



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 03:11 PM UTC

PDB ID : 5H2F / pdb_00005h2f
Title : Crystal structure of the PsbM-deletion mutant of photosystem II
Authors : Uto, S.; Kawakami, K.; Umena, Y.; Iwai, M.; Ikeuchi, M.; Shen, J.R.; Kamiya, N.
Deposited on : 2016-10-15
Resolution : 2.20 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 ⓘ 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 ⓘ](#)) 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

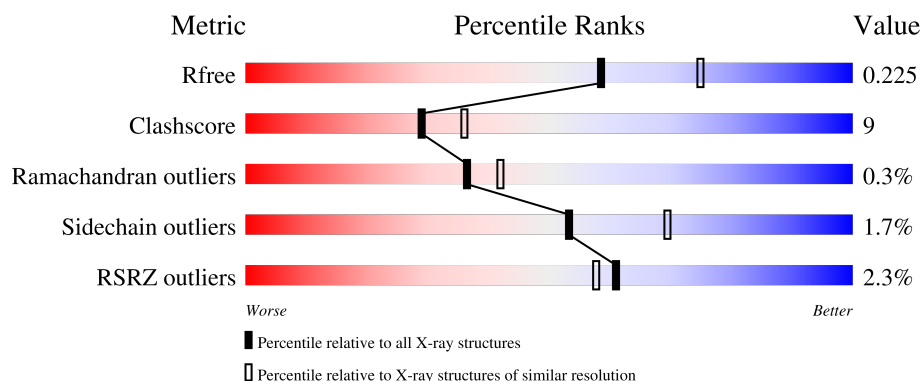
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



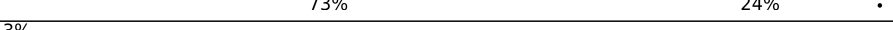
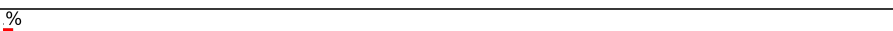
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	334	2% 87% 13% .
1	a	334	10% 84% 16% .
2	B	505	3% 86% 14% .
2	b	505	% 82% 14% .
3	C	455	% 85% 15% .

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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	80	
5	e	80	
6	F	33	
6	f	33	
7	H	63	
7	h	63	
8	I	36	
8	i	36	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	35	
11	l	35	
12	O	243	
12	o	243	
13	T	30	
13	t	30	
14	U	97	
14	u	97	
15	V	137	
15	v	137	

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Mol	Chain	Length	Quality of chain
16	Y	29	
16	y	29	
17	X	37	
17	x	37	
18	Z	62	
18	z	62	

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
22	CLA	A	405	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	407	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	902	X	-	-	-
22	CLA	c	903	X	-	-	-
22	CLA	c	906	X	-	-	-
22	CLA	c	907	X	-	-	-
22	CLA	c	908	X	-	-	-
22	CLA	c	910	X	-	-	-
22	CLA	c	911	X	-	-	-
22	CLA	c	913	X	-	-	-
22	CLA	d	402	X	-	-	-
31	DMS	B	631	-	-	X	-
31	DMS	B	638	-	-	X	-
31	DMS	O	303	-	-	X	-
31	DMS	O	304	-	-	X	-
31	DMS	O	312	-	-	X	-
31	DMS	V	212	-	-	X	-
31	DMS	a	425	-	-	X	-
31	DMS	b	638	-	-	X	-
31	DMS	c	924	-	-	X	-
31	DMS	d	415	-	-	X	-
31	DMS	f	103	-	-	X	-
31	DMS	o	304	-	-	X	-
31	DMS	o	308	-	-	X	-
31	DMS	u	205	-	-	X	-
34	HTG	D	415	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 51892 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 II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2598	1706	428	449	15			
1	a	334	Total	C	N	O	S	0	1	0
			2555	1675	427	438	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	3	0
			3950	2596	661	680	13			
2	b	483	Total	C	N	O	S	0	1	0
			3780	2484	631	652	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3470	2274	580	603	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2732	1814	442	464	12			
4	d	341	Total	C	N	O	S	0	2	0
			2717	1805	441	459	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	79	Total	C	N	O	0	0	0
			635	417	101	117			
5	e	79	Total	C	N	O	0	0	0
			636	418	101	117			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	3	0
			522	347	87	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			288	196	45	46	1			
8	i	36	Total	C	N	O	S	0	0	0
			293	199	46	47	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			277	186	41	49	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	35	Total	C	N	O	0	0	0
			287	192	46	49			
11	l	35	Total	C	N	O	0	0	0
			287	192	46	49			

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	O	243	Total	C	N	O	S	0	1	0
			1853	1160	311	378	4			
12	o	243	Total	C	N	O	S	0	0	0
			1833	1149	305	375	4			

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	T	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			
13	t	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	U	97	Total	C	N	O	0	1	0
			782	496	132	154			
14	u	97	Total	C	N	O	0	0	0
			766	487	129	150			

- Molecule 15 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	V	137	Total	C	N	O	S	0	1	0
			1066	677	177	208	4			
15	v	137	Total	C	N	O	S	0	1	0
			1058	671	175	208	4			

- Molecule 16 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
16	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

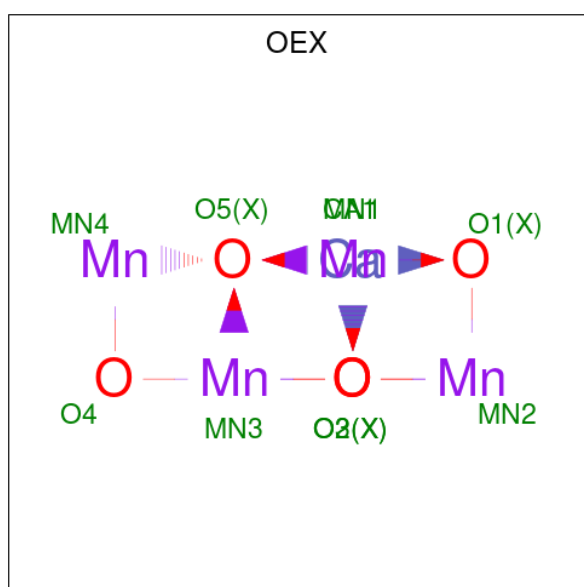
- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	37	Total	C	N	O	0	1	0
			269	183	40	46			
17	x	36	Total	C	N	O	0	0	0
			253	172	37	44			

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			453	311	68	72	2			
18	z	61	Total	C	N	O	S	0	0	0
			436	299	67	69	1			

- Molecule 19 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
19	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

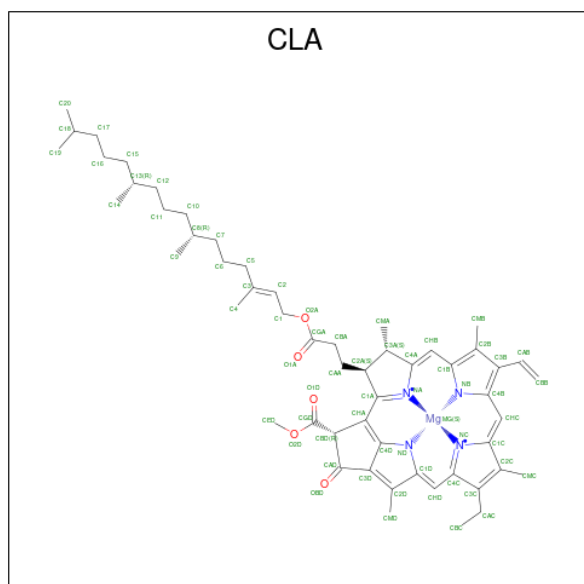
- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		
20	a	1	Total	Fe	0	0
			1	1		

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	0
			2	2		
21	a	2	Total	Cl	0	0
			2	2		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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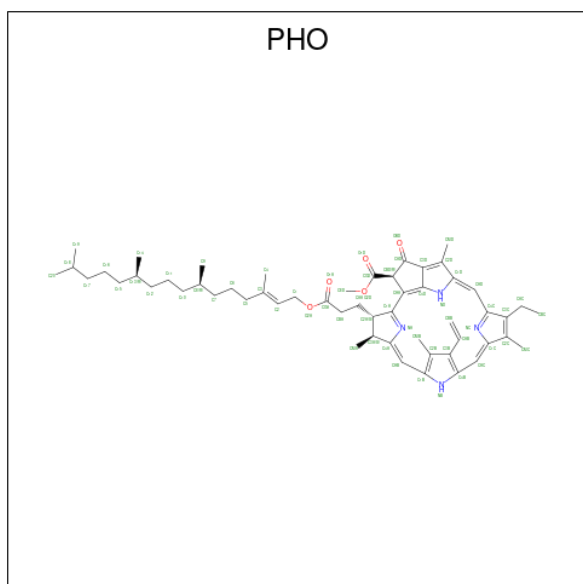
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
22	b	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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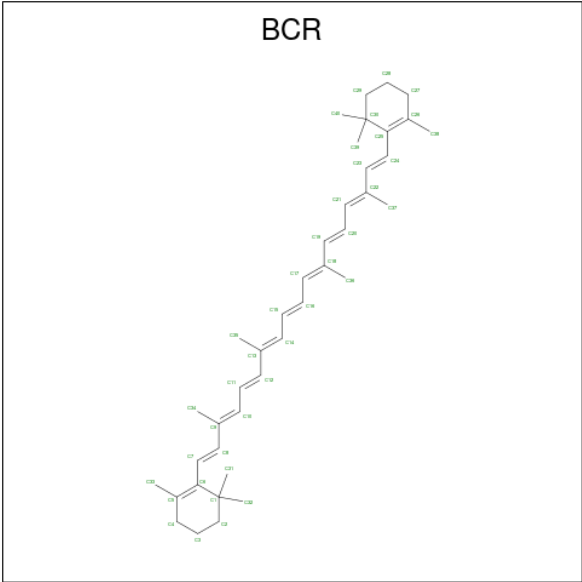
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



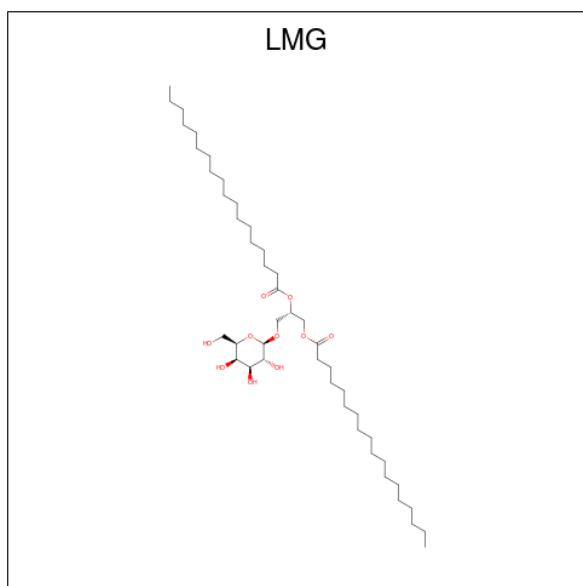
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 19 19	0	0
24	B	1	Total C 30 30	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	Y	1	Total C 39 39	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 20 20	0	0
24	b	1	Total C 31 31	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



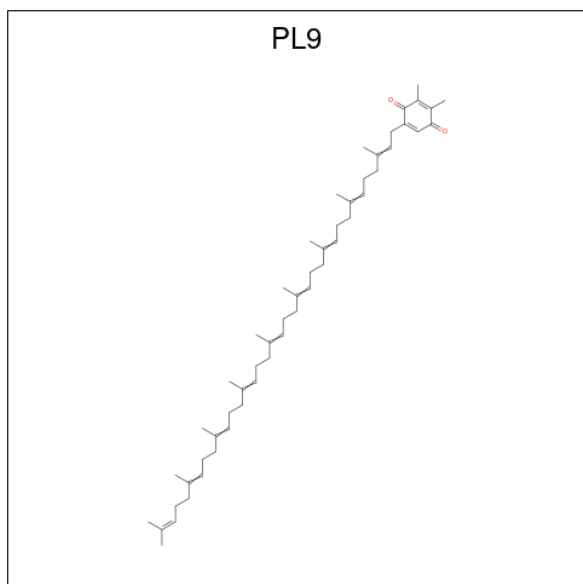
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 51 41 10	0	0
25	B	1	Total C O 40 30 10	0	0
25	C	1	Total C O 51 41 10	0	0
25	C	1	Total C O 40 30 10	0	0
25	D	1	Total C O 46 36 10	0	0
25	J	1	Total C O 45 35 10	0	0
25	b	1	Total C O 43 33 10	0	0

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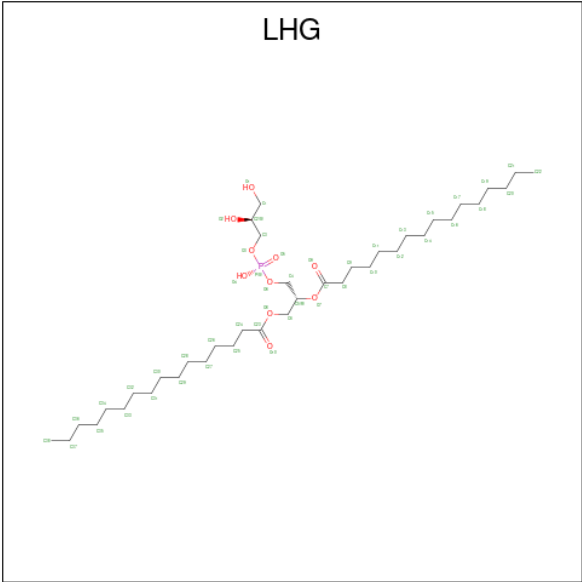
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	c	1	Total	C	O	0	0
			51	41	10		
25	c	1	Total	C	O	0	0
			49	39	10		
25	d	1	Total	C	O	0	0
			47	37	10		
25	i	1	Total	C	O	0	0
			51	41	10		
25	j	1	Total	C	O	0	0
			47	37	10		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



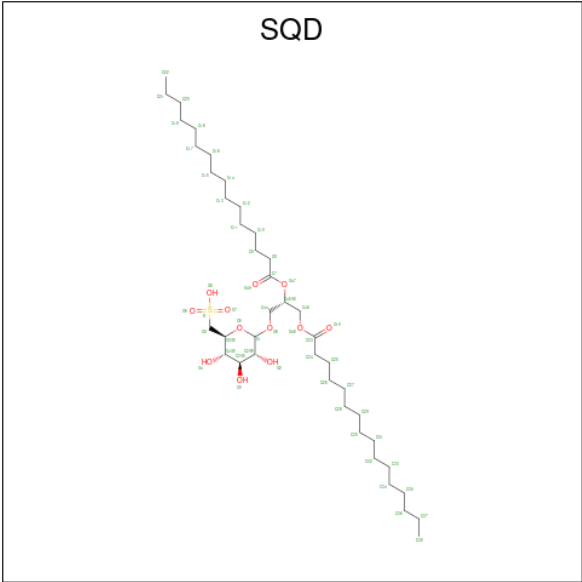
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			55	53	2		
26	D	1	Total	C	O	0	0
			55	53	2		
26	a	1	Total	C	O	0	0
			55	53	2		
26	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



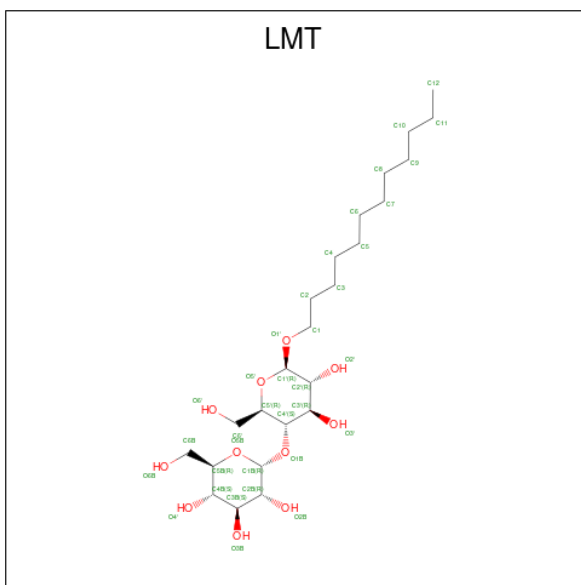
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			31	22	8	1		
27	C	1	Total	C	O	P	0	0
			30	21	8	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			45	34	10	1		
27	L	1	Total	C	O	P	0	0
			40	29	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			45	34	10	1		
27	d	1	Total	C	O	P	0	0
			33	24	8	1		
27	d	1	Total	C	O	P	0	0
			49	38	10	1		
27	d	1	Total	C	O	P	0	0
			46	35	10	1		
27	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			49	36	12	1		
28	C	1	Total	C	O	S	0	0
			54	41	12	1		
28	D	1	Total	C	O	S	0	0
			20	9	10	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			51	38	12	1		
28	b	1	Total	C	O	S	0	0
			38	26	11	1		
28	f	1	Total	C	O	S	0	0
			14	6	7	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total 35	C 24	O 11	0	0
29	B	1	Total 24	C 18	O 6	0	0
29	E	1	Total 24	C 18	O 6	0	0
29	I	1	Total 35	C 24	O 11	0	0
29	T	1	Total 24	C 18	O 6	0	0
29	Z	1	Total 35	C 24	O 11	0	0
29	a	1	Total 35	C 24	O 11	0	0
29	c	1	Total 35	C 24	O 11	0	0
29	c	1	Total 24	C 18	O 6	0	0
29	f	1	Total 25	C 19	O 6	0	0
29	t	1	Total 24	C 18	O 6	0	0

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

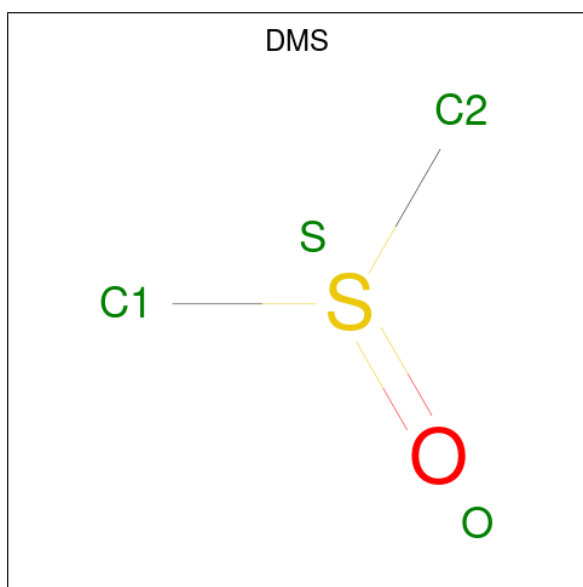
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	2	Total C 23 23	0	0
30	D	1	Total C 16 16	0	0
30	I	3	Total C 45 45	0	0
30	J	1	Total C 16 16	0	0
30	O	1	Total C 16 16	0	0
30	T	1	Total C 13 13	0	0
30	U	1	Total C 14 14	0	0
30	X	1	Total C 16 16	0	0
30	Z	1	Total C 9 9	0	0
30	a	2	Total C 16 16	0	0
30	b	2	Total C 27 27	0	0
30	c	1	Total C 10 10	0	0
30	d	1	Total C 16 16	0	0
30	i	4	Total C 58 58	0	0
30	j	1	Total C 16 16	0	0
30	t	1	Total C 16 16	0	0
30	u	1	Total C 11 11	0	0
30	x	1	Total C 15 15	0	0

- Molecule 31 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	L	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0

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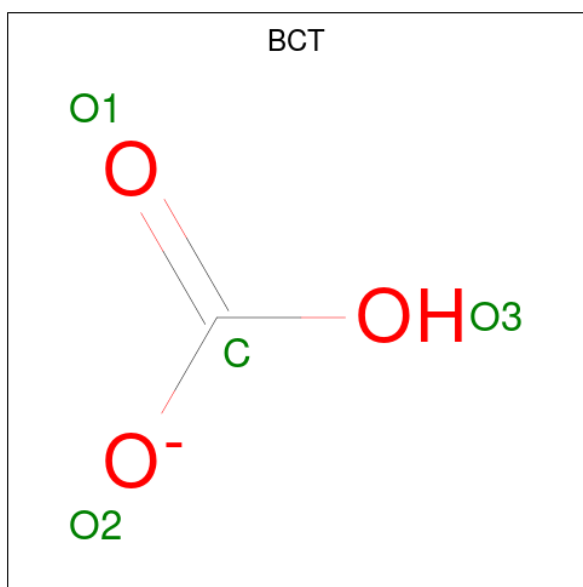
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	f	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).

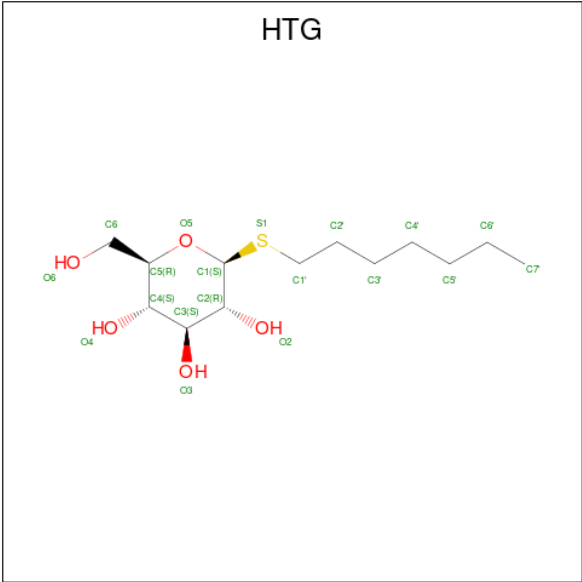


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			8	2	6		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		
33	c	1	Total	Ca	0	0
			1	1		
33	o	1	Total	Ca	0	0
			1	1		

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



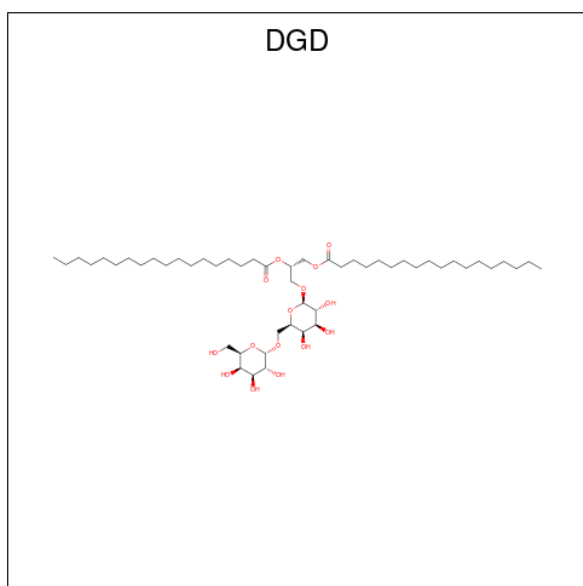
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	S		0	0
			9	8	1			
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			19	13	5	1		
34	V	1	Total	C	O	S	0	0
			14	8	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total	C	O	S	0	0
			19	13	5	1		
34	l	1	Total	C	O	S	0	0
			19	13	5	1		
34	v	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



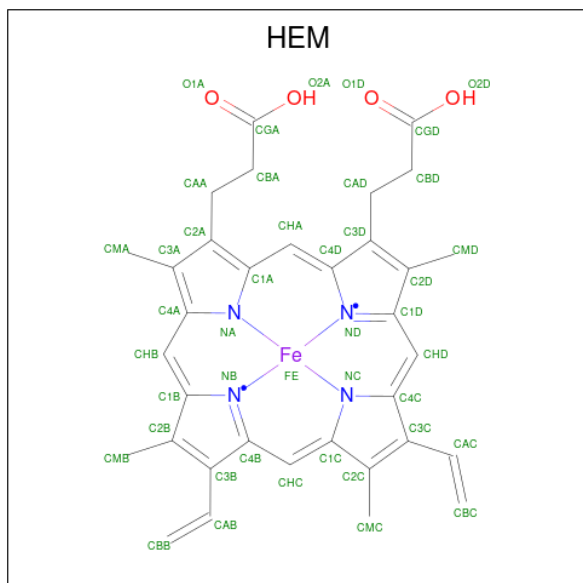
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	D	1	Total	C	O		0	0
			50	41	9			
35	H	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			

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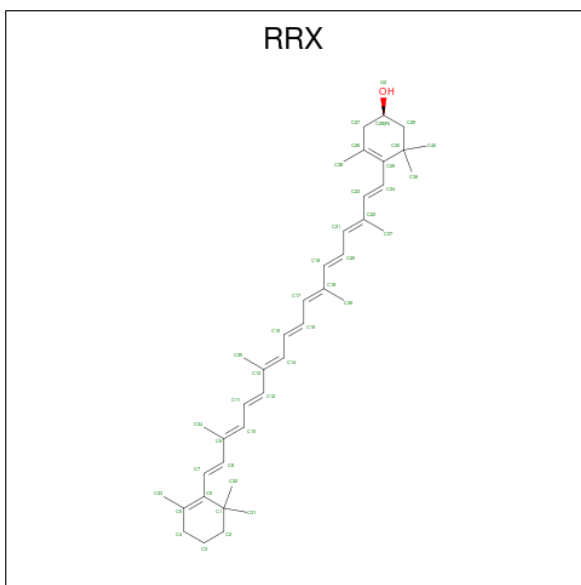
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	d	1	Total	C	O	0	0
			43	37	6		
35	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
36	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).

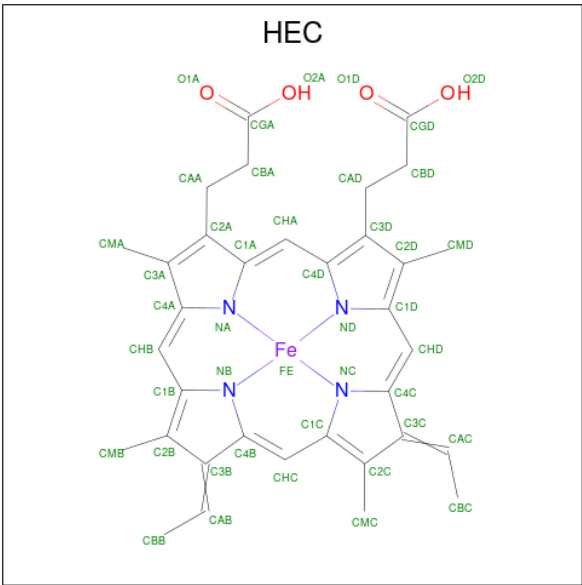


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	H	1	Total	C	O	0	0
			41	40	1		
37	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	J	1	Total	Mg	0	0
			1	1		
38	K	1	Total	Mg	0	0
			1	1		
38	j	1	Total	Mg	0	0
			1	1		
38	k	1	Total	Mg	0	0
			1	1		

- Molecule 39 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
39	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
39	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	132	Total	O	0	0
			132	132		
40	B	256	Total	O	0	6
			262	262		
40	C	174	Total	O	0	4
			178	178		
40	D	130	Total	O	0	1
			131	131		
40	E	33	Total	O	0	2
			35	35		
40	F	4	Total	O	0	0
			4	4		
40	H	39	Total	O	0	0
			39	39		
40	I	5	Total	O	0	0
			5	5		
40	J	15	Total	O	0	1
			16	16		
40	K	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	L	18	Total O 19 19	0	1
40	O	161	Total O 166 166	0	5
40	T	12	Total O 12 12	0	0
40	U	72	Total O 74 74	0	2
40	V	110	Total O 113 113	0	3
40	Y	7	Total O 8 8	0	1
40	X	15	Total O 16 16	0	1
40	Z	5	Total O 5 5	0	0
40	a	122	Total O 123 123	0	1
40	b	251	Total O 261 261	0	10
40	c	216	Total O 220 220	0	4
40	d	115	Total O 115 115	0	0
40	e	16	Total O 17 17	0	1
40	f	4	Total O 4 4	0	0
40	h	31	Total O 31 31	0	0
40	i	5	Total O 5 5	0	0
40	j	10	Total O 10 10	0	0
40	k	9	Total O 10 10	0	1
40	l	14	Total O 15 15	0	1
40	o	153	Total O 156 156	0	3
40	t	10	Total O 10 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	u	75	Total 75	O 75	0	0
40	v	77	Total 82	O 82	0	5
40	y	1	Total 1	O 1	0	0
40	x	5	Total 5	O 5	0	0
40	z	8	Total 8	O 8	0	0

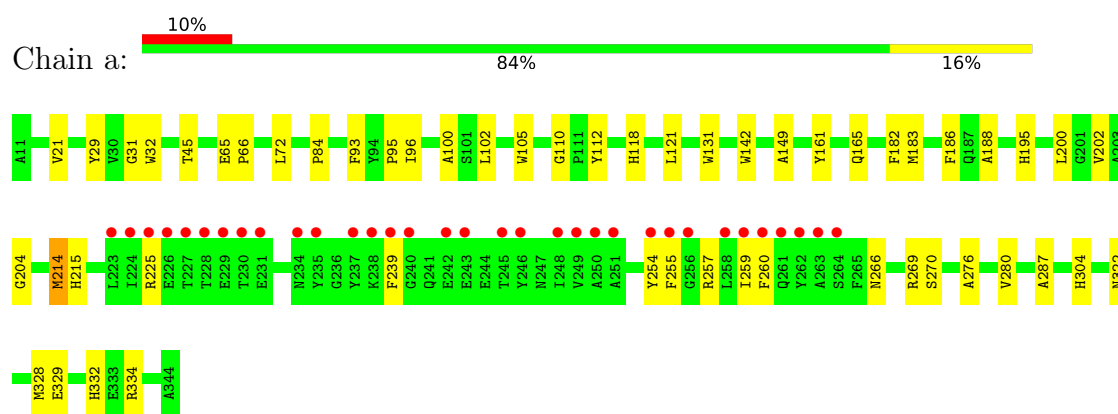
3 Residue-property plots

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.

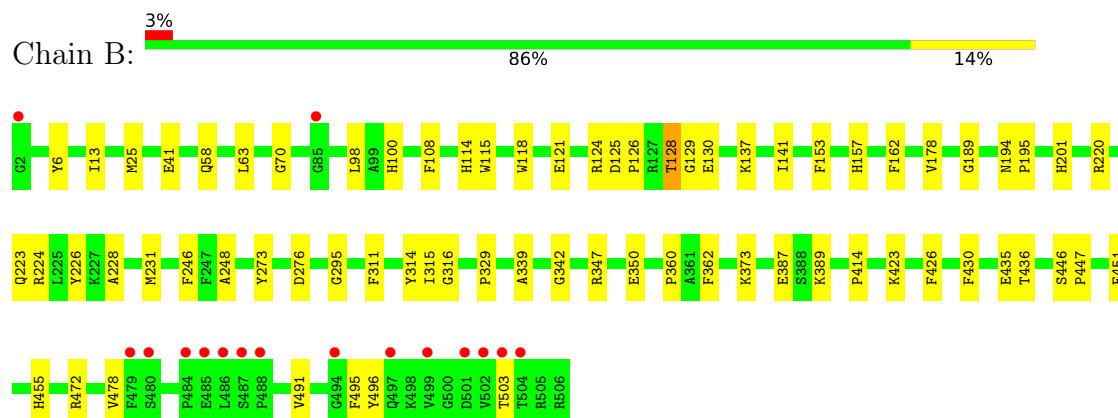
• Molecule 1: Photosystem II protein D1 1



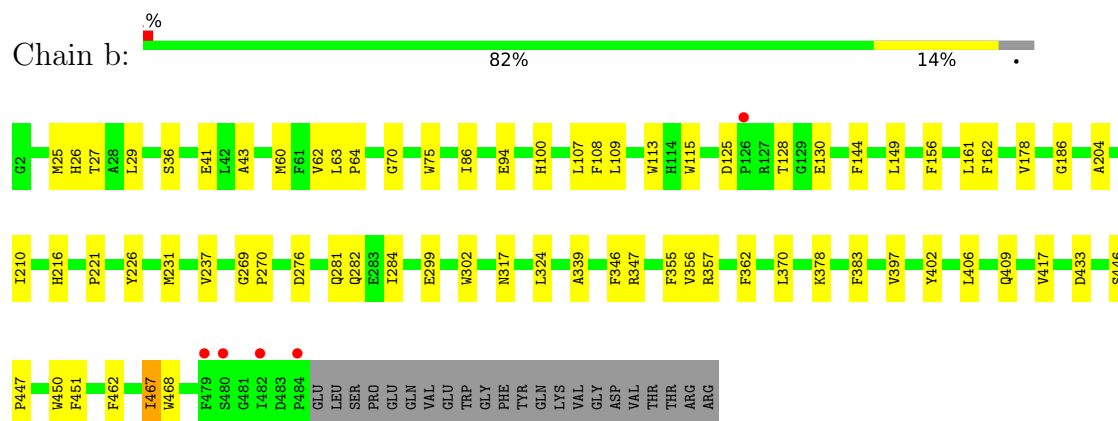
• Molecule 1: Photosystem II protein D1 1



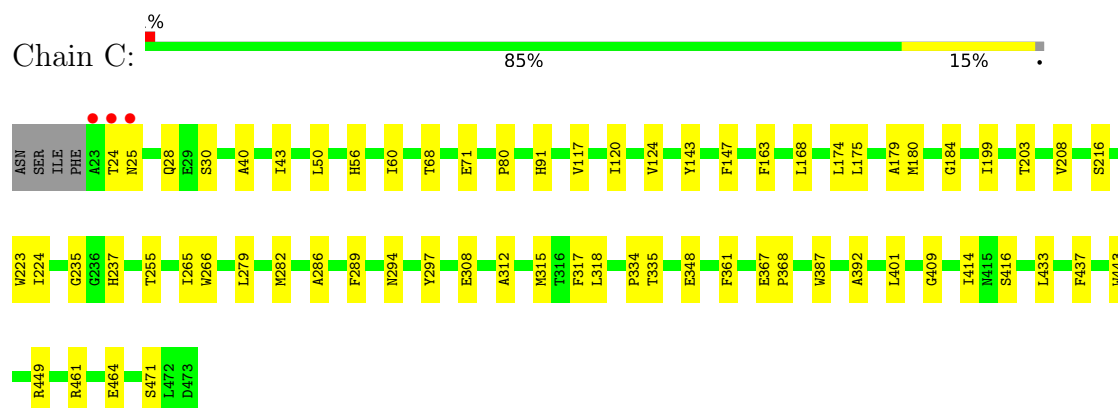
• Molecule 2: Photosystem II CP47 reaction center protein



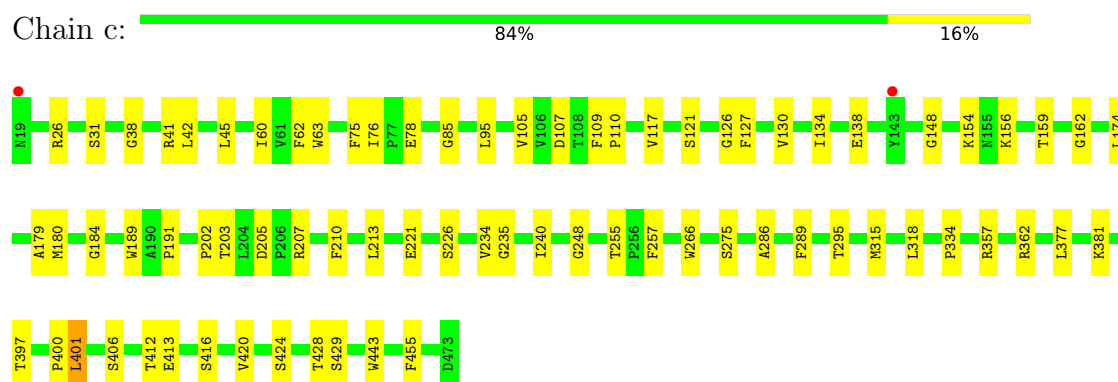
- Molecule 2: Photosystem II CP47 reaction center protein



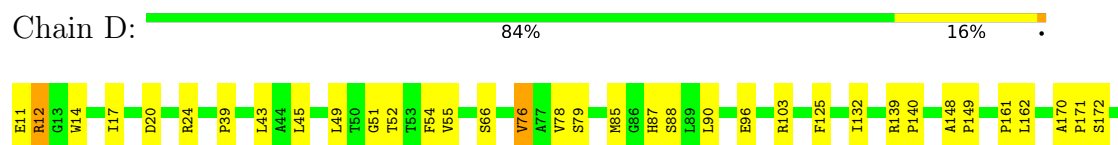
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein

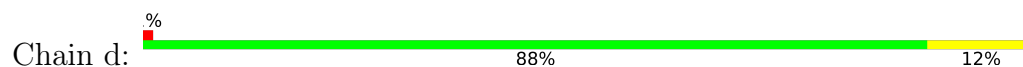


- Molecule 4: Photosystem II D2 protein

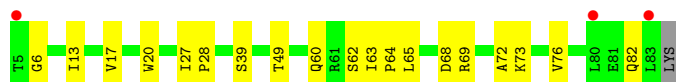
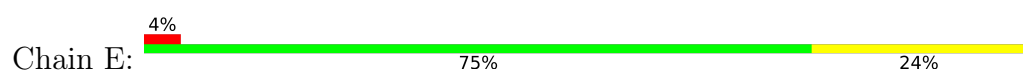




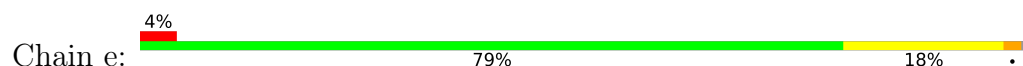
- Molecule 4: Photosystem II D2 protein



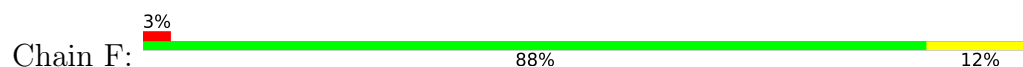
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



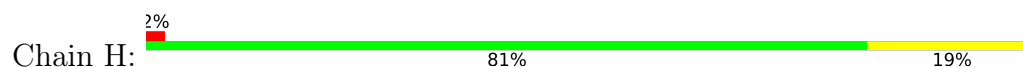
- Molecule 6: Cytochrome b559 subunit beta



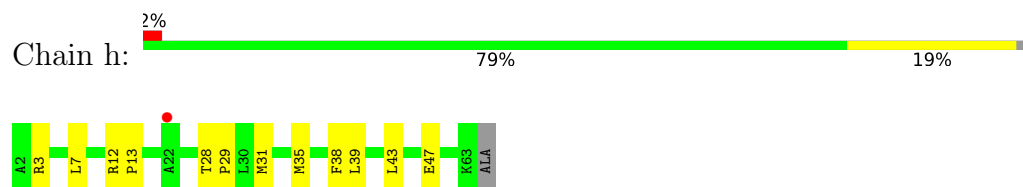
- Molecule 6: Cytochrome b559 subunit beta



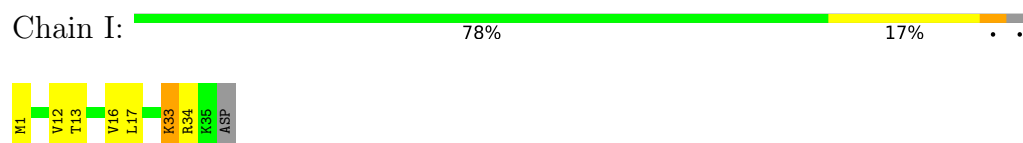
- Molecule 7: Photosystem II reaction center protein H



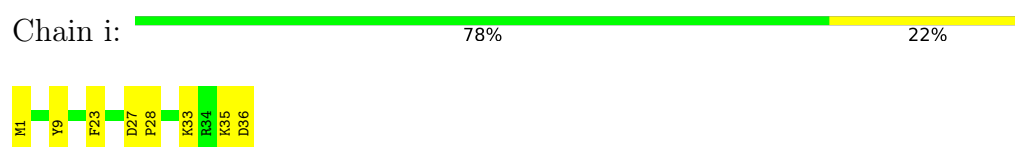
- Molecule 7: Photosystem II reaction center protein H



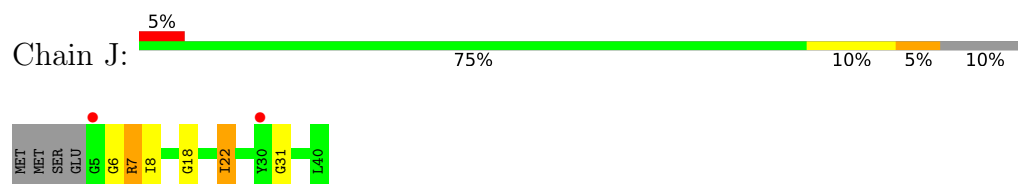
- Molecule 8: Photosystem II reaction center protein I



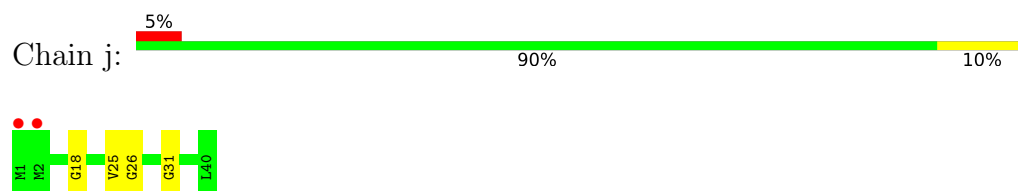
- Molecule 8: Photosystem II reaction center protein I



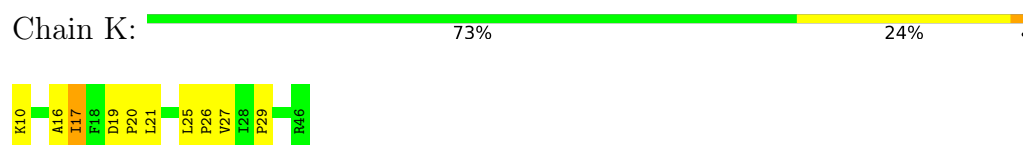
- Molecule 9: Photosystem II reaction center protein J



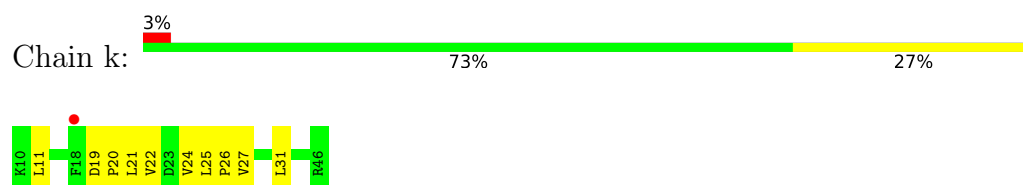
- Molecule 9: Photosystem II reaction center protein J



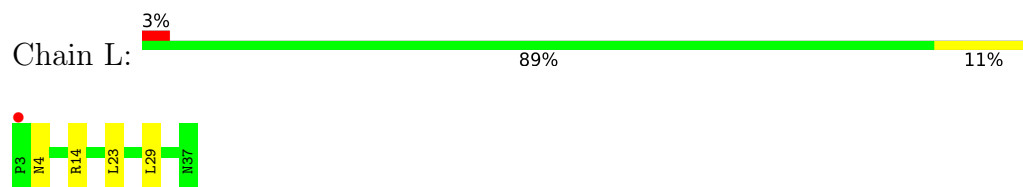
- Molecule 10: Photosystem II reaction center protein K



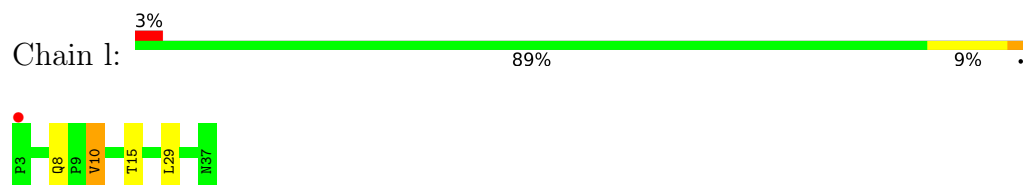
- Molecule 10: Photosystem II reaction center protein K



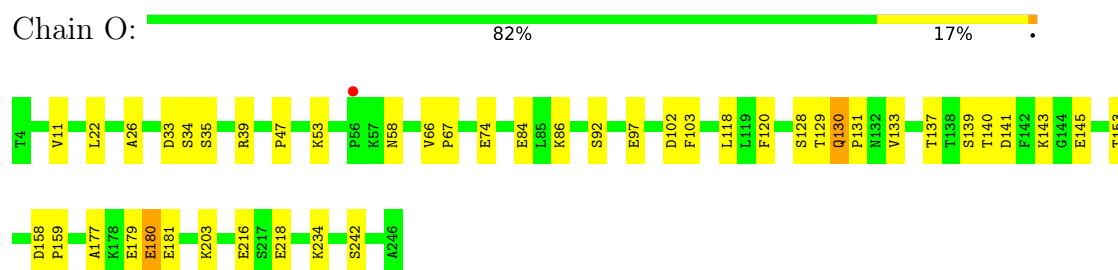
- Molecule 11: Photosystem II reaction center protein L



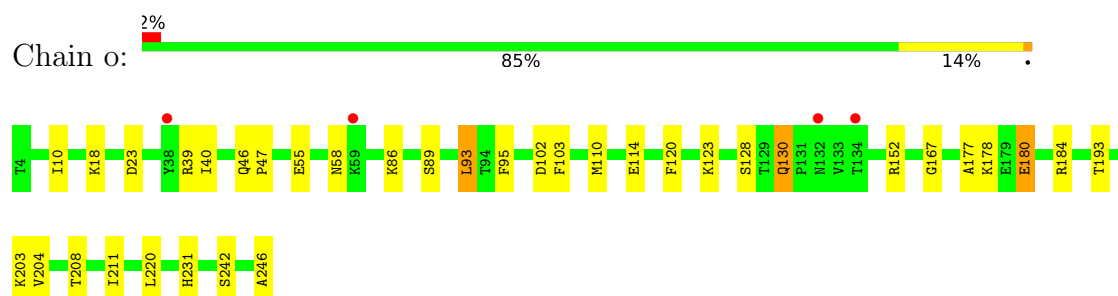
- Molecule 11: Photosystem II reaction center protein L



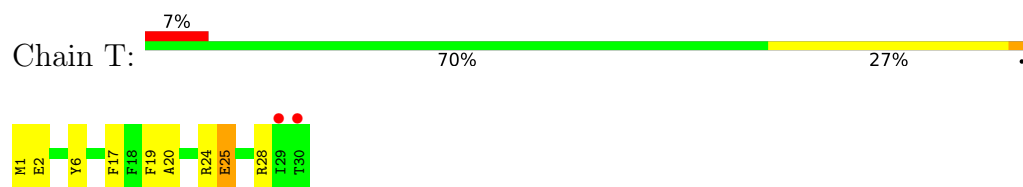
- Molecule 12: Photosystem II manganese-stabilizing polypeptide



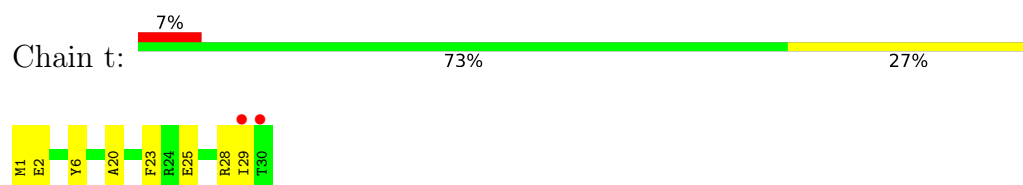
- Molecule 12: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II reaction center protein T



- Molecule 13: Photosystem II reaction center protein T



- Molecule 14: Photosystem II 12 kDa extrinsic protein

Chain U:  88% 12%



- Molecule 14: Photosystem II 12 kDa extrinsic protein

Chain u:  % 85% 15%



- Molecule 15: Cytochrome c-550

Chain V:  87% 12% .



- Molecule 15: Cytochrome c-550

Chain v:  82% 17% .



- Molecule 16: Photosystem II reaction center protein Ycf12

Chain Y:  3% 76% 24%



- Molecule 16: Photosystem II reaction center protein Ycf12

Chain y:  3% 72% 28%

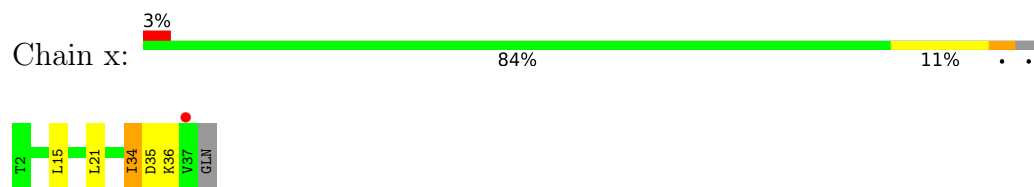


- Molecule 17: Photosystem II reaction center X protein

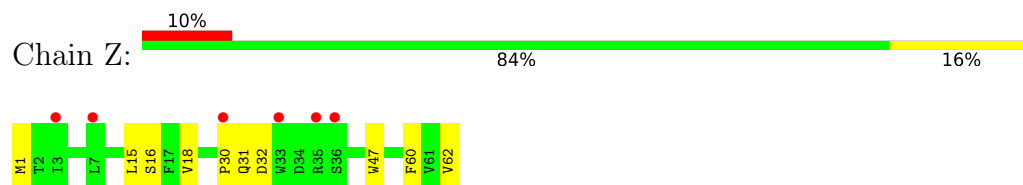
Chain X:  3% 81% 16%



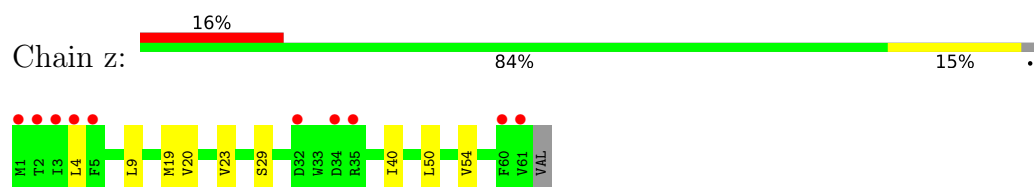
• Molecule 17: Photosystem II reaction center X protein



• Molecule 18: Photosystem II reaction center protein Z



• Molecule 18: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.95Å 226.99Å 285.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.20) 96.3 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.226 0.174 , 0.225	Depositor DCC
R_{free} test set	19357 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51892	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: UNL, CLA, BCT, BCR, HEM, RRX, DMS, SQD, HEC, FME, LMT, CL, LHG, LMG, MG, PHO, HTG, PL9, OEX, CA, FE2, DGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.09	3/2686 (0.1%)	1.03	6/3666 (0.2%)
1	a	1.13	8/2640 (0.3%)	1.05	3/3604 (0.1%)
2	B	1.07	3/4099 (0.1%)	1.03	4/5591 (0.1%)
2	b	1.06	2/3917 (0.1%)	1.02	3/5342 (0.1%)
3	C	1.03	5/3583 (0.1%)	1.00	2/4880 (0.0%)
3	c	1.01	2/3638 (0.1%)	1.04	3/4953 (0.1%)
4	D	1.10	2/2836 (0.1%)	0.99	1/3866 (0.0%)
4	d	1.04	0/2818	1.00	4/3842 (0.1%)
5	E	0.91	0/654	1.04	1/895 (0.1%)
5	e	0.89	0/655	1.05	3/896 (0.3%)
6	F	0.99	0/278	0.87	0/379
6	f	0.90	0/257	0.94	0/349
7	H	0.90	0/541	0.94	1/737 (0.1%)
7	h	0.90	0/517	0.93	0/704
8	I	0.89	0/285	1.00	0/385
8	i	0.82	0/290	0.93	0/392
9	J	0.94	0/257	1.08	1/349 (0.3%)
9	j	0.88	0/283	1.01	0/384
10	K	0.90	0/303	1.13	2/416 (0.5%)
10	k	0.85	0/296	1.05	0/408
11	L	0.97	0/294	1.03	1/399 (0.3%)
11	l	0.93	0/294	1.08	0/399
12	O	0.95	0/1887	1.02	1/2561 (0.0%)
12	o	0.86	0/1864	1.03	5/2535 (0.2%)
13	T	0.92	0/252	1.04	2/342 (0.6%)
13	t	0.89	0/252	1.02	1/342 (0.3%)
14	U	0.96	0/796	1.01	1/1078 (0.1%)
14	u	0.94	0/777	1.07	1/1054 (0.1%)
15	V	1.05	1/1090 (0.1%)	1.04	0/1480
15	v	0.95	0/1082	1.03	2/1472 (0.1%)
16	Y	0.80	0/216	1.04	0/289

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	y	0.69	0/208	1.05	0/278
17	X	0.73	0/275	1.10	0/373
17	x	0.77	0/256	1.05	0/349
18	Z	0.83	0/463	1.04	0/636
18	z	0.75	0/447	1.06	0/614
All	All	1.01	26/41286 (0.1%)	1.02	48/56239 (0.1%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	87	HIS	CG-CD2	8.02	1.44	1.35
1	A	56	PRO	CA-C	6.77	1.58	1.52
1	a	195	HIS	ND1-CE1	6.00	1.38	1.32
1	A	159	LEU	CA-C	5.80	1.58	1.52
1	a	195	HIS	CG-CD2	5.78	1.42	1.35
4	D	87	HIS	ND1-CE1	5.71	1.38	1.32
3	c	295	THR	CA-C	5.60	1.59	1.53
2	b	100	HIS	CG-ND1	-5.56	1.32	1.38
1	a	332	HIS	CG-CD2	5.51	1.42	1.35
15	V	69	ILE	C-O	5.51	1.30	1.24
3	C	317	PHE	N-CA	5.45	1.53	1.46
3	c	401	LEU	CA-C	-5.45	1.45	1.52
2	B	414	PRO	CA-C	5.41	1.57	1.52
3	C	56	HIS	CG-CD2	5.40	1.41	1.35
2	B	114	HIS	CG-CD2	5.27	1.41	1.35
2	b	26	HIS	CG-CD2	5.25	1.41	1.35
1	a	304	HIS	CG-CD2	5.21	1.41	1.35
1	a	332	HIS	ND1-CE1	5.20	1.37	1.32
1	a	118	HIS	CG-CD2	5.19	1.41	1.35
2	B	100	HIS	ND1-CE1	5.15	1.37	1.32
1	a	110	GLY	CA-C	5.14	1.55	1.51
3	C	387	TRP	CD2-CE2	5.12	1.50	1.41
1	A	198	HIS	ND1-CE1	5.11	1.37	1.32
3	C	56	HIS	CE1-NE2	5.08	1.37	1.32
3	C	91	HIS	CG-CD2	5.03	1.41	1.35
1	a	149	ALA	N-CA	-5.00	1.43	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	142	TRP	N-CA-C	7.31	121.91	112.92
2	B	342	GLY	N-CA-C	-7.27	104.63	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	269	GLY	CA-C-N	6.76	127.15	119.92
2	b	269	GLY	C-N-CA	6.76	127.15	119.92
5	E	76	VAL	N-CA-C	-6.39	104.11	110.62
1	A	167	SER	N-CA-C	6.36	118.06	108.46
12	o	130	GLN	CA-C-N	-6.29	114.30	120.52
12	o	130	GLN	C-N-CA	-6.29	114.30	120.52
1	A	110	GLY	CA-C-N	-6.07	112.31	119.05
1	A	110	GLY	C-N-CA	-6.07	112.31	119.05
2	B	295	GLY	N-CA-C	6.00	121.93	114.37
4	d	271	MET	N-CA-C	6.00	117.82	111.28
12	o	46	GLN	CA-C-N	5.89	125.65	119.76
12	o	46	GLN	C-N-CA	5.89	125.65	119.76
2	b	417	VAL	N-CA-C	-5.82	104.84	110.72
4	d	170	ALA	CA-C-N	-5.82	113.94	119.76
4	d	170	ALA	C-N-CA	-5.82	113.94	119.76
15	v	105	ARG	N-CA-C	5.72	118.25	111.33
3	c	377	LEU	N-CA-C	5.66	118.18	111.33
1	A	298	ASN	N-CA-C	5.64	118.69	110.17
3	c	357	ARG	N-CA-C	-5.53	106.03	112.89
13	T	25	GLU	CA-C-N	-5.50	114.72	120.38
13	T	25	GLU	C-N-CA	-5.50	114.72	120.38
2	B	478	VAL	N-CA-C	5.45	117.44	111.77
11	L	23	LEU	N-CA-C	-5.45	105.24	111.07
9	J	7	ARG	N-CA-C	5.45	117.66	111.02
5	e	38	VAL	N-CA-C	5.43	117.34	111.58
1	a	149	ALA	CA-C-N	-5.42	113.03	119.05
1	a	149	ALA	C-N-CA	-5.42	113.03	119.05
14	u	41	LEU	N-CA-C	5.41	118.34	111.69
3	C	71	GLU	N-CA-C	-5.40	105.47	111.36
5	e	34	GLY	N-CA-C	-5.38	105.98	112.49
13	t	20	ALA	N-CA-C	-5.37	106.23	112.89
15	v	10	VAL	N-CA-C	5.36	115.06	109.01
5	e	58	GLN	N-CA-C	5.31	117.07	111.28
2	B	189	GLY	N-CA-C	-5.29	108.39	115.32
1	A	131	TRP	CA-CB-CG	-5.18	103.75	113.60
12	O	128	SER	N-CA-C	5.17	118.01	109.85
10	K	25	LEU	CA-C-N	-5.15	114.31	119.56
10	K	25	LEU	C-N-CA	-5.15	114.31	119.56
4	d	262	SER	N-CA-C	-5.15	107.67	114.31
3	c	76	ILE	N-CA-C	-5.12	102.12	107.60
14	U	98	TYR	N-CA-C	5.10	117.96	111.69
3	C	120	ILE	N-CA-C	-5.07	105.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	o	86	LYS	N-CA-C	5.06	116.82	110.24
1	A	214	MET	N-CA-C	5.02	116.44	110.97
7	H	52	THR	N-CA-C	-5.02	106.32	112.90
4	D	76	VAL	CB-CA-C	-5.01	105.84	111.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2598	0	2484	42	0
1	a	2555	0	2420	41	0
2	B	3950	0	3776	54	0
2	b	3780	0	3636	70	0
3	C	3470	0	3380	46	0
3	c	3521	0	3439	60	0
4	D	2732	0	2640	57	0
4	d	2717	0	2628	37	0
5	E	635	0	613	12	0
5	e	636	0	609	9	0
6	F	269	0	277	3	0
6	f	250	0	261	12	0
7	H	522	0	547	13	0
7	h	501	0	526	12	0
8	I	288	0	307	3	0
8	i	293	0	309	7	0
9	J	251	0	257	8	0
9	j	277	0	277	4	0
10	K	293	0	305	9	0
10	k	286	0	285	9	0
11	L	287	0	299	3	0
11	l	287	0	299	6	0
12	O	1853	0	1819	36	0
12	o	1833	0	1783	29	0
13	T	253	0	247	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	t	253	0	247	3	0
14	U	782	0	786	7	0
14	u	766	0	765	12	0
15	V	1066	0	1075	22	0
15	v	1058	0	1053	18	0
16	Y	215	0	246	3	0
16	y	207	0	221	9	0
17	X	269	0	297	6	0
17	x	253	0	274	4	0
18	Z	453	0	471	5	0
18	z	436	0	431	5	0
19	A	10	0	0	0	0
19	a	10	0	0	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	185	0	193	10	0
22	B	1014	0	1091	25	0
22	C	836	0	915	32	0
22	D	195	0	216	5	0
22	a	256	0	277	11	0
22	b	1016	0	1096	47	0
22	c	845	0	936	32	0
22	d	130	0	144	3	0
23	A	64	0	74	0	0
23	D	64	0	74	5	0
23	a	128	0	148	10	0
24	A	40	0	56	1	0
24	B	89	0	121	4	0
24	C	80	0	112	5	0
24	D	40	0	56	1	0
24	K	40	0	56	0	0
24	Y	39	0	53	2	0
24	a	40	0	56	1	0
24	b	91	0	123	11	0
24	c	80	0	112	8	0
24	d	40	0	56	2	0
24	k	40	0	56	2	0
24	y	40	0	56	3	0
25	A	51	0	72	2	0
25	B	40	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	91	0	122	3	0
25	D	46	0	62	5	0
25	J	45	0	60	1	0
25	b	43	0	56	1	0
25	c	100	0	140	4	0
25	d	47	0	64	4	0
25	i	51	0	72	3	0
25	j	47	0	64	2	0
26	A	55	0	80	10	0
26	D	55	0	80	5	0
26	a	55	0	80	10	0
26	d	55	0	80	5	0
27	A	31	0	36	1	0
27	C	30	0	33	1	0
27	D	143	0	211	18	0
27	L	40	0	53	7	0
27	a	94	0	137	7	0
27	d	128	0	178	6	0
27	l	49	0	74	3	0
28	A	49	0	64	2	0
28	C	54	0	78	6	0
28	D	20	0	16	0	0
28	a	105	0	147	6	0
28	b	38	0	47	2	0
28	f	14	0	8	1	0
28	l	54	0	78	1	0
29	A	35	0	46	6	0
29	B	24	0	35	3	0
29	E	24	0	35	1	0
29	I	35	0	46	0	0
29	T	24	0	35	1	0
29	Z	35	0	46	1	0
29	a	35	0	46	7	0
29	c	59	0	81	1	0
29	f	25	0	35	0	0
29	t	24	0	35	2	0
30	A	5	0	0	0	0
30	B	23	0	0	0	0
30	D	16	0	0	0	0
30	I	45	0	0	1	0
30	J	16	0	0	0	0
30	O	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	T	13	0	0	0	0
30	U	14	0	0	1	0
30	X	16	0	0	1	0
30	Z	9	0	0	0	0
30	a	16	0	0	0	0
30	b	27	0	0	0	0
30	c	10	0	0	0	0
30	d	16	0	0	0	0
30	i	58	0	0	0	0
30	j	16	0	0	1	0
30	t	16	0	0	0	0
30	u	11	0	0	0	0
30	x	15	0	0	0	0
31	A	20	0	30	4	0
31	B	60	0	90	20	0
31	C	60	0	90	6	0
31	D	12	0	18	3	0
31	F	4	0	6	0	0
31	H	4	0	6	1	0
31	I	8	0	12	0	0
31	L	4	0	6	0	0
31	O	48	0	72	22	0
31	U	8	0	12	1	0
31	V	40	0	60	20	0
31	a	20	0	30	8	0
31	b	36	0	54	14	0
31	c	76	0	114	23	0
31	d	20	0	30	8	0
31	f	4	0	6	4	0
31	i	4	0	6	1	0
31	l	12	0	18	1	0
31	o	28	0	42	15	0
31	t	12	0	18	0	0
31	u	16	0	24	6	0
31	v	36	0	54	8	0
32	A	8	0	0	1	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	57	0	78	3	0
34	C	47	0	67	2	0
34	D	38	0	52	11	0
34	V	14	0	13	0	0
34	b	95	0	130	7	0
34	c	19	0	26	0	0
34	l	19	0	26	3	0
34	v	16	0	17	0	0
35	C	186	0	246	3	0
35	D	50	0	69	0	0
35	H	62	0	82	2	0
35	c	186	0	246	9	0
35	d	43	0	62	0	0
35	h	62	0	82	2	0
36	E	43	0	30	1	0
36	e	43	0	30	6	0
37	H	41	0	56	4	0
37	h	41	0	56	8	0
38	J	1	0	0	0	0
38	K	1	0	0	0	0
38	j	1	0	0	0	0
38	k	1	0	0	0	0
39	V	43	0	30	0	0
39	v	43	0	30	1	0
40	A	132	0	0	1	0
40	B	262	0	0	6	0
40	C	178	0	0	1	0
40	D	131	0	0	5	0
40	E	35	0	0	0	0
40	F	4	0	0	0	0
40	H	39	0	0	1	0
40	I	5	0	0	0	0
40	J	16	0	0	0	0
40	K	7	0	0	0	0
40	L	19	0	0	0	0
40	O	166	0	0	10	0
40	T	12	0	0	0	0
40	U	74	0	0	2	0
40	V	113	0	0	4	0
40	X	16	0	0	0	0
40	Y	8	0	0	0	0
40	Z	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	a	123	0	0	1	0
40	b	261	0	0	11	0
40	c	220	0	0	7	0
40	d	115	0	0	0	0
40	e	17	0	0	1	0
40	f	4	0	0	0	0
40	h	31	0	0	0	0
40	i	5	0	0	0	0
40	j	10	0	0	0	0
40	k	10	0	0	0	0
40	l	15	0	0	0	0
40	o	156	0	0	5	0
40	t	10	0	0	0	0
40	u	75	0	0	3	0
40	v	82	0	0	4	0
40	x	5	0	0	0	0
40	y	1	0	0	0	0
40	z	8	0	0	0	0
All	All	51892	0	50274	868	0

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 9.

All (868) 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)
3:c:362:ARG:HD3	31:c:924:DMS:H22	1.29	1.13
1:a:214:MET:HG2	26:a:415:PL9:H102	1.31	1.12
22:b:608:CLA:H92	22:b:608:CLA:H52	1.14	1.10
2:b:347[B]:ARG:NH2	40:b:845[B]:HOH:O	1.79	1.07
3:c:362:ARG:HH11	31:c:924:DMS:H23	1.19	1.07
22:b:608:CLA:H52	22:b:608:CLA:C9	1.85	1.05
12:O:66:VAL:HG13	12:O:67:PRO:HD2	1.37	1.05
2:b:125:ASP:HB3	2:b:128:THR:CG2	1.86	1.05
26:D:406:PL9:C33	27:L:101:LHG:H223	1.87	1.04
31:f:103:DMS:H12	31:v:206:DMS:H21	1.35	1.02
1:A:214:MET:HG2	26:A:411:PL9:H102	1.37	1.02
3:c:362:ARG:NH1	31:c:924:DMS:H23	1.74	1.02
4:d:85:MET:HE2	4:d:90[A]:LEU:HD21	1.43	1.00
16:y:23:THR:HG22	16:y:27:MET:HE2	1.42	0.99
31:O:310:DMS:H13	40:O:501:HOH:O	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:17:ILE:HD12	10:K:17:ILE:H	1.27	0.96
22:b:608:CLA:H92	22:b:608:CLA:C5	1.96	0.96
10:k:21:LEU:HD13	16:y:24:MET:HE3	1.49	0.94
12:o:208:THR:O	31:o:305:DMS:H13	1.66	0.94
2:b:355:PHE:HA	31:b:638:DMS:H21	1.51	0.93
25:d:409:LMG:O2	25:d:409:LMG:HC71	1.69	0.92
2:b:125:ASP:HB3	2:b:128:THR:HG22	1.50	0.92
27:D:411:LHG:H161	27:D:411:LHG:H322	1.52	0.91
31:f:103:DMS:C1	31:v:206:DMS:H21	2.00	0.91
12:O:133:VAL:HG22	31:O:304:DMS:C2	2.02	0.90
31:B:628:DMS:H12	40:D:502:HOH:O	1.70	0.90
1:A:103:ASP:OD1	31:A:419:DMS:H22	1.73	0.89
2:b:357:ARG:HE	31:d:415:DMS:H22	1.38	0.89
15:V:5:PRO:HD3	31:V:205:DMS:H13	1.54	0.88
3:c:362:ARG:HH11	31:c:924:DMS:C2	1.87	0.86
2:B:347[A]:ARG:NH2	40:B:701:HOH:O	2.09	0.86
31:B:638:DMS:H22	31:D:416:DMS:H11	1.57	0.86
12:O:66:VAL:CG1	12:O:67:PRO:HD2	2.04	0.86
10:K:17:ILE:H	10:K:17:ILE:CD1	1.88	0.85
24:b:618:BCR:HC31	28:b:621:SQD:C7	2.05	0.85
22:c:904:CLA:HBA1	22:c:904:CLA:HBD	1.59	0.85
24:b:620:BCR:H331	24:b:620:BCR:HC8	1.59	0.84
4:D:338:ASN:HB3	40:D:614:HOH:O	1.77	0.83
10:K:17:ILE:HD12	10:K:17:ILE:N	1.93	0.83
27:A:412:LHG:H352	30:I:105:UNL:C3	2.09	0.82
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.61	0.81
1:A:214:MET:HG2	26:A:411:PL9:C10	2.10	0.81
28:C:501:SQD:H381	9:J:22:ILE:HD11	1.63	0.81
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.61	0.80
1:A:304:HIS:HE1	31:V:212:DMS:C1	1.95	0.80
31:o:302:DMS:H11	40:o:473:HOH:O	1.81	0.79
3:c:148:GLY:O	3:c:156:LYS:NZ	2.14	0.79
34:B:623:HTG:H1'1	31:B:635:DMS:H22	1.62	0.79
2:B:360:PRO:HA	31:B:628:DMS:H11	1.65	0.79
31:o:308:DMS:H11	40:u:374:HOH:O	1.82	0.79
13:t:2:GLU:HG2	13:t:6:TYR:CE2	2.18	0.78
24:b:620:BCR:H331	24:b:620:BCR:C8	2.12	0.78
22:A:405:CLA:HMB3	22:A:405:CLA:HBB1	1.67	0.77
4:d:242:GLU:HG3	4:d:244:TYR:O	1.83	0.77
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.65	0.77
14:u:87:VAL:HG11	31:u:205:DMS:H12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:208:THR:O	31:o:305:DMS:C1	2.33	0.77
10:K:19:ASP:HB3	10:K:20:PRO:HD3	1.67	0.76
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.67	0.76
3:C:40:ALA:O	3:C:43:ILE:HG13	1.86	0.76
31:c:925:DMS:H21	15:v:100:ILE:O	1.86	0.76
22:c:903:CLA:H61	22:c:913:CLA:H42	1.66	0.76
15:v:129[B]:LYS:HB3	31:v:210:DMS:S	2.26	0.76
12:O:133:VAL:HG22	31:O:304:DMS:H21	1.66	0.75
1:a:214:MET:CG	26:a:415:PL9:H102	2.13	0.75
14:u:9:LEU:HA	40:u:332:HOH:O	1.87	0.75
1:A:304:HIS:CE1	31:V:212:DMS:H13	2.22	0.75
12:o:208:THR:C	31:o:305:DMS:H13	2.11	0.75
14:u:87:VAL:HG21	31:u:205:DMS:H13	1.67	0.74
27:D:411:LHG:H142	27:D:411:LHG:H331	1.68	0.74
4:D:343[B]:GLU:OE2	34:D:415:HTG:H2	1.87	0.74
29:A:414:LMT:H2B	4:D:304:ARG:HH22	1.53	0.74
27:d:408:LHG:H332	27:d:408:LHG:H141	1.70	0.74
27:D:409:LHG:O9	27:L:101:LHG:HC81	1.88	0.73
2:b:125:ASP:CB	2:b:128:THR:HG22	2.19	0.73
31:B:638:DMS:C2	31:D:416:DMS:H11	2.19	0.73
31:c:933:DMS:H13	15:v:90:GLU:HB2	1.70	0.73
12:O:143:LYS:HE3	31:O:306:DMS:H22	1.71	0.72
2:b:125:ASP:HB3	2:b:128:THR:HG23	1.71	0.72
26:d:405:PL9:C33	27:l:102:LHG:H222	2.19	0.72
15:V:126:LEU:O	15:V:129[A]:LYS:HD2	1.89	0.72
22:B:608:CLA:H203	27:D:409:LHG:H122	1.71	0.72
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.25	0.71
15:V:27:LEU:HD21	31:V:206:DMS:C1	2.20	0.71
2:b:125:ASP:OD2	2:b:128:THR:HG22	1.89	0.71
2:b:299:GLU:HG3	40:b:879:HOH:O	1.89	0.71
22:b:608:CLA:H203	31:l:104:DMS:H21	1.73	0.71
31:O:310:DMS:H11	40:O:427:HOH:O	1.90	0.71
31:O:312:DMS:H22	40:O:467:HOH:O	1.89	0.71
31:B:642:DMS:H11	40:B:853:HOH:O	1.91	0.70
4:d:332:GLN:HG2	31:d:411:DMS:H22	1.72	0.70
1:a:65:GLU:HA	31:a:425:DMS:H12	1.71	0.70
2:b:282:GLN:NE2	40:b:701:HOH:O	2.24	0.70
2:b:383:PHE:CZ	12:o:167:GLY:HA2	2.27	0.70
3:c:362:ARG:HD3	31:c:924:DMS:C2	2.13	0.70
3:C:461:ARG:HG3	40:D:534:HOH:O	1.91	0.70
36:e:101:HEM:HBA2	36:e:101:HEM:HHA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:85:MET:HE2	4:D:90[A]:LEU:HD21	1.74	0.69
12:O:133:VAL:HG22	31:O:304:DMS:H22	1.72	0.69
3:c:138:GLU:HG3	31:c:935:DMS:H12	1.75	0.69
3:c:413:GLU:OE2	40:c:1001:HOH:O	2.11	0.69
31:B:632:DMS:H12	31:B:636:DMS:H22	1.75	0.69
4:D:14:TRP:CD1	34:D:414:HTG:H61	2.28	0.69
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.75	0.68
2:B:446:SER:HB2	2:B:447:PRO:CD	2.22	0.68
36:e:101:HEM:HMC2	6:f:31:ILE:HG13	1.74	0.68
1:A:121[A]:LEU:HD23	25:A:410:LMG:H202	1.74	0.68
2:b:36:SER:OG	24:b:619:BCR:H362	1.93	0.68
18:z:19:MET:HA	18:z:19:MET:HE2	1.74	0.68
4:D:343[A]:GLU:OE2	40:D:501:HOH:O	2.11	0.68
15:V:136:TYR:OH	40:V:301:HOH:O	2.10	0.68
3:C:279:LEU:HD22	22:C:510:CLA:HED2	1.76	0.67
1:A:304:HIS:HE1	31:V:212:DMS:H13	1.58	0.67
2:b:356:VAL:HG23	31:b:638:DMS:H22	1.76	0.67
4:d:338:ASN:O	31:d:415:DMS:H23	1.95	0.67
1:A:304:HIS:CE1	31:V:212:DMS:C1	2.76	0.67
1:a:215:HIS:HA	26:a:415:PL9:O1	1.95	0.67
10:K:16:ALA:O	10:K:19:ASP:HB2	1.94	0.67
7:H:2:ALA:N	40:H:201:HOH:O	2.28	0.67
31:B:640:DMS:H12	7:H:3[B]:ARG:NH2	2.10	0.66
2:b:467:ILE:HG13	4:d:126:MET:CE	2.25	0.66
15:V:27:LEU:HD21	31:V:206:DMS:H11	1.77	0.66
3:C:414:ILE:HD13	31:V:212:DMS:H12	1.77	0.66
11:L:14:ARG:HH22	28:b:621:SQD:H3	1.59	0.66
40:b:829:HOH:O	31:o:304:DMS:H12	1.96	0.66
12:o:178:LYS:HG2	31:o:304:DMS:C2	2.26	0.66
15:v:124:LYS:HE2	40:v:356:HOH:O	1.96	0.66
5:E:68:ASP:O	5:E:72:ALA:HB2	1.96	0.66
31:a:425:DMS:H11	40:o:513:HOH:O	1.95	0.66
27:D:409:LHG:HC12	27:L:101:LHG:O5	1.96	0.65
27:a:423:LHG:HC91	27:l:102:LHG:HC92	1.77	0.65
31:o:308:DMS:C1	40:u:374:HOH:O	2.40	0.65
25:B:621:LMG:H112	25:B:621:LMG:H312	1.79	0.65
31:c:924:DMS:H21	40:c:1006:HOH:O	1.96	0.65
27:D:411:LHG:H331	27:D:411:LHG:C14	2.25	0.65
12:o:178:LYS:HG2	31:o:304:DMS:H21	1.78	0.65
31:c:937:DMS:H21	31:c:942:DMS:H22	1.78	0.64
2:B:25:MET:HE1	2:B:108:PHE:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:177:ALA:O	31:O:312:DMS:H11	1.97	0.64
22:B:605:CLA:H43	22:B:606:CLA:H2	1.80	0.64
18:z:50:LEU:O	18:z:54:VAL:HG23	1.97	0.64
3:c:127:PHE:CE1	29:c:931:LMT:H51	2.32	0.64
22:a:409:CLA:HMB2	22:d:402:CLA:H122	1.80	0.64
3:C:279:LEU:HD12	3:C:282:MET:CE	2.27	0.64
3:C:367:GLU:HB2	31:C:530:DMS:H11	1.78	0.63
17:x:34:ILE:C	17:x:36:LYS:H	2.06	0.63
14:u:87:VAL:HG21	31:u:205:DMS:C1	2.29	0.63
1:a:214:MET:SD	23:a:411:PHO:HED3	2.39	0.63
37:h:101:RRX:H55	37:h:101:RRX:H46	1.81	0.63
14:U:9:LEU:HA	40:U:301:HOH:O	1.98	0.63
3:c:179:ALA:O	3:c:184:GLY:HA2	1.98	0.62
2:b:356:VAL:H	31:b:638:DMS:H22	1.64	0.62
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.80	0.62
1:A:304:HIS:HE1	31:V:212:DMS:H11	1.63	0.62
4:D:85:MET:CE	4:D:96:GLU:HG2	2.28	0.62
3:C:80:PRO:HA	31:C:527:DMS:H22	1.82	0.62
31:c:925:DMS:C2	15:v:100:ILE:O	2.48	0.62
2:B:350:GLU:HG3	31:B:631:DMS:C1	2.30	0.62
5:e:68:ASP:O	5:e:72:ALA:HB2	1.99	0.62
12:O:74[A]:GLU:OE2	40:O:401:HOH:O	2.16	0.62
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.82	0.61
22:c:904:CLA:HBA1	22:c:904:CLA:CBD	2.29	0.61
1:a:183:MET:HA	22:a:407:CLA:HMD1	1.82	0.61
12:o:177:ALA:O	31:o:307:DMS:H11	2.00	0.61
26:A:411:PL9:H403	6:F:22:ALA:HB2	1.82	0.61
2:B:276:ASP:OD1	31:B:641:DMS:H23	2.00	0.61
5:e:22:ILE:O	5:e:25:ILE:HG22	2.01	0.61
12:o:102:ASP:OD1	12:o:123:LYS:NZ	2.32	0.61
1:A:265:PHE:HE2	26:A:411:PL9:H122	1.64	0.61
15:V:5:PRO:CD	31:V:205:DMS:H13	2.26	0.61
1:A:215:HIS:HA	26:A:411:PL9:O1	2.01	0.60
5:E:20:TRP:CD1	9:J:8:ILE:HD13	2.35	0.60
6:f:15:ILE:HG23	6:f:15:ILE:O	2.01	0.60
34:D:415:HTG:H3	15:V:55:ARG:HH12	1.66	0.60
37:h:101:RRX:H46	37:h:101:RRX:C33	2.32	0.60
2:b:25:MET:HE1	2:b:108:PHE:CD2	2.36	0.60
12:o:18:LYS:HE3	40:o:490:HOH:O	2.01	0.60
31:B:638:DMS:H22	31:D:416:DMS:C1	2.32	0.60
2:b:356:VAL:H	31:b:638:DMS:C2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:429:SER:HB3	35:c:918:DGD:HBT2	1.83	0.60
31:a:425:DMS:H21	40:o:500:HOH:O	2.01	0.59
2:b:378:LYS:HE3	31:b:636:DMS:H23	1.84	0.59
31:o:308:DMS:H12	14:u:9:LEU:HD21	1.83	0.59
25:D:412:LMG:H352	34:D:414:HTG:H6'2	1.84	0.59
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.85	0.59
12:O:216:GLU:CD	12:O:234:LYS:HD2	2.28	0.59
22:D:401:CLA:HMB1	22:D:401:CLA:HBB1	1.85	0.59
1:A:223:LEU:HD22	4:D:265:ARG:HG2	1.84	0.59
22:B:606:CLA:C14	22:B:611:CLA:HED2	2.33	0.58
26:D:406:PL9:C32	27:L:101:LHG:H223	2.32	0.58
12:O:47:PRO:HG3	12:O:120:PHE:CE1	2.38	0.58
1:a:270:SER:HB2	28:a:414:SQD:O49	2.03	0.58
22:b:615:CLA:HED3	11:l:8:GLN:O	2.04	0.58
7:h:3[A]:ARG:HH11	7:h:3[A]:ARG:HB2	1.69	0.58
24:c:916:BCR:C3	8:i:23:PHE:HB3	2.33	0.58
7:h:3[A]:ARG:HB2	7:h:3[A]:ARG:NH1	2.17	0.58
4:D:49:LEU:HD21	25:J:101:LMG:H341	1.84	0.58
14:U:92:VAL:HG21	31:U:203:DMS:H21	1.84	0.58
31:c:940:DMS:H11	40:c:1203:HOH:O	2.03	0.58
25:d:409:LMG:HC71	25:d:409:LMG:HO2	1.66	0.57
2:B:137:LYS:O	2:B:141:ILE:HG13	2.04	0.57
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.85	0.57
22:b:606:CLA:HHC	22:b:606:CLA:HBB1	1.86	0.57
2:B:223:GLN:NE2	40:B:703:HOH:O	2.37	0.57
3:c:38:GLY:HA3	22:c:912:CLA:HMD2	1.85	0.57
37:h:101:RRX:C23	37:h:101:RRX:H17	2.33	0.57
15:v:78:ASN:OD1	15:v:96:ARG:NH1	2.33	0.57
27:D:409:LHG:HC92	27:L:101:LHG:HC92	1.86	0.57
31:a:425:DMS:H11	12:o:152:ARG:HH21	1.70	0.57
24:b:620:BCR:HC8	24:b:620:BCR:C33	2.34	0.57
4:d:192:THR:HG23	22:d:402:CLA:HBC2	1.86	0.57
24:A:409:BCR:H401	31:A:419:DMS:H12	1.87	0.57
29:A:414:LMT:H2B	4:D:304:ARG:NH2	2.18	0.57
3:c:156:LYS:HE2	31:c:939:DMS:H12	1.87	0.57
12:O:39:ARG:HD3	40:O:413:HOH:O	2.04	0.56
31:O:310:DMS:C1	40:O:427:HOH:O	2.52	0.56
4:d:85:MET:CE	4:d:96:GLU:HG2	2.33	0.56
1:a:200:LEU:HD23	35:c:919:DGD:HAE1	1.87	0.56
2:b:29:LEU:HD11	24:b:618:BCR:H12C	1.87	0.56
26:A:411:PL9:H221	23:D:402:PHO:HMA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:411:PHO:HHD	23:a:411:PHO:HBC2	1.87	0.56
31:b:638:DMS:C1	40:b:867[B]:HOH:O	2.53	0.56
1:a:322:ASN:OD1	3:c:412:THR:HA	2.06	0.56
1:a:200:LEU:CD2	35:c:919:DGD:HAE1	2.36	0.56
1:a:329:GLU:HG3	40:a:617:HOH:O	2.04	0.56
2:B:248:ALA:HB2	22:B:604:CLA:H51	1.87	0.56
34:D:415:HTG:C3	15:V:55:ARG:HH12	2.19	0.56
4:d:90[B]:LEU:HG	4:d:109:GLY:HA2	1.87	0.56
5:e:13:ILE:HG21	36:e:101:HEM:HAD2	1.88	0.56
12:O:39:ARG:NH1	40:O:404:HOH:O	2.39	0.56
2:b:125:ASP:CG	2:b:128:THR:HG22	2.30	0.56
22:c:911:CLA:H192	22:c:911:CLA:HBC3	1.87	0.56
22:b:609:CLA:H203	22:b:610:CLA:H191	1.87	0.56
12:O:145:GLU:CB	31:O:303:DMS:H21	2.36	0.56
29:B:622:LMT:H11	25:D:412:LMG:HC92	1.88	0.55
15:v:4:THR:HG22	31:v:205:DMS:H23	1.88	0.55
15:V:27:LEU:HD21	31:V:206:DMS:H12	1.87	0.55
29:a:419:LMT:H6'1	4:d:304:ARG:HH22	1.72	0.55
9:j:18:GLY:HA3	24:y:101:BCR:H371	1.87	0.55
12:O:58:ASN:HB3	2:b:339:ALA:HB2	1.89	0.55
10:k:21:LEU:HB2	16:y:24:MET:HE2	1.88	0.55
24:C:515:BCR:H331	24:C:515:BCR:C8	2.36	0.55
16:Y:20:ALA:O	16:Y:24:MET:HG2	2.07	0.55
2:b:125:ASP:CB	2:b:128:THR:CG2	2.73	0.55
40:b:704:HOH:O	31:o:304:DMS:H13	2.06	0.55
2:B:350:GLU:HG3	31:B:631:DMS:H11	1.88	0.55
40:b:910:HOH:O	31:d:415:DMS:H11	2.05	0.55
22:B:611:CLA:HHC	22:B:611:CLA:HBB1	1.87	0.55
2:b:281:GLN:NE2	40:b:702:HOH:O	2.39	0.55
22:b:608:CLA:H2	25:b:622:LMG:H151	1.89	0.55
3:c:126:GLY:O	3:c:130:VAL:HG23	2.07	0.55
8:I:13:THR:O	8:I:17:LEU:HG	2.07	0.55
15:V:129[B]:LYS:HB3	31:V:212:DMS:S	2.47	0.55
1:A:183:MET:HA	22:A:405:CLA:HMD1	1.88	0.55
31:A:420:DMS:H12	40:A:559:HOH:O	2.06	0.55
10:K:20:PRO:HB3	16:Y:21:GLN:HG3	1.88	0.55
2:b:63:LEU:N	2:b:64:PRO:HD2	2.21	0.55
36:e:101:HEM:CMC	6:f:31:ILE:HG13	2.37	0.55
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.88	0.55
2:B:389:LYS:NZ	34:D:415:HTG:H2'2	2.22	0.54
27:D:411:LHG:H161	27:D:411:LHG:C32	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:408:LHG:H132	27:d:408:LHG:H341	1.89	0.54
1:A:265:PHE:CE2	26:A:411:PL9:H122	2.42	0.54
35:c:918:DGD:HAT2	35:c:919:DGD:HBN2	1.88	0.54
2:b:324:LEU:HA	4:d:293[B]:LEU:HG	1.89	0.54
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.90	0.54
2:b:128:THR:HG23	2:b:130:GLU:H	1.72	0.54
25:d:409:LMG:H221	7:h:35:MET:HE2	1.89	0.54
28:A:413:SQD:H272	2:b:109:LEU:HD13	1.90	0.54
22:b:611:CLA:H152	22:b:611:CLA:OBD	2.07	0.54
28:C:501:SQD:H302	22:C:509:CLA:H71	1.90	0.54
25:D:412:LMG:O9	25:D:412:LMG:O2	2.19	0.54
12:O:66:VAL:CG1	12:O:67:PRO:CD	2.83	0.54
22:B:608:CLA:H191	26:D:406:PL9:H303	1.89	0.54
13:T:2:GLU:HG2	13:T:6:TYR:CE2	2.43	0.54
9:J:18:GLY:O	9:J:22:ILE:HD12	2.08	0.54
12:O:179:GLU:HG3	31:O:312:DMS:H12	1.90	0.54
3:c:191:PRO:O	40:c:1002:HOH:O	2.18	0.54
12:o:55:GLU:OE2	12:o:231:HIS:CD2	2.61	0.54
4:D:11:GLU:O	4:D:12:ARG:CB	2.56	0.53
1:a:334:ARG:HD3	4:d:320:LEU:HD13	1.89	0.53
24:c:916:BCR:HC32	8:i:23:PHE:HB3	1.88	0.53
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.89	0.53
25:d:409:LMG:O2	25:d:409:LMG:C7	2.51	0.53
2:B:314:TYR:CE1	2:B:316:GLY:HA3	2.43	0.53
22:C:505:CLA:H112	35:C:519:DGD:HBF1	1.89	0.53
24:C:516:BCR:H331	24:C:516:BCR:C8	2.39	0.53
27:a:423:LHG:C18	22:b:608:CLA:C14	2.87	0.53
4:d:272:LEU:C	4:d:272:LEU:HD23	2.32	0.53
31:f:103:DMS:H12	31:v:206:DMS:C2	2.25	0.53
15:v:129[A]:LYS:HB3	31:v:210:DMS:S	2.48	0.53
29:B:622:LMT:H11	25:D:412:LMG:C9	2.39	0.53
27:a:423:LHG:O9	27:l:102:LHG:HC81	2.07	0.53
2:b:467:ILE:HG13	4:d:126:MET:HE2	1.89	0.53
17:X:23:LEU:O	17:X:27:VAL:HG23	2.08	0.53
14:u:58:VAL:HG12	14:u:79:LEU:HD22	1.91	0.53
1:A:221:SER:HB2	4:D:139:ARG:O	2.09	0.53
18:z:9:LEU:HD13	18:z:54:VAL:HG11	1.90	0.53
27:D:410:LHG:H171	27:L:101:LHG:H201	1.91	0.53
15:V:126:LEU:O	15:V:129[A]:LYS:CD	2.56	0.53
4:D:272:LEU:C	4:D:272:LEU:HD23	2.34	0.53
30:U:201:UNL:C4	40:U:346:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.43	0.53
2:b:355:PHE:O	2:b:370:LEU:HA	2.08	0.53
22:b:603:CLA:H201	35:h:102:DGD:HBT1	1.91	0.53
35:c:917:DGD:HA82	25:i:101:LMG:H211	1.91	0.53
14:U:38:TYR:HB2	14:U:41:LEU:HD12	1.91	0.52
22:b:616:CLA:H161	7:h:7:LEU:HD21	1.90	0.52
4:D:85:MET:CE	4:D:90[A]:LEU:HD21	2.38	0.52
2:b:41:GLU:HB3	2:b:60:MET:SD	2.50	0.52
8:i:33:LYS:O	8:i:35:LYS:HG3	2.09	0.52
22:B:614:CLA:HBB1	22:B:614:CLA:HMB1	1.91	0.52
3:C:28:GLN:NE2	28:C:501:SQD:O7	2.36	0.52
22:C:505:CLA:H42	35:C:518:DGD:HB42	1.91	0.52
12:O:158:ASP:HB2	12:O:159:PRO:CD	2.39	0.52
1:a:266:ASN:HD22	4:d:237:PRO:HG3	1.74	0.52
22:b:605:CLA:H43	22:b:606:CLA:H2	1.91	0.52
22:b:609:CLA:HMB2	4:d:126:MET:HG2	1.91	0.52
36:e:101:HEM:HBA2	36:e:101:HEM:CHA	2.38	0.52
1:a:287:ALA:HA	22:a:407:CLA:CED	2.40	0.52
22:A:405:CLA:HBB1	22:A:405:CLA:CMB	2.38	0.52
22:c:904:CLA:HAB	22:c:913:CLA:H41	1.91	0.52
5:e:7:GLU:HG2	6:f:19:ARG:CZ	2.39	0.52
31:c:927:DMS:H11	15:v:99:ASP:O	2.10	0.52
34:D:415:HTG:H7'3	14:U:37:GLN:HE22	1.74	0.52
12:O:145:GLU:HB2	31:O:303:DMS:H21	1.91	0.52
4:d:123:ILE:HD11	35:h:102:DGD:HAW1	1.91	0.52
31:b:638:DMS:H13	40:b:867[B]:HOH:O	2.08	0.52
22:C:514:CLA:C4B	24:C:515:BCR:H383	2.40	0.52
22:a:408:CLA:HED1	26:d:405:PL9:H371	1.92	0.52
12:o:40:ILE:HD12	12:o:95:PHE:CD2	2.44	0.52
29:a:419:LMT:C6B	4:d:304:ARG:HH22	2.22	0.51
3:c:134:ILE:HD12	22:c:912:CLA:H43	1.92	0.51
6:f:45:ARG:HG2	31:f:103:DMS:O	2.09	0.51
27:d:407:LHG:HC62	11:l:15:THR:HG23	1.92	0.51
2:b:451:PHE:CD1	2:b:451:PHE:C	2.89	0.51
3:c:205:ASP:OD2	3:c:207:ARG:NH1	2.43	0.51
12:o:39:ARG:HG3	12:o:246:ALA:HB2	1.92	0.51
1:A:63:ILE:HB	3:C:335:THR:HG21	1.92	0.51
22:B:608:CLA:H193	4:D:281:MET:SD	2.50	0.51
4:D:343[B]:GLU:CD	34:D:415:HTG:H2	2.36	0.51
8:I:12:VAL:O	8:I:16:VAL:HG23	2.11	0.51
35:c:919:DGD:HA32	25:j:101:LMG:H111	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ARG:HG3	7:H:20:LYS:HG2	1.93	0.51
31:c:933:DMS:H12	15:v:91:VAL:HG22	1.93	0.51
22:b:602:CLA:C9	37:h:101:RRX:H25	2.40	0.51
34:D:415:HTG:H62	40:V:301:HOH:O	2.11	0.51
2:B:128:THR:HB	2:B:130:GLU:H	1.75	0.51
3:C:143:TYR:HE2	34:C:532:HTG:H61	1.76	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
3:c:159:THR:HG21	31:c:939:DMS:H21	1.92	0.51
22:c:910:CLA:HMB1	22:c:910:CLA:HBB1	1.93	0.51
4:d:332:GLN:HG2	31:d:411:DMS:C2	2.40	0.51
22:d:403:CLA:H192	17:x:15:LEU:HB2	1.93	0.51
24:k:101:BCR:H331	24:k:101:BCR:C8	2.40	0.51
3:C:147:PHE:CD2	22:C:514:CLA:H3A	2.46	0.51
15:v:2:GLU:HG3	31:v:205:DMS:H12	1.93	0.51
3:C:223:TRP:CG	3:C:224:ILE:H	2.29	0.50
14:u:45:LEU:HD21	14:u:71:GLN:HB3	1.94	0.50
16:y:34:MET:HA	16:y:34:MET:HE2	1.93	0.50
2:B:121:GLU:HA	7:H:2:ALA:HB1	1.93	0.50
2:b:299:GLU:HG2	2:b:402:TYR:HD1	1.75	0.50
3:C:334:PRO:HA	12:O:153:THR:OG1	2.11	0.50
31:b:630:DMS:H11	14:u:17:LEU:CD2	2.42	0.50
24:d:404:BCR:H331	24:d:404:BCR:C8	2.42	0.50
29:A:414:LMT:H12	34:b:623:HTG:H5	1.93	0.50
2:B:115:TRP:CD2	24:B:618:BCR:HC21	2.47	0.50
3:C:60:ILE:HG22	22:C:504:CLA:HHD	1.94	0.50
12:O:133:VAL:HG13	31:O:304:DMS:H21	1.93	0.50
1:A:223:LEU:CD2	4:D:265:ARG:HG2	2.42	0.50
2:b:357:ARG:NE	31:d:415:DMS:H22	2.18	0.50
22:b:614:CLA:HMB1	22:b:614:CLA:HBB1	1.94	0.50
10:k:25:LEU:N	10:k:26:PRO:CD	2.75	0.50
12:o:103:PHE:HA	12:o:120:PHE:O	2.12	0.50
29:A:414:LMT:H32	2:b:43:ALA:HA	1.93	0.49
22:b:609:CLA:H111	4:d:120:PHE:CE1	2.48	0.49
3:c:400:PRO:C	3:c:401:LEU:HD12	2.37	0.49
22:b:606:CLA:HHC	22:b:606:CLA:CBB	2.42	0.49
24:d:404:BCR:C40	9:j:25:VAL:HG21	2.42	0.49
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.47	0.49
18:Z:62:VAL:C	40:Z:203:HOH:O	2.55	0.49
27:a:423:LHG:H372	22:b:614:CLA:H43	1.94	0.49
2:B:495:PHE:C	2:B:496:TYR:HD1	2.21	0.49
2:b:446:SER:HB2	2:b:447:PRO:CD	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:202:DMS:H12	31:u:205:DMS:H22	1.95	0.49
3:C:180:MET:HG2	3:C:199:ILE:O	2.12	0.49
2:b:221:PRO:HA	22:b:610:CLA:HED3	1.93	0.49
16:y:38:LEU:O	16:y:42:ARG:HG2	2.13	0.49
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.49
35:C:519:DGD:HBN1	27:D:411:LHG:H222	1.95	0.49
3:c:174:LEU:HB3	22:c:903:CLA:H161	1.94	0.49
22:c:904:CLA:HMB1	22:c:904:CLA:HBB1	1.93	0.49
22:B:606:CLA:HBB1	22:B:607:CLA:C5	2.43	0.49
3:C:308:GLU:HB2	3:C:361:PHE:CE2	2.47	0.49
12:O:129:THR:HA	12:O:141:ASP:O	2.13	0.49
2:b:62:VAL:HB	22:b:606:CLA:HED3	1.95	0.49
1:A:237:TYR:CB	4:D:265:ARG:HD2	2.43	0.49
22:B:608:CLA:HMB1	22:B:608:CLA:HBB1	1.94	0.49
26:a:415:PL9:H403	6:f:22:ALA:HB2	1.95	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.48
29:a:419:LMT:H6'1	4:d:304:ARG:NH2	2.28	0.48
22:b:615:CLA:OBD	11:l:10:VAL:CG2	2.61	0.48
1:A:121[B]:LEU:HD11	22:C:506:CLA:H152	1.94	0.48
26:A:411:PL9:H272	26:A:411:PL9:H251	1.66	0.48
34:B:623:HTG:H1	29:a:419:LMT:H21	1.95	0.48
31:B:638:DMS:H11	40:B:778:HOH:O	2.13	0.48
3:C:50:LEU:HD12	22:C:513:CLA:HMD2	1.94	0.48
26:D:406:PL9:H401	11:L:29:LEU:HD23	1.94	0.48
3:c:31:SER:CB	3:c:41:ARG:HG2	2.44	0.48
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.96	0.48
26:A:411:PL9:H301	4:D:45:LEU:HD22	1.96	0.48
29:a:419:LMT:C11	29:t:101:LMT:H122	2.43	0.48
27:a:423:LHG:C18	22:b:608:CLA:H141	2.43	0.48
4:d:267:LEU:C	4:d:267:LEU:HD23	2.38	0.48
37:H:101:RRX:H55	37:H:101:RRX:H46	1.95	0.48
35:c:917:DGD:HA71	25:i:101:LMG:H361	1.96	0.48
1:A:249:VAL:HG12	2:B:491:VAL:HG23	1.95	0.48
3:C:117:VAL:HG12	25:C:531:LMG:H222	1.95	0.48
23:a:410:PHO:HED2	4:d:257:PHE:CD2	2.49	0.48
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.95	0.48
12:o:193:THR:HG21	12:o:220:LEU:HD12	1.94	0.48
15:v:72:LEU:HD12	15:v:120:LEU:HD11	1.95	0.48
1:a:131:TRP:CH2	22:c:906:CLA:HAA2	2.49	0.48
12:o:114:GLU:OE1	31:o:303:DMS:H12	2.13	0.48
40:B:878:HOH:O	31:O:311:DMS:H13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:LEU:HB3	22:C:503:CLA:H161	1.95	0.48
27:D:410:LHG:H192	13:T:17:PHE:HZ	1.79	0.48
31:V:207:DMS:H23	40:V:380:HOH:O	2.14	0.48
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.48
4:d:73:PHE:CZ	25:j:101:LMG:H182	2.49	0.48
18:z:23:VAL:HG22	18:z:40:ILE:HG12	1.95	0.48
29:a:419:LMT:O2B	29:t:101:LMT:H6E	2.13	0.48
22:B:610:CLA:H42	25:D:412:LMG:H171	1.95	0.47
3:C:461:ARG:HD2	4:D:225:ASP:OD1	2.14	0.47
2:b:162:PHE:O	22:b:607:CLA:HHD	2.14	0.47
3:c:45:LEU:HD12	22:c:912:CLA:HED3	1.96	0.47
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.95	0.47
16:y:42:ARG:HD2	18:z:29:SER:OG	2.13	0.47
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.49	0.47
31:B:633:DMS:H22	4:D:140:PRO:HD2	1.96	0.47
27:a:416:LHG:H122	27:a:416:LHG:H242	1.97	0.47
2:b:462:PHE:CE1	22:b:614:CLA:HMB3	2.49	0.47
4:d:236:ASN:O	4:d:239:GLN:HG2	2.14	0.47
7:h:38:PHE:HB2	37:h:101:RRX:C10	2.43	0.47
12:o:55:GLU:OE2	12:o:231:HIS:HD2	1.96	0.47
1:A:304:HIS:CE1	31:V:212:DMS:H11	2.46	0.47
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.50	0.47
2:b:25:MET:HE3	24:b:618:BCR:C5	2.44	0.47
22:b:604:CLA:H18	22:b:610:CLA:H91	1.96	0.47
22:b:609:CLA:H142	7:h:39:LEU:HD21	1.97	0.47
3:c:202:PRO:HB3	3:c:234:VAL:HG12	1.96	0.47
24:c:916:BCR:HC31	8:i:23:PHE:HB3	1.96	0.47
14:u:27:LEU:HD22	14:u:49:ILE:HG21	1.96	0.47
3:C:414:ILE:HD13	31:V:212:DMS:C1	2.44	0.47
17:x:34:ILE:O	17:x:36:LYS:N	2.35	0.47
2:B:13:ILE:O	31:B:630:DMS:H11	2.14	0.47
2:B:228:ALA:HB2	29:B:622:LMT:H21	1.96	0.47
7:h:28:THR:HB	7:h:29:PRO:HD3	1.97	0.47
12:o:47:PRO:HG3	12:o:120:PHE:CE1	2.50	0.47
1:A:223:LEU:HD12	4:D:139:ARG:HH12	1.79	0.47
24:B:618:BCR:H331	24:B:618:BCR:C8	2.43	0.47
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.96	0.47
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.96	0.47
22:D:401:CLA:HBC2	22:D:401:CLA:CMC	2.45	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
24:Y:101:BCR:H312	18:Z:16:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.80	0.47
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.47
6:f:17:THR:HA	28:f:101:SQD:H62	1.97	0.47
31:B:638:DMS:C1	40:B:778:HOH:O	2.63	0.47
1:a:100:ALA:HB2	31:a:401:DMS:H12	1.97	0.47
18:Z:47:TRP:CD2	29:Z:101:LMT:H111	2.50	0.47
1:a:204:GLY:N	28:a:414:SQD:H221	2.30	0.47
1:A:270:SER:HB2	28:C:501:SQD:O49	2.16	0.47
1:a:257:ARG:O	4:d:128:ARG:NH2	2.48	0.47
24:k:101:BCR:H24C	24:k:101:BCR:H371	1.75	0.47
1:A:73:TYR:CD1	29:A:414:LMT:H3B	2.50	0.46
1:A:237:TYR:HD2	1:A:245:THR:HB	1.78	0.46
4:D:52:THR:HB	4:D:76:VAL:CG2	2.45	0.46
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.97	0.46
12:O:180:GLU:CD	12:O:180:GLU:H	2.24	0.46
31:b:630:DMS:H11	14:u:17:LEU:HD21	1.96	0.46
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.15	0.46
4:D:343[B]:GLU:HG3	40:V:301:HOH:O	2.14	0.46
27:D:411:LHG:H162	27:D:411:LHG:H111	1.96	0.46
1:a:29:TYR:CE1	1:a:31:GLY:HA3	2.50	0.46
22:c:908:CLA:H141	22:c:908:CLA:H161	1.70	0.46
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.98	0.46
22:C:507:CLA:HMC2	22:C:508:CLA:H102	1.96	0.46
4:D:178:ILE:O	4:D:181:PHE:HB3	2.15	0.46
2:b:276:ASP:O	31:b:629:DMS:H22	2.16	0.46
3:c:397:THR:HA	31:v:201:DMS:H13	1.97	0.46
3:C:368:PRO:HD3	31:C:530:DMS:H21	1.96	0.46
22:C:505:CLA:H201	27:D:411:LHG:C34	2.46	0.46
22:C:511:CLA:H192	22:C:511:CLA:HBC3	1.98	0.46
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.45	0.46
2:b:357:ARG:HE	31:d:415:DMS:C2	2.18	0.46
2:b:450:TRP:CZ3	4:d:293[B]:LEU:HD21	2.51	0.46
22:C:509:CLA:C2B	22:C:511:CLA:HBA1	2.45	0.46
22:C:513:CLA:C11	22:C:514:CLA:H141	2.46	0.46
15:V:79:PRO:HD3	15:V:94:SER:HB3	1.97	0.46
28:a:414:SQD:H361	24:y:101:BCR:H392	1.98	0.46
2:b:216:HIS:HE1	22:b:610:CLA:C1A	2.29	0.46
2:B:25:MET:HE1	2:B:108:PHE:HD2	1.77	0.46
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.46
22:C:503:CLA:H61	22:C:513:CLA:H42	1.98	0.46
22:C:513:CLA:H92	22:C:514:CLA:H203	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:11:PHE:O	17:X:15[A]:LEU:HG	2.16	0.46
22:C:505:CLA:H191	27:D:411:LHG:C34	2.46	0.46
4:D:55:VAL:O	4:D:66:SER:HB3	2.15	0.46
4:D:162:LEU:HD21	35:H:102:DGD:HA21	1.97	0.46
31:a:425:DMS:C1	12:o:152:ARG:NH2	2.79	0.46
3:c:406:SER:HA	3:c:420:VAL:HG23	1.98	0.46
31:c:940:DMS:H13	40:c:1150:HOH:O	2.15	0.46
37:h:101:RRX:H47	37:h:101:RRX:H48	1.77	0.46
2:B:350:GLU:HG3	31:B:631:DMS:S	2.56	0.46
1:a:269:ARG:HD2	4:d:235:PHE:HB2	1.98	0.46
2:b:406:LEU:O	2:b:409:GLN:HG3	2.16	0.45
34:b:623:HTG:O4	31:b:633:DMS:H21	2.16	0.45
4:D:39:PRO:O	4:D:43:LEU:HG	2.17	0.45
18:Z:1:MET:HE3	18:Z:60:PHE:CD1	2.50	0.45
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.97	0.45
2:b:186:GLY:HA3	40:b:839:HOH:O	2.14	0.45
22:b:602:CLA:H151	22:b:602:CLA:H203	1.98	0.45
12:o:184:ARG:HD2	31:o:308:DMS:H22	1.99	0.45
10:K:21:LEU:HD13	16:Y:24:MET:HE2	1.99	0.45
28:a:414:SQD:H271	27:d:408:LHG:H151	1.98	0.45
3:c:95:LEU:HD21	22:c:902:CLA:OBD	2.15	0.45
3:c:154:LYS:HG2	3:c:266:TRP:CE3	2.52	0.45
3:c:257:PHE:CZ	31:c:934:DMS:H11	2.52	0.45
2:B:162:PHE:O	22:B:607:CLA:HHD	2.17	0.45
22:B:607:CLA:H102	22:B:607:CLA:H61	1.61	0.45
12:O:145:GLU:HB3	31:O:303:DMS:H21	1.99	0.45
26:a:415:PL9:H371	26:a:415:PL9:H351	1.60	0.45
22:b:602:CLA:H161	37:h:101:RRX:C16	2.47	0.45
3:c:203:THR:O	3:c:235:GLY:HA3	2.15	0.45
12:o:93:LEU:O	12:o:128:SER:HA	2.16	0.45
15:v:129[B]:LYS:HE3	15:v:136:TYR:O	2.16	0.45
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.51	0.45
3:C:443:TRP:CZ2	22:C:509:CLA:HMD1	2.52	0.45
22:C:514:CLA:NB	24:C:515:BCR:H383	2.31	0.45
15:V:30:LYS:HG3	15:V:118:HIS:CE1	2.52	0.45
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.46	0.45
12:O:92:SER:HB3	12:O:131:PRO:HA	1.99	0.45
9:j:26:GLY:HA2	30:j:103:UNL:C10	2.47	0.45
12:O:218:GLU:HG3	31:O:306:DMS:H13	1.98	0.45
23:a:410:PHO:ND	23:a:410:PHO:NC	2.64	0.45
4:d:332:GLN:HA	31:d:411:DMS:H23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.97	0.45
12:o:110:MET:HE2	31:o:303:DMS:H23	1.99	0.45
3:C:294:ASN:HA	3:C:297:TYR:O	2.17	0.45
4:D:79:SER:HA	4:D:172:SER:HB3	1.97	0.45
26:D:406:PL9:H322	27:L:101:LHG:H223	1.98	0.45
5:E:20:TRP:HD1	9:J:8:ILE:HD13	1.82	0.45
22:b:612:CLA:HBB1	22:b:612:CLA:HMB3	1.98	0.45
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.97	0.45
26:d:405:PL9:H411	11:l:29:LEU:CD2	2.47	0.45
10:k:20:PRO:HB3	16:y:21:GLN:HG3	1.99	0.45
2:B:360:PRO:CA	31:B:628:DMS:H11	2.43	0.45
22:B:606:CLA:HBB1	22:B:607:CLA:H51	1.99	0.45
4:D:52:THR:HB	4:D:76:VAL:HG21	1.97	0.45
12:O:86:LYS:HE3	40:O:549:HOH:O	2.15	0.45
2:b:346:PHE:HD2	31:b:638:DMS:H23	1.81	0.45
22:b:609:CLA:C14	7:h:39:LEU:HD21	2.46	0.45
3:c:443:TRP:CZ2	22:c:909:CLA:HMD1	2.52	0.45
24:c:915:BCR:C8	24:c:915:BCR:H331	2.44	0.45
14:u:53:ALA:HB1	14:u:54:PRO:HA	1.98	0.45
17:x:34:ILE:C	17:x:36:LYS:N	2.74	0.45
4:D:266:TRP:CG	27:D:410:LHG:HC2	2.51	0.45
24:c:916:BCR:H15C	24:c:916:BCR:H351	1.75	0.45
22:B:611:CLA:HHC	22:B:611:CLA:CBB	2.46	0.44
3:C:318:LEU:C	3:C:318:LEU:HD23	2.42	0.44
22:C:507:CLA:CMB	22:C:507:CLA:HBB1	2.47	0.44
15:V:41:HIS:HA	15:V:45:ILE:O	2.17	0.44
17:X:23:LEU:C	17:X:23:LEU:HD12	2.41	0.44
3:c:189:TRP:CE3	31:c:929:DMS:H21	2.52	0.44
12:o:180:GLU:CD	12:o:180:GLU:H	2.25	0.44
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.99	0.44
15:V:2:GLU:OE2	31:V:207:DMS:H12	2.16	0.44
3:c:154:LYS:NZ	40:c:1012:HOH:O	2.44	0.44
27:d:408:LHG:H342	27:d:408:LHG:H312	1.72	0.44
22:B:612:CLA:H112	22:B:612:CLA:H72	1.68	0.44
22:a:408:CLA:HBA1	22:a:408:CLA:C4A	2.47	0.44
23:a:411:PHO:CMB	23:a:411:PHO:HBB1	2.46	0.44
3:c:362:ARG:CD	31:c:924:DMS:H22	2.22	0.44
27:d:408:LHG:H111	27:d:408:LHG:H142	1.65	0.44
2:B:118:TRP:CZ2	11:L:4:ASN:HA	2.52	0.44
15:V:118:HIS:CE1	15:V:122:GLU:HG2	2.53	0.44
4:d:52:THR:O	4:d:66:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:620:BCR:H331	24:B:620:BCR:C8	2.48	0.44
3:C:68:THR:OG1	22:C:504:CLA:HED1	2.17	0.44
3:C:266:TRP:CZ3	22:C:508:CLA:HAC2	2.52	0.44
25:C:520:LMG:H241	9:J:22:ILE:HG12	1.99	0.44
25:C:531:LMG:HC1	25:C:531:LMG:HC8	1.77	0.44
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.99	0.44
5:E:39:SER:HB3	29:E:101:LMT:H6E	1.99	0.44
12:o:110:MET:HE3	12:o:110:MET:HB3	1.88	0.44
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.84	0.44
3:C:464:GLU:OE2	4:D:245:SER:OG	2.30	0.44
31:C:527:DMS:H11	15:V:102:PRO:HG2	2.00	0.44
4:D:24:ARG:NH2	17:X:35:ASP:OD2	2.51	0.44
5:E:60:GLN:NE2	5:E:62:SER:O	2.49	0.44
12:O:97:GLU:OE2	12:O:102:ASP:OD2	2.36	0.44
15:V:41:HIS:O	15:V:42:VAL:C	2.61	0.44
22:c:902:CLA:HBB2	22:c:908:CLA:H92	2.00	0.44
4:D:24:ARG:HH2	17:X:35:ASP:CG	2.26	0.44
12:O:133:VAL:CG2	31:O:304:DMS:H21	2.42	0.44
2:b:237:VAL:HG11	22:b:611:CLA:H201	1.98	0.44
22:b:602:CLA:H91	37:h:101:RRX:H25	1.99	0.44
22:A:408:CLA:H203	22:C:507:CLA:H101	2.00	0.44
2:B:226:TYR:HA	2:B:231:MET:HG3	1.99	0.44
2:B:339:ALA:HB2	12:o:58:ASN:HB3	2.00	0.44
2:B:423:LYS:HZ2	31:O:311:DMS:H22	1.83	0.44
22:B:606:CLA:H141	22:B:611:CLA:HED2	1.98	0.44
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.48	0.44
2:b:86:ILE:C	2:b:86:ILE:HD12	2.43	0.44
22:b:612:CLA:H72	22:b:612:CLA:H112	1.68	0.44
31:u:202:DMS:H23	31:u:203:DMS:H22	1.98	0.44
2:B:315:ILE:HG22	2:B:426:PHE:HB3	2.00	0.44
2:B:350:GLU:CG	31:B:631:DMS:H11	2.48	0.44
22:B:603:CLA:H41	7:H:46:LEU:HA	1.98	0.44
22:B:606:CLA:H122	22:B:611:CLA:HMA2	2.00	0.44
3:C:348:GLU:OE2	12:O:11:VAL:HA	2.17	0.44
28:C:501:SQD:H111	27:C:522:LHG:H261	2.00	0.44
37:H:101:RRX:H43	37:H:101:RRX:H47	1.77	0.44
15:V:2:GLU:OE2	31:V:207:DMS:C1	2.66	0.44
34:b:632:HTG:H1	40:v:315:HOH:O	2.18	0.44
22:c:904:CLA:H101	22:c:904:CLA:H62	1.80	0.44
7:h:43:LEU:O	7:h:47:GLU:HG3	2.18	0.44
1:A:308:ASP:OD1	1:A:308:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:433:ASP:OD1	2:b:433:ASP:C	2.60	0.43
35:c:917:DGD:HAH2	35:c:917:DGD:HAT2	1.87	0.43
7:h:3[A]:ARG:HH11	7:h:3[A]:ARG:CB	2.31	0.43
8:i:36:ASP:HB3	31:i:106:DMS:H13	2.00	0.43
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.99	0.43
22:A:406:CLA:HMB2	23:D:402:PHO:H152	2.01	0.43
22:B:606:CLA:CMA	22:B:607:CLA:HMA2	2.48	0.43
28:C:501:SQD:H132	28:C:501:SQD:H162	1.40	0.43
4:D:90[A]:LEU:HA	4:D:90[A]:LEU:HD23	1.41	0.43
40:D:630:HOH:O	30:X:101:UNL:C1	2.66	0.43
22:a:408:CLA:H203	22:a:408:CLA:H162	1.80	0.43
23:a:411:PHO:HBB1	23:a:411:PHO:HMB1	1.99	0.43
22:b:614:CLA:HBB1	22:b:614:CLA:CMB	2.49	0.43
3:c:63:TRP:HB2	22:c:911:CLA:HAC2	2.00	0.43
22:c:905:CLA:H62	22:c:905:CLA:H41	1.72	0.43
1:A:202:VAL:HG11	22:A:406:CLA:C3D	2.47	0.43
22:B:614:CLA:H121	25:B:621:LMG:H232	1.99	0.43
3:C:437:PHE:CE1	22:C:511:CLA:HMB2	2.53	0.43
5:E:17:VAL:HG23	9:J:7:ARG:CB	2.49	0.43
24:b:618:BCR:H353	34:l:106:HTG:H7'1	2.00	0.43
22:B:608:CLA:H112	22:B:608:CLA:H91	1.76	0.43
22:C:503:CLA:H193	34:C:521:HTG:H2'1	2.00	0.43
9:J:18:GLY:O	9:J:22:ILE:CD1	2.67	0.43
12:O:140:THR:HG23	31:O:304:DMS:H23	2.00	0.43
26:a:415:PL9:H303	4:d:45:LEU:HD22	2.00	0.43
2:B:224:ARG:HG3	7:H:25:TRP:CD2	2.53	0.43
2:B:423:LYS:NZ	31:O:311:DMS:H22	2.33	0.43
23:D:402:PHO:HBC2	23:D:402:PHO:HHD	2.01	0.43
2:b:27:THR:HG22	2:b:107:LEU:HD13	1.99	0.43
15:v:41:HIS:CD2	39:v:202:HEC:NB	2.85	0.43
1:A:210:LEU:C	1:A:210:LEU:HD23	2.44	0.43
32:A:421[B]:BCT:O3	4:D:214:HIS:CE1	2.71	0.43
10:K:26:PRO:O	10:K:29:PRO:HD2	2.18	0.43
23:a:411:PHO:H42	23:a:411:PHO:H11	1.84	0.43
24:c:915:BCR:H351	24:c:915:BCR:H15C	1.77	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.54	0.43
2:B:153:PHE:O	2:B:157:HIS:HB3	2.19	0.43
3:C:208:VAL:HG13	31:C:536:DMS:H21	2.00	0.43
1:a:102:LEU:HD23	1:a:102:LEU:HA	1.82	0.43
22:a:409:CLA:HBB1	23:a:411:PHO:H122	2.00	0.43
24:a:413:BCR:H24C	24:a:413:BCR:H371	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:62:PHE:CD1	3:c:62:PHE:C	2.96	0.43
3:c:121:SER:HB2	25:c:930:LMG:H241	1.99	0.43
12:o:204:VAL:HG13	12:o:211:ILE:HG22	2.00	0.43
4:D:170:ALA:HB1	4:D:171:PRO:HD2	2.01	0.43
1:a:161:TYR:CZ	1:a:165:GLN:HG3	2.54	0.43
22:b:611:CLA:CBB	22:b:611:CLA:HH C	2.49	0.43
31:b:638:DMS:H12	40:b:710:HOH:O	2.18	0.43
5:E:13:ILE:HG21	36:E:102:HEM:HAD2	2.00	0.43
31:O:303:DMS:H23	40:O:550:HOH:O	2.17	0.43
18:Z:15:LEU:O	18:Z:18:VAL:HG22	2.19	0.43
3:c:180:MET:HE2	3:c:180:MET:HB3	1.91	0.43
3:C:163:PHE:CD2	22:C:513:CLA:HAB	2.54	0.43
22:b:615:CLA:OBD	11:l:10:VAL:HG22	2.18	0.43
5:e:6:GLY:HA2	40:e:216:HOH:O	2.18	0.43
31:u:203:DMS:H22	31:u:205:DMS:H22	2.00	0.43
27:a:423:LHG:HC61	2:b:468:TRP:CH2	2.54	0.42
2:b:115:TRP:CD2	24:b:618:BCR:HC21	2.54	0.42
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.54	0.42
22:b:602:CLA:H2	22:b:602:CLA:H72	2.01	0.42
5:e:53:ASP:OD2	5:e:53:ASP:C	2.61	0.42
25:A:410:LMG:H291	3:C:216:SER:HA	2.01	0.42
3:C:312:ALA:HB1	3:C:392:ALA:O	2.19	0.42
27:D:409:LHG:H361	27:D:409:LHG:HC82	2.00	0.42
7:H:39:LEU:C	7:H:39:LEU:HD23	2.45	0.42
1:a:239:PHE:O	13:t:29:ILE:HA	2.18	0.42
2:b:284:ILE:CG2	2:b:302:TRP:CZ3	3.02	0.42
3:c:424:SER:O	3:c:428:THR:HG23	2.19	0.42
3:C:124:VAL:HB	24:C:515:BCR:H362	2.00	0.42
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.55	0.42
1:a:72:LEU:HD11	29:a:419:LMT:H52	2.00	0.42
2:b:108:PHE:HE2	24:b:618:BCR:H333	1.84	0.42
22:c:914:CLA:H152	22:c:914:CLA:H111	1.57	0.42
4:D:291:LEU:HD21	35:H:102:DGD:CGB	2.50	0.42
23:a:411:PHO:ND	23:a:411:PHO:NC	2.67	0.42
3:c:138:GLU:HG3	31:c:935:DMS:C1	2.46	0.42
3:c:210:PHE:HA	3:c:213:LEU:HD12	2.02	0.42
26:d:405:PL9:H362	26:d:405:PL9:H402	2.01	0.42
5:e:63:ILE:HG23	5:e:64:PRO:HD2	2.02	0.42
15:v:31:ARG:HG2	15:v:31:ARG:HH11	1.85	0.42
31:C:540:DMS:H12	40:C:638:HOH:O	2.19	0.42
22:b:616:CLA:H152	22:b:616:CLA:H112	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:74:GLN:CD	5:e:74:GLN:H	2.27	0.42
10:k:11:LEU:HD11	10:k:22:VAL:HG21	2.02	0.42
16:y:34:MET:HE2	16:y:34:MET:CA	2.50	0.42
22:B:611:CLA:H152	22:B:611:CLA:OBD	2.18	0.42
27:D:409:LHG:H121	27:D:409:LHG:H332	2.00	0.42
7:H:25:TRP:HB2	31:H:103:DMS:H23	2.01	0.42
1:a:66:PRO:HD2	31:a:425:DMS:H13	2.02	0.42
23:a:411:PHO:HMA2	26:a:415:PL9:H221	2.00	0.42
28:a:414:SQD:H191	28:a:414:SQD:H222	1.69	0.42
2:b:144:PHE:CE2	2:b:210:ILE:HG23	2.54	0.42
3:c:117:VAL:HG12	25:c:930:LMG:H221	2.00	0.42
25:i:101:LMG:H151	25:i:101:LMG:H182	1.80	0.42
1:A:218:LEU:HD12	26:A:411:PL9:C3	2.49	0.42
10:K:19:ASP:HB3	10:K:20:PRO:CD	2.45	0.42
14:U:36:ILE:HG13	14:U:42:TYR:CG	2.55	0.42
2:b:94:GLU:HG2	34:b:623:HTG:H2'1	2.01	0.42
3:c:318:LEU:C	3:c:318:LEU:HD23	2.45	0.42
15:v:26:TYR:CE2	15:v:118:HIS:HD2	2.38	0.42
1:A:73:TYR:HD1	29:A:414:LMT:H3B	1.83	0.42
2:B:98:LEU:HB2	34:B:623:HTG:H7'3	2.02	0.42
2:B:201:HIS:CD2	2:B:201:HIS:C	2.94	0.42
31:B:629:DMS:H12	34:D:415:HTG:H7'2	2.02	0.42
22:D:401:CLA:H162	22:D:401:CLA:H203	1.75	0.42
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.20	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.56	0.42
1:a:121[A]:LEU:HD11	22:c:906:CLA:H203	2.01	0.42
1:a:202:VAL:HG11	22:a:409:CLA:C3D	2.50	0.42
2:b:113:TRP:CD1	22:b:617:CLA:HBA2	2.55	0.42
26:d:405:PL9:H411	11:l:29:LEU:HD23	2.01	0.42
12:o:23:ASP:O	12:o:203:LYS:HE3	2.20	0.42
22:A:408:CLA:C20	22:C:507:CLA:H101	2.49	0.42
2:B:387:GLU:HG2	34:D:415:HTG:H5'1	2.02	0.42
3:C:409:GLY:HA2	31:V:201:DMS:S	2.59	0.42
7:H:42:LEU:HD23	7:H:42:LEU:HA	1.93	0.42
12:O:22:LEU:O	12:O:203:LYS:NZ	2.45	0.42
1:a:45:THR:HG23	22:a:408:CLA:H201	2.02	0.42
22:b:606:CLA:H143	22:b:611:CLA:HED2	2.01	0.42
3:c:275:SER:HB3	22:c:910:CLA:HED3	2.02	0.42
35:c:918:DGD:HBF2	35:c:918:DGD:HBE2	1.85	0.42
3:c:121:SER:CB	25:c:930:LMG:H241	2.50	0.42
25:c:920:LMG:H142	10:k:24:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:101:HEM:CAC	6:f:27:ALA:HB1	2.50	0.42
6:f:19:ARG:O	6:f:23:VAL:HG23	2.20	0.42
1:A:323:ARG:HB3	4:D:329:MET:HA	2.02	0.41
4:D:52:THR:O	4:D:66:SER:HA	2.20	0.41
3:c:26:ARG:NH2	16:y:46:LEU:OXT	2.41	0.41
3:c:85:GLY:O	22:c:905:CLA:HED2	2.20	0.41
22:A:406:CLA:HAB	22:A:406:CLA:HHC	1.80	0.41
3:C:25:ASN:HA	3:C:30:SER:CB	2.50	0.41
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.41
12:O:33:ASP:C	12:O:35:SER:H	2.28	0.41
34:b:632:HTG:H3	40:v:315:HOH:O	2.20	0.41
3:c:60:ILE:HG22	22:c:904:CLA:HHD	2.02	0.41
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.56	0.41
3:c:189:TRP:HE3	31:c:929:DMS:H21	1.86	0.41
28:l:101:SQD:O6	13:t:23:PHE:HD1	2.03	0.41
1:a:255:PHE:CZ	26:a:415:PL9:H101	2.55	0.41
8:i:27:ASP:N	8:i:28:PRO:CD	2.84	0.41
24:y:101:BCR:HC8	24:y:101:BCR:H311	2.01	0.41
2:B:451:PHE:CD1	2:B:451:PHE:C	2.99	0.41
13:T:19:PHE:CZ	24:b:618:BCR:H332	2.56	0.41
13:T:28:ARG:HD3	13:T:28:ARG:HA	1.87	0.41
1:a:21:VAL:HG11	1:a:32:TRP:CE3	2.54	0.41
1:a:259:ILE:HG22	1:a:260:PHE:N	2.36	0.41
28:a:414:SQD:H322	22:c:909:CLA:H18	2.03	0.41
22:b:615:CLA:HBD	34:l:106:HTG:H1	2.02	0.41
34:b:626:HTG:O2	34:b:627:HTG:S1	2.78	0.41
3:c:42:LEU:HD21	22:c:912:CLA:H2A	2.01	0.41
3:c:455:PHE:HA	40:c:1070:HOH:O	2.19	0.41
22:A:405:CLA:H193	22:A:405:CLA:H161	1.70	0.41
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.55	0.41
37:H:101:RRX:H32	37:H:101:RRX:H28	1.89	0.41
2:b:75:TRP:CH2	34:b:626:HTG:H2'1	2.55	0.41
3:c:95:LEU:HD11	22:c:904:CLA:HAA1	2.01	0.41
22:c:902:CLA:H101	24:c:916:BCR:H17C	2.01	0.41
2:B:6:TYR:OH	27:D:409:LHG:HC11	2.21	0.41
2:B:124:ARG:HD2	2:B:129:GLY:O	2.20	0.41
3:C:168:LEU:HD21	22:C:510:CLA:H62	2.02	0.41
3:C:433:LEU:HD13	22:C:503:CLA:CHC	2.50	0.41
15:V:118:HIS:CE1	15:V:122:GLU:CG	3.04	0.41
1:a:93:PHE:HZ	22:a:412:CLA:HAA1	1.84	0.41
22:a:412:CLA:H11	8:i:9:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:255:THR:HG22	31:c:934:DMS:O	2.21	0.41
7:h:12:ARG:O	7:h:13:PRO:C	2.63	0.41
22:B:608:CLA:H2	25:B:621:LMG:H161	2.01	0.41
22:C:507:CLA:HBB1	22:C:507:CLA:HMB3	2.02	0.41
14:U:43:PRO:HD2	15:V:83:ASP:CG	2.46	0.41
2:b:156:PHE:HB3	2:b:162:PHE:HB3	2.03	0.41
24:c:916:BCR:H11C	24:c:916:BCR:H341	1.92	0.41
2:B:446:SER:CB	2:B:447:PRO:CD	2.91	0.41
4:D:54:PHE:O	5:E:49:THR:OG1	2.36	0.41
4:D:236:ASN:O	4:D:239:GLN:HG2	2.19	0.41
23:D:402:PHO:NC	23:D:402:PHO:ND	2.68	0.41
24:D:405:BCR:C8	24:D:405:BCR:H331	2.50	0.41
12:O:137:THR:C	12:O:139:SER:H	2.29	0.41
2:b:270:PRO:HG2	2:b:317:ASN:O	2.21	0.41
7:h:31:MET:O	7:h:35:MET:HG3	2.20	0.41
10:k:31:LEU:HD23	10:k:31:LEU:HA	1.86	0.41
15:v:41:HIS:HA	15:v:45:ILE:O	2.21	0.41
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.50	0.41
7:H:25:TRP:O	7:H:26:GLY:C	2.63	0.41
14:U:45:LEU:O	14:U:49:ILE:HG13	2.20	0.41
1:a:21:VAL:HG11	1:a:32:TRP:CZ3	2.56	0.41
1:a:182:PHE:O	1:a:186:PHE:HB2	2.21	0.41
22:b:615:CLA:HBA2	34:l:106:HTG:H2'1	2.02	0.41
22:b:617:CLA:H91	22:b:617:CLA:H112	1.82	0.41
3:C:286:ALA:HB2	22:C:503:CLA:HMD2	2.02	0.41
7:H:63:LYS:O	7:H:64:ALA:C	2.64	0.41
31:O:312:DMS:C2	40:O:467:HOH:O	2.59	0.41
26:a:415:PL9:HC2	26:a:415:PL9:H103	2.03	0.41
2:b:346:PHE:CD2	31:b:638:DMS:H23	2.55	0.41
22:c:902:CLA:C3D	22:c:904:CLA:H2	2.50	0.41
10:k:21:LEU:O	10:k:25:LEU:HG	2.21	0.41
1:A:42:LEU:HD23	28:A:413:SQD:H192	2.02	0.40
2:B:121:GLU:CA	7:H:2:ALA:HB1	2.50	0.40
2:B:224:ARG:HG2	7:H:24:GLY:O	2.22	0.40
2:B:273:TYR:HA	2:B:276:ASP:HB2	2.03	0.40
3:C:179:ALA:O	3:C:184:GLY:HA2	2.21	0.40
12:O:58:ASN:HB3	2:b:339:ALA:CB	2.51	0.40
3:c:109:PHE:N	3:c:110:PRO:CD	2.84	0.40
3:c:286:ALA:HB2	22:c:903:CLA:HMD2	2.04	0.40
22:c:910:CLA:HAB	22:c:910:CLA:HHC	1.86	0.40
1:A:72:LEU:HD21	29:T:102:LMT:H41	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TRP:CZ3	24:B:618:BCR:H322	2.57	0.40
2:B:435:GLU:O	2:B:436:THR:C	2.64	0.40
22:B:613:CLA:HHC	22:B:613:CLA:HAB	1.91	0.40
12:O:130:GLN:NE2	12:O:141:ASP:H	2.20	0.40
1:a:259:ILE:HG13	26:a:415:PL9:H253	2.03	0.40
31:a:425:DMS:H11	12:o:152:ARG:NH2	2.33	0.40
4:d:103:ARG:O	4:d:107:LEU:HG	2.21	0.40
2:B:194:ASN:HA	2:B:195:PRO:HD2	1.90	0.40
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.09	0.40
13:T:20:ALA:O	13:T:24:ARG:HB3	2.21	0.40
15:V:129[A]:LYS:HB3	31:V:212:DMS:S	2.61	0.40
15:v:124:LYS:CE	40:v:356:HOH:O	2.63	0.40
2:B:41:GLU:OE1	2:B:63:LEU:HB2	2.21	0.40
37:H:101:RRX:H3	17:X:2:THR:N	2.20	0.40
12:O:103:PHE:HA	12:O:120:PHE:O	2.21	0.40
1:a:276:ALA:O	1:a:280:VAL:HG23	2.22	0.40
12:o:130:GLN:HG2	40:o:480:HOH:O	2.21	0.40
14:u:83:THR:OG1	14:u:84:VAL:N	2.54	0.40
1:A:66:PRO:O	31:A:420:DMS:H22	2.22	0.40
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.03	0.40
22:A:408:CLA:H61	22:A:408:CLA:H41	1.70	0.40
4:D:17:ILE:O	4:D:20:ASP:HB2	2.22	0.40
4:D:125:PHE:CE1	23:D:402:PHO:HBD	2.57	0.40
22:D:401:CLA:HBB1	22:D:401:CLA:CMB	2.50	0.40
1:a:254:TYR:CD1	1:a:254:TYR:C	2.98	0.40
2:b:149:LEU:HB2	22:b:605:CLA:H171	2.04	0.40
2:b:204:ALA:CB	22:b:603:CLA:HAB	2.51	0.40
3:c:107:ASP:O	3:c:110:PRO:HD2	2.22	0.40
3:c:221:GLU:O	3:c:226:SER:HB3	2.22	0.40
22:c:913:CLA:H91	22:c:914:CLA:H141	2.03	0.40
6:f:15:ILE:O	6:f:15:ILE:CG2	2.68	0.40

There are no symmetry-related clashes.

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	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	36	42
1	a	333/334 (100%)	321 (96%)	11 (3%)	1 (0%)	36	42
2	B	506/505 (100%)	495 (98%)	11 (2%)	0	100	100
2	b	482/505 (95%)	465 (96%)	17 (4%)	0	100	100
3	C	449/455 (99%)	434 (97%)	13 (3%)	2 (0%)	30	34
3	c	454/455 (100%)	435 (96%)	18 (4%)	1 (0%)	43	51
4	D	343/342 (100%)	336 (98%)	6 (2%)	1 (0%)	36	42
4	d	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
5	E	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	8
5	e	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
6	F	31/33 (94%)	31 (100%)	0	0	100	100
6	f	29/33 (88%)	29 (100%)	0	0	100	100
7	H	64/63 (102%)	60 (94%)	4 (6%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	3	2
9	j	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	0	100	100
11	l	33/35 (94%)	33 (100%)	0	0	100	100
12	O	242/243 (100%)	228 (94%)	12 (5%)	2 (1%)	16	16
12	o	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
13	T	28/30 (93%)	28 (100%)	0	0	100	100
13	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	U	96/97 (99%)	92 (96%)	4 (4%)	0	100	100
14	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
15	v	136/137 (99%)	126 (93%)	9 (7%)	1 (1%)	18	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
16	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
17	X	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
17	x	34/37 (92%)	31 (91%)	1 (3%)	2 (6%)	1	0
18	Z	60/62 (97%)	56 (93%)	1 (2%)	3 (5%)	1	0
18	z	59/62 (95%)	55 (93%)	4 (7%)	0	100	100
All	All	5100/5190 (98%)	4921 (96%)	163 (3%)	16 (0%)	36	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
3	C	24	THR
3	C	416	SER
5	E	6	GLY
18	Z	31	GLN
18	Z	32	ASP
3	c	416	SER
15	v	19	ILE
17	x	35	ASP
9	J	6	GLY
12	O	34	SER
18	Z	30	PRO
1	a	225	ARG
12	O	26	ALA
1	A	259	ILE
17	x	34	ILE

5.3.2 Protein sidechains ⓘ

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	263/270 (97%)	259 (98%)	4 (2%)	57	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	252/270 (93%)	251 (100%)	1 (0%)	84	92
2	B	391/403 (97%)	385 (98%)	6 (2%)	57	73
2	b	378/403 (94%)	375 (99%)	3 (1%)	73	85
3	C	347/356 (98%)	343 (99%)	4 (1%)	63	78
3	c	356/356 (100%)	350 (98%)	6 (2%)	53	69
4	D	278/277 (100%)	278 (100%)	0	100	100
4	d	276/277 (100%)	275 (100%)	1 (0%)	84	92
5	E	68/71 (96%)	66 (97%)	2 (3%)	37	51
5	e	67/71 (94%)	65 (97%)	2 (3%)	36	49
6	F	27/27 (100%)	27 (100%)	0	100	100
6	f	25/27 (93%)	24 (96%)	1 (4%)	28	38
7	H	56/53 (106%)	56 (100%)	0	100	100
7	h	54/53 (102%)	54 (100%)	0	100	100
8	I	31/32 (97%)	30 (97%)	1 (3%)	34	47
8	i	31/32 (97%)	31 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	26	35
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	7
10	k	28/30 (93%)	27 (96%)	1 (4%)	31	42
11	L	33/33 (100%)	33 (100%)	0	100	100
11	l	33/33 (100%)	32 (97%)	1 (3%)	36	49
12	O	203/206 (98%)	196 (97%)	7 (3%)	32	44
12	o	199/206 (97%)	194 (98%)	5 (2%)	42	56
13	T	24/26 (92%)	23 (96%)	1 (4%)	26	36
13	t	24/26 (92%)	22 (92%)	2 (8%)	10	11
14	U	85/84 (101%)	84 (99%)	1 (1%)	63	78
14	u	82/84 (98%)	81 (99%)	1 (1%)	63	78
15	V	117/117 (100%)	114 (97%)	3 (3%)	40	55
15	v	115/117 (98%)	111 (96%)	4 (4%)	32	43
16	Y	22/22 (100%)	18 (82%)	4 (18%)	2	1
16	y	19/22 (86%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	X	29/30 (97%)	27 (93%)	2 (7%)	14	16
17	x	27/30 (90%)	26 (96%)	1 (4%)	30	41
18	Z	45/52 (86%)	45 (100%)	0	100	100
18	z	40/52 (77%)	38 (95%)	2 (5%)	22	28
All	All	4103/4234 (97%)	4033 (98%)	70 (2%)	53	69

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	LEU
1	A	224	ILE
1	A	238	LYS
1	A	248	ILE
2	B	128	THR
2	B	246	PHE
2	B	362	PHE
2	B	373	LYS
2	B	472	ARG
2	B	503	THR
3	C	255	THR
3	C	289	PHE
3	C	315	MET
3	C	471	SER
5	E	65	LEU
5	E	82	GLN
8	I	33	LYS
9	J	22	ILE
10	K	10	LYS
10	K	17	ILE
10	K	27	VAL
12	O	53	LYS
12	O	84	GLU
12	O	118	LEU
12	O	130	GLN
12	O	180	GLU
12	O	181	GLU
12	O	242	SER
13	T	25	GLU
14	U	86	GLU
15	V	30	LYS
15	V	129[A]	LYS

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Mol	Chain	Res	Type
15	V	129[B]	LYS
16	Y	19	ILE
16	Y	25	ILE
16	Y	30	ILE
16	Y	43	ARG
17	X	23	LEU
17	X	33	GLN
1	a	214	MET
2	b	161	LEU
2	b	362	PHE
2	b	467	ILE
3	c	78	GLU
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	334	PRO
3	c	381	LYS
4	d	329	MET
5	e	7	GLU
5	e	25	ILE
6	f	15	ILE
10	k	27	VAL
11	l	10	VAL
12	o	10	ILE
12	o	89	SER
12	o	93	LEU
12	o	180	GLU
12	o	242	SER
13	t	25	GLU
13	t	28	ARG
14	u	39	ARG
15	v	6	GLU
15	v	19	ILE
15	v	28	GLU
15	v	30	LYS
17	x	21	LEU
18	z	4	LEU
18	z	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	304	HIS
2	B	53	ASN
2	B	223	GLN
2	B	331	ASN
2	B	394	GLN
3	C	44	ASN
3	C	418	ASN
4	D	186	GLN
4	D	255	GLN
4	D	332	GLN
6	F	44	GLN
12	O	58	ASN
12	O	88	ASN
12	O	104	GLN
12	O	155	ASN
14	U	37	GLN
14	U	71	GLN
14	U	78	ASN
14	U	81	HIS
15	V	34	GLN
18	Z	58	ASN
1	a	165	GLN
1	a	266	ASN
1	a	296	ASN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
3	c	201	ASN
4	d	186	GLN
4	d	332	GLN
10	k	40	GLN
11	l	6	ASN
12	o	82	GLN
12	o	104	GLN
12	o	124	ASN
12	o	147	ASN
12	o	231	HIS
14	u	37	GLN
14	u	73	GLN

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Mol	Chain	Res	Type
15	v	34	GLN
15	v	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.93	0	8,9,11	1.23	1 (12%)
13	FME	T	1	13	8,9,10	0.62	0	8,9,11	1.24	1 (12%)
8	FME	i	1	8	8,9,10	0.56	0	8,9,11	1.23	1 (12%)
13	FME	t	1	13	8,9,10	0.62	0	8,9,11	1.65	2 (25%)

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
8	FME	I	1	8	-	1/7/9/11	-
13	FME	T	1	13	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
13	FME	t	1	13	-	2/7/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	t	1	FME	CB-CA-N	-3.07	104.92	110.52
13	t	1	FME	CE-SD-CG	2.61	113.85	100.32
8	i	1	FME	O-C-CA	-2.36	118.69	124.77
13	T	1	FME	C-CA-N	2.03	113.42	109.50
8	I	1	FME	O-C-CA	-2.03	119.54	124.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
13	T	1	FME	O1-CN-N-CA
13	t	1	FME	O1-CN-N-CA
13	T	1	FME	CA-CB-CG-SD
13	t	1	FME	CA-CB-CG-SD
8	i	1	FME	O1-CN-N-CA
8	i	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 352 ligands modelled in this entry, 15 are monoatomic and 27 are unknown - leaving 310 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	$\# Z > 2$
22	CLA	b	612	-	69,73,73	2.17	20 (28%)	82,113,113	2.27	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	412	-	69,73,73	2.28	22 (31%)	82,113,113	2.24	31 (37%)
31	DMS	u	204	-	3,3,3	2.86	1 (33%)	3,3,3	0.83	0
37	RRX	h	101	-	42,42,42	0.97	1 (2%)	56,58,58	1.21	5 (8%)
31	DMS	c	944	-	3,3,3	2.78	1 (33%)	3,3,3	0.81	0
22	CLA	c	914	-	69,73,73	2.35	19 (27%)	82,113,113	2.23	27 (32%)
22	CLA	B	617	-	59,63,73	2.20	16 (27%)	70,101,113	2.64	30 (42%)
27	LHG	d	407	-	48,48,48	0.76	2 (4%)	51,54,54	1.08	3 (5%)
31	DMS	V	201	-	3,3,3	2.70	1 (33%)	3,3,3	0.92	0
34	HTG	B	627	-	19,19,19	0.95	1 (5%)	23,24,24	1.83	3 (13%)
29	LMT	a	419	-	36,36,36	0.78	0	47,47,47	1.38	4 (8%)
31	DMS	b	636	-	3,3,3	2.73	1 (33%)	3,3,3	0.72	0
31	DMS	O	306	-	3,3,3	2.76	1 (33%)	3,3,3	0.78	0
35	DGD	c	918	-	63,63,67	0.94	5 (7%)	77,77,81	1.03	4 (5%)
22	CLA	C	510	-	69,73,73	2.15	18 (26%)	82,113,113	2.38	28 (34%)
24	BCR	d	404	-	41,41,41	1.06	3 (7%)	56,56,56	1.79	13 (23%)
25	LMG	D	412	-	46,46,55	1.14	3 (6%)	54,54,63	1.13	2 (3%)
27	LHG	L	101	-	39,39,48	1.05	2 (5%)	42,45,54	1.21	4 (9%)
28	SQD	l	101	-	52,54,54	1.09	3 (5%)	62,65,65	1.44	8 (12%)
23	PHO	D	402	-	58,69,69	2.83	10 (17%)	55,99,99	2.80	16 (29%)
35	DGD	C	517	-	63,63,67	0.85	3 (4%)	77,77,81	1.32	12 (15%)
39	HEC	V	202	15	46,50,50	2.05	8 (17%)	58,82,82	1.26	7 (12%)
24	BCR	B	619	-	30,30,41	0.94	0	39,39,56	1.33	8 (20%)
31	DMS	l	103	-	3,3,3	2.77	1 (33%)	3,3,3	0.68	0
22	CLA	b	609	-	69,73,73	2.22	19 (27%)	82,113,113	2.09	27 (32%)
35	DGD	c	917	-	63,63,67	0.97	3 (4%)	77,77,81	1.01	3 (3%)
22	CLA	b	615	-	56,60,73	2.73	21 (37%)	65,97,113	2.41	29 (44%)
31	DMS	I	101	-	3,3,3	2.77	1 (33%)	3,3,3	0.71	0
28	SQD	a	414	-	52,54,54	1.02	2 (3%)	62,65,65	1.96	12 (19%)
24	BCR	K	101	-	41,41,41	0.85	0	56,56,56	1.21	5 (8%)
31	DMS	B	639	-	3,3,3	2.82	1 (33%)	3,3,3	0.73	0
31	DMS	C	537	-	3,3,3	2.81	1 (33%)	3,3,3	0.72	0
22	CLA	b	606	-	69,73,73	2.23	19 (27%)	82,113,113	2.31	27 (32%)
24	BCR	c	916	-	41,41,41	0.87	0	56,56,56	1.55	10 (17%)
22	CLA	B	602	40	69,73,73	2.78	22 (31%)	82,113,113	2.35	28 (34%)
31	DMS	v	209	-	3,3,3	2.70	1 (33%)	3,3,3	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	v	207	-	3,3,3	2.78	1 (33%)	3,3,3	0.67	0
29	LMT	B	622	-	24,24,36	0.64	1 (4%)	29,29,47	0.85	1 (3%)
25	LMG	J	101	38	45,45,55	0.99	2 (4%)	53,53,63	1.03	6 (11%)
31	DMS	o	303	-	3,3,3	2.76	1 (33%)	3,3,3	0.83	0
31	DMS	c	924	-	3,3,3	2.88	1 (33%)	3,3,3	1.35	1 (33%)
31	DMS	o	308	-	3,3,3	2.85	1 (33%)	3,3,3	0.85	0
25	LMG	C	531	-	40,40,55	1.19	3 (7%)	48,48,63	1.14	3 (6%)
31	DMS	u	205	-	3,3,3	3.14	1 (33%)	3,3,3	1.22	0
29	LMT	Z	101	-	36,36,36	0.68	1 (2%)	47,47,47	1.16	3 (6%)
25	LMG	d	409	-	47,47,55	1.09	3 (6%)	55,55,63	1.48	9 (16%)
19	OEX	A	401	40,3,1	0,15,15	-	-	-	-	-
31	DMS	B	631	-	3,3,3	2.62	1 (33%)	3,3,3	0.63	0
34	HTG	D	415	-	19,19,19	1.09	1 (5%)	23,24,24	2.48	7 (30%)
31	DMS	V	212	-	3,3,3	2.84	1 (33%)	3,3,3	1.21	0
31	DMS	O	313	-	3,3,3	2.69	1 (33%)	3,3,3	0.49	0
31	DMS	C	533	-	3,3,3	2.80	1 (33%)	3,3,3	0.77	0
31	DMS	O	307	-	3,3,3	2.86	1 (33%)	3,3,3	0.93	0
31	DMS	d	412	-	3,3,3	2.62	1 (33%)	3,3,3	0.85	0
27	LHG	d	408	-	45,45,48	1.04	2 (4%)	48,51,54	0.74	0
22	CLA	B	612	-	69,73,73	2.16	17 (24%)	82,113,113	2.25	32 (39%)
22	CLA	b	607	-	69,73,73	2.24	23 (33%)	82,113,113	2.49	27 (32%)
31	DMS	b	630	-	3,3,3	2.72	1 (33%)	3,3,3	0.30	0
32	BCT	A	421[A]	20	3,3,3	1.52	1 (33%)	2,3,3	0.16	0
22	CLA	C	507	-	69,73,73	2.27	20 (28%)	82,113,113	2.18	23 (28%)
31	DMS	C	534	-	3,3,3	2.76	1 (33%)	3,3,3	0.57	0
31	DMS	I	106	-	3,3,3	2.75	1 (33%)	3,3,3	0.77	0
22	CLA	d	402	-	69,73,73	2.06	21 (30%)	82,113,113	2.36	28 (34%)
27	LHG	l	102	-	48,48,48	0.93	2 (4%)	51,54,54	1.09	3 (5%)
31	DMS	v	210	-	3,3,3	2.91	1 (33%)	3,3,3	0.81	0
31	DMS	c	938	-	3,3,3	2.83	1 (33%)	3,3,3	0.85	0
36	HEM	E	102	5,6	50,50,50	2.01	8 (16%)	67,82,82	1.50	10 (14%)
31	DMS	b	634	-	3,3,3	2.78	1 (33%)	3,3,3	0.60	0
22	CLA	B	615	-	57,61,73	2.63	19 (33%)	67,98,113	2.82	31 (46%)
31	DMS	V	211	-	3,3,3	2.88	1 (33%)	3,3,3	0.78	0
22	CLA	A	405	-	69,73,73	2.39	18 (26%)	82,113,113	2.05	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	C	536	-	3,3,3	2.75	1 (33%)	3,3,3	0.47	0
25	LMG	j	101	38	47,47,55	1.01	2 (4%)	55,55,63	1.18	7 (12%)
31	DMS	c	941	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
22	CLA	C	512	3	69,73,73	2.54	21 (30%)	82,113,113	2.28	31 (37%)
31	DMS	o	304	-	3,3,3	2.88	1 (33%)	3,3,3	1.17	0
31	DMS	C	525	-	3,3,3	2.50	1 (33%)	3,3,3	0.64	0
27	LHG	D	411	-	44,44,48	0.98	2 (4%)	47,50,54	1.05	3 (6%)
31	DMS	B	634	-	3,3,3	2.87	1 (33%)	3,3,3	0.67	0
31	DMS	c	943	-	3,3,3	2.76	1 (33%)	3,3,3	0.83	0
19	OEX	a	403	40,3,1	0,15,15	-	-	-	-	-
31	DMS	c	935	-	3,3,3	2.72	1 (33%)	3,3,3	0.91	0
24	BCR	a	413	-	41,41,41	1.15	2 (4%)	56,56,56	1.18	8 (14%)
34	HTG	C	521	-	19,19,19	0.87	2 (10%)	23,24,24	1.47	2 (8%)
34	HTG	D	414	-	19,19,19	0.81	1 (5%)	23,24,24	1.59	1 (4%)
31	DMS	v	211	-	3,3,3	2.82	1 (33%)	3,3,3	0.78	0
29	LMT	c	921	-	36,36,36	0.68	1 (2%)	47,47,47	1.04	4 (8%)
27	LHG	d	401	-	32,32,48	1.24	2 (6%)	35,37,54	1.17	4 (11%)
31	DMS	A	417	-	3,3,3	2.73	1 (33%)	3,3,3	0.49	0
22	CLA	C	505	40	69,73,73	3.00	22 (31%)	82,113,113	2.12	24 (29%)
22	CLA	D	401	40	69,73,73	1.89	17 (24%)	82,113,113	2.43	29 (35%)
37	RRX	H	101	-	42,42,42	0.84	0	56,58,58	1.52	9 (16%)
26	PL9	D	406	-	55,55,55	0.94	3 (5%)	68,69,69	1.54	14 (20%)
31	DMS	O	304	-	3,3,3	2.63	1 (33%)	3,3,3	0.43	0
31	DMS	u	202	-	3,3,3	2.68	1 (33%)	3,3,3	1.07	0
31	DMS	t	104	-	3,3,3	2.77	1 (33%)	3,3,3	0.61	0
31	DMS	V	210	-	3,3,3	2.83	1 (33%)	3,3,3	0.90	0
35	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.21	10 (12%)
26	PL9	A	411	-	55,55,55	0.96	4 (7%)	68,69,69	1.71	13 (19%)
31	DMS	b	633	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
31	DMS	V	205	-	3,3,3	2.68	1 (33%)	3,3,3	0.66	0
31	DMS	C	528	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
31	DMS	C	539	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
31	DMS	B	630	-	3,3,3	2.88	1 (33%)	3,3,3	0.94	0
31	DMS	c	923	-	3,3,3	2.56	1 (33%)	3,3,3	0.41	0
31	DMS	B	633	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LMG	i	101	-	51,51,55	0.99	2 (3%)	59,59,63	1.18	7 (11%)
29	LMT	A	414	-	36,36,36	0.79	0	47,47,47	1.14	3 (6%)
22	CLA	c	906	-	69,73,73	2.38	21 (30%)	82,113,113	2.08	25 (30%)
31	DMS	C	540	-	3,3,3	2.85	1 (33%)	3,3,3	0.91	0
22	CLA	B	607	-	69,73,73	2.36	19 (27%)	82,113,113	2.38	32 (39%)
31	DMS	D	417	-	3,3,3	2.82	1 (33%)	3,3,3	0.61	0
31	DMS	c	936	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
27	LHG	C	522	-	29,29,48	1.31	2 (6%)	32,34,54	1.36	3 (9%)
31	DMS	B	638	-	3,3,3	2.71	1 (33%)	3,3,3	0.41	0
29	LMT	c	931	-	24,24,36	0.80	1 (4%)	29,29,47	0.87	2 (6%)
35	DGD	d	406	-	42,42,67	1.25	3 (7%)	44,45,81	1.10	3 (6%)
31	DMS	D	418	-	3,3,3	2.46	1 (33%)	3,3,3	0.69	0
22	CLA	c	904	-	69,73,73	2.59	20 (28%)	82,113,113	2.39	30 (36%)
22	CLA	b	605	-	69,73,73	2.49	22 (31%)	82,113,113	2.22	22 (26%)
31	DMS	O	310	-	3,3,3	2.68	1 (33%)	3,3,3	0.87	0
31	DMS	d	411	-	3,3,3	2.77	1 (33%)	3,3,3	0.96	0
25	LMG	A	410	-	51,51,55	0.96	2 (3%)	59,59,63	1.10	5 (8%)
22	CLA	b	611	40	69,73,73	2.54	21 (30%)	82,113,113	2.22	26 (31%)
35	DGD	h	102	-	63,63,67	0.98	3 (4%)	77,77,81	1.14	4 (5%)
31	DMS	V	207	-	3,3,3	2.82	1 (33%)	3,3,3	0.92	0
31	DMS	O	314	-	3,3,3	2.80	1 (33%)	3,3,3	0.78	0
28	SQD	f	101	-	12,13,54	2.28	1 (8%)	14,16,65	1.13	2 (14%)
23	PHO	A	407	-	58,69,69	2.45	13 (22%)	55,99,99	2.74	16 (29%)
22	CLA	c	911	-	69,73,73	2.23	20 (28%)	82,113,113	2.15	28 (34%)
22	CLA	C	513	-	60,64,73	2.84	21 (35%)	71,102,113	2.39	24 (33%)
22	CLA	A	408	-	69,73,73	2.15	20 (28%)	82,113,113	2.23	31 (37%)
31	DMS	t	105	-	3,3,3	2.77	1 (33%)	3,3,3	0.63	0
24	BCR	C	516	-	41,41,41	0.93	0	56,56,56	1.37	7 (12%)
31	DMS	o	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.60	0
34	HTG	C	523	-	8,8,19	0.40	0	7,7,24	1.02	1 (14%)
31	DMS	c	934	-	3,3,3	2.72	1 (33%)	3,3,3	0.69	0
35	DGD	c	919	-	63,63,67	0.99	4 (6%)	77,77,81	1.16	6 (7%)
31	DMS	C	538	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
22	CLA	b	610	-	69,73,73	2.58	21 (30%)	82,113,113	2.05	27 (32%)
31	DMS	V	204	-	3,3,3	2.79	1 (33%)	3,3,3	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	907	-	69,73,73	2.36	20 (28%)	82,113,113	2.17	30 (36%)
27	LHG	a	423	-	44,44,48	1.02	2 (4%)	47,50,54	1.10	4 (8%)
31	DMS	t	103	-	3,3,3	2.77	1 (33%)	3,3,3	0.66	0
31	DMS	O	311	-	3,3,3	3.04	1 (33%)	3,3,3	0.93	0
31	DMS	V	209	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
26	PL9	a	415	-	55,55,55	0.95	3 (5%)	68,69,69	1.48	9 (13%)
29	LMT	E	101	-	24,24,36	0.64	0	29,29,47	0.99	1 (3%)
31	DMS	v	204	-	3,3,3	2.73	1 (33%)	3,3,3	0.70	0
32	BCT	A	421[B]	20	3,3,3	1.54	1 (33%)	2,3,3	0.37	0
31	DMS	c	927	-	3,3,3	2.70	1 (33%)	3,3,3	0.43	0
31	DMS	f	103	-	3,3,3	2.77	1 (33%)	3,3,3	0.94	0
31	DMS	A	418	-	3,3,3	2.47	1 (33%)	3,3,3	1.28	0
31	DMS	l	105	-	3,3,3	2.80	1 (33%)	3,3,3	0.74	0
31	DMS	v	205	-	3,3,3	2.72	1 (33%)	3,3,3	0.86	0
31	DMS	d	413	-	3,3,3	2.60	1 (33%)	3,3,3	0.41	0
22	CLA	c	909	-	69,73,73	3.20	23 (33%)	82,113,113	2.24	25 (30%)
27	LHG	D	409	-	48,48,48	1.02	2 (4%)	51,54,54	1.39	5 (9%)
25	LMG	c	930	-	49,49,55	1.10	3 (6%)	57,57,63	1.07	4 (7%)
31	DMS	u	203	-	3,3,3	2.79	1 (33%)	3,3,3	0.78	0
34	HTG	B	623	-	19,19,19	1.07	1 (5%)	23,24,24	1.60	2 (8%)
24	BCR	k	101	-	41,41,41	0.92	0	56,56,56	1.25	6 (10%)
31	DMS	c	937	-	3,3,3	2.95	1 (33%)	3,3,3	0.84	0
31	DMS	C	535	-	3,3,3	2.80	1 (33%)	3,3,3	0.81	0
34	HTG	b	626	-	19,19,19	0.77	1 (5%)	23,24,24	1.47	4 (17%)
31	DMS	B	637	-	3,3,3	2.84	1 (33%)	3,3,3	0.73	0
24	BCR	C	515	-	41,41,41	0.82	1 (2%)	56,56,56	1.50	9 (16%)
31	DMS	O	308	-	3,3,3	2.85	1 (33%)	3,3,3	0.64	0
22	CLA	C	503	-	69,73,73	2.40	20 (28%)	82,113,113	2.20	22 (26%)
31	DMS	d	414	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
34	HTG	B	626	-	19,19,19	0.69	0	23,24,24	1.65	5 (21%)
23	PHO	a	411	-	58,69,69	2.60	11 (18%)	55,99,99	3.14	13 (23%)
31	DMS	B	636	-	3,3,3	2.66	1 (33%)	3,3,3	0.65	0
31	DMS	c	942	-	3,3,3	2.80	1 (33%)	3,3,3	0.74	0
22	CLA	B	605	-	69,73,73	2.09	20 (28%)	82,113,113	2.36	36 (43%)
28	SQD	C	501	-	52,54,54	0.99	2 (3%)	62,65,65	1.87	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	C	518	-	63,63,67	0.97	3 (4%)	77,77,81	1.27	10 (12%)
22	CLA	C	504	-	69,73,73	2.67	22 (31%)	82,113,113	2.28	30 (36%)
28	SQD	D	408	-	18,20,54	0.85	1 (5%)	26,29,65	1.87	7 (26%)
31	DMS	C	529	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
31	DMS	b	635	-	3,3,3	2.82	1 (33%)	3,3,3	0.56	0
25	LMG	b	622	-	43,43,55	1.36	4 (9%)	51,51,63	1.90	12 (23%)
23	PHO	a	410	-	58,69,69	2.62	12 (20%)	55,99,99	2.66	12 (21%)
34	HTG	b	632	-	19,19,19	1.05	2 (10%)	23,24,24	2.36	7 (30%)
34	HTG	b	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.28	4 (17%)
31	DMS	i	106	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
22	CLA	c	908	40	69,73,73	2.71	17 (24%)	82,113,113	2.35	23 (28%)
31	DMS	U	203	-	3,3,3	2.84	1 (33%)	3,3,3	1.25	0
24	BCR	c	915	-	41,41,41	0.86	1 (2%)	56,56,56	1.40	7 (12%)
22	CLA	B	606	-	69,73,73	2.79	19 (27%)	82,113,113	2.36	29 (35%)
22	CLA	C	509	-	69,73,73	2.40	19 (27%)	82,113,113	2.14	24 (29%)
24	BCR	B	618	-	19,19,41	0.95	1 (5%)	26,26,56	1.45	5 (19%)
22	CLA	C	508	40	69,73,73	2.27	20 (28%)	82,113,113	2.29	25 (30%)
22	CLA	B	609	-	69,73,73	2.56	21 (30%)	82,113,113	2.25	26 (31%)
31	DMS	a	401	-	3,3,3	2.81	1 (33%)	3,3,3	0.83	0
31	DMS	V	206	-	3,3,3	2.76	1 (33%)	3,3,3	0.56	0
31	DMS	b	638	-	3,3,3	3.05	1 (33%)	3,3,3	0.71	0
31	DMS	o	302	-	3,3,3	2.74	1 (33%)	3,3,3	0.96	0
29	LMT	T	102	-	24,24,36	0.73	1 (4%)	29,29,47	1.28	3 (10%)
24	BCR	b	619	-	30,31,41	1.02	1 (3%)	38,40,56	1.37	6 (15%)
24	BCR	D	405	-	41,41,41	1.00	1 (2%)	56,56,56	2.01	15 (26%)
34	HTG	C	532	-	19,19,19	1.06	2 (10%)	23,24,24	1.66	1 (4%)
27	LHG	D	410	-	48,48,48	0.80	2 (4%)	51,54,54	1.10	5 (9%)
22	CLA	B	604	-	69,73,73	2.23	18 (26%)	82,113,113	2.28	32 (39%)
31	DMS	C	526	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
28	SQD	A	413	-	47,49,54	0.99	2 (4%)	57,60,65	1.71	9 (15%)
31	DMS	d	415	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
31	DMS	o	306	-	3,3,3	2.71	1 (33%)	3,3,3	0.61	0
31	DMS	b	637	-	3,3,3	2.78	1 (33%)	3,3,3	0.63	0
22	CLA	b	613	-	69,73,73	2.56	20 (28%)	82,113,113	2.24	29 (35%)
28	SQD	b	621	-	36,38,54	0.98	1 (2%)	45,48,65	1.46	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	H	102	-	63,63,67	1.03	3 (4%)	77,77,81	1.17	7 (9%)
32	BCT	a	422	20	3,3,3	1.80	1 (33%)	2,3,3	1.11	0
31	DMS	B	642	-	3,3,3	2.72	1 (33%)	3,3,3	1.04	0
34	HTG	c	922	-	19,19,19	0.78	1 (5%)	23,24,24	1.53	2 (8%)
22	CLA	C	511	-	69,73,73	2.35	19 (27%)	82,113,113	2.06	25 (30%)
24	BCR	B	620	-	41,41,41	0.99	3 (7%)	56,56,56	1.51	11 (19%)
22	CLA	B	608	40	69,73,73	2.18	20 (28%)	82,113,113	2.25	33 (40%)
22	CLA	b	603	-	69,73,73	2.79	19 (27%)	82,113,113	2.29	30 (36%)
31	DMS	F	101	-	3,3,3	2.72	1 (33%)	3,3,3	0.62	0
34	HTG	v	203	-	16,16,19	0.97	1 (6%)	20,21,24	2.82	7 (35%)
31	DMS	O	309	-	3,3,3	2.59	1 (33%)	3,3,3	0.61	0
31	DMS	D	416	-	3,3,3	2.56	1 (33%)	3,3,3	0.65	0
31	DMS	B	628	-	3,3,3	2.87	1 (33%)	3,3,3	0.78	0
31	DMS	V	208	-	3,3,3	2.66	1 (33%)	3,3,3	0.41	0
22	CLA	b	616	-	69,73,73	2.37	20 (28%)	82,113,113	2.14	27 (32%)
31	DMS	A	419	-	3,3,3	2.73	1 (33%)	3,3,3	0.84	0
22	CLA	c	905	40	69,73,73	2.64	20 (28%)	82,113,113	2.26	28 (34%)
31	DMS	a	425	-	3,3,3	3.08	1 (33%)	3,3,3	0.89	0
31	DMS	v	201	-	3,3,3	2.65	1 (33%)	3,3,3	0.88	0
29	LMT	I	102	-	36,36,36	0.69	1 (2%)	47,47,47	1.39	4 (8%)
31	DMS	c	929	-	3,3,3	2.87	1 (33%)	3,3,3	0.85	0
24	BCR	b	618	-	20,20,41	0.95	1 (5%)	27,27,56	1.76	5 (18%)
31	DMS	l	104	-	3,3,3	2.83	1 (33%)	3,3,3	0.59	0
22	CLA	C	514	-	69,73,73	2.64	20 (28%)	82,113,113	2.27	25 (30%)
24	BCR	A	409	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
31	DMS	O	303	-	3,3,3	2.81	1 (33%)	3,3,3	0.79	0
31	DMS	O	305	-	3,3,3	2.97	1 (33%)	3,3,3	0.86	0
25	LMG	C	520	-	51,51,55	1.08	2 (3%)	59,59,63	1.24	6 (10%)
31	DMS	v	208	-	3,3,3	2.69	1 (33%)	3,3,3	0.54	0
22	CLA	c	903	-	69,73,73	2.02	18 (26%)	82,113,113	2.30	26 (31%)
22	CLA	D	404	-	69,73,73	2.41	18 (26%)	82,113,113	2.03	23 (28%)
31	DMS	A	420	-	3,3,3	2.81	1 (33%)	3,3,3	1.37	0
22	CLA	c	910	-	69,73,73	2.17	18 (26%)	82,113,113	2.29	31 (37%)
31	DMS	b	629	-	3,3,3	2.33	1 (33%)	3,3,3	1.12	0
31	DMS	B	640	-	3,3,3	2.69	1 (33%)	3,3,3	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	c	925	-	3,3,3	2.72	1 (33%)	3,3,3	1.13	0
24	BCR	y	101	-	41,41,41	0.91	0	56,56,56	1.63	13 (23%)
22	CLA	b	608	40	69,73,73	2.42	21 (30%)	82,113,113	2.22	25 (30%)
31	DMS	B	635	-	3,3,3	2.84	1 (33%)	3,3,3	0.71	0
31	DMS	C	524	-	3,3,3	2.54	1 (33%)	3,3,3	0.87	0
31	DMS	a	421	-	3,3,3	2.72	1 (33%)	3,3,3	0.62	0
22	CLA	b	604	-	69,73,73	2.60	20 (28%)	82,113,113	2.27	27 (32%)
22	CLA	D	403	-	69,73,73	2.04	19 (27%)	82,113,113	2.43	28 (34%)
31	DMS	L	102	-	3,3,3	2.81	1 (33%)	3,3,3	0.97	0
27	LHG	A	412	-	30,30,48	1.41	2 (6%)	33,35,54	1.48	4 (12%)
31	DMS	A	416	-	3,3,3	2.73	1 (33%)	3,3,3	1.08	0
22	CLA	B	613	-	69,73,73	2.63	22 (31%)	82,113,113	2.09	32 (39%)
31	DMS	C	527	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
31	DMS	U	202	-	3,3,3	2.84	1 (33%)	3,3,3	1.31	0
22	CLA	b	617	-	64,68,73	2.88	21 (32%)	76,107,113	2.49	31 (40%)
22	CLA	B	611	40	69,73,73	2.90	20 (28%)	82,113,113	2.32	23 (28%)
25	LMG	B	621	-	40,40,55	1.26	3 (7%)	48,48,63	1.40	8 (16%)
22	CLA	B	610	-	69,73,73	2.38	21 (30%)	82,113,113	2.14	24 (29%)
34	HTG	V	203	-	14,14,19	0.65	0	18,19,24	2.97	7 (38%)
29	LMT	t	101	-	24,24,36	0.45	0	29,29,47	1.33	3 (10%)
34	HTG	b	627	-	19,19,19	0.97	2 (10%)	23,24,24	1.66	3 (13%)
25	LMG	c	920	-	51,51,55	0.99	2 (3%)	59,59,63	1.10	6 (10%)
22	CLA	c	912	3	69,73,73	2.87	18 (26%)	82,113,113	2.11	25 (30%)
22	CLA	B	603	-	69,73,73	2.57	23 (33%)	82,113,113	2.36	35 (42%)
31	DMS	c	940	-	3,3,3	2.79	1 (33%)	3,3,3	0.59	0
22	CLA	a	407	-	69,73,73	2.32	20 (28%)	82,113,113	2.11	29 (35%)
22	CLA	a	408	40	69,73,73	2.55	20 (28%)	82,113,113	2.43	31 (37%)
31	DMS	B	632	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
31	DMS	b	631	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
22	CLA	B	616	-	69,73,73	2.64	21 (30%)	82,113,113	2.20	26 (31%)
22	CLA	b	602	40	69,73,73	3.32	19 (27%)	82,113,113	2.39	23 (28%)
22	CLA	b	614	-	63,67,73	2.36	19 (30%)	74,105,113	2.39	25 (33%)
22	CLA	d	403	-	69,73,73	2.89	21 (30%)	82,113,113	2.12	26 (31%)
22	CLA	C	506	-	69,73,73	2.57	19 (27%)	82,113,113	2.15	24 (29%)
22	CLA	c	902	-	69,73,73	2.45	19 (27%)	82,113,113	2.36	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	D	407	-	50,50,67	1.18	3 (6%)	58,58,81	1.32	6 (10%)
31	DMS	c	939	-	3,3,3	2.83	1 (33%)	3,3,3	0.67	0
27	LHG	a	416	-	48,48,48	1.13	2 (4%)	51,54,54	1.20	4 (7%)
31	DMS	o	305	-	3,3,3	2.66	1 (33%)	3,3,3	0.68	0
22	CLA	C	502	-	69,73,73	2.11	21 (30%)	82,113,113	2.29	26 (31%)
31	DMS	C	530	-	3,3,3	2.74	1 (33%)	3,3,3	0.86	0
24	BCR	Y	101	-	40,40,41	0.91	1 (2%)	52,54,56	1.73	15 (28%)
22	CLA	B	614	-	65,69,73	2.30	17 (26%)	77,108,113	2.09	26 (33%)
34	HTG	l	106	-	19,19,19	0.93	2 (10%)	23,24,24	1.85	3 (13%)
31	DMS	O	312	-	3,3,3	2.69	1 (33%)	3,3,3	0.98	0
26	PL9	d	405	-	55,55,55	1.05	4 (7%)	68,69,69	1.45	8 (11%)
22	CLA	A	406	40	59,63,73	2.29	21 (35%)	70,101,113	2.58	32 (45%)
31	DMS	B	629	-	3,3,3	2.60	1 (33%)	3,3,3	1.21	0
31	DMS	c	933	-	3,3,3	2.90	1 (33%)	3,3,3	0.94	0
22	CLA	c	913	-	69,73,73	2.49	24 (34%)	82,113,113	2.17	27 (32%)
28	SQD	a	418	-	49,51,54	1.10	2 (4%)	59,62,65	1.47	8 (13%)
36	HEM	e	101	5,6	50,50,50	2.05	9 (18%)	67,82,82	1.34	6 (8%)
31	DMS	c	926	-	3,3,3	2.66	1 (33%)	3,3,3	0.80	0
31	DMS	B	641	-	3,3,3	2.82	1 (33%)	3,3,3	0.86	0
39	HEC	v	202	15	46,50,50	2.11	7 (15%)	58,82,82	1.37	8 (13%)
22	CLA	a	409	40	65,69,73	2.15	20 (30%)	77,108,113	2.59	33 (42%)
29	LMT	f	102	-	25,25,36	1.02	1 (4%)	30,30,47	1.25	5 (16%)
31	DMS	a	424	-	3,3,3	2.78	1 (33%)	3,3,3	1.05	0
31	DMS	c	928	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
31	DMS	v	206	-	3,3,3	2.75	1 (33%)	3,3,3	0.75	0
34	HTG	b	624	-	19,19,19	1.00	1 (5%)	23,24,24	1.99	6 (26%)
24	BCR	b	620	-	41,41,41	0.86	1 (2%)	56,56,56	1.37	8 (14%)
31	DMS	H	103	-	3,3,3	2.98	1 (33%)	3,3,3	1.22	0
31	DMS	a	402	-	3,3,3	2.44	1 (33%)	3,3,3	0.74	0

