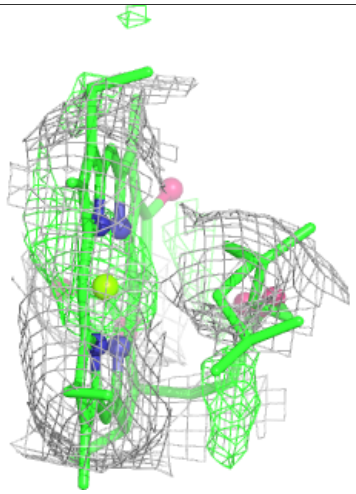


Electron density around CLA 1 1003:

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

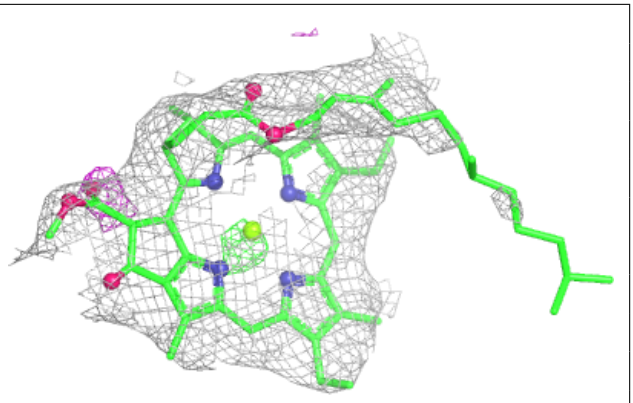


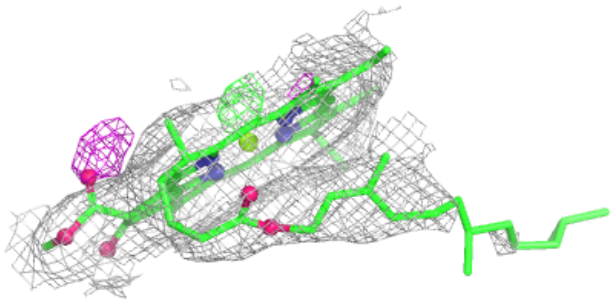


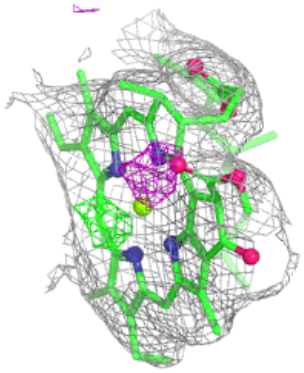


Electron density around CLA 2 2001:

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

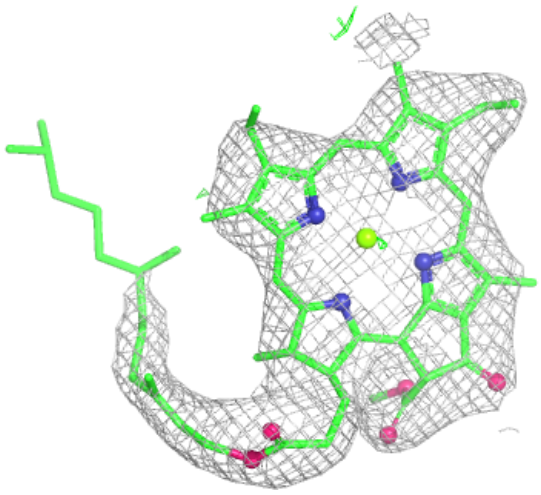


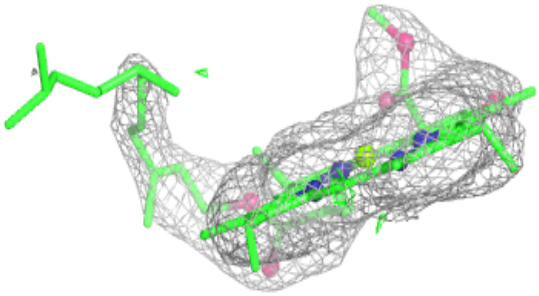




Electron density around CLA A 1111:

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

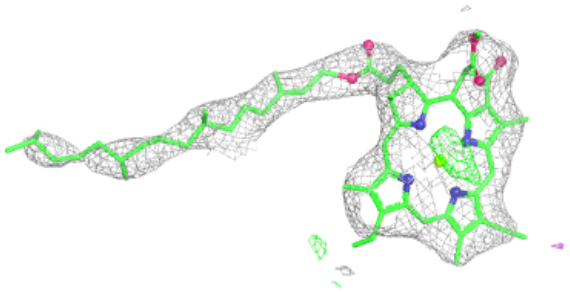






Electron density around CLA A 1132:

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

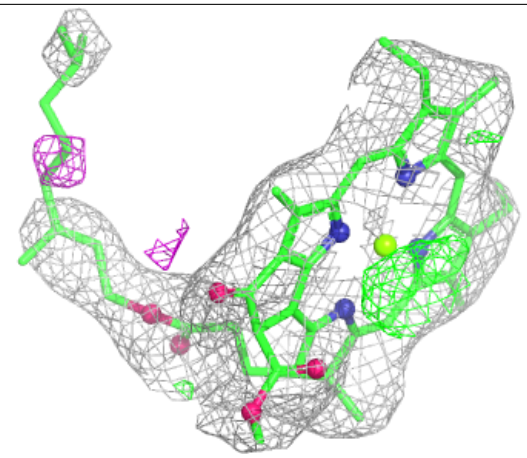


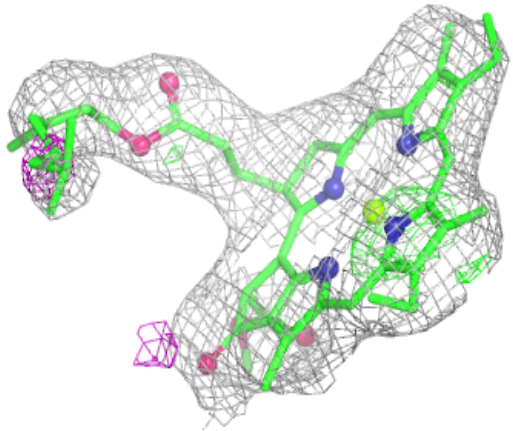


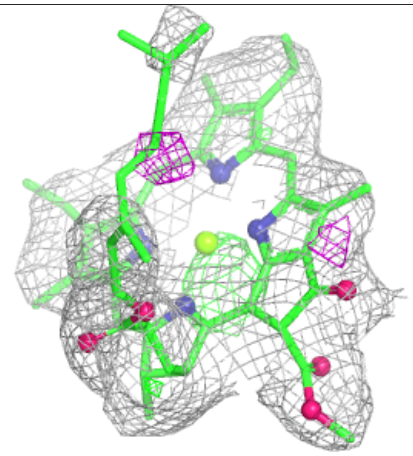


Electron density around CLA B 1236:

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

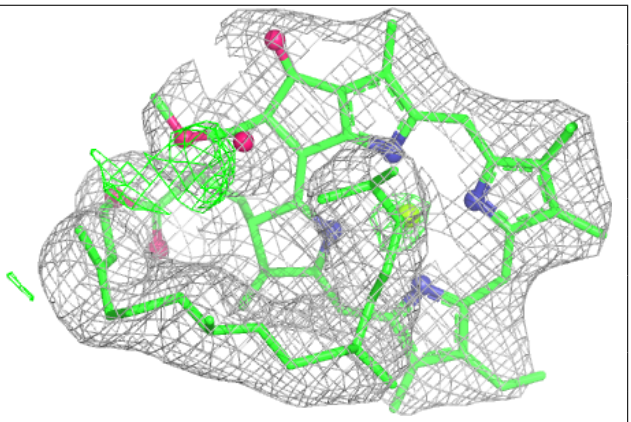


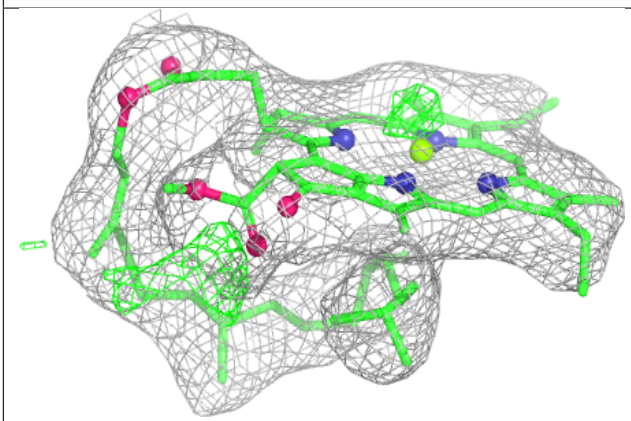


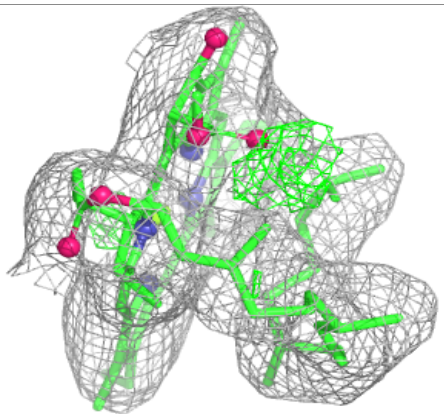


Electron density around CLA A 1104:

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

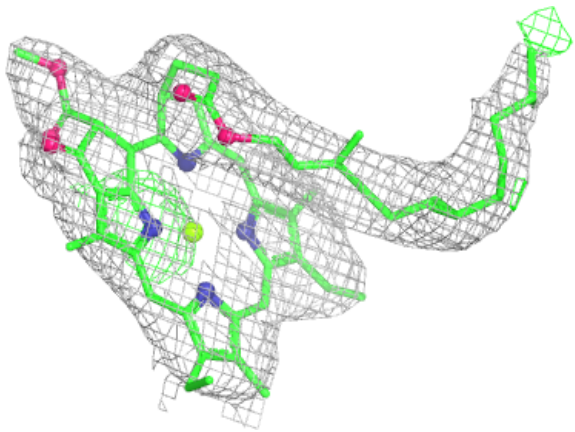


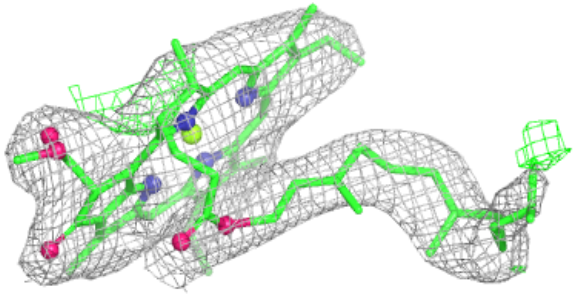


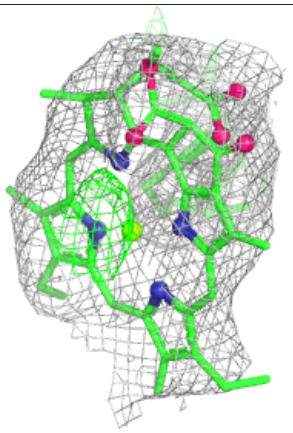


Electron density around CLA A 1237:

