



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:33 PM UTC

PDB ID : 6DHH / pdb_00006dhh
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.2 Angstrom resolution
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2018-05-20
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

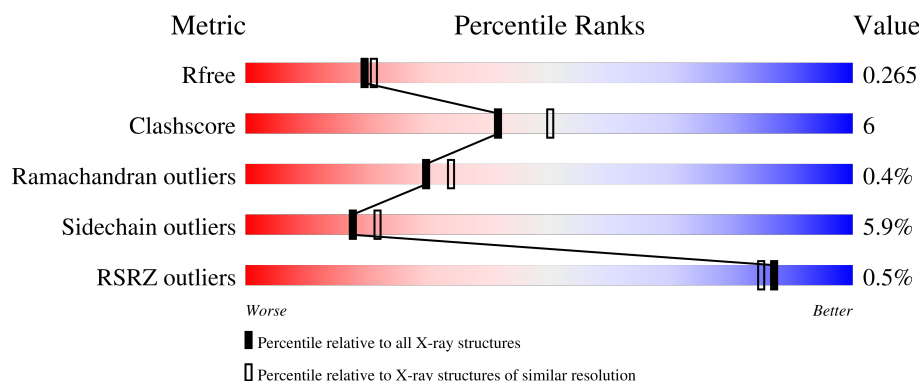
1 Overall quality at a glance

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	85% 15%

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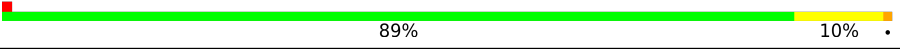
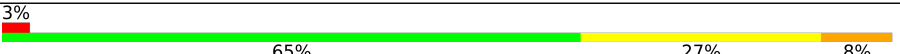
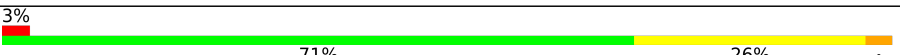
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	a	334	% 83% 16% .
2	B	505	85% 14% .
2	b	505	% 83% 17%
3	C	451	86% 12% .
3	c	451	86% 14%
4	D	341	87% 13%
4	d	341	85% 15%
5	E	82	73% 24% ..
5	e	82	61% 38% .
6	F	34	3% 85% 12% .
6	f	34	71% 26% .
7	H	65	85% 12% .
7	h	65	2% 82% 14% . .
8	I	36	78% 17% 6%
8	i	36	72% 28%
9	J	36	78% 22%
9	j	36	83% 17%
10	K	37	57% 43%
10	k	37	59% 38% .
11	L	37	86% 14%
11	l	37	84% 14% .
12	M	33	73% 24% .
12	m	33	79% 18% .
13	O	244	75% 23% .
13	o	244	81% 16% .

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Mol	Chain	Length	Quality of chain
14	T	30	
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	h	101	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103673 atoms, of which 51476 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	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	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	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	0	0
			6752	2244	3335	570	590	13			
3	c	451	Total	C	H	N	O	S	0	1	0
			6901	2286	3407	587	608	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1030	338	523	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			516	172	261	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3730	1174	1850	317	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	H	N	O	0	0	0
			519	181	261	36	39			
14	t	30	Total	C	H	N	O	0	0	0
			512	180	256	36	38			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	Y	27	Total	C	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O		0	0	0
			593	188	312	45	48				
18	x	38	Total	C	H	N	O		0	0	0
			593	188	312	45	48				

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	R	34	Total	C	H	N	O		0	0	0
			569	184	298	47	40				
20	r	31	Total	C	H	N	O		0	0	0
			461	154	234	40	33				

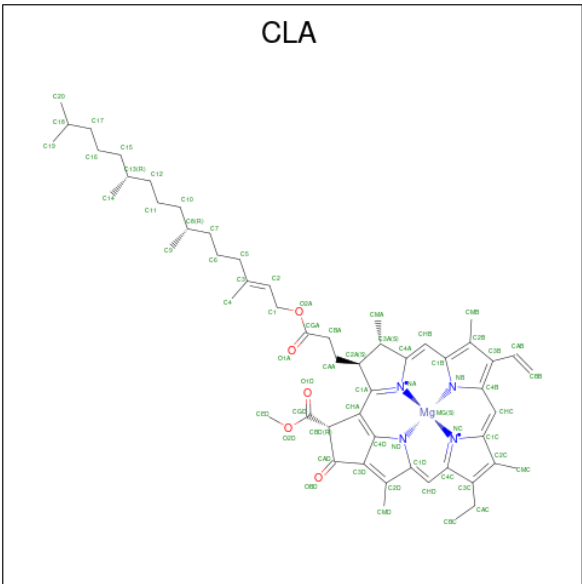
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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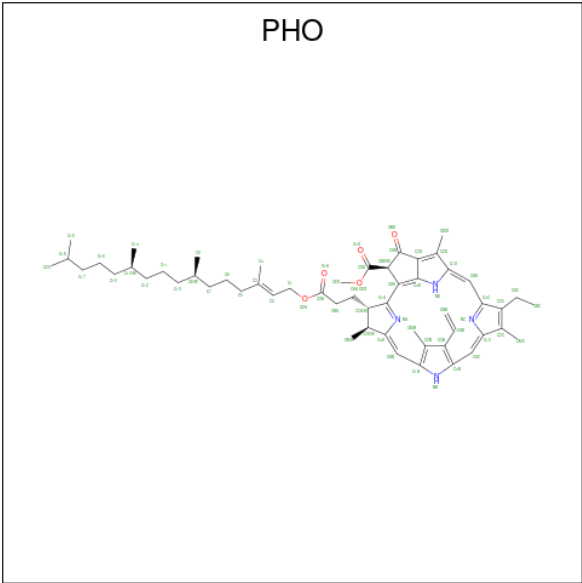
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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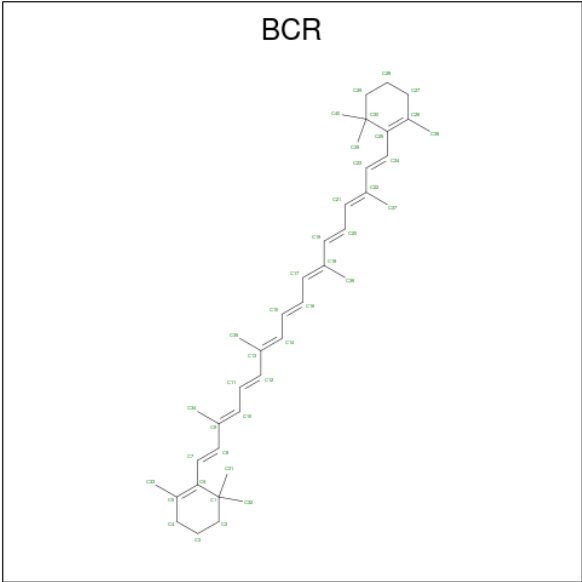
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	h	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



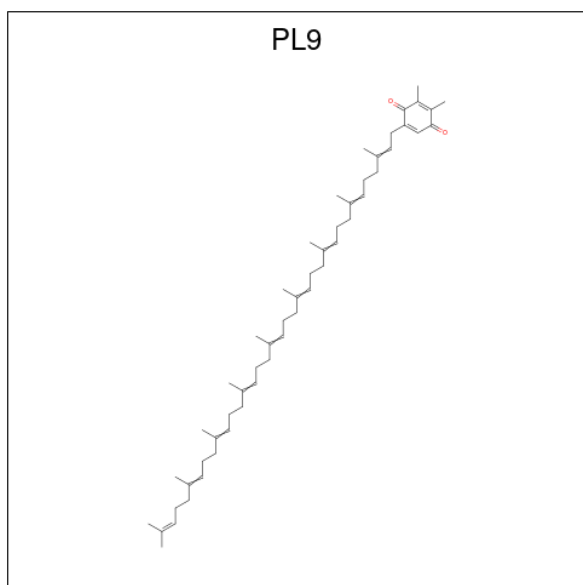
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total	C	H	0	0
			96	40	56		
25	H	1	Total	C	H	0	0
			96	40	56		
25	K	1	Total	C	H	0	0
			96	40	56		
25	T	1	Total	C	H	0	0
			96	40	56		
25	a	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	b	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	d	1	Total	C	H	0	0
			96	40	56		
25	h	1	Total	C	H	0	0
			96	40	56		
25	t	1	Total	C	H	0	0
			96	40	56		
25	y	1	Total	C	H	0	0
			96	40	56		

- 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: C₅₃H₈₀O₂).



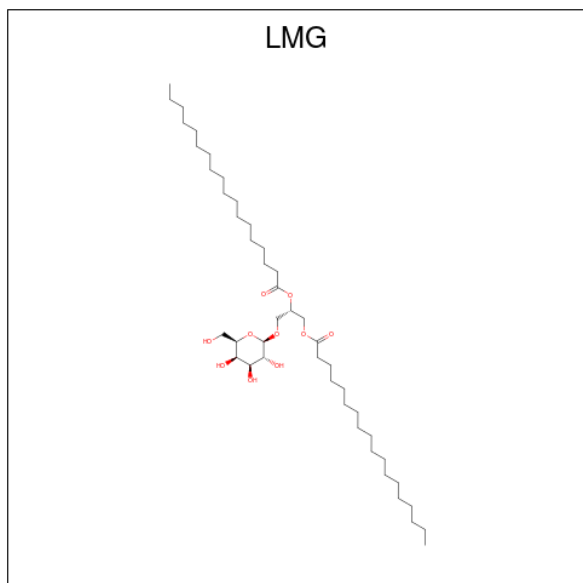
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



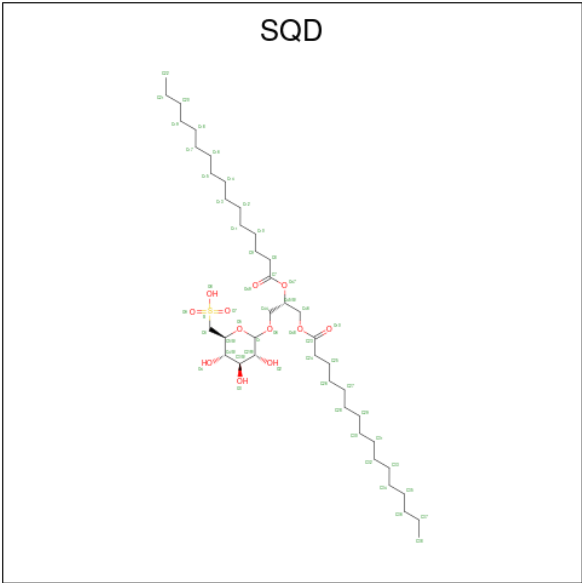
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			123	41	72	10		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			57	21	34	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

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



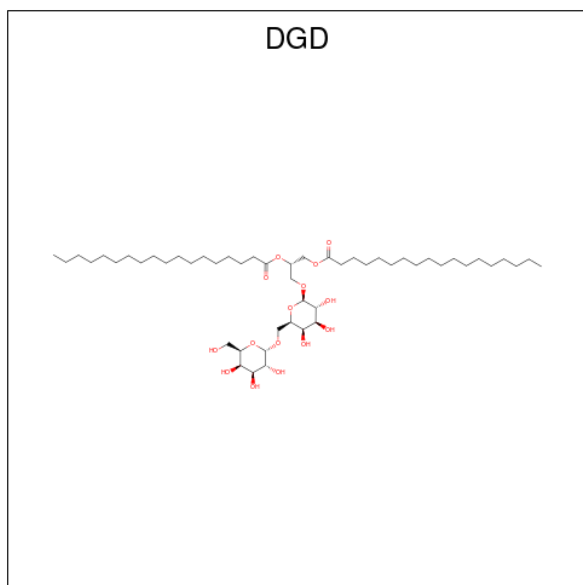
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		

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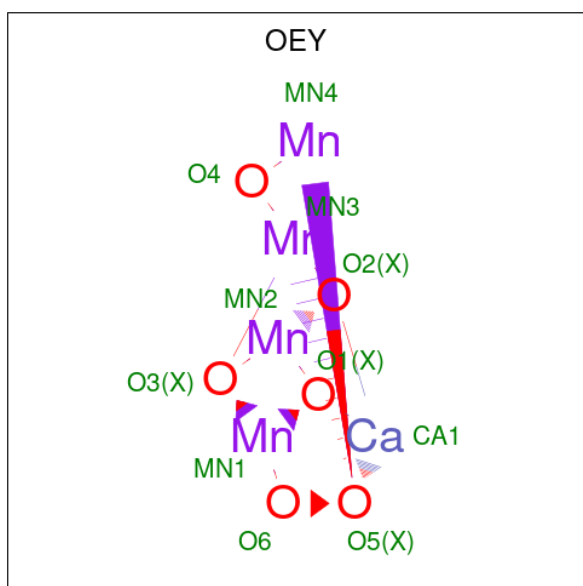
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



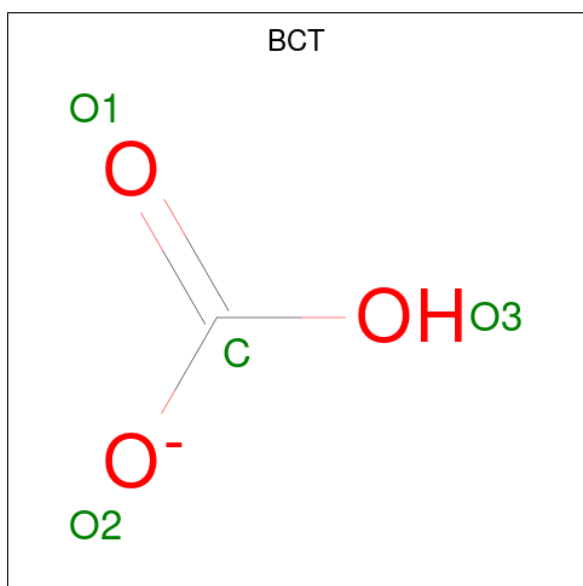
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O		0	0
			162	51	96	15			
29	C	1	Total	C	H	O		0	0
			144	47	82	15			
29	C	1	Total	C	H	O		0	0
			144	47	82	15			
29	C	1	Total	C	H	O		0	0
			144	47	82	15			
29	H	1	Total	C	H	O		0	0
			144	47	82	15			
29	a	1	Total	C	H	O		0	0
			119	39	75	5			
29	c	1	Total	C	H	O		0	0
			144	47	82	15			
29	c	1	Total	C	H	O		0	0
			144	47	82	15			
29	c	1	Total	C	H	O		0	0
			144	47	82	15			
29	h	1	Total	C	H	O		0	0
			144	47	82	15			

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	0
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	0
			11	1	4	6		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			5	1	1	3		

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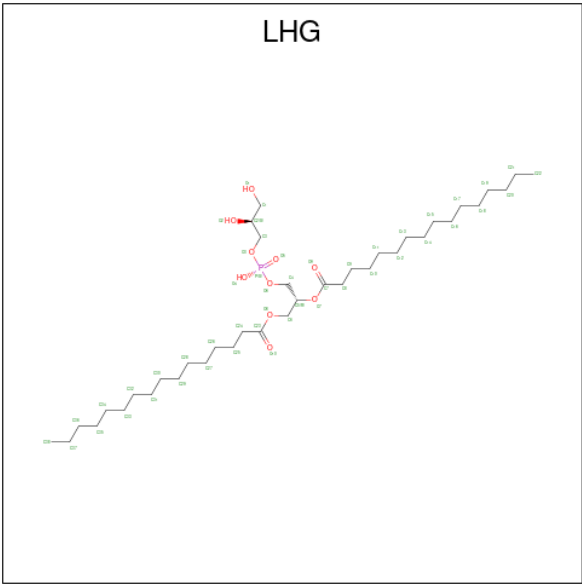
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

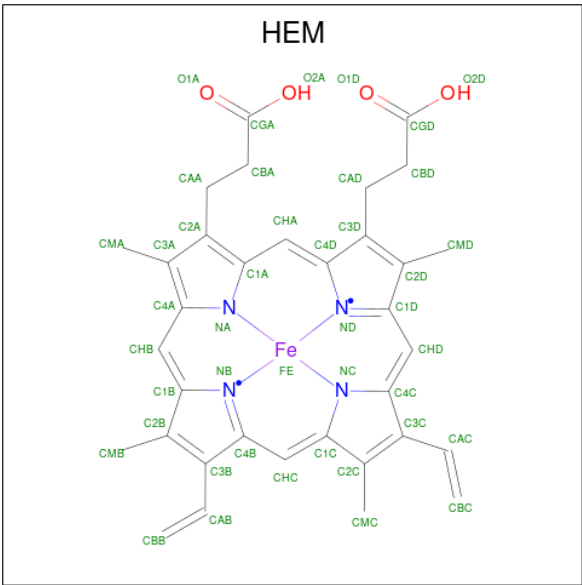
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	5	Total	C	H	O	0	0
			180	63	109	8		
32	C	3	Total	C	H	O	0	0
			103	36	63	4		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	E	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			
32	I	1	Total	C	H		0	0
			41	15	26			
32	J	1	Total	C	H	O	0	0
			28	10	16	2		
32	M	2	Total	C	H	O	0	0
			63	23	38	2		
32	T	1	Total	C	H		0	0
			44	15	29			
32	a	1	Total	C	H	O	0	0
			28	10	16	2		
32	b	5	Total	C	H	O	0	0
			223	76	141	6		
32	c	2	Total	C	H	O	0	0
			83	28	51	4		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	2	Total	C	H	O	0	0
			72	26	44	2		
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



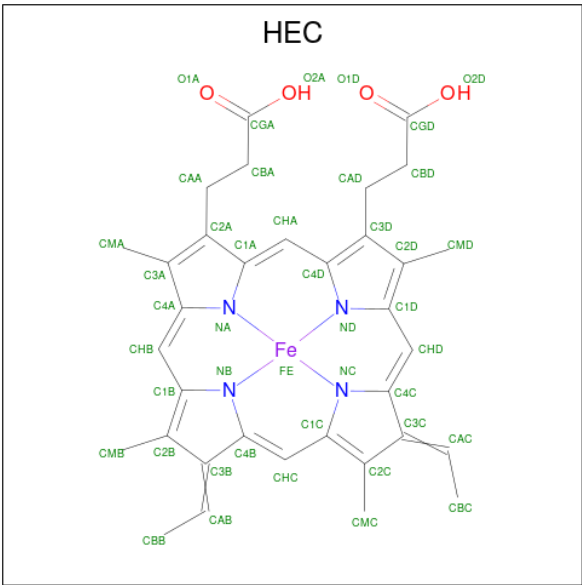
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	a	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	138	Total O 138 138	0	0
36	B	221	Total O 221 221	0	0
36	C	191	Total O 191 191	0	0
36	D	142	Total O 142 142	0	0
36	E	31	Total O 31 31	0	0
36	F	11	Total O 11 11	0	0
36	H	25	Total O 25 25	0	0
36	I	14	Total O 14 14	0	0
36	J	15	Total O 15 15	0	0
36	K	2	Total O 2 2	0	0
36	L	7	Total O 7 7	0	0
36	M	5	Total O 5 5	0	0
36	O	121	Total O 121 121	0	0
36	T	12	Total O 12 12	0	0
36	U	51	Total O 51 51	0	0
36	V	68	Total O 68 68	0	0
36	Y	5	Total O 5 5	0	0
36	X	8	Total O 8 8	0	0
36	Z	5	Total O 5 5	0	0
36	R	3	Total O 3 3	0	0
36	a	121	Total O 121 121	0	0

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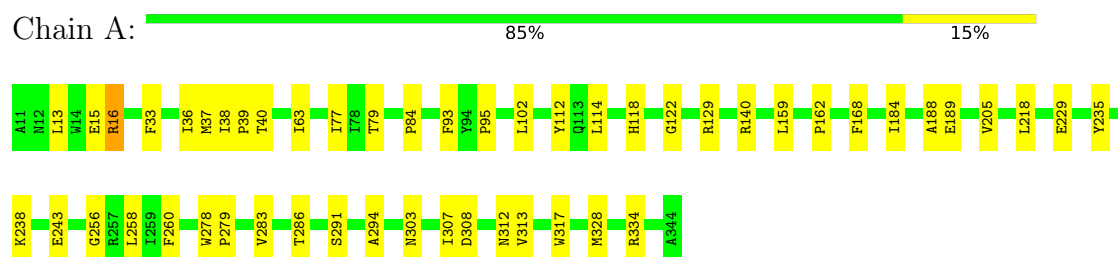
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	b	190	Total 190	O 190	0	0
36	c	154	Total 154	O 154	0	0
36	d	127	Total 127	O 127	0	0
36	e	20	Total 20	O 20	0	0
36	f	6	Total 6	O 6	0	0
36	h	17	Total 17	O 17	0	0
36	i	12	Total 12	O 12	0	0
36	j	7	Total 7	O 7	0	0
36	k	6	Total 6	O 6	0	0
36	l	11	Total 11	O 11	0	0
36	m	6	Total 6	O 6	0	0
36	o	117	Total 117	O 117	0	0
36	t	12	Total 12	O 12	0	0
36	u	50	Total 50	O 50	0	0
36	v	63	Total 63	O 63	0	0
36	y	4	Total 4	O 4	0	0
36	x	11	Total 11	O 11	0	0
36	z	1	Total 1	O 1	0	0
36	r	6	Total 6	O 6	0	0

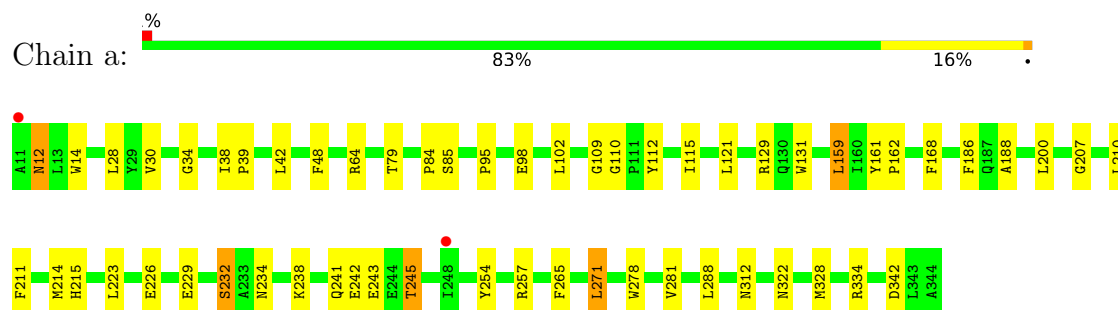
3 Residue-property plots

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.

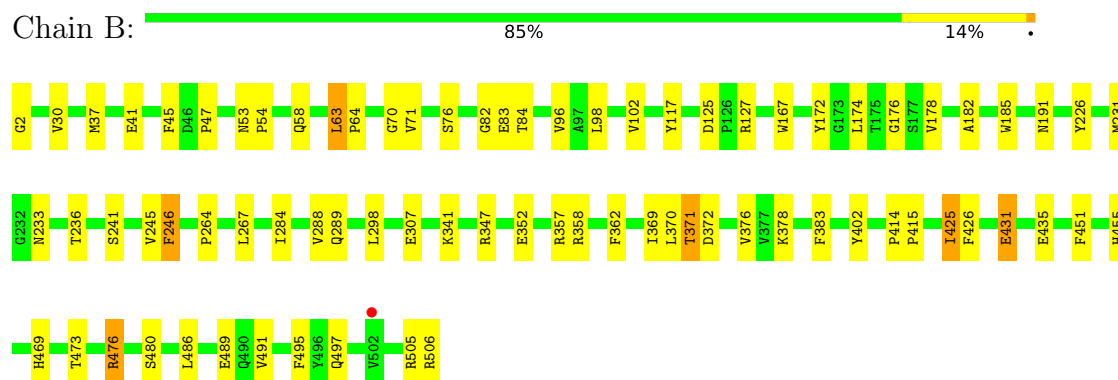
- Molecule 1: Photosystem II protein D1 1



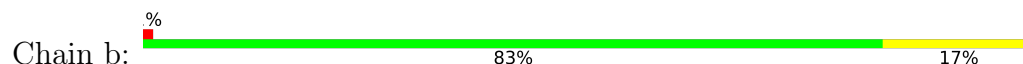
- Molecule 1: Photosystem II protein D1 1

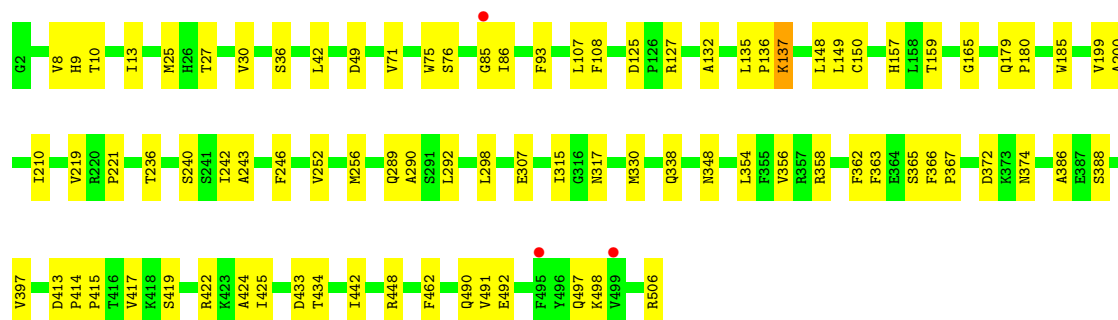


- Molecule 2: Photosystem II CP47 reaction center protein



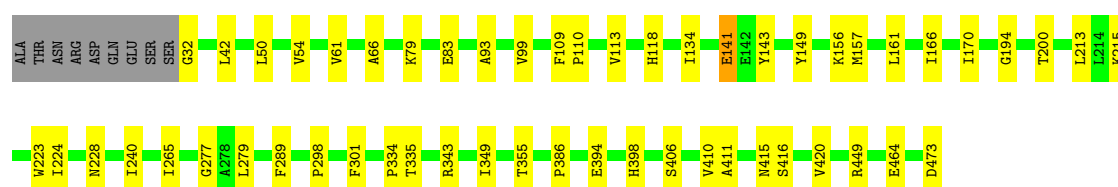
- Molecule 2: Photosystem II CP47 reaction center protein





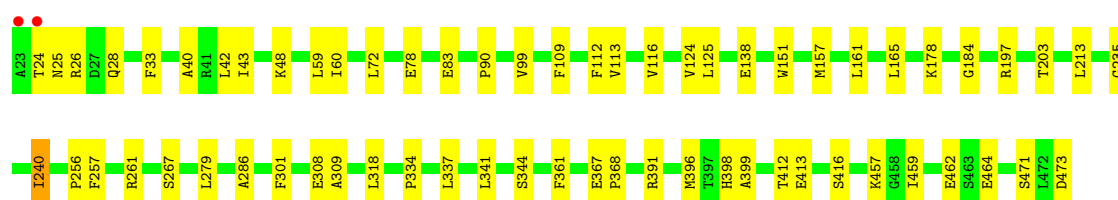
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 12%



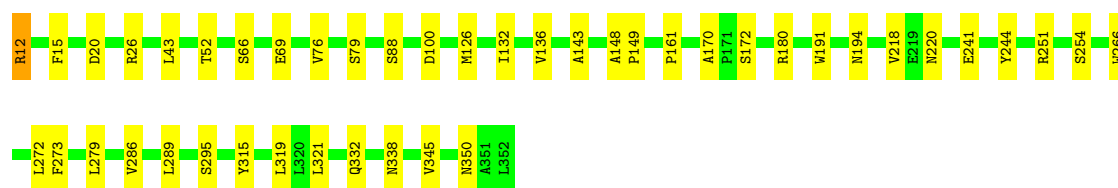
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 86% 14%



• Molecule 4: Photosystem II D2 protein

Chain D: 87% 13%



• Molecule 4: Photosystem II D2 protein

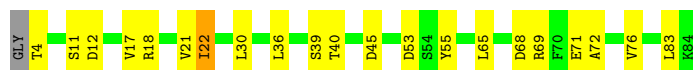
Chain d: 85% 15%





- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 73% 24% ..



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 61% 38% .



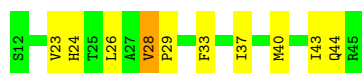
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 3% 85% 12% .



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 71% 26% .



- Molecule 7: Photosystem II reaction center protein H

Chain H: 85% 12% .



- Molecule 7: Photosystem II reaction center protein H

Chain h: 2% 82% 14% . .



- Molecule 8: Photosystem II reaction center protein I

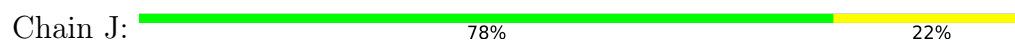
Chain I: 78% 17% 6%



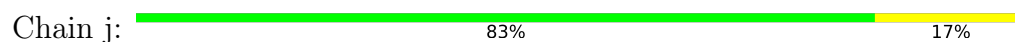
• Molecule 8: Photosystem II reaction center protein I



• Molecule 9: Photosystem II reaction center protein J



• Molecule 9: Photosystem II reaction center protein J



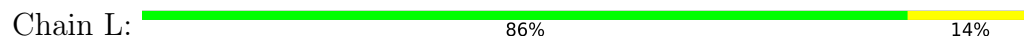
• Molecule 10: Photosystem II reaction center protein K



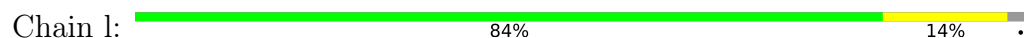
• Molecule 10: Photosystem II reaction center protein K



• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L





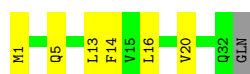
- Molecule 12: Photosystem II reaction center protein M

Chain M: 73% 24%



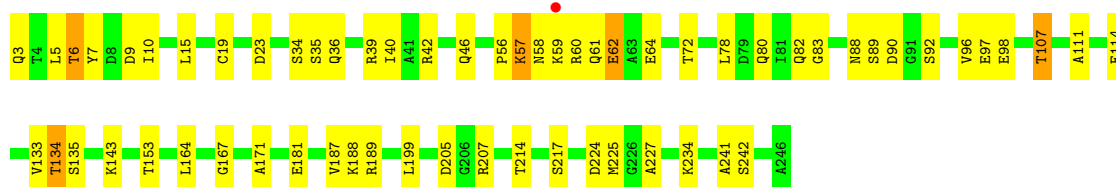
- Molecule 12: Photosystem II reaction center protein M

Chain m: 79% 18%



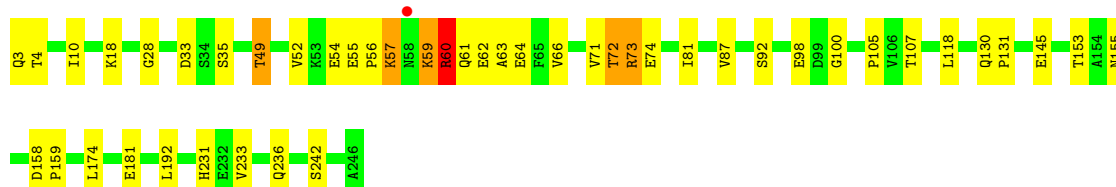
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 75% 23%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 81% 16%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 80% 17%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 87% 10%



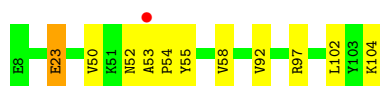
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 78% 21% .



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 89% 10% .



- Molecule 16: Cytochrome c-550

Chain V: 79% 18% .



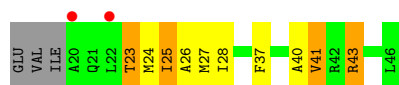
- Molecule 16: Cytochrome c-550

Chain v: 77% 23% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 7% 57% 20% 13% 10%



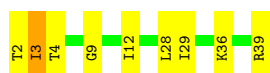
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 60% 30% 10%



- Molecule 18: Photosystem II reaction center X protein

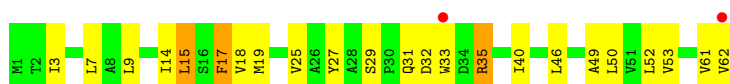
Chain X: 76% 21% .



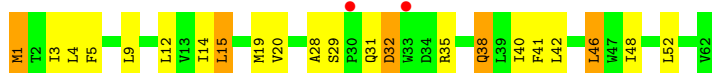
• Molecule 18: Photosystem II reaction center X protein



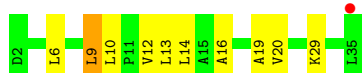
• Molecule 19: Photosystem II reaction center protein Z



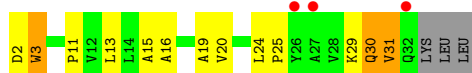
• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.69Å 222.53Å 308.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.85 – 2.20 30.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.85-2.20) 83.6 (30.85-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.20Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.193 , 0.264 0.194 , 0.265	Depositor DCC
R_{free} test set	3620 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	103673	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FME, BCT, BCR, DGD, CL, FE2, HEM, UNL, LHG, PHO, CLA, OEY, PL9, SQD, LMG, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/2707	0.76	0/3692
1	a	0.65	1/2704 (0.0%)	0.75	1/3688 (0.0%)
2	B	0.63	0/4160	0.71	0/5668
2	b	0.59	0/4118	0.69	0/5611
3	C	0.59	0/3530	0.67	0/4807
3	c	0.54	0/3610	0.69	0/4914
4	D	0.68	0/2812	0.74	0/3832
4	d	0.62	0/2821	0.72	0/3844
5	E	0.50	0/684	0.67	0/935
5	e	0.44	0/683	0.61	0/932
6	F	0.54	0/284	0.65	0/387
6	f	0.41	0/284	0.64	0/387
7	H	0.62	0/520	0.71	0/709
7	h	0.54	0/511	0.69	0/697
8	I	0.60	0/293	0.73	0/396
8	i	0.64	0/293	0.69	0/396
9	J	0.49	0/263	0.65	0/356
9	j	0.47	0/261	0.66	0/353
10	K	0.45	0/314	0.67	0/427
10	k	0.42	0/303	0.56	0/416
11	L	0.68	0/311	0.77	0/422
11	l	0.60	0/303	0.68	0/412
12	M	0.62	0/249	0.74	0/341
12	m	0.63	0/244	0.75	0/334
13	O	0.57	0/1914	0.69	0/2596
13	o	0.58	0/1905	0.72	0/2583
14	T	0.64	0/257	0.81	0/349
14	t	0.64	0/255	0.70	0/346
15	U	0.55	0/785	0.67	0/1064
15	u	0.55	0/785	0.70	0/1064
16	V	0.55	0/1085	0.63	0/1473
16	v	0.51	0/1085	0.67	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.44	0/197	0.68	0/264
17	y	0.36	0/219	0.49	0/294
18	X	0.53	0/284	0.68	0/384
18	x	0.43	0/284	0.58	0/384
19	Z	0.44	0/490	0.60	0/669
19	z	0.38	0/488	0.55	0/666
20	R	0.38	0/277	0.65	0/380
20	r	0.32	0/233	0.56	0/323
All	All	0.59	1/42805 (0.0%)	0.70	1/58268 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	u	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	110	GLY	CA-C	-5.54	1.47	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	110	GLY	O-C-N	-8.77	117.91	121.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	52	ASN	Peptide

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	2622	2508	2519	36	0
1	a	2619	2499	2510	37	0
2	B	4004	3845	3864	47	0
2	b	3978	3811	3836	46	0
3	C	3417	3335	3348	35	0
3	c	3494	3407	3420	37	0
4	D	2717	2613	2621	33	0
4	d	2723	2619	2627	34	0
5	E	662	647	648	13	0
5	e	664	647	648	18	0
6	F	275	281	282	3	0
6	f	275	281	282	8	0
7	H	507	523	523	5	0
7	h	498	518	518	8	0
8	I	296	311	311	3	0
8	i	296	311	311	6	0
9	J	257	268	268	6	0
9	j	255	261	261	3	0
10	K	302	318	318	13	0
10	k	293	305	305	9	0
11	L	304	316	316	4	0
11	l	296	304	304	2	0
12	M	256	269	269	4	0
12	m	251	267	267	3	0
13	O	1880	1850	1852	42	0
13	o	1874	1844	1846	28	0
14	T	258	261	261	3	0
14	t	256	256	256	3	0
15	U	774	772	773	10	0
15	u	774	772	773	7	0
16	V	1064	1070	1073	19	0
16	v	1064	1070	1073	19	0
17	Y	196	208	217	6	0
17	y	218	241	241	8	0
18	X	281	312	312	5	0
18	x	281	312	312	8	0
19	Z	479	509	516	11	0
19	z	477	509	509	12	0
20	R	271	298	298	4	0
20	r	227	234	224	10	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	2	0	0	0	0
23	A	184	192	192	3	0
23	B	1035	1139	1139	13	0
23	C	839	922	922	7	0
23	D	195	216	216	4	0
23	a	195	216	216	1	0
23	b	970	1067	1067	19	0
23	c	839	919	919	13	0
23	d	195	216	216	1	0
23	h	65	72	72	5	0
24	A	64	74	74	1	0
24	D	64	74	74	1	0
24	a	64	74	74	0	0
24	d	64	74	74	1	0
25	A	40	56	56	1	0
25	B	120	168	168	6	0
25	C	120	168	168	4	0
25	D	40	56	56	2	0
25	H	40	56	56	2	0
25	K	40	56	56	3	0
25	T	40	56	56	2	0
25	a	40	56	56	2	0
25	b	120	168	168	8	0
25	c	120	168	168	8	0
25	d	40	56	56	2	0
25	h	40	56	56	3	0
25	t	40	56	56	4	0
25	y	40	56	56	1	0
26	A	55	80	80	3	0
26	D	55	80	80	1	0
26	a	55	80	80	2	0
26	d	55	80	80	1	0
27	A	48	66	66	1	0
27	B	51	72	72	3	0
27	C	48	66	66	0	0
27	D	112	157	157	3	0
27	a	49	68	68	2	0
27	b	78	120	120	0	0
27	c	85	113	113	1	0
27	d	44	58	57	0	0
27	m	51	72	72	1	0
28	A	91	135	134	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	54	78	78	2	0
28	F	36	45	45	0	0
28	a	90	134	133	3	0
28	b	49	65	64	0	0
28	f	41	49	49	2	0
29	A	66	96	96	2	0
29	C	186	246	243	0	0
29	H	62	82	80	1	0
29	a	44	75	75	2	0
29	c	186	246	240	0	0
29	h	62	82	82	0	0
30	A	11	0	0	1	0
30	a	11	0	0	1	0
31	A	4	1	1	0	0
31	a	4	1	1	0	0
32	B	71	109	0	0	0
32	C	40	63	0	0	0
32	D	20	35	0	0	0
32	E	12	16	0	0	0
32	H	18	35	0	0	0
32	I	15	26	0	0	0
32	J	12	16	0	0	0
32	M	25	38	0	0	0
32	T	15	29	0	0	0
32	a	12	16	0	0	0
32	b	82	141	0	0	0
32	c	32	51	0	0	0
32	d	17	26	0	0	0
32	j	12	16	0	0	0
32	l	18	35	0	0	0
32	m	12	16	0	0	0
32	t	28	44	0	0	0
32	x	20	35	0	0	0
33	B	49	74	74	1	0
33	D	96	141	141	4	0
33	E	49	74	74	1	0
33	L	49	74	74	2	0
33	a	49	74	74	3	0
33	d	88	125	125	2	0
33	e	42	57	57	1	0
33	l	49	74	74	1	0
34	E	43	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	e	43	30	30	3	0
35	V	43	30	30	1	0
35	v	43	30	30	0	0
36	A	138	0	0	8	0
36	B	221	0	0	13	0
36	C	191	0	0	9	0
36	D	142	0	0	5	0
36	E	31	0	0	1	0
36	F	11	0	0	0	0
36	H	25	0	0	3	0
36	I	14	0	0	0	0
36	J	15	0	0	1	0
36	K	2	0	0	0	0
36	L	7	0	0	0	0
36	M	5	0	0	0	0
36	O	121	0	0	13	1
36	R	3	0	0	0	0
36	T	12	0	0	0	0
36	U	51	0	0	3	0
36	V	68	0	0	6	0
36	X	8	0	0	1	0
36	Y	5	0	0	0	0
36	Z	5	0	0	0	0
36	a	121	0	0	6	0
36	b	190	0	0	7	0
36	c	154	0	0	4	0
36	d	127	0	0	6	0
36	e	20	0	0	0	0
36	f	6	0	0	0	0
36	h	17	0	0	5	0
36	i	12	0	0	2	0
36	j	7	0	0	0	0
36	k	6	0	0	2	0
36	l	11	0	0	1	0
36	m	6	0	0	1	0
36	o	117	0	0	6	1
36	r	6	0	0	1	0
36	t	12	0	0	0	0
36	u	50	0	0	1	0
36	v	63	0	0	3	0
36	x	11	0	0	2	0
36	y	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	z	1	0	0	0	0
All	All	52197	51476	50844	648	1

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 6.