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
25	LMG	C	520	-	-	19/46/66/70	0/1/1/1
25	LMG	j	101	38	-	13/42/62/70	0/1/1/1
22	CLA	c	903	-	1/1/15/20	9/39/115/115	-
22	CLA	D	404	-	1/1/15/20	9/39/115/115	-
34	HTG	b	626	-	-	6/10/30/30	0/1/1/1
22	CLA	b	612	-	-	9/39/115/115	-
22	CLA	C	512	3	-	1/39/115/115	-
22	CLA	a	412	-	-	13/39/115/115	-
24	BCR	C	515	-	-	3/29/63/63	0/2/2/2
22	CLA	C	503	-	1/1/15/20	8/39/115/115	-
27	LHG	D	411	-	-	11/49/49/53	-
37	RRX	h	101	-	-	8/29/65/65	0/2/2/2
22	CLA	c	914	-	-	15/39/115/115	-
24	BCR	a	413	-	-	1/29/63/63	0/2/2/2
22	CLA	B	617	-	1/1/13/20	4/27/103/115	-
22	CLA	c	910	-	1/1/15/20	16/39/115/115	-
34	HTG	B	626	-	-	2/10/30/30	0/1/1/1
34	HTG	C	521	-	-	4/10/30/30	0/1/1/1
27	LHG	d	407	-	-	19/53/53/53	-
34	HTG	B	627	-	-	7/10/30/30	0/1/1/1
34	HTG	D	414	-	-	3/10/30/30	0/1/1/1
29	LMT	a	419	-	-	14/21/61/61	0/2/2/2
23	PHO	a	411	-	-	6/37/103/103	0/5/6/6
29	LMT	c	921	-	-	11/21/61/61	0/2/2/2
35	DGD	c	918	-	-	22/51/91/95	0/2/2/2
27	LHG	d	401	-	-	15/34/34/53	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	b	608	40	1/1/15/20	15/39/115/115	-
22	CLA	C	505	40	-	4/39/115/115	-
22	CLA	D	401	40	-	4/39/115/115	-
37	RRX	H	101	-	-	1/29/65/65	0/2/2/2
26	PL9	D	406	-	-	5/53/73/73	0/1/1/1
22	CLA	B	605	-	1/1/15/20	8/39/115/115	-
22	CLA	C	510	-	1/1/15/20	11/39/115/115	-
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	D	412	-	-	15/41/61/70	0/1/1/1
27	LHG	L	101	-	-	18/44/44/53	-
28	SQD	C	501	-	-	26/49/69/69	0/1/1/1
22	CLA	b	604	-	1/1/15/20	10/39/115/115	-
28	SQD	l	101	-	-	32/49/69/69	0/1/1/1
35	DGD	C	518	-	-	22/51/91/95	0/2/2/2
35	DGD	C	519	-	-	28/51/91/95	0/2/2/2
23	PHO	D	402	-	-	6/37/103/103	0/5/6/6
22	CLA	D	403	-	1/1/15/20	0/39/115/115	-
35	DGD	C	517	-	-	17/51/91/95	0/2/2/2
22	CLA	C	504	-	-	2/39/115/115	-
28	SQD	D	408	-	-	2/12/32/69	0/1/1/1
39	HEC	V	202	15	-	6/14/54/54	-
24	BCR	B	619	-	-	0/24/41/63	0/1/1/2
22	CLA	b	609	-	-	7/39/115/115	-
35	DGD	c	917	-	-	21/51/91/95	0/2/2/2
22	CLA	b	615	-	1/1/12/20	4/24/100/115	-
27	LHG	A	412	-	-	14/33/33/53	-
26	PL9	A	411	-	-	12/53/73/73	0/1/1/1
28	SQD	a	414	-	-	27/49/69/69	0/1/1/1
25	LMG	b	622	-	-	20/38/58/70	0/1/1/1
22	CLA	B	613	-	1/1/15/20	4/39/115/115	-
23	PHO	a	410	-	-	1/37/103/103	0/5/6/6
34	HTG	b	632	-	-	5/10/30/30	0/1/1/1
34	HTG	b	623	-	-	6/10/30/30	0/1/1/1
24	BCR	K	101	-	-	3/29/63/63	0/2/2/2
22	CLA	b	606	-	1/1/15/20	4/39/115/115	-
22	CLA	b	617	-	1/1/14/20	8/33/109/115	-
22	CLA	c	908	40	1/1/15/20	12/39/115/115	-
22	CLA	B	611	40	1/1/15/20	9/39/115/115	-
24	BCR	c	916	-	-	4/29/63/63	0/2/2/2
24	BCR	c	915	-	-	1/29/63/63	0/2/2/2
22	CLA	B	602	40	1/1/15/20	23/39/115/115	-
22	CLA	B	606	-	-	10/39/115/115	-
25	LMG	i	101	-	-	26/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	A	414	-	-	14/21/61/61	0/2/2/2
22	CLA	C	509	-	1/1/15/20	9/39/115/115	-
22	CLA	c	906	-	1/1/15/20	8/39/115/115	-
29	LMT	B	622	-	-	8/15/35/61	0/1/1/2
25	LMG	B	621	-	-	23/35/55/70	0/1/1/1
22	CLA	B	610	-	1/1/15/20	2/39/115/115	-
24	BCR	B	618	-	-	0/11/28/63	0/1/1/2
25	LMG	J	101	38	-	9/40/60/70	0/1/1/1
22	CLA	C	508	40	1/1/15/20	10/39/115/115	-
22	CLA	B	609	-	-	2/39/115/115	-
34	HTG	V	203	-	-	0/5/25/30	0/1/1/1
29	LMT	t	101	-	-	10/15/35/61	0/1/1/2
22	CLA	B	607	-	1/1/15/20	12/39/115/115	-
29	LMT	T	102	-	-	10/15/35/61	0/1/1/2
27	LHG	C	522	-	-	14/31/31/53	-
24	BCR	b	619	-	-	4/26/43/63	0/1/1/2
29	LMT	c	931	-	-	11/15/35/61	0/1/1/2
34	HTG	b	627	-	-	3/10/30/30	0/1/1/1
35	DGD	d	406	-	-	31/44/44/95	-
25	LMG	c	920	-	-	21/46/66/70	0/1/1/1
22	CLA	c	912	3	-	4/39/115/115	-
22	CLA	c	904	-	-	6/39/115/115	-
24	BCR	D	405	-	-	4/29/63/63	0/2/2/2
34	HTG	C	532	-	-	6/10/30/30	0/1/1/1
22	CLA	B	603	-	1/1/15/20	4/39/115/115	-
27	LHG	D	410	-	-	10/53/53/53	-
22	CLA	b	605	-	1/1/15/20	11/39/115/115	-
22	CLA	B	604	-	1/1/15/20	6/39/115/115	-
25	LMG	C	531	-	-	13/35/55/70	0/1/1/1
25	LMG	A	410	-	-	27/46/66/70	0/1/1/1
22	CLA	b	611	40	1/1/15/20	6/39/115/115	-
35	DGD	h	102	-	-	18/51/91/95	0/2/2/2
22	CLA	a	407	-	1/1/15/20	6/39/115/115	-
28	SQD	A	413	-	-	26/44/64/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
22	CLA	a	408	40	1/1/15/20	4/39/115/115	-
28	SQD	f	101	-	-	4/12/12/69	-
25	LMG	d	409	-	-	28/42/62/70	0/1/1/1
22	CLA	B	616	-	1/1/15/20	12/39/115/115	-
23	PHO	A	407	-	-	2/37/103/103	0/5/6/6
22	CLA	c	911	-	1/1/15/20	7/39/115/115	-
22	CLA	b	602	40	1/1/15/20	22/39/115/115	-
34	HTG	D	415	-	-	8/10/30/30	0/1/1/1
22	CLA	b	614	-	1/1/13/20	5/32/108/115	-
22	CLA	b	613	-	1/1/15/20	4/39/115/115	-
22	CLA	d	403	-	-	10/39/115/115	-
28	SQD	b	621	-	-	16/32/52/69	0/1/1/1
35	DGD	H	102	-	-	17/51/91/95	0/2/2/2
22	CLA	C	506	-	1/1/15/20	5/39/115/115	-
22	CLA	C	513	-	1/1/13/20	9/29/105/115	-
22	CLA	A	408	-	1/1/15/20	13/39/115/115	-
22	CLA	c	902	-	1/1/15/20	4/39/115/115	-
35	DGD	D	407	-	-	30/44/64/95	0/1/1/2
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
34	HTG	C	523	-	-	1/6/6/30	-
35	DGD	c	919	-	-	18/51/91/95	0/2/2/2
27	LHG	a	416	-	-	27/53/53/53	-
27	LHG	d	408	-	-	17/50/50/53	-
22	CLA	B	612	-	1/1/15/20	10/39/115/115	-
22	CLA	C	502	-	1/1/15/20	6/39/115/115	-
22	CLA	b	607	-	1/1/15/20	5/39/115/115	-
24	BCR	Y	101	-	-	6/29/60/63	0/2/2/2
22	CLA	B	614	-	1/1/14/20	6/35/111/115	-
34	HTG	l	106	-	-	6/10/30/30	0/1/1/1
22	CLA	b	610	-	-	3/39/115/115	-
26	PL9	d	405	-	-	6/53/73/73	0/1/1/1
34	HTG	c	922	-	-	6/10/30/30	0/1/1/1
22	CLA	A	406	40	-	3/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	507	-	1/1/15/20	10/39/115/115	-
22	CLA	C	511	-	1/1/15/20	10/39/115/115	-
22	CLA	c	907	-	1/1/15/20	10/39/115/115	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
27	LHG	a	423	-	-	20/49/49/53	-
22	CLA	B	608	40	1/1/15/20	5/39/115/115	-
22	CLA	b	603	-	1/1/15/20	3/39/115/115	-
34	HTG	v	203	-	-	4/7/27/30	0/1/1/1
26	PL9	a	415	-	-	17/53/73/73	0/1/1/1
29	LMT	E	101	-	-	9/15/35/61	0/1/1/2
22	CLA	c	913	-	1/1/15/20	20/39/115/115	-
22	CLA	d	402	-	1/1/15/20	9/39/115/115	-
28	SQD	a	418	-	-	22/46/66/69	0/1/1/1
36	HEM	e	101	5,6	-	7/14/54/54	-
22	CLA	b	616	-	1/1/15/20	9/39/115/115	-
27	LHG	l	102	-	-	26/53/53/53	-
36	HEM	E	102	5,6	-	1/14/54/54	-
22	CLA	c	905	40	-	14/39/115/115	-
39	HEC	v	202	15	-	6/14/54/54	-
22	CLA	a	409	40	-	8/35/111/115	-
29	LMT	f	102	-	-	10/17/37/61	0/1/1/2
22	CLA	B	615	-	1/1/12/20	9/25/101/115	-
22	CLA	c	909	-	-	10/39/115/115	-
27	LHG	D	409	-	-	14/53/53/53	-
29	LMT	I	102	-	-	11/21/61/61	0/2/2/2
25	LMG	c	930	-	-	12/44/64/70	0/1/1/1
22	CLA	A	405	-	1/1/15/20	6/39/115/115	-
24	BCR	b	618	-	-	7/13/30/63	0/1/1/2
34	HTG	b	624	-	-	4/10/30/30	0/1/1/1
22	CLA	C	514	-	-	18/39/115/115	-
24	BCR	A	409	-	-	2/29/63/63	0/2/2/2
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	BCR	k	101	-	-	4/29/63/63	0/2/2/2

All (1770) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	MG-NA	19.40	2.52	2.06
22	B	606	CLA	MG-NA	15.87	2.44	2.06
22	b	617	CLA	MG-NA	15.18	2.42	2.06
22	c	912	CLA	MG-NA	14.71	2.41	2.06
22	B	602	CLA	MG-NA	14.39	2.40	2.06
22	b	603	CLA	MG-NA	14.14	2.39	2.06
22	C	505	CLA	MG-NA	13.78	2.39	2.06
22	b	604	CLA	MG-NA	13.69	2.38	2.06
22	c	908	CLA	MG-NA	13.08	2.37	2.06
22	c	905	CLA	MG-NA	12.88	2.36	2.06
22	c	904	CLA	MG-NA	12.83	2.36	2.06
22	c	909	CLA	MG-NB	12.56	2.30	2.05
22	B	613	CLA	MG-NA	12.32	2.35	2.06
22	b	613	CLA	MG-NA	12.17	2.35	2.06
22	A	405	CLA	MG-NC	11.62	2.33	2.06
22	C	506	CLA	MG-NA	11.61	2.33	2.06
22	c	909	CLA	MG-NA	11.40	2.33	2.06
22	B	611	CLA	MG-NB	11.40	2.28	2.05
22	C	512	CLA	MG-NA	11.28	2.33	2.06
22	B	611	CLA	MG-NC	11.25	2.33	2.06
22	C	514	CLA	MG-NA	10.98	2.32	2.06
22	D	404	CLA	MG-NC	10.68	2.31	2.06
22	b	615	CLA	MG-NA	10.66	2.31	2.06
22	B	616	CLA	MG-NA	10.56	2.31	2.06
22	B	609	CLA	MG-ND	10.48	2.26	2.05
23	D	402	PHO	C1B-C2B	10.21	1.50	1.39
23	a	410	PHO	C1B-C2B	10.18	1.50	1.39
22	C	503	CLA	MG-NA	10.17	2.30	2.06
22	a	408	CLA	MG-NB	10.09	2.25	2.05
22	c	902	CLA	MG-NA	9.92	2.29	2.06
22	C	505	CLA	MG-ND	9.80	2.25	2.05
22	C	504	CLA	MG-NC	9.77	2.29	2.06
22	b	610	CLA	MG-NA	9.74	2.29	2.06
22	C	513	CLA	MG-NA	9.70	2.29	2.06
22	b	614	CLA	MG-NA	9.53	2.28	2.06
22	a	408	CLA	MG-ND	-9.49	1.87	2.05
22	b	608	CLA	MG-NA	9.39	2.28	2.06
22	B	615	CLA	MG-NC	9.39	2.28	2.06
22	b	616	CLA	MG-NA	9.38	2.28	2.06
22	B	603	CLA	MG-ND	-9.34	1.87	2.05
23	a	411	PHO	C1B-C2B	9.33	1.49	1.39
22	B	616	CLA	MG-NB	9.06	2.23	2.05
22	b	605	CLA	MG-NA	9.04	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	MG-NC	9.04	2.27	2.06
22	C	509	CLA	MG-NA	8.92	2.27	2.06
22	B	614	CLA	MG-NA	8.89	2.27	2.06
23	a	411	PHO	C1D-C2D	8.88	1.49	1.39
22	b	612	CLA	MG-NA	8.87	2.27	2.06
23	a	410	PHO	C1D-C2D	8.78	1.49	1.39
23	D	402	PHO	C1D-C2D	8.74	1.49	1.39
22	b	610	CLA	MG-ND	8.55	2.22	2.05
22	B	608	CLA	MG-NA	8.51	2.26	2.06
22	c	914	CLA	MG-NC	8.49	2.26	2.06
22	d	403	CLA	MG-NA	8.48	2.26	2.06
22	b	607	CLA	MG-NA	8.43	2.26	2.06
23	A	407	PHO	C1D-C2D	8.43	1.48	1.39
22	B	610	CLA	MG-NB	8.40	2.22	2.05
22	B	604	CLA	MG-NA	8.37	2.26	2.06
22	C	513	CLA	MG-NB	8.37	2.22	2.05
22	b	611	CLA	MG-NC	8.35	2.26	2.06
22	c	909	CLA	MG-ND	-8.26	1.89	2.05
22	c	906	CLA	MG-NA	8.26	2.25	2.06
22	C	504	CLA	MG-NA	8.13	2.25	2.06
22	B	612	CLA	MG-NA	8.10	2.25	2.06
22	C	508	CLA	MG-NA	8.09	2.25	2.06
22	c	912	CLA	MG-NC	8.05	2.25	2.06
22	B	607	CLA	MG-NA	8.00	2.25	2.06
22	d	403	CLA	MG-ND	-7.95	1.90	2.05
22	B	607	CLA	MG-NC	7.92	2.25	2.06
36	e	101	HEM	C3D-C2D	7.85	1.53	1.36
36	E	102	HEM	C3D-C2D	7.83	1.53	1.36
22	C	511	CLA	MG-NA	7.83	2.24	2.06
22	a	407	CLA	MG-NA	7.78	2.24	2.06
23	A	407	PHO	C1B-C2B	7.75	1.48	1.39
22	B	609	CLA	MG-NC	7.71	2.24	2.06
22	C	507	CLA	MG-NA	7.71	2.24	2.06
22	c	907	CLA	MG-NA	7.68	2.24	2.06
22	c	913	CLA	MG-NC	7.66	2.24	2.06
22	d	403	CLA	MG-NB	7.60	2.20	2.05
22	D	403	CLA	MG-NA	7.55	2.24	2.06
22	c	909	CLA	MG-NC	7.45	2.24	2.06
23	D	402	PHO	C3B-C4B	7.43	1.49	1.41
22	B	611	CLA	MG-ND	-7.40	1.91	2.05
28	f	101	SQD	C6-S	-7.31	1.67	1.77
22	C	509	CLA	MG-NC	7.29	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	907	CLA	MG-NB	7.15	2.20	2.05
22	C	514	CLA	MG-NC	7.15	2.23	2.06
39	v	202	HEC	CAC-C3C	7.08	1.58	1.35
22	b	609	CLA	MG-NA	7.07	2.23	2.06
22	A	406	CLA	MG-NA	7.05	2.23	2.06
39	V	202	HEC	CAC-C3C	7.04	1.57	1.35
22	b	611	CLA	MG-ND	-7.03	1.91	2.05
22	b	611	CLA	MG-NB	7.03	2.19	2.05
22	c	908	CLA	MG-ND	7.02	2.19	2.05
22	C	505	CLA	MG-NC	6.94	2.22	2.06
22	c	911	CLA	MG-NA	6.94	2.22	2.06
22	c	902	CLA	MG-ND	-6.94	1.92	2.05
22	c	905	CLA	MG-NC	6.93	2.22	2.06
22	B	605	CLA	MG-NA	6.88	2.22	2.06
22	b	606	CLA	MG-NB	6.81	2.19	2.05
39	V	202	HEC	CAB-C3B	6.77	1.57	1.35
39	v	202	HEC	CAB-C3B	6.77	1.57	1.35
23	D	402	PHO	C4D-CHA	6.74	1.49	1.39
22	B	603	CLA	MG-NA	6.71	2.22	2.06
22	b	602	CLA	MG-ND	6.69	2.19	2.05
22	B	617	CLA	MG-NA	6.58	2.21	2.06
22	c	913	CLA	MG-NB	6.56	2.18	2.05
22	C	510	CLA	MG-NA	6.53	2.21	2.06
22	c	913	CLA	MG-NA	6.53	2.21	2.06
23	a	411	PHO	C3B-C4B	6.50	1.48	1.41
23	D	402	PHO	C3B-C2B	6.49	1.49	1.40
22	b	605	CLA	MG-ND	-6.49	1.92	2.05
22	B	603	CLA	MG-NC	6.45	2.21	2.06
22	C	503	CLA	MG-ND	-6.44	1.93	2.05
22	C	511	CLA	MG-ND	-6.35	1.93	2.05
22	a	412	CLA	MG-ND	6.34	2.18	2.05
22	C	508	CLA	MG-NC	6.27	2.21	2.06
22	B	613	CLA	MG-NB	6.24	2.18	2.05
22	C	513	CLA	MG-NC	6.22	2.21	2.06
23	A	407	PHO	C4D-CHA	6.19	1.48	1.39
23	a	410	PHO	C3B-C4B	6.17	1.47	1.41
22	b	605	CLA	MG-NB	6.13	2.17	2.05
22	c	910	CLA	MG-NA	6.08	2.20	2.06
22	a	412	CLA	C3C-C2C	5.99	1.49	1.36
22	C	504	CLA	MG-ND	5.99	2.17	2.05
22	c	909	CLA	C3C-C2C	5.92	1.49	1.36
22	B	610	CLA	CHC-C1C	5.92	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	616	CLA	O2D-CGD	5.91	1.47	1.33
22	C	504	CLA	CHC-C1C	5.90	1.50	1.38
22	B	614	CLA	CHC-C1C	5.90	1.50	1.38
22	a	409	CLA	MG-NA	5.88	2.20	2.06
22	d	402	CLA	MG-NA	5.86	2.20	2.06
22	b	603	CLA	C3C-C2C	5.84	1.49	1.36
22	c	912	CLA	CHD-C1D	5.82	1.49	1.38
22	c	908	CLA	CHC-C1C	5.79	1.50	1.38
22	b	608	CLA	MG-NC	5.78	2.20	2.06
22	b	602	CLA	C3C-C2C	5.78	1.49	1.36
22	c	908	CLA	C3C-C2C	5.76	1.49	1.36
36	E	102	HEM	FE-NA	5.74	2.14	1.95
22	B	606	CLA	MG-NB	5.74	2.17	2.05
22	B	611	CLA	C3C-C2C	5.73	1.49	1.36
22	C	506	CLA	CHC-C1C	5.70	1.49	1.38
22	c	913	CLA	C3C-C2C	5.70	1.49	1.36
22	C	513	CLA	C3C-C2C	5.67	1.49	1.36
22	b	606	CLA	MG-NA	5.65	2.19	2.06
22	C	503	CLA	C3C-C2C	5.63	1.48	1.36
22	B	603	CLA	C3C-C2C	5.63	1.48	1.36
22	c	904	CLA	C3C-C2C	5.63	1.48	1.36
22	B	608	CLA	CHD-C1D	5.62	1.49	1.38
22	b	602	CLA	CHC-C1C	5.61	1.49	1.38
39	v	202	HEC	C3D-C2D	5.61	1.53	1.38
22	b	608	CLA	C3C-C2C	5.61	1.48	1.36
22	B	610	CLA	MG-NA	5.60	2.19	2.06
22	B	615	CLA	CHC-C1C	5.60	1.49	1.38
23	a	411	PHO	C3B-C2B	5.59	1.47	1.40
23	D	402	PHO	O2D-CGD	5.57	1.46	1.33
22	b	602	CLA	O2D-CGD	5.56	1.46	1.33
22	c	905	CLA	O2D-CGD	5.56	1.46	1.33
22	b	603	CLA	MG-ND	5.55	2.16	2.05
22	A	408	CLA	C3C-C2C	5.55	1.48	1.36
22	b	609	CLA	C3C-C2C	5.55	1.48	1.36
22	B	615	CLA	O2A-CGA	5.54	1.49	1.33
23	A	407	PHO	C3B-C2B	5.54	1.47	1.40
22	A	408	CLA	MG-NA	5.53	2.19	2.06
22	c	912	CLA	CHC-C1C	5.52	1.49	1.38
22	b	616	CLA	C3C-C2C	5.50	1.48	1.36
22	C	514	CLA	C3C-C2C	5.50	1.48	1.36
22	b	602	CLA	O2A-CGA	5.50	1.49	1.33
22	b	603	CLA	MG-NB	-5.49	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	617	CLA	C3C-C2C	5.48	1.48	1.36
22	c	909	CLA	O2D-CGD	5.48	1.46	1.33
22	c	902	CLA	CHC-C1C	5.48	1.49	1.38
22	a	409	CLA	MG-NB	5.48	2.16	2.05
22	C	511	CLA	OBD-CAD	5.47	1.31	1.22
23	a	410	PHO	C4D-CHA	5.46	1.47	1.39
22	c	906	CLA	CHC-C1C	5.46	1.49	1.38
22	B	611	CLA	CHC-C1C	5.45	1.49	1.38
22	B	609	CLA	C3C-C2C	5.45	1.48	1.36
22	b	608	CLA	CHD-C1D	5.44	1.49	1.38
22	b	604	CLA	C3C-C2C	5.43	1.48	1.36
22	c	910	CLA	CHD-C1D	5.43	1.49	1.38
22	b	611	CLA	CHC-C1C	5.43	1.49	1.38
22	c	914	CLA	O2D-CGD	5.41	1.46	1.33
22	c	903	CLA	MG-NC	5.41	2.19	2.06
22	b	615	CLA	C3C-C2C	5.41	1.48	1.36
22	b	606	CLA	MG-ND	-5.40	1.95	2.05
22	C	505	CLA	CHD-C1D	5.40	1.49	1.38
22	c	905	CLA	C3C-C2C	5.39	1.48	1.36
22	a	407	CLA	MG-ND	5.39	2.16	2.05
22	c	914	CLA	MG-NA	5.38	2.19	2.06
22	b	617	CLA	CHC-C1C	5.36	1.49	1.38
27	A	412	LHG	O7-C7	5.36	1.47	1.35
22	C	509	CLA	C3C-C2C	5.36	1.48	1.36
22	c	912	CLA	O2D-CGD	5.35	1.46	1.33
22	b	603	CLA	O2D-CGD	5.35	1.46	1.33
22	C	505	CLA	C3C-C2C	5.35	1.48	1.36
22	B	612	CLA	C3C-C2C	5.34	1.48	1.36
22	b	606	CLA	CHC-C1C	5.34	1.49	1.38
22	C	513	CLA	O2D-CGD	5.33	1.46	1.33
22	C	514	CLA	CHC-C1C	5.32	1.49	1.38
22	a	412	CLA	O2D-CGD	5.31	1.46	1.33
22	b	602	CLA	CHD-C1D	5.29	1.48	1.38
22	a	412	CLA	CHD-C1D	5.28	1.48	1.38
22	C	512	CLA	C3C-C2C	5.28	1.48	1.36
22	b	603	CLA	CHC-C1C	5.28	1.49	1.38
31	u	205	DMS	O-S	5.28	1.85	1.50
22	B	610	CLA	MG-NC	5.27	2.18	2.06
23	a	411	PHO	C4D-CHA	5.27	1.47	1.39
22	a	407	CLA	O2D-CGD	5.26	1.46	1.33
22	B	602	CLA	O2D-CGD	5.26	1.46	1.33
22	D	404	CLA	CHC-C1C	5.25	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	617	CLA	C3C-C2C	5.24	1.48	1.36
22	d	403	CLA	O2A-CGA	5.24	1.48	1.33
22	B	607	CLA	CHC-C4B	5.23	1.51	1.39
22	C	513	CLA	CHC-C1C	5.23	1.49	1.38
22	C	506	CLA	C3C-C2C	5.23	1.48	1.36
22	B	602	CLA	CHC-C1C	5.23	1.49	1.38
22	b	610	CLA	CHC-C1C	5.23	1.49	1.38
22	D	404	CLA	C3C-C2C	5.22	1.48	1.36
23	A	407	PHO	C3D-C4D	-5.22	1.34	1.41
22	d	403	CLA	CHC-C1C	5.21	1.48	1.38
22	C	510	CLA	O2D-CGD	5.21	1.46	1.33
22	b	613	CLA	MG-ND	5.21	2.16	2.05
22	b	604	CLA	O2D-CGD	5.21	1.46	1.33
22	C	504	CLA	C3C-C2C	5.20	1.48	1.36
22	B	616	CLA	CHC-C1C	5.20	1.48	1.38
22	d	403	CLA	OBD-CAD	5.20	1.31	1.22
31	a	425	DMS	O-S	5.20	1.84	1.50
22	b	613	CLA	CHC-C1C	5.20	1.48	1.38
22	c	909	CLA	CHC-C1C	5.20	1.48	1.38
22	b	608	CLA	O2D-CGD	5.19	1.46	1.33
31	O	311	DMS	O-S	5.18	1.84	1.50
22	D	404	CLA	CHD-C1D	5.18	1.48	1.38
31	b	638	DMS	O-S	5.18	1.84	1.50
22	C	508	CLA	C3C-C2C	5.18	1.47	1.36
22	c	907	CLA	O2D-CGD	5.18	1.46	1.33
22	c	904	CLA	CHD-C1D	5.17	1.48	1.38
22	A	405	CLA	C3C-C2C	5.17	1.47	1.36
22	D	401	CLA	C3C-C2C	5.15	1.47	1.36
22	a	412	CLA	MG-NC	5.15	2.18	2.06
22	b	615	CLA	O2D-CGD	5.15	1.45	1.33
22	c	910	CLA	O2D-CGD	5.14	1.45	1.33
22	C	514	CLA	CHC-C4B	5.14	1.50	1.39
22	C	502	CLA	MG-NA	5.14	2.18	2.06
22	C	510	CLA	C3C-C2C	5.13	1.47	1.36
22	a	412	CLA	CHC-C1C	5.12	1.48	1.38
22	C	514	CLA	CHD-C1D	5.12	1.48	1.38
22	b	614	CLA	CHC-C1C	5.12	1.48	1.38
22	B	604	CLA	CHD-C1D	5.12	1.48	1.38
22	b	611	CLA	C3C-C2C	5.11	1.47	1.36
23	a	411	PHO	OBD-CAD	5.11	1.29	1.22
22	b	604	CLA	CHD-C1D	5.11	1.48	1.38
22	C	503	CLA	CHC-C1C	5.11	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C3C-C2C	5.10	1.47	1.36
22	c	902	CLA	MG-NB	5.10	2.15	2.05
22	B	609	CLA	CHD-C1D	5.10	1.48	1.38
22	b	609	CLA	CHD-C1D	5.10	1.48	1.38
22	b	609	CLA	CHC-C1C	5.09	1.48	1.38
22	C	512	CLA	O2D-CGD	5.09	1.45	1.33
22	C	508	CLA	CHC-C1C	5.08	1.48	1.38
22	b	606	CLA	C3C-C2C	5.08	1.47	1.36
22	B	612	CLA	O2D-CGD	5.07	1.45	1.33
22	B	605	CLA	CHD-C1D	5.06	1.48	1.38
22	B	607	CLA	C3C-C2C	5.06	1.47	1.36
22	d	402	CLA	CHC-C1C	5.05	1.48	1.38
22	b	603	CLA	CHD-C4C	5.04	1.50	1.39
22	a	407	CLA	CHC-C1C	5.04	1.48	1.38
22	C	507	CLA	O2D-CGD	5.04	1.45	1.33
22	B	604	CLA	C3C-C2C	5.03	1.47	1.36
23	D	402	PHO	C3D-C4D	-5.03	1.34	1.41
22	c	906	CLA	C3C-C2C	5.03	1.47	1.36
22	c	902	CLA	C3C-C2C	5.03	1.47	1.36
27	a	416	LHG	O8-C23	5.03	1.48	1.33
22	C	507	CLA	CHC-C1C	5.03	1.48	1.38
36	e	101	HEM	FE-NA	5.03	2.11	1.95
22	C	502	CLA	CHC-C1C	5.02	1.48	1.38
22	B	602	CLA	CHD-C1D	5.02	1.48	1.38
22	A	406	CLA	O2D-CGD	5.02	1.45	1.33
22	C	506	CLA	CHD-C1D	5.02	1.48	1.38
22	c	907	CLA	C3C-C2C	5.01	1.47	1.36
35	D	407	DGD	O2G-C1B	5.01	1.48	1.34
22	c	906	CLA	CHD-C1D	5.00	1.48	1.38
22	A	406	CLA	MG-NB	-5.00	1.95	2.05
22	d	403	CLA	C3C-C2C	5.00	1.47	1.36
22	C	505	CLA	CHC-C1C	4.99	1.48	1.38
22	C	502	CLA	C3C-C2C	4.99	1.47	1.36
22	C	512	CLA	MG-NB	4.99	2.15	2.05
22	b	613	CLA	O2D-CGD	4.99	1.45	1.33
22	B	604	CLA	O2D-CGD	4.98	1.45	1.33
22	a	408	CLA	CHC-C1C	4.98	1.48	1.38
25	b	622	LMG	O8-C28	4.98	1.47	1.33
22	C	505	CLA	CHD-C4C	4.97	1.50	1.39
22	c	914	CLA	CHC-C1C	4.97	1.48	1.38
31	H	103	DMS	O-S	4.95	1.82	1.50
22	c	904	CLA	CHC-C1C	4.95	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	CHD-C1D	4.95	1.48	1.38
22	c	910	CLA	OBD-CAD	4.94	1.31	1.22
22	B	615	CLA	O2D-CGD	4.94	1.45	1.33
31	O	305	DMS	O-S	4.94	1.82	1.50
22	b	602	CLA	CHB-C1B	4.94	1.50	1.39
22	B	607	CLA	CHC-C1C	4.94	1.48	1.38
31	c	937	DMS	O-S	4.94	1.82	1.50
22	b	611	CLA	O2D-CGD	4.93	1.45	1.33
22	b	615	CLA	CHD-C1D	4.93	1.48	1.38
22	b	614	CLA	C3C-C2C	4.93	1.47	1.36
22	b	607	CLA	C3C-C2C	4.93	1.47	1.36
22	B	602	CLA	O2A-CGA	4.93	1.47	1.33
22	C	514	CLA	MG-NB	4.93	2.15	2.05
31	B	628	DMS	O-S	4.92	1.82	1.50
22	B	602	CLA	C3C-C2C	4.92	1.47	1.36
22	b	614	CLA	O2D-CGD	4.92	1.45	1.33
22	c	912	CLA	C3C-C2C	4.91	1.47	1.36
22	B	606	CLA	CHC-C1C	4.91	1.48	1.38
22	b	616	CLA	O2D-CGD	4.90	1.45	1.33
25	D	412	LMG	O8-C28	4.90	1.47	1.33
22	c	911	CLA	CHC-C1C	4.90	1.48	1.38
31	c	933	DMS	O-S	4.90	1.82	1.50
31	v	210	DMS	O-S	4.89	1.82	1.50
22	C	509	CLA	CHC-C1C	4.89	1.48	1.38
31	c	924	DMS	O-S	4.89	1.82	1.50
22	A	408	CLA	O2D-CGD	4.89	1.45	1.33
36	e	101	HEM	FE-NC	4.89	2.11	1.95
22	C	514	CLA	O2D-CGD	4.88	1.45	1.33
35	d	406	DGD	O2G-C1B	4.88	1.48	1.34
22	c	907	CLA	CHD-C1D	4.88	1.47	1.38
31	B	630	DMS	O-S	4.88	1.82	1.50
22	B	609	CLA	CHC-C1C	4.87	1.48	1.38
22	B	603	CLA	MG-NB	4.87	2.15	2.05
22	d	403	CLA	CHD-C1D	4.87	1.47	1.38
22	C	511	CLA	MG-NC	4.87	2.17	2.06
22	b	612	CLA	CHB-C1B	4.86	1.50	1.39
22	b	610	CLA	O2D-CGD	4.86	1.45	1.33
22	B	613	CLA	O2D-CGD	4.86	1.45	1.33
31	o	304	DMS	O-S	4.86	1.82	1.50
22	C	511	CLA	O2D-CGD	4.86	1.45	1.33
22	c	914	CLA	C3C-C2C	4.86	1.47	1.36
22	B	616	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	406	DGD	O1G-C1A	4.85	1.47	1.33
22	a	409	CLA	MG-ND	-4.85	1.96	2.05
22	c	913	CLA	CHC-C1C	4.83	1.48	1.38
22	B	603	CLA	CHC-C1C	4.83	1.48	1.38
22	C	504	CLA	CHC-C4B	4.83	1.50	1.39
23	D	402	PHO	OBD-CAD	4.83	1.28	1.22
25	B	621	LMG	O8-C28	4.81	1.47	1.33
31	B	634	DMS	O-S	4.81	1.82	1.50
22	a	408	CLA	C3C-C2C	4.81	1.47	1.36
31	V	211	DMS	O-S	4.81	1.82	1.50
31	c	929	DMS	O-S	4.81	1.82	1.50
22	c	903	CLA	CHC-C1C	4.81	1.48	1.38
22	c	906	CLA	CHD-C4C	4.80	1.50	1.39
31	B	635	DMS	O-S	4.79	1.81	1.50
22	A	408	CLA	CHD-C1D	4.78	1.47	1.38
25	D	412	LMG	O7-C10	4.78	1.47	1.34
31	o	308	DMS	O-S	4.78	1.81	1.50
36	e	101	HEM	FE-ND	4.78	2.09	1.94
22	B	604	CLA	MG-NC	4.77	2.17	2.06
31	B	637	DMS	O-S	4.77	1.81	1.50
22	b	614	CLA	CHD-C1D	4.77	1.47	1.38
22	b	605	CLA	C3C-C2C	4.76	1.47	1.36
22	C	512	CLA	O2A-CGA	4.76	1.47	1.33
31	O	308	DMS	O-S	4.76	1.81	1.50
25	C	531	LMG	O7-C10	4.75	1.47	1.34
22	D	401	CLA	OBD-CAD	4.75	1.30	1.22
31	O	307	DMS	O-S	4.75	1.81	1.50
31	B	641	DMS	O-S	4.75	1.81	1.50
22	b	605	CLA	C4B-NB	-4.75	1.31	1.37
22	c	905	CLA	CHC-C1C	4.75	1.48	1.38
31	c	939	DMS	O-S	4.75	1.81	1.50
31	V	212	DMS	O-S	4.75	1.81	1.50
31	V	210	DMS	O-S	4.75	1.81	1.50
22	b	617	CLA	O2D-CGD	4.75	1.44	1.33
22	c	908	CLA	CHB-C1B	4.75	1.50	1.39
25	c	930	LMG	O7-C10	4.75	1.47	1.34
31	b	635	DMS	O-S	4.75	1.81	1.50
22	b	607	CLA	CHC-C1C	4.74	1.48	1.38
31	C	540	DMS	O-S	4.74	1.81	1.50
31	u	204	DMS	O-S	4.74	1.81	1.50
31	v	211	DMS	O-S	4.74	1.81	1.50
22	B	613	CLA	C3C-C2C	4.74	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	520	LMG	O8-C28	4.74	1.47	1.33
31	l	104	DMS	O-S	4.73	1.81	1.50
22	C	510	CLA	O2A-CGA	4.73	1.47	1.33
35	D	407	DGD	O1G-C1A	4.73	1.47	1.33
31	c	938	DMS	O-S	4.73	1.81	1.50
22	B	615	CLA	CHB-C1B	4.72	1.50	1.39
22	A	408	CLA	MG-NC	4.72	2.17	2.06
22	B	614	CLA	MG-ND	-4.72	1.96	2.05
31	O	303	DMS	O-S	4.72	1.81	1.50
22	C	502	CLA	MG-NC	4.72	2.17	2.06
22	d	402	CLA	C3C-C2C	4.71	1.46	1.36
27	a	416	LHG	O7-C7	4.71	1.47	1.34
31	U	203	DMS	O-S	4.71	1.81	1.50
31	D	417	DMS	O-S	4.71	1.81	1.50
31	V	206	DMS	O-S	4.71	1.81	1.50
22	b	616	CLA	CHB-C1B	4.70	1.50	1.39
22	c	914	CLA	CHB-C1B	4.70	1.50	1.39
22	c	903	CLA	C3C-C2C	4.70	1.46	1.36
22	B	613	CLA	CHD-C1D	4.69	1.47	1.38
31	C	537	DMS	O-S	4.69	1.81	1.50
22	b	612	CLA	O2D-CGD	4.69	1.44	1.33
22	C	510	CLA	CHC-C1C	4.69	1.47	1.38
31	V	207	DMS	O-S	4.69	1.81	1.50
25	i	101	LMG	O8-C28	4.69	1.47	1.33
36	E	102	HEM	FE-ND	4.69	2.09	1.94
22	c	911	CLA	CHD-C1D	4.69	1.47	1.38
31	I	101	DMS	O-S	4.69	1.81	1.50
31	B	639	DMS	O-S	4.68	1.81	1.50
22	b	610	CLA	C3C-C2C	4.68	1.46	1.36
23	a	410	PHO	C3D-C2D	4.68	1.47	1.39
25	c	920	LMG	O8-C28	4.68	1.47	1.33
31	C	533	DMS	O-S	4.68	1.81	1.50
27	C	522	LHG	O7-C7	4.68	1.47	1.34
22	C	508	CLA	CHD-C1D	4.67	1.47	1.38
22	B	603	CLA	CHD-C1D	4.67	1.47	1.38
31	a	401	DMS	O-S	4.67	1.81	1.50
31	C	535	DMS	O-S	4.67	1.81	1.50
31	l	105	DMS	O-S	4.67	1.81	1.50
22	c	908	CLA	CHC-C4B	4.67	1.49	1.39
22	c	914	CLA	CHD-C1D	4.66	1.47	1.38
31	O	314	DMS	O-S	4.66	1.81	1.50
31	c	942	DMS	O-S	4.66	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	CHD-C1D	4.66	1.47	1.38
31	L	102	DMS	O-S	4.66	1.81	1.50
31	a	424	DMS	O-S	4.66	1.81	1.50
22	C	514	CLA	CHB-C1B	4.66	1.49	1.39
31	b	637	DMS	O-S	4.66	1.81	1.50
31	c	940	DMS	O-S	4.65	1.80	1.50
31	b	634	DMS	O-S	4.65	1.80	1.50
31	u	203	DMS	O-S	4.65	1.80	1.50
27	d	401	LHG	O8-C23	4.65	1.46	1.33
31	U	202	DMS	O-S	4.65	1.80	1.50
31	V	204	DMS	O-S	4.64	1.80	1.50
31	d	411	DMS	O-S	4.64	1.80	1.50
31	O	306	DMS	O-S	4.64	1.80	1.50
39	V	202	HEC	C3D-C2D	4.64	1.51	1.38
31	C	536	DMS	O-S	4.64	1.80	1.50
31	f	103	DMS	O-S	4.64	1.80	1.50
22	B	607	CLA	O2D-CGD	4.64	1.44	1.33
31	b	630	DMS	O-S	4.64	1.80	1.50
31	t	104	DMS	O-S	4.64	1.80	1.50
28	a	414	SQD	O48-C23	4.64	1.46	1.33
31	A	419	DMS	O-S	4.63	1.80	1.50
31	c	928	DMS	O-S	4.63	1.80	1.50
22	b	615	CLA	O2A-CGA	4.63	1.46	1.33
31	c	944	DMS	O-S	4.63	1.80	1.50
31	t	103	DMS	O-S	4.63	1.80	1.50
22	b	607	CLA	O2D-CGD	4.63	1.44	1.33
31	B	633	DMS	O-S	4.63	1.80	1.50
22	B	608	CLA	O2D-CGD	4.63	1.44	1.33
31	t	105	DMS	O-S	4.62	1.80	1.50
31	l	103	DMS	O-S	4.62	1.80	1.50
31	o	302	DMS	O-S	4.62	1.80	1.50
22	C	503	CLA	CHD-C1D	4.62	1.47	1.38
31	c	943	DMS	O-S	4.62	1.80	1.50
31	v	207	DMS	O-S	4.62	1.80	1.50
22	C	509	CLA	CHD-C1D	4.61	1.47	1.38
31	A	420	DMS	O-S	4.61	1.80	1.50
22	B	607	CLA	MG-ND	-4.61	1.96	2.05
22	a	407	CLA	CHD-C1D	4.61	1.47	1.38
31	o	303	DMS	O-S	4.61	1.80	1.50
31	C	534	DMS	O-S	4.61	1.80	1.50
22	B	613	CLA	CHC-C1C	4.61	1.47	1.38
22	D	404	CLA	O2D-CGD	4.61	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	913	CLA	O2D-CGD	4.60	1.44	1.33
22	C	510	CLA	CHD-C1D	4.60	1.47	1.38
31	b	631	DMS	O-S	4.60	1.80	1.50
31	d	414	DMS	O-S	4.60	1.80	1.50
31	c	936	DMS	O-S	4.60	1.80	1.50
25	B	621	LMG	O7-C10	4.60	1.47	1.34
22	C	507	CLA	C3C-C2C	4.60	1.46	1.36
31	c	925	DMS	O-S	4.60	1.80	1.50
22	b	607	CLA	CHD-C1D	4.60	1.47	1.38
31	C	539	DMS	O-S	4.59	1.80	1.50
31	v	206	DMS	O-S	4.59	1.80	1.50
31	C	527	DMS	O-S	4.59	1.80	1.50
22	b	616	CLA	CHC-C1C	4.59	1.47	1.38
22	B	608	CLA	CHD-C4C	4.59	1.49	1.39
31	C	530	DMS	O-S	4.59	1.80	1.50
31	I	106	DMS	O-S	4.59	1.80	1.50
22	c	911	CLA	CHC-C4B	4.58	1.49	1.39
22	a	407	CLA	MG-NC	4.58	2.17	2.06
22	c	910	CLA	O2A-CGA	4.58	1.46	1.33
31	A	417	DMS	O-S	4.57	1.80	1.50
22	c	903	CLA	CHD-C1D	4.57	1.47	1.38
22	b	616	CLA	MG-NC	4.57	2.17	2.06
31	b	633	DMS	O-S	4.57	1.80	1.50
31	B	642	DMS	O-S	4.57	1.80	1.50
22	d	402	CLA	O2A-CGA	4.57	1.46	1.33
22	b	610	CLA	CHB-C1B	4.57	1.49	1.39
31	C	529	DMS	O-S	4.56	1.80	1.50
22	A	405	CLA	CHC-C1C	4.56	1.47	1.38
27	A	412	LHG	O8-C23	4.56	1.46	1.33
22	B	614	CLA	C3C-C2C	4.55	1.46	1.36
31	A	416	DMS	O-S	4.55	1.80	1.50
31	b	636	DMS	O-S	4.55	1.80	1.50
31	V	209	DMS	O-S	4.55	1.80	1.50
22	c	913	CLA	CHD-C1D	4.55	1.47	1.38
28	a	418	SQD	O48-C23	4.55	1.46	1.33
31	v	204	DMS	O-S	4.55	1.80	1.50
31	c	927	DMS	O-S	4.55	1.80	1.50
22	c	910	CLA	MG-NC	4.55	2.17	2.06
22	B	613	CLA	CHC-C4B	4.55	1.49	1.39
31	C	538	DMS	O-S	4.55	1.80	1.50
31	F	101	DMS	O-S	4.55	1.80	1.50
22	C	505	CLA	O2D-CGD	4.55	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	934	DMS	O-S	4.54	1.80	1.50
22	B	614	CLA	CHD-C1D	4.54	1.47	1.38
22	d	403	CLA	CHD-C4C	4.54	1.49	1.39
31	B	638	DMS	O-S	4.54	1.80	1.50
22	c	914	CLA	O2A-CGA	4.54	1.46	1.33
25	C	520	LMG	O7-C10	4.54	1.47	1.34
31	c	935	DMS	O-S	4.54	1.80	1.50
22	B	610	CLA	C3C-C2C	4.53	1.46	1.36
22	b	610	CLA	C1D-ND	-4.53	1.31	1.37
31	a	421	DMS	O-S	4.53	1.80	1.50
22	B	612	CLA	CHC-C1C	4.53	1.47	1.38
31	O	310	DMS	O-S	4.53	1.80	1.50
23	a	410	PHO	C3B-C2B	4.52	1.46	1.40
22	b	610	CLA	CHD-C1D	4.52	1.47	1.38
31	B	632	DMS	O-S	4.52	1.80	1.50
22	a	408	CLA	CHD-C4C	4.52	1.49	1.39
22	b	609	CLA	MG-ND	-4.52	1.96	2.05
22	B	609	CLA	O2D-CGD	4.51	1.44	1.33
22	b	613	CLA	C3C-C2C	4.51	1.46	1.36
31	o	306	DMS	O-S	4.51	1.80	1.50
31	i	106	DMS	O-S	4.51	1.80	1.50
31	v	209	DMS	O-S	4.51	1.80	1.50
31	O	312	DMS	O-S	4.51	1.80	1.50
22	b	605	CLA	O2D-CGD	4.51	1.44	1.33
22	B	615	CLA	MG-NA	4.51	2.17	2.06
31	C	526	DMS	O-S	4.50	1.79	1.50
31	C	528	DMS	O-S	4.50	1.79	1.50
31	v	205	DMS	O-S	4.50	1.79	1.50
31	O	313	DMS	O-S	4.50	1.79	1.50
31	c	926	DMS	O-S	4.50	1.79	1.50
22	C	505	CLA	CHB-C1B	4.49	1.49	1.39
22	C	504	CLA	O2A-CGA	4.49	1.46	1.33
31	v	208	DMS	O-S	4.49	1.79	1.50
22	A	408	CLA	MG-NB	-4.49	1.96	2.05
28	l	101	SQD	O48-C23	4.49	1.46	1.33
22	c	912	CLA	CHD-C4C	4.49	1.49	1.39
35	H	102	DGD	O1G-C1A	4.49	1.46	1.33
28	b	621	SQD	O48-C23	4.48	1.46	1.33
31	V	205	DMS	O-S	4.48	1.79	1.50
35	c	919	DGD	O1G-C1A	4.48	1.46	1.33
31	o	307	DMS	O-S	4.48	1.79	1.50
28	l	101	SQD	O47-C7	4.48	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	CHB-C1B	4.48	1.49	1.39
22	B	616	CLA	CHD-C1D	4.48	1.47	1.38
28	a	418	SQD	O47-C7	4.48	1.46	1.34
22	c	911	CLA	C3C-C2C	4.48	1.46	1.36
27	D	409	LHG	O8-C23	4.47	1.46	1.33
22	C	506	CLA	O2D-CGD	4.47	1.44	1.33
22	b	606	CLA	O2D-CGD	4.47	1.44	1.33
22	B	604	CLA	CHB-C1B	4.47	1.49	1.39
31	o	305	DMS	O-S	4.46	1.79	1.50
22	B	605	CLA	C3C-C2C	4.46	1.46	1.36
22	d	403	CLA	O2D-CGD	4.46	1.44	1.33
22	a	407	CLA	C3C-C2C	4.46	1.46	1.36
22	B	613	CLA	MG-ND	-4.46	1.97	2.05
22	C	512	CLA	CHC-C1C	4.46	1.47	1.38
23	A	407	PHO	O2D-CGD	4.45	1.44	1.33
22	b	611	CLA	CHD-C1D	4.45	1.47	1.38
31	B	640	DMS	O-S	4.45	1.79	1.50
22	C	504	CLA	O2D-CGD	4.45	1.44	1.33
22	c	906	CLA	O2D-CGD	4.45	1.44	1.33
25	j	101	LMG	O8-C28	4.45	1.46	1.33
31	V	201	DMS	O-S	4.44	1.79	1.50
22	c	903	CLA	O2D-CGD	4.44	1.44	1.33
31	V	208	DMS	O-S	4.44	1.79	1.50
22	C	506	CLA	MG-NC	4.44	2.16	2.06
22	C	506	CLA	CHD-C4C	4.44	1.49	1.39
31	d	415	DMS	O-S	4.44	1.79	1.50
22	c	909	CLA	CHC-C4B	4.43	1.49	1.39
22	b	615	CLA	CHB-C1B	4.43	1.49	1.39
31	c	941	DMS	O-S	4.43	1.79	1.50
23	a	411	PHO	O2D-CGD	4.43	1.44	1.33
22	b	615	CLA	MG-ND	-4.43	1.97	2.05
31	u	202	DMS	O-S	4.43	1.79	1.50
22	b	602	CLA	CHC-C4B	4.42	1.49	1.39
22	c	913	CLA	O2A-CGA	4.42	1.46	1.33
22	B	610	CLA	O2D-CGD	4.42	1.44	1.33
22	B	605	CLA	OBD-CAD	4.42	1.30	1.22
28	C	501	SQD	O47-C7	4.42	1.46	1.34
31	O	304	DMS	O-S	4.42	1.79	1.50
22	C	512	CLA	CHB-C1B	4.42	1.49	1.39
22	C	503	CLA	O2D-CGD	4.42	1.44	1.33
25	b	622	LMG	O7-C10	4.42	1.46	1.34
25	d	409	LMG	O8-C28	4.42	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	CHD-C1D	4.41	1.47	1.38
25	C	531	LMG	O8-C28	4.41	1.46	1.33
22	c	912	CLA	CHC-C4B	4.41	1.49	1.39
31	B	636	DMS	O-S	4.41	1.79	1.50
27	a	423	LHG	O8-C23	4.41	1.46	1.33
22	c	906	CLA	CHC-C4B	4.41	1.49	1.39
22	C	514	CLA	O2A-CGA	4.40	1.46	1.33
25	A	410	LMG	O8-C28	4.40	1.46	1.33
31	B	629	DMS	O-S	4.40	1.79	1.50
22	B	611	CLA	O2D-CGD	4.40	1.44	1.33
22	b	613	CLA	CHD-C1D	4.40	1.47	1.38
22	A	405	CLA	MG-ND	-4.39	1.97	2.05
22	B	611	CLA	CHB-C1B	4.39	1.49	1.39
22	b	617	CLA	MG-ND	4.38	2.14	2.05
22	A	408	CLA	CHC-C1C	4.38	1.47	1.38
22	a	407	CLA	CHB-C1B	4.38	1.49	1.39
22	c	904	CLA	O2D-CGD	4.38	1.44	1.33
22	D	401	CLA	O2D-CGD	4.38	1.44	1.33
22	b	605	CLA	MG-NC	4.37	2.16	2.06
31	v	201	DMS	O-S	4.37	1.79	1.50
31	d	413	DMS	O-S	4.37	1.79	1.50
25	c	930	LMG	O8-C28	4.37	1.46	1.33
22	B	604	CLA	CHC-C1C	4.37	1.47	1.38
22	c	911	CLA	O2D-CGD	4.37	1.44	1.33
22	A	405	CLA	O2D-CGD	4.36	1.44	1.33
22	c	908	CLA	O2D-CGD	4.36	1.44	1.33
22	B	606	CLA	CHC-C4B	4.36	1.49	1.39
27	C	522	LHG	O8-C23	4.36	1.46	1.33
22	c	909	CLA	CHD-C1D	4.35	1.46	1.38
31	B	631	DMS	O-S	4.35	1.78	1.50
23	a	410	PHO	O2D-CGD	4.35	1.43	1.33
22	B	606	CLA	CHD-C1D	4.34	1.46	1.38
22	A	406	CLA	CHC-C1C	4.34	1.47	1.38
22	b	615	CLA	CHC-C1C	4.34	1.47	1.38
31	d	412	DMS	O-S	4.34	1.78	1.50
22	b	602	CLA	CHD-C4C	4.34	1.49	1.39
35	C	518	DGD	O1G-C1A	4.34	1.46	1.33
22	c	908	CLA	O2A-CGA	4.34	1.46	1.33
22	C	508	CLA	CHC-C4B	4.33	1.49	1.39
22	B	608	CLA	CHC-C1C	4.33	1.47	1.38
22	b	613	CLA	O2A-CGA	4.33	1.46	1.33
35	h	102	DGD	O1G-C1A	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	409	CLA	O2D-CGD	4.32	1.43	1.33
22	c	912	CLA	CHB-C1B	4.32	1.49	1.39
22	b	603	CLA	O2A-CGA	4.32	1.45	1.33
22	C	513	CLA	CHD-C1D	4.32	1.46	1.38
22	c	911	CLA	MG-NC	4.32	2.16	2.06
22	b	603	CLA	CHB-C1B	4.32	1.49	1.39
22	C	511	CLA	CHD-C1D	4.32	1.46	1.38
31	O	309	DMS	O-S	4.32	1.78	1.50
31	c	923	DMS	O-S	4.32	1.78	1.50
22	B	607	CLA	O2A-CGA	4.31	1.45	1.33
22	C	507	CLA	MG-NC	4.31	2.16	2.06
31	D	416	DMS	O-S	4.31	1.78	1.50
22	A	405	CLA	CHD-C1D	4.31	1.46	1.38
22	b	608	CLA	CHC-C1C	4.30	1.47	1.38
22	B	606	CLA	C3C-C2C	4.30	1.46	1.36
22	D	403	CLA	C3C-C2C	4.30	1.46	1.36
22	b	610	CLA	O2A-CGA	4.30	1.45	1.33
22	B	611	CLA	CHD-C1D	4.30	1.46	1.38
23	D	402	PHO	O2A-CGA	4.29	1.45	1.33
22	D	404	CLA	OBD-CAD	4.29	1.29	1.22
22	C	502	CLA	CHD-C1D	4.29	1.46	1.38
22	c	904	CLA	O2A-CGA	4.29	1.45	1.33
22	a	409	CLA	CHC-C1C	4.29	1.47	1.38
22	c	902	CLA	CHD-C1D	4.28	1.46	1.38
22	B	602	CLA	CHB-C1B	4.28	1.49	1.39
22	D	404	CLA	CHB-C1B	4.28	1.49	1.39
22	D	404	CLA	C4C-C3C	4.28	1.52	1.45
22	C	507	CLA	O2A-CGA	4.28	1.45	1.33
22	B	616	CLA	C1B-NB	-4.28	1.32	1.37
22	c	906	CLA	MG-NC	4.28	2.16	2.06
22	B	616	CLA	CHB-C1B	4.27	1.49	1.39
22	c	904	CLA	OBD-CAD	4.27	1.29	1.22
22	A	405	CLA	OBD-CAD	4.27	1.29	1.22
22	b	611	CLA	CHB-C1B	4.27	1.49	1.39
22	B	605	CLA	CHC-C1C	4.27	1.47	1.38
22	d	402	CLA	CHD-C4C	4.26	1.48	1.39
22	c	907	CLA	CHC-C1C	4.26	1.47	1.38
22	C	511	CLA	CHB-C1B	4.26	1.49	1.39
22	C	508	CLA	O2D-CGD	4.26	1.43	1.33
22	D	403	CLA	CHD-C1D	4.26	1.46	1.38
22	a	409	CLA	CHD-C1D	4.26	1.46	1.38
27	d	401	LHG	O7-C7	4.26	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	CHD-C1D	4.26	1.46	1.38
22	d	403	CLA	CHC-C4B	4.25	1.49	1.39
25	i	101	LMG	O7-C10	4.25	1.46	1.34
22	B	609	CLA	O2A-CGA	4.25	1.45	1.33
22	c	909	CLA	CHB-C1B	4.25	1.48	1.39
22	B	614	CLA	MG-NC	4.24	2.16	2.06
22	C	506	CLA	C1D-ND	-4.24	1.32	1.37
22	B	611	CLA	CHC-C4B	4.24	1.48	1.39
22	C	509	CLA	O2D-CGD	4.24	1.43	1.33
22	B	606	CLA	CHB-C1B	4.24	1.48	1.39
35	h	102	DGD	O2G-C1B	4.23	1.46	1.34
22	c	910	CLA	C3C-C2C	4.23	1.45	1.36
22	B	610	CLA	CHD-C1D	4.23	1.46	1.38
22	A	406	CLA	MG-ND	4.23	2.14	2.05
28	a	414	SQD	O47-C7	4.22	1.46	1.34
31	C	524	DMS	O-S	4.22	1.78	1.50
22	b	612	CLA	CHC-C1C	4.22	1.46	1.38
22	b	613	CLA	CHC-C4B	4.22	1.48	1.39
22	B	617	CLA	O2A-CGA	4.22	1.45	1.33
22	c	907	CLA	CHD-C4C	4.22	1.48	1.39
22	B	602	CLA	CHD-C4C	4.21	1.48	1.39
22	D	401	CLA	CHC-C4B	4.21	1.48	1.39
22	B	608	CLA	CHB-C1B	4.20	1.48	1.39
22	b	604	CLA	CHC-C1C	4.20	1.46	1.38
22	B	617	CLA	CHC-C1C	4.20	1.46	1.38
22	C	506	CLA	CHC-C4B	4.20	1.48	1.39
22	c	905	CLA	CHB-C1B	4.19	1.48	1.39
22	C	511	CLA	C3C-C2C	4.19	1.45	1.36
22	b	612	CLA	C3C-C2C	4.19	1.45	1.36
22	B	603	CLA	CHD-C4C	4.18	1.48	1.39
22	B	604	CLA	O2A-CGA	4.18	1.45	1.33
27	l	102	LHG	O7-C7	4.18	1.46	1.34
22	B	617	CLA	O2D-CGD	4.18	1.43	1.33
22	C	504	CLA	CHD-C4C	4.18	1.48	1.39
22	D	401	CLA	MG-NA	4.17	2.16	2.06
22	c	907	CLA	O2A-CGA	4.17	1.45	1.33
22	b	617	CLA	O2A-CGA	4.17	1.45	1.33
22	C	507	CLA	CHD-C4C	4.17	1.48	1.39
22	c	909	CLA	CHD-C4C	4.16	1.48	1.39
25	c	920	LMG	O7-C10	4.16	1.46	1.34
22	b	614	CLA	CHB-C1B	4.16	1.48	1.39
22	C	507	CLA	CHB-C1B	4.15	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	408	LHG	O8-C23	4.15	1.45	1.33
22	d	402	CLA	O2D-CGD	4.15	1.43	1.33
22	C	508	CLA	CHB-C1B	4.14	1.48	1.39
22	c	906	CLA	O2A-CGA	4.14	1.45	1.33
22	C	502	CLA	CHD-C4C	4.14	1.48	1.39
22	b	614	CLA	CHD-C4C	4.13	1.48	1.39
23	A	407	PHO	O2A-CGA	4.13	1.45	1.33
22	b	605	CLA	CHC-C1C	4.13	1.46	1.38
22	d	402	CLA	CHD-C1D	4.13	1.46	1.38
22	B	606	CLA	MG-ND	-4.12	1.97	2.05
22	D	403	CLA	O2A-CGA	4.12	1.45	1.33
25	d	409	LMG	O7-C10	4.12	1.45	1.34
22	b	608	CLA	CHD-C4C	4.12	1.48	1.39
23	a	410	PHO	C3D-C4D	-4.11	1.35	1.41
22	b	609	CLA	O2A-CGA	4.11	1.45	1.33
22	b	616	CLA	CHD-C4C	4.11	1.48	1.39
22	b	617	CLA	CHB-C1B	4.11	1.48	1.39
28	A	413	SQD	O48-C23	4.11	1.45	1.33
22	b	616	CLA	OBD-CAD	4.10	1.29	1.22
22	B	610	CLA	CHB-C1B	4.10	1.48	1.39
22	b	612	CLA	O2A-CGA	4.10	1.45	1.33
31	a	402	DMS	O-S	4.10	1.77	1.50
22	C	511	CLA	CHC-C1C	4.10	1.46	1.38
22	b	605	CLA	CHD-C1D	4.10	1.46	1.38
22	c	902	CLA	O2D-CGD	4.10	1.43	1.33
22	B	605	CLA	CHB-C1B	4.09	1.48	1.39
22	A	406	CLA	OBD-CAD	4.09	1.29	1.22
22	B	610	CLA	O2A-CGA	4.09	1.45	1.33
31	A	418	DMS	O-S	4.09	1.77	1.50
22	d	403	CLA	CHB-C1B	4.08	1.48	1.39
22	D	403	CLA	C1B-C2B	4.08	1.52	1.43
22	b	602	CLA	MG-NB	-4.08	1.97	2.05
22	C	502	CLA	O2D-CGD	4.08	1.43	1.33
25	A	410	LMG	O7-C10	4.08	1.45	1.34
22	b	617	CLA	CHD-C1D	4.07	1.46	1.38
22	B	615	CLA	OBD-CAD	4.07	1.29	1.22
31	C	525	DMS	O-S	4.07	1.77	1.50
22	a	408	CLA	O2D-CGD	4.07	1.43	1.33
22	c	911	CLA	CHD-C4C	4.06	1.48	1.39
31	D	418	DMS	O-S	4.06	1.77	1.50
22	C	510	CLA	OBD-CAD	4.06	1.29	1.22
22	b	608	CLA	CHB-C1B	4.06	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	MG-NB	4.05	2.13	2.05
22	C	513	CLA	CHC-C4B	4.05	1.48	1.39
22	B	605	CLA	O2D-CGD	4.05	1.43	1.33
23	a	411	PHO	C3D-C4D	-4.05	1.35	1.41
22	b	610	CLA	CHC-C4B	4.05	1.48	1.39
22	C	506	CLA	O2A-CGA	4.04	1.45	1.33
22	B	602	CLA	MG-NB	4.04	2.13	2.05
22	b	606	CLA	O2A-CGA	4.04	1.45	1.33
35	C	519	DGD	O1G-C1A	4.04	1.45	1.33
22	c	913	CLA	CHB-C1B	4.03	1.48	1.39
22	B	606	CLA	C1B-NB	-4.03	1.32	1.37
22	c	905	CLA	CHC-C4B	4.03	1.48	1.39
22	c	906	CLA	CHB-C1B	4.03	1.48	1.39
22	b	616	CLA	O2A-CGA	4.03	1.45	1.33
22	a	407	CLA	CHD-C4C	4.03	1.48	1.39
22	c	904	CLA	C1B-NB	-4.03	1.32	1.37
23	D	402	PHO	C3D-C2D	4.02	1.46	1.39
22	c	911	CLA	MG-NB	4.01	2.13	2.05
23	a	411	PHO	C3D-C2D	4.00	1.46	1.39
22	b	610	CLA	OBD-CAD	4.00	1.29	1.22
22	B	614	CLA	CHB-C1B	4.00	1.48	1.39
35	H	102	DGD	O2G-C1B	4.00	1.45	1.34
22	a	412	CLA	O2A-CGA	4.00	1.45	1.33
22	B	608	CLA	C3C-C2C	4.00	1.45	1.36
22	a	412	CLA	CHB-C1B	4.00	1.48	1.39
22	B	616	CLA	CHD-C4C	4.00	1.48	1.39
22	C	512	CLA	CHD-C1D	3.99	1.46	1.38
25	J	101	LMG	O7-C10	3.99	1.45	1.34
22	b	603	CLA	CHD-C1D	3.98	1.46	1.38
22	C	502	CLA	CHB-C1B	3.98	1.48	1.39
22	b	606	CLA	CHC-C4B	3.98	1.48	1.39
22	b	605	CLA	CHC-C4B	3.98	1.48	1.39
22	C	509	CLA	CHC-C4B	3.98	1.48	1.39
22	b	613	CLA	OBD-CAD	3.98	1.29	1.22
22	C	513	CLA	O2A-CGA	3.98	1.44	1.33
22	c	909	CLA	OBD-CAD	3.98	1.29	1.22
22	C	507	CLA	CHC-C4B	3.97	1.48	1.39
22	a	412	CLA	CHD-C4C	3.97	1.48	1.39
22	C	503	CLA	CHC-C4B	3.97	1.48	1.39
22	B	604	CLA	CHD-C4C	3.97	1.48	1.39
22	B	612	CLA	OBD-CAD	3.97	1.29	1.22
22	b	614	CLA	CHC-C4B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	CHB-C1B	3.96	1.48	1.39
34	B	623	HTG	C1'-S1	-3.96	1.75	1.81
22	c	911	CLA	OBD-CAD	3.95	1.29	1.22
22	D	403	CLA	CHB-C1B	3.95	1.48	1.39
22	B	614	CLA	OBD-CAD	3.94	1.29	1.22
22	b	610	CLA	MG-NC	3.94	2.15	2.06
25	J	101	LMG	O8-C28	3.94	1.44	1.33
22	B	608	CLA	OBD-CAD	3.94	1.29	1.22
22	b	611	CLA	C1D-ND	-3.93	1.32	1.37
22	C	509	CLA	CHD-C4C	3.93	1.48	1.39
22	C	502	CLA	O2A-CGA	3.93	1.44	1.33
22	B	602	CLA	CHC-C4B	3.92	1.48	1.39
22	B	614	CLA	O2A-CGA	3.92	1.44	1.33
28	A	413	SQD	O47-C7	3.92	1.45	1.34
22	B	605	CLA	CHD-C4C	3.92	1.48	1.39
27	L	101	LHG	O8-C23	3.92	1.44	1.33
35	c	918	DGD	O1G-C1A	3.91	1.44	1.33
22	c	904	CLA	CHB-C1B	3.91	1.48	1.39
27	l	102	LHG	O8-C23	3.90	1.44	1.33
22	c	911	CLA	C3D-C2D	3.90	1.49	1.39
22	b	615	CLA	CHD-C4C	3.90	1.48	1.39
22	c	903	CLA	MG-NA	3.90	2.15	2.06
22	a	408	CLA	O2A-CGA	3.90	1.44	1.33
22	B	610	CLA	CHC-C4B	3.89	1.48	1.39
22	B	603	CLA	O2D-CGD	3.89	1.42	1.33
22	B	609	CLA	MG-NB	-3.89	1.98	2.05
22	B	615	CLA	CHC-C4B	3.89	1.48	1.39
22	a	409	CLA	O2A-CGA	3.89	1.44	1.33
22	D	404	CLA	CHD-C4C	3.89	1.48	1.39
27	D	411	LHG	O7-C7	3.89	1.45	1.34
22	C	502	CLA	CHC-C4B	3.88	1.48	1.39
22	c	908	CLA	OBD-CAD	3.88	1.29	1.22
35	c	917	DGD	O2G-C1B	3.88	1.45	1.34
22	B	602	CLA	C4C-C3C	3.87	1.51	1.45
22	B	611	CLA	CHD-C4C	3.87	1.48	1.39
22	D	404	CLA	O2A-CGA	3.87	1.44	1.33
22	c	903	CLA	CHB-C1B	3.87	1.48	1.39
27	a	423	LHG	O7-C7	3.87	1.45	1.34
22	C	512	CLA	CHD-C4C	3.87	1.48	1.39
22	B	614	CLA	O2D-CGD	3.87	1.42	1.33
22	C	511	CLA	CHD-C4C	3.86	1.48	1.39
22	c	902	CLA	CHC-C4B	3.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	501	SQD	O48-C23	3.86	1.44	1.33
22	c	914	CLA	CHD-C4C	3.85	1.48	1.39
22	A	406	CLA	CHC-C4B	3.85	1.48	1.39
31	b	629	DMS	O-S	3.85	1.75	1.50
27	L	101	LHG	O7-C7	3.85	1.45	1.34
22	B	603	CLA	O2A-CGA	3.84	1.44	1.33
22	b	611	CLA	CHC-C4B	3.84	1.48	1.39
22	C	509	CLA	CHB-C1B	3.84	1.48	1.39
22	c	914	CLA	MG-ND	3.84	2.13	2.05
27	D	409	LHG	O7-C7	3.83	1.45	1.34
36	E	102	HEM	FE-NC	3.83	2.07	1.95
22	b	607	CLA	CHC-C4B	3.83	1.48	1.39
22	b	608	CLA	CHC-C4B	3.83	1.48	1.39
22	b	608	CLA	C3D-C2D	3.82	1.49	1.39
22	a	408	CLA	OBD-CAD	3.82	1.29	1.22
22	A	408	CLA	CHD-C4C	3.82	1.47	1.39
22	b	609	CLA	OBD-CAD	3.82	1.29	1.22
22	b	612	CLA	CHD-C1D	3.82	1.45	1.38
22	d	403	CLA	C3D-C2D	3.82	1.49	1.39
22	C	504	CLA	CHB-C1B	3.82	1.48	1.39
22	C	505	CLA	CHC-C4B	3.81	1.48	1.39
22	C	513	CLA	CHD-C4C	3.81	1.47	1.39
22	B	616	CLA	O2A-CGA	3.81	1.44	1.33
22	c	909	CLA	O2A-CGA	3.81	1.44	1.33
22	C	509	CLA	O2A-CGA	3.80	1.44	1.33
22	c	910	CLA	CHD-C4C	3.80	1.47	1.39
22	c	914	CLA	CHC-C4B	3.80	1.47	1.39
22	C	512	CLA	OBD-CAD	3.80	1.29	1.22
22	c	913	CLA	MG-ND	-3.79	1.98	2.05
22	C	503	CLA	O2A-CGA	3.79	1.44	1.33
22	B	606	CLA	O2D-CGD	3.79	1.42	1.33
22	b	602	CLA	C3D-C2D	3.78	1.49	1.39
22	b	613	CLA	CHB-C1B	3.77	1.47	1.39
22	C	510	CLA	C4B-NB	-3.77	1.32	1.37
22	C	510	CLA	C3D-C2D	3.77	1.49	1.39
22	b	604	CLA	C1B-NB	-3.76	1.32	1.37
22	C	506	CLA	C4C-C3C	3.76	1.51	1.45
25	j	101	LMG	O7-C10	3.76	1.44	1.34
22	D	401	CLA	CHD-C4C	3.76	1.47	1.39
22	b	609	CLA	O2D-CGD	3.76	1.42	1.33
22	b	606	CLA	CHD-C1D	3.76	1.45	1.38
22	A	405	CLA	CHC-C4B	3.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	C3D-C2D	3.75	1.49	1.39
22	C	504	CLA	OBD-CAD	3.75	1.28	1.22
22	C	506	CLA	OBD-CAD	3.75	1.28	1.22
22	B	612	CLA	O2A-CGA	3.75	1.44	1.33
22	C	514	CLA	CHD-C4C	3.75	1.47	1.39
22	D	404	CLA	CHC-C4B	3.74	1.47	1.39
22	b	609	CLA	CHC-C4B	3.74	1.47	1.39
22	B	612	CLA	CHD-C4C	3.73	1.47	1.39
22	b	602	CLA	OBD-CAD	3.73	1.28	1.22
22	c	908	CLA	CHD-C1D	3.73	1.45	1.38
22	B	617	CLA	CHC-C4B	3.72	1.47	1.39
22	b	604	CLA	C1D-ND	-3.72	1.33	1.37
22	a	409	CLA	CHD-C4C	3.72	1.47	1.39
35	c	919	DGD	O2G-C1B	3.72	1.44	1.34
22	c	903	CLA	CHD-C4C	3.72	1.47	1.39
39	v	202	HEC	CBC-CAC	-3.72	1.35	1.49
22	b	604	CLA	MG-ND	3.71	2.13	2.05
22	b	609	CLA	CHB-C1B	3.71	1.47	1.39
22	d	403	CLA	C4C-C3C	3.69	1.51	1.45
22	c	904	CLA	CHD-C4C	3.69	1.47	1.39
22	b	614	CLA	O2A-CGA	3.69	1.44	1.33
22	c	907	CLA	C1D-ND	-3.69	1.33	1.37
22	c	908	CLA	CHD-C4C	3.69	1.47	1.39
22	a	408	CLA	CHD-C1D	3.68	1.45	1.38
35	c	917	DGD	O1G-C1A	3.68	1.44	1.33
22	A	406	CLA	CHD-C4C	3.68	1.47	1.39
22	C	508	CLA	CHD-C4C	3.68	1.47	1.39
22	b	606	CLA	CHD-C4C	3.67	1.47	1.39
22	B	612	CLA	CHC-C4B	3.67	1.47	1.39
22	b	607	CLA	CHB-C1B	3.67	1.47	1.39
22	B	617	CLA	CHD-C1D	3.67	1.45	1.38
22	a	407	CLA	C4B-NB	-3.67	1.33	1.37
22	c	913	CLA	CHD-C4C	3.67	1.47	1.39
22	B	613	CLA	C1B-NB	-3.67	1.33	1.37
22	b	615	CLA	C3D-C2D	3.67	1.49	1.39
22	D	403	CLA	C3B-C4B	3.67	1.53	1.42
22	B	617	CLA	CHB-C1B	3.66	1.47	1.39
22	b	605	CLA	CHB-C1B	3.66	1.47	1.39
27	D	411	LHG	O8-C23	3.66	1.44	1.33
22	B	612	CLA	C3B-C4B	3.66	1.53	1.42
22	b	611	CLA	CHD-C4C	3.65	1.47	1.39
23	a	411	PHO	O2A-CGA	3.65	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	617	CLA	C1D-ND	-3.65	1.33	1.37
22	B	613	CLA	O2A-CGA	3.65	1.44	1.33
22	B	607	CLA	CHD-C1D	3.64	1.45	1.38
22	A	408	CLA	OBD-CAD	3.64	1.28	1.22
22	D	403	CLA	O2D-CGD	3.63	1.42	1.33
22	B	617	CLA	C3D-C2D	3.63	1.48	1.39
22	B	613	CLA	CHB-C1B	3.63	1.47	1.39
22	c	911	CLA	O2A-CGA	3.63	1.43	1.33
22	a	409	CLA	CHB-C1B	3.63	1.47	1.39
22	b	611	CLA	O2A-CGA	3.63	1.43	1.33
22	b	609	CLA	C4B-NB	-3.63	1.33	1.37
22	c	902	CLA	CHB-C1B	3.63	1.47	1.39
22	C	511	CLA	O2A-CGA	3.63	1.43	1.33
22	B	617	CLA	MG-ND	3.63	2.13	2.05
22	B	617	CLA	CHD-C4C	3.63	1.47	1.39
22	B	615	CLA	CHD-C4C	3.62	1.47	1.39
22	b	604	CLA	CHD-C4C	3.62	1.47	1.39
23	A	407	PHO	C3A-C2A	-3.62	1.51	1.54
22	b	617	CLA	C4D-CHA	3.62	1.50	1.38
22	D	403	CLA	C1D-ND	-3.62	1.33	1.37
22	C	512	CLA	CHC-C4B	3.62	1.47	1.39
22	c	911	CLA	CHB-C1B	3.61	1.47	1.39
22	b	604	CLA	CHC-C4B	3.61	1.47	1.39
22	b	603	CLA	CHC-C4B	3.61	1.47	1.39
22	c	910	CLA	CHB-C1B	3.61	1.47	1.39
22	c	902	CLA	O2A-CGA	3.61	1.43	1.33
22	c	913	CLA	CHC-C4B	3.61	1.47	1.39
22	c	905	CLA	MG-NB	3.60	2.12	2.05
22	b	615	CLA	CHC-C4B	3.60	1.47	1.39
22	a	412	CLA	C4B-NB	-3.60	1.33	1.37
22	C	503	CLA	CHB-C1B	3.60	1.47	1.39
22	B	611	CLA	C3D-C2D	3.59	1.48	1.39
22	a	407	CLA	O2A-CGA	3.59	1.43	1.33
22	c	905	CLA	C3D-C2D	3.59	1.48	1.39
23	a	410	PHO	O2A-CGA	3.59	1.43	1.33
22	a	412	CLA	C1D-ND	-3.59	1.33	1.37
22	c	903	CLA	CHC-C4B	3.59	1.47	1.39
22	c	907	CLA	OBD-CAD	3.59	1.28	1.22
22	d	402	CLA	MG-NC	3.58	2.14	2.06
35	c	918	DGD	O2G-C1B	3.58	1.44	1.34
22	A	408	CLA	O2A-CGA	3.58	1.43	1.33
22	b	616	CLA	CHC-C4B	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	409	CLA	C3C-C2C	3.57	1.44	1.36
22	B	609	CLA	C1D-ND	-3.57	1.33	1.37
22	C	504	CLA	C3D-C2D	3.56	1.48	1.39
22	B	613	CLA	CHD-C4C	3.56	1.47	1.39
22	B	605	CLA	MG-ND	3.56	2.12	2.05
22	c	910	CLA	CHC-C1C	3.56	1.45	1.38
22	c	902	CLA	OBD-CAD	3.56	1.28	1.22
25	b	622	LMG	O1-C1	3.55	1.46	1.40
22	c	913	CLA	OBD-CAD	3.55	1.28	1.22
22	b	605	CLA	C4D-CHA	3.55	1.50	1.38
22	B	609	CLA	CHD-C4C	3.54	1.47	1.39
22	a	407	CLA	CHC-C4B	3.54	1.47	1.39
22	b	605	CLA	O2A-CGA	3.54	1.43	1.33
27	d	408	LHG	O7-C7	3.53	1.44	1.34
22	b	602	CLA	C4D-CHA	3.53	1.50	1.38
22	A	406	CLA	O2A-CGA	3.53	1.43	1.33
22	c	903	CLA	O2A-CGA	3.53	1.43	1.33
22	a	408	CLA	MG-NA	3.53	2.14	2.06
22	b	607	CLA	O2A-CGA	3.52	1.43	1.33
22	b	606	CLA	C1B-C2B	3.52	1.51	1.43
22	b	608	CLA	MG-NB	3.52	2.12	2.05
22	c	905	CLA	CHD-C1D	3.52	1.45	1.38
22	B	611	CLA	O2A-CGA	3.51	1.43	1.33
22	C	511	CLA	CHC-C4B	3.51	1.47	1.39
22	a	408	CLA	C1D-ND	-3.51	1.33	1.37
22	B	603	CLA	CHC-C4B	3.51	1.47	1.39
22	B	605	CLA	O2A-CGA	3.50	1.43	1.33
22	A	408	CLA	CHC-C4B	3.50	1.47	1.39
22	c	910	CLA	C4C-C3C	3.50	1.51	1.45
22	c	905	CLA	O2A-CGA	3.50	1.43	1.33
22	d	402	CLA	CHB-C1B	3.49	1.47	1.39
22	B	606	CLA	O2A-CGA	3.49	1.43	1.33
22	C	509	CLA	MG-NB	3.48	2.12	2.05
22	C	504	CLA	C4D-CHA	3.48	1.50	1.38
22	B	606	CLA	C1D-ND	-3.48	1.33	1.37
22	B	609	CLA	CHC-C4B	3.47	1.47	1.39
22	c	903	CLA	C3D-C2D	3.46	1.48	1.39
22	C	503	CLA	C3D-C2D	3.46	1.48	1.39
22	D	403	CLA	CHD-C4C	3.46	1.47	1.39
22	c	910	CLA	C3D-C2D	3.46	1.48	1.39
22	B	610	CLA	C4D-CHA	3.45	1.50	1.38
22	b	611	CLA	C4C-C3C	3.45	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	C4C-C3C	3.45	1.50	1.45
22	b	612	CLA	CHC-C4B	3.45	1.47	1.39
22	b	609	CLA	MG-NC	3.44	2.14	2.06
22	b	617	CLA	CHC-C4B	3.44	1.47	1.39
22	b	613	CLA	C3D-C2D	3.44	1.48	1.39
22	B	609	CLA	C3D-C2D	3.44	1.48	1.39
34	C	532	HTG	C1'-S1	-3.44	1.76	1.81
22	C	513	CLA	OBD-CAD	3.43	1.28	1.22
22	c	908	CLA	C4D-CHA	3.43	1.50	1.38
22	b	607	CLA	C1D-ND	-3.42	1.33	1.37
22	c	908	CLA	C3D-C2D	3.42	1.48	1.39
22	c	907	CLA	CHC-C4B	3.42	1.47	1.39
22	C	514	CLA	C4D-CHA	3.42	1.50	1.38
22	B	603	CLA	OBD-CAD	3.42	1.28	1.22
22	B	609	CLA	CHB-C1B	3.42	1.47	1.39
22	b	617	CLA	OBD-CAD	3.41	1.28	1.22
22	C	505	CLA	MG-NB	3.41	2.12	2.05
22	C	508	CLA	O2A-CGA	3.41	1.43	1.33
35	C	517	DGD	O1G-C1A	3.41	1.43	1.33
22	c	912	CLA	OBD-CAD	3.41	1.28	1.22
22	C	505	CLA	C4D-CHA	3.41	1.50	1.38
22	a	408	CLA	CHC-C4B	3.41	1.47	1.39
22	C	512	CLA	C4D-CHA	3.41	1.50	1.38
22	b	610	CLA	CHD-C4C	3.41	1.47	1.39
39	V	202	HEC	CBB-CAB	-3.40	1.36	1.49
22	C	503	CLA	OBD-CAD	3.40	1.28	1.22
22	c	912	CLA	O2A-CGA	3.40	1.43	1.33
22	D	403	CLA	C4C-C3C	3.40	1.50	1.45
22	C	502	CLA	C3D-C2D	3.40	1.48	1.39
22	c	905	CLA	MG-ND	-3.40	1.99	2.05
22	B	602	CLA	OBD-CAD	3.39	1.28	1.22
22	B	610	CLA	C3D-C2D	3.38	1.48	1.39
22	c	907	CLA	CHB-C1B	3.38	1.47	1.39
23	A	407	PHO	OBD-CAD	3.38	1.26	1.22
22	B	610	CLA	C1B-NB	-3.38	1.33	1.37
39	v	202	HEC	CBB-CAB	-3.37	1.37	1.49
22	b	608	CLA	O2A-CGA	3.37	1.43	1.33
22	c	902	CLA	CHD-C4C	3.37	1.46	1.39
22	A	406	CLA	C1D-ND	-3.36	1.33	1.37
34	b	623	HTG	C1'-S1	-3.36	1.76	1.81
22	B	611	CLA	C4C-C3C	3.36	1.50	1.45
22	C	510	CLA	CHD-C4C	3.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	913	CLA	C3D-C2D	3.36	1.48	1.39
22	B	610	CLA	C1D-ND	-3.36	1.33	1.37
22	B	603	CLA	C1B-C2B	3.35	1.51	1.43
22	B	616	CLA	CHC-C4B	3.35	1.46	1.39
22	A	405	CLA	CHB-C1B	3.34	1.46	1.39
22	D	401	CLA	CHD-C1D	3.34	1.44	1.38
23	A	407	PHO	C4B-NB	-3.34	1.32	1.38
22	c	912	CLA	C4D-CHA	3.34	1.49	1.38
22	c	909	CLA	C4C-C3C	3.33	1.50	1.45
22	A	405	CLA	C1D-ND	-3.33	1.33	1.37
23	a	410	PHO	OBD-CAD	3.32	1.26	1.22
22	b	610	CLA	C3D-C2D	3.32	1.48	1.39
39	V	202	HEC	CBC-CAC	-3.31	1.37	1.49
22	c	907	CLA	C1B-NB	-3.31	1.33	1.37
27	D	410	LHG	O7-C7	3.31	1.43	1.34
22	c	906	CLA	C3D-C2D	3.31	1.48	1.39
22	c	905	CLA	CHD-C4C	3.31	1.46	1.39
22	C	512	CLA	C1B-C2B	3.30	1.50	1.43
22	C	511	CLA	C4C-C3C	3.30	1.50	1.45
22	C	505	CLA	O2A-CGA	3.30	1.43	1.33
22	A	406	CLA	C1B-NB	-3.30	1.33	1.37
22	B	616	CLA	C4D-CHA	3.30	1.49	1.38
22	b	613	CLA	CHD-C4C	3.29	1.46	1.39
22	B	612	CLA	C1B-C2B	3.29	1.50	1.43
22	B	617	CLA	C1B-NB	-3.29	1.33	1.37
22	C	508	CLA	OBD-CAD	3.28	1.28	1.22
22	b	607	CLA	C1B-NB	-3.28	1.33	1.37
36	E	102	HEM	CAC-C3C	3.28	1.56	1.47
22	b	604	CLA	C3D-C2D	3.27	1.47	1.39
22	a	408	CLA	CHB-C1B	3.27	1.46	1.39
22	C	503	CLA	C4D-CHA	3.27	1.49	1.38
22	B	609	CLA	C1B-NB	-3.27	1.33	1.37
22	b	617	CLA	C3D-C2D	3.27	1.47	1.39
22	C	512	CLA	C4C-C3C	3.27	1.50	1.45
27	D	410	LHG	O8-C23	3.26	1.42	1.33
22	B	610	CLA	CHD-C4C	3.26	1.46	1.39
22	b	605	CLA	C3D-C2D	3.26	1.47	1.39
22	D	401	CLA	C3D-C2D	3.26	1.47	1.39
22	B	602	CLA	C4D-CHA	3.26	1.49	1.38
22	b	604	CLA	C4D-CHA	3.25	1.49	1.38
22	b	611	CLA	C4D-CHA	3.24	1.49	1.38
22	c	914	CLA	C3D-C2D	3.24	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CHB-C1B	3.24	1.46	1.39
22	c	914	CLA	OBD-CAD	3.24	1.28	1.22
22	a	409	CLA	C1B-C2B	3.24	1.50	1.43
22	C	506	CLA	C1B-NB	-3.23	1.33	1.37
23	A	407	PHO	C3D-C2D	3.23	1.45	1.39
22	B	607	CLA	C4D-CHA	3.23	1.49	1.38
22	b	617	CLA	C1C-NC	-3.23	1.32	1.37
22	c	906	CLA	C3B-C4B	3.23	1.52	1.42
22	C	512	CLA	C3D-C2D	3.23	1.47	1.39
22	c	905	CLA	C4C-C3C	3.22	1.50	1.45
22	b	616	CLA	C4C-C3C	3.22	1.50	1.45
22	A	405	CLA	C3D-C2D	3.22	1.47	1.39
22	B	616	CLA	C3D-C2D	3.22	1.47	1.39
22	C	514	CLA	C3D-C2D	3.22	1.47	1.39
22	b	607	CLA	CHD-C4C	3.21	1.46	1.39
22	b	605	CLA	C3B-C4B	3.21	1.52	1.42
22	D	404	CLA	C3D-C2D	3.21	1.47	1.39
22	c	903	CLA	C4D-CHA	3.20	1.49	1.38
22	d	402	CLA	C4C-C3C	3.20	1.50	1.45
22	A	406	CLA	CHD-C1D	3.20	1.44	1.38
22	A	405	CLA	CHD-C4C	3.20	1.46	1.39
22	B	614	CLA	C3D-C2D	3.20	1.47	1.39
22	b	606	CLA	C1B-NB	-3.20	1.33	1.37
22	D	403	CLA	CHC-C4B	3.19	1.46	1.39
22	D	404	CLA	C1D-ND	-3.19	1.33	1.37
22	B	609	CLA	C4D-CHA	3.19	1.49	1.38
22	c	904	CLA	CHC-C4B	3.19	1.46	1.39
22	b	605	CLA	C1B-NB	-3.18	1.33	1.37
22	B	604	CLA	CHC-C4B	3.18	1.46	1.39
22	B	613	CLA	C1D-ND	-3.18	1.33	1.37
22	C	509	CLA	C1C-NC	-3.18	1.32	1.37
22	a	407	CLA	C3D-C2D	3.18	1.47	1.39
22	b	612	CLA	C3D-C2D	3.18	1.47	1.39
22	b	608	CLA	C4D-CHA	3.17	1.49	1.38
22	B	602	CLA	C3D-C2D	3.17	1.47	1.39
22	c	904	CLA	C4D-CHA	3.16	1.49	1.38
22	B	605	CLA	C4C-C3C	3.16	1.50	1.45
34	v	203	HTG	C1'-S1	-3.16	1.77	1.81
22	c	906	CLA	MG-NB	3.16	2.12	2.05
36	E	102	HEM	CAB-C3B	3.16	1.55	1.47
22	b	615	CLA	MG-NC	3.15	2.13	2.06
22	B	602	CLA	C1D-ND	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	CHB-C1B	3.15	1.46	1.39
22	C	510	CLA	C1B-NB	-3.15	1.33	1.37
22	D	403	CLA	MG-NC	3.15	2.13	2.06
22	c	906	CLA	C4D-CHA	3.14	1.49	1.38
22	b	608	CLA	OBD-CAD	3.14	1.27	1.22
36	e	101	HEM	CAB-C3B	3.13	1.55	1.47
22	C	506	CLA	C4D-CHA	3.13	1.49	1.38
22	a	407	CLA	OBD-CAD	3.13	1.27	1.22
22	C	511	CLA	C3D-C2D	3.13	1.47	1.39
22	B	604	CLA	MG-NB	-3.13	1.99	2.05
22	B	615	CLA	C3D-C2D	3.13	1.47	1.39
22	A	405	CLA	O2A-CGA	3.13	1.42	1.33
22	b	606	CLA	C1D-ND	-3.12	1.33	1.37
22	c	907	CLA	C4D-CHA	3.12	1.49	1.38
22	B	606	CLA	CHD-C4C	3.12	1.46	1.39
22	C	505	CLA	C3B-C4B	3.12	1.51	1.42
22	B	615	CLA	C4D-CHA	3.11	1.49	1.38
22	C	510	CLA	CHC-C4B	3.11	1.46	1.39
22	b	613	CLA	C4D-CHA	3.11	1.49	1.38
22	C	510	CLA	C4C-C3C	3.10	1.50	1.45
22	A	406	CLA	CHB-C1B	3.10	1.46	1.39
22	a	408	CLA	C3D-C2D	3.10	1.47	1.39
22	c	904	CLA	C4B-NB	-3.10	1.33	1.37
22	B	616	CLA	C1D-ND	-3.10	1.33	1.37
22	b	612	CLA	C1B-C2B	3.10	1.50	1.43
22	C	506	CLA	C3D-C2D	3.10	1.47	1.39
22	C	513	CLA	C4D-CHA	3.10	1.49	1.38
22	D	401	CLA	C1B-C2B	3.09	1.50	1.43
22	b	615	CLA	C4D-CHA	3.09	1.49	1.38
22	C	512	CLA	C1D-ND	-3.09	1.33	1.37
22	c	913	CLA	C1D-ND	-3.09	1.33	1.37
22	C	508	CLA	C4D-CHA	3.09	1.49	1.38
22	b	611	CLA	C3D-C2D	3.09	1.47	1.39
22	B	606	CLA	C1C-C2C	3.09	1.50	1.44
22	b	609	CLA	C4D-CHA	3.09	1.49	1.38
22	C	507	CLA	C3D-C2D	3.09	1.47	1.39
22	b	617	CLA	C1B-C2B	3.09	1.50	1.43
22	C	510	CLA	CHB-C1B	3.09	1.46	1.39
35	C	518	DGD	O3G-C1D	3.09	1.45	1.40
22	B	608	CLA	CHC-C4B	3.08	1.46	1.39
22	b	612	CLA	CHD-C4C	3.08	1.46	1.39
22	B	616	CLA	C1C-NC	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	907	CLA	C4C-C3C	3.08	1.50	1.45
22	d	402	CLA	OBD-CAD	3.07	1.27	1.22
22	B	611	CLA	OBD-CAD	3.07	1.27	1.22
22	B	613	CLA	OBD-CAD	3.07	1.27	1.22
22	C	503	CLA	C3B-C4B	3.07	1.51	1.42
22	C	507	CLA	C4D-CHA	3.07	1.48	1.38
22	B	605	CLA	C4D-CHA	3.07	1.48	1.38
22	B	605	CLA	CHC-C4B	3.06	1.46	1.39
22	D	401	CLA	CHC-C1C	3.06	1.44	1.38
22	A	405	CLA	C4C-C3C	3.06	1.50	1.45
22	B	615	CLA	CHD-C1D	3.06	1.44	1.38
22	D	401	CLA	CHB-C1B	3.06	1.46	1.39
22	b	607	CLA	MG-NC	3.06	2.13	2.06
34	l	106	HTG	C1'-S1	-3.06	1.77	1.81
22	a	412	CLA	OBD-CAD	3.06	1.27	1.22
29	f	102	LMT	O1'-C1'	3.06	1.45	1.40
22	A	408	CLA	C4C-C3C	3.06	1.50	1.45
22	c	909	CLA	C3B-C4B	3.05	1.51	1.42
27	d	407	LHG	O7-C7	3.05	1.42	1.34
22	B	610	CLA	C1B-C2B	3.05	1.50	1.43
22	B	605	CLA	C1B-C2B	3.05	1.50	1.43
22	C	502	CLA	C4D-CHA	3.05	1.48	1.38
22	C	507	CLA	OBD-CAD	3.05	1.27	1.22
22	C	505	CLA	C3D-C2D	3.04	1.47	1.39
22	A	408	CLA	C4D-CHA	3.04	1.48	1.38
22	B	616	CLA	MG-NC	3.04	2.13	2.06
22	a	412	CLA	C4D-CHA	3.04	1.48	1.38
26	a	415	PL9	C6-C5	3.03	1.50	1.35
22	B	614	CLA	CHD-C4C	3.03	1.46	1.39
22	C	513	CLA	C3D-C2D	3.03	1.47	1.39
22	a	407	CLA	C4D-CHA	3.03	1.48	1.38
22	a	408	CLA	MG-NC	3.03	2.13	2.06
22	b	606	CLA	C4D-CHA	3.03	1.48	1.38
35	C	517	DGD	O2G-C1B	3.03	1.42	1.34
22	b	612	CLA	C1B-NB	-3.03	1.33	1.37
22	b	616	CLA	C3D-C2D	3.02	1.47	1.39
22	c	911	CLA	C4D-CHA	3.01	1.48	1.38
22	B	608	CLA	O2A-CGA	3.01	1.42	1.33
22	b	616	CLA	MG-ND	3.01	2.11	2.05
22	B	613	CLA	C3D-C2D	3.01	1.47	1.39
22	C	506	CLA	C3B-C4B	3.01	1.51	1.42
22	c	909	CLA	C4D-CHA	3.01	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	411	PHO	C3A-C2A	-3.00	1.52	1.54
22	b	616	CLA	C4D-CHA	3.00	1.48	1.38
22	B	612	CLA	C3D-C2D	3.00	1.47	1.39
22	B	610	CLA	C4B-NB	-3.00	1.33	1.37
22	b	614	CLA	C4D-CHA	3.00	1.48	1.38
22	a	409	CLA	CHC-C4B	2.99	1.46	1.39
22	c	902	CLA	C4C-C3C	2.99	1.50	1.45
22	B	613	CLA	MG-NC	-2.99	1.99	2.06
35	H	102	DGD	O5D-C1E	2.99	1.45	1.40
22	C	507	CLA	C1D-ND	-2.98	1.33	1.37
22	c	912	CLA	C3D-C2D	2.98	1.47	1.39
26	A	411	PL9	C2-C3	2.98	1.42	1.34
22	C	514	CLA	C1C-C2C	2.98	1.50	1.44
22	B	617	CLA	C4D-CHA	2.98	1.48	1.38
22	b	604	CLA	CHB-C1B	2.98	1.46	1.39
22	c	908	CLA	MG-NB	-2.97	1.99	2.05
22	C	508	CLA	C3D-C2D	2.97	1.47	1.39
22	C	513	CLA	C1B-C2B	2.97	1.50	1.43
22	b	614	CLA	OBD-CAD	2.97	1.27	1.22
22	b	609	CLA	C3D-C2D	2.97	1.47	1.39
22	B	615	CLA	MG-ND	-2.96	1.99	2.05
22	B	602	CLA	C1C-NC	-2.96	1.33	1.37
22	C	509	CLA	OBD-CAD	2.96	1.27	1.22
22	C	506	CLA	CHB-C1B	2.96	1.46	1.39
22	A	408	CLA	CHB-C1B	2.95	1.46	1.39
22	B	605	CLA	MG-NC	2.95	2.13	2.06
22	D	401	CLA	C3B-C4B	2.95	1.51	1.42
22	C	507	CLA	MG-NB	2.95	2.11	2.05
22	c	909	CLA	C3D-C2D	2.95	1.47	1.39
22	B	613	CLA	C1B-C2B	2.95	1.50	1.43
22	B	608	CLA	C3D-C2D	2.95	1.47	1.39
22	b	616	CLA	MG-NB	2.94	2.11	2.05
22	C	511	CLA	C4D-CHA	2.94	1.48	1.38
22	b	606	CLA	C3D-C2D	2.94	1.47	1.39
22	C	505	CLA	C1C-NC	-2.93	1.33	1.37
22	c	910	CLA	C1B-C2B	2.93	1.50	1.43
22	c	906	CLA	C1B-C2B	2.93	1.50	1.43
22	C	502	CLA	OBD-CAD	2.93	1.27	1.22
22	C	509	CLA	C4D-CHA	2.92	1.48	1.38
22	b	616	CLA	C1B-C2B	2.92	1.50	1.43
22	b	603	CLA	C1B-C2B	2.92	1.50	1.43
22	a	409	CLA	OBD-CAD	2.92	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	913	CLA	C4D-CHA	2.92	1.48	1.38
34	D	415	HTG	C1'-S1	-2.92	1.77	1.81
22	B	603	CLA	C1C-NC	-2.92	1.33	1.37
22	b	613	CLA	C3B-C4B	2.91	1.51	1.42
22	b	603	CLA	C3D-C2D	2.91	1.46	1.39
22	C	504	CLA	C1C-C2C	2.91	1.50	1.44
22	D	401	CLA	O2A-CGA	2.91	1.41	1.33
22	C	514	CLA	OBD-CAD	2.91	1.27	1.22
22	c	911	CLA	C1C-NC	-2.91	1.33	1.37
34	b	624	HTG	C1'-S1	-2.90	1.77	1.81
22	A	405	CLA	C4D-CHA	2.90	1.48	1.38
22	c	902	CLA	C1C-C2C	2.90	1.50	1.44
22	b	614	CLA	C4C-C3C	2.90	1.50	1.45
22	b	608	CLA	C1B-C2B	2.90	1.49	1.43
22	a	412	CLA	C1B-NB	-2.89	1.34	1.37
22	b	607	CLA	C3B-C4B	2.89	1.51	1.42
22	c	902	CLA	C4D-CHA	2.89	1.48	1.38
22	b	617	CLA	C4B-NB	-2.89	1.34	1.37
32	a	422	BCT	O1-C	2.89	1.35	1.25
39	V	202	HEC	CMC-C2C	2.89	1.56	1.50
22	C	506	CLA	C1B-C2B	2.88	1.49	1.43
22	B	614	CLA	CHC-C4B	2.88	1.45	1.39
22	c	913	CLA	C4B-NB	-2.88	1.34	1.37
22	c	906	CLA	OBD-CAD	2.88	1.27	1.22
22	B	611	CLA	C3B-C4B	2.88	1.51	1.42
22	d	403	CLA	C4D-CHA	2.88	1.48	1.38
22	B	602	CLA	C1B-NB	-2.88	1.34	1.37
22	c	906	CLA	C1C-NC	-2.88	1.33	1.37
22	a	409	CLA	C4D-CHA	2.88	1.48	1.38
35	C	519	DGD	O2G-C1B	2.88	1.42	1.34
22	b	603	CLA	C4D-CHA	2.87	1.48	1.38
24	b	618	BCR	C14-C13	2.87	1.35	1.33
22	C	510	CLA	C4D-CHA	2.87	1.48	1.38
22	c	905	CLA	C4D-CHA	2.87	1.48	1.38
27	d	407	LHG	O8-C23	2.86	1.41	1.33
22	B	608	CLA	C4D-CHA	2.86	1.48	1.38
22	b	612	CLA	OBD-CAD	2.86	1.27	1.22
22	C	505	CLA	C1B-C2B	2.86	1.49	1.43
22	b	616	CLA	C1D-ND	-2.85	1.34	1.37
22	d	403	CLA	C1C-NC	-2.85	1.33	1.37
22	A	406	CLA	C3B-C4B	2.85	1.51	1.42
22	b	607	CLA	C1C-C2C	2.85	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	C1D-ND	-2.85	1.34	1.37
22	b	602	CLA	C3B-C4B	2.85	1.51	1.42
22	C	514	CLA	C3B-C4B	2.85	1.51	1.42
22	d	402	CLA	CHC-C4B	2.84	1.45	1.39
22	b	615	CLA	C1C-NC	-2.84	1.33	1.37
36	e	101	HEM	CAC-C3C	2.84	1.55	1.47
22	B	615	CLA	C4C-C3C	2.84	1.49	1.45
22	B	615	CLA	C1C-C2C	2.84	1.50	1.44
22	b	603	CLA	C3B-C4B	2.84	1.51	1.42
22	a	409	CLA	C3D-C2D	2.83	1.46	1.39
22	B	611	CLA	C1C-C2C	2.83	1.50	1.44
22	B	615	CLA	C1D-ND	-2.83	1.34	1.37
22	c	913	CLA	C4C-C3C	2.83	1.49	1.45
22	C	512	CLA	C3B-C4B	2.82	1.50	1.42
22	c	904	CLA	C3D-C2D	2.82	1.46	1.39
22	b	604	CLA	C4C-C3C	2.82	1.49	1.45
22	b	614	CLA	MG-NC	2.82	2.13	2.06
22	b	609	CLA	CHD-C4C	2.82	1.45	1.39
26	d	405	PL9	C6-C5	2.82	1.49	1.35
22	b	614	CLA	C3D-C2D	2.82	1.46	1.39
22	d	402	CLA	MG-NB	-2.82	2.00	2.05
22	b	606	CLA	C3B-C4B	2.81	1.50	1.42
22	c	911	CLA	C1B-NB	-2.81	1.34	1.37
22	b	605	CLA	CHD-C4C	2.81	1.45	1.39
22	B	608	CLA	C4C-C3C	2.81	1.49	1.45
22	b	614	CLA	C1B-C2B	2.81	1.49	1.43
22	B	614	CLA	C4D-CHA	2.81	1.48	1.38
22	b	610	CLA	C4D-CHA	2.81	1.48	1.38
22	a	412	CLA	C1B-C2B	2.81	1.49	1.43
24	A	409	BCR	C19-C18	2.80	1.52	1.46
22	b	608	CLA	C1B-NB	-2.80	1.34	1.37
22	b	602	CLA	C1C-C2C	2.80	1.50	1.44
39	v	202	HEC	CMD-C2D	2.80	1.56	1.50
22	A	406	CLA	C4D-CHA	2.80	1.48	1.38
22	c	903	CLA	C1B-C2B	2.80	1.49	1.43
22	B	605	CLA	C1B-NB	-2.80	1.34	1.37
22	D	403	CLA	C4D-CHA	2.80	1.48	1.38
22	B	613	CLA	C4C-C3C	2.80	1.49	1.45
22	b	611	CLA	OBD-CAD	2.80	1.27	1.22
22	B	607	CLA	C3D-C2D	2.79	1.46	1.39
34	b	632	HTG	O5-C1	2.79	1.46	1.42
22	C	513	CLA	MG-ND	-2.79	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	C3B-C4B	2.79	1.50	1.42
22	b	613	CLA	C4B-NB	-2.79	1.34	1.37
26	A	411	PL9	C6-C5	2.78	1.48	1.35
22	a	412	CLA	CHC-C4B	2.78	1.45	1.39
22	D	404	CLA	C4D-CHA	2.78	1.47	1.38
22	b	611	CLA	C1B-NB	-2.78	1.34	1.37
22	B	604	CLA	C4D-CHA	2.78	1.47	1.38
22	b	613	CLA	C1D-ND	-2.78	1.34	1.37
22	b	612	CLA	MG-NC	2.77	2.12	2.06
22	c	910	CLA	MG-NB	-2.77	2.00	2.05
22	b	606	CLA	CHB-C1B	2.77	1.45	1.39
22	C	505	CLA	C1D-ND	-2.76	1.34	1.37
22	D	401	CLA	C4D-CHA	2.76	1.47	1.38
22	B	604	CLA	C3D-C2D	2.76	1.46	1.39
22	A	406	CLA	C3C-C2C	2.76	1.42	1.36
22	c	914	CLA	C1C-C2C	2.76	1.50	1.44
22	a	412	CLA	C3D-C2D	2.76	1.46	1.39
22	c	912	CLA	C3B-C4B	2.76	1.50	1.42
26	a	415	PL9	C2-C3	2.76	1.41	1.34
22	b	609	CLA	MG-NB	2.76	2.11	2.05
22	d	402	CLA	C3B-C4B	2.75	1.50	1.42
22	b	615	CLA	OBD-CAD	2.75	1.27	1.22
29	I	102	LMT	O1'-C1'	2.75	1.44	1.40
22	C	512	CLA	C1C-C2C	2.75	1.50	1.44
22	c	910	CLA	C3B-C4B	2.75	1.50	1.42
22	b	605	CLA	C1B-C2B	2.75	1.49	1.43
22	c	903	CLA	C3B-C4B	2.74	1.50	1.42
35	C	517	DGD	O5D-C1E	2.74	1.44	1.40
22	b	607	CLA	C1B-C2B	2.73	1.49	1.43
22	B	615	CLA	C1C-NC	-2.73	1.33	1.37
22	c	907	CLA	C3D-C2D	2.73	1.46	1.39
22	a	408	CLA	C4D-CHA	2.73	1.47	1.38
39	V	202	HEC	CMA-C3A	2.72	1.56	1.50
22	B	611	CLA	C4D-CHA	2.72	1.47	1.38
22	C	509	CLA	C3B-C4B	2.72	1.50	1.42
22	a	412	CLA	MG-NA	2.71	2.12	2.06
22	b	612	CLA	C4D-CHA	2.71	1.47	1.38
22	c	904	CLA	C1D-ND	-2.71	1.34	1.37
22	c	909	CLA	C1B-C2B	2.71	1.49	1.43
36	E	102	HEM	CMA-C3A	2.71	1.56	1.50
22	c	904	CLA	C1C-NC	-2.71	1.33	1.37
22	c	910	CLA	CHC-C4B	2.71	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	C1C-C2C	2.70	1.50	1.44
22	D	401	CLA	C1D-ND	-2.70	1.34	1.37
23	A	407	PHO	C3B-C4B	2.70	1.44	1.41
22	a	407	CLA	C1D-ND	-2.70	1.34	1.37
22	C	507	CLA	C4C-C3C	2.70	1.49	1.45
22	c	904	CLA	MG-NC	2.69	2.12	2.06
22	b	615	CLA	C1C-C2C	2.69	1.50	1.44
22	c	904	CLA	C4C-C3C	2.69	1.49	1.45
22	c	905	CLA	C1B-NB	-2.69	1.34	1.37
22	C	504	CLA	C3B-C4B	2.69	1.50	1.42
29	c	921	LMT	O1'-C1'	2.69	1.44	1.40
39	v	202	HEC	CMC-C2C	2.69	1.56	1.50
24	d	404	BCR	C12-C13	2.69	1.51	1.46
25	d	409	LMG	O1-C1	2.68	1.44	1.40
22	b	607	CLA	C4D-CHA	2.68	1.47	1.38
29	c	931	LMT	O1'-C1'	2.68	1.44	1.40
23	a	410	PHO	CBD-CGD	-2.68	1.49	1.52
22	c	914	CLA	C4D-CHA	2.68	1.47	1.38
34	C	521	HTG	C1'-S1	-2.68	1.77	1.81
22	b	602	CLA	C1B-C2B	2.68	1.49	1.43
22	c	902	CLA	C3B-C4B	2.68	1.50	1.42
22	b	608	CLA	C1D-ND	-2.68	1.34	1.37
24	D	405	BCR	C8-C9	2.68	1.51	1.46
22	A	406	CLA	C4B-NB	-2.68	1.34	1.37
22	B	608	CLA	MG-NB	-2.68	2.00	2.05
35	c	917	DGD	O5D-C1E	2.67	1.44	1.40
26	A	411	PL9	C7-C3	2.67	1.54	1.51
22	b	607	CLA	MG-NB	2.67	2.11	2.05
22	c	910	CLA	C4D-CHA	2.67	1.47	1.38
22	C	513	CLA	C3B-C4B	2.66	1.50	1.42
22	c	908	CLA	MG-NC	2.66	2.12	2.06
26	d	405	PL9	C18-C19	2.66	1.39	1.33
22	c	904	CLA	C1B-C2B	2.65	1.49	1.43
36	e	101	HEM	CMD-C2D	2.65	1.56	1.50
22	b	612	CLA	MG-NB	2.65	2.11	2.05
22	b	602	CLA	C4C-C3C	2.65	1.49	1.45
22	B	604	CLA	OBD-CAD	2.65	1.27	1.22
22	B	603	CLA	C3B-C4B	2.65	1.50	1.42
22	b	613	CLA	C1B-C2B	2.64	1.49	1.43
22	D	403	CLA	MG-ND	-2.64	2.00	2.05
22	B	616	CLA	OBD-CAD	2.64	1.27	1.22
22	b	603	CLA	OBD-CAD	2.64	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	627	HTG	C1'-S1	-2.64	1.77	1.81
22	B	605	CLA	C3D-C2D	2.63	1.46	1.39
34	B	627	HTG	C1'-S1	-2.62	1.77	1.81
22	B	606	CLA	C3B-C4B	2.62	1.50	1.42
22	b	603	CLA	MG-NC	2.61	2.12	2.06
22	b	610	CLA	C1B-C2B	2.61	1.49	1.43
22	C	502	CLA	C1B-NB	-2.61	1.34	1.37
22	a	409	CLA	C3D-C4D	-2.60	1.38	1.44
22	B	610	CLA	C3B-C4B	2.60	1.50	1.42
22	B	617	CLA	C1D-ND	-2.60	1.34	1.37
35	C	518	DGD	O2G-C1B	2.60	1.41	1.34
22	c	910	CLA	MG-ND	-2.60	2.00	2.05
22	b	609	CLA	C1D-ND	-2.59	1.34	1.37
22	b	609	CLA	C1C-NC	-2.59	1.33	1.37
36	e	101	HEM	CMB-C2B	2.59	1.56	1.50
22	b	607	CLA	C3D-C2D	2.59	1.46	1.39
22	b	604	CLA	OBD-CAD	2.59	1.26	1.22
22	c	911	CLA	C3B-C4B	2.59	1.50	1.42
29	Z	101	LMT	O1'-C1'	2.58	1.44	1.40
22	B	612	CLA	C4D-CHA	2.58	1.47	1.38
22	B	606	CLA	C1B-C2B	2.58	1.49	1.43
22	C	509	CLA	C4C-C3C	2.58	1.49	1.45
22	c	912	CLA	C4C-C3C	2.58	1.49	1.45
22	b	617	CLA	C1C-C2C	2.58	1.49	1.44
24	a	413	BCR	C5-C6	2.57	1.38	1.34
22	C	505	CLA	C4B-NB	-2.57	1.34	1.37
22	d	402	CLA	C4D-CHA	2.57	1.47	1.38
23	A	407	PHO	CBD-CGD	-2.57	1.49	1.52
22	d	403	CLA	C1C-C2C	2.56	1.49	1.44
22	B	607	CLA	C3D-C4D	-2.56	1.38	1.44
22	B	607	CLA	C1D-ND	-2.56	1.34	1.37
22	A	406	CLA	C3D-C2D	2.56	1.46	1.39
22	b	613	CLA	C1A-CHA	2.56	1.53	1.43
22	B	603	CLA	C3D-C4D	-2.56	1.38	1.44
22	B	603	CLA	C1D-ND	-2.55	1.34	1.37
22	C	507	CLA	C3B-C4B	2.55	1.50	1.42
22	c	909	CLA	C1C-C2C	2.55	1.49	1.44
22	b	604	CLA	O2A-CGA	2.55	1.40	1.33
22	B	605	CLA	C3B-C4B	2.55	1.50	1.42
22	b	610	CLA	C3B-C4B	2.54	1.50	1.42
22	A	408	CLA	C3D-C2D	2.54	1.45	1.39
22	b	604	CLA	C3B-C4B	2.54	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	C1B-C2B	2.54	1.49	1.43
22	B	603	CLA	C4D-CHA	2.54	1.47	1.38
22	c	908	CLA	C3B-C2B	2.53	1.49	1.41
22	c	909	CLA	C1D-ND	-2.53	1.34	1.37
22	C	508	CLA	C3B-C4B	2.53	1.50	1.42
22	B	603	CLA	C3D-C2D	2.52	1.45	1.39
22	B	607	CLA	C1C-C2C	2.52	1.49	1.44
22	c	912	CLA	C1C-NC	-2.52	1.33	1.37
22	a	407	CLA	C1B-NB	-2.51	1.34	1.37
22	b	612	CLA	C1D-ND	-2.51	1.34	1.37
22	c	903	CLA	OBD-CAD	2.51	1.26	1.22
22	B	616	CLA	C1B-C2B	2.50	1.49	1.43
22	C	502	CLA	C4C-C3C	2.50	1.49	1.45
22	b	614	CLA	C1C-NC	-2.50	1.34	1.37
22	b	612	CLA	CBD-CAD	-2.50	1.45	1.56
35	c	919	DGD	O5D-C1E	2.49	1.44	1.40
23	a	410	PHO	C1B-NB	-2.49	1.34	1.38
22	c	906	CLA	C4B-NB	-2.49	1.34	1.37
22	C	504	CLA	C1B-C2B	2.49	1.49	1.43
22	a	412	CLA	MG-NB	2.49	2.10	2.05
26	D	406	PL9	C6-C5	2.49	1.47	1.35
22	C	510	CLA	MG-NC	2.48	2.12	2.06
22	d	403	CLA	C3B-C4B	2.48	1.50	1.42
22	c	911	CLA	C1D-ND	-2.48	1.34	1.37
22	d	402	CLA	C3D-C2D	2.47	1.45	1.39
22	b	607	CLA	MG-ND	2.47	2.10	2.05
24	A	409	BCR	C12-C13	2.47	1.51	1.46
22	b	605	CLA	C4C-C3C	2.47	1.49	1.45
22	A	405	CLA	C1B-C2B	2.47	1.48	1.43
22	b	617	CLA	C1B-NB	-2.47	1.34	1.37
22	b	606	CLA	MG-NC	2.47	2.12	2.06
22	A	408	CLA	C3B-C4B	2.46	1.49	1.42
22	c	909	CLA	C1C-NC	-2.46	1.34	1.37
22	b	604	CLA	C1B-C2B	2.45	1.48	1.43
24	d	404	BCR	C30-C25	-2.45	1.50	1.53
22	b	607	CLA	C4C-C3C	2.45	1.49	1.45
22	c	905	CLA	C1B-C2B	2.45	1.48	1.43
22	C	503	CLA	C4B-NB	-2.45	1.34	1.37
22	a	409	CLA	C1D-ND	-2.44	1.34	1.37
22	B	605	CLA	C1D-ND	-2.44	1.34	1.37
22	C	503	CLA	CHD-C4C	2.44	1.44	1.39
22	B	617	CLA	C3B-C4B	2.44	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	MG-ND	-2.44	2.01	2.05
22	c	907	CLA	C3B-C4B	2.43	1.49	1.42
22	B	614	CLA	C1B-C2B	2.43	1.48	1.43
34	b	626	HTG	C1'-S1	-2.43	1.78	1.81
22	C	507	CLA	C1C-C2C	2.43	1.49	1.44
22	c	906	CLA	C1D-ND	-2.43	1.34	1.37
22	a	409	CLA	C4B-NB	-2.42	1.34	1.37
22	D	403	CLA	CHC-C1C	2.42	1.43	1.38
24	d	404	BCR	C23-C22	2.42	1.51	1.46
22	C	514	CLA	C1B-C2B	2.42	1.48	1.43
22	B	609	CLA	C4C-C3C	2.41	1.49	1.45
22	B	609	CLA	CBD-CAD	-2.41	1.45	1.56
22	B	602	CLA	C1B-C2B	2.41	1.48	1.43
22	b	605	CLA	C1C-NC	-2.41	1.34	1.37
22	B	606	CLA	C1C-NC	-2.40	1.34	1.37
32	A	421[A]	BCT	O1-C	2.40	1.34	1.25
35	D	407	DGD	O3G-C1D	2.40	1.44	1.40
22	C	508	CLA	C1D-ND	-2.39	1.34	1.37
22	C	514	CLA	C1D-ND	-2.39	1.34	1.37
35	d	406	DGD	O3G-C1D	2.39	1.44	1.40
22	D	401	CLA	C4B-NB	-2.39	1.34	1.37
22	b	613	CLA	C1C-NC	-2.39	1.34	1.37
22	b	610	CLA	C1B-NB	-2.39	1.34	1.37
22	B	607	CLA	C4C-C3C	2.39	1.49	1.45
22	B	614	CLA	C4C-C3C	2.39	1.49	1.45
22	B	602	CLA	C1C-C2C	2.39	1.49	1.44
22	c	912	CLA	C1B-C2B	2.38	1.48	1.43
22	C	511	CLA	C1B-NB	-2.38	1.34	1.37
22	a	409	CLA	C3B-C4B	2.38	1.49	1.42
28	D	408	SQD	O6-C1	2.38	1.44	1.40
22	c	912	CLA	C1B-NB	-2.38	1.34	1.37
22	a	407	CLA	C3B-C4B	2.38	1.49	1.42
22	c	908	CLA	C4C-C3C	2.38	1.49	1.45
22	C	502	CLA	C1D-ND	-2.37	1.34	1.37
22	A	408	CLA	C1B-NB	-2.37	1.34	1.37
22	B	608	CLA	C1B-C2B	2.37	1.48	1.43
22	A	406	CLA	MG-NC	-2.37	2.00	2.06
22	B	612	CLA	MG-NB	2.37	2.10	2.05
22	C	508	CLA	C1B-NB	-2.37	1.34	1.37
34	D	414	HTG	C1'-S1	-2.37	1.78	1.81
22	b	617	CLA	C3B-C2B	2.36	1.49	1.41
22	b	611	CLA	C1C-C2C	2.36	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	402	CLA	C1B-NB	-2.36	1.34	1.37
25	B	621	LMG	O1-C1	2.36	1.44	1.40
22	b	616	CLA	C3B-C2B	2.36	1.49	1.41
24	Y	101	BCR	C5-C6	2.36	1.36	1.33
22	d	403	CLA	C1B-C2B	2.35	1.48	1.43
22	b	614	CLA	C1C-C2C	2.35	1.49	1.44
22	b	603	CLA	C1D-ND	-2.35	1.34	1.37
22	b	611	CLA	C1B-C2B	2.35	1.48	1.43
34	c	922	HTG	C1'-S1	-2.35	1.78	1.81
22	B	603	CLA	C1C-C2C	2.35	1.49	1.44
22	b	615	CLA	C3B-C4B	2.35	1.49	1.42
29	B	622	LMT	O1'-C1'	2.35	1.44	1.40
28	l	101	SQD	O6-C1	2.34	1.44	1.40
22	C	513	CLA	C1D-ND	-2.34	1.34	1.37
22	b	617	CLA	C3B-C4B	2.34	1.49	1.42
22	B	607	CLA	CHD-C4C	2.34	1.44	1.39
22	C	504	CLA	C1B-NB	-2.34	1.34	1.37
22	C	513	CLA	C1C-C2C	2.34	1.49	1.44
22	B	608	CLA	C3B-C4B	2.34	1.49	1.42
22	c	914	CLA	C1B-C2B	2.34	1.48	1.43
22	B	606	CLA	OBD-CAD	2.34	1.26	1.22
22	C	505	CLA	C3D-C4D	-2.33	1.38	1.44
32	A	421[B]	BCT	O1-C	2.33	1.33	1.25
22	b	603	CLA	C1B-NB	-2.32	1.34	1.37
22	d	402	CLA	MG-ND	-2.32	2.01	2.05
22	a	409	CLA	C4C-C3C	2.32	1.49	1.45
36	e	101	HEM	CMA-C3A	2.32	1.55	1.50
22	C	507	CLA	C1C-NC	-2.32	1.34	1.37
24	b	619	BCR	C12-C13	2.32	1.50	1.46
26	D	406	PL9	C2-C3	2.32	1.40	1.34
22	B	606	CLA	C4D-CHA	2.32	1.46	1.38
22	b	607	CLA	O2A-C1	-2.32	1.39	1.46
22	c	911	CLA	C1B-C2B	2.32	1.48	1.43
22	b	608	CLA	C4C-C3C	2.31	1.49	1.45
22	c	913	CLA	C3B-C4B	2.31	1.49	1.42
22	C	508	CLA	C1B-C2B	2.31	1.48	1.43
22	C	503	CLA	C1B-C2B	2.31	1.48	1.43
25	C	531	LMG	O1-C1	2.30	1.44	1.40
22	b	614	CLA	MG-ND	2.30	2.10	2.05
22	C	511	CLA	C3D-C4D	-2.30	1.39	1.44
22	A	405	CLA	C3A-C2A	-2.30	1.48	1.54
22	C	508	CLA	C1C-C2C	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	905	CLA	C1C-NC	-2.29	1.34	1.37
22	C	514	CLA	C3B-C2B	2.29	1.48	1.41
22	c	903	CLA	C4C-C3C	2.29	1.48	1.45
22	B	609	CLA	C1C-C2C	2.29	1.49	1.44
22	B	608	CLA	C1B-NB	-2.29	1.34	1.37
22	C	508	CLA	C3B-C2B	2.29	1.48	1.41
22	D	403	CLA	OBD-CAD	2.29	1.26	1.22
22	C	510	CLA	C1B-C2B	2.29	1.48	1.43
22	B	607	CLA	C3B-C2B	2.28	1.48	1.41
22	C	502	CLA	C4B-NB	-2.28	1.34	1.37
22	B	607	CLA	OBD-CAD	2.28	1.26	1.22
22	B	611	CLA	C1B-NB	-2.28	1.34	1.37
22	C	503	CLA	C4C-C3C	2.27	1.48	1.45
22	c	903	CLA	CBD-CAD	-2.27	1.46	1.56
22	b	611	CLA	C3B-C4B	2.27	1.49	1.42
22	b	612	CLA	C4B-NB	-2.27	1.34	1.37
22	b	605	CLA	C1D-ND	-2.27	1.34	1.37
22	c	907	CLA	C1B-C2B	2.26	1.48	1.43
22	c	911	CLA	CBD-CAD	-2.26	1.46	1.56
22	C	504	CLA	C1C-NC	-2.26	1.34	1.37
22	c	914	CLA	C1D-ND	-2.26	1.34	1.37
22	c	907	CLA	C3D-C4D	-2.26	1.39	1.44
22	b	616	CLA	C3B-C4B	2.26	1.49	1.42
22	a	408	CLA	C1D-C2D	2.26	1.49	1.45
22	b	602	CLA	C3B-C2B	2.25	1.48	1.41
22	b	611	CLA	C3D-C4D	-2.25	1.39	1.44
22	c	914	CLA	C4C-C3C	2.25	1.48	1.45
22	B	609	CLA	OBD-CAD	2.25	1.26	1.22
24	a	413	BCR	C12-C13	2.25	1.50	1.46
22	B	613	CLA	C3D-C4D	-2.25	1.39	1.44
22	c	909	CLA	C4B-NB	-2.25	1.34	1.37
22	c	913	CLA	C1B-NB	-2.25	1.34	1.37
22	B	616	CLA	C3B-C4B	2.25	1.49	1.42
24	C	515	BCR	C19-C18	2.24	1.50	1.46
22	a	412	CLA	C3B-C4B	2.24	1.49	1.42
22	b	615	CLA	MG-NB	-2.24	2.01	2.05
22	B	609	CLA	C3D-C4D	-2.23	1.39	1.44
22	B	604	CLA	C1C-NC	-2.23	1.34	1.37
22	D	403	CLA	C3D-C2D	2.23	1.45	1.39
22	b	610	CLA	C1C-NC	-2.23	1.34	1.37
22	B	613	CLA	C4B-NB	-2.23	1.34	1.37
22	c	913	CLA	C1B-C2B	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	902	CLA	C1D-ND	-2.22	1.34	1.37
22	c	913	CLA	C3B-C2B	2.21	1.48	1.41
22	C	512	CLA	C1B-NB	-2.21	1.35	1.37
22	C	513	CLA	C1B-NB	-2.20	1.35	1.37
22	c	903	CLA	C1D-ND	-2.20	1.35	1.37
22	c	902	CLA	C3D-C2D	2.20	1.45	1.39
22	b	615	CLA	C1B-C2B	2.20	1.48	1.43
34	C	532	HTG	C1-S1	-2.20	1.77	1.80
26	d	405	PL9	C23-C24	2.20	1.38	1.33
22	B	604	CLA	C3B-C4B	2.20	1.49	1.42
22	A	408	CLA	C3D-C4D	-2.20	1.39	1.44
22	c	906	CLA	C4C-C3C	2.20	1.48	1.45
22	C	502	CLA	C3B-C4B	2.20	1.49	1.42
22	b	617	CLA	CHD-C4C	2.19	1.44	1.39
22	b	604	CLA	C4B-NB	-2.19	1.35	1.37
22	A	406	CLA	C3D-C4D	-2.19	1.39	1.44
22	c	914	CLA	C3B-C4B	2.19	1.49	1.42
35	c	919	DGD	O2G-C2G	-2.19	1.41	1.46
22	C	513	CLA	C4C-C3C	2.19	1.48	1.45
22	B	615	CLA	C1B-C2B	2.18	1.48	1.43
22	C	505	CLA	CBD-CAD	-2.18	1.46	1.56
22	c	909	CLA	C3D-C4D	-2.18	1.39	1.44
22	b	606	CLA	C1C-NC	-2.17	1.34	1.37
22	A	408	CLA	CHB-C4A	-2.17	1.32	1.37
22	C	514	CLA	C4C-C3C	2.17	1.48	1.45
22	B	610	CLA	C1C-C2C	2.17	1.48	1.44
22	B	609	CLA	C1B-C2B	2.16	1.48	1.43
22	d	402	CLA	C1B-C2B	2.16	1.48	1.43
24	c	915	BCR	C23-C22	2.16	1.50	1.46
26	D	406	PL9	C7-C3	2.16	1.54	1.51
22	c	905	CLA	C1D-ND	-2.15	1.35	1.37
22	b	608	CLA	C3B-C4B	2.15	1.49	1.42
22	b	610	CLA	C1C-C2C	2.15	1.48	1.44
29	T	102	LMT	O1'-C1'	2.15	1.43	1.40
22	b	605	CLA	OBD-CAD	2.15	1.26	1.22
22	b	614	CLA	C3B-C4B	2.15	1.49	1.42
22	a	407	CLA	C1C-NC	-2.14	1.34	1.37
22	C	508	CLA	C4C-C3C	2.14	1.48	1.45
24	B	620	BCR	C26-C25	2.14	1.38	1.34
22	C	511	CLA	C1C-C2C	2.14	1.48	1.44
22	C	507	CLA	C4B-NB	-2.13	1.35	1.37
22	B	613	CLA	C4D-CHA	2.13	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	918	DGD	O3G-C1D	2.13	1.43	1.40
22	c	904	CLA	C3D-C4D	-2.13	1.39	1.44
22	C	503	CLA	C1C-C2C	2.13	1.48	1.44
22	a	412	CLA	C3D-C4D	-2.13	1.39	1.44
34	l	106	HTG	C1-S1	-2.13	1.77	1.80
22	B	612	CLA	C4B-NB	-2.12	1.35	1.37
22	C	510	CLA	MG-NB	-2.12	2.01	2.05
22	b	607	CLA	CBD-CAD	-2.12	1.47	1.56
22	B	608	CLA	C1C-NC	-2.12	1.34	1.37
35	c	918	DGD	O5D-C1E	2.12	1.43	1.40
22	A	405	CLA	C3B-C4B	2.12	1.48	1.42
22	C	504	CLA	C3B-C2B	2.12	1.48	1.41
22	b	613	CLA	C4C-C3C	2.12	1.48	1.45
22	C	503	CLA	C1D-ND	-2.11	1.35	1.37
22	c	907	CLA	MG-ND	-2.11	2.01	2.05
22	b	608	CLA	C3D-C4D	-2.11	1.39	1.44
22	D	404	CLA	C1C-C2C	2.11	1.48	1.44
22	B	604	CLA	CBD-CAD	-2.11	1.47	1.56
22	B	610	CLA	C4C-C3C	2.11	1.48	1.45
22	B	617	CLA	C4B-NB	-2.11	1.35	1.37
22	B	611	CLA	C1B-C2B	2.11	1.48	1.43
22	a	408	CLA	C1B-C2B	2.10	1.48	1.43
22	b	609	CLA	C3B-C4B	2.10	1.48	1.42
22	b	615	CLA	C3D-C4D	-2.10	1.39	1.44
22	d	402	CLA	C4B-NB	-2.10	1.35	1.37
25	D	412	LMG	O1-C1	2.10	1.43	1.40
36	E	102	HEM	CMD-C2D	2.10	1.55	1.50
22	C	511	CLA	C3B-C4B	2.10	1.48	1.42
25	c	930	LMG	O1-C1	2.10	1.43	1.40
22	B	605	CLA	CBD-CAD	-2.10	1.47	1.56
26	a	415	PL9	C7-C3	2.09	1.54	1.51
22	B	602	CLA	C3B-C2B	2.08	1.48	1.41
22	C	504	CLA	C4C-C3C	2.08	1.48	1.45
22	C	509	CLA	C4B-NB	-2.08	1.35	1.37
22	a	408	CLA	C4C-C3C	2.08	1.48	1.45
22	b	612	CLA	C3D-C4D	-2.08	1.39	1.44
22	d	402	CLA	C3D-C4D	-2.07	1.39	1.44
24	b	620	BCR	C30-C25	-2.07	1.51	1.53
22	a	408	CLA	C3B-C2B	2.07	1.48	1.41
22	a	407	CLA	C4C-C3C	2.07	1.48	1.45
22	D	401	CLA	C1B-NB	-2.07	1.35	1.37
22	C	512	CLA	CBD-CAD	-2.07	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C4C-C3C	2.07	1.48	1.45
22	C	502	CLA	C1C-C2C	2.07	1.48	1.44
39	V	202	HEC	C3B-C2B	-2.07	1.34	1.41
22	c	913	CLA	C1C-C2C	2.06	1.48	1.44
26	d	405	PL9	C28-C29	2.06	1.37	1.33
22	B	611	CLA	CBD-CAD	-2.06	1.47	1.56
24	B	620	BCR	C19-C18	2.06	1.50	1.46
22	C	512	CLA	MG-NC	2.06	2.11	2.06
22	c	913	CLA	C3D-C4D	-2.06	1.39	1.44
22	b	608	CLA	C4B-NB	-2.06	1.35	1.37
22	B	602	CLA	C3B-C4B	2.05	1.48	1.42
26	A	411	PL9	C6-C1	2.05	1.52	1.48
22	b	610	CLA	C4C-C3C	2.05	1.48	1.45
35	h	102	DGD	O5D-C1E	2.05	1.43	1.40
24	B	620	BCR	C30-C25	-2.05	1.51	1.53
22	B	612	CLA	C1D-ND	-2.05	1.35	1.37
35	c	918	DGD	O2G-C2G	-2.04	1.41	1.46
22	C	505	CLA	C3B-C2B	2.04	1.48	1.41
22	A	408	CLA	CBD-CAD	-2.04	1.47	1.56
22	B	616	CLA	C4C-C3C	2.04	1.48	1.45
25	b	622	LMG	C4-C5	2.04	1.57	1.53
22	c	906	CLA	C3B-C2B	2.04	1.48	1.41
22	B	608	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	608	CLA	CBD-CAD	-2.03	1.47	1.56
22	B	613	CLA	C3B-C4B	2.03	1.48	1.42
22	B	603	CLA	C4C-C3C	2.03	1.48	1.45
22	B	602	CLA	C3D-C4D	-2.03	1.39	1.44
22	C	506	CLA	C1A-CHA	2.03	1.51	1.43
37	h	101	RRX	C24-C25	2.03	1.52	1.45
34	C	521	HTG	C1-S1	-2.03	1.77	1.80
22	C	503	CLA	C1C-NC	-2.03	1.34	1.37
22	c	902	CLA	C1B-C2B	2.03	1.47	1.43
22	A	406	CLA	C1B-C2B	2.02	1.47	1.43
24	B	618	BCR	C5-C6	2.02	1.37	1.34
34	b	627	HTG	O5-C1	2.02	1.45	1.42
22	b	607	CLA	OBD-CAD	2.02	1.26	1.22
22	C	502	CLA	C1B-C2B	2.02	1.47	1.43
22	B	603	CLA	C1B-NB	-2.02	1.35	1.37
22	a	412	CLA	CBD-CAD	-2.02	1.47	1.56
22	c	905	CLA	C3B-C4B	2.02	1.48	1.42
22	d	403	CLA	C1D-C2D	2.02	1.49	1.45
22	B	616	CLA	C4B-NB	-2.02	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C1C-C2C	2.01	1.48	1.44
22	B	610	CLA	OBD-CAD	2.01	1.25	1.22
34	b	632	HTG	C1'-S1	-2.00	1.78	1.81
22	D	404	CLA	C4B-NB	-2.00	1.35	1.37
22	B	614	CLA	C1C-C2C	2.00	1.48	1.44