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

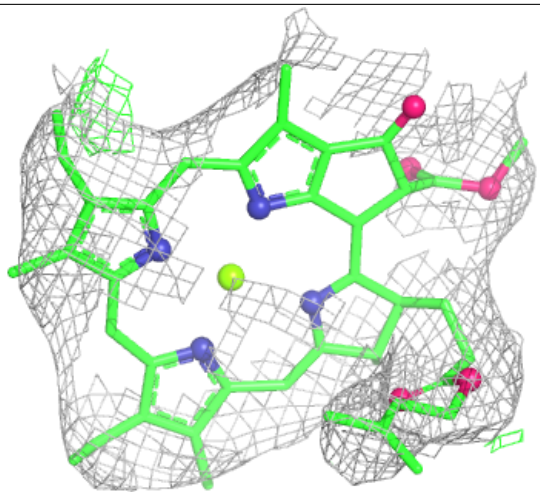


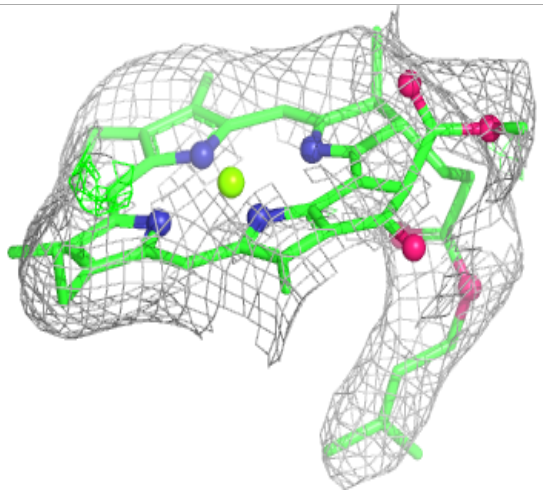




Electron density around CLA 1 1012:

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

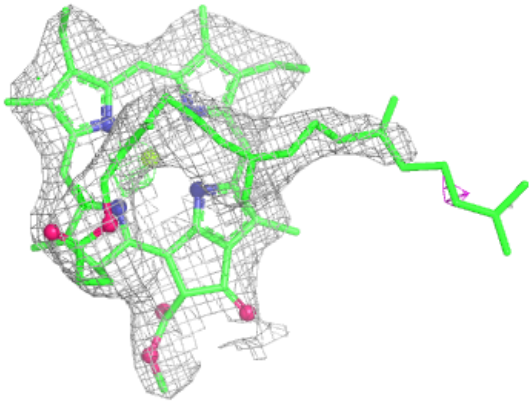


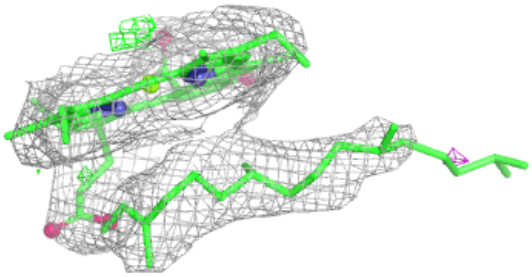


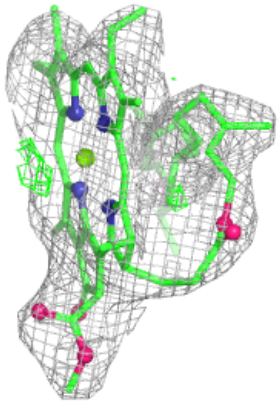


Electron density around CLA B 1224:

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

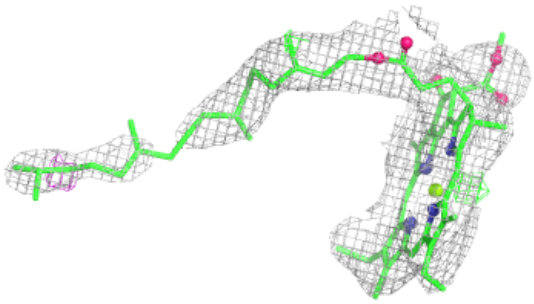


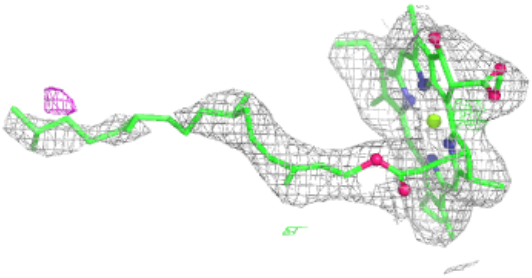


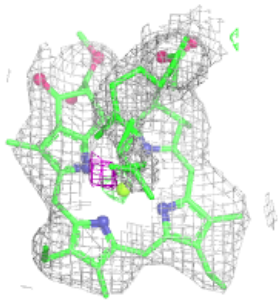


Electron density around CLA B 1226:

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

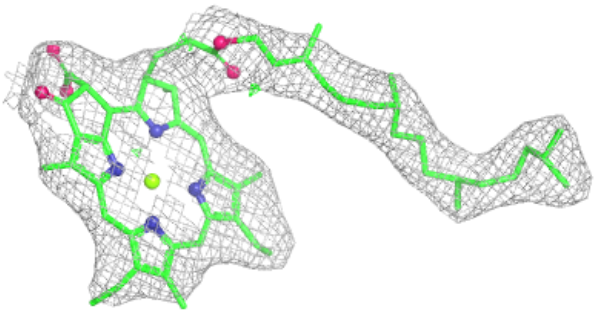


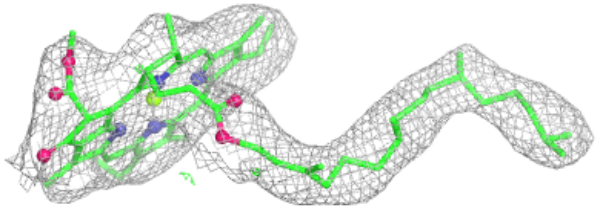


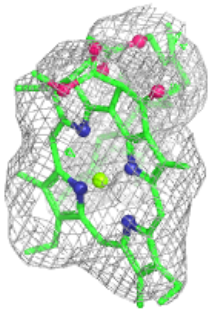


Electron density around CLA A 1106:

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

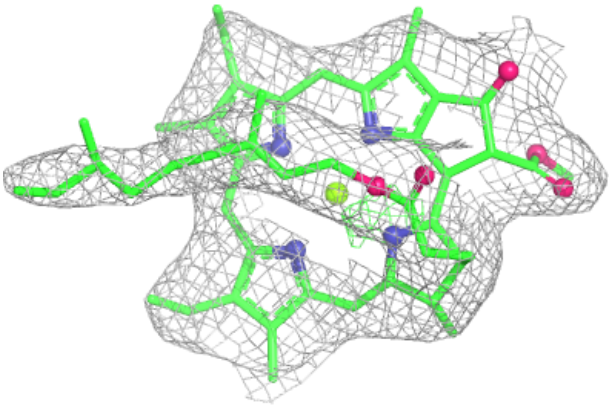


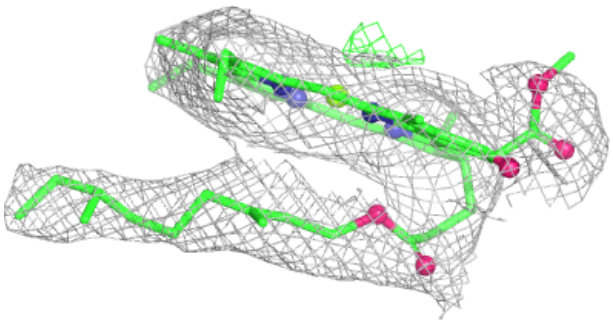


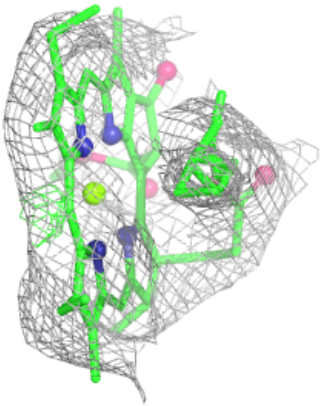


Electron density around CLA A 1136:

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

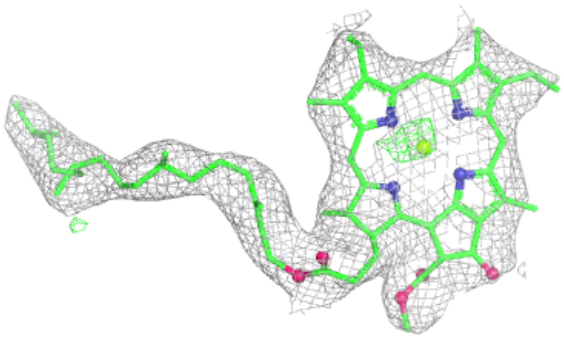


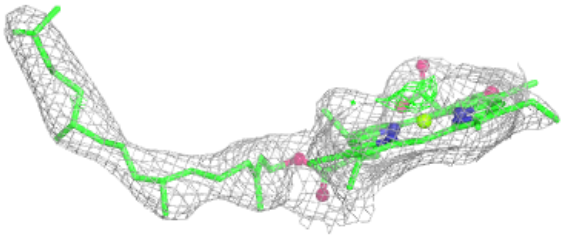




Electron density around CLA B 1023:

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

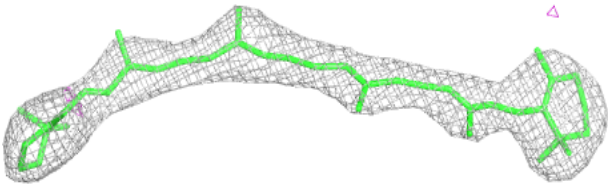


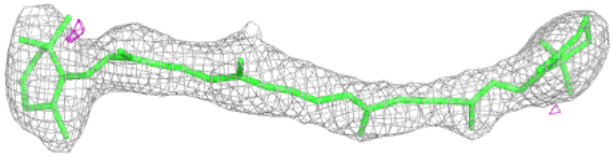


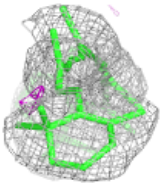


Electron density around BCR F 6014:

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

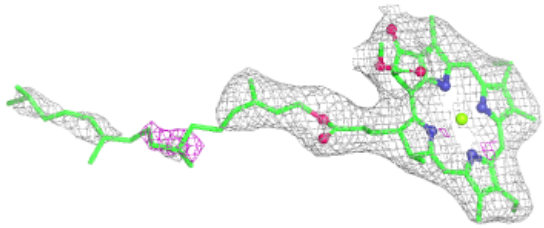


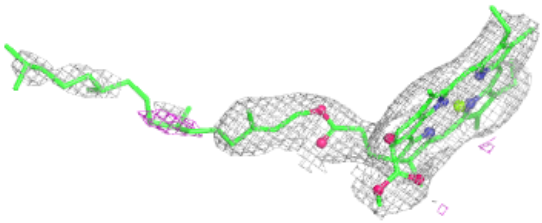


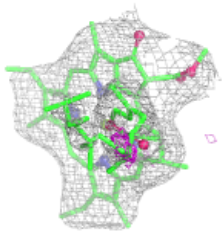


Electron density around CLA A 1107:

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

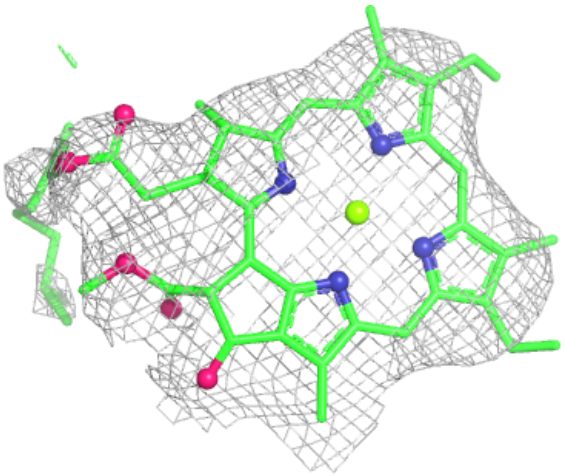


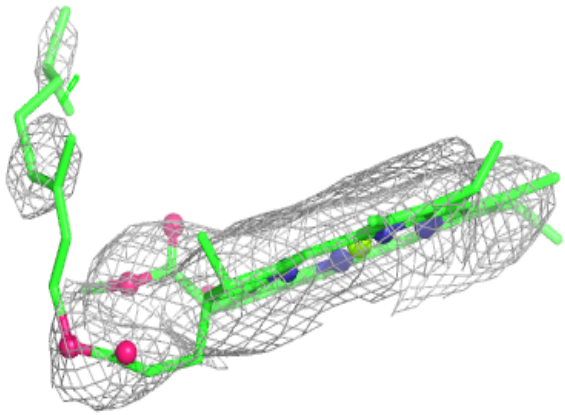


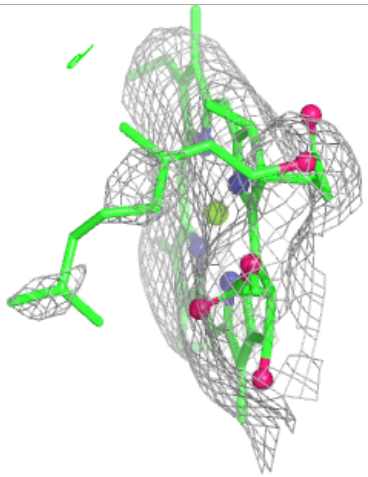


Electron density around CLA 3 3005:

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

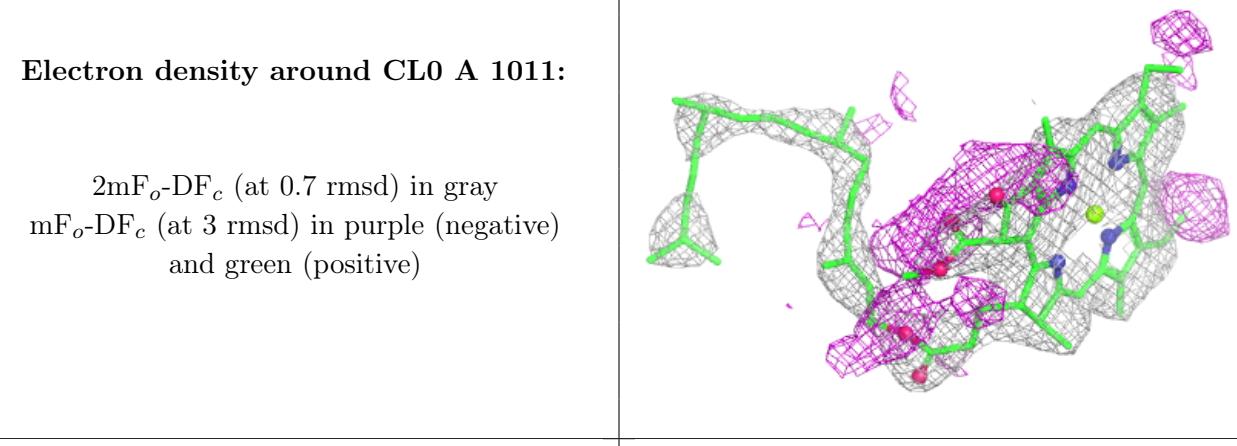






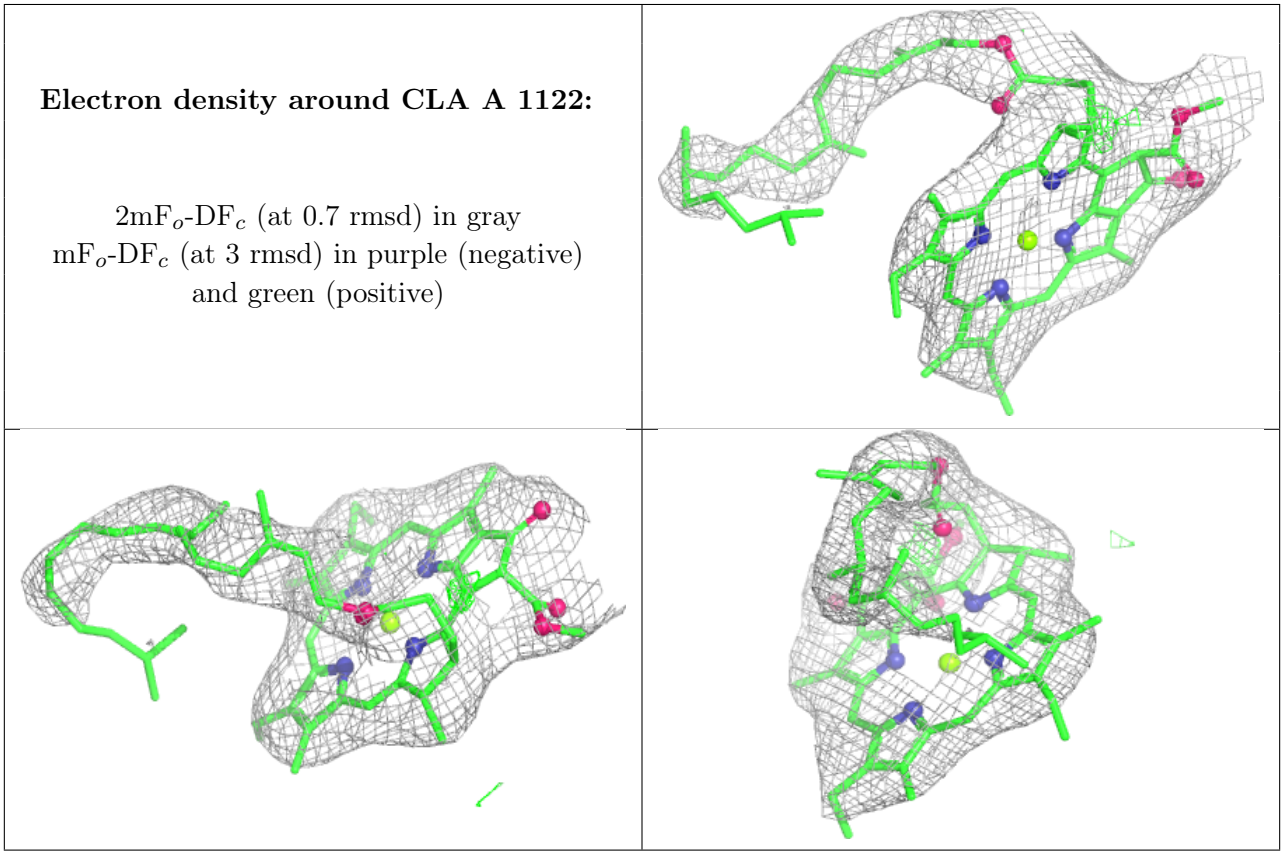
Electron density around CL0 A 1011:

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



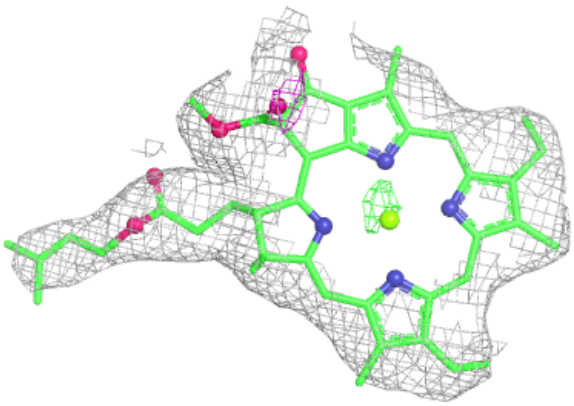
Electron density around CLA A 1122:

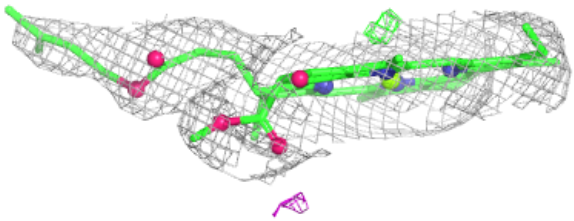
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

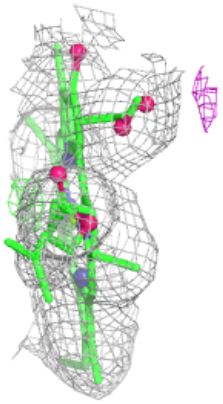


Electron density around CLA F 1302:

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

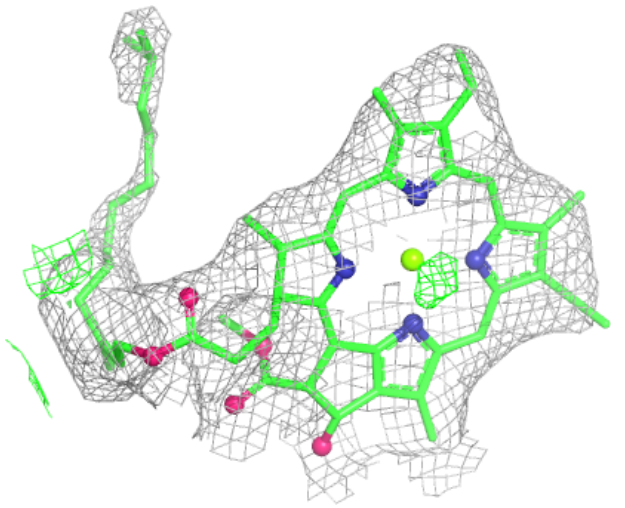


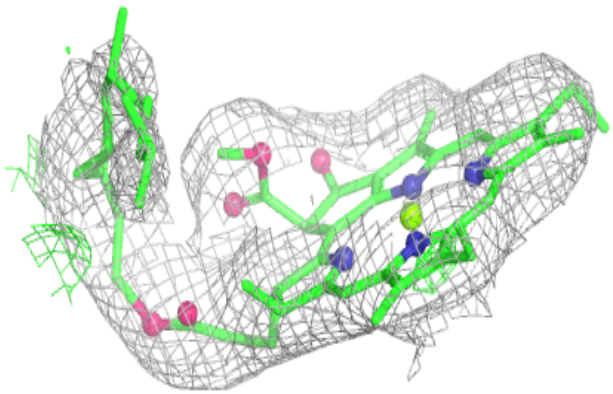




Electron density around CLA 4 4005:

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

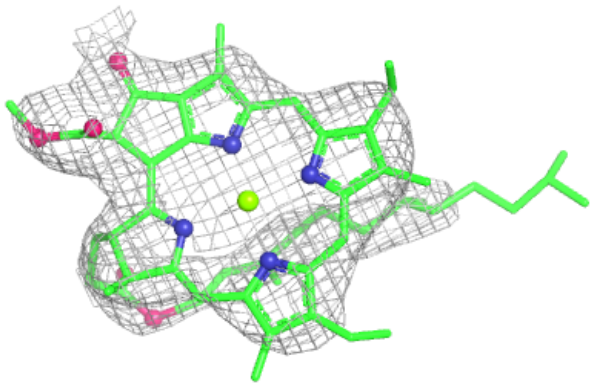


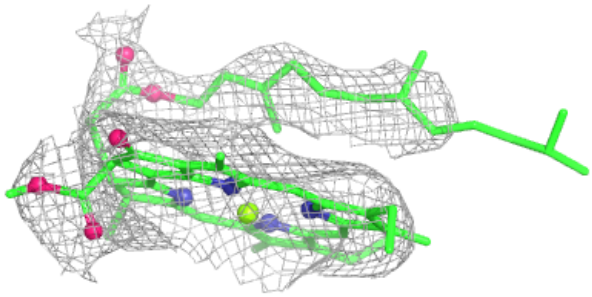


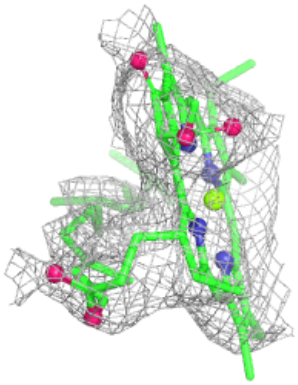


Electron density around CLA A 1116:

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

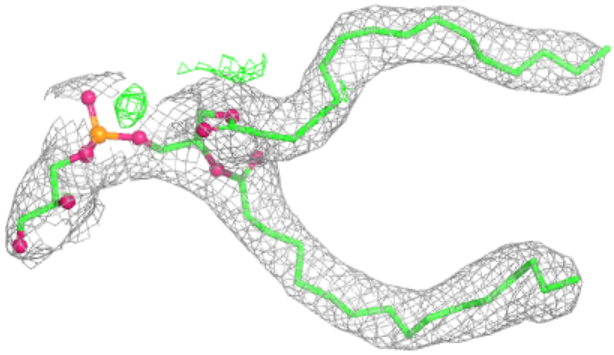


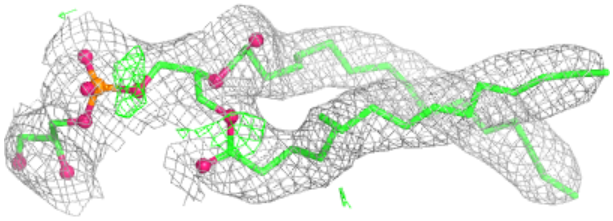


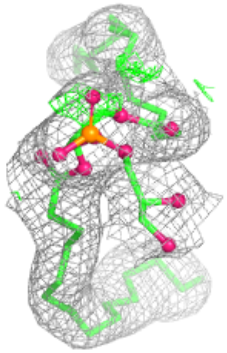


Electron density around LHG A 7001:

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

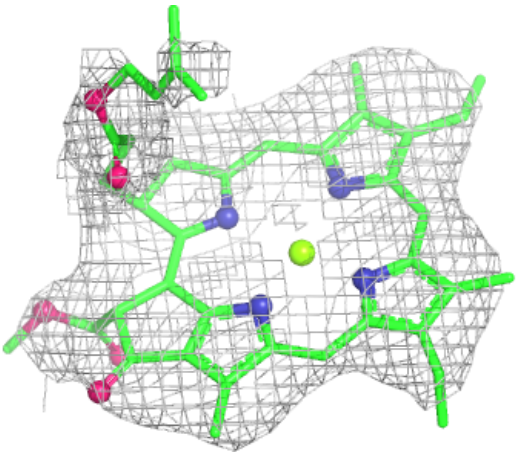


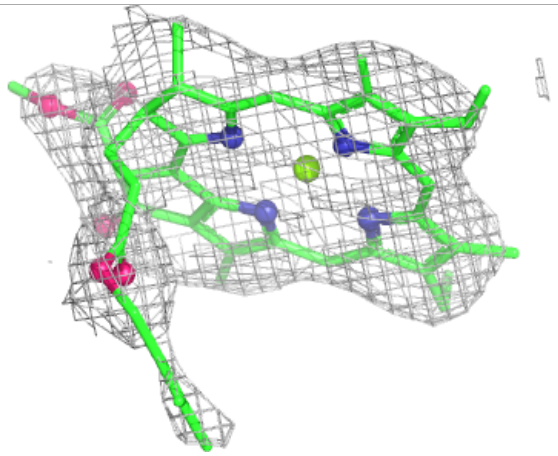


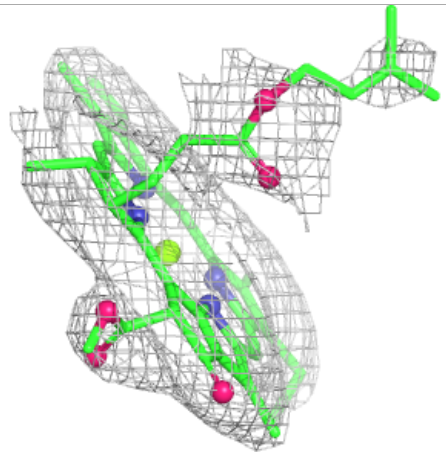


Electron density around CLA A 1130:

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

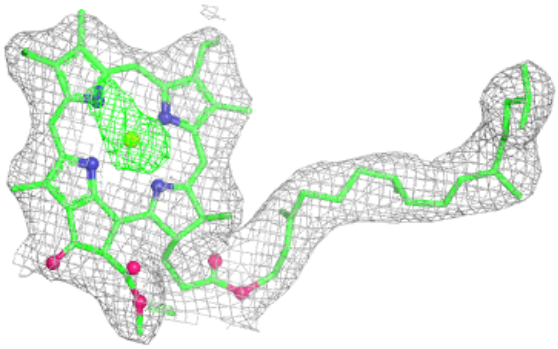


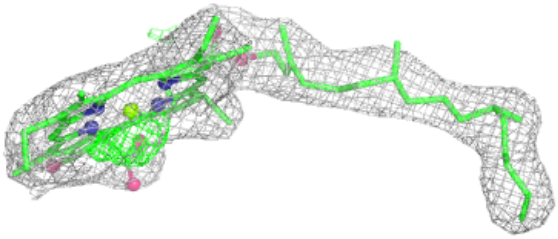


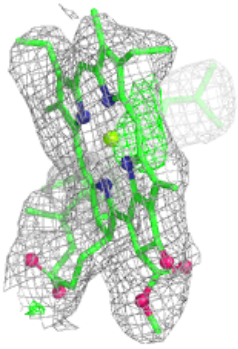


Electron density around CLA A 1013:

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

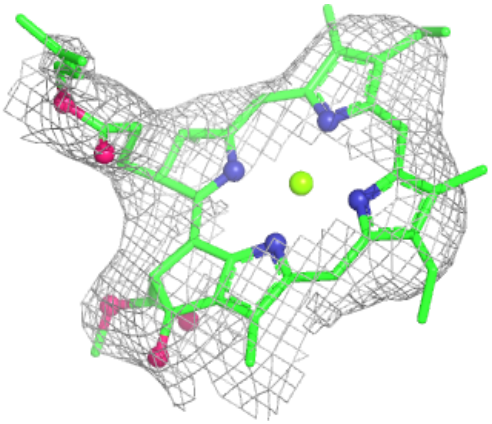


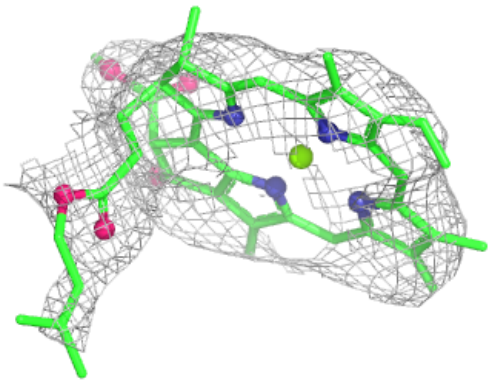


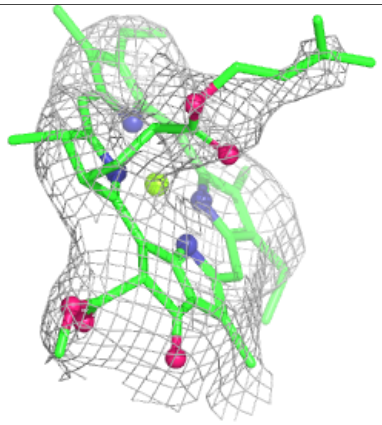


Electron density around CLA 2 2008:

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

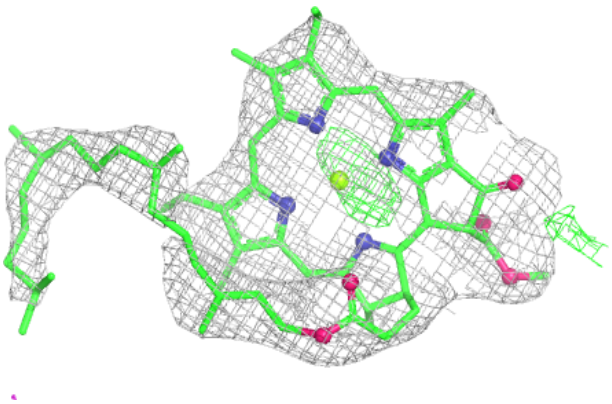


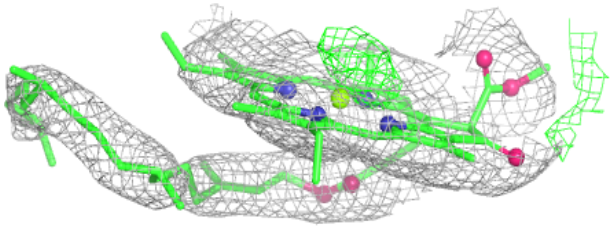




Electron density around CLA A 1117:

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

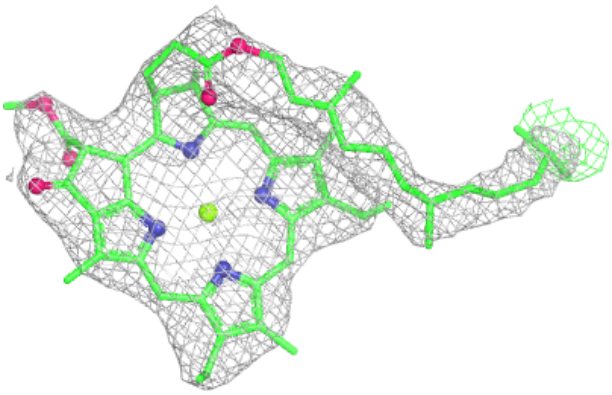


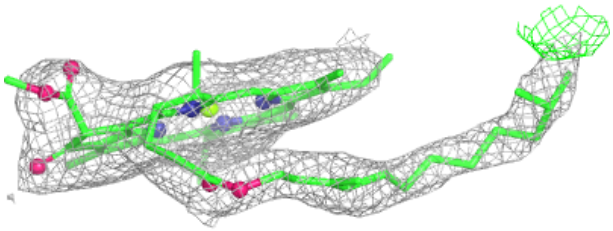


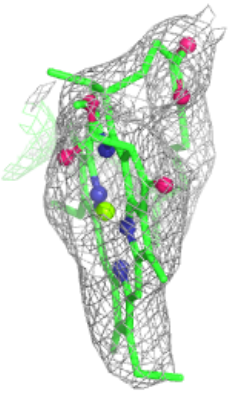


Electron density around CLA B 1215:

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

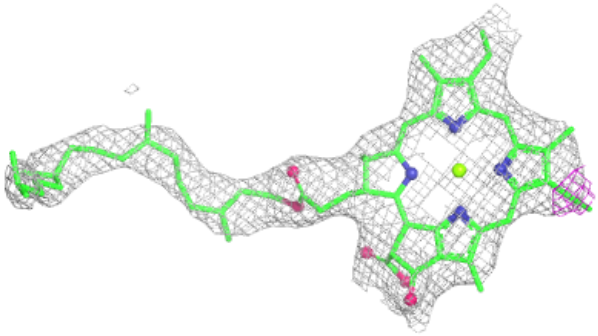


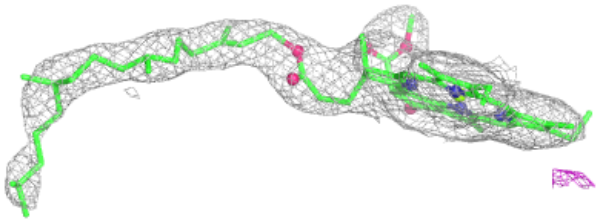


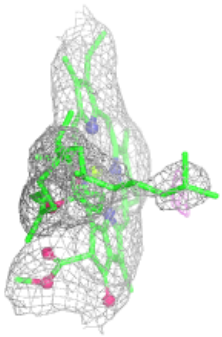


Electron density around CLA A 1103:

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

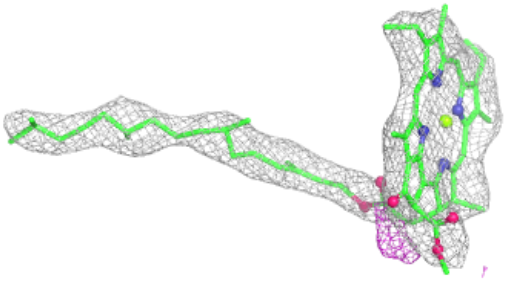


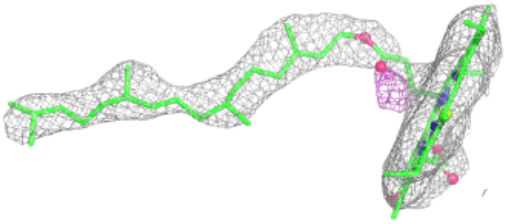


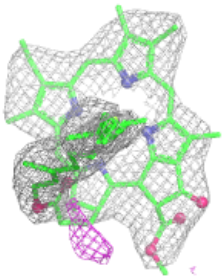


Electron density around CLA B 1225:

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

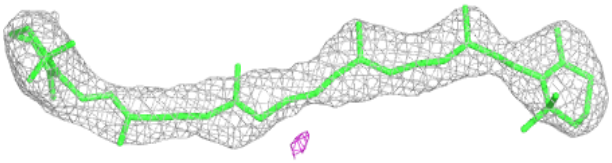


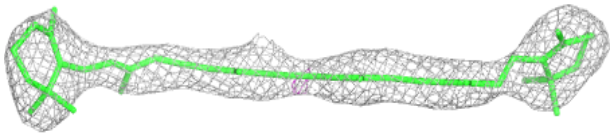


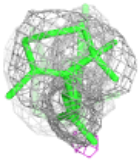


Electron density around BCR A 6017:

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

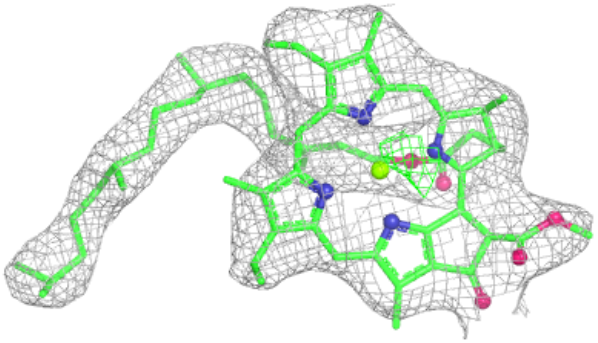


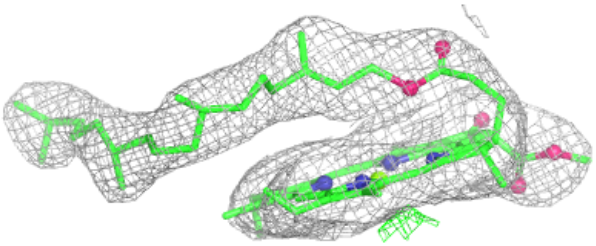




Electron density around CLA B 1235:

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

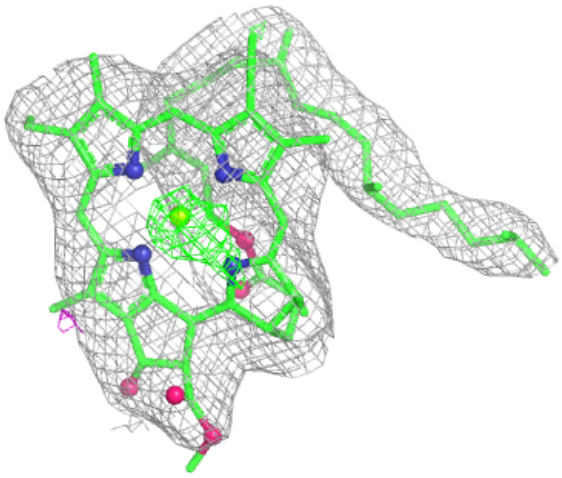


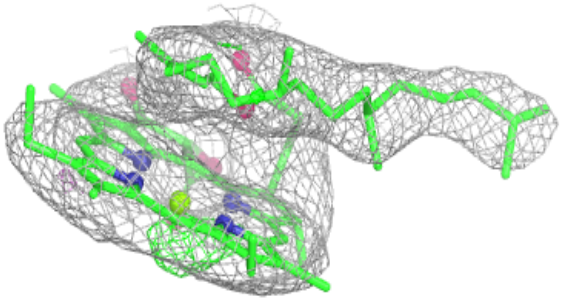


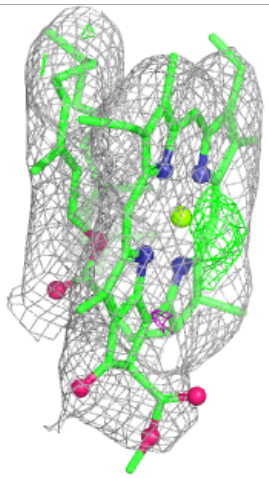


Electron density around CLA B 1205:

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

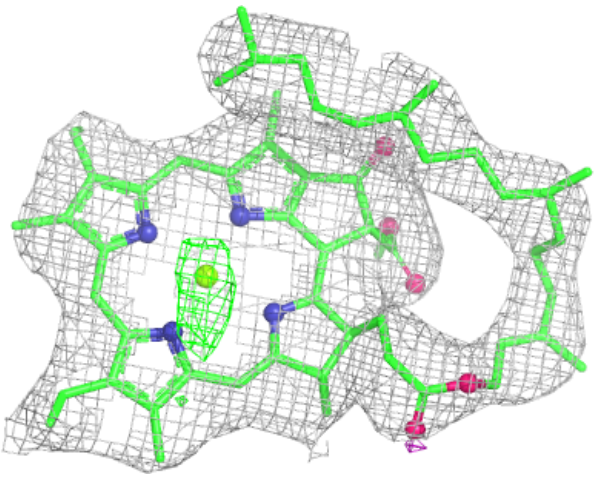


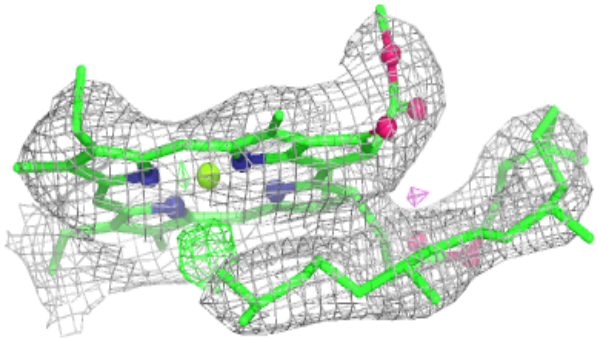


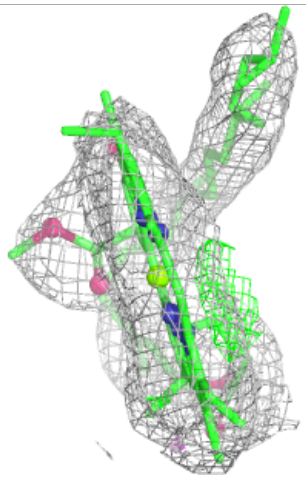


Electron density around CLA B 1202:

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

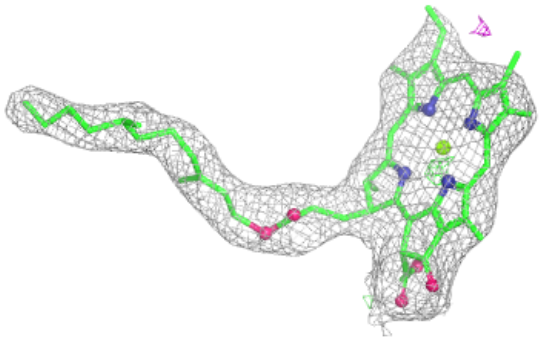


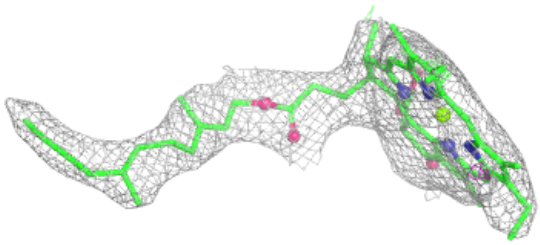


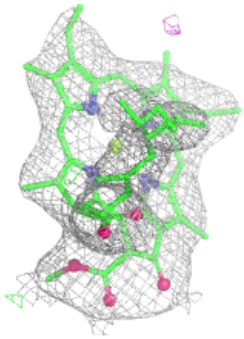


Electron density around CLA B 1230:

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

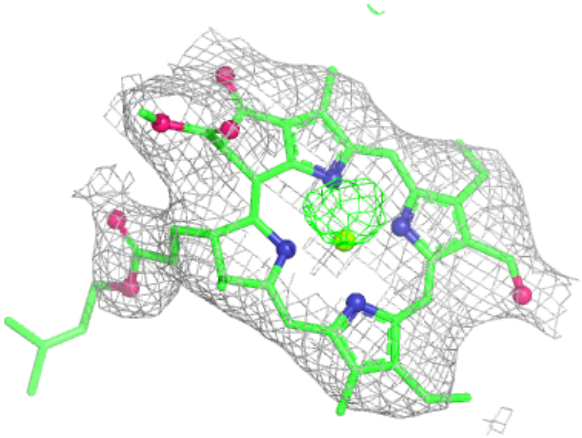


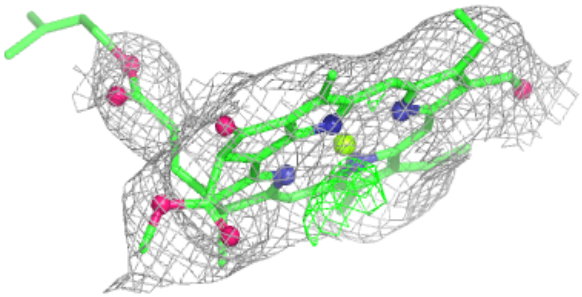


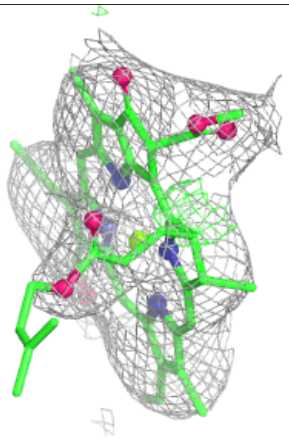


Electron density around CHL 4 4011:

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

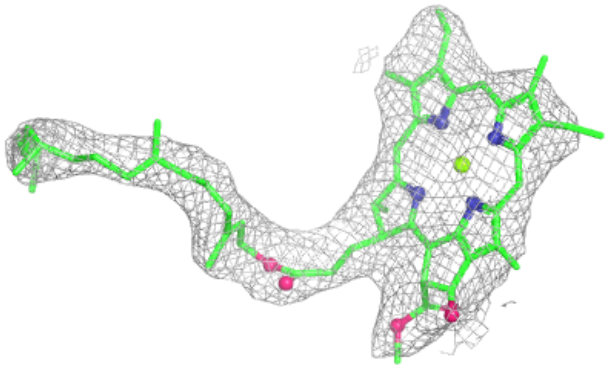


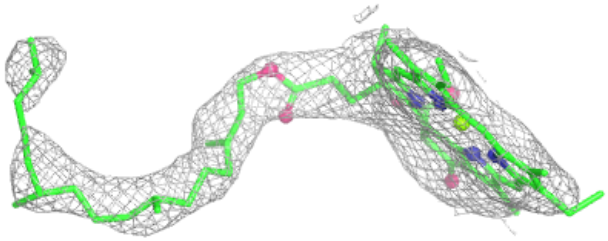


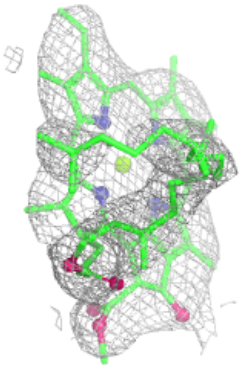


Electron density around CLA B 1206:

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

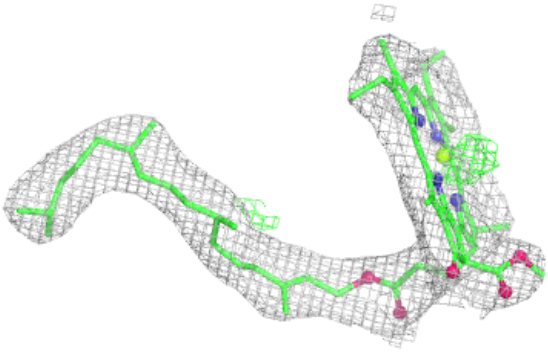


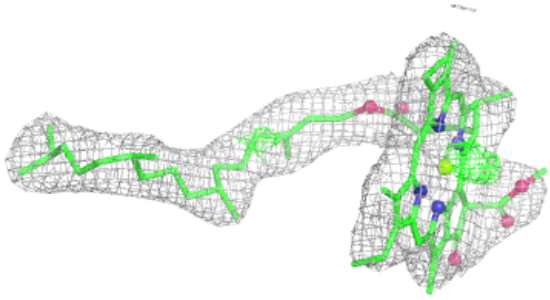


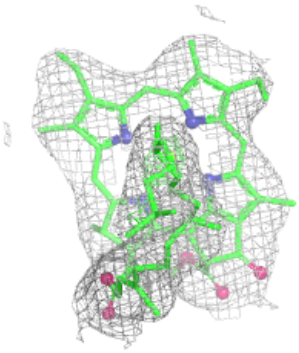


Electron density around CLA A 1128:

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

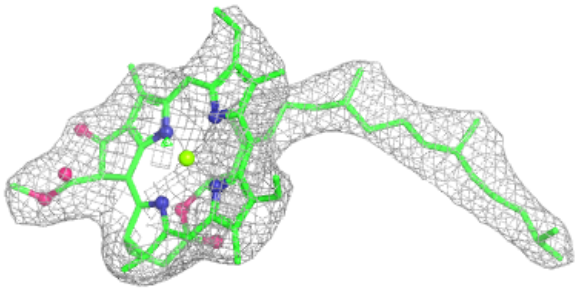


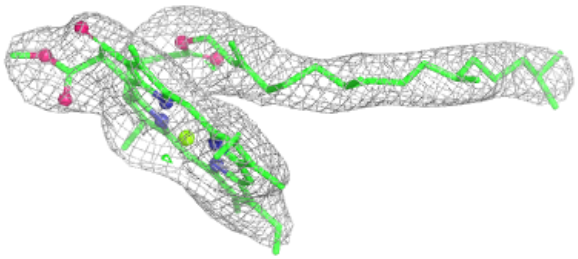


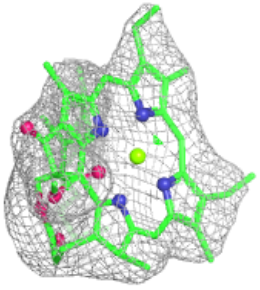


Electron density around CLA A 1140:

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

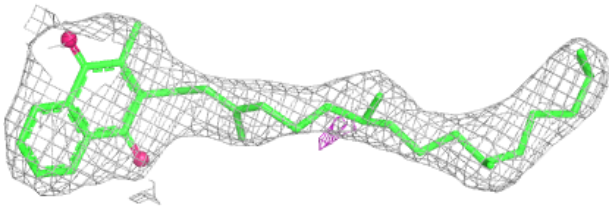


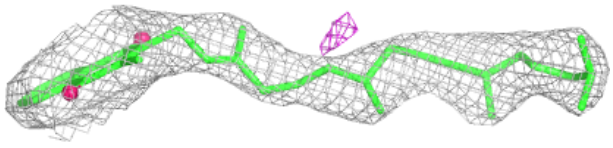


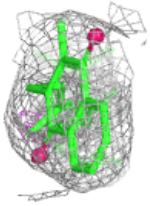


Electron density around PQN A 5001:

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

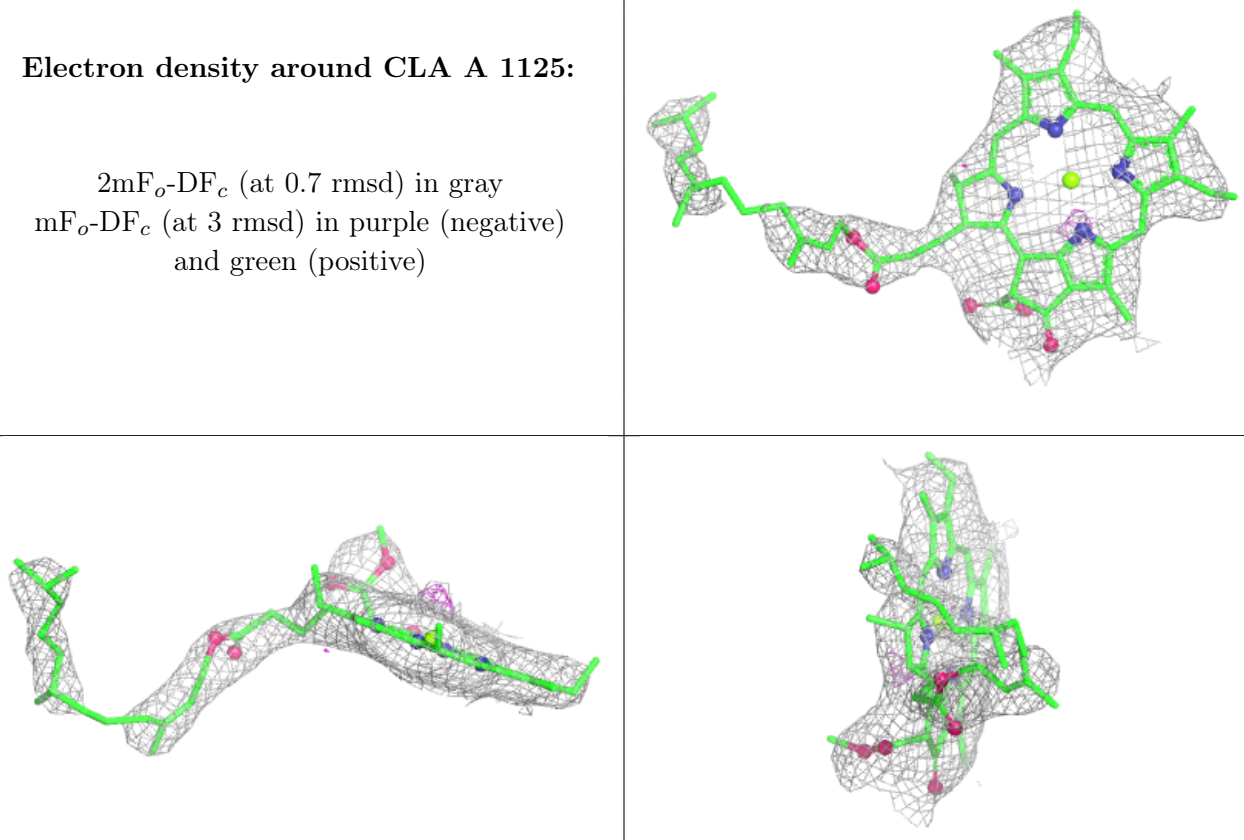






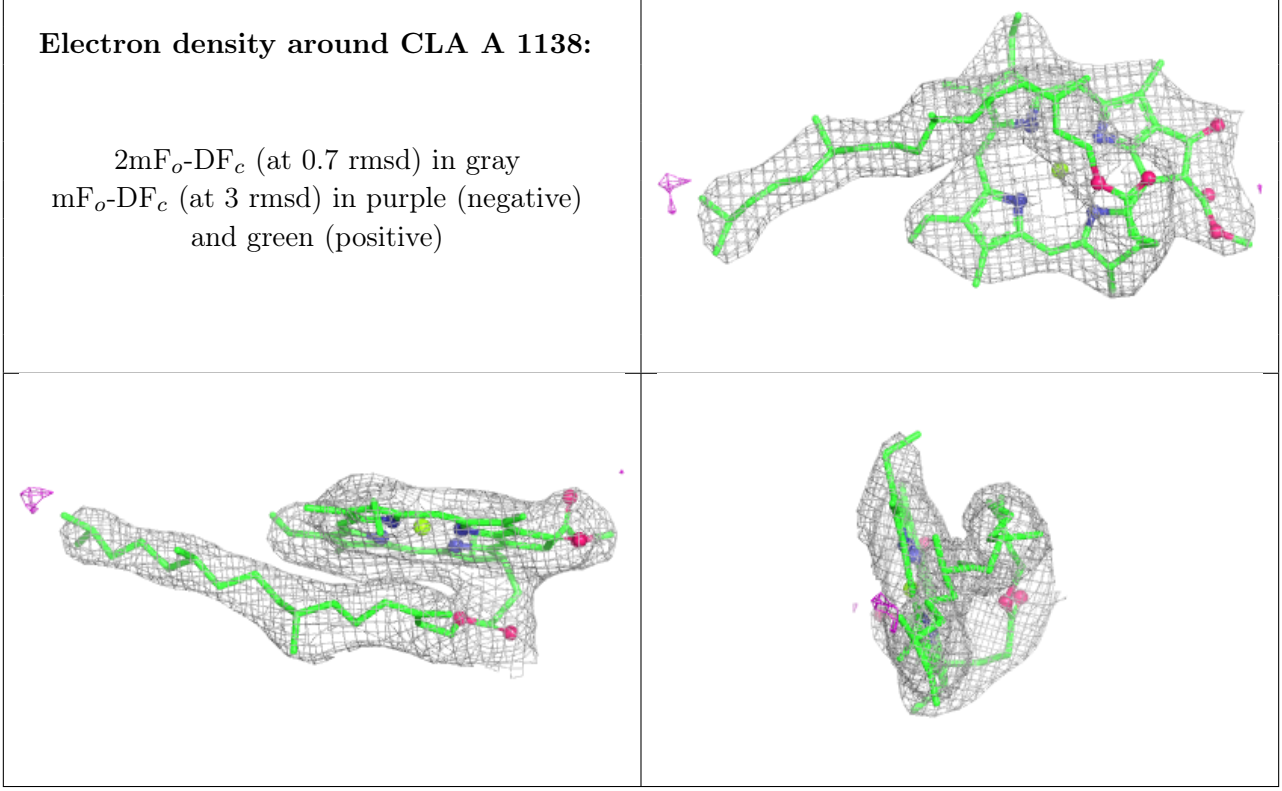
Electron density around CLA A 1125:

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



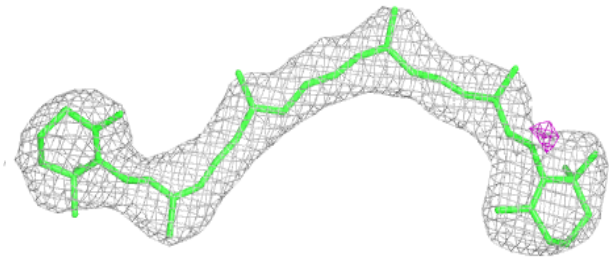
Electron density around CLA A 1138:

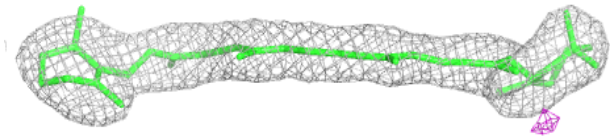
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

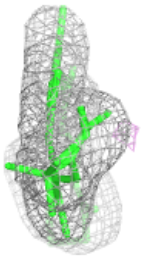


Electron density around BCR A 6011:

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

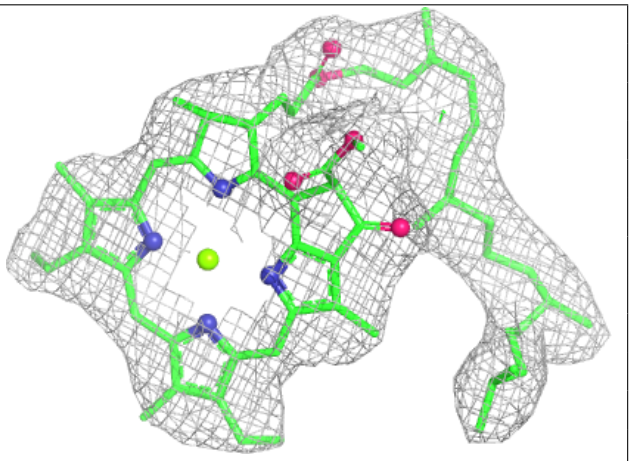


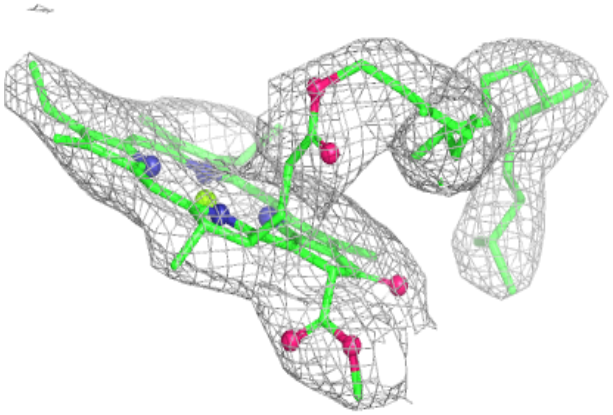


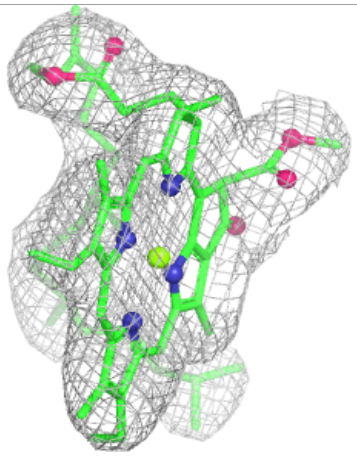


Electron density around CLA B 1229:

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

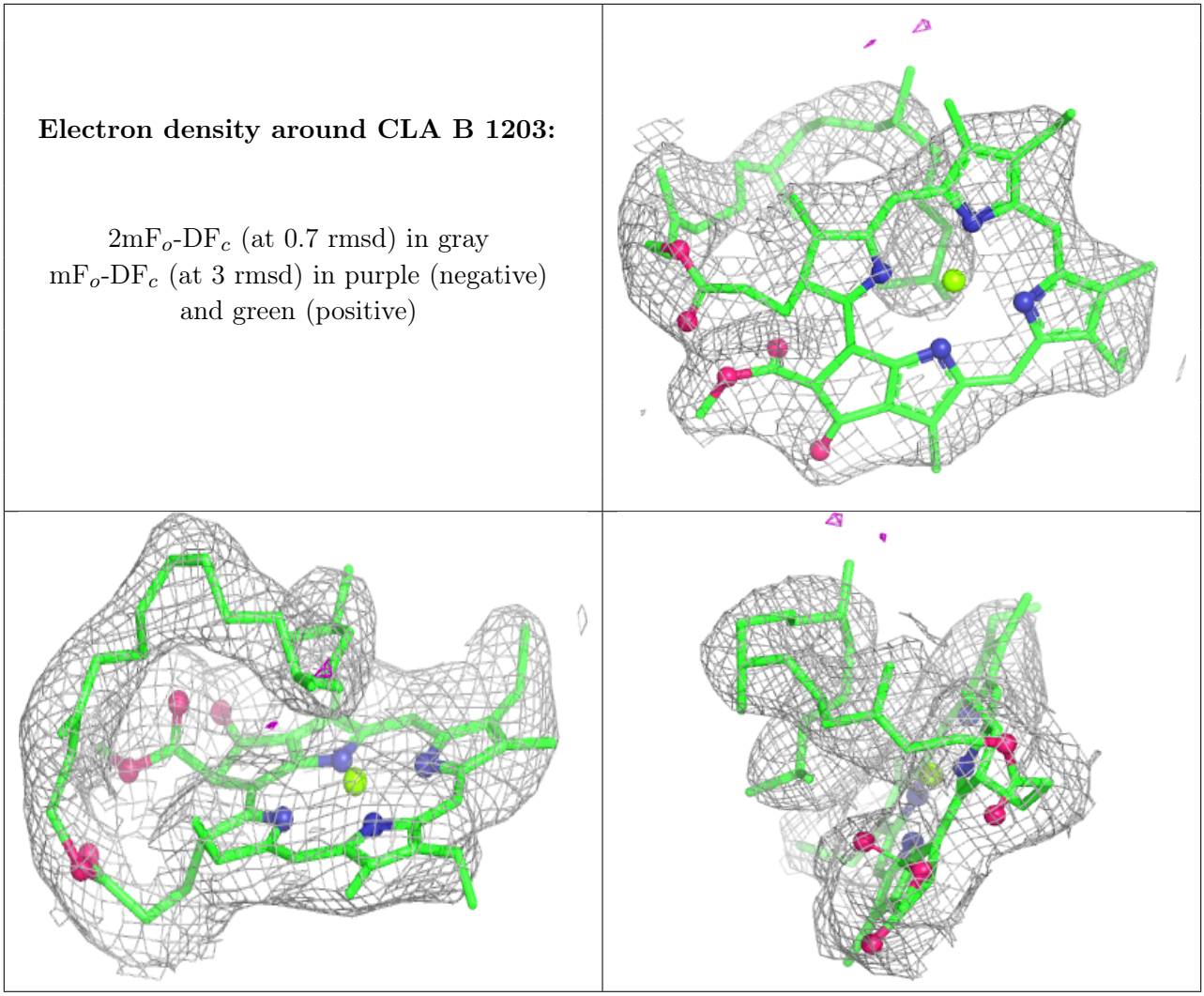






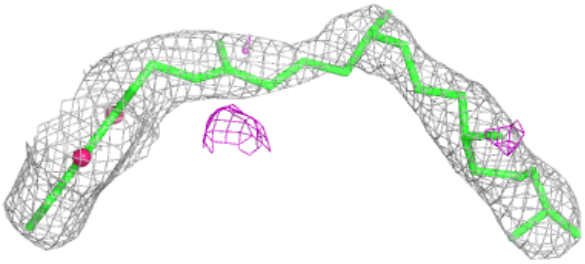
Electron density around CLA B 1203:

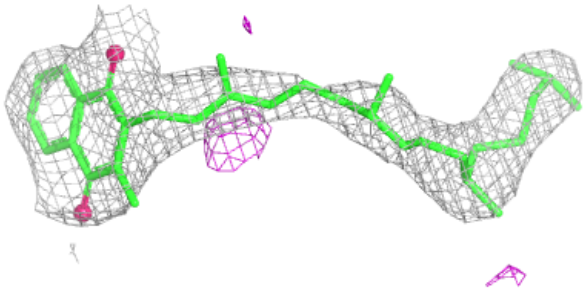
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

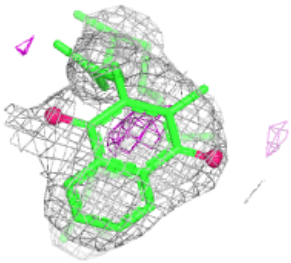


Electron density around PQN B 5002:

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

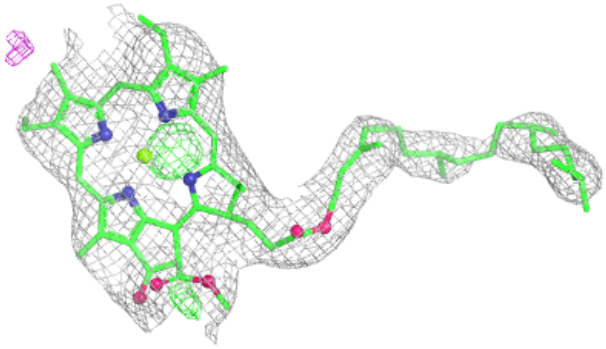


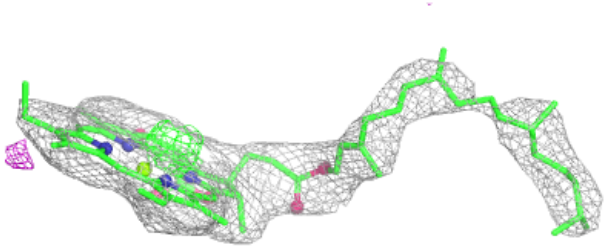


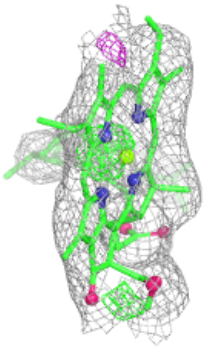


Electron density around CLA B 1210:

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

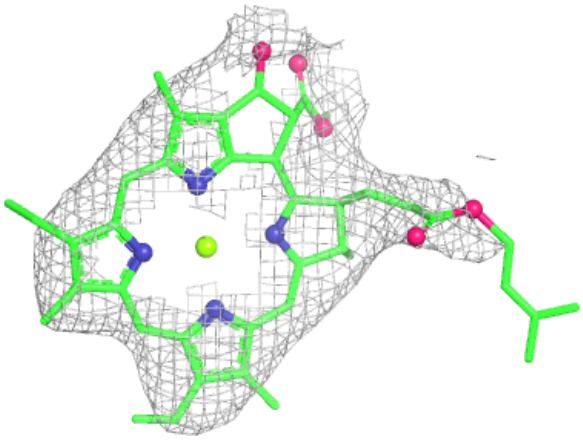


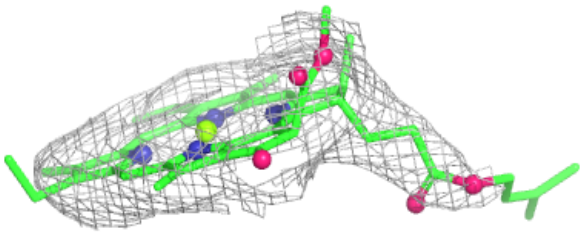


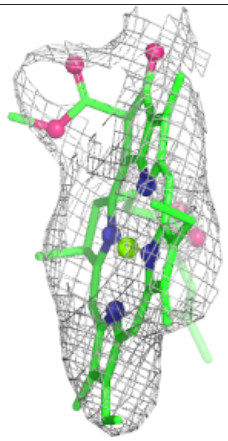


Electron density around CLA 4 4009:

$2mF_o$-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

There are no such residues in this entry.