All (648) 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)
13:O:90:ASP:OD1	36:O:301:HOH:O	1.60	1.15
4:D:332:GLN:O	36:D:501:HOH:O	1.79	0.99
2:b:358:ARG:O	36:b:701:HOH:O	1.83	0.96
1:a:243:GLU:OE1	36:a:501:HOH:O	1.86	0.93
2:B:2:GLY:N	36:B:701:HOH:O	2.04	0.91
10:k:19:ASP:OD1	36:k:101:HOH:O	1.88	0.90
30:a:416:OEY:O6	30:a:416:OEY:O5	1.92	0.87
3:C:464:GLU:O	36:C:601:HOH:O	1.93	0.86
2:b:307:GLU:OE1	36:b:702:HOH:O	1.93	0.85
3:c:391[A]:ARG:NH1	36:c:601:HOH:O	2.08	0.85
3:C:194:GLY:N	36:C:602:HOH:O	2.09	0.84
3:C:156:LYS:NZ	36:C:603:HOH:O	2.11	0.84
4:d:241:GLU:OE2	36:d:501:HOH:O	1.95	0.83
7:H:56:ASP:OD1	18:X:2:THR:N	2.12	0.83
13:o:62:GLU:OE2	13:o:63:ALA:N	2.13	0.82
4:D:286:VAL:HG21	23:D:403:CLA:HED2	1.65	0.77
13:o:28:GLY:O	36:o:301:HOH:O	2.01	0.77
3:c:78:GLU:OE1	16:v:106:ASN:ND2	2.17	0.77
2:B:473:THR:O	2:B:476:ARG:NH1	2.18	0.76
23:A:405:CLA:H92	27:D:407:LMG:C25	2.15	0.76
13:O:88:ASN:ND2	13:O:92:SER:OG	2.19	0.76
9:J:36:LEU:O	36:J:201:HOH:O	2.04	0.74
33:D:408:LHG:O2	36:D:502:HOH:O	2.04	0.74
2:b:292:LEU:O	36:b:703:HOH:O	2.06	0.73
2:b:434:THR:N	36:b:705:HOH:O	2.22	0.72
5:e:61:ARG:NH2	16:v:125:ILE:O	2.22	0.72
5:E:17:VAL:HG23	9:J:7:ARG:HG3	1.73	0.71
2:B:58:GLN:OE1	36:B:702:HOH:O	2.07	0.71
25:b:620:BCR:C8	25:b:620:BCR:H331	2.20	0.70
2:B:341:LYS:NZ	36:B:703:HOH:O	2.12	0.70
16:v:103:LYS:NZ	36:v:302:HOH:O	2.25	0.70
8:i:14:PHE:CZ	8:i:18:LEU:HD11	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:701:HOH:O	11:L:11:GLU:OE2	2.10	0.69
5:E:45:ASP:OD2	36:E:201:HOH:O	2.11	0.69
19:z:1:MET:SD	19:z:1:MET:N	2.62	0.69
25:C:515:BCR:H331	25:C:515:BCR:C8	2.22	0.68
12:m:5:GLN:O	36:m:201:HOH:O	2.09	0.68
13:o:98:GLU:OE1	36:o:302:HOH:O	2.12	0.67
20:r:2:ASP:N	36:r:101:HOH:O	2.27	0.66
34:e:102:HEM:HHC	34:e:102:HEM:HBB2	1.76	0.66
3:C:194:GLY:O	36:C:602:HOH:O	2.14	0.66
34:E:102:HEM:HHD	34:E:102:HEM:HBC2	1.77	0.66
16:v:55:ARG:NH2	36:v:304:HOH:O	2.28	0.66
15:U:18:GLY:O	36:U:201:HOH:O	2.14	0.65
7:h:24:GLY:N	36:h:201:HOH:O	2.30	0.65
13:O:80:GLN:OE1	36:O:303:HOH:O	2.14	0.65
15:U:54:PRO:O	36:U:202:HOH:O	2.15	0.64
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.79	0.64
3:C:334:PRO:HA	13:O:153:THR:OG1	1.98	0.64
19:z:32:ASP:HB2	19:z:35:ARG:HB3	1.80	0.64
13:o:145:GLU:OE2	36:o:303:HOH:O	2.15	0.64
4:d:91:LEU:O	36:d:502:HOH:O	2.14	0.63
23:b:615:CLA:H141	23:b:615:CLA:H172	1.80	0.63
3:c:473:ASP:OXT	14:t:28:ARG:NH1	2.31	0.63
1:a:232:SER:OG	33:l:101:LHG:O5	2.16	0.63
20:r:29:LYS:O	20:r:31:VAL:N	2.31	0.63
3:c:40:ALA:O	3:c:43:ILE:HD12	1.98	0.63
13:O:56:PRO:O	13:O:58:ASN:N	2.30	0.63
18:X:2:THR:OG1	18:X:3:ILE:N	2.23	0.63
13:O:143:LYS:NZ	36:O:305:HOH:O	2.20	0.62
29:A:413:DGD:HD5	2:b:75:TRP:HB3	1.79	0.62
3:C:228:ASN:O	36:C:604:HOH:O	2.16	0.62
13:O:59:LYS:O	13:O:61:GLN:N	2.32	0.62
4:d:25:ASP:OD1	36:d:503:HOH:O	2.16	0.62
23:c:505:CLA:HBB1	23:c:505:CLA:HMB1	1.82	0.62
16:V:9:THR:O	36:V:301:HOH:O	2.16	0.61
23:b:604:CLA:H2	23:b:606:CLA:H91	1.82	0.61
6:f:40:MET:HA	6:f:43:ILE:HD13	1.82	0.61
1:a:334:ARG:NH2	36:a:505:HOH:O	2.32	0.61
1:a:342:ASP:O	36:a:502:HOH:O	2.16	0.61
3:c:151:TRP:HA	3:c:157:MET:HE3	1.81	0.61
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.83	0.61
33:D:408:LHG:O1	33:L:101:LHG:O4	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.82	0.61
25:C:520:BCR:H372	10:K:32:PHE:CD1	2.36	0.61
25:c:515:BCR:C8	25:c:515:BCR:H331	2.31	0.61
16:V:87:GLU:OE1	16:V:96:ARG:NH1	2.34	0.61
25:b:619:BCR:H331	25:b:619:BCR:C8	2.31	0.60
16:v:3:LEU:HD23	16:v:23:GLU:HG3	1.84	0.60
5:E:17:VAL:O	5:E:21:VAL:HG23	2.01	0.60
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.83	0.60
13:O:187:VAL:O	13:O:189:ARG:NH1	2.34	0.60
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.83	0.60
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.83	0.60
20:R:9:LEU:O	20:R:12:VAL:HG22	2.02	0.60
3:C:93:ALA:HB1	3:C:99:VAL:HG11	1.85	0.59
25:C:515:BCR:H331	25:C:515:BCR:HC8	1.84	0.59
13:O:111:ALA:O	36:O:304:HOH:O	2.17	0.59
4:d:126:MET:HE3	4:d:143:ALA:O	2.03	0.59
13:o:56:PRO:HD3	13:o:63:ALA:HB2	1.85	0.59
15:u:104:LYS:HE3	16:v:45:ILE:HG22	1.84	0.59
16:V:106:ASN:OD1	16:V:106:ASN:N	2.35	0.59
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.02	0.58
2:b:30:VAL:HG12	23:b:606:CLA:HHD	1.85	0.58
4:d:246:MET:HE3	4:d:264:LYS:CG	2.33	0.58
25:c:514:BCR:H382	25:c:514:BCR:H23C	1.85	0.58
3:c:257:PHE:O	3:c:261:ARG:HG3	2.04	0.57
15:u:50:VAL:O	15:u:53:ALA:HB2	2.04	0.57
2:b:221:PRO:HB3	23:b:610:CLA:O1D	2.05	0.57
25:t:101:BCR:HC8	25:t:101:BCR:H311	1.87	0.57
3:C:473:ASP:OD2	14:T:24:ARG:HD3	2.04	0.57
13:O:181:GLU:N	13:O:181:GLU:OE1	2.38	0.57
17:Y:25:ILE:O	17:Y:28:ILE:N	2.32	0.57
6:f:26:LEU:O	6:f:29:PRO:HD2	2.03	0.57
29:H:102:DGD:O2D	36:H:201:HOH:O	2.17	0.56
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.36	0.56
23:b:615:CLA:H141	23:b:615:CLA:C17	2.35	0.56
16:V:57:GLU:OE2	36:V:302:HOH:O	2.18	0.56
2:B:63:LEU:N	2:B:64:PRO:HD2	2.21	0.56
3:C:406:SER:HA	3:C:420:VAL:HG23	1.86	0.56
3:c:178:LYS:NZ	3:c:184:GLY:O	2.39	0.56
1:A:283:VAL:HA	1:A:286:THR:HG22	1.87	0.56
2:B:37:MET:O	2:B:41:GLU:HG3	2.04	0.55
3:c:413:GLU:OE2	36:c:603:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:SER:O	2:B:245:VAL:HG23	2.06	0.55
2:B:506:ARG:HD3	36:B:706:HOH:O	2.05	0.55
25:t:101:BCR:H23C	25:t:101:BCR:H382	1.88	0.55
15:u:53:ALA:O	15:u:55:TYR:CD2	2.59	0.55
1:a:234:ASN:ND2	33:a:410:LHG:O1	2.40	0.55
23:D:402:CLA:HBB1	23:D:402:CLA:HMB3	1.89	0.55
3:c:116:VAL:HG13	25:c:521:BCR:H332	1.87	0.55
4:D:254:SER:OG	14:T:24:ARG:NH2	2.39	0.55
13:o:57:LYS:O	13:o:60:ARG:N	2.39	0.54
25:t:101:BCR:HC8	25:t:101:BCR:H321	1.89	0.54
16:V:28:GLU:OE2	16:V:31:ARG:NH2	2.39	0.54
2:B:45:PHE:CE2	2:B:47:PRO:HB3	2.43	0.54
2:B:476:ARG:HD3	36:B:806:HOH:O	2.07	0.54
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.43	0.54
13:O:225:MET:HE1	36:O:308:HOH:O	2.08	0.54
3:C:79:LYS:NZ	36:C:614:HOH:O	2.41	0.53
2:b:36:SER:OG	25:b:619:BCR:H362	2.08	0.53
19:z:32:ASP:OD1	19:z:32:ASP:N	2.42	0.53
2:B:451:PHE:CE1	2:B:455:HIS:CE1	2.96	0.53
8:i:5:LYS:NZ	36:i:101:HOH:O	2.40	0.53
16:v:10:VAL:HG23	16:v:69:ILE:HD11	1.89	0.53
19:Z:32:ASP:OD1	19:Z:35:ARG:N	2.41	0.53
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.91	0.53
20:R:16:ALA:O	20:R:20:VAL:HG23	2.09	0.53
25:H:101:BCR:H331	25:H:101:BCR:C8	2.38	0.53
5:e:68:ASP:O	5:e:72:ALA:HB2	2.08	0.53
7:h:24:GLY:CA	36:h:201:HOH:O	2.57	0.53
1:a:102:LEU:HD12	29:a:413:DGD:HG2	1.91	0.53
2:B:370:LEU:N	2:B:370:LEU:HD12	2.24	0.52
10:K:43:VAL:HG21	10:K:46[A]:ARG:CZ	2.39	0.52
4:d:267:LEU:C	4:d:267:LEU:HD23	2.34	0.52
34:e:102:HEM:HMC2	34:e:102:HEM:HBC2	1.91	0.52
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.45	0.52
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.45	0.52
2:b:27:THR:HG22	2:b:107:LEU:HD13	1.91	0.52
6:f:43:ILE:HD12	6:f:43:ILE:N	2.23	0.52
6:F:45:ARG:NH1	9:J:40:LEU:OXT	2.38	0.52
1:A:184:ILE:HG21	4:D:321:LEU:HD13	1.92	0.52
5:e:8:ARG:NH2	5:e:12:ASP:OD2	2.42	0.52
2:B:30:VAL:HG12	23:B:605:CLA:HMD3	1.91	0.52
5:E:36:LEU:O	5:E:40:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:133:VAL:C	13:O:134:THR:HG23	2.35	0.52
23:b:616:CLA:C1B	23:b:616:CLA:H191	2.40	0.51
25:d:405:BCR:H331	25:d:405:BCR:C8	2.39	0.51
3:C:298:PRO:HG2	3:C:301:PHE:CD2	2.46	0.51
8:I:35:LYS:HD2	8:I:35:LYS:N	2.25	0.51
5:e:33:ALA:HB2	20:r:11:PRO:HG2	1.92	0.51
25:y:101:BCR:H23C	25:y:101:BCR:H382	1.91	0.51
33:B:622:LHG:H222	12:M:18:PRO:HG3	1.92	0.51
9:J:19:MET:O	9:J:23:VAL:HG23	2.10	0.51
33:d:407:LHG:H321	14:t:21:ILE:HD11	1.92	0.51
1:A:16:ARG:CZ	36:A:525:HOH:O	2.59	0.51
23:B:607:CLA:HBB1	23:B:607:CLA:HMB3	1.92	0.51
15:U:69:GLU:OE1	15:U:72:LYS:NZ	2.42	0.51
1:a:64:ARG:NH1	13:o:105:PRO:O	2.44	0.51
4:d:194:ASN:HA	4:d:295:SER:OG	2.10	0.51
6:f:29:PRO:O	6:f:33:PHE:HD2	1.94	0.51
1:A:303:ASN:O	3:C:415:ASN:ND2	2.40	0.50
28:A:412:SQD:H312	25:b:620:BCR:H363	1.92	0.50
3:C:83:GLU:OE1	16:V:103:LYS:NZ	2.44	0.50
29:A:413:DGD:O2D	36:A:501:HOH:O	2.20	0.50
2:B:264:PRO:HG2	2:B:267:LEU:HD12	1.93	0.50
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.46	0.50
25:t:101:BCR:H311	25:t:101:BCR:C8	2.40	0.50
5:E:53:ASP:O	16:V:1:ALA:N	2.45	0.50
19:z:48:ILE:O	19:z:52:LEU:HG	2.12	0.50
1:A:184:ILE:CG2	4:D:321:LEU:HD13	2.41	0.50
1:A:334:ARG:NH2	36:A:514:HOH:O	2.43	0.50
2:B:357:ARG:NH2	36:B:707:HOH:O	2.27	0.50
3:C:50:LEU:O	3:C:54:VAL:HG23	2.12	0.50
26:D:406:PL9:H412	11:L:29:LEU:HD23	1.92	0.50
16:v:110:LYS:O	16:v:113:VAL:HG22	2.12	0.50
2:B:185:TRP:HB3	23:B:601:CLA:HMA3	1.93	0.50
3:C:394:GLU:O	3:C:398:HIS:ND1	2.39	0.50
13:O:57:LYS:HE2	2:b:338:GLN:O	2.10	0.50
13:O:189:ARG:NE	36:O:302:HOH:O	2.14	0.50
19:z:38:GLN:O	19:z:42:LEU:HD13	2.12	0.50
1:A:40:THR:O	1:A:118:HIS:HB3	2.11	0.50
3:C:143:TYR:CE1	23:C:513:CLA:HED3	2.47	0.50
13:O:36:GLN:OE1	13:O:36:GLN:HA	2.11	0.50
11:l:20:GLY:O	11:l:24:ILE:HG12	2.12	0.50
15:u:23:GLU:OE2	36:u:201:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:38:VAL:CG2	25:K:101:BCR:H21C	2.41	0.50
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.92	0.50
5:e:22:ILE:O	5:e:26:THR:HG23	2.12	0.50
12:M:17:VAL:HB	12:M:18:PRO:HD3	1.92	0.49
6:f:37:ILE:HG22	9:j:28:PHE:CE1	2.46	0.49
2:b:413:ASP:O	2:b:417:VAL:HG23	2.12	0.49
23:b:617:CLA:HED2	23:b:617:CLA:H2A	1.94	0.49
13:o:18:LYS:NZ	13:o:74:GLU:OE1	2.45	0.49
2:b:137:LYS:HE3	36:b:719:HOH:O	2.12	0.49
1:a:159:LEU:C	1:a:162:PRO:HD2	2.37	0.49
1:A:308:ASP:OD1	1:A:312:ASN:N	2.42	0.49
13:O:92:SER:N	36:O:301:HOH:O	2.37	0.49
25:a:408:BCR:C8	25:a:408:BCR:H331	2.43	0.49
2:b:150:CYS:HB2	23:b:604:CLA:CMC	2.42	0.49
9:j:18:GLY:O	9:j:21:VAL:HG22	2.12	0.49
6:F:27:ALA:O	6:F:28:VAL:C	2.56	0.49
13:O:189:ARG:NH2	36:O:302:HOH:O	2.37	0.49
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.94	0.49
19:Z:49:ALA:O	19:Z:53:VAL:HG23	2.13	0.49
33:a:410:LHG:O4	4:d:141:TYR:OH	2.28	0.49
16:v:41:HIS:HA	16:v:45:ILE:O	2.13	0.49
17:y:23:THR:O	17:y:27:MET:HE2	2.13	0.49
1:A:218:LEU:HD12	26:A:409:PL9:C3	2.43	0.49
1:A:129:ARG:NH1	36:A:509:HOH:O	2.42	0.49
23:b:614:CLA:H142	27:m:101:LMG:C25	2.43	0.49
11:l:14:ARG:N	36:l:201:HOH:O	2.36	0.49
36:A:552:HOH:O	4:D:350:ASN:HB2	2.13	0.48
18:X:4:THR:HB	36:X:107:HOH:O	2.12	0.48
4:D:194:ASN:HA	4:D:295:SER:OG	2.13	0.48
25:T:101:BCR:H19C	25:b:619:BCR:H363	1.94	0.48
15:U:58:VAL:O	15:U:61:VAL:HG22	2.12	0.48
3:c:26:ARG:O	10:k:46:ARG:HD2	2.13	0.48
8:i:14:PHE:CE2	8:i:18:LEU:HD11	2.48	0.48
23:c:506:CLA:O1A	23:c:506:CLA:C2	2.61	0.48
13:O:88:ASN:HB2	36:O:301:HOH:O	2.13	0.48
13:o:55:GLU:OE1	13:o:231:HIS:CD2	2.67	0.48
13:O:224:ASP:HB3	13:O:227:ALA:HB3	1.95	0.48
19:Z:32:ASP:OD2	19:Z:35:ARG:NE	2.32	0.48
2:b:498:LYS:HD2	4:d:20:ASP:HA	1.96	0.48
1:a:95:PRO:HD2	1:a:98:GLU:CG	2.44	0.48
5:e:4:THR:HG23	5:e:4:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:24:HIS:O	6:f:28:VAL:HG13	2.14	0.48
13:o:59:LYS:C	13:o:60:ARG:HG3	2.39	0.48
13:O:107:THR:HG22	36:O:346:HOH:O	2.14	0.48
2:b:185:TRP:HB3	23:h:101:CLA:HMA3	1.96	0.48
3:c:318:LEU:C	3:c:318:LEU:HD23	2.38	0.48
23:c:509:CLA:H141	23:c:512:CLA:HMD3	1.94	0.48
5:e:13:ILE:HG22	5:e:19:TYR:CD2	2.49	0.48
16:v:26:TYR:OH	16:v:122:GLU:OE2	2.30	0.48
4:d:170:ALA:HB1	4:d:171:PRO:CD	2.44	0.48
13:o:59:LYS:O	13:o:60:ARG:NH1	2.46	0.48
18:x:29:ILE:HG23	36:x:208:HOH:O	2.13	0.48
25:D:405:BCR:H331	25:D:405:BCR:C8	2.44	0.47
10:K:15:TYR:O	10:K:17:ILE:N	2.47	0.47
3:c:90:PRO:HB3	3:c:301:PHE:HB3	1.95	0.47
4:d:217:THR:HG21	26:d:406:PL9:C1	2.44	0.47
10:K:38:VAL:HG23	25:K:101:BCR:H21C	1.95	0.47
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.94	0.47
2:B:497:GLN:OE1	36:B:704:HOH:O	2.20	0.47
4:D:79:SER:HA	4:D:172:SER:HB3	1.95	0.47
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.96	0.47
1:a:312:ASN:OD1	36:a:503:HOH:O	2.20	0.47
2:b:414:PRO:N	2:b:415:PRO:HD2	2.29	0.47
19:z:14:ILE:O	19:z:15:LEU:HB2	2.15	0.47
13:O:58:ASN:HB3	36:b:702:HOH:O	2.13	0.47
2:b:413:ASP:OD2	2:b:413:ASP:N	2.44	0.47
3:c:334:PRO:HA	13:o:153:THR:OG1	2.14	0.47
13:o:33:ASP:OD1	13:o:33:ASP:C	2.58	0.47
2:B:369:ILE:C	2:B:370:LEU:HD12	2.39	0.47
4:D:272:LEU:C	4:D:272:LEU:HD23	2.39	0.47
3:c:203:THR:O	3:c:235:GLY:HA3	2.15	0.47
16:v:122:GLU:N	16:v:123:PRO:HD2	2.28	0.47
19:z:14:ILE:O	19:z:14:ILE:HG22	2.14	0.47
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.50	0.47
15:U:45:LEU:HD21	15:U:71:GLN:HG2	1.96	0.47
26:a:409:PL9:H261	33:e:101:LHG:H201	1.96	0.47
2:b:71:VAL:HG23	23:b:607:CLA:HMA2	1.96	0.47
23:b:604:CLA:HMD3	23:b:607:CLA:HBB1	1.96	0.47
1:A:33:PHE:HE1	23:C:505:CLA:H92	1.78	0.47
2:B:102:VAL:HA	25:B:618:BCR:C40	2.44	0.47
15:U:39:ARG:NH2	16:V:60:ALA:O	2.46	0.47
16:V:102:PRO:HA	16:V:105:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:386:ALA:HB3	15:u:102:LEU:HD22	1.94	0.47
7:h:3:ARG:NH2	36:h:204:HOH:O	2.47	0.47
10:k:26:PRO:O	10:k:29:PRO:HD2	2.15	0.47
17:y:19:ILE:O	17:y:23:THR:HG22	2.14	0.47
7:H:50:ASN:OD1	7:H:52:THR:CG2	2.63	0.47
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.96	0.47
2:b:442:ILE:HD11	13:o:174:LEU:HD23	1.97	0.47
36:A:611:HOH:O	3:C:410:VAL:HA	2.14	0.47
23:b:615:CLA:C2B	25:b:618:BCR:H373	2.44	0.47
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.97	0.46
5:e:17:VAL:O	5:e:18:ARG:C	2.57	0.46
10:k:18:PHE:CE2	19:z:9:LEU:HD23	2.51	0.46
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.49	0.46
2:B:284:ILE:O	2:B:288:VAL:HG23	2.16	0.46
13:O:98:GLU:CG	36:O:335:HOH:O	2.64	0.46
1:a:215:HIS:HA	26:a:409:PL9:O1	2.15	0.46
13:O:92:SER:CB	36:O:301:HOH:O	2.58	0.46
16:V:77:LYS:NZ	36:V:307:HOH:O	2.49	0.46
13:o:71:VAL:HG22	13:o:107:THR:O	2.14	0.46
13:o:72:THR:O	13:o:73:ARG:HB2	2.14	0.46
23:A:405:CLA:C9	27:D:407:LMG:C25	2.89	0.46
3:C:32:GLY:N	36:C:625:HOH:O	2.48	0.46
4:D:26:ARG:NH1	36:D:509:HOH:O	2.46	0.46
4:D:286:VAL:CG2	23:D:403:CLA:HED2	2.41	0.46
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.98	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
12:M:11:THR:O	12:M:15:VAL:HG23	2.15	0.46
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.98	0.46
2:B:357:ARG:NE	36:B:707:HOH:O	2.39	0.46
23:B:601:CLA:H92	25:H:101:BCR:H19C	1.97	0.46
17:y:18:VAL:O	17:y:22:LEU:HD22	2.16	0.46
1:A:159:LEU:C	1:A:162:PRO:HD2	2.40	0.46
1:a:84:PRO:HA	1:a:112:TYR:CG	2.51	0.46
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.97	0.46
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.50	0.46
23:h:101:CLA:C9	25:h:102:BCR:H23C	2.46	0.46
17:y:27:MET:O	17:y:30:ILE:HG22	2.16	0.46
13:o:3:GLN:NE2	36:o:315:HOH:O	2.49	0.46
16:v:23:GLU:O	16:v:27:LEU:HG	2.16	0.46
26:A:409:PL9:H361	6:F:25:THR:HG21	1.98	0.46
8:I:4:LEU:HD22	8:I:8:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:367:GLU:N	3:c:368:PRO:CD	2.79	0.46
18:x:3:ILE:N	18:x:3:ILE:HD12	2.30	0.46
1:A:189:GLU:CD	30:A:414:OEY:O6	2.58	0.46
15:U:24:LYS:HE2	36:U:204:HOH:O	2.14	0.46
15:U:68:THR:O	15:U:71:GLN:N	2.49	0.46
19:Z:14:ILE:O	19:Z:18:VAL:HG23	2.16	0.46
2:b:157:HIS:C	2:b:157:HIS:CD2	2.94	0.46
4:d:24:ARG:HH22	18:x:35:ASP:CG	2.25	0.45
5:e:14:ILE:O	5:e:20:TRP:NE1	2.46	0.45
36:A:618:HOH:O	3:C:411:ALA:HA	2.15	0.45
13:O:39:ARG:HH21	13:O:82:GLN:NE2	2.15	0.45
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.73	0.45
23:h:101:CLA:CHA	23:h:101:CLA:HBA2	2.45	0.45
17:y:41:VAL:C	17:y:43:ARG:H	2.24	0.45
33:D:408:LHG:HC62	11:L:15:THR:HG23	1.99	0.45
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.52	0.45
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.51	0.45
5:e:68:ASP:OD1	5:e:71:GLU:HG2	2.16	0.45
16:v:77:LYS:O	16:v:96:ARG:HB2	2.16	0.45
2:B:172:TYR:O	2:B:174:LEU:HG	2.17	0.45
25:B:617:BCR:H24C	25:B:617:BCR:H371	1.82	0.45
3:C:61:VAL:HG12	3:C:118:HIS:O	2.16	0.45
4:D:20:ASP:OD2	18:X:39:ARG:NH2	2.46	0.45
23:D:403:CLA:HBC3	23:D:403:CLA:HHD	1.98	0.45
13:O:171:ALA:C	36:O:316:HOH:O	2.60	0.45
18:X:9:GLY:HA2	18:X:12:ILE:HD12	1.99	0.45
16:v:100:ILE:C	16:v:102:PRO:HD3	2.42	0.45
3:C:109:PHE:CE2	3:C:113:VAL:CG2	2.99	0.45
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.52	0.45
4:d:330:ALA:N	4:d:331:PRO:CD	2.80	0.45
20:r:3:TRP:CD1	20:r:3:TRP:C	2.94	0.45
13:O:6:THR:HG22	13:O:9:ASP:CG	2.41	0.45
1:a:207:GLY:O	1:a:211:PHE:CD2	2.70	0.45
2:b:433:ASP:OD1	2:b:433:ASP:C	2.60	0.45
5:e:74:GLN:O	5:e:78:THR:HG23	2.16	0.45
13:o:52:VAL:O	13:o:66:VAL:HG22	2.16	0.45
16:v:17:LYS:NZ	36:v:312:HOH:O	2.50	0.45
2:B:167:TRP:CZ2	2:B:176:GLY:HA3	2.52	0.45
3:C:215:LYS:NZ	36:C:623:HOH:O	2.47	0.45
4:D:218:VAL:HG13	4:D:244:TYR:CD2	2.51	0.45
8:I:2:GLU:O	8:I:6:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:19:ASP:N	10:K:20:PRO:HD2	2.32	0.45
16:V:3:LEU:HD23	16:V:3:LEU:HA	1.87	0.45
2:b:356:VAL:HG21	2:b:424:ALA:HB3	1.99	0.45
2:B:191:ASN:OD1	2:B:191:ASN:C	2.60	0.45
2:B:376:VAL:HG12	2:B:378:LYS:HD2	1.98	0.45
3:C:279:LEU:CD1	23:C:509:CLA:HED2	2.46	0.45
10:K:28:ILE:N	10:K:29:PRO:CD	2.79	0.45
29:a:413:DGD:O1B	29:a:413:DGD:O1G	2.35	0.45
3:c:116:VAL:CG1	25:c:521:BCR:H332	2.47	0.45
5:E:68:ASP:O	5:E:72:ALA:HB2	2.16	0.45
3:c:286:ALA:HB2	23:c:502:CLA:HMD1	1.98	0.45
3:c:309:ALA:HB1	3:c:399:ALA:HB2	1.99	0.45
5:e:22:ILE:HG23	20:r:19:ALA:HB2	1.99	0.45
18:x:39:ARG:C	36:x:209:HOH:O	2.59	0.45
2:B:469:HIS:CE1	23:B:611:CLA:NA	2.85	0.45
2:B:506:ARG:NH1	36:B:706:HOH:O	2.27	0.45
13:O:83:GLY:HA2	13:O:98:GLU:HG3	1.99	0.45
3:c:60:ILE:HG22	23:c:503:CLA:HHD	1.99	0.45
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.98	0.45
2:B:53:ASN:N	2:B:54:PRO:CD	2.80	0.44
2:B:233:ASN:O	2:B:236:THR:HG22	2.17	0.44
1:a:242:GLU:CD	1:a:242:GLU:H	2.25	0.44
4:D:332:GLN:NE2	36:D:504:HOH:O	2.35	0.44
1:a:214:MET:SD	24:d:401:PHO:CAD	3.05	0.44
2:b:366:PHE:CG	2:b:367:PRO:HD2	2.52	0.44
2:b:165:GLY:HA3	2:b:179:GLN:O	2.18	0.44
2:B:451:PHE:CD2	2:B:451:PHE:C	2.95	0.44
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.99	0.44
5:E:22[A]:ILE:HD11	34:E:102:HEM:CHB	2.48	0.44
5:E:36:LEU:HA	5:E:39:SER:OG	2.17	0.44
7:H:63:LYS:NZ	36:H:203:HOH:O	2.38	0.44
10:K:17:ILE:N	10:K:17:ILE:HD12	2.33	0.44
16:V:41:HIS:HA	16:V:45:ILE:O	2.17	0.44
25:c:521:BCR:H20C	25:c:521:BCR:H361	1.85	0.44
4:d:320:LEU:HD11	13:o:159:PRO:O	2.16	0.44
7:h:12:ARG:NH2	7:h:15:ASN:O	2.48	0.44
1:a:281:VAL:HG11	28:a:411:SQD:H181	2.00	0.44
33:a:410:LHG:H222	23:b:614:CLA:H203	1.99	0.44
2:b:422:ARG:O	2:b:425:ILE:HG12	2.18	0.44
10:k:40:GLN:HA	10:k:43:VAL:HG22	1.99	0.44
5:E:22[A]:ILE:HD12	20:R:19:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:12:ASN:OD1	1:a:12:ASN:C	2.60	0.44
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.00	0.44
1:A:218:LEU:HD12	26:A:409:PL9:C4	2.48	0.44
27:B:620:LMG:HC71	27:B:620:LMG:O9	2.18	0.44
13:O:5:LEU:HD13	13:O:10:ILE:HD11	2.00	0.44
36:a:567:HOH:O	16:v:1:ALA:CB	2.66	0.44
1:A:37:MET:HG3	1:A:122:GLY:O	2.17	0.44
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.99	0.44
4:D:266:TRP:CD1	33:D:408:LHG:HC31	2.52	0.44
19:Z:27:TYR:HE2	19:Z:33:TRP:CH2	2.35	0.44
1:a:64:ARG:HD2	36:o:322:HOH:O	2.17	0.44
1:a:161:TYR:CE1	1:a:186:PHE:CE2	3.06	0.44
23:c:512:CLA:H92	23:c:512:CLA:H61	1.90	0.44
23:h:101:CLA:H101	23:h:101:CLA:H142	2.00	0.44
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.48	0.44
3:C:343:ARG:HG2	3:C:349:ILE:HD13	2.00	0.44
10:K:24:VAL:O	10:K:24:VAL:CG1	2.65	0.44
2:b:135:LEU:N	2:b:136:PRO:CD	2.81	0.44
2:b:242:ILE:HG23	2:b:462:PHE:HD1	1.82	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.43
13:O:5:LEU:CD1	13:O:10:ILE:HD11	2.47	0.43
13:O:10:ILE:HD12	13:O:15:LEU:HD12	1.99	0.43
2:b:363:PHE:HB3	2:b:365:SER:O	2.19	0.43
3:c:112:PHE:O	3:c:116:VAL:HG23	2.18	0.43
2:B:341:LYS:HE3	2:B:431:GLU:HB2	1.99	0.43
7:H:9:ASP:OD2	36:H:202:HOH:O	2.21	0.43
2:B:371:THR:HG23	2:B:372:ASP:O	2.18	0.43
5:E:18:ARG:O	5:E:22[A]:ILE:HG22	2.19	0.43
1:a:322:ASN:OD1	3:c:412:THR:HA	2.18	0.43
3:c:459:ILE:HG21	3:c:464:GLU:HG3	2.00	0.43
4:d:71:CYS:HB2	4:d:76:VAL:HG12	1.99	0.43
2:B:182:ALA:HB3	36:B:780:HOH:O	2.17	0.43
17:Y:25:ILE:O	17:Y:27:MET:N	2.51	0.43
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.18	0.43
23:c:508:CLA:HMD3	33:d:408:LHG:H102	2.00	0.43
4:d:346:LEU:HD23	4:d:346:LEU:HA	1.85	0.43
28:f:101:SQD:H312	18:x:27:VAL:HG11	2.00	0.43
1:a:12:ASN:OD1	1:a:14:TRP:N	2.51	0.43
4:d:62:GLY:O	4:d:63:LEU:HD23	2.18	0.43
7:h:3:ARG:HB2	7:h:3:ARG:NH1	2.33	0.43
10:k:25:LEU:N	10:k:26:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ASP:OD2	2:B:125:ASP:C	2.61	0.43
2:B:425:ILE:HD11	2:B:426:PHE:CE2	2.53	0.43
23:B:601:CLA:H62	23:B:601:CLA:H93	1.81	0.43
25:B:617:BCR:H383	28:B:623:SQD:H131	2.00	0.43
15:U:16:LYS:HE3	15:U:85:THR:OG1	2.18	0.43
2:b:317:ASN:HA	2:b:330:MET:HE1	2.01	0.43
4:d:79:SER:HA	4:d:172:SER:HB3	2.00	0.43
4:d:246:MET:HE3	4:d:264:LYS:HG2	2.00	0.43
5:e:5:THR:OG1	5:e:7:GLU:OE1	2.33	0.43
12:m:16:LEU:O	12:m:20:VAL:HG23	2.19	0.43
27:a:414:LMG:HC3	36:i:101:HOH:O	2.19	0.43
3:c:59:LEU:HD21	10:k:32:PHE:CD1	2.54	0.43
7:h:3:ARG:CZ	36:h:204:HOH:O	2.67	0.43
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.83	0.43
1:a:254:TYR:OH	4:d:129:GLN:HB3	2.19	0.43
4:d:13:GLY:HA3	36:d:530:HOH:O	2.19	0.43
20:r:16:ALA:O	20:r:20:VAL:N	2.49	0.43
24:A:406:PHO:H141	24:A:406:PHO:H162	1.80	0.43
1:a:85:SER:HA	1:a:109:GLY:HA3	2.01	0.43
3:c:184:GLY:HA3	3:c:197:ARG:O	2.19	0.43
23:c:505:CLA:HBB1	23:c:505:CLA:CMB	2.48	0.43
19:z:1:MET:HB2	19:z:4:LEU:HD23	2.01	0.43
20:r:20:VAL:O	20:r:24:LEU:HB2	2.19	0.43
20:r:24:LEU:N	20:r:25:PRO:HD2	2.34	0.43
3:C:279:LEU:HD12	23:C:509:CLA:HED2	2.00	0.43
13:O:164:LEU:HB2	13:O:188:LYS:HB2	2.00	0.43
25:h:102:BCR:H15C	25:h:102:BCR:H351	1.89	0.43
8:i:7:THR:O	8:i:11:VAL:HG23	2.18	0.43
17:y:23:THR:HG23	17:y:24:MET:HE2	2.01	0.43
13:O:6:THR:O	13:O:9:ASP:N	2.51	0.42
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.84	0.42
13:o:52:VAL:HG22	13:o:233:VAL:HG22	2.01	0.42
20:r:29:LYS:O	20:r:30:GLN:C	2.60	0.42
2:B:117:TYR:HA	11:L:1:MET:HE1	2.01	0.42
4:D:69:GLU:HG2	5:E:55:TYR:OH	2.20	0.42
25:K:101:BCR:H322	19:Z:17:PHE:CE1	2.54	0.42
4:d:174:GLY:O	4:d:178:ILE:HG12	2.19	0.42
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.54	0.42
25:A:408:BCR:H24C	25:A:408:BCR:H371	1.76	0.42
3:C:277:GLY:C	23:C:505:CLA:HBC2	2.44	0.42
13:O:133:VAL:HG12	13:O:135:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:514:BCR:C23	25:c:514:BCR:C38	2.97	0.42
14:t:1:FME:O1	14:t:4:ILE:HG13	2.19	0.42
2:B:347:ARG:HA	2:B:352:GLU:O	2.19	0.42
23:B:606:CLA:C9	28:a:412:SQD:H223	2.49	0.42
13:O:83:GLY:HA3	13:O:96:VAL:O	2.20	0.42
19:Z:15:LEU:HD22	19:Z:19:MET:HG3	2.00	0.42
23:a:404:CLA:HBB1	23:a:404:CLA:HMB1	2.01	0.42
5:e:63:ILE:HD12	5:e:63:ILE:N	2.34	0.42
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.42
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.54	0.42
2:b:10:THR:HB	2:b:13:ILE:HD12	2.00	0.42
23:b:616:CLA:H2	23:b:617:CLA:HBB2	2.02	0.42
17:y:39:LEU:HD21	19:z:28:ALA:HB3	2.01	0.42
1:A:15:GLU:OE2	1:A:15:GLU:HA	2.19	0.42
1:A:307:ILE:HA	1:A:312:ASN:O	2.19	0.42
23:B:602:CLA:H161	23:B:602:CLA:H141	1.87	0.42
23:B:613:CLA:H143	27:B:620:LMG:H232	2.01	0.42
3:C:109:PHE:N	3:C:110:PRO:CD	2.83	0.42
4:D:100:ASP:OD1	4:D:100:ASP:C	2.62	0.42
12:M:9:ILE:HG13	12:M:13:LEU:HD22	2.01	0.42
16:V:119:ILE:O	16:V:123:PRO:HD2	2.19	0.42
19:Z:29:SER:HB3	19:Z:31:GLN:HG3	2.00	0.42
1:a:131:TRP:CH2	23:c:505:CLA:HAA2	2.55	0.42
27:a:414:LMG:O9	27:a:414:LMG:C9	2.66	0.42
8:i:31:ASN:HB2	8:i:32:PRO:HD2	2.01	0.42
10:k:46:ARG:O	36:k:102:HOH:O	2.21	0.42
1:A:235:TYR:O	1:A:238:LYS:NZ	2.53	0.42
1:A:258:LEU:HA	4:D:132:ILE:CD1	2.50	0.42
4:D:273:PHE:CE1	33:L:101:LHG:H121	2.54	0.42
4:D:319:LEU:HD21	36:D:606:HOH:O	2.19	0.42
3:c:83:GLU:OE2	3:c:398:HIS:NE2	2.50	0.42
4:d:40:CYS:HB3	4:d:117:HIS:O	2.19	0.42
4:d:272:LEU:C	4:d:272:LEU:HD23	2.45	0.42
13:o:54:GLU:HG2	13:o:64:GLU:O	2.19	0.42
19:z:42:LEU:O	19:z:46:LEU:HB2	2.20	0.42
9:J:15:THR:HG22	9:J:19:MET:CE	2.50	0.42
10:K:18:PHE:CE2	19:Z:9:LEU:HD21	2.55	0.42
2:b:159:THR:O	2:b:180:PRO:HB3	2.19	0.42
2:b:199:VAL:O	2:b:200:ALA:C	2.63	0.42
1:A:188:ALA:HB2	1:A:328:MET:CB	2.50	0.42
5:E:30:LEU:HD23	20:R:12:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:19:CYS:SG	13:O:46:GLN:HB2	2.60	0.42
13:O:205:ASP:OD1	13:O:207:ARG:NH1	2.52	0.42
16:V:92:HIS:CD2	35:V:201:HEC:ND	2.87	0.42
2:b:256:MET:O	2:b:448:ARG:HD3	2.20	0.42
25:C:515:BCR:HC8	25:C:515:BCR:C33	2.49	0.42
4:D:126:MET:HE3	4:D:143:ALA:O	2.20	0.42
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.01	0.42
3:c:48:LYS:HG3	3:c:138:GLU:HA	2.01	0.42
2:B:307:GLU:OE1	13:o:59:LYS:HG3	2.20	0.41
7:H:36:GLY:O	7:H:40:VAL:HG23	2.20	0.41
23:b:610:CLA:C2B	25:h:102:BCR:H323	2.50	0.41
3:c:391[B]:ARG:CZ	36:c:668:HOH:O	2.68	0.41
23:c:504:CLA:C15	27:c:519:LMG:C43	2.98	0.41
4:d:243:THR:HG22	36:d:515:HOH:O	2.19	0.41
4:D:136:VAL:O	4:D:136:VAL:HG12	2.20	0.41
13:O:6:THR:O	13:O:7:TYR:C	2.63	0.41
16:V:123:PRO:HG3	36:V:311:HOH:O	2.20	0.41
17:Y:41:VAL:HG12	17:Y:41:VAL:O	2.21	0.41
1:a:278:TRP:CD1	1:a:278:TRP:C	2.98	0.41
4:d:12:ARG:HA	36:d:585:HOH:O	2.19	0.41
36:h:213:HOH:O	18:x:10:PHE:HA	2.20	0.41
1:A:36:ILE:HG23	23:A:407:CLA:HBB1	2.03	0.41
17:Y:40:ALA:O	17:Y:41:VAL:HB	2.21	0.41
1:a:48:PHE:HA	1:a:115:ILE:HD11	2.03	0.41
1:a:129:ARG:NH2	36:a:518:HOH:O	2.53	0.41
4:d:218:VAL:HG22	4:d:244:TYR:CZ	2.54	0.41
23:B:608:CLA:C1A	23:B:608:CLA:CGA	2.98	0.41
3:C:398:HIS:HE1	36:V:318:HOH:O	2.02	0.41
17:Y:37:PHE:O	17:Y:40:ALA:O	2.38	0.41
1:a:265:PHE:CD2	1:a:271:LEU:HD23	2.55	0.41
2:b:125:ASP:HB2	2:b:132:ALA:HB3	2.01	0.41
36:b:720:HOH:O	7:h:3:ARG:NH2	2.53	0.41
3:c:42:LEU:HD21	23:c:511:CLA:H2A	2.01	0.41
3:c:457:LYS:HD3	4:d:228:GLY:O	2.20	0.41
8:i:8:VAL:O	8:i:12:VAL:HG23	2.21	0.41
2:B:358:ARG:HD2	36:B:724:HOH:O	2.20	0.41
3:C:66:ALA:HB1	10:K:25:LEU:HB3	2.03	0.41
25:D:405:BCR:H24C	25:D:405:BCR:H371	1.92	0.41
13:O:61:GLN:O	13:O:62:GLU:O	2.39	0.41
23:b:613:CLA:H43	23:b:616:CLA:H12	2.02	0.41
3:c:28:GLN:HA	3:c:33:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:HA	36:A:506:HOH:O	2.19	0.41
2:B:82:GLY:HA2	36:B:818:HOH:O	2.21	0.41
23:B:614:CLA:H141	23:B:614:CLA:H161	1.87	0.41
25:B:617:BCR:H20C	25:B:617:BCR:H361	1.94	0.41
25:B:619:BCR:H382	28:a:412:SQD:H82	2.02	0.41
2:b:148:LEU:HD23	2:b:210:ILE:HD11	2.01	0.41
2:b:289:GLN:O	2:b:290:ALA:C	2.63	0.41
28:f:101:SQD:O49	28:f:101:SQD:C46	2.67	0.41
1:A:291:SER:O	1:A:294:ALA:HB3	2.20	0.41
27:A:410:LMG:O10	27:A:410:LMG:HC8	2.20	0.41
3:C:223:TRP:CG	3:C:224:ILE:H	2.38	0.41
10:K:27:VAL:HG12	10:K:27:VAL:O	2.20	0.41
5:e:30:LEU:HD11	34:e:102:HEM:CBB	2.50	0.41
18:x:9:GLY:O	18:x:10:PHE:C	2.63	0.41
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.03	0.41
2:B:246:PHE:CD2	2:B:246:PHE:C	2.99	0.41
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.03	0.41
5:e:17:VAL:HG23	9:j:7:ARG:HB2	2.02	0.41
15:u:92:VAL:HG12	15:u:97:ARG:HD2	2.02	0.41
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.03	0.41
1:A:256:GLY:O	1:A:260:PHE:CA	2.69	0.41
4:D:15:PHE:CD2	4:D:15:PHE:C	2.99	0.41
27:D:407:LMG:C43	33:E:101:LHG:H131	2.51	0.41
13:O:42:ARG:O	13:O:241:ALA:HA	2.21	0.41
16:V:99:ASP:OD1	16:V:99:ASP:N	2.51	0.41
16:V:132:GLY:HA3	16:V:136:TYR:HD2	1.86	0.41
19:Z:61:VAL:O	19:Z:62:VAL:C	2.64	0.41
1:a:30:VAL:O	1:a:34:GLY:HA3	2.20	0.41
23:b:615:CLA:OBD	23:b:615:CLA:HED3	2.21	0.41
23:c:510:CLA:HBD	23:c:510:CLA:HAA2	2.03	0.41
4:d:241:GLU:CD	4:d:241:GLU:N	2.79	0.41
23:h:101:CLA:H91	23:h:101:CLA:H111	1.90	0.41
13:o:158:ASP:HB2	13:o:159:PRO:CD	2.51	0.41
1:A:114:LEU:C	1:A:114:LEU:HD23	2.46	0.41
25:B:617:BCR:H322	27:B:620:LMG:H111	2.03	0.41
1:a:95:PRO:HG2	1:a:98:GLU:HG2	2.03	0.41
25:a:408:BCR:H351	25:a:408:BCR:H15C	1.78	0.41
23:b:616:CLA:H191	23:b:616:CLA:CHB	2.50	0.41
3:c:256:PRO:HA	23:c:506:CLA:HED3	2.03	0.41
23:B:605:CLA:HBB1	23:B:606:CLA:C5	2.51	0.40
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:623:SQD:H45	28:B:623:SQD:O10	2.21	0.40
4:D:12:ARG:HA	4:D:12:ARG:NE	2.37	0.40
4:D:279:LEU:HD22	24:D:401:PHO:HBC3	2.03	0.40
1:a:257:ARG:NH1	2:b:491:VAL:O	2.47	0.40
2:b:49:ASP:C	2:b:49:ASP:OD1	2.62	0.40
15:u:53:ALA:N	15:u:54:PRO:CD	2.84	0.40
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.03	0.40
2:B:71:VAL:HG21	2:B:96:VAL:HG21	2.03	0.40
4:D:52:THR:O	4:D:66:SER:HA	2.21	0.40
13:O:111:ALA:HA	2:b:76:SER:O	2.21	0.40
17:Y:23:THR:O	17:Y:27:MET:CE	2.70	0.40
2:b:372:ASP:C	2:b:374:ASN:N	2.78	0.40
3:c:213:LEU:HD21	25:c:515:BCR:C20	2.51	0.40
4:d:45:LEU:HD12	4:d:45:LEU:HA	1.81	0.40
23:d:404:CLA:HBB1	23:d:404:CLA:HMB3	2.03	0.40
5:e:26:THR:HA	20:r:15:ALA:HB1	2.03	0.40
17:y:27:MET:HA	17:y:30:ILE:HG22	2.03	0.40
1:A:63:ILE:HB	3:C:335:THR:HG21	2.02	0.40
9:J:5:GLY:N	9:J:7:ARG:HG2	2.36	0.40
23:b:616:CLA:C17	23:b:616:CLA:H121	2.51	0.40
3:c:344:SER:HA	36:c:638:HOH:O	2.21	0.40
12:m:14:PHE:CD2	12:m:14:PHE:C	3.00	0.40
10:K:15:TYR:C	10:K:17:ILE:N	2.78	0.40
14:T:14:ILE:O	14:T:17:PHE:HB2	2.21	0.40
16:V:2:GLU:HB2	36:V:363:HOH:O	2.21	0.40
16:V:64:PRO:O	16:V:66:ARG:HG2	2.21	0.40
13:o:92:SER:HB3	13:o:131:PRO:HA	2.03	0.40
16:v:28:GLU:OE1	16:v:28:GLU:HA	2.21	0.40
19:z:40:ILE:HG13	19:z:41:PHE:N	2.36	0.40
3:C:141:GLU:CG	36:C:665:HOH:O	2.70	0.40
3:C:149:TYR:CD1	3:C:157:MET:HE1	2.57	0.40
1:a:79:THR:HG22	4:d:315:TYR:HB2	2.03	0.40
2:b:42:LEU:HD11	2:b:93:PHE:HB3	2.04	0.40
25:b:619:BCR:H20C	25:b:619:BCR:H361	1.96	0.40
3:c:109:PHE:CE2	3:c:113:VAL:CG2	3.05	0.40
3:c:337:LEU:HD23	13:o:105:PRO:HG3	2.02	0.40
25:c:521:BCR:C21	10:k:32:PHE:CE2	3.05	0.40
25:d:405:BCR:H20C	25:d:405:BCR:H361	1.89	0.40
6:f:43:ILE:N	6:f:43:ILE:CD1	2.85	0.40
7:h:46:LEU:HD12	7:h:46:LEU:O	2.21	0.40
13:o:155:ASN:HB3	36:o:364:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:x:34:ILE:HG22	18:x:35:ASP:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:362:HOH:O	36:o:304:HOH:O[1_655]	1.86	0.34