All (2581) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	C4A-NA-C1A	11.60	111.97	106.68
22	C	506	CLA	C4A-NA-C1A	11.09	111.74	106.68
22	B	602	CLA	C4A-NA-C1A	10.85	111.63	106.68
23	a	410	PHO	C3B-C4B-NB	10.46	114.28	107.46
22	c	912	CLA	C4A-NA-C1A	10.25	111.36	106.68
22	c	909	CLA	C4A-NA-C1A	9.88	111.19	106.68
23	A	407	PHO	C3B-C4B-NB	9.79	113.85	107.46
22	c	904	CLA	C4A-NA-C1A	9.73	111.12	106.68
22	b	608	CLA	C4A-NA-C1A	9.70	111.11	106.68
22	c	908	CLA	C4A-NA-C1A	9.61	111.06	106.68
22	C	514	CLA	C4A-NA-C1A	9.60	111.06	106.68
23	a	411	PHO	O2D-CGD-CBD	9.43	121.31	110.95
22	c	905	CLA	C4A-NA-C1A	9.15	110.85	106.68
22	B	606	CLA	C4A-NA-C1A	8.78	110.68	106.68
28	a	414	SQD	O6-C1-C2	8.75	121.56	108.27
23	D	402	PHO	C2D-C1D-ND	8.72	115.73	109.43
22	C	507	CLA	C4A-NA-C1A	8.65	110.63	106.68
22	B	615	CLA	C4A-NA-C1A	8.65	110.62	106.68
23	a	411	PHO	C2B-C1B-NB	8.56	115.62	109.43
22	b	617	CLA	C4A-NA-C1A	8.47	110.54	106.68
22	B	616	CLA	C4A-NA-C1A	8.47	110.54	106.68
22	C	505	CLA	C4A-NA-C1A	8.40	110.51	106.68
23	D	402	PHO	C3B-C4B-NB	8.38	112.92	107.46
22	C	504	CLA	C4A-NA-C1A	8.37	110.50	106.68
23	a	411	PHO	C2D-C1D-ND	8.33	115.45	109.43
22	C	513	CLA	C4A-NA-C1A	8.32	110.48	106.68
34	V	203	HTG	O5-C1-C2	-8.22	98.98	110.32
22	B	611	CLA	O2D-CGD-CBD	8.07	125.33	111.23
22	C	512	CLA	C4A-NA-C1A	8.02	110.34	106.68
23	A	407	PHO	C2B-C1B-NB	7.96	115.18	109.43
22	b	614	CLA	C4A-NA-C1A	7.92	110.29	106.68
22	C	508	CLA	C4A-NA-C1A	7.85	110.26	106.68
22	D	403	CLA	C4A-NA-C1A	7.82	110.25	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	411	PHO	C1-C2-C3	-7.79	113.43	126.20
23	a	410	PHO	O2D-CGD-CBD	7.74	119.45	110.95
23	A	407	PHO	O2D-CGD-CBD	7.57	119.27	110.95
22	b	605	CLA	C4A-NA-C1A	7.56	110.13	106.68
22	b	606	CLA	CHD-C4C-C3C	-7.56	113.75	124.77
22	d	403	CLA	C4A-NA-C1A	7.51	110.11	106.68
22	b	615	CLA	C4A-NA-C1A	7.44	110.07	106.68
22	B	604	CLA	O2D-CGD-CBD	7.44	124.23	111.23
22	B	605	CLA	C4A-NA-C1A	7.43	110.07	106.68
22	b	603	CLA	O2D-CGD-CBD	7.36	124.10	111.23
23	a	411	PHO	C3B-C4B-NB	7.34	112.25	107.46
22	b	616	CLA	C4A-NA-C1A	7.28	110.00	106.68
34	l	106	HTG	C1'-S1-C1	7.27	116.14	100.45
22	B	612	CLA	C4A-NA-C1A	7.19	109.96	106.68
22	C	509	CLA	C4A-NA-C1A	7.13	109.93	106.68
34	C	532	HTG	C1'-S1-C1	7.10	115.79	100.45
22	B	615	CLA	C2D-C1D-ND	7.08	117.14	110.13
34	v	203	HTG	O5-C1-C2	-7.06	100.58	110.32
22	C	502	CLA	O2D-CGD-O1D	-7.00	110.22	123.85
28	C	501	SQD	O6-C1-C2	7.00	118.90	108.27
22	b	612	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	B	611	CLA	C4A-NA-C1A	6.92	109.84	106.68
22	D	403	CLA	C2C-C1C-NC	6.91	117.24	109.98
34	D	414	HTG	C1'-S1-C1	6.90	115.35	100.45
23	a	410	PHO	C2D-C1D-ND	6.90	114.41	109.43
22	B	610	CLA	C4A-NA-C1A	6.89	109.82	106.68
22	b	602	CLA	O2D-CGD-CBD	6.86	123.22	111.23
23	D	402	PHO	C2B-C1B-NB	6.81	114.35	109.43
22	a	409	CLA	C2C-C1C-NC	6.78	117.10	109.98
22	c	902	CLA	C4A-NA-C1A	6.77	109.77	106.68
34	b	632	HTG	C1'-S1-C1	6.72	114.97	100.45
22	C	508	CLA	O2D-CGD-CBD	6.70	122.94	111.23
22	B	608	CLA	C4D-CHA-C1A	-6.67	113.28	121.24
22	D	403	CLA	C1C-C2C-C3C	-6.66	99.97	106.98
22	C	502	CLA	O2D-CGD-CBD	6.61	122.79	111.23
22	c	913	CLA	C4A-NA-C1A	6.57	109.67	106.68
34	b	624	HTG	C1'-S1-C1	6.49	114.47	100.45
22	C	502	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	a	409	CLA	C1C-C2C-C3C	-6.45	100.19	106.98
22	D	401	CLA	C1C-C2C-C3C	-6.40	100.25	106.98
34	D	415	HTG	C1'-S1-C1	6.40	114.27	100.45
22	D	401	CLA	C2B-C1B-NB	6.38	116.94	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	b	613	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
23	a	411	PHO	C4D-ND-C1D	-6.35	101.27	108.87
22	B	609	CLA	O2D-CGD-CBD	6.34	122.32	111.23
23	D	402	PHO	C4D-ND-C1D	-6.32	101.30	108.87
22	B	615	CLA	CHD-C4C-C3C	-6.32	115.56	124.77
24	D	405	BCR	C24-C23-C22	-6.27	116.96	126.23
22	A	406	CLA	C1C-C2C-C3C	-6.26	100.39	106.98
22	B	610	CLA	CHD-C4C-C3C	-6.26	115.65	124.77
22	B	617	CLA	O2D-CGD-CBD	6.26	122.17	111.23
22	b	607	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
34	v	203	HTG	C1'-S1-C1	6.23	113.91	100.45
22	b	607	CLA	O2D-CGD-CBD	6.19	122.06	111.23
25	b	622	LMG	O1-C1-C2	6.18	117.66	108.27
22	a	412	CLA	O2D-CGD-CBD	6.16	121.99	111.23
22	a	408	CLA	CHD-C4C-C3C	-6.15	115.81	124.77
23	D	402	PHO	O2D-CGD-CBD	6.12	117.67	110.95
34	D	415	HTG	O5-C1-C2	-6.12	101.88	110.32
23	D	402	PHO	C3D-C4D-ND	6.12	115.55	107.71
22	c	914	CLA	C4A-NA-C1A	6.11	109.47	106.68
22	B	617	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
22	c	914	CLA	C4D-CHA-C1A	-6.11	113.96	121.24
23	A	407	PHO	C2D-C1D-ND	6.09	113.83	109.43
22	B	607	CLA	O2D-CGD-O1D	-6.07	112.03	123.85
23	a	410	PHO	C2B-C1B-NB	6.05	113.81	109.43
27	A	412	LHG	O7-C7-C8	6.05	121.88	111.09
34	B	627	HTG	C1'-S1-C1	6.04	113.50	100.45
22	b	617	CLA	O2D-CGD-CBD	6.02	121.75	111.23
22	B	602	CLA	O2D-CGD-CBD	6.01	121.74	111.23
22	C	510	CLA	C2C-C1C-NC	5.99	116.28	109.98
22	b	605	CLA	C4D-CHA-C1A	-5.99	114.10	121.24
22	A	406	CLA	C2C-C1C-NC	5.99	116.27	109.98
22	b	607	CLA	C4A-NA-C1A	5.98	109.41	106.68
34	b	627	HTG	C1'-S1-C1	5.97	113.35	100.45
22	D	401	CLA	C2C-C1C-NC	5.96	116.24	109.98
22	b	612	CLA	CHD-C4C-C3C	-5.92	116.15	124.77
22	B	607	CLA	O2D-CGD-CBD	5.91	121.55	111.23
23	a	411	PHO	C3D-C4D-ND	5.86	115.23	107.71
22	b	611	CLA	O2D-CGD-CBD	5.80	121.38	111.23
22	C	510	CLA	C3B-C2B-C1B	-5.80	100.33	107.17
22	d	402	CLA	C4D-CHA-C1A	-5.79	114.34	121.24
22	a	408	CLA	C4D-CHA-C1A	-5.77	114.36	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	903	CLA	C1-C2-C3	-5.76	116.77	126.20
25	d	409	LMG	O1-C1-C2	5.75	117.01	108.27
22	b	608	CLA	C4D-CHA-C1A	-5.74	114.40	121.24
22	b	604	CLA	CHD-C4C-C3C	-5.74	116.41	124.77
22	D	401	CLA	CHD-C4C-C3C	-5.73	116.41	124.77
22	b	613	CLA	C4A-NA-C1A	5.73	109.29	106.68
22	B	607	CLA	CHD-C4C-C3C	-5.72	116.44	124.77
22	c	904	CLA	C4D-CHA-C1A	-5.71	114.44	121.24
22	b	614	CLA	CMB-C2B-C1B	5.71	134.11	125.42
22	b	607	CLA	O2D-CGD-O1D	-5.71	112.74	123.85
22	c	910	CLA	C4A-NA-C1A	5.71	109.28	106.68
27	D	409	LHG	O7-C7-C8	5.70	123.81	111.48
22	D	401	CLA	C3B-C2B-C1B	-5.69	100.46	107.17
22	D	403	CLA	C1-C2-C3	-5.64	116.95	126.20
23	A	407	PHO	C3D-C4D-ND	5.63	114.93	107.71
34	B	623	HTG	C1'-S1-C1	5.63	112.61	100.45
23	D	402	PHO	C1-C2-C3	-5.60	117.02	126.20
28	a	414	SQD	O9-S-C6	5.60	115.12	106.76
22	b	604	CLA	C2C-C1C-NC	5.58	115.84	109.98
22	c	913	CLA	C1-C2-C3	-5.55	117.10	126.20
22	c	908	CLA	O2D-CGD-CBD	5.55	120.93	111.23
22	b	617	CLA	CHD-C4C-C3C	-5.55	116.69	124.77
22	B	605	CLA	C2C-C1C-NC	5.54	115.81	109.98
22	d	402	CLA	C2B-C1B-NB	5.54	116.07	110.33
22	b	610	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
22	d	402	CLA	O2D-CGD-CBD	5.53	120.91	111.23
22	a	412	CLA	C4D-CHA-C1A	-5.52	114.66	121.24
22	c	902	CLA	C2D-C1D-ND	5.52	115.59	110.13
34	V	203	HTG	C1'-S1-C1	5.51	110.71	100.16
22	C	510	CLA	C4D-CHA-C1A	-5.51	114.67	121.24
22	B	609	CLA	CHD-C4C-C3C	-5.50	116.76	124.77
25	b	622	LMG	O7-C10-C11	5.50	123.37	111.48
27	a	416	LHG	O7-C7-C8	5.48	123.33	111.48
22	a	412	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
34	c	922	HTG	C1'-S1-C1	5.47	112.25	100.45
22	C	510	CLA	C2B-C1B-NB	5.46	115.98	110.33
22	B	615	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
34	C	521	HTG	C1'-S1-C1	5.45	112.23	100.45
24	D	405	BCR	C7-C8-C9	-5.43	118.21	126.23
22	B	606	CLA	CHD-C4C-C3C	-5.43	116.86	124.77
22	b	617	CLA	C2D-C1D-ND	5.42	115.49	110.13
22	c	914	CLA	CHD-C4C-C3C	-5.41	116.89	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	910	CLA	C2C-C1C-NC	5.40	115.65	109.98
22	B	613	CLA	C4A-NA-C1A	5.38	109.13	106.68
22	a	408	CLA	CHD-C4C-NC	5.37	132.56	124.23
22	c	906	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
28	l	101	SQD	O6-C1-C2	5.35	116.40	108.27
22	c	903	CLA	C4A-NA-C1A	5.34	109.12	106.68
22	b	611	CLA	C4A-NA-C1A	5.33	109.11	106.68
22	c	902	CLA	CMD-C2D-C1D	5.31	134.08	124.73
22	b	607	CLA	C1-C2-C3	-5.31	117.50	126.20
22	A	405	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
36	E	102	HEM	CBD-CAD-C3D	-5.29	97.91	112.53
22	a	408	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
22	b	611	CLA	C2D-C1D-ND	5.28	115.35	110.13
22	c	907	CLA	C2C-C1C-NC	5.28	115.53	109.98
22	C	503	CLA	C2B-C1B-NB	5.27	115.80	110.33
22	C	504	CLA	C3B-C2B-C1B	-5.27	100.95	107.17
22	c	903	CLA	CHD-C4C-C3C	-5.26	117.11	124.77
22	A	406	CLA	CHC-C4B-NB	5.25	131.92	124.05
24	d	404	BCR	C7-C8-C9	-5.25	118.47	126.23
34	b	632	HTG	O5-C5-C4	5.24	119.15	109.70
22	C	510	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
22	b	611	CLA	CHD-C4C-C3C	-5.24	117.13	124.77
22	b	615	CLA	C4D-CHA-C1A	-5.24	114.99	121.24
22	B	605	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
22	c	906	CLA	C4A-NA-C1A	5.23	109.06	106.68
34	B	626	HTG	C1'-S1-C1	5.22	111.73	100.45
22	B	616	CLA	CHD-C4C-C3C	-5.22	117.16	124.77
22	D	404	CLA	C4A-NA-C1A	5.21	109.05	106.68
22	C	510	CLA	C4A-NA-C1A	5.19	109.05	106.68
22	c	913	CLA	O2D-CGD-CBD	5.19	120.30	111.23
22	C	511	CLA	C2C-C1C-NC	5.18	115.43	109.98
22	c	902	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
22	b	604	CLA	O2D-CGD-CBD	5.17	120.28	111.23
22	c	910	CLA	C4D-CHA-C1A	-5.17	115.07	121.24
22	c	902	CLA	CHD-C1D-ND	-5.16	117.55	124.80
22	c	902	CLA	CHD-C4C-C3C	-5.15	117.26	124.77
35	d	406	DGD	O2G-C1B-C2B	5.15	122.63	111.48
22	a	407	CLA	C4A-NA-C1A	5.14	109.02	106.68
22	A	406	CLA	C2B-C1B-NB	5.14	115.66	110.33
22	c	911	CLA	C2B-C1B-NB	5.13	115.65	110.33
28	a	414	SQD	O47-C7-C8	5.12	122.56	111.48
22	c	906	CLA	O2D-CGD-CBD	5.11	120.16	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	C2C-C1C-NC	5.11	115.34	109.98
22	a	409	CLA	C4D-CHA-C1A	-5.10	115.16	121.24
22	B	609	CLA	C4D-CHA-C1A	-5.10	115.16	121.24
22	C	514	CLA	CHD-C4C-C3C	-5.10	117.34	124.77
22	d	402	CLA	C2D-C1D-ND	5.09	115.16	110.13
22	C	503	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
22	c	910	CLA	C2B-C1B-NB	5.08	115.60	110.33
22	C	512	CLA	C2B-C1B-NB	5.07	115.58	110.33
22	B	617	CLA	O2D-CGD-O1D	-5.06	114.00	123.85
22	C	503	CLA	O2D-CGD-CBD	5.06	120.08	111.23
22	A	405	CLA	C2C-C1C-NC	5.05	115.29	109.98
22	c	907	CLA	O2D-CGD-CBD	5.05	120.06	111.23
22	b	609	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
22	b	606	CLA	CHD-C4C-NC	5.04	132.05	124.23
22	A	405	CLA	C2D-C1D-ND	5.04	115.12	110.13
22	c	903	CLA	O2D-CGD-O1D	-5.04	114.04	123.85
22	b	613	CLA	CAC-C3C-C4C	5.04	131.35	124.79
22	c	911	CLA	C4A-NA-C1A	5.04	108.98	106.68
22	C	504	CLA	CHD-C4C-C3C	-5.03	117.44	124.77
22	c	911	CLA	CHD-C4C-C3C	-5.02	117.45	124.77
22	c	913	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
29	I	102	LMT	O1B-C4'-C3'	5.02	119.99	107.23
28	D	408	SQD	O6-C1-C2	5.01	115.89	108.27
22	b	613	CLA	C4D-CHA-C1A	-5.00	115.28	121.24
22	A	408	CLA	C2C-C1C-NC	4.99	115.22	109.98
22	B	608	CLA	C2C-C1C-NC	4.99	115.22	109.98
22	c	908	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
22	B	617	CLA	C2C-C1C-NC	4.97	115.20	109.98
22	B	603	CLA	CHD-C4C-C3C	-4.96	117.54	124.77
22	C	512	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
23	A	407	PHO	C4D-ND-C1D	-4.95	102.94	108.87
28	a	418	SQD	C1-O5-C5	-4.95	104.05	113.72
22	A	405	CLA	C1C-C2C-C3C	-4.95	101.78	106.98
22	b	606	CLA	O2D-CGD-CBD	4.94	119.87	111.23
22	B	607	CLA	C2C-C1C-NC	4.94	115.17	109.98
24	b	618	BCR	C3-C4-C5	-4.94	105.25	114.06
22	C	503	CLA	O2D-CGD-O1D	-4.94	114.24	123.85
22	C	503	CLA	C2D-C1D-ND	4.94	115.01	110.13
22	b	612	CLA	C4D-CHA-C1A	-4.93	115.36	121.24
22	B	603	CLA	C4D-CHA-C1A	-4.92	115.37	121.24
22	B	611	CLA	CHD-C4C-C3C	-4.92	117.60	124.77
22	C	503	CLA	C4D-CHA-C1A	-4.92	115.38	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	409	CLA	C2B-C1B-NB	4.91	115.42	110.33
28	C	501	SQD	O9-S-C6	4.91	114.09	106.76
22	b	605	CLA	C3B-C2B-C1B	-4.91	101.39	107.17
22	A	406	CLA	CHD-C4C-C3C	-4.91	117.62	124.77
22	C	503	CLA	C4A-NA-C1A	4.90	108.91	106.68
22	b	609	CLA	CHD-C4C-C3C	-4.90	117.63	124.77
22	B	604	CLA	C2C-C1C-NC	4.90	115.12	109.98
23	a	411	PHO	O2D-CGD-O1D	-4.89	114.32	123.85
22	b	604	CLA	C1C-C2C-C3C	-4.89	101.83	106.98
22	C	513	CLA	CHD-C4C-C3C	-4.89	117.64	124.77
22	a	409	CLA	C2D-C1D-ND	4.89	114.96	110.13
28	A	413	SQD	O48-C23-C24	4.88	126.72	111.83
22	b	612	CLA	C2D-C1D-ND	4.88	114.96	110.13
27	C	522	LHG	O7-C7-C8	4.88	122.04	111.48
22	c	910	CLA	CHC-C4B-NB	4.87	131.35	124.05
22	c	908	CLA	CHD-C1D-ND	-4.87	117.95	124.80
24	C	515	BCR	C33-C5-C6	-4.87	119.17	124.48
22	B	611	CLA	O2D-CGD-O1D	-4.86	114.38	123.85
22	b	606	CLA	C4D-CHA-C1A	-4.86	115.45	121.24
22	B	612	CLA	C4D-CHA-C1A	-4.85	115.45	121.24
22	a	409	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
22	c	911	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
22	C	510	CLA	O2D-CGD-CBD	4.85	119.71	111.23
34	v	203	HTG	C1-C2-C3	-4.84	101.08	110.55
22	a	408	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
22	B	617	CLA	C2B-C1B-NB	4.82	115.33	110.33
22	B	609	CLA	C2C-C1C-NC	4.82	115.04	109.98
22	a	409	CLA	O2D-CGD-CBD	4.81	119.64	111.23
22	a	408	CLA	C2C-C1C-NC	4.81	115.03	109.98
22	b	603	CLA	CHA-C4D-ND	4.80	142.46	132.55
22	B	603	CLA	C2C-C1C-NC	4.80	115.02	109.98
22	A	408	CLA	C2B-C1B-NB	4.79	115.30	110.33
22	A	408	CLA	C2D-C1D-ND	4.79	114.87	110.13
22	b	604	CLA	C4-C3-C5	4.79	123.53	115.23
22	b	607	CLA	C2B-C1B-NB	4.78	115.29	110.33
22	c	910	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
22	d	402	CLA	C1D-ND-C4D	-4.77	102.96	106.31
22	D	404	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
22	C	507	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
22	b	617	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
22	A	405	CLA	C2B-C1B-NB	4.77	115.27	110.33
22	c	908	CLA	O2D-CGD-O1D	-4.77	114.57	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	l	101	SQD	O47-C7-C8	4.77	121.80	111.48
22	B	613	CLA	C4D-CHA-C1A	-4.77	115.56	121.24
22	C	507	CLA	CHD-C4C-C3C	-4.76	117.83	124.77
22	a	407	CLA	O2D-CGD-CBD	4.75	119.54	111.23
22	C	508	CLA	CHD-C4C-C3C	-4.75	117.85	124.77
22	a	408	CLA	CHD-C1D-ND	-4.75	118.12	124.80
35	c	919	DGD	O2G-C1B-C2B	4.74	121.74	111.48
28	a	418	SQD	O6-C1-C2	4.74	115.47	108.27
36	E	102	HEM	C4D-ND-C1D	4.74	110.81	105.21
22	B	608	CLA	C2B-C1B-NB	4.73	115.23	110.33
22	B	605	CLA	C2D-C1D-ND	4.73	114.81	110.13
22	c	907	CLA	C4A-NA-C1A	4.73	108.84	106.68
22	b	607	CLA	C4D-CHA-C1A	-4.73	115.60	121.24
22	C	513	CLA	O2D-CGD-CBD	4.73	119.49	111.23
22	b	603	CLA	CHD-C1D-ND	-4.72	118.16	124.80
22	B	607	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
22	C	512	CLA	C1-O2A-CGA	4.72	128.08	116.65
22	C	509	CLA	O2D-CGD-CBD	4.72	119.48	111.23
22	b	610	CLA	C2C-C1C-NC	4.72	114.94	109.98
22	C	505	CLA	C1C-C2C-C3C	-4.72	102.02	106.98
22	B	612	CLA	C2B-C1B-NB	4.71	115.21	110.33
22	B	607	CLA	C4D-CHA-C1A	-4.71	115.63	121.24
22	A	408	CLA	C1C-C2C-C3C	-4.70	102.03	106.98
22	c	907	CLA	CHD-C1D-ND	-4.70	118.18	124.80
22	a	408	CLA	C2B-C1B-NB	4.70	115.20	110.33
22	C	505	CLA	O2D-CGD-CBD	4.70	119.44	111.23
22	a	412	CLA	C2C-C1C-NC	4.69	114.91	109.98
22	C	504	CLA	CHA-C4D-ND	4.69	142.23	132.55
22	B	615	CLA	O2D-CGD-CBD	4.69	119.43	111.23
26	A	411	PL9	C7-C3-C4	4.69	120.77	116.91
22	B	607	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
22	c	907	CLA	C2B-C1B-NB	4.68	115.18	110.33
22	b	616	CLA	C2D-C1D-ND	4.68	114.76	110.13
24	Y	101	BCR	C38-C26-C25	-4.67	119.39	124.48
22	B	604	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
22	B	604	CLA	CHC-C4B-NB	4.67	131.05	124.05
23	a	410	PHO	C4D-ND-C1D	-4.67	103.28	108.87
22	d	403	CLA	C1-O2A-CGA	4.67	127.95	116.65
22	D	404	CLA	C2B-C1B-NB	4.66	115.16	110.33
24	y	101	BCR	C33-C5-C6	-4.66	119.39	124.48
22	C	511	CLA	C1C-C2C-C3C	-4.66	102.08	106.98
22	B	605	CLA	O2D-CGD-CBD	4.65	119.36	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	BCR	C38-C26-C25	-4.65	119.41	124.48
22	a	412	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
22	b	610	CLA	CHD-C4C-C3C	-4.64	118.00	124.77
22	B	603	CLA	C4A-NA-C1A	4.64	108.80	106.68
22	B	607	CLA	CHC-C4B-NB	4.63	131.00	124.05
22	B	611	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	c	904	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
22	b	605	CLA	C2D-C1D-ND	4.63	114.71	110.13
22	C	512	CLA	CHD-C4C-C3C	-4.63	118.03	124.77
22	D	401	CLA	CHD-C4C-NC	4.62	131.40	124.23
22	B	613	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
34	V	203	HTG	O2-C2-C1	4.62	118.51	110.30
22	c	903	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
23	a	410	PHO	C3D-C4D-ND	4.62	113.63	107.71
22	d	403	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
22	B	609	CLA	C2D-C1D-ND	4.61	114.69	110.13
22	B	612	CLA	CHD-C4C-C3C	-4.61	118.06	124.77
22	b	605	CLA	C2C-C1C-NC	4.60	114.82	109.98
22	d	402	CLA	C2C-C1C-NC	4.60	114.82	109.98
22	d	402	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
22	a	409	CLA	CHD-C4C-C3C	-4.60	118.06	124.77
22	a	412	CLA	C4-C3-C5	4.60	123.21	115.23
22	B	609	CLA	CHD-C1D-ND	-4.60	118.33	124.80
22	B	603	CLA	CHC-C4B-NB	4.60	130.95	124.05
22	b	606	CLA	CHD-C1D-ND	-4.60	118.33	124.80
28	A	413	SQD	O6-C1-C2	4.59	115.25	108.27
34	b	626	HTG	C1'-S1-C1	4.59	110.35	100.45
22	b	607	CLA	CHD-C1D-ND	-4.58	118.35	124.80
22	B	612	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
22	D	401	CLA	CMB-C2B-C1B	4.58	132.39	125.42
22	C	505	CLA	C2C-C1C-NC	4.57	114.78	109.98
22	b	606	CLA	C2D-C1D-ND	4.57	114.65	110.13
29	I	102	LMT	C1'-O5'-C5'	4.57	122.64	113.72
22	B	604	CLA	C3B-C2B-C1B	-4.56	101.80	107.17
22	c	908	CLA	C2D-C1D-ND	4.55	114.63	110.13
22	B	614	CLA	CHC-C4B-NB	4.55	130.87	124.05
22	C	507	CLA	C2C-C1C-NC	4.54	114.75	109.98
22	A	408	CLA	C4A-NA-C1A	4.54	108.75	106.68
22	A	406	CLA	C4-C3-C5	4.53	123.09	115.23
22	b	602	CLA	C1-O2A-CGA	4.53	127.61	116.65
22	b	609	CLA	C4A-NA-C1A	4.53	108.74	106.68
22	a	408	CLA	CHC-C4B-NB	4.52	130.83	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	617	CLA	C1-O2A-CGA	4.52	127.59	116.65
22	B	611	CLA	C2D-C1D-ND	4.52	114.60	110.13
22	c	909	CLA	C1C-C2C-C3C	-4.52	102.23	106.98
22	B	606	CLA	C4D-CHA-C1A	-4.52	115.86	121.24
22	c	914	CLA	C1C-C2C-C3C	-4.51	102.23	106.98
22	d	402	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
22	c	909	CLA	O2D-CGD-CBD	4.51	119.11	111.23
22	B	608	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
22	b	616	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
22	D	404	CLA	O2D-CGD-CBD	4.50	119.10	111.23
22	b	605	CLA	C2B-C1B-NB	4.50	114.99	110.33
22	C	502	CLA	CHD-C4C-C3C	-4.50	118.22	124.77
22	b	608	CLA	C2C-C1C-NC	4.49	114.70	109.98
22	b	614	CLA	CAC-C3C-C4C	4.49	130.63	124.79
22	c	909	CLA	C3B-C2B-C1B	-4.48	101.88	107.17
22	b	614	CLA	CHD-C4C-C3C	-4.48	118.24	124.77
22	a	407	CLA	C2D-C1D-ND	4.48	114.56	110.13
22	B	617	CLA	C4D-CHA-C1A	-4.48	115.91	121.24
22	c	903	CLA	C2B-C1B-NB	4.48	114.97	110.33
22	C	514	CLA	CHC-C4B-NB	4.47	130.75	124.05
36	e	101	HEM	C4D-ND-C1D	4.47	110.50	105.21
22	B	614	CLA	C4D-CHA-C1A	-4.47	115.92	121.24
22	B	614	CLA	C2D-C1D-ND	4.46	114.54	110.13
22	a	408	CLA	C2D-C1D-ND	4.46	114.54	110.13
28	C	501	SQD	C1-O5-C5	-4.46	105.01	113.72
22	C	502	CLA	C2C-C1C-NC	4.45	114.66	109.98
22	B	603	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
22	c	907	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
22	C	502	CLA	C2D-C1D-ND	4.45	114.53	110.13
24	c	916	BCR	C15-C14-C13	-4.45	121.04	127.28
22	C	503	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
22	C	505	CLA	CHD-C1D-ND	-4.44	118.55	124.80
22	a	407	CLA	CAC-C3C-C4C	4.44	130.57	124.79
22	c	902	CLA	O2D-CGD-CBD	4.44	119.00	111.23
22	c	910	CLA	CAC-C3C-C4C	4.44	130.56	124.79
22	c	910	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
22	b	613	CLA	O2D-CGD-CBD	4.43	118.97	111.23
22	C	513	CLA	C1-O2A-CGA	4.43	127.36	116.65
25	C	520	LMG	O8-C28-C29	4.43	125.33	111.83
22	b	616	CLA	CHC-C4B-NB	4.43	130.69	124.05
22	B	612	CLA	C2D-C1D-ND	4.42	114.50	110.13
22	c	908	CLA	C1C-C2C-C3C	-4.42	102.33	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	610	CLA	CHC-C4B-NB	4.42	130.68	124.05
22	c	902	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
22	c	905	CLA	C2B-C1B-NB	4.42	114.91	110.33
22	B	617	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
22	b	615	CLA	O2D-CGD-CBD	4.41	118.94	111.23
22	a	407	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
22	C	514	CLA	C3B-C2B-C1B	-4.41	101.98	107.17
35	H	102	DGD	O1G-C1A-O1A	-4.40	112.61	123.63
22	b	603	CLA	C4A-NA-C1A	4.40	108.69	106.68
22	b	617	CLA	CBC-CAC-C3C	-4.40	100.49	112.42
22	B	610	CLA	CHD-C4C-NC	4.40	131.05	124.23
22	b	605	CLA	O2D-CGD-CBD	4.40	118.92	111.23
22	b	614	CLA	CHD-C1D-ND	-4.40	118.61	124.80
22	b	607	CLA	C2D-C1D-ND	4.39	114.47	110.13
22	B	606	CLA	C2D-C1D-ND	4.39	114.47	110.13
22	c	904	CLA	C2C-C1C-NC	4.39	114.59	109.98
22	A	406	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
22	B	609	CLA	C1C-C2C-C3C	-4.39	102.37	106.98
22	C	509	CLA	C2D-C1D-ND	4.38	114.46	110.13
22	b	612	CLA	C2C-C1C-NC	4.38	114.58	109.98
22	a	409	CLA	CHD-C1D-ND	-4.38	118.64	124.80
22	b	604	CLA	C2B-C1B-NB	4.37	114.86	110.33
22	c	908	CLA	CHD-C4C-NC	4.37	131.00	124.23
28	C	501	SQD	C1-C2-C3	-4.36	100.83	110.01
22	B	611	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
22	B	602	CLA	O2D-CGD-O1D	-4.36	115.37	123.85
22	B	617	CLA	O2A-CGA-CBA	4.36	125.11	111.83
24	c	915	BCR	C33-C5-C6	-4.35	119.74	124.48
22	C	511	CLA	CHD-C4C-C3C	-4.35	118.44	124.77
22	c	906	CLA	C2B-C1B-NB	4.34	114.83	110.33
28	A	413	SQD	O9-S-C6	4.34	113.24	106.76
22	b	614	CLA	CMD-C2D-C1D	4.34	132.37	124.73
22	b	614	CLA	CHC-C4B-NB	4.34	130.56	124.05
23	D	402	PHO	C4-C3-C5	4.34	122.76	115.23
35	D	407	DGD	C4D-C3D-C2D	4.34	118.44	110.83
22	c	911	CLA	CHD-C4C-NC	4.33	130.95	124.23
22	b	609	CLA	O2D-CGD-CBD	4.33	118.80	111.23
22	C	504	CLA	C2D-C1D-ND	4.32	114.41	110.13
22	B	605	CLA	CHD-C4C-C3C	-4.32	118.47	124.77
22	C	513	CLA	C2D-C1D-ND	4.32	114.40	110.13
35	D	407	DGD	O2G-C1B-C2B	4.32	120.82	111.48
22	b	602	CLA	C1C-C2C-C3C	-4.32	102.44	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	C4D-CHA-C1A	-4.32	116.10	121.24
37	H	101	RRX	C24-C23-C22	-4.31	119.86	126.23
22	b	603	CLA	CMD-C2D-C1D	4.31	132.32	124.73
22	B	603	CLA	C2B-C1B-NB	4.31	114.79	110.33
22	B	603	CLA	O2D-CGD-CBD	4.31	118.76	111.23
22	C	507	CLA	C2B-C1B-NB	4.30	114.78	110.33
27	l	102	LHG	O7-C7-C8	4.30	120.78	111.48
22	B	614	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
22	C	503	CLA	CMB-C2B-C1B	4.30	131.96	125.42
22	B	617	CLA	CHD-C4C-NC	4.29	130.89	124.23
25	D	412	LMG	O7-C10-C11	4.29	120.76	111.48
22	b	603	CLA	C2B-C1B-NB	4.29	114.77	110.33
22	B	617	CLA	C2D-C1D-ND	4.29	114.37	110.13
25	d	409	LMG	O7-C10-C11	4.28	120.75	111.48
22	b	609	CLA	C2B-C1B-NB	4.28	114.77	110.33
22	B	606	CLA	CHC-C1C-NC	-4.28	117.86	124.31
22	a	409	CLA	C3B-C4B-NB	4.28	114.35	110.53
22	b	611	CLA	C4D-CHA-C1A	-4.28	116.14	121.24
22	c	905	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
34	D	415	HTG	O5-C5-C4	4.27	117.40	109.70
22	a	408	CLA	O2D-CGD-CBD	4.27	118.70	111.23
22	B	610	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
22	C	504	CLA	O2D-CGD-O1D	-4.27	115.53	123.85
22	c	903	CLA	C2C-C1C-NC	4.26	114.46	109.98
22	c	913	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
22	B	604	CLA	C2B-C1B-NB	4.26	114.75	110.33
22	b	610	CLA	CHD-C1D-ND	-4.26	118.81	124.80
22	C	508	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
36	e	101	HEM	CBD-CAD-C3D	-4.25	100.77	112.53
22	b	612	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
22	B	616	CLA	C2D-C1D-ND	4.25	114.33	110.13
22	b	614	CLA	C2C-C1C-NC	4.25	114.44	109.98
34	b	632	HTG	C1-O5-C5	4.24	120.17	112.56
25	B	621	LMG	O7-C10-C11	4.24	120.65	111.48
22	D	403	CLA	C2D-C1D-ND	4.24	114.32	110.13
28	a	414	SQD	C1-C2-C3	-4.24	101.10	110.01
22	b	608	CLA	CHA-C4D-ND	4.23	141.29	132.55
22	d	403	CLA	C2C-C1C-NC	4.23	114.42	109.98
22	c	902	CLA	C2C-C1C-NC	4.22	114.42	109.98
22	C	511	CLA	O2D-CGD-O1D	-4.22	115.63	123.85
22	b	611	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
22	a	407	CLA	C1C-C2C-C3C	-4.22	102.55	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	SQD	O47-C7-C8	4.21	120.60	111.48
22	b	617	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
22	b	608	CLA	C1C-C2C-C3C	-4.21	102.56	106.98
22	C	507	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
22	c	903	CLA	CHA-C4D-ND	4.20	141.22	132.55
22	B	602	CLA	O1D-CGD-CBD	-4.20	116.23	124.52
22	A	408	CLA	C4-C3-C5	4.20	122.52	115.23
28	A	413	SQD	O47-C7-C8	4.20	120.57	111.48
22	B	611	CLA	CHD-C1D-ND	-4.20	118.89	124.80
22	C	506	CLA	CAC-C3C-C4C	4.20	130.25	124.79
22	c	904	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
22	b	603	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
22	D	403	CLA	C4D-CHA-C1A	-4.19	116.24	121.24
22	c	902	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	B	608	CLA	C3B-C2B-C1B	-4.18	102.24	107.17
22	C	514	CLA	O2D-CGD-O1D	-4.18	115.70	123.85
22	C	508	CLA	C2D-C1D-ND	4.18	114.27	110.13
22	B	604	CLA	C2D-C1D-ND	4.18	114.26	110.13
22	c	907	CLA	CHD-C4C-C3C	-4.18	118.68	124.77
27	D	409	LHG	O7-C7-O9	-4.17	113.94	123.70
22	B	602	CLA	CAC-C3C-C4C	4.17	130.22	124.79
22	b	606	CLA	O2D-CGD-O1D	-4.17	115.73	123.85
22	c	903	CLA	C2D-C1D-ND	4.17	114.25	110.13
22	c	906	CLA	CHD-C4C-C3C	-4.17	118.69	124.77
24	b	618	BCR	C33-C5-C6	-4.17	119.94	124.48
22	C	507	CLA	C2D-C1D-ND	4.16	114.25	110.13
22	b	602	CLA	CHD-C4C-C3C	-4.16	118.70	124.77
22	D	401	CLA	C2D-C1D-ND	4.16	114.25	110.13
35	c	917	DGD	O2G-C1B-C2B	4.16	120.49	111.48
22	b	606	CLA	C2C-C1C-NC	4.16	114.36	109.98
27	d	407	LHG	O8-C23-O10	-4.16	113.22	123.63
22	B	606	CLA	CMC-C2C-C1C	4.16	131.53	125.03
22	B	617	CLA	CHD-C1D-ND	-4.16	118.95	124.80
35	C	517	DGD	O3G-C3G-C2G	-4.16	100.71	110.82
22	C	502	CLA	C1C-C2C-C3C	-4.15	102.61	106.98
22	b	607	CLA	C2C-C1C-NC	4.15	114.34	109.98
22	b	607	CLA	C1C-C2C-C3C	-4.15	102.62	106.98
22	a	409	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	a	410	PHO	O2D-CGD-O1D	-4.15	115.78	123.85
26	d	405	PL9	O1-C4-C3	-4.14	116.36	120.73
22	a	412	CLA	O2D-CGD-O1D	-4.14	115.78	123.85
22	B	613	CLA	CHD-C4C-C3C	-4.14	118.73	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	914	CLA	C2D-C1D-ND	4.14	114.22	110.13
22	c	912	CLA	CHC-C4B-NB	4.14	130.26	124.05
22	d	403	CLA	O2D-CGD-CBD	4.13	118.45	111.23
22	C	513	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
22	B	610	CLA	C4D-CHA-C1A	-4.13	116.32	121.24
22	B	609	CLA	O2D-CGD-O1D	-4.13	115.81	123.85
25	C	520	LMG	O7-C10-C11	4.13	120.41	111.48
22	C	514	CLA	CHA-C4D-ND	4.13	141.06	132.55
22	B	605	CLA	C4D-CHA-C1A	-4.12	116.33	121.24
22	c	912	CLA	CHA-C4D-ND	4.12	141.04	132.55
22	D	404	CLA	CAC-C3C-C4C	4.11	130.14	124.79
22	a	409	CLA	C4A-NA-C1A	4.11	108.56	106.68
22	B	606	CLA	O2D-CGD-O1D	-4.11	115.85	123.85
22	c	911	CLA	O2D-CGD-CBD	4.11	118.41	111.23
22	B	615	CLA	CHD-C4C-NC	4.11	130.60	124.23
22	c	911	CLA	CMC-C2C-C1C	4.10	131.44	125.03
22	c	903	CLA	O2D-CGD-CBD	4.10	118.39	111.23
22	B	616	CLA	CHD-C4C-NC	4.09	130.58	124.23
22	c	905	CLA	CHD-C4C-C3C	-4.09	118.81	124.77
22	A	408	CLA	C1D-ND-C4D	-4.09	103.44	106.31
22	b	607	CLA	C1-O2A-CGA	4.09	126.55	116.65
22	C	509	CLA	C2B-C1B-NB	4.09	114.56	110.33
22	c	905	CLA	C2D-C1D-ND	4.09	114.17	110.13
22	c	904	CLA	C1-C2-C3	-4.09	119.50	126.20
24	B	620	BCR	C2-C1-C6	4.08	116.37	110.44
22	c	909	CLA	C2B-C1B-NB	4.08	114.56	110.33
22	b	616	CLA	CHD-C4C-C3C	-4.08	118.83	124.77
22	b	609	CLA	C2C-C1C-NC	4.08	114.26	109.98
22	B	615	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
22	B	613	CLA	C2C-C1C-NC	4.07	114.26	109.98
22	B	604	CLA	O2D-CGD-O1D	-4.07	115.92	123.85
22	C	509	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
22	C	512	CLA	C2C-C1C-NC	4.07	114.26	109.98
22	b	604	CLA	C3B-C2B-C1B	-4.07	102.38	107.17
22	A	406	CLA	C4D-CHA-C1A	-4.07	116.39	121.24
22	B	611	CLA	C2C-C1C-NC	4.07	114.25	109.98
22	B	609	CLA	CHA-C4D-ND	4.07	140.94	132.55
22	b	615	CLA	C2C-C1C-NC	4.06	114.25	109.98
22	B	616	CLA	O2D-CGD-CBD	4.06	118.33	111.23
26	A	411	PL9	C53-C6-C1	4.06	123.60	115.28
22	B	602	CLA	CHC-C4B-NB	4.06	130.14	124.05
22	c	903	CLA	C1D-CHD-C4C	-4.06	117.39	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	627	HTG	C1-O5-C5	4.06	119.84	112.56
22	B	616	CLA	CHD-C1D-ND	-4.06	119.09	124.80
22	B	613	CLA	CAC-C3C-C4C	4.06	130.07	124.79
22	d	403	CLA	C3B-C2B-C1B	-4.05	102.39	107.17
22	B	615	CLA	CHC-C4B-NB	4.05	130.13	124.05
22	b	607	CLA	C3B-C2B-C1B	-4.05	102.39	107.17
22	b	611	CLA	C3B-C2B-C1B	-4.05	102.40	107.17
22	b	605	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
26	D	406	PL9	C40-C39-C41	4.04	122.24	115.23
22	C	506	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
22	c	913	CLA	O2D-CGD-O1D	-4.04	115.99	123.85
22	d	402	CLA	O2A-CGA-CBA	4.04	124.14	111.83
22	d	402	CLA	O2D-CGD-O1D	-4.03	116.00	123.85
37	H	101	RRX	C31-C1-C6	-4.03	103.93	110.24
22	b	615	CLA	CHD-C4C-C3C	-4.03	118.90	124.77
26	d	405	PL9	C35-C34-C36	4.03	122.22	115.23
22	B	604	CLA	CHD-C4C-C3C	-4.02	118.91	124.77
22	b	609	CLA	CHA-C4D-ND	4.02	140.85	132.55
28	A	413	SQD	O48-C23-O10	-4.02	113.57	123.63
22	c	905	CLA	C2C-C1C-NC	4.02	114.20	109.98
22	C	511	CLA	C4A-NA-C1A	4.02	108.51	106.68
22	b	612	CLA	CHD-C4C-NC	4.02	130.46	124.23
22	D	401	CLA	C1D-CHD-C4C	-4.01	117.49	126.02
22	C	503	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
22	A	406	CLA	C1D-CHD-C4C	-4.01	117.50	126.02
22	C	512	CLA	C2D-C1D-ND	4.01	114.09	110.13
22	c	913	CLA	CHD-C4C-C3C	-4.01	118.93	124.77
22	C	514	CLA	O2D-CGD-CBD	4.01	118.23	111.23
22	B	615	CLA	C3B-C2B-C1B	-4.00	102.45	107.17
22	A	406	CLA	C2D-C1D-ND	4.00	114.08	110.13
22	d	403	CLA	C2B-C1B-NB	4.00	114.47	110.33
22	b	603	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
23	a	411	PHO	C4-C3-C5	3.99	122.15	115.23
22	c	911	CLA	CHC-C4B-NB	3.99	130.03	124.05
22	D	404	CLA	CHD-C1D-ND	-3.99	119.19	124.80
22	B	610	CLA	C2C-C1C-NC	3.98	114.17	109.98
22	c	902	CLA	C2B-C1B-NB	3.98	114.46	110.33
22	A	408	CLA	O2D-CGD-CBD	3.98	118.19	111.23
22	B	612	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
22	D	404	CLA	CHC-C4B-NB	3.98	130.02	124.05
22	a	412	CLA	C2B-C1B-NB	3.97	114.44	110.33
25	C	531	LMG	O7-C10-C11	3.97	120.07	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	C2D-C1D-ND	3.96	114.04	110.13
34	V	203	HTG	C1-C2-C3	-3.96	102.81	110.55
35	C	517	DGD	C3G-C2G-C1G	-3.96	102.56	111.78
22	c	905	CLA	C3B-C4B-NB	3.96	114.06	110.53
22	C	509	CLA	CHC-C4B-NB	3.95	129.98	124.05
22	C	514	CLA	C4D-CHA-C1A	-3.95	116.53	121.24
22	a	412	CLA	CHD-C4C-C3C	-3.95	119.01	124.77
22	b	605	CLA	CHD-C4C-C3C	-3.95	119.02	124.77
22	B	607	CLA	C4-C3-C5	3.94	122.08	115.23
22	c	914	CLA	C3B-C2B-C1B	-3.94	102.52	107.17
22	C	507	CLA	CHD-C1D-ND	-3.94	119.25	124.80
22	C	509	CLA	C4D-CHA-C1A	-3.94	116.54	121.24
22	c	909	CLA	C4D-CHA-C1A	-3.94	116.54	121.24
22	B	615	CLA	C1-O2A-CGA	3.94	126.19	116.65
22	c	910	CLA	O2D-CGD-CBD	3.94	118.11	111.23
22	B	612	CLA	C2C-C1C-NC	3.94	114.12	109.98
35	h	102	DGD	O1G-C1A-C2A	3.94	123.84	111.83
22	b	608	CLA	CGD-CBD-CAD	-3.93	98.13	110.85
22	c	904	CLA	CMD-C2D-C1D	3.93	131.65	124.73
22	b	615	CLA	CHC-C4B-NB	3.93	129.94	124.05
22	B	608	CLA	O2D-CGD-CBD	3.93	118.09	111.23
22	C	513	CLA	C1C-C2C-C3C	-3.92	102.85	106.98
22	b	603	CLA	O2D-CGD-O1D	-3.92	116.21	123.85
22	B	603	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
24	d	404	BCR	C30-C25-C26	-3.92	117.28	122.64
22	c	904	CLA	CHA-C4D-ND	3.92	140.64	132.55
22	c	908	CLA	CHC-C4B-NB	3.92	129.93	124.05
22	D	403	CLA	CHC-C4B-NB	3.92	129.92	124.05
22	C	504	CLA	CHC-C4B-NB	3.91	129.92	124.05
35	H	102	DGD	O1G-C1A-C2A	3.91	123.76	111.83
22	C	511	CLA	CHA-C4D-ND	3.91	140.62	132.55
22	B	607	CLA	CHA-C4D-ND	3.91	140.62	132.55
22	c	914	CLA	O2D-CGD-O1D	-3.91	116.24	123.85
22	c	914	CLA	CMC-C2C-C1C	3.91	131.14	125.03
22	c	903	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
22	C	508	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
22	C	511	CLA	O2D-CGD-CBD	3.90	118.05	111.23
24	Y	101	BCR	C16-C15-C14	-3.90	115.54	123.52
25	c	920	LMG	O8-C28-C29	3.90	123.72	111.83
22	c	912	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
25	c	930	LMG	O7-C10-C11	3.89	119.90	111.48
22	b	612	CLA	C3D-C2D-C1D	-3.89	100.52	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
22	B	610	CLA	O2D-CGD-CBD	3.89	118.03	111.23
22	b	616	CLA	C1C-C2C-C3C	-3.88	102.89	106.98
22	B	608	CLA	CGD-CBD-CAD	-3.88	98.27	110.85
22	b	611	CLA	C3D-C2D-C1D	-3.88	100.53	105.83
27	a	423	LHG	O7-C7-C8	3.88	119.88	111.48
22	B	615	CLA	C2C-C1C-NC	3.88	114.06	109.98
22	b	607	CLA	CMD-C2D-C1D	3.88	131.56	124.73
29	a	419	LMT	C4B-C3B-C2B	-3.88	104.02	110.83
22	B	603	CLA	C2D-C1D-ND	3.88	113.96	110.13
22	C	510	CLA	CMB-C2B-C1B	3.88	131.32	125.42
22	c	912	CLA	C3B-C2B-C1B	-3.88	102.60	107.17
22	b	610	CLA	CMC-C2C-C1C	3.88	131.09	125.03
22	C	502	CLA	CHD-C1D-ND	-3.87	119.36	124.80
22	a	408	CLA	CED-O2D-CGD	3.87	124.69	115.92
22	C	512	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
22	C	514	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
22	c	906	CLA	C4D-CHA-C1A	-3.86	116.64	121.24
22	a	408	CLA	C4A-NA-C1A	3.86	108.44	106.68
22	b	610	CLA	C4A-NA-C1A	3.86	108.44	106.68
22	b	614	CLA	C2D-C1D-ND	3.86	113.94	110.13
22	B	606	CLA	C3B-C2B-C1B	-3.86	102.62	107.17
22	b	610	CLA	C3B-C2B-C1B	-3.85	102.63	107.17
22	a	409	CLA	C4-C3-C5	3.85	121.91	115.23
22	b	613	CLA	CHD-C4C-NC	3.85	130.20	124.23
22	C	504	CLA	O2D-CGD-CBD	3.85	117.96	111.23
22	c	906	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
22	c	903	CLA	C4D-CHA-C1A	-3.85	116.66	121.24
22	B	611	CLA	O2A-CGA-CBA	3.85	123.56	111.83
22	B	612	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
22	B	602	CLA	CHA-C4D-ND	3.84	140.48	132.55
22	b	614	CLA	O2D-CGD-CBD	3.84	117.94	111.23
22	a	409	CLA	C1-C2-C3	-3.84	119.91	126.20
22	b	609	CLA	CHC-C4B-NB	3.84	129.80	124.05
22	c	906	CLA	C1-O2A-CGA	3.83	125.92	116.65
22	b	614	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
22	B	617	CLA	C3B-C2B-C1B	-3.83	102.66	107.17
22	B	608	CLA	CBC-CAC-C3C	-3.83	102.04	112.42
29	T	102	LMT	C1'-C2'-C3'	3.83	118.06	110.01
22	A	406	CLA	CHD-C1D-ND	-3.83	119.42	124.80
22	c	909	CLA	CHD-C4C-C3C	-3.83	119.20	124.77
22	c	913	CLA	C2B-C1B-NB	3.82	114.29	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C2D-C1D-ND	3.82	113.91	110.13
22	b	611	CLA	C2B-C1B-NB	3.82	114.29	110.33
24	c	915	BCR	C15-C14-C13	-3.82	121.92	127.28
22	C	512	CLA	CMB-C2B-C1B	3.81	131.23	125.42
22	A	408	CLA	CHC-C4B-NB	3.81	129.77	124.05
22	c	914	CLA	C2C-C1C-NC	3.81	113.99	109.98
22	b	607	CLA	CHD-C4C-NC	3.81	130.14	124.23
22	B	606	CLA	CAC-C3C-C4C	3.81	129.75	124.79
22	b	607	CLA	C3D-C2D-C1D	-3.81	100.63	105.83
22	c	913	CLA	CHC-C4B-NB	3.80	129.75	124.05
22	C	510	CLA	CHA-C4D-ND	3.80	140.40	132.55
22	C	510	CLA	CHC-C4B-NB	3.80	129.75	124.05
22	C	504	CLA	C2B-C1B-NB	3.80	114.27	110.33
22	b	603	CLA	C2D-C1D-ND	3.80	113.89	110.13
22	D	403	CLA	C3B-C4B-NB	3.80	113.92	110.53
22	B	604	CLA	C4A-NA-C1A	3.80	108.41	106.68
22	B	609	CLA	CAC-C3C-C4C	3.80	129.73	124.79
22	B	605	CLA	CMC-C2C-C1C	3.80	130.97	125.03
22	C	505	CLA	C3B-C2B-C1B	-3.79	102.70	107.17
22	b	608	CLA	CHC-C4B-NB	3.79	129.73	124.05
22	C	509	CLA	CHD-C4C-C3C	-3.79	119.25	124.77
22	B	613	CLA	C2B-C1B-NB	3.79	114.25	110.33
22	D	401	CLA	CBC-CAC-C3C	-3.79	102.16	112.42
22	d	403	CLA	CHC-C4B-NB	3.79	129.73	124.05
22	A	408	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
22	B	612	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
22	c	907	CLA	C3B-C2B-C1B	-3.78	102.72	107.17
22	b	605	CLA	CHA-C4D-ND	3.78	140.34	132.55
22	B	616	CLA	C3D-C2D-C1D	-3.78	100.68	105.83
22	C	507	CLA	C3D-C2D-C1D	-3.78	100.68	105.83
22	B	603	CLA	C3B-C2B-C1B	-3.78	102.72	107.17
22	c	914	CLA	CHC-C4B-NB	3.77	129.71	124.05
22	c	906	CLA	C2D-C1D-ND	3.77	113.86	110.13
22	c	914	CLA	CHD-C4C-NC	3.77	130.08	124.23
28	l	101	SQD	O7-S-C6	3.77	112.38	106.76
22	c	905	CLA	C3D-C2D-C1D	-3.77	100.69	105.83
22	B	611	CLA	CMD-C2D-C1D	3.76	131.36	124.73
22	C	506	CLA	C2C-C1C-NC	3.76	113.94	109.98
22	C	509	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
22	B	606	CLA	CHC-C4B-NB	3.76	129.69	124.05
22	B	615	CLA	C2B-C1B-NB	3.76	114.22	110.33
22	a	407	CLA	C4-C3-C5	3.76	121.75	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	415	PL9	C53-C6-C1	3.75	122.96	115.28
22	D	404	CLA	C1C-C2C-C3C	-3.75	103.03	106.98
22	b	608	CLA	C3B-C2B-C1B	-3.75	102.75	107.17
22	A	406	CLA	CMC-C2C-C1C	3.75	130.90	125.03
22	b	612	CLA	C3B-C2B-C1B	-3.75	102.75	107.17
22	c	911	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
22	c	902	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
22	a	409	CLA	CHC-C4B-NB	3.75	129.67	124.05
22	c	911	CLA	CHD-C1D-ND	-3.75	119.53	124.80
22	c	913	CLA	C2D-C1D-ND	3.74	113.83	110.13
25	b	622	LMG	C3-C4-C5	3.74	117.02	110.23
22	b	606	CLA	C2B-C1B-NB	3.74	114.21	110.33
22	D	401	CLA	C4D-CHA-C1A	-3.74	116.78	121.24
24	k	101	BCR	C24-C23-C22	-3.74	120.70	126.23
22	A	408	CLA	C4D-CHA-C1A	-3.74	116.78	121.24
22	a	407	CLA	C2C-C1C-NC	3.74	113.91	109.98
22	c	904	CLA	CHB-C1B-NB	-3.74	118.44	124.05
22	A	408	CLA	CHD-C1D-ND	-3.74	119.54	124.80
22	b	615	CLA	CHA-C4D-ND	3.74	140.26	132.55
22	c	905	CLA	CHC-C4B-NB	3.74	129.65	124.05
22	c	904	CLA	O2A-CGA-CBA	3.73	123.22	111.83
22	B	609	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
22	b	617	CLA	C2C-C1C-NC	3.73	113.90	109.98
22	c	913	CLA	C2C-C1C-NC	3.73	113.90	109.98
24	d	404	BCR	C16-C15-C14	-3.73	115.88	123.52
22	c	912	CLA	C2B-C1B-NB	3.73	114.19	110.33
22	A	408	CLA	C3B-C2B-C1B	-3.73	102.78	107.17
24	A	409	BCR	C15-C16-C17	-3.73	115.90	123.52
22	C	508	CLA	C3B-C2B-C1B	-3.72	102.78	107.17
22	C	507	CLA	CHC-C4B-NB	3.72	129.63	124.05
22	C	513	CLA	C3D-C2D-C1D	-3.72	100.75	105.83
22	D	403	CLA	C2B-C1B-NB	3.72	114.18	110.33
22	C	504	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
22	B	617	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
22	b	606	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
22	B	603	CLA	C3D-C2D-C1D	-3.71	100.76	105.83
22	b	613	CLA	C3B-C2B-C1B	-3.71	102.79	107.17
22	c	911	CLA	C2D-C1D-ND	3.71	113.80	110.13
22	B	607	CLA	C1-C2-C3	-3.71	120.11	126.20
24	b	620	BCR	C7-C8-C9	-3.71	120.74	126.23
22	A	408	CLA	CHD-C4C-C3C	-3.71	119.36	124.77
22	c	902	CLA	CHD-C4C-NC	3.71	129.98	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	911	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
22	C	513	CLA	CHA-C4D-ND	3.71	140.20	132.55
22	b	612	CLA	CHA-C4D-ND	3.71	140.20	132.55
22	C	505	CLA	CHD-C4C-C3C	-3.71	119.37	124.77
22	b	604	CLA	C2D-C1D-ND	3.70	113.79	110.13
22	B	602	CLA	C1-O2A-CGA	3.70	125.61	116.65
24	C	515	BCR	C38-C26-C25	-3.70	120.45	124.48
22	C	508	CLA	C2C-C1C-NC	3.70	113.87	109.98
22	B	605	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
22	B	606	CLA	C2B-C1B-NB	3.70	114.16	110.33
22	b	616	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
22	B	614	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
22	b	604	CLA	C4A-NA-C1A	3.69	108.36	106.68
22	C	506	CLA	C2B-C1B-NB	3.69	114.16	110.33
26	D	406	PL9	C7-C8-C9	-3.69	120.47	126.83
22	b	604	CLA	CHD-C4C-NC	3.69	129.96	124.23
22	b	604	CLA	CMC-C2C-C1C	3.69	130.80	125.03
24	B	618	BCR	C3-C4-C5	-3.69	107.48	114.06
22	b	602	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
22	b	615	CLA	C3D-C2D-C1D	-3.69	100.80	105.83
22	b	615	CLA	C2D-C1D-ND	3.68	113.77	110.13
22	C	503	CLA	C3D-C2D-C1D	-3.68	100.80	105.83
27	D	411	LHG	O8-C23-O10	-3.68	114.42	123.63
22	B	614	CLA	C2B-C1B-NB	3.68	114.14	110.33
22	b	617	CLA	CHA-C4D-ND	3.68	140.14	132.55
22	b	617	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
22	B	612	CLA	CMD-C2D-C1D	3.68	131.20	124.73
22	c	906	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
22	B	605	CLA	CAC-C3C-C4C	3.67	129.57	124.79
22	B	615	CLA	CHD-C1D-ND	-3.67	119.63	124.80
28	C	501	SQD	O8-S-C6	3.67	113.06	105.97
22	c	909	CLA	CHA-C4D-ND	3.67	140.13	132.55
22	C	509	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
22	b	616	CLA	O2D-CGD-CBD	3.67	117.64	111.23
34	b	624	HTG	C1-C2-C3	3.67	117.72	110.55
22	B	608	CLA	C4A-NA-C1A	3.67	108.35	106.68
22	B	613	CLA	CHD-C1D-ND	-3.67	119.64	124.80
22	a	407	CLA	C3D-C2D-C1D	-3.66	100.83	105.83
22	B	613	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
22	B	617	CLA	CHC-C4B-NB	3.66	129.54	124.05
22	B	614	CLA	CHD-C4C-C3C	-3.66	119.44	124.77
22	C	511	CLA	C2B-C1B-NB	3.66	114.12	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	607	CLA	C2D-C1D-ND	3.66	113.74	110.13
22	B	616	CLA	CHA-C4D-ND	3.66	140.09	132.55
22	C	508	CLA	CMD-C2D-C1D	3.66	131.16	124.73
28	a	418	SQD	O47-C7-C8	3.65	119.39	111.48
26	a	415	PL9	C7-C3-C4	3.65	119.92	116.91
22	B	607	CLA	C4A-NA-C1A	3.65	108.34	106.68
22	b	613	CLA	C2C-C1C-NC	3.65	113.81	109.98
22	b	617	CLA	CHC-C4B-NB	3.65	129.52	124.05
22	C	508	CLA	CHD-C1D-ND	-3.65	119.67	124.80
22	B	603	CLA	C7-C6-C5	-3.65	103.55	113.26
22	b	606	CLA	C4A-NA-C1A	3.65	108.34	106.68
22	b	604	CLA	C3D-C2D-C1D	-3.64	100.86	105.83
22	B	608	CLA	CHA-C4D-ND	3.64	140.06	132.55
22	D	404	CLA	C2C-C1C-NC	3.64	113.81	109.98
22	A	406	CLA	CHD-C4C-NC	3.64	129.87	124.23
22	b	613	CLA	C3D-C2D-C1D	-3.64	100.87	105.83
22	d	403	CLA	CMD-C2D-C1D	3.64	131.13	124.73
22	C	507	CLA	O2D-CGD-CBD	3.64	117.59	111.23
39	v	202	HEC	C4D-ND-C1D	3.63	111.75	105.82
22	b	608	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
22	B	616	CLA	C3B-C2B-C1B	-3.63	102.89	107.17
22	D	403	CLA	C2A-C1A-CHA	-3.63	117.57	123.87
22	B	616	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
22	B	611	CLA	C2B-C1B-NB	3.63	114.09	110.33
22	b	614	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
22	C	514	CLA	O2A-CGA-CBA	3.62	122.88	111.83
22	A	406	CLA	CHA-C4D-ND	3.62	140.02	132.55
22	B	608	CLA	C4-C3-C5	3.62	121.51	115.23
22	D	401	CLA	CHC-C4B-NB	3.62	129.48	124.05
22	B	616	CLA	C2C-C1C-NC	3.62	113.78	109.98
22	B	614	CLA	O2D-CGD-O1D	-3.62	116.81	123.85
22	D	401	CLA	O2D-CGD-CBD	3.62	117.55	111.23
25	b	622	LMG	C7-O1-C1	3.61	121.53	113.80
22	b	612	CLA	CMD-C2D-C1D	3.60	131.08	124.73
22	C	514	CLA	CHD-C4C-NC	3.60	129.82	124.23
22	B	604	CLA	C3D-C2D-C1D	-3.60	100.92	105.83
22	B	617	CLA	C4A-NA-C1A	3.60	108.32	106.68
22	c	903	CLA	CHD-C4C-NC	3.60	129.81	124.23
22	b	602	CLA	C2D-C1D-ND	3.60	113.69	110.13
22	B	602	CLA	CHD-C1D-ND	-3.60	119.74	124.80
22	b	608	CLA	O2D-CGD-CBD	3.60	117.52	111.23
22	c	906	CLA	C2C-C1C-NC	3.60	113.76	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	612	CLA	CMB-C2B-C1B	3.59	130.89	125.42
24	D	405	BCR	C28-C27-C26	-3.59	107.65	114.06
22	B	602	CLA	CMD-C2D-C1D	3.59	131.05	124.73
22	c	903	CLA	CHC-C4B-NB	3.59	129.43	124.05
22	c	910	CLA	C2D-C1D-ND	3.59	113.68	110.13
22	C	513	CLA	O1D-CGD-CBD	-3.59	117.44	124.52
22	c	914	CLA	C3D-C2D-C1D	-3.59	100.94	105.83
24	D	405	BCR	C29-C30-C25	3.59	115.65	110.44
22	C	504	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
22	b	606	CLA	C4-C3-C5	3.58	121.45	115.23
22	c	910	CLA	CHA-C4D-ND	3.58	139.94	132.55
35	h	102	DGD	O1G-C1A-O1A	-3.58	114.66	123.63
22	b	617	CLA	C3C-C4C-NC	3.58	115.02	110.43
34	b	624	HTG	O5-C1-C2	3.58	115.25	110.32
22	C	505	CLA	CMD-C2D-C1D	3.58	131.03	124.73
22	b	614	CLA	C3B-C2B-C1B	-3.58	102.95	107.17
35	c	918	DGD	O2G-C1B-C2B	3.58	119.22	111.48
35	C	519	DGD	O6D-C1D-O3G	-3.58	101.59	110.04
22	c	905	CLA	CHA-C4D-ND	3.57	139.91	132.55
22	b	605	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
22	c	904	CLA	C2B-C1B-NB	3.57	114.03	110.33
27	d	401	LHG	O7-C7-C8	3.56	119.19	111.48
24	K	101	BCR	C24-C23-C22	-3.56	120.96	126.23
22	b	602	CLA	C3B-C2B-C1B	-3.56	102.97	107.17
22	C	512	CLA	CHA-C4D-ND	3.56	139.89	132.55
24	c	916	BCR	C33-C5-C6	-3.56	120.60	124.48
22	d	402	CLA	C4-C3-C5	3.56	121.40	115.23
22	a	407	CLA	CHD-C1D-ND	-3.56	119.80	124.80
22	b	606	CLA	C3B-C2B-C1B	-3.56	102.98	107.17
22	d	402	CLA	CHD-C4C-C3C	-3.56	119.59	124.77
22	B	615	CLA	C4-C3-C5	3.56	121.40	115.23
22	c	908	CLA	C3B-C2B-C1B	-3.55	102.98	107.17
27	D	411	LHG	O8-C23-C24	3.55	122.67	111.83
22	b	602	CLA	O2A-CGA-CBA	3.55	122.66	111.83
35	h	102	DGD	O2G-C1B-C2B	3.55	119.16	111.48
34	B	627	HTG	O5-C1-C2	3.55	115.21	110.32
22	b	609	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
22	b	605	CLA	C3D-C2D-C1D	-3.54	101.00	105.83
28	a	414	SQD	C1-O5-C5	-3.54	106.80	113.72
22	C	505	CLA	CHA-C4D-ND	3.54	139.86	132.55
22	b	606	CLA	C1-C2-C3	-3.54	120.39	126.20
25	b	622	LMG	O6-C1-O1	3.54	118.41	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	C2B-C1B-NB	3.54	114.00	110.33
27	L	101	LHG	O7-C7-C8	3.54	119.14	111.48
22	B	611	CLA	O2A-CGA-O1A	-3.54	114.78	123.63
22	c	905	CLA	C4D-CHA-C1A	-3.54	117.02	121.24
22	b	604	CLA	CHA-C4D-ND	3.54	139.85	132.55
22	B	613	CLA	C2D-C1D-ND	3.54	113.63	110.13
22	B	606	CLA	CHA-C4D-ND	3.54	139.85	132.55
22	C	508	CLA	C2B-C1B-NB	3.54	113.99	110.33
22	b	602	CLA	CHA-C4D-ND	3.54	139.84	132.55
24	y	101	BCR	C21-C20-C19	-3.53	112.96	123.20
22	B	611	CLA	CHA-C4D-ND	3.53	139.84	132.55
22	b	613	CLA	C4-C3-C5	3.53	121.36	115.23
22	B	602	CLA	C2C-C1C-NC	3.53	113.69	109.98
22	C	510	CLA	CHD-C4C-C3C	-3.53	119.63	124.77
27	D	409	LHG	O8-C23-C24	3.53	122.60	111.83
22	c	910	CLA	C2A-C1A-CHA	-3.52	117.75	123.87
22	b	615	CLA	C1C-C2C-C3C	-3.52	103.27	106.98
22	B	610	CLA	CHD-C1D-ND	-3.52	119.84	124.80
29	a	419	LMT	C2'-C3'-C4'	3.52	117.68	109.68
22	b	616	CLA	C2C-C1C-NC	3.52	113.68	109.98
22	C	507	CLA	CAC-C3C-C4C	3.52	129.37	124.79
22	D	403	CLA	O2D-CGD-CBD	3.52	117.38	111.23
22	c	908	CLA	C4-C3-C5	3.51	121.33	115.23
22	b	607	CLA	CHA-C4D-ND	3.51	139.78	132.55
22	c	903	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
22	C	508	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
22	c	904	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
22	B	602	CLA	C3B-C2B-C1B	-3.50	103.04	107.17
22	b	617	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
22	C	505	CLA	CHD-C4C-NC	3.50	129.66	124.23
22	B	607	CLA	CMD-C2D-C1D	3.50	130.89	124.73
22	c	909	CLA	C2C-C1C-NC	3.50	113.66	109.98
22	b	610	CLA	CHD-C4C-NC	3.50	129.65	124.23
22	B	605	CLA	CHC-C4B-NB	3.49	129.29	124.05
22	C	508	CLA	CHA-C4D-ND	3.49	139.76	132.55
22	D	403	CLA	CHD-C4C-C3C	-3.49	119.68	124.77
26	d	405	PL9	C7-C8-C9	-3.49	120.82	126.83
35	C	519	DGD	O1G-C1A-C2A	3.49	122.47	111.83
22	c	904	CLA	CHD-C4C-C3C	-3.49	119.69	124.77
22	c	912	CLA	O2D-CGD-CBD	3.48	117.32	111.23
22	b	608	CLA	CHD-C4C-C3C	-3.48	119.70	124.77
22	b	617	CLA	O1D-CGD-CBD	-3.48	117.65	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	C3B-C2B-C1B	-3.48	103.07	107.17
22	B	612	CLA	CMB-C2B-C1B	3.48	130.72	125.42
28	a	418	SQD	O48-C23-C24	3.48	122.43	111.83
29	f	102	LMT	O1'-C1'-C2'	3.47	113.55	108.27
22	C	506	CLA	CHC-C4B-NB	3.47	129.26	124.05
22	A	405	CLA	CHC-C4B-NB	3.47	129.26	124.05
22	C	504	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
22	B	604	CLA	CHA-C4D-ND	3.47	139.71	132.55
22	B	613	CLA	C2A-C1A-CHA	-3.47	117.85	123.87
22	b	604	CLA	C1D-CHD-C4C	-3.47	118.65	126.02
22	a	407	CLA	CHA-C4D-ND	3.46	139.69	132.55
22	B	609	CLA	C3B-C2B-C1B	-3.46	103.09	107.17
24	b	619	BCR	C29-C30-C25	3.46	115.46	110.44
22	B	614	CLA	CHA-C4D-ND	3.46	139.68	132.55
22	d	403	CLA	CHA-C4D-ND	3.45	139.67	132.55
22	B	607	CLA	C3D-C2D-C1D	-3.45	101.12	105.83
22	C	513	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
29	E	101	LMT	O5'-C5'-C6'	3.45	114.98	106.44
22	c	904	CLA	C2D-C1D-ND	3.45	113.54	110.13
25	b	622	LMG	C4-C3-C2	3.45	116.88	110.83
22	b	612	CLA	CHD-C1D-ND	-3.44	119.96	124.80
25	A	410	LMG	O7-C10-C11	3.44	118.93	111.48
22	B	607	CLA	CHC-C1C-NC	-3.44	119.13	124.31
22	b	603	CLA	C1-C2-C3	-3.44	120.56	126.20
22	c	908	CLA	CBC-CAC-C3C	-3.44	103.09	112.42
22	b	614	CLA	CAA-CBA-CGA	-3.44	103.45	113.21
22	B	603	CLA	CHC-C1C-NC	-3.43	119.14	124.31
22	b	616	CLA	CHD-C4C-NC	3.43	129.55	124.23
22	c	907	CLA	C4B-C3B-C2B	-3.43	103.03	107.30
22	B	605	CLA	CHD-C1D-ND	-3.43	119.97	124.80
22	C	511	CLA	C3B-C2B-C1B	-3.43	103.13	107.17
34	v	203	HTG	O4-C4-C3	-3.43	102.30	110.38
22	b	606	CLA	CHA-C4D-ND	3.42	139.62	132.55
22	c	904	CLA	CMB-C2B-C1B	3.42	130.63	125.42
22	c	910	CLA	C1-O2A-CGA	3.42	124.94	116.65
22	c	912	CLA	O2A-CGA-O1A	-3.42	115.08	123.63
22	b	603	CLA	CHC-C4B-NB	3.42	129.17	124.05
22	b	612	CLA	CHC-C4B-NB	3.42	129.17	124.05
22	b	615	CLA	CAC-C3C-C4C	3.42	129.24	124.79
35	C	518	DGD	O2G-C1B-C2B	3.42	118.87	111.48
22	B	608	CLA	CHC-C4B-NB	3.41	129.17	124.05
22	C	508	CLA	C4D-CHA-C1A	-3.41	117.17	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	604	CLA	CHD-C1D-ND	-3.41	120.00	124.80
22	B	604	CLA	CHD-C1D-ND	-3.41	120.00	124.80
22	C	502	CLA	CAC-C3C-C4C	3.41	129.22	124.79
22	a	412	CLA	C1-C2-C3	-3.41	120.61	126.20
22	C	514	CLA	CMC-C2C-C1C	3.41	130.36	125.03
22	d	403	CLA	C4D-CHA-C1A	-3.40	117.18	121.24
22	b	609	CLA	C1D-CHD-C4C	-3.40	118.79	126.02
22	b	604	CLA	O2A-CGA-O1A	-3.40	115.12	123.63
22	C	506	CLA	O2D-CGD-CBD	3.40	117.17	111.23
26	D	406	PL9	C20-C19-C21	3.39	121.12	115.23
22	a	409	CLA	CMC-C2C-C1C	3.39	130.34	125.03
37	H	101	RRX	C7-C8-C9	-3.39	121.21	126.23
22	a	412	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
22	B	605	CLA	CHA-C4D-ND	3.39	139.55	132.55
22	a	409	CLA	CHD-C4C-NC	3.39	129.49	124.23
22	B	615	CLA	O2A-CGA-CBA	3.39	122.18	111.83
22	C	511	CLA	C4D-CHA-C1A	-3.39	117.20	121.24
22	d	402	CLA	C3D-C2D-C1D	-3.39	101.21	105.83
22	A	406	CLA	C4A-NA-C1A	3.39	108.22	106.68
22	B	617	CLA	C4B-C3B-C2B	-3.39	103.09	107.30
22	B	603	CLA	C1-C2-C3	-3.39	120.65	126.20
22	c	907	CLA	C3B-C4B-NB	3.38	113.55	110.53
24	y	101	BCR	C24-C23-C22	-3.38	121.23	126.23
25	b	622	LMG	O6-C5-C6	3.38	114.82	106.44
22	a	408	CLA	CBC-CAC-C3C	-3.38	103.25	112.42
22	c	911	CLA	C4D-CHA-C1A	-3.38	117.21	121.24
22	C	507	CLA	CHA-C4D-ND	3.38	139.52	132.55
22	B	611	CLA	C3B-C2B-C1B	-3.38	103.19	107.17
22	b	609	CLA	C1C-C2C-C3C	-3.38	103.43	106.98
22	C	512	CLA	CHD-C1D-ND	-3.38	120.05	124.80
22	B	606	CLA	O2D-CGD-CBD	3.38	117.13	111.23
22	B	612	CLA	CHD-C1D-ND	-3.37	120.05	124.80
22	B	616	CLA	C4D-CHA-C1A	-3.37	117.22	121.24
22	B	603	CLA	CHA-C4D-ND	3.37	139.50	132.55
22	b	613	CLA	C4C-C3C-C2C	-3.37	101.99	106.89
22	B	615	CLA	CED-O2D-CGD	3.37	123.56	115.92
22	B	608	CLA	CAC-C3C-C4C	3.37	129.17	124.79
22	B	607	CLA	C2B-C1B-NB	3.37	113.82	110.33
22	d	402	CLA	O2A-CGA-O1A	-3.37	115.20	123.63
22	C	510	CLA	C2D-C1D-ND	3.36	113.45	110.13
22	c	902	CLA	CMB-C2B-C1B	3.36	130.54	125.42
35	C	519	DGD	O2G-C1B-C2B	3.36	118.75	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	408	CLA	CMD-C2D-C1D	3.35	130.64	124.73
22	C	514	CLA	CHC-C1C-NC	-3.35	119.26	124.31
22	B	606	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
26	D	406	PL9	C53-C6-C1	3.35	122.13	115.28
22	c	914	CLA	CHA-C4D-ND	3.35	139.45	132.55
39	V	202	HEC	CBD-CAD-C3D	-3.34	103.28	112.53
22	b	614	CLA	C4-C3-C5	3.34	121.03	115.23
22	b	609	CLA	C4D-CHA-C1A	-3.34	117.26	121.24
22	c	909	CLA	C2D-C1D-ND	3.34	113.43	110.13
22	d	402	CLA	CHA-C4D-ND	3.34	139.44	132.55
22	D	401	CLA	C3D-C2D-C1D	-3.34	101.28	105.83
35	D	407	DGD	C3D-C4D-C5D	3.33	114.88	109.81
22	B	605	CLA	C3B-C2B-C1B	-3.33	103.24	107.17
22	b	617	CLA	C4C-C3C-C2C	-3.33	102.04	106.89
27	a	423	LHG	O8-C23-C24	3.33	122.00	111.83
22	C	513	CLA	CHD-C4C-NC	3.33	129.40	124.23
22	B	605	CLA	CMD-C2D-C1D	3.33	130.59	124.73
22	c	907	CLA	CMD-C2D-C1D	3.33	130.59	124.73
22	B	610	CLA	C3B-C2B-C1B	-3.33	103.25	107.17
22	c	914	CLA	O2D-CGD-CBD	3.33	117.05	111.23
22	C	508	CLA	CHD-C4C-NC	3.33	129.39	124.23
22	B	613	CLA	CMD-C2D-C1D	3.33	130.59	124.73
22	c	905	CLA	O2D-CGD-CBD	3.32	117.04	111.23
22	C	511	CLA	C1D-CHD-C4C	-3.32	118.96	126.02
28	b	621	SQD	O7-S-C6	3.32	111.72	106.76
22	b	602	CLA	CHC-C4B-NB	3.32	129.02	124.05
22	b	617	CLA	C2B-C1B-NB	3.31	113.76	110.33
22	B	615	CLA	C1D-ND-C4D	-3.31	103.99	106.31
22	A	406	CLA	O2D-CGD-CBD	3.31	117.02	111.23
22	B	605	CLA	CHD-C4C-NC	3.31	129.36	124.23
22	B	612	CLA	C2A-C1A-CHA	-3.31	118.13	123.87
22	b	611	CLA	CHA-C4D-ND	3.31	139.37	132.55
22	c	908	CLA	C2C-C1C-NC	3.30	113.45	109.98
29	Z	101	LMT	C3B-C4B-C5B	3.30	116.22	110.23
22	C	509	CLA	O2A-CGA-O1A	-3.30	115.37	123.63
22	B	614	CLA	C2C-C1C-NC	3.30	113.45	109.98
35	c	919	DGD	O1G-C1A-C2A	3.30	121.90	111.83
22	b	602	CLA	C2C-C1C-NC	3.30	113.45	109.98
22	b	616	CLA	CED-O2D-CGD	3.30	123.40	115.92
22	c	902	CLA	C4D-CHA-C1A	-3.30	117.31	121.24
22	a	408	CLA	C3D-C2D-C1D	-3.30	101.33	105.83
22	B	615	CLA	O1D-CGD-CBD	-3.30	118.02	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	910	CLA	O2A-CGA-CBA	3.29	121.88	111.83
22	A	408	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
22	C	505	CLA	C2B-C1B-NB	3.29	113.74	110.33
22	a	407	CLA	CHC-C4B-NB	3.29	128.99	124.05
22	b	603	CLA	CHD-C4C-C3C	-3.29	119.98	124.77
22	C	502	CLA	C3B-C2B-C1B	-3.29	103.29	107.17
28	b	621	SQD	O5-C1-C2	-3.29	103.61	110.37
22	d	403	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
22	b	612	CLA	C7-C6-C5	-3.28	104.51	113.26
22	a	407	CLA	C4D-CHA-C1A	-3.28	117.33	121.24
22	A	405	CLA	C3D-C2D-C1D	-3.28	101.36	105.83
22	C	503	CLA	C2C-C1C-NC	3.28	113.43	109.98
22	B	610	CLA	CHA-C4D-ND	3.28	139.31	132.55
22	c	907	CLA	CHD-C4C-NC	3.27	129.31	124.23
22	c	908	CLA	C3D-C2D-C1D	-3.27	101.36	105.83
22	b	616	CLA	CHD-C1D-ND	-3.27	120.19	124.80
22	B	614	CLA	C3D-C2D-C1D	-3.27	101.37	105.83
22	C	509	CLA	C2C-C1C-NC	3.27	113.41	109.98
22	B	615	CLA	CMD-C2D-C1D	3.27	130.48	124.73
22	B	617	CLA	CHA-C4D-ND	3.26	139.28	132.55
24	y	101	BCR	C38-C26-C25	-3.26	120.92	124.48
22	b	610	CLA	C2B-C1B-NB	3.26	113.71	110.33
22	B	603	CLA	O2A-CGA-CBA	3.26	121.78	111.83
22	B	604	CLA	C4D-CHA-C1A	-3.26	117.35	121.24
22	C	512	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
22	b	610	CLA	C1-C2-C3	-3.26	120.86	126.20
22	B	603	CLA	C3B-C4B-NB	3.26	113.44	110.53
22	d	402	CLA	CMB-C2B-C1B	3.26	130.38	125.42
22	D	401	CLA	CMC-C2C-C1C	3.26	130.12	125.03
22	C	513	CLA	CHC-C4B-NB	3.26	128.93	124.05
22	a	407	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
22	b	603	CLA	C3D-C2D-C1D	-3.25	101.39	105.83
27	d	407	LHG	O8-C23-C24	3.25	121.76	111.83
22	C	511	CLA	C2D-C1D-ND	3.25	113.35	110.13
35	c	919	DGD	O2G-C1B-O1B	-3.25	116.10	123.70
22	c	905	CLA	C3B-C2B-C1B	-3.25	103.34	107.17
22	a	408	CLA	CHA-C4D-ND	3.25	139.25	132.55
28	D	408	SQD	O6-C44-C45	3.25	114.96	108.81
22	b	606	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
22	A	408	CLA	CHA-C4D-ND	3.25	139.25	132.55
22	c	907	CLA	C4D-CHA-C1A	-3.25	117.37	121.24
22	b	610	CLA	CBC-CAC-C3C	-3.24	103.62	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	CHB-C4A-NA	3.24	129.08	124.40
22	b	604	CLA	CHC-C4B-NB	3.24	128.91	124.05
37	h	101	RRX	C7-C8-C9	-3.24	121.44	126.23
22	C	506	CLA	C1-O2A-CGA	3.24	124.49	116.65
28	b	621	SQD	O6-C1-C2	3.24	113.19	108.27
22	C	512	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
22	A	405	CLA	CHD-C1D-ND	-3.23	120.26	124.80
22	B	606	CLA	C2C-C1C-NC	3.22	113.37	109.98
22	c	902	CLA	C4-C3-C5	3.22	120.82	115.23
26	A	411	PL9	C22-C23-C24	-3.22	120.25	127.62
22	a	412	CLA	CHA-C4D-ND	3.22	139.19	132.55
22	c	907	CLA	C3D-C2D-C1D	-3.22	101.44	105.83
22	D	404	CLA	CHA-C4D-ND	3.22	139.19	132.55
22	C	510	CLA	C1-C2-C3	-3.21	120.93	126.20
22	c	914	CLA	C1-O2A-CGA	3.21	124.43	116.65
26	A	411	PL9	C32-C33-C34	-3.21	120.27	127.62
22	b	603	CLA	C4-C3-C5	3.21	120.80	115.23
22	D	403	CLA	CHC-C1C-NC	-3.21	119.47	124.31
22	B	607	CLA	CHD-C4C-NC	3.21	129.21	124.23
22	C	509	CLA	CMB-C2B-C1B	3.21	130.31	125.42
24	d	404	BCR	C21-C20-C19	-3.21	113.90	123.20
22	b	613	CLA	O2A-CGA-CBA	3.21	121.62	111.83
22	b	616	CLA	CHA-C4D-ND	3.21	139.17	132.55
39	v	202	HEC	CBB-CAB-C3B	-3.21	121.02	127.43
22	B	615	CLA	CHA-C4D-ND	3.21	139.16	132.55
22	C	510	CLA	O2A-CGA-CBA	3.20	121.61	111.83
22	b	616	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
22	d	402	CLA	C3B-C4B-NB	3.20	113.39	110.53
22	B	611	CLA	CHD-C4C-NC	3.20	129.19	124.23
22	B	610	CLA	C1-C2-C3	-3.20	120.95	126.20
25	B	621	LMG	O8-C28-C29	3.20	121.59	111.83
22	b	615	CLA	C2B-C1B-NB	3.20	113.64	110.33
25	C	520	LMG	O8-C28-O10	-3.20	115.62	123.63
22	C	503	CLA	CAC-C3C-C4C	3.20	128.95	124.79
22	C	507	CLA	CMC-C2C-C1C	3.20	130.03	125.03
22	B	602	CLA	CHD-C4C-C3C	-3.20	120.11	124.77
22	d	403	CLA	CHD-C4C-C3C	-3.20	120.11	124.77
22	B	609	CLA	CHD-C4C-NC	3.19	129.19	124.23
22	D	404	CLA	C1-O2A-CGA	3.19	124.38	116.65
22	D	403	CLA	C3D-C2D-C1D	-3.19	101.48	105.83
22	B	612	CLA	O2D-CGD-CBD	3.19	116.81	111.23
22	b	605	CLA	CAC-C3C-C4C	3.18	128.93	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	912	CLA	C4-C3-C5	3.18	120.75	115.23
22	D	404	CLA	CMD-C2D-C1D	3.18	130.32	124.73
22	c	905	CLA	CHD-C4C-NC	3.17	129.15	124.23
22	B	605	CLA	C2B-C1B-NB	3.17	113.62	110.33
22	C	509	CLA	C3D-C2D-C1D	-3.17	101.51	105.83
22	B	617	CLA	C3B-C4B-NB	3.17	113.36	110.53
26	a	415	PL9	C35-C34-C36	3.17	120.73	115.23
22	c	902	CLA	CHA-C4D-ND	3.17	139.08	132.55
22	b	615	CLA	C1-O2A-CGA	3.16	124.30	116.65
22	C	513	CLA	CMB-C2B-C1B	3.16	130.23	125.42
22	B	617	CLA	O2A-CGA-O1A	-3.16	115.72	123.63
22	C	502	CLA	CHC-C4B-NB	3.16	128.79	124.05
22	a	409	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
25	c	920	LMG	O7-C10-C11	3.15	118.29	111.48
22	C	511	CLA	O2A-CGA-O1A	-3.15	115.75	123.63
22	a	409	CLA	C1-O2A-CGA	3.15	124.27	116.65
39	V	202	HEC	CHD-C4C-NC	3.14	127.88	124.45
24	B	620	BCR	C38-C26-C25	-3.14	121.06	124.48
22	b	602	CLA	C3D-C2D-C1D	-3.14	101.55	105.83
22	C	513	CLA	C4D-CHA-C1A	-3.14	117.50	121.24
28	l	101	SQD	O48-C23-C24	3.13	121.39	111.83
22	D	403	CLA	CMC-C2C-C1C	3.13	129.93	125.03
22	c	913	CLA	CHD-C1D-ND	-3.13	120.40	124.80
22	b	612	CLA	CAC-C3C-C4C	3.13	128.86	124.79
22	C	512	CLA	C3D-C2D-C1D	-3.13	101.56	105.83
22	B	606	CLA	C3D-C2D-C1D	-3.13	101.56	105.83
24	C	516	BCR	C7-C8-C9	-3.13	121.61	126.23
22	b	603	CLA	C2C-C1C-NC	3.13	113.27	109.98
22	b	606	CLA	CMB-C2B-C1B	3.12	130.18	125.42
22	c	913	CLA	CHA-C4D-ND	3.12	139.00	132.55
28	b	621	SQD	O48-C23-C24	3.12	121.36	111.83
22	C	504	CLA	C4-C3-C5	3.12	120.65	115.23
22	C	506	CLA	CHA-C4D-ND	3.12	138.99	132.55
39	v	202	HEC	C2A-C1A-NA	-3.12	107.31	110.32
22	c	908	CLA	CHA-C4D-ND	3.12	138.99	132.55
22	b	610	CLA	CHC-C1C-NC	-3.12	119.61	124.31
22	A	405	CLA	O2A-CGA-O1A	-3.12	115.83	123.63
37	h	101	RRX	C11-C10-C9	-3.12	122.91	127.28
22	c	905	CLA	C4B-C3B-C2B	-3.12	103.43	107.30
22	c	907	CLA	CHC-C4B-NB	3.12	128.72	124.05
23	D	402	PHO	C4D-CHA-CBD	3.11	109.95	108.45
24	B	618	BCR	C2-C3-C4	-3.11	104.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	904	CLA	CAC-C3C-C4C	3.11	128.84	124.79
22	B	602	CLA	C1C-C2C-C3C	-3.11	103.71	106.98
29	t	101	LMT	O5'-C5'-C4'	3.11	115.30	109.70
27	a	416	LHG	O8-C23-C24	3.11	121.32	111.83
22	b	602	CLA	CHD-C4C-NC	3.11	129.05	124.23
22	c	909	CLA	C3D-C2D-C1D	-3.11	101.59	105.83
22	D	403	CLA	C3B-C2B-C1B	-3.11	103.51	107.17
22	B	606	CLA	C3C-C4C-NC	3.11	114.41	110.43
35	C	518	DGD	O6E-C1E-C2E	3.11	116.75	110.37
22	C	503	CLA	CHC-C4B-NB	3.11	128.71	124.05
34	c	922	HTG	C1-O5-C5	3.10	118.13	112.56
29	t	101	LMT	C1'-C2'-C3'	-3.10	103.48	110.01
22	b	604	CLA	C2A-C3A-C4A	-3.10	96.86	101.87
22	C	506	CLA	C4D-CHA-C1A	-3.10	117.54	121.24
22	b	604	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
22	c	904	CLA	C7-C6-C5	-3.10	105.00	113.26
22	B	605	CLA	C6-C5-C3	-3.10	105.92	113.47
22	B	608	CLA	C3B-C4B-NB	3.10	113.30	110.53
22	B	616	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
37	H	101	RRX	C10-C11-C12	-3.10	114.22	123.20
22	C	514	CLA	C2D-C1D-ND	3.10	113.19	110.13
22	a	409	CLA	C2A-C1A-CHA	-3.10	118.49	123.87
22	c	905	CLA	C4-C3-C5	3.09	120.60	115.23
22	b	615	CLA	C3B-C2B-C1B	-3.09	103.52	107.17
22	D	403	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	B	620	BCR	C7-C8-C9	-3.09	121.67	126.23
24	C	515	BCR	C7-C8-C9	-3.09	121.67	126.23
24	Y	101	BCR	C37-C22-C23	3.09	122.80	118.09
24	y	101	BCR	C16-C15-C14	-3.08	117.21	123.52
34	v	203	HTG	O3-C3-C2	3.08	117.64	110.38
22	C	505	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
22	C	511	CLA	C4D-C3D-CAD	3.08	111.45	108.11
28	a	414	SQD	O48-C23-C24	3.08	121.23	111.83
22	B	608	CLA	C2D-C1D-ND	3.08	113.17	110.13
24	B	620	BCR	C32-C1-C6	-3.08	105.42	110.24
22	a	408	CLA	C4B-CHC-C1C	-3.08	119.01	126.25
22	B	605	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
22	C	508	CLA	CHC-C4B-NB	3.07	128.66	124.05
22	c	910	CLA	C1D-CHD-C4C	-3.07	119.49	126.02
25	C	531	LMG	O8-C28-C29	3.07	121.19	111.83
22	B	608	CLA	CMB-C2B-C1B	3.07	130.09	125.42
22	A	405	CLA	CHD-C4C-C3C	-3.07	120.30	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	C3C-C4C-NC	3.07	114.36	110.43
22	B	610	CLA	CBC-CAC-C3C	-3.06	104.12	112.42
22	c	911	CLA	CAC-C3C-C4C	3.06	128.77	124.79
22	C	509	CLA	C4-C3-C5	3.06	120.54	115.23
22	c	911	CLA	CHA-C4D-ND	3.06	138.86	132.55
25	A	410	LMG	O8-C28-C29	3.06	121.15	111.83
22	b	609	CLA	C4-C3-C5	3.05	120.52	115.23
39	V	202	HEC	C4D-ND-C1D	3.05	110.79	105.82
24	D	405	BCR	C33-C5-C6	-3.05	121.16	124.48
22	b	609	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
22	C	502	CLA	CHA-C4D-ND	3.05	138.84	132.55
37	H	101	RRX	C16-C17-C18	-3.04	123.01	127.28
22	A	405	CLA	C7-C6-C5	-3.04	105.15	113.26
22	C	513	CLA	C4-C3-C5	3.04	120.51	115.23
22	c	909	CLA	CHD-C4C-NC	3.04	128.95	124.23
22	b	609	CLA	C3C-C4C-NC	3.04	114.33	110.43
22	b	615	CLA	C4-C3-C5	3.04	120.51	115.23
27	D	409	LHG	C5-O7-C7	-3.04	110.52	117.80
22	C	511	CLA	CAC-C3C-C4C	3.04	128.75	124.79
22	b	610	CLA	C2D-C1D-ND	3.04	113.14	110.13
22	C	505	CLA	C3D-C2D-C1D	-3.04	101.68	105.83
22	c	905	CLA	CHD-C1D-ND	-3.04	120.52	124.80
22	C	513	CLA	C2C-C1C-NC	3.04	113.17	109.98
22	c	908	CLA	CMD-C2D-C1D	3.04	130.08	124.73
22	b	613	CLA	C2B-C1B-NB	3.04	113.48	110.33
22	D	404	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
22	C	502	CLA	C3D-C2D-C1D	-3.03	101.69	105.83
22	c	910	CLA	CMC-C2C-C1C	3.03	129.78	125.03
22	D	404	CLA	C2D-C1D-ND	3.03	113.13	110.13
22	c	909	CLA	CHC-C4B-NB	3.03	128.59	124.05
22	a	409	CLA	CMD-C2D-C1D	3.03	130.06	124.73
22	b	602	CLA	C2B-C1B-NB	3.02	113.46	110.33
22	D	401	CLA	C1-C2-C3	-3.02	121.24	126.20
24	C	516	BCR	C11-C10-C9	-3.02	123.04	127.28
22	B	603	CLA	CMD-C2D-C1D	3.02	130.05	124.73
24	D	405	BCR	C38-C26-C25	-3.02	121.19	124.48
22	b	613	CLA	C11-C12-C13	-3.02	105.92	115.97
22	B	609	CLA	CHC-C4B-NB	3.02	128.58	124.05
24	c	915	BCR	C7-C8-C9	-3.02	121.77	126.23
22	C	505	CLA	C4D-CHA-C1A	-3.02	117.64	121.24
22	c	914	CLA	CHC-C1C-NC	-3.02	119.77	124.31
22	B	608	CLA	C3D-C2D-C1D	-3.02	101.72	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	SQD	O48-C23-O10	-3.02	116.08	123.63
22	b	607	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
22	b	617	CLA	CHD-C1D-ND	-3.01	120.57	124.80
22	a	408	CLA	CHB-C4A-NA	3.01	128.74	124.40
22	B	610	CLA	C3D-C2D-C1D	-3.01	101.73	105.83
22	c	909	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
27	A	412	LHG	O8-C23-C24	3.00	121.00	111.83
35	H	102	DGD	O2G-C1B-C2B	3.00	117.98	111.48
22	B	617	CLA	CBC-CAC-C3C	-3.00	104.28	112.42
29	t	101	LMT	O1'-C1'-C2'	3.00	112.83	108.27
35	C	518	DGD	O3G-C1D-C2D	3.00	112.83	108.27
28	A	413	SQD	C1-O5-C5	-3.00	107.86	113.72
22	b	612	CLA	C2B-C1B-NB	3.00	113.44	110.33
22	b	611	CLA	CHD-C1D-ND	-3.00	120.58	124.80
22	C	513	CLA	C2B-C1B-NB	3.00	113.44	110.33
22	b	616	CLA	C2B-C1B-NB	3.00	113.43	110.33
26	A	411	PL9	C45-C44-C46	2.99	120.42	115.23
22	C	504	CLA	C2C-C1C-NC	2.99	113.12	109.98
22	B	615	CLA	C4D-CHA-C1A	-2.99	117.67	121.24
22	c	913	CLA	C3D-C2D-C1D	-2.99	101.75	105.83
22	B	607	CLA	C3C-C4C-NC	2.99	114.26	110.43
22	c	907	CLA	CHA-C4D-ND	2.99	138.72	132.55
26	a	415	PL9	C42-C43-C44	-2.99	120.78	127.62
22	B	613	CLA	C1-O2A-CGA	2.99	123.89	116.65
22	b	614	CLA	CHA-C4D-ND	2.99	138.71	132.55
22	B	604	CLA	C1D-CHD-C4C	-2.99	119.67	126.02
22	c	909	CLA	C1-C2-C3	-2.99	121.30	126.20
24	d	404	BCR	C37-C22-C23	2.99	122.65	118.09
39	V	202	HEC	CBC-CAC-C3C	-2.99	121.47	127.43
22	b	613	CLA	C3C-C4C-NC	2.99	114.25	110.43
22	b	608	CLA	C4-C3-C5	2.98	120.41	115.23
22	b	603	CLA	O2A-CGA-CBA	2.98	120.93	111.83
22	C	511	CLA	CHD-C4C-NC	2.98	128.86	124.23
22	c	909	CLA	CMB-C2B-C1B	2.98	129.96	125.42
22	c	906	CLA	CHA-C4D-ND	2.98	138.70	132.55
24	c	916	BCR	C11-C10-C9	-2.98	123.10	127.28
22	c	902	CLA	C3B-C2B-C1B	-2.98	103.66	107.17
22	a	412	CLA	CBC-CAC-C3C	-2.98	104.35	112.42
22	a	409	CLA	C1D-ND-C4D	-2.97	104.23	106.31
22	B	612	CLA	C1D-ND-C4D	-2.97	104.23	106.31
24	c	916	BCR	C38-C26-C25	-2.97	121.24	124.48
22	b	611	CLA	C3C-C4C-NC	2.97	114.24	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	101	LMG	O8-C28-O10	-2.97	116.20	123.63
22	c	905	CLA	CMD-C2D-C1D	2.97	129.96	124.73
22	C	503	CLA	CHA-C4D-ND	2.97	138.67	132.55
22	B	602	CLA	C3D-C2D-C1D	-2.97	101.78	105.83
22	D	401	CLA	C3B-C4B-NB	2.96	113.17	110.53
22	b	613	CLA	CHC-C4B-NB	2.96	128.49	124.05
22	B	609	CLA	C2B-C1B-NB	2.96	113.40	110.33
22	b	609	CLA	O2A-CGA-O1A	-2.96	116.22	123.63
22	A	406	CLA	C4D-C3D-CAD	2.96	111.32	108.11
22	d	403	CLA	CHD-C1D-ND	-2.96	120.64	124.80
22	C	509	CLA	CHD-C4C-NC	2.96	128.82	124.23
25	b	622	LMG	O8-C28-C29	2.96	120.86	111.83
22	C	514	CLA	C3D-C2D-C1D	-2.96	101.79	105.83
24	B	619	BCR	C28-C27-C26	-2.96	108.78	114.06
22	c	909	CLA	C1-O2A-CGA	2.96	123.81	116.65
22	C	513	CLA	C1-C2-C3	-2.96	121.35	126.20
22	C	510	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	b	603	CLA	C4D-CHA-C1A	-2.96	117.72	121.24
22	b	610	CLA	C3D-C2D-C1D	-2.96	101.80	105.83
22	B	610	CLA	CMC-C2C-C1C	2.96	129.65	125.03
22	a	412	CLA	CHB-C1B-NB	-2.95	119.62	124.05
34	b	632	HTG	C3-C4-C5	2.95	115.59	110.23
22	a	412	CLA	CHD-C4C-NC	2.95	128.81	124.23
22	c	907	CLA	C2D-C1D-ND	2.95	113.05	110.13
22	B	614	CLA	O2D-CGD-CBD	2.95	116.39	111.23
22	C	509	CLA	CHB-C4A-NA	2.95	128.66	124.40
22	B	605	CLA	CMB-C2B-C1B	2.95	129.91	125.42
22	C	502	CLA	CMB-C2B-C1B	2.95	129.91	125.42
22	c	912	CLA	C2C-C1C-NC	2.95	113.08	109.98
22	c	910	CLA	C3B-C4B-NB	2.95	113.16	110.53
22	d	403	CLA	CMB-C2B-C1B	2.94	129.90	125.42
35	D	407	DGD	O1G-C1A-C2A	2.94	120.81	111.83
22	D	401	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	C	513	CLA	CHD-C1D-ND	-2.94	120.66	124.80
22	c	905	CLA	CAC-C3C-C4C	2.94	128.62	124.79
37	h	101	RRX	C16-C17-C18	-2.94	123.15	127.28
22	A	408	CLA	O2A-CGA-O1A	-2.94	116.27	123.63
34	D	415	HTG	O5-C1-S1	2.94	118.01	109.94
22	C	502	CLA	C1D-CHD-C4C	-2.94	119.78	126.02
22	B	610	CLA	C1-O2A-CGA	2.93	123.75	116.65
22	c	902	CLA	C1-O2A-CGA	2.93	123.75	116.65
34	C	521	HTG	C1-O5-C5	2.93	117.82	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	617	CLA	CAC-C3C-C4C	2.93	128.60	124.79
22	b	613	CLA	CED-O2D-CGD	2.93	122.56	115.92
22	C	514	CLA	CMB-C2B-C1B	2.93	129.87	125.42
22	B	613	CLA	CHB-C1B-NB	-2.93	119.66	124.05
22	c	902	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
22	A	405	CLA	C4-C3-C5	2.92	120.30	115.23
24	K	101	BCR	C33-C5-C6	-2.92	121.30	124.48
22	a	407	CLA	CMD-C2D-C1D	2.92	129.87	124.73
26	D	406	PL9	C10-C9-C11	2.92	120.29	115.23
24	B	620	BCR	C23-C24-C25	-2.92	119.20	127.00
22	d	402	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
22	b	607	CLA	C3C-C4C-NC	2.91	114.16	110.43
22	B	603	CLA	CHD-C4C-NC	2.91	128.74	124.23
22	C	504	CLA	C3C-C4C-NC	2.91	114.16	110.43
24	Y	101	BCR	C24-C23-C22	-2.91	121.93	126.23
22	d	402	CLA	C2A-C1A-CHA	-2.91	118.82	123.87
27	d	401	LHG	O8-C23-C24	2.91	120.70	111.83
28	A	413	SQD	O3-C3-C2	2.91	117.22	110.38
25	i	101	LMG	O8-C28-C29	2.90	120.69	111.83
24	k	101	BCR	C32-C1-C6	-2.90	105.69	110.24
22	b	610	CLA	CHA-C4D-ND	2.90	138.54	132.55
26	A	411	PL9	C37-C36-C34	-2.90	103.56	113.19
22	C	503	CLA	CHD-C4C-NC	2.90	128.73	124.23
22	b	608	CLA	C3D-C2D-C1D	-2.90	101.87	105.83
24	D	405	BCR	C10-C11-C12	-2.90	114.80	123.20
24	Y	101	BCR	C1-C6-C7	2.90	123.51	115.65
27	D	410	LHG	O8-C6-C5	-2.90	100.04	108.40
22	b	606	CLA	C3C-C4C-NC	2.90	114.14	110.43
22	c	903	CLA	C6-C5-C3	-2.90	106.41	113.47
22	B	606	CLA	CHD-C4C-NC	2.90	128.72	124.23
24	d	404	BCR	C30-C25-C24	2.90	123.50	115.65
22	A	406	CLA	CAC-C3C-C4C	2.90	128.56	124.79
22	B	606	CLA	C4-C3-C5	2.89	120.25	115.23
22	c	906	CLA	CHD-C1D-ND	-2.89	120.73	124.80
22	c	909	CLA	CHD-C1D-ND	-2.89	120.73	124.80
22	b	609	CLA	CAC-C3C-C4C	2.89	128.56	124.79
22	c	911	CLA	O2A-CGA-O1A	-2.89	116.39	123.63
22	c	908	CLA	C1-C2-C3	-2.89	121.46	126.20
29	A	414	LMT	C1'-C2'-C3'	-2.89	103.92	110.01
22	b	615	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
22	c	905	CLA	C5-C3-C2	-2.89	114.68	121.17
22	b	606	CLA	CMC-C2C-C1C	2.89	129.55	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	913	CLA	CHD-C4C-NC	2.89	128.71	124.23
22	C	502	CLA	C2B-C1B-NB	2.89	113.32	110.33
22	B	613	CLA	C3D-C2D-C1D	-2.88	101.89	105.83
24	C	515	BCR	C29-C30-C25	2.88	114.63	110.44
22	C	509	CLA	CHA-C4D-ND	2.88	138.50	132.55
22	a	412	CLA	C3B-C4B-NB	2.88	113.10	110.53
22	c	906	CLA	CHD-C4C-NC	2.88	128.70	124.23
22	b	605	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
22	A	406	CLA	C1-C2-C3	-2.88	121.48	126.20
22	c	914	CLA	CHD-C1D-ND	-2.87	120.76	124.80
28	C	501	SQD	O5-C1-C2	-2.87	104.46	110.37
22	B	606	CLA	C1D-ND-C4D	-2.87	104.30	106.31
24	k	101	BCR	C2-C1-C6	2.87	114.61	110.44
22	B	617	CLA	CAC-C3C-C4C	2.87	128.52	124.79
24	A	409	BCR	C38-C26-C25	-2.87	121.36	124.48
25	i	101	LMG	O6-C1-C2	-2.86	104.49	110.37
34	V	203	HTG	O5-C1-S1	2.86	117.80	109.94
24	b	618	BCR	C11-C10-C9	-2.86	123.26	127.28
22	c	908	CLA	CED-O2D-CGD	-2.86	109.43	115.92
22	b	612	CLA	C3B-C4B-NB	2.86	113.08	110.53
22	D	403	CLA	C4-C3-C5	2.86	120.19	115.23
22	b	611	CLA	O2A-CGA-CBA	2.86	120.55	111.83
22	b	609	CLA	C1-C2-C3	-2.86	121.52	126.20
26	A	411	PL9	C20-C19-C21	2.86	120.19	115.23
24	D	405	BCR	C16-C17-C18	-2.86	123.27	127.28
22	b	613	CLA	C1-C2-C3	-2.86	121.52	126.20
22	B	605	CLA	CGD-CBD-CAD	-2.86	101.60	110.85
22	C	511	CLA	CMD-C2D-C1D	2.85	129.75	124.73
22	c	912	CLA	O2A-CGA-CBA	2.85	120.53	111.83
22	C	506	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
22	b	615	CLA	CED-O2D-CGD	2.85	122.38	115.92
22	c	912	CLA	C4D-CHA-C1A	-2.85	117.85	121.24
22	C	502	CLA	C2A-C1A-CHA	-2.85	118.93	123.87
22	C	512	CLA	CHC-C4B-NB	2.85	128.32	124.05
28	a	414	SQD	O9-S-O7	-2.85	104.57	113.82
39	v	202	HEC	CBD-CAD-C3D	-2.84	104.67	112.53
22	C	510	CLA	CAC-C3C-C4C	2.84	128.49	124.79
22	B	612	CLA	C7-C6-C5	-2.84	105.69	113.26
22	B	616	CLA	O2A-CGA-O1A	-2.84	116.52	123.63
22	C	502	CLA	C1-O2A-CGA	2.84	123.53	116.65
22	B	609	CLA	C1D-CHD-C4C	-2.84	119.98	126.02
22	B	613	CLA	CHC-C4B-NB	2.84	128.31	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	402	CLA	CMA-C3A-C2A	-2.84	103.02	113.98
28	b	621	SQD	O48-C23-O10	-2.84	116.54	123.63
22	b	607	CLA	C3B-C4B-NB	2.83	113.06	110.53
22	B	609	CLA	C3C-C4C-NC	2.83	114.06	110.43
29	Z	101	LMT	O5B-C5B-C4B	2.83	114.80	109.70
22	B	616	CLA	O1D-CGD-CBD	-2.83	118.94	124.52
22	B	608	CLA	CED-O2D-CGD	2.83	122.33	115.92
22	b	611	CLA	CHD-C4C-NC	2.83	128.62	124.23
22	B	608	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	a	410	PHO	C7-C6-C5	-2.83	105.73	113.26
24	b	620	BCR	C24-C23-C22	-2.83	122.05	126.23
24	C	516	BCR	C37-C22-C23	2.83	122.40	118.09
22	D	401	CLA	CHB-C1B-NB	-2.82	119.81	124.05
22	A	406	CLA	O1D-CGD-CBD	-2.82	118.95	124.52
22	B	604	CLA	O2A-CGA-CBA	2.82	120.44	111.83
22	c	910	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
34	b	623	HTG	C2'-C1'-S1	-2.82	102.86	112.36
23	A	407	PHO	CMA-C3A-C4A	-2.82	108.53	114.61
22	C	511	CLA	CHC-C4B-NB	2.82	128.28	124.05
28	l	101	SQD	O5-C1-C2	-2.82	104.58	110.37
22	B	615	CLA	CHC-C1C-NC	-2.82	120.07	124.31
22	B	604	CLA	CHC-C1C-NC	-2.82	120.07	124.31
22	B	609	CLA	CHB-C4A-NA	2.82	128.46	124.40
22	b	616	CLA	O1D-CGD-CBD	-2.81	118.97	124.52
22	c	908	CLA	O2A-CGA-CBA	2.81	120.41	111.83
26	d	405	PL9	C22-C23-C24	-2.81	121.19	127.62
22	A	405	CLA	C4D-CHA-C1A	-2.81	117.89	121.24
24	y	101	BCR	C1-C6-C7	2.81	123.28	115.65
22	D	403	CLA	CHD-C1D-ND	-2.81	120.85	124.80
22	B	612	CLA	CHD-C4C-NC	2.81	128.59	124.23
22	C	510	CLA	C1D-CHD-C4C	-2.81	120.05	126.02
35	C	517	DGD	O2G-C1B-O1B	-2.81	117.14	123.70
22	d	403	CLA	C4D-C3D-CAD	2.81	111.16	108.11
26	a	415	PL9	C20-C19-C21	2.81	120.10	115.23
22	b	608	CLA	C1D-ND-C4D	2.81	108.28	106.31
22	c	903	CLA	CHD-C1D-ND	-2.81	120.85	124.80
22	a	407	CLA	CHD-C4C-C3C	-2.81	120.68	124.77
22	A	405	CLA	CHC-C1C-NC	-2.81	120.08	124.31
25	d	409	LMG	C8-O7-C10	-2.81	111.08	117.80
22	C	504	CLA	CHD-C1D-ND	-2.80	120.86	124.80
22	a	407	CLA	O2A-CGA-O1A	-2.80	116.61	123.63
27	L	101	LHG	C6-C5-C4	-2.80	105.25	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	607	CLA	C14-C13-C12	-2.80	101.29	111.27
22	C	510	CLA	C3B-C4B-NB	2.80	113.03	110.53
22	B	602	CLA	O2A-CGA-CBA	2.80	120.38	111.83
23	A	407	PHO	O1D-CGD-CBD	-2.80	120.48	124.72
22	C	514	CLA	O2A-CGA-O1A	-2.80	116.62	123.63
35	C	518	DGD	O5D-C6D-C5D	2.80	115.73	109.42
22	a	412	CLA	C2D-C1D-ND	2.80	112.90	110.13
22	b	616	CLA	O2A-CGA-O1A	-2.80	116.63	123.63
22	c	907	CLA	O2A-CGA-CBA	2.80	120.36	111.83
22	C	510	CLA	C3D-C2D-C1D	-2.80	102.01	105.83
22	c	913	CLA	C2A-C1A-CHA	-2.80	119.01	123.87
22	b	617	CLA	C1D-CHD-C4C	-2.80	120.08	126.02
22	a	412	CLA	C2A-C1A-CHA	-2.80	119.02	123.87
22	a	409	CLA	CAC-C3C-C4C	2.79	128.43	124.79
22	A	406	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
22	B	603	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
22	b	603	CLA	C1-O2A-CGA	2.79	123.41	116.65
22	D	403	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
22	B	607	CLA	CBC-CAC-C3C	-2.79	104.85	112.42
35	c	918	DGD	O1G-C1A-C2A	2.79	120.34	111.83
22	C	512	CLA	CMD-C2D-C1D	2.79	129.64	124.73
29	c	921	LMT	O1'-C1'-C2'	2.79	112.51	108.27
36	E	102	HEM	C3B-C2B-C1B	2.78	108.50	106.41
22	B	604	CLA	C2A-C3A-C4A	-2.78	97.37	101.87
22	c	911	CLA	CBC-CAC-C3C	-2.78	104.88	112.42
22	B	602	CLA	CMC-C2C-C1C	2.78	129.38	125.03
22	C	510	CLA	C1-O2A-CGA	2.78	123.38	116.65
22	C	504	CLA	O2A-CGA-CBA	2.78	120.31	111.83
22	C	511	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
26	A	411	PL9	C25-C24-C26	2.78	120.05	115.23
22	C	505	CLA	C7-C6-C5	-2.78	105.86	113.26
22	b	616	CLA	O2A-CGA-CBA	2.77	120.30	111.83
22	c	906	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
22	c	907	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
26	D	406	PL9	C37-C38-C39	-2.77	121.28	127.62
22	C	502	CLA	CHD-C4C-NC	2.77	128.53	124.23
34	D	415	HTG	C3-C4-C5	2.77	115.25	110.23
22	B	607	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
22	c	907	CLA	CHB-C1B-NB	-2.77	119.90	124.05
22	c	914	CLA	CMD-C2D-C1D	2.77	129.60	124.73
22	B	614	CLA	C1-C2-C3	-2.77	121.66	126.20
22	b	606	CLA	CAC-C3C-C4C	2.77	128.39	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	621	LMG	C3-C4-C5	2.76	115.24	110.23
22	c	903	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
22	B	608	CLA	C1-O2A-CGA	2.76	123.33	116.65
22	C	508	CLA	O2A-CGA-CBA	2.76	120.24	111.83
22	B	610	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
22	B	609	CLA	C6-C5-C3	-2.76	106.75	113.47
22	C	512	CLA	C3B-C4B-NB	2.76	112.99	110.53
27	D	411	LHG	O7-C7-C8	2.76	117.44	111.48
23	a	411	PHO	CMB-C2B-C3B	2.76	130.19	124.68
26	D	406	PL9	C12-C13-C14	-2.75	121.32	127.62
22	C	504	CLA	C4C-C3C-C2C	-2.75	102.88	106.89
34	v	203	HTG	O5-C1-S1	2.75	117.50	109.94
22	b	606	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
29	c	931	LMT	O5'-C5'-C6'	2.75	113.26	106.44
22	c	914	CLA	O1D-CGD-CBD	-2.75	119.09	124.52
22	c	904	CLA	C4D-C3D-CAD	2.75	111.09	108.11
25	b	622	LMG	O7-C10-O9	-2.75	117.28	123.70
22	c	906	CLA	O2A-CGA-CBA	2.75	120.21	111.83
35	C	517	DGD	O6E-C1E-C2E	-2.75	104.73	110.37
23	a	410	PHO	OBD-CAD-C3D	-2.74	123.61	127.89
22	b	604	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
28	D	408	SQD	O7-S-C6	2.74	110.85	106.76
36	E	102	HEM	CBA-CAA-C2A	-2.74	104.95	112.53
22	A	408	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
22	c	911	CLA	O2A-CGA-CBA	2.74	120.19	111.83
22	c	910	CLA	CHD-C4C-C3C	-2.74	120.78	124.77
22	c	910	CLA	CHC-C4B-C3B	-2.74	115.49	127.37
22	b	609	CLA	CMD-C2D-C1D	2.74	129.55	124.73
25	i	101	LMG	O7-C10-C11	2.74	117.40	111.48
23	A	407	PHO	CBC-CAC-C3C	-2.74	108.96	112.87
23	D	402	PHO	C1A-C2A-C3A	-2.73	100.24	102.84
24	D	405	BCR	C29-C28-C27	-2.73	105.27	111.28
34	D	415	HTG	C1-C2-C3	-2.73	105.20	110.55
22	b	602	CLA	CED-O2D-CGD	2.73	122.12	115.92
22	c	911	CLA	C3D-C2D-C1D	-2.73	102.10	105.83
27	a	423	LHG	O8-C23-O10	-2.73	116.79	123.63
22	B	614	CLA	O2A-CGA-CBA	2.73	120.16	111.83
26	A	411	PL9	C3-C4-C5	2.73	121.97	118.57
22	B	613	CLA	O2D-CGD-CBD	2.73	116.00	111.23
22	C	514	CLA	CHD-C1D-ND	-2.73	120.97	124.80
22	B	612	CLA	CHA-C4D-ND	2.73	138.17	132.55
22	B	613	CLA	O2A-CGA-CBA	2.72	120.14	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	903	CLA	O2A-CGA-O1A	-2.72	116.81	123.63
22	B	608	CLA	CHD-C4C-C3C	-2.72	120.80	124.77
22	b	612	CLA	CMC-C2C-C1C	2.72	129.29	125.03
25	j	101	LMG	C7-O1-C1	-2.72	107.96	113.80
22	c	912	CLA	CHD-C4C-C3C	-2.72	120.81	124.77
26	d	405	PL9	C53-C6-C1	2.72	120.85	115.28
27	D	409	LHG	O8-C23-O10	-2.72	116.83	123.63
22	b	613	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
34	b	627	HTG	C3-C4-C5	2.72	115.16	110.23
34	B	626	HTG	C3-C4-C5	2.71	115.15	110.23
22	a	408	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
24	d	404	BCR	C24-C23-C22	-2.71	122.22	126.23
22	C	512	CLA	CHD-C4C-NC	2.71	128.44	124.23
22	b	610	CLA	C7-C6-C5	-2.71	106.04	113.26
22	C	508	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
22	B	603	CLA	CHC-C4B-C3B	-2.71	115.61	127.37
25	j	101	LMG	O8-C28-C29	2.71	120.10	111.83
35	C	518	DGD	O1G-C1A-O1A	-2.71	116.85	123.63
28	a	414	SQD	O2-C2-C1	2.71	116.53	110.08
22	B	606	CLA	C7-C6-C5	-2.71	106.05	113.26
22	C	508	CLA	C4-C3-C5	2.71	119.92	115.23
22	b	616	CLA	C1D-CHD-C4C	-2.71	120.27	126.02
22	C	512	CLA	C4D-CHA-C1A	-2.70	118.02	121.24
22	b	613	CLA	CHD-C1D-ND	-2.70	121.00	124.80
22	A	408	CLA	CHD-C4C-NC	2.70	128.41	124.23
22	c	914	CLA	C2B-C1B-NB	2.70	113.12	110.33
22	b	613	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
22	b	617	CLA	C1-O2A-CGA	2.70	123.18	116.65
24	C	516	BCR	C33-C5-C6	-2.70	121.54	124.48
22	C	509	CLA	O2A-CGA-CBA	2.69	120.05	111.83
22	C	513	CLA	C1D-CHD-C4C	-2.69	120.30	126.02
22	D	404	CLA	C2A-C1A-CHA	-2.69	119.19	123.87
22	C	510	CLA	CHB-C1B-NB	-2.69	120.01	124.05
22	B	604	CLA	CMD-C2D-C1D	2.69	129.47	124.73
22	C	505	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
22	C	504	CLA	CHD-C4C-NC	2.69	128.40	124.23
35	c	919	DGD	O1G-C1A-O1A	-2.69	116.90	123.63
24	b	620	BCR	C3-C4-C5	-2.69	109.26	114.06
26	a	415	PL9	C32-C33-C34	-2.69	121.47	127.62
22	B	608	CLA	CHD-C1D-ND	-2.69	121.02	124.80
22	D	401	CLA	CHA-C4D-ND	2.69	138.09	132.55
22	a	412	CLA	O2A-CGA-CBA	2.68	120.02	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	911	CLA	C2C-C1C-NC	2.68	112.80	109.98
22	B	602	CLA	C4D-CHA-C1A	-2.68	118.05	121.24
22	B	615	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
22	C	507	CLA	CHD-C4C-NC	2.68	128.39	124.23
25	j	101	LMG	C9-C8-C7	-2.68	105.54	111.78
26	A	411	PL9	C37-C38-C39	-2.68	121.49	127.62
34	b	632	HTG	O5-C1-S1	2.68	117.29	109.94
35	C	518	DGD	O2G-C1B-O1B	-2.67	117.45	123.70
22	c	904	CLA	CHD-C1D-ND	-2.67	121.04	124.80
25	d	409	LMG	O7-C10-O9	-2.67	117.46	123.70
28	C	501	SQD	O48-C23-C24	2.67	119.97	111.83
22	b	616	CLA	CMC-C2C-C1C	2.66	129.20	125.03
22	C	502	CLA	O2A-CGA-CBA	2.66	119.96	111.83
22	D	403	CLA	O2A-CGA-CBA	2.66	119.96	111.83
22	C	507	CLA	C4-C3-C5	2.66	119.85	115.23
29	c	921	LMT	O2'-C2'-C3'	-2.66	104.10	110.38
29	f	102	LMT	C3'-C4'-C5'	-2.66	105.03	110.93
25	d	409	LMG	O2-C2-C1	2.66	116.41	110.08
22	b	611	CLA	C4C-C3C-C2C	-2.66	103.02	106.89
22	B	615	CLA	C3C-C4C-NC	2.66	113.84	110.43
24	b	618	BCR	C7-C8-C9	-2.66	122.30	126.23
24	C	515	BCR	C8-C7-C6	-2.66	119.90	127.00
25	J	101	LMG	C7-O1-C1	-2.66	108.10	113.80
22	C	514	CLA	C2B-C1B-NB	2.66	113.08	110.33
22	B	602	CLA	C4C-C3C-C2C	-2.66	103.03	106.89
24	D	405	BCR	C36-C18-C19	2.66	122.14	118.09
22	c	909	CLA	CMD-C2D-C1D	2.66	129.40	124.73
22	c	914	CLA	O2A-CGA-CBA	2.65	119.93	111.83
22	b	614	CLA	CHD-C4C-NC	2.65	128.35	124.23
23	A	407	PHO	CED-O2D-CGD	2.65	121.94	115.92
22	b	608	CLA	C2B-C1B-NB	2.65	113.08	110.33
22	d	403	CLA	CHD-C4C-NC	2.65	128.34	124.23
22	B	603	CLA	C1-O2A-CGA	2.65	123.07	116.65
22	C	508	CLA	CBC-CAC-C3C	-2.65	105.23	112.42
22	b	613	CLA	CHB-C4A-NA	2.65	128.23	124.40
22	b	610	CLA	O2D-CGD-CBD	2.65	115.86	111.23
22	a	407	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
22	C	514	CLA	C1D-CHD-C4C	-2.65	120.39	126.02
28	a	414	SQD	O47-C7-O49	-2.65	117.52	123.70
22	C	511	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
24	a	413	BCR	C28-C27-C26	-2.65	109.34	114.06
22	b	602	CLA	CHC-C1C-NC	-2.64	120.33	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
22	B	604	CLA	O1D-CGD-CBD	-2.64	119.31	124.52
22	A	405	CLA	CHA-C4D-ND	2.64	137.99	132.55
24	y	101	BCR	C7-C6-C5	-2.64	115.48	121.56
23	A	407	PHO	CMB-C2B-C3B	2.64	129.95	124.68
25	D	412	LMG	O8-C28-C29	2.64	119.87	111.83
22	b	614	CLA	CED-O2D-CGD	2.64	121.89	115.92
22	D	404	CLA	C4-C3-C5	2.64	119.80	115.23
22	B	616	CLA	O2A-CGA-CBA	2.63	119.87	111.83
22	B	609	CLA	C11-C12-C13	-2.63	107.21	115.97
22	b	608	CLA	CHD-C4C-NC	2.63	128.31	124.23
22	B	613	CLA	CMC-C2C-C1C	2.63	129.15	125.03
22	B	613	CLA	CHD-C4C-NC	2.63	128.31	124.23
34	B	623	HTG	O4-C4-C3	-2.63	104.17	110.38
22	C	502	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
22	A	405	CLA	C1D-ND-C4D	-2.63	104.47	106.31
34	b	626	HTG	C3-C4-C5	2.63	115.00	110.23
22	a	407	CLA	C2B-C1B-NB	2.63	113.05	110.33
22	A	406	CLA	CHC-C4B-C3B	-2.63	115.97	127.37
22	a	409	CLA	CHC-C4B-C3B	-2.63	115.97	127.37
22	b	604	CLA	CHC-C1C-NC	-2.63	120.36	124.31
26	D	406	PL9	C50-C49-C48	-2.62	114.78	122.66
22	b	605	CLA	C1D-CHD-C4C	-2.62	120.45	126.02
22	c	903	CLA	O2A-CGA-CBA	2.62	119.82	111.83
22	A	408	CLA	C1D-CHD-C4C	-2.62	120.45	126.02
22	C	509	CLA	CHD-C1D-ND	-2.62	121.12	124.80
22	c	906	CLA	CAC-C3C-C4C	2.62	128.19	124.79
22	b	615	CLA	CMD-C2D-C1D	2.62	129.34	124.73
28	l	101	SQD	O47-C7-O49	-2.62	117.59	123.70
22	b	617	CLA	CHD-C4C-NC	2.62	128.29	124.23
25	j	101	LMG	O7-C10-C11	2.61	117.14	111.48
24	d	404	BCR	C37-C22-C21	-2.61	118.58	122.82
22	C	511	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
22	b	611	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
22	b	603	CLA	CAA-CBA-CGA	-2.61	105.80	113.21
22	C	507	CLA	C3C-C4C-NC	2.61	113.77	110.43
27	a	423	LHG	O7-C7-O9	-2.61	117.61	123.70
22	A	406	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
24	K	101	BCR	C20-C21-C22	-2.61	123.62	127.28
22	B	616	CLA	C6-C7-C8	-2.61	107.30	115.97
27	L	101	LHG	O7-C7-O9	-2.60	117.61	123.70
22	a	407	CLA	O2A-CGA-CBA	2.60	119.78	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	CAA-CBA-CGA	-2.60	105.81	113.21
22	b	602	CLA	C4-C3-C5	2.60	119.75	115.23
22	B	606	CLA	CMD-C2D-C1D	2.60	129.31	124.73
22	C	508	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
24	D	405	BCR	C15-C14-C13	-2.60	123.63	127.28
22	B	610	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
26	a	415	PL9	C10-C9-C11	2.60	119.74	115.23
22	B	611	CLA	O1D-CGD-CBD	-2.60	119.40	124.52
24	B	620	BCR	C10-C11-C12	-2.60	115.68	123.20
22	D	403	CLA	CHC-C4B-C3B	-2.59	116.11	127.37
22	d	402	CLA	CMD-C2D-C1D	2.59	129.29	124.73
28	C	501	SQD	O9-S-O7	-2.59	105.39	113.82
22	C	509	CLA	C5-C3-C2	-2.59	115.35	121.17
22	B	613	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
29	a	419	LMT	O5B-C5B-C6B	2.59	112.86	106.44
34	B	626	HTG	O5-C1-C2	-2.59	106.75	110.32
23	A	407	PHO	C4B-NB-C1B	-2.59	105.04	108.82
22	B	608	CLA	C1-C2-C3	-2.59	121.95	126.20
25	c	930	LMG	O8-C28-C29	2.59	119.73	111.83
22	C	504	CLA	C4D-CHA-C1A	-2.59	118.16	121.24
22	c	912	CLA	C2D-C1D-ND	2.59	112.69	110.13
22	b	609	CLA	C11-C12-C13	-2.58	107.37	115.97
22	b	614	CLA	C4C-C3C-C2C	-2.58	103.13	106.89
22	c	913	CLA	C4D-CHA-C1A	-2.58	118.16	121.24
22	B	605	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
22	c	907	CLA	C4-C3-C5	2.58	119.71	115.23
26	D	406	PL9	C25-C24-C26	2.58	119.70	115.23
22	c	910	CLA	CMB-C2B-C1B	2.58	129.34	125.42
22	c	914	CLA	CED-O2D-CGD	2.58	121.76	115.92
22	c	902	CLA	CMC-C2C-C1C	2.58	129.06	125.03
22	d	403	CLA	CED-O2D-CGD	2.57	121.75	115.92
22	b	612	CLA	CBC-CAC-C3C	-2.57	105.44	112.42
22	A	406	CLA	CMD-C2D-C1D	2.57	129.26	124.73
22	b	610	CLA	C2A-C1A-CHA	-2.57	119.40	123.87
22	C	507	CLA	CMB-C2B-C1B	2.57	129.33	125.42
22	b	610	CLA	CAC-C3C-C4C	2.57	128.13	124.79
28	D	408	SQD	C3-C4-C5	2.57	114.89	110.23
22	c	907	CLA	CMB-C2B-C1B	2.57	129.33	125.42
22	B	606	CLA	C4C-C3C-C2C	-2.57	103.16	106.89
22	B	613	CLA	CHA-C4D-ND	2.57	137.84	132.55
22	b	616	CLA	C4D-CHA-C1A	-2.57	118.18	121.24
22	C	506	CLA	C4-C3-C5	2.57	119.68	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	i	101	LMG	C1-O6-C5	-2.56	108.71	113.72
35	D	407	DGD	O1G-C1G-C2G	2.56	115.78	108.40
26	a	415	PL9	C40-C39-C41	2.56	119.68	115.23
23	a	410	PHO	O2A-CGA-CBA	2.56	119.65	111.83
35	C	519	DGD	O3G-C3G-C2G	-2.56	104.59	110.82
23	a	411	PHO	C4B-NB-C1B	-2.56	105.08	108.82
24	D	405	BCR	C32-C1-C6	2.56	114.26	110.24
22	B	610	CLA	CMB-C2B-C1B	2.56	129.32	125.42
22	a	412	CLA	CED-O2D-CGD	2.56	121.72	115.92
22	C	513	CLA	CMD-C2D-C1D	2.56	129.23	124.73
22	D	403	CLA	CHA-C4D-ND	2.56	137.83	132.55
25	j	101	LMG	O2-C2-C1	-2.56	103.98	110.08
22	A	408	CLA	C3B-C4B-NB	2.56	112.81	110.53
22	D	401	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	B	603	CLA	C3C-C4C-NC	2.56	113.70	110.43
22	c	905	CLA	CHC-C4B-C3B	-2.56	116.28	127.37
24	Y	101	BCR	C34-C9-C8	2.56	121.99	118.09
24	D	405	BCR	C30-C25-C24	2.56	122.58	115.65
22	B	609	CLA	O2A-CGA-CBA	2.55	119.62	111.83
22	d	402	CLA	CHC-C4B-NB	2.55	127.88	124.05
24	c	916	BCR	C16-C17-C18	-2.55	123.70	127.28
22	c	904	CLA	C4C-C3C-C2C	-2.55	103.18	106.89
22	C	502	CLA	CMC-C2C-C1C	2.55	129.02	125.03
22	B	604	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
22	D	404	CLA	C4D-CHA-C1A	-2.55	118.20	121.24
24	Y	101	BCR	C7-C8-C9	-2.55	122.46	126.23
28	D	408	SQD	O8-S-C6	2.55	110.89	105.97
35	c	919	DGD	C2G-O2G-C1B	-2.55	111.70	117.80
22	b	611	CLA	CHC-C1C-NC	-2.55	120.47	124.31
22	C	512	CLA	CHB-C1B-NB	-2.55	120.23	124.05
24	B	619	BCR	C15-C16-C17	-2.55	118.31	123.52
22	B	612	CLA	CHB-C4A-NA	2.55	128.07	124.40
22	B	602	CLA	C2D-C1D-ND	2.55	112.64	110.13
22	C	512	CLA	C4C-C3C-C2C	-2.54	103.19	106.89
22	B	607	CLA	OBD-CAD-C3D	-2.54	122.47	128.42
24	K	101	BCR	C16-C17-C18	-2.54	123.71	127.28
22	C	514	CLA	C2C-C1C-NC	2.54	112.65	109.98
22	c	904	CLA	CAA-CBA-CGA	-2.54	105.99	113.21
28	f	101	SQD	O8-S-C6	2.54	110.97	106.00
22	C	504	CLA	CMC-C2C-C1C	2.54	129.00	125.03
22	b	607	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
22	B	616	CLA	O2D-CGD-O1D	-2.54	118.91	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	404	CLA	C3D-C2D-C1D	-2.54	102.37	105.83
27	D	410	LHG	C14-C13-C12	-2.54	101.55	114.37
22	C	505	CLA	C1-O2A-CGA	2.53	122.79	116.65
22	b	611	CLA	C1D-CHD-C4C	-2.53	120.63	126.02
22	c	903	CLA	CMC-C2C-C1C	2.53	128.99	125.03
22	B	603	CLA	OBD-CAD-C3D	-2.53	122.50	128.42
22	B	605	CLA	C1D-CHD-C4C	-2.53	120.64	126.02
22	C	504	CLA	CHC-C1C-NC	-2.53	120.50	124.31
22	c	906	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
22	b	613	CLA	C4B-C3B-C2B	-2.53	104.16	107.30
22	b	617	CLA	O2A-CGA-CBA	2.53	119.55	111.83
22	C	506	CLA	CHD-C1D-ND	-2.53	121.24	124.80
22	a	409	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
22	C	509	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
22	a	412	CLA	CMC-C2C-C1C	2.53	128.99	125.03
22	d	402	CLA	CAC-C3C-C4C	2.53	128.08	124.79
22	B	610	CLA	CAC-C3C-C4C	2.53	128.08	124.79
22	b	612	CLA	C1D-CHD-C4C	-2.53	120.65	126.02
26	A	411	PL9	C30-C29-C31	2.53	119.61	115.23
22	A	405	CLA	C1D-CHD-C4C	-2.52	120.65	126.02
35	c	917	DGD	O2G-C1B-O1B	-2.52	117.80	123.70
22	a	407	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
22	C	502	CLA	C4D-CHA-C1A	-2.52	118.23	121.24
35	C	518	DGD	C3B-C2B-C1B	-2.52	104.45	113.69
24	k	101	BCR	C11-C10-C9	-2.52	123.74	127.28
22	c	913	CLA	C1-O2A-CGA	2.52	122.75	116.65
29	f	102	LMT	O5'-C5'-C6'	2.52	112.69	106.44
22	a	409	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
22	C	505	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
25	B	621	LMG	O7-C10-O9	-2.52	117.82	123.70
22	b	613	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
25	d	409	LMG	C3-C4-C5	2.52	114.79	110.23
22	B	608	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
22	A	405	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
22	c	914	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	Y	101	BCR	C8-C9-C10	-2.51	115.06	119.01
25	A	410	LMG	C8-O7-C10	-2.51	111.79	117.80
22	c	910	CLA	CHB-C1B-NB	-2.51	120.28	124.05
22	C	508	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
39	V	202	HEC	CBB-CAB-C3B	-2.51	122.42	127.43
24	C	516	BCR	C38-C26-C25	-2.51	121.75	124.48
34	D	415	HTG	O2-C2-C3	2.51	116.28	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	SQD	O2-C2-C1	2.51	116.05	110.08
22	a	408	CLA	O2A-CGA-CBA	2.51	119.48	111.83
28	D	408	SQD	C4-C3-C2	2.50	115.23	110.83
23	A	407	PHO	C4D-CHA-CBD	2.50	109.66	108.45
22	b	603	CLA	CMB-C2B-C3B	2.50	132.44	126.55
22	b	604	CLA	C3C-C4C-NC	2.50	113.63	110.43
22	B	611	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
22	A	408	CLA	CMC-C2C-C1C	2.50	128.94	125.03
22	c	911	CLA	C1D-CHD-C4C	-2.50	120.71	126.02
22	a	408	CLA	CBB-CAB-C3B	-2.50	115.05	127.53
35	C	518	DGD	C6D-C5D-C4D	2.50	117.31	112.07
22	c	912	CLA	CHC-C1C-NC	-2.50	120.55	124.31
22	a	408	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
22	D	404	CLA	CBC-CAC-C3C	-2.49	105.66	112.42
22	b	612	CLA	C1-C2-C3	-2.49	122.11	126.20
25	d	409	LMG	O8-C28-C29	2.49	119.43	111.83
22	b	615	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
22	C	507	CLA	C1-O2A-CGA	2.49	122.68	116.65
28	C	501	SQD	C45-O47-C7	-2.49	111.84	117.80
35	C	519	DGD	O2G-C1B-O1B	-2.49	117.89	123.70
22	B	610	CLA	C1D-CHD-C4C	-2.49	120.73	126.02
22	b	614	CLA	C2B-C1B-NB	2.49	112.90	110.33
22	d	402	CLA	C1D-CHD-C4C	-2.48	120.74	126.02
22	A	408	CLA	CAC-C3C-C4C	2.48	128.02	124.79
34	b	623	HTG	C1-O5-C5	2.48	117.01	112.56
34	v	203	HTG	O2-C2-C1	2.48	114.71	110.30
22	C	512	CLA	O2D-CGD-CBD	2.48	115.57	111.23
22	c	907	CLA	CHB-C4A-NA	2.48	127.98	124.40
39	v	202	HEC	C3D-C4D-ND	-2.48	107.40	110.15
22	b	603	CLA	C4D-C3D-CAD	2.48	110.80	108.11
22	d	403	CLA	C2D-C1D-ND	2.48	112.58	110.13
28	a	414	SQD	C44-O6-C1	-2.48	108.48	113.80
22	D	401	CLA	C4-C3-C5	2.48	119.53	115.23
22	B	613	CLA	C3D-C4D-ND	2.48	114.01	109.99
22	b	603	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
29	c	921	LMT	C1B-O1B-C4'	-2.48	112.11	117.98
24	Y	101	BCR	C24-C25-C26	-2.47	115.86	121.56
25	c	930	LMG	O7-C10-O9	-2.47	117.92	123.70
22	c	914	CLA	CAC-C3C-C4C	2.47	128.01	124.79
35	d	406	DGD	O2G-C1B-O1B	-2.47	117.93	123.70
22	b	604	CLA	C4D-CHA-C1A	-2.47	118.30	121.24
29	c	931	LMT	O1'-C1'-C2'	2.47	112.02	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
22	B	616	CLA	CHB-C4A-NA	2.47	127.96	124.40
25	i	101	LMG	C31-C30-C29	-2.47	104.06	113.13
35	h	102	DGD	C3D-C4D-C5D	-2.47	105.76	110.23
22	b	615	CLA	O2A-CGA-CBA	2.47	119.36	111.83
22	B	603	CLA	C4C-C3C-C2C	-2.47	103.30	106.89
26	D	406	PL9	C51-C49-C50	2.47	120.27	114.59
22	B	617	CLA	C4-C3-C5	2.47	119.51	115.23
22	c	912	CLA	CMC-C2C-C1C	2.47	128.89	125.03
22	D	403	CLA	C4-C3-C2	-2.47	117.29	123.63
22	d	402	CLA	CHD-C1D-ND	-2.46	121.33	124.80
22	B	602	CLA	CHC-C1C-NC	-2.46	120.60	124.31
22	C	503	CLA	C6-C5-C3	-2.46	107.47	113.47
37	H	101	RRX	C38-C26-C25	-2.46	121.80	124.48
22	C	514	CLA	C1-O2A-CGA	2.46	122.61	116.65
27	d	401	LHG	O8-C23-O10	-2.46	117.47	123.63
22	c	911	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
22	b	612	CLA	C1D-ND-C4D	-2.46	104.59	106.31
22	a	408	CLA	CHC-C4B-C3B	-2.46	116.71	127.37
22	B	615	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
35	c	918	DGD	O1G-C1A-O1A	-2.46	117.49	123.63
22	B	606	CLA	C2A-C1A-CHA	-2.45	119.61	123.87
22	B	604	CLA	C1D-ND-C4D	-2.45	104.59	106.31
22	b	609	CLA	CHD-C4C-NC	2.45	128.03	124.23
22	B	614	CLA	CHC-C4B-C3B	-2.45	116.73	127.37
22	c	904	CLA	OBD-CAD-C3D	-2.45	122.69	128.42
22	c	908	CLA	C2B-C1B-NB	2.45	112.86	110.33
22	C	503	CLA	CMC-C2C-C1C	2.45	128.86	125.03
24	a	413	BCR	C40-C30-C25	-2.44	106.41	110.24
24	B	620	BCR	C33-C5-C6	-2.44	121.82	124.48
22	C	514	CLA	CMD-C2D-C1D	2.44	129.03	124.73
22	A	408	CLA	C5-C3-C2	-2.44	115.69	121.17
25	J	101	LMG	O8-C28-C29	2.44	119.28	111.83
22	a	412	CLA	OBD-CAD-C3D	-2.44	122.71	128.42
22	b	602	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	A	408	CLA	O2A-CGA-CBA	2.44	119.28	111.83
23	a	410	PHO	C4B-NB-C1B	-2.44	105.26	108.82
24	d	404	BCR	C35-C13-C14	-2.44	118.87	122.82
22	B	616	CLA	CHB-C1B-NB	-2.44	120.39	124.05
22	B	605	CLA	C4-C3-C5	2.44	119.46	115.23
22	b	606	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
27	d	401	LHG	O4-P-O5	2.44	120.33	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	407	CLA	CMC-C2C-C1C	2.43	128.84	125.03
22	b	612	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
22	B	605	CLA	CAA-C2A-C3A	-2.43	106.42	113.00
22	c	913	CLA	C6-C5-C3	-2.43	107.54	113.47
35	D	407	DGD	C1D-C2D-C3D	2.43	115.13	110.01
22	b	607	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
22	c	906	CLA	CHC-C4B-NB	2.43	127.69	124.05
22	B	612	CLA	CAC-C3C-C4C	2.43	127.95	124.79
22	b	614	CLA	C4D-CHA-C1A	-2.43	118.35	121.24
22	b	609	CLA	C2D-C1D-ND	2.43	112.53	110.13
24	c	915	BCR	C38-C26-C25	-2.43	121.84	124.48
22	B	605	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	a	408	CLA	C1D-ND-C4D	-2.42	104.61	106.31
26	d	405	PL9	C42-C43-C44	-2.42	122.08	127.62
22	b	609	CLA	C4D-C3D-CAD	2.42	110.74	108.11
22	c	910	CLA	C4D-C3D-CAD	2.42	110.74	108.11
22	B	604	CLA	CBC-CAC-C3C	-2.42	105.86	112.42
22	c	912	CLA	CAC-C3C-C4C	2.42	127.94	124.79
27	a	416	LHG	O7-C7-O9	-2.42	118.05	123.70
22	B	605	CLA	C4D-C3D-CAD	2.42	110.73	108.11
22	b	612	CLA	O2A-CGA-CBA	2.42	119.21	111.83
22	C	504	CLA	CMD-C2D-C1D	2.42	128.99	124.73
22	B	605	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
24	A	409	BCR	C33-C5-C6	-2.42	121.85	124.48
22	c	908	CLA	C4D-CHA-C1A	-2.42	118.36	121.24
22	C	512	CLA	C3C-C4C-NC	2.42	113.53	110.43
22	C	510	CLA	C4-C3-C5	2.42	119.42	115.23
22	b	615	CLA	CHC-C1C-NC	-2.42	120.67	124.31
22	B	608	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
24	Y	101	BCR	C15-C14-C13	-2.42	123.89	127.28
22	B	617	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	C	506	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
24	a	413	BCR	C23-C24-C25	-2.41	120.56	127.00
22	b	617	CLA	C4-C3-C5	2.41	119.41	115.23
22	C	507	CLA	C1D-CHD-C4C	-2.41	120.90	126.02
22	B	605	CLA	O2A-CGA-CBA	2.41	119.18	111.83
39	v	202	HEC	CHA-C1A-NA	2.41	127.08	124.45
28	b	621	SQD	C3-C4-C5	2.41	114.60	110.23
29	T	102	LMT	O5'-C1'-C2'	2.41	115.32	110.37
22	C	506	CLA	C2D-C1D-ND	2.41	112.51	110.13
22	b	615	CLA	C2A-C1A-CHA	-2.41	119.69	123.87
22	B	609	CLA	C1-O2A-CGA	2.41	122.47	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	616	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
22	c	912	CLA	CMD-C2D-C1D	2.40	128.96	124.73
22	A	406	CLA	CHB-C1B-NB	-2.40	120.44	124.05
22	C	510	CLA	C11-C10-C8	-2.40	107.98	115.97
24	d	404	BCR	C15-C14-C13	-2.40	123.91	127.28
22	A	405	CLA	O2A-CGA-CBA	2.40	119.15	111.83
22	B	617	CLA	C1-C2-C3	-2.40	122.27	126.20
24	c	916	BCR	C36-C18-C19	2.40	121.75	118.09
22	A	405	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
36	E	102	HEM	CHB-C1B-NB	2.40	127.33	124.37
35	C	517	DGD	O2G-C1B-C2B	2.40	116.67	111.48
26	D	406	PL9	C40-C39-C38	-2.40	117.47	123.63
22	C	505	CLA	CHC-C4B-NB	2.40	127.64	124.05
22	D	404	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
22	b	616	CLA	CAC-C3C-C4C	2.40	127.91	124.79
22	a	408	CLA	C6-C5-C3	-2.40	107.63	113.47
22	b	604	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
24	a	413	BCR	C8-C7-C6	-2.40	120.60	127.00
23	a	411	PHO	CMA-C3A-C4A	-2.39	109.45	114.61
22	b	605	CLA	CGD-CBD-CAD	-2.39	103.10	110.85
22	C	502	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
22	b	610	CLA	CMB-C2B-C1B	2.39	129.06	125.42
25	i	101	LMG	O1-C1-C2	2.39	111.90	108.27
22	b	614	CLA	O2A-CGA-CBA	2.39	119.12	111.83
22	B	604	CLA	CMC-C2C-C1C	2.39	128.77	125.03
22	D	401	CLA	C6-C5-C3	-2.39	107.65	113.47
22	C	506	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
34	V	203	HTG	C1-O5-C5	-2.39	108.28	112.56
24	B	619	BCR	C24-C23-C22	-2.38	122.71	126.23
22	C	508	CLA	CHC-C1C-NC	-2.38	120.72	124.31
34	l	106	HTG	C1-C2-C3	-2.38	105.89	110.55
22	B	602	CLA	CED-O2D-CGD	2.38	121.31	115.92
37	h	101	RRX	C10-C11-C12	-2.38	116.31	123.20
22	C	511	CLA	O2A-CGA-CBA	2.38	119.08	111.83
22	b	610	CLA	CMD-C2D-C1D	2.38	128.91	124.73
22	c	905	CLA	CED-O2D-CGD	2.38	121.30	115.92
22	b	612	CLA	C4B-C3B-C2B	-2.37	104.35	107.30
37	h	101	RRX	C2-C1-C6	2.37	113.89	110.44
35	C	517	DGD	O5D-C6D-C5D	-2.37	104.07	109.42
22	c	904	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
22	B	617	CLA	CHC-C4B-C3B	-2.37	117.08	127.37
24	d	404	BCR	C10-C11-C12	-2.37	116.33	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	919	DGD	O2E-C2E-C3E	-2.37	104.79	110.38
28	a	414	SQD	O5-C1-C2	-2.37	105.50	110.37
22	B	613	CLA	CHC-C1C-NC	-2.37	120.75	124.31
24	D	405	BCR	C38-C26-C27	2.37	118.64	113.60
22	b	611	CLA	CHC-C4B-NB	2.37	127.60	124.05
22	a	412	CLA	CMB-C2B-C1B	2.37	129.02	125.42
28	D	408	SQD	C1-O5-C5	-2.37	109.10	113.72
25	C	531	LMG	O6-C5-C6	2.36	112.30	106.44
24	b	618	BCR	C1-C6-C7	2.36	122.06	115.65
22	c	912	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	b	617	CLA	CHC-C1C-NC	-2.36	120.76	124.31
22	B	612	CLA	CHC-C4B-NB	2.36	127.59	124.05
22	C	510	CLA	CMD-C2D-C1D	2.36	128.88	124.73
22	b	605	CLA	O2A-CGA-CBA	2.35	119.01	111.83
22	a	407	CLA	C1D-CHD-C4C	-2.35	121.02	126.02
22	b	617	CLA	C4D-CHA-C1A	-2.35	118.44	121.24
22	a	412	CLA	CMD-C2D-C3D	2.35	133.09	127.69
34	C	523	HTG	C1-S1-C1'	2.35	112.50	100.32
25	J	101	LMG	O3-C3-C2	-2.35	104.83	110.38
27	C	522	LHG	O8-C23-C24	2.35	119.00	111.83
22	d	403	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
24	B	620	BCR	C40-C30-C25	-2.35	106.56	110.24
22	b	610	CLA	C16-C15-C13	-2.35	108.16	115.97
24	c	916	BCR	C35-C13-C14	-2.35	119.01	122.82
24	B	619	BCR	C23-C24-C25	-2.35	120.73	127.00
22	B	617	CLA	C1D-CHD-C4C	-2.35	121.03	126.02
22	c	912	CLA	CMB-C2B-C1B	2.35	128.99	125.42
22	c	910	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
22	C	510	CLA	C3C-C4C-NC	2.35	113.44	110.43
22	a	407	CLA	C7-C6-C5	-2.34	107.01	113.26
23	D	402	PHO	OBD-CAD-C3D	-2.34	124.23	127.89
27	a	416	LHG	C6-O8-C23	2.34	125.69	117.12
22	C	507	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
22	c	906	CLA	C4C-C3C-C2C	-2.34	103.48	106.89
25	B	621	LMG	O1-C1-C2	2.34	111.83	108.27
22	B	602	CLA	CMB-C2B-C1B	2.34	128.98	125.42
34	b	627	HTG	C1-O5-C5	2.34	116.76	112.56
22	a	412	CLA	CHC-C4B-NB	2.34	127.56	124.05
22	C	510	CLA	CHC-C4B-C3B	-2.34	117.22	127.37
22	D	401	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
22	b	606	CLA	C3B-C4B-NB	2.34	112.62	110.53
22	b	612	CLA	C4B-CHC-C1C	-2.34	120.75	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	617	CLA	C4-C3-C2	-2.34	117.62	123.63
22	B	603	CLA	C1D-CHD-C4C	-2.34	121.05	126.02
22	B	613	CLA	CMB-C2B-C1B	2.34	128.98	125.42
22	C	512	CLA	C3A-C2A-C1A	2.33	104.83	101.34
25	c	930	LMG	C1-O6-C5	2.33	118.28	113.72
22	b	608	CLA	CMB-C2B-C1B	2.33	128.97	125.42
22	B	603	CLA	C5-C3-C2	-2.33	115.93	121.17
25	B	621	LMG	O6-C5-C4	2.33	113.90	109.70
22	c	907	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
22	D	401	CLA	CHC-C4B-C3B	-2.33	117.26	127.37
24	B	620	BCR	C15-C14-C13	-2.33	124.01	127.28
34	b	624	HTG	C1-O5-C5	2.33	116.74	112.56
22	C	507	CLA	C4C-C3C-C2C	-2.33	103.50	106.89
22	b	614	CLA	CHC-C4B-C3B	-2.33	117.27	127.37
22	c	907	CLA	CAC-C3C-C4C	2.33	127.82	124.79
22	B	609	CLA	CMC-C2C-C1C	2.33	128.67	125.03
22	b	614	CLA	C3C-C4C-NC	2.33	113.41	110.43
22	b	606	CLA	CHC-C1C-NC	-2.33	120.81	124.31
22	b	611	CLA	C4B-C3B-C2B	-2.32	104.41	107.30
24	y	101	BCR	C15-C14-C13	-2.32	124.02	127.28
22	A	406	CLA	CED-O2D-CGD	2.32	121.19	115.92
22	C	502	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
22	D	403	CLA	C1D-ND-C4D	-2.32	104.68	106.31
22	D	401	CLA	CAC-C3C-C4C	2.32	127.81	124.79
22	A	406	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
31	c	924	DMS	O-S-C2	2.32	118.11	106.49
24	B	620	BCR	C15-C16-C17	-2.32	118.77	123.52
22	B	612	CLA	CBC-CAC-C3C	-2.32	106.13	112.42
22	B	606	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	D	403	CLA	CAC-C3C-C4C	2.32	127.81	124.79
24	b	620	BCR	C33-C5-C6	-2.32	121.95	124.48
22	c	909	CLA	CMC-C2C-C3C	2.32	132.42	126.15
22	b	611	CLA	CMC-C2C-C1C	2.32	128.66	125.03
22	b	604	CLA	O2A-CGA-CBA	2.32	118.90	111.83
22	d	402	CLA	CHB-C1B-NB	-2.32	120.57	124.05
22	B	603	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	B	614	CLA	C1D-CHD-C4C	-2.32	121.10	126.02
24	B	619	BCR	C20-C21-C22	-2.31	124.03	127.28
22	C	512	CLA	C4D-C3D-CAD	2.31	110.62	108.11
22	C	510	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
22	c	912	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
22	a	409	CLA	CHA-C4D-ND	2.31	137.31	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	511	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
22	B	604	CLA	CHD-C4C-NC	2.31	127.81	124.23
22	C	503	CLA	C4C-C3C-C2C	-2.31	103.53	106.89
22	c	912	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
26	D	406	PL9	C22-C23-C24	-2.30	122.35	127.62
22	B	608	CLA	C4-C3-C2	-2.30	117.71	123.63
22	a	408	CLA	CMD-C2D-C1D	2.30	128.78	124.73
24	a	413	BCR	C24-C23-C22	-2.30	122.83	126.23
22	B	602	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
24	Y	101	BCR	C21-C20-C19	-2.30	116.53	123.20
24	a	413	BCR	C32-C1-C31	-2.30	102.04	108.63
22	c	913	CLA	O2A-CGA-CBA	2.30	118.85	111.83
22	a	412	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
22	c	907	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
22	A	408	CLA	CHC-C4B-C3B	-2.30	117.39	127.37
22	b	615	CLA	C3B-C4B-NB	2.30	112.58	110.53
22	a	412	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
22	B	612	CLA	C1-C2-C3	-2.30	122.43	126.20
22	B	607	CLA	C1-O2A-CGA	2.30	122.22	116.65
22	c	905	CLA	C7-C6-C5	-2.30	107.14	113.26
24	y	101	BCR	C10-C11-C12	-2.30	116.54	123.20
22	B	613	CLA	C1D-ND-C4D	-2.30	104.70	106.31
22	b	612	CLA	C3C-C4C-NC	2.30	113.37	110.43
22	C	506	CLA	CHB-C4A-NA	2.30	127.72	124.40
25	B	621	LMG	C4-C3-C2	2.30	114.86	110.83
24	Y	101	BCR	C10-C11-C12	-2.30	116.55	123.20
24	B	618	BCR	C35-C13-C12	2.30	120.65	118.57
22	B	611	CLA	C1D-CHD-C4C	-2.29	121.14	126.02
22	d	402	CLA	CMC-C2C-C1C	2.29	128.62	125.03
22	B	607	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
27	D	410	LHG	O8-C23-O10	-2.29	117.89	123.63
22	c	914	CLA	CMB-C2B-C1B	2.29	128.91	125.42
22	B	603	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
22	B	604	CLA	CHC-C4B-C3B	-2.29	117.43	127.37
24	c	916	BCR	C21-C20-C19	-2.29	116.57	123.20
22	b	617	CLA	CMD-C2D-C1D	2.29	128.76	124.73
22	B	604	CLA	C2A-C1A-CHA	-2.29	119.90	123.87
22	a	409	CLA	O2A-CGA-CBA	2.29	118.81	111.83
22	d	402	CLA	CHD-C4C-NC	2.29	127.78	124.23
22	C	508	CLA	C1D-CHD-C4C	-2.29	121.16	126.02
22	c	904	CLA	C6-C5-C3	-2.28	107.90	113.47
22	b	605	CLA	CMB-C2B-C1B	2.28	128.90	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	H	102	DGD	C3B-C2B-C1B	-2.28	105.32	113.69
22	b	613	CLA	CMC-C2C-C1C	2.28	128.60	125.03
22	b	615	CLA	CHD-C4C-NC	2.28	127.77	124.23
22	b	603	CLA	OBD-CAD-C3D	-2.28	123.08	128.42
22	b	615	CLA	CHC-C4B-C3B	-2.28	117.47	127.37
22	c	907	CLA	C1D-CHD-C4C	-2.28	121.17	126.02
35	H	102	DGD	C2G-O2G-C1B	-2.28	112.34	117.80
29	I	102	LMT	C2'-C3'-C4'	-2.28	104.51	109.68
22	A	408	CLA	CMB-C2B-C1B	2.28	128.89	125.42
26	A	411	PL9	C10-C9-C11	2.28	119.18	115.23
22	B	614	CLA	CMB-C2B-C1B	2.28	128.88	125.42
22	b	607	CLA	C4C-C3C-C2C	-2.27	103.58	106.89
24	c	916	BCR	C7-C8-C9	-2.27	122.87	126.23
22	c	913	CLA	CBC-CAC-C3C	-2.27	106.26	112.42
22	B	606	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
22	b	610	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
22	b	604	CLA	CAC-C3C-C4C	2.27	127.75	124.79
22	B	613	CLA	C4C-C3C-C2C	-2.27	103.59	106.89
22	B	608	CLA	CHC-C4B-C3B	-2.27	117.52	127.37
22	B	615	CLA	CHC-C4B-C3B	-2.27	117.52	127.37
28	b	621	SQD	O9-S-C6	2.27	110.14	106.76
22	c	912	CLA	C4D-C3D-CAD	2.27	110.57	108.11
24	Y	101	BCR	C36-C18-C19	2.27	121.55	118.09
22	b	617	CLA	CHB-C1B-NB	-2.26	120.65	124.05
22	B	602	CLA	CHD-C4C-NC	2.26	127.74	124.23
24	b	619	BCR	C30-C25-C24	2.26	121.79	115.65
22	d	403	CLA	CAC-C3C-C4C	2.26	127.73	124.79
22	b	613	CLA	CMD-C2D-C3D	2.26	132.88	127.69
23	D	402	PHO	O2D-CGD-O1D	-2.26	119.44	123.85
22	B	608	CLA	CHB-C4A-NA	2.26	127.66	124.40
22	B	615	CLA	CAA-CBA-CGA	-2.26	106.79	113.21
22	c	904	CLA	C4-C3-C5	2.26	119.15	115.23
26	D	406	PL9	C42-C43-C44	-2.26	122.46	127.62
22	b	609	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
22	c	913	CLA	CMD-C2D-C1D	2.26	128.70	124.73
22	b	605	CLA	C1-O2A-CGA	2.26	122.11	116.65
22	B	605	CLA	C3B-C4B-NB	2.26	112.54	110.53
22	a	412	CLA	CHD-C1D-ND	-2.25	121.63	124.80
22	A	405	CLA	C3C-C4C-NC	2.25	113.31	110.43
22	B	612	CLA	C3C-C4C-NC	2.25	113.31	110.43
22	A	408	CLA	CHC-C1C-NC	-2.25	120.92	124.31
35	C	517	DGD	O3D-C3D-C2D	-2.25	105.07	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	904	CLA	CHC-C4B-NB	2.25	127.42	124.05
22	C	504	CLA	OBD-CAD-C3D	-2.25	123.16	128.42
22	B	607	CLA	CMC-C2C-C1C	2.25	128.55	125.03
22	a	409	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
22	c	905	CLA	CMB-C2B-C1B	2.25	128.84	125.42
35	C	519	DGD	O1G-C1A-O1A	-2.25	118.01	123.63
22	a	412	CLA	C3D-C2D-C1D	-2.25	102.77	105.83
24	b	619	BCR	C24-C25-C26	-2.25	116.38	121.56
22	B	606	CLA	CMB-C2B-C1B	2.25	128.84	125.42
22	B	612	CLA	C3D-C4D-ND	2.25	113.64	109.99
24	B	619	BCR	C11-C12-C13	-2.25	120.21	126.36
35	d	406	DGD	O1G-C1A-C2A	2.24	118.68	111.83
22	c	906	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
23	A	407	PHO	C1A-C2A-C3A	-2.24	100.70	102.84
25	C	520	LMG	O8-C9-C8	2.24	114.86	108.40
22	b	606	CLA	OBD-CAD-C3D	-2.24	123.17	128.42
22	B	617	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
22	b	611	CLA	C9-C8-C10	-2.24	103.28	111.27
22	c	906	CLA	CHB-C1B-NB	-2.24	120.69	124.05
22	C	512	CLA	CED-O2D-CGD	2.24	121.00	115.92
22	B	610	CLA	C3C-C4C-NC	2.24	113.30	110.43
22	B	616	CLA	C3B-C4B-NB	2.24	112.53	110.53
23	a	411	PHO	C11-C12-C13	-2.24	108.52	115.97
22	b	602	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
22	B	602	CLA	C4B-C3B-C2B	-2.24	104.52	107.30
22	B	603	CLA	C1D-ND-C4D	-2.24	104.74	106.31
24	D	405	BCR	C2-C1-C6	2.24	113.69	110.44
22	B	616	CLA	C4C-C3C-C2C	-2.24	103.64	106.89
22	B	608	CLA	CMC-C2C-C1C	2.23	128.53	125.03
22	D	401	CLA	O2A-CGA-CBA	2.23	118.65	111.83
22	B	602	CLA	C2B-C1B-NB	2.23	112.64	110.33
22	c	910	CLA	CED-O2D-CGD	2.23	120.98	115.92
22	C	506	CLA	C3A-C2A-C1A	2.23	104.68	101.34
22	B	603	CLA	C6-C7-C8	-2.23	108.54	115.97
22	B	607	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
34	l	106	HTG	O5-C1-C2	-2.23	107.24	110.32
22	B	612	CLA	CHB-C1B-NB	-2.23	120.70	124.05
34	b	632	HTG	C4-C3-C2	-2.23	106.92	110.83
24	c	915	BCR	C8-C7-C6	-2.23	121.04	127.00
24	k	101	BCR	C38-C26-C25	-2.23	122.05	124.48
29	f	102	LMT	C1-O1'-C1'	2.23	117.49	113.68
25	c	920	LMG	O8-C9-C8	2.23	114.82	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	C1-O2A-CGA	2.23	122.04	116.65
22	B	614	CLA	CHD-C4C-NC	2.23	127.69	124.23
22	b	615	CLA	C3C-C4C-NC	2.23	113.28	110.43
22	b	611	CLA	C1D-ND-C4D	-2.23	104.75	106.31
22	B	614	CLA	C7-C6-C5	-2.23	107.33	113.26
24	y	101	BCR	C34-C9-C8	2.23	121.49	118.09
22	b	612	CLA	CHC-C4B-C3B	-2.23	117.71	127.37
22	B	616	CLA	CMD-C2D-C1D	2.22	128.65	124.73
22	C	506	CLA	CHD-C4C-C3C	-2.22	121.53	124.77
22	a	407	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
22	C	513	CLA	CED-O2D-CGD	2.22	120.96	115.92
22	c	907	CLA	CHC-C4B-C3B	-2.22	117.72	127.37
22	B	612	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
25	j	101	LMG	O4-C4-C5	-2.22	103.85	109.32
35	C	519	DGD	O4D-C4D-C3D	-2.22	105.14	110.38
22	C	504	CLA	CED-O2D-CGD	2.22	120.95	115.92
22	B	616	CLA	CHC-C4B-NB	2.22	127.38	124.05
22	C	504	CLA	C5-C3-C2	-2.22	116.19	121.17
22	B	609	CLA	CMD-C2D-C1D	2.22	128.63	124.73
22	B	604	CLA	C3C-C4C-NC	2.22	113.27	110.43
22	c	906	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
22	b	616	CLA	CHB-C4A-NA	2.22	127.60	124.40
24	C	515	BCR	C36-C18-C19	2.22	121.47	118.09
26	a	415	PL9	C51-C49-C50	2.21	119.69	114.59
22	b	605	CLA	C4B-C3B-C2B	-2.21	104.55	107.30
36	e	101	HEM	C3B-C4B-NB	-2.21	107.88	109.47
22	c	909	CLA	CHC-C1C-NC	-2.21	120.98	124.31
25	d	409	LMG	O6-C5-C6	2.21	111.92	106.44
25	j	101	LMG	O8-C28-O10	-2.21	118.09	123.63
29	T	102	LMT	O1'-C1-C2	2.21	116.87	109.37
22	a	408	CLA	C4-C3-C5	2.21	119.07	115.23
22	a	409	CLA	CHB-C4A-NA	2.21	127.59	124.40
22	B	609	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
22	D	404	CLA	CMB-C2B-C1B	2.21	128.78	125.42
36	E	102	HEM	CMD-C2D-C1D	2.21	128.48	125.03
22	a	412	CLA	CAC-C3C-C4C	2.21	127.66	124.79
22	A	406	CLA	CHC-C1C-C2C	-2.20	120.68	126.95
28	A	413	SQD	C45-O47-C7	-2.20	112.52	117.80
24	b	620	BCR	C16-C17-C18	-2.20	124.19	127.28
29	A	414	LMT	O1'-C1'-C2'	2.20	111.62	108.27
26	D	406	PL9	C2-C1-C6	2.20	121.62	119.00
22	B	610	CLA	CHC-C4B-NB	2.20	127.35	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	515	BCR	C24-C23-C22	-2.20	122.98	126.23
22	C	512	CLA	C6-C7-C8	-2.20	108.65	115.97
22	D	401	CLA	CMD-C2D-C3D	2.20	132.74	127.69
24	Y	101	BCR	C30-C25-C24	2.20	121.62	115.65
22	B	617	CLA	C3C-C4C-NC	2.20	113.25	110.43
22	C	502	CLA	C3C-C4C-NC	2.20	113.25	110.43
22	C	504	CLA	C1-C2-C3	-2.20	122.60	126.20
22	C	505	CLA	C2D-C1D-ND	2.20	112.30	110.13
22	b	608	CLA	CBC-CAC-C3C	-2.20	106.46	112.42
35	C	517	DGD	C4E-C3E-C2E	-2.20	106.97	110.83
22	C	509	CLA	C1D-ND-C4D	-2.20	104.77	106.31
22	c	909	CLA	O2A-CGA-CBA	2.20	118.53	111.83
22	d	403	CLA	O2A-CGA-CBA	2.20	118.53	111.83
22	B	615	CLA	CMB-C2B-C1B	2.19	128.76	125.42
22	c	903	CLA	CMD-C2D-C1D	2.19	128.59	124.73
22	C	506	CLA	CMC-C2C-C1C	2.19	128.46	125.03
22	B	604	CLA	C6-C5-C3	2.19	118.81	113.47
22	B	610	CLA	C2B-C1B-NB	2.19	112.60	110.33
22	B	607	CLA	C1D-CHD-C4C	-2.19	121.36	126.02
34	b	624	HTG	O5-C5-C6	2.19	111.87	106.44
22	b	608	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
22	a	408	CLA	CMC-C2C-C3C	2.19	132.07	126.15
28	f	101	SQD	O7-S-C6	2.19	110.03	106.73
22	B	612	CLA	C3B-C4B-NB	2.19	112.48	110.53
22	c	912	CLA	CHD-C4C-NC	2.19	127.62	124.23
22	c	910	CLA	CMD-C2D-C1D	2.19	128.58	124.73
22	C	503	CLA	CHB-C1B-C2B	-2.19	121.08	127.43
22	b	615	CLA	C1D-CHD-C4C	-2.19	121.38	126.02
22	B	608	CLA	CHD-C4C-NC	2.18	127.62	124.23
35	C	519	DGD	O6E-C5E-C6E	2.18	111.85	106.44
22	B	615	CLA	CMC-C2C-C1C	2.18	128.44	125.03
28	a	418	SQD	O48-C23-O10	-2.18	118.17	123.63
22	c	908	CLA	C1D-CHD-C4C	-2.18	121.39	126.02
25	B	621	LMG	O6-C1-O1	2.18	115.19	110.04
22	b	602	CLA	C4B-C3B-C2B	-2.18	104.59	107.30
24	b	620	BCR	C32-C1-C6	-2.18	106.83	110.24
22	c	913	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
22	b	610	CLA	CHC-C4B-C3B	-2.18	117.92	127.37
23	A	407	PHO	C7-C6-C5	-2.18	107.46	113.26
22	C	504	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
22	a	407	CLA	C11-C10-C8	-2.17	108.74	115.97
22	A	408	CLA	C2A-C1A-CHA	-2.17	120.10	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	CMC-C2C-C1C	2.17	128.43	125.03
22	c	913	CLA	C1D-CHD-C4C	-2.17	121.40	126.02
22	b	603	CLA	CAC-C3C-C4C	2.17	127.61	124.79
26	d	405	PL9	C10-C9-C11	2.17	119.00	115.23
22	A	405	CLA	CMB-C2B-C1B	2.17	128.72	125.42
34	b	623	HTG	C4'-C3'-C2'	-2.17	103.41	114.37
22	b	616	CLA	C6-C7-C8	-2.17	108.76	115.97
22	c	911	CLA	C16-C15-C13	-2.17	108.76	115.97
25	A	410	LMG	O6-C1-C2	-2.17	105.92	110.37
22	B	607	CLA	C4B-CHC-C1C	-2.17	121.15	126.25
22	C	514	CLA	C2A-C1A-CHA	-2.17	120.11	123.87
22	B	608	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
35	C	517	DGD	O6D-C1D-O3G	-2.17	104.92	110.04
22	d	403	CLA	CHC-C1C-NC	-2.17	121.05	124.31
24	b	620	BCR	C15-C14-C13	-2.17	124.24	127.28
25	b	622	LMG	C9-O8-C28	2.17	125.04	117.12
35	C	518	DGD	O1G-C1A-C2A	2.17	118.44	111.83
36	E	102	HEM	C4C-NC-C1C	2.17	109.35	105.82
22	c	911	CLA	C1-O2A-CGA	2.17	121.89	116.65
28	a	418	SQD	C44-O6-C1	-2.17	109.15	113.80
34	B	626	HTG	O5-C5-C4	2.16	113.60	109.70
25	A	410	LMG	O8-C28-O10	-2.16	118.22	123.63
22	D	403	CLA	CED-O2D-CGD	2.16	120.82	115.92
22	b	616	CLA	CHC-C4B-C3B	-2.16	118.00	127.37
22	C	511	CLA	CMC-C2C-C1C	2.16	128.41	125.03
22	B	611	CLA	C3C-C4C-NC	2.16	113.19	110.43
22	B	613	CLA	CBA-CAA-C2A	-2.16	107.37	113.79
24	y	101	BCR	C8-C9-C10	-2.16	115.61	119.01
34	b	632	HTG	O2-C2-C3	2.16	115.46	110.38
28	a	418	SQD	O5-C1-O6	2.16	115.14	110.04
22	b	608	CLA	CMD-C2D-C1D	2.16	128.52	124.73
22	A	406	CLA	C2A-C1A-CHA	-2.15	120.13	123.87
22	b	609	CLA	CHD-C1D-ND	-2.15	121.77	124.80
22	a	408	CLA	C3B-C4B-NB	2.15	112.45	110.53
24	y	101	BCR	C23-C24-C25	-2.15	121.25	127.00
22	b	606	CLA	CMD-C2D-C1D	2.15	128.52	124.73
27	A	412	LHG	C6-O8-C23	2.15	124.99	117.12
24	A	409	BCR	C35-C13-C12	2.15	121.38	118.09
22	C	505	CLA	C6-C5-C3	2.15	118.71	113.47
23	D	402	PHO	CED-O2D-CGD	2.15	120.80	115.92
22	b	617	CLA	C4B-C3B-C2B	-2.15	104.63	107.30
24	A	409	BCR	C36-C18-C17	-2.15	119.33	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
22	c	905	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
22	B	604	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
22	c	911	CLA	CHB-C4A-NA	2.15	127.50	124.40
22	c	910	CLA	C3C-C4C-NC	2.15	113.18	110.43
28	l	101	SQD	O9-S-C6	2.15	109.96	106.76
22	a	408	CLA	C1D-CHD-C4C	-2.15	121.46	126.02
22	b	613	CLA	CMB-C2B-C1B	2.15	128.69	125.42
29	f	102	LMT	O1B-C4'-C5'	2.15	116.04	109.00
22	a	407	CLA	C5-C3-C2	-2.14	116.35	121.17
22	B	614	CLA	C2A-C1A-CHA	-2.14	120.14	123.87
34	B	626	HTG	O5-C5-C6	2.14	111.75	106.44
24	Y	101	BCR	C11-C12-C13	-2.14	120.49	126.36
22	c	910	CLA	C4C-C3C-C2C	-2.14	103.77	106.89
22	d	403	CLA	CHC-C4B-C3B	-2.14	118.08	127.37
22	B	616	CLA	C1-C2-C3	-2.14	122.69	126.20
22	B	612	CLA	C4B-C3B-C2B	-2.14	104.64	107.30
22	b	608	CLA	OBD-CAD-C3D	-2.14	123.41	128.42
22	B	605	CLA	C1D-ND-C4D	-2.14	104.81	106.31
22	B	608	CLA	CHB-C1B-NB	-2.14	120.84	124.05
24	k	101	BCR	C15-C16-C17	-2.14	119.14	123.52
22	c	913	CLA	CBB-CAB-C3B	-2.14	116.84	127.53
22	C	513	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
22	b	603	CLA	C1D-CHD-C4C	-2.14	121.48	126.02
24	C	515	BCR	C11-C12-C13	-2.14	120.50	126.36
22	c	904	CLA	CAA-C2A-C3A	-2.14	107.23	113.00
27	A	412	LHG	O7-C7-O9	-2.14	118.87	122.99
22	c	904	CLA	C4B-C3B-C2B	-2.13	104.65	107.30
22	B	614	CLA	CMD-C2D-C1D	2.13	128.49	124.73
22	b	611	CLA	C2A-C1A-CHA	-2.13	120.16	123.87
22	B	603	CLA	C4D-C3D-CAD	2.13	110.42	108.11
24	B	618	BCR	C1-C6-C5	-2.13	119.72	122.64
22	D	404	CLA	CHC-C4B-C3B	-2.13	118.12	127.37
27	l	102	LHG	C6-O8-C23	2.13	124.90	117.12
22	B	615	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
23	A	407	PHO	O2A-CGA-CBA	2.12	118.31	111.83
22	c	907	CLA	C1-C2-C3	-2.12	122.72	126.20
22	c	909	CLA	CAC-C3C-C2C	2.12	131.46	127.56
22	D	403	CLA	C3C-C4C-NC	2.12	113.15	110.43
25	c	920	LMG	O3-C3-C4	-2.12	105.37	110.38
37	H	101	RRX	C20-C21-C22	-2.12	124.30	127.28
22	b	604	CLA	C5-C3-C2	-2.12	116.40	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	CHC-C4B-C3B	-2.12	118.17	127.37
22	c	902	CLA	C3B-C4B-NB	2.12	112.42	110.53
29	I	102	LMT	C3'-C4'-C5'	-2.12	106.23	110.93
22	a	412	CLA	C5-C3-C2	-2.12	116.41	121.17
36	e	101	HEM	CHA-C4D-ND	2.12	126.99	124.37
22	B	611	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
27	d	407	LHG	O7-C7-C8	2.12	116.06	111.48
22	B	607	CLA	O2A-CGA-CBA	2.12	118.29	111.83
27	D	410	LHG	C34-C33-C32	-2.12	103.67	114.37
22	a	409	CLA	CMB-C2B-C3B	2.12	131.53	126.55
22	A	406	CLA	C5-C3-C2	-2.12	116.42	121.17
22	a	407	CLA	C3C-C4C-NC	2.12	113.14	110.43
22	c	902	CLA	C4D-C3D-CAD	2.11	110.40	108.11
22	C	504	CLA	C2A-C1A-CHA	-2.11	120.20	123.87
22	b	608	CLA	CHC-C4B-C3B	-2.11	118.21	127.37
24	a	413	BCR	C16-C15-C14	-2.11	119.20	123.52
34	V	203	HTG	O5-C5-C6	2.11	111.67	106.44
22	c	909	CLA	OBD-CAD-C3D	-2.11	123.48	128.42
22	c	903	CLA	C16-C15-C13	-2.11	108.95	115.97
22	c	912	CLA	C1-O2A-CGA	2.11	121.76	116.65
22	b	614	CLA	C1-C2-C3	-2.11	122.74	126.20
22	a	409	CLA	C1D-CHD-C4C	-2.11	121.54	126.02
22	b	603	CLA	C4B-C3B-C2B	-2.11	104.68	107.30
36	e	101	HEM	CAA-C2A-C1A	2.11	129.05	124.94
22	b	617	CLA	CHC-C4B-C3B	-2.11	118.23	127.37
23	D	402	PHO	CAC-C3C-C4C	2.11	129.44	124.03
34	b	623	HTG	O5-C1-C2	2.11	113.22	110.32
24	B	619	BCR	C29-C30-C25	2.11	113.50	110.44
34	b	626	HTG	C2'-C1'-S1	-2.10	105.27	112.36
24	b	619	BCR	C23-C24-C25	-2.10	121.38	127.00
22	c	910	CLA	C1D-ND-C4D	-2.10	104.84	106.31
24	a	413	BCR	C15-C16-C17	-2.10	119.22	123.52
22	A	406	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
22	B	614	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
22	c	907	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
24	c	915	BCR	C15-C16-C17	-2.10	119.22	123.52
22	b	607	CLA	C1D-ND-C4D	-2.10	104.84	106.31
22	B	611	CLA	C2A-C1A-CHA	-2.10	120.23	123.87
22	b	602	CLA	CMC-C2C-C1C	2.10	128.31	125.03
22	C	512	CLA	C4B-C3B-C2B	-2.10	104.70	107.30
22	b	610	CLA	C4D-CHA-C1A	-2.09	118.75	121.24
24	y	101	BCR	C35-C13-C12	2.09	121.29	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	618	BCR	C32-C1-C6	-2.09	106.96	110.24
29	a	419	LMT	O4'-C4B-C5B	2.09	114.48	109.32
28	a	414	SQD	O48-C23-O10	-2.09	118.39	123.63
35	c	917	DGD	O4D-C4D-C5D	-2.09	104.17	109.32
22	B	614	CLA	C3B-C4B-NB	2.09	112.40	110.53
22	B	613	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
22	C	512	CLA	CHB-C4A-NA	2.09	127.42	124.40
22	a	407	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
22	c	906	CLA	C1-C2-C3	-2.09	122.78	126.20
22	b	603	CLA	CED-O2D-CGD	2.09	120.65	115.92
28	A	413	SQD	C1-C2-C3	-2.09	105.62	110.01
22	C	507	CLA	CMD-C2D-C1D	2.09	128.40	124.73
35	C	517	DGD	O1G-C1A-O1A	-2.08	118.42	123.63
29	A	414	LMT	O3B-C3B-C2B	2.08	115.29	110.38
22	b	610	CLA	O2A-CGA-CBA	2.08	118.19	111.83
36	E	102	HEM	C2A-C1A-NA	-2.08	107.84	110.15
22	C	509	CLA	CHC-C4B-C3B	-2.08	118.33	127.37
22	c	904	CLA	CBB-CAB-C3B	-2.08	117.12	127.53
22	b	603	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	b	615	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
34	b	626	HTG	C4'-C3'-C2'	-2.08	103.86	114.37
22	B	604	CLA	CAC-C3C-C4C	2.08	127.49	124.79
22	A	405	CLA	C4C-C3C-C2C	-2.08	103.87	106.89
25	b	622	LMG	O8-C9-C8	2.08	114.38	108.40
22	b	617	CLA	CMB-C2B-C1B	2.07	128.58	125.42
28	b	621	SQD	C1-C2-C3	-2.07	105.65	110.01
35	H	102	DGD	C1D-O6D-C5D	-2.07	109.67	113.72
29	B	622	LMT	O5'-C5'-C4'	2.07	113.44	109.70
22	c	902	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	a	409	CLA	CED-O2D-CGD	2.07	120.62	115.92
37	H	101	RRX	C33-C5-C6	-2.07	122.22	124.48
29	c	921	LMT	C1B-O5B-C5B	2.07	117.77	113.72
22	D	404	CLA	CMC-C2C-C1C	2.07	128.27	125.03
22	c	913	CLA	CMB-C2B-C1B	2.07	128.57	125.42
29	Z	101	LMT	O3B-C3B-C2B	-2.07	105.49	110.38
22	c	908	CLA	C4B-C3B-C2B	-2.07	104.73	107.30
22	B	603	CLA	CAA-CBA-CGA	-2.07	107.33	113.21
22	a	408	CLA	CBA-CAA-C2A	-2.07	107.64	113.79
22	c	905	CLA	CHC-C1C-NC	-2.07	121.19	124.31
22	c	911	CLA	CHB-C1B-NB	-2.07	120.95	124.05
37	H	101	RRX	C2-C1-C6	2.07	113.44	110.44
39	V	202	HEC	O2D-CGD-CBD	2.07	120.53	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	914	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
24	b	619	BCR	C20-C21-C22	-2.06	124.38	127.28
25	c	920	LMG	O4-C4-C3	-2.06	105.51	110.38
22	B	604	CLA	CED-O2D-CGD	2.06	120.59	115.92
27	l	102	LHG	O8-C23-C24	2.06	118.12	111.83
28	l	101	SQD	O48-C23-O10	-2.06	118.47	123.63
22	B	605	CLA	C6-C7-C8	-2.06	109.12	115.97
22	C	505	CLA	CHC-C1C-NC	-2.06	121.21	124.31
27	L	101	LHG	O8-C23-O10	-2.06	118.47	123.63
27	C	522	LHG	O4-P-O5	2.06	118.86	110.83
24	B	619	BCR	C15-C14-C13	-2.06	124.39	127.28
22	B	605	CLA	CHB-C1B-NB	-2.06	120.96	124.05
35	c	918	DGD	C3A-C2A-C1A	-2.06	106.16	113.69
22	C	511	CLA	CHD-C1D-ND	-2.06	121.91	124.80
22	A	405	CLA	CHB-C4A-NA	2.06	127.37	124.40
22	c	913	CLA	C4C-C3C-C2C	-2.06	103.90	106.89
22	b	609	CLA	O2A-CGA-CBA	2.05	118.10	111.83
35	C	517	DGD	O6E-C5E-C6E	2.05	111.53	106.44
25	i	101	LMG	C6-C5-C4	2.05	118.06	113.02
22	C	505	CLA	CMC-C2C-C3C	2.05	131.70	126.15
24	c	915	BCR	C24-C23-C22	-2.05	123.20	126.23
34	b	624	HTG	C4-C3-C2	2.05	114.43	110.83
22	b	608	CLA	CBB-CAB-C3B	-2.05	117.28	127.53
22	b	606	CLA	CHC-C4B-NB	2.05	127.12	124.05
22	B	617	CLA	O2A-C1-C2	2.05	115.99	108.11
26	d	405	PL9	C22-C21-C19	2.05	119.97	113.19
22	A	408	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
23	D	402	PHO	C4-C3-C2	-2.05	118.37	123.63
25	C	520	LMG	O6-C5-C6	2.05	111.52	106.44
36	E	102	HEM	O1D-CGD-CBD	-2.05	116.60	123.09
22	c	906	CLA	CMB-C2B-C3B	2.05	131.37	126.55
22	c	905	CLA	C1D-CHD-C4C	-2.05	121.67	126.02
35	C	517	DGD	C6D-C5D-C4D	2.05	116.36	112.07
22	C	506	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	D	401	CLA	C4A-NA-C1A	2.05	107.61	106.68
25	J	101	LMG	C9-C8-C7	-2.04	107.02	111.78
36	e	101	HEM	C1D-C2D-C3D	-2.04	104.83	106.98
22	B	614	CLA	CAC-C3C-C4C	2.04	127.45	124.79
22	b	608	CLA	CMC-C2C-C3C	2.04	131.68	126.15
22	B	614	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
22	c	903	CLA	C3C-C4C-NC	2.04	113.05	110.43
22	B	603	CLA	C2A-C1A-CHA	-2.04	120.33	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	622	LMG	O6-C5-C4	2.04	113.38	109.70
22	B	608	CLA	C2A-C1A-CHA	-2.04	120.33	123.87
22	B	606	CLA	C16-C15-C13	-2.04	109.19	115.97
22	B	612	CLA	C1-O2A-CGA	2.04	121.59	116.65
25	C	520	LMG	O7-C10-O9	-2.04	118.94	123.70
24	B	620	BCR	C24-C23-C22	-2.04	123.22	126.23
22	B	611	CLA	CMC-C2C-C1C	2.04	128.22	125.03
35	C	519	DGD	O6D-C1D-C2D	-2.04	106.18	110.37
22	B	607	CLA	CHD-C1D-ND	-2.04	121.94	124.80
22	b	607	CLA	C1D-CHD-C4C	-2.04	121.69	126.02
22	C	506	CLA	C7-C6-C5	-2.03	107.84	113.26
22	d	403	CLA	O1D-CGD-CBD	-2.03	120.50	124.52
22	c	909	CLA	C4C-C3C-C2C	-2.03	103.93	106.89
22	c	910	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
22	d	403	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
23	D	402	PHO	CMB-C2B-C3B	2.03	128.74	124.68
27	D	410	LHG	O8-C23-C24	2.03	118.03	111.83
24	C	516	BCR	C8-C7-C6	-2.03	121.57	127.00
24	K	101	BCR	C7-C8-C9	-2.03	123.23	126.23
22	c	905	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
22	C	503	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	B	613	CLA	C4-C3-C5	2.03	118.75	115.23
22	c	910	CLA	C4-C3-C5	2.03	118.75	115.23
22	c	914	CLA	C3C-C4C-NC	2.03	113.03	110.43
22	C	505	CLA	C3B-C4B-NB	2.03	112.34	110.53
39	v	202	HEC	C1D-C2D-C3D	-2.03	104.49	106.82
35	C	519	DGD	C6D-C5D-C4D	2.03	116.32	112.07
24	b	620	BCR	C23-C24-C25	-2.03	121.58	127.00
25	c	920	LMG	O8-C28-O10	-2.03	118.56	123.63
24	C	516	BCR	C23-C24-C25	-2.03	121.59	127.00
24	b	619	BCR	C38-C26-C25	-2.02	122.28	124.48
26	A	411	PL9	C35-C34-C36	2.02	118.74	115.23
22	C	514	CLA	C4C-C3C-C2C	-2.02	103.94	106.89
22	c	911	CLA	CHC-C4B-C3B	-2.02	118.59	127.37
22	c	904	CLA	C1D-CHD-C4C	-2.02	121.72	126.02
24	C	515	BCR	C32-C1-C6	-2.02	107.07	110.24
39	v	202	HEC	CBC-CAC-C3C	-2.02	123.39	127.43
22	B	612	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
39	V	202	HEC	CMD-C2D-C1D	2.02	128.49	125.42
28	a	418	SQD	C4-C3-C2	2.02	114.38	110.83
22	B	613	CLA	C3B-C4B-NB	2.02	112.33	110.53
22	b	609	CLA	CBB-CAB-C3B	-2.02	117.44	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	607	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
24	c	916	BCR	C35-C13-C12	2.02	121.17	118.09
22	b	616	CLA	CMD-C2D-C3D	2.02	132.31	127.69
22	C	512	CLA	C6-C5-C3	-2.02	108.56	113.47
22	b	613	CLA	C1C-C2C-C3C	-2.01	104.86	106.98
22	B	613	CLA	C4D-C3D-CAD	2.01	110.29	108.11
23	a	410	PHO	CAC-C3C-C2C	2.01	131.25	127.56
22	A	406	CLA	CHB-C4A-NA	2.01	127.30	124.40
22	B	605	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
22	b	607	CLA	O2A-CGA-CBA	2.01	117.97	111.83
22	b	605	CLA	CHD-C1D-C2D	-2.01	121.31	125.49
22	c	903	CLA	CHC-C4B-C3B	-2.01	118.65	127.37
35	C	518	DGD	O3D-C3D-C2D	-2.01	105.64	110.38
22	B	605	CLA	C5-C3-C2	-2.01	116.66	121.17
24	d	404	BCR	C12-C13-C14	2.01	122.17	119.01
22	C	503	CLA	C16-C15-C13	-2.01	109.29	115.97
22	C	506	CLA	CHC-C4B-C3B	-2.01	118.65	127.37
25	J	101	LMG	O7-C10-C11	2.01	115.83	111.48
22	B	606	CLA	C6-C5-C3	-2.01	108.58	113.47
35	H	102	DGD	O5D-C1E-C2E	2.01	111.32	108.27
22	B	607	CLA	CHC-C4B-C3B	-2.01	118.67	127.37
22	C	504	CLA	CHB-C1B-NB	-2.00	121.04	124.05
25	d	409	LMG	O1-C7-C8	2.00	115.69	110.82
22	B	615	CLA	C3B-C4B-NB	2.00	112.32	110.53
22	B	602	CLA	CHC-C4B-C3B	-2.00	118.68	127.37
22	c	911	CLA	CHC-C1C-NC	-2.00	121.30	124.31
36	E	102	HEM	O2A-CGA-CBA	2.00	120.32	114.00
22	C	512	CLA	CHC-C4B-C3B	-2.00	118.69	127.37

All (51) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	405	CLA	ND
22	A	408	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	B	617	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	513	CLA	ND
22	D	403	CLA	ND
22	D	404	CLA	ND
22	a	407	CLA	ND
22	a	408	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	611	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	b	617	CLA	ND
22	c	902	CLA	ND
22	c	903	CLA	ND
22	c	906	CLA	ND
22	c	907	CLA	ND
22	c	908	CLA	ND
22	c	910	CLA	ND
22	c	911	CLA	ND
22	c	913	CLA	ND
22	d	402	CLA	ND

All (1705) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	602	CLA	C11-C10-C8-C9
22	B	606	CLA	C4B-C3B-CAB-CBB
22	B	610	CLA	C4B-C3B-CAB-CBB
22	B	615	CLA	C2-C1-O2A-CGA
22	B	615	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	b	602	CLA	C2-C1-O2A-CGA
22	b	602	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	b	617	CLA	CHA-CBD-CGD-O2D
22	c	903	CLA	CAD-CBD-CGD-O1D
22	c	904	CLA	C1A-C2A-CAA-CBA
22	c	908	CLA	CHA-CBD-CGD-O1D
22	c	914	CLA	C11-C12-C13-C15
23	a	411	PHO	C4C-C3C-CAC-CBC
24	D	405	BCR	C21-C22-C23-C24
24	D	405	BCR	C37-C22-C23-C24
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C21-C22-C23-C24
24	b	618	BCR	C7-C8-C9-C10
24	b	618	BCR	C7-C8-C9-C34
24	b	619	BCR	C7-C8-C9-C10
24	b	619	BCR	C7-C8-C9-C34
24	d	404	BCR	C21-C22-C23-C24
24	d	404	BCR	C37-C22-C23-C24
24	d	404	BCR	C23-C24-C25-C26
24	y	101	BCR	C7-C8-C9-C10
25	B	621	LMG	C2-C1-O1-C7
25	D	412	LMG	C11-C10-O7-C8
25	d	409	LMG	C2-C1-O1-C7
25	d	409	LMG	O6-C1-O1-C7
26	A	411	PL9	C26-C27-C28-C29
27	A	412	LHG	C4-O6-P-O3
27	A	412	LHG	C4-O6-P-O4
27	A	412	LHG	C4-O6-P-O5
27	A	412	LHG	C8-C7-O7-C5
27	L	101	LHG	C4-O6-P-O3
27	a	416	LHG	C3-O3-P-O5
27	a	416	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
27	a	423	LHG	O1-C1-C2-C3
27	a	423	LHG	C4-O6-P-O5
27	d	401	LHG	C4-O6-P-O3
27	d	401	LHG	C4-O6-P-O4
27	d	401	LHG	C5-C4-O6-P
27	d	401	LHG	O10-C23-O8-C6
27	d	401	LHG	C24-C23-O8-C6
27	d	407	LHG	C3-O3-P-O5
27	d	407	LHG	C4-O6-P-O4
27	l	102	LHG	O1-C1-C2-C3
27	l	102	LHG	C3-O3-P-O4
27	l	102	LHG	C3-O3-P-O6
28	A	413	SQD	C2-C1-O6-C44
28	A	413	SQD	C5-C6-S-O7
28	A	413	SQD	C5-C6-S-O8
28	A	413	SQD	C5-C6-S-O9
28	D	408	SQD	O6-C44-C45-C46
28	D	408	SQD	O6-C44-C45-O47
28	a	414	SQD	C5-C6-S-O7
28	a	414	SQD	C5-C6-S-O8
28	a	414	SQD	C5-C6-S-O9
28	a	418	SQD	C2-C1-O6-C44
28	a	418	SQD	O6-C44-C45-O47
28	l	101	SQD	O5-C5-C6-S
29	B	622	LMT	C2-C1-O1'-C1'
29	E	101	LMT	C2'-C1'-O1'-C1
29	I	102	LMT	C3'-C4'-O1B-C1B
29	I	102	LMT	O5'-C1'-O1'-C1
29	a	419	LMT	O5'-C1'-O1'-C1
29	c	931	LMT	C2'-C1'-O1'-C1
29	c	931	LMT	O5'-C1'-O1'-C1
29	f	102	LMT	C2'-C1'-O1'-C1
29	f	102	LMT	O5'-C1'-O1'-C1
29	t	101	LMT	C2-C1-O1'-C1'
34	B	627	HTG	O5-C1-S1-C1'
34	C	521	HTG	O5-C1-S1-C1'
34	C	532	HTG	O5-C1-S1-C1'
34	D	415	HTG	O5-C1-S1-C1'
34	b	632	HTG	O5-C1-S1-C1'
34	c	922	HTG	C2-C1-S1-C1'
34	l	106	HTG	C2-C1-S1-C1'
34	l	106	HTG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
35	D	407	DGD	O1G-C1G-C2G-O2G
35	D	407	DGD	C2D-C1D-O3G-C3G
35	D	407	DGD	O6D-C1D-O3G-C3G
35	d	406	DGD	C2B-C1B-O2G-C2G
37	h	101	RRX	C7-C8-C9-C10
37	h	101	RRX	C7-C8-C9-C34
39	V	202	HEC	C2C-C3C-CAC-CBC
39	V	202	HEC	C4C-C3C-CAC-CBC
39	v	202	HEC	C2B-C3B-CAB-CBB
39	v	202	HEC	C4B-C3B-CAB-CBB
39	v	202	HEC	C2C-C3C-CAC-CBC
39	v	202	HEC	C4C-C3C-CAC-CBC
27	A	412	LHG	O9-C7-O7-C5
22	B	617	CLA	O1A-CGA-O2A-C1
22	b	602	CLA	O1A-CGA-O2A-C1
25	A	410	LMG	O10-C28-O8-C9
25	B	621	LMG	O10-C28-O8-C9
28	l	101	SQD	O10-C23-O48-C46
23	a	411	PHO	O1D-CGD-O2D-CED
22	C	514	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	C5-C6-C7-C8
25	D	412	LMG	O9-C10-O7-C8
22	C	510	CLA	C3-C5-C6-C7
22	C	513	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
22	c	913	CLA	C3-C5-C6-C7
22	b	602	CLA	CBA-CGA-O2A-C1
28	l	101	SQD	C24-C23-O48-C46
35	d	406	DGD	C2A-C1A-O1G-C1G
29	c	921	LMT	C4'-C5'-C6'-O6'
22	C	514	CLA	CBD-CGD-O2D-CED
22	c	912	CLA	CBD-CGD-O2D-CED
23	a	411	PHO	CBD-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
22	c	914	CLA	O1D-CGD-O2D-CED
22	A	408	CLA	C4-C3-C5-C6
22	B	606	CLA	C4-C3-C5-C6
22	B	615	CLA	C4-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
26	A	411	PL9	C25-C24-C26-C27
26	a	415	PL9	C35-C34-C36-C37
22	B	606	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C2-C3-C5-C6
22	c	913	CLA	CBD-CGD-O2D-CED
22	A	408	CLA	C3-C5-C6-C7
22	B	602	CLA	C3-C5-C6-C7
22	b	605	CLA	C3-C5-C6-C7
22	B	617	CLA	CBA-CGA-O2A-C1
25	A	410	LMG	C29-C28-O8-C9
25	B	621	LMG	C29-C28-O8-C9
28	b	621	SQD	C24-C23-O48-C46
34	c	922	HTG	O5-C5-C6-O6
29	A	414	LMT	O5B-C5B-C6B-O6B
29	c	921	LMT	O5'-C5'-C6'-O6'
22	B	615	CLA	O1A-CGA-O2A-C1
25	D	412	LMG	O10-C28-O8-C9
28	b	621	SQD	O10-C23-O48-C46
25	b	622	LMG	O9-C10-O7-C8
35	d	406	DGD	O1B-C1B-O2G-C2G
25	D	412	LMG	O6-C5-C6-O5
29	a	419	LMT	C4'-C5'-C6'-O6'
29	c	931	LMT	C4'-C5'-C6'-O6'
22	a	412	CLA	C3-C5-C6-C7
25	d	409	LMG	C8-C9-O8-C28
23	a	411	PHO	C2C-C3C-CAC-CBC
22	a	407	CLA	C2C-C3C-CAC-CBC
29	t	101	LMT	O5'-C5'-C6'-O6'
34	b	627	HTG	O5-C5-C6-O6
35	d	406	DGD	O1A-C1A-O1G-C1G
34	b	626	HTG	C4-C5-C6-O6
29	a	419	LMT	O5'-C5'-C6'-O6'
29	c	931	LMT	O5'-C5'-C6'-O6'
22	c	910	CLA	CBD-CGD-O2D-CED
25	b	622	LMG	C11-C10-O7-C8
25	d	409	LMG	C11-C10-O7-C8
27	C	522	LHG	C8-C7-O7-C5
29	f	102	LMT	C4'-C5'-C6'-O6'
34	D	415	HTG	O5-C5-C6-O6
25	D	412	LMG	C4-C5-C6-O5
22	B	615	CLA	CBA-CGA-O2A-C1
25	D	412	LMG	C29-C28-O8-C9
22	A	408	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
26	A	411	PL9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
26	a	415	PL9	C33-C34-C36-C37
34	b	626	HTG	O5-C5-C6-O6
22	C	513	CLA	O1D-CGD-O2D-CED
26	A	411	PL9	C9-C11-C12-C13
26	D	406	PL9	C39-C41-C42-C43
26	a	415	PL9	C9-C11-C12-C13
26	a	415	PL9	C14-C16-C17-C18
26	a	415	PL9	C34-C36-C37-C38
36	e	101	HEM	C1A-C2A-CAA-CBA
29	I	102	LMT	O5B-C5B-C6B-O6B
34	c	922	HTG	C4-C5-C6-O6
36	e	101	HEM	C3A-C2A-CAA-CBA
28	b	621	SQD	O5-C1-O6-C44
22	b	617	CLA	CBD-CGD-O2D-CED
29	A	414	LMT	C4B-C5B-C6B-O6B
34	b	627	HTG	C4-C5-C6-O6
29	T	102	LMT	C4'-C5'-C6'-O6'
34	l	106	HTG	C4-C5-C6-O6
28	C	501	SQD	C13-C14-C15-C16
28	a	414	SQD	C17-C18-C19-C20
22	c	902	CLA	CBD-CGD-O2D-CED
34	b	624	HTG	S1-C1'-C2'-C3'
29	t	101	LMT	C4'-C5'-C6'-O6'
27	a	423	LHG	C1-C2-C3-O3
22	B	602	CLA	CBA-CGA-O2A-C1
22	c	913	CLA	CBA-CGA-O2A-C1
25	C	531	LMG	C29-C28-O8-C9
25	b	622	LMG	C29-C28-O8-C9
25	i	101	LMG	C29-C28-O8-C9
35	D	407	DGD	C2A-C1A-O1G-C1G
27	d	408	LHG	C11-C12-C13-C14
35	D	407	DGD	CCB-CDB-CEB-CFB
35	c	918	DGD	C8B-C9B-CAB-CBB
22	b	616	CLA	O1D-CGD-O2D-CED
34	v	203	HTG	C1'-C2'-C3'-C4'
22	B	602	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
22	b	608	CLA	C6-C7-C8-C9
22	c	905	CLA	C14-C13-C15-C16
22	c	910	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	912	CLA	C11-C10-C8-C9
22	c	913	CLA	C6-C7-C8-C9
35	c	917	DGD	C1B-C2B-C3B-C4B
22	c	913	CLA	O1A-CGA-O2A-C1
34	C	532	HTG	C4-C5-C6-O6
24	Y	101	BCR	C37-C22-C23-C24
24	k	101	BCR	C11-C12-C13-C35
24	y	101	BCR	C7-C8-C9-C34
24	y	101	BCR	C37-C22-C23-C24
34	C	532	HTG	S1-C1'-C2'-C3'
34	l	106	HTG	S1-C1'-C2'-C3'
29	T	102	LMT	O5'-C5'-C6'-O6'
29	f	102	LMT	O5'-C5'-C6'-O6'
24	b	618	BCR	C11-C12-C13-C14
28	l	101	SQD	C23-C24-C25-C26
25	C	531	LMG	O10-C28-O8-C9
22	c	911	CLA	O1D-CGD-O2D-CED
27	a	423	LHG	C24-C23-O8-C6
22	c	907	CLA	C5-C6-C7-C8
27	a	416	LHG	C7-C8-C9-C10
22	c	910	CLA	C2-C1-O2A-CGA
22	B	607	CLA	O1D-CGD-O2D-CED
22	D	401	CLA	C2C-C3C-CAC-CBC
22	b	612	CLA	C13-C15-C16-C17
27	a	423	LHG	O1-C1-C2-O2
22	B	616	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
25	b	622	LMG	O10-C28-O8-C9
34	l	106	HTG	O5-C5-C6-O6
29	t	101	LMT	O1'-C1-C2-C3
22	c	905	CLA	C4-C3-C5-C6
25	c	920	LMG	C28-C29-C30-C31
35	c	918	DGD	C1A-C2A-C3A-C4A
24	k	101	BCR	C9-C10-C11-C12
28	f	101	SQD	O6-C1-O5-C5
25	d	409	LMG	O9-C10-O7-C8
27	C	522	LHG	O9-C7-O7-C5
35	C	517	DGD	O6E-C5E-C6E-O5E
26	a	415	PL9	C19-C21-C22-C23
26	a	415	PL9	C24-C26-C27-C28
29	A	414	LMT	C4'-C5'-C6'-O6'
22	C	502	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C8-C10-C11-C12
25	c	930	LMG	O6-C5-C6-O5
25	A	410	LMG	C28-C29-C30-C31
25	C	520	LMG	C10-C11-C12-C13
28	A	413	SQD	C23-C24-C25-C26
35	C	518	DGD	C1A-C2A-C3A-C4A
25	i	101	LMG	O10-C28-O8-C9
22	A	408	CLA	C13-C15-C16-C17
22	B	607	CLA	C13-C15-C16-C17
22	C	510	CLA	C10-C11-C12-C13
22	b	604	CLA	C5-C6-C7-C8
22	b	617	CLA	C5-C6-C7-C8
22	c	910	CLA	C13-C15-C16-C17
22	B	606	CLA	C13-C15-C16-C17
22	B	616	CLA	C8-C10-C11-C12
22	b	602	CLA	C10-C11-C12-C13
22	d	403	CLA	C8-C10-C11-C12
25	j	101	LMG	O6-C5-C6-O5
25	d	409	LMG	C10-C11-C12-C13
27	A	412	LHG	C23-C24-C25-C26
27	a	423	LHG	C23-C24-C25-C26
28	C	501	SQD	C7-C8-C9-C10
35	d	406	DGD	C1B-C2B-C3B-C4B
22	C	504	CLA	O1D-CGD-O2D-CED
25	B	621	LMG	O6-C1-O1-C7
28	A	413	SQD	O5-C1-O6-C44
28	a	418	SQD	O5-C1-O6-C44
29	E	101	LMT	O5'-C1'-O1'-C1
35	H	102	DGD	C6B-C7B-C8B-C9B
22	A	405	CLA	C15-C16-C17-C18
22	B	605	CLA	C13-C15-C16-C17
22	B	607	CLA	C15-C16-C17-C18
22	B	616	CLA	C5-C6-C7-C8
22	C	507	CLA	C10-C11-C12-C13
22	C	510	CLA	C15-C16-C17-C18
22	D	404	CLA	C15-C16-C17-C18
22	b	609	CLA	C13-C15-C16-C17
22	b	612	CLA	C10-C11-C12-C13
27	D	411	LHG	C12-C13-C14-C15
22	B	602	CLA	O1A-CGA-O2A-C1
35	D	407	DGD	O1A-C1A-O1G-C1G
25	c	930	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
35	c	918	DGD	C1B-C2B-C3B-C4B
28	a	418	SQD	C32-C33-C34-C35
29	f	102	LMT	O1'-C1-C2-C3
22	C	512	CLA	O1D-CGD-O2D-CED
22	A	408	CLA	C10-C11-C12-C13
22	B	602	CLA	C13-C15-C16-C17
35	C	519	DGD	O6E-C5E-C6E-O5E
28	b	621	SQD	C23-C24-C25-C26
35	C	518	DGD	C1B-C2B-C3B-C4B
22	C	503	CLA	O1D-CGD-O2D-CED
27	d	401	LHG	C8-C7-O7-C5
34	b	623	HTG	S1-C1'-C2'-C3'
27	C	522	LHG	C7-C8-C9-C10
34	B	623	HTG	C4-C5-C6-O6
22	b	616	CLA	C5-C6-C7-C8
35	H	102	DGD	C2B-C3B-C4B-C5B
24	b	618	BCR	C9-C10-C11-C12
22	B	609	CLA	C13-C15-C16-C17
22	b	608	CLA	C10-C11-C12-C13
22	c	910	CLA	C15-C16-C17-C18
27	d	401	LHG	O9-C7-O7-C5
22	B	612	CLA	C15-C16-C17-C18
22	C	514	CLA	C15-C16-C17-C18
22	c	908	CLA	C5-C6-C7-C8
22	c	912	CLA	O1D-CGD-O2D-CED
22	c	903	CLA	O1D-CGD-O2D-CED
25	B	621	LMG	C28-C29-C30-C31
22	B	604	CLA	C5-C6-C7-C8
22	b	605	CLA	C13-C15-C16-C17
22	b	608	CLA	C15-C16-C17-C18
25	b	622	LMG	C4-C5-C6-O5
34	C	532	HTG	O5-C5-C6-O6
34	B	627	HTG	S1-C1'-C2'-C3'
22	A	408	CLA	C8-C10-C11-C12
22	B	611	CLA	C15-C16-C17-C18
22	C	509	CLA	C13-C15-C16-C17
22	d	403	CLA	C15-C16-C17-C18
22	b	616	CLA	C10-C11-C12-C13
22	c	909	CLA	CBD-CGD-O2D-CED
35	D	407	DGD	C2B-C1B-O2G-C2G
35	D	407	DGD	O1B-C1B-O2G-C2G
25	C	531	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	a	415	PL9	C39-C41-C42-C43
34	b	624	HTG	C1'-C2'-C3'-C4'
34	l	106	HTG	C1'-C2'-C3'-C4'
27	d	407	LHG	O2-C2-C3-O3
25	d	409	LMG	C29-C28-O8-C9
27	a	423	LHG	O10-C23-O8-C6
22	c	905	CLA	C10-C11-C12-C13
22	c	909	CLA	C10-C11-C12-C13
24	K	101	BCR	C11-C12-C13-C35
24	Y	101	BCR	C36-C18-C19-C20
24	b	618	BCR	C11-C12-C13-C35
24	c	916	BCR	C37-C22-C23-C24
37	h	101	RRX	C37-C22-C23-C24
22	B	608	CLA	C8-C10-C11-C12
27	D	409	LHG	O1-C1-C2-C3
27	D	410	LHG	O1-C1-C2-C3
27	d	407	LHG	O1-C1-C2-C3
27	D	409	LHG	C23-C24-C25-C26
22	C	507	CLA	C16-C17-C18-C20
22	C	508	CLA	C16-C17-C18-C20
22	a	407	CLA	C16-C17-C18-C19
22	c	906	CLA	C16-C17-C18-C19
22	c	907	CLA	C16-C17-C18-C19
22	c	913	CLA	C16-C17-C18-C19
22	c	914	CLA	C16-C17-C18-C19
27	d	408	LHG	C31-C32-C33-C34
29	T	102	LMT	O1'-C1-C2-C3
25	B	621	LMG	C11-C10-O7-C8
22	B	608	CLA	O1D-CGD-O2D-CED
25	b	622	LMG	C10-C11-C12-C13
34	b	626	HTG	S1-C1'-C2'-C3'
22	C	510	CLA	C2-C1-O2A-CGA
22	C	503	CLA	C16-C17-C18-C19
22	C	508	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C20
22	c	914	CLA	C16-C17-C18-C20
29	I	102	LMT	C1-C2-C3-C4
29	t	101	LMT	C1-C2-C3-C4
27	a	423	LHG	C26-C27-C28-C29
35	c	918	DGD	C3A-C4A-C5A-C6A
22	C	509	CLA	CBD-CGD-O2D-CED
29	B	622	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	J	101	LMG	C30-C31-C32-C33
25	b	622	LMG	C19-C20-C21-C22
25	c	920	LMG	C15-C16-C17-C18
25	c	930	LMG	C35-C36-C37-C38
25	d	409	LMG	C20-C21-C22-C23
25	i	101	LMG	C11-C12-C13-C14
25	j	101	LMG	C30-C31-C32-C33
29	B	622	LMT	C6-C7-C8-C9
35	C	517	DGD	C2B-C3B-C4B-C5B
35	C	517	DGD	C5B-C6B-C7B-C8B
35	C	519	DGD	C5B-C6B-C7B-C8B
35	d	406	DGD	CAA-CBA-CCA-CDA
27	l	102	LHG	C7-C8-C9-C10
25	C	531	LMG	C13-C14-C15-C16
28	C	501	SQD	C17-C18-C19-C20
35	h	102	DGD	C8A-C9A-CAA-CBA
35	h	102	DGD	C5B-C6B-C7B-C8B
29	B	622	LMT	C1-C2-C3-C4
25	A	410	LMG	C16-C17-C18-C19
25	B	621	LMG	C14-C15-C16-C17
25	d	409	LMG	C19-C20-C21-C22
27	d	407	LHG	C14-C15-C16-C17
27	d	408	LHG	C10-C11-C12-C13
27	l	102	LHG	C26-C27-C28-C29
28	a	418	SQD	C15-C16-C17-C18
28	l	101	SQD	C17-C18-C19-C20
35	C	519	DGD	CAB-CBB-CCB-CDB
35	c	917	DGD	C7B-C8B-C9B-CAB
35	d	406	DGD	C5B-C6B-C7B-C8B
35	d	406	DGD	CBB-CCB-CDB-CEB
27	D	410	LHG	O1-C1-C2-O2
28	C	501	SQD	C15-C16-C17-C18
28	l	101	SQD	C24-C25-C26-C27
35	D	407	DGD	C8B-C9B-CAB-CBB
22	C	513	CLA	C4B-C3B-CAB-CBB
35	C	519	DGD	C1A-C2A-C3A-C4A
34	C	521	HTG	C1'-C2'-C3'-C4'
25	c	930	LMG	C37-C38-C39-C40
27	l	102	LHG	C32-C33-C34-C35
28	l	101	SQD	C34-C35-C36-C37
22	A	408	CLA	C16-C17-C18-C20
22	B	611	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	C16-C17-C18-C19
22	C	514	CLA	C16-C17-C18-C19
22	a	407	CLA	C16-C17-C18-C20
22	b	608	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C20
22	b	616	CLA	C16-C17-C18-C19
22	c	906	CLA	C16-C17-C18-C20
22	B	607	CLA	C2A-CAA-CBA-CGA
27	l	102	LHG	C10-C11-C12-C13
28	a	418	SQD	C13-C14-C15-C16
22	c	905	CLA	C15-C16-C17-C18
28	l	101	SQD	C8-C7-O47-C45
25	d	409	LMG	C29-C30-C31-C32
22	b	607	CLA	C6-C7-C8-C10
27	d	401	LHG	C27-C28-C29-C30
34	b	632	HTG	C2'-C3'-C4'-C5'
35	H	102	DGD	CCB-CDB-CEB-CFB
27	a	423	LHG	C7-C8-C9-C10
25	c	920	LMG	C35-C36-C37-C38
25	j	101	LMG	C37-C38-C39-C40
28	A	413	SQD	C9-C10-C11-C12
28	a	418	SQD	C12-C13-C14-C15
28	b	621	SQD	C31-C32-C33-C34
34	C	523	HTG	C2'-C3'-C4'-C5'
35	C	519	DGD	C7B-C8B-C9B-CAB
35	C	519	DGD	CBB-CCB-CDB-CEB
22	b	602	CLA	C3-C5-C6-C7
25	A	410	LMG	C29-C30-C31-C32
25	C	520	LMG	C31-C32-C33-C34
25	b	622	LMG	C31-C32-C33-C34
27	a	416	LHG	C34-C35-C36-C37
28	A	413	SQD	C26-C27-C28-C29
28	a	418	SQD	C27-C28-C29-C30
22	c	905	CLA	C2-C3-C5-C6
29	I	102	LMT	C5-C6-C7-C8
22	A	405	CLA	C13-C15-C16-C17
22	b	617	CLA	C10-C11-C12-C13
22	c	907	CLA	C15-C16-C17-C18
35	d	406	DGD	C6A-C7A-C8A-C9A
22	A	408	CLA	C16-C17-C18-C19
22	B	606	CLA	C16-C17-C18-C20
22	C	514	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	c	908	CLA	C16-C17-C18-C20
22	c	909	CLA	C16-C17-C18-C19
29	Z	101	LMT	C1-C2-C3-C4
28	a	418	SQD	C24-C25-C26-C27
29	Z	101	LMT	C4-C5-C6-C7
29	c	921	LMT	C2-C3-C4-C5
35	d	406	DGD	C8B-C9B-CAB-CBB
28	f	101	SQD	O5-C1-O6-C44
25	b	622	LMG	C21-C22-C23-C24
25	c	920	LMG	C20-C21-C22-C23
27	D	411	LHG	C29-C30-C31-C32
27	l	102	LHG	C27-C28-C29-C30
27	d	407	LHG	C1-C2-C3-O3
22	c	904	CLA	CBA-CGA-O2A-C1
26	a	415	PL9	C44-C46-C47-C48
28	C	501	SQD	O6-C44-C45-C46
27	a	416	LHG	C15-C16-C17-C18
28	l	101	SQD	C14-C15-C16-C17
35	C	518	DGD	CBB-CCB-CDB-CEB
35	c	918	DGD	C3B-C4B-C5B-C6B
28	a	418	SQD	C7-C8-C9-C10
22	B	605	CLA	C10-C11-C12-C13
25	A	410	LMG	C20-C21-C22-C23
25	A	410	LMG	C38-C39-C40-C41
25	d	409	LMG	C12-C13-C14-C15
27	a	416	LHG	C11-C12-C13-C14
27	l	102	LHG	C28-C29-C30-C31
28	a	414	SQD	C15-C16-C17-C18
28	a	418	SQD	C29-C30-C31-C32
29	f	102	LMT	C2-C3-C4-C5
35	C	519	DGD	C5A-C6A-C7A-C8A
35	h	102	DGD	C2B-C3B-C4B-C5B
35	h	102	DGD	C3B-C4B-C5B-C6B
25	d	409	LMG	O10-C28-O8-C9
24	Y	101	BCR	C1-C6-C7-C8
25	C	520	LMG	C16-C17-C18-C19
25	c	930	LMG	C32-C33-C34-C35
28	l	101	SQD	C12-C13-C14-C15
29	c	931	LMT	C2-C3-C4-C5
34	b	624	HTG	C3'-C4'-C5'-C6'
35	c	918	DGD	CAB-CBB-CCB-CDB
22	c	910	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	C	501	SQD	C18-C19-C20-C21
28	a	418	SQD	C18-C19-C20-C21
25	B	621	LMG	C15-C16-C17-C18
27	d	407	LHG	C26-C27-C28-C29
28	C	501	SQD	C30-C31-C32-C33
28	a	414	SQD	C29-C30-C31-C32
28	a	414	SQD	C31-C32-C33-C34
22	A	406	CLA	C6-C7-C8-C9
22	B	606	CLA	C16-C17-C18-C19
22	B	606	CLA	C2B-C3B-CAB-CBB
22	B	610	CLA	C2B-C3B-CAB-CBB
24	b	618	BCR	C1-C6-C7-C8
24	b	618	BCR	C5-C6-C7-C8
24	d	404	BCR	C23-C24-C25-C30
37	h	101	RRX	C1-C6-C7-C8
37	h	101	RRX	C5-C6-C7-C8
28	a	418	SQD	C17-C18-C19-C20
22	B	605	CLA	C3-C5-C6-C7
25	C	520	LMG	C18-C19-C20-C21
27	l	102	LHG	C16-C17-C18-C19
22	a	407	CLA	C4C-C3C-CAC-CBC
25	j	101	LMG	C36-C37-C38-C39
27	a	416	LHG	C32-C33-C34-C35
27	d	407	LHG	C30-C31-C32-C33
35	D	407	DGD	C3B-C4B-C5B-C6B
22	a	408	CLA	C15-C16-C17-C18
22	c	913	CLA	C15-C16-C17-C18
35	C	517	DGD	C4A-C5A-C6A-C7A
35	D	407	DGD	C4A-C5A-C6A-C7A
35	c	919	DGD	C4A-C5A-C6A-C7A
26	A	411	PL9	C4-C3-C7-C8
27	C	522	LHG	C24-C25-C26-C27
27	d	408	LHG	C15-C16-C17-C18
29	a	419	LMT	C11-C10-C9-C8
35	h	102	DGD	CBB-CCB-CDB-CEB
25	B	621	LMG	O9-C10-O7-C8
28	l	101	SQD	O49-C7-O47-C45
25	A	410	LMG	C39-C40-C41-C42
27	A	412	LHG	C26-C27-C28-C29
27	D	411	LHG	C13-C14-C15-C16
25	J	101	LMG	O6-C5-C6-O5
34	b	632	HTG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
25	C	520	LMG	C34-C35-C36-C37
25	b	622	LMG	C17-C18-C19-C20
25	d	409	LMG	C34-C35-C36-C37
27	D	411	LHG	C18-C19-C20-C21
28	C	501	SQD	C9-C10-C11-C12
28	a	418	SQD	C28-C29-C30-C31
35	c	917	DGD	C7A-C8A-C9A-CAA
35	c	919	DGD	C2A-C3A-C4A-C5A
34	D	415	HTG	C1'-C2'-C3'-C4'
28	C	501	SQD	C14-C15-C16-C17
35	d	406	DGD	C3B-C4B-C5B-C6B
25	J	101	LMG	C12-C13-C14-C15
25	c	920	LMG	C18-C19-C20-C21
28	b	621	SQD	C28-C29-C30-C31
29	A	414	LMT	C6-C7-C8-C9
35	C	519	DGD	C2A-C3A-C4A-C5A
35	H	102	DGD	C7A-C8A-C9A-CAA
25	C	520	LMG	C20-C21-C22-C23
25	b	622	LMG	C14-C15-C16-C17
29	I	102	LMT	C6-C7-C8-C9
35	C	518	DGD	C2A-C3A-C4A-C5A
22	B	614	CLA	O1D-CGD-O2D-CED
25	D	412	LMG	C2-C1-O1-C7
22	c	904	CLA	O1A-CGA-O2A-C1
25	A	410	LMG	C21-C22-C23-C24
28	A	413	SQD	C27-C28-C29-C30
25	d	409	LMG	C28-C29-C30-C31
29	a	419	LMT	C1-C2-C3-C4
29	Z	101	LMT	O5B-C5B-C6B-O6B
25	d	409	LMG	C32-C33-C34-C35
25	i	101	LMG	C14-C15-C16-C17
28	a	414	SQD	C16-C17-C18-C19
35	c	919	DGD	C9A-CAA-CBA-CCA
27	a	416	LHG	C25-C26-C27-C28
27	l	102	LHG	C13-C14-C15-C16
28	A	413	SQD	C11-C12-C13-C14
29	a	419	LMT	C2-C3-C4-C5
35	C	517	DGD	C4B-C5B-C6B-C7B
35	d	406	DGD	C4B-C5B-C6B-C7B
22	B	603	CLA	C3-C5-C6-C7
22	b	610	CLA	C3-C5-C6-C7
28	l	101	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	A	410	LMG	C11-C10-O7-C8
25	i	101	LMG	C11-C10-O7-C8
27	a	416	LHG	C8-C7-O7-C5
25	C	520	LMG	C28-C29-C30-C31
27	D	410	LHG	C14-C15-C16-C17
27	a	416	LHG	C29-C30-C31-C32
29	I	102	LMT	C7-C8-C9-C10
25	i	101	LMG	C34-C35-C36-C37
27	D	409	LHG	C10-C11-C12-C13
24	A	409	BCR	C36-C18-C19-C20
25	i	101	LMG	C10-C11-C12-C13
27	d	401	LHG	C11-C12-C13-C14
28	b	621	SQD	C29-C30-C31-C32
35	c	917	DGD	C8A-C9A-CAA-CBA
35	C	518	DGD	C2G-C3G-O3G-C1D
27	d	401	LHG	C26-C27-C28-C29
29	c	931	LMT	C7-C8-C9-C10
35	C	518	DGD	CCA-CDA-CEA-CFA
35	D	407	DGD	CAA-CBA-CCA-CDA
22	c	907	CLA	C16-C17-C18-C20
22	c	908	CLA	C16-C17-C18-C19
22	c	913	CLA	C16-C17-C18-C20
25	d	409	LMG	C11-C12-C13-C14
27	D	409	LHG	C31-C32-C33-C34
27	a	416	LHG	C10-C11-C12-C13
28	a	414	SQD	C13-C14-C15-C16
28	a	414	SQD	C32-C33-C34-C35
29	t	101	LMT	C7-C8-C9-C10
35	c	919	DGD	C6A-C7A-C8A-C9A
35	c	919	DGD	CCB-CDB-CEB-CFB
29	c	921	LMT	C1-C2-C3-C4
25	C	520	LMG	C15-C16-C17-C18
28	A	413	SQD	C28-C29-C30-C31
35	C	518	DGD	C7A-C8A-C9A-CAA
22	B	607	CLA	C10-C11-C12-C13
27	a	423	LHG	C29-C30-C31-C32
28	a	414	SQD	C18-C19-C20-C21
29	Z	101	LMT	C3-C4-C5-C6
35	C	518	DGD	CAA-CBA-CCA-CDA
22	B	608	CLA	C15-C16-C17-C18
22	C	502	CLA	C15-C16-C17-C18
27	C	522	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	C3B-C4B-C5B-C6B
27	d	408	LHG	C28-C29-C30-C31
27	a	423	LHG	O6-C4-C5-O7
35	C	519	DGD	O6D-C5D-C6D-O5D
25	A	410	LMG	C17-C18-C19-C20
27	D	409	LHG	C15-C16-C17-C18
28	A	413	SQD	C17-C18-C19-C20
29	a	419	LMT	C6-C7-C8-C9
35	d	406	DGD	CCA-CDA-CEA-CFA
22	B	612	CLA	C13-C15-C16-C17
22	A	406	CLA	C6-C7-C8-C10
22	B	611	CLA	C16-C17-C18-C19
27	D	409	LHG	C29-C30-C31-C32
25	C	520	LMG	C39-C40-C41-C42
28	a	414	SQD	C27-C28-C29-C30
35	C	518	DGD	C6A-C7A-C8A-C9A
22	a	409	CLA	C8-C10-C11-C12
22	c	904	CLA	C8-C10-C11-C12
22	c	906	CLA	C13-C15-C16-C17
22	c	908	CLA	C13-C15-C16-C17
22	a	412	CLA	O1D-CGD-O2D-CED
35	D	407	DGD	C2B-C3B-C4B-C5B
28	A	413	SQD	O6-C44-C45-O47
28	C	501	SQD	O6-C44-C45-O47
28	a	414	SQD	O6-C44-C45-O47
35	d	406	DGD	O2G-C2G-C3G-O3G
25	i	101	LMG	C30-C31-C32-C33
27	a	416	LHG	C12-C13-C14-C15
27	l	102	LHG	C29-C30-C31-C32
35	c	919	DGD	C4B-C5B-C6B-C7B
22	B	602	CLA	O1D-CGD-O2D-CED
25	J	101	LMG	C34-C35-C36-C37
25	c	920	LMG	C30-C31-C32-C33
25	b	622	LMG	C18-C19-C20-C21
27	d	408	LHG	C13-C14-C15-C16
28	a	414	SQD	C24-C25-C26-C27
28	b	621	SQD	C24-C25-C26-C27
35	H	102	DGD	CAB-CBB-CCB-CDB
35	c	918	DGD	CAA-CBA-CCA-CDA
25	i	101	LMG	C12-C13-C14-C15
27	C	522	LHG	C9-C10-C11-C12
29	a	419	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
35	c	917	DGD	O6E-C5E-C6E-O5E
22	c	910	CLA	C8-C10-C11-C12
27	a	416	LHG	C9-C10-C11-C12
28	l	101	SQD	C28-C29-C30-C31
29	f	102	LMT	C11-C10-C9-C8
35	c	918	DGD	CBA-CCA-CDA-CEA
35	d	406	DGD	C9A-CAA-CBA-CCA
22	c	914	CLA	C4-C3-C5-C6
22	b	608	CLA	C8-C10-C11-C12
27	C	522	LHG	C12-C13-C14-C15
28	C	501	SQD	C12-C13-C14-C15
35	D	407	DGD	C2A-C3A-C4A-C5A
35	D	407	DGD	C5A-C6A-C7A-C8A
35	d	406	DGD	C2A-C3A-C4A-C5A
22	b	607	CLA	C2A-CAA-CBA-CGA
25	c	930	LMG	C34-C35-C36-C37
28	a	414	SQD	C30-C31-C32-C33
28	a	418	SQD	C31-C32-C33-C34
28	l	101	SQD	C26-C27-C28-C29
29	c	921	LMT	C4-C5-C6-C7
25	j	101	LMG	C31-C32-C33-C34
35	C	518	DGD	C5A-C6A-C7A-C8A
25	B	621	LMG	C12-C13-C14-C15
27	L	101	LHG	C13-C14-C15-C16
28	l	101	SQD	C11-C12-C13-C14
29	I	102	LMT	C4-C5-C6-C7
35	c	919	DGD	C8A-C9A-CAA-CBA
22	a	412	CLA	C15-C16-C17-C18
22	A	406	CLA	O1D-CGD-O2D-CED
25	C	520	LMG	C12-C13-C14-C15
35	D	407	DGD	C6B-C7B-C8B-C9B
22	C	507	CLA	C1A-C2A-CAA-CBA
22	c	909	CLA	C1A-C2A-CAA-CBA
22	D	404	CLA	C8-C10-C11-C12
25	i	101	LMG	C16-C17-C18-C19
28	A	413	SQD	C16-C17-C18-C19
25	c	920	LMG	C19-C20-C21-C22
28	a	418	SQD	C16-C17-C18-C19
35	D	407	DGD	C7B-C8B-C9B-CAB
29	c	921	LMT	O1'-C1-C2-C3
22	C	507	CLA	C5-C6-C7-C8
27	a	416	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	B	621	LMG	C13-C14-C15-C16
22	B	602	CLA	C11-C10-C8-C7
22	B	602	CLA	C12-C13-C15-C16
22	B	605	CLA	C11-C12-C13-C15
22	B	607	CLA	C12-C13-C15-C16
22	B	612	CLA	C12-C13-C15-C16
22	B	616	CLA	C11-C12-C13-C15
22	a	407	CLA	C12-C13-C15-C16
22	a	409	CLA	C11-C10-C8-C7
22	a	412	CLA	C11-C12-C13-C15
22	b	605	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C10-C8-C7
22	c	903	CLA	C11-C12-C13-C15
22	c	910	CLA	C11-C10-C8-C7
25	A	410	LMG	C33-C34-C35-C36
27	l	102	LHG	C34-C35-C36-C37
28	C	501	SQD	C34-C35-C36-C37
34	D	414	HTG	C2'-C3'-C4'-C5'
22	C	503	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	B	602	CLA	C10-C11-C12-C13
22	c	910	CLA	C10-C11-C12-C13
34	B	623	HTG	O5-C5-C6-O6
23	D	402	PHO	C2C-C3C-CAC-CBC
28	A	413	SQD	C25-C26-C27-C28
35	C	518	DGD	O6D-C5D-C6D-O5D
22	b	602	CLA	C13-C15-C16-C17
25	c	920	LMG	C11-C12-C13-C14
28	A	413	SQD	C18-C19-C20-C21
22	b	604	CLA	C2-C3-C5-C6
35	c	917	DGD	C9A-CAA-CBA-CCA
22	d	403	CLA	CBD-CGD-O2D-CED
28	C	501	SQD	C8-C7-O47-C45
22	A	408	CLA	C11-C10-C8-C9
22	B	607	CLA	C11-C12-C13-C14
22	C	514	CLA	C11-C10-C8-C9
22	D	404	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
25	A	410	LMG	C18-C19-C20-C21
28	A	413	SQD	C15-C16-C17-C18
34	b	626	HTG	C3'-C4'-C5'-C6'
35	c	919	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	C6A-C7A-C8A-C9A
35	C	517	DGD	CAA-CBA-CCA-CDA
25	c	920	LMG	C32-C33-C34-C35
29	E	101	LMT	O5'-C5'-C6'-O6'
25	i	101	LMG	O9-C10-O7-C8
25	b	622	LMG	C2-C1-O1-C7
28	l	101	SQD	C31-C32-C33-C34
29	c	921	LMT	C6-C7-C8-C9
25	B	621	LMG	C7-C8-C9-O8
25	D	412	LMG	O1-C7-C8-C9
25	d	409	LMG	C7-C8-C9-O8
27	d	408	LHG	C4-C5-C6-O8
28	A	413	SQD	O6-C44-C45-C46
28	a	414	SQD	O6-C44-C45-C46
35	D	407	DGD	C1G-C2G-C3G-O3G
28	l	101	SQD	C33-C34-C35-C36
22	B	612	CLA	C10-C11-C12-C13
25	J	101	LMG	C17-C18-C19-C20
27	D	409	LHG	C28-C29-C30-C31
27	D	410	LHG	C32-C33-C34-C35
27	L	101	LHG	C24-C25-C26-C27
27	l	102	LHG	C30-C31-C32-C33
22	C	513	CLA	CBA-CGA-O2A-C1
22	C	509	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
22	c	909	CLA	C16-C17-C18-C20
25	i	101	LMG	C35-C36-C37-C38
22	c	911	CLA	C8-C10-C11-C12
25	A	410	LMG	C35-C36-C37-C38
25	J	101	LMG	C16-C17-C18-C19
29	E	101	LMT	C11-C10-C9-C8
22	D	401	CLA	O1D-CGD-O2D-CED
23	a	411	PHO	CHA-CBD-CGD-O2D
27	d	408	LHG	C25-C26-C27-C28
28	C	501	SQD	C33-C34-C35-C36
27	C	522	LHG	C23-C24-C25-C26
28	a	414	SQD	C7-C8-C9-C10
35	D	407	DGD	C3A-C4A-C5A-C6A
22	B	612	CLA	C4-C3-C5-C6
26	d	405	PL9	C40-C39-C41-C42
29	T	102	LMT	C1-C2-C3-C4
22	B	612	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	c	914	CLA	C2-C3-C5-C6
26	d	405	PL9	C38-C39-C41-C42
27	a	423	LHG	C14-C15-C16-C17
23	D	402	PHO	C8-C10-C11-C12
29	c	921	LMT	O5B-C5B-C6B-O6B
25	A	410	LMG	O9-C10-O7-C8
25	c	920	LMG	C17-C18-C19-C20
25	C	531	LMG	C12-C13-C14-C15
28	l	101	SQD	C9-C10-C11-C12
25	C	531	LMG	O6-C5-C6-O5
22	B	612	CLA	C8-C10-C11-C12
35	D	407	DGD	CCA-CDA-CEA-CFA
27	A	412	LHG	C3-O3-P-O5
27	D	409	LHG	C16-C17-C18-C19
28	C	501	SQD	C28-C29-C30-C31
35	d	406	DGD	CAB-CBB-CCB-CDB
22	B	602	CLA	O2A-C1-C2-C3
23	a	410	PHO	O2A-C1-C2-C3
27	L	101	LHG	C16-C17-C18-C19
29	T	102	LMT	C11-C10-C9-C8
29	t	101	LMT	C11-C10-C9-C8
35	c	919	DGD	C3B-C4B-C5B-C6B
24	k	101	BCR	C19-C20-C21-C22
25	i	101	LMG	C33-C34-C35-C36
27	A	412	LHG	C27-C28-C29-C30
35	C	519	DGD	C9A-CAA-CBA-CCA
35	C	519	DGD	C2B-C3B-C4B-C5B
29	a	419	LMT	O1'-C1-C2-C3
35	c	917	DGD	C2A-C3A-C4A-C5A
25	A	410	LMG	C31-C32-C33-C34
27	d	408	LHG	C16-C17-C18-C19
27	L	101	LHG	O6-C4-C5-O7
22	b	613	CLA	C8-C10-C11-C12
22	b	614	CLA	C8-C10-C11-C12
27	A	412	LHG	C25-C26-C27-C28
22	c	914	CLA	CBA-CGA-O2A-C1
27	d	408	LHG	C19-C20-C21-C22
25	d	409	LMG	C21-C22-C23-C24
28	l	101	SQD	C10-C11-C12-C13
34	D	414	HTG	C1'-C2'-C3'-C4'
35	C	519	DGD	C4A-C5A-C6A-C7A
35	c	918	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
34	b	623	HTG	C2'-C3'-C4'-C5'
35	C	519	DGD	C9B-CAB-CBB-CCB
27	d	407	LHG	C12-C13-C14-C15
28	a	414	SQD	C14-C15-C16-C17
35	h	102	DGD	C6B-C7B-C8B-C9B
25	A	410	LMG	C22-C23-C24-C25
25	C	520	LMG	C22-C23-C24-C25
29	A	414	LMT	C9-C10-C11-C12
29	I	102	LMT	C9-C10-C11-C12
25	c	920	LMG	C12-C13-C14-C15
27	L	101	LHG	C14-C15-C16-C17
35	c	918	DGD	C2B-C3B-C4B-C5B
27	a	423	LHG	O7-C5-C6-O8
28	b	621	SQD	C35-C36-C37-C38
35	H	102	DGD	CDB-CEB-CFB-CGB
25	C	520	LMG	C17-C18-C19-C20
25	b	622	LMG	C15-C16-C17-C18
28	a	418	SQD	C24-C23-O48-C46
25	C	520	LMG	C33-C34-C35-C36
35	c	919	DGD	C6B-C7B-C8B-C9B
27	l	102	LHG	C35-C36-C37-C38
25	i	101	LMG	C18-C19-C20-C21
34	B	626	HTG	C2'-C3'-C4'-C5'
25	C	531	LMG	C14-C15-C16-C17
35	c	917	DGD	C8B-C9B-CAB-CBB
29	Z	101	LMT	C9-C10-C11-C12
27	L	101	LHG	C10-C11-C12-C13
29	I	102	LMT	C11-C10-C9-C8
22	C	513	CLA	O1A-CGA-O2A-C1
28	A	413	SQD	C19-C20-C21-C22
22	B	614	CLA	C10-C11-C12-C13
25	A	410	LMG	C11-C12-C13-C14
28	l	101	SQD	C25-C26-C27-C28
35	C	517	DGD	C3B-C4B-C5B-C6B
25	b	622	LMG	C13-C14-C15-C16
25	i	101	LMG	C13-C14-C15-C16
25	B	621	LMG	C17-C18-C19-C20
34	B	626	HTG	C3'-C4'-C5'-C6'
29	a	419	LMT	C2B-C1B-O1B-C4'
25	b	622	LMG	C12-C13-C14-C15
29	Z	101	LMT	C11-C10-C9-C8
35	d	406	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
28	l	101	SQD	C19-C20-C21-C22
34	D	415	HTG	C4'-C5'-C6'-C7'
35	h	102	DGD	CDB-CEB-CFB-CGB
28	A	413	SQD	C30-C31-C32-C33
22	c	909	CLA	C13-C15-C16-C17
22	d	403	CLA	C13-C15-C16-C17
22	B	615	CLA	O1D-CGD-O2D-CED
35	C	519	DGD	C4D-C5D-C6D-O5D
35	c	917	DGD	C4D-C5D-C6D-O5D
26	A	411	PL9	C30-C29-C31-C32
27	L	101	LHG	C19-C20-C21-C22
27	D	410	LHG	C26-C27-C28-C29
27	l	102	LHG	C9-C10-C11-C12
35	d	406	DGD	C2B-C3B-C4B-C5B
22	c	904	CLA	C5-C6-C7-C8
28	a	414	SQD	C35-C36-C37-C38
28	C	501	SQD	C11-C12-C13-C14
27	d	407	LHG	O1-C1-C2-O2
29	A	414	LMT	C2-C1-O1'-C1'
29	T	102	LMT	C2-C1-O1'-C1'
29	c	931	LMT	C2-C1-O1'-C1'
22	B	607	CLA	C14-C13-C15-C16
22	B	612	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C12-C13-C14
22	C	507	CLA	C11-C12-C13-C14
22	a	407	CLA	C14-C13-C15-C16
22	a	409	CLA	C11-C10-C8-C9
22	a	412	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
22	c	903	CLA	C11-C12-C13-C14
22	c	914	CLA	C11-C12-C13-C14
35	C	517	DGD	C6B-C7B-C8B-C9B
22	c	908	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	C8-C10-C11-C12
27	d	408	LHG	C2-C3-O3-P
22	B	602	CLA	C4B-C3B-CAB-CBB
22	C	502	CLA	C4B-C3B-CAB-CBB
25	i	101	LMG	C15-C16-C17-C18
35	H	102	DGD	O2G-C1B-C2B-C3B
27	a	416	LHG	C33-C34-C35-C36
22	b	603	CLA	C13-C15-C16-C17
25	c	920	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
27	A	412	LHG	C32-C33-C34-C35
28	l	101	SQD	C13-C14-C15-C16
35	c	919	DGD	C8B-C9B-CAB-CBB
29	A	414	LMT	C11-C10-C9-C8
35	C	518	DGD	C3A-C4A-C5A-C6A
27	d	407	LHG	C35-C36-C37-C38
29	I	102	LMT	C4B-C5B-C6B-O6B
27	L	101	LHG	O6-C4-C5-C6
27	d	407	LHG	C29-C30-C31-C32
27	d	408	LHG	C12-C13-C14-C15
34	D	414	HTG	C4'-C5'-C6'-C7'
35	C	518	DGD	CDB-CEB-CFB-CGB
35	h	102	DGD	CDA-CEA-CFA-CGA
29	a	419	LMT	O5B-C1B-O1B-C4'
22	A	408	CLA	C11-C10-C8-C7
22	B	605	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C12-C13-C15
22	B	616	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C12-C13-C15
22	C	509	CLA	C11-C10-C8-C7
22	C	514	CLA	C11-C10-C8-C7
22	D	404	CLA	C12-C13-C15-C16
22	c	905	CLA	C11-C10-C8-C7
22	c	905	CLA	C11-C12-C13-C15
22	c	908	CLA	C11-C12-C13-C15
22	c	913	CLA	C11-C12-C13-C15
22	d	402	CLA	C11-C12-C13-C15
22	c	914	CLA	C5-C6-C7-C8
22	c	914	CLA	C13-C15-C16-C17
25	c	930	LMG	C38-C39-C40-C41
29	A	414	LMT	C2-C3-C4-C5
27	L	101	LHG	O2-C2-C3-O3
29	T	102	LMT	C9-C10-C11-C12
22	D	404	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C20
22	c	911	CLA	C16-C17-C18-C20
25	B	621	LMG	C29-C30-C31-C32
35	C	517	DGD	CAB-CBB-CCB-CDB
35	c	919	DGD	CBB-CCB-CDB-CEB
29	A	414	LMT	C4-C5-C6-C7
34	C	521	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
34	D	415	HTG	C3'-C4'-C5'-C6'
35	c	917	DGD	O6D-C5D-C6D-O5D
25	j	101	LMG	C16-C17-C18-C19
26	a	415	PL9	C13-C14-C16-C17
22	a	408	CLA	C2C-C3C-CAC-CBC
25	A	410	LMG	C19-C20-C21-C22
25	d	409	LMG	C22-C23-C24-C25
22	B	605	CLA	O1D-CGD-O2D-CED
35	C	519	DGD	C2A-C1A-O1G-C1G
24	c	915	BCR	C9-C10-C11-C12
22	a	409	CLA	C10-C11-C12-C13
34	b	627	HTG	C3'-C4'-C5'-C6'
29	c	931	LMT	C4-C5-C6-C7
25	i	101	LMG	C40-C41-C42-C43
25	c	920	LMG	C33-C34-C35-C36
29	A	414	LMT	C3-C4-C5-C6
29	A	414	LMT	C5-C6-C7-C8
34	b	624	HTG	C2'-C3'-C4'-C5'
25	b	622	LMG	C32-C33-C34-C35
35	c	918	DGD	CDA-CEA-CFA-CGA
25	c	930	LMG	C11-C12-C13-C14
35	c	919	DGD	CDB-CEB-CFB-CGB
22	c	914	CLA	C10-C11-C12-C13
25	B	621	LMG	O1-C7-C8-C9
25	i	101	LMG	C7-C8-C9-O8
28	a	418	SQD	O6-C44-C45-C46
28	l	101	SQD	C44-C45-C46-O48
35	d	406	DGD	O1G-C1G-C2G-C3G
35	d	406	DGD	C1G-C2G-C3G-O3G
27	a	416	LHG	C13-C14-C15-C16
25	i	101	LMG	C22-C23-C24-C25
22	D	404	CLA	C3-C5-C6-C7
25	b	622	LMG	C16-C17-C18-C19
22	c	905	CLA	C8-C10-C11-C12
25	c	920	LMG	C31-C32-C33-C34
29	t	101	LMT	C9-C10-C11-C12
27	l	102	LHG	C11-C10-C9-C8
29	E	101	LMT	C3-C4-C5-C6
35	C	519	DGD	CDB-CEB-CFB-CGB
22	b	615	CLA	C4-C3-C5-C6
26	a	415	PL9	C45-C44-C46-C47
25	C	520	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C16-C17-C18-C19
29	f	102	LMT	C1-C2-C3-C4
22	B	609	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
25	d	409	LMG	C36-C37-C38-C39
22	C	502	CLA	C2B-C3B-CAB-CBB
24	D	405	BCR	C23-C24-C25-C30
27	a	423	LHG	O2-C2-C3-O3
22	C	514	CLA	CBA-CGA-O2A-C1
35	c	918	DGD	C5B-C6B-C7B-C8B
27	D	411	LHG	C2-C3-O3-P
25	J	101	LMG	C35-C36-C37-C38
27	a	416	LHG	C31-C32-C33-C34
35	C	519	DGD	CCB-CDB-CEB-CFB
25	j	101	LMG	C13-C14-C15-C16
22	c	903	CLA	C15-C16-C17-C18
22	b	611	CLA	CBD-CGD-O2D-CED
27	L	101	LHG	C15-C16-C17-C18
28	A	413	SQD	C11-C10-C9-C8
25	i	101	LMG	O8-C28-C29-C30
22	B	615	CLA	C2A-CAA-CBA-CGA
25	B	621	LMG	O7-C8-C9-O8
28	l	101	SQD	O47-C45-C46-O48
35	D	407	DGD	O2G-C2G-C3G-O3G
35	d	406	DGD	O1G-C1G-C2G-O2G
26	a	415	PL9	C4-C3-C7-C8
34	c	922	HTG	O5-C1-S1-C1'
34	b	626	HTG	C2'-C3'-C4'-C5'
25	i	101	LMG	C29-C30-C31-C32
22	a	409	CLA	C12-C13-C15-C16
25	B	621	LMG	C10-C11-C12-C13
35	C	518	DGD	CDA-CEA-CFA-CGA
26	a	415	PL9	C15-C14-C16-C17
25	A	410	LMG	C36-C37-C38-C39
25	i	101	LMG	C31-C32-C33-C34
28	C	501	SQD	C27-C28-C29-C30
35	C	517	DGD	C5A-C6A-C7A-C8A
22	C	508	CLA	C5-C6-C7-C8
26	A	411	PL9	C28-C29-C31-C32
35	c	917	DGD	CDA-CEA-CFA-CGA
25	c	920	LMG	C21-C22-C23-C24
34	C	532	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C16-C17-C18-C20
22	b	612	CLA	C16-C17-C18-C20
28	a	418	SQD	C9-C10-C11-C12
35	C	519	DGD	CBA-CCA-CDA-CEA
22	C	511	CLA	C8-C10-C11-C12
25	D	412	LMG	C12-C13-C14-C15
22	B	605	CLA	C11-C10-C8-C9
22	B	616	CLA	C11-C12-C13-C14
22	C	505	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	c	906	CLA	C14-C13-C15-C16
22	c	913	CLA	C11-C12-C13-C14
23	D	402	PHO	C11-C12-C13-C14
27	D	411	LHG	C16-C17-C18-C19
35	c	917	DGD	C3B-C4B-C5B-C6B
35	d	406	DGD	C4A-C5A-C6A-C7A
25	B	621	LMG	C18-C19-C20-C21
27	A	412	LHG	C33-C34-C35-C36
27	a	423	LHG	C28-C29-C30-C31
28	C	501	SQD	C35-C36-C37-C38
35	d	406	DGD	CDB-CEB-CFB-CGB
22	b	605	CLA	C16-C17-C18-C20
22	C	502	CLA	O1D-CGD-O2D-CED
27	A	412	LHG	C24-C25-C26-C27
35	c	918	DGD	C6A-C7A-C8A-C9A
29	f	102	LMT	C9-C10-C11-C12
27	L	101	LHG	C11-C10-C9-C8
35	D	407	DGD	C5B-C6B-C7B-C8B
29	t	101	LMT	C3-C4-C5-C6
22	D	401	CLA	C4C-C3C-CAC-CBC
27	D	409	LHG	O1-C1-C2-O2
25	C	520	LMG	C37-C38-C39-C40
28	C	501	SQD	C10-C11-C12-C13
29	t	101	LMT	C2-C3-C4-C5
35	C	518	DGD	C9A-CAA-CBA-CCA
22	c	914	CLA	O1A-CGA-O2A-C1
35	C	518	DGD	CBA-CCA-CDA-CEA
22	B	602	CLA	C16-C17-C18-C19
29	A	414	LMT	O5'-C5'-C6'-O6'
27	L	101	LHG	C25-C26-C27-C28
27	d	408	LHG	C32-C33-C34-C35
22	B	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C11-C10-C8-C7
22	C	505	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C15
22	b	604	CLA	C11-C10-C8-C7
22	c	906	CLA	C12-C13-C15-C16
22	c	907	CLA	C6-C7-C8-C10
22	c	913	CLA	C6-C7-C8-C10
22	c	914	CLA	C12-C13-C15-C16
22	d	403	CLA	C11-C10-C8-C7
23	D	402	PHO	C11-C12-C13-C15
27	a	416	LHG	C14-C15-C16-C17
35	c	917	DGD	C3A-C4A-C5A-C6A
25	D	412	LMG	C35-C36-C37-C38
24	y	101	BCR	C21-C22-C23-C24
37	h	101	RRX	C21-C22-C23-C24
28	a	418	SQD	O10-C23-O48-C46
25	C	531	LMG	C8-C7-O1-C1
35	c	918	DGD	C2G-C3G-O3G-C1D
35	c	918	DGD	C5D-C6D-O5D-C1E
22	d	403	CLA	C10-C11-C12-C13
22	a	409	CLA	C14-C13-C15-C16
34	b	632	HTG	C3'-C4'-C5'-C6'
36	e	101	HEM	C2C-C3C-CAC-CBC
28	C	501	SQD	C24-C25-C26-C27
28	C	501	SQD	C31-C32-C33-C34
29	Z	101	LMT	C5-C6-C7-C8
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	918	DGD	C4A-C5A-C6A-C7A
22	C	514	CLA	O2A-C1-C2-C3
23	A	407	PHO	O2A-C1-C2-C3
34	B	623	HTG	C1'-C2'-C3'-C4'
22	C	514	CLA	O1A-CGA-O2A-C1
34	c	922	HTG	S1-C1'-C2'-C3'
25	j	101	LMG	C35-C36-C37-C38
29	T	102	LMT	C5-C6-C7-C8
29	A	414	LMT	C1-C2-C3-C4
22	b	613	CLA	O1D-CGD-O2D-CED
28	f	101	SQD	O5-C5-C6-S
34	b	623	HTG	C4'-C5'-C6'-C7'
22	B	603	CLA	C13-C15-C16-C17
22	C	507	CLA	C13-C15-C16-C17
22	c	913	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	C	501	SQD	O49-C7-O47-C45
28	A	413	SQD	C13-C14-C15-C16
35	c	917	DGD	O6E-C1E-O5D-C6D
35	c	918	DGD	O6E-C1E-O5D-C6D
27	C	522	LHG	C4-C5-C6-O8
27	a	423	LHG	C4-C5-C6-O8
35	D	407	DGD	O1G-C1G-C2G-C3G
35	H	102	DGD	O1G-C1G-C2G-C3G
22	c	903	CLA	C16-C17-C18-C19
35	C	519	DGD	CAA-CBA-CCA-CDA
26	a	415	PL9	C43-C44-C46-C47
27	d	401	LHG	C31-C32-C33-C34
35	d	406	DGD	C9B-CAB-CBB-CCB
34	B	627	HTG	C2-C1-S1-C1'
34	D	415	HTG	C2-C1-S1-C1'
25	C	520	LMG	C21-C22-C23-C24
25	d	409	LMG	C13-C14-C15-C16
27	a	416	LHG	C30-C31-C32-C33
25	B	621	LMG	O1-C7-C8-O7
25	d	409	LMG	O7-C8-C9-O8
25	i	101	LMG	O7-C8-C9-O8
27	C	522	LHG	O7-C5-C6-O8
28	b	621	SQD	O47-C45-C46-O48
35	H	102	DGD	O1G-C1G-C2G-O2G
22	B	611	CLA	C11-C12-C13-C14
22	B	612	CLA	C11-C12-C13-C14
22	a	412	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	c	908	CLA	C14-C13-C15-C16
29	T	102	LMT	C2-C3-C4-C5
25	c	930	LMG	C14-C15-C16-C17
25	c	930	LMG	C33-C34-C35-C36
25	c	920	LMG	C34-C35-C36-C37
35	d	406	DGD	C3A-C4A-C5A-C6A
25	d	409	LMG	C15-C16-C17-C18
27	a	416	LHG	C27-C28-C29-C30
35	c	919	DGD	CAA-CBA-CCA-CDA
35	D	407	DGD	C8A-C9A-CAA-CBA
27	l	102	LHG	C14-C15-C16-C17
35	C	518	DGD	C4B-C5B-C6B-C7B
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	C8B-C9B-CAB-CBB
25	i	101	LMG	C36-C37-C38-C39
29	B	622	LMT	C4-C5-C6-C7
35	H	102	DGD	C7B-C8B-C9B-CAB
22	b	604	CLA	C4-C3-C5-C6
27	L	101	LHG	C1-C2-C3-O3
22	C	508	CLA	C10-C11-C12-C13
22	B	602	CLA	C16-C17-C18-C20
22	c	911	CLA	C16-C17-C18-C19
22	b	612	CLA	C8-C10-C11-C12
22	B	617	CLA	O1D-CGD-O2D-CED
35	C	518	DGD	C4D-C5D-C6D-O5D
28	a	414	SQD	C11-C10-C9-C8
27	l	102	LHG	O1-C1-C2-O2
29	f	102	LMT	C2-C1-O1'-C1'
25	C	520	LMG	C14-C15-C16-C17
22	b	602	CLA	C4B-C3B-CAB-CBB
22	c	902	CLA	C4B-C3B-CAB-CBB
27	D	410	LHG	C13-C14-C15-C16
34	b	626	HTG	C4'-C5'-C6'-C7'
24	A	409	BCR	C17-C18-C19-C20
24	c	916	BCR	C21-C22-C23-C24
24	k	101	BCR	C11-C12-C13-C14
35	C	519	DGD	O1A-C1A-O1G-C1G
27	a	423	LHG	O6-C4-C5-C6
27	A	412	LHG	C28-C29-C30-C31
25	j	101	LMG	C34-C35-C36-C37
25	b	622	LMG	C29-C30-C31-C32
25	d	409	LMG	C30-C31-C32-C33
29	E	101	LMT	C5-C6-C7-C8
22	B	602	CLA	C6-C7-C8-C10
22	B	603	CLA	C6-C7-C8-C10
22	B	604	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
22	C	510	CLA	C12-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C10
22	C	514	CLA	C11-C12-C13-C15
22	a	409	CLA	C6-C7-C8-C10
22	b	602	CLA	C11-C10-C8-C7
22	b	608	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C10-C8-C7
22	b	609	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	b	609	CLA	C11-C12-C13-C15
22	c	905	CLA	C12-C13-C15-C16
22	c	907	CLA	C11-C12-C13-C15
22	c	909	CLA	C11-C12-C13-C15
22	c	910	CLA	C6-C7-C8-C10
22	c	912	CLA	C11-C10-C8-C7
22	D	404	CLA	C16-C17-C18-C20
22	b	617	CLA	C8-C10-C11-C12
28	a	414	SQD	C12-C13-C14-C15
29	c	921	LMT	C9-C10-C11-C12
35	c	919	DGD	C2A-C1A-O1G-C1G
27	d	401	LHG	C9-C10-C11-C12
28	a	414	SQD	C25-C26-C27-C28
29	c	921	LMT	C3-C4-C5-C6
22	c	906	CLA	C8-C10-C11-C12
39	V	202	HEC	C4B-C3B-CAB-CBB
22	B	602	CLA	C11-C12-C13-C14
22	B	607	CLA	C11-C10-C8-C9
22	B	616	CLA	C14-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C9
22	b	604	CLA	C11-C10-C8-C9
22	c	905	CLA	C11-C10-C8-C9
22	d	403	CLA	C11-C10-C8-C9
27	d	407	LHG	C34-C35-C36-C37
27	d	407	LHG	C16-C17-C18-C19
24	C	515	BCR	C13-C14-C15-C16
27	D	410	LHG	C30-C31-C32-C33
28	b	621	SQD	O5-C5-C6-S
25	C	531	LMG	C29-C30-C31-C32
35	C	519	DGD	C4E-C5E-C6E-O5E
25	A	410	LMG	O1-C7-C8-O7
25	A	410	LMG	O7-C8-C9-O8
25	D	412	LMG	O1-C7-C8-O7
25	c	930	LMG	O1-C7-C8-O7
28	b	621	SQD	O6-C44-C45-O47
28	l	101	SQD	O6-C44-C45-O47
35	h	102	DGD	CCB-CDB-CEB-CFB
25	A	410	LMG	O1-C7-C8-C9
35	D	407	DGD	CDA-CEA-CFA-CGA
34	b	623	HTG	C3'-C4'-C5'-C6'
25	j	101	LMG	C39-C40-C41-C42
27	a	416	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	B	622	LMT	C11-C10-C9-C8
22	C	503	CLA	CAD-CBD-CGD-O2D
22	b	606	CLA	CAD-CBD-CGD-O2D
22	c	905	CLA	CAD-CBD-CGD-O2D
35	C	519	DGD	O6D-C1D-O3G-C3G
22	b	611	CLA	C8-C10-C11-C12
25	d	409	LMG	C14-C15-C16-C17
22	C	514	CLA	C3-C5-C6-C7
22	c	905	CLA	C3-C5-C6-C7
22	C	508	CLA	C2A-CAA-CBA-CGA
28	a	414	SQD	C33-C34-C35-C36
35	C	517	DGD	CBB-CCB-CDB-CEB
22	B	602	CLA	CAD-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	608	CLA	CAD-CBD-CGD-O1D
22	B	611	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CAD-CBD-CGD-O1D
22	C	511	CLA	CHA-CBD-CGD-O1D
22	C	513	CLA	CAD-CBD-CGD-O1D
22	b	602	CLA	CAD-CBD-CGD-O1D
22	b	605	CLA	CHA-CBD-CGD-O2D
22	b	608	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O1D
22	c	905	CLA	CAD-CBD-CGD-O1D
22	c	908	CLA	CHA-CBD-CGD-O2D
22	c	910	CLA	CHA-CBD-CGD-O1D
22	c	910	CLA	CHA-CBD-CGD-O2D
22	c	913	CLA	CHA-CBD-CGD-O1D
27	L	101	LHG	C4-O6-P-O5
27	a	416	LHG	C4-O6-P-O3
27	a	416	LHG	C4-O6-P-O4
27	d	407	LHG	C3-O3-P-O6
27	d	407	LHG	C4-O6-P-O3
27	l	102	LHG	C3-O3-P-O5
37	H	101	RRX	C9-C10-C11-C12
37	h	101	RRX	C9-C10-C11-C12
39	V	202	HEC	C2B-C3B-CAB-CBB
27	L	101	LHG	C26-C27-C28-C29
25	c	930	LMG	C28-C29-C30-C31
25	A	410	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	D	411	LHG	C15-C16-C17-C18
22	b	602	CLA	C4-C3-C5-C6
22	B	602	CLA	C2B-C3B-CAB-CBB
22	b	602	CLA	C2B-C3B-CAB-CBB
35	h	102	DGD	O2G-C1B-C2B-C3B
22	b	615	CLA	C2-C3-C5-C6
35	H	102	DGD	C5B-C6B-C7B-C8B
29	B	622	LMT	C9-C10-C11-C12
25	J	101	LMG	C18-C19-C20-C21
34	C	532	HTG	C1'-C2'-C3'-C4'
27	d	401	LHG	C11-C10-C9-C8
25	c	920	LMG	C37-C38-C39-C40
22	B	613	CLA	O1A-CGA-O2A-C1
35	c	917	DGD	C5B-C6B-C7B-C8B
28	l	101	SQD	C15-C16-C17-C18
27	d	401	LHG	C4-C5-O7-C7
27	a	416	LHG	O6-C4-C5-C6
22	C	506	CLA	C11-C12-C13-C14
22	a	409	CLA	C6-C7-C8-C9
22	b	602	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
22	c	905	CLA	C11-C12-C13-C14
22	c	907	CLA	C6-C7-C8-C9
22	c	908	CLA	C11-C12-C13-C14
22	d	402	CLA	C11-C12-C13-C14
22	C	506	CLA	C11-C12-C13-C15
22	a	412	CLA	C6-C7-C8-C10
22	b	612	CLA	C12-C13-C15-C16
29	A	414	LMT	C7-C8-C9-C10
35	c	918	DGD	CCA-CDA-CEA-CFA
35	h	102	DGD	C9A-CAA-CBA-CCA
35	c	918	DGD	C2E-C1E-O5D-C6D
34	b	632	HTG	C4'-C5'-C6'-C7'
22	b	616	CLA	C4-C3-C5-C6
25	J	101	LMG	C14-C15-C16-C17
25	c	920	LMG	C36-C37-C38-C39
27	L	101	LHG	C5-C6-O8-C23
35	h	102	DGD	C7A-C8A-C9A-CAA
27	d	408	LHG	C29-C30-C31-C32
27	d	408	LHG	O7-C5-C6-O8
35	h	102	DGD	O1G-C1G-C2G-O2G
24	K	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C2C-C3C-CAC-CBC
35	C	517	DGD	O6D-C5D-C6D-O5D
25	d	409	LMG	C18-C19-C20-C21
27	C	522	LHG	C13-C14-C15-C16
22	B	617	CLA	C2-C1-O2A-CGA
22	b	611	CLA	C16-C17-C18-C20
25	j	101	LMG	C18-C19-C20-C21
27	C	522	LHG	O7-C7-C8-C9
25	A	410	LMG	C7-C8-C9-O8
26	A	411	PL9	C39-C41-C42-C43
28	b	621	SQD	C44-C45-C46-O48
35	D	407	DGD	C4B-C5B-C6B-C7B
34	D	415	HTG	C2'-C1'-S1-C1
22	c	914	CLA	CBD-CGD-O2D-CED
35	c	917	DGD	C5D-C6D-O5D-C1E
25	b	622	LMG	C20-C21-C22-C23
22	c	910	CLA	C2A-CAA-CBA-CGA
37	h	101	RRX	C19-C20-C21-C22
35	d	406	DGD	C7A-C8A-C9A-CAA
22	B	616	CLA	C4-C3-C5-C6
22	b	602	CLA	C2-C3-C5-C6
35	c	918	DGD	C4B-C5B-C6B-C7B
22	D	404	CLA	C6-C7-C8-C9
22	c	913	CLA	C14-C13-C15-C16
22	c	914	CLA	C14-C13-C15-C16
22	C	510	CLA	O1D-CGD-O2D-CED
35	C	517	DGD	CDA-CEA-CFA-CGA
25	C	531	LMG	C21-C22-C23-C24
34	B	627	HTG	C1'-C2'-C3'-C4'
22	B	616	CLA	C13-C15-C16-C17
35	C	517	DGD	C4D-C5D-C6D-O5D
27	a	416	LHG	C17-C18-C19-C20
22	C	506	CLA	O1D-CGD-O2D-CED
34	b	623	HTG	C4-C5-C6-O6
29	E	101	LMT	C1-C2-C3-C4
25	B	621	LMG	C4-C5-C6-O5
27	l	102	LHG	C31-C32-C33-C34
36	e	101	HEM	C4C-C3C-CAC-CBC
27	a	423	LHG	C10-C11-C12-C13
29	a	419	LMT	C7-C8-C9-C10
22	A	408	CLA	C12-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	c	904	CLA	C6-C7-C8-C10
22	c	913	CLA	C12-C13-C15-C16
22	B	613	CLA	C8-C10-C11-C12
22	a	408	CLA	C4C-C3C-CAC-CBC
27	D	409	LHG	C25-C26-C27-C28
22	B	606	CLA	C8-C10-C11-C12
25	C	520	LMG	O1-C7-C8-O7
28	A	413	SQD	O47-C45-C46-O48
35	h	102	DGD	CAA-CBA-CCA-CDA
29	B	622	LMT	C3-C4-C5-C6
35	c	918	DGD	C9A-CAA-CBA-CCA
27	a	416	LHG	C35-C36-C37-C38
28	l	101	SQD	C7-C8-C9-C10
29	c	921	LMT	C5-C6-C7-C8
26	d	405	PL9	C35-C34-C36-C37
27	l	102	LHG	C1-C2-C3-O3
27	D	410	LHG	C29-C30-C31-C32
28	a	414	SQD	C28-C29-C30-C31
36	e	101	HEM	CAA-CBA-CGA-O1A
25	C	531	LMG	O1-C7-C8-C9
27	d	407	LHG	C31-C32-C33-C34
34	v	203	HTG	S1-C1'-C2'-C3'
22	A	408	CLA	C11-C12-C13-C14
22	b	608	CLA	C14-C13-C15-C16
22	b	611	CLA	C11-C12-C13-C14
22	c	907	CLA	C14-C13-C15-C16
22	c	908	CLA	C11-C10-C8-C9
22	c	909	CLA	C11-C10-C8-C9
23	D	402	PHO	C6-C7-C8-C9
27	d	401	LHG	C25-C26-C27-C28
22	b	606	CLA	O1D-CGD-O2D-CED
28	A	413	SQD	C24-C23-O48-C46
27	D	409	LHG	C11-C10-C9-C8
35	C	519	DGD	CDA-CEA-CFA-CGA
27	d	407	LHG	C28-C29-C30-C31
35	c	917	DGD	C2E-C1E-O5D-C6D
22	c	902	CLA	C2A-CAA-CBA-CGA
25	D	412	LMG	C21-C22-C23-C24
29	E	101	LMT	O1'-C1-C2-C3
22	a	412	CLA	C10-C11-C12-C13
22	C	513	CLA	C2B-C3B-CAB-CBB
22	b	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	C	515	BCR	C23-C24-C25-C30
24	D	405	BCR	C23-C24-C25-C26
24	b	619	BCR	C23-C24-C25-C30
25	C	531	LMG	C10-C11-C12-C13
36	e	101	HEM	CAA-CBA-CGA-O2A
22	b	616	CLA	C2-C3-C5-C6
25	j	101	LMG	C32-C33-C34-C35
35	c	917	DGD	CAA-CBA-CCA-CDA
22	C	506	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	508	CLA	C11-C12-C13-C15
22	C	510	CLA	C11-C10-C8-C7
22	C	511	CLA	C12-C13-C15-C16
22	D	404	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C12-C13-C15
22	c	903	CLA	C12-C13-C15-C16
27	l	102	LHG	C17-C18-C19-C20
26	d	405	PL9	C4-C3-C7-C8
28	b	621	SQD	C44-C45-O47-C7
25	C	531	LMG	C17-C18-C19-C20
34	v	203	HTG	C4-C5-C6-O6
34	B	627	HTG	C4'-C5'-C6'-C7'
22	d	402	CLA	C15-C16-C17-C18
35	C	517	DGD	C8A-C9A-CAA-CBA
22	B	616	CLA	C2-C3-C5-C6
28	a	418	SQD	C10-C11-C12-C13
35	H	102	DGD	C5A-C6A-C7A-C8A
39	V	202	HEC	CAD-CBD-CGD-O2D
27	a	416	LHG	O2-C2-C3-O3
22	c	911	CLA	O1A-CGA-O2A-C1
22	d	403	CLA	C6-C7-C8-C9
35	d	406	DGD	C2D-C1D-O3G-C3G
28	b	621	SQD	C34-C35-C36-C37
35	c	917	DGD	C6A-C7A-C8A-C9A
22	B	604	CLA	C4-C3-C5-C6
22	c	906	CLA	C2-C3-C5-C6
26	d	405	PL9	C33-C34-C36-C37
28	l	101	SQD	C11-C10-C9-C8
22	b	609	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C19
35	c	919	DGD	O1A-C1A-O1G-C1G
35	H	102	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
26	D	406	PL9	C34-C36-C37-C38
35	h	102	DGD	O1G-C1G-C2G-C3G
34	C	521	HTG	O5-C5-C6-O6
29	a	419	LMT	C4-C5-C6-C7
22	a	412	CLA	C4-C3-C5-C6
27	d	407	LHG	C11-C12-C13-C14
35	H	102	DGD	O1B-C1B-C2B-C3B
35	C	519	DGD	C4B-C5B-C6B-C7B
35	C	519	DGD	C6B-C7B-C8B-C9B
22	C	503	CLA	C4B-C3B-CAB-CBB
22	b	610	CLA	C4B-C3B-CAB-CBB
22	c	913	CLA	C4B-C3B-CAB-CBB
22	d	402	CLA	C4B-C3B-CAB-CBB
27	D	409	LHG	C19-C20-C21-C22
22	b	607	CLA	C16-C17-C18-C20
22	c	903	CLA	C16-C17-C18-C20
22	B	613	CLA	C10-C11-C12-C13
35	C	519	DGD	C8A-C9A-CAA-CBA
35	D	407	DGD	C6A-C7A-C8A-C9A
23	A	407	PHO	CHA-CBD-CGD-O1D
25	c	920	LMG	C22-C23-C24-C25
28	a	414	SQD	C10-C11-C12-C13
27	l	102	LHG	C23-C24-C25-C26
28	f	101	SQD	C45-C44-O6-C1
35	D	407	DGD	C9B-CAB-CBB-CCB
22	b	616	CLA	C8-C10-C11-C12
27	D	411	LHG	C26-C27-C28-C29
35	C	518	DGD	C8A-C9A-CAA-CBA
26	A	411	PL9	C2-C3-C7-C8
22	B	614	CLA	C11-C10-C8-C7
22	c	909	CLA	C11-C10-C8-C7
39	v	202	HEC	CAD-CBD-CGD-O2D
39	V	202	HEC	CAD-CBD-CGD-O1D
22	A	405	CLA	C14-C13-C15-C16
22	B	611	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C9
22	C	509	CLA	C14-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C14
22	b	604	CLA	C6-C7-C8-C9
28	A	413	SQD	O10-C23-O48-C46
25	A	410	LMG	C15-C16-C17-C18
28	C	501	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
28	a	418	SQD	C45-C44-O6-C1
35	d	406	DGD	C2G-C3G-O3G-C1D
25	i	101	LMG	O10-C28-C29-C30
22	C	510	CLA	C2A-CAA-CBA-CGA
22	b	616	CLA	C3A-C2A-CAA-CBA
39	v	202	HEC	CAD-CBD-CGD-O1D
35	C	518	DGD	C2E-C1E-O5D-C6D
29	c	931	LMT	O1'-C1-C2-C3
28	a	414	SQD	O47-C7-C8-C9
35	c	919	DGD	O6D-C5D-C6D-O5D
27	D	410	LHG	C35-C36-C37-C38
27	C	522	LHG	O6-C4-C5-O7
34	D	415	HTG	C4-C5-C6-O6
25	C	520	LMG	O1-C7-C8-C9
28	A	413	SQD	C44-C45-C46-O48
28	l	101	SQD	O6-C44-C45-C46
22	C	511	CLA	O1A-CGA-O2A-C1
22	d	402	CLA	C16-C17-C18-C20
27	d	408	LHG	C27-C28-C29-C30
22	C	514	CLA	C4-C3-C5-C6
29	c	931	LMT	C9-C10-C11-C12
22	C	511	CLA	C2-C3-C5-C6
22	a	408	CLA	C16-C17-C18-C20
26	d	405	PL9	C36-C37-C38-C39
35	D	407	DGD	CBB-CCB-CDB-CEB
22	C	514	CLA	C10-C11-C12-C13
22	c	913	CLA	C10-C11-C12-C13
25	D	412	LMG	C34-C35-C36-C37
29	T	102	LMT	C7-C8-C9-C10
25	j	101	LMG	C40-C41-C42-C43
27	D	411	LHG	C31-C32-C33-C34
25	D	412	LMG	O7-C8-C9-O8
22	B	604	CLA	C11-C10-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	b	609	CLA	C11-C12-C13-C14
22	c	907	CLA	C11-C12-C13-C14
22	c	909	CLA	C11-C12-C13-C14
22	b	611	CLA	C16-C17-C18-C19
27	d	408	LHG	C17-C18-C19-C20
22	c	913	CLA	CAA-CBA-CGA-O2A
35	c	917	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
22	c	911	CLA	CBA-CGA-O2A-C1
22	C	509	CLA	C5-C6-C7-C8
34	B	627	HTG	C4-C5-C6-O6
22	A	408	CLA	C11-C12-C13-C15
22	B	611	CLA	C12-C13-C15-C16
22	C	509	CLA	C12-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C15
22	b	604	CLA	C6-C7-C8-C10
22	b	608	CLA	C12-C13-C15-C16
22	c	907	CLA	C12-C13-C15-C16
22	c	908	CLA	C11-C10-C8-C7
22	c	910	CLA	C11-C12-C13-C15
22	d	403	CLA	C6-C7-C8-C10
25	A	410	LMG	C40-C41-C42-C43
22	C	503	CLA	C2B-C3B-CAB-CBB
22	b	617	CLA	C2B-C3B-CAB-CBB
22	c	913	CLA	C2B-C3B-CAB-CBB
22	d	402	CLA	C2B-C3B-CAB-CBB
24	C	515	BCR	C23-C24-C25-C26
24	a	413	BCR	C1-C6-C7-C8
24	b	619	BCR	C23-C24-C25-C26
24	c	916	BCR	C1-C6-C7-C8
24	c	916	BCR	C5-C6-C7-C8
23	a	411	PHO	C5-C6-C7-C8
22	C	507	CLA	C2-C1-O2A-CGA
22	d	402	CLA	C2-C1-O2A-CGA
35	C	518	DGD	C2B-C3B-C4B-C5B
25	B	621	LMG	C20-C21-C22-C23
22	A	405	CLA	C2C-C3C-CAC-CBC
27	D	409	LHG	C30-C31-C32-C33
22	D	401	CLA	C15-C16-C17-C18
22	a	412	CLA	C8-C10-C11-C12
35	d	406	DGD	C8A-C9A-CAA-CBA
36	e	101	HEM	C2A-CAA-CBA-CGA
35	h	102	DGD	C7B-C8B-C9B-CAB
25	B	621	LMG	C16-C17-C18-C19
34	B	627	HTG	C2'-C1'-S1-C1
34	b	623	HTG	C2'-C1'-S1-C1
34	c	922	HTG	C2'-C1'-S1-C1
34	v	203	HTG	C2'-C1'-S1-C1
22	c	902	CLA	C13-C15-C16-C17
27	a	423	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	CAA-CBA-CGA-O2A
25	d	409	LMG	O8-C28-C29-C30
27	l	102	LHG	O6-C4-C5-O7
26	A	411	PL9	C20-C19-C21-C22
26	D	406	PL9	C35-C34-C36-C37
22	C	513	CLA	CAA-CBA-CGA-O2A
35	C	519	DGD	C6A-C7A-C8A-C9A
28	l	101	SQD	O47-C7-C8-C9
35	H	102	DGD	C8A-C9A-CAA-CBA
25	c	920	LMG	C40-C41-C42-C43
22	C	510	CLA	C11-C10-C8-C9
22	C	511	CLA	C11-C10-C8-C9
22	C	514	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C10-C8-C9
22	c	910	CLA	C11-C12-C13-C14
25	c	920	LMG	C13-C14-C15-C16
29	E	101	LMT	C4-C5-C6-C7
28	b	621	SQD	O6-C44-C45-C46
35	h	102	DGD	C1G-C2G-C3G-O3G
22	b	602	CLA	C1A-C2A-CAA-CBA
22	b	608	CLA	C4B-C3B-CAB-CBB
22	b	611	CLA	C4B-C3B-CAB-CBB
22	b	604	CLA	CBD-CGD-O2D-CED
22	c	906	CLA	C4-C3-C5-C6
22	C	503	CLA	C15-C16-C17-C18
28	C	501	SQD	O47-C7-C8-C9
26	A	411	PL9	C13-C14-C16-C17
26	D	406	PL9	C11-C12-C13-C14
24	Y	101	BCR	C17-C18-C19-C20
35	h	102	DGD	CAB-CBB-CCB-CDB
22	b	613	CLA	CBA-CGA-O2A-C1
22	b	604	CLA	C2A-CAA-CBA-CGA
27	D	411	LHG	C30-C31-C32-C33
29	a	419	LMT	C5-C6-C7-C8
22	B	607	CLA	C16-C17-C18-C19
22	C	511	CLA	CAA-CBA-CGA-O2A
27	D	410	LHG	C25-C26-C27-C28
28	l	101	SQD	C16-C17-C18-C19
22	C	511	CLA	C11-C10-C8-C7
22	a	412	CLA	C12-C13-C15-C16
22	b	612	CLA	C6-C7-C8-C10
26	D	406	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	O2A-C1-C2-C3
29	Z	101	LMT	C7-C8-C9-C10
22	C	514	CLA	C8-C10-C11-C12
22	b	604	CLA	C10-C11-C12-C13
35	d	406	DGD	CDA-CEA-CFA-CGA
22	b	614	CLA	CAA-CBA-CGA-O2A
26	a	415	PL9	C3-C7-C8-C9
29	c	931	LMT	C5-C6-C7-C8
26	a	415	PL9	C25-C24-C26-C27
22	B	606	CLA	C10-C11-C12-C13
27	C	522	LHG	C27-C28-C29-C30
22	a	412	CLA	C2-C3-C5-C6
22	A	405	CLA	C4C-C3C-CAC-CBC
22	B	613	CLA	CBA-CGA-O2A-C1
22	C	502	CLA	CAA-CBA-CGA-O2A
22	b	602	CLA	CAA-CBA-CGA-O2A
22	C	513	CLA	CAA-CBA-CGA-O1A
22	c	913	CLA	CAA-CBA-CGA-O1A
27	D	411	LHG	C11-C12-C13-C14
22	B	602	CLA	C6-C7-C8-C9
22	B	603	CLA	C6-C7-C8-C9
22	B	604	CLA	C6-C7-C8-C9
22	a	412	CLA	C14-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C10-C8-C9
22	b	609	CLA	C11-C10-C8-C9
22	c	903	CLA	C14-C13-C15-C16
22	c	910	CLA	C6-C7-C8-C9
35	c	917	DGD	O1B-C1B-C2B-C3B
27	a	423	LHG	C30-C31-C32-C33
22	B	608	CLA	C13-C15-C16-C17
22	C	511	CLA	CBA-CGA-O2A-C1
28	C	501	SQD	C32-C33-C34-C35
22	c	911	CLA	CAA-CBA-CGA-O2A
25	B	621	LMG	O8-C28-C29-C30
24	K	101	BCR	C11-C12-C13-C14
25	d	409	LMG	O10-C28-C29-C30
22	B	611	CLA	C4C-C3C-CAC-CBC
35	D	407	DGD	C2G-C3G-O3G-C1D
22	d	402	CLA	CAA-CBA-CGA-O2A
27	l	102	LHG	C11-C12-C13-C14
25	D	412	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	CAA-CBA-CGA-O1A
22	b	614	CLA	CAA-CBA-CGA-O1A
28	a	414	SQD	C19-C20-C21-C22
35	c	919	DGD	CCA-CDA-CEA-CFA
22	B	611	CLA	C5-C6-C7-C8
36	E	102	HEM	C2B-C3B-CAB-CBB
22	b	607	CLA	C16-C17-C18-C19
22	b	605	CLA	CAD-CBD-CGD-O2D
22	d	403	CLA	CAD-CBD-CGD-O2D
23	D	402	PHO	CAD-CBD-CGD-O2D
35	C	519	DGD	O1G-C1A-C2A-C3A
28	l	101	SQD	O49-C7-C8-C9
22	b	613	CLA	O1A-CGA-O2A-C1
22	C	511	CLA	CAA-CBA-CGA-O1A
35	c	918	DGD	O2G-C1B-C2B-C3B
35	H	102	DGD	C3B-C4B-C5B-C6B
26	A	411	PL9	C15-C14-C16-C17
22	A	405	CLA	C12-C13-C15-C16
22	B	607	CLA	C11-C12-C13-C15
26	a	415	PL9	C2-C3-C7-C8
27	D	409	LHG	O7-C7-C8-C9
27	L	101	LHG	O7-C7-C8-C9
28	C	501	SQD	O49-C7-C8-C9
25	i	101	LMG	C21-C22-C23-C24

There are no ring outliers.

211 monomers are involved in 519 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	612	CLA	2	0
22	a	412	CLA	2	0
37	h	101	RRX	8	0
22	c	914	CLA	2	0
27	d	407	LHG	1	0
31	V	201	DMS	1	0
29	a	419	LMT	7	0
31	b	636	DMS	1	0
31	O	306	DMS	2	0
35	c	918	DGD	3	0
22	C	510	CLA	2	0
24	d	404	BCR	2	0
25	D	412	LMG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	L	101	LHG	7	0
28	l	101	SQD	1	0
23	D	402	PHO	5	0
22	b	609	CLA	5	0
35	c	917	DGD	3	0
22	b	615	CLA	5	0
28	a	414	SQD	6	0
22	b	606	CLA	5	0
24	c	916	BCR	6	0
29	B	622	LMT	3	0
25	J	101	LMG	1	0
31	o	303	DMS	2	0
31	c	924	DMS	7	0
31	o	308	DMS	4	0
25	C	531	LMG	2	0
31	u	205	DMS	5	0
29	Z	101	LMT	1	0
25	d	409	LMG	4	0
31	B	631	DMS	4	0
34	D	415	HTG	9	0
31	V	212	DMS	11	0
27	d	408	LHG	5	0
22	B	612	CLA	1	0
22	b	607	CLA	1	0
31	b	630	DMS	2	0
22	C	507	CLA	5	0
22	d	402	CLA	2	0
27	l	102	LHG	3	0
31	v	210	DMS	2	0
36	E	102	HEM	1	0
22	A	405	CLA	4	0
31	C	536	DMS	1	0
25	j	101	LMG	2	0
31	o	304	DMS	4	0
27	D	411	LHG	8	0
31	c	935	DMS	2	0
24	a	413	BCR	1	0
34	C	521	HTG	1	0
34	D	414	HTG	2	0
22	C	505	CLA	4	0
22	D	401	CLA	4	0
37	H	101	RRX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	406	PL9	5	0
31	O	304	DMS	6	0
31	u	202	DMS	2	0
35	C	519	DGD	2	0
26	A	411	PL9	10	0
31	b	633	DMS	1	0
31	V	205	DMS	2	0
31	B	630	DMS	1	0
31	B	633	DMS	1	0
25	i	101	LMG	3	0
29	A	414	LMT	6	0
22	c	906	CLA	2	0
31	C	540	DMS	1	0
22	B	607	CLA	5	0
27	C	522	LHG	1	0
31	B	638	DMS	5	0
29	c	931	LMT	1	0
22	c	904	CLA	8	0
22	b	605	CLA	2	0
31	O	310	DMS	3	0
31	d	411	DMS	3	0
25	A	410	LMG	2	0
22	b	611	CLA	4	0
35	h	102	DGD	2	0
31	V	207	DMS	3	0
28	f	101	SQD	1	0
22	c	911	CLA	2	0
22	C	513	CLA	5	0
22	A	408	CLA	3	0
24	C	516	BCR	1	0
31	o	307	DMS	1	0
31	c	934	DMS	2	0
35	c	919	DGD	4	0
22	b	610	CLA	4	0
27	a	423	LHG	6	0
31	O	311	DMS	3	0
26	a	415	PL9	10	0
29	E	101	LMT	1	0
32	A	421[B]	BCT	1	0
31	c	927	DMS	1	0
31	f	103	DMS	4	0
31	v	205	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	909	CLA	2	0
27	D	409	LHG	7	0
25	c	930	LMG	3	0
31	u	203	DMS	2	0
34	B	623	HTG	3	0
24	k	101	BCR	2	0
31	c	937	DMS	1	0
34	b	626	HTG	2	0
24	C	515	BCR	4	0
22	C	503	CLA	5	0
23	a	411	PHO	8	0
31	B	636	DMS	1	0
31	c	942	DMS	1	0
22	B	605	CLA	1	0
28	C	501	SQD	6	0
35	C	518	DGD	1	0
22	C	504	CLA	2	0
25	b	622	LMG	1	0
23	a	410	PHO	2	0
34	b	632	HTG	2	0
34	b	623	HTG	3	0
31	i	106	DMS	1	0
22	c	908	CLA	2	0
31	U	203	DMS	1	0
24	c	915	BCR	2	0
22	B	606	CLA	7	0
22	C	509	CLA	3	0
24	B	618	BCR	3	0
22	C	508	CLA	2	0
31	a	401	DMS	1	0
31	V	206	DMS	3	0
31	b	638	DMS	9	0
31	o	302	DMS	1	0
29	T	102	LMT	1	0
24	b	619	BCR	1	0
24	D	405	BCR	1	0
34	C	532	HTG	1	0
27	D	410	LHG	3	0
22	B	604	CLA	1	0
28	A	413	SQD	2	0
31	d	415	DMS	5	0
28	b	621	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	H	102	DGD	2	0
31	B	642	DMS	1	0
22	C	511	CLA	3	0
24	B	620	BCR	1	0
22	B	608	CLA	6	0
22	b	603	CLA	2	0
31	D	416	DMS	3	0
31	B	628	DMS	3	0
22	b	616	CLA	2	0
31	A	419	DMS	2	0
22	c	905	CLA	2	0
31	a	425	DMS	7	0
31	v	201	DMS	1	0
31	c	929	DMS	2	0
24	b	618	BCR	7	0
31	l	104	DMS	1	0
22	C	514	CLA	5	0
24	A	409	BCR	1	0
31	O	303	DMS	4	0
25	C	520	LMG	1	0
22	c	903	CLA	3	0
31	A	420	DMS	2	0
22	c	910	CLA	3	0
31	b	629	DMS	1	0
31	B	640	DMS	1	0
31	c	925	DMS	2	0
24	y	101	BCR	3	0
22	b	608	CLA	7	0
31	B	635	DMS	1	0
22	b	604	CLA	1	0
22	D	403	CLA	1	0
27	A	412	LHG	1	0
22	B	613	CLA	1	0
31	C	527	DMS	2	0
22	b	617	CLA	2	0
22	B	611	CLA	6	0
25	B	621	LMG	3	0
22	B	610	CLA	1	0
29	t	101	LMT	2	0
34	b	627	HTG	1	0
25	c	920	LMG	1	0
22	c	912	CLA	4	0

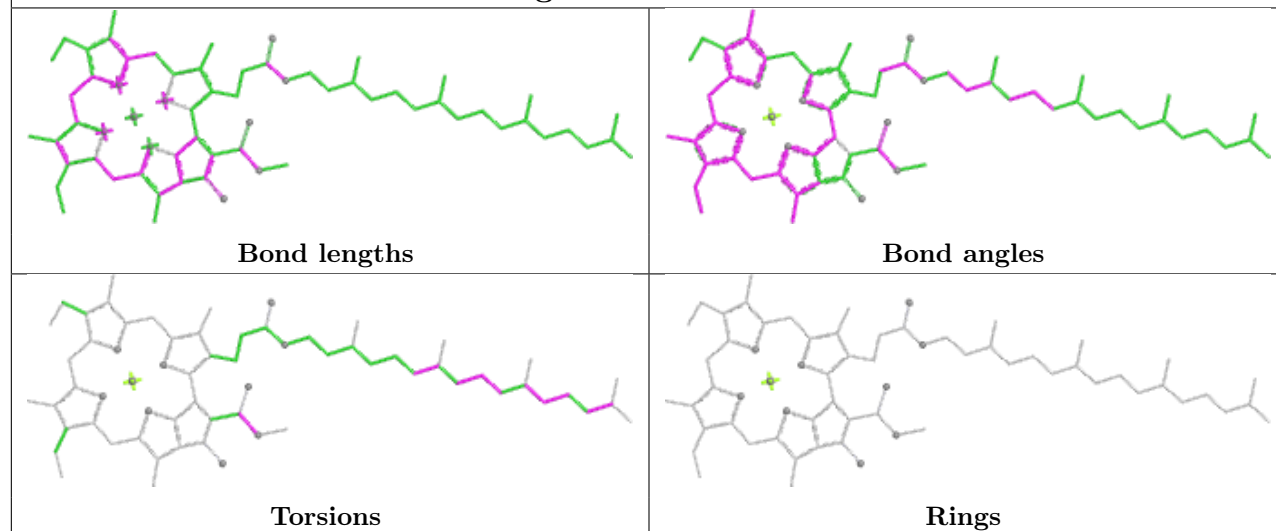
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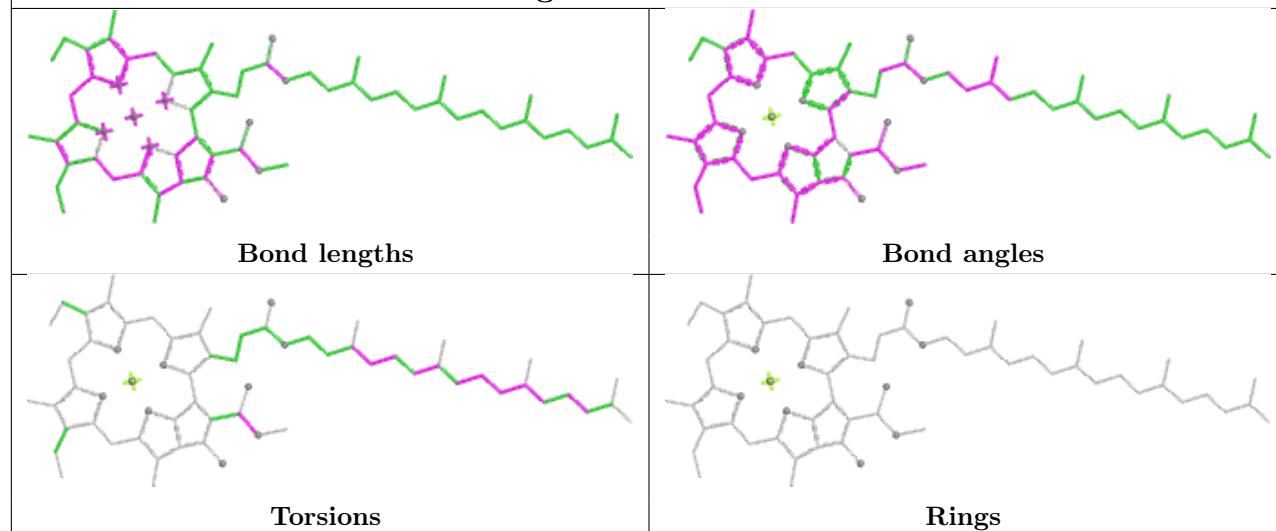
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	603	CLA	1	0
31	c	940	DMS	2	0
22	a	407	CLA	2	0
22	a	408	CLA	4	0
31	B	632	DMS	1	0
22	b	602	CLA	5	0
22	b	614	CLA	4	0
22	d	403	CLA	1	0
22	C	506	CLA	1	0
22	c	902	CLA	4	0
31	c	939	DMS	2	0
27	a	416	LHG	1	0
31	o	305	DMS	3	0
31	C	530	DMS	2	0
24	Y	101	BCR	2	0
22	B	614	CLA	2	0
34	l	106	HTG	3	0
31	O	312	DMS	4	0
26	d	405	PL9	5	0
22	A	406	CLA	3	0
31	B	629	DMS	1	0
31	c	933	DMS	2	0
22	c	913	CLA	3	0
36	e	101	HEM	6	0
31	B	641	DMS	1	0
39	v	202	HEC	1	0
22	a	409	CLA	3	0
31	v	206	DMS	3	0
24	b	620	BCR	3	0
31	H	103	DMS	1	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 than 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.

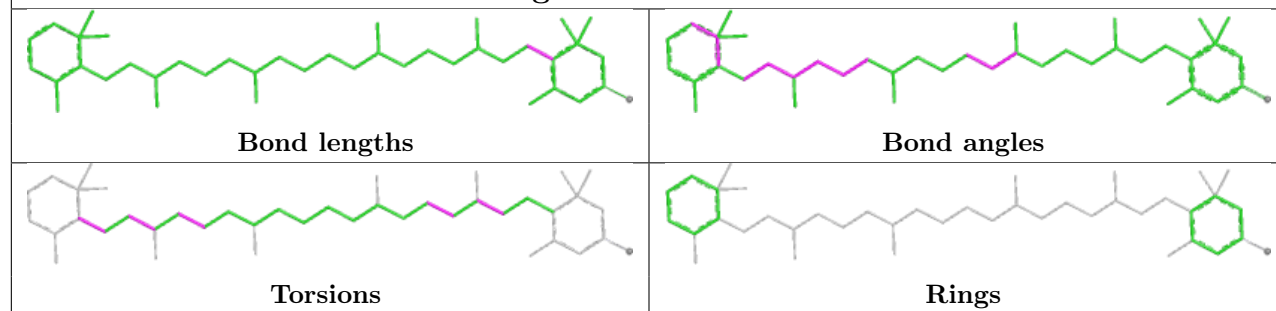
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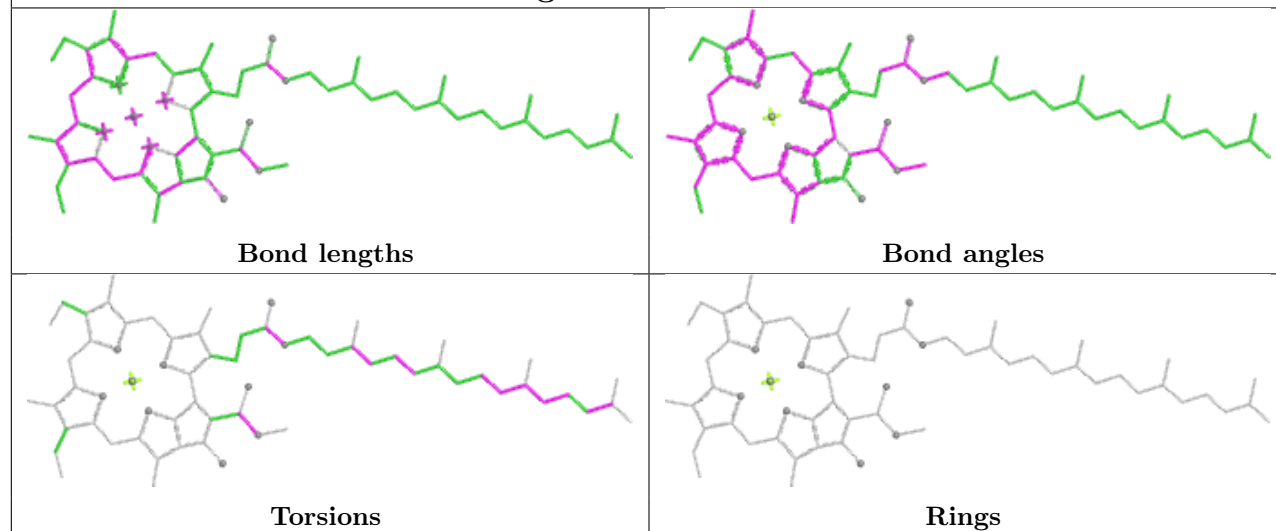
Ligand CLA a 412



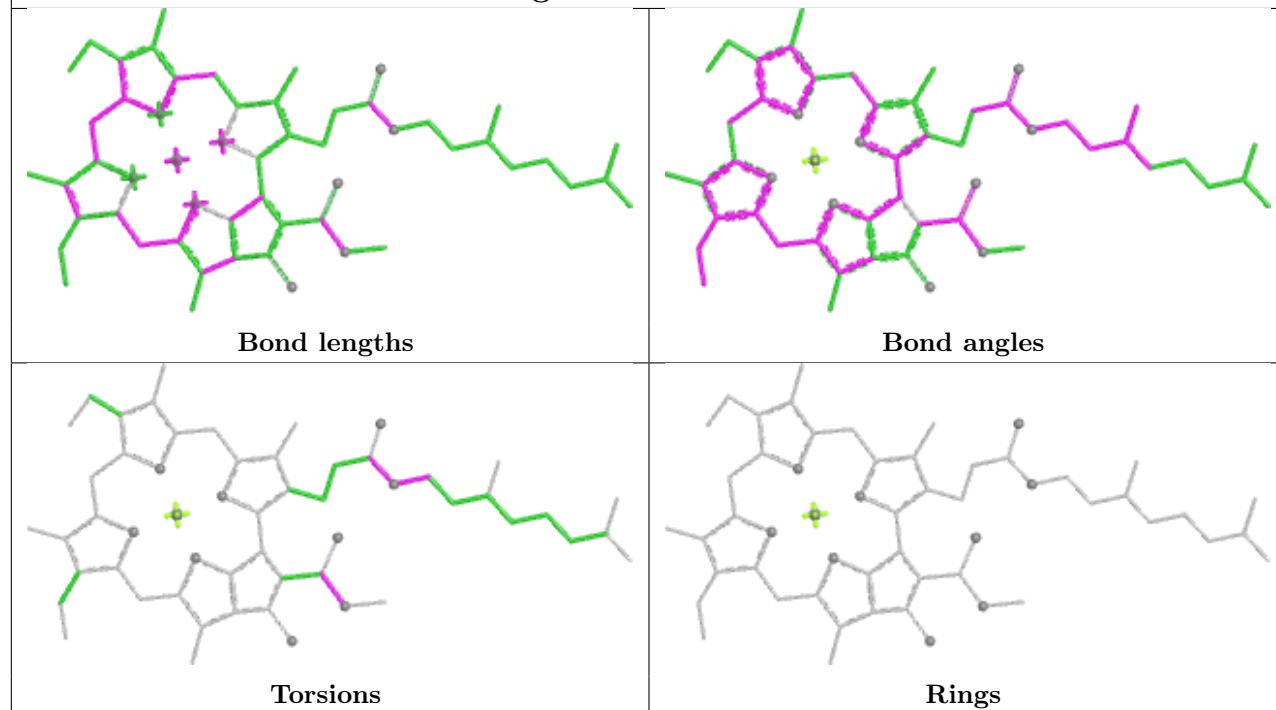
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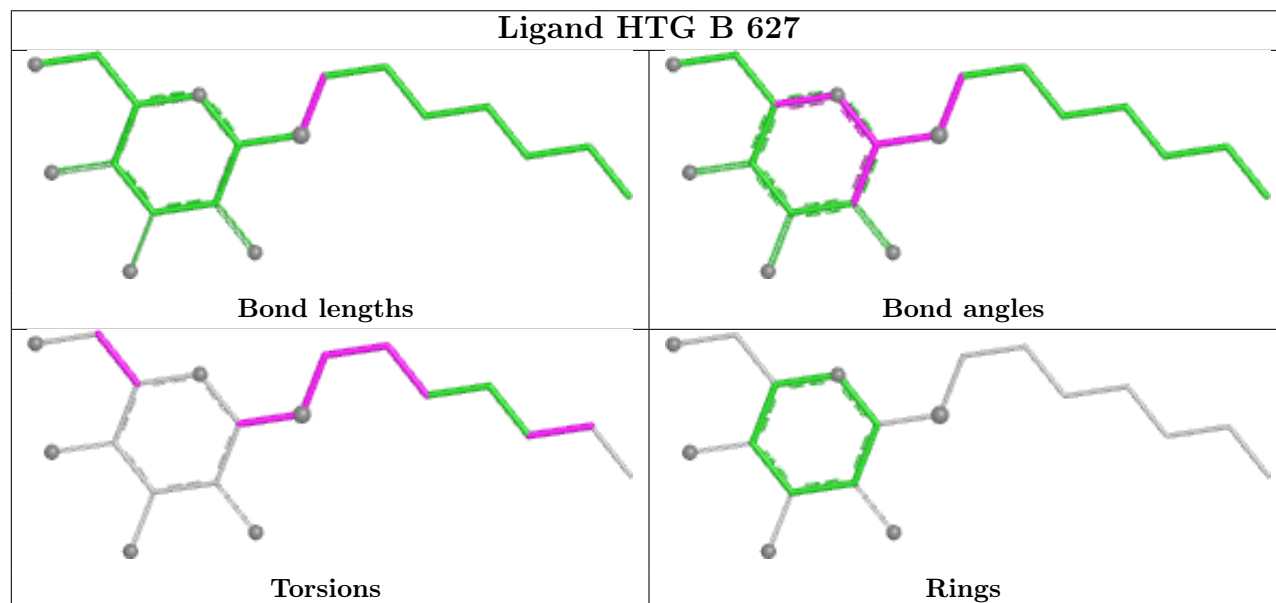
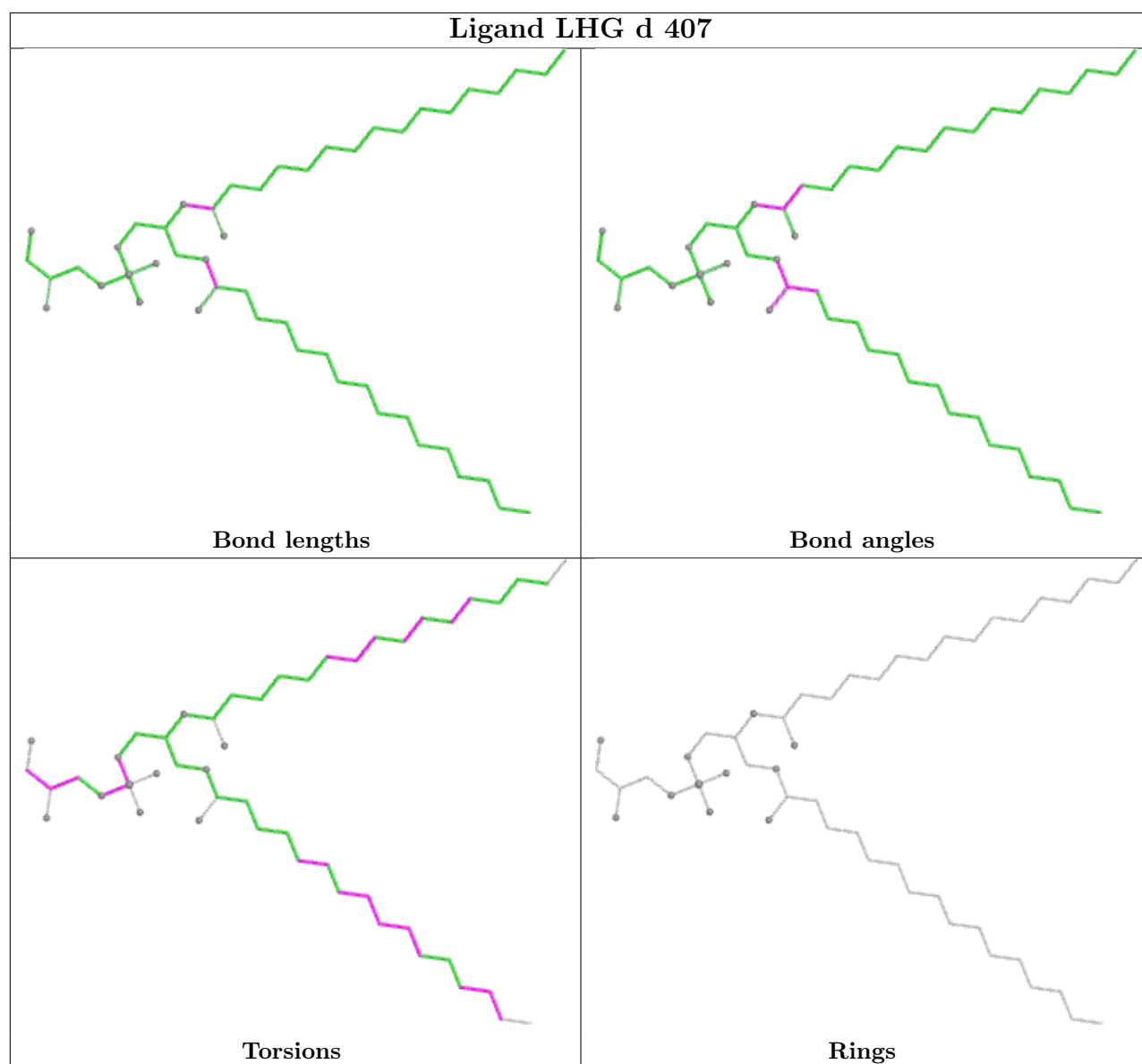


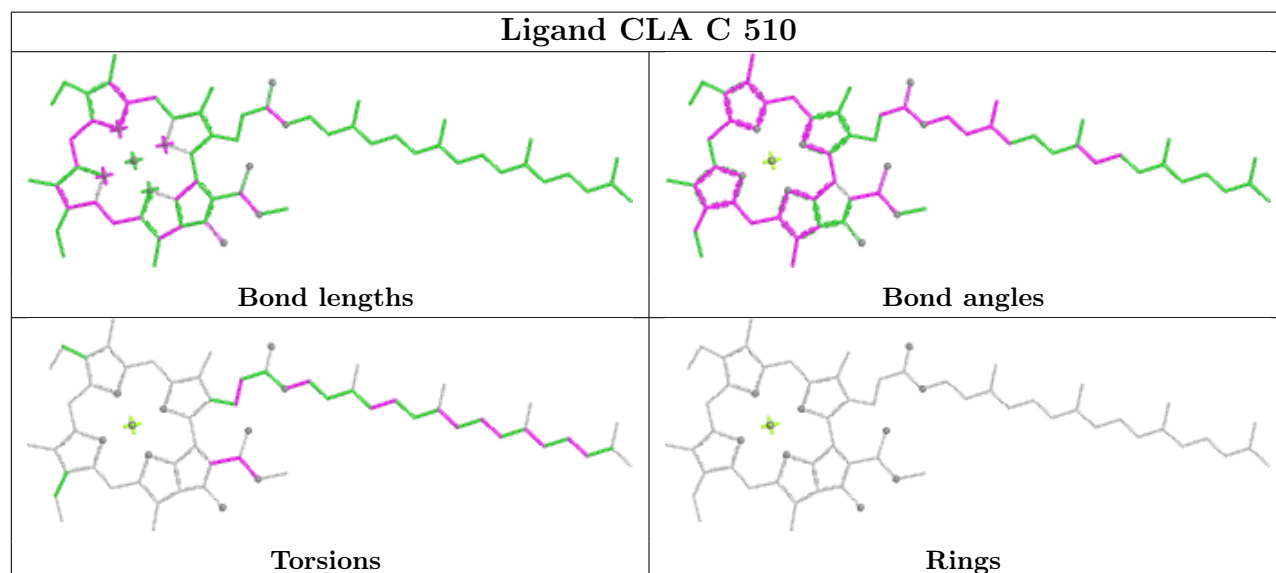
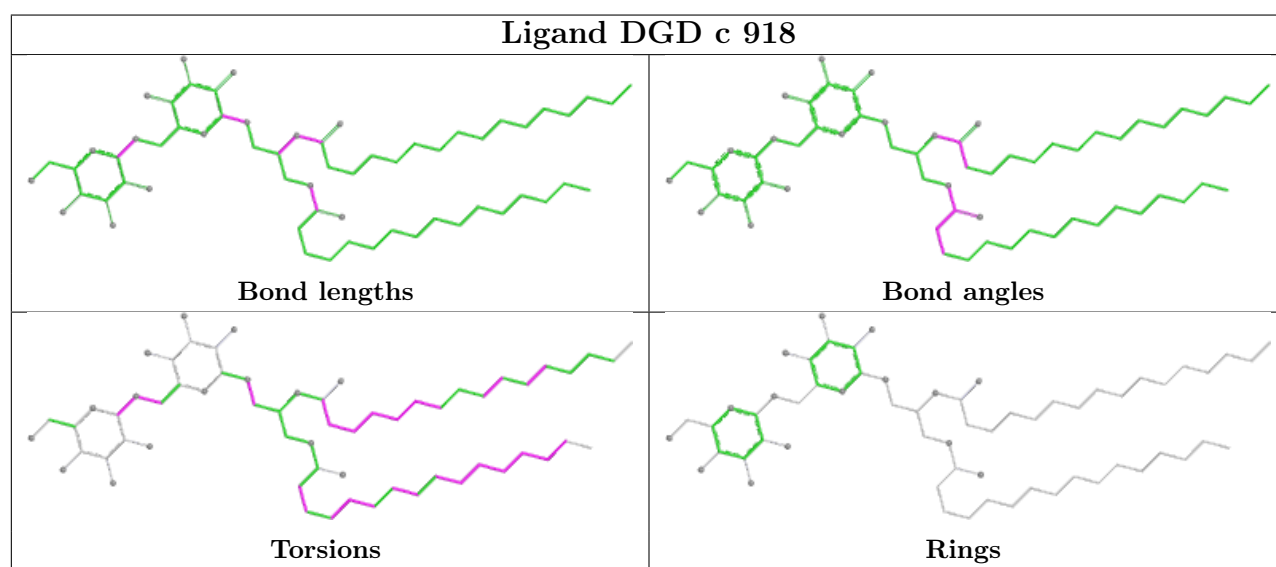
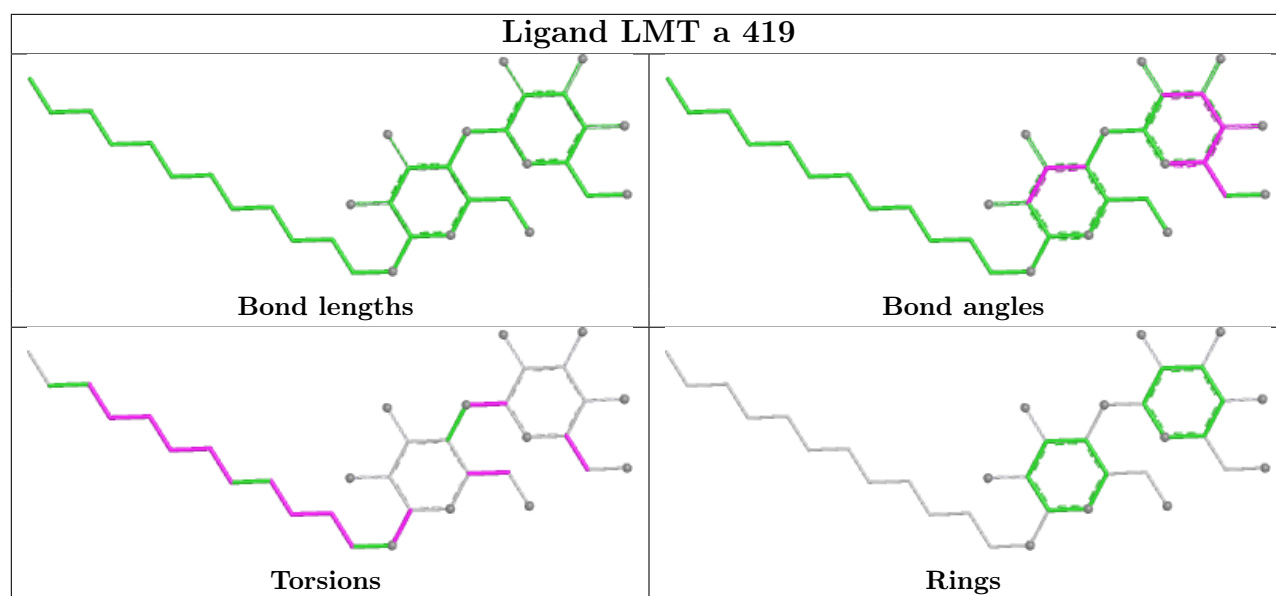
Ligand CLA c 914

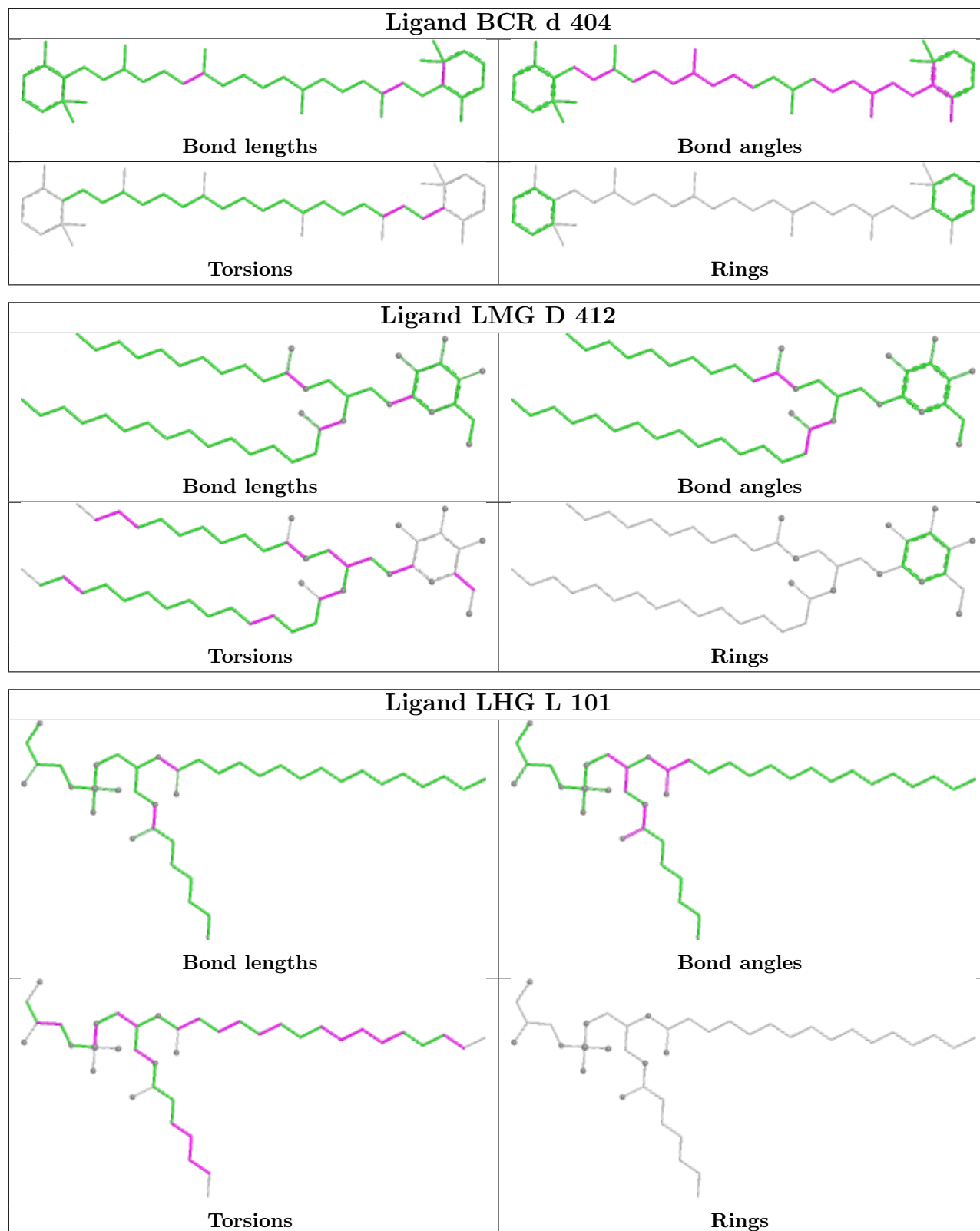


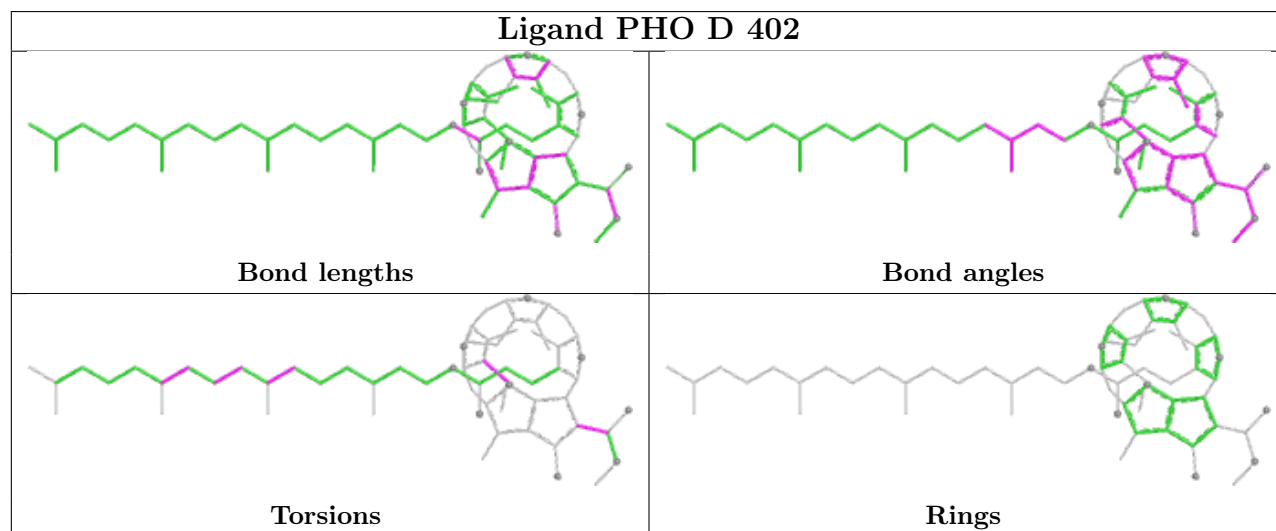
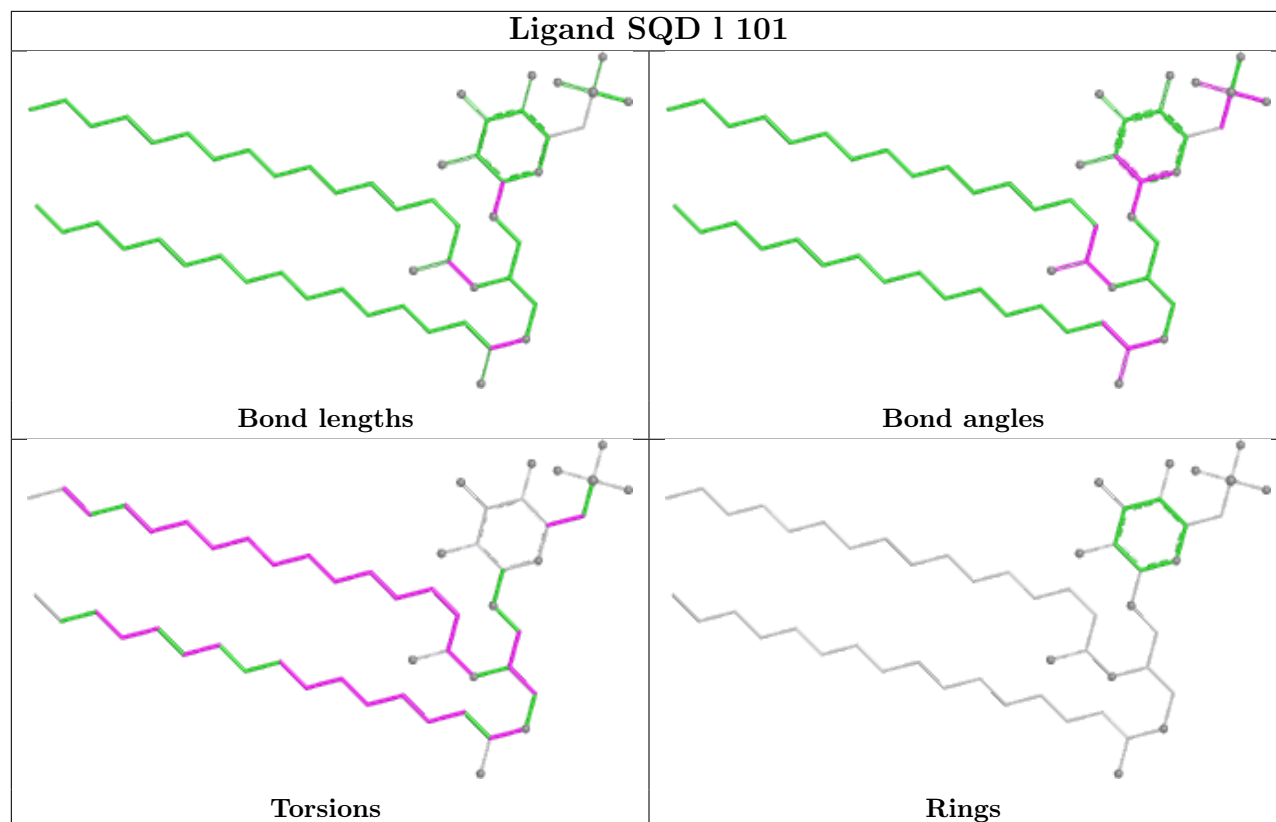
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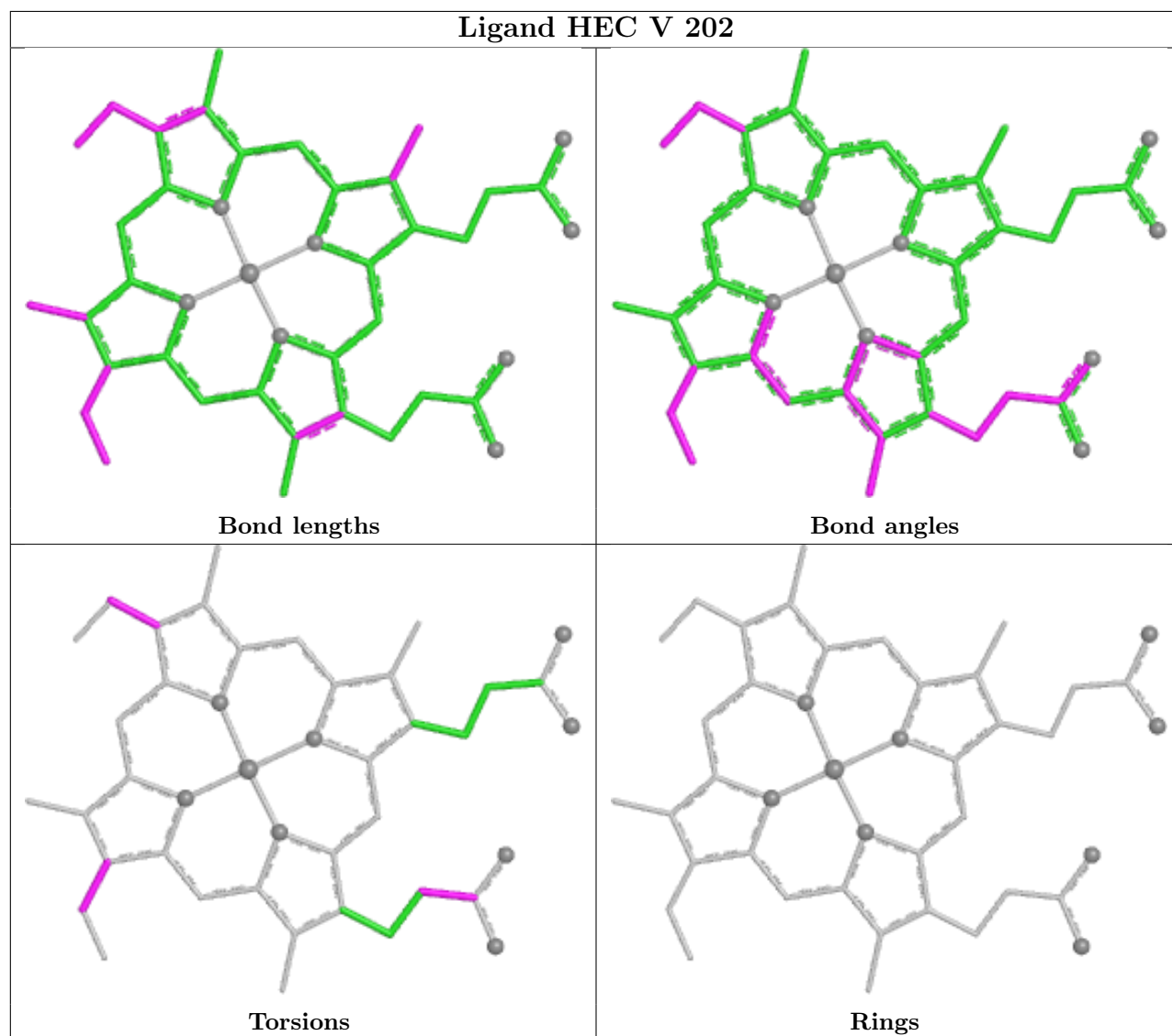
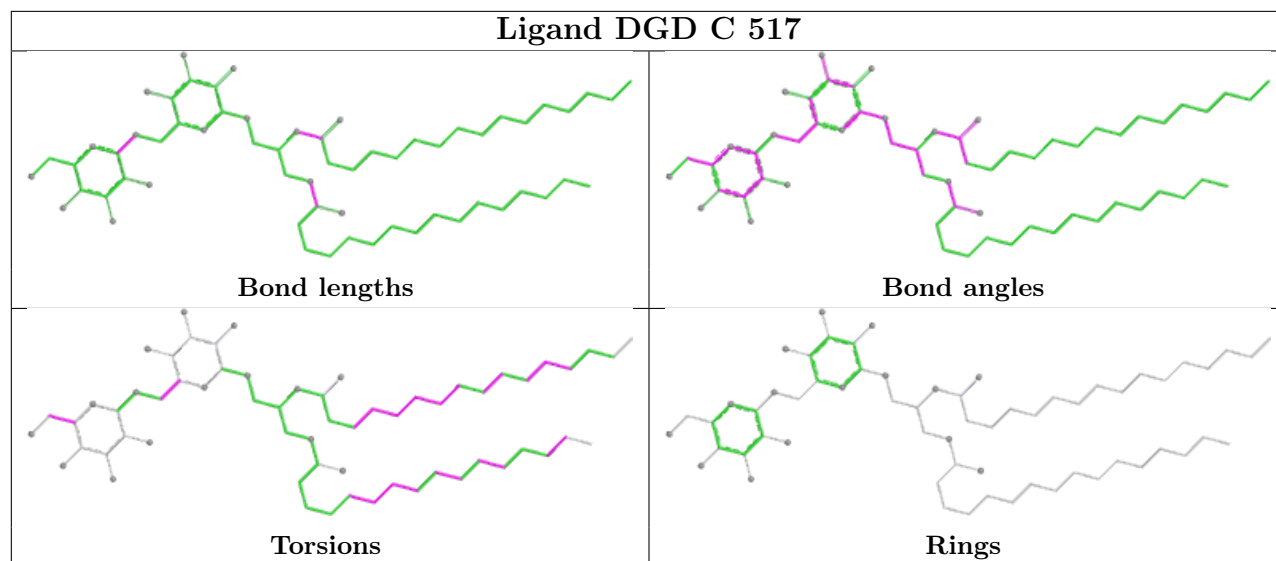


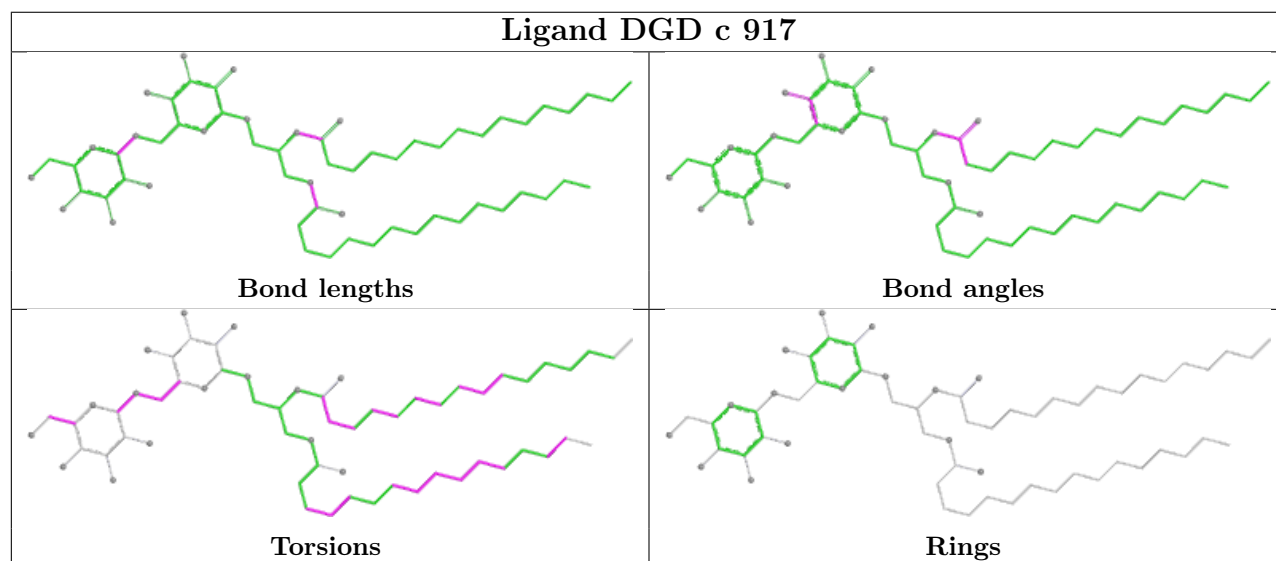
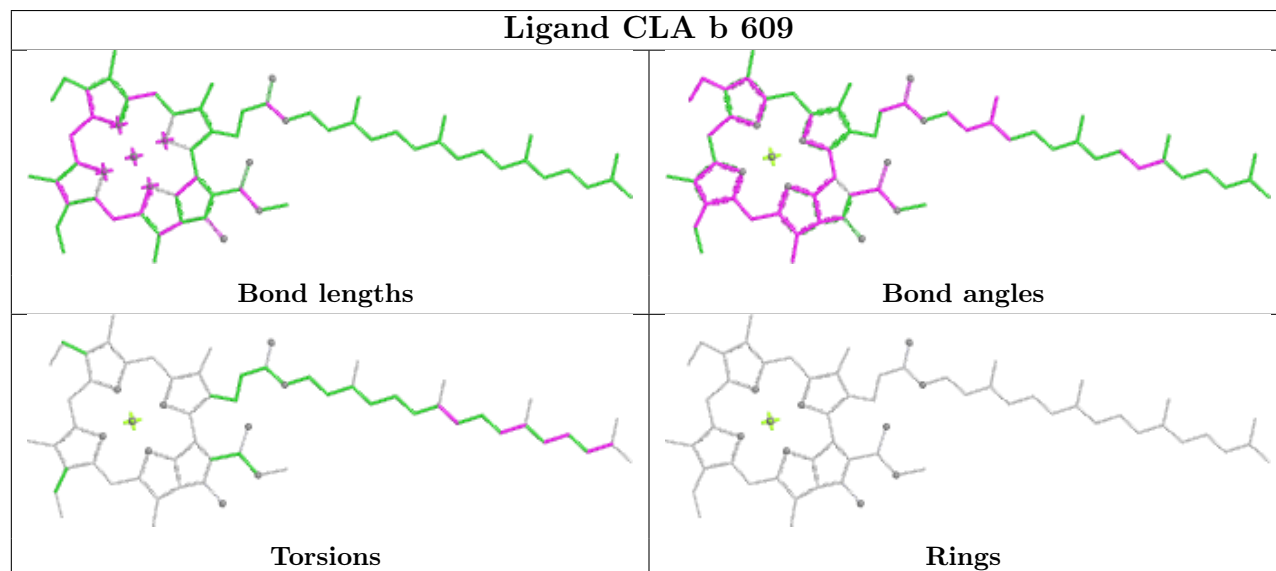
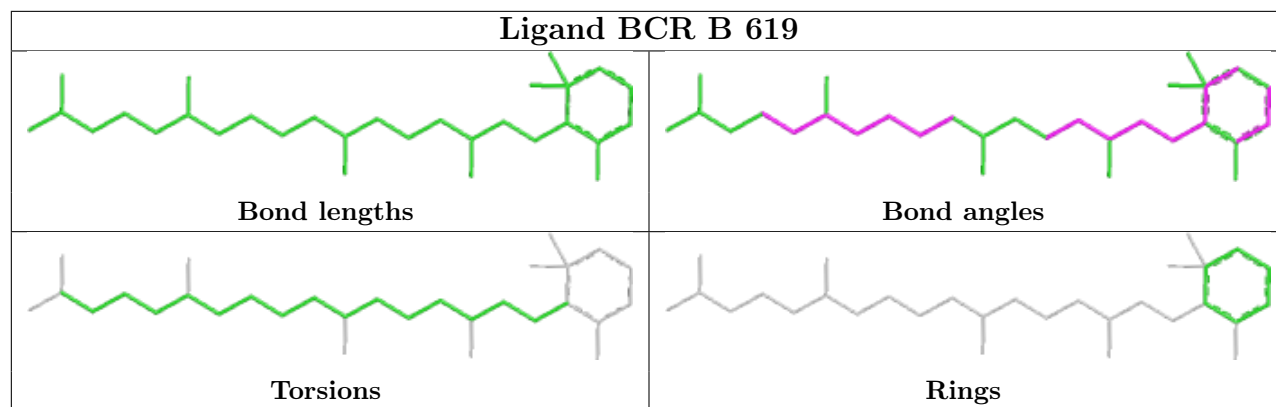