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	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
1	a	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
2	B	508/505 (101%)	490 (96%)	18 (4%)	0	100	100
2	b	503/505 (100%)	481 (96%)	20 (4%)	2 (0%)	30	34
3	C	440/451 (98%)	426 (97%)	13 (3%)	1 (0%)	43	51
3	c	450/451 (100%)	431 (96%)	18 (4%)	1 (0%)	43	51
4	D	339/341 (99%)	331 (98%)	7 (2%)	1 (0%)	36	42
4	d	340/341 (100%)	329 (97%)	10 (3%)	1 (0%)	36	42
5	E	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
5	e	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
6	f	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
7	H	63/65 (97%)	55 (87%)	8 (13%)	0	100	100
7	h	61/65 (94%)	56 (92%)	5 (8%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	28 (82%)	6 (18%)	0	100	100
9	j	34/36 (94%)	29 (85%)	5 (15%)	0	100	100
10	K	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	3	2
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	222 (91%)	19 (8%)	2 (1%)	16	16
13	o	242/244 (99%)	225 (93%)	14 (6%)	3 (1%)	10	8
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	u	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	17 (68%)	5 (20%)	3 (12%)	0	0
17	y	28/30 (93%)	25 (89%)	1 (4%)	2 (7%)	1	0
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
19	z	60/62 (97%)	51 (85%)	6 (10%)	3 (5%)	1	0
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
20	r	29/34 (85%)	25 (86%)	2 (7%)	2 (7%)	1	0
All	All	5235/5326 (98%)	4988 (95%)	225 (4%)	22 (0%)	30	34

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	60	ARG

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Mol	Chain	Res	Type
13	O	62	GLU
17	Y	41	VAL
3	c	416	SER
13	o	60	ARG
20	r	30	GLN
20	r	31	VAL
17	Y	43	ARG
19	z	15	LEU
19	z	31	GLN
17	Y	26	ALA
2	b	127	ARG
13	o	61	GLN
4	D	338	ASN
13	o	73	ARG
17	y	42	ARG
4	d	65	SER
19	z	5	PHE
2	b	85	GLY
17	y	41	VAL

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	270/270 (100%)	263 (97%)	7 (3%)	40	55
1	a	269/270 (100%)	254 (94%)	15 (6%)	19	24
2	B	407/403 (101%)	386 (95%)	21 (5%)	21	26
2	b	402/403 (100%)	385 (96%)	17 (4%)	26	36
3	C	344/352 (98%)	333 (97%)	11 (3%)	34	47
3	c	353/352 (100%)	338 (96%)	15 (4%)	26	36
4	D	276/276 (100%)	270 (98%)	6 (2%)	45	61
4	d	277/276 (100%)	270 (98%)	7 (2%)	42	56
5	E	72/72 (100%)	63 (88%)	9 (12%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	71/72 (99%)	62 (87%)	9 (13%)	4	4
6	F	28/28 (100%)	26 (93%)	2 (7%)	13	16
6	f	28/28 (100%)	25 (89%)	3 (11%)	6	6
7	H	53/54 (98%)	48 (91%)	5 (9%)	8	9
7	h	53/54 (98%)	47 (89%)	6 (11%)	5	5
8	I	32/32 (100%)	28 (88%)	4 (12%)	4	4
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	24/24 (100%)	23 (96%)	1 (4%)	26	36
9	j	23/24 (96%)	21 (91%)	2 (9%)	9	10
10	K	31/30 (103%)	30 (97%)	1 (3%)	34	47
10	k	30/30 (100%)	23 (77%)	7 (23%)	1	0
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	51
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	22
12	M	28/29 (97%)	25 (89%)	3 (11%)	6	6
12	m	28/29 (97%)	27 (96%)	1 (4%)	31	42
13	O	208/207 (100%)	188 (90%)	20 (10%)	8	8
13	o	207/207 (100%)	193 (93%)	14 (7%)	14	17
14	T	26/26 (100%)	23 (88%)	3 (12%)	5	5
14	t	25/26 (96%)	25 (100%)	0	100	100
15	U	84/84 (100%)	77 (92%)	7 (8%)	10	11
15	u	84/84 (100%)	82 (98%)	2 (2%)	43	58
16	V	117/117 (100%)	108 (92%)	9 (8%)	12	13
16	v	117/117 (100%)	111 (95%)	6 (5%)	21	27
17	Y	19/23 (83%)	15 (79%)	4 (21%)	1	1
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	3
18	X	31/31 (100%)	27 (87%)	4 (13%)	4	4
18	x	31/31 (100%)	28 (90%)	3 (10%)	8	8
19	Z	52/52 (100%)	42 (81%)	10 (19%)	1	1
19	z	51/52 (98%)	42 (82%)	9 (18%)	2	1
20	R	28/29 (97%)	22 (79%)	6 (21%)	1	1
20	r	19/29 (66%)	17 (90%)	2 (10%)	6	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4321/4348 (99%)	4064 (94%)	257 (6%)	18	22

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	16	ARG
1	A	77	ILE
1	A	102	LEU
1	A	205	VAL
1	A	229	GLU
1	A	243	GLU
2	B	63	LEU
2	B	76	SER
2	B	83	GLU
2	B	84	THR
2	B	98	LEU
2	B	127	ARG
2	B	246	PHE
2	B	289	GLN
2	B	362	PHE
2	B	371	THR
2	B	425	ILE
2	B	431	GLU
2	B	435	GLU
2	B	476	ARG
2	B	480[A]	SER
2	B	480[B]	SER
2	B	486	LEU
2	B	489	GLU
2	B	491	VAL
2	B	495	PHE
2	B	505	ARG
3	C	134	ILE
3	C	141	GLU
3	C	161	LEU
3	C	166	ILE
3	C	170	ILE
3	C	200	THR
3	C	213	LEU
3	C	240	ILE
3	C	289	PHE

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Mol	Chain	Res	Type
3	C	355	THR
3	C	386	PRO
4	D	12	ARG
4	D	43	LEU
4	D	76	VAL
4	D	241	GLU
4	D	251	ARG
4	D	345	VAL
5	E	4	THR
5	E	11	SER
5	E	12	ASP
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	65	LEU
5	E	71	GLU
5	E	76	VAL
5	E	83	LEU
6	F	12	SER
6	F	25	THR
7	H	20	LYS
7	H	45	ILE
7	H	52	THR
7	H	53	LEU
7	H	56	ASP
8	I	4	LEU
8	I	33	LYS
8	I	35	LYS
8	I	36	ASP
9	J	8	ILE
10	K	13	GLU
11	L	7	ARG
12	M	3	VAL
12	M	13	LEU
12	M	16	LEU
13	O	3	GLN
13	O	6	THR
13	O	23	ASP
13	O	34	SER
13	O	35	SER
13	O	40	ILE
13	O	57	LYS
13	O	64	GLU

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Mol	Chain	Res	Type
13	O	72	THR
13	O	78	LEU
13	O	89	SER
13	O	97	GLU
13	O	107	THR
13	O	114	GLU
13	O	134	THR
13	O	199	LEU
13	O	214	THR
13	O	217	SER
13	O	234	LYS
13	O	242	SER
14	T	2	GLU
14	T	24	ARG
14	T	25	GLU
15	U	8	GLU
15	U	23	GLU
15	U	51	LYS
15	U	59	GLU
15	U	61	VAL
15	U	67	LEU
15	U	79	LEU
16	V	3	LEU
16	V	7	VAL
16	V	21	LEU
16	V	31	ARG
16	V	86	GLN
16	V	90	GLU
16	V	99	ASP
16	V	105	ARG
16	V	106	ASN
17	Y	23	THR
17	Y	24	MET
17	Y	25	ILE
17	Y	43	ARG
18	X	3	ILE
18	X	28	LEU
18	X	29	ILE
18	X	36	LYS
19	Z	3	ILE
19	Z	7	LEU
19	Z	15	LEU

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Mol	Chain	Res	Type
19	Z	17	PHE
19	Z	25	VAL
19	Z	35	ARG
19	Z	40	ILE
19	Z	46	LEU
19	Z	50	LEU
19	Z	52	LEU
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	13	LEU
20	R	14	LEU
20	R	29	LYS
1	a	12	ASN
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159	LEU
1	a	200	LEU
1	a	210	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	232	SER
1	a	238	LYS
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	86	ILE
2	b	137	LYS
2	b	149	LEU
2	b	219	VAL
2	b	236	THR
2	b	240	SER
2	b	252	VAL
2	b	298	LEU
2	b	315	ILE
2	b	362	PHE
2	b	388	SER
2	b	397	VAL
2	b	419	SER
2	b	490	GLN

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Mol	Chain	Res	Type
2	b	492	GLU
2	b	497	GLN
2	b	506	ARG
3	c	24	THR
3	c	25	ASN
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	161	LEU
3	c	165	LEU
3	c	240	ILE
3	c	267	SER
3	c	279	LEU
3	c	341	LEU
3	c	396	MET
3	c	462	GLU
3	c	471	SER
4	d	182	LEU
4	d	272	LEU
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	16	SER
5	e	39	SER
5	e	54	SER
5	e	61	ARG
5	e	66	VAL
5	e	75	GLN
5	e	82	GLN
5	e	83	LEU
5	e	84	LYS
6	f	23	VAL
6	f	28	VAL
6	f	44	GLN
7	h	3	ARG
7	h	7	LEU
7	h	27	THR
7	h	37	LEU
7	h	40	VAL

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Mol	Chain	Res	Type
7	h	56	ASP
9	j	13	VAL
9	j	36	LEU
10	k	10	LYS
10	k	13	GLU
10	k	21	LEU
10	k	24	VAL
10	k	27	VAL
10	k	30	VAL
10	k	46	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	4	THR
13	o	10	ILE
13	o	35	SER
13	o	49	THR
13	o	57	LYS
13	o	59	LYS
13	o	60	ARG
13	o	72	THR
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	181	GLU
13	o	192	LEU
13	o	242	SER
15	u	23	GLU
15	u	58	VAL
16	v	15	GLU
16	v	19	ILE
16	v	24	LYS
16	v	52	LEU
16	v	109	GLU
16	v	110	LYS
17	y	22	LEU
17	y	27	MET
17	y	38	LEU
18	x	8	LYS
18	x	15	LEU
18	x	34	ILE
19	z	1	MET

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Mol	Chain	Res	Type
19	z	3	ILE
19	z	12	LEU
19	z	19	MET
19	z	20	VAL
19	z	29	SER
19	z	32	ASP
19	z	38	GLN
19	z	46	LEU
20	r	3	TRP
20	r	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	261	GLN
3	C	155	ASN
3	C	418	ASN
4	D	61	HIS
4	D	334	GLN
4	D	336	HIS
4	D	350	ASN
11	L	6	ASN
11	L	8	GLN
12	M	4	ASN
13	O	82	GLN
13	O	88	ASN
13	O	155	ASN
15	U	73	GLN
17	Y	21	GLN
1	a	261	GLN
2	b	409	GLN
3	c	25	ASN
3	c	322	GLN
3	c	327	ASN
3	c	418	ASN
4	d	164	GLN
4	d	236	ASN
4	d	255	GLN
4	d	334	GLN
4	d	350	ASN
13	o	58	ASN

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Mol	Chain	Res	Type
13	o	130	GLN
13	o	155	ASN
13	o	186	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.96	0	8,9,11	1.02	1 (12%)
8	FME	i	1	8	8,9,10	0.99	0	8,9,11	1.01	1 (12%)
8	FME	I	1	8	8,9,10	1.02	0	8,9,11	1.40	1 (12%)
12	FME	M	1	12	8,9,10	1.18	1 (12%)	8,9,11	1.38	2 (25%)
14	FME	t	1	14	8,9,10	0.98	1 (12%)	8,9,11	0.97	1 (12%)
14	FME	T	1	14	8,9,10	1.06	1 (12%)	8,9,11	1.99	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
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.65	1.42	1.46
14	T	1	FME	CA-N	-2.60	1.42	1.46
14	t	1	FME	CA-N	-2.06	1.43	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	-3.99	116.68	122.82
8	I	1	FME	C-CA-N	3.05	115.38	109.50
8	i	1	FME	C-CA-N	2.55	114.42	109.50
14	T	1	FME	O1-CN-N	-2.37	119.20	125.32
12	M	1	FME	C-CA-N	-2.31	105.05	109.50
12	M	1	FME	CB-CA-N	2.19	114.50	110.52
14	t	1	FME	CA-N-CN	-2.11	119.58	122.82
12	m	1	FME	CB-CA-N	2.00	114.16	110.52

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	C-CA-CB-CG
12	M	1	FME	CB-CA-N-CN
14	t	1	FME	C-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE
14	t	1	FME	N-CA-CB-CG
12	m	1	FME	CA-CB-CG-SD
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CA-CB-CG-SD
12	m	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	t	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 149 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
29	DGD	C	518	-	63,63,67	1.13	6 (9%)	77,77,81	1.49	10 (12%)
23	CLA	B	609	-	69,73,73	1.69	11 (15%)	82,113,113	1.19	7 (8%)
23	CLA	B	601	36	69,73,73	1.53	10 (14%)	82,113,113	1.65	9 (10%)
23	CLA	B	605	-	69,73,73	1.72	12 (17%)	82,113,113	1.54	15 (18%)
23	CLA	D	404	-	69,73,73	1.85	8 (11%)	82,113,113	1.17	9 (10%)
23	CLA	b	616	-	69,73,73	1.85	13 (18%)	82,113,113	1.46	15 (18%)
23	CLA	h	101	36	69,73,73	1.34	11 (15%)	82,113,113	1.38	10 (12%)
33	LHG	L	101	-	48,48,48	0.96	2 (4%)	51,54,54	1.19	3 (5%)
23	CLA	C	512	-	69,73,73	1.79	12 (17%)	82,113,113	1.29	8 (9%)
25	BCR	K	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.22	5 (8%)
23	CLA	b	614	-	69,73,73	1.23	9 (13%)	82,113,113	1.38	11 (13%)
33	LHG	E	101	-	48,48,48	1.05	5 (10%)	51,54,54	1.17	3 (5%)
28	SQD	a	412	-	35,35,54	1.14	2 (5%)	37,37,65	1.34	5 (13%)
24	PHO	d	401	-	58,69,69	2.24	10 (17%)	55,99,99	1.71	11 (20%)
23	CLA	b	611	36	69,73,73	1.24	8 (11%)	82,113,113	1.55	11 (13%)
33	LHG	D	409	-	46,46,48	1.03	4 (8%)	49,52,54	1.35	4 (8%)
23	CLA	C	506	-	69,73,73	1.65	12 (17%)	82,113,113	1.19	5 (6%)
23	CLA	B	615	-	69,73,73	1.48	11 (15%)	82,113,113	1.39	10 (12%)
23	CLA	C	503	-	69,73,73	1.31	10 (14%)	82,113,113	1.56	12 (14%)
23	CLA	b	606	-	69,73,73	1.28	6 (8%)	82,113,113	1.55	13 (15%)
28	SQD	A	412	-	38,38,54	1.16	4 (10%)	40,40,65	1.06	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	404	-	69,73,73	1.66	9 (13%)	82,113,113	1.61	12 (14%)
27	LMG	d	409	-	44,44,55	1.17	3 (6%)	52,52,63	1.42	9 (17%)
23	CLA	A	404	-	69,73,73	1.32	9 (13%)	82,113,113	1.53	15 (18%)
29	DGD	C	516	-	63,63,67	1.40	11 (17%)	77,77,81	1.37	9 (11%)
23	CLA	c	511	3	69,73,73	1.52	11 (15%)	82,113,113	1.28	5 (6%)
25	BCR	B	619	-	41,41,41	1.27	3 (7%)	56,56,56	1.37	11 (19%)
23	CLA	d	403	-	69,73,73	1.24	10 (14%)	82,113,113	1.17	6 (7%)
23	CLA	A	405	36	69,73,73	1.17	7 (10%)	82,113,113	1.34	13 (15%)
23	CLA	B	607	36	69,73,73	1.31	9 (13%)	82,113,113	1.19	7 (8%)
27	LMG	b	623	-	21,21,55	1.03	1 (4%)	20,20,63	0.90	0
28	SQD	F	101	-	34,36,54	1.06	3 (8%)	42,45,65	1.79	10 (23%)
25	BCR	a	408	-	41,41,41	1.19	4 (9%)	56,56,56	1.46	7 (12%)
28	SQD	A	411	-	50,52,54	1.07	4 (8%)	60,63,65	2.10	10 (16%)
23	CLA	B	610	36	69,73,73	1.52	12 (17%)	82,113,113	1.50	12 (14%)
23	CLA	b	603	-	69,73,73	1.25	7 (10%)	82,113,113	1.37	13 (15%)
23	CLA	a	405	36	69,73,73	1.36	7 (10%)	82,113,113	1.22	9 (10%)
23	CLA	b	613	-	69,73,73	1.50	10 (14%)	82,113,113	1.41	11 (13%)
29	DGD	c	517	-	63,63,67	1.28	11 (17%)	77,77,81	1.53	10 (12%)
23	CLA	D	403	-	69,73,73	1.58	11 (15%)	82,113,113	1.59	8 (9%)
23	CLA	c	501	-	69,73,73	1.31	10 (14%)	82,113,113	1.55	9 (10%)
27	LMG	D	410	-	31,31,55	1.16	4 (12%)	33,33,63	1.14	3 (9%)
23	CLA	B	608	-	69,73,73	1.31	9 (13%)	82,113,113	1.38	8 (9%)
25	BCR	d	405	-	41,41,41	1.16	2 (4%)	56,56,56	1.33	7 (12%)
28	SQD	f	101	-	39,41,54	1.10	4 (10%)	49,52,65	1.81	10 (20%)
23	CLA	C	502	-	69,73,73	1.46	10 (14%)	82,113,113	1.31	8 (9%)
23	CLA	b	605	-	69,73,73	1.58	10 (14%)	82,113,113	1.74	15 (18%)
27	LMG	c	522	-	48,48,55	1.27	8 (16%)	56,56,63	1.46	7 (12%)
23	CLA	b	612	-	69,73,73	1.66	11 (15%)	82,113,113	1.51	13 (15%)
23	CLA	C	504	36	63,67,73	1.24	6 (9%)	74,105,113	1.41	12 (16%)
23	CLA	b	617	-	64,68,73	1.26	10 (15%)	76,107,113	1.64	10 (13%)
23	CLA	B	613	-	69,73,73	1.57	12 (17%)	82,113,113	1.43	13 (15%)
23	CLA	D	402	36	69,73,73	1.32	10 (14%)	82,113,113	1.46	11 (13%)
29	DGD	c	518	-	63,63,67	1.25	9 (14%)	77,77,81	1.46	14 (18%)
33	LHG	d	407	-	48,48,48	0.91	3 (6%)	51,54,54	1.21	4 (7%)
23	CLA	B	604	-	69,73,73	1.41	10 (14%)	82,113,113	1.72	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	m	101	-	51,51,55	0.92	2 (3%)	59,59,63	1.57	14 (23%)
26	PL9	A	409	-	55,55,55	0.93	1 (1%)	68,69,69	1.62	12 (17%)
25	BCR	b	618	-	41,41,41	1.19	4 (9%)	56,56,56	1.43	11 (19%)
33	LHG	D	408	-	48,48,48	1.15	5 (10%)	51,54,54	1.20	4 (7%)
25	BCR	y	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.25	5 (8%)
27	LMG	D	407	-	51,51,55	1.07	2 (3%)	59,59,63	1.27	5 (8%)
23	CLA	B	602	-	69,73,73	1.46	10 (14%)	82,113,113	1.61	14 (17%)
23	CLA	c	505	-	69,73,73	1.26	7 (10%)	82,113,113	1.31	12 (14%)
27	LMG	D	411	-	26,26,55	1.04	2 (7%)	26,26,63	1.24	3 (11%)
23	CLA	C	510	-	69,73,73	1.62	10 (14%)	82,113,113	1.57	6 (7%)
25	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.37	6 (10%)
31	BCT	A	415	21	3,3,3	1.22	0	2,3,3	2.87	1 (50%)
31	BCT	a	417	21	3,3,3	1.32	0	2,3,3	2.83	2 (100%)
23	CLA	b	608	36	69,73,73	1.13	7 (10%)	82,113,113	1.25	5 (6%)
23	CLA	B	616	-	64,68,73	1.78	14 (21%)	76,107,113	1.46	10 (13%)
25	BCR	D	405	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	8 (14%)
25	BCR	b	620	-	41,41,41	1.02	3 (7%)	56,56,56	1.33	7 (12%)
28	SQD	B	623	-	52,54,54	0.91	3 (5%)	62,65,65	1.86	14 (22%)
29	DGD	a	413	-	43,43,67	1.19	3 (6%)	45,45,81	1.43	6 (13%)
23	CLA	c	504	36	64,68,73	1.84	11 (17%)	76,107,113	1.50	11 (14%)
27	LMG	a	414	-	49,49,55	0.88	2 (4%)	57,57,63	1.27	4 (7%)
23	CLA	C	505	-	69,73,73	1.43	8 (11%)	82,113,113	1.32	7 (8%)
23	CLA	a	407	-	69,73,73	1.45	11 (15%)	82,113,113	1.30	14 (17%)
23	CLA	c	512	-	69,73,73	1.45	10 (14%)	82,113,113	1.39	10 (12%)
23	CLA	c	508	-	68,72,73	1.32	8 (11%)	80,111,113	1.25	8 (10%)
23	CLA	c	510	-	69,73,73	1.24	5 (7%)	82,113,113	1.43	12 (14%)
28	SQD	a	411	-	52,54,54	1.01	5 (9%)	62,65,65	1.81	15 (24%)
23	CLA	c	503	-	69,73,73	1.15	5 (7%)	82,113,113	1.45	9 (10%)
27	LMG	B	620	-	51,51,55	0.94	3 (5%)	59,59,63	1.55	12 (20%)
33	LHG	l	101	-	48,48,48	0.85	3 (6%)	51,54,54	1.21	4 (7%)
23	CLA	C	513	-	69,73,73	1.33	7 (10%)	82,113,113	1.50	9 (10%)
25	BCR	A	408	-	41,41,41	0.99	2 (4%)	56,56,56	1.41	8 (14%)
25	BCR	H	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.43	10 (17%)
23	CLA	C	501	-	69,73,73	2.14	9 (13%)	82,113,113	1.62	9 (10%)
24	PHO	a	406	-	58,69,69	2.12	11 (18%)	55,99,99	1.42	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	508	-	69,73,73	1.35	8 (11%)	82,113,113	1.48	12 (14%)
23	CLA	b	609	-	69,73,73	1.24	7 (10%)	82,113,113	1.58	11 (13%)
29	DGD	C	517	-	63,63,67	1.28	7 (11%)	77,77,81	1.55	10 (12%)
34	HEM	e	102	5,6	50,50,50	1.46	7 (14%)	67,82,82	1.24	8 (11%)
23	CLA	b	615	-	69,73,73	1.59	8 (11%)	82,113,113	1.51	12 (14%)
27	LMG	c	519	-	37,37,55	1.10	4 (10%)	45,45,63	1.21	3 (6%)
33	LHG	B	622	-	48,48,48	0.92	2 (4%)	51,54,54	1.44	7 (13%)
23	CLA	B	614	-	69,73,73	1.49	8 (11%)	82,113,113	1.35	9 (10%)
33	LHG	d	408	-	38,38,48	0.91	1 (2%)	41,44,54	1.10	4 (9%)
33	LHG	a	410	-	48,48,48	0.80	1 (2%)	51,54,54	1.38	6 (11%)
23	CLA	B	606	-	69,73,73	1.65	9 (13%)	82,113,113	1.47	10 (12%)
23	CLA	C	511	3	69,73,73	1.63	10 (14%)	82,113,113	1.45	8 (9%)
23	CLA	c	502	-	69,73,73	1.71	8 (11%)	82,113,113	1.41	8 (9%)
25	BCR	C	520	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	2 (3%)
27	LMG	A	410	-	48,48,55	1.03	2 (4%)	56,56,63	1.24	5 (8%)
29	DGD	c	516	-	63,63,67	1.30	10 (15%)	77,77,81	1.59	14 (18%)
23	CLA	C	507	36	69,73,73	1.22	10 (14%)	82,113,113	1.20	5 (6%)
28	SQD	b	601	-	47,49,54	1.00	2 (4%)	57,60,65	2.33	16 (28%)
23	CLA	c	506	-	69,73,73	1.44	8 (11%)	82,113,113	1.55	15 (18%)
30	OEY	a	416	1,3,36	0,16,16	-	-	-	-	-
29	DGD	H	102	-	63,63,67	1.65	10 (15%)	77,77,81	1.64	15 (19%)
25	BCR	b	619	-	41,41,41	1.28	2 (4%)	56,56,56	1.33	7 (12%)
25	BCR	t	101	-	41,41,41	1.10	4 (9%)	56,56,56	1.30	7 (12%)
23	CLA	B	611	-	69,73,73	1.13	7 (10%)	82,113,113	1.34	10 (12%)
35	HEC	v	201	16	46,50,50	1.86	7 (15%)	58,82,82	1.49	6 (10%)
27	LMG	C	519	-	48,48,55	1.12	5 (10%)	56,56,63	1.35	6 (10%)
25	BCR	c	521	-	41,41,41	0.94	2 (4%)	56,56,56	1.15	4 (7%)
23	CLA	b	610	-	69,73,73	1.37	8 (11%)	82,113,113	1.32	9 (10%)
23	CLA	c	509	-	69,73,73	1.69	10 (14%)	82,113,113	1.66	12 (14%)
23	CLA	C	509	-	69,73,73	1.90	7 (10%)	82,113,113	1.31	6 (7%)
25	BCR	c	515	-	41,41,41	1.19	4 (9%)	56,56,56	1.46	11 (19%)
24	PHO	D	401	-	58,69,69	2.18	10 (17%)	55,99,99	1.46	8 (14%)
25	BCR	B	617	-	41,41,41	1.19	3 (7%)	56,56,56	1.40	8 (14%)
25	BCR	C	515	-	41,41,41	1.28	4 (9%)	56,56,56	1.40	7 (12%)
35	HEC	V	201	16	46,50,50	1.88	8 (17%)	58,82,82	1.26	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	607	-	69,73,73	1.47	5 (7%)	82,113,113	1.63	9 (10%)
23	CLA	c	507	36	69,73,73	1.37	7 (10%)	82,113,113	1.32	10 (12%)
25	BCR	T	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.40	7 (12%)
23	CLA	d	402	36	69,73,73	1.47	7 (10%)	82,113,113	1.57	8 (9%)
33	LHG	e	101	-	41,41,48	0.83	2 (4%)	44,47,54	1.30	5 (11%)
26	PL9	D	406	-	55,55,55	1.42	7 (12%)	68,69,69	1.50	11 (16%)
25	BCR	B	618	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	7 (12%)
23	CLA	d	404	-	69,73,73	1.80	10 (14%)	82,113,113	1.12	6 (7%)
26	PL9	d	406	-	55,55,55	1.32	8 (14%)	68,69,69	1.66	20 (29%)
25	BCR	h	102	-	41,41,41	1.25	2 (4%)	56,56,56	1.34	9 (16%)
29	DGD	A	413	-	67,67,67	1.29	10 (14%)	81,81,81	1.36	7 (8%)
23	CLA	A	407	-	58,62,73	1.64	10 (17%)	68,99,113	1.70	15 (22%)
30	OEY	A	414	1,3,36	0,16,16	-	-	-	-	-
23	CLA	b	604	-	69,73,73	1.55	13 (18%)	82,113,113	1.58	11 (13%)
23	CLA	B	612	-	69,73,73	1.04	4 (5%)	82,113,113	1.58	13 (15%)
23	CLA	B	603	-	69,73,73	1.24	9 (13%)	82,113,113	1.45	11 (13%)
25	BCR	C	514	-	41,41,41	1.20	2 (4%)	56,56,56	1.40	9 (16%)
27	LMG	b	622	-	55,55,55	1.08	4 (7%)	63,63,63	1.46	10 (15%)
29	DGD	h	103	-	63,63,67	1.00	4 (6%)	77,77,81	1.60	17 (22%)
24	PHO	A	406	-	58,69,69	1.99	15 (25%)	55,99,99	1.79	13 (23%)
26	PL9	a	409	-	55,55,55	1.38	6 (10%)	68,69,69	1.39	8 (11%)
23	CLA	c	513	-	69,73,73	1.23	11 (15%)	82,113,113	1.14	6 (7%)
34	HEM	E	102	5,6	50,50,50	1.44	4 (8%)	67,82,82	1.23	6 (8%)

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
29	DGD	C	518	-	-	16/51/91/95	0/2/2/2
23	CLA	B	609	-	-	10/39/115/115	-
23	CLA	B	601	36	-	17/39/115/115	-
23	CLA	B	605	-	1/1/20/20	9/39/115/115	-
23	CLA	D	404	-	-	9/39/115/115	-
23	CLA	b	616	-	1/1/20/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	h	101	36	1/1/20/20	17/39/115/115	-
33	LHG	L	101	-	-	21/53/53/53	-
23	CLA	C	512	-	1/1/20/20	11/39/115/115	-
25	BCR	K	101	-	-	9/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/20/20	5/39/115/115	-
33	LHG	E	101	-	-	27/53/53/53	-
28	SQD	a	412	-	-	21/37/37/69	-
24	PHO	d	401	-	-	3/37/103/103	0/5/6/6
23	CLA	b	611	36	1/1/20/20	8/39/115/115	-
33	LHG	D	409	-	-	24/51/51/53	-
23	CLA	C	506	-	1/1/20/20	14/39/115/115	-
23	CLA	B	615	-	1/1/20/20	9/39/115/115	-
23	CLA	C	503	-	1/1/20/20	9/39/115/115	-
23	CLA	b	606	-	1/1/20/20	5/39/115/115	-
28	SQD	A	412	-	-	17/39/39/69	-
23	CLA	a	404	-	1/1/20/20	10/39/115/115	-
27	LMG	d	409	-	-	11/39/59/70	0/1/1/1
23	CLA	A	404	-	1/1/20/20	4/39/115/115	-
29	DGD	C	516	-	-	21/51/91/95	0/2/2/2
23	CLA	c	511	3	1/1/20/20	12/39/115/115	-
25	BCR	B	619	-	-	3/29/63/63	0/2/2/2
23	CLA	A	405	36	-	2/39/115/115	-
23	CLA	d	403	-	1/1/20/20	10/39/115/115	-
23	CLA	B	607	36	1/1/20/20	11/39/115/115	-
27	LMG	b	623	-	-	12/17/17/70	-
28	SQD	F	101	-	-	14/28/48/69	0/1/1/1
25	BCR	a	408	-	-	2/29/63/63	0/2/2/2
28	SQD	A	411	-	-	19/47/67/69	0/1/1/1
23	CLA	B	610	36	1/1/20/20	6/39/115/115	-
23	CLA	b	603	-	1/1/20/20	4/39/115/115	-
23	CLA	a	405	36	1/1/20/20	10/39/115/115	-
23	CLA	b	613	-	1/1/20/20	11/39/115/115	-
29	DGD	c	517	-	-	20/51/91/95	0/2/2/2
23	CLA	D	403	-	1/1/20/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	501	-	1/1/20/20	6/39/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
23	CLA	B	608	-	-	3/39/115/115	-
25	BCR	d	405	-	-	13/29/63/63	0/2/2/2
28	SQD	f	101	-	-	12/36/56/69	0/1/1/1
23	CLA	C	502	-	-	9/39/115/115	-
23	CLA	b	605	-	1/1/20/20	12/39/115/115	-
27	LMG	c	522	-	-	21/43/63/70	0/1/1/1
23	CLA	b	612	-	-	9/39/115/115	-
23	CLA	C	504	36	1/1/18/20	8/32/108/115	-
23	CLA	b	617	-	1/1/19/20	8/33/109/115	-
23	CLA	B	613	-	1/1/20/20	9/39/115/115	-
23	CLA	D	402	36	1/1/20/20	0/39/115/115	-
29	DGD	c	518	-	-	20/51/91/95	0/2/2/2
33	LHG	d	407	-	-	23/53/53/53	-
23	CLA	B	604	-	1/1/20/20	10/39/115/115	-
27	LMG	m	101	-	-	19/46/66/70	0/1/1/1
26	PL9	A	409	-	-	21/53/73/73	0/1/1/1
25	BCR	b	618	-	-	4/29/63/63	0/2/2/2
33	LHG	D	408	-	-	24/53/53/53	-
25	BCR	y	101	-	-	8/29/63/63	0/2/2/2
27	LMG	D	407	-	-	19/46/66/70	0/1/1/1
23	CLA	B	602	-	1/1/20/20	4/39/115/115	-
23	CLA	c	505	-	1/1/20/20	14/39/115/115	-
27	LMG	D	411	-	-	13/22/22/70	-
23	CLA	C	510	-	1/1/20/20	8/39/115/115	-
25	BCR	c	514	-	-	11/29/63/63	0/2/2/2
23	CLA	b	608	36	1/1/20/20	14/39/115/115	-
23	CLA	B	616	-	1/1/19/20	8/33/109/115	-
25	BCR	D	405	-	-	12/29/63/63	0/2/2/2
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
28	SQD	B	623	-	-	19/49/69/69	0/1/1/1
29	DGD	a	413	-	-	21/45/45/95	-
23	CLA	c	504	36	1/1/19/20	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	a	414	-	-	28/44/64/70	0/1/1/1
23	CLA	C	505	-	1/1/20/20	8/39/115/115	-
23	CLA	a	407	-	1/1/20/20	9/39/115/115	-
23	CLA	c	512	-	1/1/20/20	18/39/115/115	-
23	CLA	c	508	-	-	9/38/114/115	-
23	CLA	c	510	-	1/1/20/20	18/39/115/115	-
28	SQD	a	411	-	-	18/49/69/69	0/1/1/1
23	CLA	c	503	-	-	12/39/115/115	-
27	LMG	B	620	-	-	21/46/66/70	0/1/1/1
33	LHG	l	101	-	-	19/53/53/53	-
23	CLA	C	513	-	1/1/20/20	14/39/115/115	-
25	BCR	A	408	-	-	5/29/63/63	0/2/2/2
25	BCR	H	101	-	-	7/29/63/63	0/2/2/2
23	CLA	C	501	-	1/1/20/20	4/39/115/115	-
24	PHO	a	406	-	-	5/37/103/103	0/5/6/6
23	CLA	C	508	-	-	7/39/115/115	-
23	CLA	b	609	-	-	7/39/115/115	-
29	DGD	C	517	-	-	18/51/91/95	0/2/2/2
34	HEM	e	102	5,6	-	3/14/54/54	-
23	CLA	b	615	-	1/1/20/20	14/39/115/115	-
27	LMG	c	519	-	-	10/31/51/70	0/1/1/1
33	LHG	B	622	-	-	11/53/53/53	-
23	CLA	B	614	-	1/1/20/20	10/39/115/115	-
33	LHG	d	408	-	-	14/43/43/53	-
33	LHG	a	410	-	-	19/53/53/53	-
23	CLA	B	606	-	1/1/20/20	13/39/115/115	-
23	CLA	C	511	3	-	3/39/115/115	-
23	CLA	c	502	-	-	6/39/115/115	-
25	BCR	C	520	-	-	10/29/63/63	0/2/2/2
27	LMG	A	410	-	-	20/43/63/70	0/1/1/1
29	DGD	c	516	-	-	24/51/91/95	0/2/2/2
23	CLA	C	507	36	1/1/20/20	12/39/115/115	-
28	SQD	b	601	-	-	20/44/64/69	0/1/1/1
23	CLA	c	506	-	1/1/20/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	DGD	H	102	-	-	17/51/91/95	0/2/2/2
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
25	BCR	t	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	611	-	1/1/20/20	10/39/115/115	-
35	HEC	v	201	16	-	6/14/54/54	-
27	LMG	C	519	-	-	19/43/63/70	0/1/1/1
25	BCR	c	521	-	-	4/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/20/20	10/39/115/115	-
23	CLA	b	610	-	-	4/39/115/115	-
23	CLA	C	509	-	1/1/20/20	10/39/115/115	-
25	BCR	c	515	-	-	8/29/63/63	0/2/2/2
24	PHO	D	401	-	-	4/37/103/103	0/5/6/6
25	BCR	B	617	-	-	3/29/63/63	0/2/2/2
25	BCR	C	515	-	-	4/29/63/63	0/2/2/2
35	HEC	V	201	16	-	6/14/54/54	-
23	CLA	b	607	-	1/1/20/20	9/39/115/115	-
23	CLA	c	507	36	1/1/20/20	14/39/115/115	-
25	BCR	T	101	-	-	14/29/63/63	0/2/2/2
23	CLA	d	402	36	1/1/20/20	5/39/115/115	-
33	LHG	e	101	-	-	23/46/46/53	-
26	PL9	D	406	-	-	11/53/73/73	0/1/1/1
25	BCR	B	618	-	-	11/29/63/63	0/2/2/2
23	CLA	d	404	-	1/1/20/20	7/39/115/115	-
26	PL9	d	406	-	-	21/53/73/73	0/1/1/1
25	BCR	h	102	-	-	6/29/63/63	0/2/2/2
29	DGD	A	413	-	-	31/55/95/95	0/2/2/2
23	CLA	A	407	-	1/1/17/20	2/26/102/115	-
23	CLA	b	604	-	1/1/20/20	10/39/115/115	-
23	CLA	B	612	-	1/1/20/20	10/39/115/115	-
23	CLA	B	603	-	-	16/39/115/115	-
25	BCR	C	514	-	-	15/29/63/63	0/2/2/2
27	LMG	b	622	-	-	24/50/70/70	0/1/1/1
29	DGD	h	103	-	-	15/51/91/95	0/2/2/2
24	PHO	A	406	-	-	9/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PL9	a	409	-	-	26/53/73/73	0/1/1/1
23	CLA	c	513	-	1/1/20/20	10/39/115/115	-
34	HEM	E	102	5,6	-	2/14/54/54	-