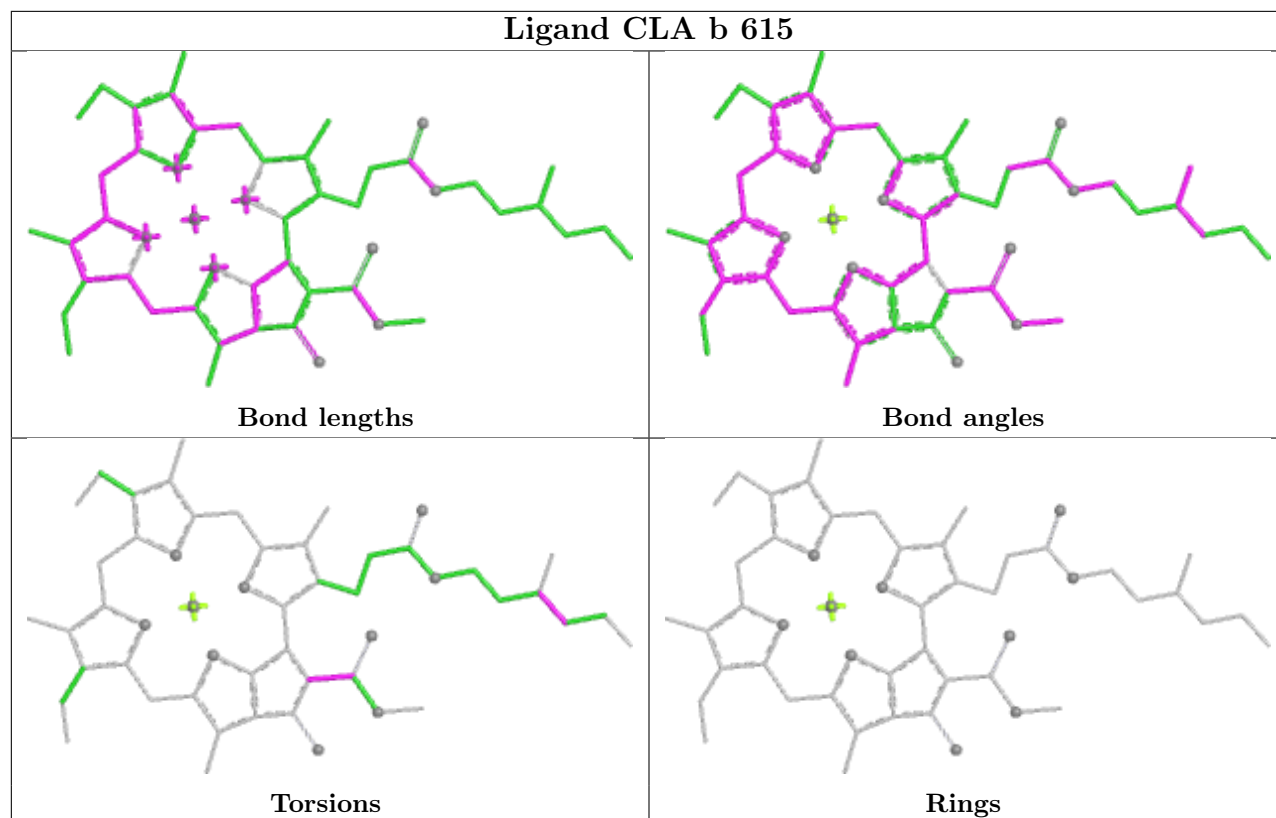




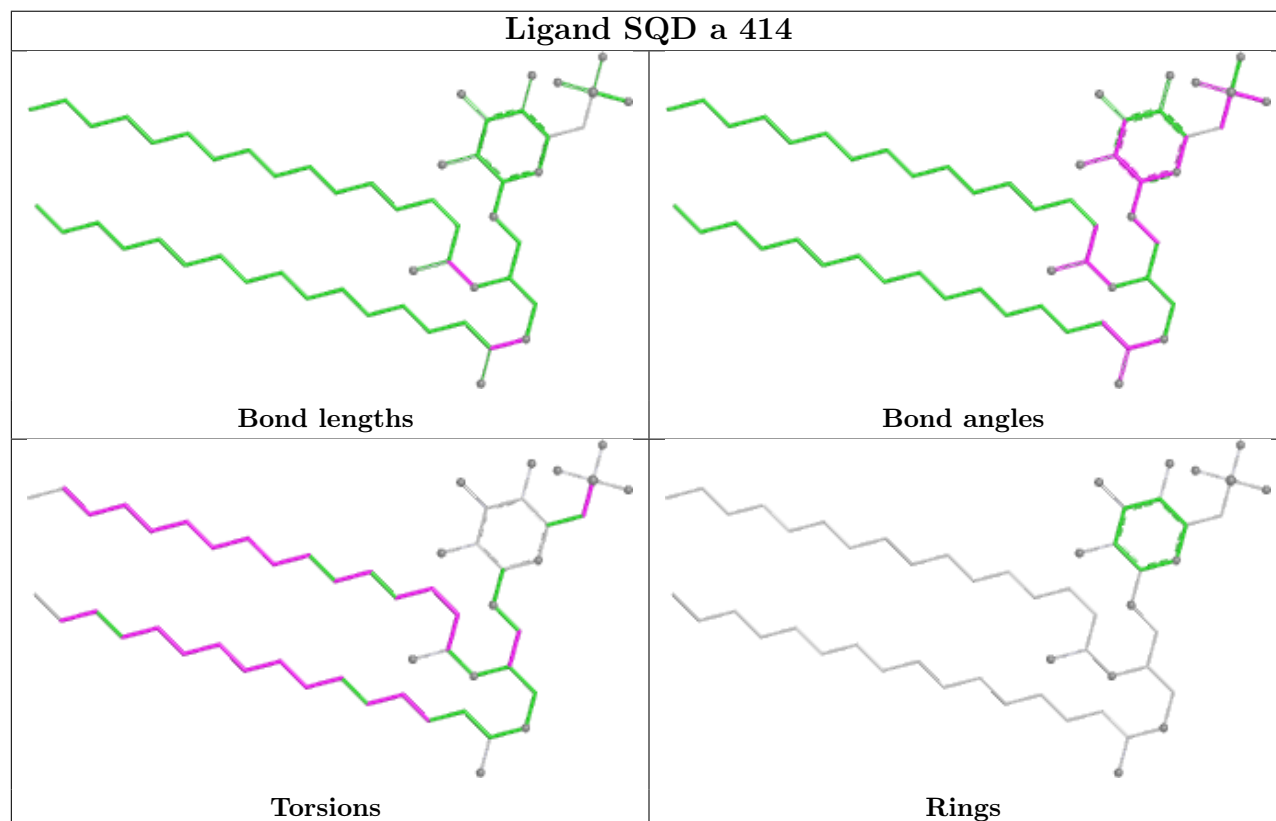


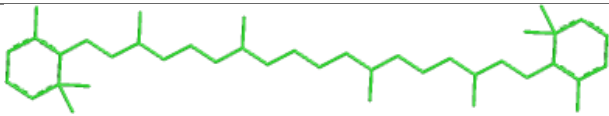
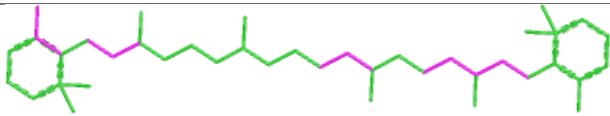
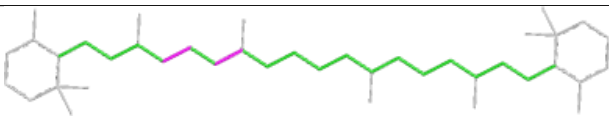
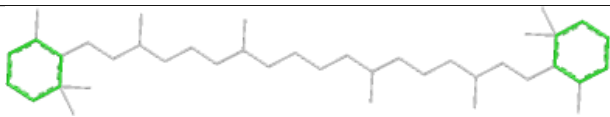


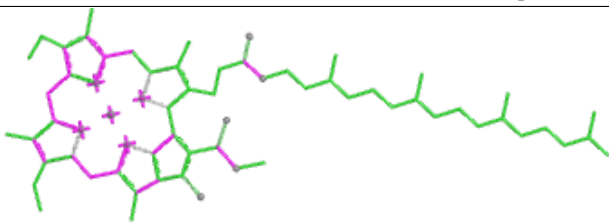
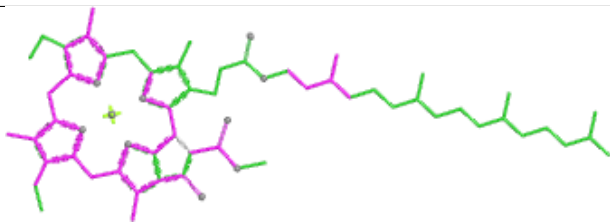
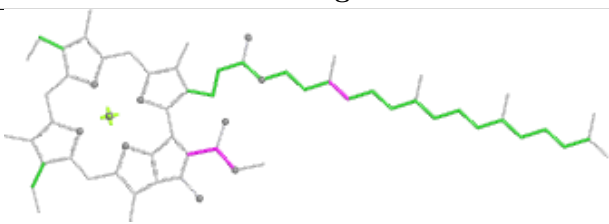
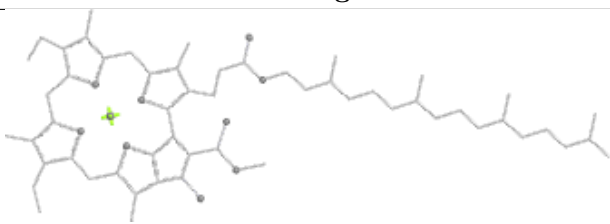
Ligand CLA b 615

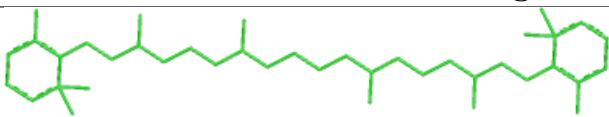
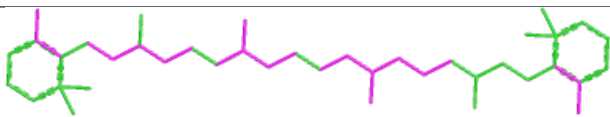
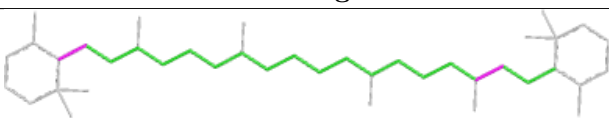
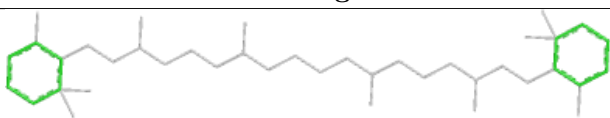


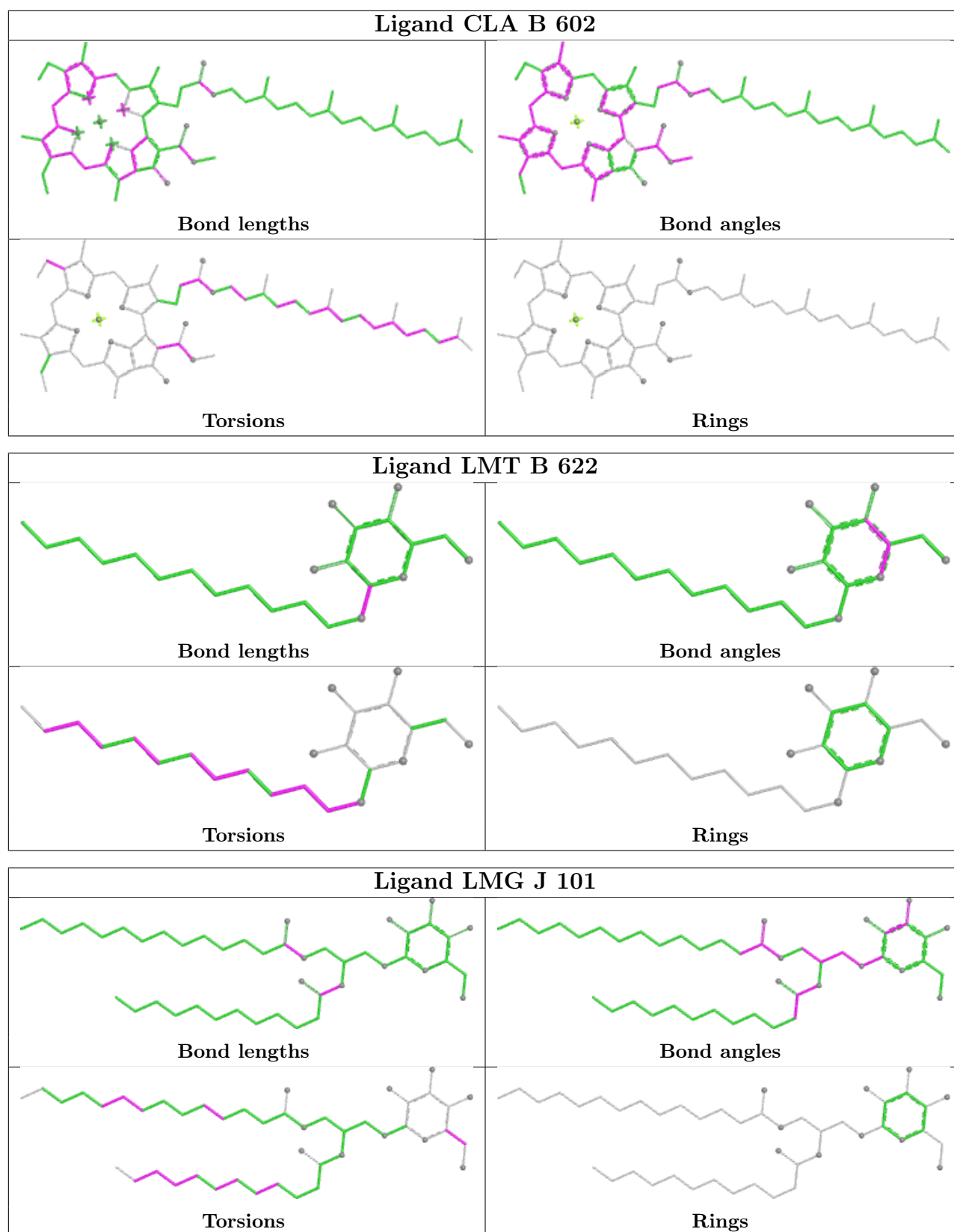
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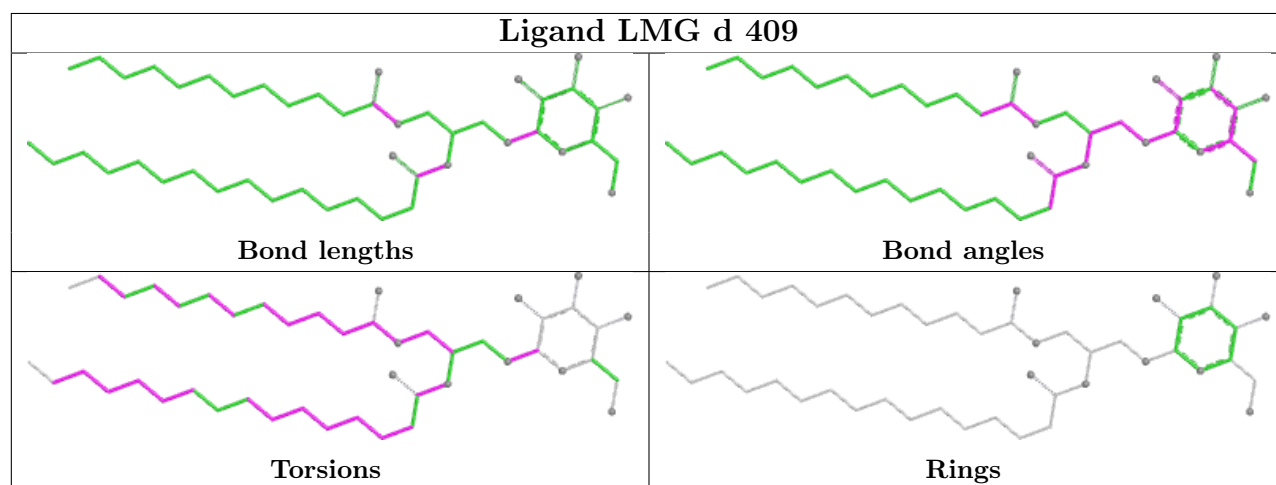
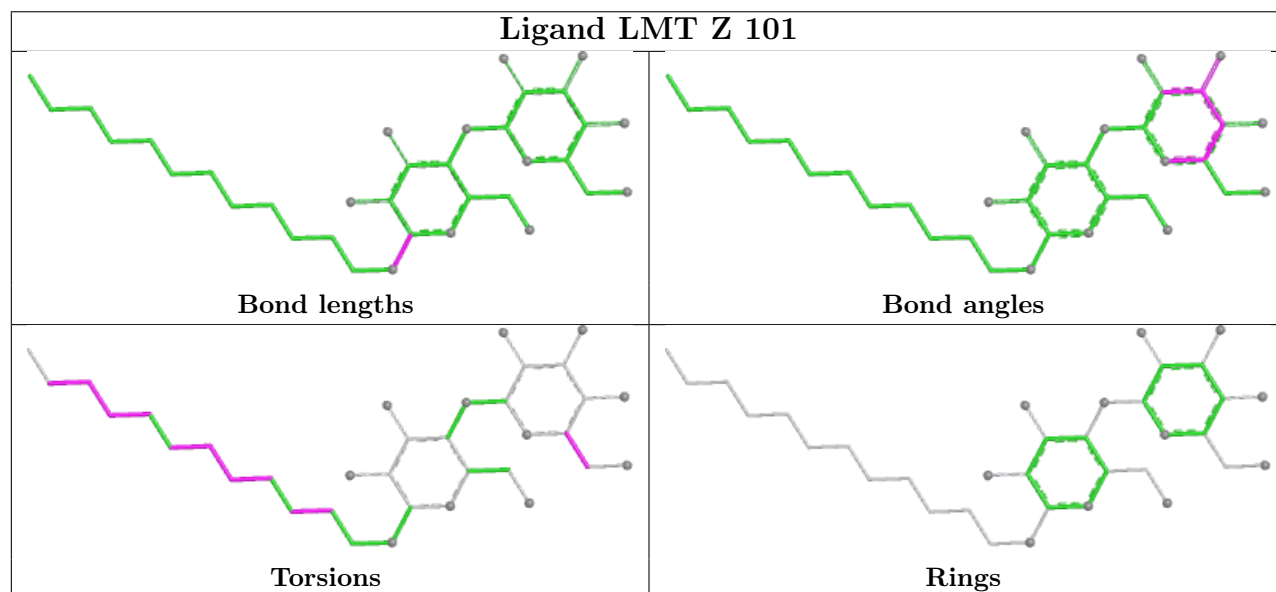
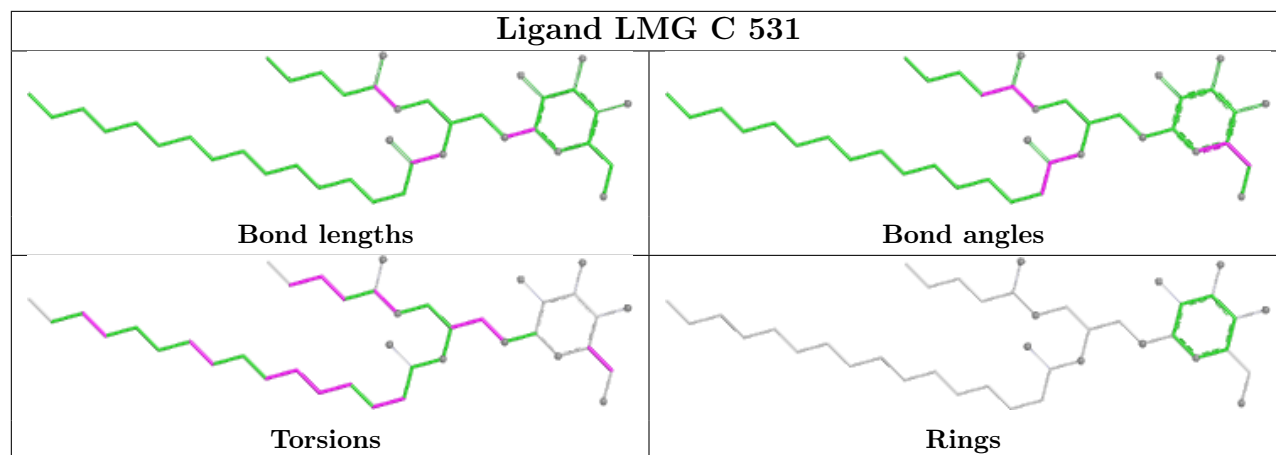


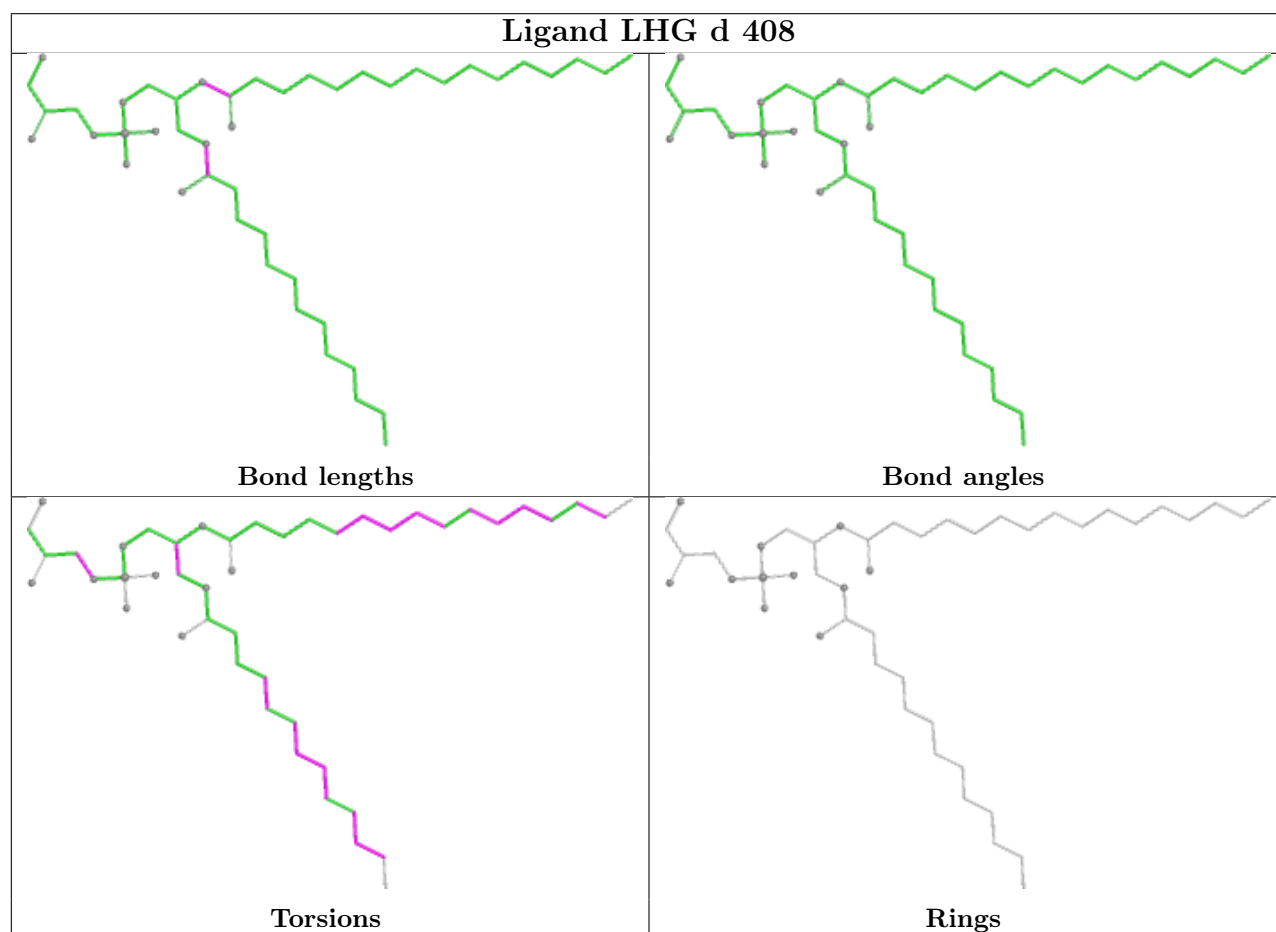
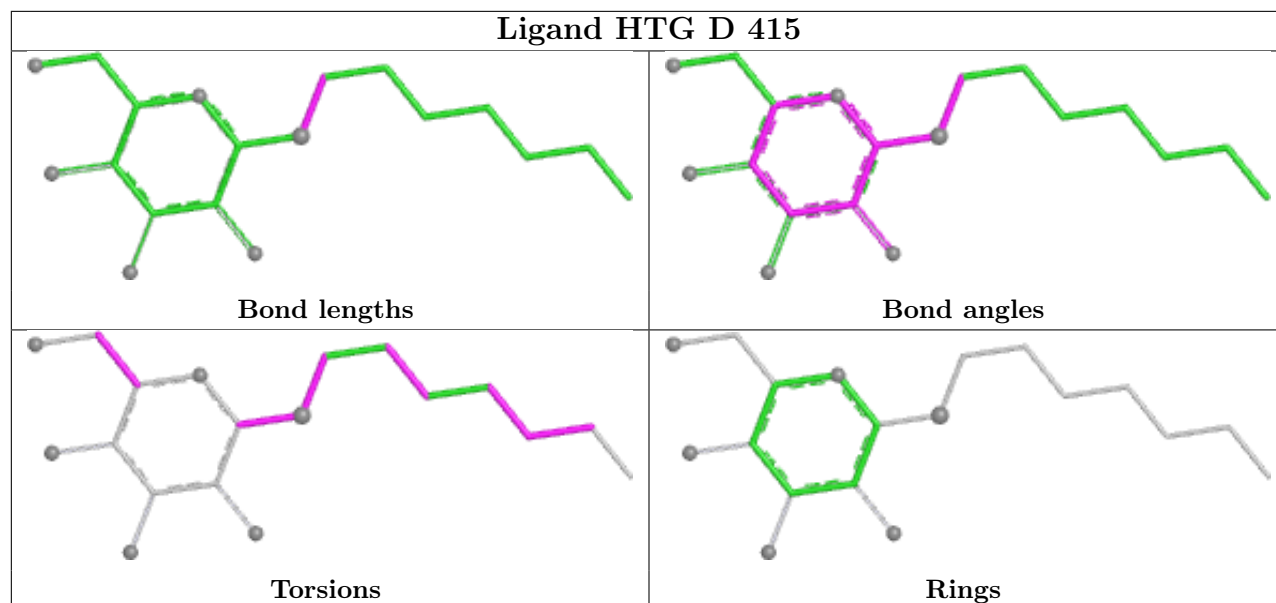
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

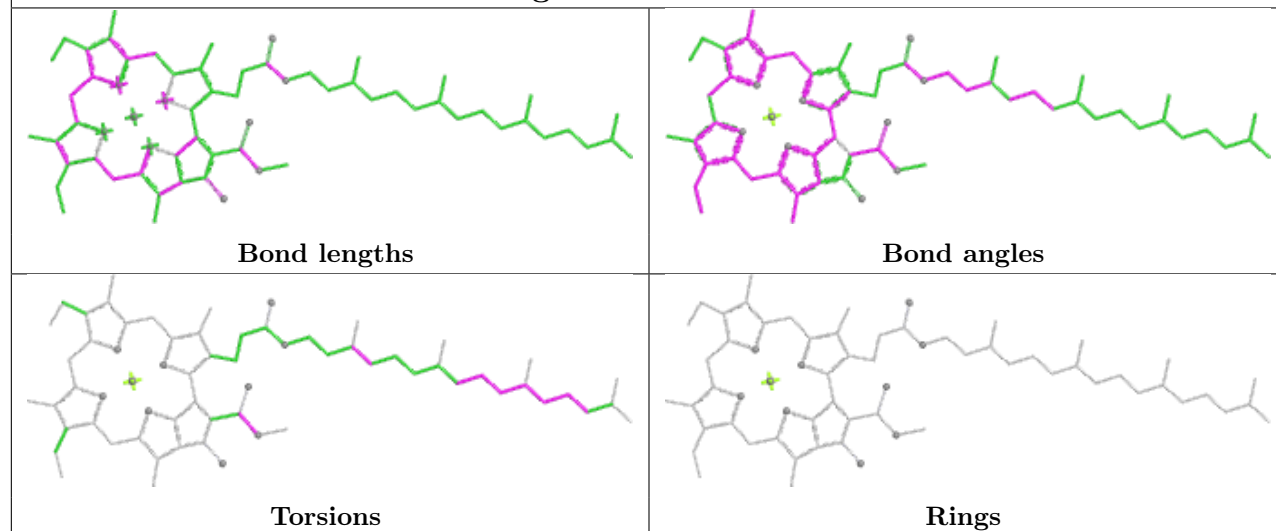
Ligand BCR c 916	
	
Bond lengths	Bond angles
	
Torsions	Rings



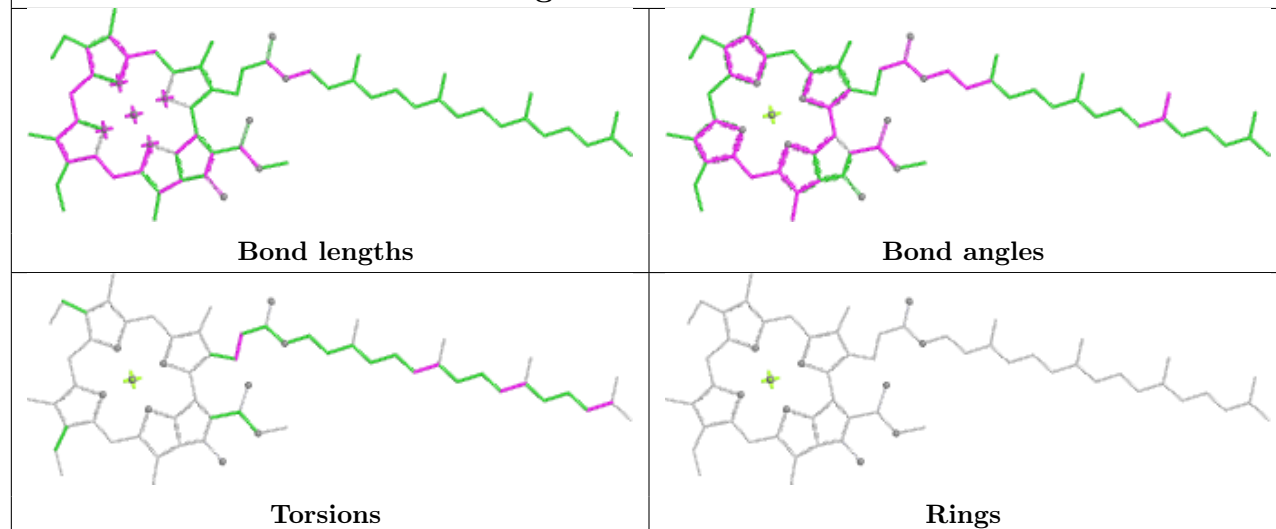




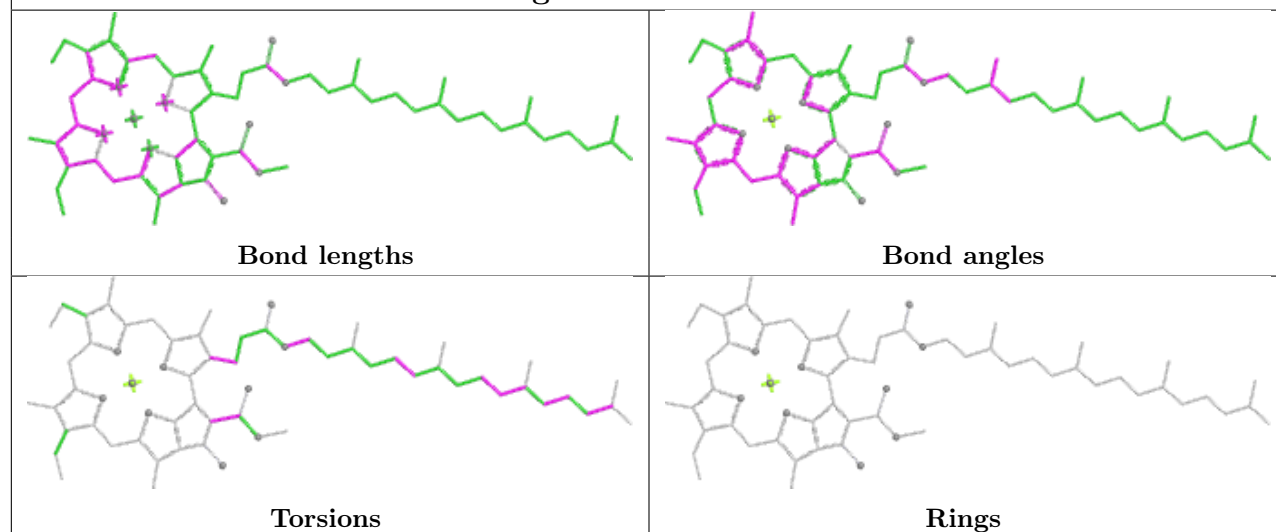
Ligand CLA B 612

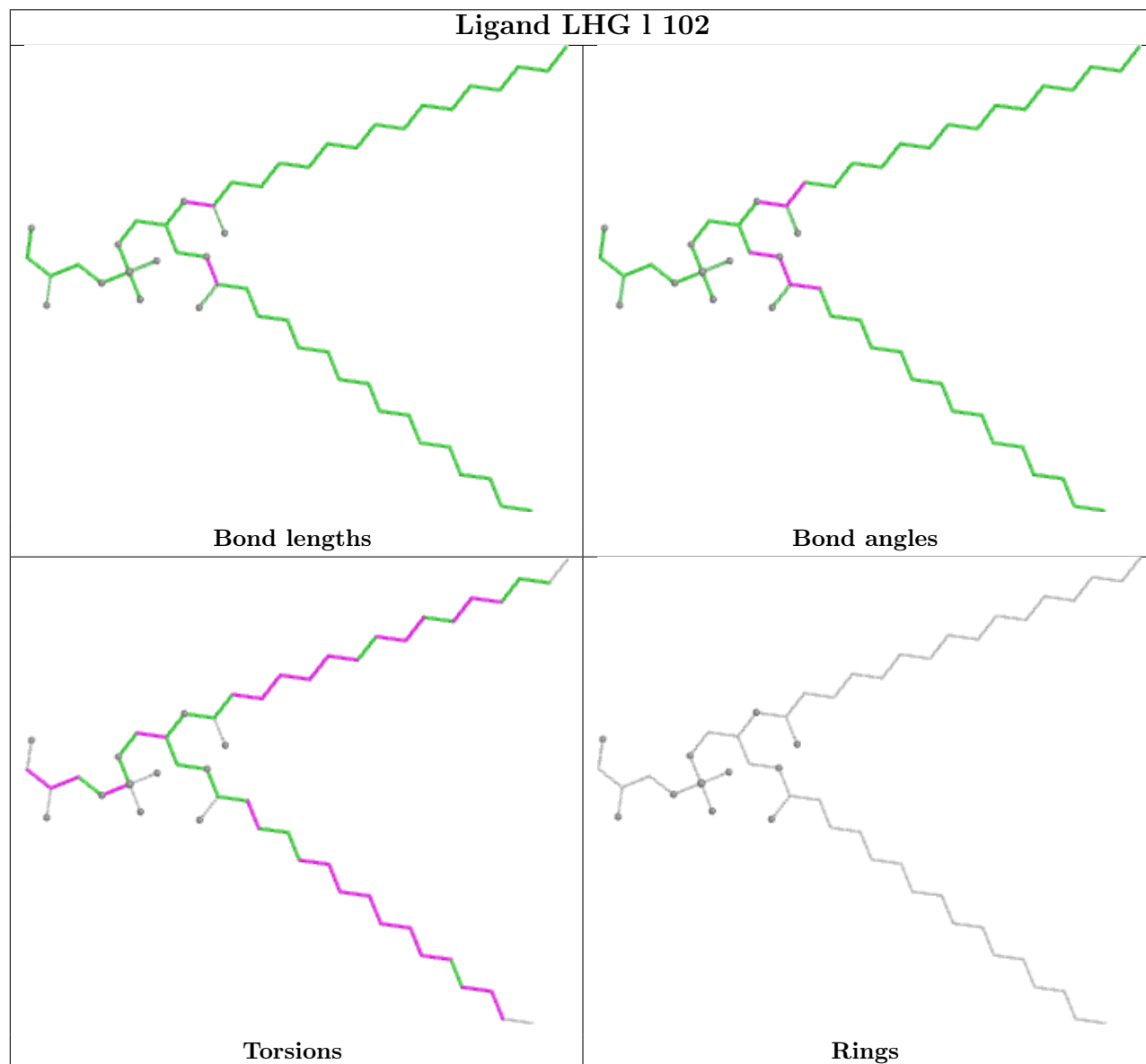
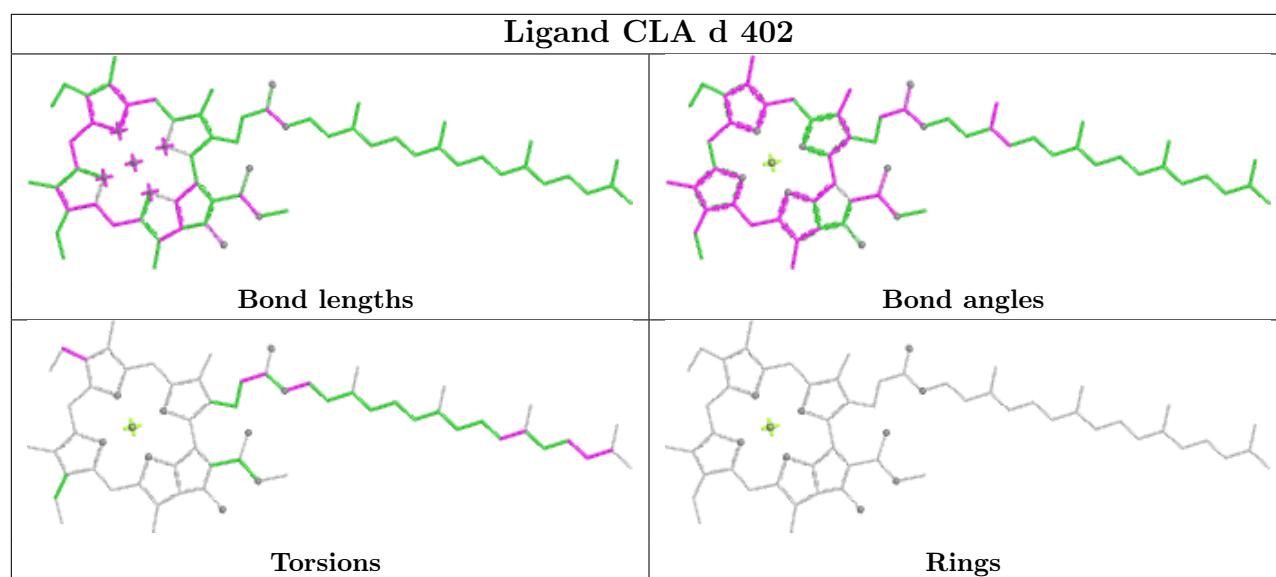


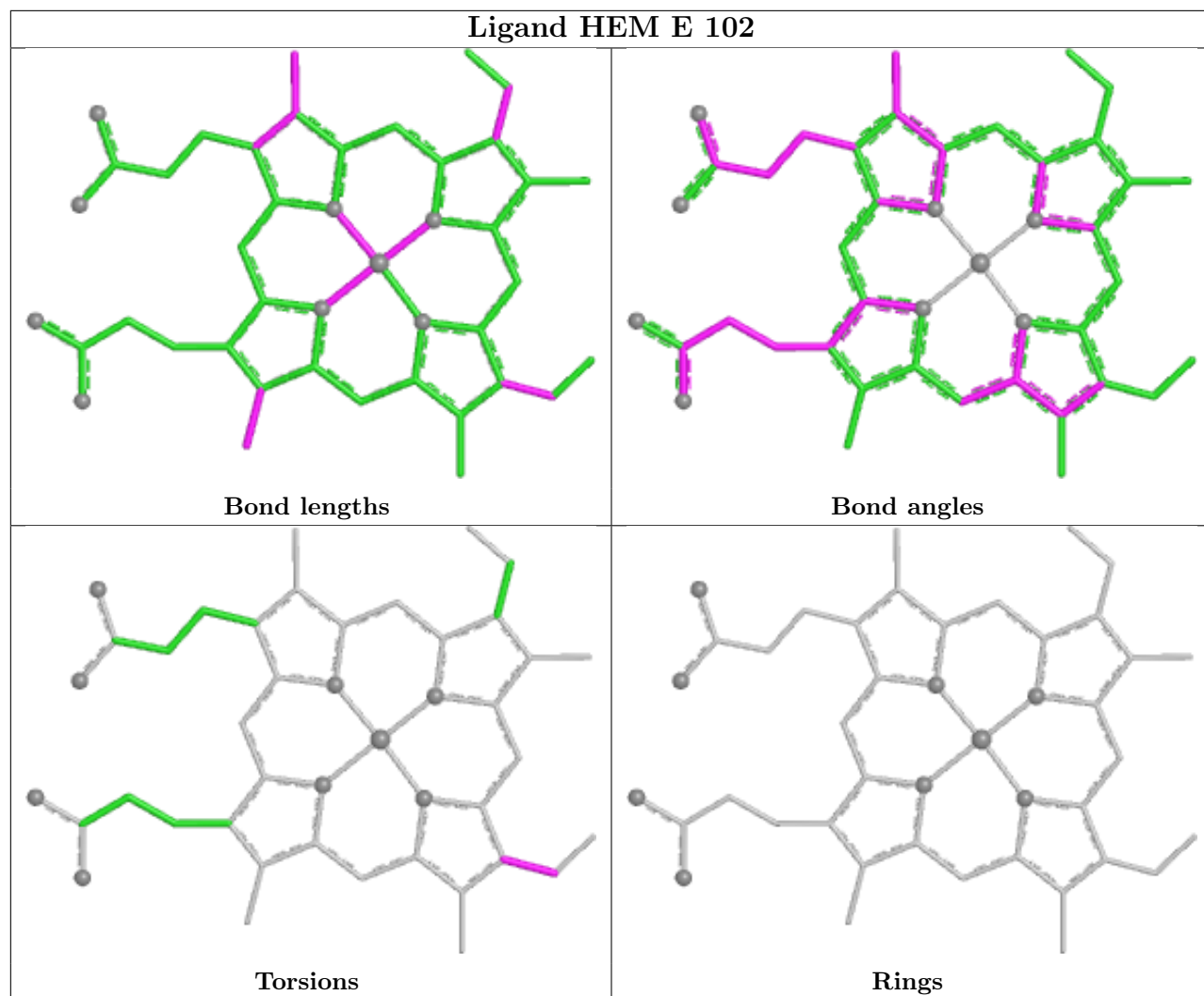
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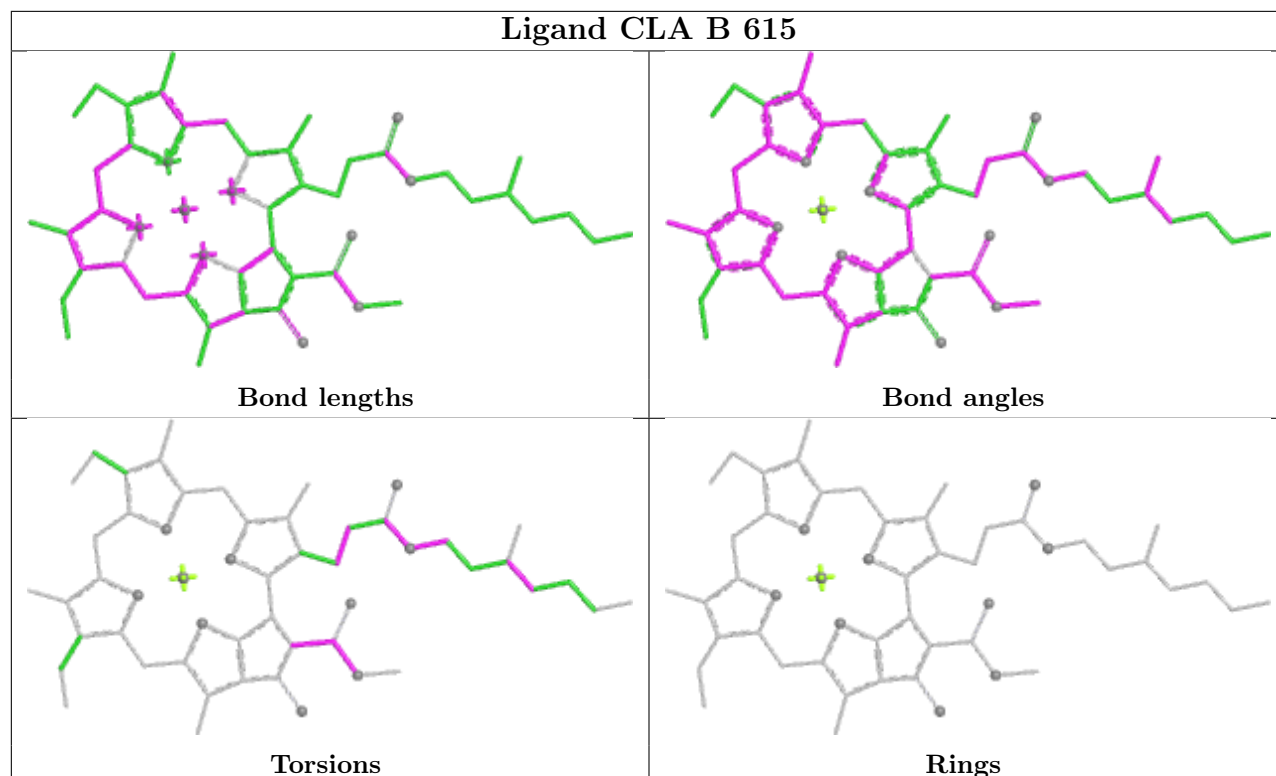
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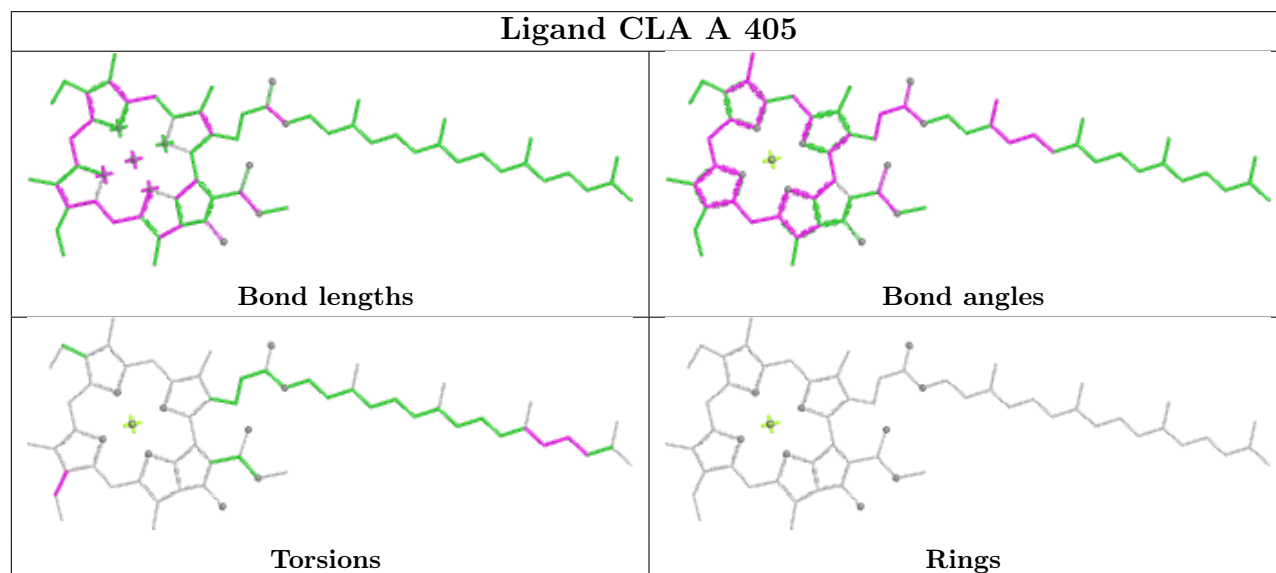




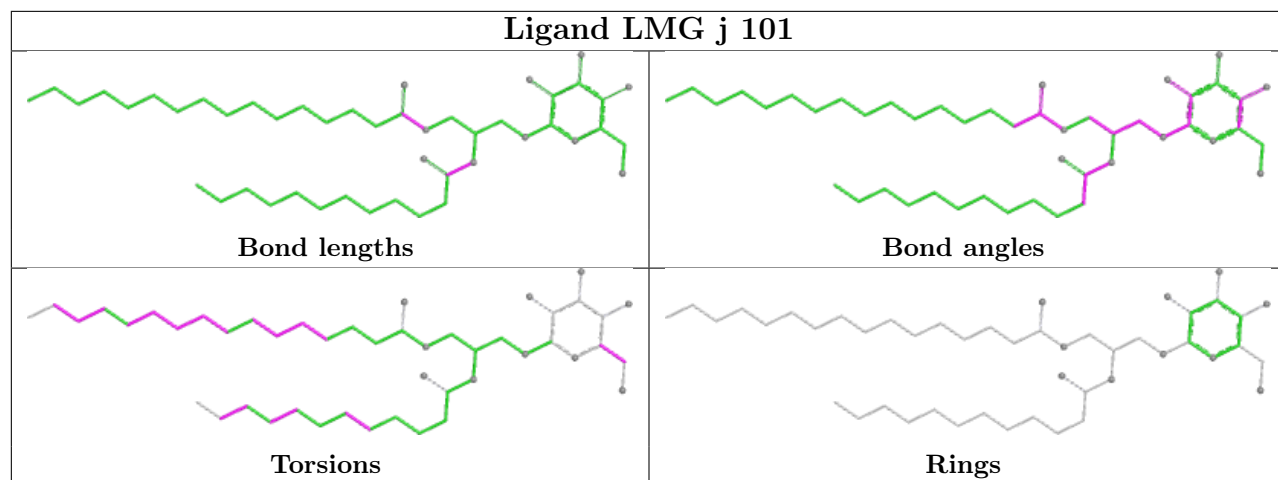
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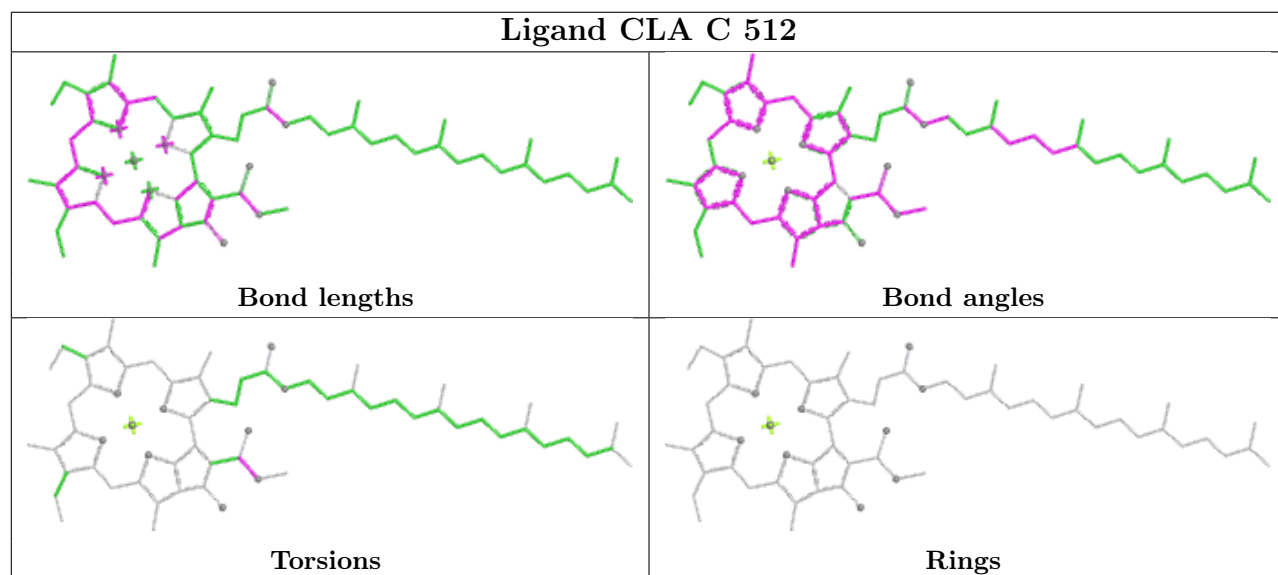
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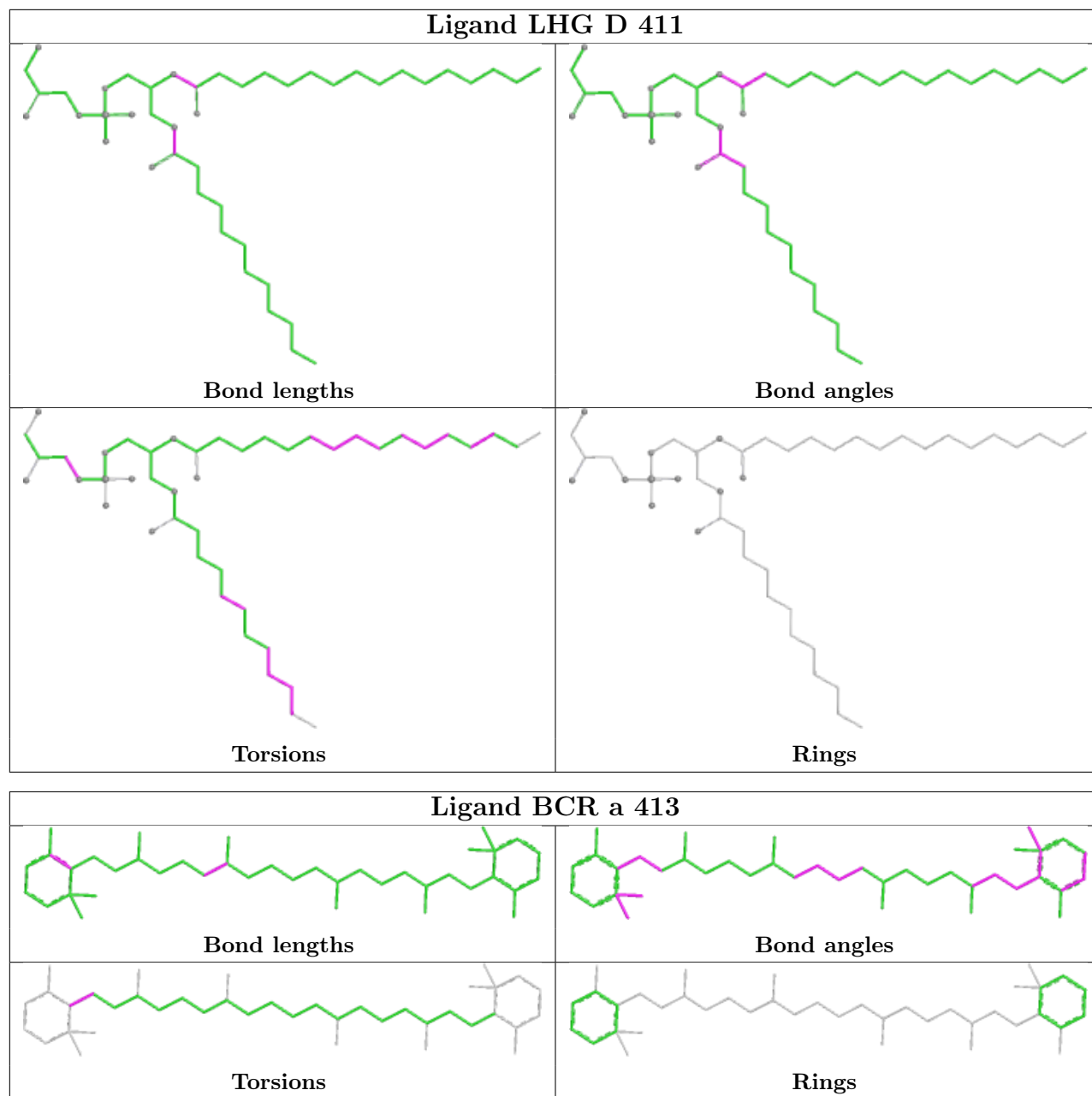


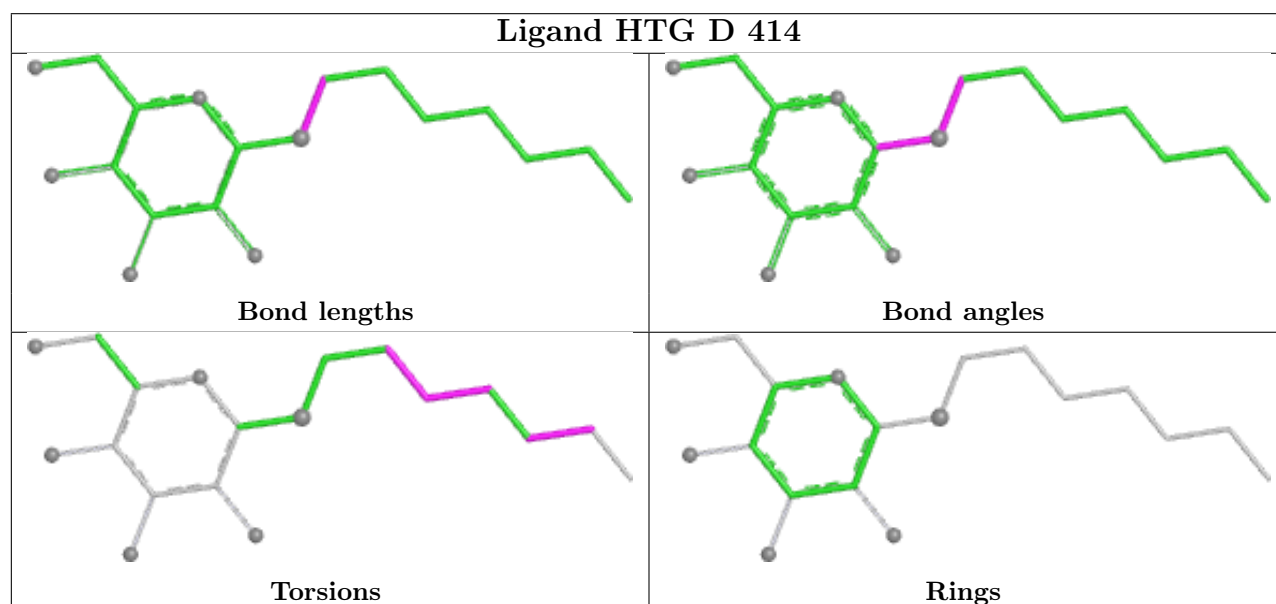
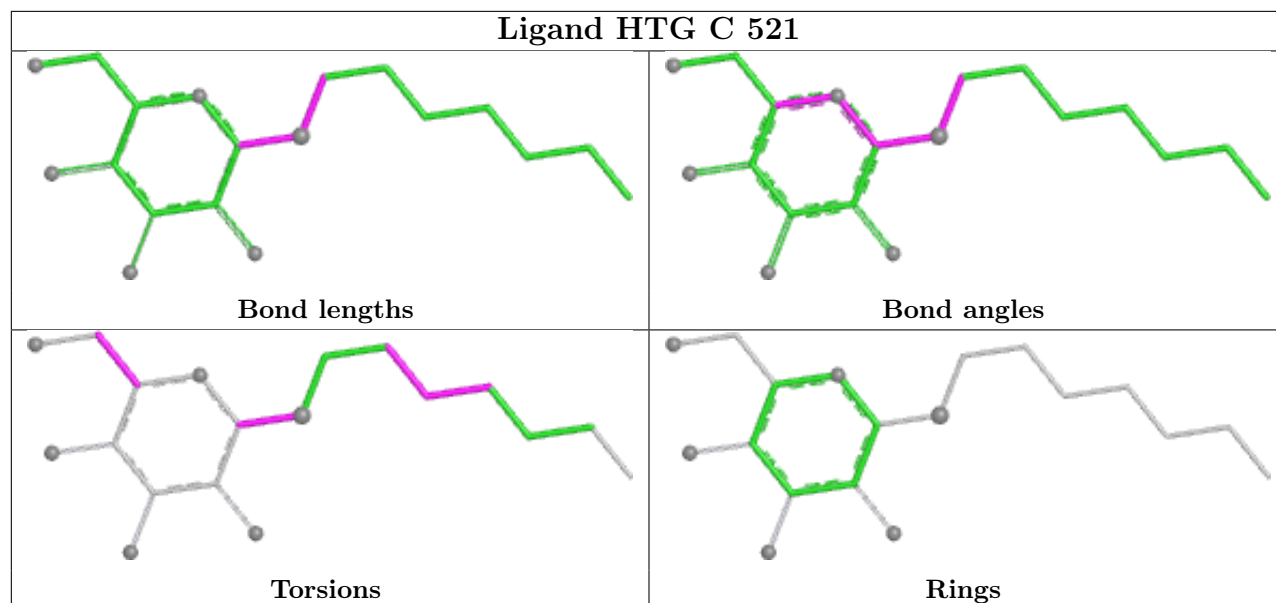
Ligand LMG j 101

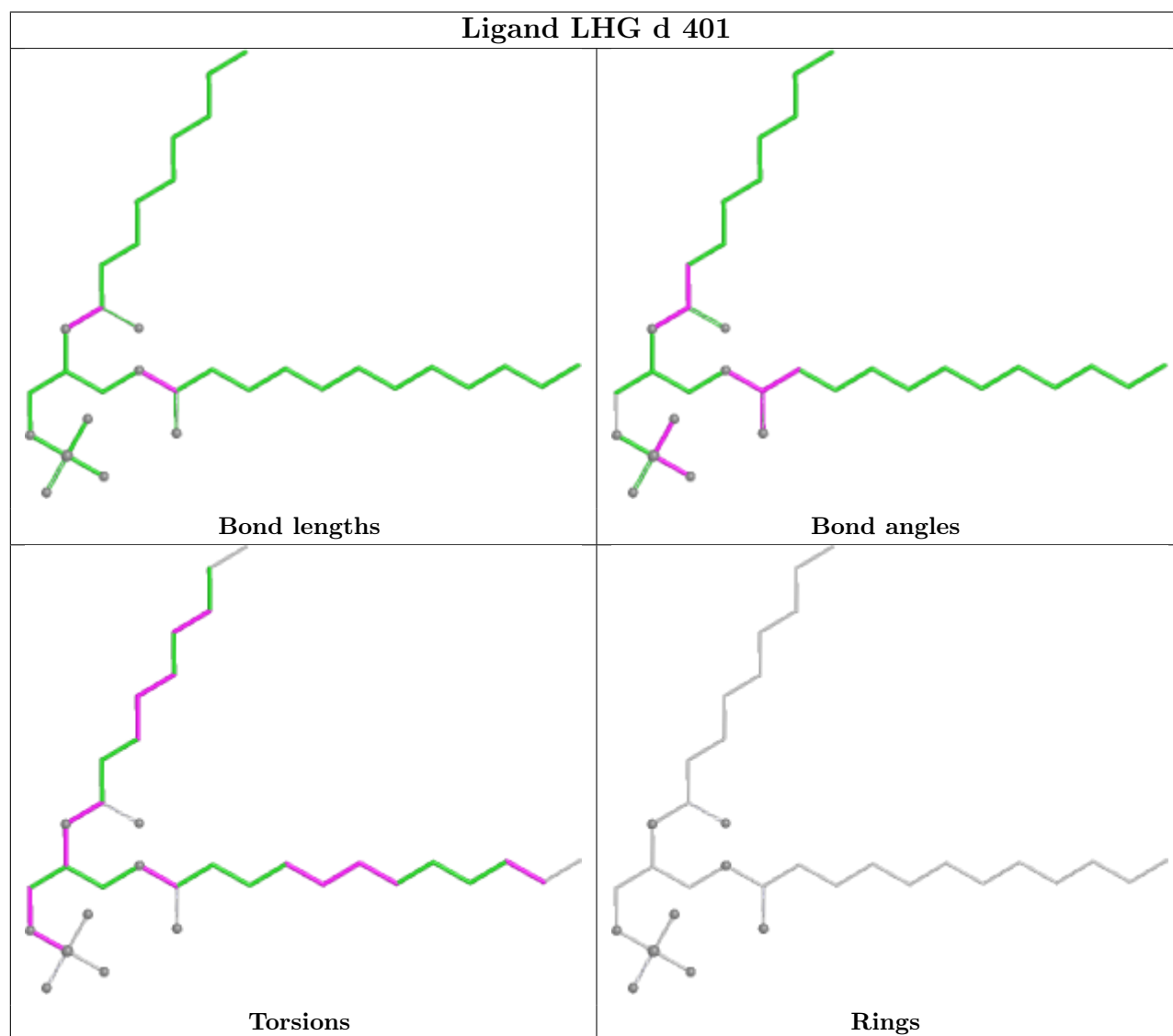
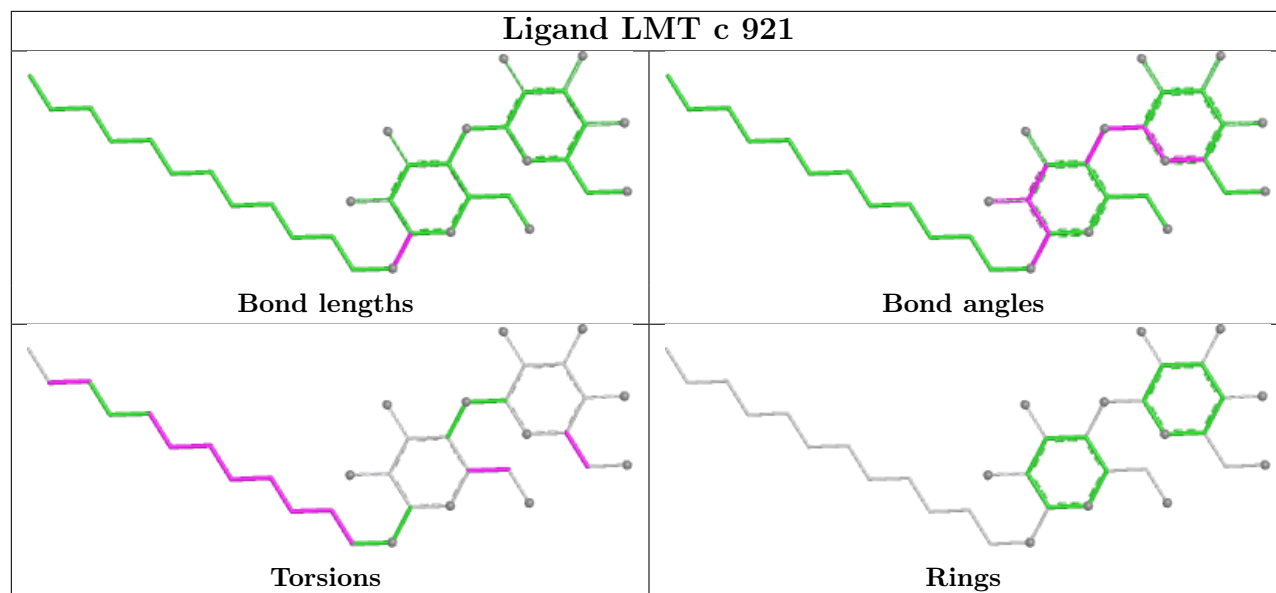


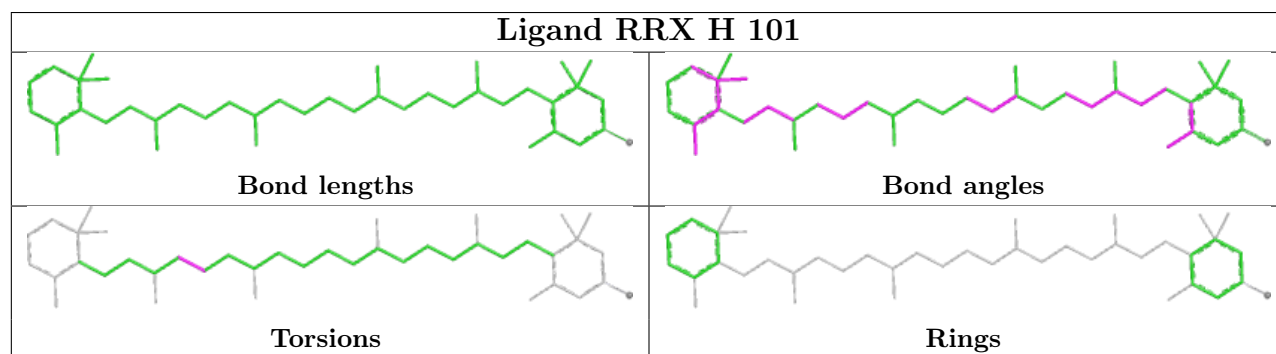
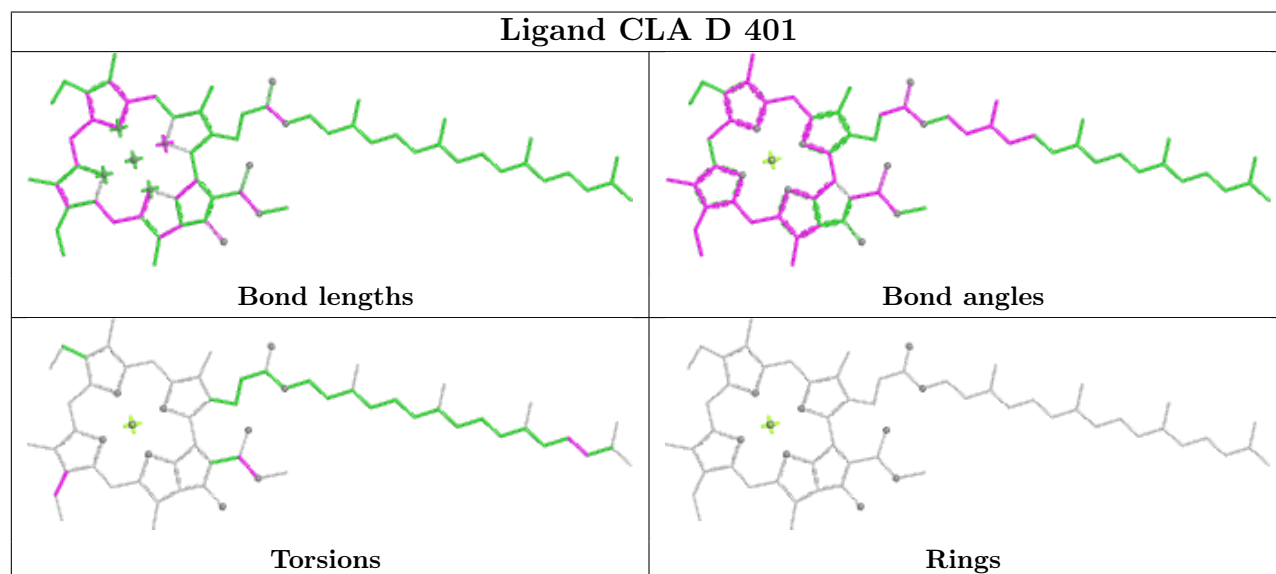
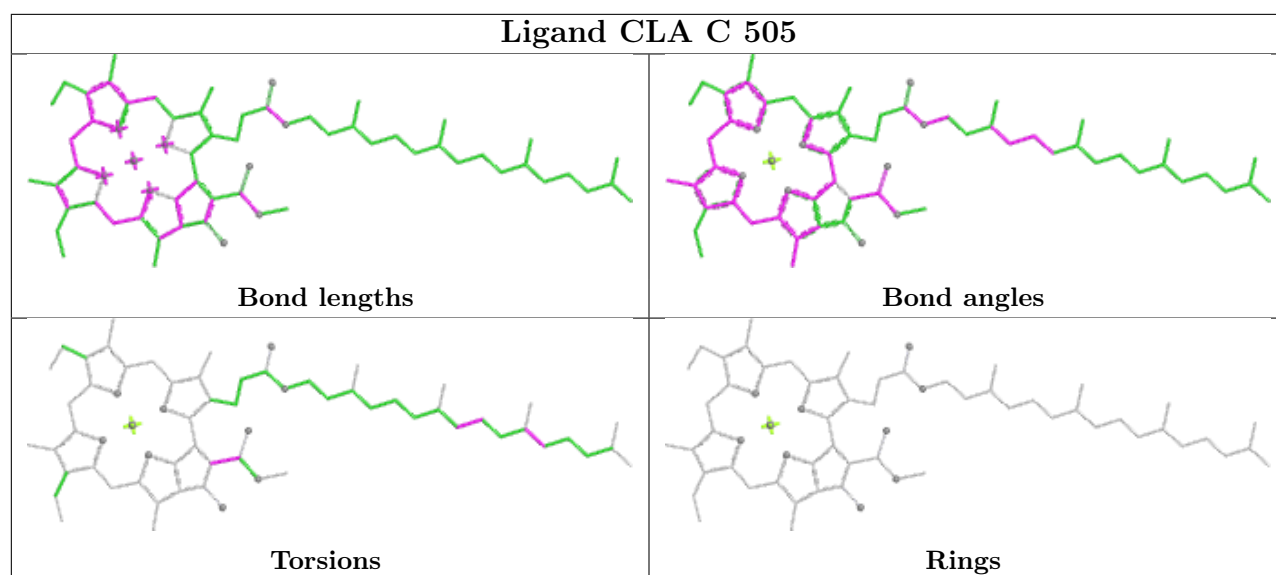
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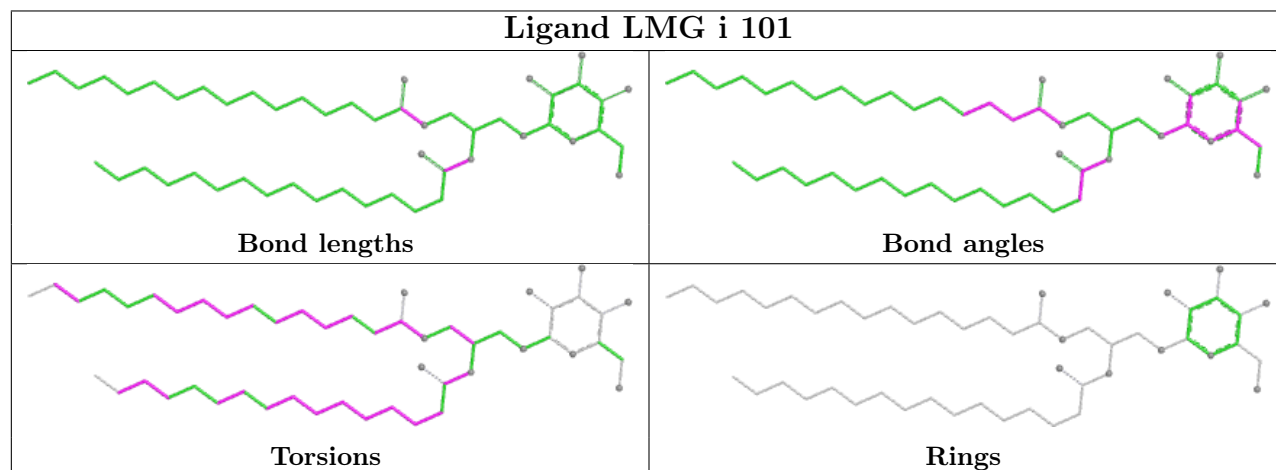
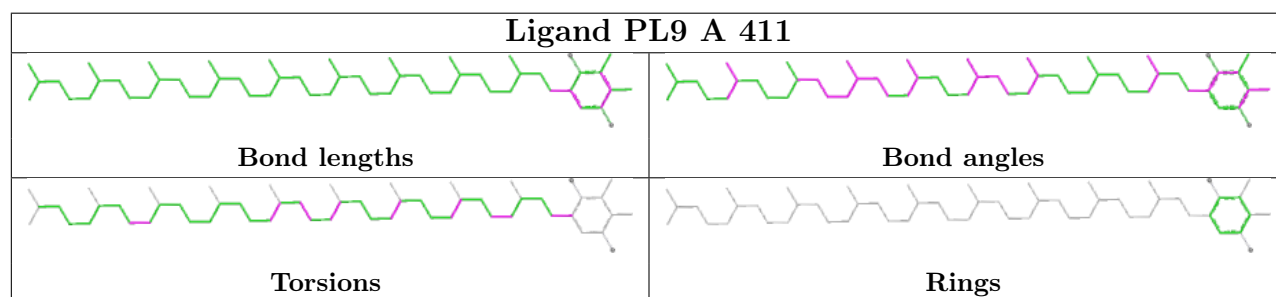
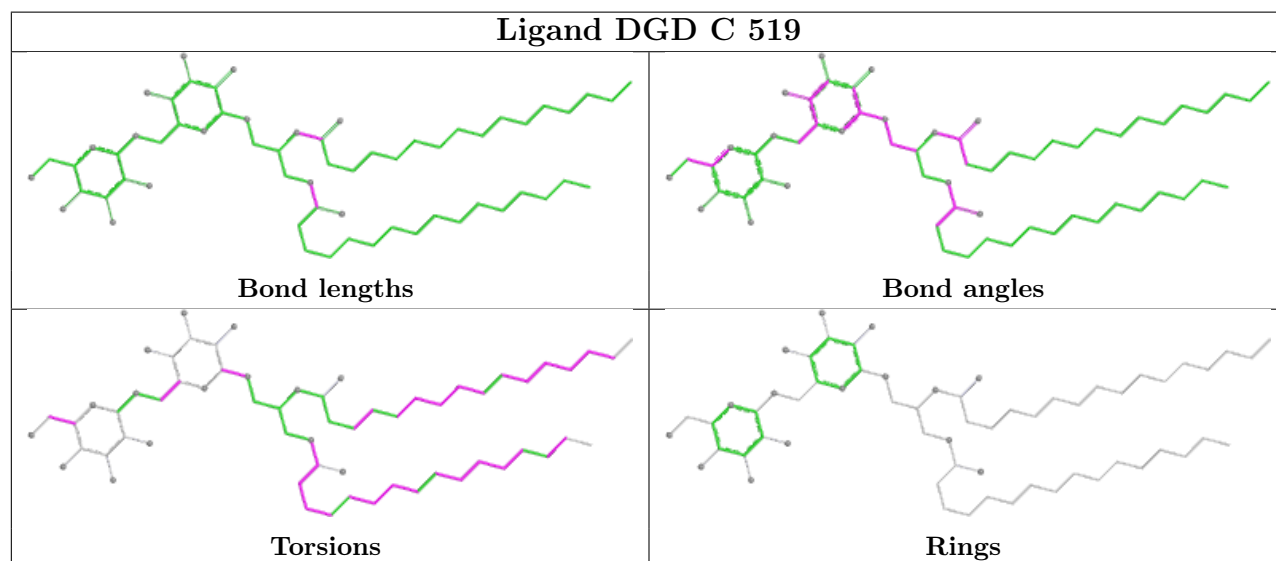
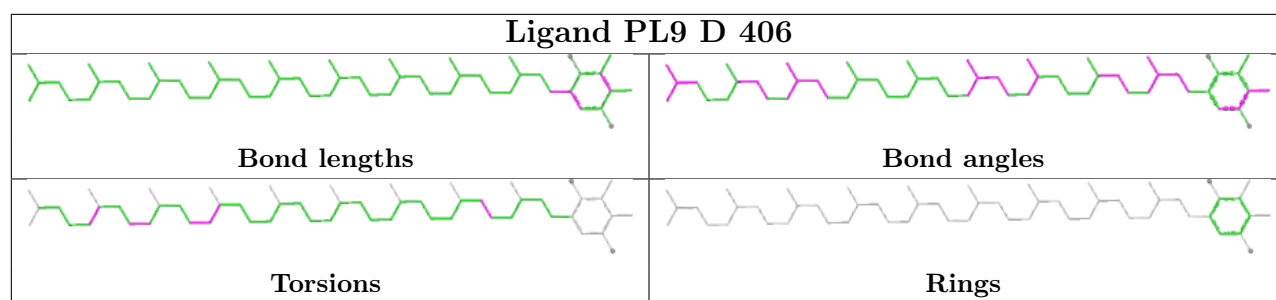


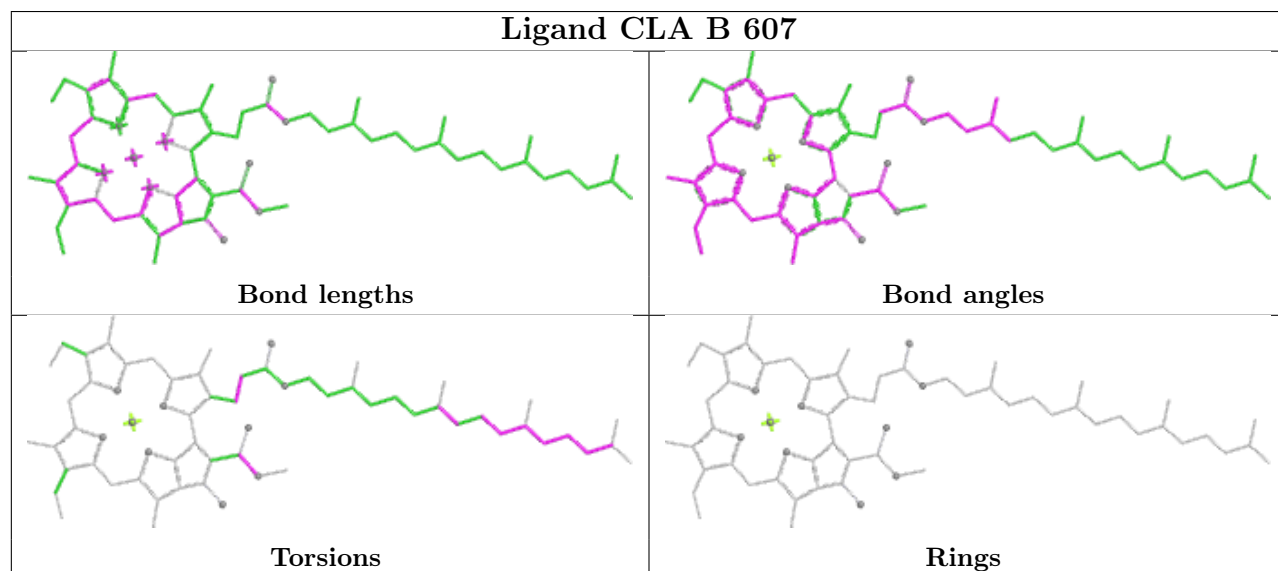
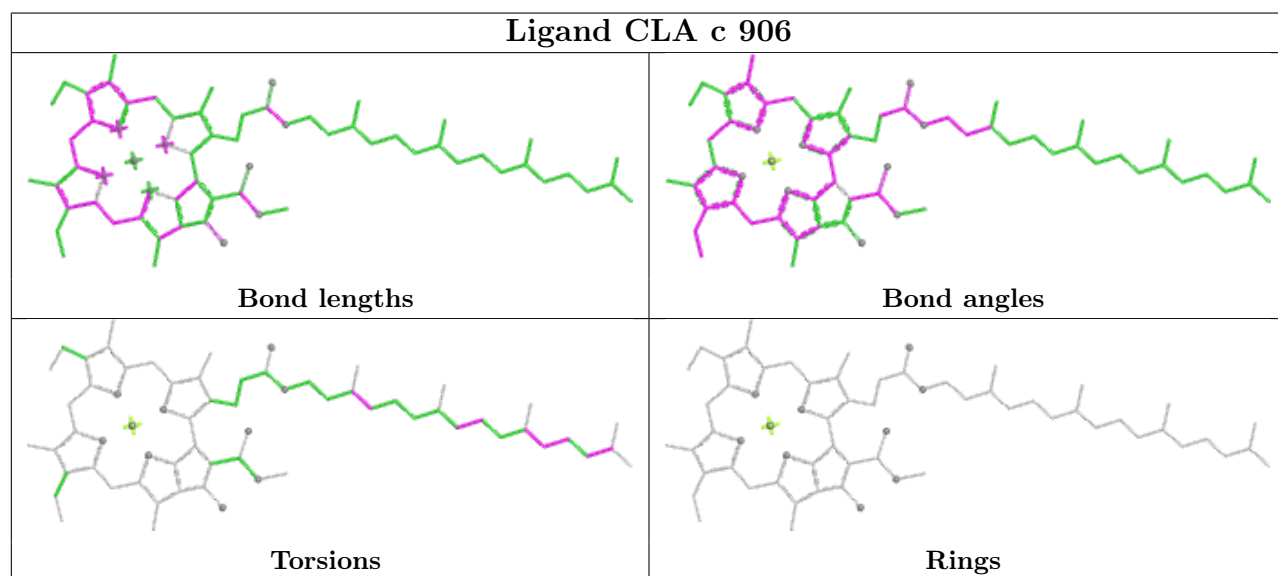
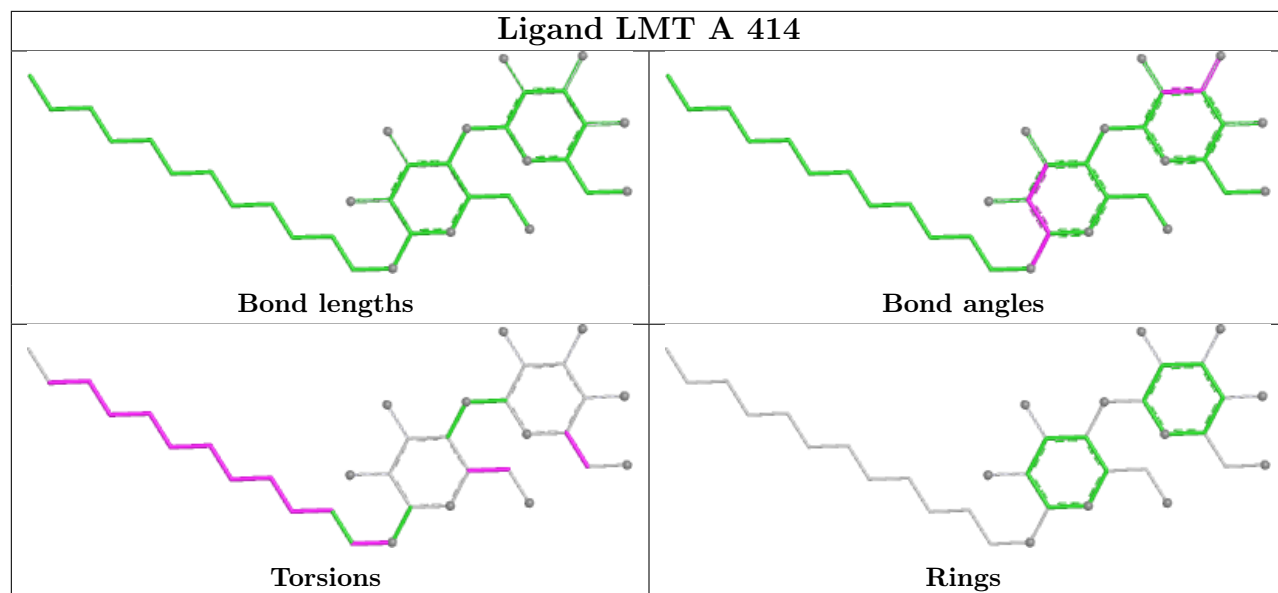


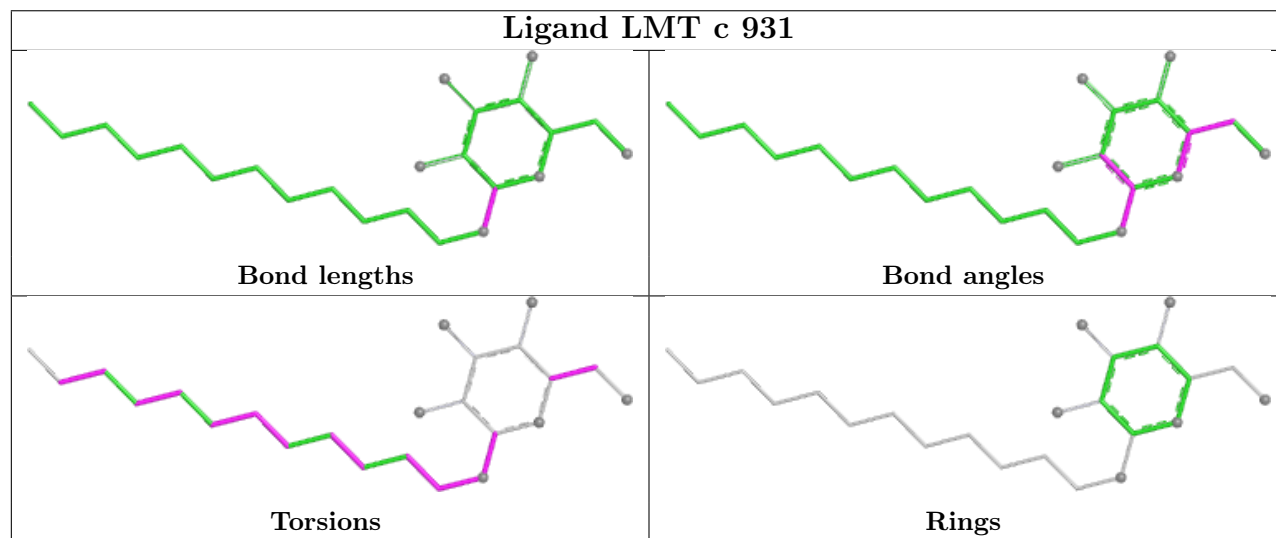
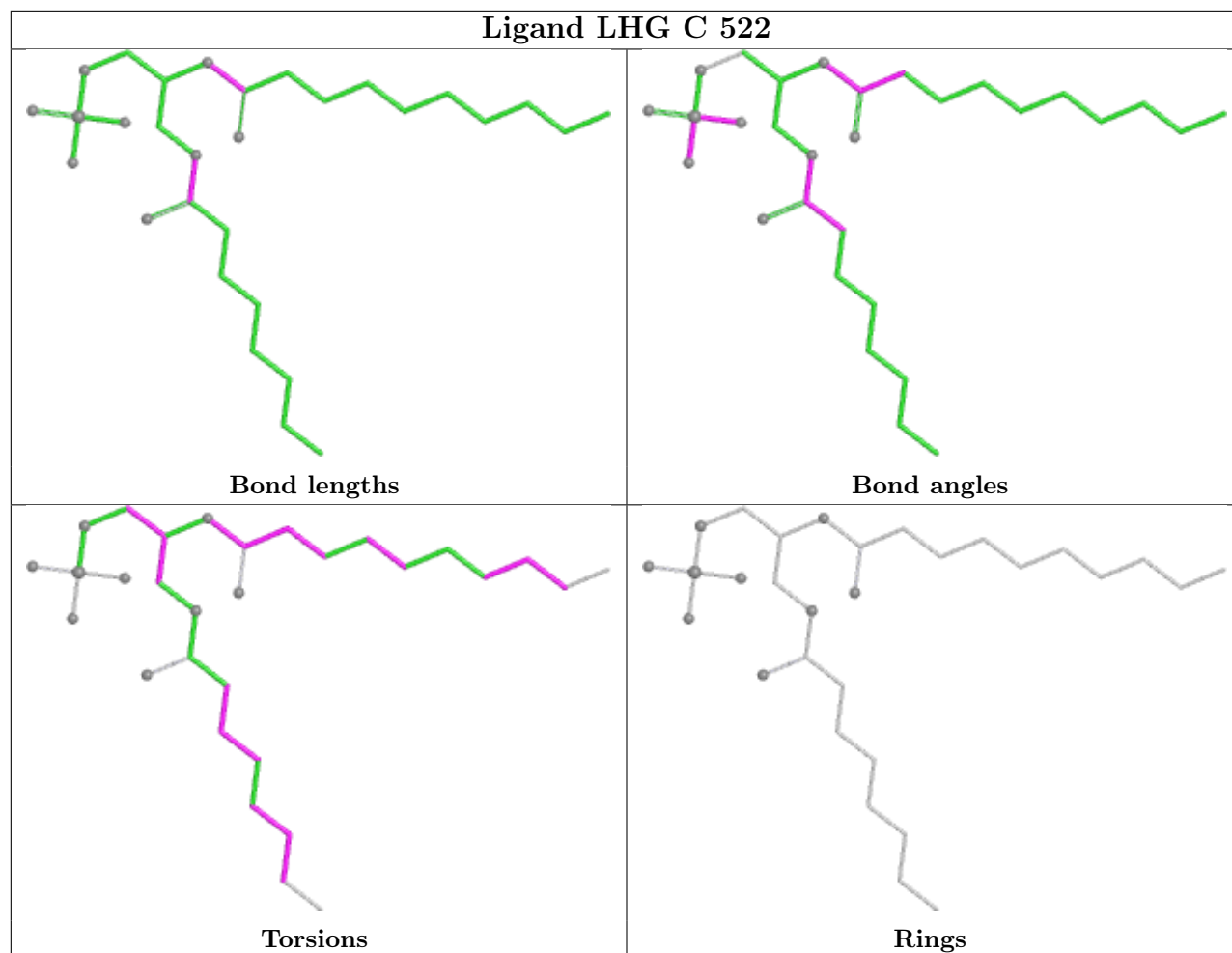


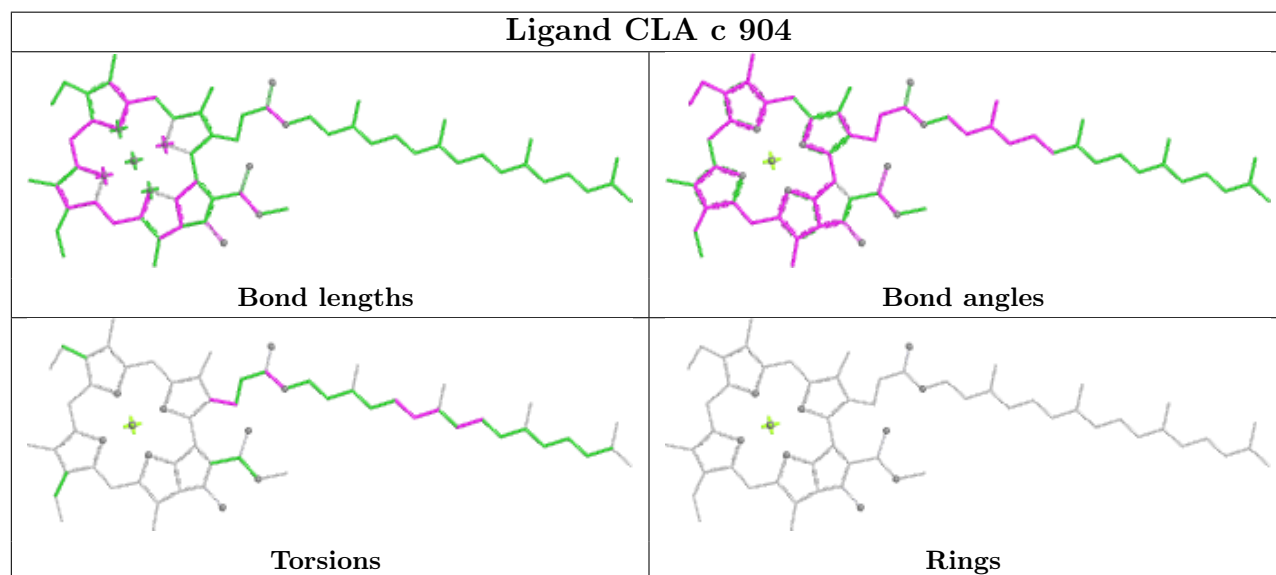
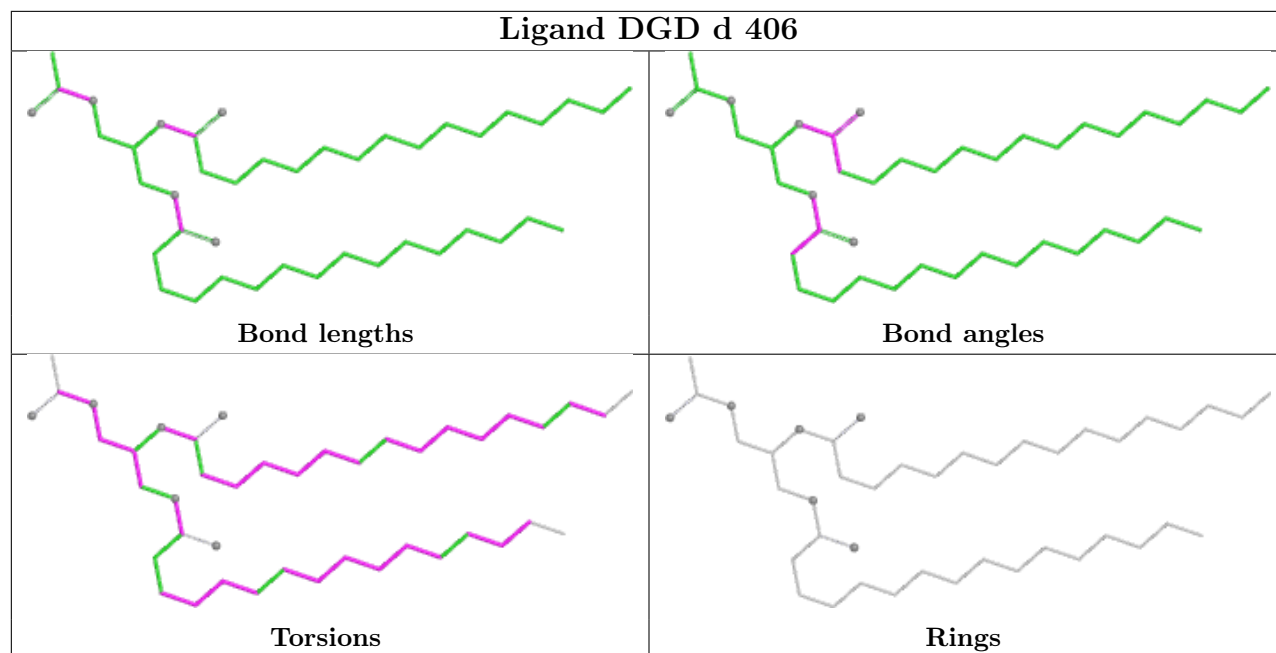




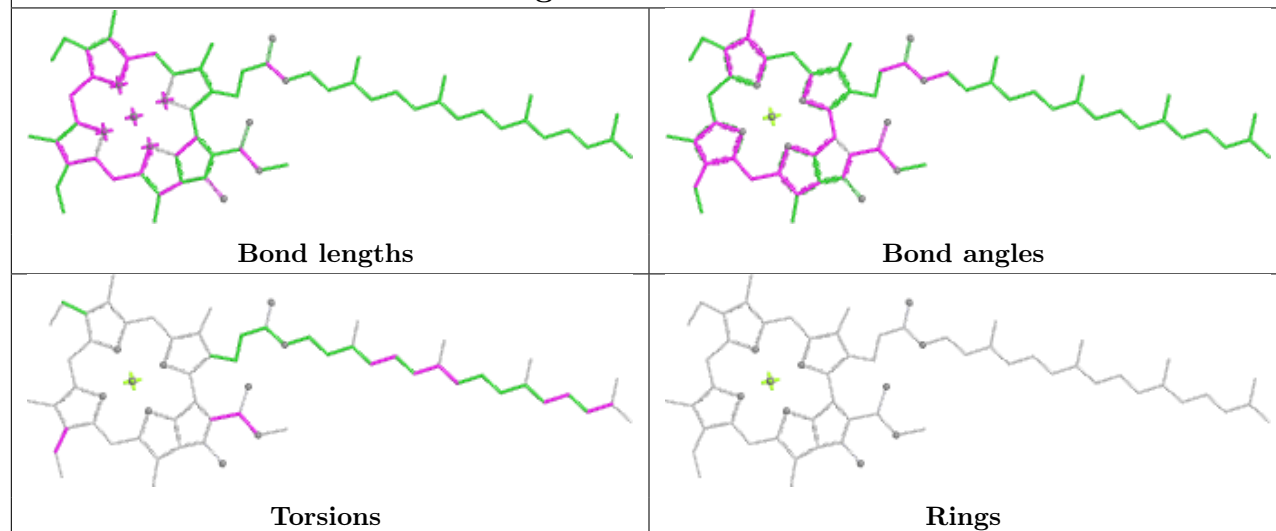




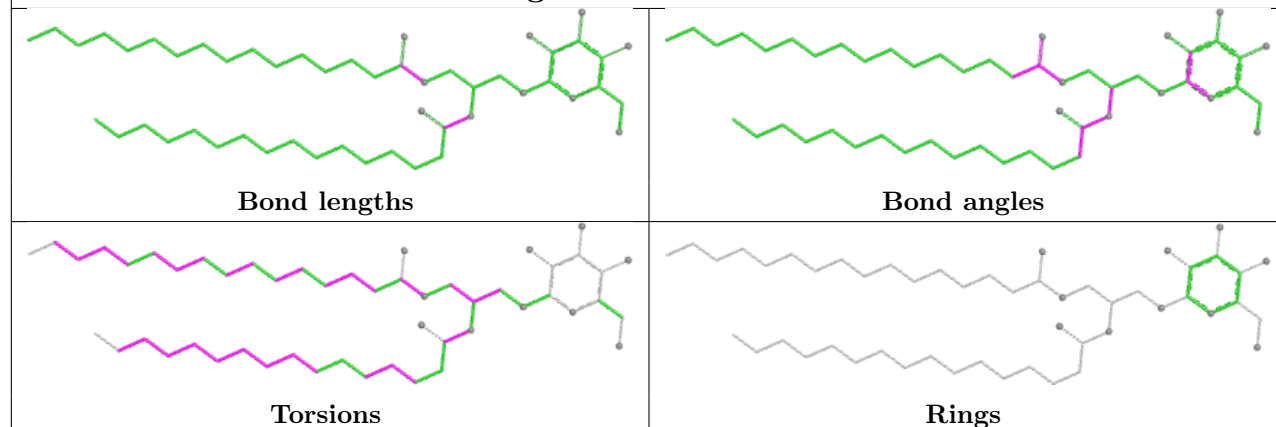




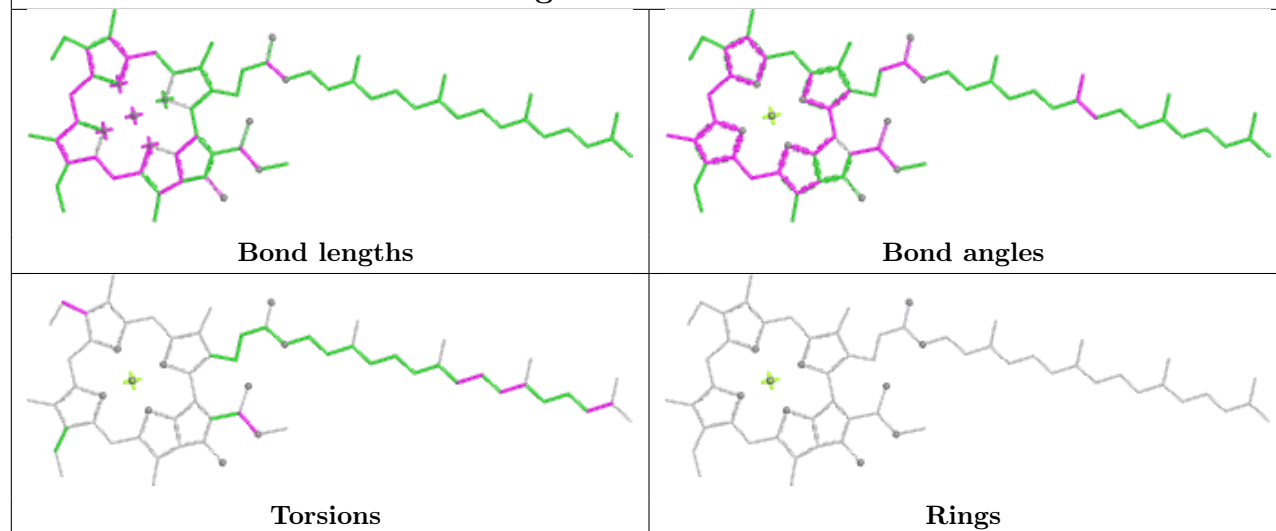
Ligand CLA b 605

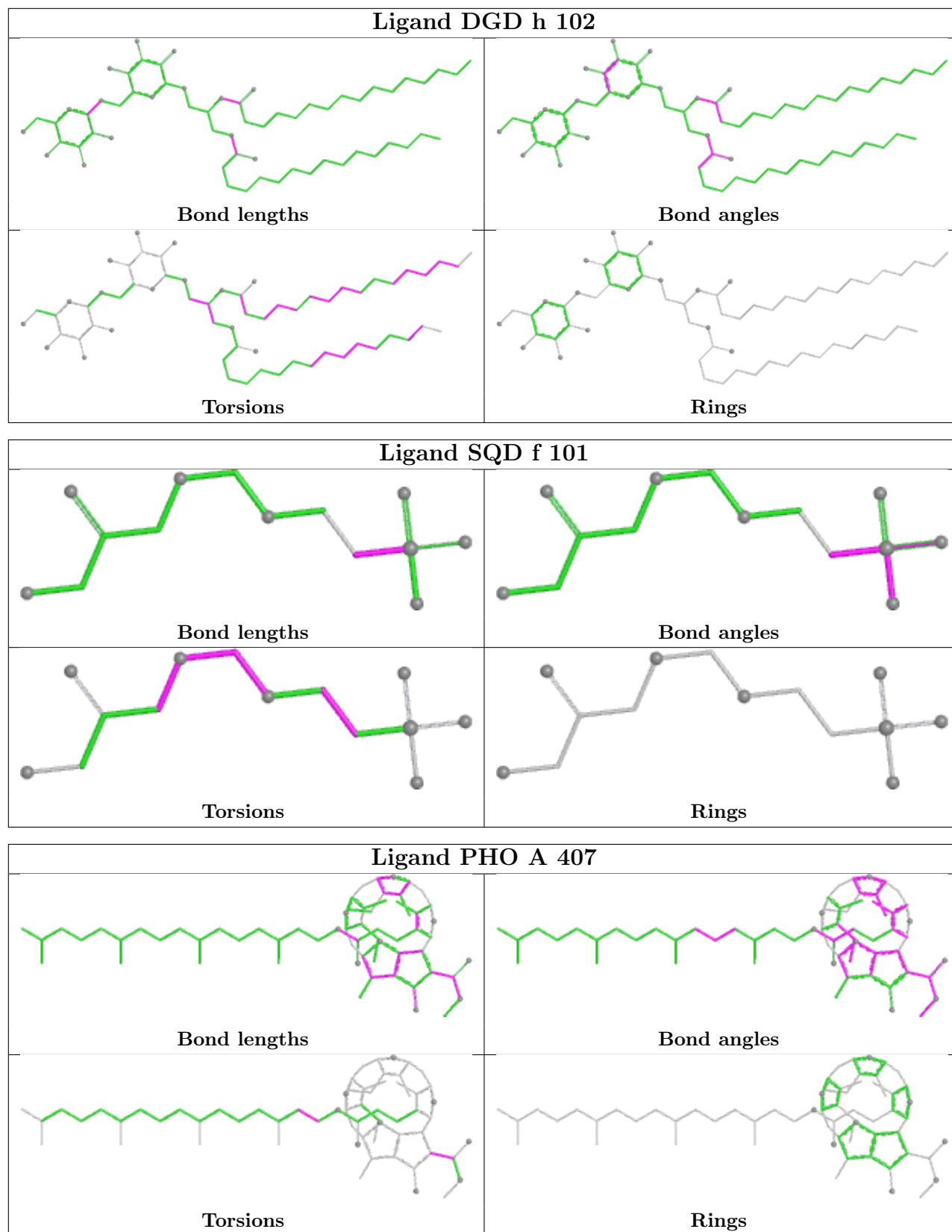


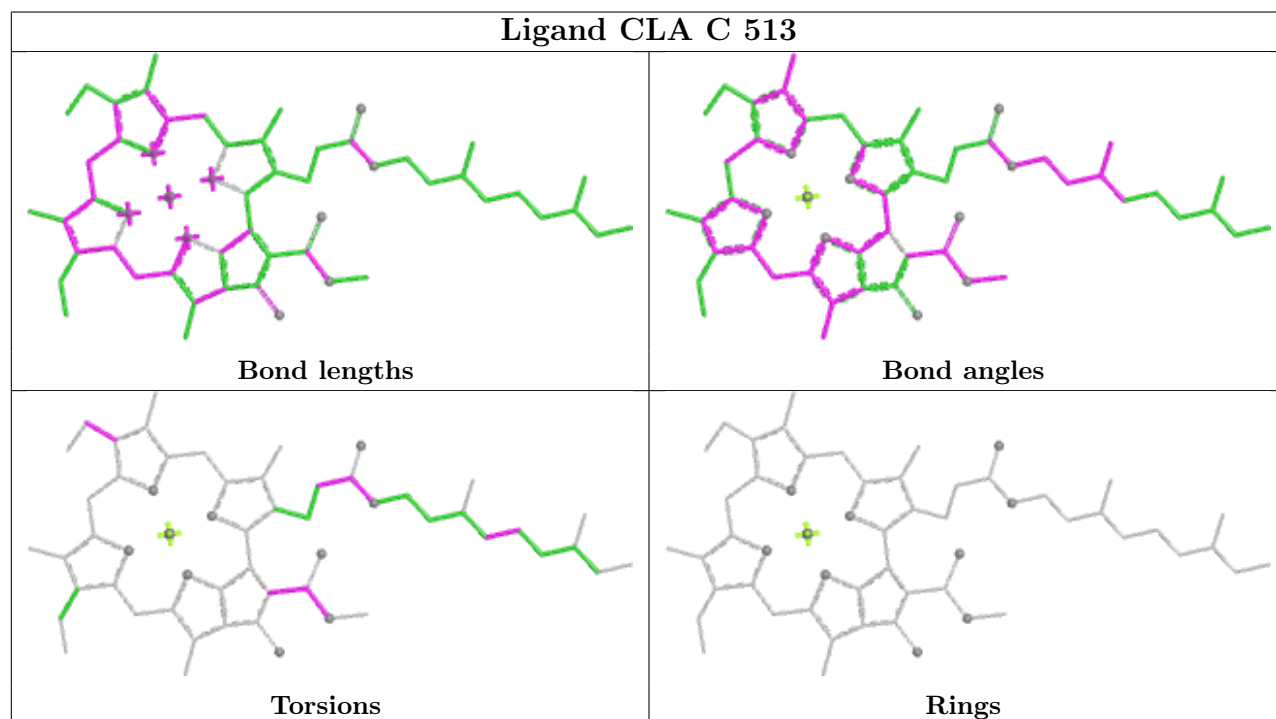
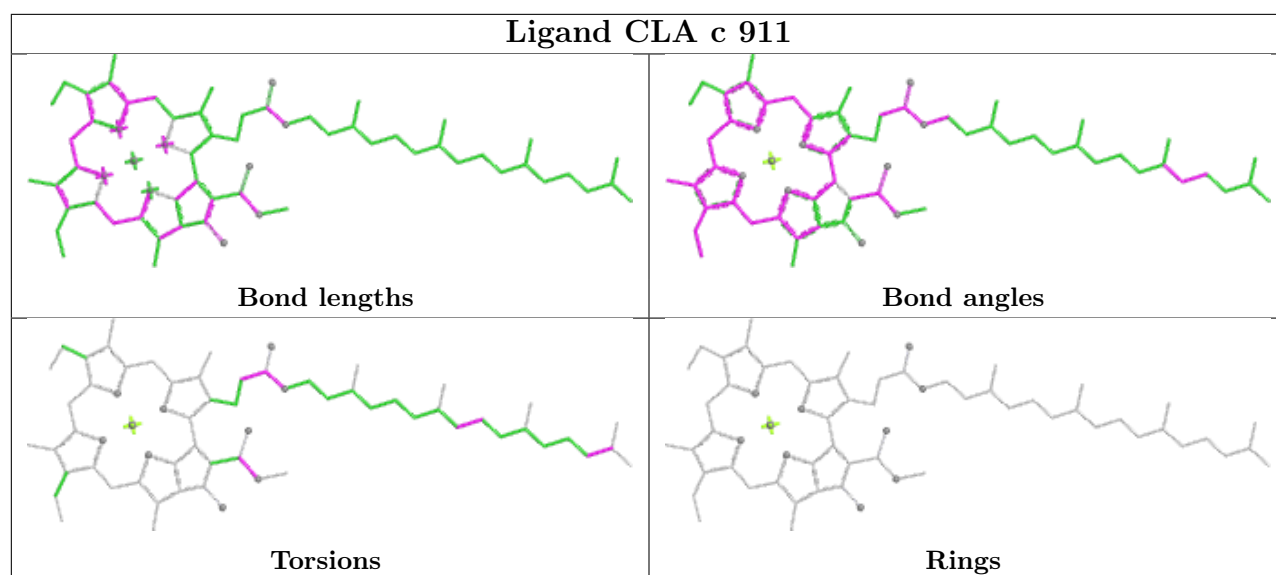
Ligand LMG A 410

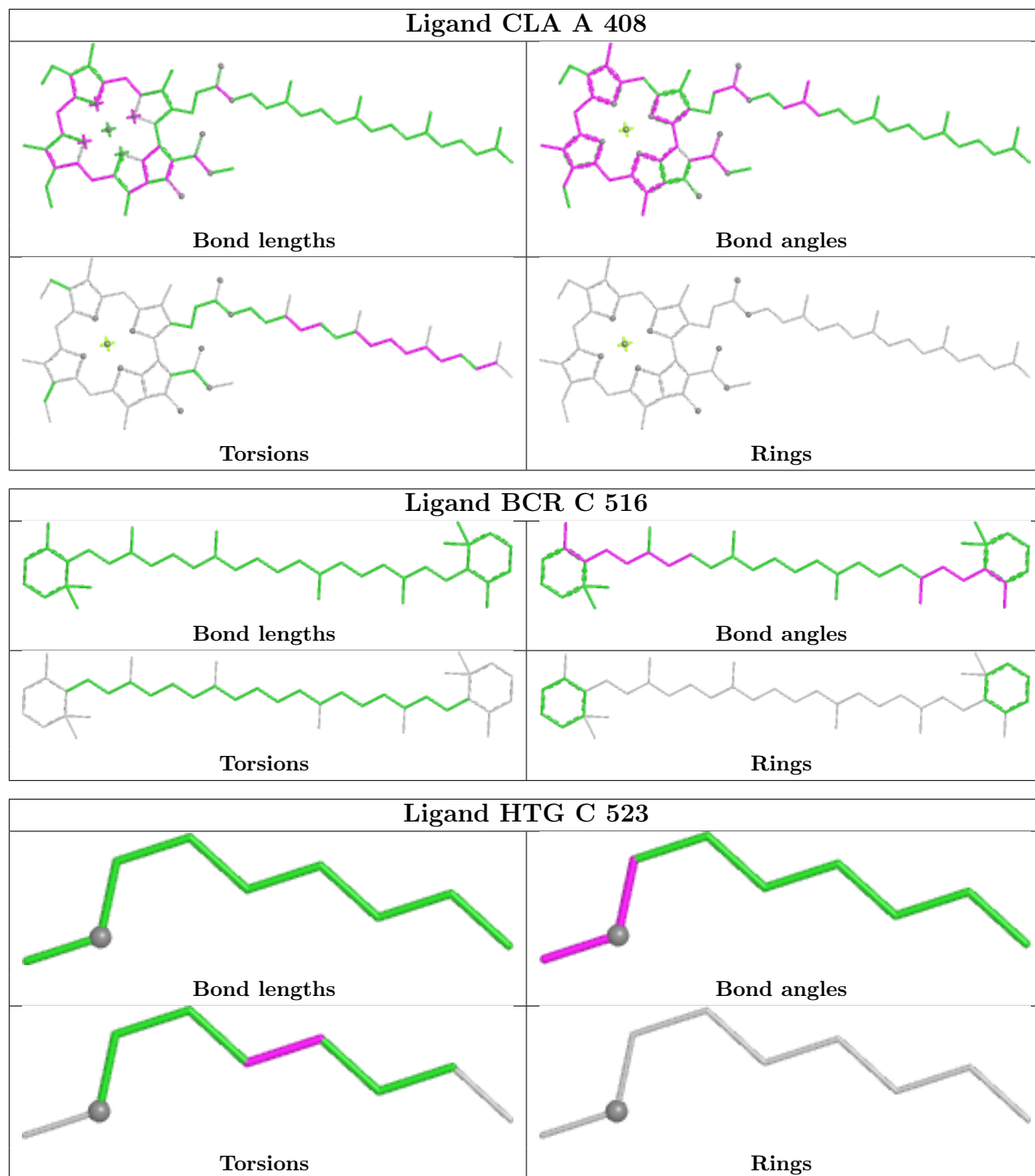


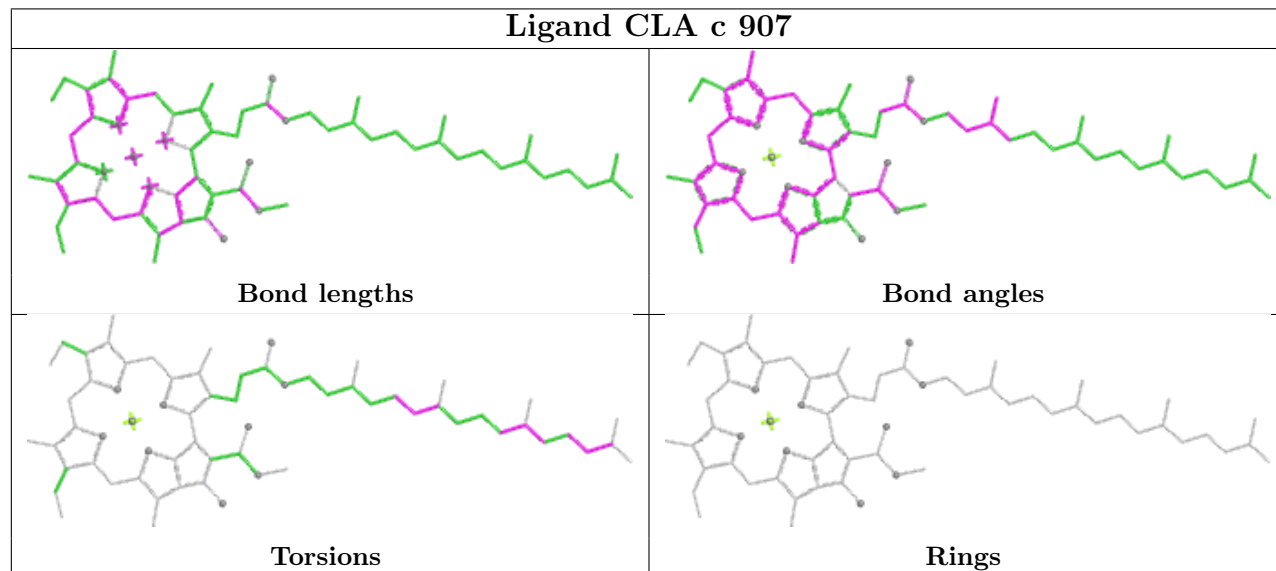
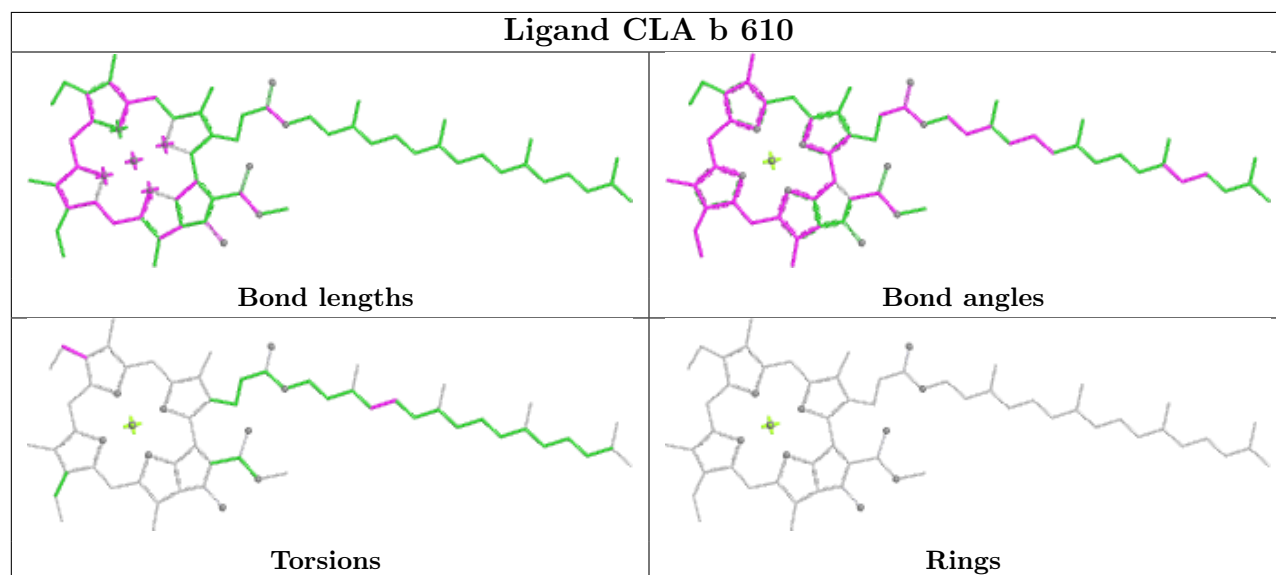
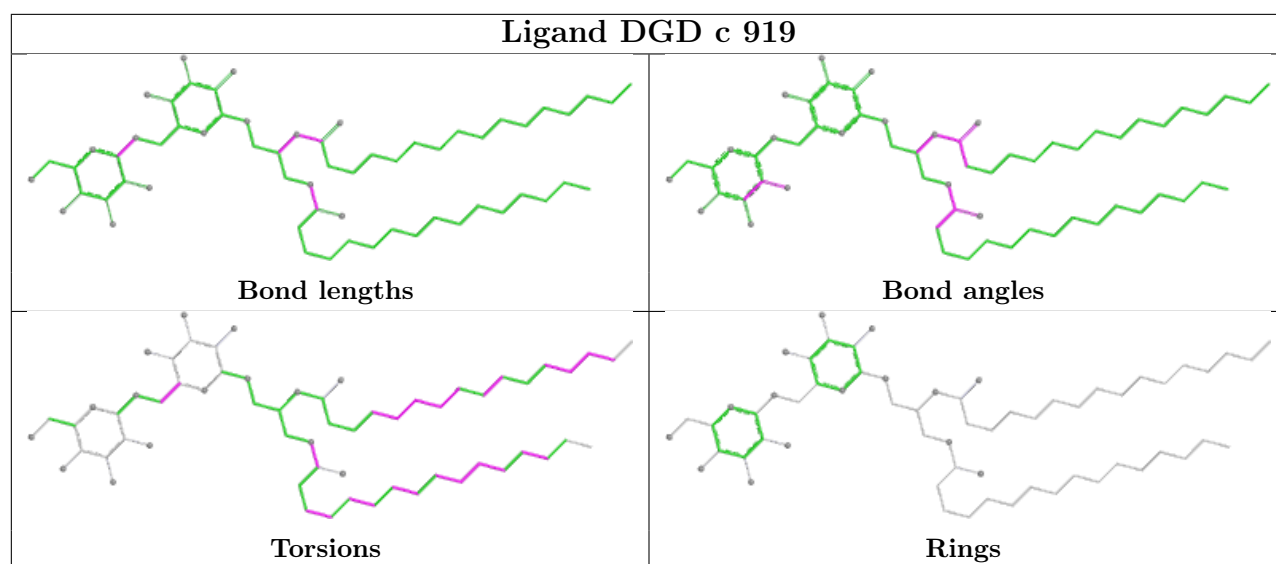
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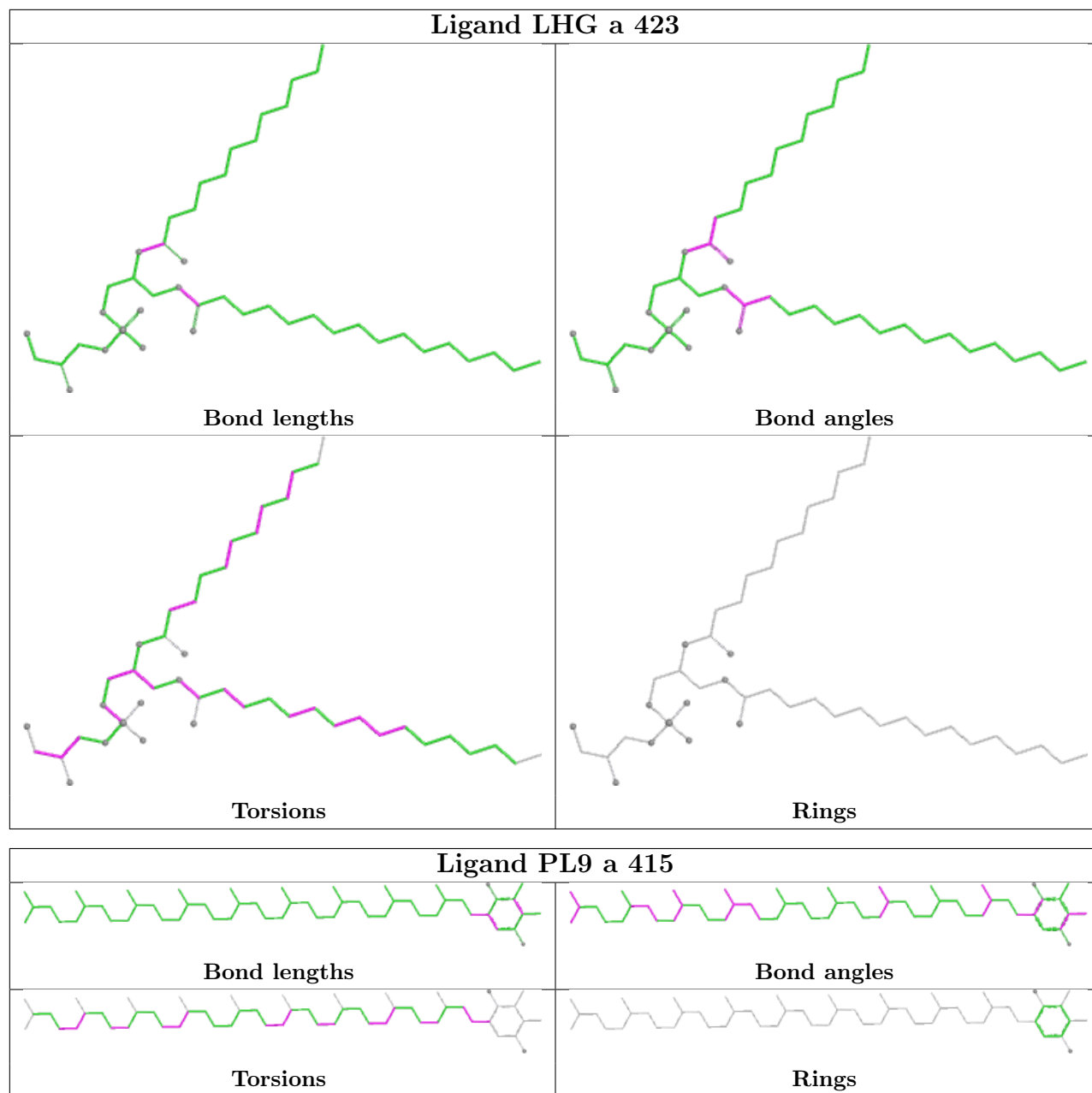


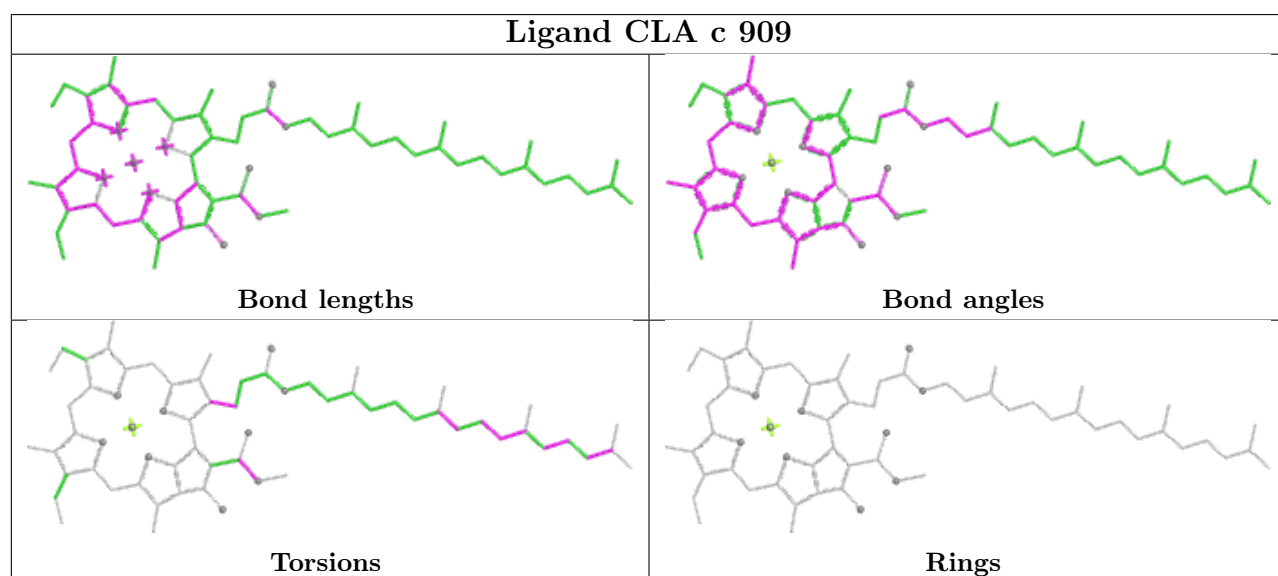
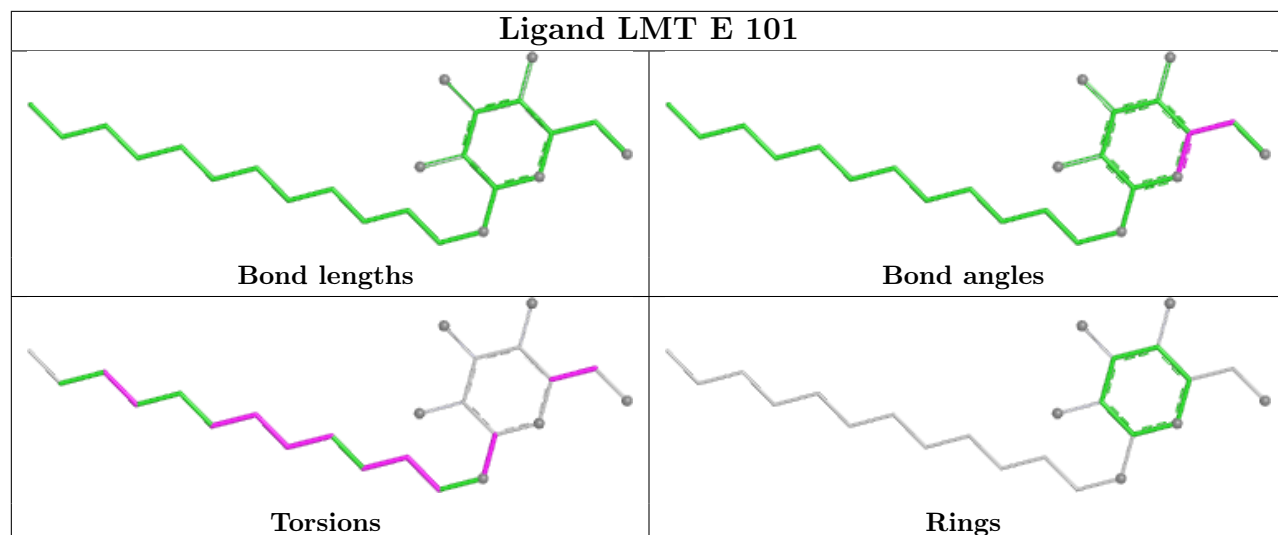


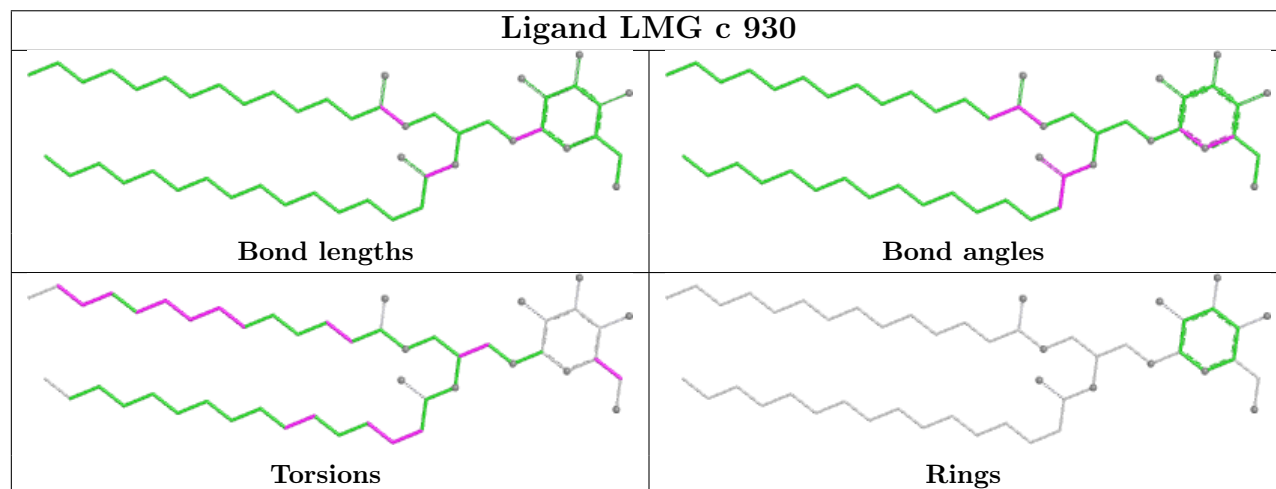
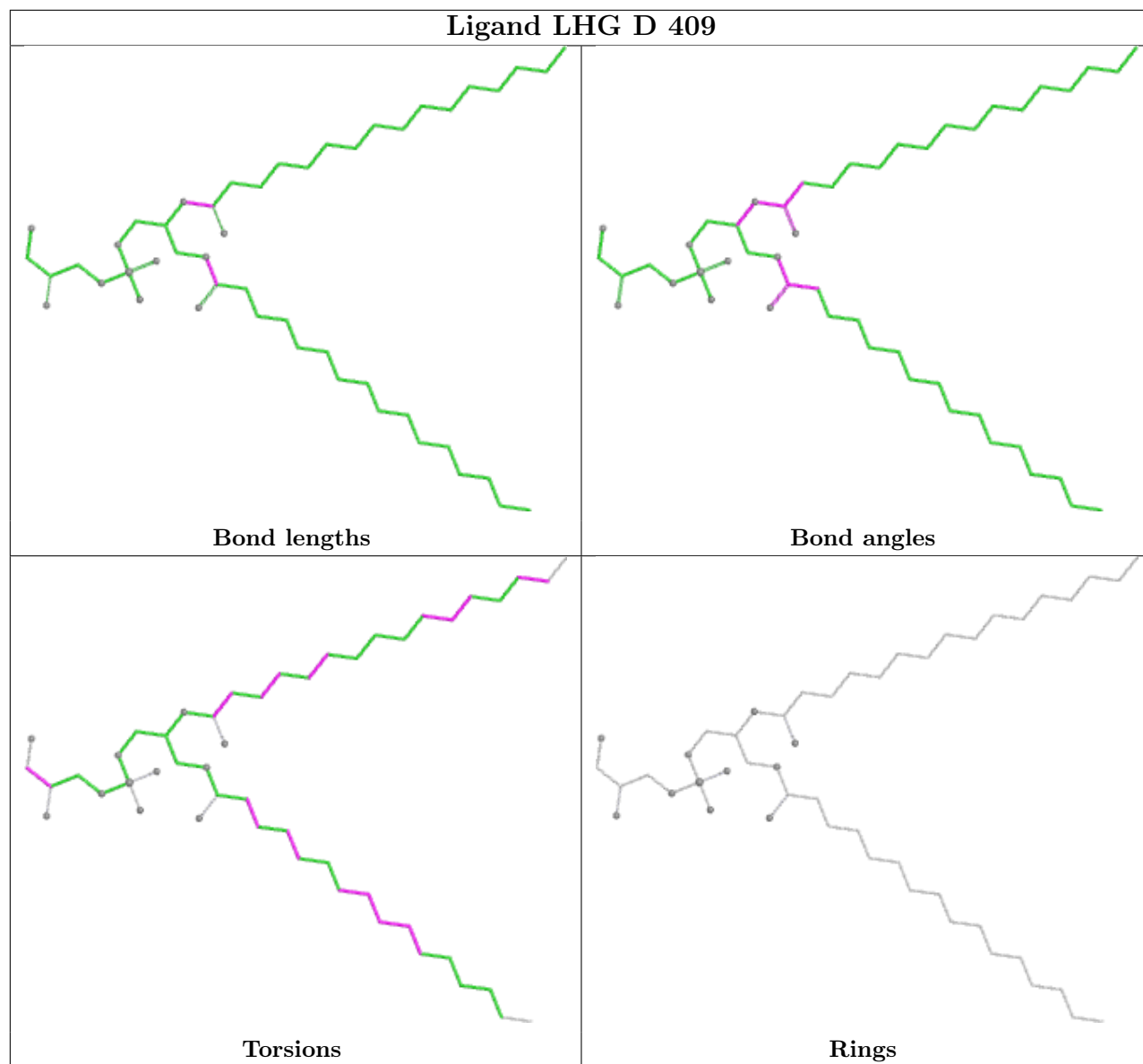


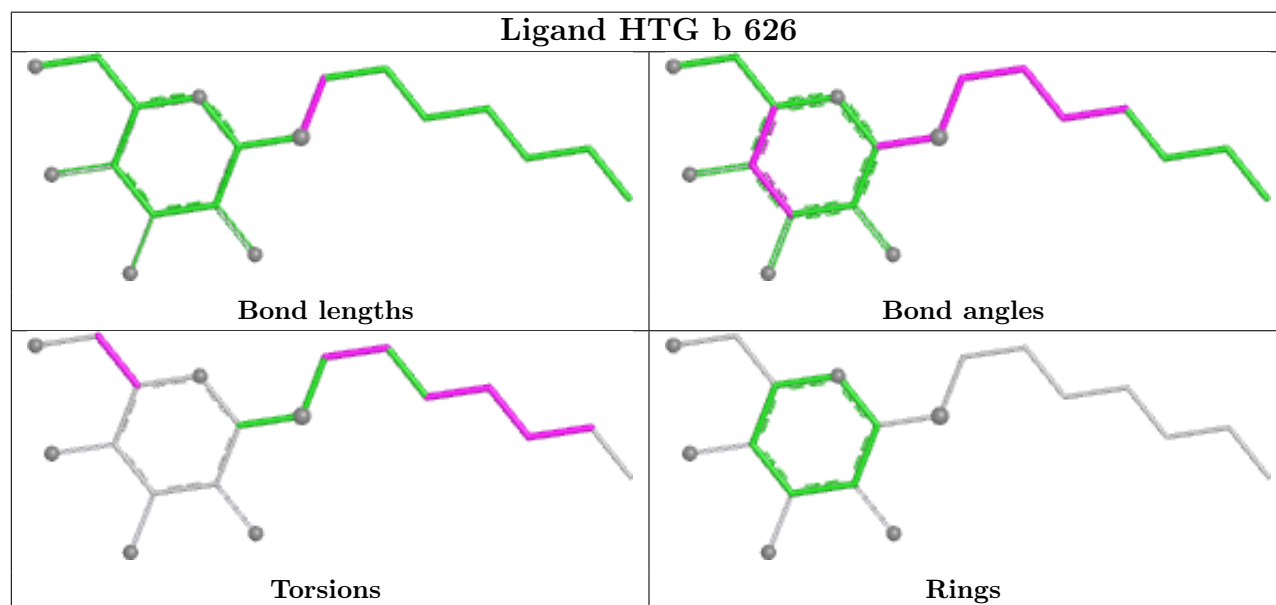
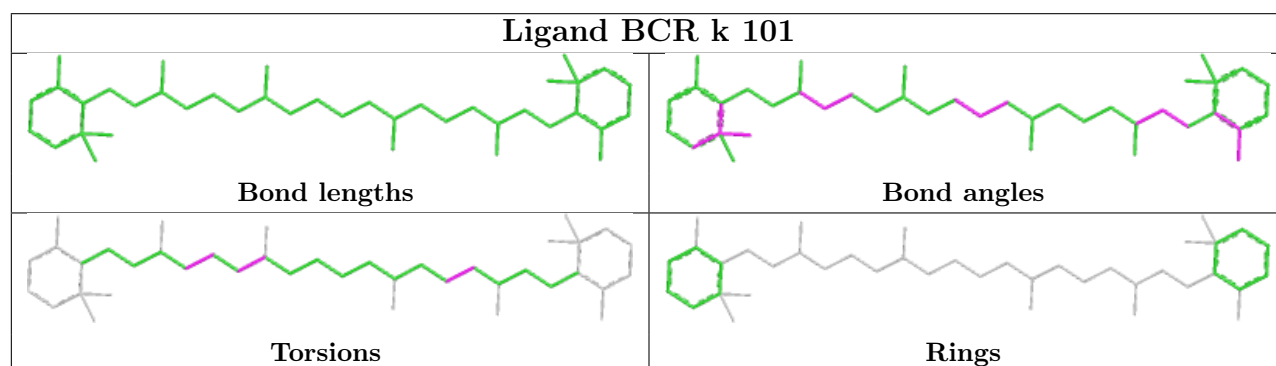
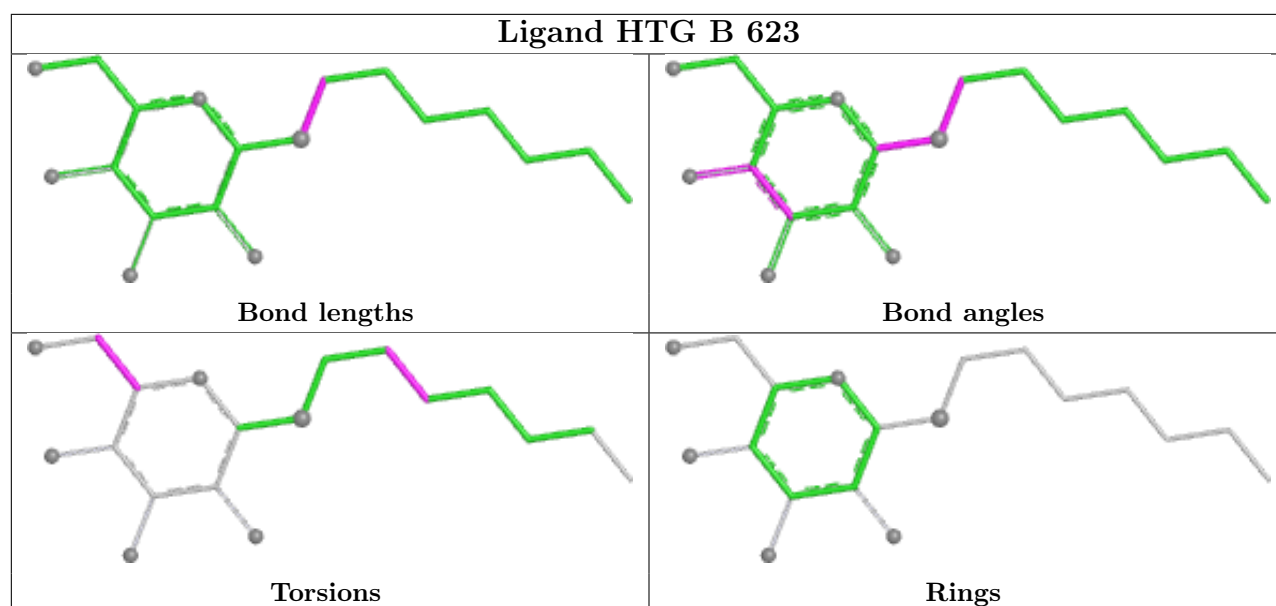


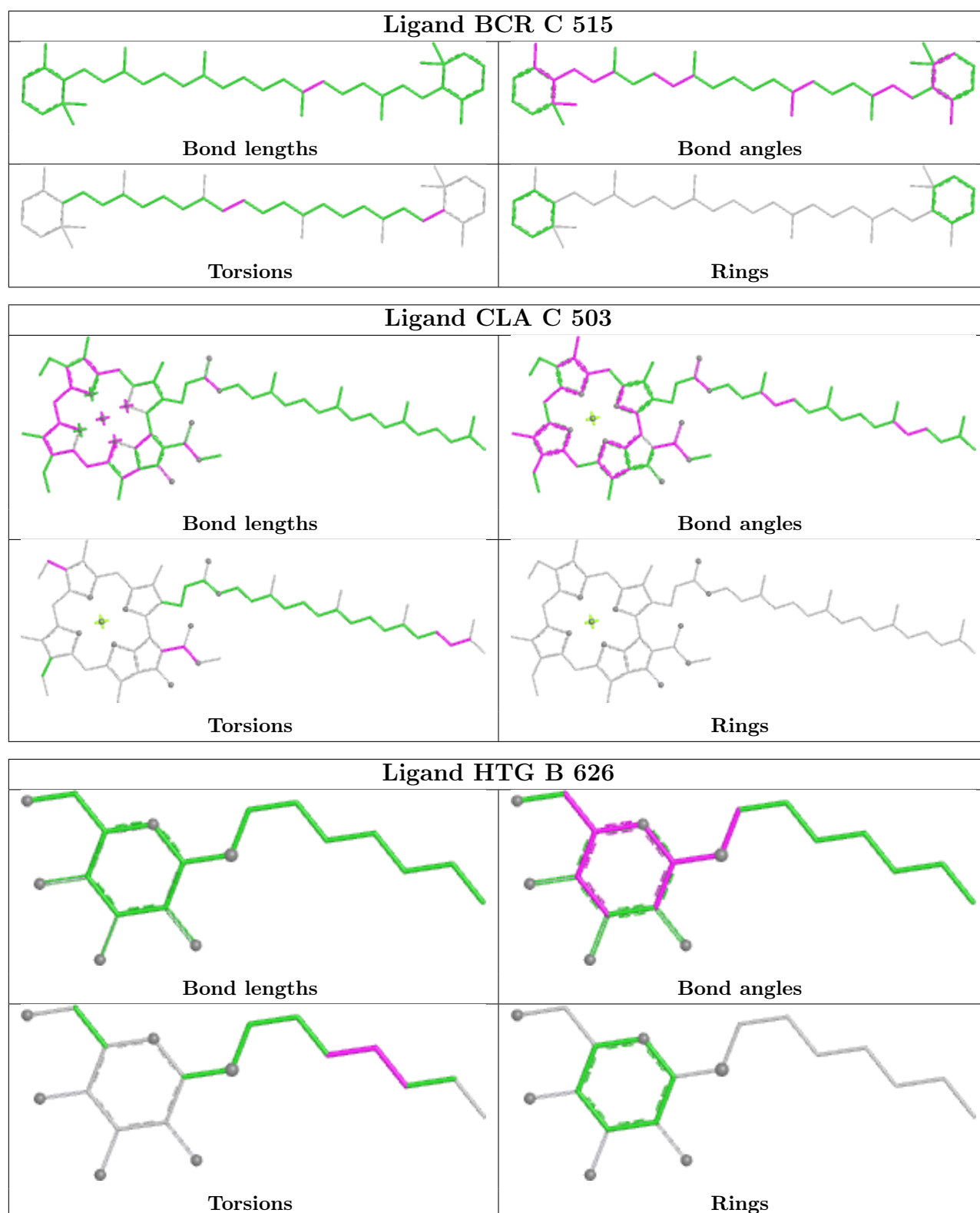


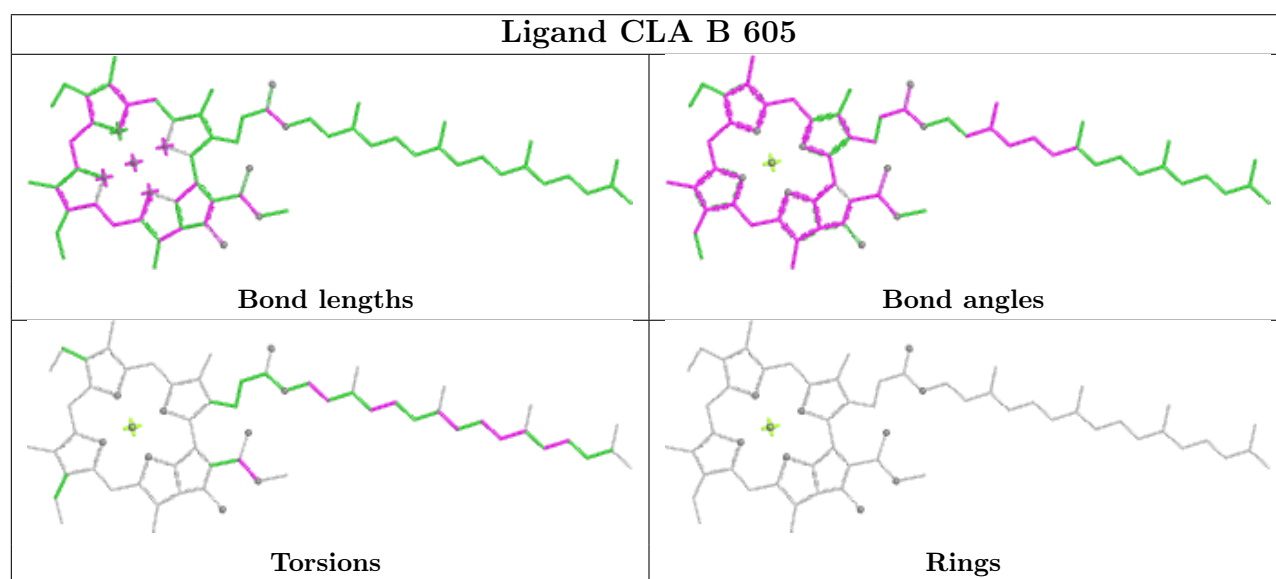
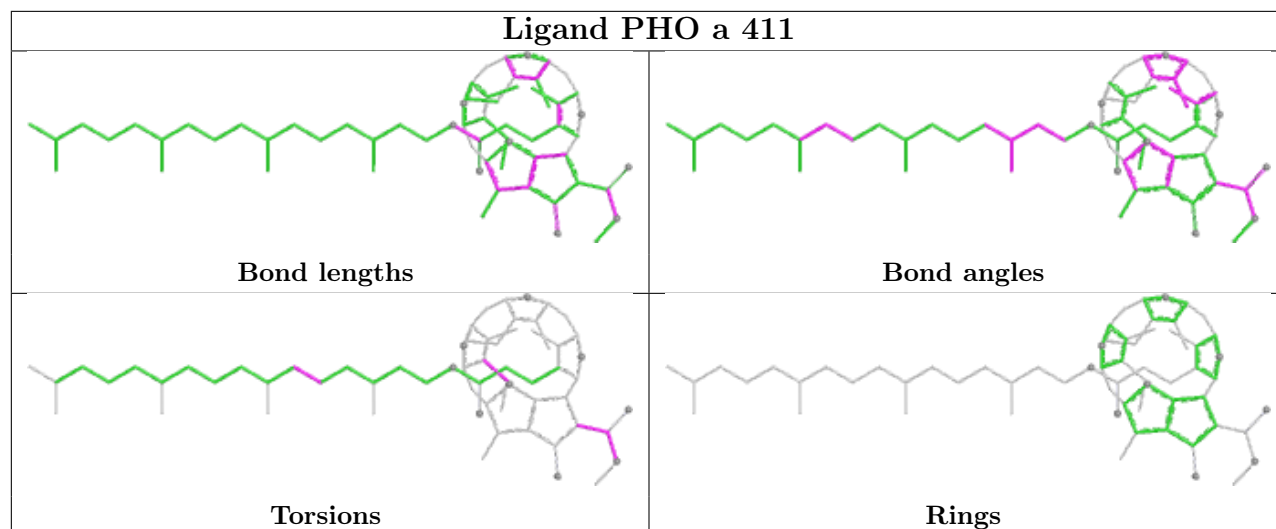


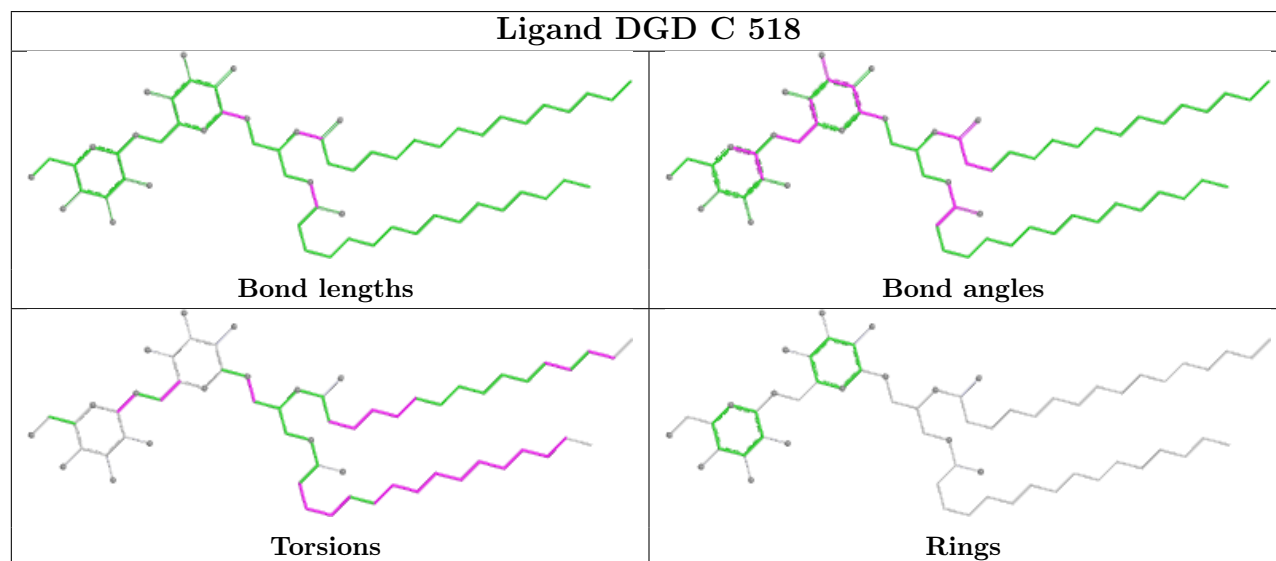
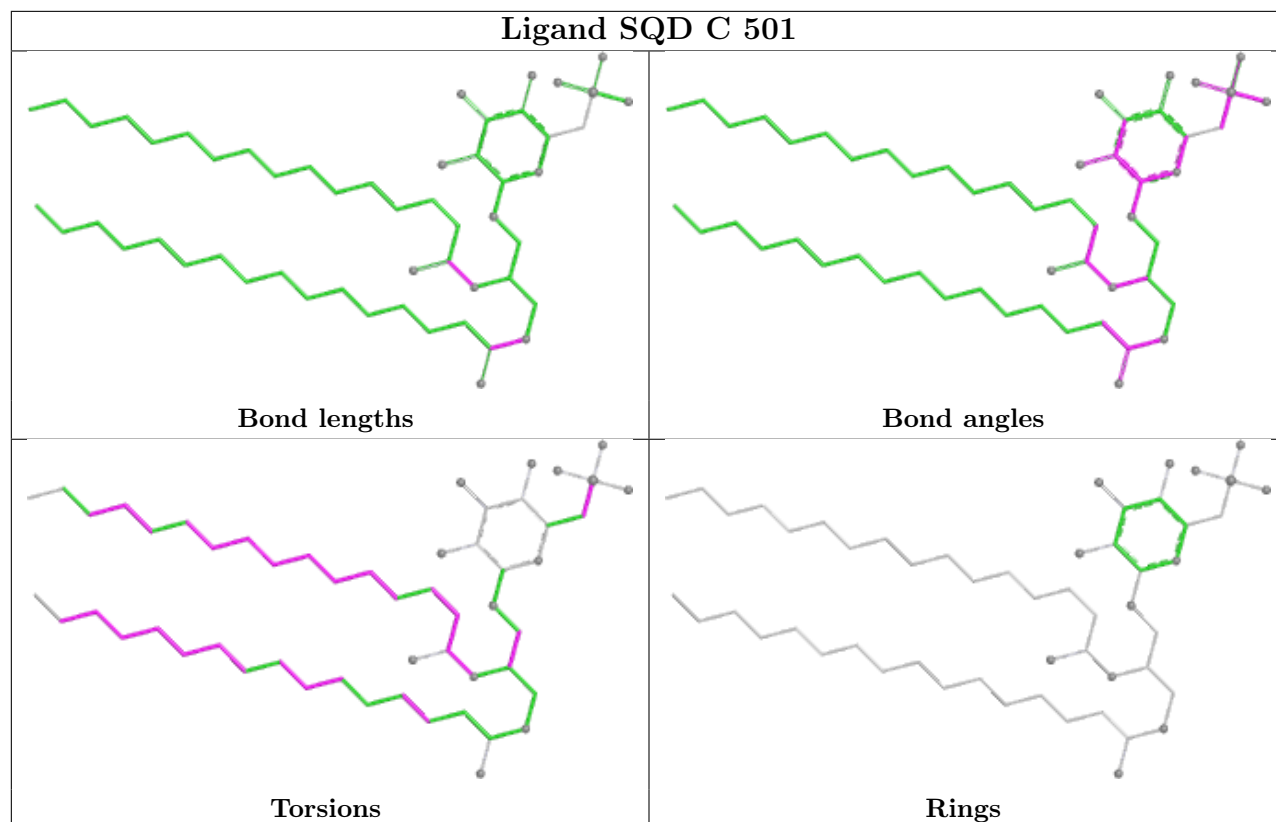




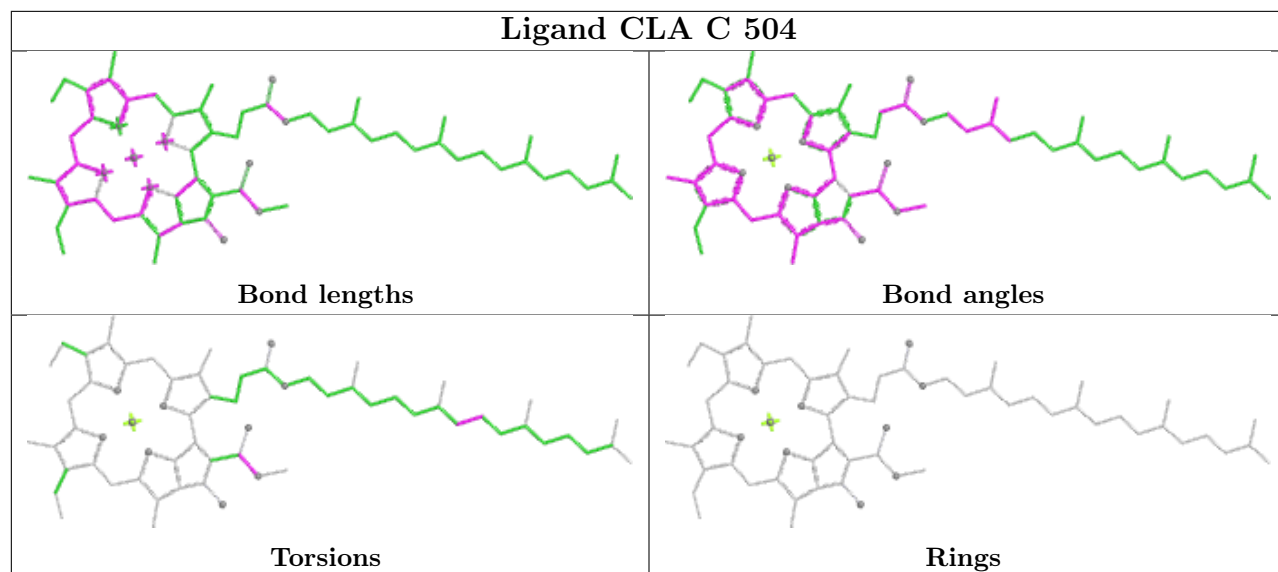




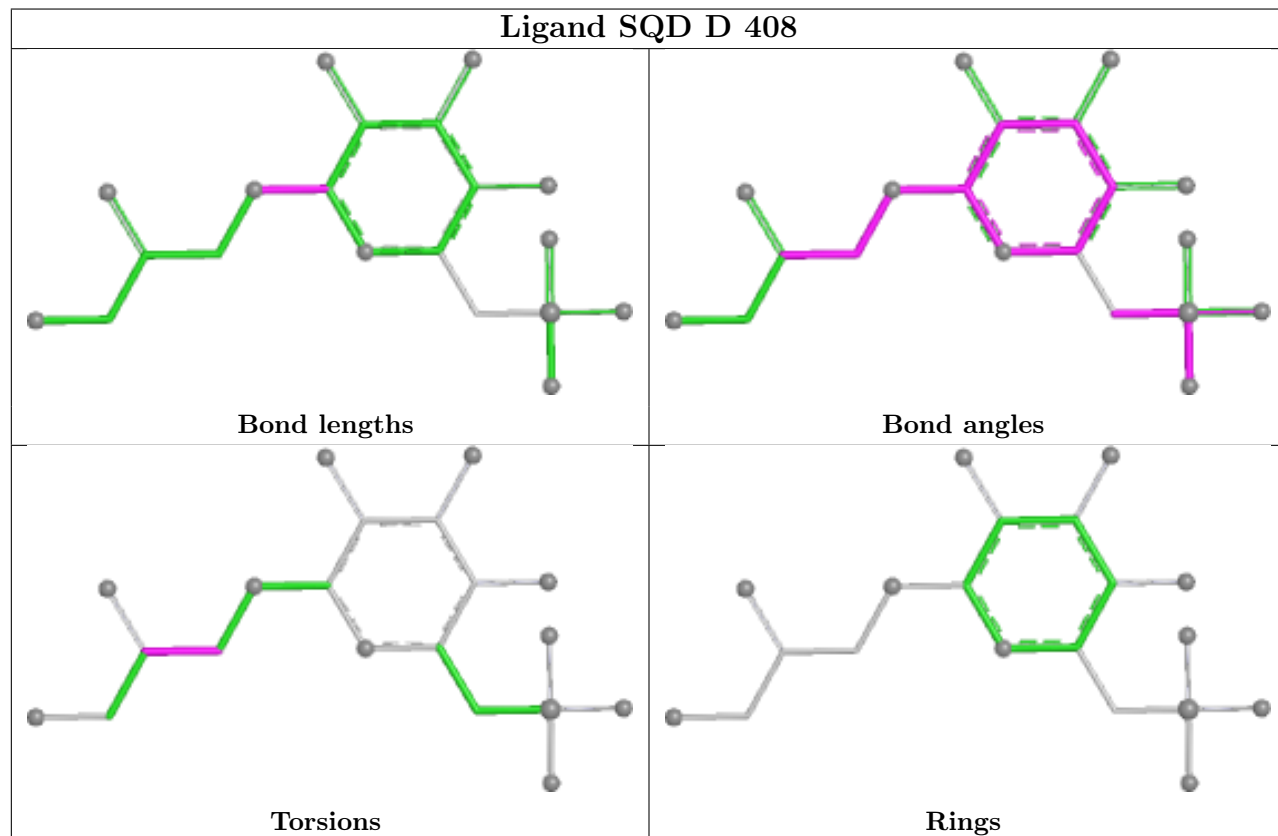


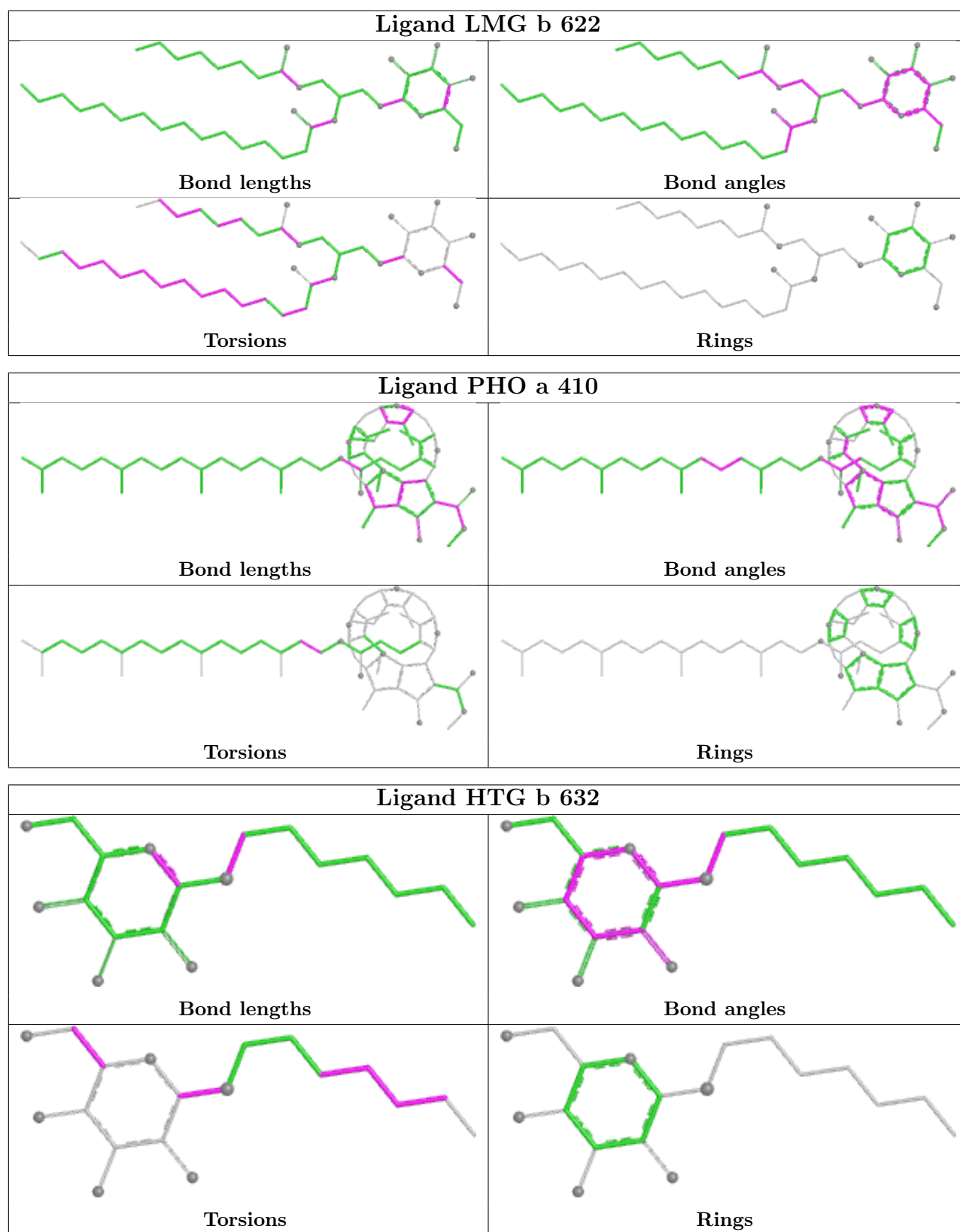


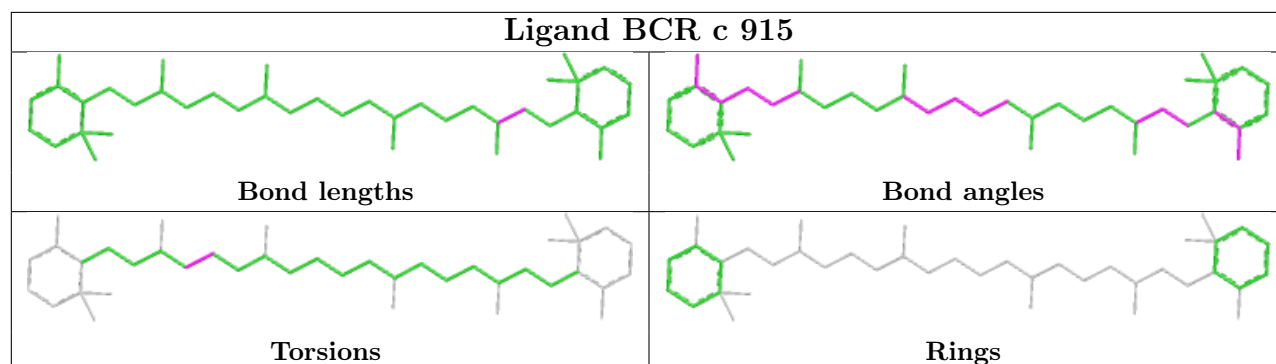
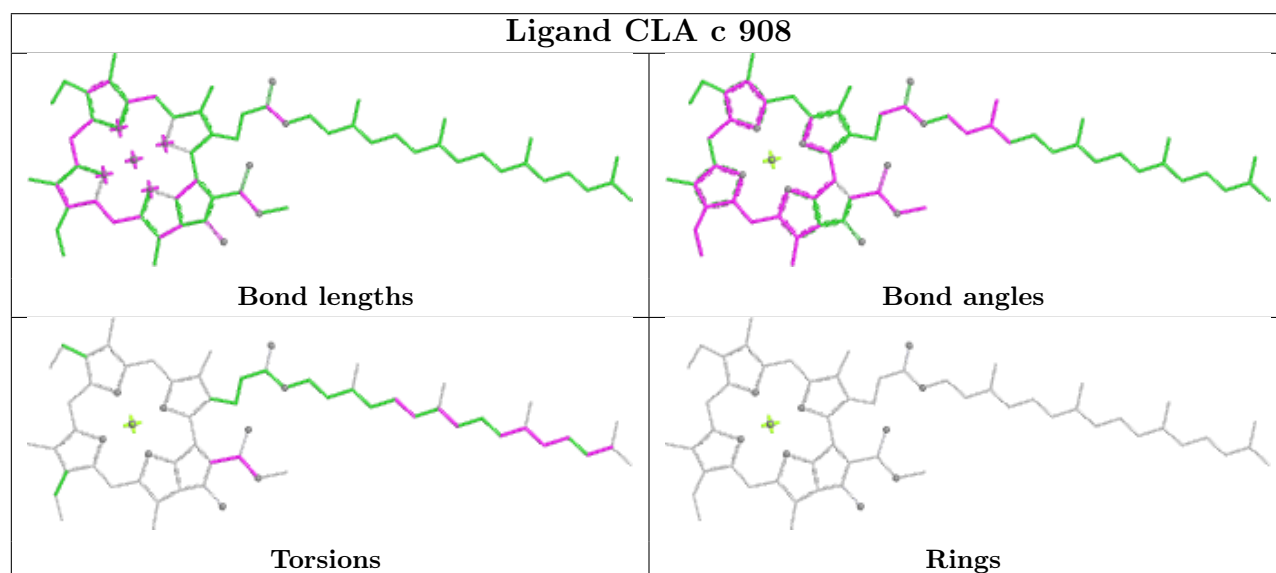
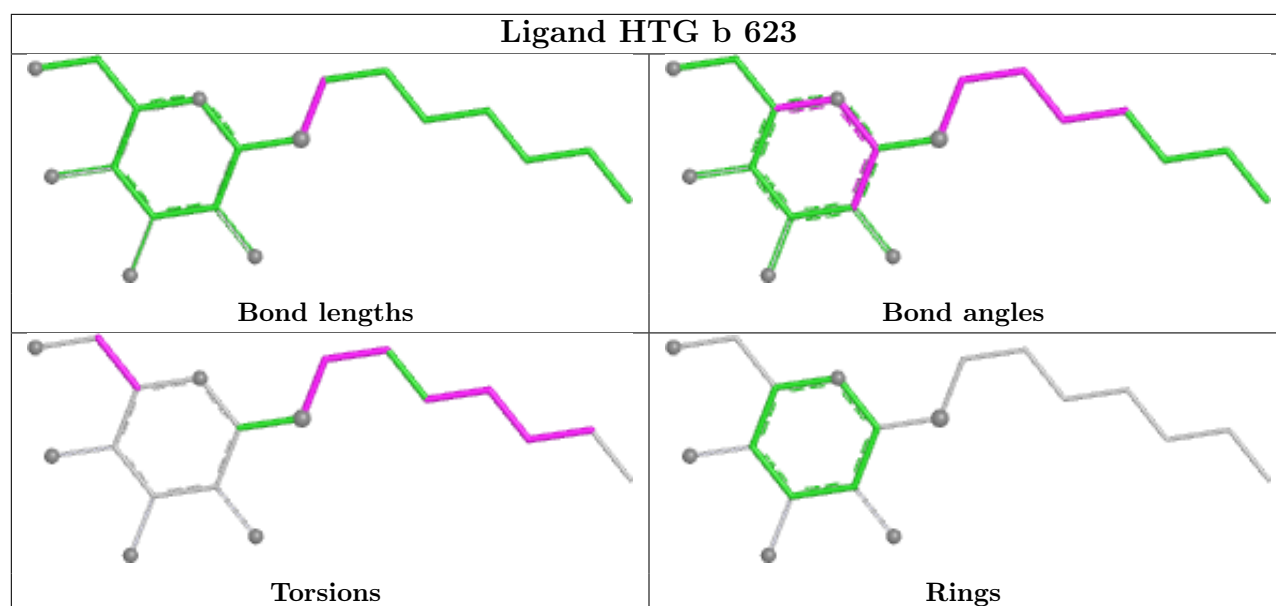
Ligand CLA C 504

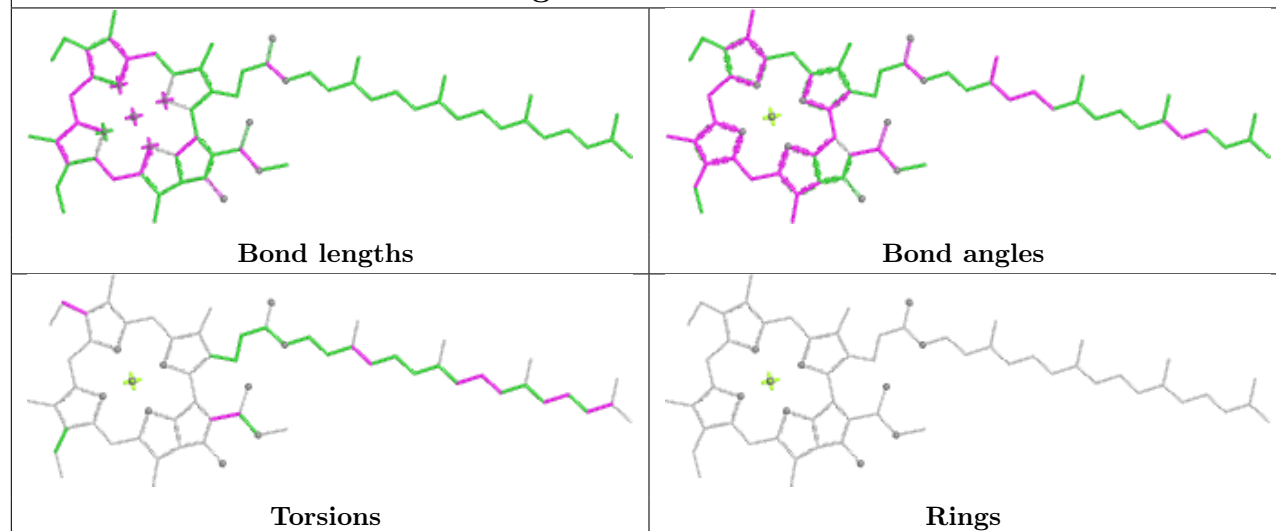
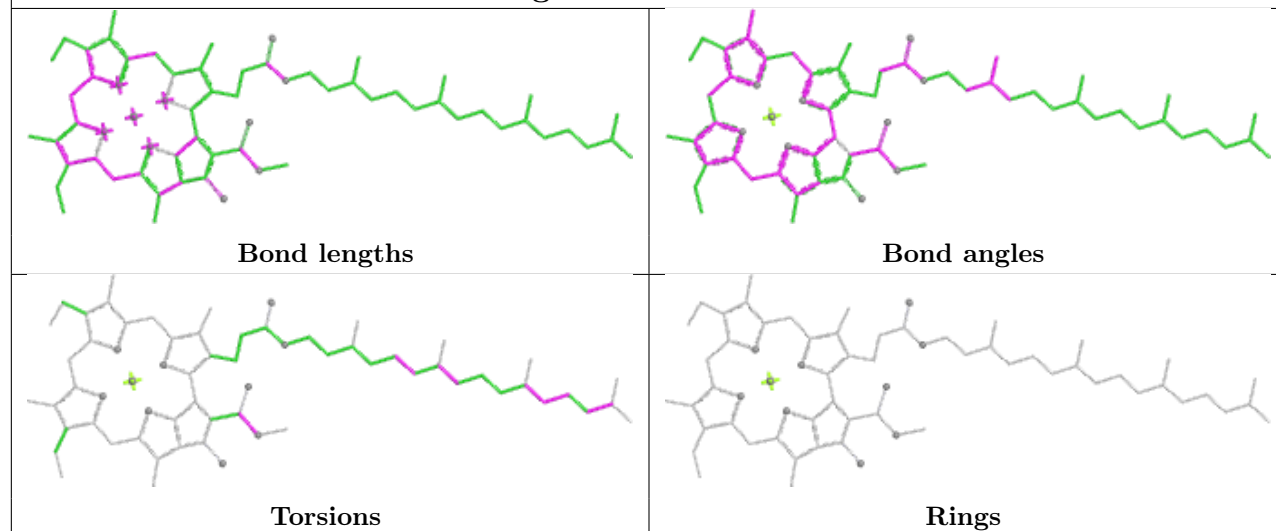


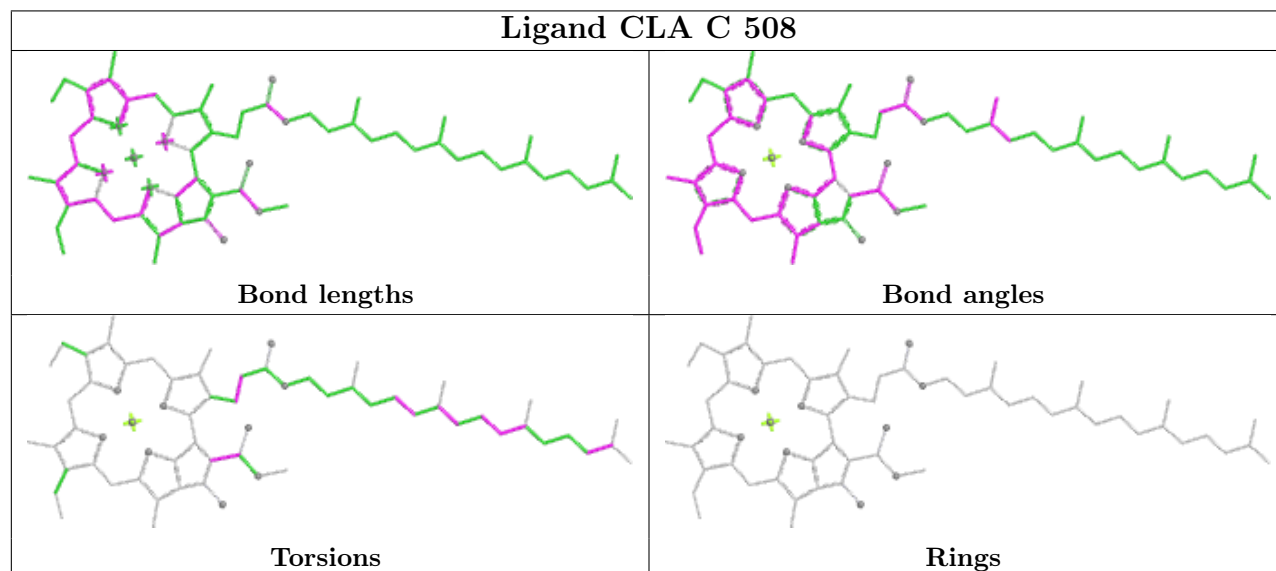
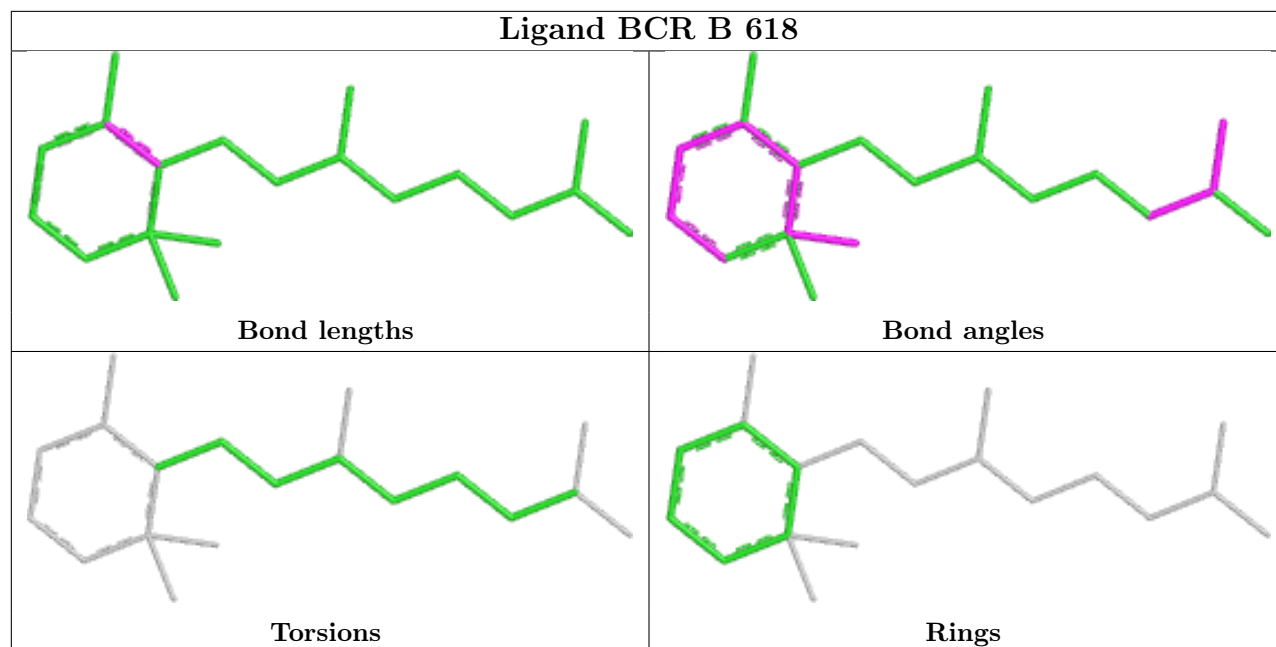
Ligand SQD D 408

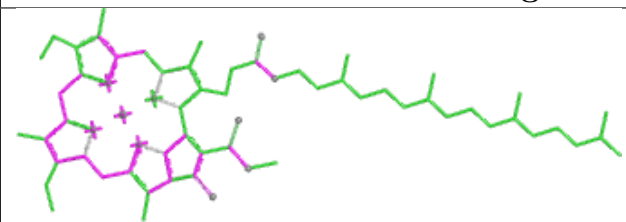
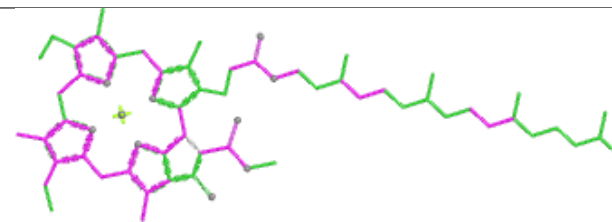
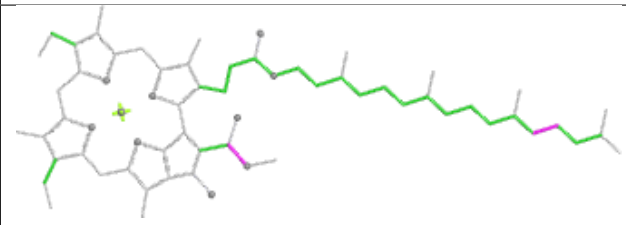
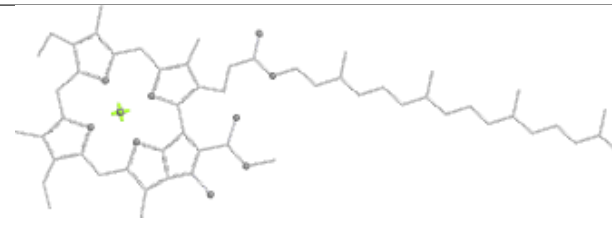




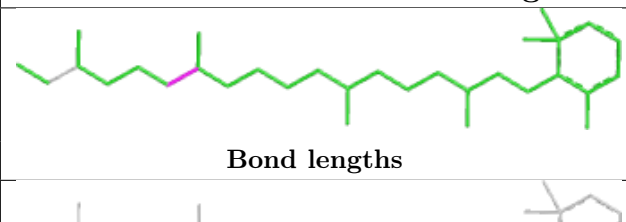
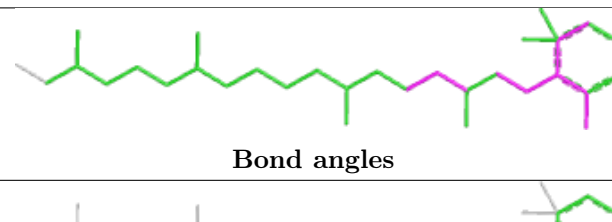


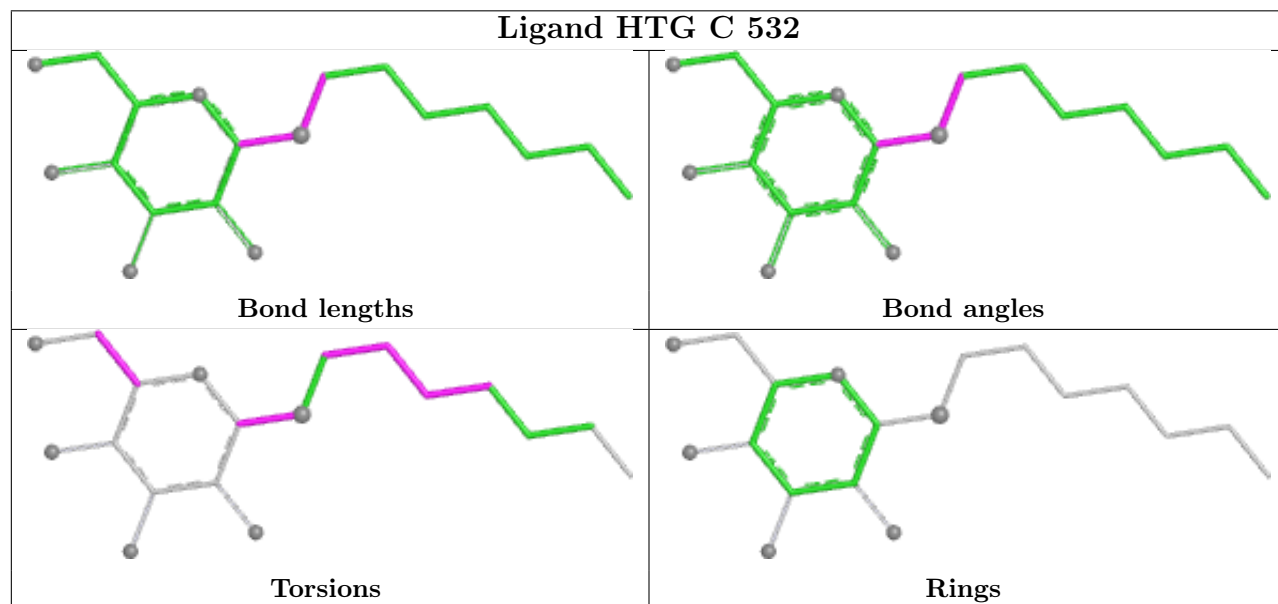
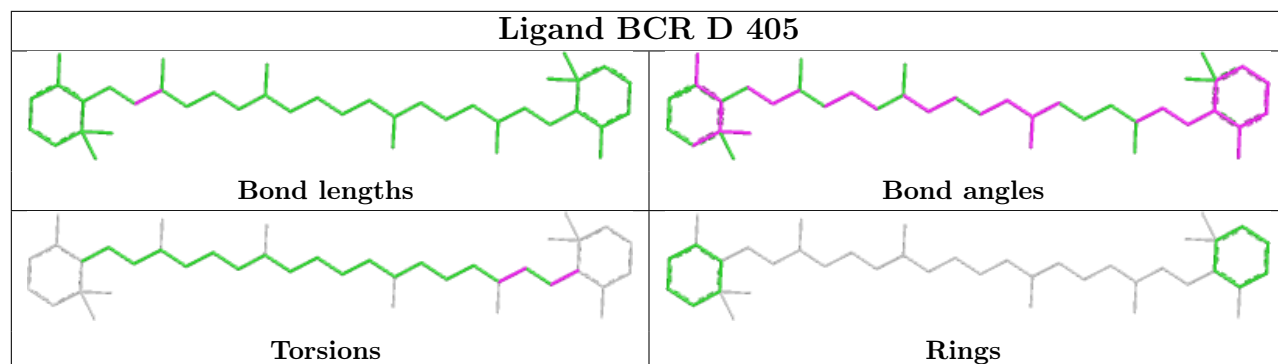
Ligand CLA B 606**Ligand CLA C 509**

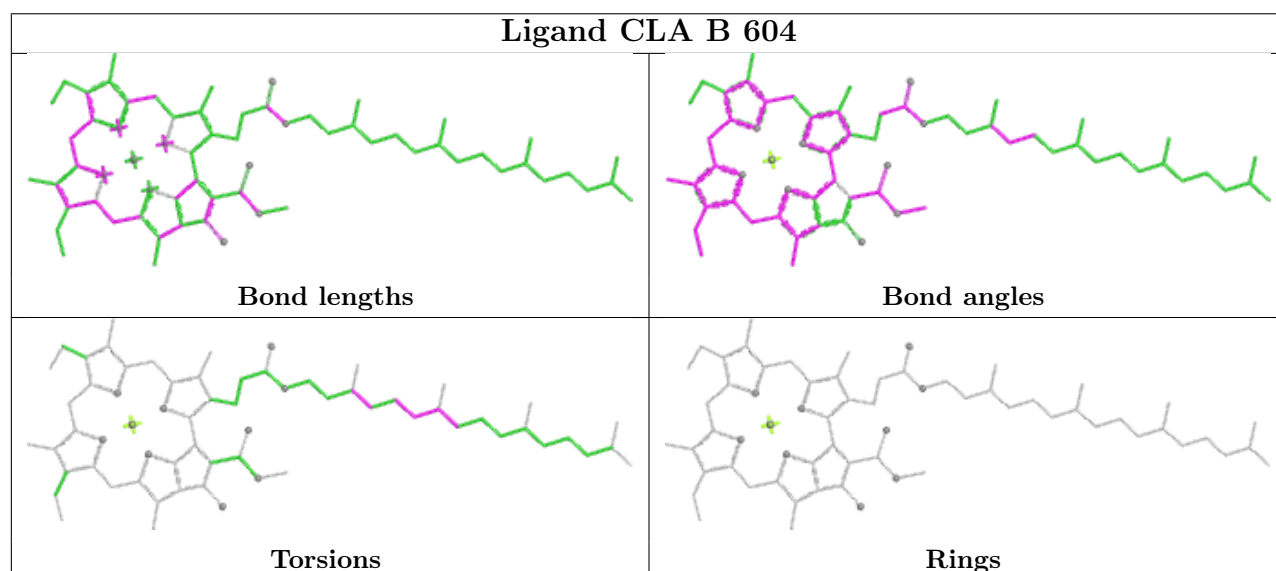
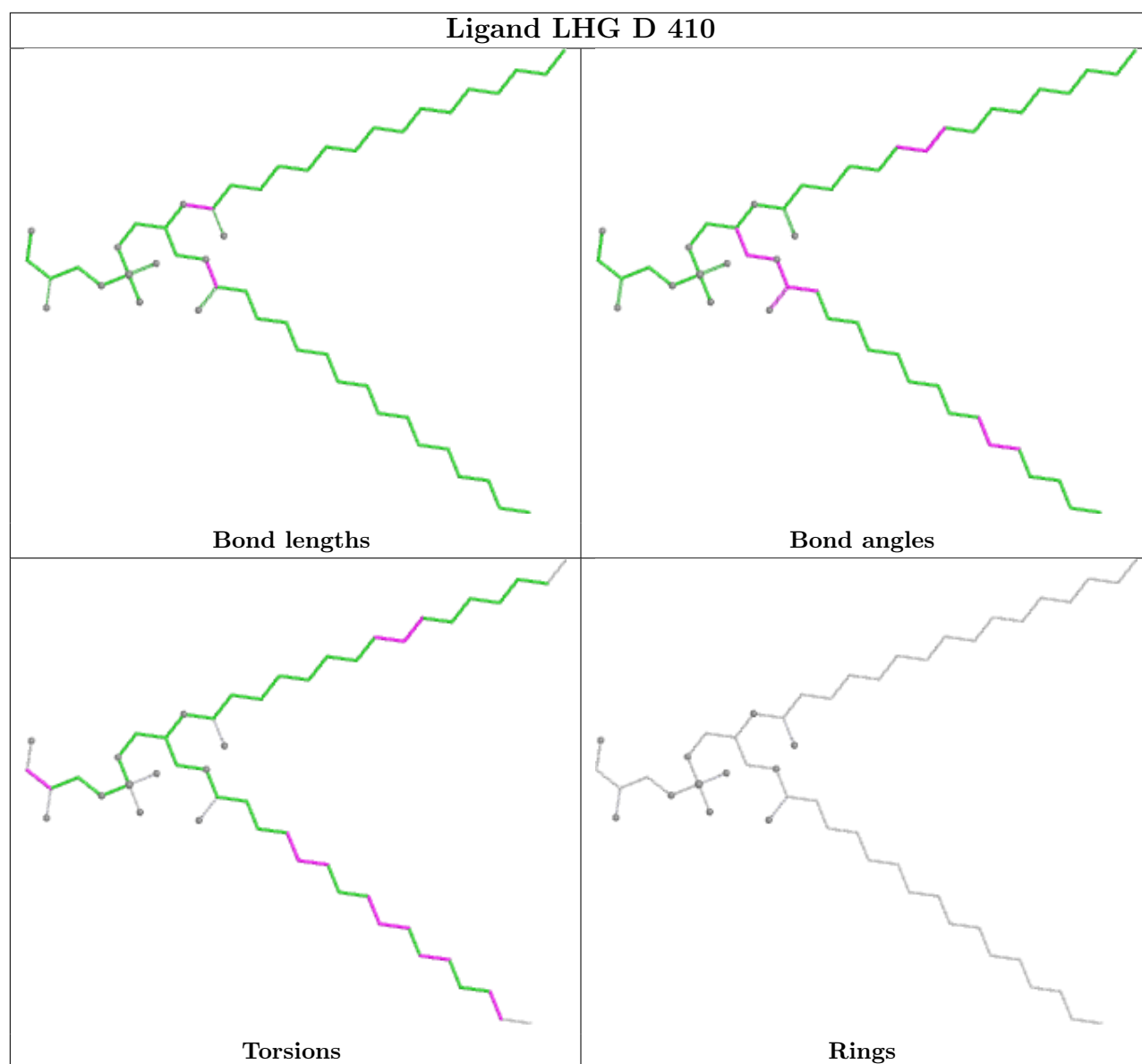


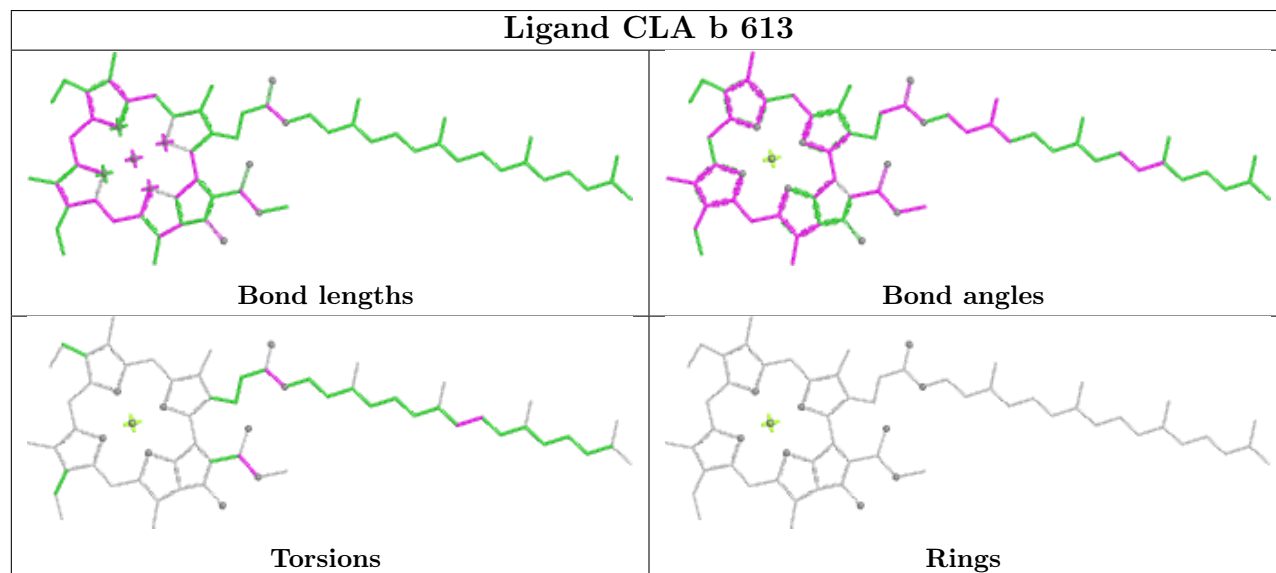
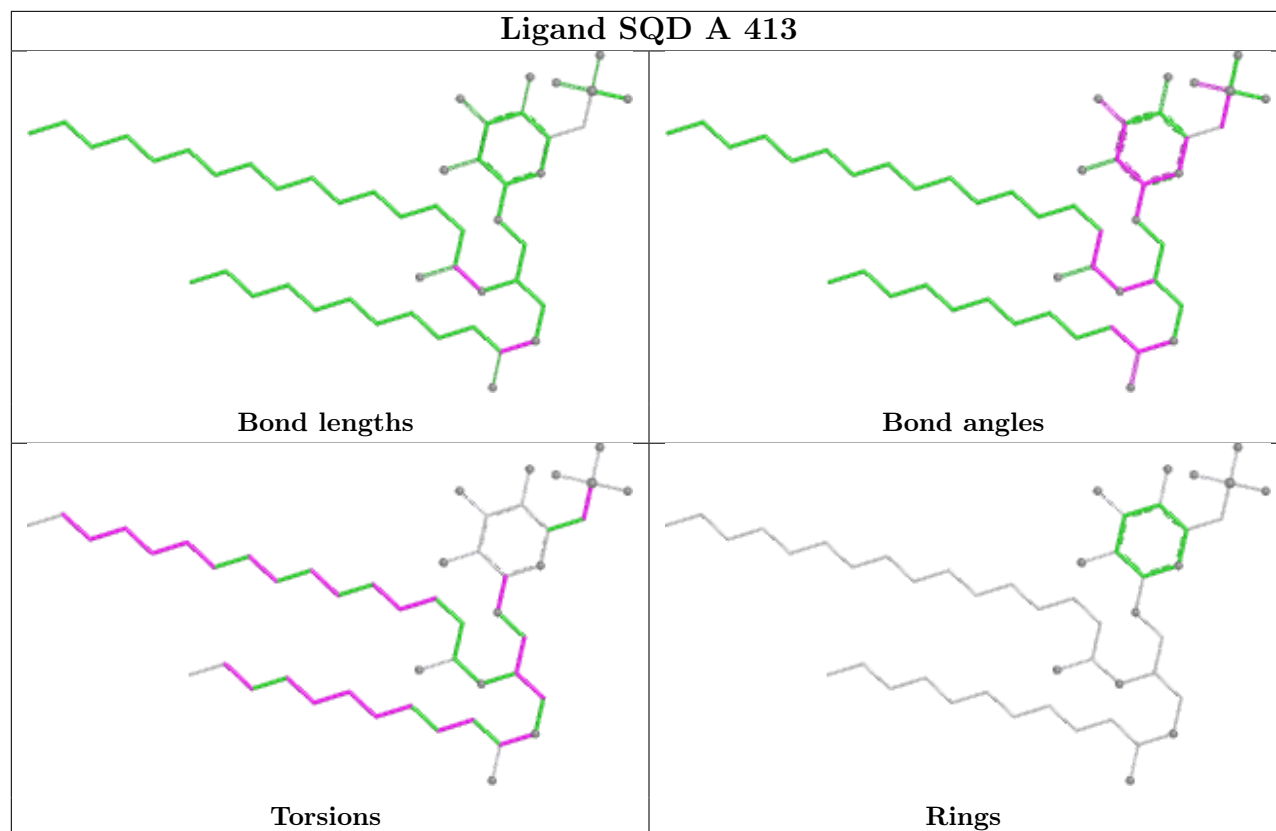
Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

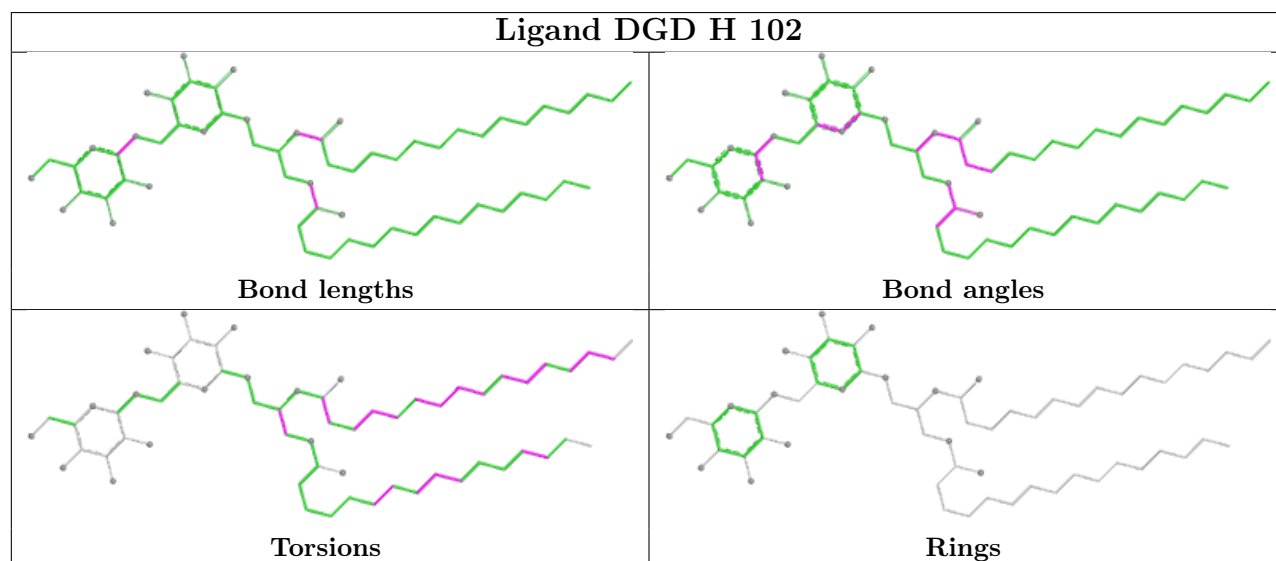
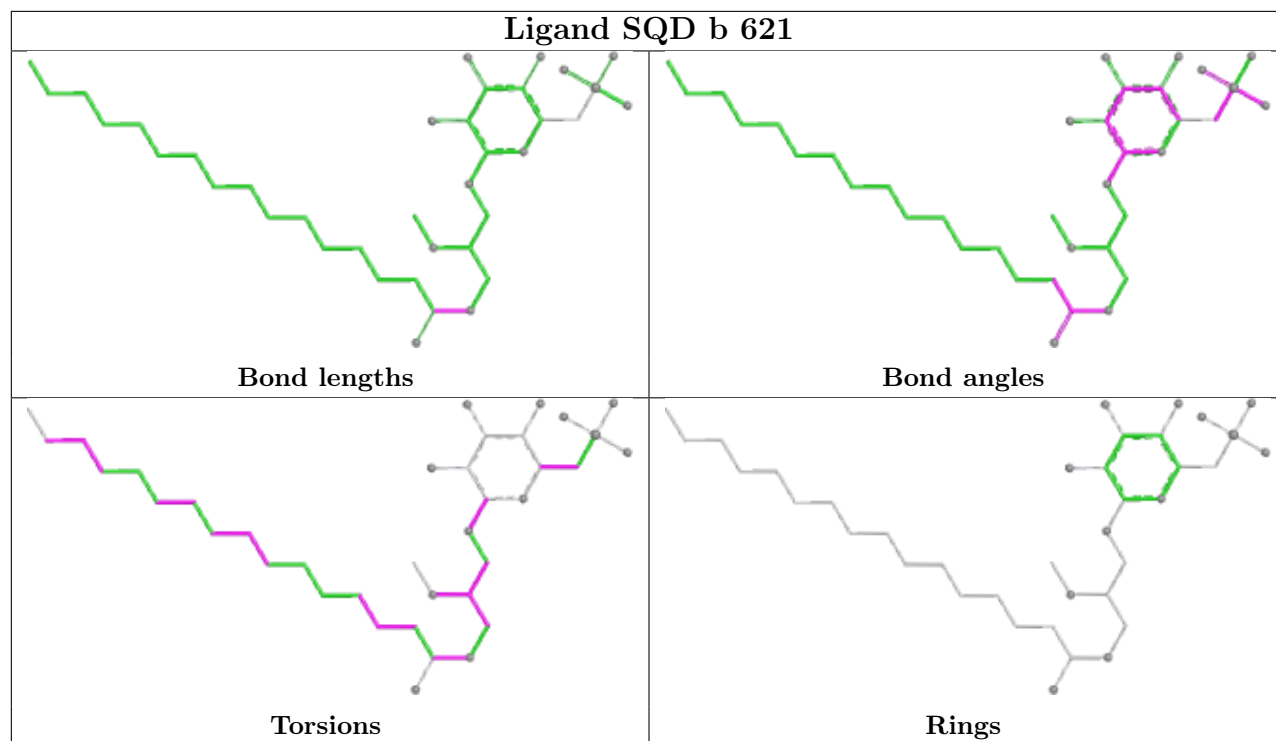
Ligand LMT T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

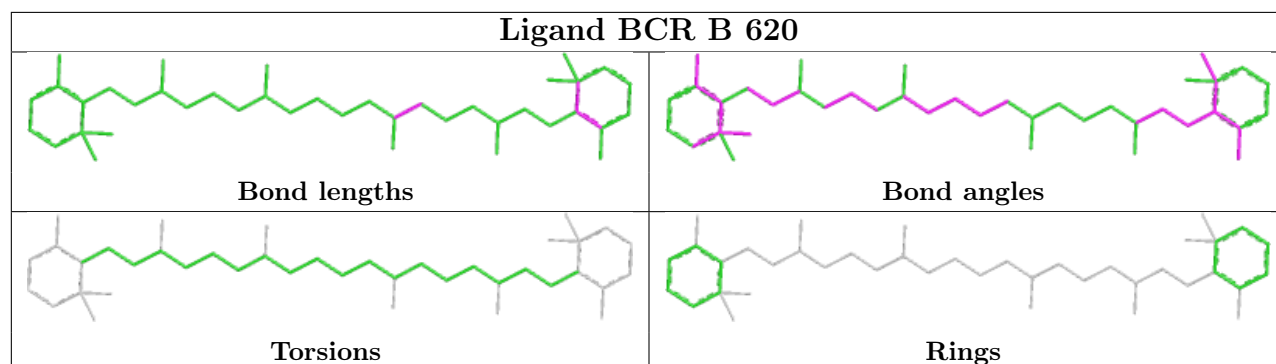
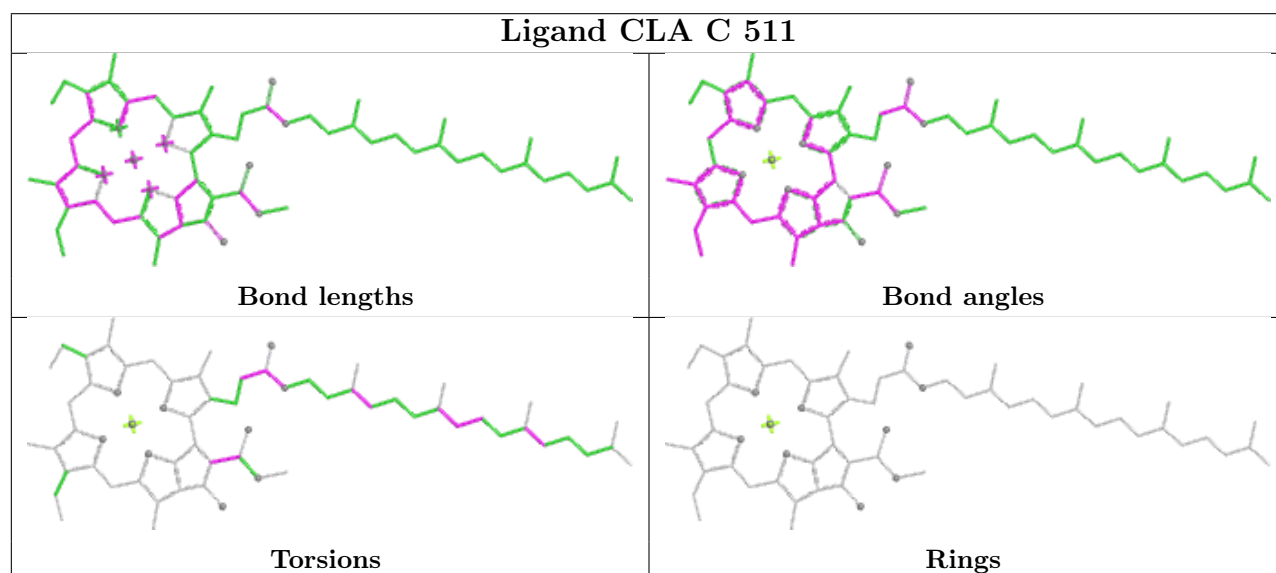
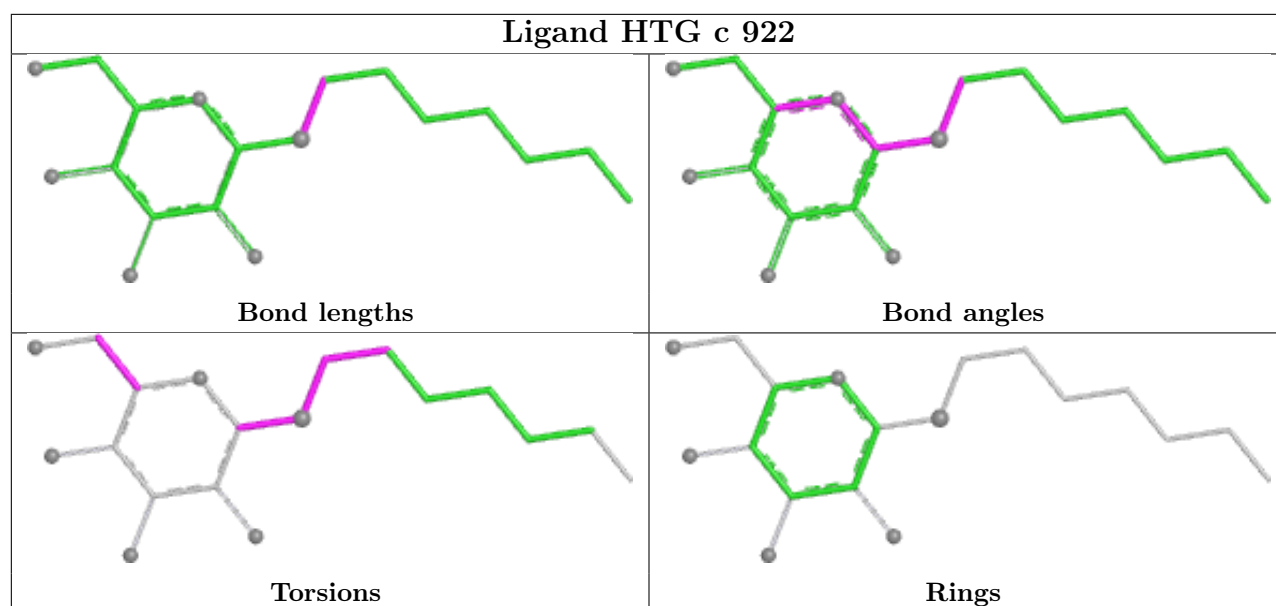
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

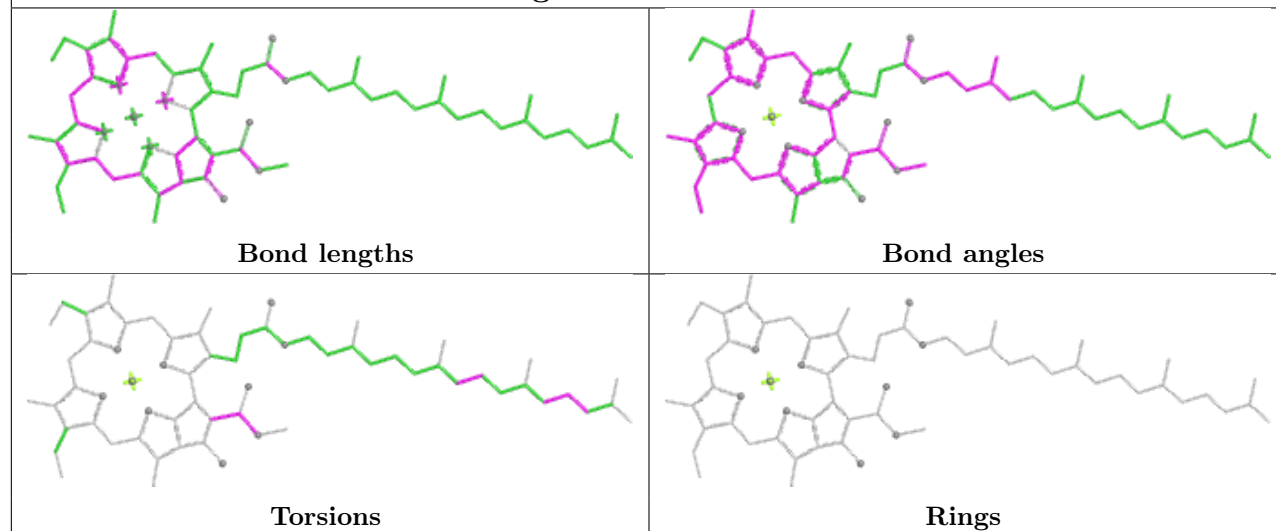
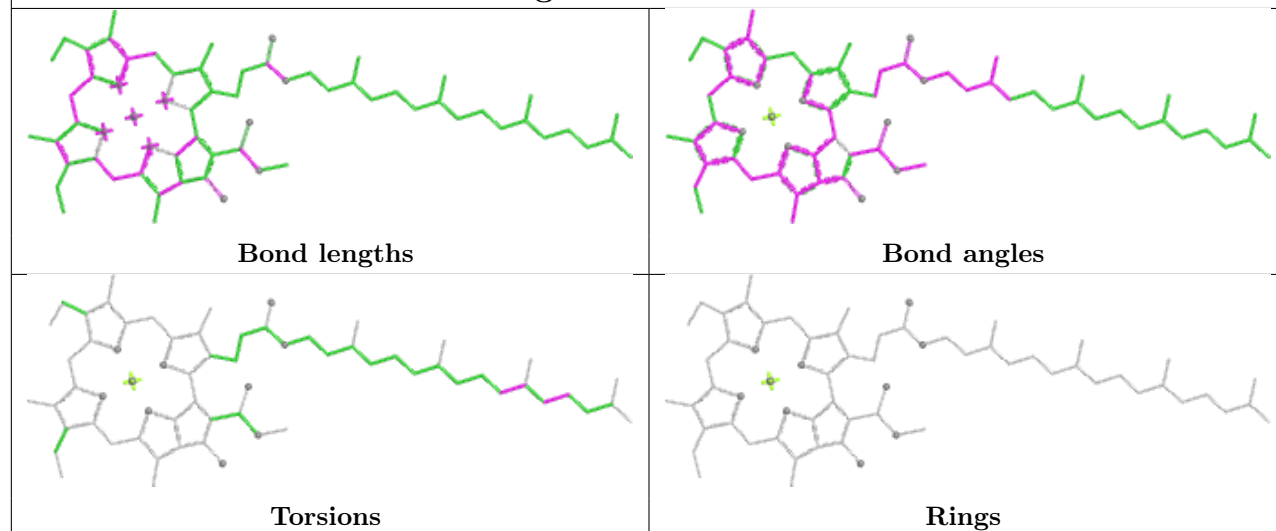


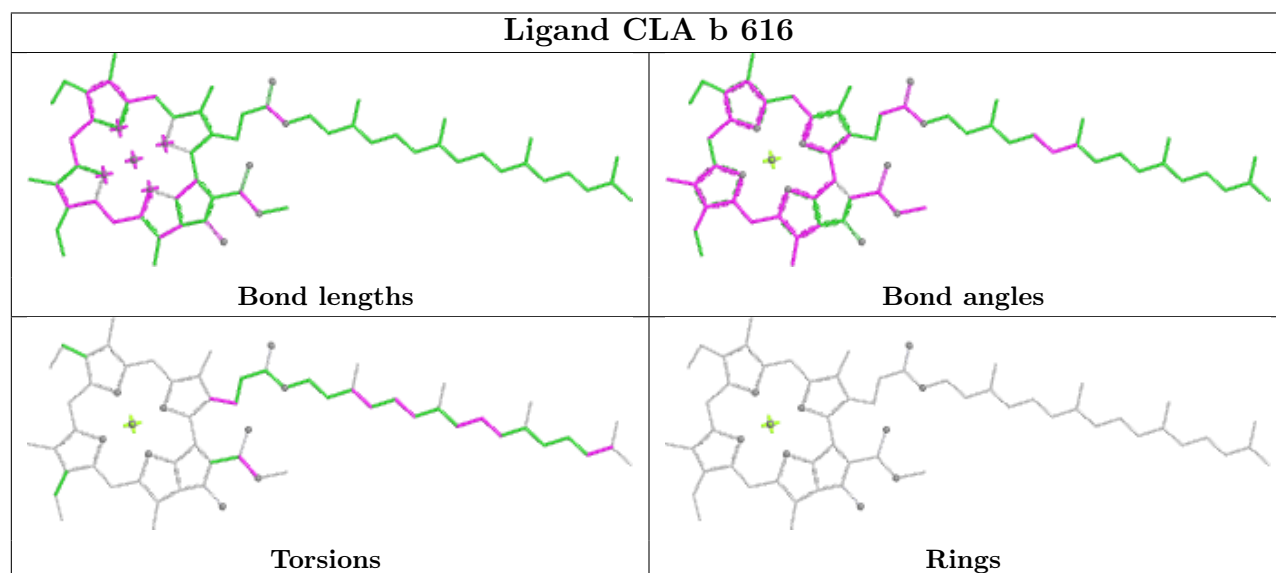
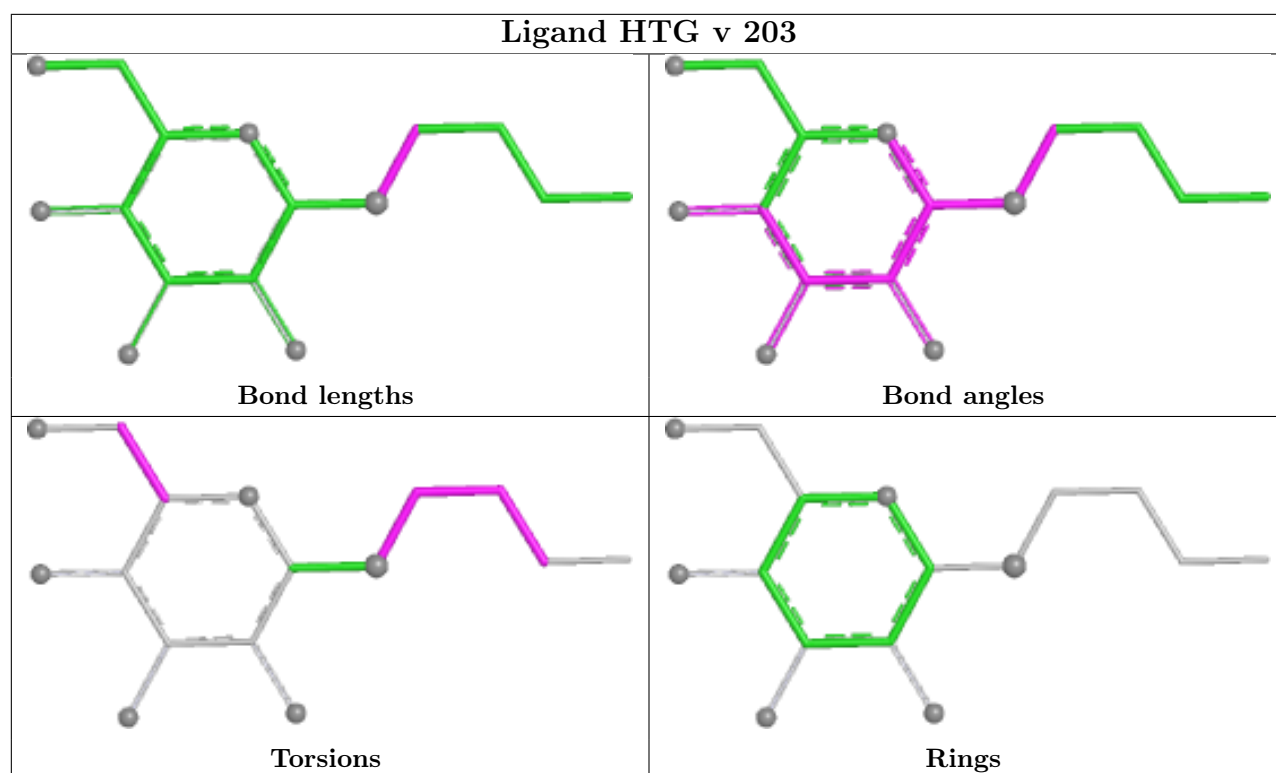




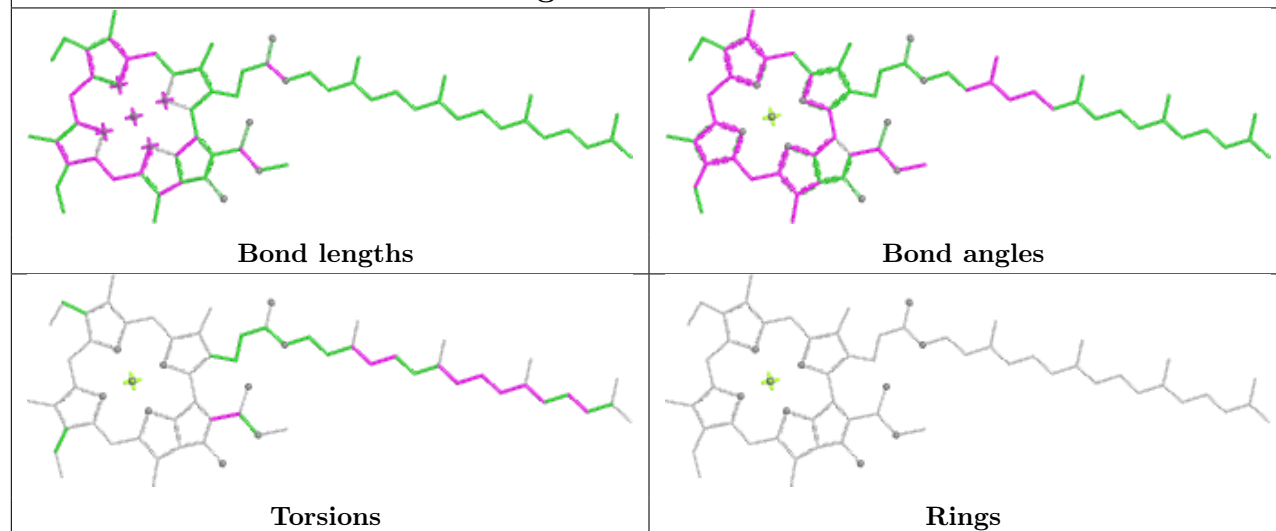




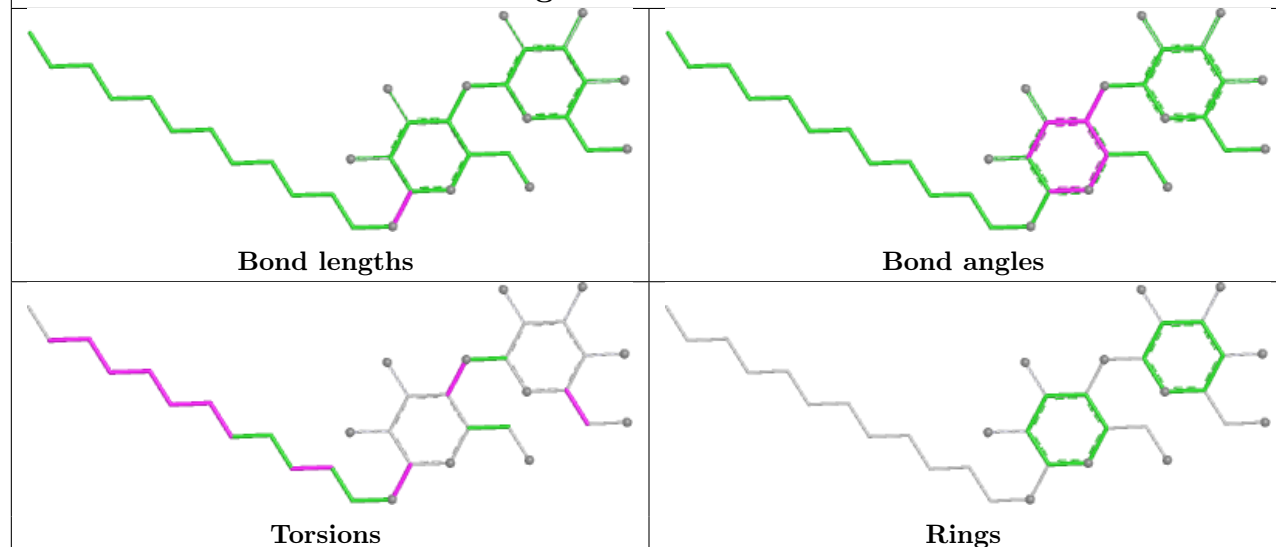
Ligand CLA B 608**Ligand CLA b 603**



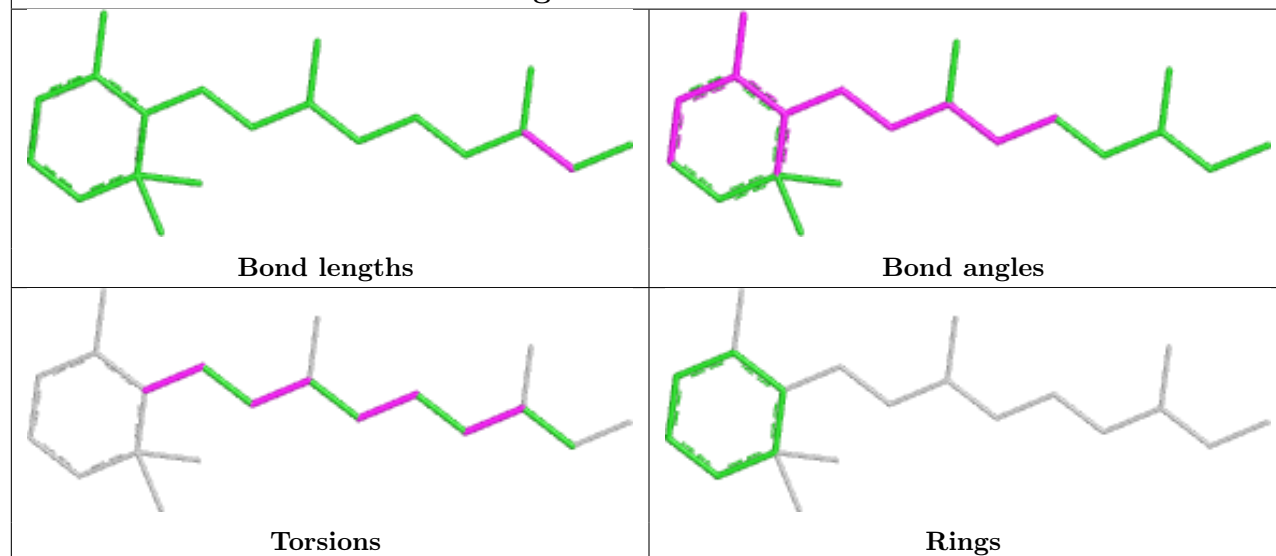
Ligand CLA c 905

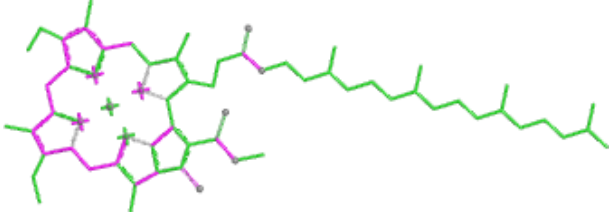
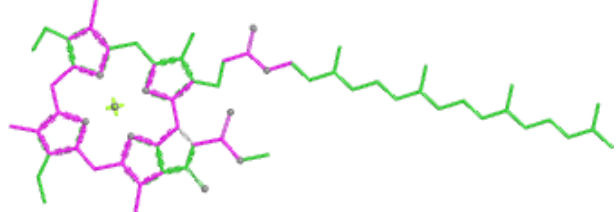
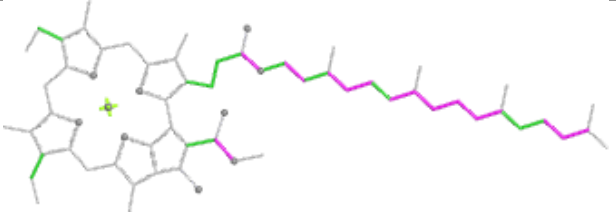
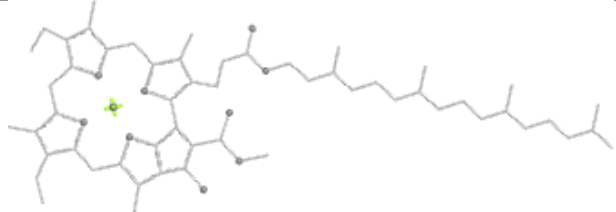
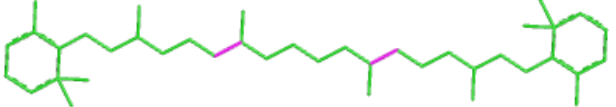
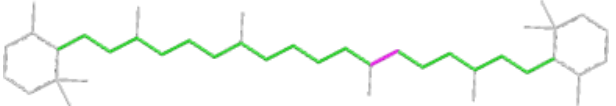
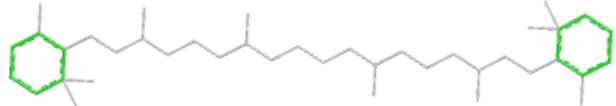
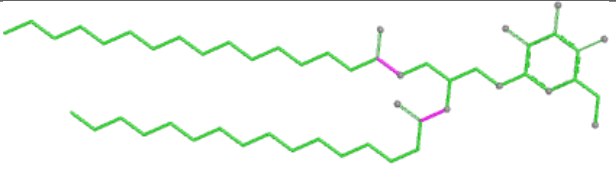
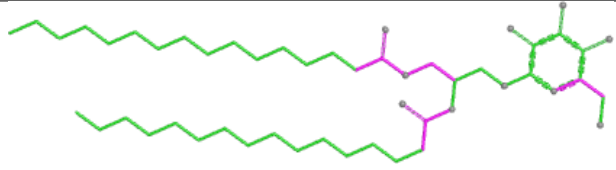
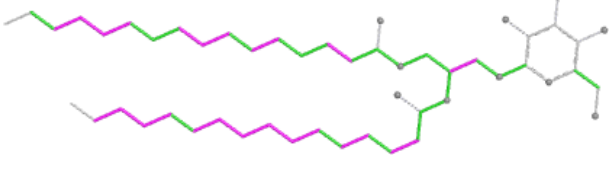
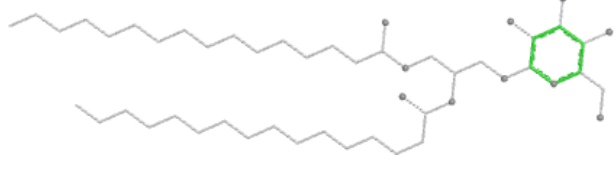


Ligand LMT I 102

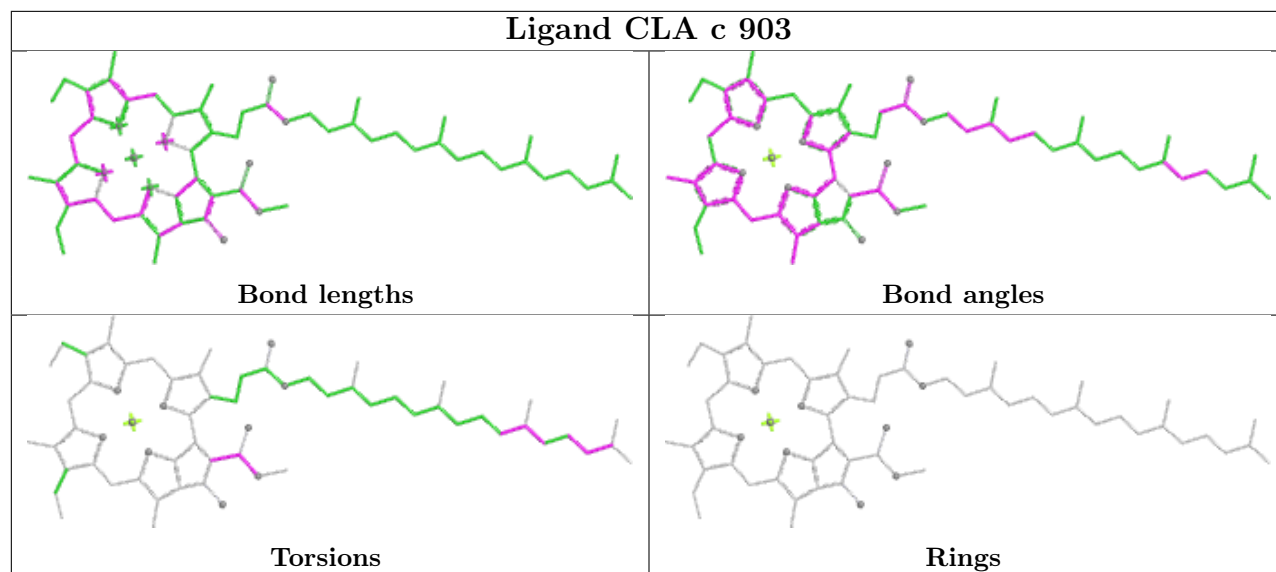


Ligand BCR b 618

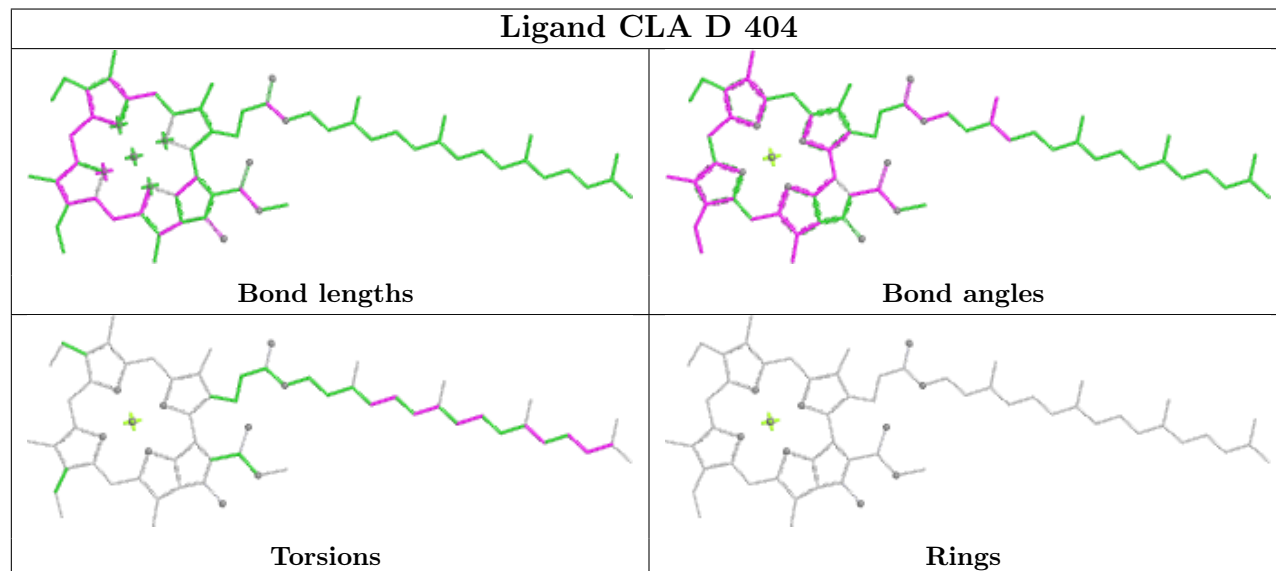


Ligand CLA C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

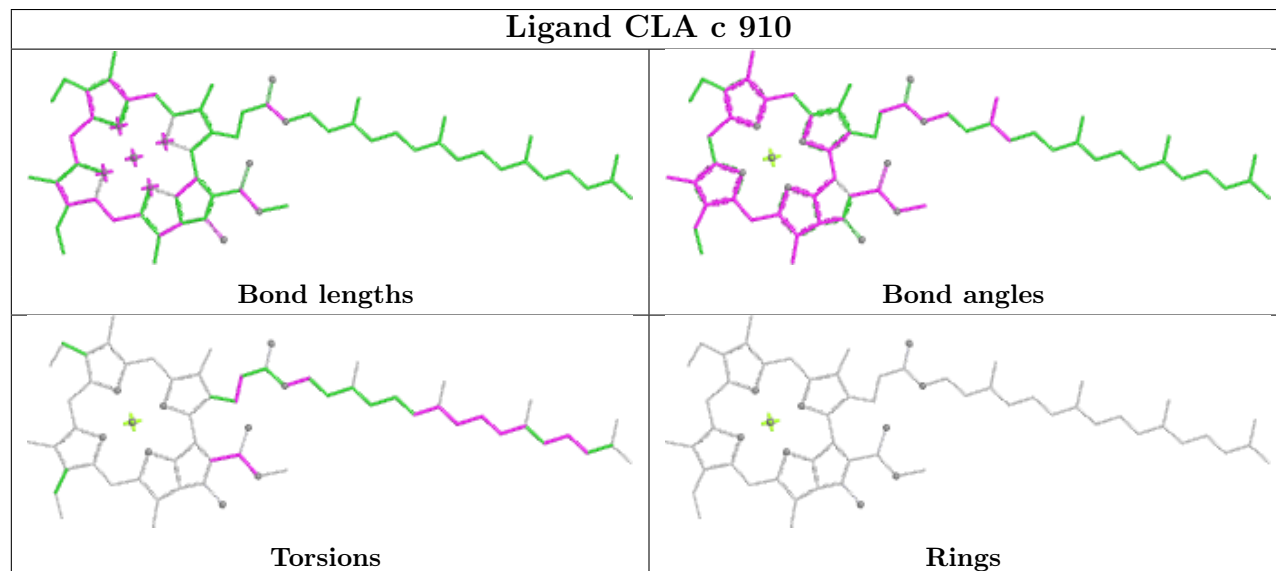
Ligand CLA c 903

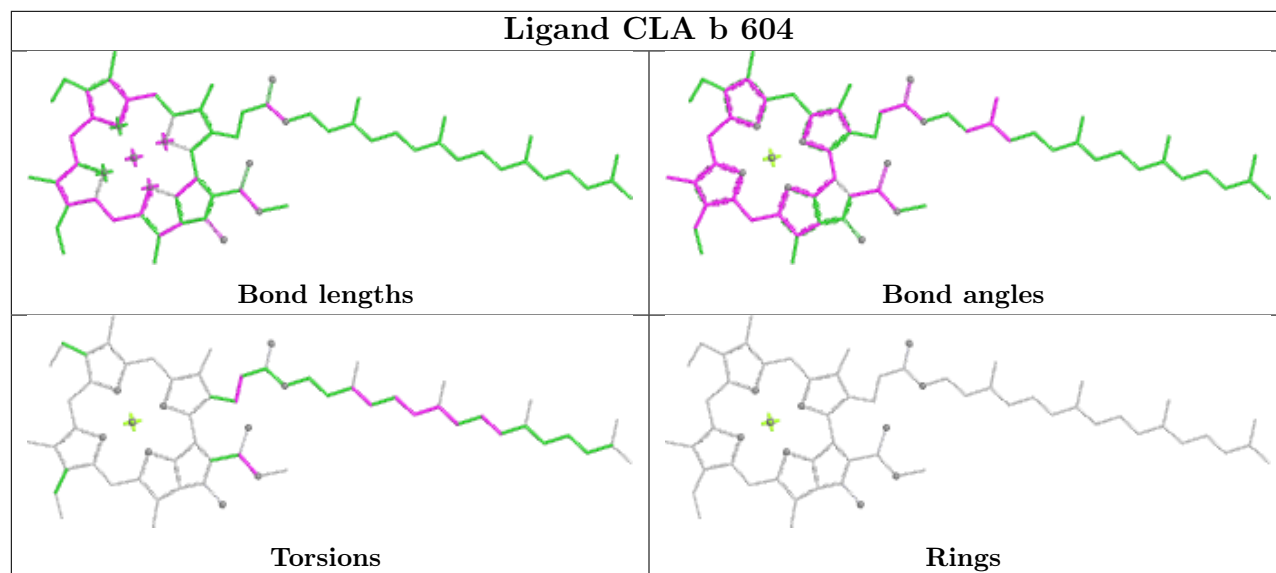
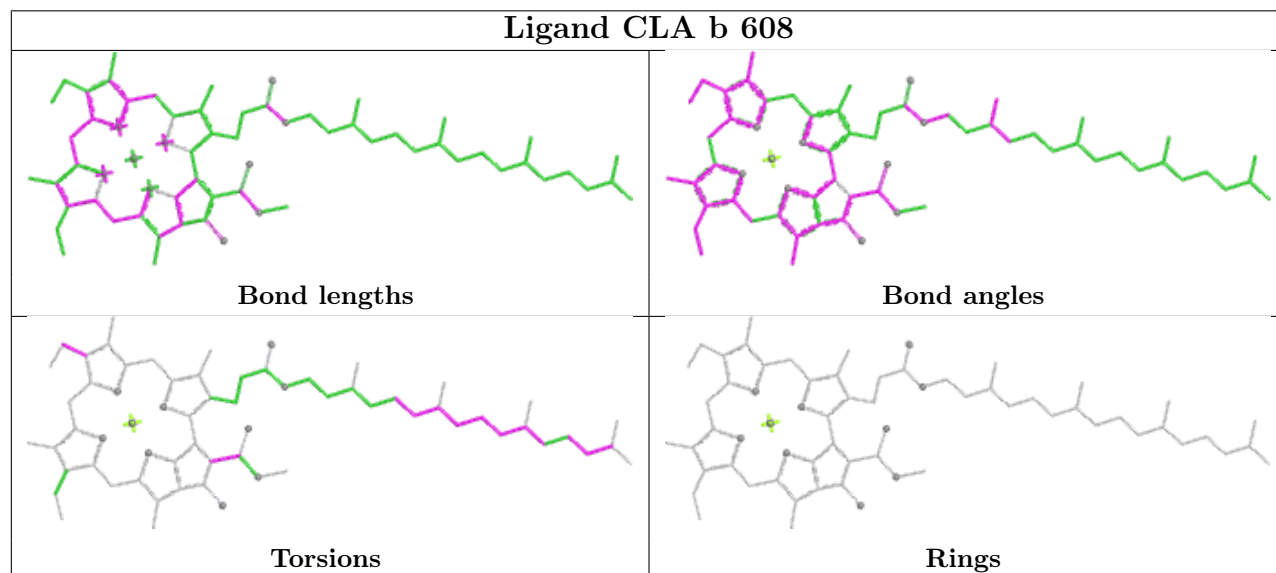
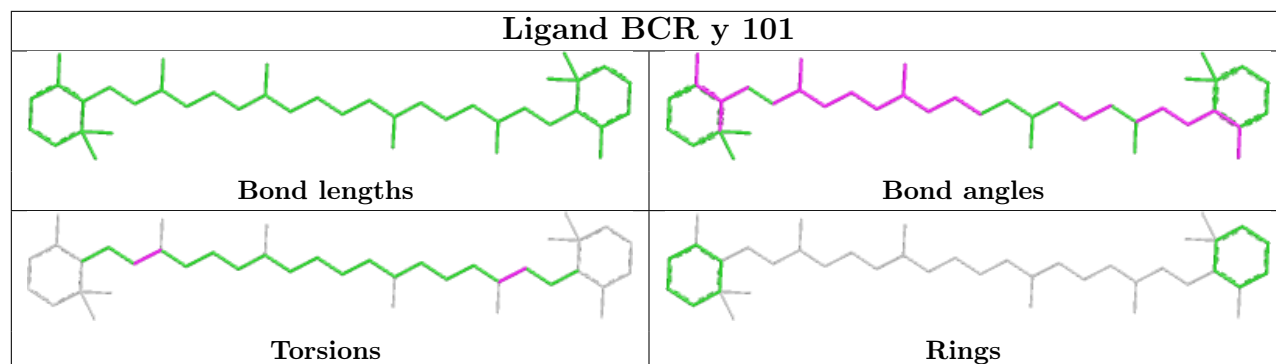


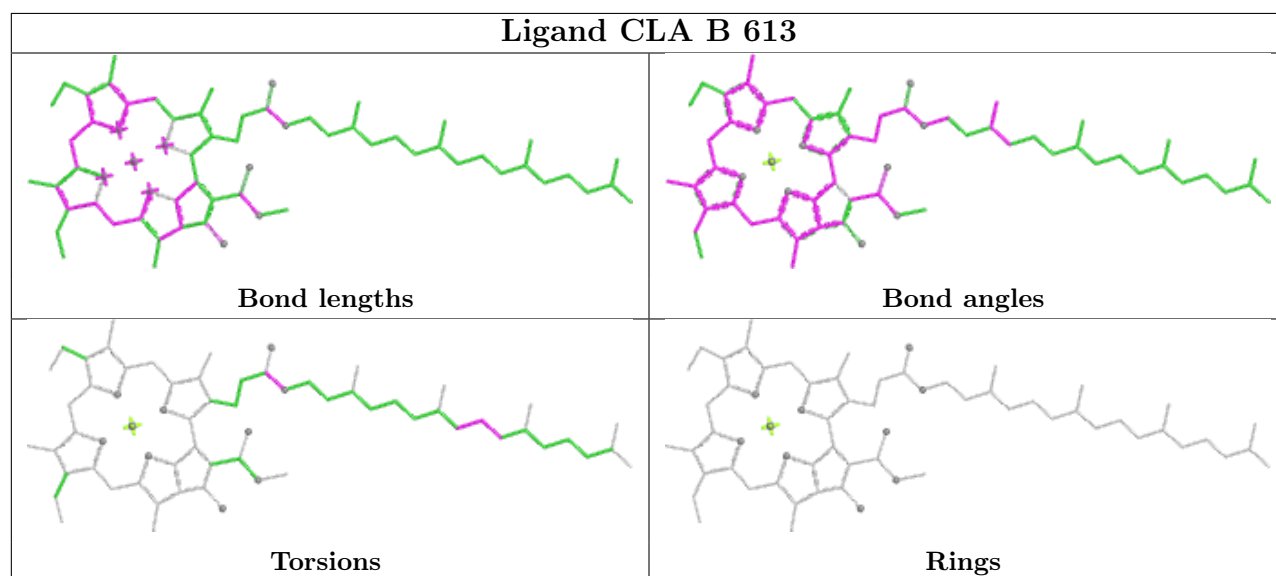
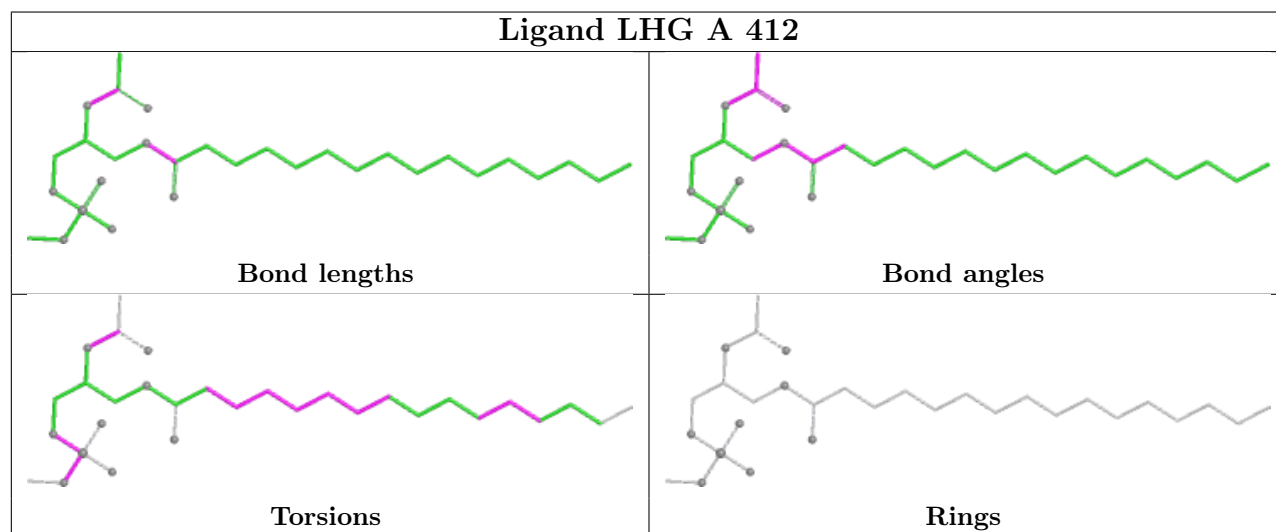
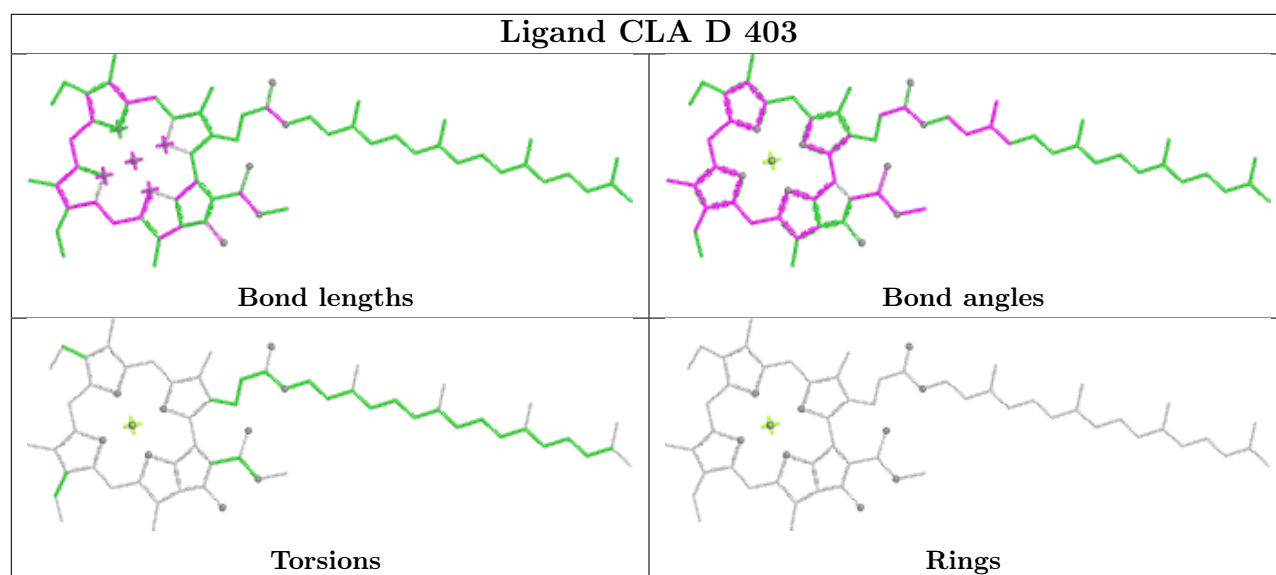
Ligand CLA D 404



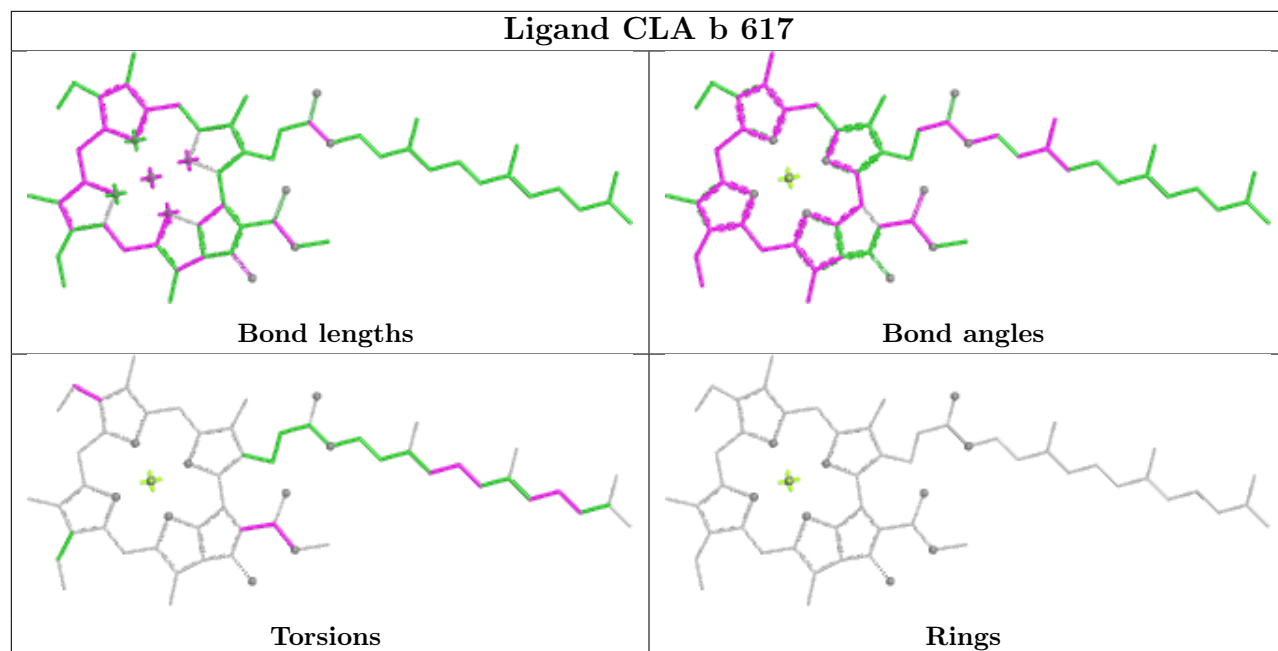
Ligand CLA c 910



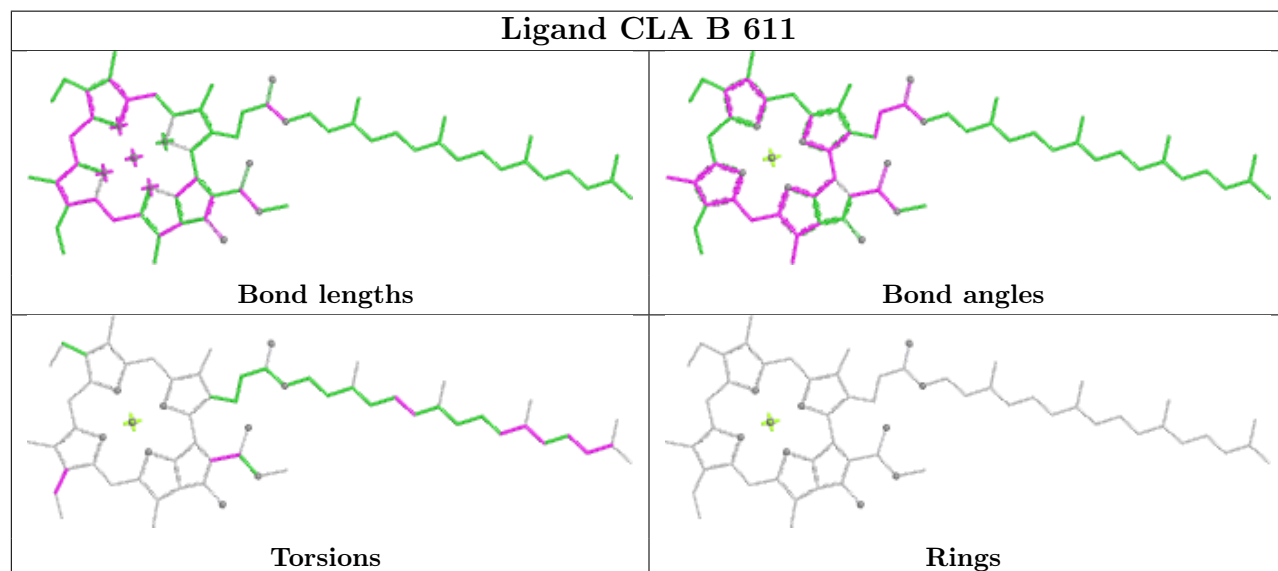




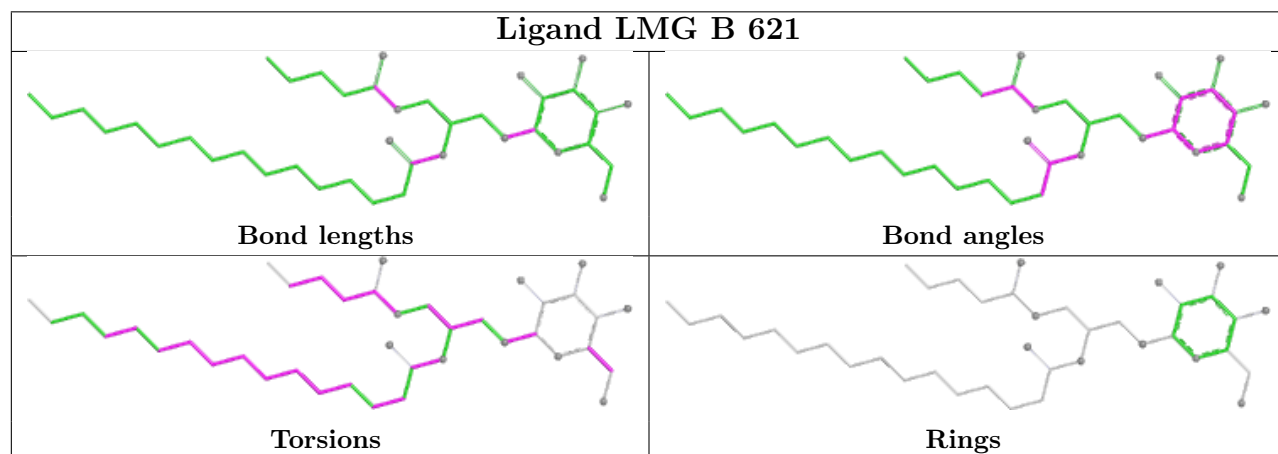
Ligand CLA b 617



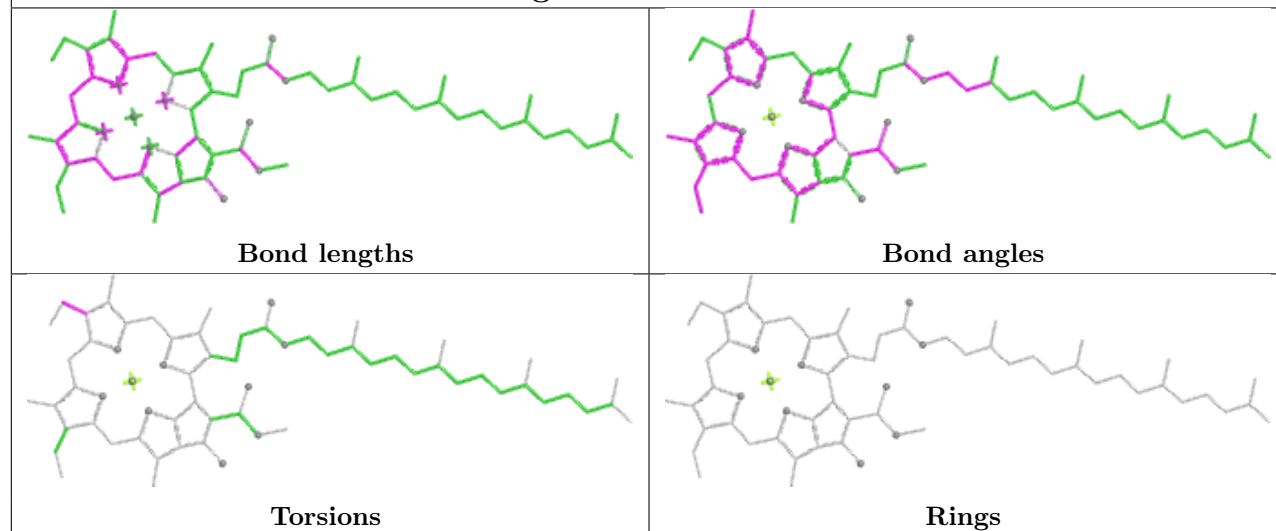
Ligand CLA B 611



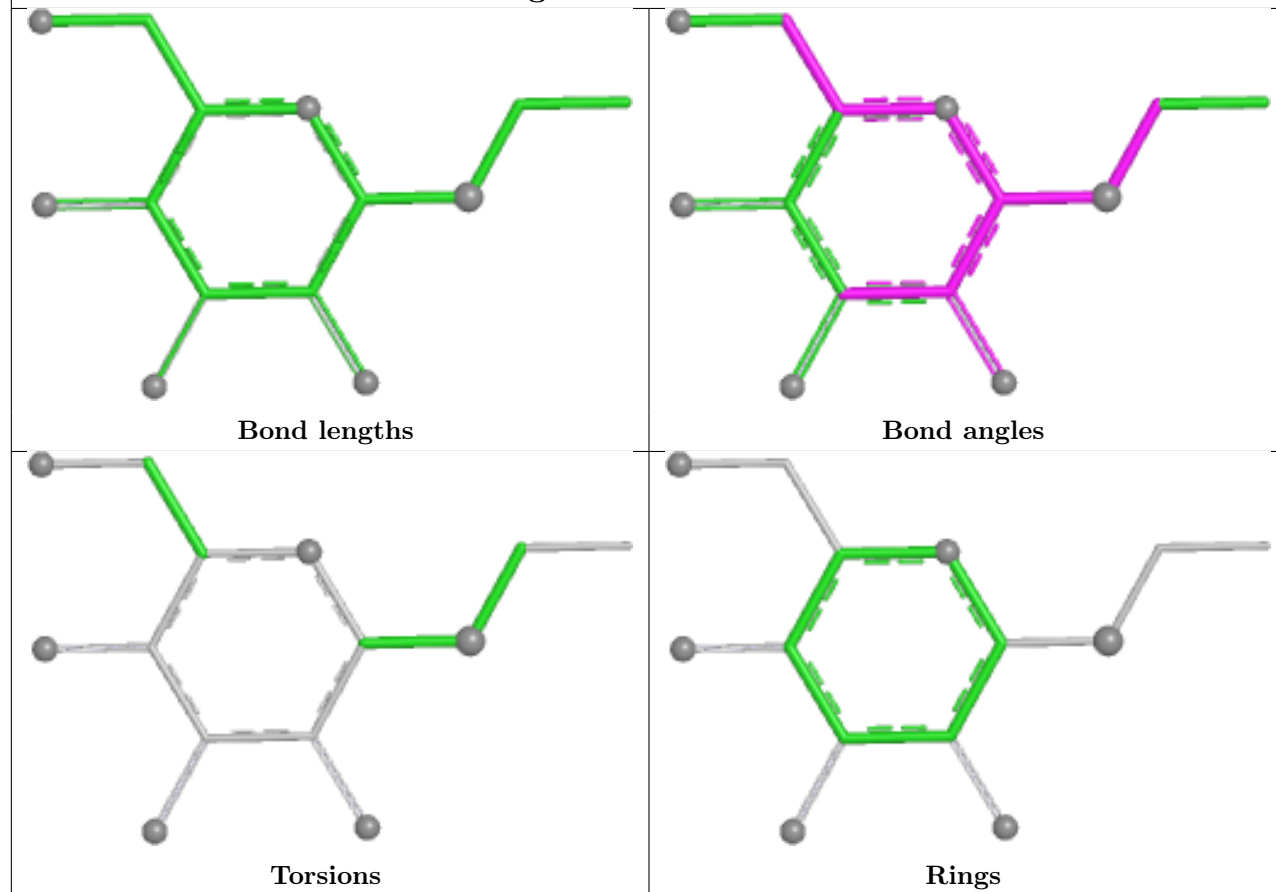
Ligand LMG B 621

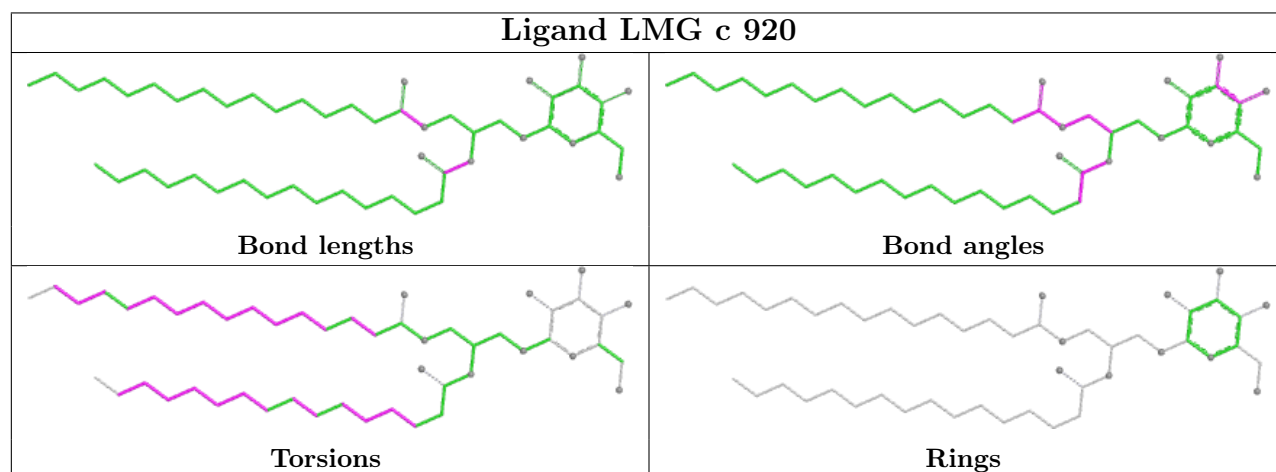
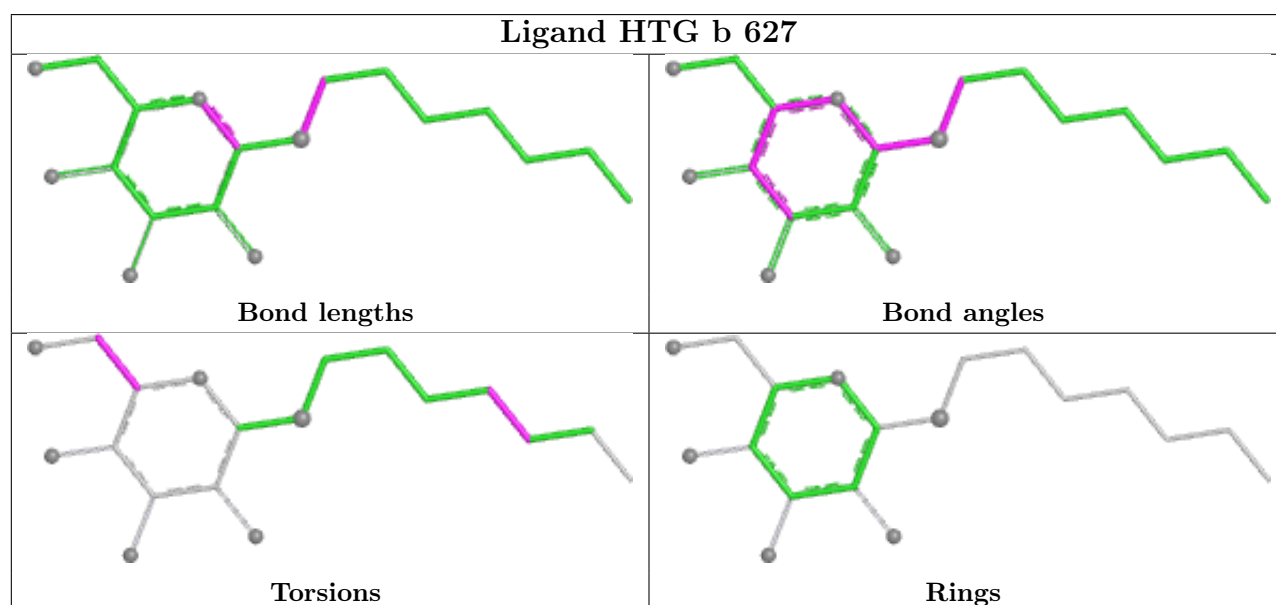
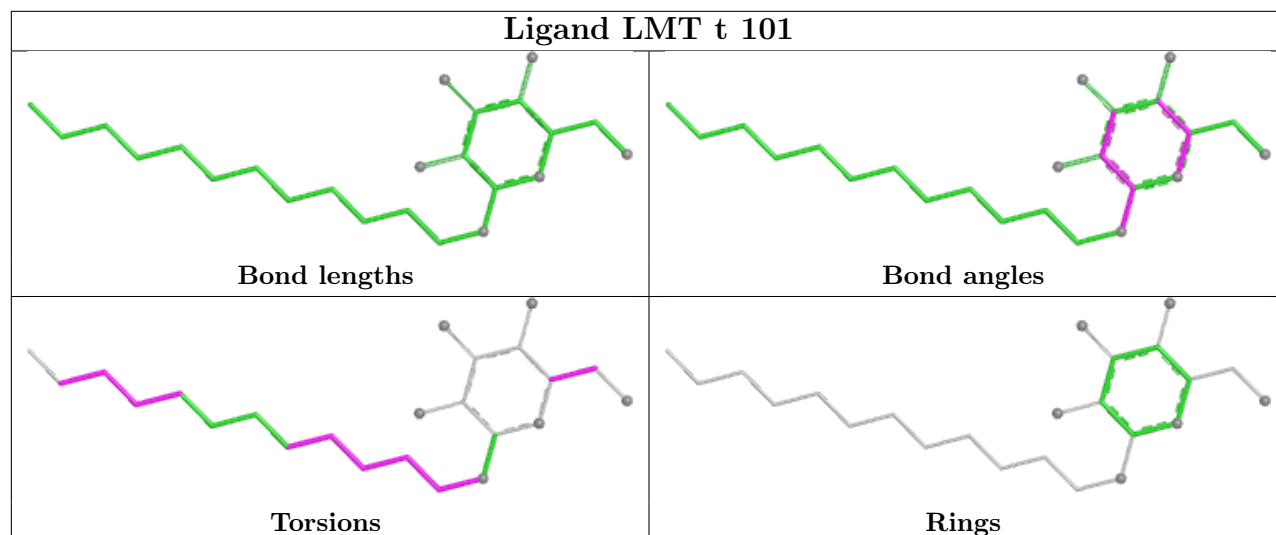


Ligand CLA B 610

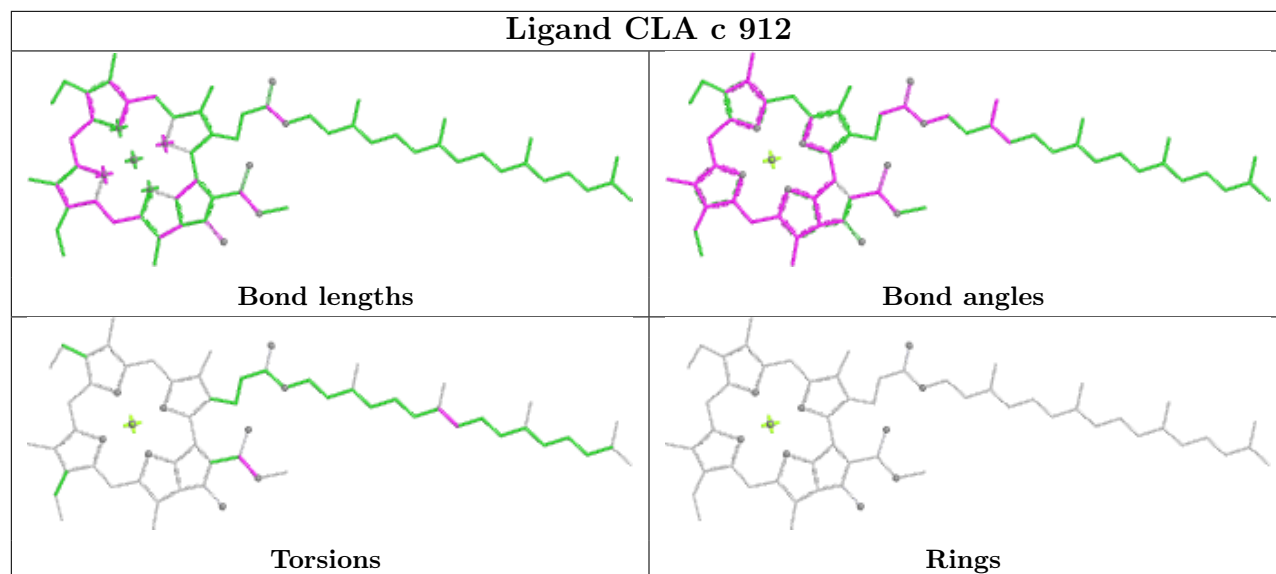


Ligand HTG V 203

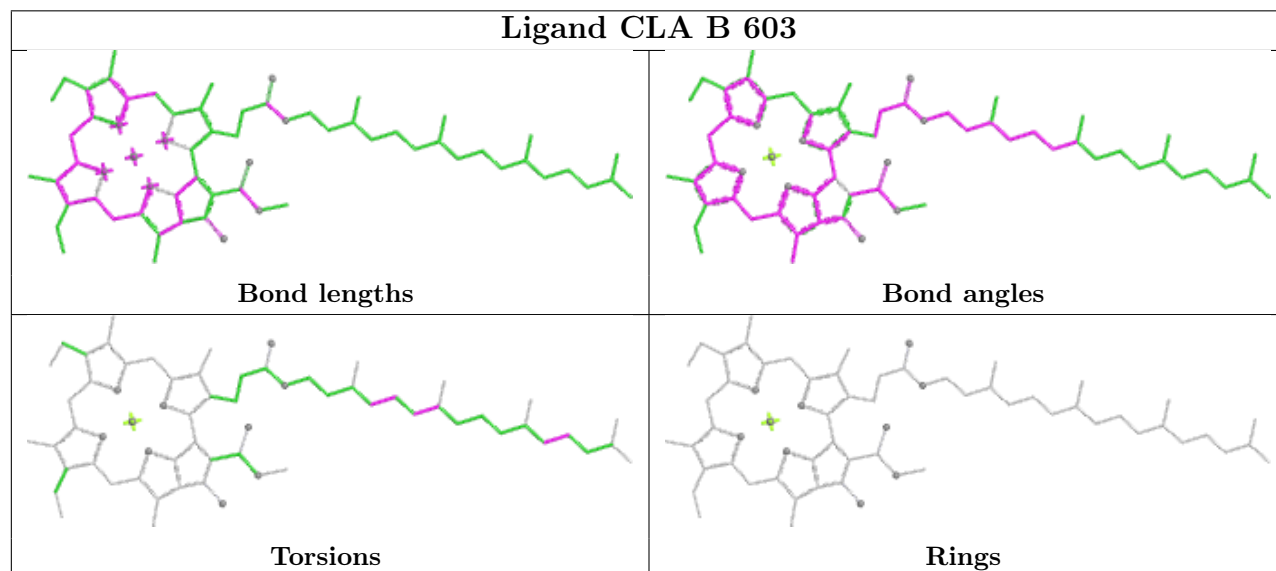




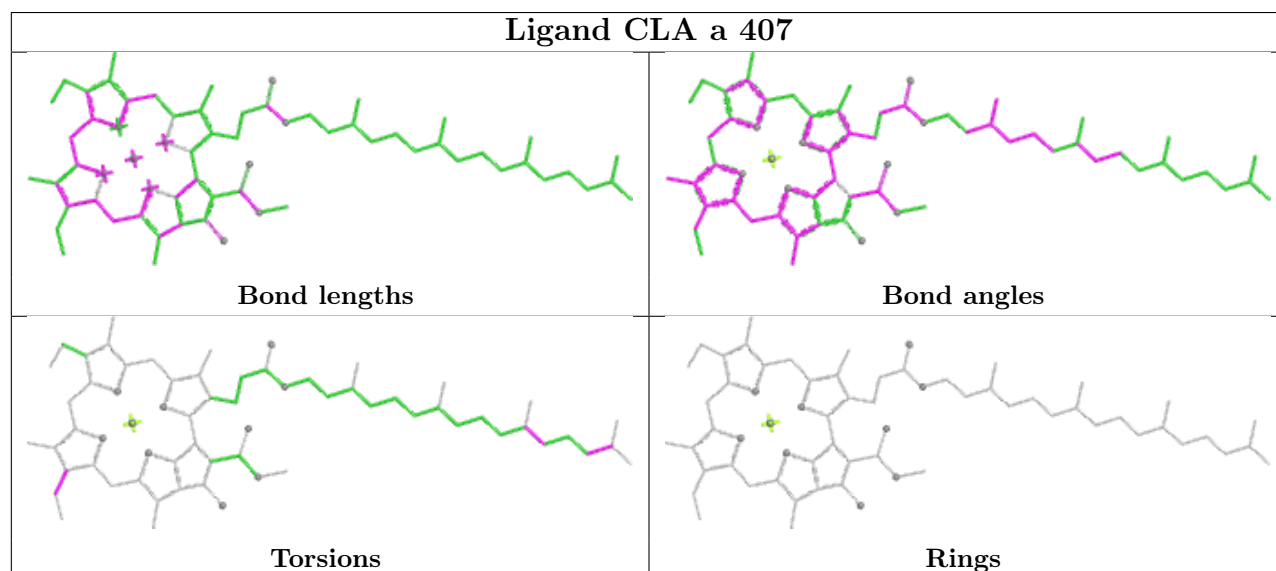
Ligand CLA c 912



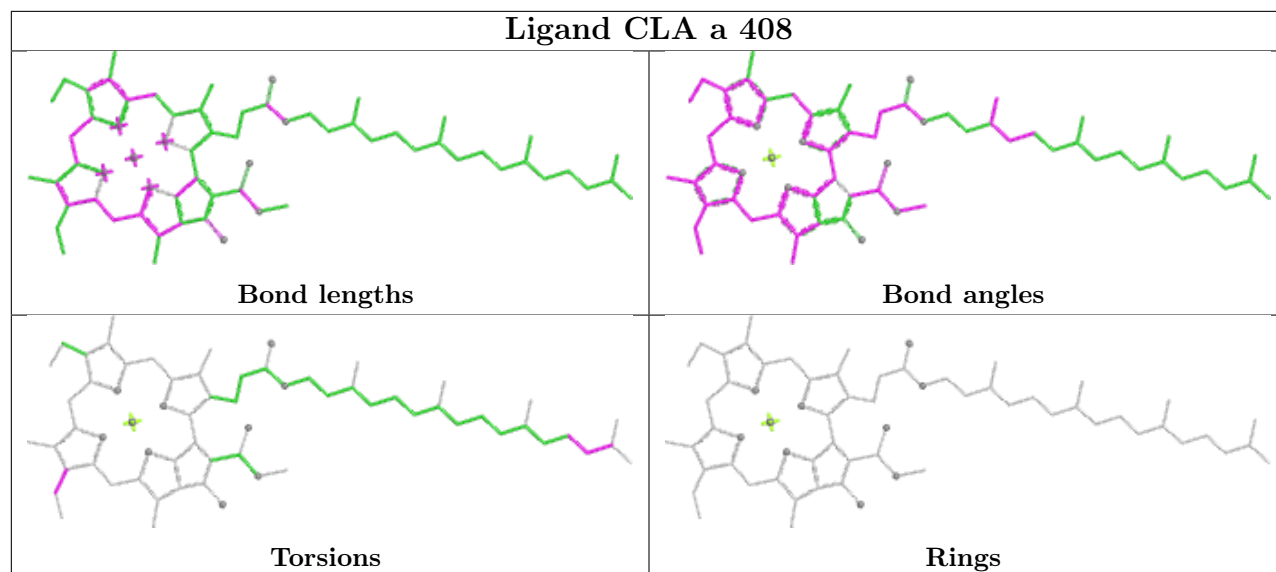
Ligand CLA B 603



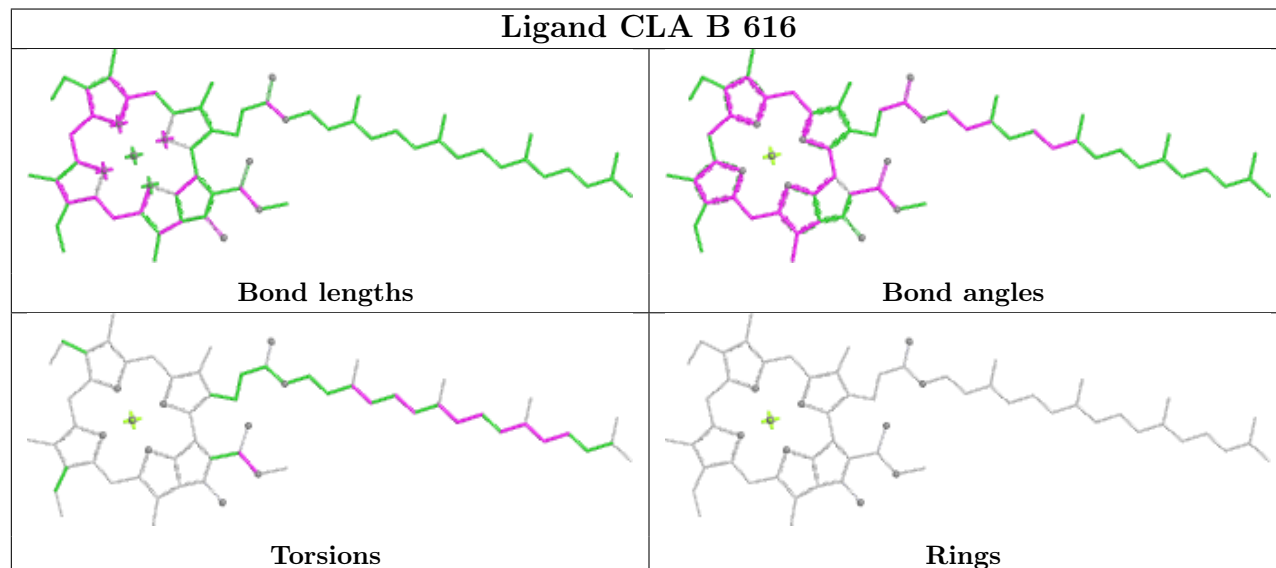
Ligand CLA a 407



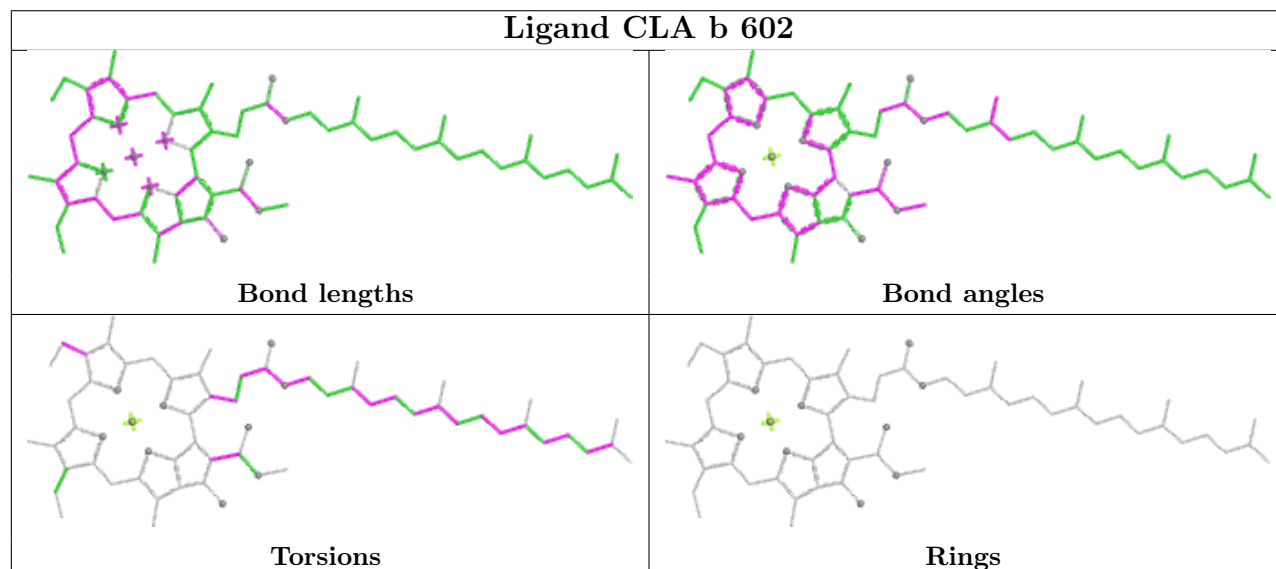
Ligand CLA a 408



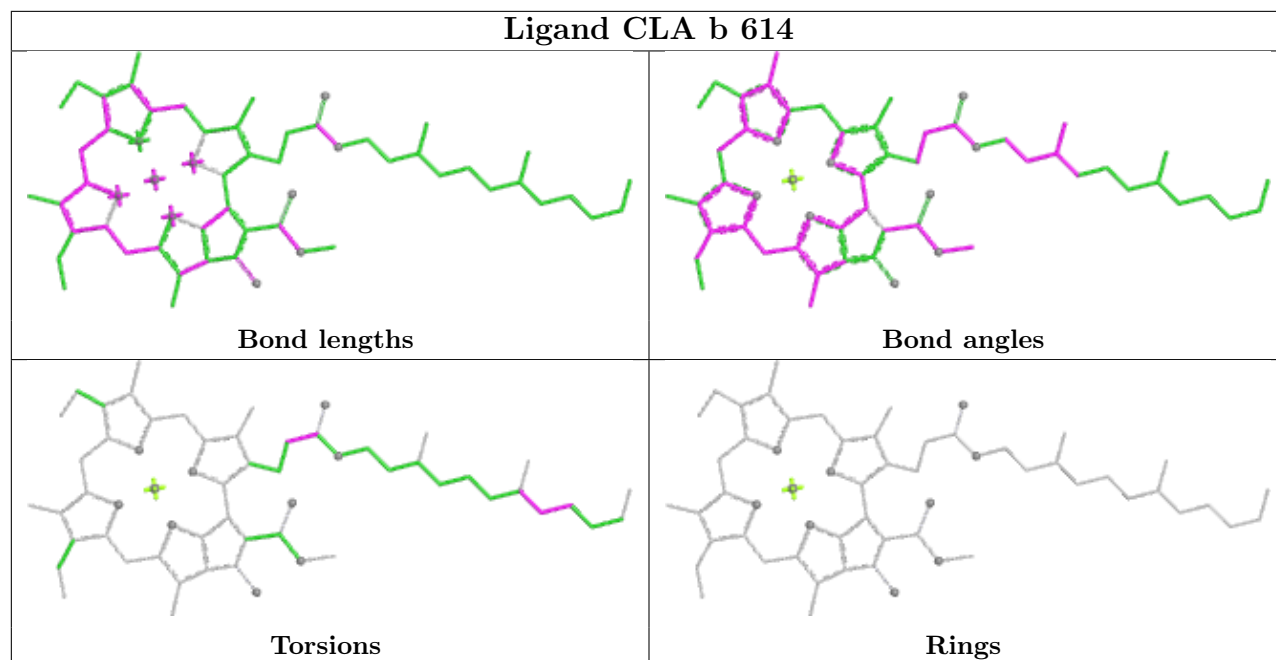
Ligand CLA B 616



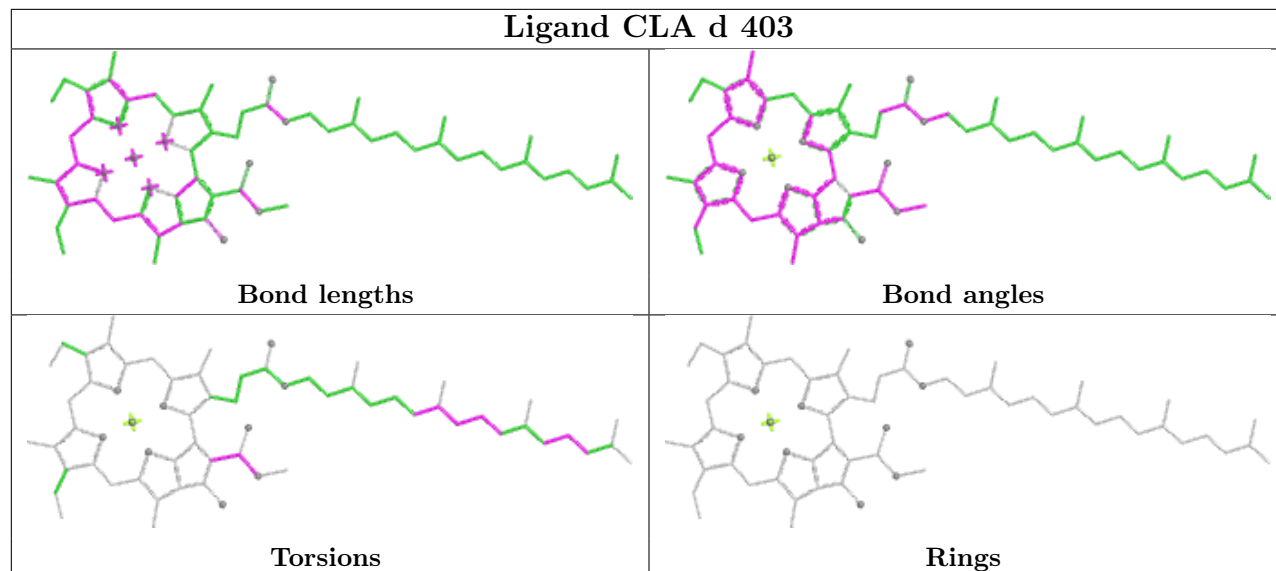
Ligand CLA b 602

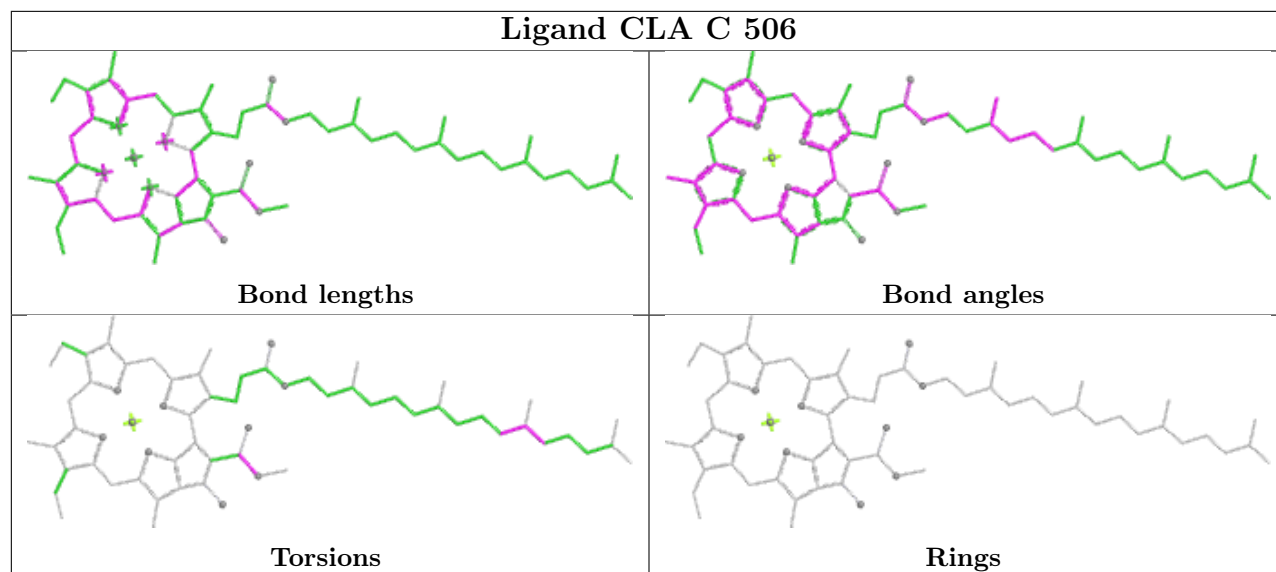
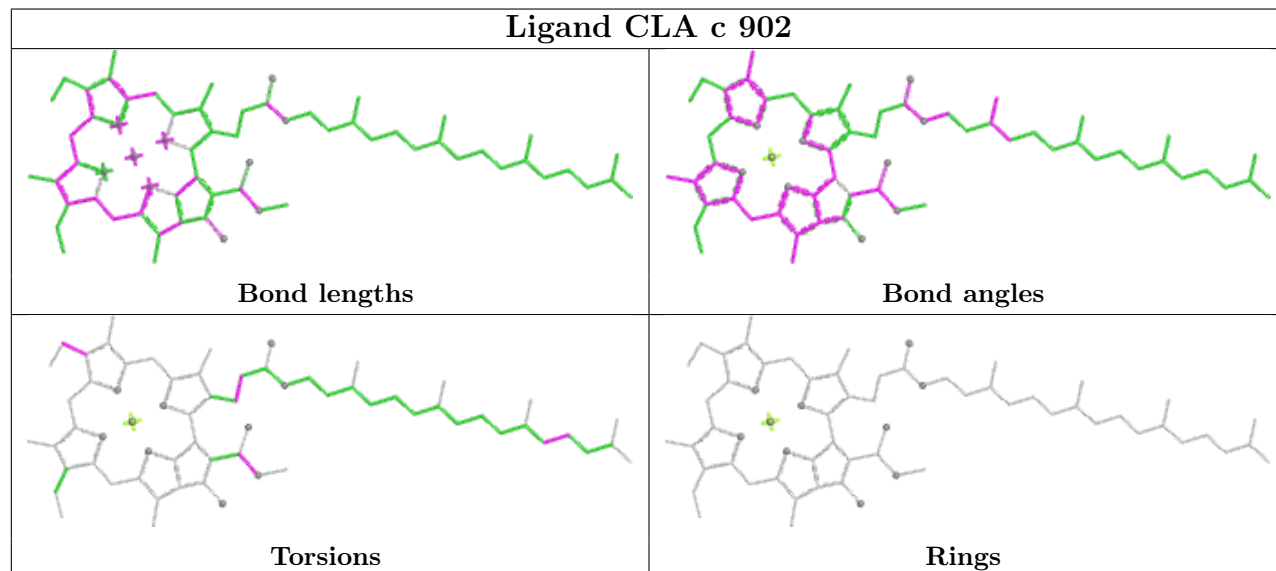


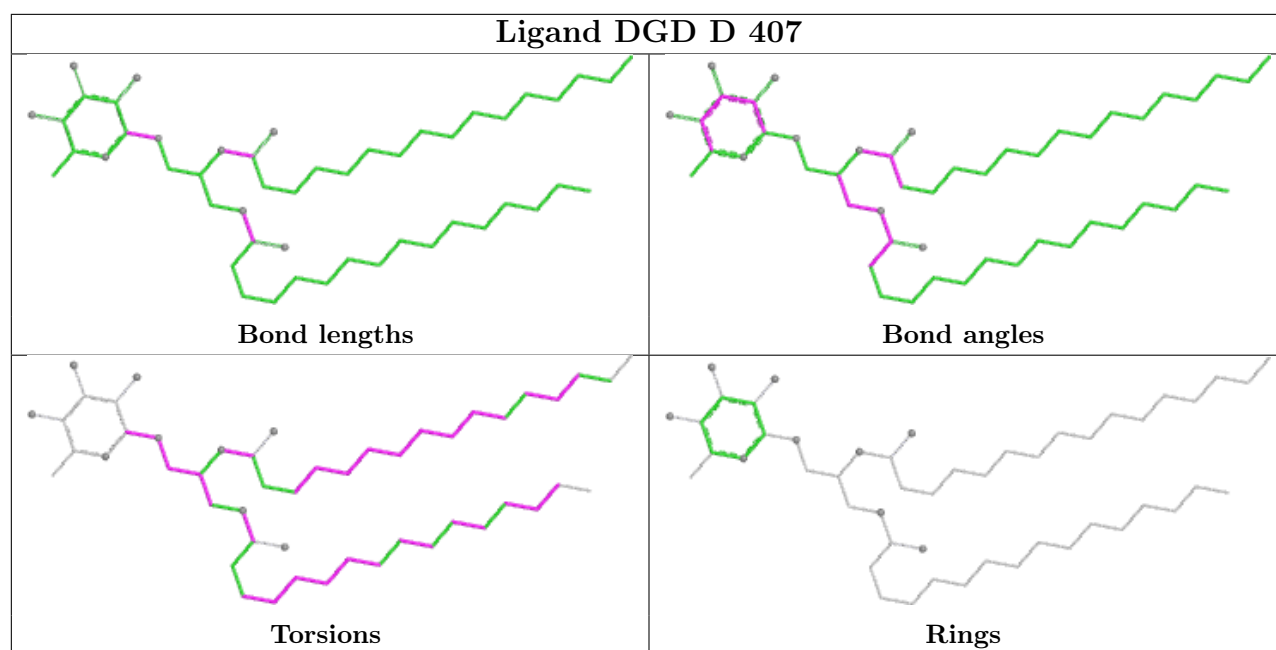
Ligand CLA b 614

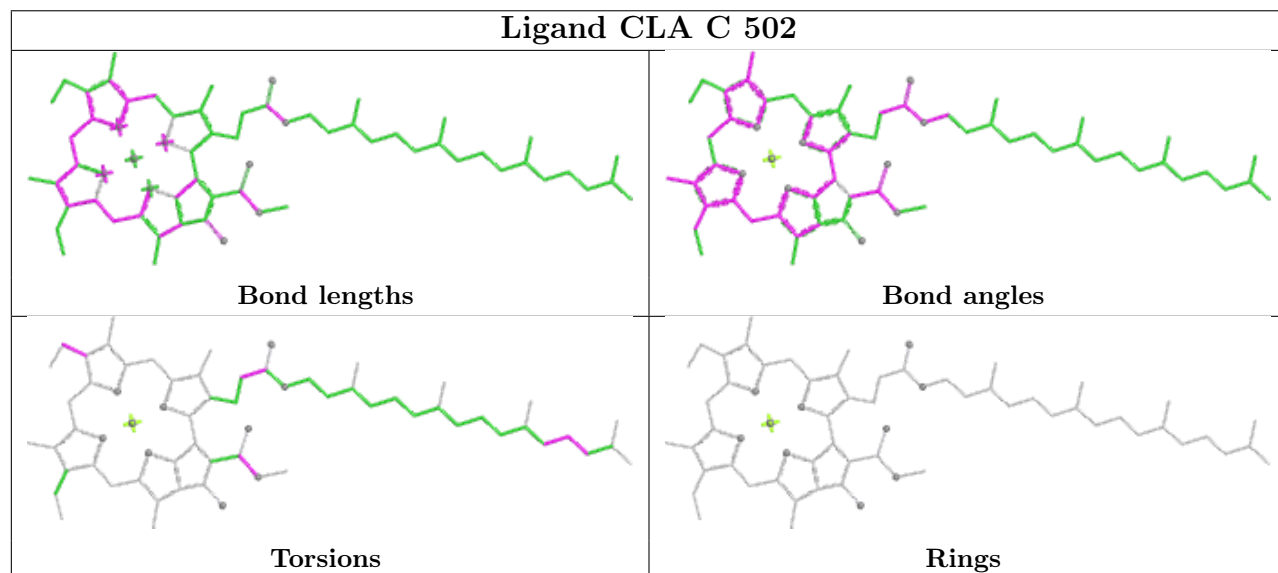
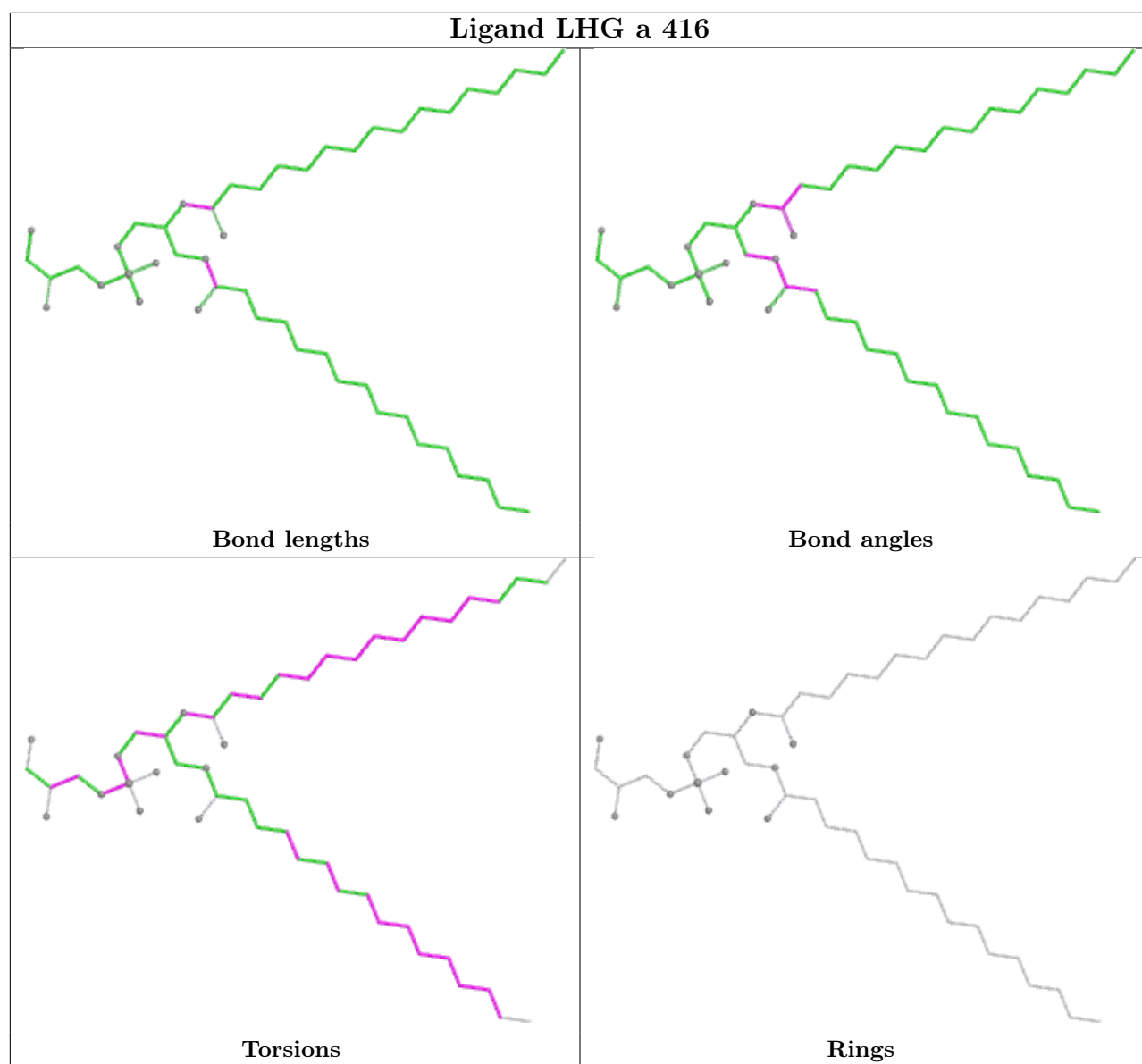


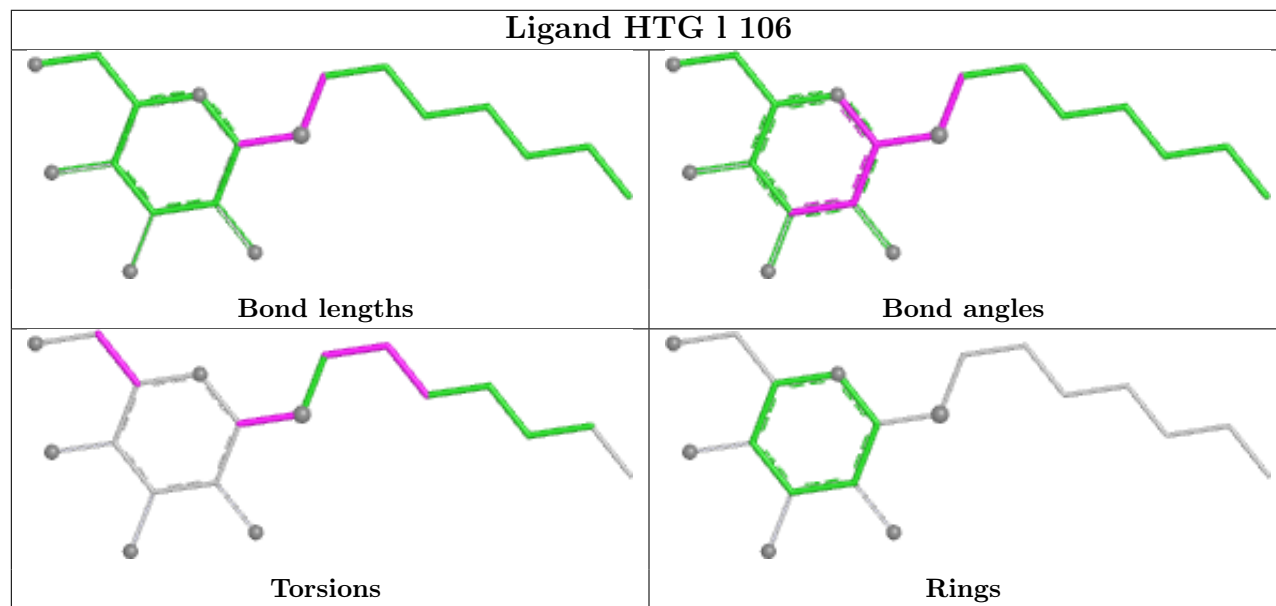
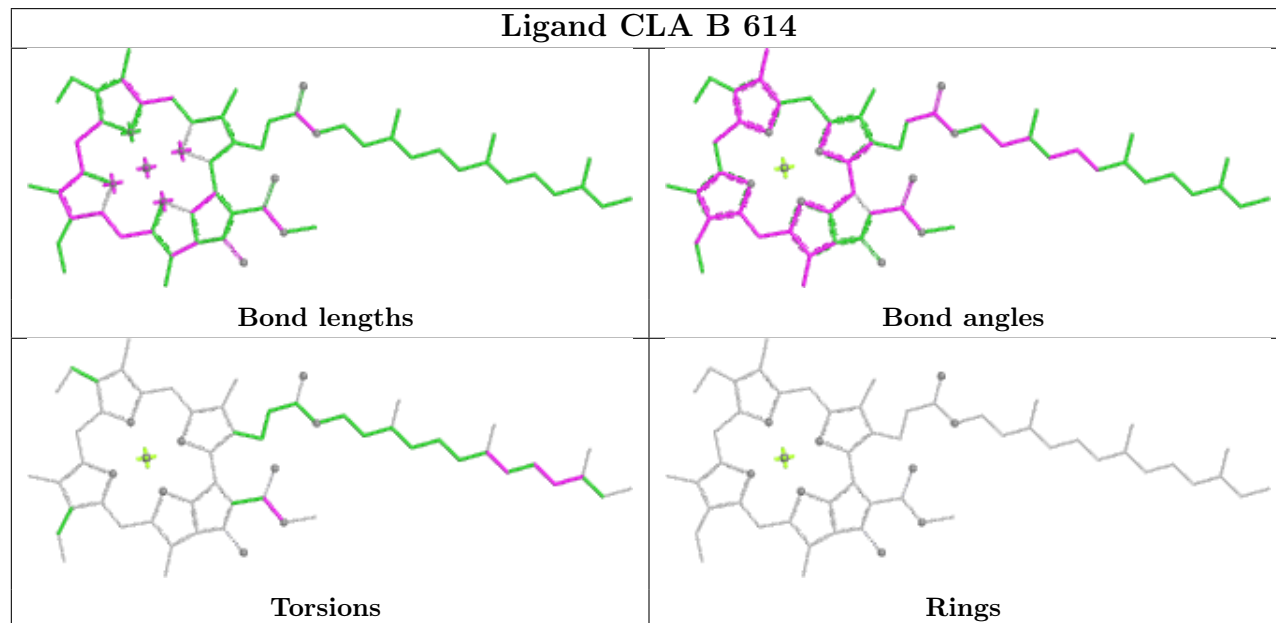
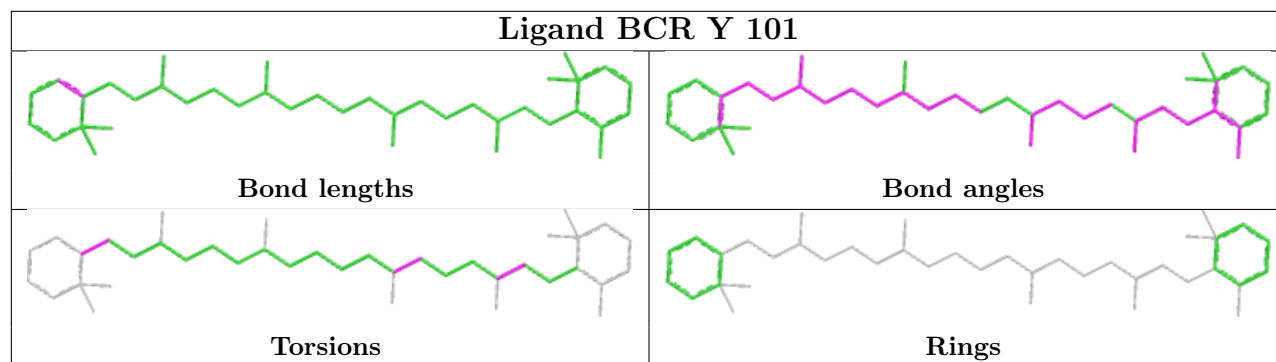
Ligand CLA d 403

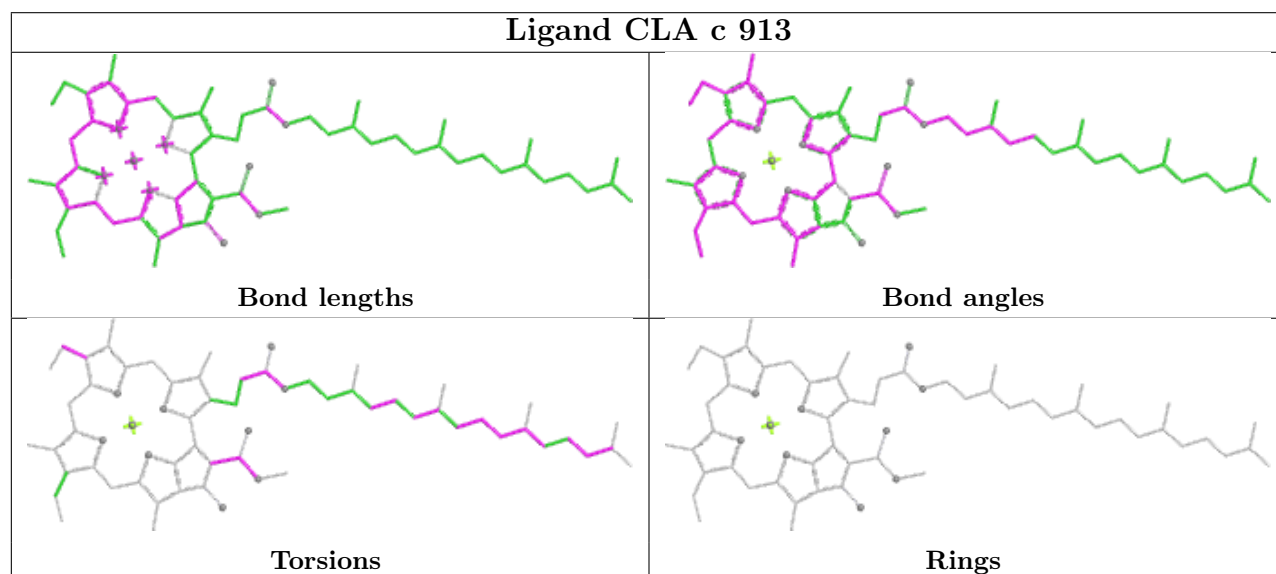
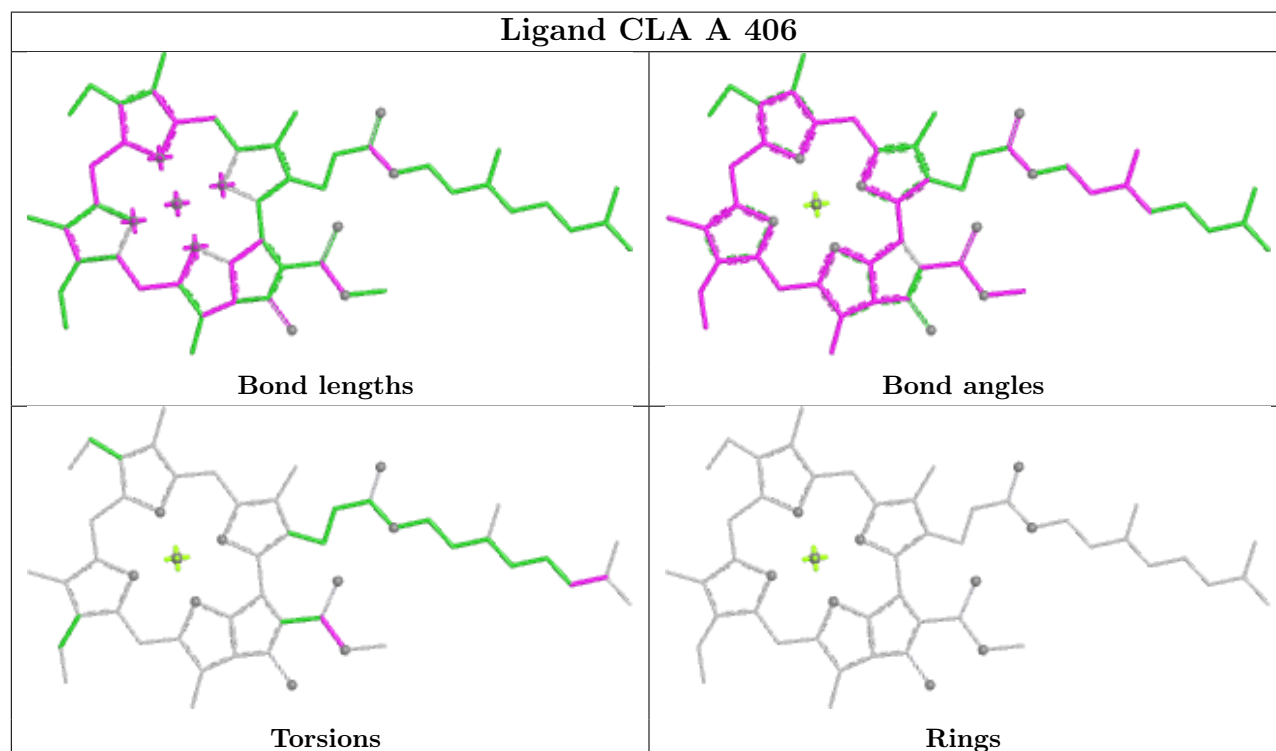
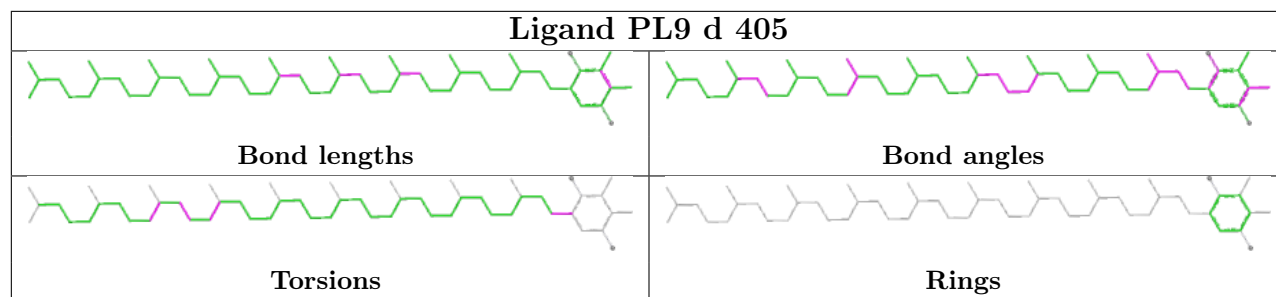