All (971) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	MG-NB	-11.83	1.82	2.05
23	D	404	CLA	MG-NB	-11.58	1.82	2.05
23	C	501	CLA	MG-ND	-11.02	1.83	2.05
24	d	401	PHO	C1B-C2B	10.83	1.51	1.39
24	D	401	PHO	C1B-C2B	9.97	1.50	1.39
23	B	605	CLA	MG-NB	9.75	2.25	2.05
24	a	406	PHO	C1B-C2B	9.37	1.49	1.39
24	D	401	PHO	C3B-C4B	9.27	1.50	1.41
23	a	404	CLA	MG-NB	8.77	2.23	2.05
23	C	511	CLA	MG-NA	8.53	2.26	2.06
23	C	501	CLA	MG-NA	8.49	2.26	2.06
23	C	512	CLA	MG-NB	8.36	2.22	2.05
23	c	502	CLA	MG-NB	-8.33	1.89	2.05
23	b	612	CLA	MG-NA	8.32	2.26	2.06
23	B	606	CLA	MG-NA	8.29	2.26	2.06
24	d	401	PHO	C3B-C4B	8.26	1.49	1.41
23	d	404	CLA	MG-NA	8.18	2.25	2.06
23	B	616	CLA	MG-NB	-8.05	1.89	2.05
23	b	616	CLA	MG-NC	-7.87	1.87	2.06
24	a	406	PHO	C3B-C4B	7.84	1.49	1.41
23	c	509	CLA	MG-ND	7.78	2.21	2.05
24	A	406	PHO	C3B-C4B	7.66	1.49	1.41
23	B	613	CLA	MG-NB	-7.46	1.91	2.05
24	A	406	PHO	C1B-C2B	7.38	1.47	1.39
23	C	506	CLA	MG-ND	-7.38	1.91	2.05
23	C	512	CLA	MG-ND	-7.30	1.91	2.05
23	b	607	CLA	MG-NA	7.25	2.23	2.06
23	b	605	CLA	MG-NB	7.03	2.19	2.05
23	B	601	CLA	MG-NA	6.76	2.22	2.06
23	c	502	CLA	MG-ND	6.72	2.19	2.05
23	d	402	CLA	MG-NA	6.68	2.22	2.06
23	B	609	CLA	MG-ND	-6.64	1.92	2.05
23	c	511	CLA	MG-NA	6.58	2.21	2.06
23	b	604	CLA	MG-ND	-6.54	1.92	2.05
23	B	610	CLA	MG-ND	-6.52	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	CLA	MG-ND	-6.52	1.92	2.05
23	C	510	CLA	MG-NA	6.45	2.21	2.06
23	b	616	CLA	MG-NA	6.43	2.21	2.06
23	B	614	CLA	MG-NA	6.38	2.21	2.06
35	V	201	HEC	CAC-C3C	6.26	1.55	1.35
35	v	201	HEC	CAB-C3B	6.22	1.55	1.35
23	c	506	CLA	MG-NA	6.18	2.21	2.06
23	c	505	CLA	MG-NC	-6.17	1.91	2.06
23	B	602	CLA	MG-ND	6.16	2.18	2.05
23	C	501	CLA	MG-NB	6.13	2.17	2.05
23	b	610	CLA	MG-NA	6.11	2.20	2.06
23	b	615	CLA	MG-ND	-6.11	1.93	2.05
23	C	509	CLA	MG-ND	6.07	2.17	2.05
23	d	404	CLA	MG-NC	-6.07	1.91	2.06
35	v	201	HEC	CAC-C3C	6.06	1.54	1.35
23	b	615	CLA	MG-NA	6.05	2.20	2.06
23	C	505	CLA	MG-NB	-6.01	1.93	2.05
23	c	509	CLA	MG-NB	-6.00	1.93	2.05
23	c	504	CLA	MG-NC	5.96	2.20	2.06
23	a	405	CLA	MG-ND	-5.94	1.94	2.05
23	D	403	CLA	MG-NB	5.91	2.17	2.05
23	c	512	CLA	MG-NC	5.87	2.20	2.06
23	c	504	CLA	MG-NA	-5.82	1.92	2.06
23	c	507	CLA	MG-NB	-5.74	1.94	2.05
23	B	615	CLA	MG-ND	5.59	2.16	2.05
23	C	513	CLA	MG-ND	5.56	2.16	2.05
23	c	504	CLA	MG-NB	5.55	2.16	2.05
23	B	609	CLA	MG-NA	5.54	2.19	2.06
23	b	606	CLA	MG-ND	5.53	2.16	2.05
23	C	510	CLA	MG-NB	5.52	2.16	2.05
35	V	201	HEC	CAB-C3B	5.49	1.52	1.35
29	H	102	DGD	O5D-C1E	5.42	1.49	1.40
23	C	502	CLA	MG-NC	5.40	2.19	2.06
23	c	501	CLA	MG-NA	5.34	2.19	2.06
23	c	504	CLA	MG-ND	-5.34	1.95	2.05
23	D	403	CLA	MG-ND	-5.30	1.95	2.05
23	a	407	CLA	MG-NB	-5.23	1.95	2.05
23	C	508	CLA	MG-NA	5.22	2.18	2.06
23	b	613	CLA	MG-NA	5.16	2.18	2.06
23	b	604	CLA	MG-NA	5.09	2.18	2.06
33	L	101	LHG	O7-C5	-4.97	1.34	1.46
25	b	619	BCR	C30-C25	-4.97	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404	CLA	MG-ND	-4.95	1.96	2.05
26	a	409	PL9	C53-C6	-4.94	1.40	1.50
25	h	102	BCR	C30-C25	-4.94	1.47	1.53
23	C	506	CLA	MG-NB	4.94	2.15	2.05
23	C	508	CLA	MG-ND	4.89	2.15	2.05
34	e	102	HEM	FE-NA	4.82	2.11	1.95
23	B	604	CLA	MG-NA	4.80	2.17	2.06
25	B	619	BCR	C1-C6	-4.79	1.47	1.53
23	D	403	CLA	MG-NA	4.72	2.17	2.06
23	B	604	CLA	MG-NB	4.71	2.15	2.05
23	c	506	CLA	MG-ND	-4.69	1.96	2.05
23	a	404	CLA	MG-NA	4.65	2.17	2.06
23	B	614	CLA	MG-ND	-4.61	1.96	2.05
23	b	616	CLA	MG-NB	4.51	2.14	2.05
23	b	611	CLA	MG-NB	-4.50	1.96	2.05
23	b	609	CLA	MG-NB	4.48	2.14	2.05
25	K	101	BCR	C30-C25	-4.46	1.48	1.53
23	b	613	CLA	MG-NB	-4.44	1.97	2.05
25	K	101	BCR	C1-C6	-4.43	1.48	1.53
23	C	503	CLA	MG-NA	4.38	2.16	2.06
29	C	516	DGD	C4E-C3E	4.36	1.63	1.52
26	D	406	PL9	C6-C1	-4.35	1.41	1.48
23	C	505	CLA	MG-NC	4.34	2.16	2.06
24	d	401	PHO	C1D-C2D	4.31	1.44	1.39
23	c	510	CLA	MG-NC	-4.30	1.96	2.06
23	b	603	CLA	C1D-ND	4.23	1.43	1.37
26	a	409	PL9	C7-C3	4.23	1.56	1.51
23	b	615	CLA	C1D-ND	4.22	1.43	1.37
23	C	506	CLA	MG-NA	4.22	2.16	2.06
34	E	102	HEM	FE-NB	4.17	2.07	1.94
23	B	608	CLA	MG-ND	4.17	2.14	2.05
23	C	502	CLA	MG-NB	-4.15	1.97	2.05
23	c	507	CLA	MG-NA	-4.14	1.96	2.06
25	C	514	BCR	C1-C6	-4.14	1.48	1.53
29	H	102	DGD	O2G-C2G	-4.13	1.36	1.46
25	C	515	BCR	C1-C6	-4.11	1.48	1.53
23	A	407	CLA	MG-NC	-4.10	1.96	2.06
25	T	101	BCR	C30-C25	-4.09	1.48	1.53
25	B	617	BCR	C1-C6	-4.08	1.48	1.53
23	c	508	CLA	MG-NB	4.07	2.13	2.05
23	B	613	CLA	CMD-C2D	-4.06	1.42	1.50
23	B	605	CLA	MG-ND	-4.03	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C4B-NB	4.03	1.43	1.37
23	d	402	CLA	C1D-ND	4.01	1.43	1.37
23	a	407	CLA	C1D-ND	4.01	1.43	1.37
29	H	102	DGD	C4D-C5D	4.01	1.61	1.53
29	H	102	DGD	C1E-C2E	3.96	1.64	1.52
23	b	615	CLA	C4B-NB	3.96	1.43	1.37
29	A	413	DGD	O3G-C1D	3.96	1.46	1.40
23	b	605	CLA	C1D-ND	3.96	1.43	1.37
23	B	615	CLA	CMB-C2B	-3.95	1.42	1.50
35	v	201	HEC	CBB-CAB	-3.94	1.34	1.49
23	h	101	CLA	MG-NA	3.94	2.15	2.06
23	C	501	CLA	C1D-ND	3.91	1.43	1.37
24	a	406	PHO	C1D-C2D	3.91	1.43	1.39
23	A	404	CLA	MG-NA	3.90	2.15	2.06
25	y	101	BCR	C30-C25	-3.89	1.48	1.53
25	b	618	BCR	C30-C25	-3.86	1.48	1.53
23	D	404	CLA	C1D-ND	3.86	1.42	1.37
23	A	404	CLA	MG-NC	-3.86	1.97	2.06
29	C	517	DGD	O2G-C2G	-3.84	1.37	1.46
26	d	406	PL9	C3-C4	-3.81	1.43	1.49
23	c	510	CLA	MG-NA	3.81	2.15	2.06
23	b	613	CLA	MG-NC	-3.80	1.97	2.06
35	V	201	HEC	CBB-CAB	-3.80	1.35	1.49
25	d	405	BCR	C1-C6	-3.79	1.48	1.53
25	c	514	BCR	C1-C6	-3.79	1.48	1.53
23	c	502	CLA	MG-NA	3.78	2.15	2.06
23	B	609	CLA	C1D-ND	3.77	1.42	1.37
23	B	609	CLA	MG-NC	-3.77	1.97	2.06
24	A	406	PHO	C1D-C2D	3.77	1.43	1.39
23	c	509	CLA	C1D-ND	3.74	1.42	1.37
29	H	102	DGD	O5D-C6D	-3.74	1.37	1.43
23	c	506	CLA	C1D-ND	3.73	1.42	1.37
23	b	612	CLA	MG-NB	3.73	2.13	2.05
23	B	616	CLA	MG-NC	3.73	2.15	2.06
27	C	519	LMG	O7-C8	-3.73	1.37	1.46
23	B	606	CLA	C1B-C2B	3.72	1.51	1.43
28	a	411	SQD	O48-C23	3.70	1.44	1.33
29	A	413	DGD	C4D-C5D	3.70	1.60	1.53
29	C	517	DGD	O5D-C1E	3.70	1.46	1.40
23	d	402	CLA	C1B-C2B	3.68	1.51	1.43
28	A	412	SQD	O48-C23	3.68	1.44	1.33
23	B	610	CLA	C4B-NB	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C1D-ND	3.68	1.42	1.37
23	D	402	CLA	MG-NC	-3.67	1.97	2.06
35	V	201	HEC	CBC-CAC	-3.66	1.35	1.49
29	c	518	DGD	C6D-C5D	3.66	1.62	1.51
23	b	613	CLA	C1D-ND	3.65	1.42	1.37
23	c	511	CLA	C4B-NB	3.65	1.42	1.37
23	B	606	CLA	MG-NC	-3.64	1.97	2.06
27	d	409	LMG	O1-C7	-3.62	1.37	1.43
23	C	503	CLA	C1B-C2B	3.62	1.51	1.43
23	C	510	CLA	C1B-C2B	3.61	1.51	1.43
23	A	404	CLA	C1B-C2B	3.61	1.51	1.43
23	C	511	CLA	C1D-ND	3.61	1.42	1.37
23	B	602	CLA	MG-NB	3.61	2.12	2.05
23	B	610	CLA	C1D-ND	3.59	1.42	1.37
25	b	618	BCR	C1-C6	-3.58	1.49	1.53
29	c	518	DGD	C4D-C3D	3.58	1.61	1.52
23	c	504	CLA	C1B-NB	-3.57	1.33	1.37
28	a	412	SQD	O48-C23	3.54	1.43	1.33
23	c	508	CLA	MG-ND	3.54	2.12	2.05
23	D	404	CLA	C4B-NB	3.54	1.42	1.37
27	b	622	LMG	C4-C3	3.51	1.61	1.52
23	B	616	CLA	MG-NA	3.51	2.14	2.06
24	A	406	PHO	C3A-C2A	3.51	1.57	1.54
23	c	509	CLA	C4B-NB	3.51	1.42	1.37
29	A	413	DGD	C1E-C2E	3.50	1.62	1.52
23	a	407	CLA	MG-ND	-3.50	1.98	2.05
23	d	403	CLA	CMB-C2B	-3.50	1.43	1.50
23	B	601	CLA	C4B-NB	3.49	1.42	1.37
28	b	601	SQD	O48-C23	3.49	1.43	1.33
26	D	406	PL9	C11-C9	-3.49	1.44	1.51
28	b	601	SQD	O47-C7	3.48	1.44	1.34
25	B	618	BCR	C30-C25	-3.48	1.49	1.53
23	b	612	CLA	CMD-C2D	-3.47	1.43	1.50
29	c	517	DGD	O3G-C1D	-3.47	1.34	1.40
23	b	613	CLA	MG-ND	-3.46	1.98	2.05
23	C	511	CLA	C1B-C2B	3.46	1.51	1.43
23	d	404	CLA	C4B-NB	3.45	1.42	1.37
23	B	616	CLA	C1D-ND	3.43	1.42	1.37
25	B	617	BCR	C30-C25	-3.43	1.49	1.53
23	b	610	CLA	C1D-ND	3.43	1.42	1.37
23	B	602	CLA	C1B-C2B	3.42	1.51	1.43
23	C	513	CLA	MG-NB	-3.42	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C1B-C2B	3.42	1.51	1.43
24	d	401	PHO	C4D-ND	-3.42	1.33	1.38
29	C	517	DGD	C4D-C3D	3.41	1.61	1.52
23	b	614	CLA	MG-NA	3.41	2.14	2.06
23	b	605	CLA	MG-NC	3.40	2.14	2.06
23	B	601	CLA	MG-ND	-3.40	1.99	2.05
23	b	605	CLA	MG-ND	-3.40	1.99	2.05
23	B	616	CLA	C4B-NB	3.40	1.42	1.37
23	b	609	CLA	CHC-C1C	3.39	1.45	1.38
33	D	409	LHG	P-O6	3.39	1.72	1.59
23	a	407	CLA	CMC-C2C	-3.38	1.43	1.50
23	A	407	CLA	CMD-C2D	-3.38	1.43	1.50
27	d	409	LMG	O7-C8	-3.35	1.38	1.46
23	B	602	CLA	C4B-NB	3.35	1.42	1.37
29	c	516	DGD	O3G-C3G	-3.33	1.38	1.43
23	h	101	CLA	C4B-NB	3.33	1.42	1.37
25	h	102	BCR	C1-C6	-3.32	1.49	1.53
23	c	509	CLA	CHC-C1C	3.31	1.45	1.38
33	d	408	LHG	P-O6	3.31	1.72	1.59
23	C	502	CLA	C1D-ND	3.30	1.42	1.37
23	B	601	CLA	C1D-ND	3.30	1.42	1.37
23	a	405	CLA	MG-NA	3.29	2.14	2.06
28	a	412	SQD	O47-C7	3.28	1.43	1.34
33	D	408	LHG	O8-C6	-3.28	1.37	1.45
25	H	101	BCR	C30-C25	-3.28	1.49	1.53
23	b	603	CLA	C1B-C2B	3.28	1.50	1.43
25	C	514	BCR	C30-C25	-3.27	1.49	1.53
23	b	611	CLA	MG-NC	3.27	2.14	2.06
23	h	101	CLA	C1B-C2B	3.27	1.50	1.43
23	B	606	CLA	C1D-ND	3.27	1.42	1.37
23	b	617	CLA	C1D-ND	3.26	1.42	1.37
23	b	610	CLA	C4B-NB	3.26	1.42	1.37
23	B	607	CLA	CHC-C4B	-3.25	1.32	1.39
23	B	605	CLA	C1B-C2B	3.25	1.50	1.43
23	C	513	CLA	C1D-ND	3.24	1.42	1.37
23	b	612	CLA	MG-NC	-3.24	1.98	2.06
23	A	407	CLA	CMB-C2B	-3.23	1.44	1.50
25	a	408	BCR	C1-C6	-3.23	1.49	1.53
23	C	502	CLA	C4B-NB	3.23	1.42	1.37
29	H	102	DGD	C4E-C5E	3.21	1.59	1.53
29	a	413	DGD	O2G-C1B	3.21	1.43	1.34
23	B	609	CLA	MG-NB	-3.21	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3B-C4B	3.20	1.52	1.42
23	a	404	CLA	C1B-C2B	3.20	1.50	1.43
25	a	408	BCR	C30-C25	-3.20	1.49	1.53
28	A	412	SQD	O47-C7	3.19	1.43	1.34
23	B	616	CLA	C1B-C2B	3.19	1.50	1.43
29	c	518	DGD	O2E-C2E	-3.19	1.35	1.43
23	b	607	CLA	C1B-C2B	3.19	1.50	1.43
35	v	201	HEC	CBC-CAC	-3.19	1.37	1.49
28	f	101	SQD	O47-C7	3.18	1.43	1.34
28	A	411	SQD	O48-C23	3.18	1.42	1.33
23	b	611	CLA	CMD-C2D	-3.18	1.44	1.50
28	F	101	SQD	O48-C23	3.17	1.42	1.33
23	B	608	CLA	CMD-C2D	-3.17	1.44	1.50
26	d	406	PL9	C16-C14	-3.17	1.44	1.51
23	B	608	CLA	C1B-NB	-3.16	1.33	1.37
29	c	516	DGD	O5D-C6D	-3.16	1.38	1.43
25	c	514	BCR	C30-C25	-3.15	1.49	1.53
29	C	516	DGD	O2E-C2E	-3.15	1.35	1.43
23	A	404	CLA	C4B-NB	3.15	1.42	1.37
23	C	504	CLA	C1B-NB	-3.14	1.33	1.37
25	b	620	BCR	C30-C25	-3.14	1.49	1.53
29	a	413	DGD	O1G-C1A	3.14	1.42	1.33
33	E	101	LHG	O8-C23	3.14	1.42	1.33
23	h	101	CLA	C1D-ND	3.13	1.42	1.37
23	B	615	CLA	C1B-C2B	3.13	1.50	1.43
27	c	522	LMG	C4-C3	3.11	1.60	1.52
29	c	517	DGD	C4E-C3E	3.10	1.60	1.52
23	c	511	CLA	C1B-C2B	3.10	1.50	1.43
23	B	610	CLA	MG-NA	3.10	2.13	2.06
25	D	405	BCR	C1-C6	-3.10	1.49	1.53
29	c	517	DGD	O4E-C4E	-3.10	1.35	1.43
23	b	603	CLA	C4B-NB	3.09	1.41	1.37
27	b	622	LMG	O6-C1	3.09	1.49	1.41
23	B	613	CLA	C1D-ND	3.09	1.41	1.37
29	H	102	DGD	O1G-C1G	-3.08	1.38	1.45
24	D	401	PHO	C1D-C2D	3.08	1.43	1.39
23	C	504	CLA	MG-NA	3.08	2.13	2.06
23	c	508	CLA	C1B-C2B	3.08	1.50	1.43
25	b	619	BCR	C1-C6	-3.08	1.49	1.53
23	c	511	CLA	C1D-ND	3.08	1.41	1.37
23	C	505	CLA	C4B-NB	3.07	1.41	1.37
23	B	606	CLA	C4B-NB	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C1B-C2B	3.06	1.50	1.43
27	c	522	LMG	O1-C1	3.06	1.45	1.40
23	B	604	CLA	C1D-ND	3.05	1.41	1.37
26	d	406	PL9	C30-C29	-3.05	1.43	1.50
23	c	513	CLA	MG-NC	-3.04	1.99	2.06
23	A	404	CLA	C3B-C4B	3.04	1.51	1.42
28	B	623	SQD	O47-C7	3.04	1.42	1.34
28	A	411	SQD	O47-C7	3.03	1.42	1.34
29	h	103	DGD	O5D-C6D	-3.02	1.38	1.43
23	c	508	CLA	C3B-C4B	3.02	1.51	1.42
24	d	401	PHO	CAC-C3C	-3.02	1.46	1.51
29	c	516	DGD	C4D-C3D	3.02	1.60	1.52
23	c	511	CLA	MG-NC	3.01	2.13	2.06
34	E	102	HEM	FE-NC	3.01	2.05	1.95
23	b	616	CLA	CAA-C2A	-3.01	1.48	1.54
23	D	403	CLA	C1B-C2B	3.00	1.50	1.43
23	B	604	CLA	CHC-C1C	3.00	1.44	1.38
23	B	613	CLA	C1B-C2B	3.00	1.50	1.43
23	B	605	CLA	MG-NC	-3.00	1.99	2.06
23	b	610	CLA	C1B-C2B	2.99	1.50	1.43
24	d	401	PHO	C4D-CHA	2.99	1.44	1.39
29	C	518	DGD	O2G-C2G	-2.99	1.39	1.46
23	b	616	CLA	CMC-C2C	-2.98	1.44	1.50
23	D	403	CLA	C1D-ND	2.98	1.41	1.37
23	b	616	CLA	C3B-C4B	2.98	1.51	1.42
23	B	603	CLA	CMC-C2C	-2.98	1.44	1.50
33	d	407	LHG	O7-C5	-2.98	1.39	1.46
29	H	102	DGD	O2D-C2D	-2.98	1.35	1.43
29	C	517	DGD	C1E-C2E	2.97	1.61	1.52
23	C	507	CLA	C1B-NB	-2.96	1.34	1.37
23	B	603	CLA	C1B-C2B	2.96	1.50	1.43
23	b	617	CLA	C4B-NB	2.95	1.41	1.37
23	C	510	CLA	C4B-NB	2.95	1.41	1.37
25	c	515	BCR	C1-C6	-2.94	1.50	1.53
23	D	402	CLA	C1B-NB	-2.94	1.34	1.37
23	b	612	CLA	C1B-C2B	2.94	1.50	1.43
23	B	607	CLA	CMB-C2B	-2.93	1.44	1.50
23	a	407	CLA	CHC-C4B	-2.93	1.32	1.39
27	B	620	LMG	C1-C2	2.93	1.61	1.52
23	C	506	CLA	C1B-NB	-2.93	1.34	1.37
29	C	516	DGD	O2G-C2G	-2.92	1.39	1.46
28	A	412	SQD	O47-C45	-2.92	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	DGD	C1D-C2D	2.92	1.61	1.52
29	c	516	DGD	O2E-C2E	-2.92	1.35	1.43
23	C	508	CLA	C1D-ND	2.91	1.41	1.37
23	c	513	CLA	CMB-C2B	-2.91	1.44	1.50
25	d	405	BCR	C30-C25	-2.91	1.50	1.53
23	b	606	CLA	C4B-NB	2.91	1.41	1.37
23	B	616	CLA	MG-ND	2.91	2.11	2.05
29	a	413	DGD	C2B-C1B	2.91	1.59	1.50
25	B	619	BCR	C30-C25	-2.91	1.50	1.53
23	B	607	CLA	MG-NA	2.90	2.13	2.06
25	c	515	BCR	C30-C25	-2.90	1.50	1.53
23	B	611	CLA	C1D-ND	2.90	1.41	1.37
23	c	504	CLA	C4B-NB	2.90	1.41	1.37
23	a	404	CLA	C3B-C4B	2.89	1.51	1.42
23	C	503	CLA	MG-ND	2.89	2.11	2.05
25	C	520	BCR	C30-C25	-2.89	1.50	1.53
23	C	507	CLA	C1B-C2B	2.89	1.49	1.43
29	C	518	DGD	O4E-C4E	-2.88	1.35	1.43
23	B	610	CLA	CMD-C2D	-2.88	1.44	1.50
23	a	407	CLA	C1B-NB	-2.88	1.34	1.37
23	C	507	CLA	C1D-ND	2.88	1.41	1.37
23	D	404	CLA	CMD-C2D	-2.87	1.44	1.50
23	D	402	CLA	MG-ND	2.86	2.11	2.05
23	A	405	CLA	CMB-C2B	-2.86	1.44	1.50
25	D	405	BCR	C30-C25	-2.86	1.50	1.53
23	b	617	CLA	CMD-C2D	-2.86	1.44	1.50
23	b	616	CLA	C4B-NB	2.85	1.41	1.37
23	c	512	CLA	C4B-NB	2.84	1.41	1.37
23	c	512	CLA	MG-NB	2.84	2.11	2.05
23	b	605	CLA	CHC-C1C	2.83	1.44	1.38
23	b	607	CLA	C1D-ND	2.83	1.41	1.37
23	c	513	CLA	C1B-C2B	2.83	1.49	1.43
29	c	516	DGD	O2G-C2G	-2.83	1.39	1.46
26	A	409	PL9	C53-C6	-2.83	1.45	1.50
23	B	605	CLA	CHC-C1C	2.82	1.44	1.38
23	a	404	CLA	CHC-C1C	2.82	1.44	1.38
23	d	404	CLA	CMD-C2D	-2.82	1.45	1.50
28	f	101	SQD	O48-C23	2.82	1.41	1.33
27	c	522	LMG	C7-C8	2.82	1.59	1.50
33	D	408	LHG	C24-C23	2.82	1.58	1.50
23	D	402	CLA	C1B-C2B	2.82	1.49	1.43
23	C	505	CLA	C1B-C2B	2.82	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C1D-ND	2.82	1.41	1.37
23	B	603	CLA	C1D-ND	2.81	1.41	1.37
23	B	606	CLA	CHC-C1C	2.81	1.44	1.38
23	d	404	CLA	CMB-C2B	-2.81	1.45	1.50
23	b	614	CLA	MG-ND	-2.81	2.00	2.05
25	B	618	BCR	C1-C6	-2.80	1.50	1.53
23	b	606	CLA	CHC-C1C	2.80	1.44	1.38
25	b	620	BCR	C1-C6	-2.80	1.50	1.53
27	d	409	LMG	O4-C4	-2.80	1.36	1.43
25	C	515	BCR	C30-C25	-2.79	1.50	1.53
23	c	503	CLA	C4B-NB	2.79	1.41	1.37
26	a	409	PL9	C6-C1	-2.79	1.43	1.48
27	c	522	LMG	C3-C2	2.79	1.59	1.52
23	C	513	CLA	C1B-C2B	2.79	1.49	1.43
23	B	607	CLA	C1D-ND	2.78	1.41	1.37
23	b	614	CLA	CMB-C2B	-2.78	1.45	1.50
28	A	411	SQD	O2-C2	-2.78	1.36	1.43
23	b	617	CLA	CMB-C2B	-2.77	1.45	1.50
23	b	608	CLA	C1B-NB	-2.77	1.34	1.37
29	c	518	DGD	O1G-C1G	-2.77	1.39	1.45
23	b	607	CLA	MG-NC	-2.77	1.99	2.06
24	D	401	PHO	C4D-ND	-2.77	1.34	1.38
23	C	512	CLA	C1B-C2B	2.77	1.49	1.43
23	c	513	CLA	MG-NA	2.77	2.12	2.06
29	c	518	DGD	O3G-C3G	-2.77	1.39	1.43
25	A	408	BCR	C1-C6	-2.76	1.50	1.53
23	B	611	CLA	CMD-C2D	-2.76	1.45	1.50
24	D	401	PHO	CMD-C2D	-2.76	1.46	1.51
23	B	602	CLA	C3B-C4B	2.76	1.50	1.42
23	c	501	CLA	C1D-ND	2.76	1.41	1.37
33	d	407	LHG	P-O3	2.76	1.70	1.59
24	a	406	PHO	CMC-C2C	-2.75	1.46	1.50
26	D	406	PL9	C5-C4	-2.75	1.37	1.47
23	A	407	CLA	C1D-ND	2.75	1.41	1.37
27	c	519	LMG	C7-C8	2.74	1.59	1.50
23	b	606	CLA	C1B-C2B	2.74	1.49	1.43
29	C	518	DGD	C1G-C2G	2.74	1.59	1.50
23	b	614	CLA	CMD-C2D	-2.74	1.45	1.50
34	E	102	HEM	CAB-C3B	2.73	1.54	1.47
23	C	506	CLA	C1B-C2B	2.73	1.49	1.43
27	D	410	LMG	C7-C8	2.73	1.57	1.51
23	d	404	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	MG-NC	2.73	2.12	2.06
23	B	602	CLA	C1D-ND	2.72	1.41	1.37
23	B	607	CLA	C1B-NB	-2.72	1.34	1.37
24	d	401	PHO	CMC-C2C	-2.72	1.46	1.50
26	D	406	PL9	C3-C4	-2.72	1.45	1.49
24	a	406	PHO	C3D-C4D	2.71	1.44	1.41
23	d	403	CLA	C1B-C2B	2.71	1.49	1.43
23	B	615	CLA	C1B-NB	-2.71	1.34	1.37
23	b	604	CLA	C4B-NB	2.71	1.41	1.37
23	c	503	CLA	MG-NC	2.71	2.12	2.06
23	B	609	CLA	C1B-C2B	2.71	1.49	1.43
33	D	408	LHG	P-O3	2.70	1.70	1.59
27	a	414	LMG	O8-C9	-2.70	1.39	1.45
23	B	614	CLA	CMB-C2B	-2.70	1.45	1.50
23	d	402	CLA	CMB-C2B	-2.70	1.45	1.50
23	b	616	CLA	CMD-C2D	-2.70	1.45	1.50
23	c	508	CLA	CHC-C1C	2.69	1.43	1.38
23	c	501	CLA	C1B-C2B	2.69	1.49	1.43
23	c	507	CLA	CHC-C4B	-2.69	1.33	1.39
34	e	102	HEM	CAB-C3B	2.69	1.54	1.47
23	h	101	CLA	CMC-C2C	-2.69	1.45	1.50
27	b	622	LMG	C6-C5	2.68	1.60	1.51
23	b	612	CLA	C1B-NB	-2.68	1.34	1.37
27	m	101	LMG	C4-C3	2.68	1.59	1.52
23	b	616	CLA	MG-ND	-2.68	2.00	2.05
23	C	512	CLA	C1D-ND	2.68	1.41	1.37
23	c	510	CLA	C1D-ND	2.67	1.41	1.37
23	C	510	CLA	CHC-C1C	2.67	1.43	1.38
23	B	611	CLA	C1B-C2B	2.67	1.49	1.43
26	d	406	PL9	C45-C44	-2.67	1.44	1.50
23	b	616	CLA	C1D-ND	2.67	1.41	1.37
24	a	406	PHO	C1D-ND	2.67	1.43	1.38
23	b	604	CLA	CMA-C3A	-2.66	1.47	1.53
23	c	511	CLA	CHC-C1C	2.66	1.43	1.38
23	B	616	CLA	CMD-C2D	-2.66	1.45	1.50
23	c	503	CLA	C1D-ND	2.66	1.41	1.37
29	c	516	DGD	C2B-C1B	-2.66	1.43	1.50
23	C	504	CLA	CMB-C2B	-2.66	1.45	1.50
23	a	405	CLA	C1D-ND	2.66	1.41	1.37
23	c	504	CLA	CHC-C1C	2.66	1.43	1.38
23	a	407	CLA	CMB-C2B	-2.66	1.45	1.50
25	t	101	BCR	C30-C25	-2.66	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C1B-C2B	2.66	1.49	1.43
23	c	506	CLA	CAC-C3C	-2.65	1.44	1.51
23	b	608	CLA	MG-NB	-2.65	2.00	2.05
23	c	508	CLA	C1D-ND	2.65	1.41	1.37
23	C	512	CLA	CHC-C1C	2.65	1.43	1.38
23	C	502	CLA	CMB-C2B	-2.65	1.45	1.50
34	E	102	HEM	CAC-C3C	2.65	1.54	1.47
23	B	609	CLA	O2D-CGD	2.65	1.39	1.33
23	c	505	CLA	C1B-C2B	2.65	1.49	1.43
23	B	603	CLA	C1B-NB	-2.65	1.34	1.37
23	D	404	CLA	CMB-C2B	-2.64	1.45	1.50
27	A	410	LMG	C7-C8	2.64	1.59	1.50
25	y	101	BCR	C1-C6	-2.64	1.50	1.53
23	B	603	CLA	CMA-C3A	-2.64	1.47	1.53
23	B	615	CLA	CHC-C1C	2.64	1.43	1.38
23	c	506	CLA	CMD-C2D	-2.63	1.45	1.50
23	b	613	CLA	C3B-C4B	2.63	1.50	1.42
23	B	616	CLA	CMC-C2C	-2.63	1.45	1.50
24	a	406	PHO	CMB-C2B	-2.63	1.46	1.51
29	c	516	DGD	O3D-C3D	-2.62	1.36	1.43
23	b	604	CLA	CMB-C2B	-2.62	1.45	1.50
23	B	608	CLA	CHC-C1C	2.62	1.43	1.38
23	c	505	CLA	C3B-C4B	2.62	1.50	1.42
25	T	101	BCR	C1-C6	-2.62	1.50	1.53
23	c	512	CLA	CMB-C2B	-2.62	1.45	1.50
23	c	512	CLA	CMD-C2D	-2.62	1.45	1.50
24	A	406	PHO	C3D-C4D	2.62	1.44	1.41
23	c	512	CLA	C1B-C2B	2.62	1.49	1.43
23	C	511	CLA	CMB-C2B	-2.61	1.45	1.50
24	A	406	PHO	CMC-C2C	-2.61	1.46	1.50
25	C	515	BCR	C33-C5	-2.61	1.46	1.50
23	C	509	CLA	C1B-C2B	2.61	1.49	1.43
25	c	515	BCR	C33-C5	-2.61	1.46	1.50
23	B	601	CLA	C1B-C2B	2.60	1.49	1.43