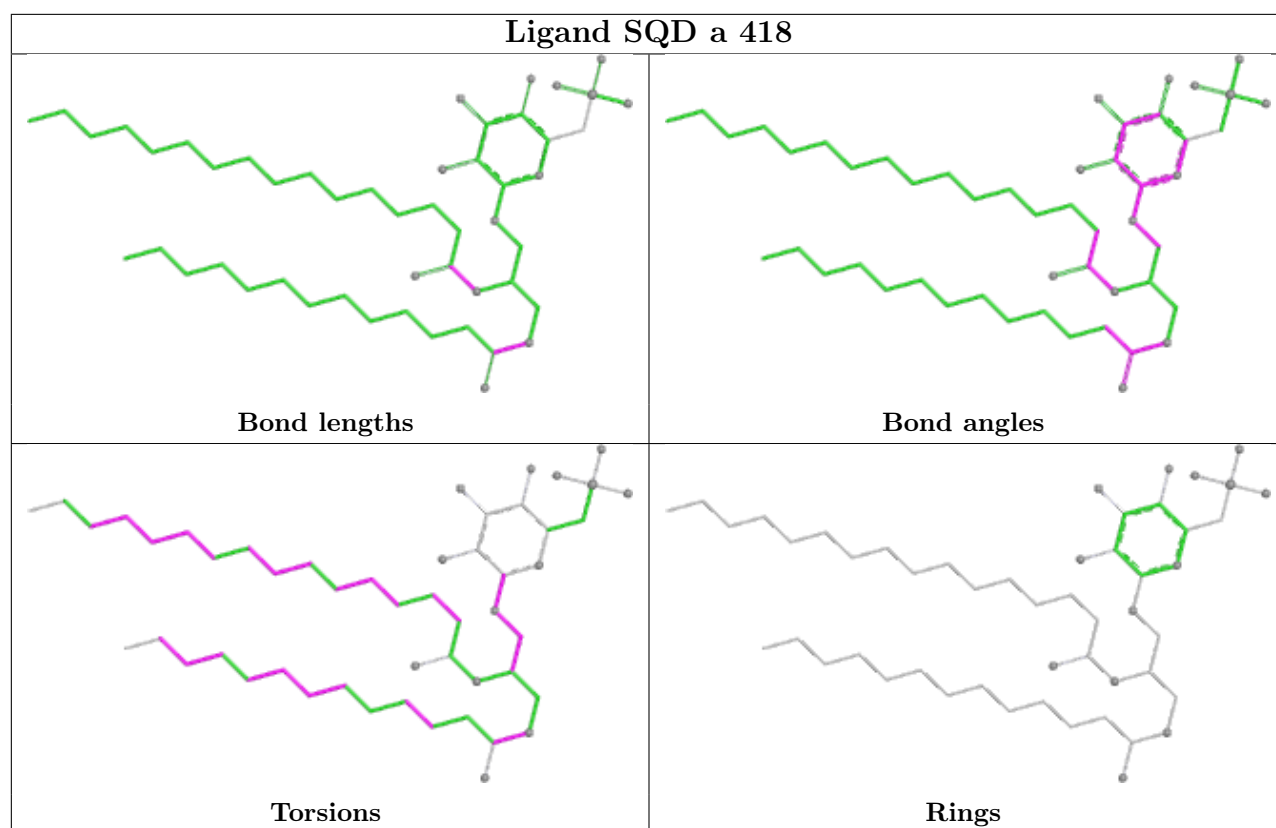
Ligand CLA C 506**Ligand CLA c 902**



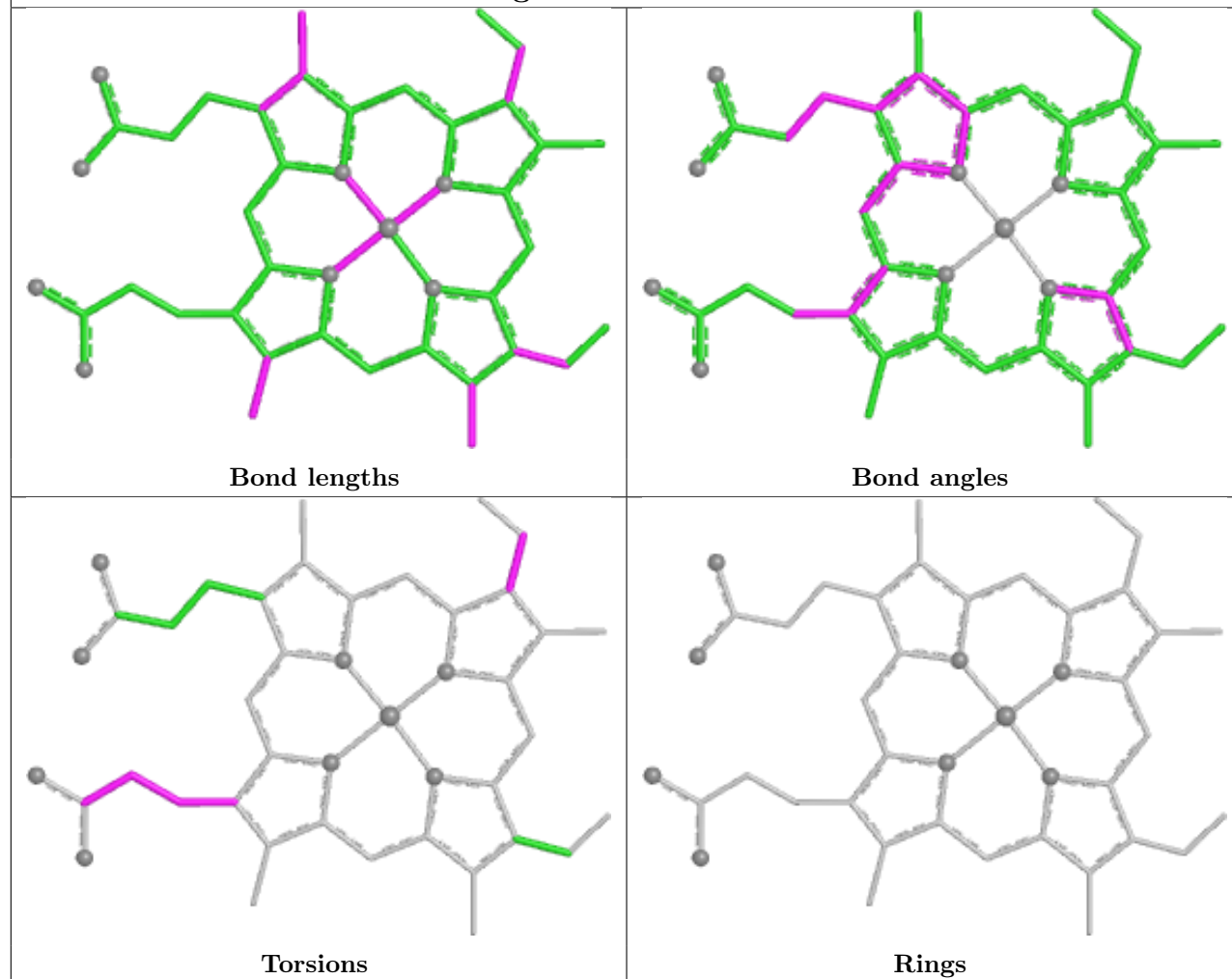




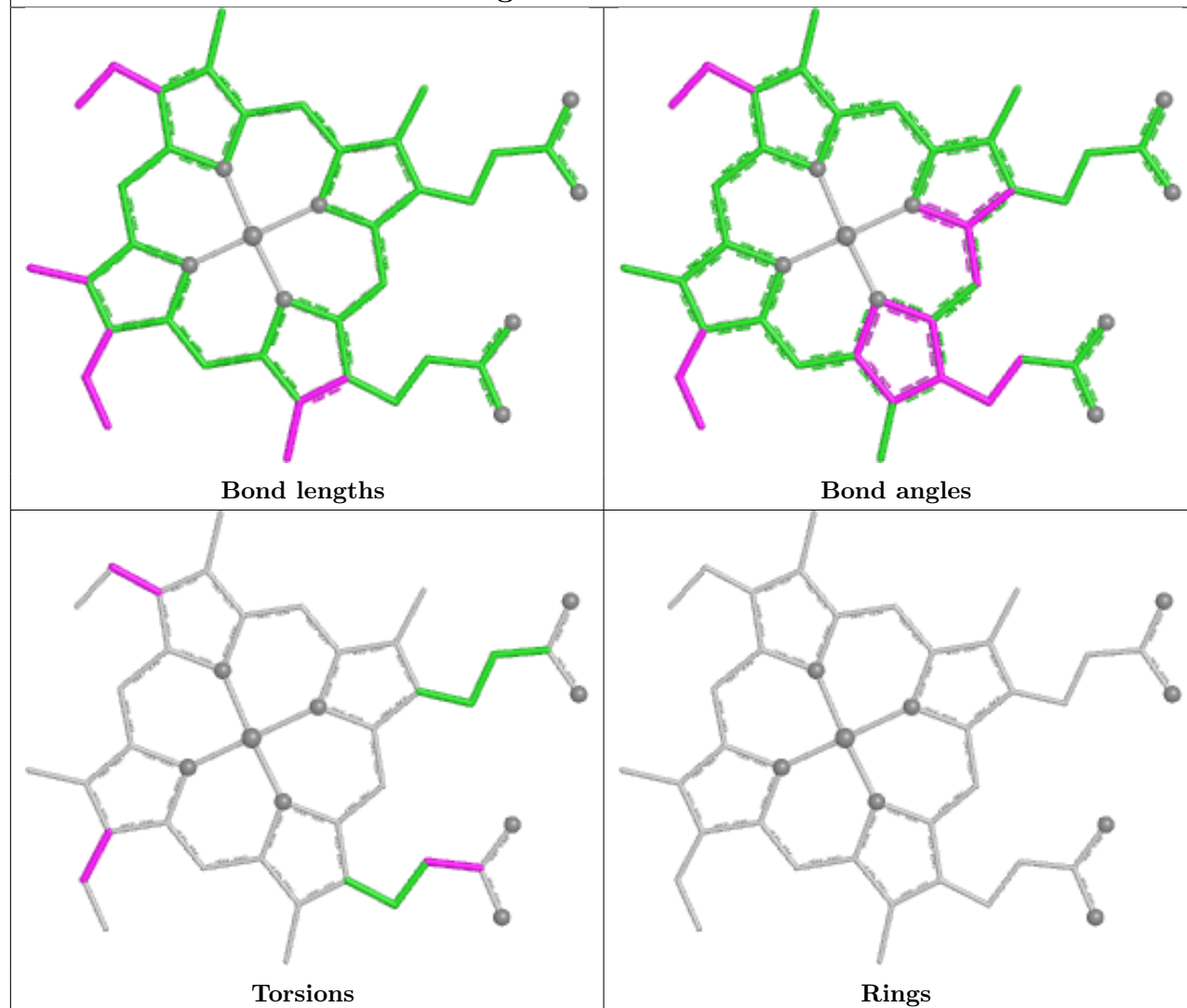




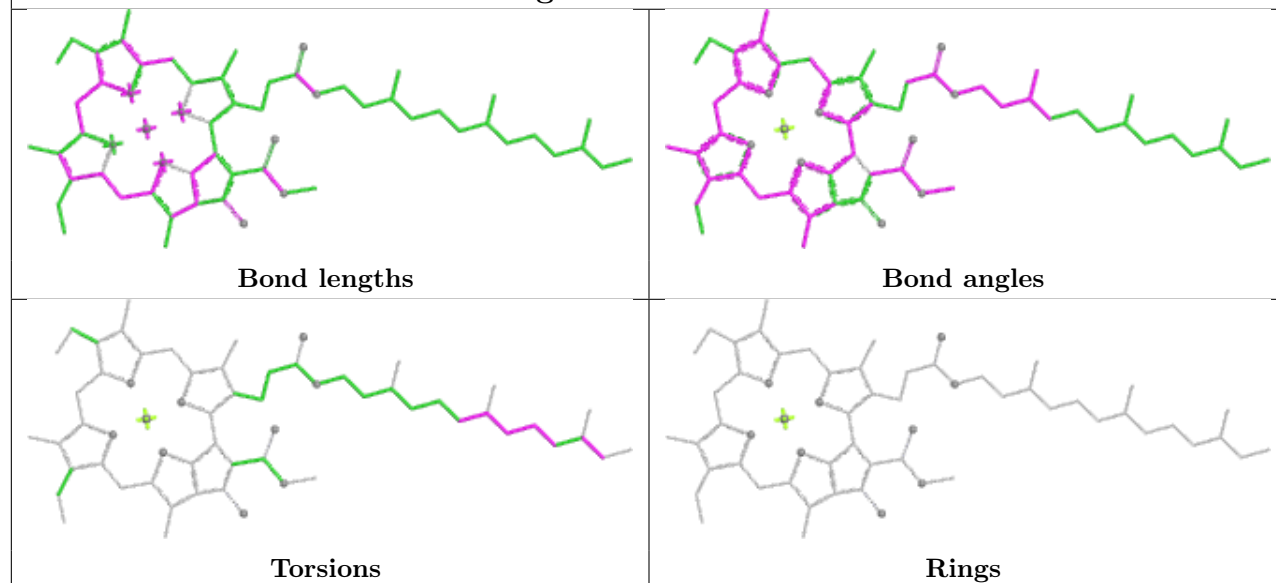
Ligand HEM e 101

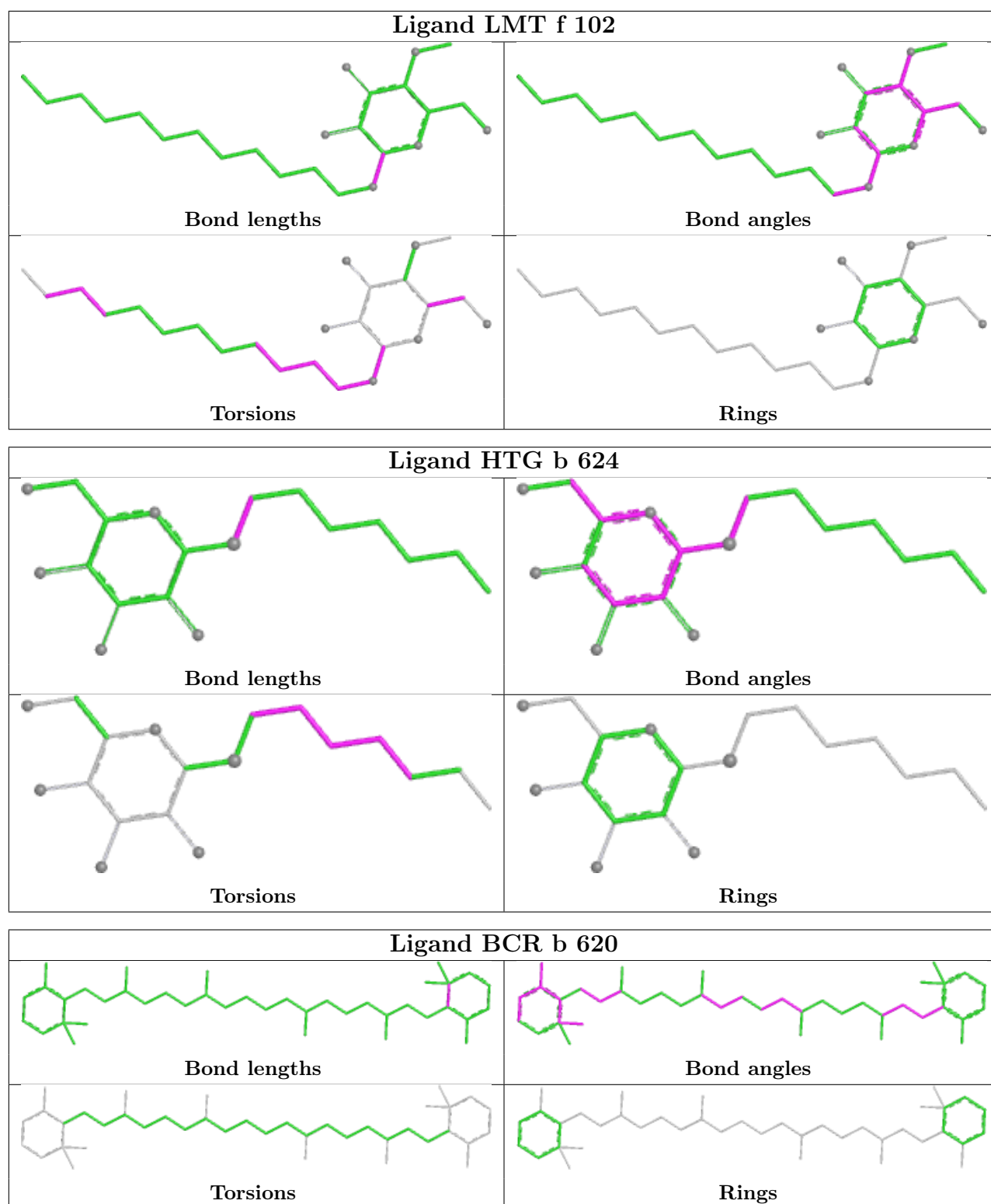


Ligand HEC v 202



Ligand CLA a 409





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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	334/334 (100%)	-0.48	7 (2%) 63 60	17, 28, 66, 87	1 (0%)
1	a	334/334 (100%)	-0.18	33 (9%) 13 10	17, 30, 96, 135	1 (0%)
2	B	505/505 (100%)	-0.32	16 (3%) 50 47	21, 33, 67, 109	3 (0%)
2	b	483/505 (95%)	-0.32	5 (1%) 79 77	19, 35, 57, 124	1 (0%)
3	C	451/455 (99%)	-0.29	3 (0%) 84 82	24, 37, 55, 106	0
3	c	455/455 (100%)	-0.14	2 (0%) 88 87	27, 41, 57, 89	1 (0%)
4	D	342/342 (100%)	-0.55	0 100 100	14, 29, 51, 86	3 (0%)
4	d	341/342 (99%)	-0.41	4 (1%) 76 74	16, 32, 59, 85	2 (0%)
5	E	79/80 (98%)	0.19	3 (3%) 44 41	30, 53, 77, 89	0
5	e	79/80 (98%)	0.43	3 (3%) 44 41	35, 54, 91, 96	0
6	F	33/33 (100%)	0.03	1 (3%) 52 49	32, 38, 68, 87	0
6	f	31/33 (93%)	0.18	1 (3%) 50 47	34, 42, 62, 95	0
7	H	63/63 (100%)	0.11	1 (1%) 70 67	22, 41, 51, 104	3 (4%)
7	h	62/63 (98%)	0.31	1 (1%) 70 67	26, 48, 62, 74	1 (1%)
8	I	34/36 (94%)	-0.08	0 100 100	33, 42, 60, 78	0
8	i	35/36 (97%)	-0.19	0 100 100	34, 43, 71, 95	0
9	J	36/40 (90%)	0.02	2 (5%) 30 27	29, 46, 73, 82	0
9	j	40/40 (100%)	0.25	2 (5%) 34 31	34, 47, 81, 92	0
10	K	37/37 (100%)	-0.11	0 100 100	36, 44, 55, 70	0
10	k	37/37 (100%)	0.18	1 (2%) 56 53	39, 47, 68, 81	0
11	L	35/35 (100%)	-0.25	1 (2%) 53 50	23, 32, 66, 78	0
11	l	35/35 (100%)	-0.04	1 (2%) 53 50	25, 35, 75, 92	0
12	O	243/243 (100%)	-0.20	1 (0%) 88 87	20, 39, 69, 104	1 (0%)
12	o	243/243 (100%)	-0.19	4 (1%) 70 67	24, 42, 71, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	T	29/30 (96%)	-0.24	2 (6%) 23 20	26, 32, 59, 89	0
13	t	29/30 (96%)	-0.16	2 (6%) 23 20	27, 34, 66, 98	0
14	U	97/97 (100%)	-0.32	0 100 100	26, 36, 58, 89	1 (1%)
14	u	97/97 (100%)	-0.31	1 (1%) 79 77	28, 37, 51, 76	0
15	V	137/137 (100%)	-0.53	0 100 100	22, 34, 50, 70	1 (0%)
15	v	137/137 (100%)	-0.11	0 100 100	24, 44, 61, 84	1 (0%)
16	Y	29/29 (100%)	0.28	1 (3%) 48 45	40, 54, 69, 81	0
16	y	29/29 (100%)	0.53	1 (3%) 48 45	51, 62, 70, 74	0
17	X	37/37 (100%)	0.31	1 (2%) 56 53	27, 50, 72, 83	1 (2%)
17	x	36/37 (97%)	0.63	1 (2%) 55 52	41, 54, 88, 89	0
18	Z	62/62 (100%)	0.70	6 (9%) 13 10	42, 54, 88, 106	0
18	z	61/62 (98%)	1.04	10 (16%) 4 3	49, 64, 98, 102	0
All	All	5147/5190 (99%)	-0.21	117 (2%) 61 58	14, 37, 70, 135	21 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	486	LEU	5.6
1	a	230	THR	5.5
17	x	37	VAL	5.2
7	H	64	ALA	4.8
1	A	246	TYR	4.6
13	t	30	THR	4.4
1	a	242	GLU	4.4
2	B	479	PHE	4.4
3	c	19	ASN	4.1
11	L	3	PRO	4.1
1	a	262	TYR	3.9
18	Z	33	TRP	3.9
1	a	235	TYR	3.7
18	z	3	ILE	3.6
1	a	240	GLY	3.6
9	j	2	MET	3.6
2	B	485	GLU	3.6
2	b	479	PHE	3.6
1	A	230	THR	3.5
13	t	29	ILE	3.5
1	a	256	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
4	d	27	PHE	3.4
13	T	29	ILE	3.4
16	y	18	VAL	3.4
1	A	245	THR	3.3
1	a	254	TYR	3.3
1	a	231	GLU	3.3
1	a	263	ALA	3.2
1	a	245	THR	3.2
11	l	3	PRO	3.2
5	E	5	THR	3.2
1	a	261	GLN	3.2
12	o	132	ASN	3.2
18	z	2	THR	3.2
1	a	228	THR	3.1
18	z	61	VAL	3.1
1	a	224	ILE	3.1
2	b	482	ILE	3.0
2	B	504	THR	3.0
1	a	229	GLU	3.0
1	a	255	PHE	3.0
1	A	231	GLU	3.0
6	F	16	PHE	2.9
2	B	487	SER	2.9
18	Z	35	ARG	2.9
2	B	499	VAL	2.9
2	b	480	SER	2.9
2	B	2	GLY	2.8
4	d	237	PRO	2.8
1	a	258	LEU	2.8
9	J	30	TYR	2.8
18	z	5	PHE	2.8
1	a	249	VAL	2.8
2	B	494	GLY	2.7
3	C	23	ALA	2.7
3	c	143	TYR	2.7
2	B	484	PRO	2.7
18	z	32	ASP	2.6
1	a	248	ILE	2.6
6	f	15	ILE	2.6
18	z	4	LEU	2.6
5	e	72	ALA	2.6
18	z	60	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
17	X	38	GLN	2.6
2	b	126	PRO	2.6
1	a	259	ILE	2.6
12	o	59	LYS	2.6
18	Z	3	ILE	2.5
1	a	246	TYR	2.5
1	a	223	LEU	2.5
18	z	34	ASP	2.5
18	z	35	ARG	2.5
2	B	501	ASP	2.5
1	a	238	LYS	2.4
2	b	484	PRO	2.4
1	a	226	GLU	2.4
1	A	11	ALA	2.3
5	e	84	LYS	2.3
1	a	264	SER	2.3
1	a	260	PHE	2.3
5	E	80	LEU	2.3
4	d	240	ALA	2.3
1	a	227	THR	2.3
16	Y	18	VAL	2.3
2	B	488	PRO	2.3
1	A	262	TYR	2.3
2	B	85	GLY	2.3
1	a	250	ALA	2.3
2	B	503	THR	2.3
1	a	243	GLU	2.3
4	d	28	VAL	2.3
5	E	83	LEU	2.3
3	C	25	ASN	2.3
18	z	1	MET	2.3
5	e	61	ARG	2.3
7	h	22	ALA	2.3
1	a	234	ASN	2.2
3	C	24	THR	2.2
14	u	8	GLU	2.2
18	Z	36	SER	2.2
10	k	18	PHE	2.2
1	a	237	TYR	2.2
18	Z	7	LEU	2.2
18	Z	30	PRO	2.2
9	J	5	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	480	SER	2.2
2	B	497	GLN	2.1
1	a	251	ALA	2.1
1	a	239	PHE	2.1
1	a	225	ARG	2.1
13	T	30	THR	2.1
1	A	247	ASN	2.1
12	O	56	PRO	2.1
2	B	502	VAL	2.1
9	j	1	MET	2.0
12	o	38	TYR	2.0
12	o	134	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
13	FME	T	1	10/11	0.88	0.14	38,42,72,75	0
13	FME	t	1	10/11	0.92	0.10	33,38,80,91	0
8	FME	I	1	10/11	0.96	0.09	33,37,40,41	0
8	FME	i	1	10/11	0.97	0.09	36,41,45,48	0

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, 95th 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
31	DMS	c	942	4/4	0.60	0.24	101,103,111,117	0
31	DMS	c	936	4/4	0.64	0.22	106,116,116,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	C	537	4/4	0.67	0.29	88,103,104,113	0
30	UNL	c	932	10/-	0.70	0.23	56,74,80,83	0
31	DMS	O	307	4/4	0.70	0.24	84,97,98,104	0
30	UNL	i	104	16/-	0.70	0.23	67,76,87,89	0
31	DMS	c	937	4/4	0.70	0.25	80,90,91,100	0
31	DMS	B	639	4/4	0.70	0.20	72,87,90,102	0
34	HTG	b	624	19/19	0.70	0.18	69,97,109,110	0
31	DMS	O	305	4/4	0.71	0.20	68,70,79,99	0
29	LMT	f	102	25/35	0.71	0.21	61,93,105,108	0
34	HTG	c	922	19/19	0.71	0.16	70,93,109,112	0
30	UNL	t	102	16/-	0.72	0.16	59,71,78,80	0
30	UNL	i	105	10/-	0.72	0.22	67,78,86,87	0
31	DMS	u	205	4/4	0.73	0.26	64,67,73,83	0
31	DMS	b	637	4/4	0.73	0.20	90,97,101,112	0
30	UNL	a	417	10/-	0.73	0.24	75,80,84,87	0
30	UNL	Z	102	9/-	0.74	0.17	57,71,79,81	0
34	HTG	b	627	19/19	0.74	0.16	50,92,108,109	0
34	HTG	D	415	19/19	0.74	0.19	39,69,80,87	0
35	DGD	d	406	43/66	0.74	0.22	58,85,139,146	0
34	HTG	D	414	19/19	0.75	0.18	63,103,114,115	0
34	HTG	b	632	19/19	0.75	0.20	56,74,91,92	0
31	DMS	b	636	4/4	0.75	0.23	88,95,109,113	0
31	DMS	c	938	4/4	0.75	0.20	86,91,98,103	0
34	HTG	B	627	19/19	0.76	0.16	51,104,113,116	0
31	DMS	v	207	4/4	0.76	0.31	84,93,97,117	0
29	LMT	I	102	35/35	0.77	0.15	76,88,100,102	0
31	DMS	d	414	4/4	0.77	0.28	102,112,113,120	0
30	UNL	I	105	16/-	0.77	0.20	70,82,88,90	0
30	UNL	a	420	6/-	0.77	0.20	56,59,60,60	0
30	UNL	b	628	11/-	0.77	0.16	58,63,78,79	0
31	DMS	V	211	4/4	0.77	0.23	77,84,85,85	0
31	DMS	u	204	4/4	0.78	0.20	50,68,69,75	0
27	LHG	A	412	31/49	0.78	0.19	66,83,107,117	0
31	DMS	v	204	4/4	0.78	0.19	87,88,90,91	0
31	DMS	a	401	4/4	0.78	0.28	75,84,85,104	0
30	UNL	u	201	11/-	0.78	0.20	47,53,69,69	0
34	HTG	v	203	16/19	0.78	0.15	52,69,81,97	0
35	DGD	D	407	50/66	0.78	0.20	60,87,120,123	0
31	DMS	l	105	4/4	0.78	0.26	100,103,110,115	0
31	DMS	c	943	4/4	0.79	0.21	77,82,87,92	0
22	CLA	b	602	65/65	0.79	0.16	49,67,89,98	0
31	DMS	l	103	4/4	0.79	0.24	91,95,97,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	c	935	4/4	0.79	0.16	71,78,81,84	0
31	DMS	u	203	4/4	0.79	0.21	56,68,72,84	0
29	LMT	A	414	35/35	0.79	0.17	59,86,109,114	0
31	DMS	C	540	4/4	0.79	0.22	82,83,91,97	0
31	DMS	H	103	4/4	0.79	0.21	63,67,69,74	0
31	DMS	v	205	4/4	0.79	0.19	70,72,78,80	0
31	DMS	L	102	4/4	0.79	0.23	79,80,91,100	0
29	LMT	T	102	24/35	0.80	0.17	42,80,98,101	0
31	DMS	f	103	4/4	0.80	0.24	87,89,90,100	0
31	DMS	O	313	4/4	0.80	0.26	89,100,100,107	0
27	LHG	a	416	49/49	0.80	0.17	60,84,100,108	0
34	HTG	V	203	14/19	0.81	0.15	48,52,79,84	0
31	DMS	c	944	4/4	0.81	0.20	79,82,89,92	0
29	LMT	Z	101	35/35	0.81	0.16	40,105,123,128	0
31	DMS	C	539	4/4	0.81	0.23	88,90,93,95	0
25	LMG	D	412	46/55	0.81	0.19	41,68,138,142	0
31	DMS	B	634	4/4	0.81	0.23	57,68,73,95	0
30	UNL	j	103	16/-	0.81	0.16	59,67,71,74	0
31	DMS	C	534	4/4	0.81	0.17	105,111,112,121	0
31	DMS	B	631	4/4	0.82	0.19	78,80,84,87	0
28	SQD	D	408	20/54	0.82	0.15	65,97,105,108	0
31	DMS	B	637	4/4	0.82	0.20	69,76,80,88	0
34	HTG	l	106	19/19	0.82	0.17	63,97,108,109	0
31	DMS	U	203	4/4	0.82	0.23	62,73,74,76	0
30	UNL	T	101	13/-	0.82	0.16	63,71,77,79	0
24	BCR	B	618	19/40	0.82	0.15	50,59,74,77	0
30	UNL	I	104	16/-	0.83	0.18	60,71,84,86	0
34	HTG	C	532	19/19	0.83	0.14	69,98,111,112	0
26	PL9	A	411	55/55	0.83	0.20	61,73,87,92	0
28	SQD	l	101	54/54	0.83	0.16	53,82,119,123	0
30	UNL	U	201	14/-	0.83	0.17	44,57,65,66	0
27	LHG	d	401	33/49	0.83	0.14	62,94,138,142	0
31	DMS	t	105	4/4	0.83	0.23	89,93,101,108	0
29	LMT	a	419	35/35	0.83	0.18	46,69,93,100	0
29	LMT	E	101	24/35	0.83	0.17	61,82,97,113	0
29	LMT	t	101	24/35	0.83	0.13	50,71,109,119	0
31	DMS	c	940	4/4	0.83	0.19	74,74,75,80	0
30	UNL	I	103	13/-	0.83	0.17	53,57,77,82	0
31	DMS	C	533	4/4	0.83	0.19	79,84,85,89	0
29	LMT	c	931	24/35	0.84	0.18	50,84,95,98	0
28	SQD	b	621	38/54	0.84	0.16	58,90,110,112	0
31	DMS	C	536	4/4	0.84	0.20	77,80,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	LMG	b	622	43/55	0.84	0.17	48,78,88,98	0
31	DMS	d	415	4/4	0.84	0.17	60,63,67,79	0
31	DMS	C	538	4/4	0.84	0.14	79,86,86,87	0
30	UNL	b	625	16/-	0.84	0.15	43,52,64,67	0
34	HTG	C	523	9/19	0.84	0.17	63,69,81,86	0
31	DMS	V	207	4/4	0.84	0.18	64,71,71,76	0
29	LMT	c	921	35/35	0.84	0.15	74,90,99,103	0
31	DMS	o	308	4/4	0.85	0.16	76,77,82,91	0
31	DMS	V	210	4/4	0.85	0.19	70,73,78,88	0
26	PL9	a	415	55/55	0.85	0.22	64,84,106,111	0
25	LMG	c	930	49/55	0.85	0.13	44,78,96,106	0
31	DMS	b	634	4/4	0.85	0.15	68,76,79,86	0
28	SQD	f	101	14/54	0.85	0.12	77,89,96,96	0
27	LHG	C	522	30/49	0.85	0.14	55,79,127,134	0
31	DMS	c	929	4/4	0.85	0.25	69,73,76,78	0
31	DMS	O	314	4/4	0.85	0.19	78,80,86,91	0
25	LMG	d	409	47/55	0.85	0.15	49,76,113,114	0
25	LMG	C	531	40/55	0.85	0.14	37,81,103,107	0
31	DMS	V	209	4/4	0.86	0.21	76,87,89,93	0
30	UNL	x	101	15/-	0.86	0.11	43,50,56,58	0
31	DMS	o	305	4/4	0.86	0.17	78,82,86,87	0
30	UNL	B	624	7/-	0.86	0.18	30,45,51,56	0
31	DMS	t	103	4/4	0.86	0.17	89,102,103,103	0
28	SQD	a	418	51/54	0.86	0.14	47,70,91,97	0
31	DMS	c	941	4/4	0.86	0.15	73,79,87,88	0
31	DMS	O	308	4/4	0.86	0.17	64,72,73,80	0
31	DMS	B	636	4/4	0.86	0.14	60,62,67,69	0
25	LMG	B	621	40/55	0.86	0.16	47,82,108,112	0
31	DMS	c	927	4/4	0.86	0.21	87,89,91,97	0
30	UNL	A	415	5/-	0.86	0.18	68,72,73,75	0
30	UNL	i	103	16/-	0.86	0.14	53,64,79,82	0
31	DMS	a	421	4/4	0.87	0.19	85,87,87,94	0
31	DMS	o	302	4/4	0.87	0.17	59,64,71,75	0
31	DMS	o	303	4/4	0.87	0.21	60,77,80,83	0
31	DMS	D	417	4/4	0.87	0.16	72,72,77,86	0
31	DMS	b	635	4/4	0.87	0.16	62,69,76,86	0
31	DMS	U	202	4/4	0.87	0.21	42,49,58,67	0
24	BCR	b	618	20/40	0.87	0.18	57,65,70,71	0
27	LHG	l	102	49/49	0.87	0.14	38,61,91,95	0
30	UNL	J	103	16/-	0.87	0.13	44,57,77,77	0
31	DMS	B	642	4/4	0.87	0.16	65,66,75,82	0
31	DMS	C	529	4/4	0.87	0.16	72,78,78,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMT	B	622	24/35	0.87	0.12	57,67,73,78	0
31	DMS	l	104	4/4	0.87	0.20	79,80,86,87	0
31	DMS	v	210	4/4	0.87	0.25	63,71,80,91	0
31	DMS	t	104	4/4	0.88	0.15	101,101,104,111	0
30	UNL	i	102	16/-	0.88	0.15	41,51,80,81	0
24	BCR	b	619	31/40	0.88	0.11	47,54,63,67	0
31	DMS	A	416	4/4	0.88	0.19	60,67,69,72	0
31	DMS	C	535	4/4	0.88	0.16	70,79,83,86	0
31	DMS	A	417	4/4	0.88	0.15	76,82,83,85	0
31	DMS	V	204	4/4	0.88	0.16	66,73,76,76	0
31	DMS	O	303	4/4	0.88	0.15	68,71,78,79	0
31	DMS	b	638	4/4	0.88	0.20	49,52,54,70	0
28	SQD	A	413	49/54	0.88	0.15	46,65,91,95	0
34	HTG	C	521	19/19	0.88	0.12	55,80,93,96	0
31	DMS	C	528	4/4	0.88	0.21	88,89,90,90	0
31	DMS	V	212	4/4	0.89	0.17	51,54,55,72	0
27	LHG	D	409	49/49	0.89	0.15	38,56,85,97	0
31	DMS	v	206	4/4	0.89	0.17	69,72,72,77	0
31	DMS	C	530	4/4	0.89	0.17	71,79,82,83	0
31	DMS	b	631	4/4	0.89	0.16	68,72,79,80	0
31	DMS	V	205	4/4	0.89	0.13	64,66,67,71	0
31	DMS	O	311	4/4	0.89	0.15	48,56,59,61	0
31	DMS	B	632	4/4	0.89	0.14	49,57,67,69	0
30	UNL	D	413	16/-	0.89	0.12	38,46,52,58	0
30	UNL	O	301	16/-	0.89	0.16	39,47,73,74	0
37	RRX	h	101	41/41	0.89	0.12	40,49,75,82	0
31	DMS	c	928	4/4	0.90	0.15	73,74,74,80	0
30	UNL	B	625	16/-	0.90	0.12	40,47,59,59	0
22	CLA	B	602	65/65	0.90	0.11	39,56,101,107	0
24	BCR	B	619	30/40	0.90	0.10	44,51,61,63	0
31	DMS	i	106	4/4	0.90	0.19	72,76,79,89	0
28	SQD	a	414	54/54	0.90	0.13	36,69,81,87	0
31	DMS	V	208	4/4	0.90	0.15	73,74,77,78	0
31	DMS	c	939	4/4	0.90	0.15	88,92,95,102	0
30	UNL	X	101	16/-	0.90	0.12	35,53,62,64	0
31	DMS	I	101	4/4	0.90	0.19	64,69,74,76	0
31	DMS	o	304	4/4	0.90	0.18	70,70,70,74	0
34	HTG	B	626	19/19	0.90	0.12	42,69,81,87	0
31	DMS	I	106	4/4	0.90	0.18	64,74,78,80	0
22	CLA	c	914	65/65	0.90	0.12	47,60,95,108	0
25	LMG	i	101	51/55	0.91	0.12	45,57,80,81	0
25	LMG	c	920	51/55	0.91	0.13	37,61,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	d	412	4/4	0.91	0.13	58,59,66,66	0
31	DMS	F	101	4/4	0.91	0.16	69,70,74,77	0
31	DMS	B	638	4/4	0.91	0.16	81,82,86,93	0
31	DMS	u	202	4/4	0.91	0.15	47,53,55,68	0
31	DMS	A	420	4/4	0.91	0.16	37,39,39,57	0
31	DMS	B	641	4/4	0.91	0.14	46,49,61,66	0
31	DMS	a	425	4/4	0.91	0.17	39,47,51,62	0
25	LMG	C	520	51/55	0.91	0.12	34,60,90,92	0
27	LHG	a	423	45/49	0.91	0.11	39,58,72,74	0
31	DMS	O	304	4/4	0.91	0.15	74,80,84,88	0
24	BCR	c	915	40/40	0.91	0.11	43,59,68,69	0
31	DMS	v	208	4/4	0.91	0.17	88,90,91,94	0
31	DMS	v	209	4/4	0.91	0.14	72,74,76,81	0
31	DMS	O	306	4/4	0.91	0.15	69,69,70,81	0
31	DMS	v	211	4/4	0.91	0.14	65,77,82,90	0
30	UNL	d	410	16/-	0.92	0.10	40,49,57,60	0
25	LMG	A	410	51/55	0.92	0.11	47,62,83,91	0
27	LHG	L	101	40/49	0.92	0.11	37,53,63,66	0
27	LHG	d	408	46/49	0.92	0.13	29,41,93,97	0
31	DMS	O	309	4/4	0.92	0.16	61,70,70,74	0
34	HTG	b	626	19/19	0.92	0.11	47,69,86,90	0
22	CLA	c	913	65/65	0.92	0.11	42,54,96,98	0
24	BCR	d	404	40/40	0.93	0.09	27,38,63,66	0
31	DMS	d	413	4/4	0.93	0.24	67,69,73,80	0
31	DMS	o	306	4/4	0.93	0.15	66,71,74,83	0
24	BCR	k	101	40/40	0.93	0.09	36,45,51,52	0
24	BCR	y	101	40/40	0.93	0.09	32,41,51,53	0
24	BCR	Y	101	39/40	0.93	0.08	34,40,48,50	0
31	DMS	C	527	4/4	0.93	0.16	74,80,80,81	0
32	BCT	a	422	4/4	0.93	0.10	51,52,56,57	0
22	CLA	C	507	65/65	0.93	0.11	37,45,85,88	0
31	DMS	c	926	4/4	0.93	0.14	63,64,67,68	0
31	DMS	B	635	4/4	0.93	0.15	61,63,66,73	0
35	DGD	c	918	62/66	0.93	0.10	34,42,98,113	0
22	CLA	b	617	60/65	0.93	0.10	32,41,75,80	0
37	RRX	H	101	41/41	0.93	0.10	32,42,58,62	0
22	CLA	C	514	65/65	0.93	0.10	44,55,83,86	0
22	CLA	B	615	53/65	0.94	0.09	31,36,71,84	0
22	CLA	b	607	65/65	0.94	0.08	29,37,58,65	0
31	DMS	a	424	4/4	0.94	0.12	38,47,50,65	0
24	BCR	C	515	40/40	0.94	0.09	37,50,58,59	0
31	DMS	B	633	4/4	0.94	0.17	65,71,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	615	52/65	0.94	0.09	36,42,71,76	0
22	CLA	B	617	55/65	0.94	0.09	28,35,72,76	0
34	HTG	b	623	19/19	0.94	0.09	42,46,54,63	0
22	CLA	c	904	65/65	0.94	0.08	32,44,50,54	0
22	CLA	c	907	65/65	0.94	0.11	39,47,102,108	0
24	BCR	c	916	40/40	0.94	0.08	33,42,48,49	0
22	CLA	c	908	65/65	0.94	0.09	34,39,53,61	0
31	DMS	B	640	4/4	0.94	0.17	47,53,57,63	0
28	SQD	C	501	54/54	0.94	0.11	32,64,83,89	0
25	LMG	j	101	47/55	0.94	0.10	33,43,69,74	0
35	DGD	C	518	62/66	0.94	0.10	29,40,89,109	0
31	DMS	c	934	4/4	0.94	0.11	64,73,74,77	0
22	CLA	B	607	65/65	0.94	0.08	28,34,56,65	0
22	CLA	B	608	65/65	0.94	0.09	24,29,64,79	0
35	DGD	h	102	62/66	0.94	0.09	28,42,53,58	0
22	CLA	d	403	65/65	0.94	0.10	35,40,85,90	0
31	DMS	A	419	4/4	0.94	0.17	58,60,70,72	0
31	DMS	c	933	4/4	0.95	0.12	57,64,66,70	0
22	CLA	b	614	59/65	0.95	0.08	26,32,76,82	0
31	DMS	O	310	4/4	0.95	0.14	66,68,68,73	0
24	BCR	B	620	40/40	0.95	0.07	30,37,49,50	0
22	CLA	C	509	65/65	0.95	0.09	29,35,81,102	0
24	BCR	C	516	40/40	0.95	0.08	32,39,47,54	0
24	BCR	D	405	40/40	0.95	0.08	26,35,62,66	0
24	BCR	K	101	40/40	0.95	0.08	31,39,43,43	0
31	DMS	V	201	4/4	0.95	0.10	46,48,54,58	0
32	BCT	A	421[A]	4/4	0.95	0.10	34,36,39,39	4
32	BCT	A	421[B]	4/4	0.95	0.10	27,29,30,34	4
26	PL9	D	406	55/55	0.95	0.07	21,30,37,51	0
33	CA	B	601	1/1	0.95	0.05	64,64,64,64	0
33	CA	O	302	1/1	0.95	0.06	59,59,59,59	0
34	HTG	B	623	19/19	0.95	0.09	41,47,64,66	0
22	CLA	C	512	65/65	0.95	0.08	31,39,48,51	0
26	PL9	d	405	55/55	0.95	0.07	23,32,39,43	0
24	BCR	a	413	40/40	0.95	0.07	26,31,38,39	0
22	CLA	c	902	65/65	0.95	0.08	34,39,50,51	0
22	CLA	C	513	56/65	0.95	0.08	37,48,62,65	0
27	LHG	D	411	45/49	0.95	0.10	31,39,90,94	0
24	BCR	b	620	40/40	0.95	0.07	33,39,48,49	0
22	CLA	c	906	65/65	0.95	0.08	30,40,50,54	0
31	DMS	D	416	4/4	0.95	0.12	55,59,60,69	0
22	CLA	B	611	65/65	0.95	0.08	26,33,41,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	D	404	65/65	0.95	0.09	30,37,94,104	0
31	DMS	b	630	4/4	0.95	0.15	56,63,63,64	0
31	DMS	B	629	4/4	0.95	0.14	48,52,58,65	0
31	DMS	b	633	4/4	0.95	0.14	68,68,70,78	0
22	CLA	c	909	65/65	0.95	0.08	31,37,80,97	0
22	CLA	c	910	65/65	0.95	0.09	28,38,58,64	0
22	CLA	c	912	65/65	0.95	0.08	35,45,50,53	0
35	DGD	C	519	62/66	0.95	0.09	23,36,76,85	0
22	CLA	a	412	65/65	0.95	0.11	27,32,102,116	0
35	DGD	H	102	62/66	0.95	0.08	28,37,46,50	0
22	CLA	B	604	65/65	0.95	0.08	26,30,40,47	0
35	DGD	c	919	62/66	0.95	0.09	29,40,73,79	0
22	CLA	C	508	65/65	0.95	0.08	32,42,55,59	0
23	PHO	a	411	64/64	0.95	0.06	26,33,40,48	0
25	LMG	J	101	45/55	0.95	0.09	28,36,71,79	0
22	CLA	b	610	65/65	0.95	0.08	32,41,45,54	0
22	CLA	A	408	65/65	0.96	0.09	19,29,99,110	0
27	LHG	d	407	49/49	0.96	0.07	28,36,56,63	0
31	DMS	d	411	4/4	0.96	0.12	60,62,64,64	0
22	CLA	b	608	65/65	0.96	0.08	27,31,73,74	0
31	DMS	B	630	4/4	0.96	0.13	63,67,68,75	0
22	CLA	b	609	65/65	0.96	0.06	27,34,42,45	0
23	PHO	A	407	64/64	0.96	0.06	20,25,30,32	0
23	PHO	D	402	64/64	0.96	0.06	25,29,35,39	0
23	PHO	a	410	64/64	0.96	0.06	21,28,32,36	0
22	CLA	B	614	61/65	0.96	0.07	25,31,70,83	0
24	BCR	A	409	40/40	0.96	0.06	25,30,37,38	0
22	CLA	b	611	65/65	0.96	0.07	28,35,40,43	0
22	CLA	b	612	65/65	0.96	0.08	27,31,72,83	0
22	CLA	B	606	65/65	0.96	0.07	24,30,42,46	0
22	CLA	C	510	65/65	0.96	0.09	31,36,59,64	0
22	CLA	b	616	65/65	0.96	0.07	30,37,53,57	0
31	DMS	c	924	4/4	0.96	0.14	37,42,47,49	0
31	DMS	c	925	4/4	0.96	0.11	51,58,60,61	0
22	CLA	C	511	65/65	0.96	0.06	31,36,41,46	0
22	CLA	B	610	65/65	0.96	0.06	30,37,42,46	0
31	DMS	O	312	4/4	0.96	0.14	37,51,56,59	0
22	CLA	C	502	65/65	0.96	0.07	33,39,52,62	0
22	CLA	c	905	65/65	0.96	0.08	30,35,62,66	0
35	DGD	C	517	62/66	0.96	0.09	24,35,80,88	0
22	CLA	C	503	65/65	0.96	0.07	28,32,47,56	0
22	CLA	C	504	65/65	0.96	0.06	29,37,42,51	0

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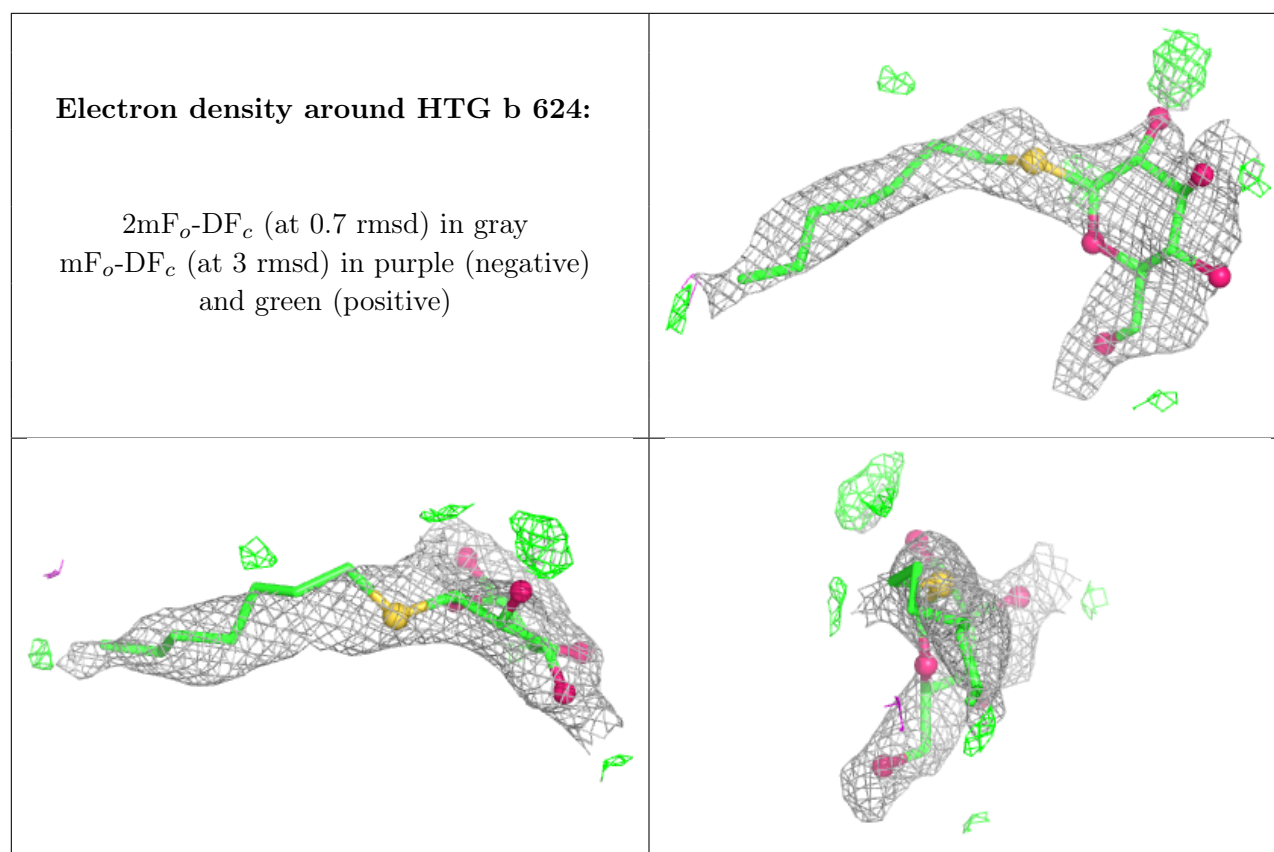
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	v	201	4/4	0.96	0.16	42,48,50,51	0
22	CLA	C	505	65/65	0.96	0.07	28,34,58,60	0
35	DGD	c	917	62/66	0.96	0.08	26,42,81,94	0
27	LHG	D	410	49/49	0.96	0.07	29,36,51,61	0
22	CLA	C	506	65/65	0.96	0.07	30,37,50,54	0
31	DMS	V	206	4/4	0.96	0.09	45,48,51,62	0
22	CLA	b	603	65/65	0.96	0.07	29,36,46,49	0
36	HEM	E	102	43/43	0.96	0.09	48,56,62,65	0
22	CLA	c	911	65/65	0.96	0.06	29,38,46,52	0
22	CLA	b	604	65/65	0.96	0.07	26,32,45,50	0
38	MG	J	102	1/1	0.96	0.06	30,30,30,30	0
22	CLA	B	609	65/65	0.97	0.06	25,30,38,39	0
31	DMS	C	526	4/4	0.97	0.09	48,48,50,51	0
22	CLA	B	616	65/65	0.97	0.06	30,36,50,57	0
22	CLA	A	406	55/65	0.97	0.06	21,27,49,60	0
31	DMS	b	629	4/4	0.97	0.09	29,31,36,45	0
22	CLA	a	408	65/65	0.97	0.05	20,26,35,41	0
22	CLA	a	409	61/65	0.97	0.07	25,29,80,87	0
22	CLA	B	603	65/65	0.97	0.06	27,36,43,47	0
22	CLA	b	613	65/65	0.97	0.06	26,32,37,40	0
22	CLA	B	612	65/65	0.97	0.06	23,29,55,60	0
22	CLA	B	613	65/65	0.97	0.06	24,30,37,40	0
22	CLA	A	405	65/65	0.97	0.06	18,23,36,54	0
22	CLA	b	605	65/65	0.97	0.07	23,29,63,65	0
22	CLA	d	402	65/65	0.97	0.05	21,27,42,50	0
36	HEM	e	101	43/43	0.97	0.09	43,55,85,93	0
31	DMS	o	307	4/4	0.97	0.19	48,56,62,64	0
22	CLA	b	606	65/65	0.97	0.06	24,28,40,40	0
22	CLA	c	903	65/65	0.97	0.07	27,34,54,65	0
38	MG	k	102	1/1	0.97	0.07	48,48,48,48	0
31	DMS	c	923	4/4	0.98	0.09	37,40,42,43	0
22	CLA	B	605	65/65	0.98	0.06	24,28,60,66	0
31	DMS	B	628	4/4	0.98	0.07	27,29,32,38	0
31	DMS	D	418	4/4	0.98	0.06	35,39,42,43	0
31	DMS	C	525	4/4	0.98	0.08	34,35,38,40	0
22	CLA	a	407	65/65	0.98	0.05	23,26,45,61	0
21	CL	A	404	1/1	0.98	0.04	28,28,28,28	0
22	CLA	D	401	65/65	0.98	0.05	19,23,31,36	0
31	DMS	A	418	4/4	0.98	0.05	29,30,31,31	0
38	MG	K	102	1/1	0.98	0.05	51,51,51,51	0
22	CLA	D	403	65/65	0.98	0.05	18,24,45,52	0
39	HEC	V	202	43/43	0.98	0.06	23,29,36,40	0

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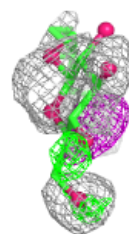
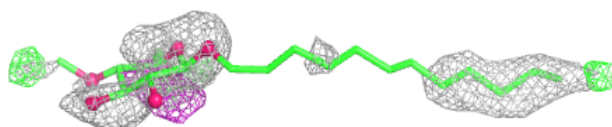
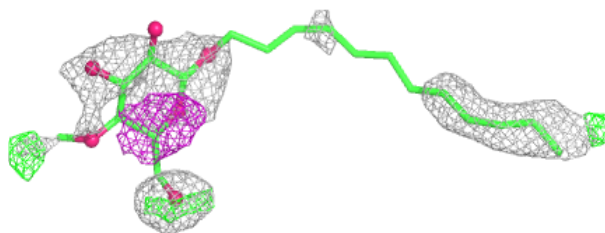
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
39	HEC	v	202	43/43	0.98	0.06	33,37,42,46	0
21	CL	a	406	1/1	0.99	0.03	32,32,32,32	0
33	CA	b	601	1/1	0.99	0.03	59,59,59,59	0
33	CA	c	901	1/1	0.99	0.05	48,48,48,48	0
33	CA	o	301	1/1	0.99	0.04	55,55,55,55	0
31	DMS	a	402	4/4	0.99	0.07	30,32,34,34	0
38	MG	j	102	1/1	0.99	0.08	40,40,40,40	0
31	DMS	C	524	4/4	0.99	0.06	38,42,43,43	0
21	CL	A	403	1/1	0.99	0.04	29,29,29,29	0
21	CL	a	405	1/1	0.99	0.04	31,31,31,31	0
19	OEX	A	401	10/10	1.00	0.05	25,27,31,32	0
19	OEX	a	403	10/10	1.00	0.03	29,31,32,33	0
20	FE2	A	402	1/1	1.00	0.01	39,39,39,39	0
20	FE2	a	404	1/1	1.00	0.01	42,42,42,42	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.

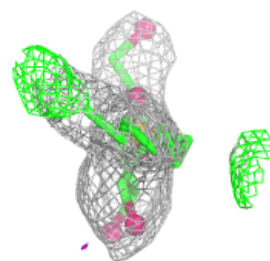
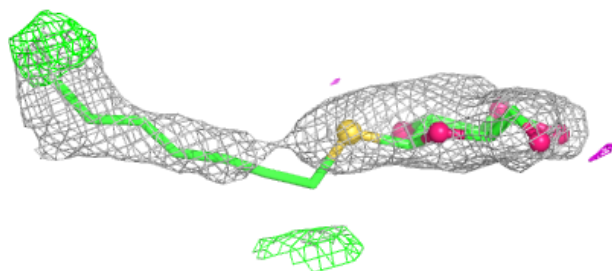
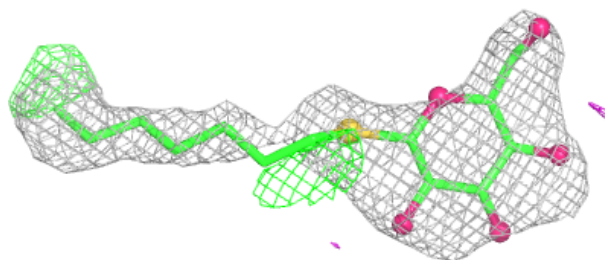


Electron density around LMT f 102:

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

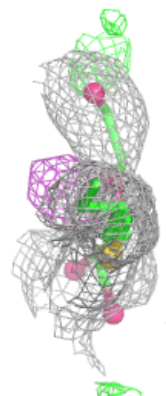
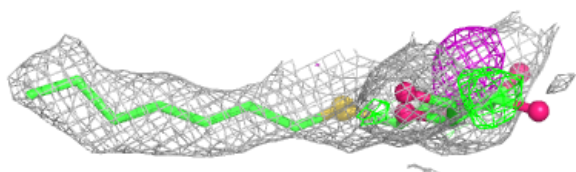
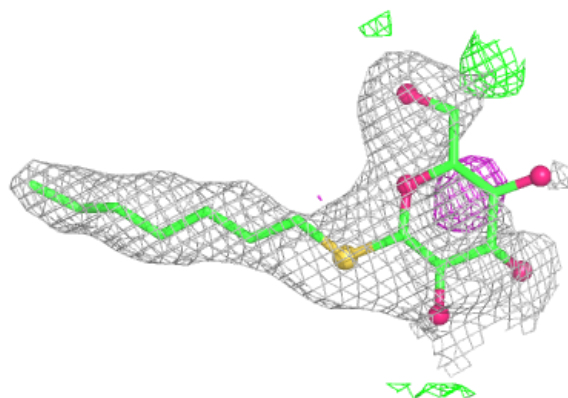
**Electron density around HTG c 922:**

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

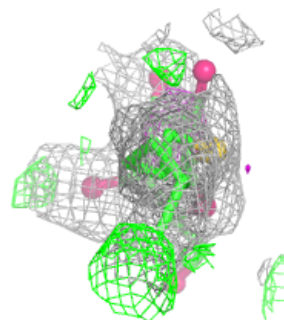
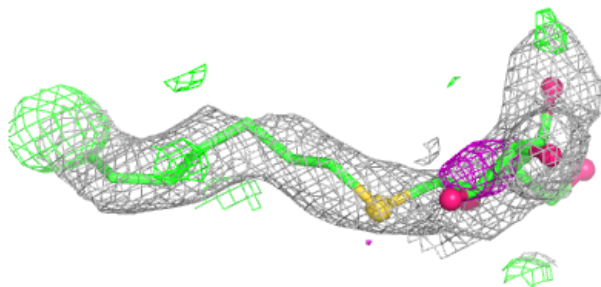
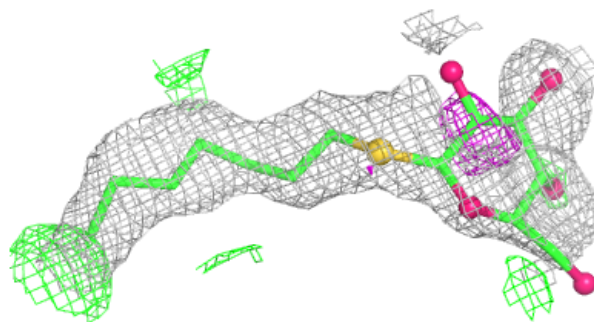


Electron density around HTG b 627:

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

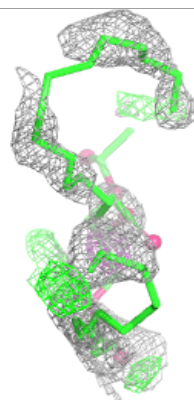
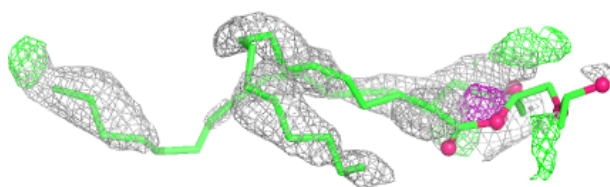
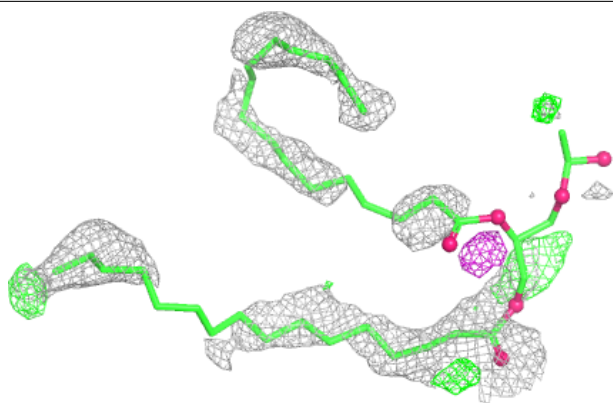
**Electron density around HTG D 415:**

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

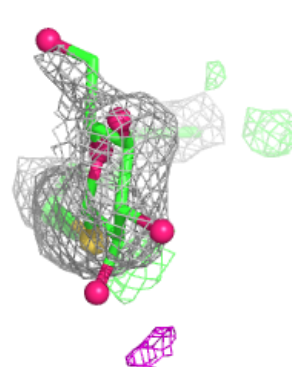
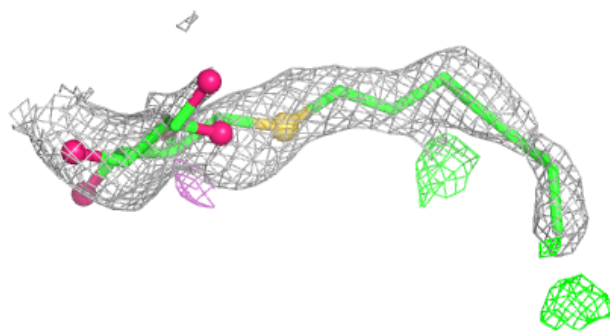
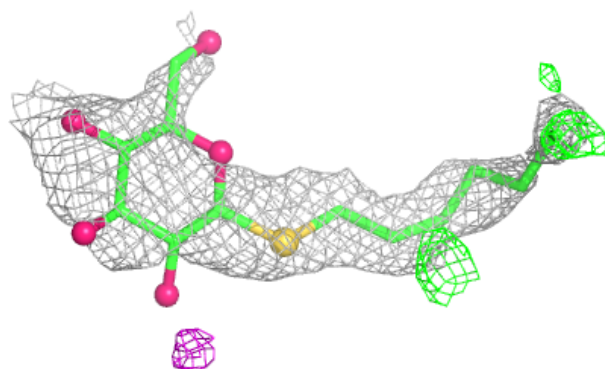


Electron density around DGD d 406:

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

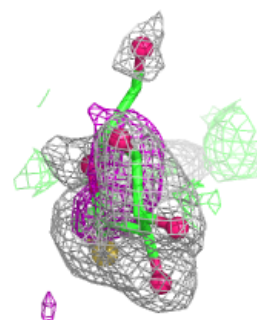
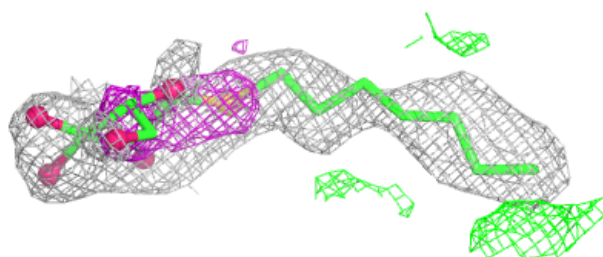
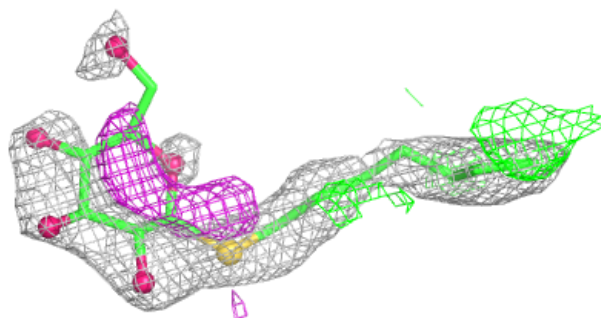
**Electron density around HTG D 414:**

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

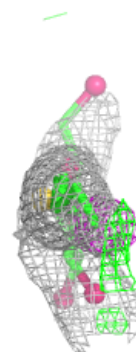
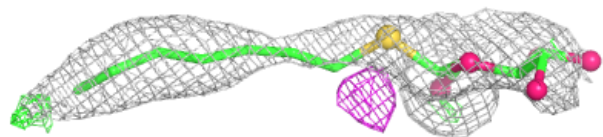
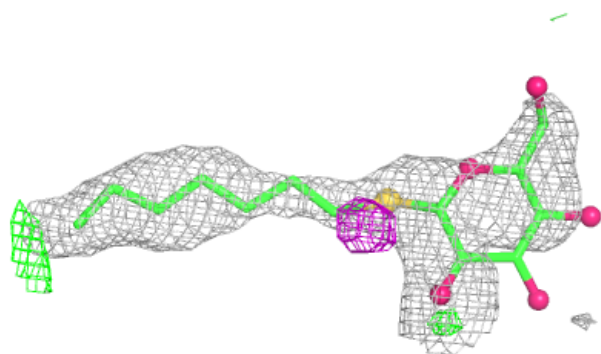


Electron density around HTG b 632:

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

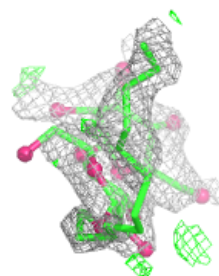
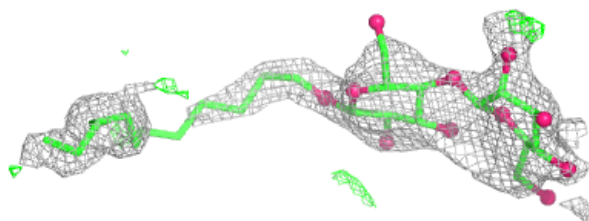
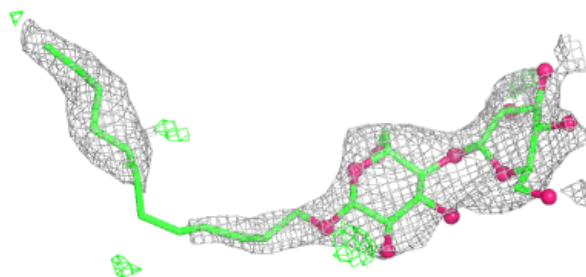
**Electron density around HTG B 627:**

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

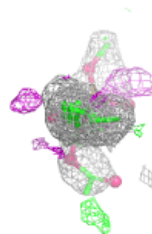
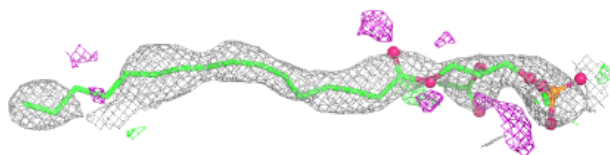
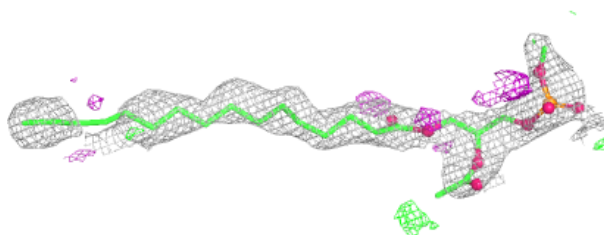


Electron density around LMT I 102:

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

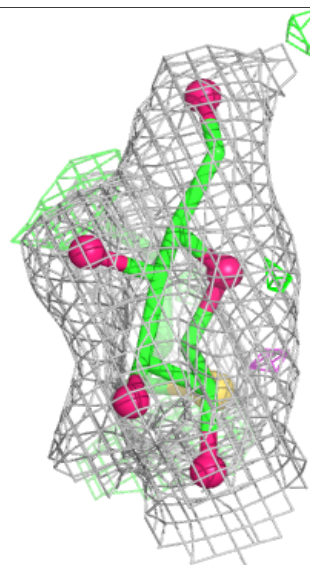
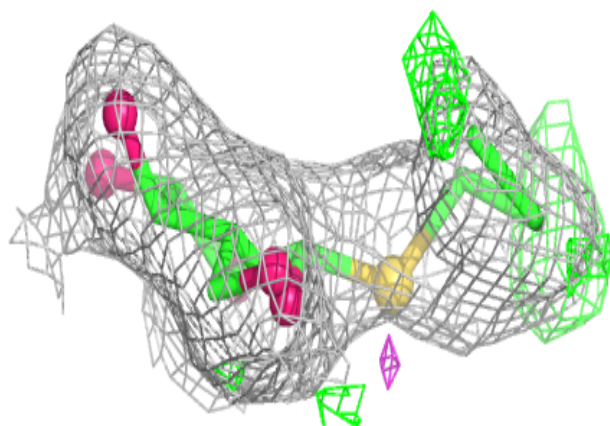
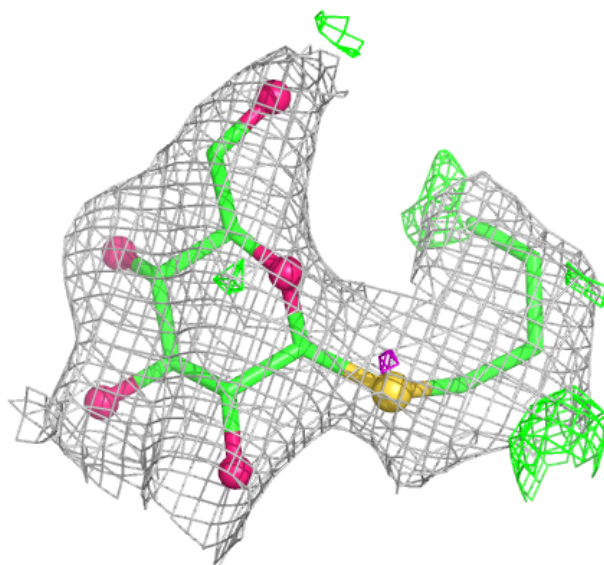
**Electron density around LHG A 412:**

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



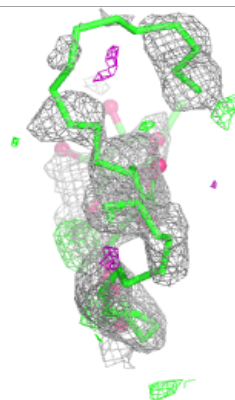
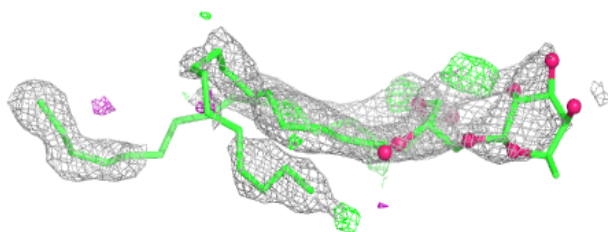
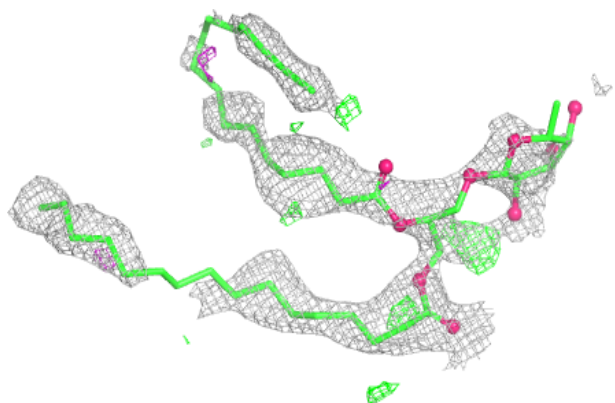
Electron density around HTG v 203:

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

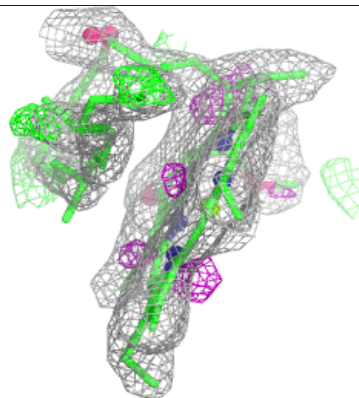
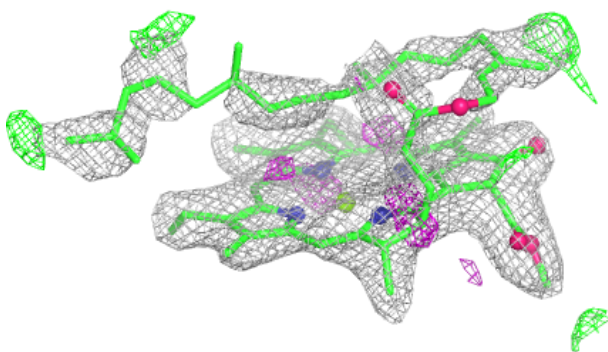
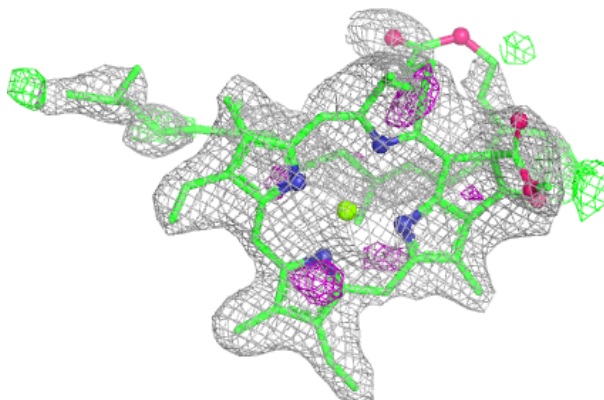


Electron density around DGD D 407:

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

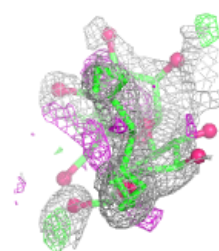
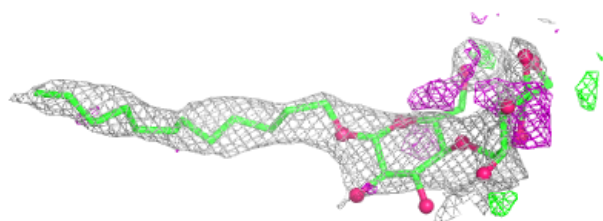
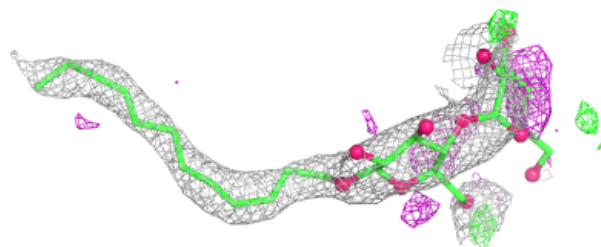
**Electron density around CLA b 602:**

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

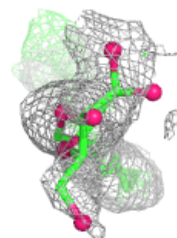
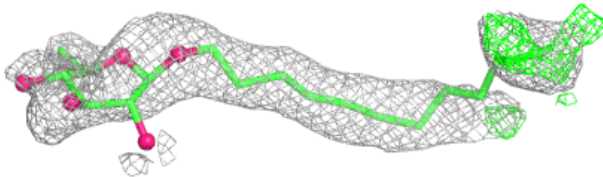
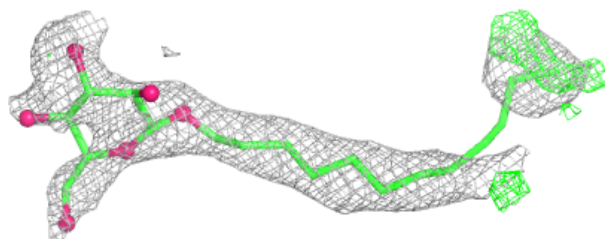


Electron density around LMT A 414:

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

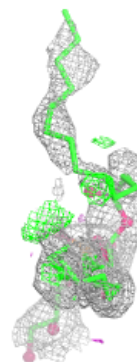
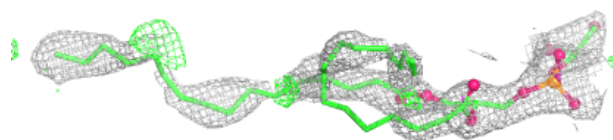
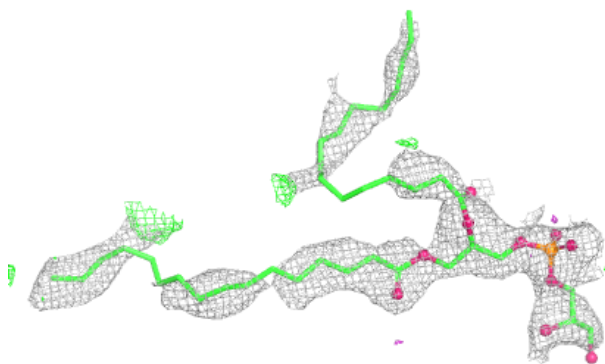
**Electron density around LMT T 102:**

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



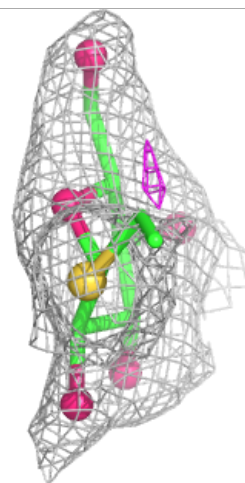
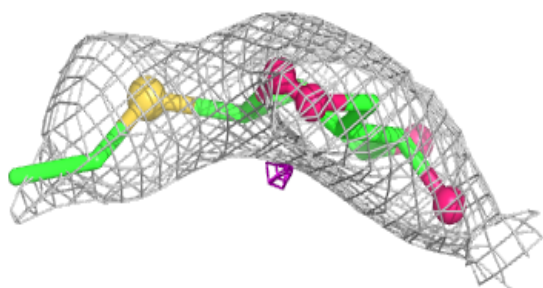
Electron density around LHG a 416:

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



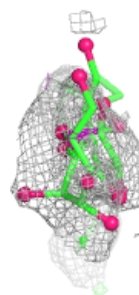
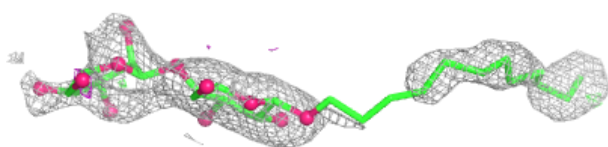
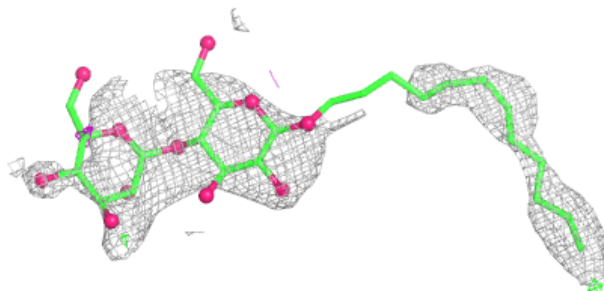
Electron density around HTG V 203:

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

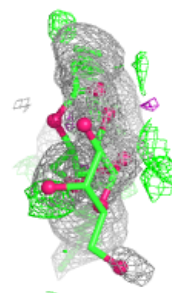
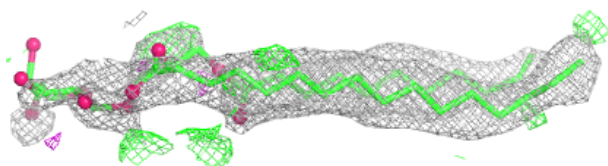
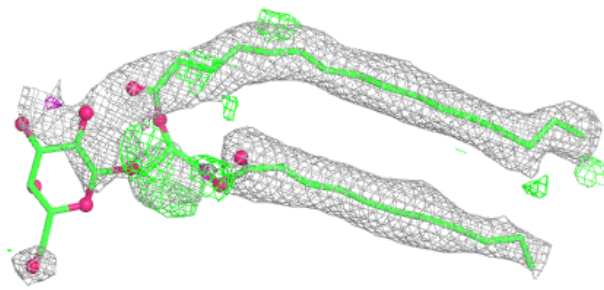


Electron density around LMT Z 101:

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

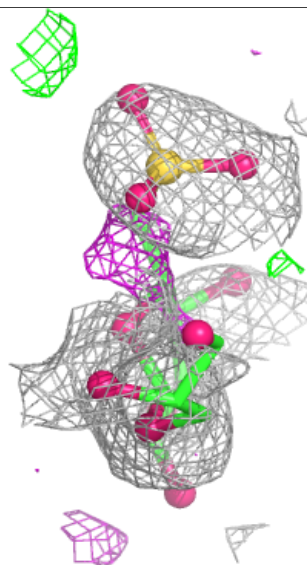
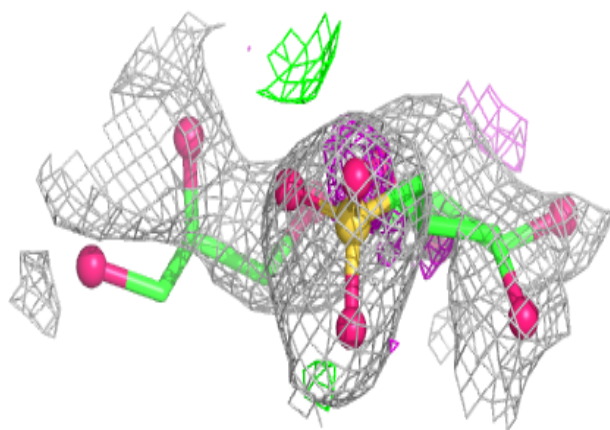
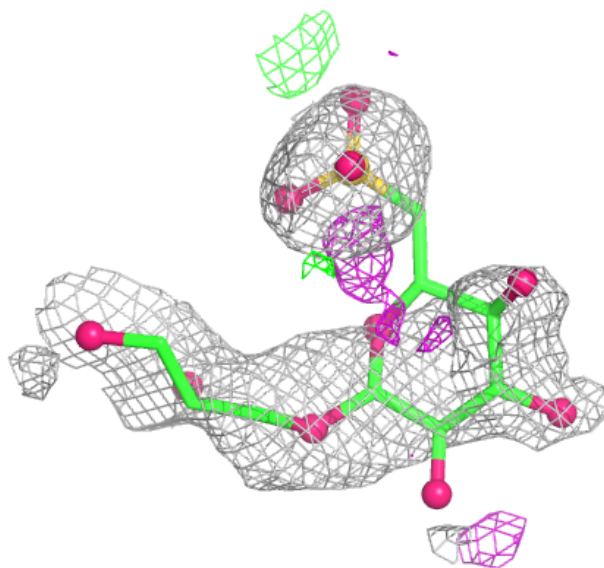
**Electron density around LMG D 412:**

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



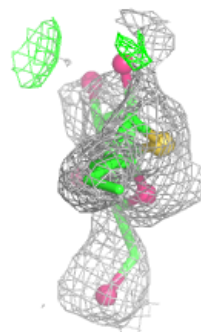
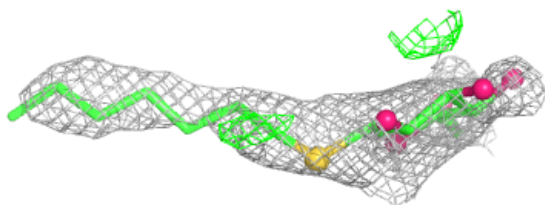
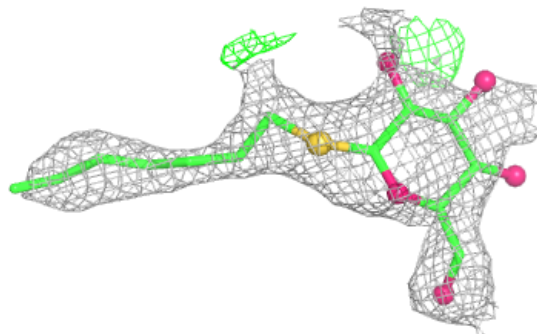
Electron density around SQD D 408:

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

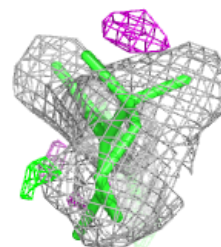
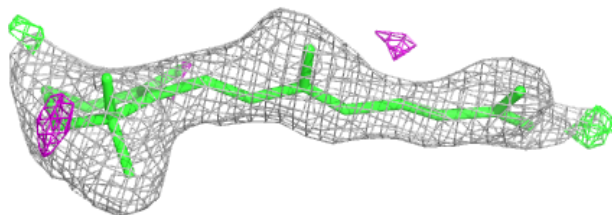
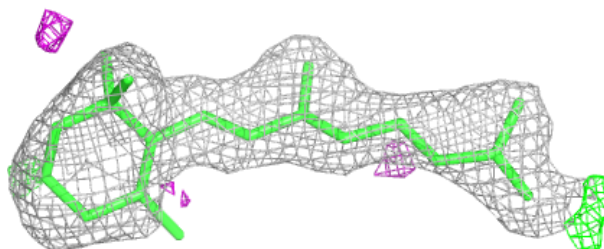


Electron density around HTG 1 106:

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

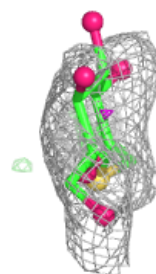
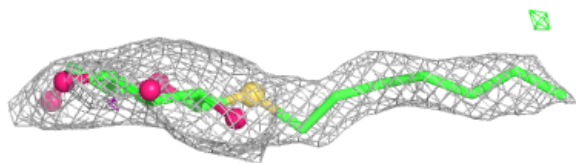
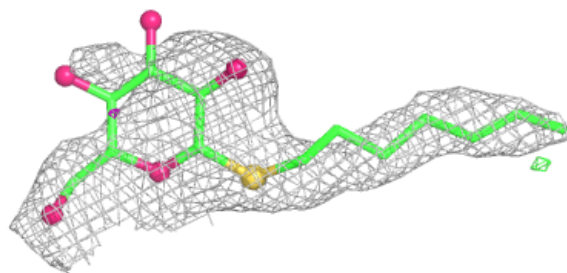
**Electron density around BCR B 618:**

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

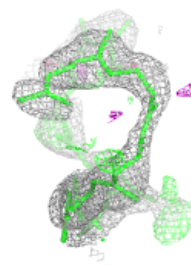
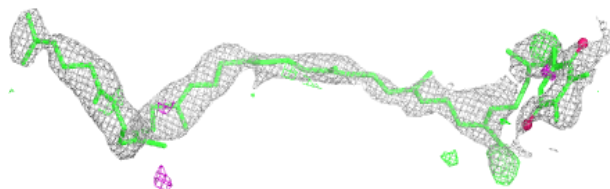
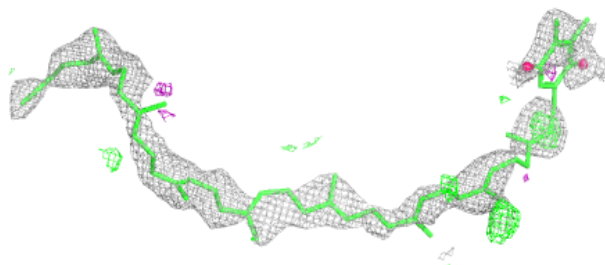


Electron density around HTG C 532:

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

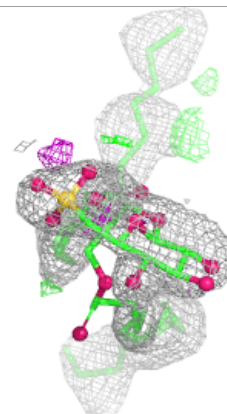
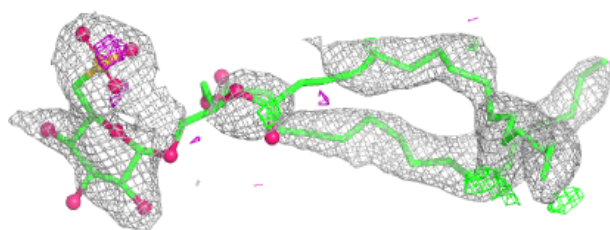
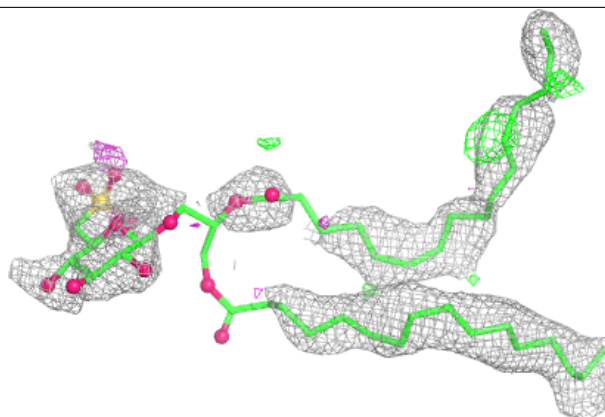
**Electron density around PL9 A 411:**

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

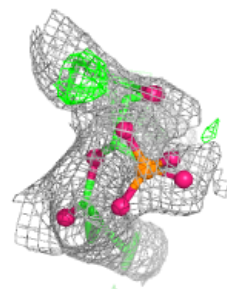
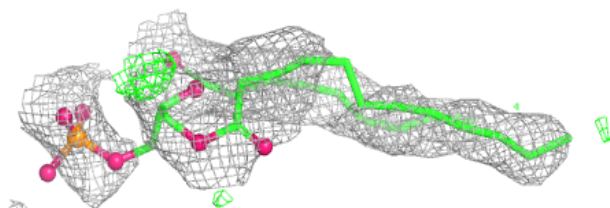
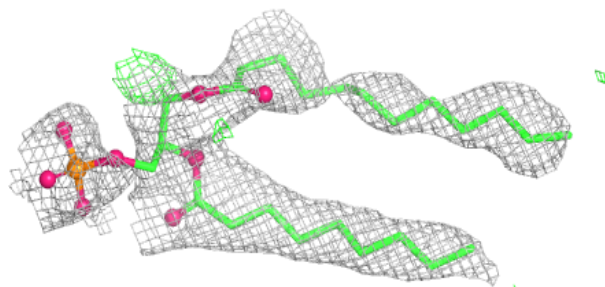


Electron density around SQD 1 101:

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

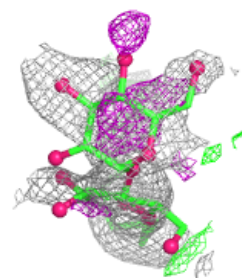
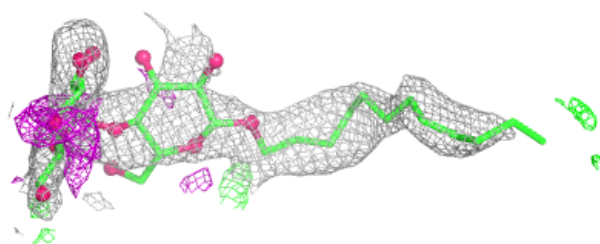
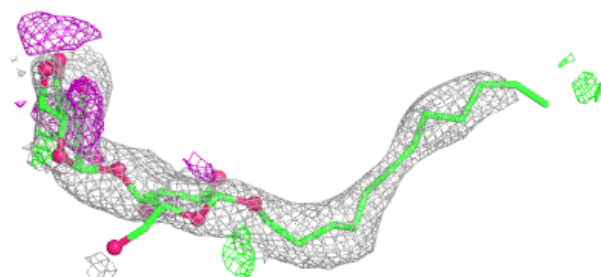
**Electron density around LHG d 401:**

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

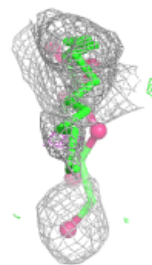
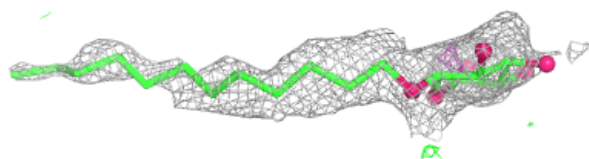
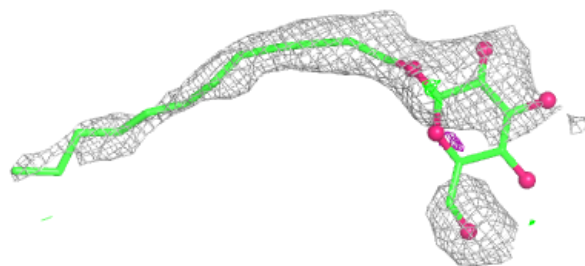


Electron density around LMT a 419:

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

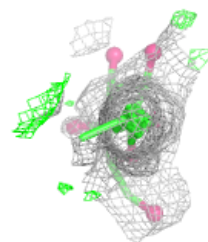
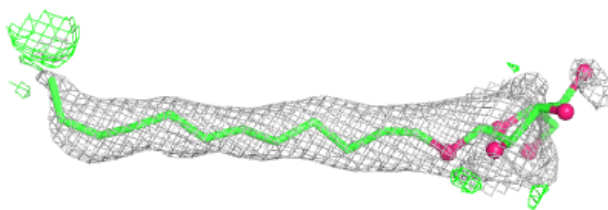
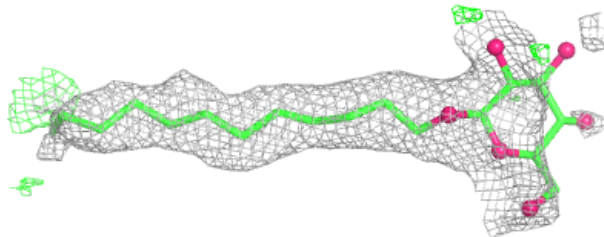
**Electron density around LMT E 101:**

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

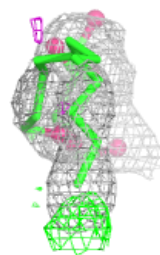
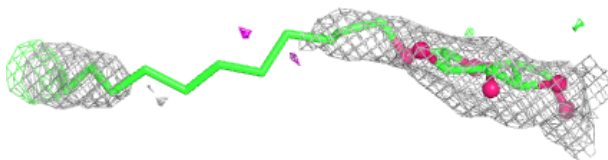
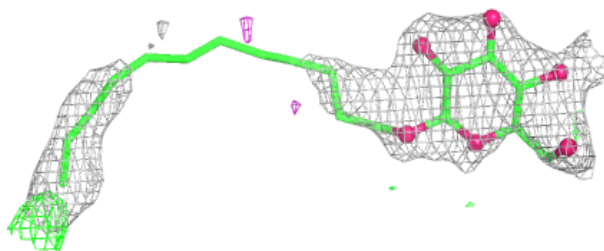


Electron density around LMT t 101:

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

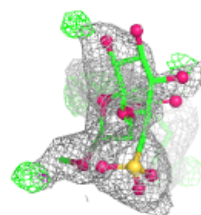
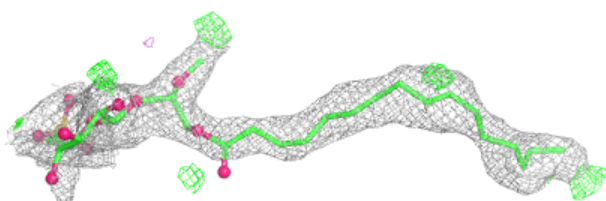
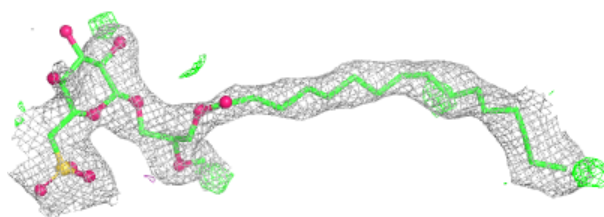
**Electron density around LMT c 931:**

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

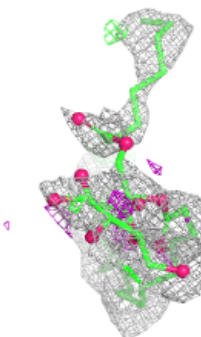
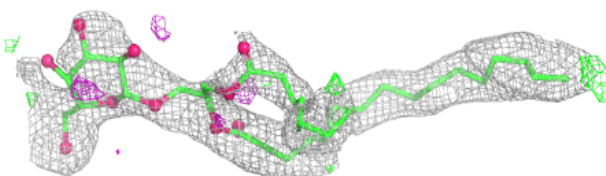
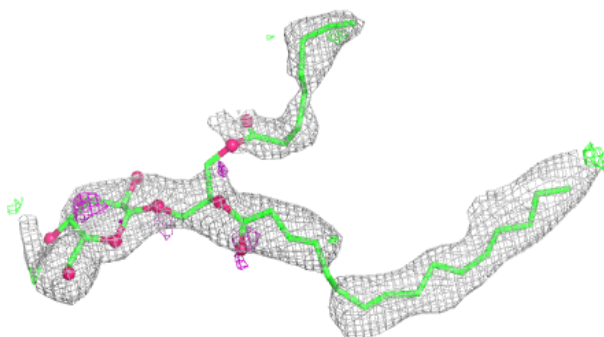


Electron density around SQD b 621:

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

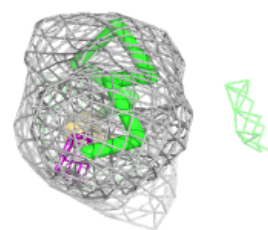
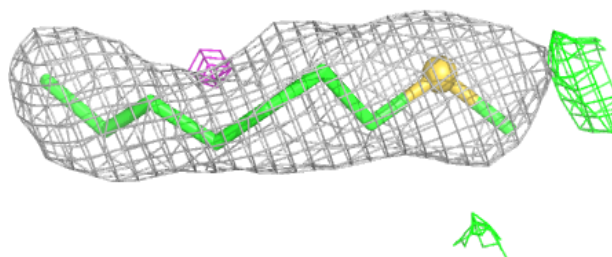
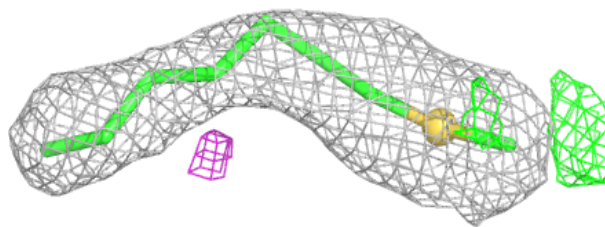
**Electron density around LMG b 622:**

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

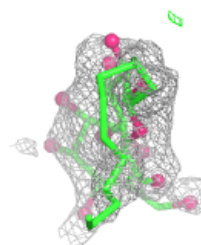
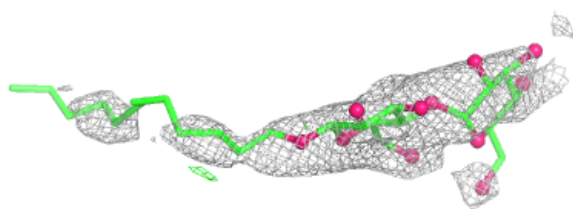
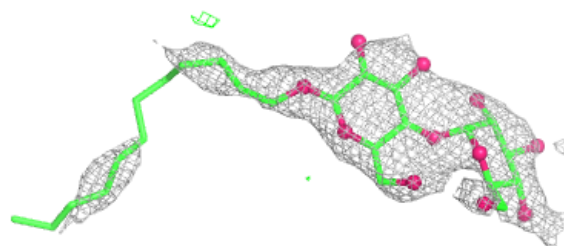


Electron density around HTG C 523:

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

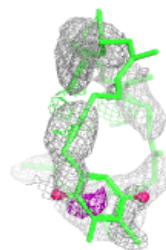
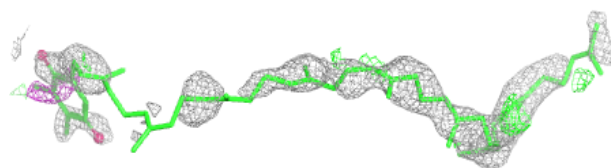
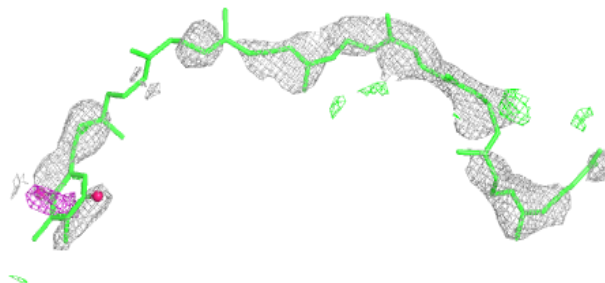
**Electron density around LMT c 921:**

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

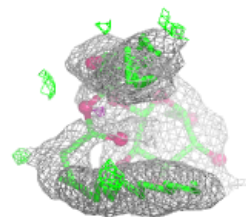
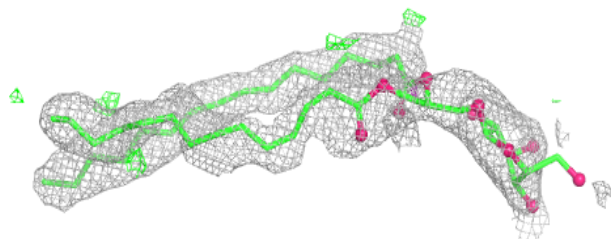
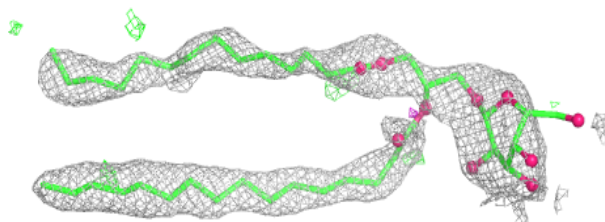


Electron density around PL9 a 415:

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

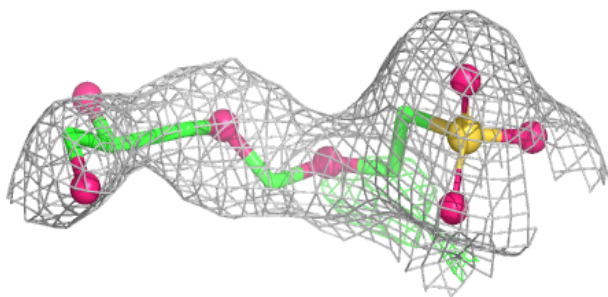
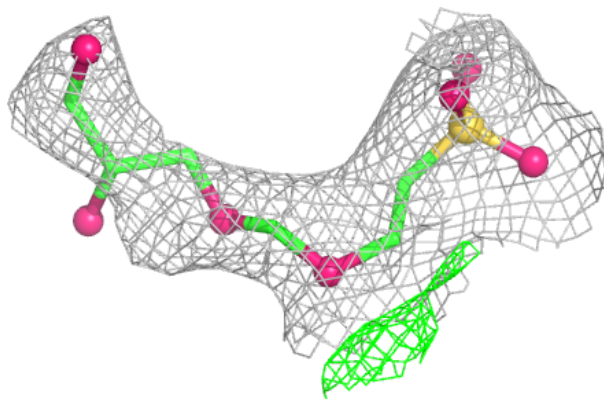
**Electron density around LMG c 930:**

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

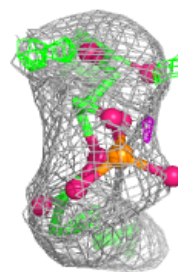
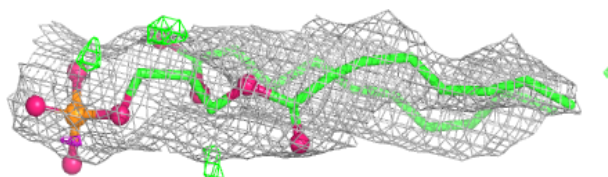
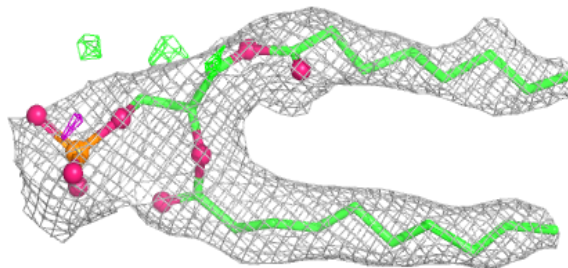


Electron density around SQD f 101:

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

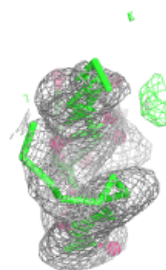
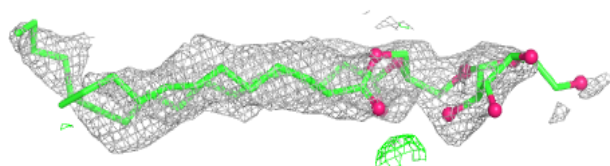
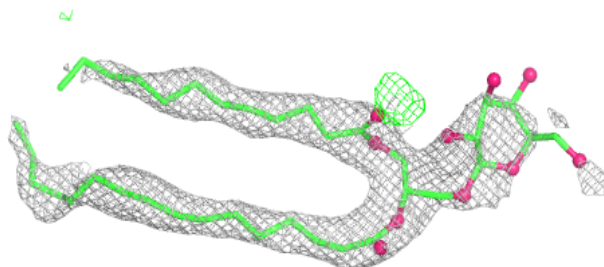
**Electron density around LHG C 522:**

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

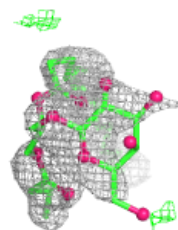
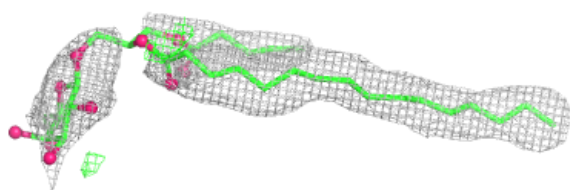
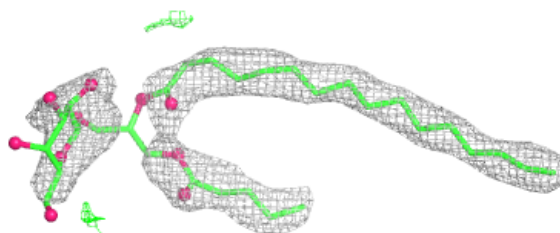


Electron density around LMG d 409:

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

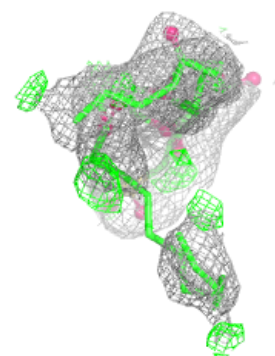
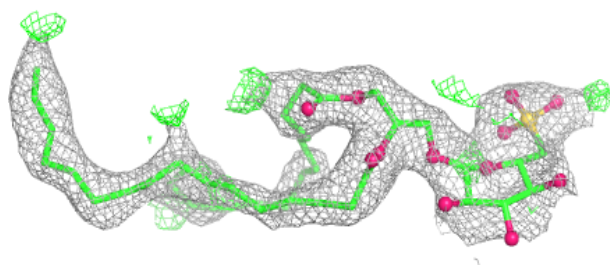
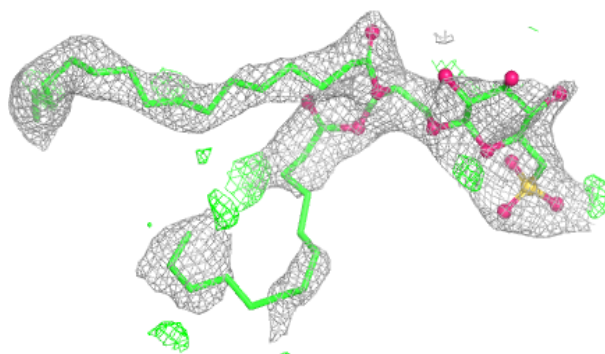
**Electron density around LMG C 531:**

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

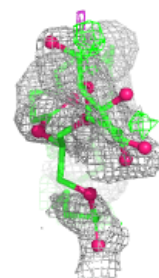
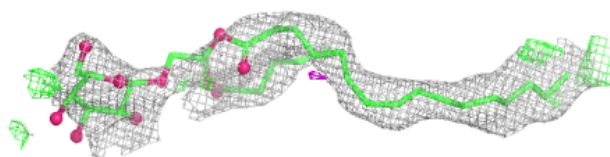
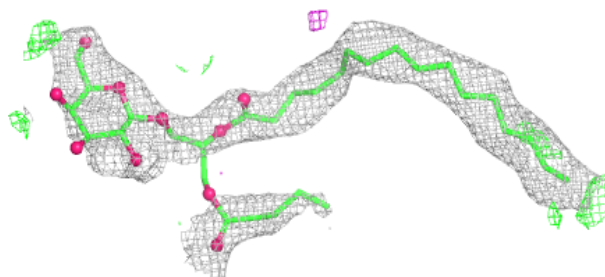


Electron density around SQD a 418:

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

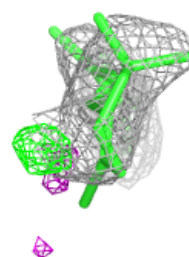
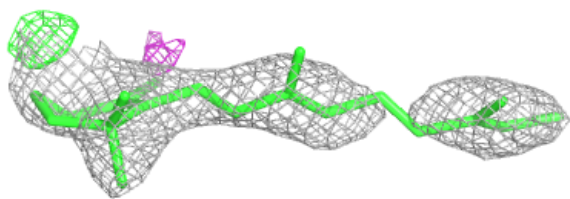
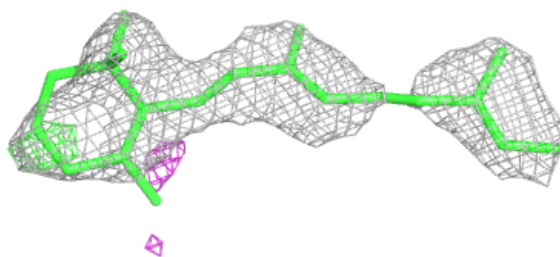
**Electron density around LMG B 621:**

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



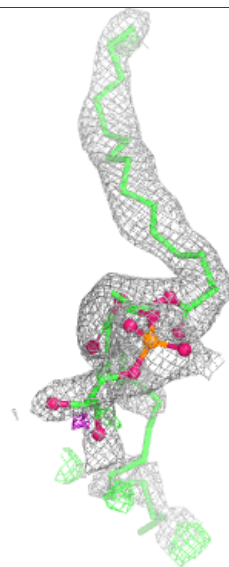
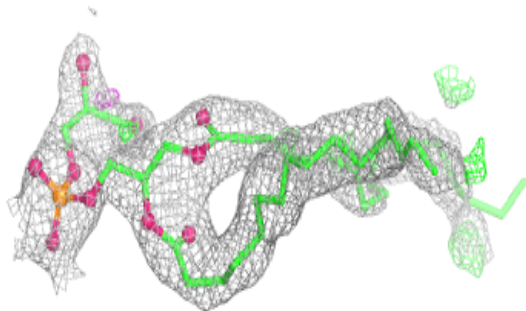
Electron density around BCR b 618:

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



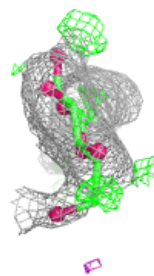
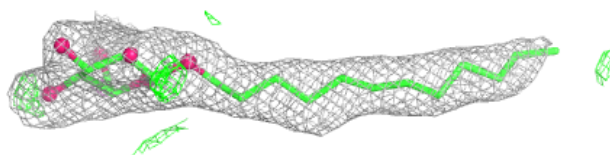
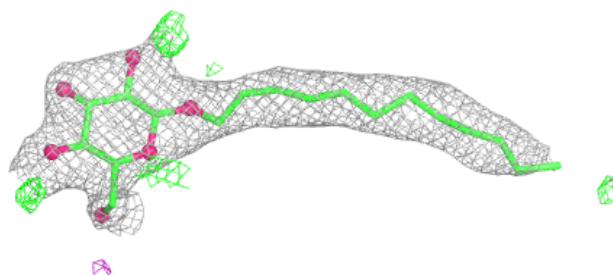
Electron density around LHG 1 102:

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

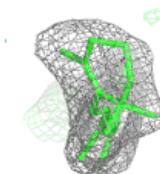
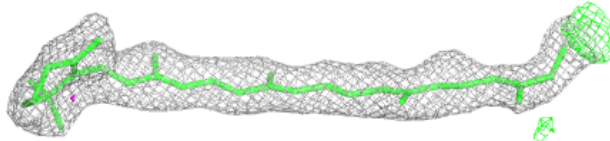
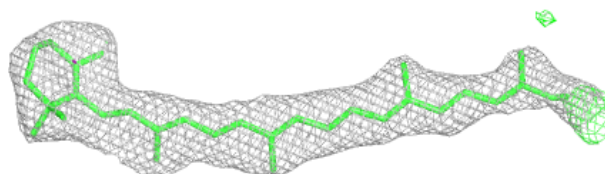


Electron density around LMT B 622:

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

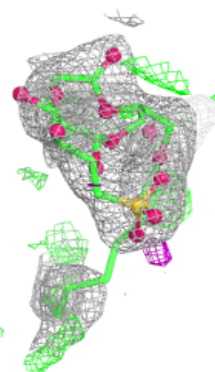
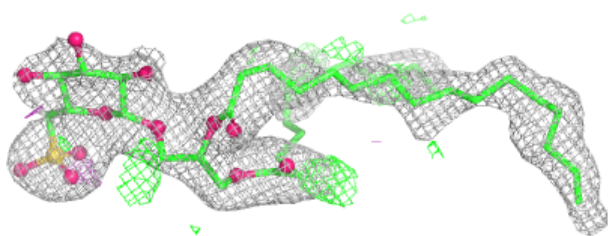
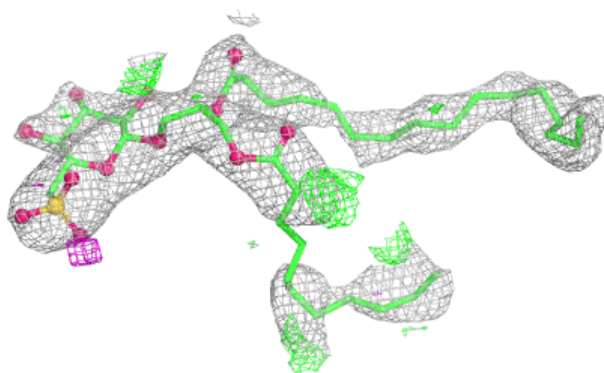
**Electron density around BCR b 619:**

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

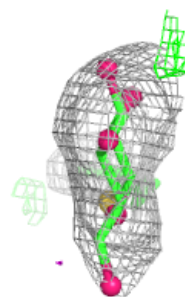
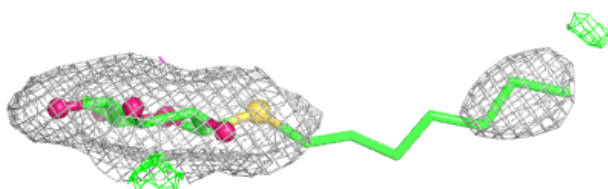
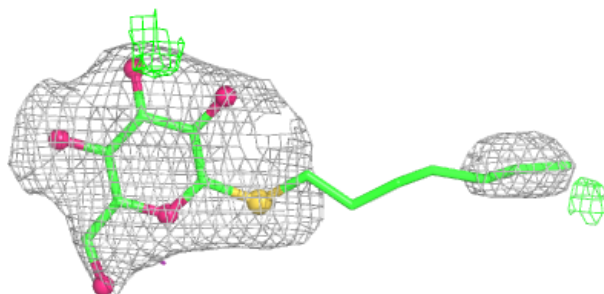


Electron density around SQD A 413:

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

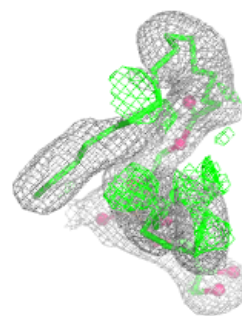
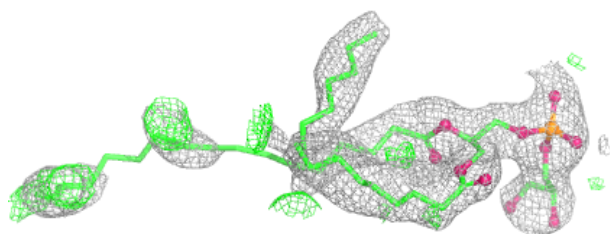
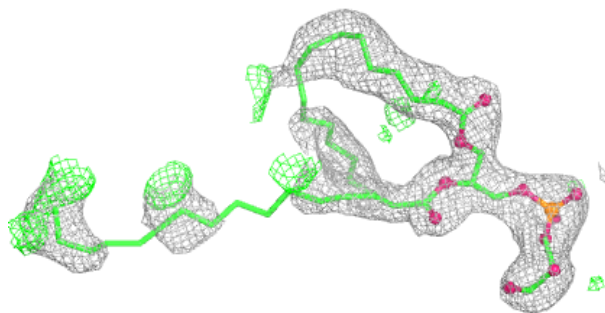
**Electron density around HTG C 521:**

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

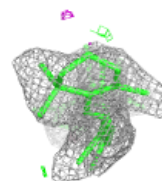
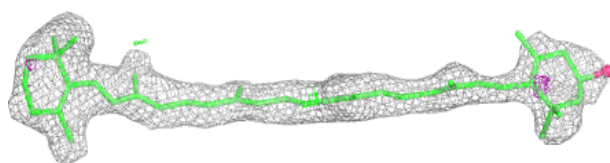
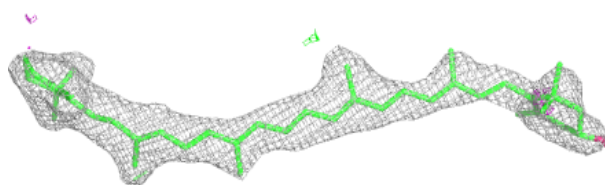


Electron density around LHG D 409:

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

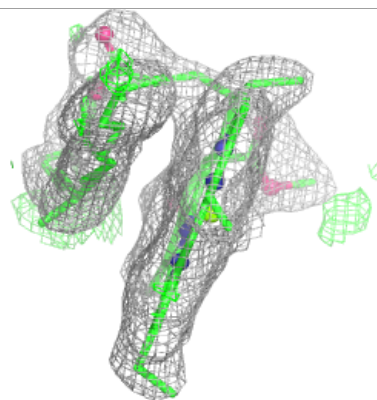
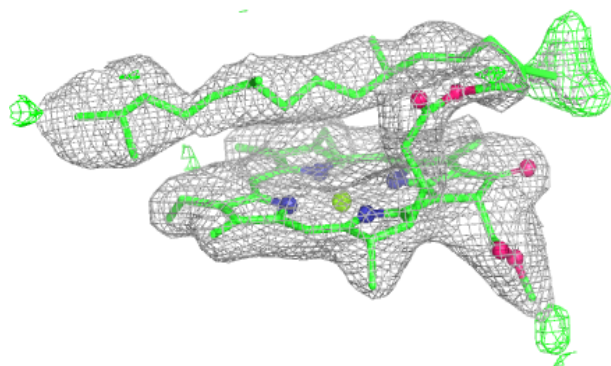
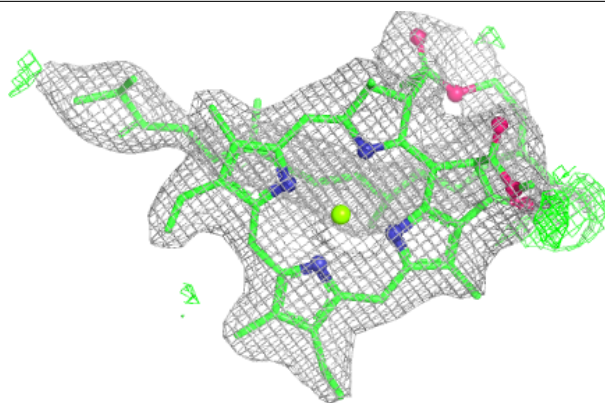
**Electron density around RRX h 101:**

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

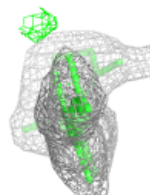
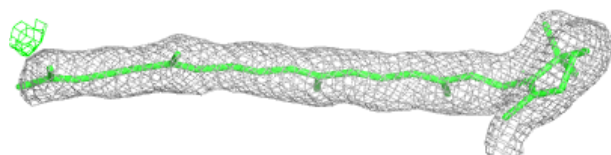
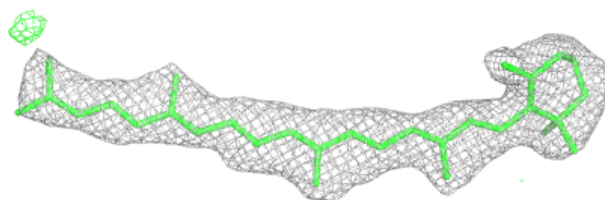


Electron density around CLA B 602:

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

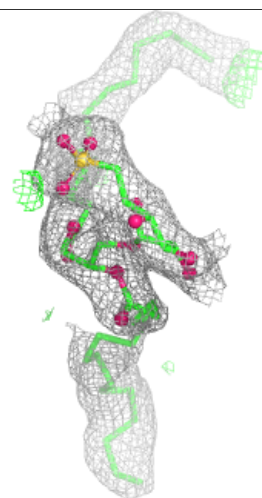
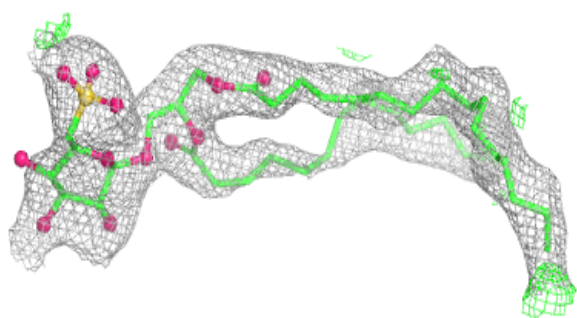
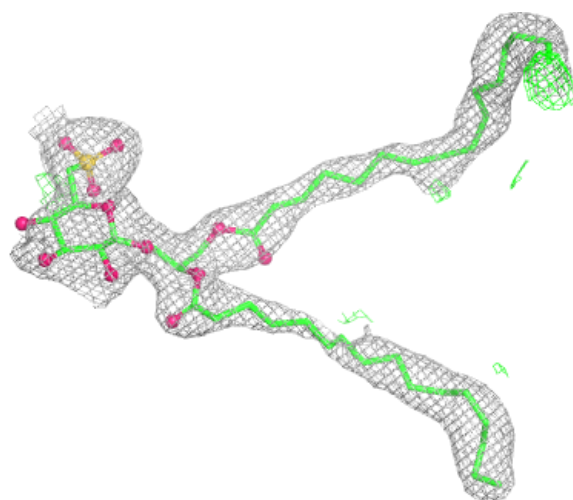
**Electron density around BCR B 619:**

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



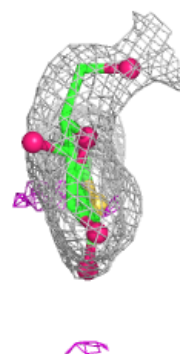
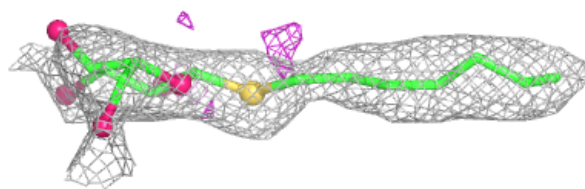
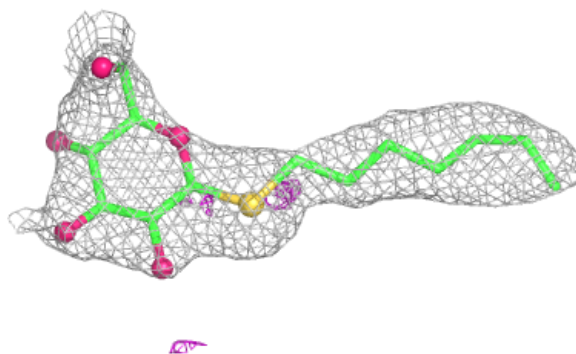
Electron density around SQD a 414:

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

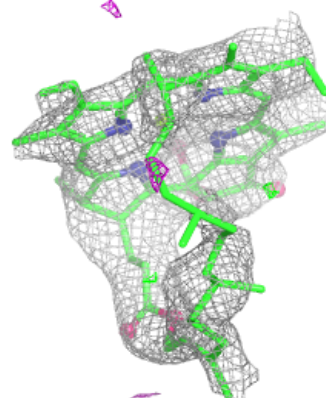
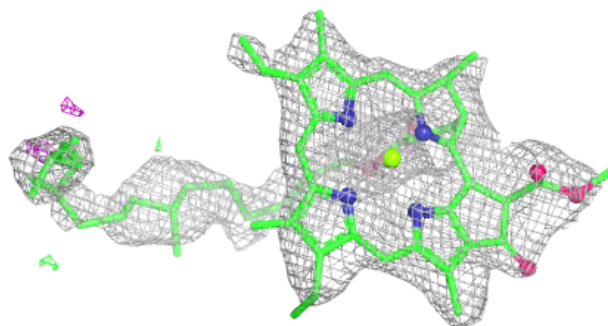
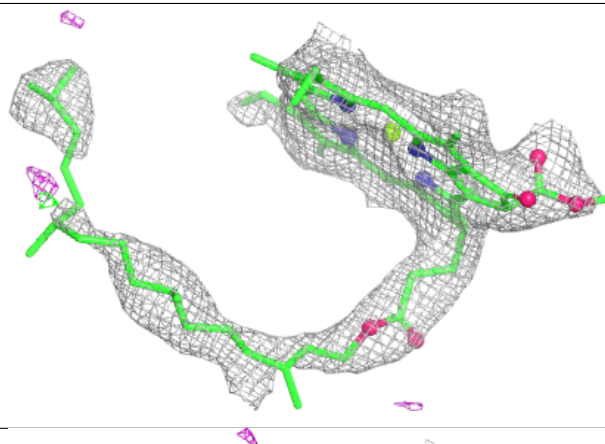


Electron density around HTG B 626:

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

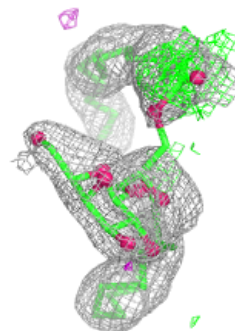
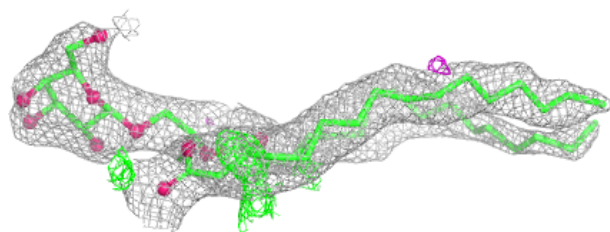
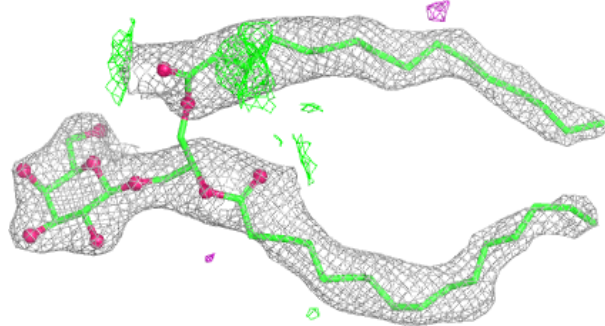
**Electron density around CLA c 914:**

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



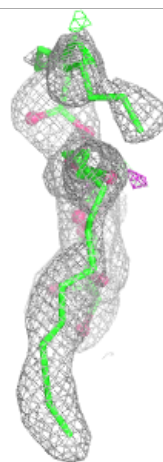
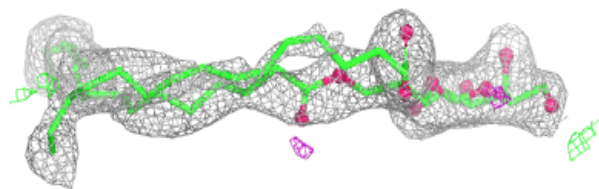
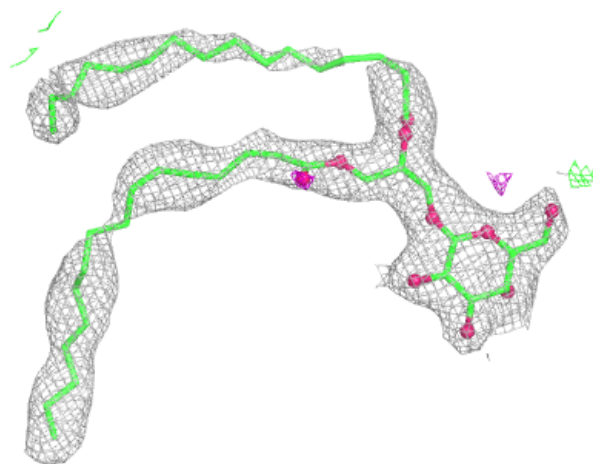
Electron density around LMG i 101:

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



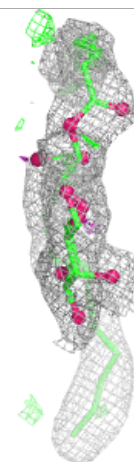
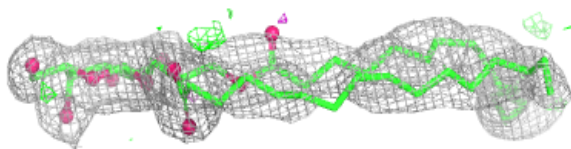
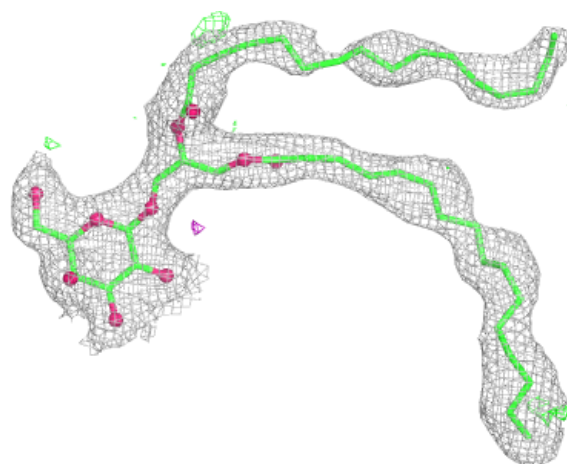
Electron density around LMG c 920:

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



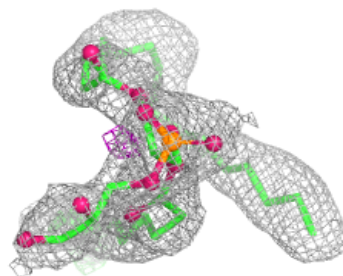
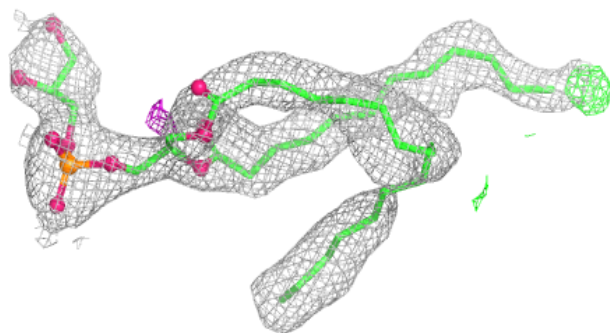
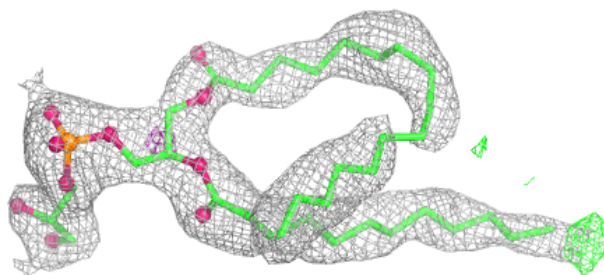
Electron density around LMG C 520:

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

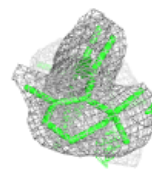
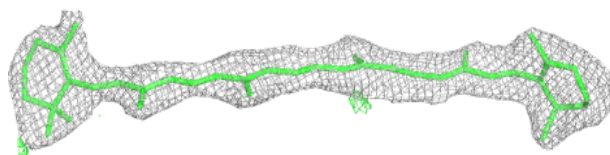
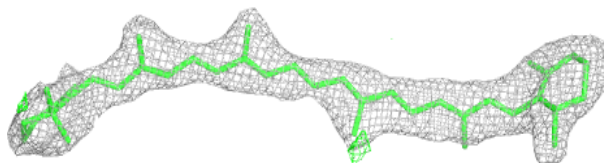


Electron density around LHG a 423:

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

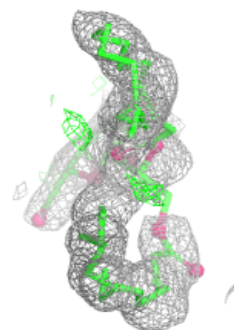
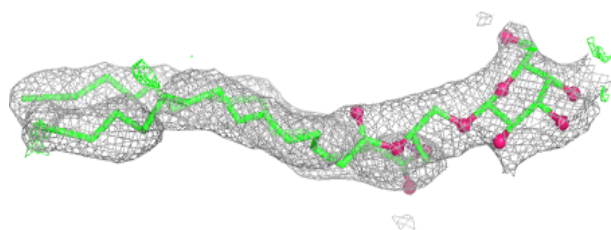
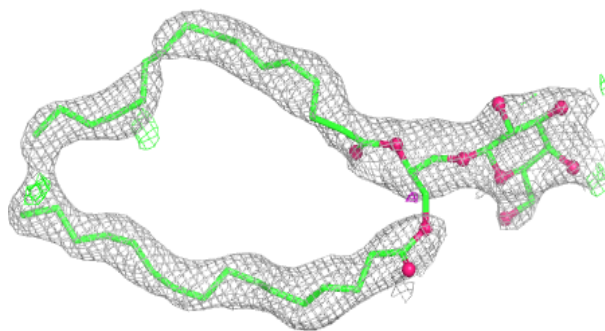
**Electron density around BCR c 915:**

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

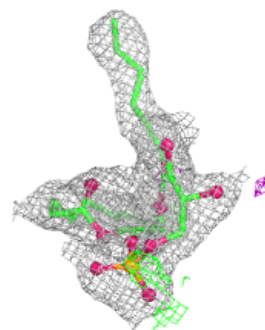
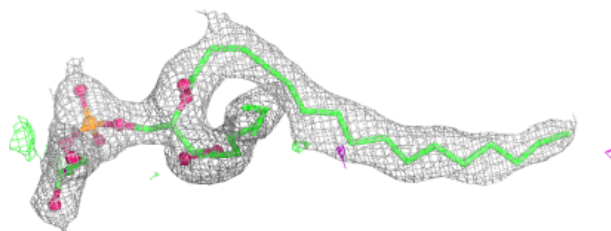
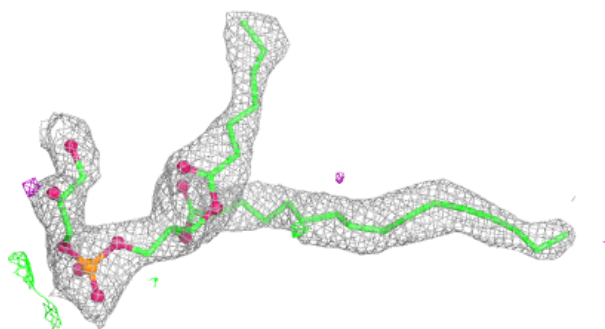


Electron density around LMG A 410:

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

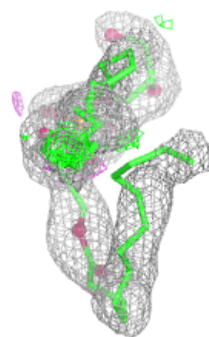
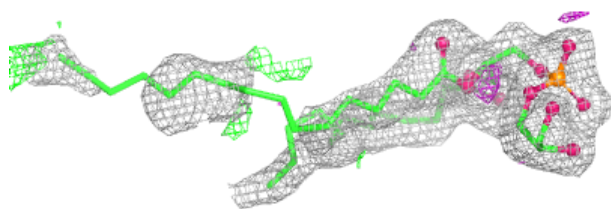
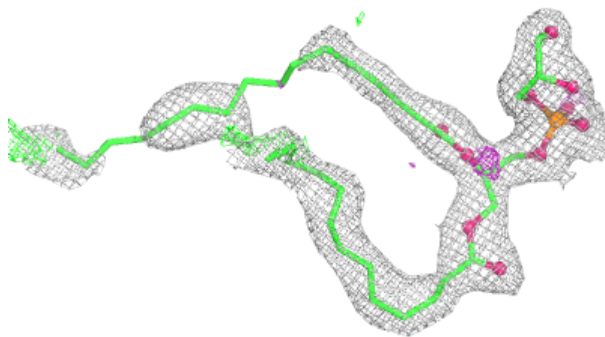
**Electron density around LHG L 101:**

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

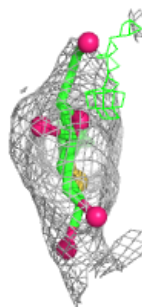
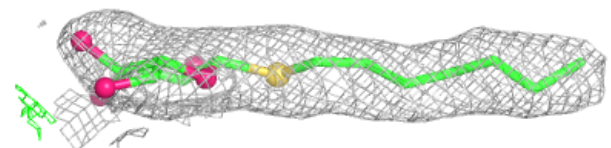
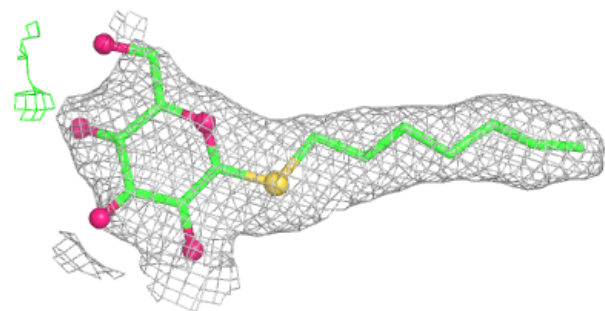


Electron density around LHG d 408:

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

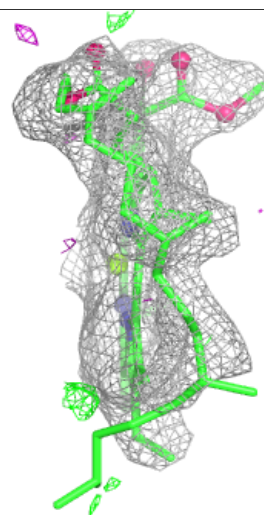
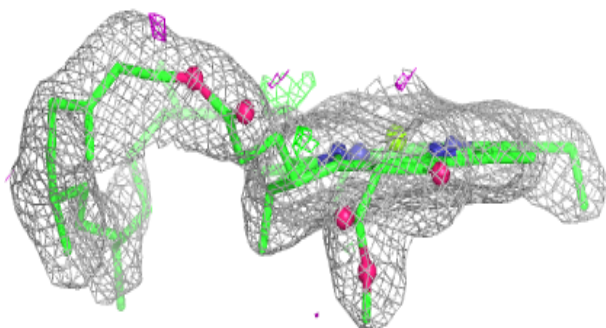
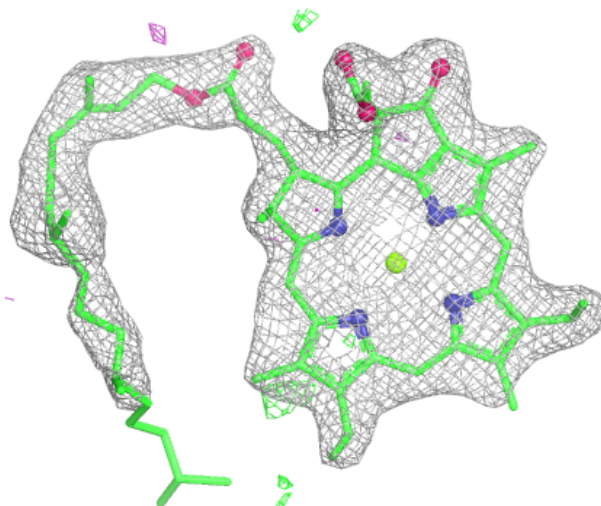
**Electron density around HTG b 626:**

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



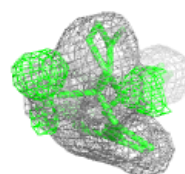
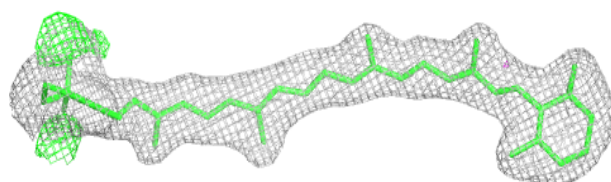
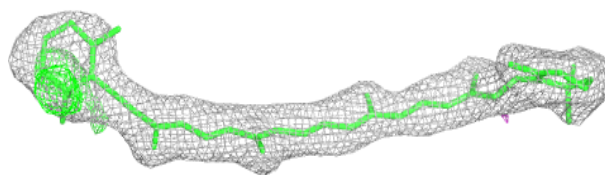
Electron density around CLA c 913:

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

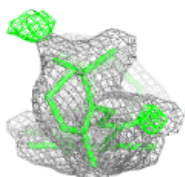
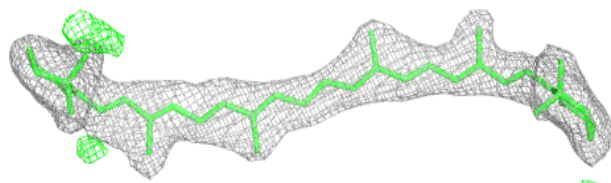
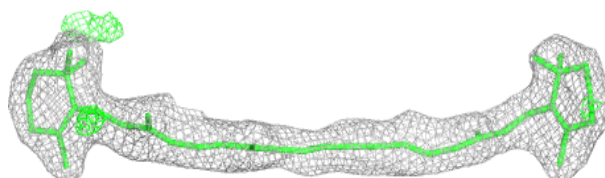


Electron density around BCR d 404:

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

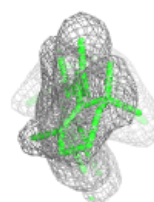
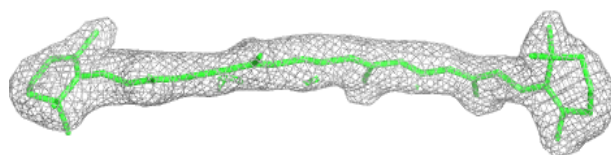
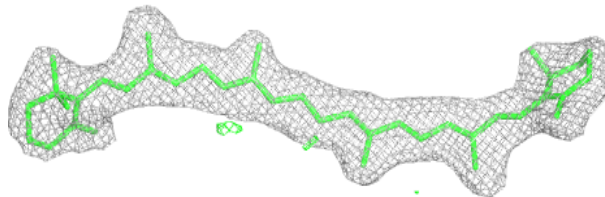
**Electron density around BCR k 101:**

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

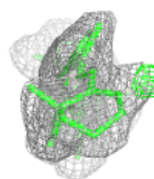
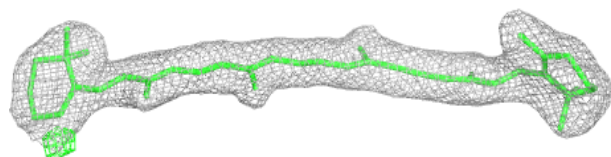
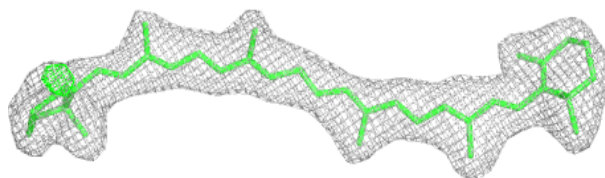


Electron density around BCR y 101:

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

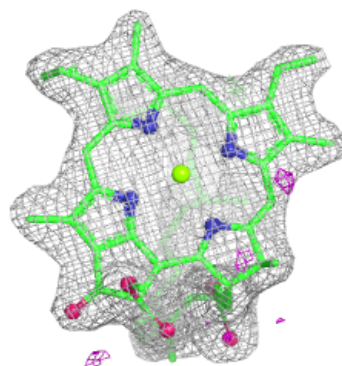
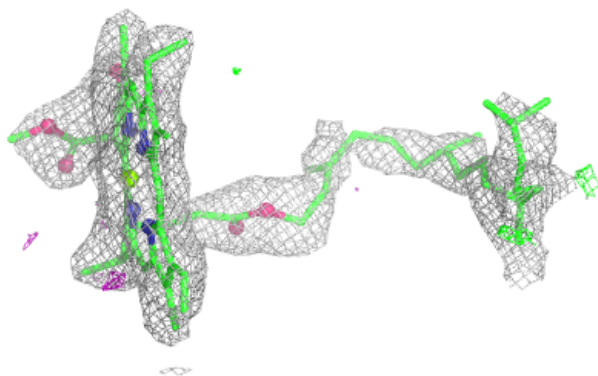
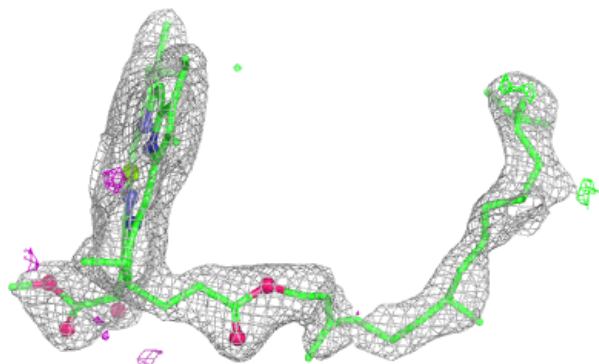
**Electron density around BCR Y 101:**

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

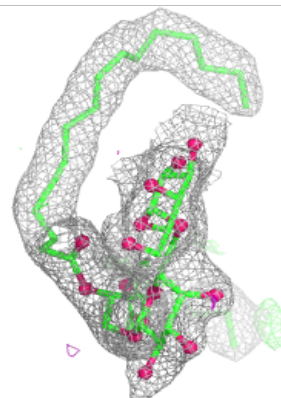
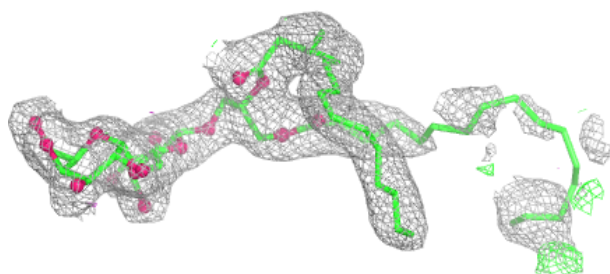
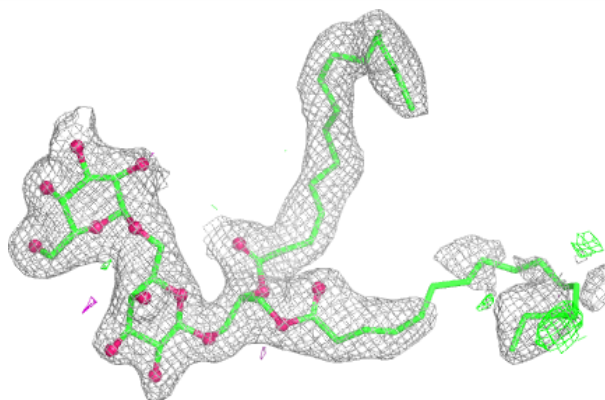


Electron density around CLA C 507:

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

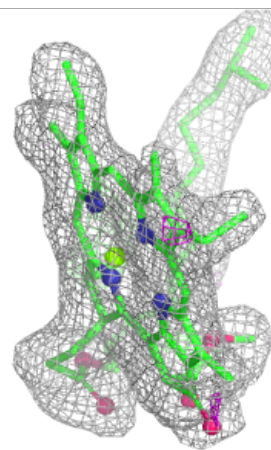
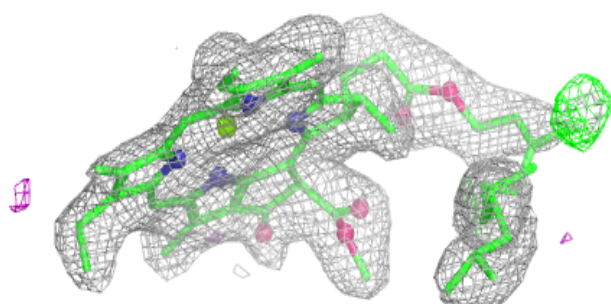
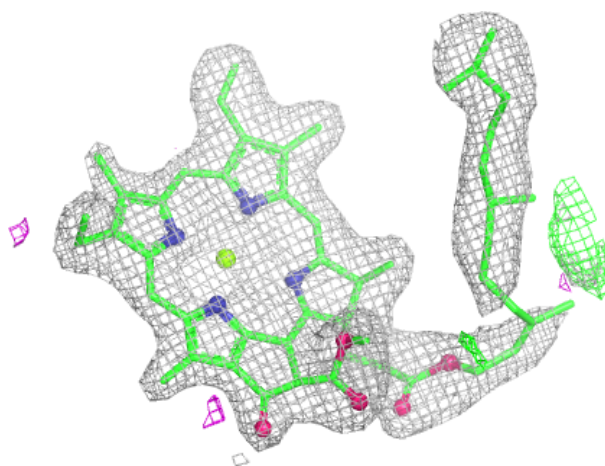
**Electron density around DGD c 918:**

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



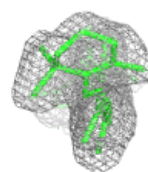
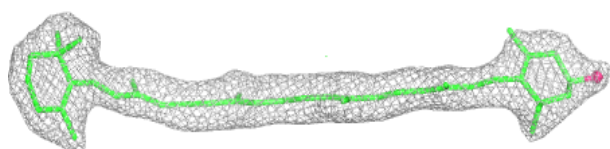
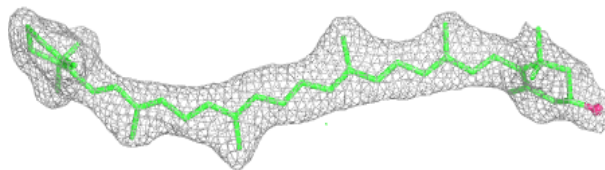
Electron density around CLA b 617:

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

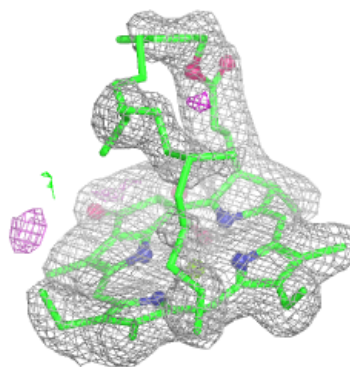
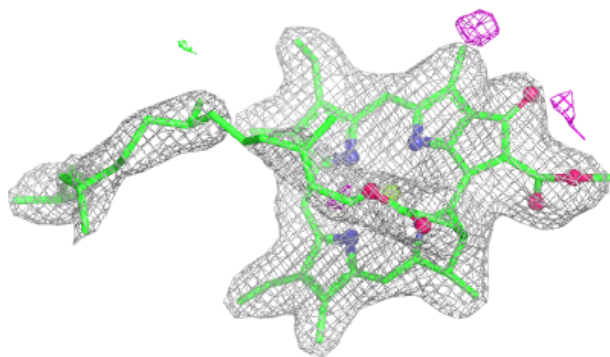
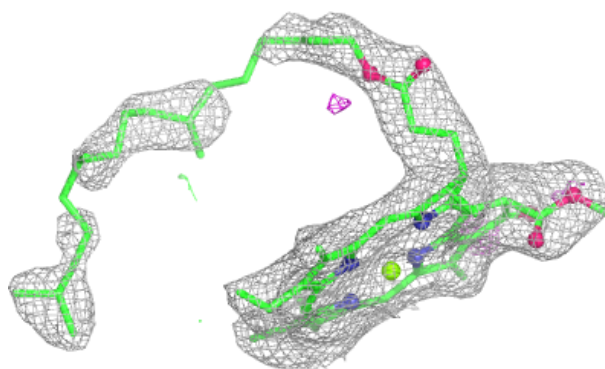


Electron density around RRX H 101:

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

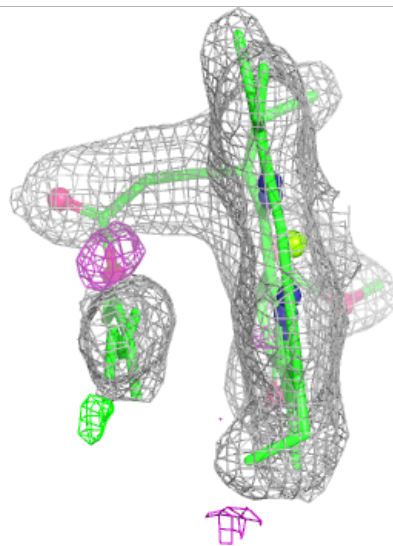
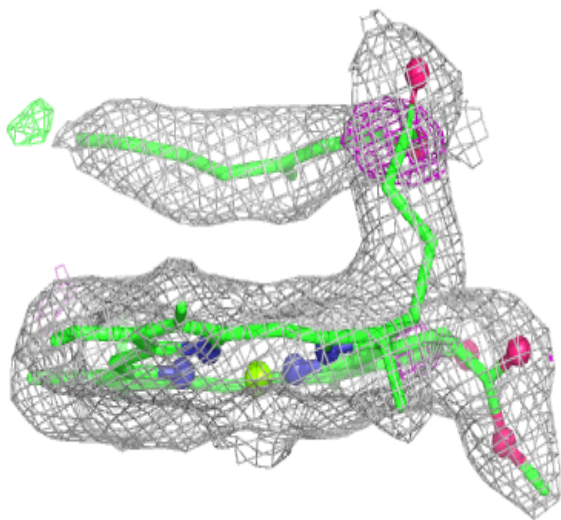
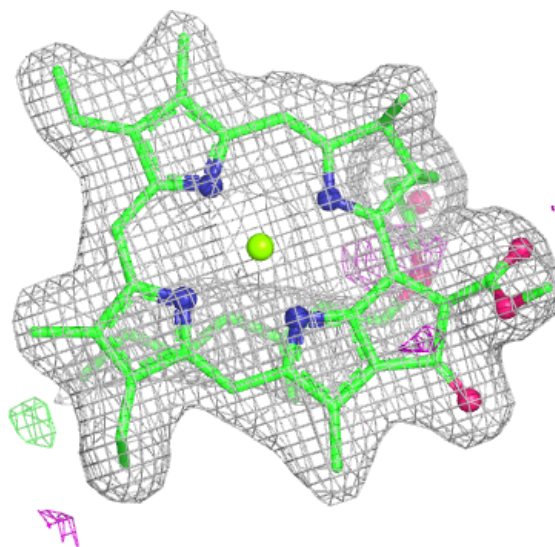
**Electron density around CLA C 514:**