23	B	615	CLA	C4B-NB	2.60	1.41	1.37
23	A	405	CLA	C1B-C2B	2.60	1.49	1.43
23	B	613	CLA	C4B-NB	2.60	1.41	1.37
33	E	101	LHG	C24-C23	2.60	1.58	1.50
29	C	518	DGD	O3G-C3G	-2.60	1.39	1.43
29	H	102	DGD	C6D-C5D	2.59	1.59	1.51
23	a	404	CLA	MG-ND	2.59	2.10	2.05
23	D	402	CLA	C3B-C4B	2.59	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	517	DGD	O3E-C3E	-2.58	1.36	1.43
23	C	511	CLA	C3B-C4B	2.58	1.50	1.42
23	b	605	CLA	C3D-C4D	2.58	1.50	1.44
23	c	507	CLA	C1D-ND	2.58	1.41	1.37
23	c	507	CLA	C1B-C2B	2.58	1.49	1.43
23	C	509	CLA	C3B-C4B	2.58	1.50	1.42
23	B	608	CLA	CMC-C2C	-2.57	1.45	1.50
23	b	608	CLA	C1D-ND	2.57	1.41	1.37
27	D	410	LMG	C9-C8	2.57	1.58	1.50
23	B	604	CLA	MG-NC	2.57	2.12	2.06
23	C	501	CLA	C1B-C2B	2.57	1.49	1.43
29	A	413	DGD	C3E-C2E	2.57	1.59	1.52
23	a	405	CLA	CMB-C2B	-2.57	1.45	1.50
23	c	501	CLA	CHC-C4B	-2.57	1.33	1.39
33	E	101	LHG	P-O6	2.56	1.69	1.59
33	e	101	LHG	O7-C5	-2.56	1.40	1.46
29	A	413	DGD	C4E-C5E	2.56	1.58	1.53
27	c	522	LMG	C9-C8	2.56	1.58	1.50
34	e	102	HEM	CMC-C2C	2.56	1.56	1.50
23	B	613	CLA	OBD-CAD	2.56	1.26	1.22
23	B	612	CLA	CHC-C4B	-2.55	1.33	1.39
27	c	519	LMG	C4-C5	2.55	1.58	1.53
23	a	404	CLA	C1D-ND	2.55	1.41	1.37
23	B	611	CLA	MG-NC	-2.54	2.00	2.06
23	B	606	CLA	MG-ND	-2.54	2.00	2.05
29	C	516	DGD	O2D-C2D	-2.54	1.36	1.43
23	C	506	CLA	C4B-NB	2.54	1.41	1.37
23	b	609	CLA	C1B-C2B	2.53	1.49	1.43
23	c	513	CLA	C1D-ND	2.53	1.41	1.37
27	m	101	LMG	O1-C7	-2.53	1.39	1.43
23	b	605	CLA	CMB-C2B	-2.53	1.45	1.50
23	b	605	CLA	CMC-C2C	-2.53	1.45	1.50
23	b	613	CLA	CMC-C2C	-2.53	1.45	1.50
28	F	101	SQD	O3-C3	-2.53	1.36	1.43
29	C	516	DGD	O5D-C1E	2.53	1.44	1.40
23	b	617	CLA	C1B-C2B	2.52	1.49	1.43
24	D	401	PHO	CMC-C2C	-2.52	1.46	1.50
35	V	201	HEC	C3D-C2D	-2.52	1.32	1.38
23	b	611	CLA	C1B-C2B	2.52	1.49	1.43
23	B	609	CLA	CMC-C2C	-2.52	1.45	1.50
26	a	409	PL9	C10-C9	-2.52	1.44	1.50
23	b	616	CLA	CHC-C1C	2.52	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	CMC-C2C	-2.52	1.45	1.50
23	b	604	CLA	CMD-C2D	-2.52	1.45	1.50
23	c	511	CLA	C3B-C4B	2.52	1.50	1.42
34	e	102	HEM	CAC-C3C	2.51	1.54	1.47
23	c	509	CLA	C3C-C2C	2.51	1.42	1.36
23	b	606	CLA	CHC-C4B	-2.51	1.33	1.39
23	B	610	CLA	C1B-NB	-2.51	1.34	1.37
23	C	501	CLA	C4B-NB	2.50	1.41	1.37
28	B	623	SQD	O48-C23	2.50	1.40	1.33
23	B	610	CLA	C1B-C2B	2.50	1.49	1.43
24	A	406	PHO	O2D-CGD	2.50	1.39	1.33
23	d	403	CLA	MG-ND	-2.50	2.00	2.05
23	A	404	CLA	C1D-ND	2.50	1.41	1.37
29	c	518	DGD	O3D-C3D	-2.50	1.36	1.43
23	b	609	CLA	C4B-NB	2.50	1.41	1.37
23	h	101	CLA	MG-NB	-2.50	2.00	2.05
23	C	510	CLA	O2A-CGA	2.50	1.40	1.33
23	B	610	CLA	C3D-C4D	2.49	1.49	1.44
23	C	501	CLA	CMD-C2D	-2.48	1.45	1.50
23	b	609	CLA	C3B-C4B	2.48	1.50	1.42
27	C	519	LMG	C4-C5	2.48	1.58	1.53
25	b	618	BCR	C33-C5	-2.48	1.47	1.50
26	d	406	PL9	C46-C44	-2.48	1.46	1.51
23	b	611	CLA	CMB-C2B	-2.48	1.45	1.50
27	A	410	LMG	C4-C3	2.47	1.58	1.52
23	B	604	CLA	C3B-C4B	2.47	1.49	1.42
23	B	605	CLA	C1D-ND	2.47	1.41	1.37
23	A	405	CLA	C1D-ND	2.47	1.41	1.37
29	C	517	DGD	C4E-C5E	2.47	1.58	1.53
23	B	609	CLA	CMD-C2D	-2.47	1.45	1.50
24	D	401	PHO	CBD-CGD	-2.46	1.49	1.52
35	V	201	HEC	C3B-C2B	-2.46	1.32	1.41
23	B	608	CLA	C1B-C2B	2.46	1.48	1.43
23	B	613	CLA	C1C-NC	-2.46	1.34	1.37
35	v	201	HEC	C3D-C2D	-2.45	1.32	1.38
23	A	405	CLA	CMD-C2D	-2.45	1.45	1.50
23	B	607	CLA	CAC-C3C	-2.45	1.44	1.51
27	D	411	LMG	O8-C28	2.45	1.38	1.30
23	c	509	CLA	C1B-C2B	2.44	1.48	1.43
23	c	501	CLA	CMC-C2C	-2.44	1.45	1.50
23	C	512	CLA	C1D-C2D	2.44	1.50	1.45
25	c	521	BCR	C30-C25	-2.44	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	619	BCR	C33-C5	-2.43	1.47	1.50
23	C	510	CLA	C3B-C4B	2.43	1.49	1.42
23	c	511	CLA	CMB-C2B	-2.43	1.45	1.50
23	B	604	CLA	C1B-C2B	2.43	1.48	1.43
29	c	517	DGD	C6E-C5E	2.43	1.59	1.51
27	b	622	LMG	C7-C8	2.43	1.58	1.50
33	D	409	LHG	C4-C5	2.42	1.58	1.50
23	b	614	CLA	C4B-NB	2.42	1.41	1.37
23	b	611	CLA	C1C-NC	-2.42	1.34	1.37
23	b	605	CLA	MG-NA	2.42	2.12	2.06
25	B	617	BCR	C33-C5	-2.42	1.47	1.50
23	b	604	CLA	MG-NC	-2.42	2.00	2.06
33	l	101	LHG	C8-C7	-2.42	1.43	1.50
23	B	612	CLA	C1D-ND	2.41	1.41	1.37
23	B	608	CLA	C3B-C4B	2.41	1.49	1.42
23	B	601	CLA	MG-NC	2.41	2.12	2.06
23	c	502	CLA	C1B-C2B	2.41	1.48	1.43
23	B	605	CLA	CMB-C2B	-2.41	1.45	1.50
23	a	407	CLA	C1B-C2B	2.41	1.48	1.43
23	c	513	CLA	C3B-C4B	2.40	1.49	1.42
25	a	408	BCR	C33-C5	-2.40	1.47	1.50
23	b	608	CLA	C3B-C4B	2.40	1.49	1.42
24	A	406	PHO	C4D-ND	-2.40	1.34	1.38
23	c	513	CLA	C1B-NB	-2.40	1.34	1.37
23	c	510	CLA	C1B-NB	-2.40	1.34	1.37
23	C	502	CLA	MG-NA	-2.39	2.00	2.06
28	a	411	SQD	O47-C7	2.39	1.41	1.34
23	C	505	CLA	C4C-C3C	2.39	1.49	1.45
33	d	407	LHG	C3-C2	2.39	1.59	1.51
23	D	402	CLA	MG-NB	2.39	2.10	2.05
25	t	101	BCR	C33-C5	-2.39	1.47	1.50
23	b	612	CLA	CHC-C1C	2.38	1.43	1.38
23	c	513	CLA	C4B-NB	2.38	1.41	1.37
23	A	404	CLA	C5-C3	-2.38	1.46	1.51
23	c	512	CLA	CHC-C1C	2.38	1.43	1.38
23	b	606	CLA	C3B-C4B	2.38	1.49	1.42
23	B	614	CLA	CMC-C2C	-2.38	1.45	1.50
23	C	502	CLA	C3B-C4B	2.37	1.49	1.42
23	b	610	CLA	CMC-C2C	-2.37	1.45	1.50
29	c	517	DGD	O1G-C1A	2.37	1.40	1.33
23	b	615	CLA	CHC-C1C	2.37	1.43	1.38
23	C	503	CLA	C1B-NB	-2.37	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	PHO	CAC-C3C	-2.37	1.47	1.51
29	A	413	DGD	C3G-C2G	2.37	1.58	1.50
23	C	505	CLA	O1D-CGD	2.37	1.27	1.21
23	B	607	CLA	O2D-CGD	2.37	1.39	1.33
24	a	406	PHO	CMD-C2D	-2.36	1.46	1.51
23	B	603	CLA	O2D-CGD	2.36	1.39	1.33
23	b	608	CLA	C1B-C2B	2.36	1.48	1.43
35	V	201	HEC	CMB-C2B	2.36	1.55	1.50
29	c	516	DGD	C4E-C3E	2.36	1.58	1.52
23	b	604	CLA	CMC-C2C	-2.36	1.45	1.50
35	v	201	HEC	C3B-C2B	-2.36	1.33	1.41
23	b	604	CLA	MG-NB	2.36	2.10	2.05
23	B	601	CLA	CMD-C2D	-2.35	1.45	1.50
23	B	613	CLA	MG-NC	2.35	2.11	2.06
23	B	605	CLA	O2D-CED	-2.35	1.40	1.45
23	b	614	CLA	MG-NB	-2.35	2.01	2.05
23	C	511	CLA	CMC-C2C	-2.35	1.46	1.50
29	A	413	DGD	O5D-C1E	2.35	1.44	1.40
23	C	508	CLA	C1B-C2B	2.35	1.48	1.43
33	D	409	LHG	O3-C3	-2.34	1.35	1.44
23	C	507	CLA	MG-NA	2.34	2.11	2.06
23	C	506	CLA	CMD-C2D	-2.34	1.46	1.50
23	b	616	CLA	CMB-C2B	-2.34	1.46	1.50
27	C	519	LMG	C3-C2	2.34	1.58	1.52
23	b	603	CLA	MG-NA	2.34	2.11	2.06
24	D	401	PHO	C4D-CHA	2.34	1.43	1.39
23	b	610	CLA	MG-ND	-2.34	2.01	2.05
33	D	408	LHG	O7-C5	-2.34	1.41	1.46
24	a	406	PHO	C4D-CHA	2.34	1.43	1.39
29	c	518	DGD	C1D-C2D	2.33	1.59	1.52
23	D	402	CLA	C1D-C2D	2.33	1.50	1.45
23	A	404	CLA	MG-ND	2.33	2.10	2.05
23	d	402	CLA	C1B-NB	-2.33	1.34	1.37
24	A	406	PHO	CMB-C2B	-2.33	1.47	1.51
23	c	508	CLA	CMC-C2C	-2.33	1.46	1.50
25	c	515	BCR	C36-C18	-2.33	1.46	1.50
23	C	505	CLA	CMB-C2B	-2.33	1.46	1.50
28	a	411	SQD	O2-C2	-2.33	1.37	1.43
23	B	610	CLA	CMB-C2B	-2.33	1.46	1.50
27	c	522	LMG	O6-C5	-2.33	1.38	1.44
29	A	413	DGD	C6E-C5E	2.33	1.59	1.51
27	C	519	LMG	O8-C9	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	CHC-C1C	2.32	1.43	1.38
34	e	102	HEM	C2A-C3A	-2.32	1.32	1.38
23	A	407	CLA	MG-NA	-2.32	2.00	2.06
27	b	623	LMG	O7-C10	2.32	1.38	1.30
23	B	605	CLA	CMC-C2C	-2.31	1.46	1.50
23	b	603	CLA	CAC-C3C	-2.31	1.45	1.51
23	B	610	CLA	CHC-C1C	2.31	1.43	1.38
23	B	611	CLA	CMB-C2B	-2.31	1.46	1.50
23	B	614	CLA	CHC-C1C	2.31	1.43	1.38
25	A	408	BCR	C33-C5	-2.31	1.47	1.50
23	C	504	CLA	C3B-C4B	2.31	1.49	1.42
23	B	602	CLA	CMD-C2D	-2.31	1.46	1.50
23	A	405	CLA	CHC-C4B	-2.30	1.34	1.39
23	c	513	CLA	CHC-C1C	2.30	1.43	1.38
23	B	601	CLA	MG-NB	-2.30	2.01	2.05
28	a	411	SQD	O47-C45	-2.30	1.41	1.46
23	C	513	CLA	C3B-C4B	2.30	1.49	1.42
29	h	103	DGD	C3D-C2D	2.30	1.58	1.52
23	d	403	CLA	C1D-ND	2.29	1.40	1.37
23	B	603	CLA	MG-ND	2.29	2.10	2.05
29	C	517	DGD	O3E-C3E	-2.29	1.37	1.43
23	C	503	CLA	MG-NB	2.29	2.10	2.05
23	c	501	CLA	C4B-NB	2.29	1.40	1.37
24	a	406	PHO	CAC-C3C	-2.29	1.47	1.51
25	C	515	BCR	C38-C26	-2.29	1.47	1.50
29	c	517	DGD	O1G-C1G	-2.29	1.40	1.45
23	C	511	CLA	C4B-NB	2.29	1.40	1.37
28	a	411	SQD	O5-C5	-2.29	1.38	1.44
23	C	509	CLA	CMB-C2B	-2.29	1.46	1.50
33	l	101	LHG	O8-C23	2.28	1.40	1.33
27	B	620	LMG	C9-C8	2.28	1.58	1.50
26	D	406	PL9	C27-C28	-2.28	1.43	1.50
23	c	505	CLA	MG-ND	2.28	2.10	2.05
33	B	622	LHG	O6-C4	-2.28	1.36	1.44
27	c	522	LMG	C1-C2	2.28	1.59	1.52
24	a	406	PHO	C1A-C2A	2.27	1.54	1.51
33	a	410	LHG	O7-C5	-2.27	1.41	1.46
23	a	405	CLA	C1B-C2B	2.27	1.48	1.43
24	A	406	PHO	CMD-C2D	-2.27	1.47	1.51
23	D	402	CLA	C1D-ND	2.27	1.40	1.37
23	c	512	CLA	C3B-C4B	2.27	1.49	1.42
23	c	501	CLA	CMB-C2B	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C1D-ND	2.27	1.40	1.37
24	d	401	PHO	CMD-C2D	-2.26	1.47	1.51
23	C	509	CLA	C4B-NB	2.26	1.40	1.37
23	B	609	CLA	C3B-C4B	2.26	1.49	1.42
23	B	614	CLA	C1B-C2B	2.26	1.48	1.43
23	C	507	CLA	CMB-C2B	-2.26	1.46	1.50
23	c	511	CLA	C1B-NB	-2.26	1.34	1.37
23	B	601	CLA	CMB-C2B	-2.26	1.46	1.50
23	a	405	CLA	CMD-C2D	-2.26	1.46	1.50
23	B	605	CLA	CMD-C2D	-2.26	1.46	1.50
23	B	601	CLA	CMC-C2C	-2.26	1.46	1.50
23	d	403	CLA	C4B-NB	2.25	1.40	1.37
27	c	522	LMG	C4-C5	2.25	1.57	1.53
23	B	606	CLA	MG-NB	2.25	2.10	2.05
23	B	602	CLA	CAC-C3C	-2.25	1.45	1.51
23	b	604	CLA	C3B-C4B	2.25	1.49	1.42
29	C	518	DGD	C4D-C5D	2.25	1.57	1.53
29	C	516	DGD	O3E-C3E	-2.25	1.37	1.43
23	c	513	CLA	CMD-C2D	-2.25	1.46	1.50
23	B	603	CLA	MG-NC	2.24	2.11	2.06
23	A	405	CLA	CHC-C1C	2.24	1.43	1.38
29	H	102	DGD	C6E-C5E	2.24	1.59	1.51
29	c	516	DGD	O1G-C1G	-2.24	1.40	1.45
23	b	613	CLA	CMB-C2B	-2.23	1.46	1.50
23	B	604	CLA	CMC-C2C	-2.23	1.46	1.50
23	B	613	CLA	C5-C3	-2.23	1.46	1.51
23	b	614	CLA	C5-C3	-2.23	1.46	1.51
23	C	510	CLA	MG-NC	2.23	2.11	2.06
23	c	502	CLA	CHC-C4B	-2.23	1.34	1.39
33	B	622	LHG	O7-C5	-2.23	1.41	1.46
23	C	509	CLA	CMD-C2D	-2.23	1.46	1.50
23	b	617	CLA	O2D-CED	-2.23	1.40	1.45
23	c	504	CLA	C3B-C4B	2.23	1.49	1.42
23	A	405	CLA	C3B-C4B	2.23	1.49	1.42
24	d	401	PHO	CMA-C3A	-2.22	1.49	1.53
23	b	615	CLA	MG-NC	2.22	2.11	2.06
23	C	508	CLA	C3B-C4B	2.22	1.49	1.42
23	D	403	CLA	C1C-NC	-2.22	1.34	1.37
24	A	406	PHO	C1D-ND	2.22	1.42	1.38
29	c	517	DGD	O3G-C3G	-2.22	1.39	1.43
28	f	101	SQD	O3-C3	-2.22	1.37	1.43
23	b	608	CLA	CMD-C2D	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	411	LMG	O7-C10	2.22	1.38	1.30
33	D	409	LHG	C3-C2	2.22	1.58	1.51
26	d	406	PL9	C46-C47	-2.22	1.46	1.53
23	C	501	CLA	CMC-C2C	-2.22	1.46	1.50
27	c	519	LMG	C3-C2	2.21	1.58	1.52
23	C	502	CLA	CHC-C1C	2.21	1.42	1.38
23	B	605	CLA	C1B-NB	-2.21	1.35	1.37
23	b	612	CLA	CMA-C3A	-2.21	1.48	1.53
23	b	615	CLA	CMC-C2C	-2.21	1.46	1.50
23	A	407	CLA	C1A-CHA	-2.21	1.34	1.43
23	B	610	CLA	CMC-C2C	-2.21	1.46	1.50
23	C	512	CLA	C1A-CHA	-2.21	1.34	1.43
23	c	510	CLA	C3B-C4B	2.21	1.49	1.42
29	c	517	DGD	C1D-C2D	2.21	1.59	1.52
26	a	409	PL9	C40-C39	-2.21	1.45	1.50
23	C	512	CLA	C3B-C4B	2.20	1.49	1.42
27	C	519	LMG	C1-C2	2.20	1.59	1.52
23	B	608	CLA	CMB-C2B	-2.20	1.46	1.50
27	D	410	LMG	C32-C31	2.20	1.62	1.51
23	B	615	CLA	C1D-ND	2.20	1.40	1.37
23	B	613	CLA	C1B-NB	-2.19	1.35	1.37
23	B	615	CLA	CAC-C3C	-2.19	1.45	1.51
23	d	403	CLA	MG-NA	2.19	2.11	2.06
23	d	403	CLA	CMC-C2C	-2.19	1.46	1.50
23	c	502	CLA	O2A-CGA	2.19	1.39	1.33
23	B	610	CLA	C3B-C4B	2.19	1.49	1.42
29	h	103	DGD	O2D-C2D	-2.19	1.37	1.43
23	d	404	CLA	C1B-NB	-2.19	1.35	1.37
23	c	511	CLA	C3C-C2C	2.18	1.41	1.36
23	b	609	CLA	C1D-C2D	2.18	1.49	1.45
29	C	516	DGD	O1G-C1A	2.18	1.39	1.33
23	d	404	CLA	C3B-C4B	2.18	1.49	1.42
23	c	508	CLA	CMB-C2B	-2.18	1.46	1.50
23	c	506	CLA	CHC-C1C	2.18	1.42	1.38
23	D	403	CLA	C4B-NB	2.18	1.40	1.37
27	D	410	LMG	O8-C28	2.18	1.39	1.33
25	y	101	BCR	C33-C5	-2.17	1.47	1.50
23	a	407	CLA	MG-NC	-2.17	2.01	2.06
23	D	403	CLA	CMD-C2D	-2.17	1.46	1.50
25	a	408	BCR	C27-C26	-2.17	1.47	1.51
23	B	606	CLA	C3B-C4B	2.17	1.49	1.42
33	e	101	LHG	P-O6	2.17	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	CMB-C2B	-2.17	1.46	1.50
24	A	406	PHO	C1A-C2A	2.16	1.54	1.51
23	c	507	CLA	CMB-C2B	-2.16	1.46	1.50
23	D	404	CLA	C1B-NB	-2.16	1.35	1.37
23	c	501	CLA	MG-ND	-2.16	2.01	2.05
23	B	616	CLA	C2-C3	2.16	1.38	1.33
28	A	411	SQD	O47-C45	-2.16	1.41	1.46
23	c	509	CLA	CMB-C2B	-2.16	1.46	1.50
23	B	613	CLA	CMC-C2C	-2.16	1.46	1.50
23	b	611	CLA	CMC-C2C	-2.15	1.46	1.50
33	D	408	LHG	C8-C7	-2.15	1.44	1.50
24	D	401	PHO	CMB-C2B	-2.15	1.47	1.51
28	F	101	SQD	O2-C2	-2.15	1.37	1.43
23	D	402	CLA	C3D-C4D	2.15	1.49	1.44
29	c	518	DGD	C4E-C5E	-2.15	1.48	1.53
23	b	604	CLA	C1B-NB	-2.15	1.35	1.37
23	b	613	CLA	CMD-C2D	-2.15	1.46	1.50
23	B	616	CLA	C3B-C4B	2.14	1.49	1.42
23	D	404	CLA	C1B-C2B	2.14	1.48	1.43
23	B	612	CLA	C1C-NC	-2.14	1.34	1.37
23	h	101	CLA	C3B-C4B	2.14	1.49	1.42
23	C	503	CLA	C1D-ND	2.14	1.40	1.37
23	d	403	CLA	CMD-C2D	-2.14	1.46	1.50
23	C	507	CLA	C4B-NB	2.14	1.40	1.37
23	C	512	CLA	CMD-C2D	-2.14	1.46	1.50
23	c	506	CLA	CMB-C2B	-2.14	1.46	1.50
25	c	521	BCR	C38-C26	-2.14	1.47	1.50
29	A	413	DGD	O2G-C1B	2.14	1.40	1.34
28	B	623	SQD	O2-C2	-2.13	1.37	1.43
23	b	603	CLA	C3B-C4B	2.13	1.49	1.42
23	c	512	CLA	CMC-C2C	-2.13	1.46	1.50
23	C	512	CLA	CAA-C2A	-2.13	1.50	1.54
23	c	505	CLA	CMB-C2B	-2.13	1.46	1.50
29	C	516	DGD	C3D-C2D	2.13	1.57	1.52
28	f	101	SQD	O2-C2	-2.13	1.37	1.43
23	a	407	CLA	CAC-C3C	-2.13	1.45	1.51
23	D	402	CLA	C4C-C3C	2.13	1.48	1.45
27	D	407	LMG	C30-C29	2.11	1.59	1.52
29	C	516	DGD	O5D-C6D	-2.11	1.40	1.43
23	C	508	CLA	C4B-NB	2.11	1.40	1.37
23	B	616	CLA	C4C-C3C	2.11	1.48	1.45
24	A	406	PHO	CBD-CGD	-2.11	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	t	101	BCR	C1-C6	-2.11	1.51	1.53
24	d	401	PHO	C3D-CAD	-2.11	1.43	1.47
23	b	603	CLA	CMD-C2D	-2.10	1.46	1.50
23	B	607	CLA	C4B-NB	2.10	1.40	1.37
23	b	608	CLA	CHC-C1C	2.10	1.42	1.38
23	C	503	CLA	C3B-C4B	2.10	1.48	1.42
25	C	520	BCR	C1-C6	-2.10	1.51	1.53
29	C	518	DGD	C2A-C1A	-2.10	1.44	1.50
23	B	615	CLA	MG-NC	2.10	2.11	2.06
29	c	517	DGD	C3E-C2E	2.10	1.57	1.52
23	C	504	CLA	C1D-ND	2.10	1.40	1.37
23	D	403	CLA	CHC-C1C	2.10	1.42	1.38
23	c	505	CLA	CHC-C1C	2.10	1.42	1.38
23	c	509	CLA	C3D-C4D	2.10	1.48	1.44
23	B	611	CLA	C3B-C4B	2.10	1.48	1.42
23	c	502	CLA	CMC-C2C	-2.09	1.46	1.50
23	d	402	CLA	C3B-C4B	2.09	1.48	1.42
33	E	101	LHG	P-O3	2.09	1.67	1.59
29	c	516	DGD	C6D-C5D	2.09	1.57	1.51
23	B	615	CLA	MG-NB	2.09	2.09	2.05
25	y	101	BCR	C38-C26	-2.09	1.47	1.50
23	C	504	CLA	CMA-C3A	-2.09	1.48	1.53
23	C	512	CLA	C5-C3	-2.09	1.47	1.51
23	b	612	CLA	C3B-C4B	2.09	1.48	1.42
23	D	404	CLA	C1A-CHA	-2.09	1.34	1.43
23	C	512	CLA	O2D-CED	-2.09	1.40	1.45
23	c	504	CLA	CAC-C3C	-2.09	1.45	1.51
23	b	610	CLA	CMD-C2D	-2.09	1.46	1.50
23	C	506	CLA	CHC-C1C	2.08	1.42	1.38
23	B	611	CLA	CHC-C4B	-2.08	1.34	1.39
23	d	403	CLA	C3B-C4B	2.08	1.48	1.42
23	B	609	CLA	C1B-NB	-2.08	1.35	1.37
27	D	407	LMG	O2-C2	-2.08	1.37	1.43
23	c	501	CLA	CAC-C3C	-2.08	1.45	1.51
23	c	504	CLA	C1D-ND	2.08	1.40	1.37
23	B	608	CLA	C3C-C2C	2.08	1.41	1.36
23	c	511	CLA	C1D-C2D	2.08	1.49	1.45
23	h	101	CLA	O2A-CGA	2.08	1.39	1.33
23	b	609	CLA	CAB-C3B	-2.07	1.41	1.47
23	b	611	CLA	C3B-C4B	2.07	1.48	1.42
23	b	617	CLA	CAB-C3B	-2.07	1.41	1.47
33	E	101	LHG	C1-C2	2.07	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C1B-C2B	2.07	1.48	1.43
23	a	404	CLA	CMC-C2C	-2.07	1.46	1.50
23	B	614	CLA	C3B-C4B	2.07	1.48	1.42
23	d	404	CLA	CMC-C2C	-2.07	1.46	1.50
27	a	414	LMG	C4-C5	2.07	1.57	1.53
23	h	101	CLA	CMD-C2D	-2.07	1.46	1.50
23	a	405	CLA	C4B-NB	2.07	1.40	1.37
23	c	509	CLA	C3B-C4B	2.07	1.48	1.42
23	C	508	CLA	C1D-C2D	2.07	1.49	1.45
23	C	511	CLA	CHC-C4B	-2.07	1.34	1.39
23	h	101	CLA	C3D-C4D	2.07	1.48	1.44
34	e	102	HEM	CMA-C3A	2.07	1.55	1.50
23	A	407	CLA	CHD-C1D	-2.07	1.34	1.38
23	b	612	CLA	CHC-C4B	-2.07	1.34	1.39
23	D	403	CLA	CMC-C2C	-2.06	1.46	1.50
23	C	513	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	513	CLA	C4B-NB	2.06	1.40	1.37
23	c	505	CLA	C1D-ND	2.06	1.40	1.37
23	C	508	CLA	CHC-C1C	2.06	1.42	1.38
29	c	517	DGD	C1E-C2E	2.06	1.58	1.52
23	a	404	CLA	O2D-CED	-2.06	1.40	1.45
35	V	201	HEC	CMC-C2C	2.06	1.55	1.50
29	h	103	DGD	C4D-C5D	2.06	1.57	1.53
23	B	616	CLA	CMB-C2B	-2.05	1.46	1.50
23	d	402	CLA	C1D-C2D	2.05	1.49	1.45
23	b	604	CLA	C1D-ND	2.05	1.40	1.37
25	t	101	BCR	C27-C26	-2.05	1.47	1.51
29	C	517	DGD	O1G-C1G	-2.05	1.40	1.45
23	C	511	CLA	C3D-C4D	2.05	1.48	1.44
23	c	506	CLA	C1B-C2B	2.05	1.47	1.43
27	B	620	LMG	C6-C5	2.05	1.58	1.51
23	A	404	CLA	CMC-C2C	-2.05	1.46	1.50
24	A	406	PHO	O2A-CGA	2.05	1.39	1.33
25	b	618	BCR	C38-C26	-2.05	1.47	1.50
26	d	406	PL9	C20-C19	-2.05	1.45	1.50
25	b	620	BCR	C38-C26	-2.05	1.47	1.50
23	B	612	CLA	C3B-C4B	2.04	1.48	1.42
23	b	617	CLA	MG-ND	-2.04	2.01	2.05
33	l	101	LHG	C6-C5	2.04	1.57	1.50
23	C	506	CLA	CAC-C3C	-2.04	1.45	1.51
23	c	501	CLA	CMD-C2D	-2.04	1.46	1.50
23	c	503	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	CHC-C4B	-2.04	1.34	1.39
27	c	519	LMG	C4-C3	2.04	1.57	1.52
23	C	510	CLA	CMD-C2D	-2.04	1.46	1.50
23	C	506	CLA	CMC-C2C	-2.04	1.46	1.50
23	h	101	CLA	MG-NC	-2.04	2.01	2.06
25	H	101	BCR	C33-C5	-2.04	1.47	1.50
26	D	406	PL9	C45-C44	-2.04	1.45	1.50
23	C	506	CLA	O2D-CGD	2.04	1.38	1.33
26	a	409	PL9	C5-C4	-2.04	1.40	1.47
23	C	511	CLA	CHC-C1C	2.03	1.42	1.38
23	C	503	CLA	C4B-NB	2.03	1.40	1.37
23	c	504	CLA	C1B-C2B	2.03	1.47	1.43
23	C	503	CLA	CMB-C2B	-2.03	1.46	1.50
23	b	612	CLA	CMB-C2B	-2.03	1.46	1.50
23	C	505	CLA	C1D-ND	2.03	1.40	1.37
23	C	502	CLA	C1B-NB	-2.03	1.35	1.37
23	b	610	CLA	CAC-C3C	-2.03	1.45	1.51
23	B	604	CLA	O2A-CGA	2.03	1.39	1.33
29	c	518	DGD	C6E-C5E	-2.03	1.45	1.51
23	a	407	CLA	CMD-C2D	-2.03	1.46	1.50
23	A	407	CLA	CHC-C4B	-2.03	1.34	1.39
23	C	507	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	604	CLA	CHC-C1C	2.02	1.42	1.38
26	D	406	PL9	C52-C5	-2.02	1.46	1.50
23	A	407	CLA	C3D-C4D	2.02	1.48	1.44
23	C	503	CLA	CHC-C4B	-2.02	1.34	1.39
28	A	412	SQD	C46-C45	2.02	1.55	1.50
23	B	613	CLA	CMB-C2B	-2.02	1.46	1.50
23	B	603	CLA	C3B-C4B	2.02	1.48	1.42
26	d	406	PL9	C8-C9	2.02	1.37	1.33
23	c	513	CLA	CMC-C2C	-2.02	1.46	1.50
23	C	507	CLA	CHC-C4B	-2.02	1.34	1.39
23	b	614	CLA	C1D-ND	2.02	1.40	1.37
23	b	607	CLA	MG-ND	2.02	2.09	2.05
23	d	403	CLA	CAB-C3B	-2.02	1.42	1.47
23	B	616	CLA	CHC-C4B	-2.02	1.34	1.39
23	c	502	CLA	C1D-ND	2.01	1.40	1.37
25	T	101	BCR	C27-C26	-2.01	1.47	1.51
23	B	602	CLA	CHC-C1C	2.01	1.42	1.38
23	b	614	CLA	C1C-NC	-2.01	1.34	1.37
23	b	613	CLA	C3D-C4D	2.01	1.48	1.44
23	B	604	CLA	O2D-CED	-2.01	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	MG-ND	-2.01	2.01	2.05
24	A	406	PHO	OBD-CAD	2.01	1.24	1.22
23	b	615	CLA	C3D-C4D	2.01	1.48	1.44
33	L	101	LHG	O7-C7	2.01	1.39	1.34
34	e	102	HEM	C3B-C2B	-2.01	1.33	1.37
23	B	615	CLA	C3B-C4B	2.01	1.48	1.42
23	b	605	CLA	CBD-CGD	-2.00	1.46	1.52
23	C	507	CLA	CAA-C2A	-2.00	1.50	1.54
23	D	403	CLA	C3B-C4B	2.00	1.48	1.42
35	v	201	HEC	CMC-C2C	2.00	1.54	1.50
29	C	516	DGD	C2B-C1B	-2.00	1.44	1.50
29	A	413	DGD	C4D-C3D	2.00	1.57	1.52

All (1306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C4A-NA-C1A	10.48	111.46	106.68
23	d	402	CLA	C4A-NA-C1A	10.08	111.28	106.68
28	b	601	SQD	O6-C1-C2	10.06	123.55	108.27
23	C	510	CLA	C4A-NA-C1A	9.86	111.18	106.68
23	b	607	CLA	C4A-NA-C1A	9.86	111.18	106.68
23	b	605	CLA	C4A-NA-C1A	9.34	110.94	106.68
28	A	411	SQD	O6-C1-C2	9.29	122.38	108.27
23	D	403	CLA	C4A-NA-C1A	9.03	110.80	106.68
23	C	511	CLA	C4A-NA-C1A	8.40	110.51	106.68
23	C	501	CLA	C4A-NA-C1A	8.12	110.39	106.68
23	c	509	CLA	C4A-NA-C1A	8.11	110.38	106.68
28	a	411	SQD	O6-C1-C2	7.81	120.13	108.27
23	C	513	CLA	C4A-NA-C1A	7.77	110.23	106.68
23	B	606	CLA	C4A-NA-C1A	7.66	110.17	106.68
23	C	503	CLA	C4A-NA-C1A	7.65	110.17	106.68
23	B	612	CLA	C4A-NA-C1A	7.61	110.15	106.68
23	B	601	CLA	C4A-NA-C1A	7.57	110.13	106.68
23	b	617	CLA	C4A-NA-C1A	7.43	110.07	106.68
23	c	503	CLA	C4A-NA-C1A	7.42	110.06	106.68
23	b	604	CLA	C4A-NA-C1A	7.26	109.99	106.68
23	c	501	CLA	C4A-NA-C1A	7.17	109.95	106.68
28	A	411	SQD	O7-S-C6	7.09	117.34	106.76
23	b	615	CLA	C4A-NA-C1A	6.92	109.84	106.68
23	a	404	CLA	C4A-NA-C1A	6.91	109.83	106.68
23	b	612	CLA	C4A-NA-C1A	6.84	109.80	106.68
23	c	502	CLA	C4A-NA-C1A	6.76	109.76	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C4A-NA-C1A	6.63	109.70	106.68
23	c	506	CLA	C4A-NA-C1A	6.57	109.67	106.68
23	b	609	CLA	C3B-C4B-NB	-6.55	104.68	110.53
26	A	409	PL9	C7-C3-C4	6.46	122.23	116.91
23	B	615	CLA	C4A-NA-C1A	6.42	109.61	106.68
23	B	616	CLA	C4A-NA-C1A	6.41	109.60	106.68
23	A	404	CLA	C4A-NA-C1A	6.36	109.58	106.68
24	A	406	PHO	C4D-CHA-CBD	-6.31	105.43	108.45
23	b	611	CLA	C4A-NA-C1A	6.31	109.56	106.68
29	c	517	DGD	O3G-C3G-C2G	-6.24	95.63	110.82
23	c	511	CLA	C4A-NA-C1A	6.08	109.45	106.68
28	f	101	SQD	O6-C1-C2	5.98	117.36	108.27
23	c	504	CLA	C4A-NA-C1A	5.93	109.38	106.68
23	c	512	CLA	C4A-NA-C1A	5.80	109.33	106.68
29	H	102	DGD	O3G-C3G-C2G	-5.77	96.77	110.82
23	C	509	CLA	C4A-NA-C1A	5.77	109.31	106.68
23	B	610	CLA	O2D-CGD-O1D	-5.71	112.73	123.85
29	C	517	DGD	O3G-C3G-C2G	-5.69	96.98	110.82
23	B	607	CLA	C4A-NA-C1A	5.68	109.27	106.68
23	B	601	CLA	O2D-CGD-O1D	-5.68	112.79	123.85
23	B	602	CLA	C4A-NA-C1A	5.62	109.24	106.68
35	v	201	HEC	CBC-CAC-C3C	-5.61	116.23	127.43
28	f	101	SQD	O9-S-C6	5.60	115.11	106.76
24	d	401	PHO	C4D-CHA-CBD	-5.53	105.80	108.45
23	c	501	CLA	O2D-CGD-O1D	-5.50	113.14	123.85
23	c	508	CLA	C4A-NA-C1A	5.50	109.19	106.68
23	B	603	CLA	C4A-NA-C1A	5.45	109.16	106.68
23	B	605	CLA	C4A-NA-C1A	5.44	109.16	106.68
26	a	409	PL9	C7-C3-C4	5.43	121.38	116.91
23	A	407	CLA	C1D-ND-C4D	-5.42	102.51	106.31
23	D	402	CLA	C4A-NA-C1A	5.35	109.12	106.68
28	F	101	SQD	O6-C1-C2	5.31	116.33	108.27
23	B	602	CLA	CHB-C4A-NA	5.30	132.05	124.40
27	b	622	LMG	O1-C1-C2	-5.24	100.31	108.27
23	C	507	CLA	C4A-NA-C1A	5.23	109.06	106.68
23	b	610	CLA	C4A-NA-C1A	5.20	109.05	106.68
29	a	413	DGD	O3G-C3G-C2G	-5.20	98.40	111.77
23	B	614	CLA	O2D-CGD-O1D	-5.18	113.76	123.85
23	b	611	CLA	O2D-CGD-O1D	-5.16	113.80	123.85
28	a	412	SQD	O47-C7-C8	5.06	122.43	111.48
23	b	604	CLA	O2D-CGD-O1D	-5.00	114.11	123.85
23	A	405	CLA	O2D-CGD-O1D	-5.00	114.12	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	PHO	O1D-CGD-CBD	4.97	132.26	124.72
35	V	201	HEC	CBC-CAC-C3C	-4.94	117.55	127.43
23	B	613	CLA	C1-C2-C3	-4.93	118.12	126.20
28	b	601	SQD	C45-O47-C7	4.92	129.58	117.80
23	B	601	CLA	O1D-CGD-CBD	4.86	134.10	124.52
23	c	509	CLA	C3B-C4B-NB	-4.84	106.21	110.53
23	h	101	CLA	C4A-NA-C1A	4.77	108.86	106.68
28	b	601	SQD	C1-C2-C3	-4.70	100.11	110.01
23	C	502	CLA	O2D-CGD-O1D	-4.65	114.80	123.85
23	C	506	CLA	C4A-NA-C1A	4.65	108.80	106.68
33	D	409	LHG	O4-P-O5	4.64	134.05	112.44
23	b	609	CLA	CHB-C4A-NA	4.64	131.10	124.40
28	B	623	SQD	O6-C1-C2	4.63	115.31	108.27
29	h	103	DGD	O3G-C3G-C2G	-4.61	99.60	110.82
28	B	623	SQD	O7-S-C6	4.61	113.64	106.76
23	b	608	CLA	O2D-CGD-O1D	-4.61	114.87	123.85
29	c	516	DGD	O3G-C3G-C2G	-4.61	99.60	110.82
33	d	407	LHG	O4-P-O5	4.61	133.89	112.44
35	V	201	HEC	CBB-CAB-C3B	-4.57	118.29	127.43
29	H	102	DGD	C1D-C2D-C3D	-4.56	100.41	110.01
23	d	403	CLA	C4A-NA-C1A	4.55	108.76	106.68
23	b	606	CLA	C4A-NA-C1A	4.50	108.73	106.68
28	A	411	SQD	C1-C2-C3	-4.48	100.59	110.01
33	a	410	LHG	O4-P-O5	4.46	133.21	112.44
23	B	614	CLA	C3B-C4B-NB	-4.46	106.55	110.53
33	B	622	LHG	O4-P-O5	4.44	133.09	112.44
35	v	201	HEC	CBB-CAB-C3B	-4.43	118.58	127.43
23	C	505	CLA	CAC-C3C-C4C	4.42	130.55	124.79
23	b	613	CLA	C4A-NA-C1A	4.38	108.68	106.68
28	B	623	SQD	O9-S-O7	-4.36	99.63	113.82
29	C	517	DGD	O5D-C1E-C2E	4.36	114.89	108.27
24	A	406	PHO	C2B-C1B-NB	-4.35	106.28	109.43
23	b	617	CLA	O2D-CGD-O1D	-4.35	115.38	123.85
33	d	408	LHG	O4-P-O5	4.33	132.58	112.44
33	e	101	LHG	O4-P-O5	4.32	132.55	112.44
23	B	608	CLA	C3B-C4B-NB	-4.30	106.69	110.53
23	B	610	CLA	C4A-NA-C1A	4.30	108.64	106.68
23	b	609	CLA	O2D-CGD-CBD	4.29	118.72	111.23
23	C	501	CLA	C3B-C4B-NB	-4.28	106.71	110.53
23	B	602	CLA	O2D-CGD-O1D	-4.28	115.52	123.85
23	b	605	CLA	C3B-C4B-NB	-4.27	106.72	110.53
23	b	609	CLA	C4A-NA-C1A	4.27	108.62	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	PL9	C7-C3-C2	-4.26	118.37	123.39
29	c	517	DGD	O6D-C1D-O3G	-4.25	100.00	110.04
29	c	516	DGD	O2D-C2D-C1D	-4.24	99.97	110.08
23	b	615	CLA	O2D-CGD-CBD	4.23	118.62	111.23
23	D	403	CLA	C3B-C4B-NB	-4.20	106.78	110.53
23	B	612	CLA	CAC-C3C-C4C	4.19	130.25	124.79
28	a	411	SQD	O9-S-C6	4.18	112.99	106.76
23	b	614	CLA	O2D-CGD-O1D	-4.17	115.73	123.85
23	c	508	CLA	CHB-C4A-NA	4.16	130.40	124.40
26	D	406	PL9	C7-C3-C4	4.14	120.32	116.91
33	E	101	LHG	O4-P-O5	4.13	131.67	112.44
33	D	408	LHG	O4-P-O5	4.12	131.60	112.44
23	B	602	CLA	O2D-CGD-CBD	4.12	118.42	111.23
24	d	401	PHO	O1D-CGD-CBD	4.11	130.96	124.72
23	b	606	CLA	C4D-CHA-C1A	4.11	126.14	121.24
23	b	616	CLA	C3B-C4B-NB	-4.10	106.87	110.53
23	b	605	CLA	C1-C2-C3	-4.10	119.48	126.20
26	d	406	PL9	C37-C38-C39	-4.07	118.31	127.62
23	b	604	CLA	O2D-CGD-CBD	4.06	118.33	111.23
28	B	623	SQD	O47-C7-C8	4.06	120.26	111.48
28	B	623	SQD	C3-C4-C5	4.04	117.56	110.23
28	b	601	SQD	O2-C2-C1	4.03	119.69	110.08
23	a	405	CLA	C4A-NA-C1A	4.03	108.52	106.68
23	B	611	CLA	O2D-CGD-O1D	-4.01	116.04	123.85
28	A	411	SQD	O47-C7-C8	4.01	120.15	111.48
29	C	518	DGD	O3E-C3E-C2E	-4.00	100.94	110.38
25	B	617	BCR	C2-C1-C6	4.00	116.24	110.44
28	F	101	SQD	O9-S-C6	4.00	112.72	106.76
23	b	603	CLA	CHB-C4A-NA	3.99	130.15	124.40
25	b	618	BCR	C2-C1-C6	3.98	116.22	110.44
23	c	505	CLA	C4A-NA-C1A	3.97	108.49	106.68
24	a	406	PHO	C2B-C1B-NB	-3.97	106.56	109.43
23	C	504	CLA	C3B-C4B-NB	-3.96	106.99	110.53
23	B	604	CLA	CHB-C4A-NA	3.96	130.12	124.40
33	l	101	LHG	O4-P-O5	3.96	130.85	112.44
29	C	516	DGD	O3G-C3G-C2G	-3.94	101.23	110.82
23	c	510	CLA	O2D-CGD-O1D	-3.94	116.19	123.85
23	D	402	CLA	CHB-C4A-NA	3.93	130.07	124.40
23	C	512	CLA	O2D-CGD-O1D	-3.91	116.24	123.85
23	B	614	CLA	O2D-CGD-CBD	3.91	118.06	111.23
23	C	512	CLA	CHB-C4A-NA	3.91	130.04	124.40
23	h	101	CLA	O2D-CGD-O1D	-3.91	116.24	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C4D-C3D-CAD	-3.89	103.88	108.11
23	C	501	CLA	CAC-C3C-C4C	3.88	129.84	124.79
23	b	611	CLA	O1D-CGD-CBD	3.88	132.16	124.52
23	b	615	CLA	CMB-C2B-C1B	-3.85	119.55	125.42
23	B	610	CLA	O2A-CGA-O1A	-3.84	114.02	123.63
23	B	608	CLA	C6-C5-C3	-3.84	104.11	113.47
26	D	406	PL9	C37-C38-C39	-3.83	118.85	127.62
23	A	407	CLA	CMB-C2B-C1B	-3.83	119.59	125.42
23	B	608	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
23	b	611	CLA	CAC-C3C-C4C	3.82	129.76	124.79
23	c	501	CLA	O2D-CGD-CBD	3.81	117.89	111.23
24	a	406	PHO	C4D-CHA-CBD	-3.81	106.63	108.45
24	D	401	PHO	O2D-CGD-CBD	-3.79	106.78	110.95
28	b	601	SQD	O9-S-O7	-3.79	101.51	113.82
23	C	513	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
23	c	509	CLA	O2A-CGA-O1A	-3.77	114.19	123.63
23	B	610	CLA	O2D-CGD-CBD	3.77	117.82	111.23
29	C	518	DGD	O3G-C3G-C2G	-3.77	101.65	110.82
23	c	505	CLA	CHD-C1D-ND	-3.77	119.50	124.80
28	A	412	SQD	O47-C7-C8	3.76	119.62	111.48
23	C	502	CLA	C4A-NA-C1A	3.76	108.39	106.68
23	b	617	CLA	O2D-CGD-CBD	3.75	117.79	111.23
27	c	522	LMG	O6-C1-O1	-3.75	101.19	110.04
23	c	513	CLA	C4A-NA-C1A	3.73	108.38	106.68
23	B	606	CLA	CGD-CBD-CAD	-3.73	98.76	110.85
28	b	601	SQD	O48-C23-C24	3.73	123.21	111.83
29	c	516	DGD	O3G-C1D-C2D	-3.72	102.62	108.27
24	d	401	PHO	C2B-C1B-NB	-3.72	106.74	109.43
23	b	613	CLA	CMB-C2B-C1B	-3.72	119.76	125.42
23	b	615	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
23	c	510	CLA	C3B-C4B-NB	-3.70	107.23	110.53
23	h	101	CLA	O2D-CGD-CBD	3.69	117.68	111.23
23	c	504	CLA	C3B-C4B-NB	-3.68	107.24	110.53
23	c	506	CLA	CBC-CAC-C3C	-3.68	102.44	112.42
33	B	622	LHG	O8-C23-C24	3.68	123.06	111.83
23	B	604	CLA	C3B-C4B-NB	-3.68	107.25	110.53
31	A	415	BCT	O2-C-O1	3.67	129.07	119.68
23	B	603	CLA	O2D-CGD-CBD	3.67	117.65	111.23
28	B	623	SQD	O48-C23-C24	3.67	123.03	111.83
23	b	617	CLA	CHB-C4A-NA	3.67	129.70	124.40
23	B	613	CLA	C1D-ND-C4D	-3.67	103.74	106.31
23	a	404	CLA	O1D-CGD-CBD	3.66	131.75	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	L	101	LHG	O4-P-O5	3.66	129.46	112.44
29	h	103	DGD	C3D-C4D-C5D	-3.64	103.63	110.23
23	b	614	CLA	C4A-NA-C1A	3.63	108.34	106.68
28	b	601	SQD	C3-C4-C5	3.62	116.80	110.23
23	b	608	CLA	O1D-CGD-CBD	3.62	131.66	124.52
25	T	101	BCR	C27-C26-C25	3.61	127.58	122.70
25	b	618	BCR	C27-C26-C25	3.61	127.58	122.70
33	a	410	LHG	O8-C23-C24	3.59	122.79	111.83
25	y	101	BCR	C27-C26-C25	3.59	127.56	122.70
23	B	612	CLA	CHB-C4A-NA	3.59	129.58	124.40
33	B	622	LHG	O8-C23-O10	-3.59	114.66	123.63
23	a	404	CLA	C3B-C4B-NB	-3.59	107.33	110.53
25	b	620	BCR	C38-C26-C25	-3.57	120.58	124.48
28	b	601	SQD	O7-S-C6	3.57	112.08	106.76
28	b	601	SQD	O9-S-C6	3.56	112.08	106.76
28	a	411	SQD	O9-S-O7	-3.56	102.24	113.82
23	c	512	CLA	C3B-C4B-NB	-3.55	107.36	110.53
23	C	512	CLA	C3B-C4B-NB	-3.55	107.36	110.53
25	T	101	BCR	C7-C8-C9	-3.54	121.00	126.23
28	F	101	SQD	O8-S-C6	3.53	112.79	105.97
35	V	201	HEC	CHB-C4A-NA	3.52	128.28	124.45
23	c	505	CLA	O2D-CGD-CBD	3.51	117.37	111.23
29	A	413	DGD	O5D-C1E-C2E	3.51	113.60	108.27
29	a	413	DGD	C1G-C2G-C3G	-3.50	103.71	111.80
23	C	509	CLA	CHD-C1D-ND	-3.50	119.88	124.80
23	D	402	CLA	C3B-C4B-NB	-3.48	107.43	110.53
33	D	409	LHG	O8-C23-C24	3.47	122.42	111.83
23	B	609	CLA	C4A-NA-C1A	3.47	108.26	106.68
28	B	623	SQD	C1-O5-C5	-3.47	106.95	113.72
28	a	411	SQD	O47-C7-C8	3.46	118.97	111.48
23	C	510	CLA	C3B-C4B-NB	-3.46	107.44	110.53
23	c	509	CLA	O1D-CGD-CBD	3.45	131.32	124.52
23	c	504	CLA	CHB-C4A-NA	3.45	129.38	124.40
25	C	514	BCR	C33-C5-C6	-3.45	120.72	124.48
23	c	507	CLA	C4A-NA-C1A	3.45	108.25	106.68
26	d	406	PL9	C8-C7-C3	3.44	120.93	112.03
23	d	403	CLA	C4-C3-C5	3.43	121.18	115.23
24	a	406	PHO	C1-C2-C3	-3.42	120.59	126.20
23	b	614	CLA	C7-C6-C5	-3.42	104.15	113.26
27	D	410	LMG	O1-C7-C8	-3.42	102.98	111.77
25	c	514	BCR	C27-C26-C25	3.41	127.32	122.70
23	d	403	CLA	C3B-C4B-NB	-3.41	107.48	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C27-C26-C25	3.41	127.31	122.70
23	C	501	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
23	b	613	CLA	CAC-C3C-C4C	3.39	129.20	124.79
27	c	522	LMG	C4-C3-C2	3.39	116.78	110.83
23	b	616	CLA	C1D-ND-C4D	-3.38	103.94	106.31
23	B	603	CLA	CHB-C4A-NA	3.38	129.28	124.40
23	b	603	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
23	B	605	CLA	C3B-C4B-NB	-3.38	107.51	110.53
23	D	403	CLA	O2D-CGD-CBD	3.38	117.14	111.23
23	B	608	CLA	C4A-NA-C1A	3.38	108.22	106.68
23	B	610	CLA	C3B-C4B-NB	-3.38	107.52	110.53
23	b	606	CLA	CHD-C1D-ND	-3.38	120.05	124.80
28	B	623	SQD	O5-C5-C4	3.37	115.78	109.70
25	c	514	BCR	C15-C16-C17	-3.37	116.62	123.52
29	c	518	DGD	O3G-C3G-C2G	-3.37	102.62	110.82
23	c	504	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
23	C	503	CLA	CHD-C1D-ND	-3.37	120.06	124.80
27	m	101	LMG	O7-C10-O9	-3.37	115.83	123.70
23	b	604	CLA	C3B-C4B-NB	-3.37	107.53	110.53
23	A	404	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
23	B	605	CLA	O1D-CGD-CBD	3.36	131.15	124.52
28	B	623	SQD	O48-C23-O10	-3.36	115.22	123.63
23	c	507	CLA	CHB-C4A-NA	3.36	129.24	124.40
23	B	615	CLA	CHB-C4A-NA	3.35	129.24	124.40
25	C	515	BCR	C15-C14-C13	-3.35	122.58	127.28
35	v	201	HEC	CMC-C2C-C1C	-3.35	120.32	125.42
23	B	616	CLA	C1-O2A-CGA	3.35	124.75	116.65
23	D	402	CLA	CHD-C1D-ND	-3.35	120.09	124.80
25	c	521	BCR	C27-C26-C25	3.34	127.22	122.70
25	h	102	BCR	C38-C26-C25	-3.34	120.84	124.48
23	C	508	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
23	B	609	CLA	CHA-C1A-NA	-3.34	118.82	126.39
23	c	507	CLA	C2C-C1C-NC	3.34	113.49	109.98
29	c	518	DGD	O5E-C6E-C5E	-3.34	99.98	111.33
25	B	617	BCR	C29-C30-C25	3.33	115.27	110.44
25	a	408	BCR	C2-C1-C6	3.31	115.25	110.44
25	H	101	BCR	C2-C1-C6	3.31	115.25	110.44
28	A	411	SQD	O9-S-O7	-3.31	103.06	113.82
29	h	103	DGD	C3G-C2G-C1G	-3.30	104.08	111.78
27	d	409	LMG	O1-C1-C2	-3.30	103.25	108.27
28	a	412	SQD	O48-C23-C24	3.30	121.89	111.83
23	D	403	CLA	CHB-C4A-NA	3.29	129.15	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C4-C3-C5	3.29	120.93	115.23
29	H	102	DGD	C3E-C4E-C5E	-3.28	104.28	110.23
23	b	606	CLA	C1-C2-C3	-3.28	120.83	126.20
23	B	613	CLA	OBD-CAD-C3D	3.27	136.05	128.42
23	b	614	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	h	102	BCR	C27-C26-C25	3.25	127.10	122.70
23	b	613	CLA	CMB-C2B-C3B	3.25	134.19	126.55
23	C	508	CLA	C3B-C4B-NB	-3.24	107.64	110.53
25	b	619	BCR	C35-C13-C14	-3.24	117.56	122.82
26	d	406	PL9	O1-C4-C3	-3.24	117.31	120.73
23	B	601	CLA	CHB-C4A-NA	3.24	129.07	124.40
23	c	512	CLA	CHB-C4A-NA	3.24	129.07	124.40
24	A	406	PHO	CMA-C3A-C4A	-3.24	107.64	114.61
27	a	414	LMG	C1-O6-C5	-3.23	107.42	113.72
25	H	101	BCR	C27-C26-C25	3.22	127.06	122.70
23	b	616	CLA	CHD-C4C-C3C	-3.21	120.09	124.77
25	t	101	BCR	C15-C16-C17	-3.21	116.95	123.52
25	K	101	BCR	C39-C30-C25	-3.21	105.21	110.24
25	a	408	BCR	C27-C26-C25	3.20	127.03	122.70
23	B	610	CLA	CHB-C4A-NA	3.20	129.02	124.40
23	c	513	CLA	CHB-C4A-NA	3.20	129.02	124.40
28	f	101	SQD	O9-S-O7	-3.20	103.41	113.82
23	a	405	CLA	C3B-C4B-NB	-3.20	107.67	110.53
23	B	616	CLA	C2C-C1C-NC	3.19	113.34	109.98
27	D	411	LMG	O7-C10-O9	-3.19	115.12	123.33
23	b	616	CLA	CHB-C1B-NB	3.19	128.84	124.05
23	c	505	CLA	CHB-C4A-NA	3.19	129.00	124.40
31	a	417	BCT	O2-C-O1	3.19	127.83	119.68
28	b	601	SQD	O5-C5-C4	3.19	115.45	109.70
29	A	413	DGD	C3G-C2G-C1G	-3.18	104.36	111.78
23	c	504	CLA	CMB-C2B-C1B	-3.18	120.57	125.42
23	a	404	CLA	C3A-C2A-C1A	3.18	106.10	101.34
26	A	409	PL9	C20-C19-C21	3.18	120.74	115.23
23	B	606	CLA	O2D-CGD-CBD	3.17	116.77	111.23
23	B	601	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
26	d	406	PL9	C22-C23-C24	-3.16	120.40	127.62
27	B	620	LMG	O6-C1-O1	-3.15	102.59	110.04
27	c	522	LMG	O7-C10-O9	-3.15	116.35	123.70
27	C	519	LMG	O1-C7-C8	-3.14	103.17	110.82
25	D	405	BCR	C24-C23-C22	-3.14	121.59	126.23
24	D	401	PHO	C4D-CHA-CBD	-3.14	106.95	108.45
23	d	402	CLA	O2D-CGD-O1D	-3.14	117.74	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	518	DGD	O3G-C1D-C2D	-3.13	103.52	108.27
29	C	516	DGD	O6D-C1D-O3G	-3.13	102.65	110.04
23	A	407	CLA	C4-C3-C5	3.13	120.66	115.23
23	A	404	CLA	C3B-C4B-NB	-3.13	107.74	110.53
23	A	405	CLA	O2D-CGD-CBD	3.12	116.69	111.23
23	A	407	CLA	C3D-C4D-ND	3.12	115.07	109.99
23	B	605	CLA	CHB-C4A-NA	3.12	128.91	124.40
23	b	607	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
23	c	510	CLA	C4A-NA-C1A	3.12	108.10	106.68
23	c	510	CLA	C7-C6-C5	-3.12	104.95	113.26
23	b	613	CLA	C11-C12-C13	-3.12	105.60	115.97
23	A	404	CLA	CAA-CBA-CGA	-3.12	104.36	113.21
23	D	402	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
29	C	518	DGD	O6D-C1D-O3G	-3.11	102.69	110.04
25	b	620	BCR	C27-C26-C25	3.11	126.91	122.70
23	b	605	CLA	C4-C3-C5	3.10	120.62	115.23
34	E	102	HEM	CBD-CAD-C3D	-3.10	103.95	112.53
33	E	101	LHG	O8-C23-C24	3.10	121.28	111.83
29	h	103	DGD	C1E-O6E-C5E	3.09	119.76	113.72
28	f	101	SQD	O5-C5-C4	3.09	115.27	109.70
23	C	504	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
23	c	506	CLA	O1D-CGD-CBD	3.09	130.61	124.52
25	A	408	BCR	C11-C10-C9	-3.09	122.95	127.28
23	b	617	CLA	CHC-C4B-NB	3.09	128.68	124.05
23	b	610	CLA	O1D-CGD-CBD	3.09	130.60	124.52
23	C	508	CLA	CHD-C1D-ND	-3.08	120.46	124.80
26	a	409	PL9	C22-C23-C24	-3.08	120.57	127.62
23	b	609	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
23	B	604	CLA	C2D-C1D-ND	-3.08	107.08	110.13
23	D	404	CLA	C1D-ND-C4D	-3.08	104.15	106.31
24	A	406	PHO	CMB-C2B-C3B	3.08	130.84	124.68
23	A	407	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
23	c	503	CLA	C3B-C4B-NB	-3.07	107.79	110.53
23	c	506	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	B	608	CLA	O2D-CGD-CBD	3.06	116.58	111.23
23	A	407	CLA	CHD-C1D-ND	-3.06	120.50	124.80
26	d	406	PL9	C7-C3-C4	3.05	119.42	116.91
28	a	411	SQD	O7-S-C6	3.05	111.31	106.76
25	B	618	BCR	C27-C26-C25	3.05	126.83	122.70
29	c	518	DGD	C3G-C2G-C1G	-3.05	104.67	111.78
27	d	409	LMG	O6-C1-O1	-3.05	102.84	110.04
27	m	101	LMG	O8-C28-O10	-3.05	116.00	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C3B-C4B-NB	-3.05	107.81	110.53
28	F	101	SQD	C1-C2-C3	-3.04	103.61	110.01
23	B	602	CLA	CHC-C1C-NC	3.04	128.89	124.31
26	D	406	PL9	C8-C7-C3	3.04	119.89	112.03
25	B	619	BCR	C29-C30-C25	3.04	114.85	110.44
29	c	517	DGD	CDB-CCB-CBB	-3.03	99.04	114.37
23	B	614	CLA	CBC-CAC-C3C	-3.03	104.20	112.42
23	b	616	CLA	C4A-NA-C1A	3.03	108.06	106.68
25	b	619	BCR	C15-C14-C13	-3.03	123.03	127.28
23	B	612	CLA	C1-O2A-CGA	3.03	123.98	116.65
23	B	611	CLA	O2D-CGD-CBD	3.03	116.52	111.23
26	a	409	PL9	C7-C3-C2	-3.02	119.83	123.39
29	h	103	DGD	C6D-C5D-C4D	3.02	118.40	112.07
23	b	603	CLA	O2D-CGD-CBD	3.02	116.50	111.23
23	C	505	CLA	C3B-C4B-NB	-3.01	107.84	110.53
23	c	512	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
25	B	617	BCR	C15-C14-C13	-3.01	123.06	127.28
23	a	405	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
24	a	406	PHO	O2D-CGD-O1D	-3.00	118.00	123.85
34	E	102	HEM	CHC-C4B-NB	3.00	127.65	124.42
28	B	623	SQD	O9-S-C6	2.99	111.23	106.76
23	B	608	CLA	CHB-C4A-NA	2.99	128.72	124.40
23	c	510	CLA	CAA-CBA-CGA	-2.99	104.72	113.21
23	B	605	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
26	D	406	PL9	C22-C23-C24	-2.99	120.79	127.62
23	B	603	CLA	O2A-CGA-O1A	-2.98	116.16	123.63
23	D	404	CLA	C4-C3-C5	2.98	120.40	115.23
27	c	522	LMG	O3-C3-C2	-2.98	103.35	110.38
28	A	411	SQD	O48-C23-C24	2.98	120.92	111.83
23	B	605	CLA	C4D-C3D-CAD	-2.98	104.87	108.11
23	c	512	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
23	c	503	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
23	B	604	CLA	O2A-CGA-O1A	-2.98	116.19	123.63
23	b	604	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
27	A	410	LMG	O6-C1-O1	-2.97	103.02	110.04
25	y	101	BCR	C30-C25-C26	-2.97	118.58	122.64
23	c	507	CLA	CHD-C1D-ND	-2.97	120.63	124.80
25	d	405	BCR	C38-C26-C25	-2.97	121.25	124.48
26	d	406	PL9	O2-C1-C6	2.96	125.20	120.48
23	A	407	CLA	CMB-C2B-C3B	2.96	133.51	126.55
23	b	603	CLA	C3C-C4C-NC	-2.96	106.64	110.43
23	h	101	CLA	C3B-C4B-NB	-2.96	107.89	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CHD-C1D-ND	-2.95	120.64	124.80
23	b	613	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
29	c	516	DGD	C3G-C2G-C1G	-2.95	104.91	111.78
25	b	620	BCR	C2-C1-C6	2.95	114.72	110.44
23	b	616	CLA	CHC-C1C-NC	2.94	128.74	124.31
23	C	509	CLA	C1-C2-C3	-2.94	121.38	126.20
24	d	401	PHO	CMB-C2B-C3B	2.94	130.56	124.68
29	C	516	DGD	O3E-C3E-C2E	-2.94	103.44	110.38
33	D	409	LHG	O8-C23-O10	-2.94	116.28	123.63
33	a	410	LHG	O8-C23-O10	-2.94	116.28	123.63
23	c	506	CLA	C4-C3-C5	2.94	120.32	115.23
23	b	603	CLA	C4A-NA-C1A	2.93	108.02	106.68
23	C	501	CLA	O2A-CGA-O1A	-2.93	116.29	123.63
23	C	503	CLA	C4-C3-C5	2.93	120.32	115.23
23	C	512	CLA	O1D-CGD-CBD	2.93	130.30	124.52
29	H	102	DGD	O2D-C2D-C1D	-2.93	103.09	110.08
23	B	615	CLA	C4-C3-C5	-2.93	110.14	115.23
23	c	502	CLA	C1-O2A-CGA	2.93	123.74	116.65
25	c	515	BCR	C30-C25-C26	-2.93	118.63	122.64
23	B	605	CLA	CHD-C4C-C3C	-2.93	120.50	124.77
23	c	508	CLA	CHD-C1D-ND	-2.92	120.69	124.80
24	d	401	PHO	CBC-CAC-C3C	2.92	117.05	112.87
23	a	404	CLA	CHC-C1C-NC	2.92	128.71	124.31
29	H	102	DGD	C6D-C5D-C4D	2.92	118.19	112.07
23	B	613	CLA	C3B-C4B-NB	-2.91	107.93	110.53
29	C	517	DGD	C1D-C2D-C3D	-2.91	103.89	110.01
23	A	405	CLA	CAC-C3C-C4C	2.91	128.57	124.79
24	A	406	PHO	CBC-CAC-C3C	2.91	117.03	112.87
25	A	408	BCR	C16-C15-C14	-2.90	117.58	123.52
23	a	407	CLA	C4A-NA-C1A	2.90	108.00	106.68
23	A	405	CLA	C3A-C2A-C1A	2.90	105.68	101.34
28	b	601	SQD	O8-S-C6	2.90	111.57	105.97
23	B	613	CLA	C4A-NA-C1A	2.90	108.00	106.68
23	b	605	CLA	CHC-C1C-NC	2.90	128.68	124.31
23	d	404	CLA	CHD-C1D-ND	-2.89	120.73	124.80
26	D	406	PL9	C7-C3-C2	-2.89	119.98	123.39
25	a	408	BCR	C35-C13-C14	-2.89	118.13	122.82
23	b	606	CLA	CHD-C4C-NC	2.89	128.71	124.23
27	D	407	LMG	O8-C28-O10	-2.89	116.41	123.63
23	c	510	CLA	CHB-C4A-NA	2.89	128.56	124.40
23	c	502	CLA	CHC-C4B-NB	2.88	128.37	124.05
23	c	509	CLA	O2D-CGD-O1D	-2.88	118.24	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	CAA-CBA-CGA	-2.88	105.03	113.21
23	B	602	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	c	513	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	A	409	PL9	C27-C28-C29	-2.87	121.05	127.62
23	c	508	CLA	O2A-CGA-O1A	-2.87	116.45	123.63
23	A	404	CLA	CHB-C4A-NA	2.87	128.54	124.40
23	B	605	CLA	CHD-C1D-ND	-2.87	120.77	124.80
23	b	607	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
23	b	604	CLA	C4-C3-C5	2.86	120.20	115.23
23	C	513	CLA	CHB-C4A-NA	2.86	128.53	124.40
23	B	601	CLA	CHA-C4D-ND	2.86	138.45	132.55
23	C	505	CLA	C4A-NA-C1A	2.86	107.98	106.68
26	A	409	PL9	C22-C23-C24	-2.85	121.09	127.62
33	d	407	LHG	O8-C23-C24	2.85	120.53	111.83
23	C	512	CLA	C4A-NA-C1A	2.85	107.98	106.68
26	D	406	PL9	C12-C13-C14	-2.85	121.10	127.62
23	d	402	CLA	C3B-C4B-NB	-2.85	107.98	110.53
29	C	517	DGD	O6D-C1D-O3G	-2.85	103.32	110.04
27	m	101	LMG	O7-C10-C11	2.85	117.64	111.48
23	c	510	CLA	CHD-C1D-ND	-2.84	120.80	124.80
27	D	407	LMG	O3-C3-C2	-2.84	103.67	110.38
23	b	606	CLA	C3B-C4B-NB	-2.84	108.00	110.53
23	a	404	CLA	CHD-C1D-ND	-2.84	120.81	124.80
23	B	613	CLA	C3D-C4D-ND	2.83	114.59	109.99
29	h	103	DGD	O3E-C3E-C2E	-2.83	103.69	110.38
23	B	613	CLA	CHC-C4B-NB	2.83	128.30	124.05
23	B	616	CLA	C1-C2-C3	2.83	130.83	126.20
25	d	405	BCR	C16-C15-C14	-2.83	117.73	123.52
23	D	402	CLA	O2D-CGD-CBD	2.83	116.17	111.23
23	B	616	CLA	CAC-C3C-C4C	2.82	128.46	124.79
25	T	101	BCR	C35-C13-C14	-2.82	118.25	122.82
29	C	518	DGD	C3G-C2G-C1G	-2.82	105.22	111.78
23	b	610	CLA	CMB-C2B-C1B	-2.82	121.13	125.42
27	m	101	LMG	O3-C3-C2	-2.81	103.75	110.38
24	A	406	PHO	O2D-CGD-CBD	2.81	114.03	110.95
24	A	406	PHO	C1A-C2A-C3A	-2.80	100.17	102.84
24	a	406	PHO	CMB-C2B-C3B	2.80	130.28	124.68
25	B	618	BCR	C37-C22-C21	-2.80	118.28	122.82
29	h	103	DGD	O6E-C5E-C4E	2.80	114.74	109.70
27	C	519	LMG	O7-C10-O9	-2.79	117.17	123.70
29	C	518	DGD	CDB-CCB-CBB	-2.79	100.26	114.37
28	A	411	SQD	C1-O5-C5	-2.79	108.27	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	C1-O2A-CGA	2.79	123.40	116.65
23	B	612	CLA	O1D-CGD-CBD	2.79	130.02	124.52
23	h	101	CLA	O2A-CGA-O1A	-2.78	116.66	123.63
25	H	101	BCR	C38-C26-C25	-2.78	121.45	124.48
29	c	516	DGD	C3D-C4D-C5D	-2.78	105.18	110.23
27	B	620	LMG	C4-C3-C2	-2.78	105.95	110.83
29	H	102	DGD	O2G-C1B-O1B	-2.78	117.22	123.70
23	b	611	CLA	CHB-C4A-NA	2.77	128.40	124.40
25	A	408	BCR	C40-C30-C25	2.77	114.59	110.24
24	A	406	PHO	CED-O2D-CGD	2.77	122.20	115.92
27	a	414	LMG	O6-C1-O1	-2.77	103.50	110.04
23	b	617	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	b	615	CLA	CMB-C2B-C3B	2.77	133.06	126.55
25	H	101	BCR	C16-C15-C14	-2.76	117.86	123.52
23	d	403	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
25	A	408	BCR	C27-C26-C25	2.76	126.44	122.70
23	c	509	CLA	CMB-C2B-C1B	-2.76	121.21	125.42
23	b	612	CLA	CHD-C1D-C2D	2.76	131.23	125.49
23	C	504	CLA	CHD-C4C-NC	2.76	128.51	124.23
23	C	511	CLA	CHB-C4A-NA	2.76	128.38	124.40
25	b	619	BCR	C8-C7-C6	-2.76	119.63	127.00
23	c	512	CLA	C1-C2-C3	-2.76	121.68	126.20
23	c	509	CLA	CHB-C4A-NA	2.75	128.38	124.40
25	C	515	BCR	C15-C16-C17	-2.75	117.89	123.52
29	c	517	DGD	C3G-O3G-C1D	2.75	119.69	113.80
27	B	620	LMG	O7-C10-O9	-2.75	117.28	123.70
23	B	606	CLA	CHB-C4A-NA	2.74	128.36	124.40
25	K	101	BCR	C27-C26-C25	2.74	126.41	122.70
29	h	103	DGD	C1D-O6D-C5D	-2.74	108.37	113.72
23	B	611	CLA	C2C-C1C-NC	2.74	112.86	109.98
34	e	102	HEM	CBD-CAD-C3D	-2.74	104.96	112.53
23	C	513	CLA	CHD-C1D-ND	-2.74	120.95	124.80
29	c	517	DGD	C8B-C7B-C6B	-2.74	100.52	114.37
27	b	622	LMG	C1-O6-C5	-2.74	108.37	113.72
25	H	101	BCR	C24-C23-C22	-2.74	122.19	126.23
28	A	411	SQD	O48-C23-O10	-2.73	116.79	123.63
23	b	605	CLA	CHB-C4A-NA	2.73	128.34	124.40
25	c	515	BCR	C35-C13-C14	-2.73	118.39	122.82
29	C	517	DGD	O6E-C1E-O5D	-2.73	103.59	110.04
23	c	501	CLA	CED-O2D-CGD	-2.73	109.73	115.92
25	b	618	BCR	C32-C1-C6	-2.72	105.97	110.24
23	c	507	CLA	CHC-C4B-NB	2.72	128.14	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	406	PL9	C50-C49-C48	-2.72	114.48	122.66
27	d	409	LMG	O6-C5-C4	2.72	114.61	109.70
26	D	406	PL9	C42-C43-C44	-2.72	121.39	127.62
33	e	101	LHG	O8-C23-C24	2.72	120.13	111.83
34	e	102	HEM	CBA-CAA-C2A	-2.72	105.02	112.53
23	d	404	CLA	CHA-C1A-NA	-2.72	120.24	126.39
27	c	519	LMG	O6-C1-O1	-2.72	103.62	110.04
23	a	405	CLA	CHB-C4A-NA	2.72	128.32	124.40
23	D	402	CLA	CED-O2D-CGD	-2.71	109.76	115.92
26	d	406	PL9	C7-C3-C2	-2.71	120.19	123.39
27	d	409	LMG	C6-C5-C4	-2.71	106.36	113.02
33	L	101	LHG	O8-C23-C24	2.71	120.10	111.83
23	C	503	CLA	C7-C6-C5	-2.71	106.04	113.26
34	e	102	HEM	CHB-C1B-NB	2.70	127.71	124.37
28	F	101	SQD	O48-C23-C24	2.70	120.07	111.83
33	d	407	LHG	C20-C19-C18	-2.70	100.74	114.37
23	c	512	CLA	CMB-C2B-C3B	2.70	132.89	126.55
25	H	101	BCR	C29-C30-C25	2.69	114.35	110.44
23	D	403	CLA	CED-O2D-CGD	2.69	122.01	115.92
28	F	101	SQD	O48-C23-O10	-2.69	116.91	123.63
25	B	619	BCR	C12-C13-C14	-2.68	114.79	119.01
28	B	623	SQD	C4-C3-C2	2.68	115.54	110.83
25	C	520	BCR	C29-C30-C25	2.68	114.33	110.44
28	a	411	SQD	C1-C2-C3	-2.68	104.37	110.01
25	B	617	BCR	C35-C13-C14	-2.68	118.48	122.82
23	A	407	CLA	O2D-CGD-CBD	2.68	115.91	111.23
33	a	410	LHG	C11-C10-C9	-2.68	100.83	114.37
33	e	101	LHG	O8-C23-O10	-2.67	116.94	123.63
23	B	613	CLA	CHB-C4A-NA	2.67	128.26	124.40
23	D	404	CLA	CHB-C1B-NB	2.67	128.06	124.05
27	m	101	LMG	C40-C39-C38	-2.67	100.88	114.37
23	c	507	CLA	O2A-CGA-O1A	-2.67	116.96	123.63
25	c	515	BCR	C38-C26-C25	-2.67	121.58	124.48
23	b	617	CLA	C2C-C1C-NC	2.67	112.78	109.98
23	B	615	CLA	C6-C7-C8	-2.67	107.11	115.97
23	c	503	CLA	CAC-C3C-C4C	2.66	128.25	124.79
25	C	514	BCR	C2-C1-C6	2.66	114.30	110.44
24	a	406	PHO	O1D-CGD-CBD	2.66	128.75	124.72
23	b	616	CLA	CAA-CBA-CGA	-2.65	105.68	113.21
25	c	514	BCR	C39-C30-C25	2.65	114.40	110.24
34	e	102	HEM	CHC-C1C-NC	2.65	127.34	124.45
25	A	408	BCR	C2-C1-C6	2.65	114.28	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	O2D-CGD-CBD	2.65	115.86	111.23
25	a	408	BCR	C15-C14-C13	-2.64	123.57	127.28
25	t	101	BCR	C27-C26-C25	2.64	126.28	122.70
23	c	505	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
23	C	502	CLA	O2D-CGD-CBD	2.63	115.84	111.23
29	c	516	DGD	CDB-CCB-CBB	-2.63	101.06	114.37
23	b	603	CLA	CHD-C1D-ND	-2.63	121.10	124.80
23	B	603	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
29	a	413	DGD	C2G-O2G-C1B	2.63	124.09	117.80
23	c	508	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
23	b	616	CLA	CHD-C4C-NC	2.63	128.31	124.23
23	A	405	CLA	CED-O2D-CGD	-2.63	109.95	115.92
23	C	503	CLA	CHD-C1D-C2D	2.63	130.96	125.49
29	C	518	DGD	CBB-CAB-C9B	-2.63	101.08	114.37
23	b	608	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
25	c	515	BCR	C2-C1-C6	2.63	114.26	110.44
25	h	102	BCR	C33-C5-C6	-2.63	121.62	124.48
23	B	612	CLA	C11-C12-C13	-2.63	107.23	115.97
28	B	623	SQD	O47-C7-O49	-2.63	117.57	123.70
23	C	505	CLA	O1D-CGD-CBD	2.63	129.70	124.52
26	a	409	PL9	C37-C38-C39	-2.62	121.62	127.62
23	b	611	CLA	C3B-C4B-NB	-2.62	108.19	110.53
29	H	102	DGD	C3G-C2G-C1G	-2.62	105.67	111.78
28	F	101	SQD	O5-C5-C4	2.62	114.43	109.70
23	b	616	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
23	C	504	CLA	C11-C10-C8	-2.62	107.25	115.97
26	d	406	PL9	C11-C9-C8	-2.62	115.28	121.17
27	m	101	LMG	C9-C8-C7	-2.62	105.68	111.78
23	b	606	CLA	C1D-ND-C4D	2.62	108.15	106.31
28	a	411	SQD	O8-S-C6	2.62	111.03	105.97
23	b	612	CLA	C2D-C1D-ND	-2.62	107.54	110.13
23	c	509	CLA	CMB-C2B-C3B	2.62	132.70	126.55
23	C	510	CLA	C1D-ND-C4D	2.61	108.14	106.31
26	d	406	PL9	C40-C39-C38	-2.61	116.92	123.63
29	H	102	DGD	C4D-C3D-C2D	-2.61	106.25	110.83
23	b	610	CLA	CHC-C4B-NB	2.60	127.95	124.05
23	C	508	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
27	B	620	LMG	C38-C37-C36	-2.60	101.21	114.37
23	B	601	CLA	CHC-C4B-NB	2.60	127.95	124.05
27	B	620	LMG	C40-C39-C38	-2.60	101.22	114.37
23	B	602	CLA	CHD-C1D-C2D	2.60	130.90	125.49
25	a	408	BCR	C38-C26-C27	-2.60	108.05	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	BCR	C24-C23-C22	-2.60	122.39	126.23
33	D	408	LHG	O8-C23-O10	-2.60	117.14	123.63
23	b	607	CLA	CHD-C4C-NC	2.59	128.25	124.23
24	d	401	PHO	CMA-C3A-C4A	-2.59	109.02	114.61
25	c	515	BCR	C36-C18-C17	-2.59	118.61	122.82
23	C	504	CLA	CHD-C1D-ND	-2.59	121.15	124.80
28	B	623	SQD	O47-C45-C46	2.59	117.64	108.34
25	d	405	BCR	C29-C30-C25	2.59	114.20	110.44
25	d	405	BCR	C33-C5-C6	-2.59	121.66	124.48
27	m	101	LMG	O1-C7-C8	-2.59	104.53	110.82
23	B	613	CLA	O1D-CGD-CBD	2.59	129.62	124.52
25	H	101	BCR	C8-C9-C10	2.58	123.08	119.01
23	C	511	CLA	CAC-C3C-C4C	2.58	128.15	124.79
23	C	508	CLA	O2D-CGD-CBD	2.58	115.74	111.23
25	D	405	BCR	C2-C1-C6	2.58	114.18	110.44
25	C	515	BCR	C29-C30-C25	2.58	114.18	110.44
33	B	622	LHG	C11-C10-C9	-2.58	101.35	114.37
35	v	201	HEC	CHC-C1C-NC	2.57	128.53	123.86
23	B	602	CLA	CHD-C1D-ND	-2.57	121.18	124.80
23	a	407	CLA	CMD-C2D-C1D	-2.57	120.20	124.73
23	b	603	CLA	C1-O2A-CGA	2.57	122.88	116.65
25	C	514	BCR	C24-C23-C22	-2.57	122.43	126.23
23	B	607	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
23	b	612	CLA	CHD-C1D-ND	-2.57	121.19	124.80
23	b	614	CLA	CHB-C4A-NA	2.57	128.10	124.40
23	D	404	CLA	O2A-CGA-O1A	-2.56	117.21	123.63
23	B	604	CLA	O1D-CGD-CBD	2.56	129.58	124.52
23	B	616	CLA	CHC-C4B-NB	2.56	127.89	124.05
29	C	516	DGD	O5D-C6D-C5D	-2.56	103.64	109.42
23	B	614	CLA	CHB-C1B-NB	2.56	127.89	124.05
23	B	603	CLA	C3B-C4B-NB	-2.56	108.25	110.53
23	c	503	CLA	O1D-CGD-CBD	2.56	129.57	124.52
23	C	508	CLA	CHB-C4A-NA	2.56	128.09	124.40
29	C	517	DGD	CDB-CCB-CBB	-2.56	101.44	114.37
25	b	618	BCR	C15-C14-C13	-2.56	123.69	127.28
29	c	518	DGD	O6E-C5E-C6E	-2.55	100.11	106.44
25	d	405	BCR	C27-C26-C25	2.55	126.15	122.70
25	c	515	BCR	C29-C30-C25	2.55	114.14	110.44
23	C	505	CLA	CHC-C4B-NB	2.55	127.88	124.05
25	b	619	BCR	C30-C25-C26	-2.55	119.15	122.64
25	C	515	BCR	C2-C1-C6	2.55	114.14	110.44
33	l	101	LHG	O8-C23-O10	-2.55	117.25	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C1-O2A-CGA	-2.55	110.48	116.65
23	c	504	CLA	O2D-CGD-CBD	2.54	115.68	111.23
23	b	612	CLA	C1-C2-C3	-2.54	122.03	126.20