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



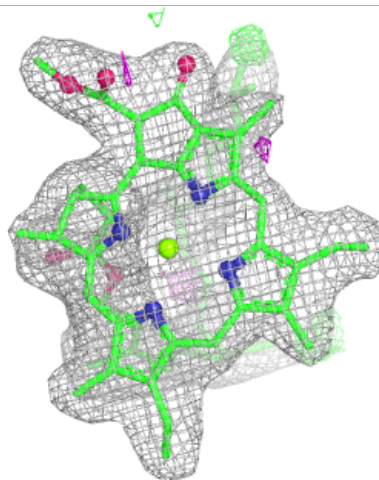
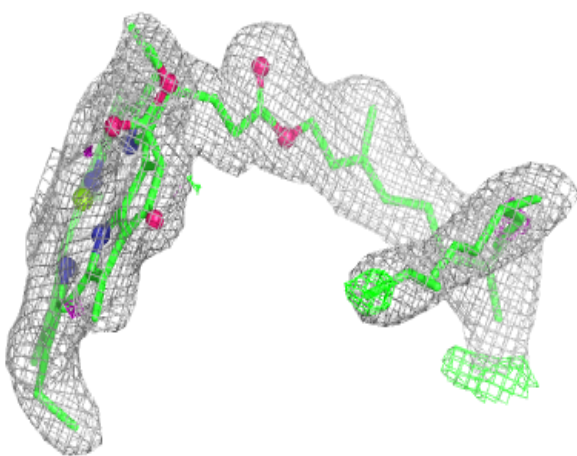
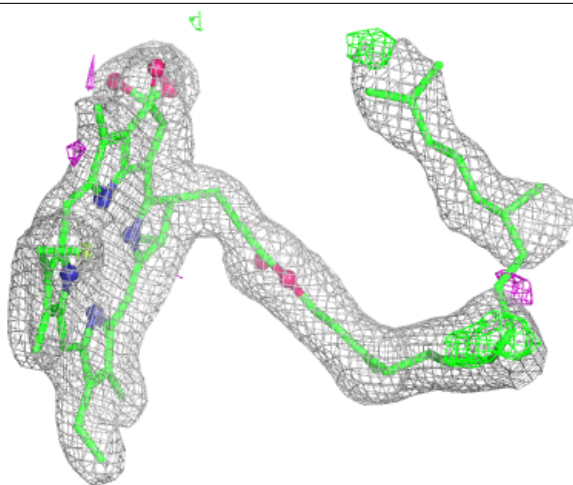
Electron density around CLA B 615:

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



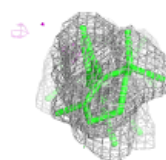
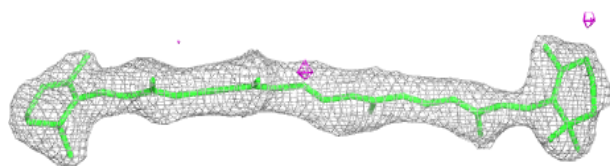
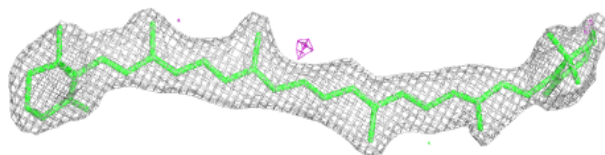
Electron density around CLA b 607:

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

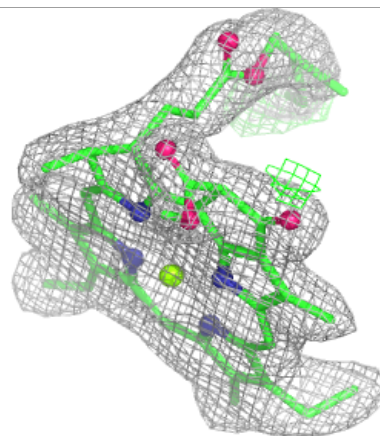
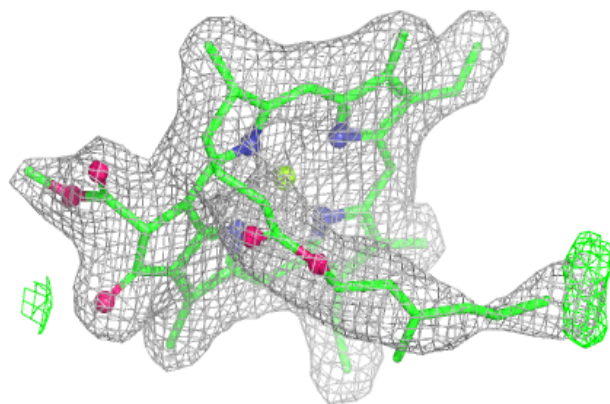
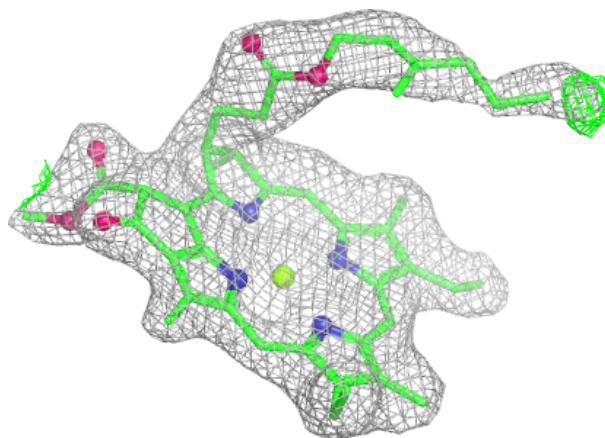


Electron density around BCR C 515:

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

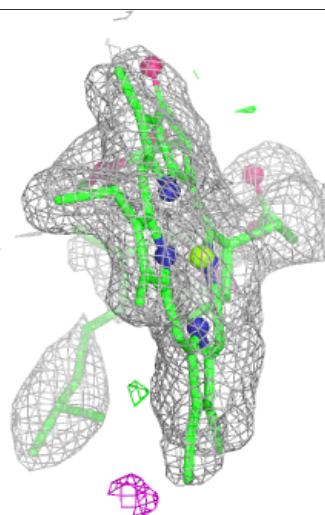
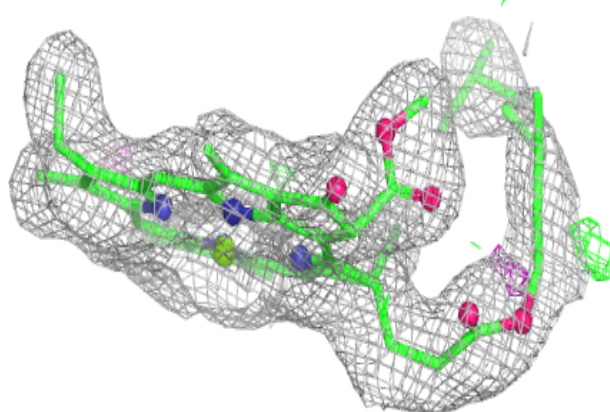
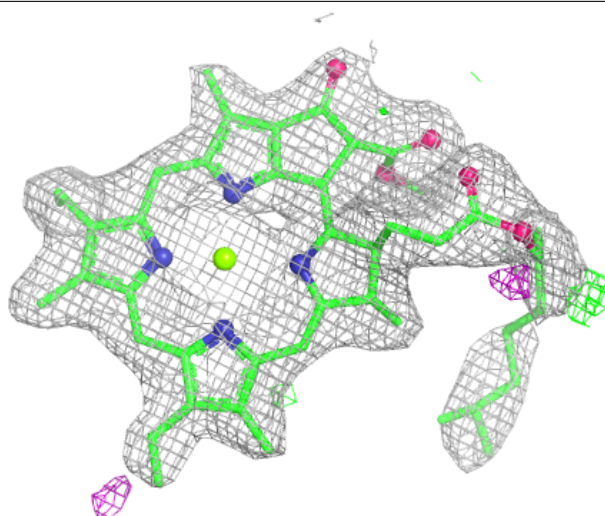
**Electron density around CLA b 615:**

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



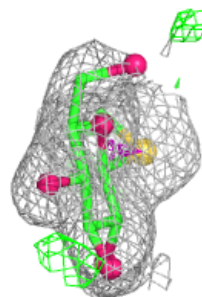
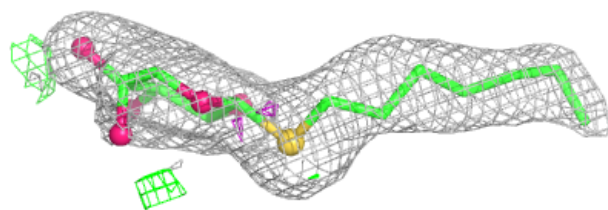
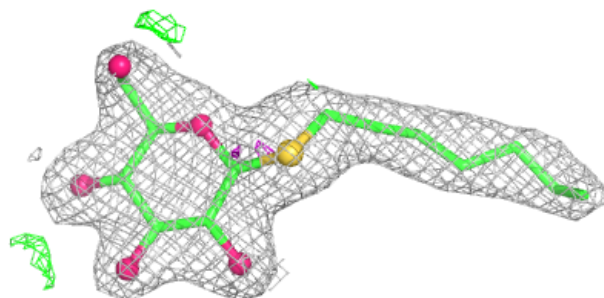
Electron density around CLA B 617:

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



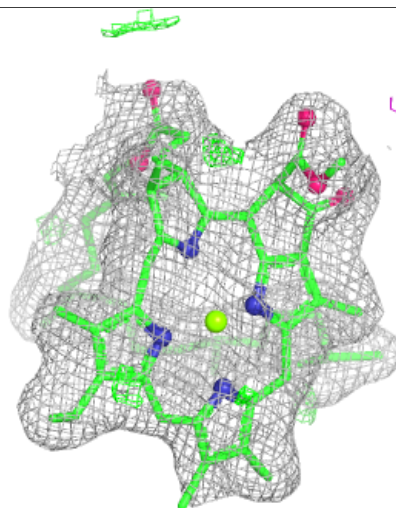
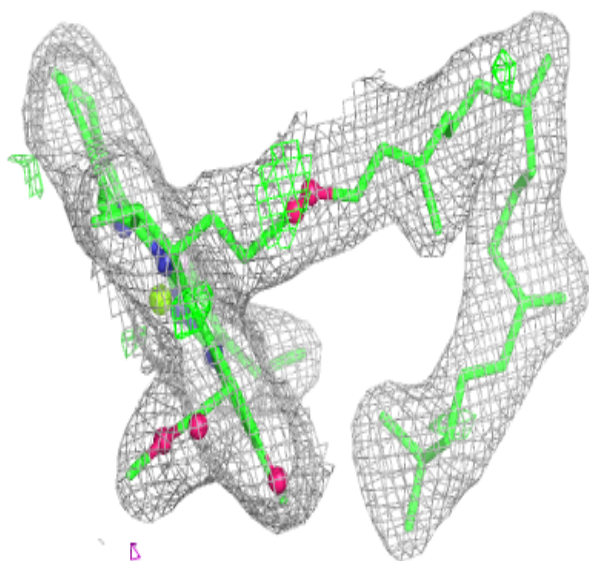
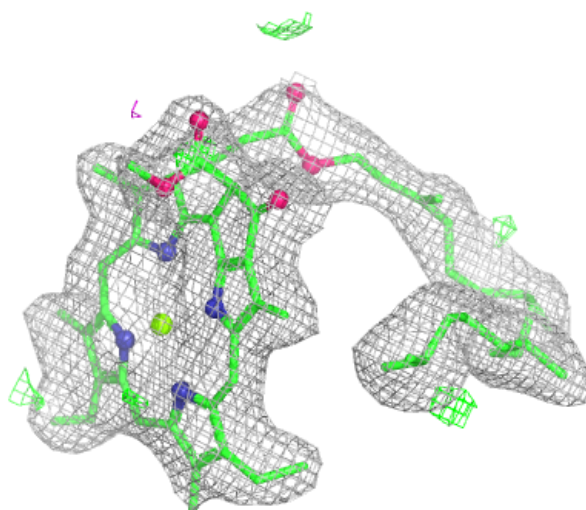
Electron density around HTG b 623:

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



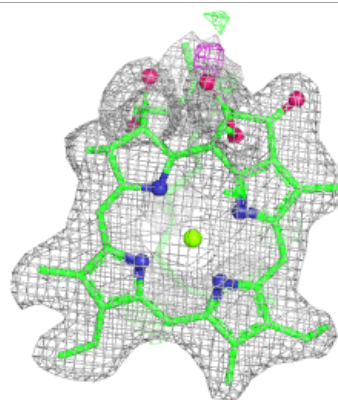
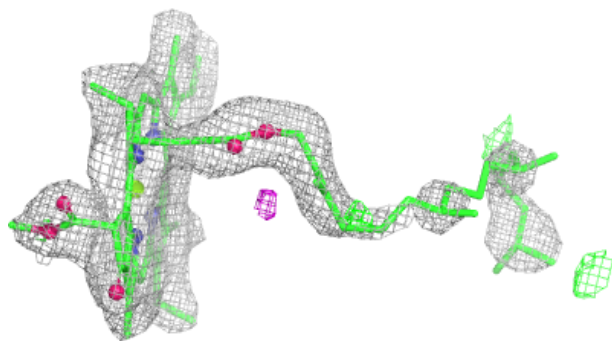
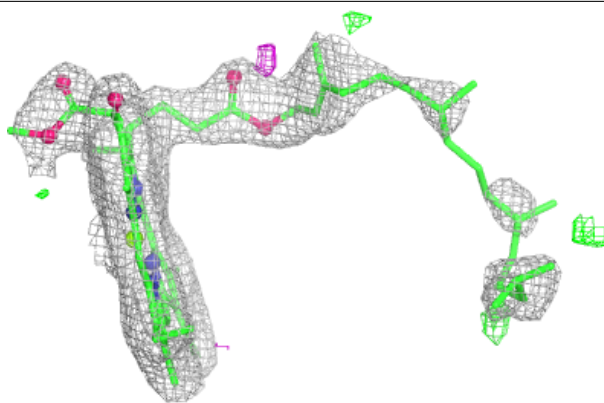
Electron density around CLA c 904:

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

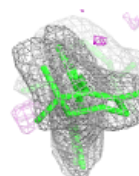
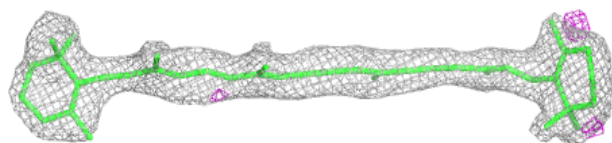
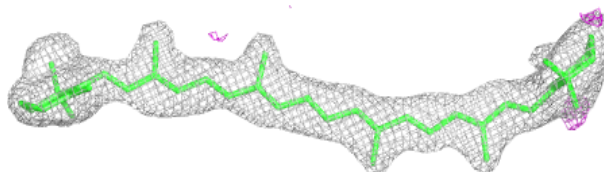


Electron density around CLA c 907:

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

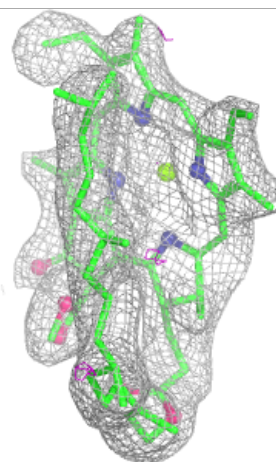
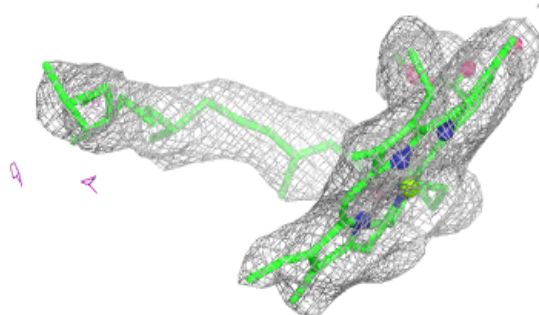
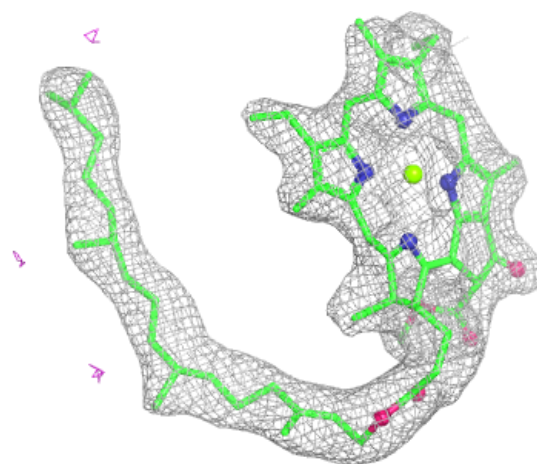
**Electron density around BCR c 916:**

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



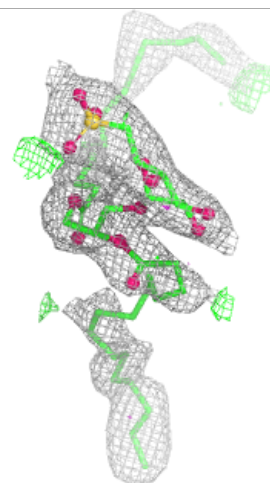
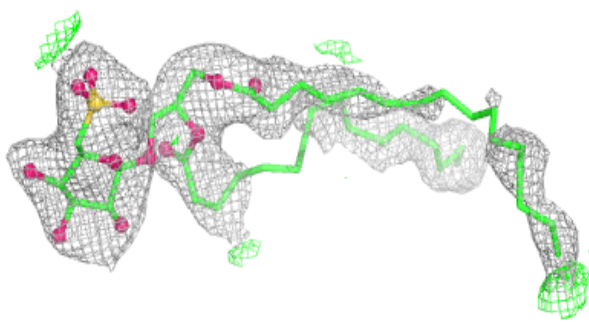
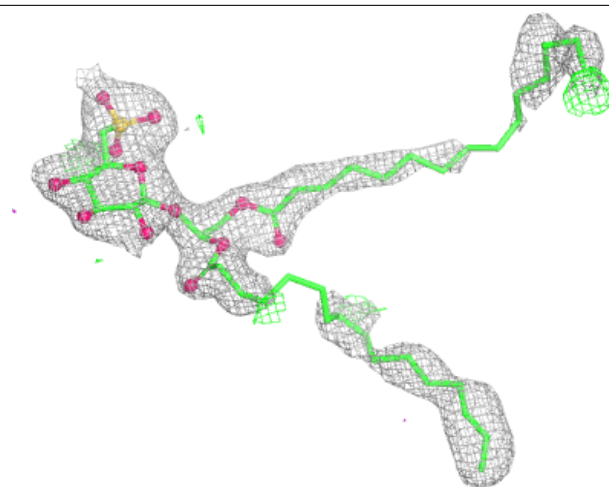
Electron density around CLA c 908:

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



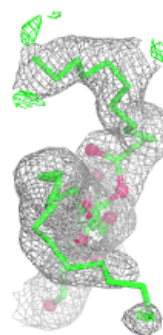
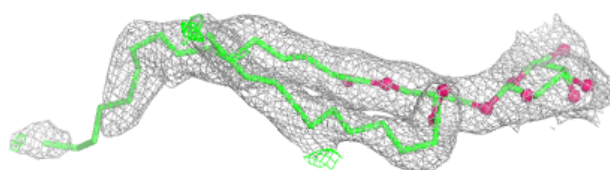
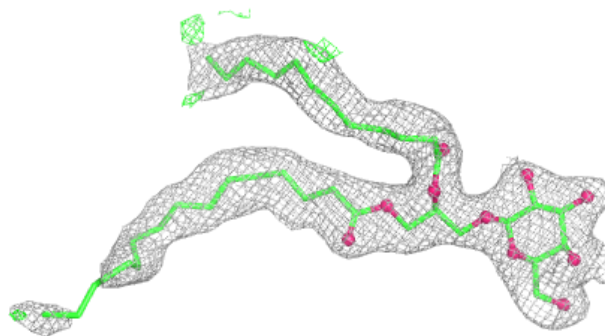
Electron density around SQD C 501:

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

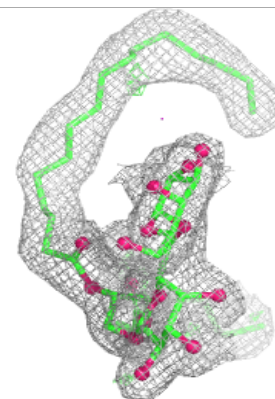
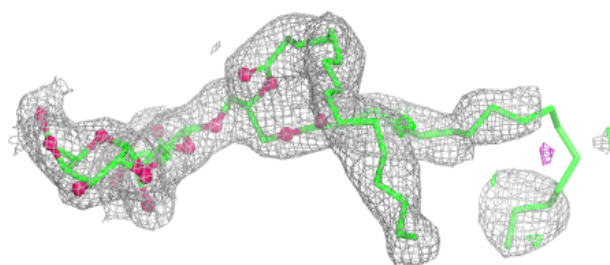
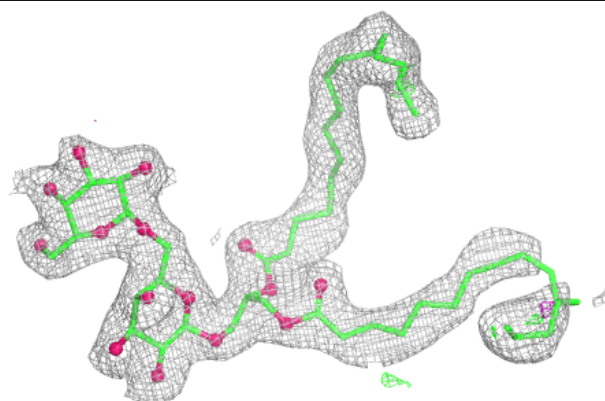


Electron density around LMG j 101:

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

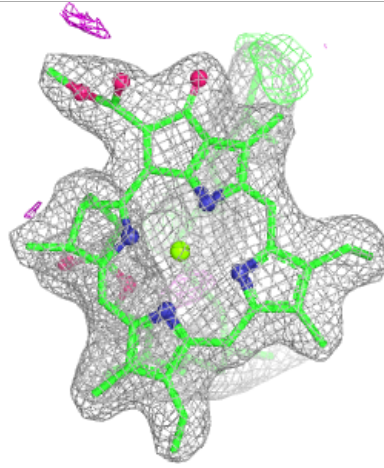
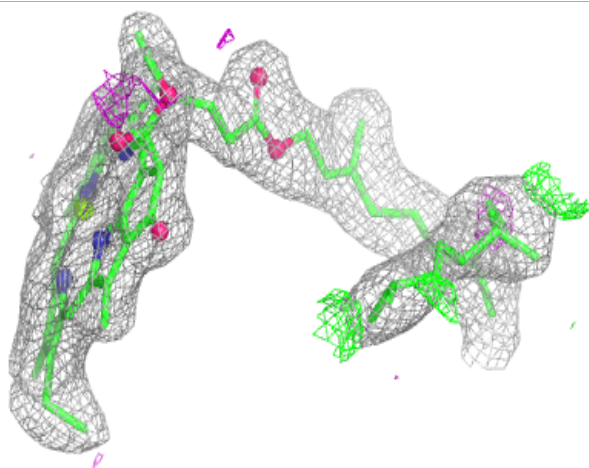
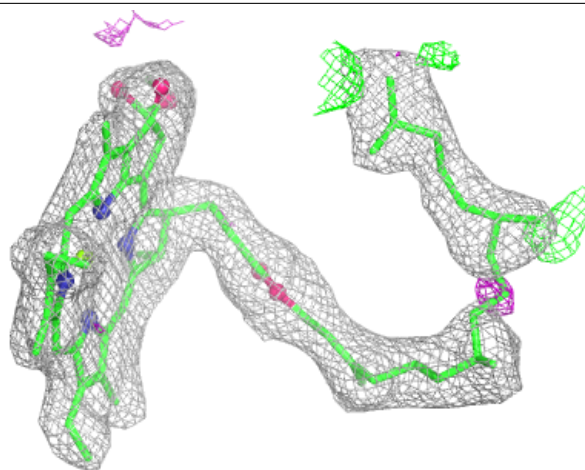
**Electron density around DGD C 518:**

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



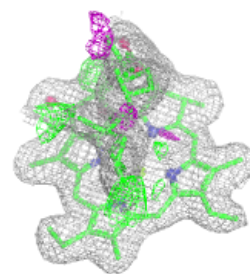
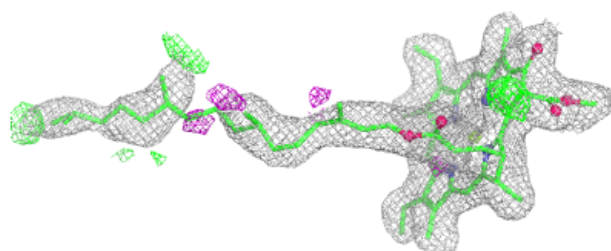
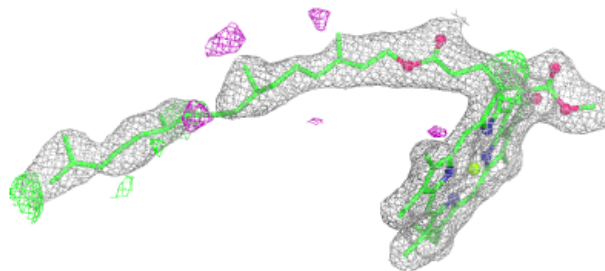
Electron density around CLA B 607:

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

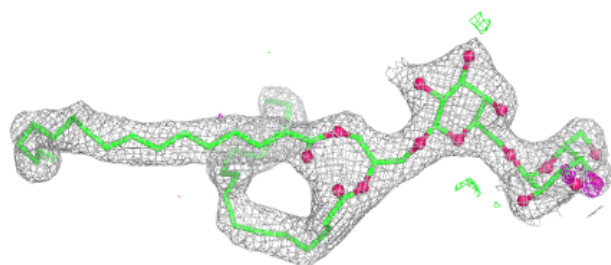
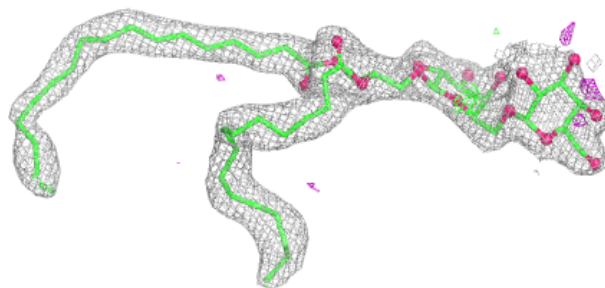


Electron density around CLA B 608:

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

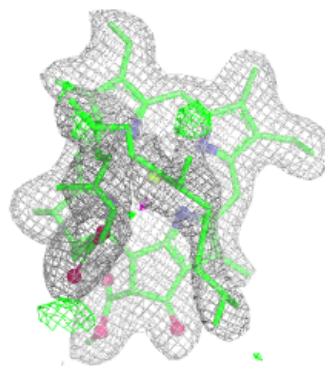
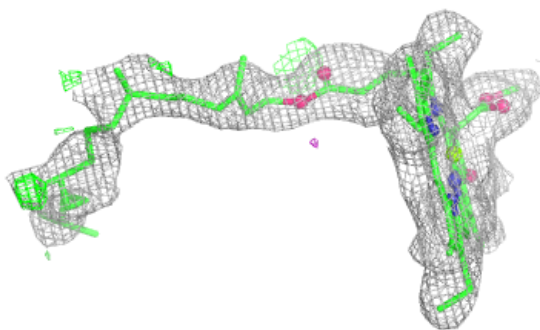
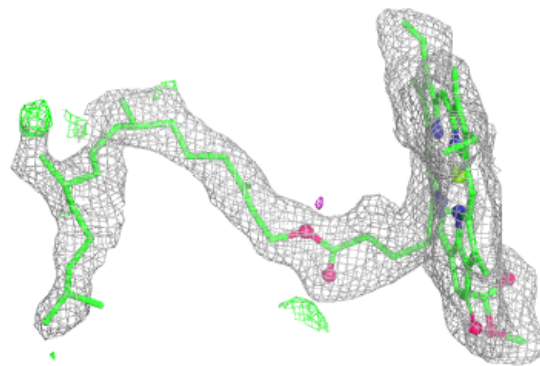
**Electron density around DGD h 102:**

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



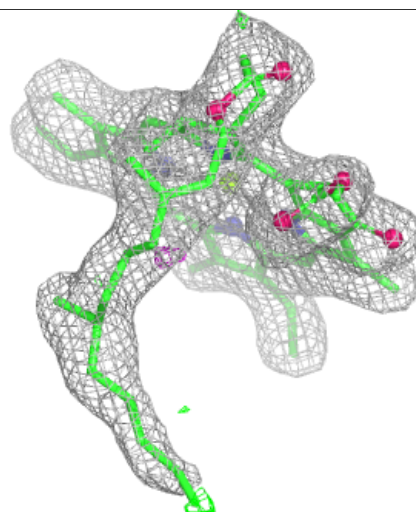
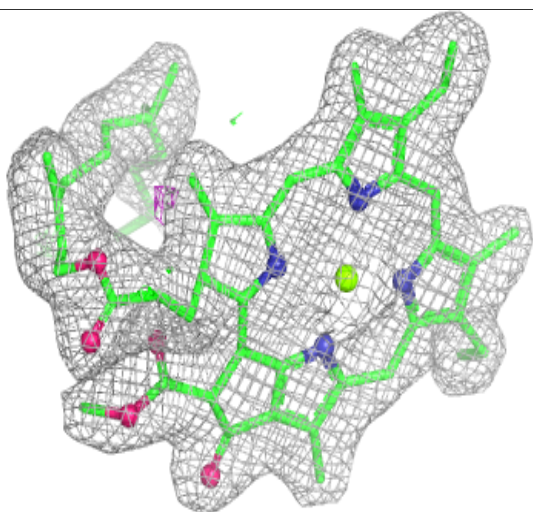
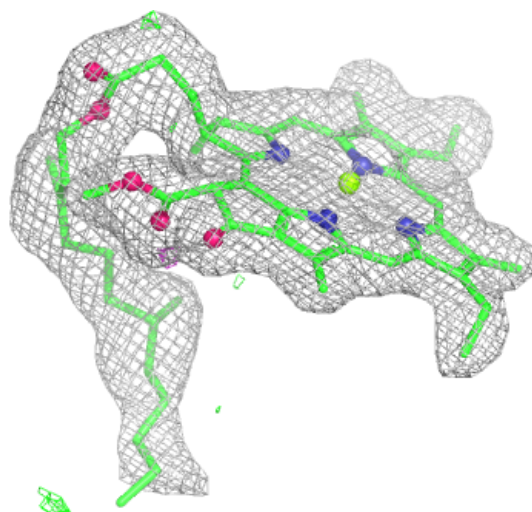
Electron density around CLA d 403:

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



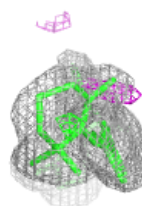
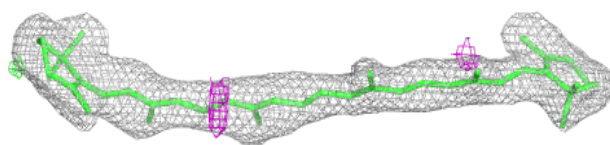
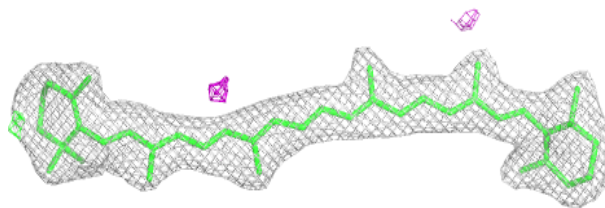
Electron density around CLA b 614:

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

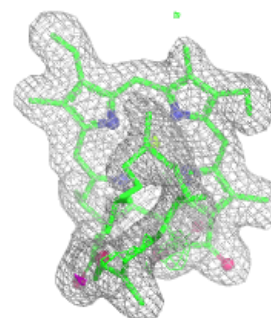
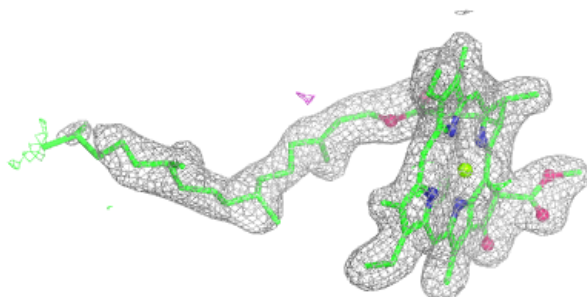
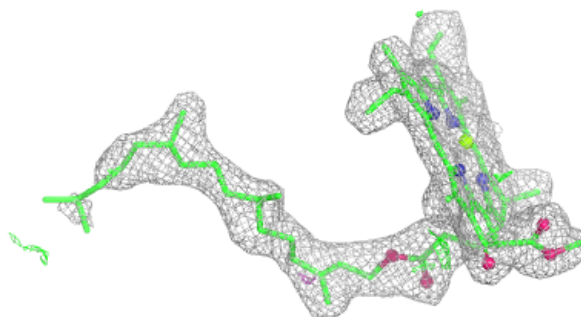


Electron density around BCR B 620:

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

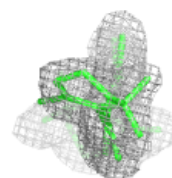
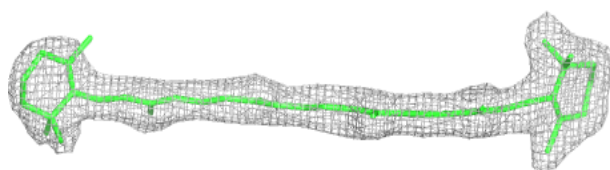
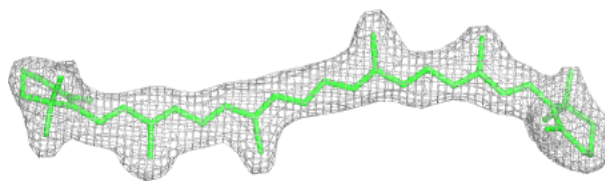
**Electron density around CLA C 509:**

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

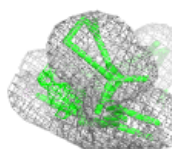
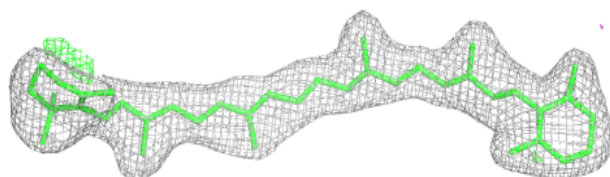
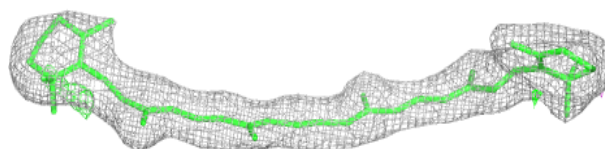


Electron density around BCR C 516:

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

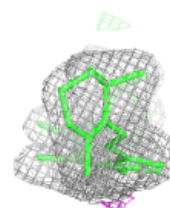
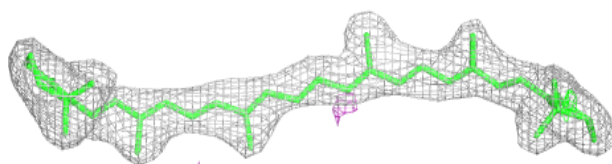
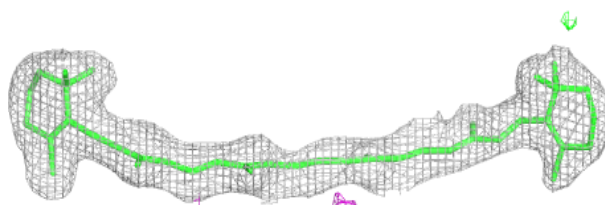
**Electron density around BCR D 405:**

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

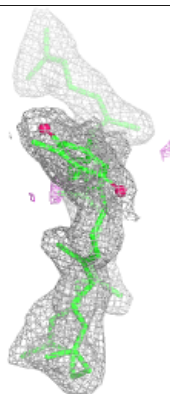
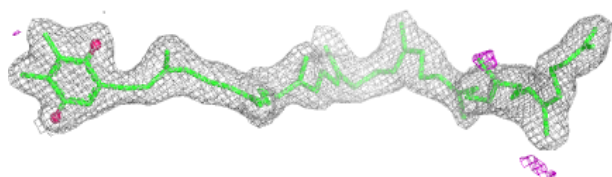
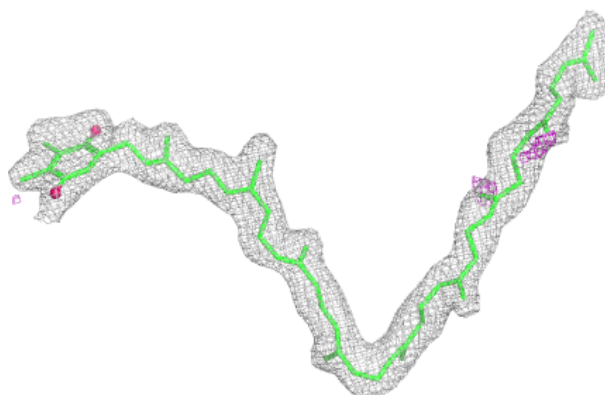


Electron density around BCR K 101:

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

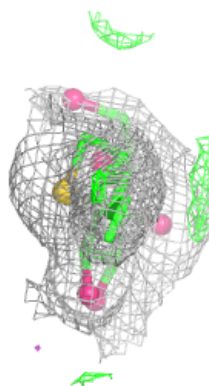
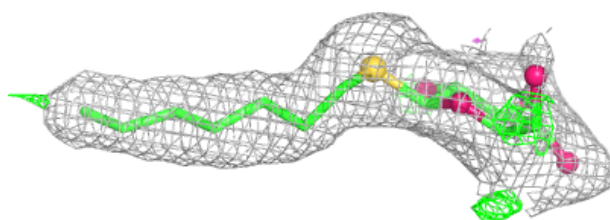
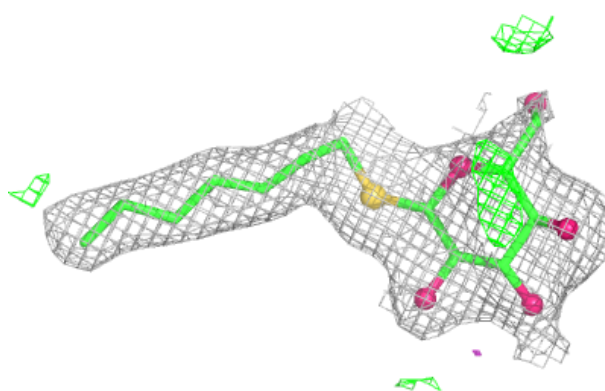
**Electron density around PL9 D 406:**

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

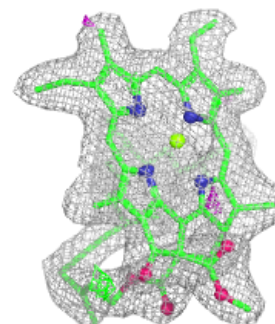
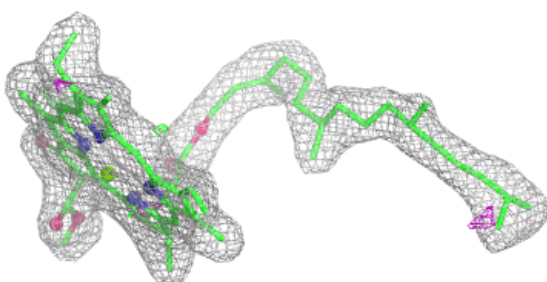
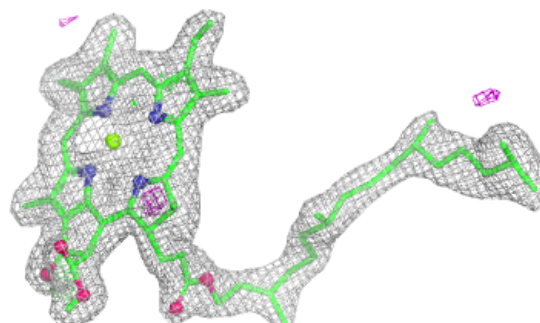


Electron density around HTG B 623:

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

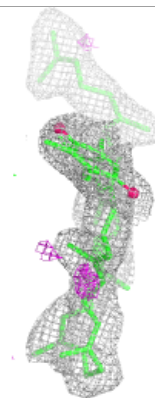
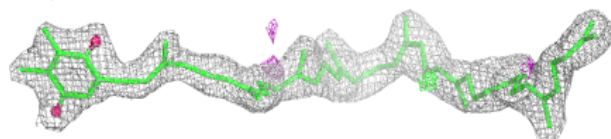
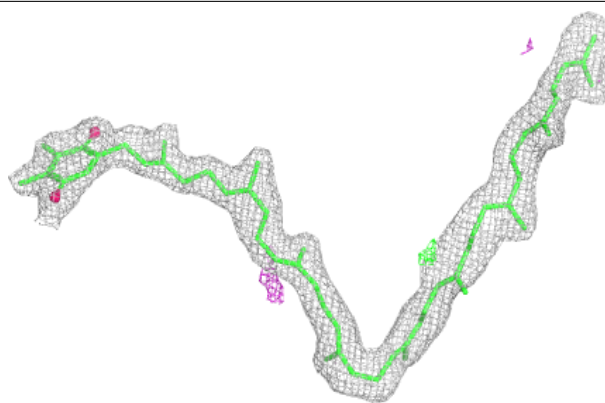
**Electron density around CLA C 512:**

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

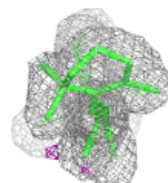
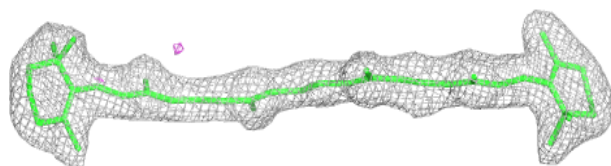
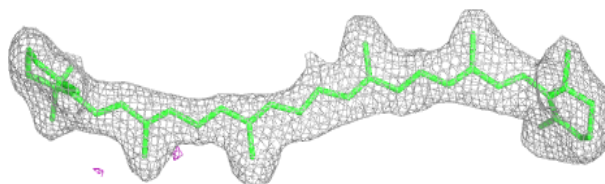


Electron density around PL9 d 405:

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

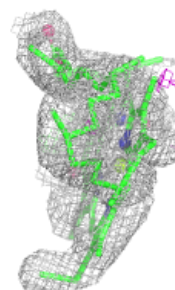
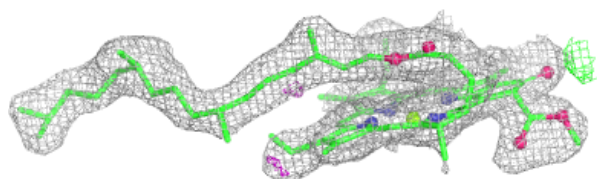
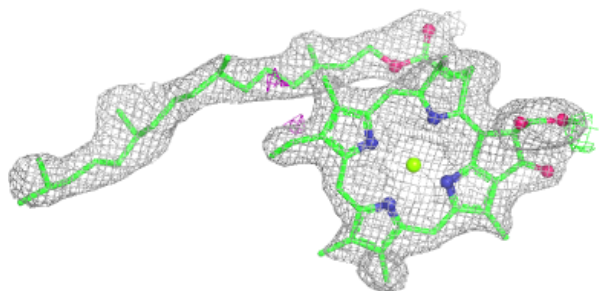
**Electron density around BCR a 413:**

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



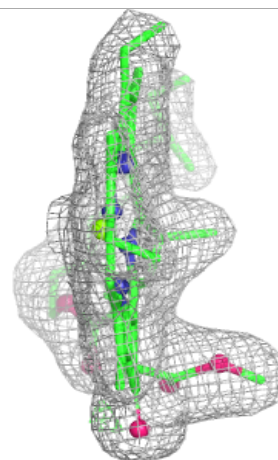
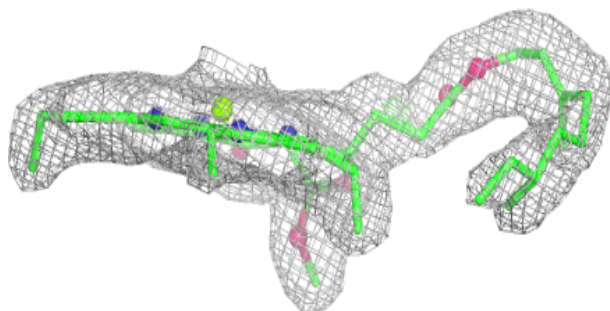
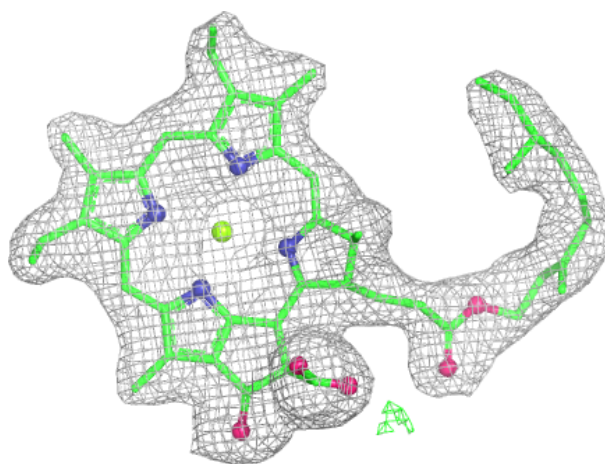
Electron density around CLA c 902:

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



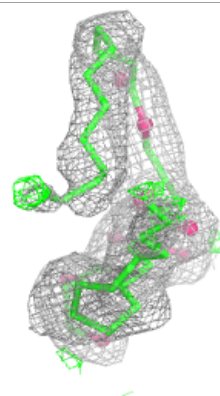
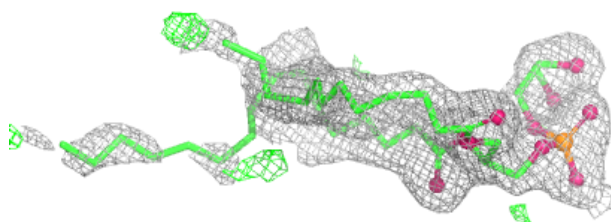
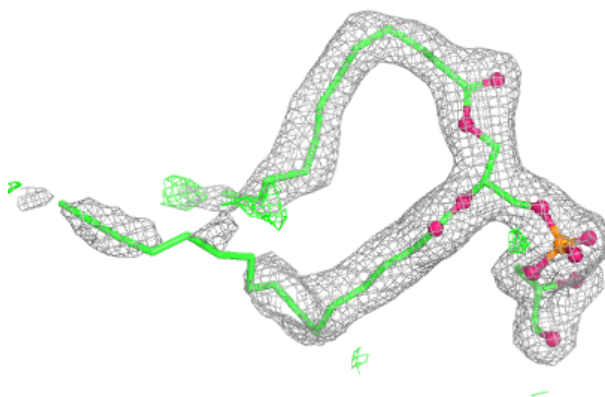
Electron density around CLA C 513:

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

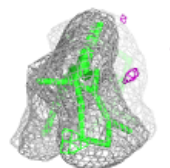
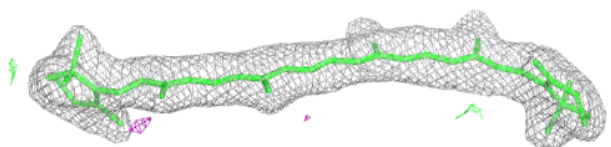
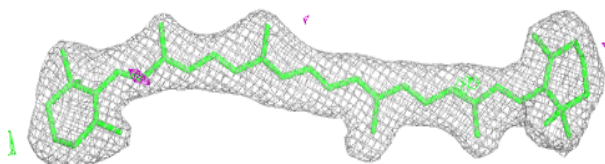


Electron density around LHG D 411:

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

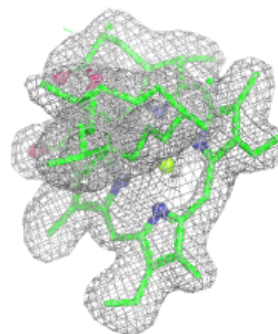
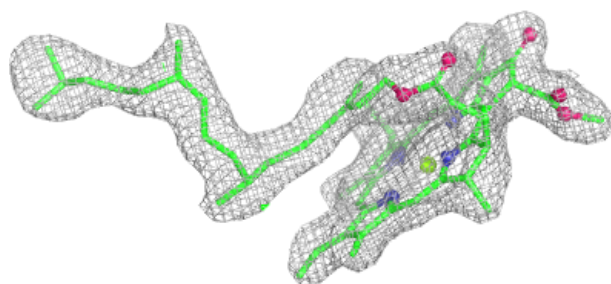
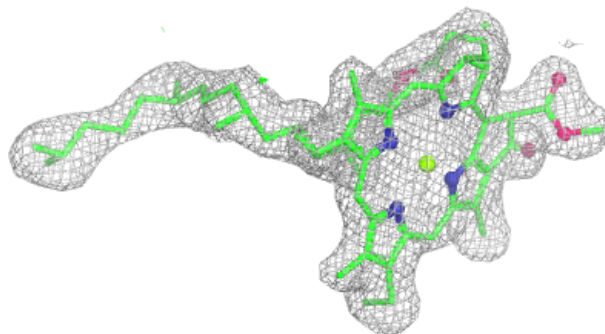
**Electron density around BCR b 620:**

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



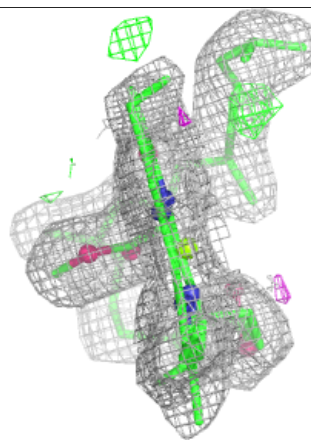
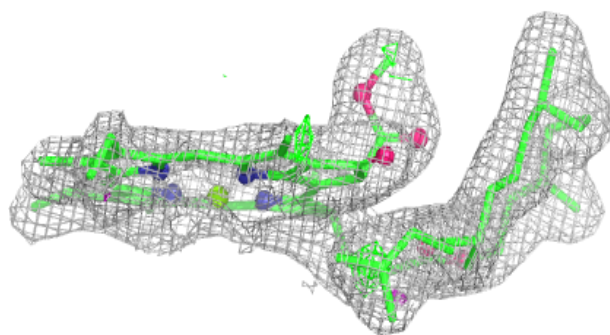
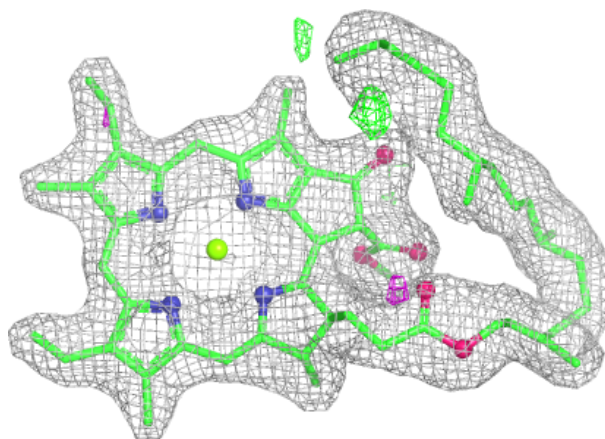
Electron density around CLA c 906:

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



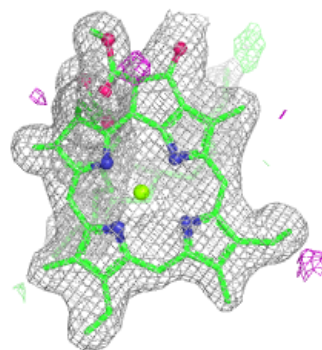
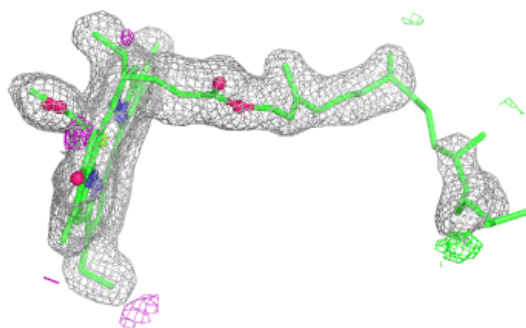
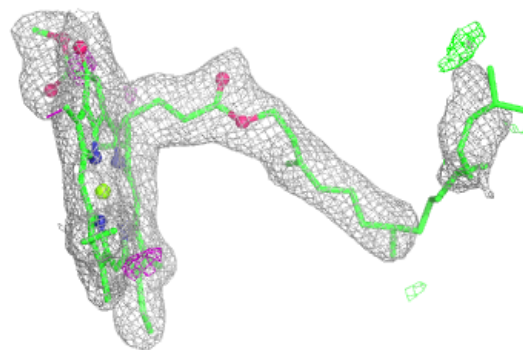
Electron density around CLA B 611:

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

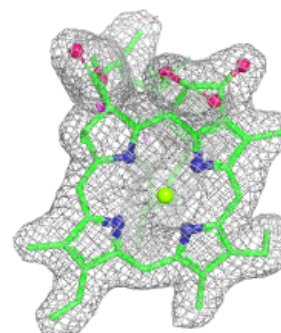
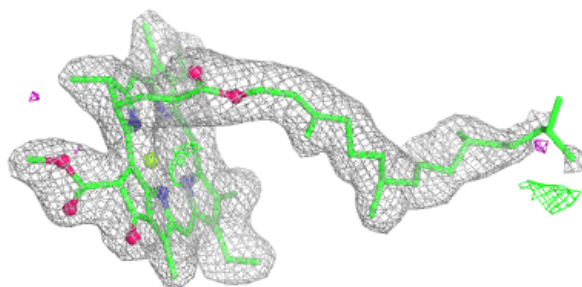
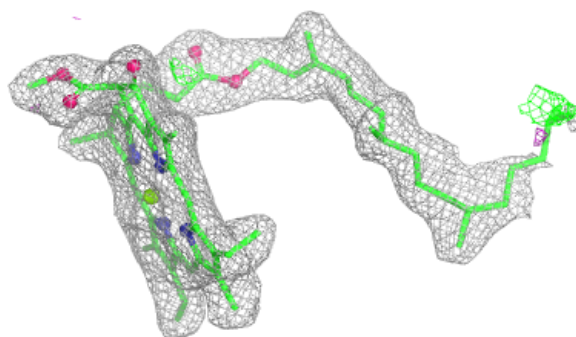


Electron density around CLA D 404:

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

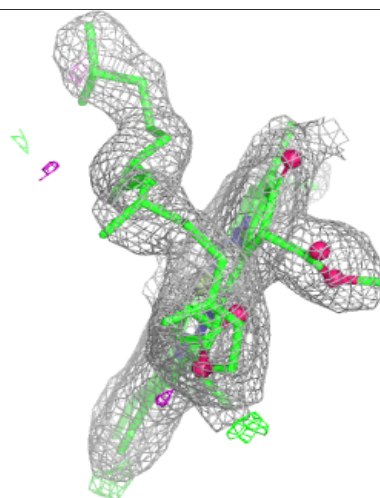
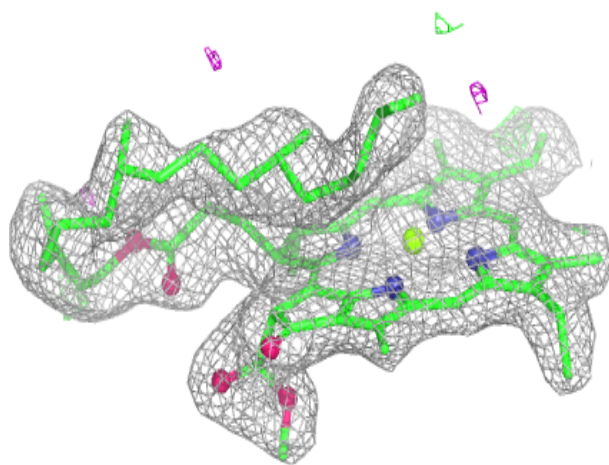
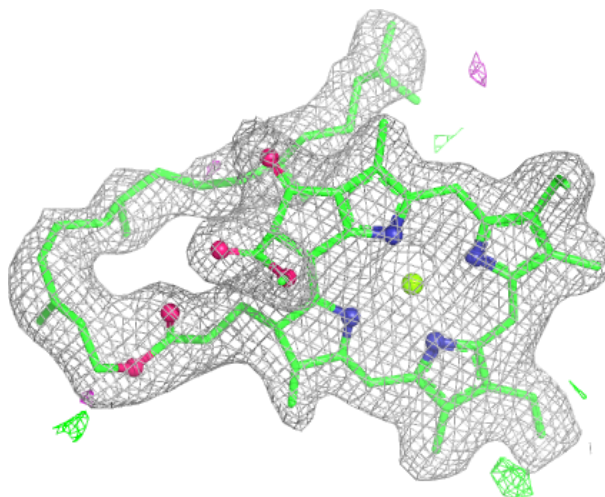
**Electron density around CLA c 909:**

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



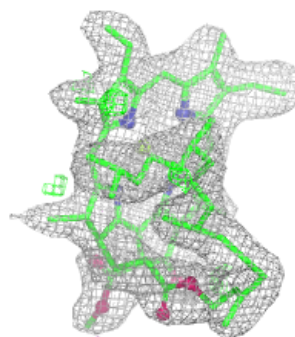
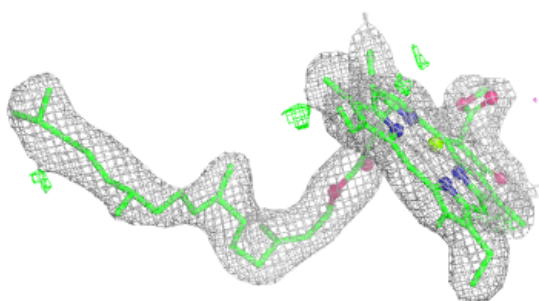
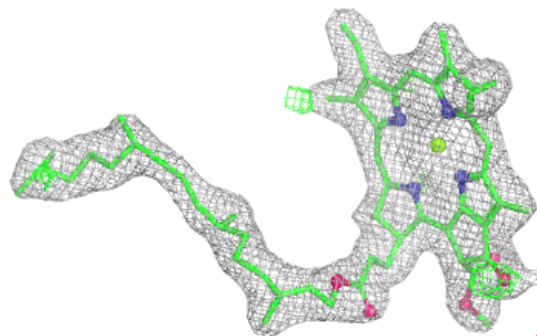
Electron density around CLA c 910:

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

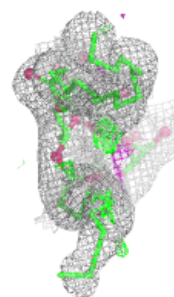
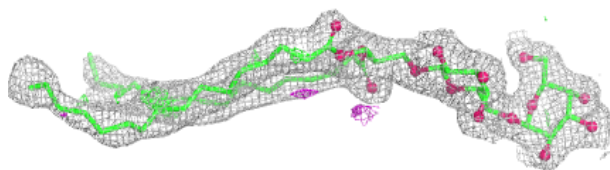
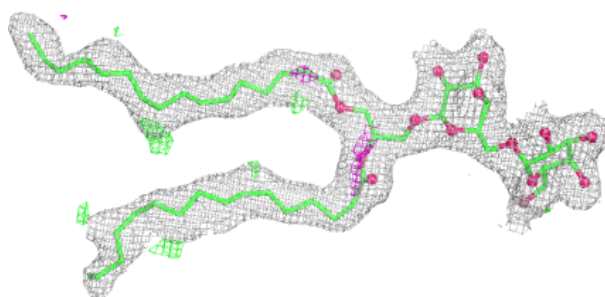


Electron density around CLA c 912:

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

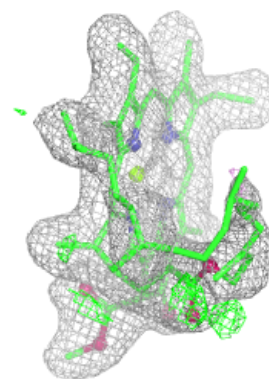
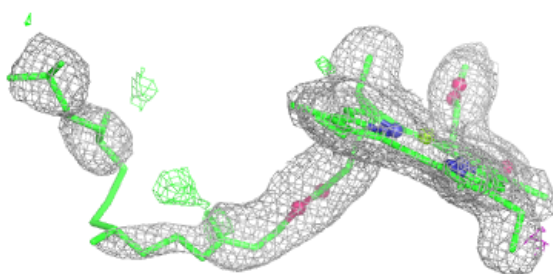
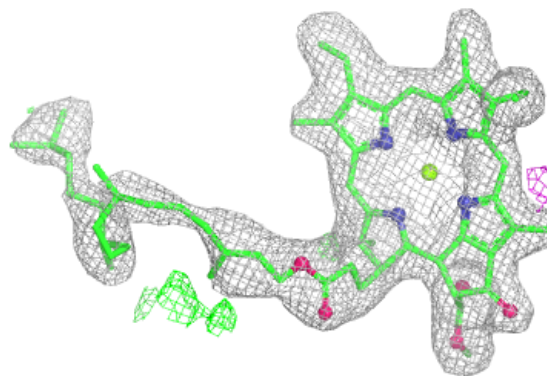
**Electron density around DGD C 519:**

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

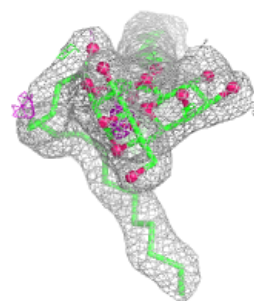
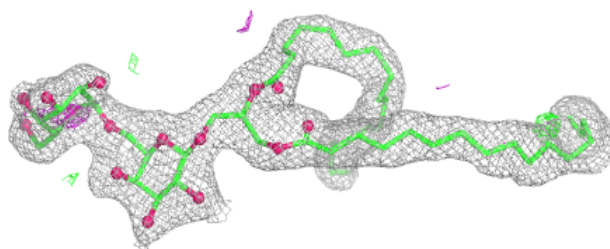
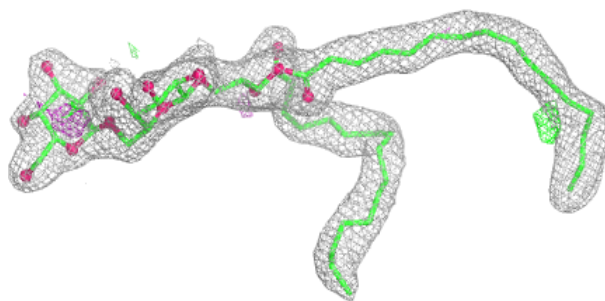


Electron density around CLA a 412:

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

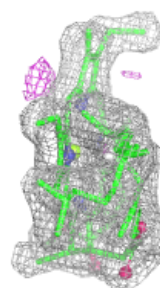
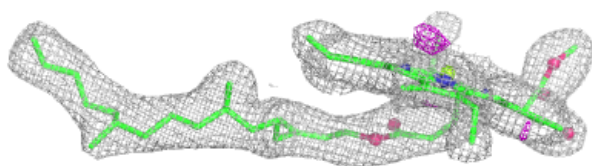
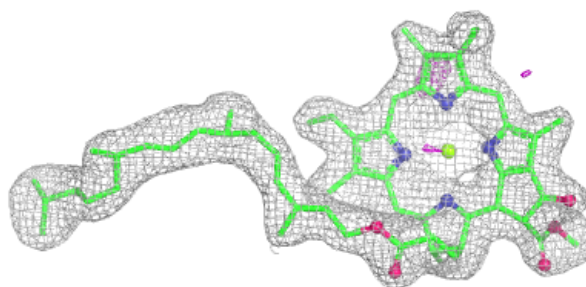
**Electron density around DGD H 102:**

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

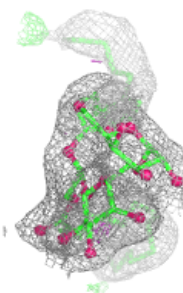
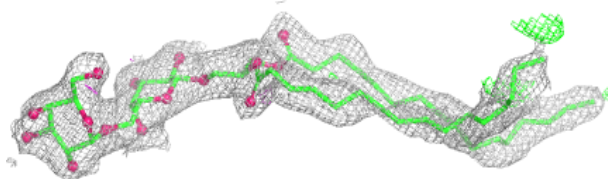
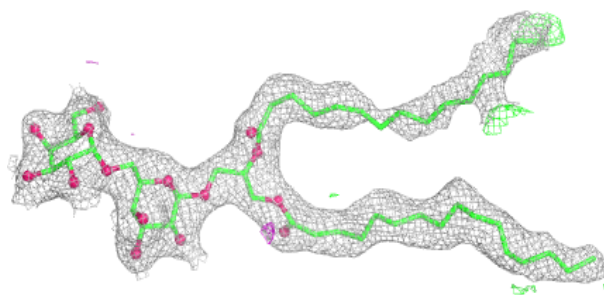


Electron density around CLA B 604:

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

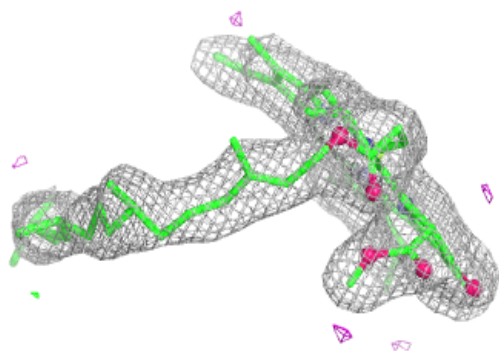
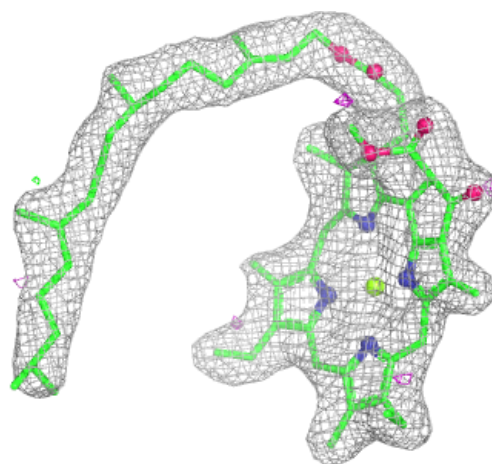
**Electron density around DGD c 919:**

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



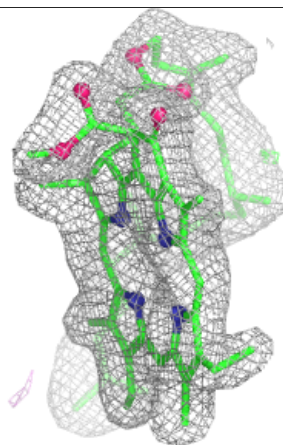
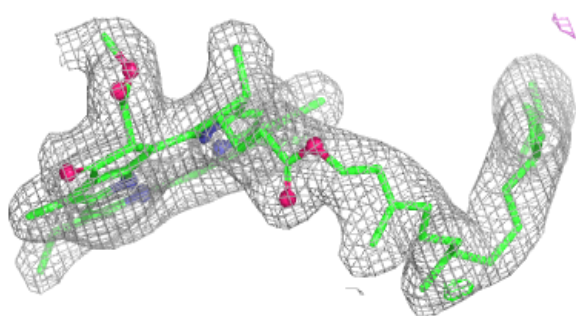
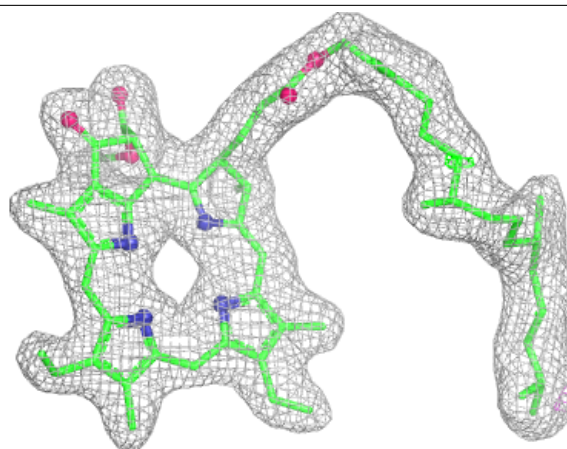
Electron density around CLA C 508:

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

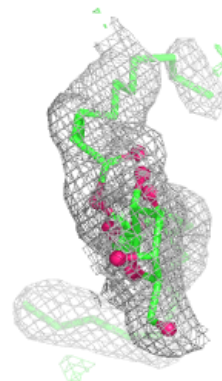
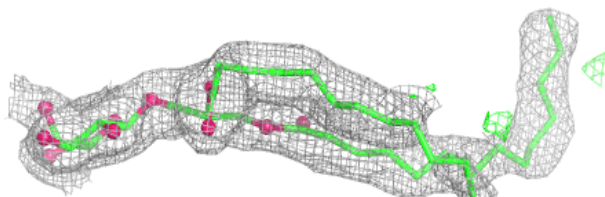
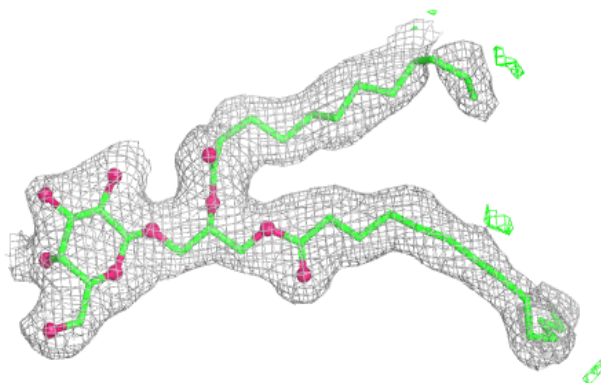


Electron density around PHO a 411:

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

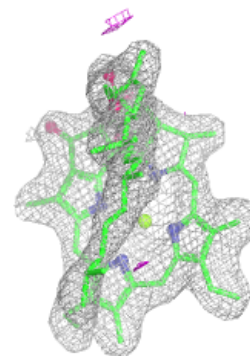
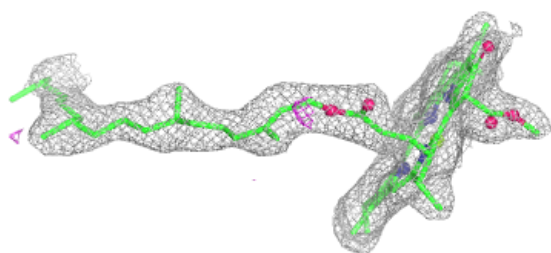
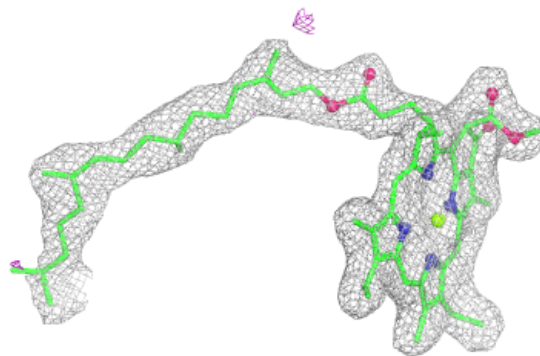
**Electron density around LMG J 101:**

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

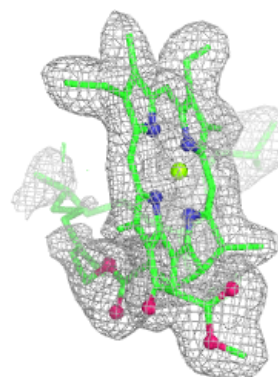
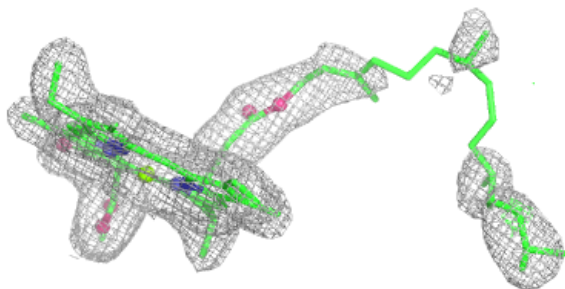
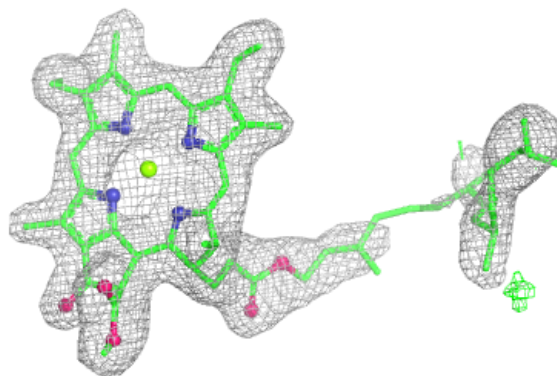


Electron density around CLA b 610:

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

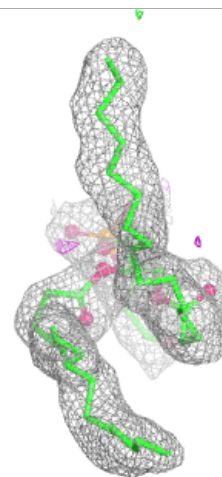
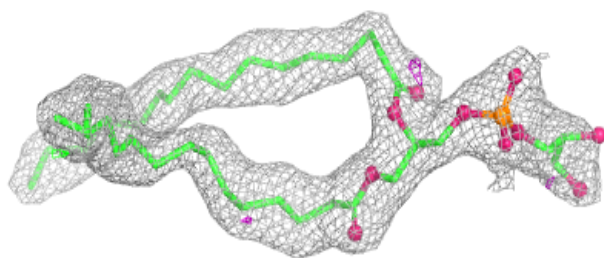
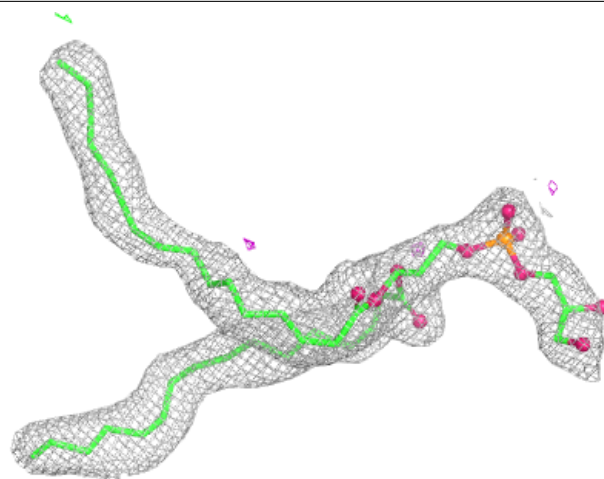
**Electron density around CLA A 408:**

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



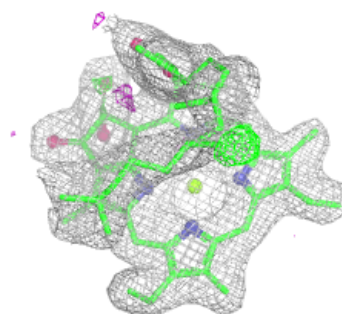
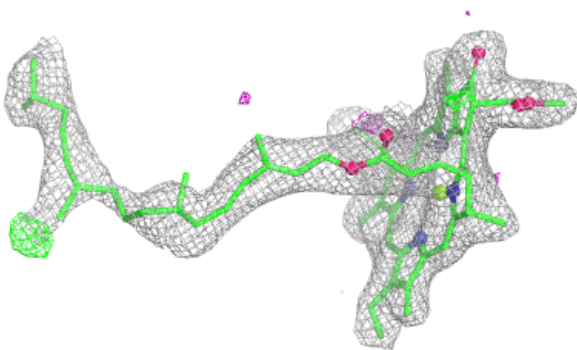
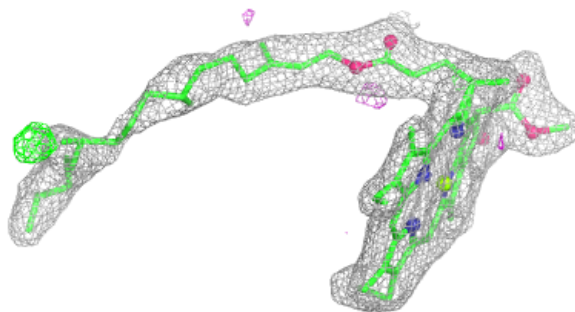
Electron density around LHG d 407:

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

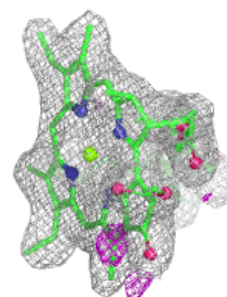
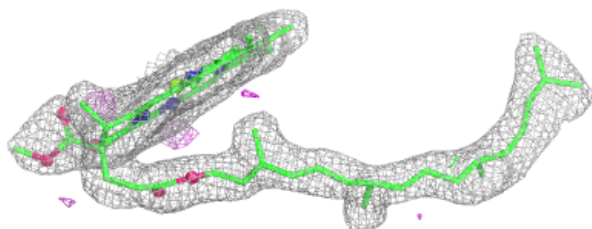
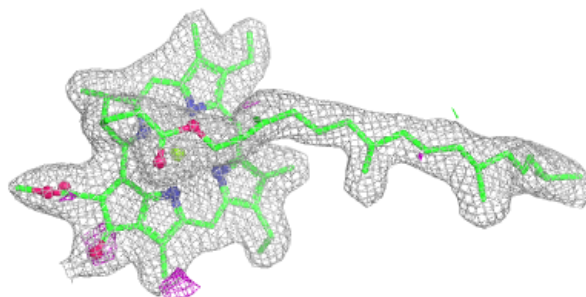


Electron density around CLA b 608:

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

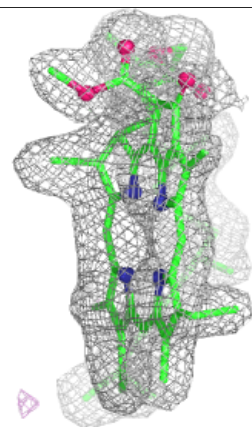
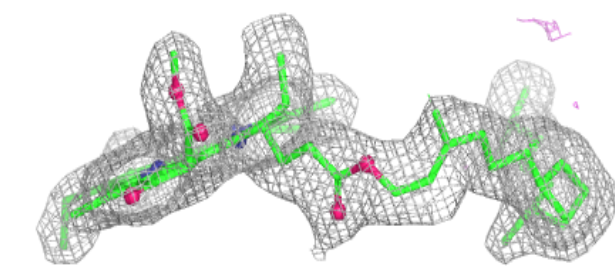
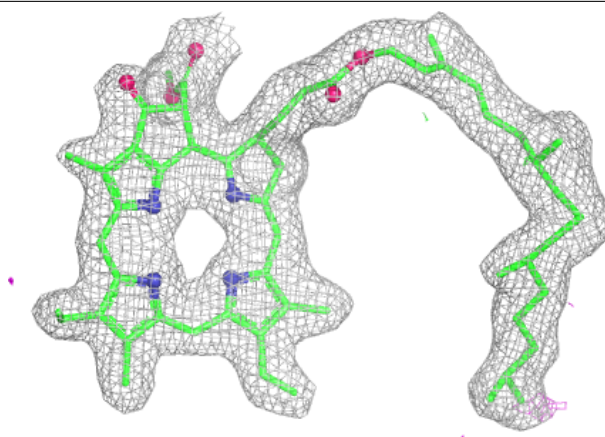
**Electron density around CLA b 609:**

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



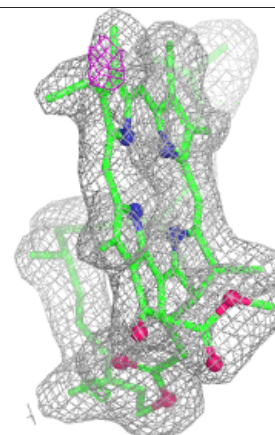
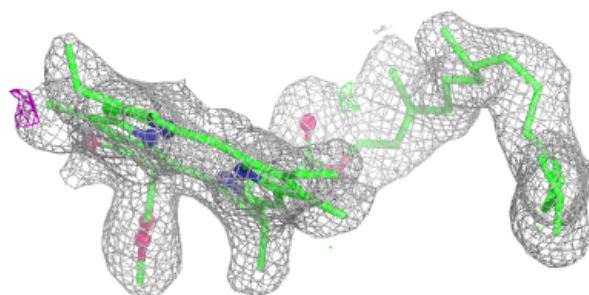
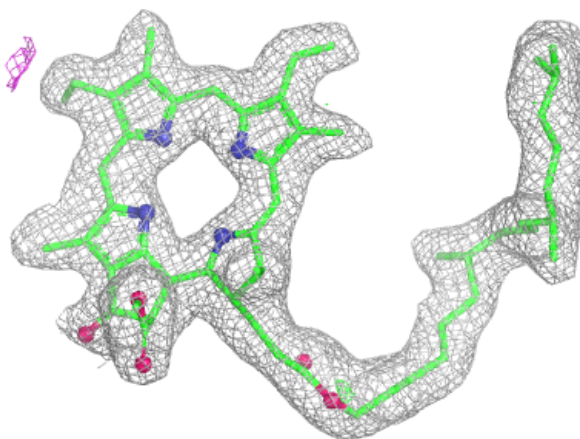
Electron density around PHO A 407:

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



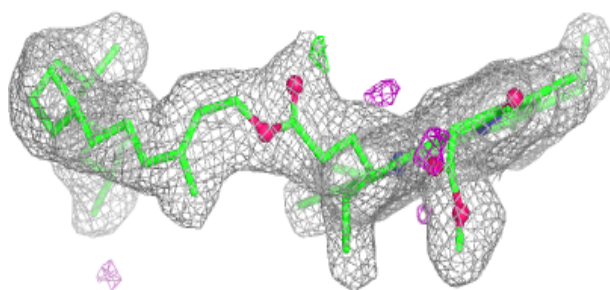
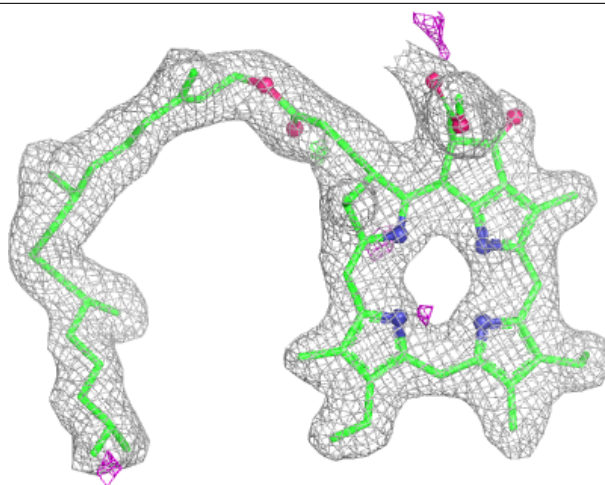
Electron density around PHO D 402:

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



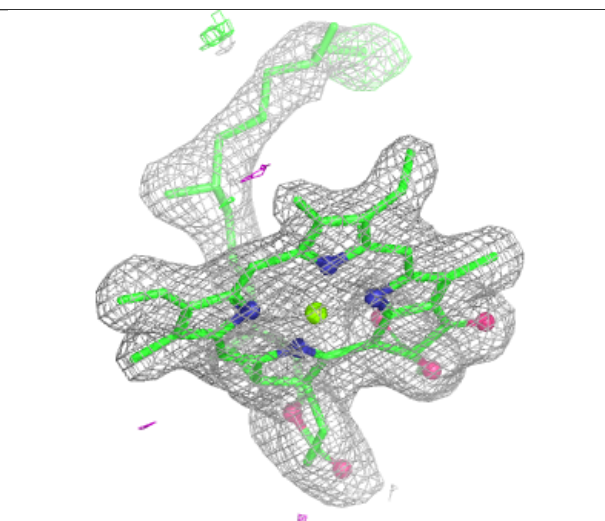
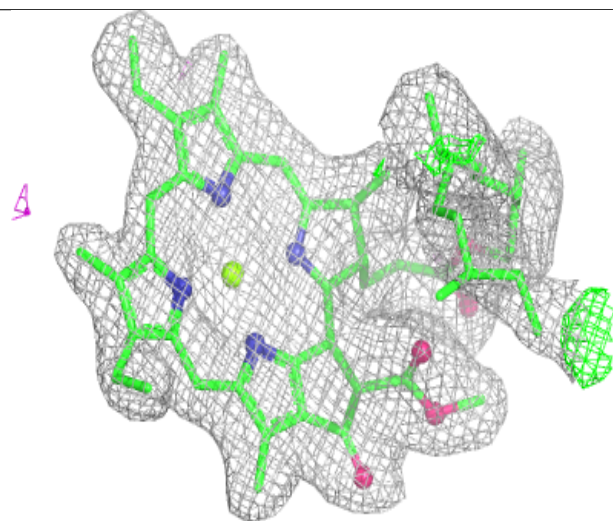
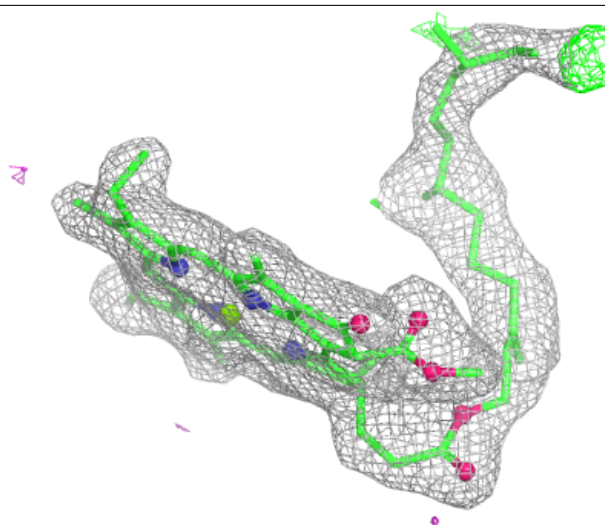
Electron density around PHO a 410:

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



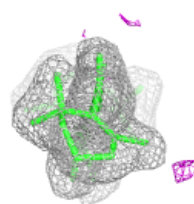
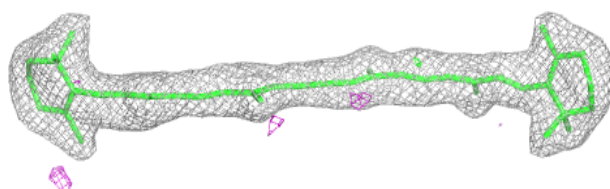
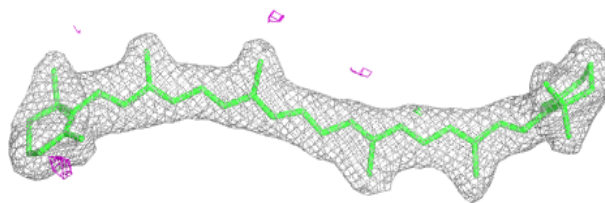
Electron density around CLA B 614:

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



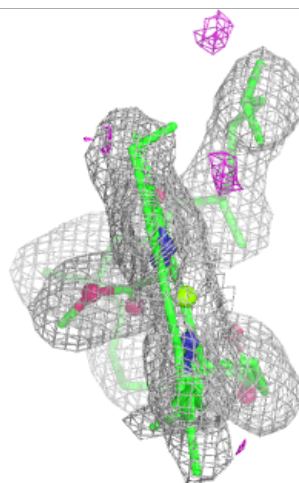
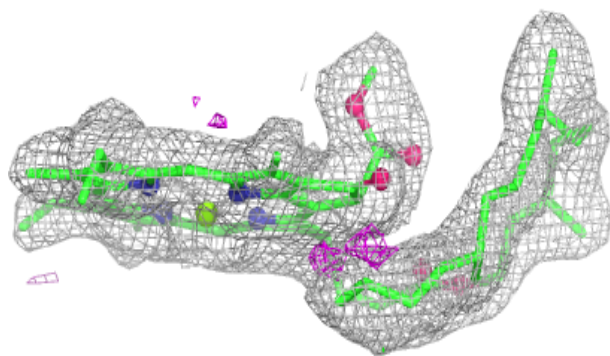
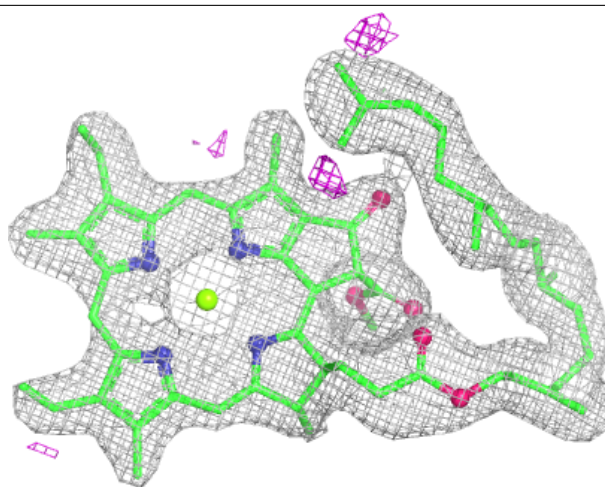
Electron density around BCR A 409:

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



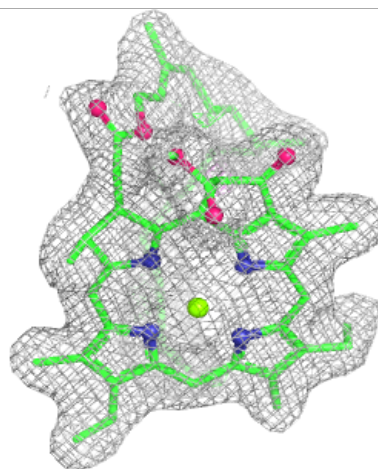
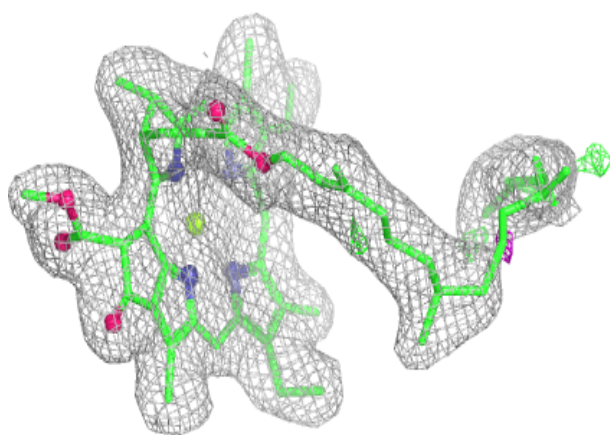
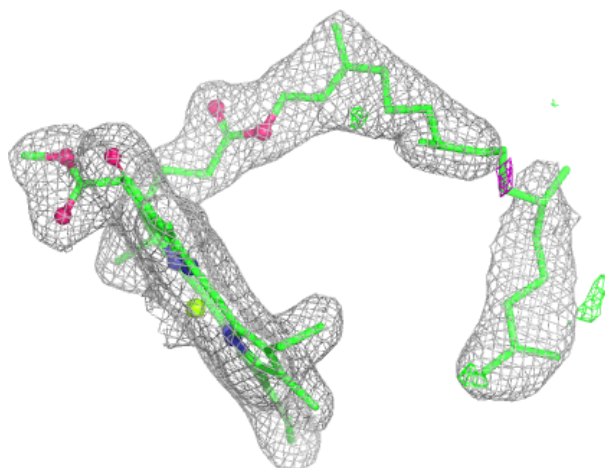
Electron density around CLA b 611:

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



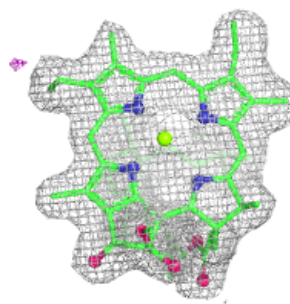
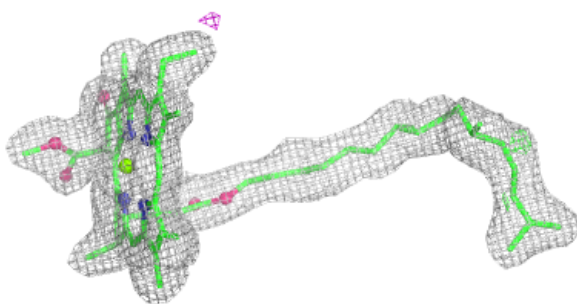
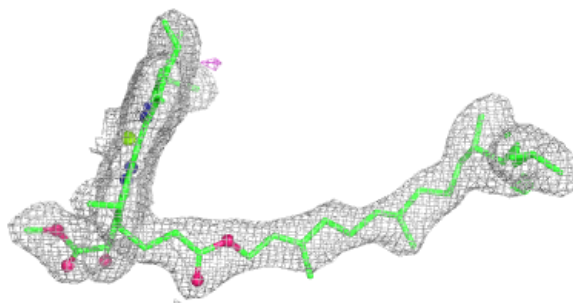
Electron density around CLA b 612:

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



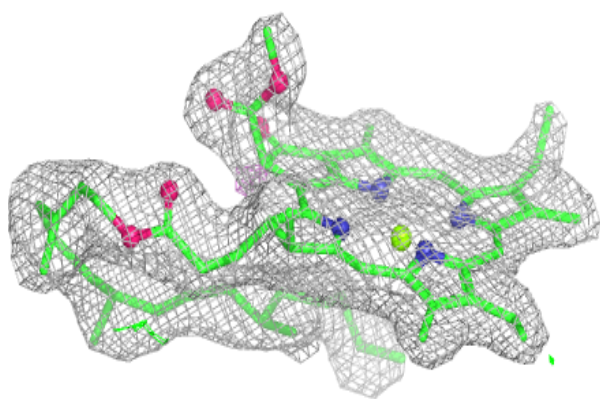
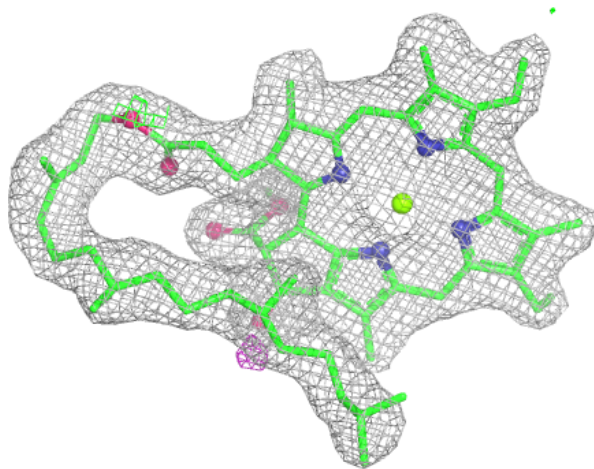
Electron density around CLA B 606:

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



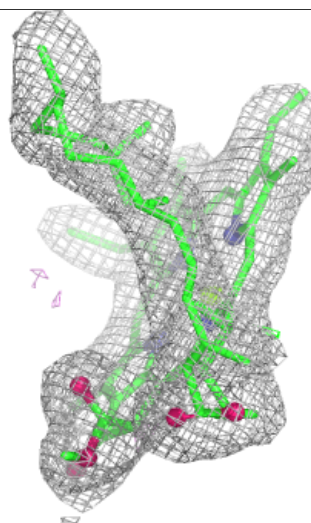
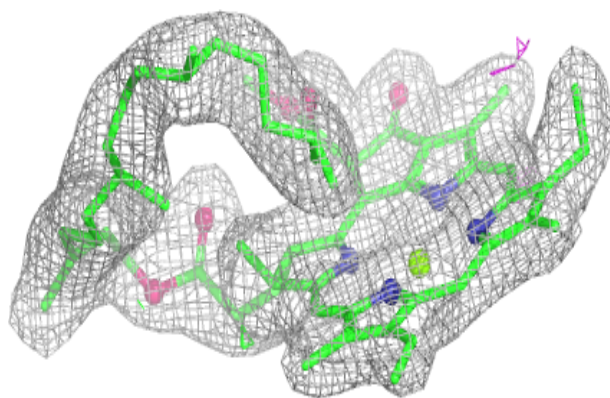
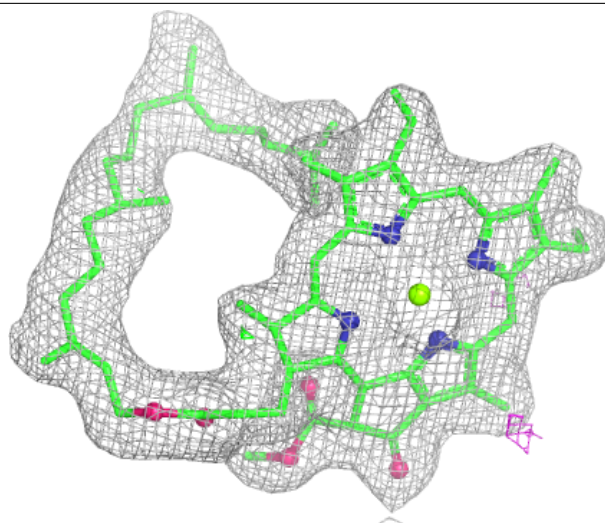
Electron density around CLA C 510:

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



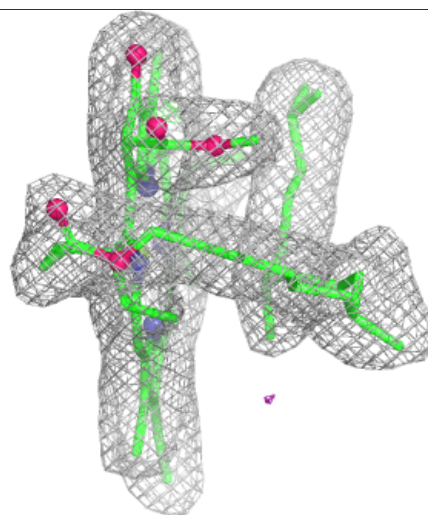
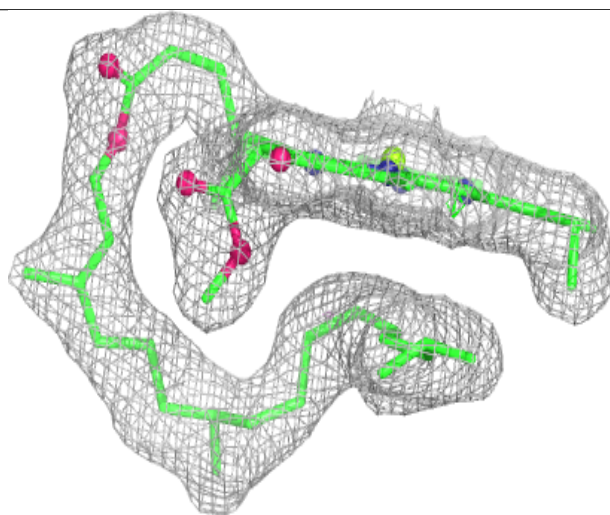
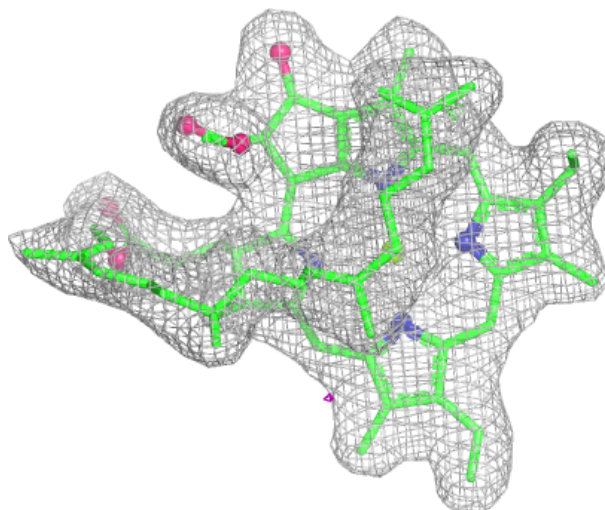
Electron density around CLA b 616:

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



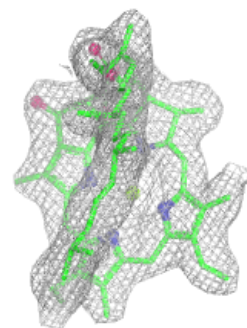
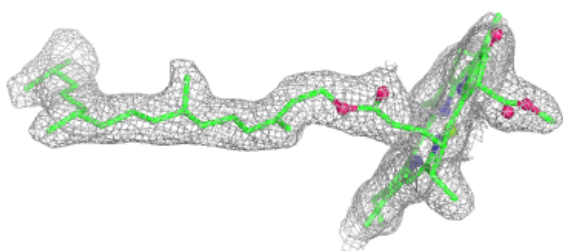
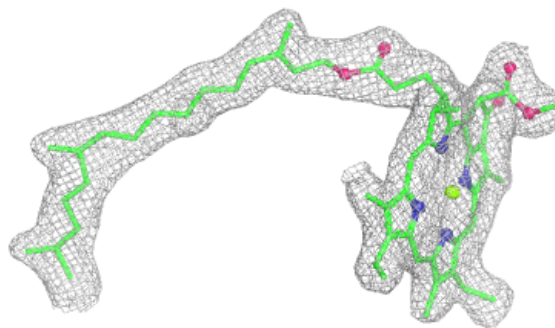
Electron density around CLA C 511:

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

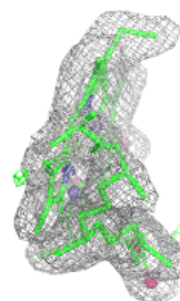
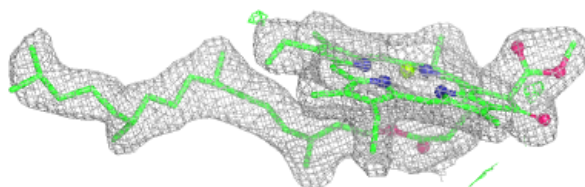
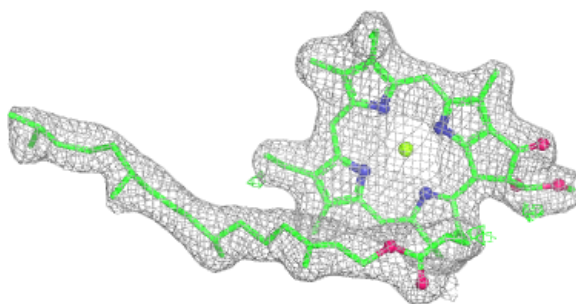


Electron density around CLA B 610:

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

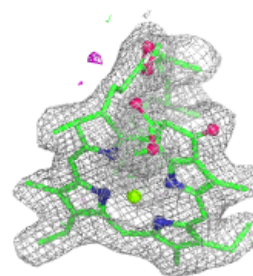
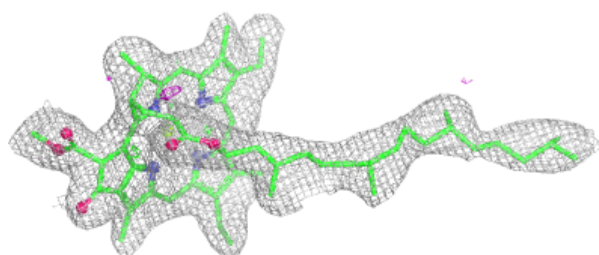
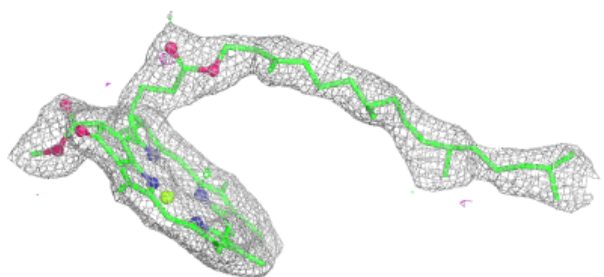
**Electron density around CLA C 502:**

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

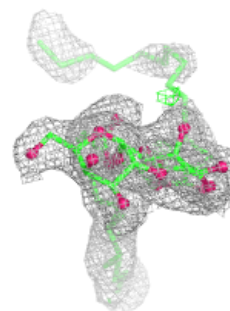
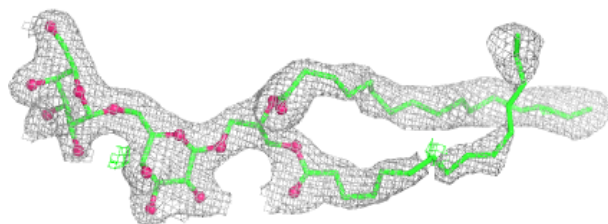
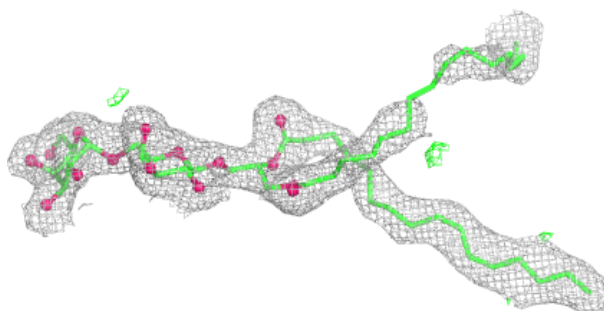


Electron density around CLA c 905:

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

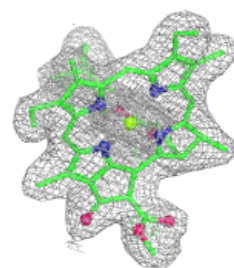
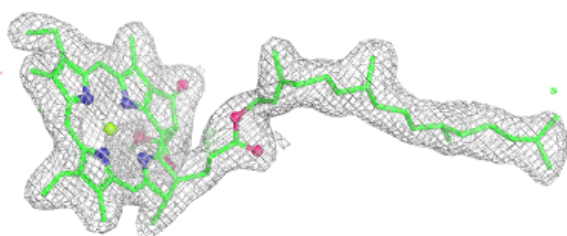
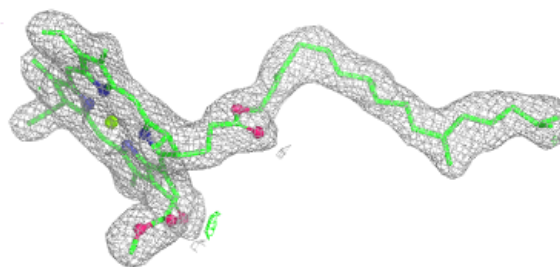
**Electron density around DGD C 517:**

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



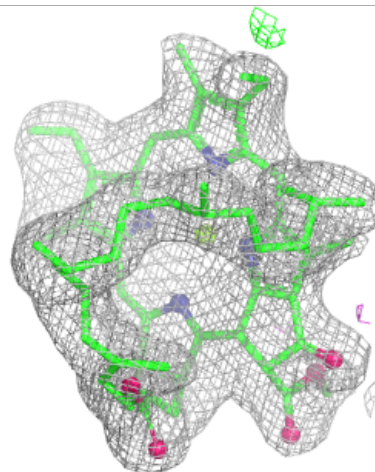
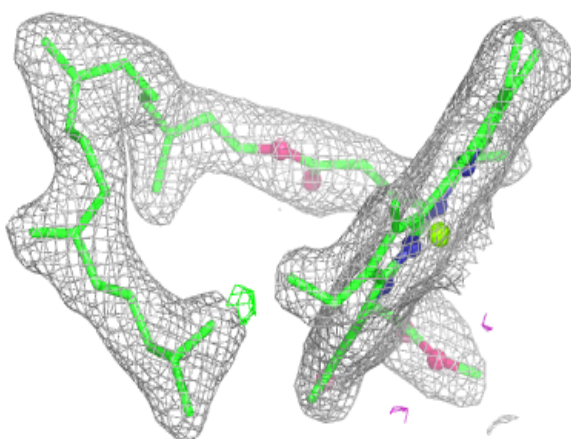
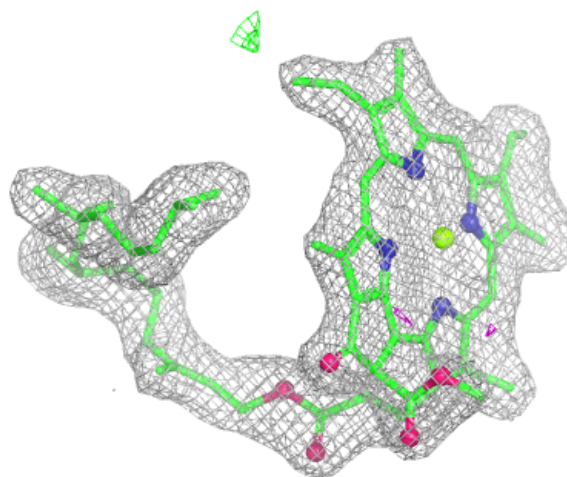
Electron density around CLA C 503:

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



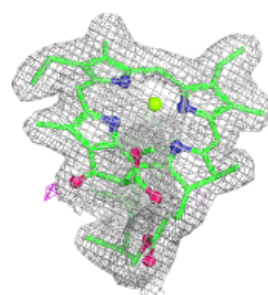
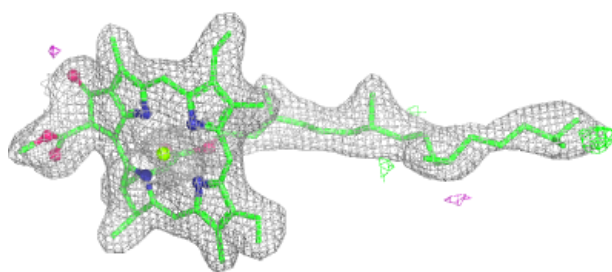
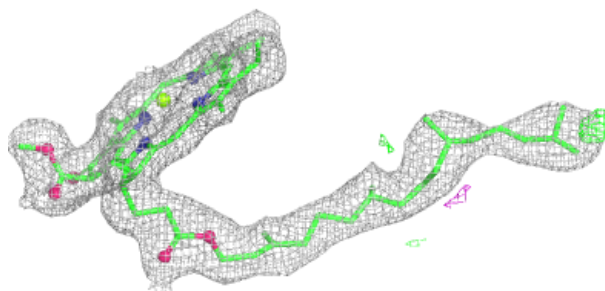
Electron density around CLA C 504:

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

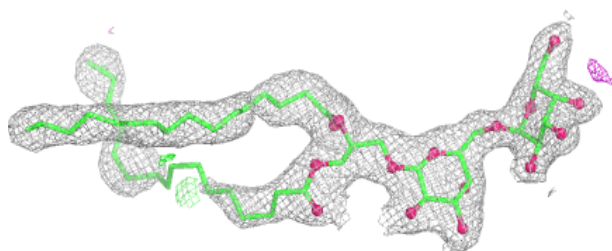
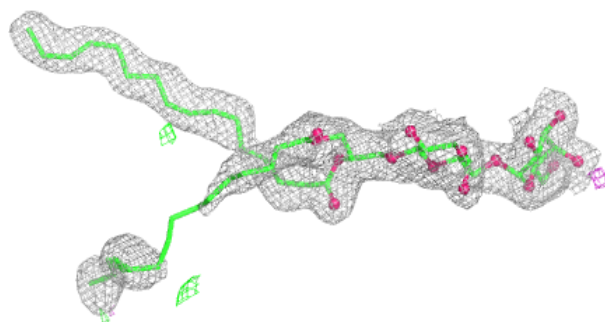


Electron density around CLA C 505:

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

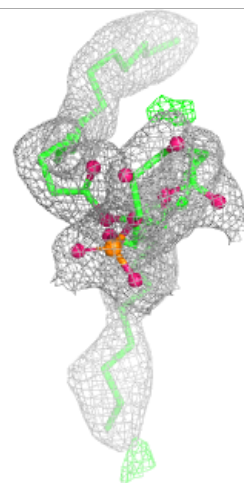
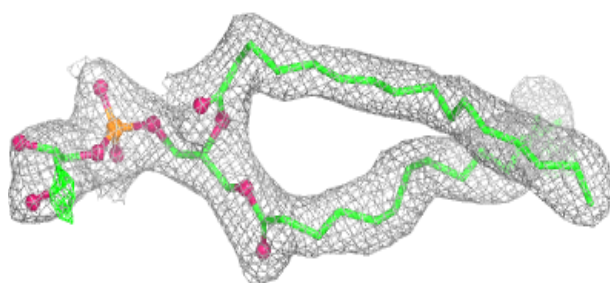
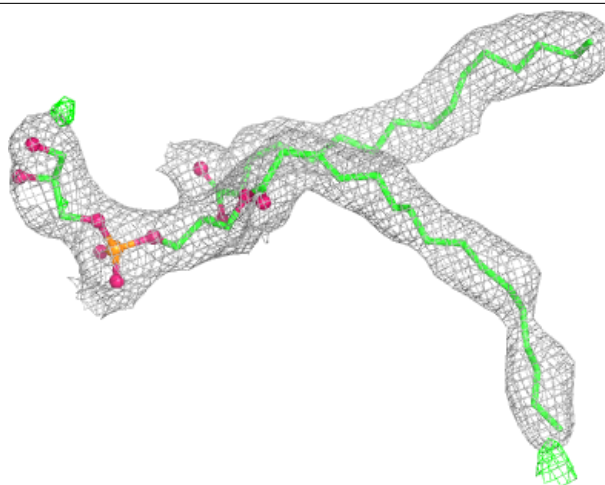
**Electron density around DGD c 917:**

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



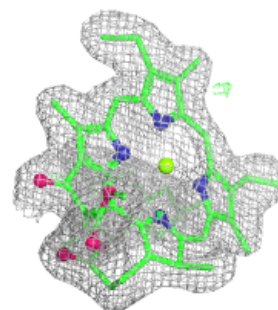
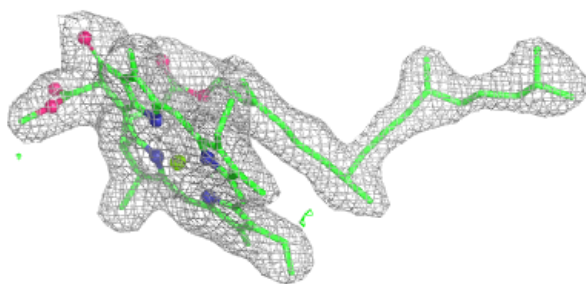
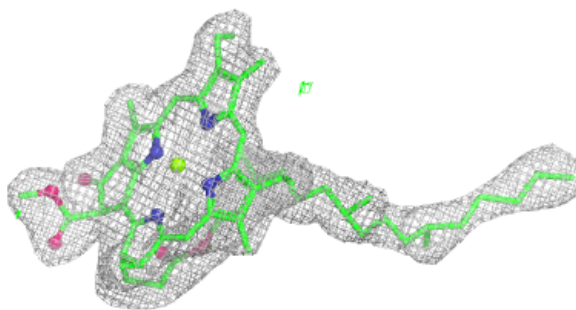
Electron density around LHG D 410:

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

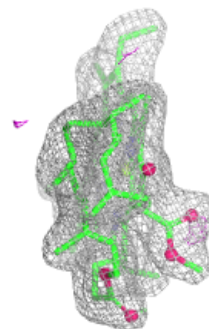
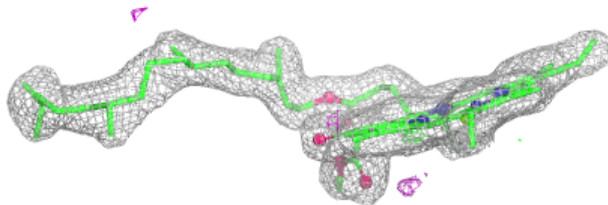
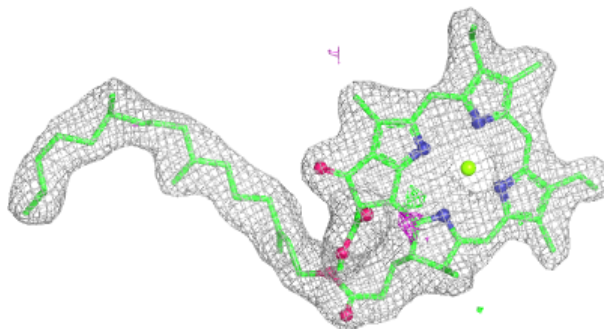


Electron density around CLA C 506:

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

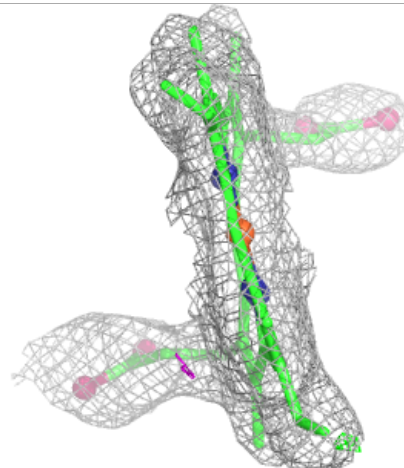
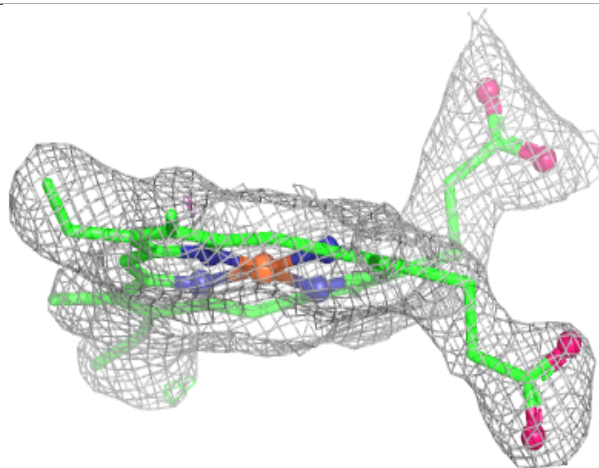
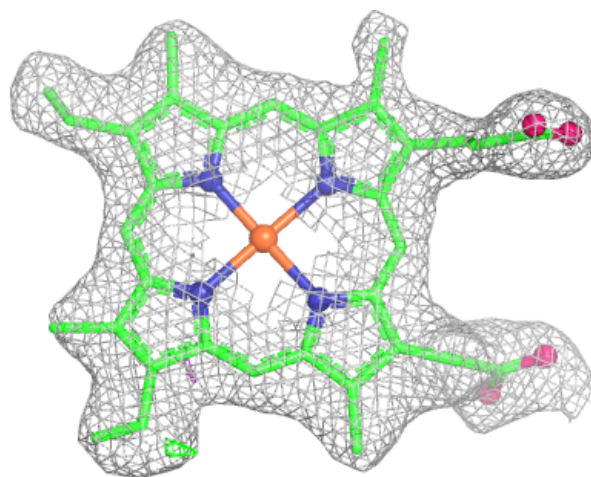
**Electron density around CLA b 603:**

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



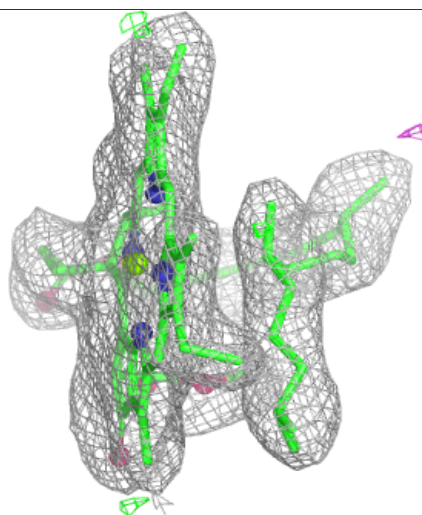
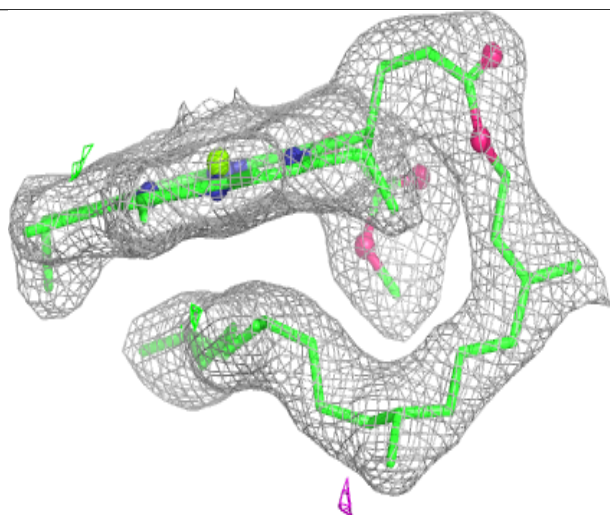
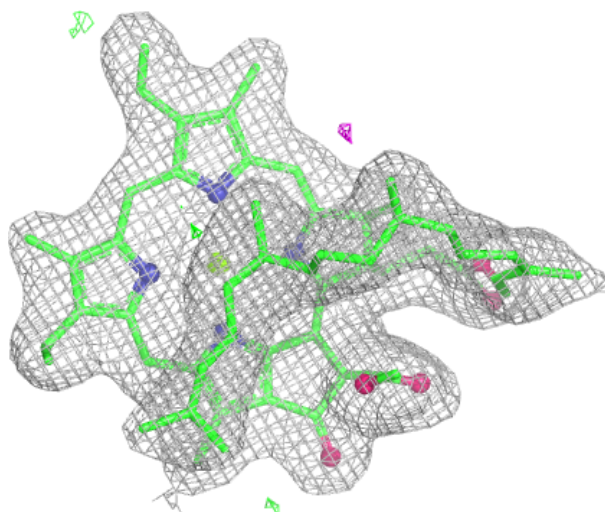
Electron density around HEM E 102:

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



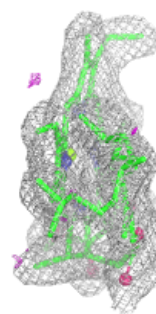
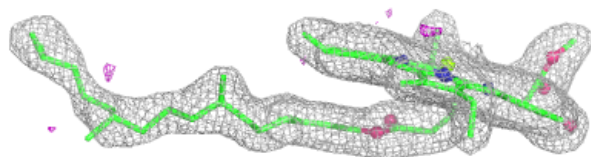
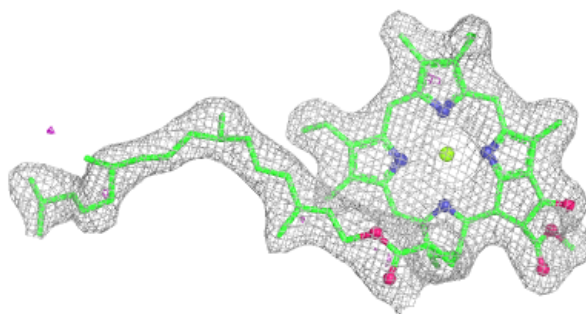
Electron density around CLA c 911:

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

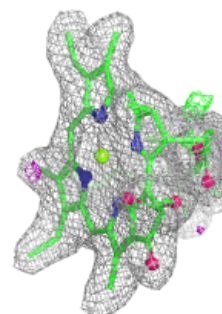
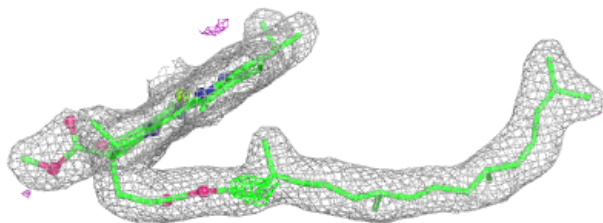
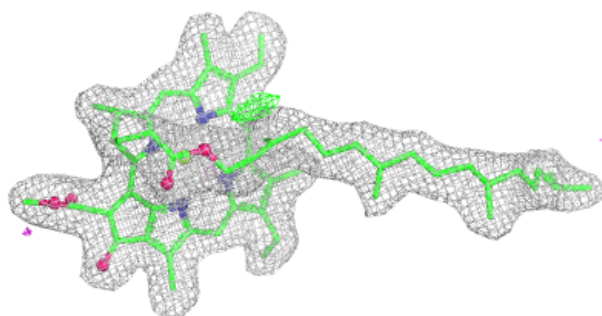


Electron density around CLA b 604:

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

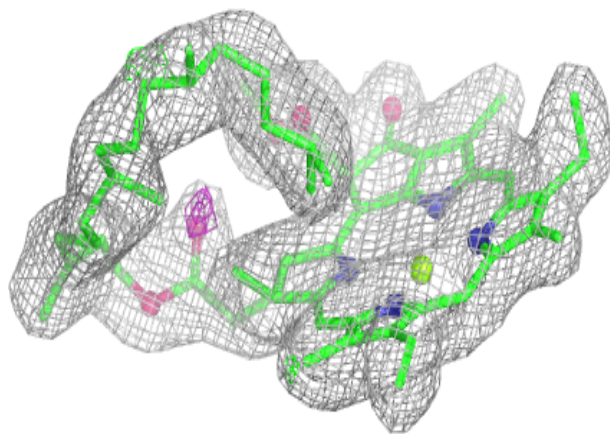
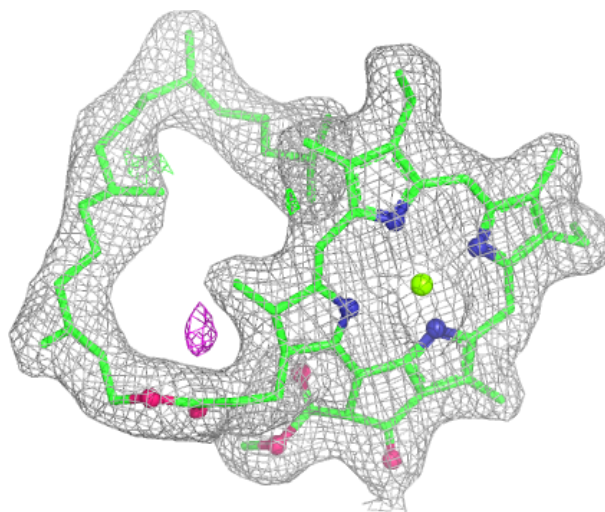
**Electron density around CLA B 609:**

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



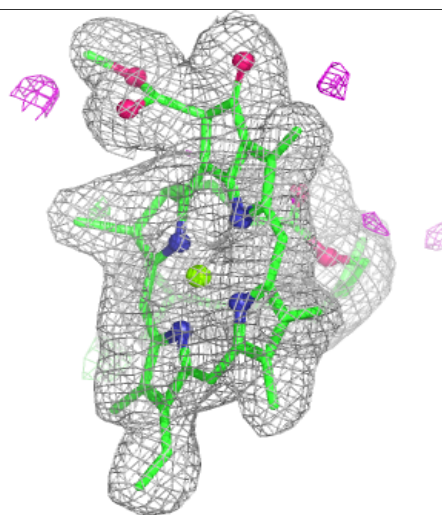
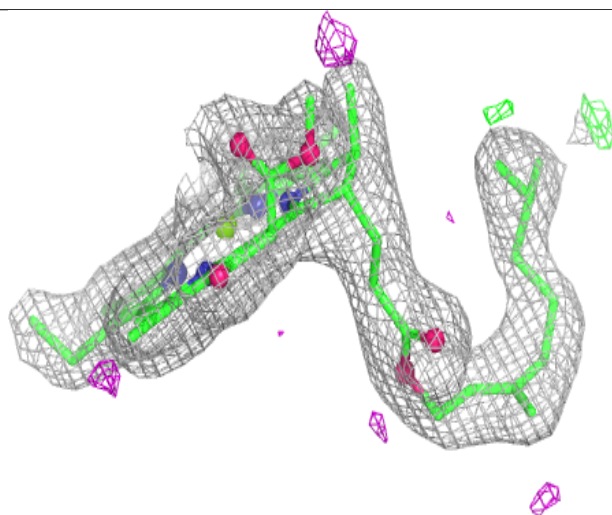
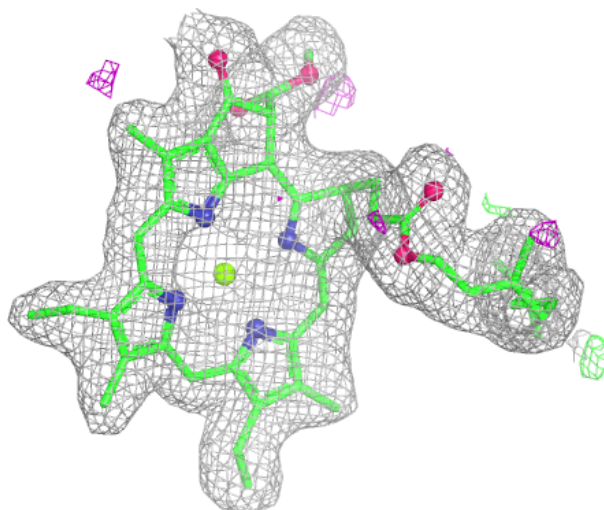
Electron density around CLA B 616:

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



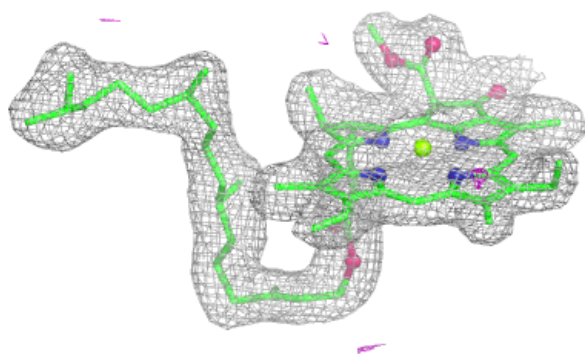
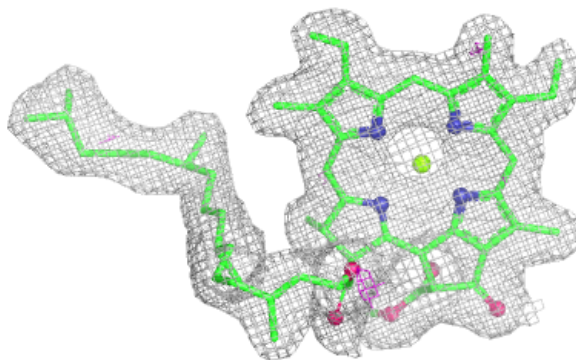
Electron density around CLA A 406:

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

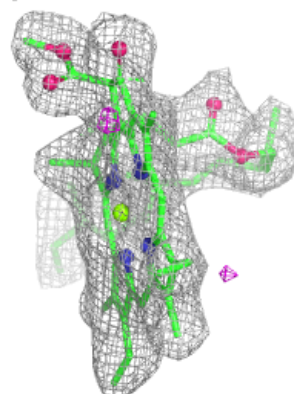
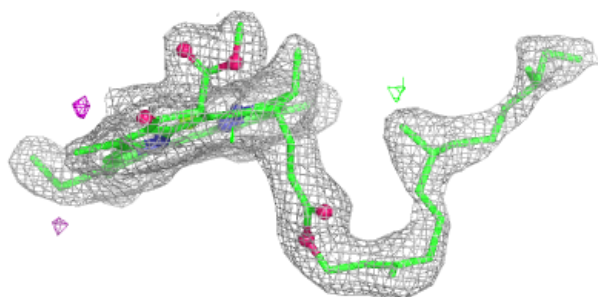
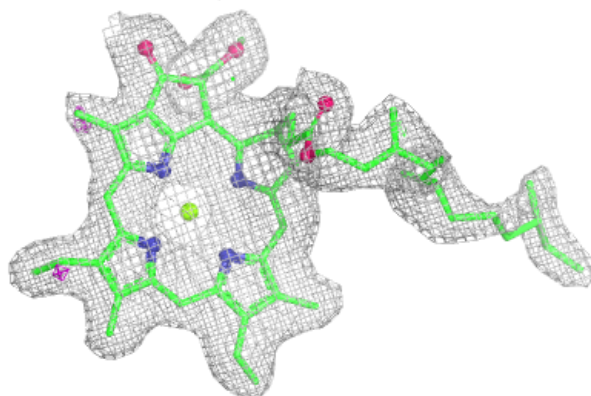


Electron density around CLA a 408:

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

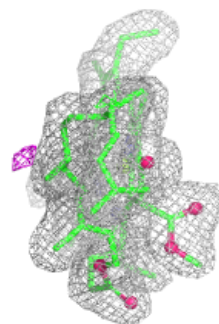
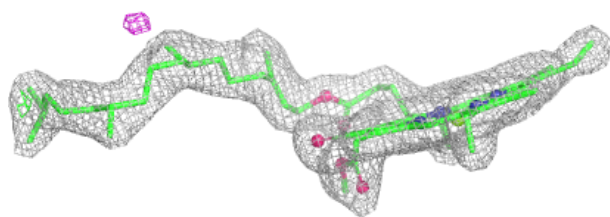
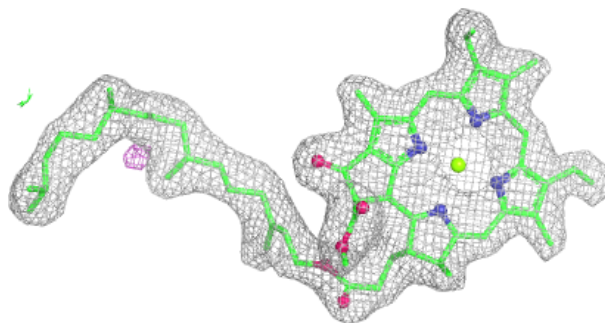
**Electron density around CLA a 409:**

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

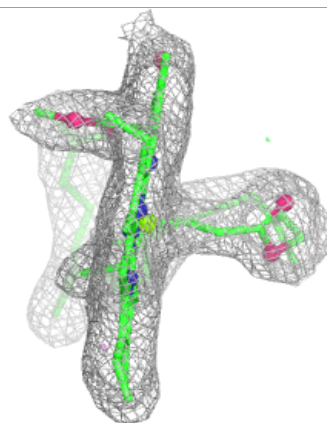
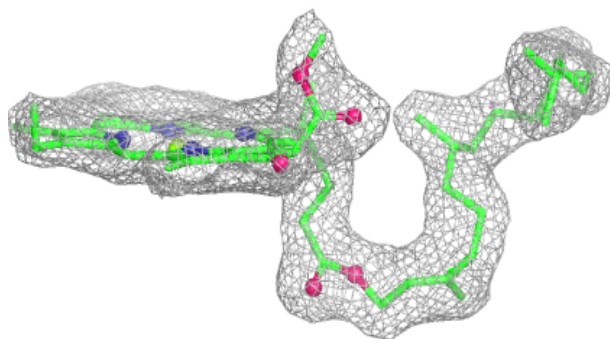
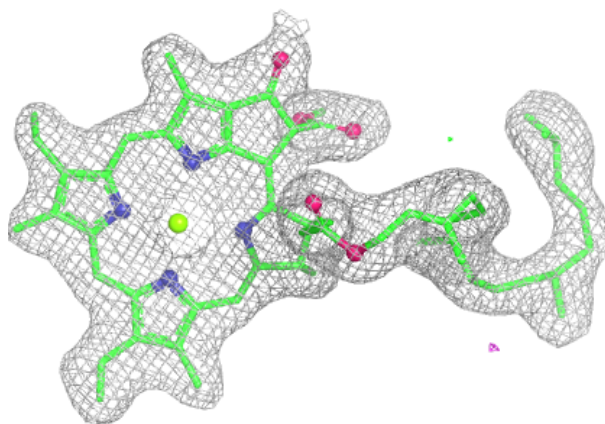


Electron density around CLA B 603:

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

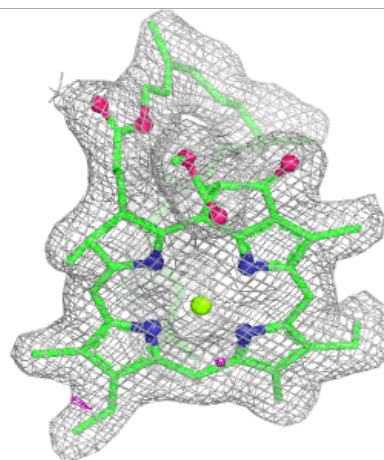
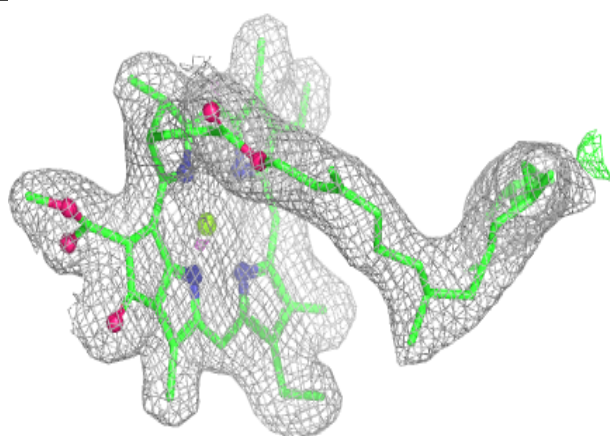
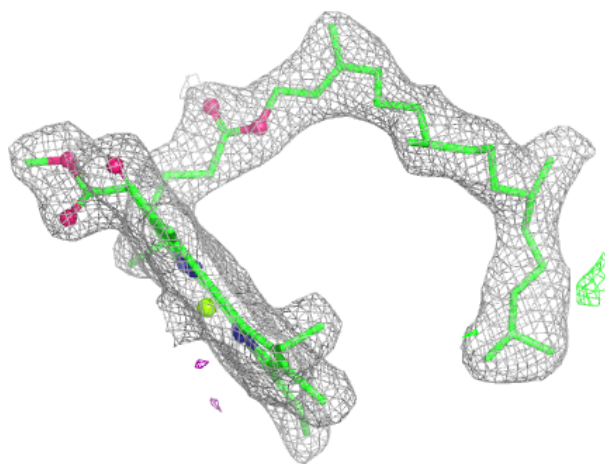
**Electron density around CLA b 613:**

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



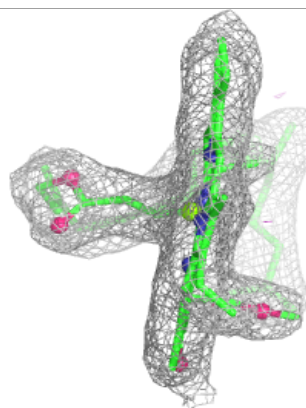
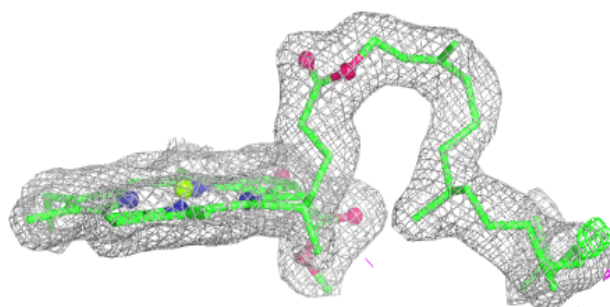
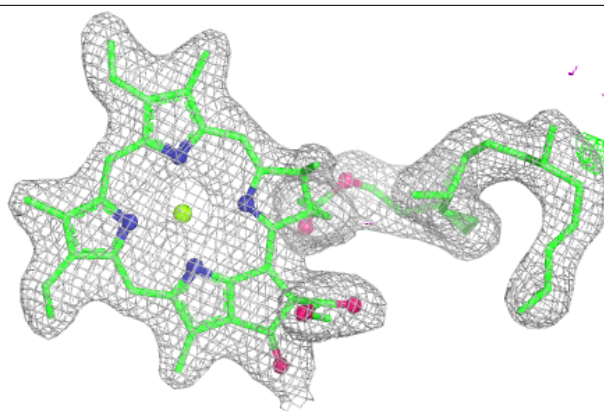
Electron density around CLA B 612:

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

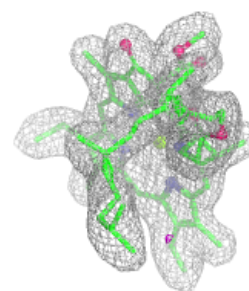
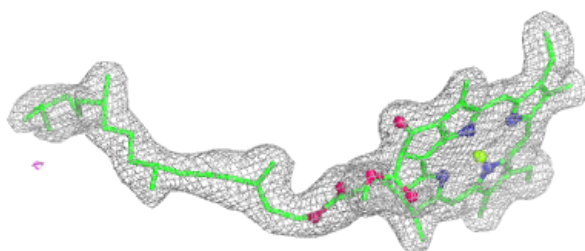
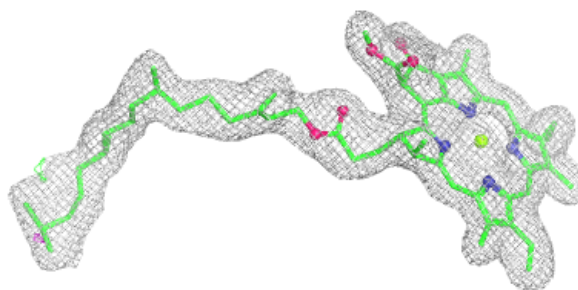


Electron density around CLA B 613:

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

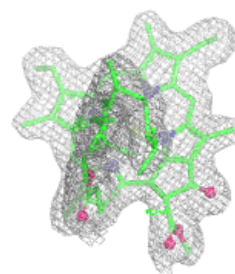
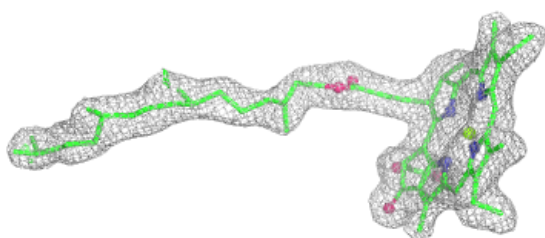
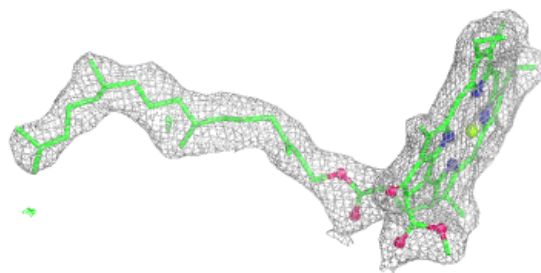
**Electron density around CLA A 405:**

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

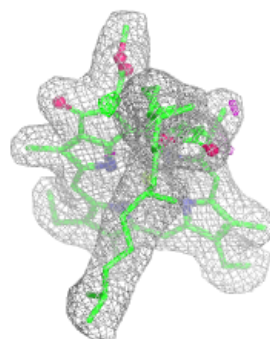
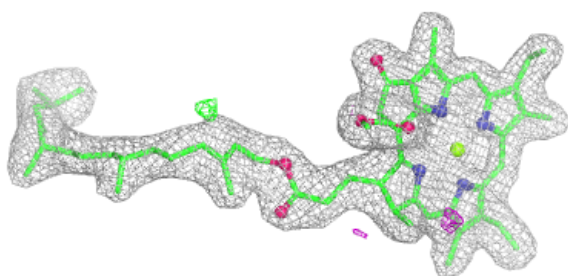
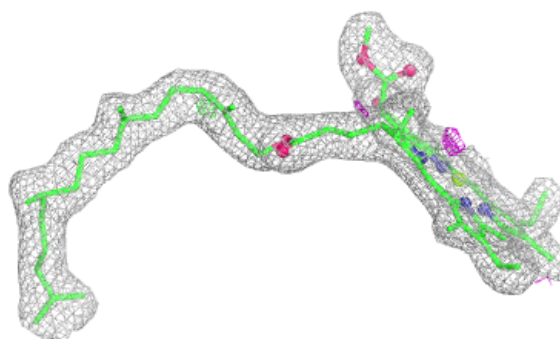


Electron density around CLA b 605:

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

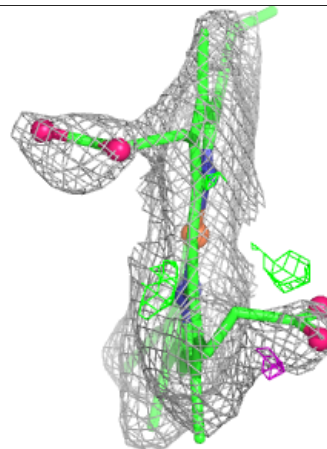
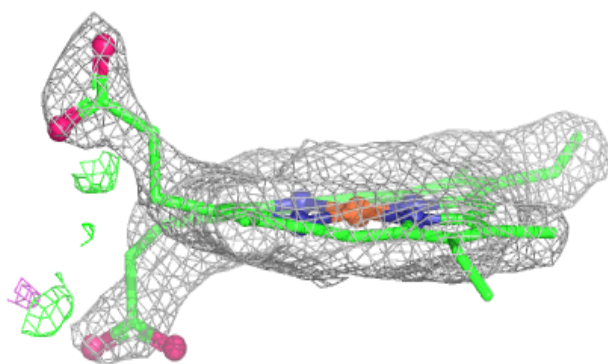
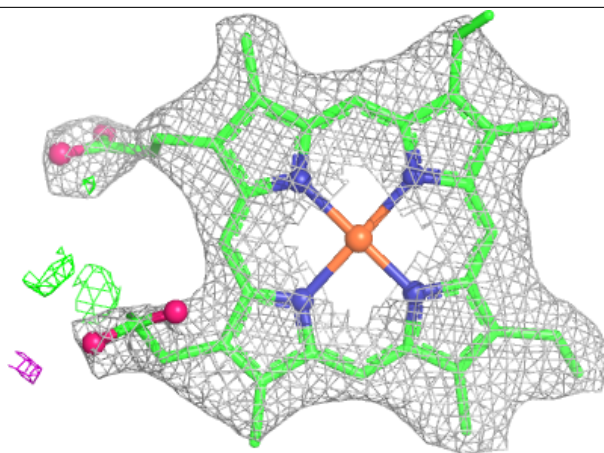
**Electron density around CLA d 402:**

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



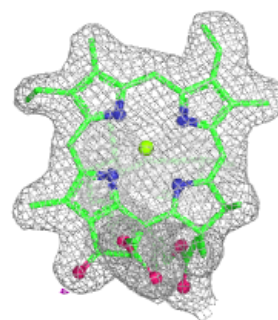
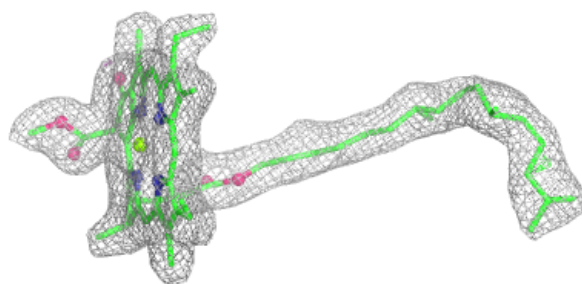
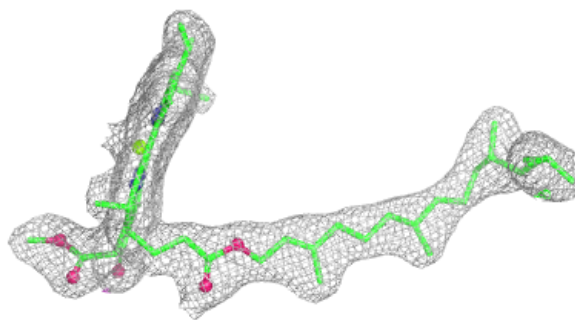
Electron density around HEM e 101:

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

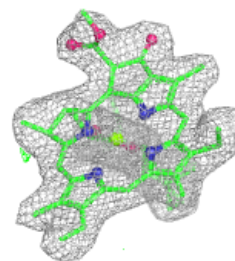
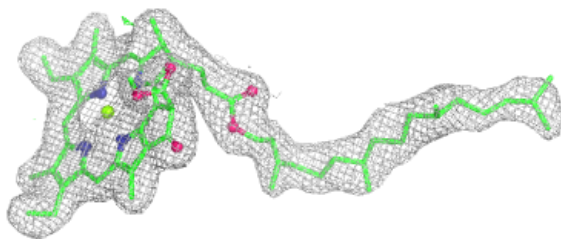
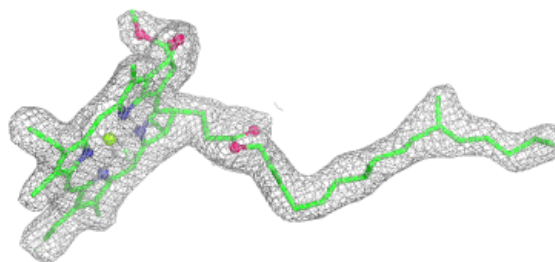


Electron density around CLA b 606:

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

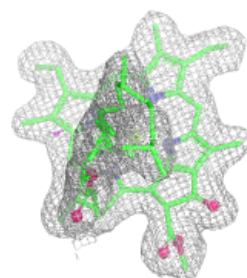
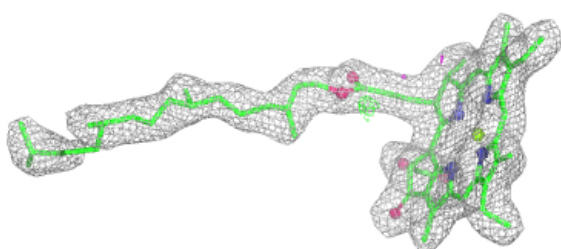
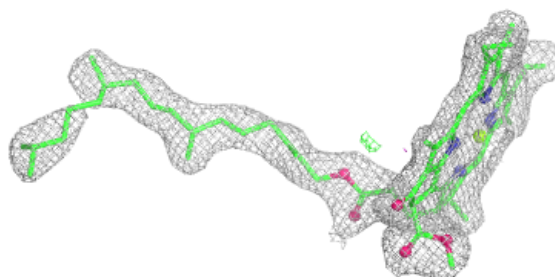
**Electron density around CLA c 903:**

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

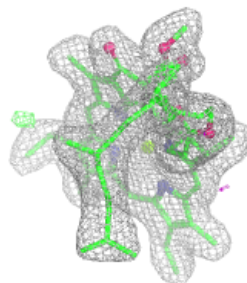
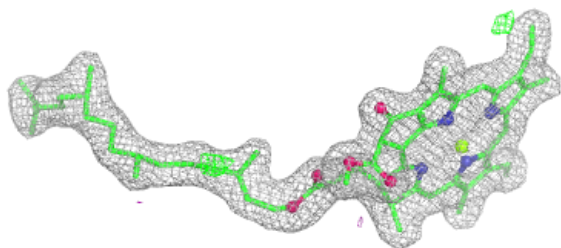
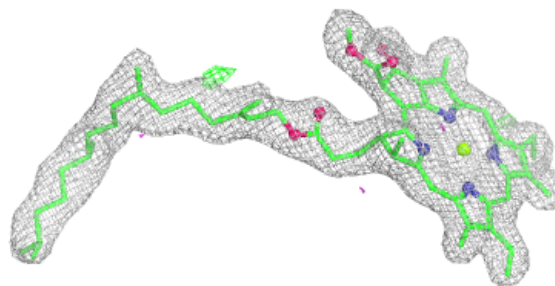


Electron density around CLA B 605:

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

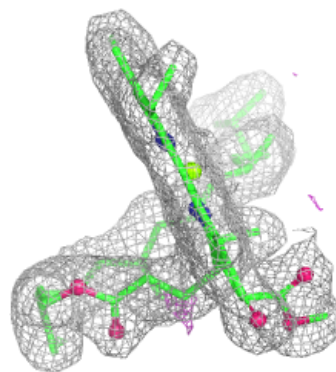
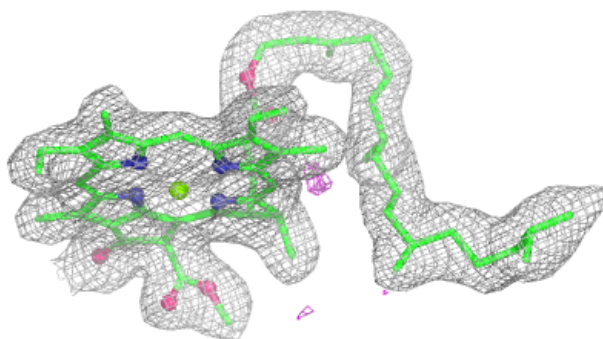
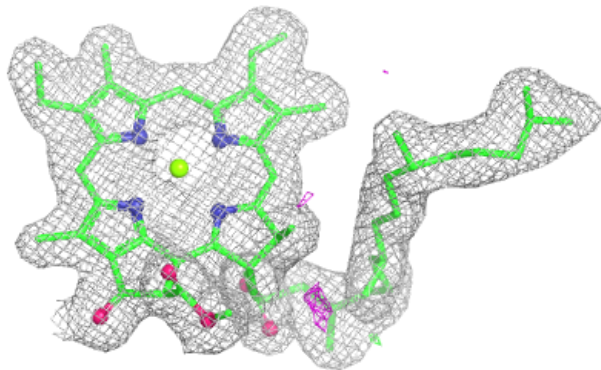
**Electron density around CLA a 407:**

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

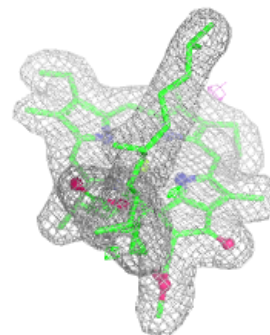
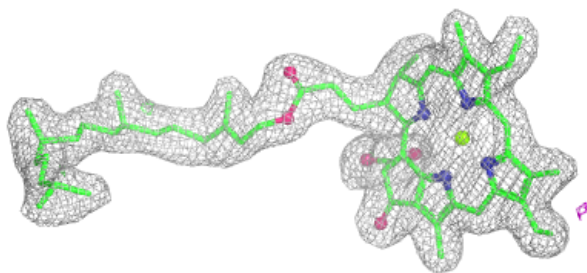
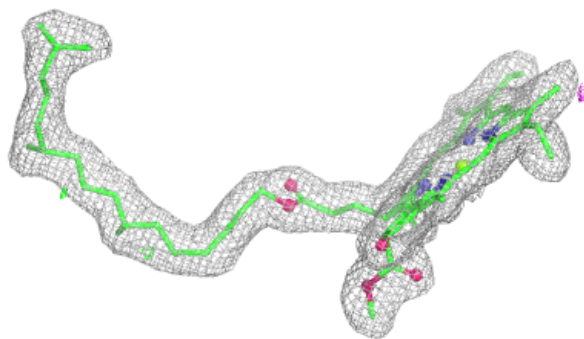


Electron density around CLA D 401:

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

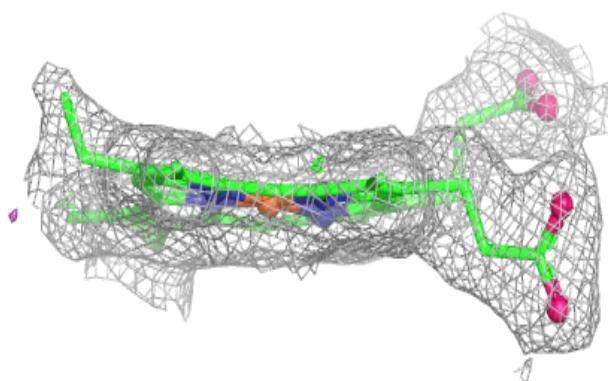
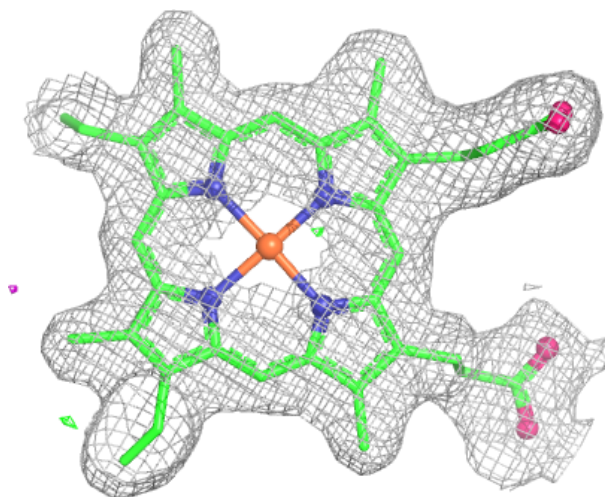
**Electron density around CLA D 403:**

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



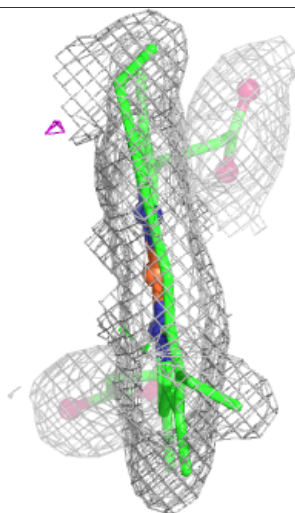
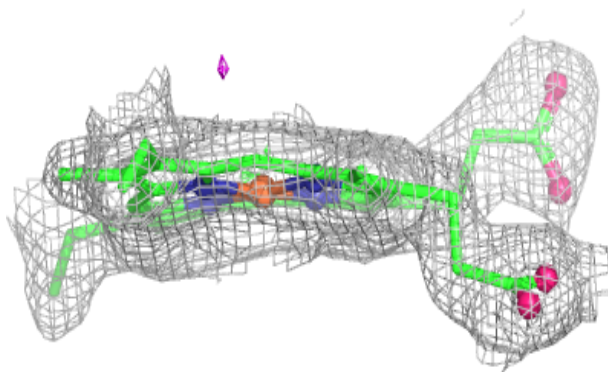
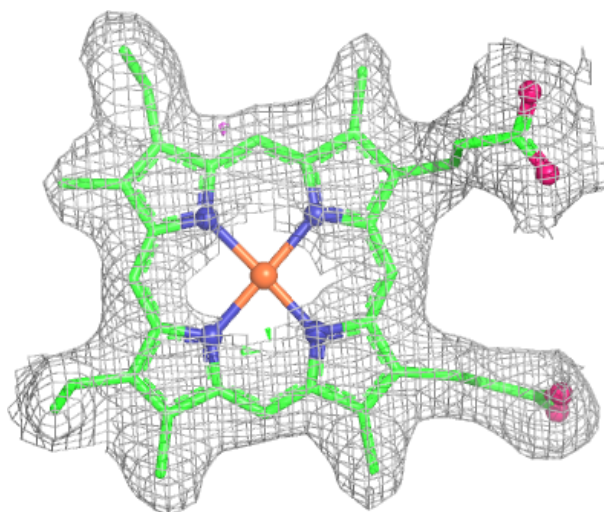
Electron density around HEC V 202:

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



Electron density around HEC v 202:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.