27	D	407	LMG	O2-C2-C1	-2.54	104.02	110.08
23	c	506	CLA	CHB-C4A-NA	2.54	128.07	124.40
23	c	502	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
23	C	503	CLA	C4D-CHA-C1A	2.54	124.27	121.24
23	d	402	CLA	O2D-CGD-CBD	2.54	115.67	111.23
23	a	404	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
29	c	517	DGD	O2E-C2E-C1E	-2.54	104.03	110.08
27	B	620	LMG	C1-C2-C3	-2.54	104.67	110.01
23	b	608	CLA	CHD-C1D-ND	-2.54	121.23	124.80
23	c	504	CLA	CMB-C2B-C3B	2.54	132.51	126.55
23	c	505	CLA	CHC-C1C-NC	2.53	128.13	124.31
25	c	515	BCR	C34-C9-C10	-2.53	118.71	122.82
23	c	507	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
23	a	407	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
23	a	407	CLA	CHA-C1A-NA	-2.53	120.66	126.39
23	B	605	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
23	b	616	CLA	CHD-C1D-ND	-2.53	121.24	124.80
25	B	618	BCR	C30-C25-C26	-2.53	119.18	122.64
24	D	401	PHO	CMB-C2B-C3B	2.53	129.73	124.68
29	C	518	DGD	O3D-C3D-C4D	-2.53	104.42	110.38
24	D	401	PHO	O2A-CGA-O1A	-2.52	117.31	123.63
23	B	611	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
33	D	408	LHG	O8-C23-C24	2.52	119.53	111.83
23	B	611	CLA	C1-C2-C3	-2.52	122.06	126.20
25	b	618	BCR	C3-C4-C5	-2.52	109.56	114.06
26	A	409	PL9	O2-C1-C2	-2.52	116.10	121.83
25	K	101	BCR	C38-C26-C25	-2.52	121.74	124.48
23	B	613	CLA	C7-C6-C5	-2.52	106.55	113.26
23	h	101	CLA	CBA-CAA-C2A	2.51	121.27	113.79
25	t	101	BCR	C36-C18-C19	2.51	121.92	118.09
25	H	101	BCR	C1-C6-C5	-2.51	119.20	122.64
29	A	413	DGD	CDB-CCB-CBB	-2.51	101.68	114.37
24	D	401	PHO	C1-C2-C3	-2.51	122.09	126.20
25	h	102	BCR	C8-C9-C10	2.50	122.95	119.01
23	D	404	CLA	CHD-C1D-ND	-2.50	121.28	124.80
23	h	101	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	c	507	CLA	CHD-C4C-NC	2.50	128.11	124.23
29	c	518	DGD	C1D-C2D-C3D	-2.50	104.75	110.01
23	C	506	CLA	O2A-CGA-O1A	-2.50	117.37	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	e	102	HEM	CHA-C4D-ND	2.50	127.46	124.37
29	H	102	DGD	C1D-O6D-C5D	-2.50	108.84	113.72
23	B	601	CLA	C1-C2-C3	-2.50	122.10	126.20
24	d	401	PHO	CGD-CBD-CAD	2.50	118.94	110.85
28	A	411	SQD	O9-S-C6	2.50	110.49	106.76
27	A	410	LMG	C38-C37-C36	-2.50	101.74	114.37
23	a	405	CLA	CHC-C4B-NB	2.50	127.80	124.05
23	C	513	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
26	d	406	PL9	C20-C19-C21	2.50	119.56	115.23
23	a	407	CLA	CHB-C4A-NA	2.49	128.00	124.40
23	c	511	CLA	C3B-C4B-NB	-2.49	108.31	110.53
27	m	101	LMG	C31-C30-C29	-2.49	103.99	113.13
23	B	614	CLA	CHC-C4B-NB	2.49	127.78	124.05
25	b	620	BCR	C11-C10-C9	-2.48	123.79	127.28
25	b	619	BCR	C27-C26-C25	2.48	126.06	122.70
27	d	409	LMG	C40-C39-C38	-2.48	101.81	114.37
23	B	608	CLA	CHD-C1D-ND	-2.48	121.31	124.80
25	c	515	BCR	C11-C10-C9	-2.48	123.80	127.28
23	B	610	CLA	O1D-CGD-CBD	2.48	129.41	124.52
29	h	103	DGD	C4D-C3D-C2D	-2.48	106.48	110.83
23	B	607	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
23	C	509	CLA	CHB-C4A-NA	2.48	127.97	124.40
25	C	515	BCR	C27-C26-C25	2.48	126.05	122.70
26	d	406	PL9	O2-C1-C2	-2.48	116.20	121.83
28	a	412	SQD	O49-C7-C8	-2.48	114.10	123.78
23	C	508	CLA	CHB-C1B-NB	2.48	127.76	124.05
23	c	511	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
23	B	615	CLA	C3B-C4B-NB	-2.47	108.32	110.53
29	C	516	DGD	CDB-CCB-CBB	-2.47	101.88	114.37
25	c	521	BCR	C29-C30-C25	2.47	114.03	110.44
23	b	611	CLA	C1-C2-C3	-2.47	122.15	126.20
23	A	407	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
23	B	606	CLA	CHD-C1D-ND	-2.46	121.34	124.80
23	b	612	CLA	C3B-C4B-NB	-2.46	108.33	110.53
23	b	606	CLA	OBD-CAD-C3D	2.46	134.17	128.42
33	B	622	LHG	O3-P-O5	-2.46	99.18	108.94
29	c	517	DGD	O3D-C3D-C4D	-2.46	104.58	110.38
27	C	519	LMG	O1-C1-C2	-2.46	104.54	108.27
29	A	413	DGD	O5D-C6D-C5D	-2.46	103.88	109.42
23	C	502	CLA	O1D-CGD-CBD	2.46	129.37	124.52
25	b	619	BCR	C2-C1-C6	2.46	114.01	110.44
23	B	606	CLA	C3B-C4B-NB	-2.46	108.34	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
26	A	409	PL9	C12-C13-C14	-2.45	122.02	127.62
23	C	504	CLA	C4-C3-C5	2.45	119.48	115.23
25	c	514	BCR	C15-C14-C13	-2.45	123.85	127.28
33	d	408	LHG	C25-C24-C23	2.45	122.66	113.69
23	C	501	CLA	CHC-C4B-NB	2.45	127.72	124.05
23	c	501	CLA	C2C-C1C-NC	2.44	112.55	109.98
23	C	511	CLA	CHA-C1A-NA	-2.44	120.86	126.39
25	H	101	BCR	C35-C13-C14	-2.44	118.86	122.82
25	c	514	BCR	C30-C25-C26	-2.44	119.30	122.64
25	C	514	BCR	C34-C9-C10	-2.44	118.86	122.82
23	C	504	CLA	CMB-C2B-C1B	-2.44	121.71	125.42
23	A	407	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	C	514	BCR	C11-C10-C9	-2.44	123.86	127.28
28	B	623	SQD	C25-C24-C23	-2.44	104.77	113.69
25	D	405	BCR	C38-C26-C25	-2.44	121.83	124.48
25	a	408	BCR	C3-C4-C5	-2.43	109.72	114.06
23	a	405	CLA	O2D-CGD-CBD	2.43	115.48	111.23
23	b	604	CLA	CED-O2D-CGD	-2.43	110.40	115.92
29	C	516	DGD	C6D-O5D-C1E	2.43	119.01	113.80
28	f	101	SQD	O8-S-C6	2.43	110.66	105.97
23	b	604	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	C	507	CLA	CHB-C4A-NA	2.42	127.90	124.40
23	b	617	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
26	d	406	PL9	C40-C39-C41	2.42	119.43	115.23
27	B	620	LMG	C3-C4-C5	-2.42	105.85	110.23
25	h	102	BCR	C34-C9-C8	-2.42	114.39	118.09
23	C	505	CLA	C1-C2-C3	-2.42	122.24	126.20
23	c	505	CLA	CHD-C1D-C2D	2.42	130.51	125.49
29	C	516	DGD	O2D-C2D-C1D	-2.42	104.32	110.08
23	C	503	CLA	C6-C7-C8	-2.42	107.94	115.97
23	a	404	CLA	CMA-C3A-C4A	2.42	118.27	111.77
23	C	510	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
29	c	516	DGD	C5B-C4B-C3B	-2.41	102.16	114.37
27	b	622	LMG	O7-C10-O9	-2.41	118.06	123.70
23	b	607	CLA	CHC-C4B-NB	2.41	127.67	124.05
23	B	605	CLA	CHD-C4C-NC	2.41	127.97	124.23
23	b	615	CLA	C3B-C4B-NB	-2.41	108.38	110.53
23	B	612	CLA	C9-C8-C7	-2.41	102.68	111.27
29	c	518	DGD	O3G-C1D-C2D	-2.41	104.61	108.27
23	b	606	CLA	CMD-C2D-C3D	2.41	133.22	127.69
23	B	609	CLA	O2A-CGA-O1A	-2.41	117.60	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C7-C6-C5	-2.41	106.84	113.26
28	f	101	SQD	O47-C7-C8	2.41	119.78	110.93
23	c	507	CLA	CHD-C4C-C3C	-2.41	121.26	124.77
23	A	405	CLA	C1-O2A-CGA	2.41	122.48	116.65
27	b	622	LMG	C8-O7-C10	2.41	123.56	117.80
31	a	417	BCT	O3-C-O1	-2.41	113.52	119.68
23	b	614	CLA	C1D-ND-C4D	-2.40	104.62	106.31
29	h	103	DGD	O6E-C5E-C6E	-2.40	100.49	106.44
23	b	615	CLA	CHB-C1B-NB	2.40	127.65	124.05
25	B	619	BCR	C30-C25-C26	-2.39	119.36	122.64
25	C	514	BCR	C7-C8-C9	-2.39	122.69	126.23
27	d	409	LMG	O3-C3-C2	-2.39	104.73	110.38
25	h	102	BCR	C7-C8-C9	-2.39	122.69	126.23
23	B	612	CLA	CHD-C1D-ND	-2.39	121.44	124.80
23	b	605	CLA	CAC-C3C-C4C	2.39	127.90	124.79
25	b	619	BCR	C11-C10-C9	-2.39	123.93	127.28
29	C	517	DGD	O3D-C3D-C4D	-2.39	104.75	110.38
23	C	501	CLA	O2D-CGD-CBD	2.39	115.40	111.23
28	F	101	SQD	O9-S-O7	-2.38	106.07	113.82
23	C	502	CLA	C3B-C4B-NB	-2.38	108.40	110.53
23	B	602	CLA	C1-O2A-CGA	2.38	122.42	116.65
28	f	101	SQD	O48-C23-O10	-2.38	117.67	123.63
23	b	614	CLA	C2A-C3A-C4A	2.38	105.71	101.87
23	C	508	CLA	CHD-C1D-C2D	2.38	130.43	125.49
23	A	404	CLA	C1-O2A-CGA	-2.38	110.90	116.65
27	c	519	LMG	O2-C2-C1	-2.37	104.42	110.08
28	b	601	SQD	O5-C1-C2	-2.37	105.50	110.37
23	A	405	CLA	O1D-CGD-CBD	2.37	129.19	124.52
23	c	506	CLA	CHA-C1A-NA	-2.37	121.03	126.39
25	b	618	BCR	C33-C5-C6	-2.36	121.91	124.48
24	D	401	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
26	A	409	PL9	C36-C34-C33	-2.36	115.87	121.17
23	b	609	CLA	CHC-C4B-NB	2.36	127.59	124.05
23	C	507	CLA	C2A-C1A-CHA	2.36	127.96	123.87
23	c	509	CLA	C3A-C2A-C1A	2.36	104.87	101.34
23	c	510	CLA	C16-C15-C13	-2.36	108.14	115.97
23	C	511	CLA	C2A-C1A-CHA	2.35	127.95	123.87
25	C	520	BCR	C27-C26-C25	2.35	125.88	122.70
23	b	609	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
27	C	519	LMG	C9-C8-C7	-2.35	106.30	111.78
29	c	518	DGD	C6D-O5D-C1E	2.35	118.83	113.80
29	c	516	DGD	O6E-C5E-C4E	2.35	113.93	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	620	LMG	O1-C7-C8	-2.35	105.10	110.82
23	b	606	CLA	CHD-C1D-C2D	2.35	130.37	125.49
23	C	503	CLA	C5-C3-C2	-2.35	115.89	121.17
23	c	506	CLA	C3B-C4B-NB	-2.35	108.43	110.53
23	A	404	CLA	O1D-CGD-CBD	2.35	129.15	124.52
25	t	101	BCR	C1-C6-C5	-2.35	119.43	122.64
23	c	501	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
23	b	606	CLA	CBC-CAC-C3C	-2.34	106.07	112.42
27	b	622	LMG	C40-C39-C38	-2.34	102.52	114.37
23	c	506	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
29	c	516	DGD	C8B-C7B-C6B	-2.34	102.55	114.37
23	b	609	CLA	CHD-C1D-ND	-2.34	121.51	124.80
23	b	605	CLA	OBD-CAD-C3D	2.34	133.88	128.42
23	B	612	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
23	B	606	CLA	CHD-C4C-NC	2.34	127.86	124.23
25	B	618	BCR	C15-C16-C17	-2.34	118.74	123.52
23	B	601	CLA	C3B-C4B-NB	-2.34	108.44	110.53
28	a	412	SQD	C45-O47-C7	2.33	123.38	117.80
25	c	514	BCR	C33-C5-C6	-2.33	121.94	124.48
23	b	612	CLA	C1D-ND-C4D	2.33	107.95	106.31
23	A	405	CLA	CMD-C2D-C3D	2.33	133.03	127.69
29	c	516	DGD	C4D-C3D-C2D	-2.33	106.74	110.83
23	B	610	CLA	CGD-CBD-CAD	-2.33	103.30	110.85
24	d	401	PHO	C6-C7-C8	-2.33	108.22	115.97
23	b	611	CLA	C4-C3-C5	2.33	119.27	115.23
29	c	518	DGD	CDB-CCB-CBB	-2.33	102.60	114.37
23	a	405	CLA	CED-O2D-CGD	-2.33	110.64	115.92
25	h	102	BCR	C30-C25-C26	-2.32	119.46	122.64
28	a	411	SQD	O10-C23-C24	-2.32	114.69	123.78
23	D	403	CLA	CHC-C4B-NB	2.32	127.53	124.05
23	A	405	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
23	d	404	CLA	CHD-C1D-C2D	2.32	130.31	125.49
33	e	101	LHG	C11-C10-C9	-2.32	102.64	114.37
23	c	502	CLA	CHD-C1D-ND	-2.32	121.54	124.80
29	A	413	DGD	C1E-O6E-C5E	2.32	118.25	113.72
23	a	407	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
25	B	619	BCR	C1-C6-C5	-2.32	119.47	122.64
23	b	613	CLA	C2C-C1C-NC	2.32	112.41	109.98
23	b	609	CLA	C6-C7-C8	-2.32	108.27	115.97
26	a	409	PL9	C32-C33-C34	-2.31	122.33	127.62
23	D	402	CLA	CHD-C1D-C2D	2.31	130.30	125.49
23	C	508	CLA	CMB-C2B-C3B	2.31	131.99	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C1-C2-C3	-2.31	122.41	126.20
23	A	404	CLA	CAA-C2A-C1A	-2.31	104.40	111.97
25	A	408	BCR	C8-C7-C6	-2.31	120.82	127.00
23	A	407	CLA	CHD-C4C-NC	2.31	127.81	124.23
26	D	406	PL9	C35-C34-C36	2.31	119.23	115.23
29	C	517	DGD	O4D-C4D-C5D	-2.31	103.64	109.32
23	C	506	CLA	C3B-C4B-NB	-2.31	108.47	110.53
23	c	503	CLA	C3A-C2A-C1A	2.30	104.79	101.34
25	B	619	BCR	C11-C10-C9	-2.30	124.05	127.28
23	b	615	CLA	CAC-C3C-C4C	2.30	127.79	124.79
24	d	401	PHO	C1-C2-C3	-2.30	122.42	126.20
23	C	505	CLA	CHB-C4A-NA	2.30	127.72	124.40
25	b	620	BCR	C29-C30-C25	2.30	113.78	110.44
25	C	514	BCR	C15-C16-C17	-2.30	118.81	123.52
23	b	603	CLA	CHC-C1C-NC	2.30	127.78	124.31
27	b	622	LMG	C42-C41-C40	-2.30	102.74	114.37
23	d	404	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
27	m	101	LMG	O1-C1-C2	-2.30	104.79	108.27
23	B	610	CLA	CED-O2D-CGD	-2.29	110.71	115.92
23	B	609	CLA	CHA-C4D-ND	2.29	137.28	132.55
25	c	521	BCR	C31-C1-C6	2.29	113.84	110.24
23	B	602	CLA	C2D-C1D-ND	-2.29	107.86	110.13
27	c	522	LMG	O2-C2-C1	-2.29	104.61	110.08
23	b	615	CLA	CHB-C4A-NA	2.29	127.70	124.40
29	A	413	DGD	C4E-C3E-C2E	-2.29	106.81	110.83
23	A	407	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
28	a	411	SQD	O47-C7-O49	-2.29	118.36	123.70
23	b	612	CLA	CHB-C4A-NA	2.29	127.70	124.40
23	c	510	CLA	O2D-CGD-CBD	2.29	115.23	111.23
28	a	411	SQD	C3-C4-C5	2.29	114.38	110.23
23	a	404	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
27	C	519	LMG	O2-C2-C1	-2.28	104.63	110.08
27	C	519	LMG	O6-C1-O1	-2.28	104.65	110.04
23	B	605	CLA	CAA-CBA-CGA	-2.28	106.73	113.21
23	b	605	CLA	CGD-CBD-CAD	-2.28	103.46	110.85
24	A	406	PHO	OBD-CAD-C3D	2.28	131.45	127.89
25	C	515	BCR	C1-C6-C5	-2.28	119.52	122.64
34	E	102	HEM	CHD-C4C-C3C	2.28	129.05	125.21
26	A	409	PL9	C31-C29-C28	2.28	126.28	121.17
23	C	511	CLA	CHD-C4C-C3C	2.28	128.10	124.77
23	c	504	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
34	e	102	HEM	C3B-C2B-C1B	2.28	108.12	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C11-C10-C8	-2.28	108.40	115.97
23	d	402	CLA	C2B-C1B-NB	-2.27	107.97	110.33
34	E	102	HEM	CHC-C1C-NC	2.27	126.93	124.45
23	B	603	CLA	CHD-C1D-ND	-2.27	121.61	124.80
27	m	101	LMG	C1-O6-C5	-2.27	109.28	113.72
27	d	409	LMG	O1-C7-C8	-2.27	105.30	110.82
23	B	614	CLA	C2B-C1B-NB	-2.27	107.97	110.33
29	H	102	DGD	C4E-C3E-C2E	-2.27	106.85	110.83
23	c	506	CLA	C4-C3-C2	-2.27	117.80	123.63
23	B	615	CLA	C2B-C1B-NB	-2.27	107.97	110.33
23	c	511	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
26	A	409	PL9	C21-C19-C18	-2.27	116.08	121.17
23	C	513	CLA	O1D-CGD-CBD	2.27	128.99	124.52
25	B	619	BCR	C33-C5-C6	-2.27	122.01	124.48
25	t	101	BCR	C2-C1-C6	2.27	113.73	110.44
26	a	409	PL9	C27-C28-C29	-2.27	122.44	127.62
23	c	505	CLA	CHD-C4C-NC	2.26	127.74	124.23
23	B	604	CLA	OBD-CAD-C3D	2.26	133.71	128.42
25	B	619	BCR	C2-C1-C6	2.26	113.73	110.44
28	a	411	SQD	O48-C23-C24	2.26	118.74	111.83
29	C	517	DGD	O5E-C6E-C5E	-2.26	103.63	111.33
27	A	410	LMG	O7-C10-O9	-2.26	118.42	123.70
28	F	101	SQD	C44-O6-C1	2.26	117.54	113.68
25	B	618	BCR	C38-C26-C27	-2.26	108.78	113.60
23	c	504	CLA	C7-C6-C5	-2.26	107.24	113.26
25	b	618	BCR	C8-C7-C6	-2.26	120.96	127.00
23	c	504	CLA	C3D-C4D-ND	2.26	113.66	109.99
25	a	408	BCR	C29-C30-C25	2.26	113.72	110.44
23	B	615	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
23	b	614	CLA	C1-O2A-CGA	2.25	122.11	116.65
33	a	410	LHG	C5-O7-C7	-2.25	112.41	117.80
23	a	407	CLA	C4-C3-C5	2.25	119.14	115.23
23	D	404	CLA	C3D-C4D-ND	2.25	113.65	109.99
23	B	603	CLA	C6-C7-C8	-2.25	108.49	115.97
27	c	519	LMG	C40-C39-C38	-2.25	103.01	114.37
23	B	614	CLA	CHD-C1D-ND	-2.25	121.64	124.80
23	b	610	CLA	CMB-C2B-C3B	2.25	131.83	126.55
33	B	622	LHG	C18-C17-C16	-2.24	103.02	114.37
25	B	619	BCR	C32-C1-C6	-2.24	106.72	110.24
23	b	608	CLA	C3B-C4B-NB	-2.24	108.53	110.53
23	C	509	CLA	CED-O2D-CGD	2.24	121.00	115.92
33	D	408	LHG	C20-C19-C18	-2.24	103.03	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C4A-NA-C1A	2.24	107.70	106.68
23	B	616	CLA	CHA-C1A-NA	-2.24	121.31	126.39
24	A	406	PHO	C4B-NB-C1B	2.24	112.08	108.82
25	B	619	BCR	C34-C9-C10	-2.24	119.19	122.82
23	c	509	CLA	CHD-C1D-ND	-2.24	121.65	124.80
29	c	518	DGD	O6D-C1D-O3G	-2.24	104.75	110.04
25	y	101	BCR	C23-C22-C21	-2.24	115.48	119.01
23	b	603	CLA	CHD-C1D-C2D	2.24	130.15	125.49
27	D	407	LMG	O6-C1-O1	-2.24	104.75	110.04
23	c	501	CLA	O1D-CGD-CBD	2.24	128.94	124.52
23	B	610	CLA	C6-C5-C3	2.24	118.92	113.47
23	d	402	CLA	C3A-C2A-C1A	2.24	104.69	101.34
23	D	404	CLA	C1-C2-C3	-2.24	122.53	126.20
26	D	406	PL9	C7-C8-C9	-2.24	122.98	126.83
23	a	407	CLA	CGD-CBD-CAD	-2.24	103.60	110.85
26	a	409	PL9	C8-C7-C3	2.24	117.81	112.03
25	T	101	BCR	C36-C18-C17	-2.24	119.19	122.82
23	c	507	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
23	c	505	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
28	b	601	SQD	O47-C7-C8	2.23	116.31	111.48
23	C	503	CLA	O1D-CGD-CBD	2.23	128.92	124.52
23	B	611	CLA	C9-C8-C10	-2.23	103.32	111.27
23	b	603	CLA	CHD-C4C-NC	2.23	127.69	124.23
23	D	404	CLA	CHB-C1B-C2B	-2.23	120.96	127.43
23	c	508	CLA	C3B-C4B-NB	-2.23	108.54	110.53
23	h	101	CLA	CHC-C4B-NB	2.23	127.39	124.05
25	c	515	BCR	C8-C9-C10	2.22	122.51	119.01
23	c	509	CLA	CHD-C4C-NC	2.22	127.68	124.23
27	B	620	LMG	C9-C8-C7	-2.22	106.60	111.78
23	c	512	CLA	CGD-CBD-CAD	2.22	118.04	110.85
34	E	102	HEM	CHD-C1D-ND	2.22	126.81	124.42
27	D	411	LMG	O8-C28-O10	-2.22	117.62	123.33
23	B	613	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
23	b	613	CLA	C1-C2-C3	-2.22	122.56	126.20
23	B	615	CLA	C2A-C3A-C4A	2.22	105.45	101.87
23	C	513	CLA	CHD-C1D-C2D	2.22	130.10	125.49
27	B	620	LMG	C8-O7-C10	2.22	123.10	117.80
23	C	512	CLA	CHD-C1D-ND	-2.22	121.68	124.80
23	C	504	CLA	CHB-C1B-NB	2.22	127.37	124.05
23	b	613	CLA	C3B-C4B-NB	-2.22	108.55	110.53
29	C	516	DGD	O3D-C3D-C4D	-2.21	105.16	110.38
23	d	404	CLA	CHB-C4A-NA	2.21	127.59	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CHB-C1B-C2B	-2.21	121.01	127.43
23	a	407	CLA	CMD-C2D-C3D	2.21	132.76	127.69
25	D	405	BCR	C28-C27-C26	-2.21	110.12	114.06
28	b	601	SQD	O47-C45-C46	2.21	116.27	108.34
29	A	413	DGD	C2G-O2G-C1B	2.21	123.08	117.80
23	A	405	CLA	CHB-C4A-NA	2.21	127.58	124.40
29	H	102	DGD	C8B-C7B-C6B	-2.21	103.22	114.37
27	b	622	LMG	O6-C5-C6	2.21	111.91	106.44
23	B	602	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
23	C	504	CLA	C6-C5-C3	2.20	118.84	113.47
23	C	513	CLA	C1-O2A-CGA	-2.20	111.32	116.65
29	H	102	DGD	O5D-C1E-C2E	2.20	111.62	108.27
23	b	610	CLA	C3B-C4B-NB	-2.20	108.56	110.53
23	b	616	CLA	CHB-C4A-NA	2.20	127.58	124.40
27	b	622	LMG	O2-C2-C1	-2.20	104.83	110.08
23	b	612	CLA	CHD-C4C-NC	2.20	127.64	124.23
33	L	101	LHG	C11-C10-C9	-2.20	103.25	114.37
23	c	508	CLA	CHD-C1D-C2D	2.20	130.06	125.49
25	D	405	BCR	C7-C8-C9	-2.19	122.99	126.23
25	b	618	BCR	C16-C15-C14	-2.19	119.03	123.52
23	B	616	CLA	C5-C3-C2	2.19	126.09	121.17
23	a	405	CLA	CHA-C1A-NA	-2.19	121.43	126.39
23	c	501	CLA	C7-C6-C5	-2.19	107.43	113.26
23	C	509	CLA	C4-C3-C5	2.19	119.03	115.23
23	B	611	CLA	C3B-C4B-NB	-2.19	108.58	110.53
23	d	402	CLA	CHC-C4B-NB	2.19	127.33	124.05
24	A	406	PHO	C3D-C4D-ND	2.19	110.51	107.71
29	C	518	DGD	C4A-C3A-C2A	-2.18	105.10	113.13
23	b	616	CLA	CHB-C1B-C2B	-2.18	121.08	127.43
23	B	616	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
23	A	405	CLA	CMD-C2D-C1D	-2.18	120.88	124.73
23	a	404	CLA	CAC-C3C-C4C	2.18	127.63	124.79
23	A	405	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
33	E	101	LHG	C27-C26-C25	-2.18	103.34	114.37
25	C	514	BCR	C15-C14-C13	-2.18	124.22	127.28
23	b	611	CLA	C11-C12-C13	-2.18	108.72	115.97
27	m	101	LMG	C1-C2-C3	-2.18	105.43	110.01
23	C	504	CLA	CHB-C4A-NA	2.18	127.54	124.40
25	H	101	BCR	C34-C9-C8	-2.18	114.76	118.09
27	m	101	LMG	C6-C5-C4	-2.18	107.67	113.02
23	B	603	CLA	C14-C13-C15	-2.18	103.52	111.27
23	B	602	CLA	CHC-C1C-C2C	-2.18	120.76	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	516	DGD	O5E-C6E-C5E	-2.18	103.92	111.33
25	B	617	BCR	C24-C23-C22	-2.18	123.02	126.23
23	c	504	CLA	C1C-C2C-C3C	-2.17	104.69	106.98
24	D	401	PHO	OBD-CAD-CBD	-2.17	122.64	125.82
23	C	502	CLA	CHB-C1B-NB	2.17	127.31	124.05
23	C	504	CLA	CMC-C2C-C1C	2.17	128.43	125.03
23	C	510	CLA	CHB-C4A-NA	2.17	127.53	124.40
23	a	407	CLA	O2D-CGD-CBD	2.17	115.02	111.23
23	a	407	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
26	d	406	PL9	C27-C28-C29	-2.17	122.66	127.62
26	d	406	PL9	C30-C29-C28	-2.17	118.06	123.63
26	d	406	PL9	C31-C29-C28	2.17	126.03	121.17
23	B	606	CLA	CMD-C2D-C1D	2.17	128.54	124.73
23	D	403	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	b	603	CLA	CMD-C2D-C1D	2.16	128.53	124.73
23	b	606	CLA	C16-C15-C13	-2.16	108.78	115.97
25	B	619	BCR	C15-C16-C17	-2.16	119.10	123.52
25	y	101	BCR	C2-C1-C6	2.16	113.58	110.44
26	a	409	PL9	C35-C34-C36	2.16	118.98	115.23
23	c	510	CLA	CMB-C2B-C3B	2.16	131.63	126.55
23	a	407	CLA	CHC-C1C-NC	2.16	127.56	124.31
23	B	605	CLA	C16-C15-C13	-2.16	108.78	115.97
23	B	602	CLA	C3C-C4C-NC	-2.16	107.66	110.43
29	a	413	DGD	CDB-CCB-CBB	-2.16	103.45	114.37
23	a	404	CLA	CHB-C4A-NA	2.16	127.52	124.40
25	b	618	BCR	C30-C25-C26	-2.16	119.69	122.64
23	b	615	CLA	CHD-C1D-ND	-2.16	121.77	124.80
25	b	620	BCR	C15-C16-C17	-2.16	119.11	123.52
23	b	614	CLA	CHA-C1A-NA	-2.16	121.51	126.39
28	a	411	SQD	C10-C9-C8	-2.15	105.21	113.13
23	a	404	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
25	b	618	BCR	C35-C13-C14	-2.15	119.33	122.82
23	C	510	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
29	h	103	DGD	C1D-C2D-C3D	-2.15	105.49	110.01
27	A	410	LMG	O3-C3-C2	-2.15	105.31	110.38
23	B	607	CLA	C2C-C1C-NC	2.15	112.24	109.98
24	a	406	PHO	C5-C3-C2	2.15	125.99	121.17
25	A	408	BCR	C38-C26-C27	-2.15	109.01	113.60
29	c	516	DGD	C4E-C3E-C2E	-2.15	107.06	110.83
23	B	612	CLA	C16-C15-C13	-2.15	108.83	115.97
33	B	622	LHG	C15-C14-C13	-2.15	103.51	114.37
29	c	517	DGD	O2G-C1B-O1B	-2.15	118.68	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	C4E-C3E-C2E	-2.15	107.06	110.83
24	A	406	PHO	O2D-CGD-O1D	-2.15	119.67	123.85
23	B	610	CLA	CBC-CAC-C3C	-2.15	106.60	112.42
27	d	409	LMG	O2-C2-C1	-2.15	104.96	110.08
23	c	513	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
25	B	617	BCR	C15-C16-C17	-2.14	119.13	123.52
23	c	502	CLA	C4D-CHA-C1A	2.14	123.80	121.24
29	c	516	DGD	CBB-CAB-C9B	-2.14	103.54	114.37
23	b	615	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
23	d	402	CLA	CHB-C4A-NA	2.14	127.49	124.40
29	c	518	DGD	CAB-C9B-C8B	-2.14	103.56	114.37
23	c	511	CLA	C2D-C1D-ND	-2.14	108.01	110.13
26	d	406	PL9	C45-C44-C46	-2.14	111.52	115.23
23	b	611	CLA	CHD-C4C-C3C	2.14	127.89	124.77
23	c	509	CLA	O2A-CGA-CBA	2.14	118.35	111.83
29	C	518	DGD	O6E-C5E-C4E	2.13	113.55	109.70
29	h	103	DGD	CDB-CCB-CBB	-2.13	103.58	114.37
25	T	101	BCR	C8-C9-C10	2.13	122.36	119.01
23	b	604	CLA	CHD-C1D-ND	-2.13	121.80	124.80
23	b	612	CLA	C11-C12-C13	-2.13	108.88	115.97
23	C	512	CLA	C6-C5-C3	-2.13	108.28	113.47
33	d	407	LHG	C11-C10-C9	-2.13	103.60	114.37
25	c	515	BCR	C33-C5-C6	-2.13	122.16	124.48
24	A	406	PHO	C3B-C4B-NB	-2.13	106.08	107.46
23	A	407	CLA	CED-O2D-CGD	-2.13	111.09	115.92
25	y	101	BCR	C33-C5-C6	-2.12	122.17	124.48
23	b	616	CLA	CMB-C2B-C3B	2.12	131.54	126.55
23	B	605	CLA	CHD-C1D-C2D	2.12	129.90	125.49
27	c	522	LMG	C17-C16-C15	-2.12	103.64	114.37
23	C	508	CLA	C3C-C4C-NC	-2.12	107.71	110.43
23	A	404	CLA	C6-C5-C3	2.12	118.64	113.47
23	B	611	CLA	C4A-NA-C1A	2.12	107.65	106.68
23	b	605	CLA	O1A-CGA-CBA	2.12	132.08	123.78
25	B	618	BCR	C2-C1-C6	2.12	113.52	110.44
23	b	609	CLA	C11-C10-C8	-2.12	108.92	115.97
23	C	501	CLA	CAC-C3C-C2C	-2.12	123.66	127.56
25	d	405	BCR	C8-C7-C6	-2.12	121.34	127.00
23	A	404	CLA	C4D-C3D-CAD	-2.12	105.80	108.11
34	e	102	HEM	CMC-C2C-C1C	-2.12	121.00	124.73
25	c	521	BCR	C33-C5-C6	-2.12	122.17	124.48
23	b	610	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	b	609	CLA	C4B-C3B-C2B	2.12	109.94	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	408	LHG	O8-C23-O10	-2.12	118.33	123.63
23	B	612	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
23	A	407	CLA	OBD-CAD-C3D	2.12	133.36	128.42
23	B	616	CLA	O2D-CGD-CBD	2.12	114.93	111.23
23	B	612	CLA	C7-C6-C5	-2.12	107.62	113.26
27	c	522	LMG	C9-C8-C7	-2.12	106.85	111.78
23	c	512	CLA	CHA-C1A-NA	-2.11	121.61	126.39
23	B	604	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
23	C	503	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
29	c	517	DGD	C1D-C2D-C3D	-2.11	105.56	110.01
23	B	615	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
29	c	517	DGD	C3G-C2G-C1G	-2.11	106.86	111.78
23	b	603	CLA	CGD-CBD-CAD	-2.11	104.01	110.85
23	C	501	CLA	CHA-C1A-NA	-2.11	121.61	126.39
23	B	606	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
26	A	409	PL9	C40-C39-C38	-2.11	118.21	123.63
23	C	511	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
23	B	611	CLA	CHD-C4C-NC	2.11	127.50	124.23
26	D	406	PL9	C27-C28-C29	-2.11	122.80	127.62
33	a	410	LHG	C20-C19-C18	-2.11	103.71	114.37
25	t	101	BCR	C11-C10-C9	-2.11	124.32	127.28
23	C	513	CLA	CHD-C4C-NC	2.11	127.50	124.23
26	D	406	PL9	C15-C14-C13	-2.10	118.22	123.63
27	D	410	LMG	O7-C10-O9	-2.10	118.78	123.70
29	c	518	DGD	C3E-C4E-C5E	-2.10	106.42	110.23
25	d	405	BCR	C40-C30-C25	2.10	113.54	110.24
29	h	103	DGD	CCB-CBB-CAB	-2.10	103.73	114.37
23	b	617	CLA	C2A-C3A-C4A	2.10	105.27	101.87
34	e	102	HEM	CAB-C3B-C2B	-2.10	121.60	128.43
23	b	605	CLA	C2A-C1A-CHA	2.10	127.52	123.87
23	h	101	CLA	CHD-C1D-ND	-2.10	121.84	124.80
23	C	507	CLA	C3A-C2A-C1A	2.10	104.48	101.34
23	A	407	CLA	C3B-C4B-NB	-2.10	108.66	110.53
23	d	404	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
23	b	612	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
23	b	612	CLA	C11-C10-C8	-2.10	109.00	115.97
29	h	103	DGD	CBB-CAB-C9B	-2.10	103.77	114.37
25	b	618	BCR	C15-C16-C17	-2.10	119.23	123.52
23	b	610	CLA	CHA-C1A-NA	-2.09	121.65	126.39
23	c	506	CLA	CHA-C4D-ND	2.09	136.87	132.55
23	A	404	CLA	C3A-C2A-C1A	2.09	104.47	101.34
23	C	506	CLA	CHB-C4A-NA	2.09	127.42	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C9-C8-C7	2.09	118.73	111.27
23	b	605	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
23	D	404	CLA	CHA-C1A-NA	-2.09	121.66	126.39
23	b	604	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
25	T	101	BCR	C1-C6-C5	-2.09	119.78	122.64
27	b	622	LMG	C3-C4-C5	-2.09	106.45	110.23
24	a	406	PHO	O2D-CGD-CBD	2.09	113.24	110.95
25	K	101	BCR	C8-C7-C6	-2.09	121.43	127.00
23	b	603	CLA	CMB-C2B-C3B	2.08	131.45	126.55
29	a	413	DGD	CFB-CEB-CDB	-2.08	103.84	114.37
23	c	508	CLA	O2D-CGD-CBD	2.08	114.87	111.23
27	D	411	LMG	C38-C37-C36	-2.08	103.85	114.37
28	f	101	SQD	C1-O5-C5	-2.08	109.66	113.72
23	d	403	CLA	C5-C3-C2	-2.08	116.50	121.17
23	D	402	CLA	C16-C15-C13	-2.08	109.06	115.97
29	c	518	DGD	C1E-O6E-C5E	-2.08	109.66	113.72
23	B	610	CLA	CHA-C1A-NA	-2.08	121.69	126.39
25	K	101	BCR	C30-C25-C26	-2.08	119.80	122.64
34	E	102	HEM	CHA-C1A-NA	2.08	127.63	123.86
24	a	406	PHO	O2A-CGA-O1A	-2.08	118.43	123.63
23	B	611	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
23	B	607	CLA	CHB-C4A-NA	2.08	127.40	124.40
23	b	605	CLA	C7-C6-C5	-2.08	107.73	113.26
27	m	101	LMG	C19-C18-C17	-2.08	103.88	114.37
35	v	201	HEC	CHA-C4D-ND	2.07	127.62	123.86
25	D	405	BCR	C16-C15-C14	-2.07	119.28	123.52
29	a	413	DGD	C5B-C4B-C3B	-2.07	103.88	114.37
28	b	601	SQD	O10-C23-C24	-2.07	115.67	123.78
23	b	616	CLA	C4-C3-C5	2.07	118.83	115.23
25	h	102	BCR	C35-C13-C14	-2.07	119.46	122.82
23	b	607	CLA	O2D-CGD-CBD	2.07	114.85	111.23
25	b	620	BCR	C31-C1-C6	2.07	113.49	110.24
25	B	617	BCR	C3-C4-C5	-2.07	110.37	114.06
23	B	612	CLA	C3B-C4B-NB	-2.07	108.69	110.53
29	h	103	DGD	O5E-C6E-C5E	-2.07	104.30	111.33
23	B	602	CLA	CHD-C4C-NC	2.07	127.43	124.23
33	l	101	LHG	C20-C19-C18	-2.06	103.93	114.37
23	c	506	CLA	C2A-C1A-CHA	2.06	127.45	123.87
29	h	103	DGD	O2D-C2D-C1D	-2.06	105.16	110.08
23	c	513	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
27	B	620	LMG	O8-C28-O10	-2.06	118.47	123.63
25	T	101	BCR	C38-C26-C27	-2.06	109.20	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	405	BCR	C27-C26-C25	2.06	125.49	122.70
26	d	406	PL9	C45-C44-C43	-2.06	118.34	123.63
23	c	510	CLA	O1D-CGD-CBD	2.06	128.58	124.52
25	h	102	BCR	C39-C30-C25	-2.06	107.02	110.24
23	B	613	CLA	C2C-C1C-NC	2.06	112.14	109.98
23	b	607	CLA	C2C-C1C-NC	2.06	112.14	109.98
23	a	405	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
23	C	512	CLA	CHA-C4D-ND	2.06	136.79	132.55
23	C	503	CLA	CHB-C4A-NA	2.05	127.36	124.40
25	D	405	BCR	C29-C30-C25	2.05	113.42	110.44
23	c	503	CLA	CHD-C1D-C2D	2.05	129.76	125.49
26	d	406	PL9	C32-C33-C34	-2.05	122.92	127.62
23	b	613	CLA	CHB-C1B-NB	2.05	127.13	124.05
23	C	507	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
23	c	506	CLA	C3C-C4C-NC	-2.05	107.80	110.43
27	B	620	LMG	C37-C36-C35	-2.05	104.00	114.37
29	c	518	DGD	C9B-C8B-C7B	-2.05	104.00	114.37
23	b	604	CLA	CMB-C2B-C3B	2.05	131.37	126.55
23	B	609	CLA	C2A-C1A-CHA	2.05	127.42	123.87
28	f	101	SQD	C1-C2-C3	-2.05	105.70	110.01
23	b	616	CLA	C3A-C2A-C1A	2.05	104.41	101.34
23	A	404	CLA	CHD-C4C-NC	2.05	127.41	124.23
23	B	614	CLA	C1-C2-C3	-2.05	122.84	126.20
23	c	513	CLA	CHD-C1D-ND	-2.05	121.92	124.80
23	C	506	CLA	C1-C2-C3	-2.05	122.85	126.20
23	a	407	CLA	CAA-C2A-C3A	-2.04	107.47	113.00
28	A	411	SQD	C45-O47-C7	2.04	122.69	117.80
25	C	515	BCR	C39-C30-C25	2.04	113.44	110.24
23	c	506	CLA	CHC-C4B-NB	2.04	127.11	124.05
23	A	404	CLA	CMB-C2B-C3B	2.04	131.35	126.55
23	A	404	CLA	CHD-C1D-ND	-2.04	121.93	124.80
29	c	516	DGD	C1D-C2D-C3D	-2.04	105.72	110.01
25	B	619	BCR	C37-C22-C21	-2.04	119.52	122.82
23	b	605	CLA	CHB-C1B-NB	2.04	127.10	124.05
23	D	402	CLA	C7-C6-C5	-2.04	107.83	113.26
27	D	407	LMG	C3-C4-C5	-2.04	106.54	110.23
28	b	601	SQD	O49-C7-C8	-2.04	115.82	123.78
23	C	502	CLA	C1-O2A-CGA	2.04	121.58	116.65
29	c	518	DGD	O1G-C1A-C2A	-2.04	105.63	111.83
25	t	101	BCR	C29-C30-C25	2.03	113.39	110.44
23	b	605	CLA	CAA-CBA-CGA	-2.03	107.43	113.21
29	C	516	DGD	C8B-C7B-C6B	-2.03	104.09	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	617	CLA	C6-C5-C3	2.03	118.42	113.47
24	d	401	PHO	CAA-CBA-CGA	-2.03	107.44	113.21
23	A	404	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
29	H	102	DGD	C7B-C6B-C5B	-2.03	104.10	114.37
28	f	101	SQD	O48-C23-C24	2.03	118.03	111.83
23	B	609	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	D	402	CLA	CAC-C3C-C4C	2.03	127.43	124.79
25	B	617	BCR	C31-C1-C6	-2.03	107.06	110.24
27	d	409	LMG	O2-C2-C3	-2.03	105.59	110.38
23	b	615	CLA	CHA-C4D-ND	2.03	136.73	132.55
23	B	607	CLA	CHA-C1A-NA	-2.03	121.80	126.39
23	B	604	CLA	C1D-ND-C4D	2.03	107.73	106.31
33	d	408	LHG	O8-C6-C5	-2.03	102.55	108.40
25	B	618	BCR	C15-C14-C13	-2.03	124.44	127.28
23	B	613	CLA	C2A-C3A-C4A	2.03	105.14	101.87
23	c	502	CLA	CHD-C4C-NC	2.02	127.37	124.23
33	e	101	LHG	C5-O7-C7	-2.02	112.95	117.80
23	B	607	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
26	A	409	PL9	O2-C1-C6	2.02	123.70	120.48
23	c	502	CLA	CHB-C1B-NB	2.02	127.08	124.05
27	m	101	LMG	O2-C2-C1	-2.02	105.26	110.08
23	C	503	CLA	O2A-C1-C2	-2.02	100.33	108.11
23	b	612	CLA	O2D-CGD-CBD	2.02	114.76	111.23
25	C	514	BCR	C27-C26-C25	2.02	125.43	122.70
28	a	411	SQD	O8-S-O9	-2.02	106.35	111.40
27	b	622	LMG	C1-C2-C3	-2.02	105.76	110.01
23	h	101	CLA	O2A-C1-C2	2.02	115.88	108.11
28	F	101	SQD	C46-C45-C44	-2.02	107.15	113.67
23	b	614	CLA	CAA-C2A-C1A	2.02	118.59	111.97
33	l	101	LHG	C27-C26-C25	-2.02	104.17	114.37
35	v	201	HEC	O2A-CGA-CBA	2.02	120.37	114.00
23	B	603	CLA	C2A-C1A-CHA	2.02	127.37	123.87
28	a	411	SQD	C1-O5-C5	-2.02	109.78	113.72
23	b	610	CLA	C16-C15-C13	-2.01	109.27	115.97
23	b	613	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
23	a	407	CLA	C2A-C1A-CHA	2.01	127.36	123.87
29	h	103	DGD	O6D-C1D-O3G	-2.01	105.29	110.04
28	a	412	SQD	O48-C23-O10	-2.01	118.59	123.63
24	d	401	PHO	O2A-CGA-O1A	-2.01	118.59	123.63
35	V	201	HEC	C4A-C3A-C2A	2.01	109.96	106.97
27	a	414	LMG	O5-C6-C5	-2.01	104.48	111.33
23	c	503	CLA	C2D-C1D-ND	-2.01	108.14	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C6-C7-C8	-2.01	109.28	115.97
27	a	414	LMG	O2-C2-C3	-2.01	105.64	110.38
27	D	410	LMG	C8-O7-C10	2.01	122.61	117.80
23	b	607	CLA	C4D-CHA-C1A	2.01	123.64	121.24
23	c	501	CLA	CHA-C1A-NA	-2.01	121.84	126.39
23	c	512	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
23	B	603	CLA	C4D-CHA-C1A	2.01	123.64	121.24
33	D	409	LHG	C11-C10-C9	-2.01	104.22	114.37
23	C	511	CLA	CMC-C2C-C3C	2.01	131.58	126.15
29	H	102	DGD	CAB-C9B-C8B	-2.01	104.23	114.37
28	a	411	SQD	O5-C1-C2	-2.01	106.25	110.37
23	c	503	CLA	CHC-C4B-NB	2.01	127.06	124.05
23	C	502	CLA	CHA-C1A-NA	-2.00	121.85	126.39
27	A	410	LMG	C36-C35-C34	-2.00	104.23	114.37
23	A	405	CLA	O1A-CGA-CBA	2.00	131.62	123.78
29	H	102	DGD	O6E-C5E-C4E	2.00	113.31	109.70
23	d	403	CLA	C11-C12-C13	-2.00	109.31	115.97
26	d	406	PL9	C42-C43-C44	-2.00	123.04	127.62
23	c	510	CLA	CHA-C4D-ND	2.00	136.68	132.55
23	B	606	CLA	CHA-C4D-ND	2.00	136.68	132.55

All (55) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	602	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	402	CLA	ND
23	D	403	CLA	ND
23	a	404	CLA	ND
23	a	405	CLA	ND
23	a	407	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	611	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	c	501	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND
23	d	404	CLA	ND
23	h	101	CLA	ND

All (1710) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C2B-C3B-CAB-CBB
23	B	605	CLA	C4B-C3B-CAB-CBB
23	B	606	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	C2B-C3B-CAB-CBB
23	B	609	CLA	C4B-C3B-CAB-CBB
23	B	616	CLA	CBD-CGD-O2D-CED
23	C	501	CLA	C2B-C3B-CAB-CBB
23	C	501	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C4-C3-C5-C6
23	C	506	CLA	C1A-C2A-CAA-CBA
23	C	506	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	C14-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C9
23	a	405	CLA	C2B-C3B-CAB-CBB
23	a	405	CLA	C4B-C3B-CAB-CBB
23	a	407	CLA	C1A-C2A-CAA-CBA
23	b	611	CLA	C2B-C3B-CAB-CBB
23	b	611	CLA	C4B-C3B-CAB-CBB
23	b	615	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	b	615	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	C11-C10-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C10-C8-C9
23	c	511	CLA	C14-C13-C15-C16
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	CBD-CGD-O2D-CED
23	h	101	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	C3A-C2A-CAA-CBA
23	h	101	CLA	CBD-CGD-O2D-CED
23	h	101	CLA	C11-C10-C8-C9
25	B	617	BCR	C11-C12-C13-C35
25	B	617	BCR	C12-C13-C14-C15
25	B	617	BCR	C35-C13-C14-C15
25	B	618	BCR	C17-C18-C19-C20
25	B	618	BCR	C18-C19-C20-C21
25	B	618	BCR	C20-C21-C22-C37
25	B	618	BCR	C22-C23-C24-C25
25	B	619	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	C	514	BCR	C11-C10-C9-C8
25	C	514	BCR	C11-C12-C13-C14
25	C	514	BCR	C16-C17-C18-C36
25	C	514	BCR	C20-C21-C22-C37
25	C	520	BCR	C11-C10-C9-C8
25	C	520	BCR	C11-C10-C9-C34
25	C	520	BCR	C10-C11-C12-C13
25	D	405	BCR	C35-C13-C14-C15
25	D	405	BCR	C14-C15-C16-C17
25	D	405	BCR	C16-C17-C18-C19
25	D	405	BCR	C16-C17-C18-C36
25	H	101	BCR	C23-C24-C25-C26
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C21-C22-C23-C24
25	T	101	BCR	C1-C6-C7-C8
25	T	101	BCR	C5-C6-C7-C8
25	T	101	BCR	C7-C8-C9-C10
25	T	101	BCR	C11-C12-C13-C35
25	T	101	BCR	C16-C17-C18-C36
25	T	101	BCR	C20-C21-C22-C23
25	T	101	BCR	C37-C22-C23-C24
25	c	514	BCR	C11-C10-C9-C34
25	c	514	BCR	C35-C13-C14-C15
25	c	514	BCR	C18-C19-C20-C21
25	c	515	BCR	C35-C13-C14-C15
25	c	515	BCR	C16-C17-C18-C36
25	c	515	BCR	C17-C18-C19-C20
25	d	405	BCR	C16-C17-C18-C19
25	d	405	BCR	C16-C17-C18-C36
25	d	405	BCR	C37-C22-C23-C24
25	h	102	BCR	C18-C19-C20-C21
25	t	101	BCR	C11-C10-C9-C34
25	y	101	BCR	C7-C8-C9-C34
25	y	101	BCR	C11-C10-C9-C34
25	y	101	BCR	C20-C21-C22-C37
26	A	409	PL9	C9-C11-C12-C13
26	A	409	PL9	C12-C13-C14-C15
26	A	409	PL9	C12-C13-C14-C16
26	A	409	PL9	C22-C23-C24-C25
26	A	409	PL9	C22-C23-C24-C26
26	A	409	PL9	C32-C33-C34-C36
26	A	409	PL9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C37-C38-C39-C41
26	D	406	PL9	C12-C13-C14-C16
26	D	406	PL9	C32-C33-C34-C35
26	D	406	PL9	C32-C33-C34-C36
26	a	409	PL9	C7-C8-C9-C10
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C28-C29-C31-C32
26	a	409	PL9	C32-C33-C34-C35
26	a	409	PL9	C37-C38-C39-C41
26	d	406	PL9	C27-C28-C29-C31
26	d	406	PL9	C32-C33-C34-C35
26	d	406	PL9	C42-C43-C44-C46
27	A	410	LMG	O9-C10-O7-C8
27	C	519	LMG	C11-C10-O7-C8
27	D	410	LMG	O1-C7-C8-C9
27	D	410	LMG	O1-C7-C8-O7
27	a	414	LMG	O6-C1-O1-C7
27	b	622	LMG	C2-C1-O1-C7
27	b	622	LMG	O9-C10-O7-C8
27	b	622	LMG	C11-C10-O7-C8
28	A	412	SQD	C46-C45-O47-C7
28	B	623	SQD	C2-C1-O6-C44
28	B	623	SQD	O5-C1-O6-C44
28	B	623	SQD	O6-C44-C45-O47
28	B	623	SQD	O49-C7-O47-C45
28	B	623	SQD	C8-C7-O47-C45
28	F	101	SQD	O10-C23-O48-C46
28	a	411	SQD	O47-C45-C46-O48
28	a	412	SQD	O6-C44-C45-C46
28	a	412	SQD	O6-C44-C45-O47
28	a	412	SQD	C8-C7-O47-C45
28	b	601	SQD	O10-C23-O48-C46
28	b	601	SQD	C5-C6-S-O7
28	b	601	SQD	C5-C6-S-O8
28	b	601	SQD	C5-C6-S-O9
28	f	101	SQD	C2-C1-O6-C44
28	f	101	SQD	O5-C1-O6-C44
29	A	413	DGD	O1B-C1B-O2G-C2G
33	D	408	LHG	O1-C1-C2-C3
33	D	408	LHG	C3-O3-P-O4
33	D	408	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
33	D	408	LHG	C4-O6-P-O4
33	D	409	LHG	O2-C2-C3-O3
33	D	409	LHG	C3-O3-P-O5
33	D	409	LHG	C3-O3-P-O6
33	D	409	LHG	C4-O6-P-O3
33	D	409	LHG	C4-O6-P-O4
33	E	101	LHG	C4-O6-P-O3
33	E	101	LHG	O10-C23-O8-C6
33	E	101	LHG	C24-C23-O8-C6
33	L	101	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O5
33	a	410	LHG	O1-C1-C2-C3
33	a	410	LHG	C1-C2-C3-O3
33	d	407	LHG	O1-C1-C2-C3
33	d	407	LHG	C3-O3-P-O4
33	d	407	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O3
33	d	407	LHG	C4-O6-P-O4
33	e	101	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O4
33	e	101	LHG	O10-C23-O8-C6
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O5
35	V	201	HEC	C2B-C3B-CAB-CBB
35	V	201	HEC	C4B-C3B-CAB-CBB
35	V	201	HEC	C2C-C3C-CAC-CBC
35	V	201	HEC	C4C-C3C-CAC-CBC
35	v	201	HEC	C2B-C3B-CAB-CBB
35	v	201	HEC	C4B-C3B-CAB-CBB
35	v	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C4C-C3C-CAC-CBC
23	b	617	CLA	O1D-CGD-O2D-CED
23	h	101	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	O1D-CGD-O2D-CED
23	B	614	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
24	a	406	PHO	CBD-CGD-O2D-CED
27	a	414	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
26	d	406	PL9	C47-C48-C49-C50
26	d	406	PL9	C47-C48-C49-C51
27	a	414	LMG	C29-C28-O8-C9
28	b	601	SQD	C24-C23-O48-C46
33	e	101	LHG	C24-C23-O8-C6
27	c	522	LMG	O10-C28-O8-C9
28	a	412	SQD	O10-C23-O48-C46
29	a	413	DGD	O1A-C1A-O1G-C1G
23	c	510	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	O1D-CGD-O2D-CED
27	C	519	LMG	O9-C10-O7-C8
27	D	410	LMG	O9-C10-O7-C8
27	c	522	LMG	O9-C10-O7-C8
28	a	412	SQD	O49-C7-O47-C45
29	a	413	DGD	O1B-C1B-O2G-C2G
33	e	101	LHG	O9-C7-O7-C5
23	B	616	CLA	C3-C5-C6-C7
23	b	605	CLA	C3-C5-C6-C7
23	c	506	CLA	O1D-CGD-O2D-CED
28	a	412	SQD	C24-C23-O48-C46
29	a	413	DGD	C2A-C1A-O1G-C1G
23	B	610	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	C11-C10-O7-C8
29	A	413	DGD	C2B-C1B-O2G-C2G
23	B	606	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
23	A	407	CLA	C4-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
26	a	409	PL9	C30-C29-C31-C32
23	A	407	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	B	614	CLA	C2-C3-C5-C6
23	C	504	CLA	C2-C3-C5-C6
23	b	604	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
26	A	409	PL9	C18-C19-C21-C22
26	a	409	PL9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
26	d	406	PL9	C38-C39-C41-C42
24	a	406	PHO	O1D-CGD-O2D-CED
23	h	101	CLA	C2A-CAA-CBA-CGA
27	c	522	LMG	C29-C28-O8-C9
28	F	101	SQD	C24-C23-O48-C46
26	A	409	PL9	C42-C43-C44-C45
26	a	409	PL9	C42-C43-C44-C45
26	d	406	PL9	C42-C43-C44-C45
26	a	409	PL9	C32-C33-C34-C36
26	d	406	PL9	C32-C33-C34-C36
23	C	505	CLA	C2C-C3C-CAC-CBC
23	B	604	CLA	C13-C15-C16-C17
23	C	512	CLA	C3-C5-C6-C7
23	b	603	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
33	a	410	LHG	O2-C2-C3-O3
28	F	101	SQD	C44-C45-C46-O48
23	B	614	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CBA-CGA-O2A-C1
29	A	413	DGD	O6E-C5E-C6E-O5E
29	C	516	DGD	O6E-C5E-C6E-O5E
23	B	607	CLA	CBD-CGD-O2D-CED
27	D	410	LMG	C11-C10-O7-C8
33	e	101	LHG	C8-C7-O7-C5
23	c	512	CLA	CBD-CGD-O2D-CED
23	b	615	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
27	B	620	LMG	O10-C28-O8-C9
27	c	522	LMG	O6-C5-C6-O5
26	A	409	PL9	C34-C36-C37-C38
26	A	409	PL9	C44-C46-C47-C48
26	a	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C29-C31-C32-C33
26	a	409	PL9	C34-C36-C37-C38
26	d	406	PL9	C44-C46-C47-C48
23	c	511	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	C3-C5-C6-C7
23	D	403	CLA	C3-C5-C6-C7
27	A	410	LMG	O6-C1-O1-C7
27	b	622	LMG	O6-C1-O1-C7
27	c	519	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
28	f	101	SQD	C24-C23-O48-C46
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	614	CLA	CBD-CGD-O2D-CED
27	a	414	LMG	O6-C5-C6-O5
23	B	601	CLA	O1A-CGA-O2A-C1
29	A	413	DGD	C4E-C5E-C6E-O5E
29	C	516	DGD	C4E-C5E-C6E-O5E
27	c	522	LMG	C11-C10-O7-C8
23	C	502	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	O1D-CGD-O2D-CED
27	a	414	LMG	C4-C5-C6-O5
29	h	103	DGD	C4E-C5E-C6E-O5E
23	b	615	CLA	C2-C3-C5-C6
23	c	503	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	C11-C10-C8-C9
23	B	605	CLA	C11-C10-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	C	503	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	607	CLA	C14-C13-C15-C16
23	b	611	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C12-C13-C14
23	c	510	CLA	C11-C12-C13-C14
23	c	512	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C12-C13-C14
27	a	414	LMG	C2-C1-O1-C7
29	c	517	DGD	C2E-C1E-O5D-C6D
33	D	408	LHG	O2-C2-C3-O3
28	a	411	SQD	C12-C13-C14-C15
25	B	618	BCR	C7-C8-C9-C34
25	C	514	BCR	C11-C12-C13-C35
25	C	520	BCR	C7-C8-C9-C34
25	C	520	BCR	C37-C22-C23-C24
25	H	101	BCR	C11-C12-C13-C35
25	H	101	BCR	C37-C22-C23-C24
25	K	101	BCR	C37-C22-C23-C24
25	T	101	BCR	C7-C8-C9-C34
25	b	620	BCR	C37-C22-C23-C24
25	c	514	BCR	C11-C12-C13-C35
25	c	514	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	c	515	BCR	C11-C12-C13-C35
25	d	405	BCR	C7-C8-C9-C34
25	d	405	BCR	C11-C12-C13-C35
25	y	101	BCR	C7-C8-C9-C10
33	E	101	LHG	C23-C24-C25-C26
23	b	604	CLA	O1D-CGD-O2D-CED
23	C	508	CLA	CBD-CGD-O2D-CED
28	A	411	SQD	C23-C24-C25-C26
25	c	515	BCR	C14-C15-C16-C17
23	C	505	CLA	C5-C6-C7-C8
23	C	510	CLA	C15-C16-C17-C18
33	D	408	LHG	O1-C1-C2-O2
29	c	516	DGD	C1B-C2B-C3B-C4B
33	E	101	LHG	C7-C8-C9-C10
23	c	503	CLA	C15-C16-C17-C18
29	h	103	DGD	O6E-C5E-C6E-O5E
23	B	606	CLA	C6-C7-C8-C10
29	a	413	DGD	C1A-C2A-C3A-C4A
29	C	517	DGD	O6E-C5E-C6E-O5E
26	A	409	PL9	C29-C31-C32-C33
26	a	409	PL9	C44-C46-C47-C48
26	d	406	PL9	C29-C31-C32-C33
29	C	518	DGD	C4E-C5E-C6E-O5E
23	b	604	CLA	C8-C10-C11-C12
23	b	612	CLA	C15-C16-C17-C18
29	H	102	DGD	C4E-C5E-C6E-O5E
27	D	410	LMG	C10-C11-C12-C13
27	D	411	LMG	C28-C29-C30-C31
27	c	522	LMG	C10-C11-C12-C13
27	d	409	LMG	C28-C29-C30-C31
27	m	101	LMG	C10-C11-C12-C13
28	A	411	SQD	C7-C8-C9-C10
28	A	412	SQD	C7-C8-C9-C10
29	c	516	DGD	C1A-C2A-C3A-C4A
29	c	518	DGD	C1A-C2A-C3A-C4A
28	a	411	SQD	O10-C23-O48-C46
23	D	403	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	C10-C11-C12-C13
23	C	512	CLA	C15-C16-C17-C18
23	b	610	CLA	C15-C16-C17-C18
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	b	611	CLA	C2A-CAA-CBA-CGA
25	D	405	BCR	C18-C19-C20-C21
23	b	605	CLA	C10-C11-C12-C13
23	b	617	CLA	C10-C11-C12-C13
23	c	506	CLA	C5-C6-C7-C8
33	a	410	LHG	C7-C8-C9-C10
33	a	410	LHG	C23-C24-C25-C26
33	e	101	LHG	C7-C8-C9-C10
29	c	518	DGD	O1A-C1A-O1G-C1G
29	c	517	DGD	O6E-C1E-O5D-C6D
23	B	602	CLA	C8-C10-C11-C12
23	B	604	CLA	C10-C11-C12-C13
23	B	606	CLA	C15-C16-C17-C18
23	B	611	CLA	C13-C15-C16-C17
23	C	503	CLA	C5-C6-C7-C8
23	C	512	CLA	C8-C10-C11-C12
23	a	407	CLA	C10-C11-C12-C13
23	b	608	CLA	C10-C11-C12-C13
23	b	612	CLA	C13-C15-C16-C17
23	c	507	CLA	C8-C10-C11-C12
29	c	517	DGD	C4E-C5E-C6E-O5E
28	B	623	SQD	C23-C24-C25-C26
23	B	607	CLA	C5-C6-C7-C8
23	c	505	CLA	C15-C16-C17-C18
23	c	512	CLA	O1D-CGD-O2D-CED
29	H	102	DGD	O6E-C5E-C6E-O5E
26	a	409	PL9	C47-C48-C49-C50
26	d	406	PL9	C22-C23-C24-C25
23	B	601	CLA	C5-C6-C7-C8
23	a	407	CLA	C13-C15-C16-C17
23	c	513	CLA	C8-C10-C11-C12
23	h	101	CLA	C13-C15-C16-C17
24	d	401	PHO	CBD-CGD-O2D-CED
33	l	101	LHG	C23-C24-C25-C26
29	c	517	DGD	O6E-C5E-C6E-O5E
23	D	404	CLA	C5-C6-C7-C8
23	b	608	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
24	D	401	PHO	CBD-CGD-O2D-CED
29	a	413	DGD	C2B-C1B-O2G-C2G
23	B	603	CLA	C10-C11-C12-C13
23	B	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	B	609	CLA	C3-C5-C6-C7
23	b	609	CLA	C13-C15-C16-C17
33	D	409	LHG	C7-C8-C9-C10
27	A	410	LMG	C29-C28-O8-C9
27	B	620	LMG	C29-C28-O8-C9
23	B	602	CLA	C13-C15-C16-C17
23	C	512	CLA	C10-C11-C12-C13
23	a	407	CLA	C5-C6-C7-C8
23	b	612	CLA	C8-C10-C11-C12
23	b	615	CLA	C5-C6-C7-C8
23	b	615	CLA	C15-C16-C17-C18
23	c	508	CLA	C13-C15-C16-C17
23	A	404	CLA	C15-C16-C17-C18
23	B	607	CLA	C13-C15-C16-C17
23	B	611	CLA	C15-C16-C17-C18
23	B	614	CLA	C13-C15-C16-C17
23	b	603	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
23	c	506	CLA	C13-C15-C16-C17
23	c	509	CLA	C10-C11-C12-C13
23	C	505	CLA	C4C-C3C-CAC-CBC
23	C	509	CLA	C13-C15-C16-C17
23	b	607	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
23	c	509	CLA	C15-C16-C17-C18
23	c	512	CLA	C13-C15-C16-C17
23	h	101	CLA	C15-C16-C17-C18
23	c	510	CLA	C8-C10-C11-C12
23	c	510	CLA	C15-C16-C17-C18
23	C	511	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	C11-C10-C8-C9
23	b	608	CLA	O1A-CGA-O2A-C1
29	C	517	DGD	C2E-C1E-O5D-C6D
29	c	517	DGD	C2D-C1D-O3G-C3G
27	C	519	LMG	C4-C5-C6-O5
25	B	618	BCR	C16-C17-C18-C36
25	C	514	BCR	C35-C13-C14-C15
25	C	520	BCR	C20-C21-C22-C37
25	D	405	BCR	C20-C21-C22-C37
25	H	101	BCR	C16-C17-C18-C36
25	K	101	BCR	C11-C10-C9-C34
25	a	408	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
25	d	405	BCR	C35-C13-C14-C15
25	h	102	BCR	C11-C10-C9-C34
25	t	101	BCR	C16-C17-C18-C36
29	A	413	DGD	C1A-C2A-C3A-C4A
33	d	408	LHG	C24-C25-C26-C27
23	B	607	CLA	O1D-CGD-O2D-CED
23	b	614	CLA	C10-C11-C12-C13
25	B	618	BCR	C37-C22-C23-C24
25	B	619	BCR	C7-C8-C9-C34
25	C	514	BCR	C7-C8-C9-C34
25	C	514	BCR	C37-C22-C23-C24
25	A	408	BCR	C17-C18-C19-C20
23	B	609	CLA	C13-C15-C16-C17
23	b	616	CLA	C5-C6-C7-C8
33	E	101	LHG	O1-C1-C2-C3
33	d	408	LHG	O1-C1-C2-C3
27	c	519	LMG	C11-C10-O7-C8
23	B	615	CLA	C16-C17-C18-C20
23	b	608	CLA	C16-C17-C18-C20
23	c	502	CLA	C16-C17-C18-C19
23	c	507	CLA	C16-C17-C18-C20
23	b	605	CLA	C8-C10-C11-C12
25	B	618	BCR	C11-C10-C9-C8
25	C	514	BCR	C16-C17-C18-C19
25	H	101	BCR	C11-C10-C9-C8
25	H	101	BCR	C16-C17-C18-C19
25	K	101	BCR	C11-C10-C9-C8
25	K	101	BCR	C20-C21-C22-C23
25	T	101	BCR	C16-C17-C18-C19
25	b	620	BCR	C11-C10-C9-C8
25	c	514	BCR	C16-C17-C18-C19
25	c	514	BCR	C20-C21-C22-C23
25	c	515	BCR	C12-C13-C14-C15
25	d	405	BCR	C11-C10-C9-C8
25	h	102	BCR	C11-C10-C9-C8
25	t	101	BCR	C16-C17-C18-C19
29	C	517	DGD	O6E-C1E-O5D-C6D
29	c	517	DGD	O6D-C1D-O3G-C3G
29	c	516	DGD	C4D-C5D-C6D-O5D
23	b	614	CLA	O1D-CGD-O2D-CED
29	c	516	DGD	O6D-C5D-C6D-O5D
23	B	601	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
27	A	410	LMG	O10-C28-O8-C9
28	f	101	SQD	O10-C23-O48-C46
27	D	407	LMG	O6-C5-C6-O5
27	A	410	LMG	C16-C17-C18-C19
28	A	411	SQD	C28-C29-C30-C31
28	a	412	SQD	C12-C13-C14-C15
33	L	101	LHG	C14-C15-C16-C17
25	d	405	BCR	C14-C15-C16-C17
27	D	411	LMG	C32-C33-C34-C35
28	A	411	SQD	C30-C31-C32-C33
28	a	412	SQD	C16-C17-C18-C19
29	H	102	DGD	C3B-C4B-C5B-C6B
29	h	103	DGD	C5B-C6B-C7B-C8B
27	D	407	LMG	C19-C20-C21-C22
27	a	414	LMG	C29-C30-C31-C32
28	A	411	SQD	C11-C12-C13-C14
28	b	601	SQD	C16-C17-C18-C19
33	d	407	LHG	C29-C30-C31-C32
27	B	620	LMG	C12-C13-C14-C15
27	a	414	LMG	C12-C13-C14-C15
29	c	518	DGD	CCA-CDA-CEA-CFA
33	D	409	LHG	C27-C28-C29-C30
33	e	101	LHG	C17-C18-C19-C20
33	d	407	LHG	O1-C1-C2-O2
27	D	411	LMG	C33-C34-C35-C36
27	c	519	LMG	C36-C37-C38-C39
23	c	511	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	C4B-C3B-CAB-CBB
23	B	606	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
23	d	403	CLA	C4B-C3B-CAB-CBB
29	c	516	DGD	C4A-C5A-C6A-C7A
33	D	409	LHG	C32-C33-C34-C35
23	B	613	CLA	C16-C17-C18-C19
23	b	608	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
27	D	407	LMG	C11-C12-C13-C14
28	a	412	SQD	C11-C12-C13-C14
29	H	102	DGD	C4B-C5B-C6B-C7B
33	E	101	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
27	b	622	LMG	C31-C32-C33-C34
23	B	615	CLA	C11-C12-C13-C15
23	C	507	CLA	C11-C10-C8-C7
23	D	403	CLA	C12-C13-C15-C16
28	A	412	SQD	C32-C33-C34-C35
28	a	412	SQD	C10-C11-C12-C13
29	c	518	DGD	C5B-C6B-C7B-C8B
23	c	505	CLA	C5-C6-C7-C8
27	b	622	LMG	C19-C20-C21-C22
29	H	102	DGD	C7B-C8B-C9B-CAB
33	E	101	LHG	C28-C29-C30-C31
33	a	410	LHG	C25-C26-C27-C28
23	a	407	CLA	C3A-C2A-CAA-CBA
23	c	512	CLA	C3A-C2A-CAA-CBA
29	A	413	DGD	C5B-C6B-C7B-C8B
29	C	517	DGD	C9A-CAA-CBA-CCA
33	E	101	LHG	C33-C34-C35-C36
33	L	101	LHG	C32-C33-C34-C35
23	B	605	CLA	C15-C16-C17-C18
23	B	612	CLA	C10-C11-C12-C13
23	C	507	CLA	C10-C11-C12-C13
27	c	519	LMG	C4-C5-C6-O5
25	c	514	BCR	C13-C14-C15-C16
23	B	609	CLA	C16-C17-C18-C19
23	c	502	CLA	C16-C17-C18-C20
23	c	511	CLA	O1A-CGA-O2A-C1
33	D	408	LHG	C11-C10-C9-C8
33	B	622	LHG	C31-C32-C33-C34
23	C	503	CLA	CBA-CGA-O2A-C1
23	b	615	CLA	CBA-CGA-O2A-C1
33	l	101	LHG	C24-C23-O8-C6
27	D	407	LMG	C14-C15-C16-C17
29	C	517	DGD	C5B-C6B-C7B-C8B
29	a	413	DGD	C4A-C5A-C6A-C7A
29	c	516	DGD	C8B-C9B-CAB-CBB
33	d	407	LHG	C32-C33-C34-C35
33	e	101	LHG	C23-C24-C25-C26
27	B	620	LMG	C36-C37-C38-C39
27	C	519	LMG	C30-C31-C32-C33
27	a	414	LMG	C16-C17-C18-C19
27	b	623	LMG	C11-C12-C13-C14
28	b	601	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
29	C	518	DGD	C5A-C6A-C7A-C8A
29	a	413	DGD	C2A-C3A-C4A-C5A
33	D	408	LHG	C15-C16-C17-C18
33	L	101	LHG	C18-C19-C20-C21
33	d	407	LHG	C11-C12-C13-C14
33	d	408	LHG	C26-C27-C28-C29
33	e	101	LHG	C14-C15-C16-C17
33	e	101	LHG	C26-C27-C28-C29
28	B	623	SQD	C28-C29-C30-C31
28	F	101	SQD	C25-C26-C27-C28
29	a	413	DGD	C7B-C8B-C9B-CAB
33	L	101	LHG	C27-C28-C29-C30
33	a	410	LHG	C16-C17-C18-C19
27	D	411	LMG	C16-C17-C18-C19
27	m	101	LMG	C31-C32-C33-C34
28	A	412	SQD	C14-C15-C16-C17
29	c	516	DGD	C4B-C5B-C6B-C7B
33	D	409	LHG	C9-C10-C11-C12
33	E	101	LHG	C15-C16-C17-C18
26	a	409	PL9	C17-C18-C19-C20
23	c	513	CLA	C16-C17-C18-C20
23	B	601	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	512	CLA	C2B-C3B-CAB-CBB
25	D	405	BCR	C23-C24-C25-C26
25	D	405	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C30
25	K	101	BCR	C1-C6-C7-C8
25	b	618	BCR	C1-C6-C7-C8
25	b	618	BCR	C5-C6-C7-C8
27	b	622	LMG	C15-C16-C17-C18
27	c	519	LMG	C31-C32-C33-C34
28	B	623	SQD	C34-C35-C36-C37
23	D	403	CLA	O1D-CGD-O2D-CED
23	b	611	CLA	C15-C16-C17-C18
27	D	410	LMG	C33-C34-C35-C36
33	l	101	LHG	C27-C28-C29-C30
33	d	408	LHG	C23-C24-C25-C26
33	E	101	LHG	C11-C10-C9-C8
26	D	406	PL9	C4-C3-C7-C8
27	A	410	LMG	C14-C15-C16-C17
27	D	407	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	A	411	SQD	C11-C10-C9-C8
33	B	622	LHG	C25-C26-C27-C28
33	L	101	LHG	C30-C31-C32-C33
29	A	413	DGD	C2B-C3B-C4B-C5B
29	C	517	DGD	CAB-CBB-CCB-CDB
25	B	618	BCR	C10-C11-C12-C13
25	D	405	BCR	C10-C11-C12-C13
25	d	405	BCR	C10-C11-C12-C13
23	B	609	CLA	C16-C17-C18-C20
27	c	522	LMG	C38-C39-C40-C41
27	m	101	LMG	C29-C30-C31-C32
28	a	411	SQD	C10-C11-C12-C13
29	A	413	DGD	C2A-C3A-C4A-C5A
29	A	413	DGD	CAA-CBA-CCA-CDA
29	C	518	DGD	C3A-C4A-C5A-C6A
33	B	622	LHG	C9-C10-C11-C12
29	C	516	DGD	C1B-C2B-C3B-C4B
23	c	506	CLA	CBA-CGA-O2A-C1
23	b	607	CLA	C6-C7-C8-C9
23	d	402	CLA	C14-C13-C15-C16
27	B	620	LMG	C14-C15-C16-C17
27	C	519	LMG	C11-C12-C13-C14
23	B	613	CLA	C8-C10-C11-C12
27	a	414	LMG	C32-C33-C34-C35
27	b	623	LMG	C37-C38-C39-C40
33	D	409	LHG	C30-C31-C32-C33
25	D	405	BCR	C22-C23-C24-C25
27	b	623	LMG	C32-C33-C34-C35
28	A	411	SQD	C14-C15-C16-C17
29	c	518	DGD	C4B-C5B-C6B-C7B
23	c	501	CLA	C8-C10-C11-C12
23	C	503	CLA	O1A-CGA-O2A-C1
27	D	411	LMG	C14-C15-C16-C17
27	D	411	LMG	C31-C32-C33-C34
27	b	622	LMG	C18-C19-C20-C21
28	A	412	SQD	C12-C13-C14-C15
23	D	403	CLA	C15-C16-C17-C18
29	c	518	DGD	C2A-C1A-O1G-C1G
27	B	620	LMG	O6-C5-C6-O5
27	D	407	LMG	C38-C39-C40-C41
29	a	413	DGD	C8B-C9B-CAB-CBB
23	c	512	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	c	516	DGD	O1B-C1B-O2G-C2G
33	E	101	LHG	O9-C7-O7-C5
27	a	414	LMG	C39-C40-C41-C42
33	l	101	LHG	C9-C10-C11-C12
25	b	618	BCR	C11-C12-C13-C35
29	c	517	DGD	C1A-C2A-C3A-C4A
27	B	620	LMG	C19-C20-C21-C22
33	D	408	LHG	C32-C33-C34-C35
33	e	101	LHG	C16-C17-C18-C19
23	B	601	CLA	C16-C17-C18-C19
28	f	101	SQD	C31-C32-C33-C34
29	C	518	DGD	C6B-C7B-C8B-C9B
33	D	408	LHG	C30-C31-C32-C33
33	a	410	LHG	C30-C31-C32-C33
23	C	505	CLA	C4-C3-C5-C6
23	C	510	CLA	C4-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
26	d	406	PL9	C12-C11-C9-C8
27	b	622	LMG	C23-C24-C25-C26
28	a	412	SQD	C15-C16-C17-C18
27	D	407	LMG	C34-C35-C36-C37
23	b	615	CLA	O1A-CGA-O2A-C1
27	c	522	LMG	C37-C38-C39-C40
28	A	411	SQD	C33-C34-C35-C36
29	h	103	DGD	C2B-C3B-C4B-C5B
33	d	408	LHG	C29-C30-C31-C32
33	D	409	LHG	C23-C24-C25-C26
33	a	410	LHG	C10-C11-C12-C13
33	e	101	LHG	C13-C14-C15-C16
27	B	620	LMG	C17-C18-C19-C20
27	D	407	LMG	C20-C21-C22-C23
27	b	622	LMG	C11-C12-C13-C14
23	a	405	CLA	C8-C10-C11-C12
33	a	410	LHG	C17-C18-C19-C20
27	a	414	LMG	C28-C29-C30-C31
23	B	605	CLA	C5-C6-C7-C8
23	C	506	CLA	C15-C16-C17-C18
24	d	401	PHO	O1D-CGD-O2D-CED
29	A	413	DGD	CDB-CEB-CFB-CGB
29	c	516	DGD	O6E-C5E-C6E-O5E
23	h	101	CLA	C3-C5-C6-C7
27	A	410	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
28	A	411	SQD	O6-C44-C45-O47
29	A	413	DGD	O2G-C2G-C3G-O3G
23	C	504	CLA	C11-C12-C13-C14
28	A	412	SQD	C28-C29-C30-C31
29	c	517	DGD	CAA-CBA-CCA-CDA
23	C	513	CLA	CBA-CGA-O2A-C1
27	D	407	LMG	C35-C36-C37-C38
28	A	412	SQD	C30-C31-C32-C33
28	F	101	SQD	C27-C28-C29-C30
29	c	517	DGD	C7B-C8B-C9B-CAB
29	h	103	DGD	C3B-C4B-C5B-C6B
23	C	513	CLA	C5-C6-C7-C8
27	d	409	LMG	C14-C15-C16-C17
29	h	103	DGD	C7A-C8A-C9A-CAA
33	D	408	LHG	C12-C13-C14-C15
28	A	411	SQD	C12-C13-C14-C15
28	A	412	SQD	C15-C16-C17-C18
28	f	101	SQD	C25-C26-C27-C28
29	C	518	DGD	CAA-CBA-CCA-CDA
23	b	617	CLA	C2-C1-O2A-CGA
23	B	615	CLA	C16-C17-C18-C19
29	A	413	DGD	C8B-C9B-CAB-CBB
23	b	612	CLA	C2-C3-C5-C6
26	D	406	PL9	C13-C14-C16-C17
33	D	409	LHG	C1-C2-C3-O3
33	d	407	LHG	C1-C2-C3-O3
27	c	522	LMG	C16-C17-C18-C19
23	B	603	CLA	CBD-CGD-O2D-CED
27	D	407	LMG	C16-C17-C18-C19
27	d	409	LMG	C32-C33-C34-C35
28	B	623	SQD	C11-C12-C13-C14
29	c	518	DGD	C8A-C9A-CAA-CBA
33	d	407	LHG	C28-C29-C30-C31
23	C	502	CLA	O1D-CGD-O2D-CED
27	c	522	LMG	C36-C37-C38-C39
23	a	404	CLA	C15-C16-C17-C18
28	f	101	SQD	C28-C29-C30-C31
33	E	101	LHG	O1-C1-C2-O2
33	a	410	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
23	c	506	CLA	O1A-CGA-O2A-C1
23	C	503	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
33	B	622	LHG	C12-C13-C14-C15
27	D	410	LMG	C11-C12-C13-C14
29	A	413	DGD	C6B-C7B-C8B-C9B
29	h	103	DGD	CAB-CBB-CCB-CDB
23	C	513	CLA	C13-C15-C16-C17
23	c	511	CLA	C13-C15-C16-C17
27	C	519	LMG	O6-C5-C6-O5
23	B	604	CLA	C11-C10-C8-C7
23	B	604	CLA	C11-C12-C13-C15
23	C	506	CLA	C12-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C7
23	C	509	CLA	C12-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	608	CLA	C6-C7-C8-C10
23	b	608	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C12-C13-C15
23	c	504	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C12-C13-C15-C16
23	h	101	CLA	C11-C10-C8-C7
24	a	406	PHO	C6-C7-C8-C10
23	a	404	CLA	C16-C17-C18-C20
33	B	622	LHG	C29-C30-C31-C32
23	B	609	CLA	CBD-CGD-O2D-CED
27	C	519	LMG	C31-C32-C33-C34
33	D	408	LHG	C33-C34-C35-C36
23	B	615	CLA	C4-C3-C5-C6
23	B	609	CLA	C2-C3-C5-C6
23	C	510	CLA	C2-C3-C5-C6
26	A	409	PL9	C28-C29-C31-C32
33	L	101	LHG	C17-C18-C19-C20
23	c	503	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C11-C10-C8-C9
23	B	604	CLA	C11-C12-C13-C14
23	B	615	CLA	C6-C7-C8-C9
23	C	508	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C14-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C10-C8-C9
23	b	607	CLA	C11-C10-C8-C9
23	c	501	CLA	C11-C12-C13-C14
23	c	506	CLA	C11-C10-C8-C9
23	c	508	CLA	C14-C13-C15-C16
23	c	509	CLA	C14-C13-C15-C16
24	a	406	PHO	C6-C7-C8-C9
29	H	102	DGD	CBA-CCA-CDA-CEA
33	E	101	LHG	C25-C26-C27-C28
27	c	522	LMG	C34-C35-C36-C37
29	C	516	DGD	C4A-C5A-C6A-C7A
23	c	503	CLA	CBA-CGA-O2A-C1
29	c	516	DGD	C2A-C1A-O1G-C1G
33	d	408	LHG	C24-C23-O8-C6
33	d	407	LHG	C30-C31-C32-C33
23	b	606	CLA	C5-C6-C7-C8
28	A	411	SQD	O6-C44-C45-C46
28	B	623	SQD	O6-C44-C45-C46
28	a	411	SQD	C44-C45-C46-O48
28	b	601	SQD	C44-C45-C46-O48
29	A	413	DGD	C1G-C2G-C3G-O3G
27	D	410	LMG	C14-C15-C16-C17
29	A	413	DGD	CBB-CCB-CDB-CEB
33	a	410	LHG	C32-C33-C34-C35
33	d	407	LHG	O2-C2-C3-O3
27	C	519	LMG	C18-C19-C20-C21
28	a	411	SQD	C25-C26-C27-C28
28	b	601	SQD	C14-C15-C16-C17
23	B	614	CLA	CBA-CGA-O2A-C1
27	C	519	LMG	C29-C28-O8-C9
28	A	412	SQD	C23-C24-C25-C26
27	A	410	LMG	O6-C5-C6-O5
27	d	409	LMG	O6-C5-C6-O5
29	C	518	DGD	O6E-C5E-C6E-O5E
27	A	410	LMG	C38-C39-C40-C41
27	b	622	LMG	C16-C17-C18-C19
29	C	517	DGD	CCB-CDB-CEB-CFB
24	d	401	PHO	C2C-C3C-CAC-CBC
29	c	518	DGD	CBB-CCB-CDB-CEB
25	T	101	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	b	619	BCR	C20-C21-C22-C37
25	c	521	BCR	C20-C21-C22-C37
23	B	612	CLA	C13-C15-C16-C17
27	a	414	LMG	C38-C39-C40-C41
27	m	101	LMG	C32-C33-C34-C35
28	a	411	SQD	C23-C24-C25-C26
33	d	407	LHG	C7-C8-C9-C10
23	b	612	CLA	C4-C3-C5-C6
23	b	611	CLA	C2C-C3C-CAC-CBC
23	C	505	CLA	C2-C3-C5-C6
28	B	623	SQD	C9-C10-C11-C12
33	l	101	LHG	C16-C17-C18-C19
23	B	603	CLA	C16-C17-C18-C20
27	m	101	LMG	C19-C20-C21-C22
33	B	622	LHG	C32-C33-C34-C35
33	d	408	LHG	C27-C28-C29-C30
33	l	101	LHG	C24-C25-C26-C27
27	b	622	LMG	O6-C5-C6-O5
33	e	101	LHG	C11-C10-C9-C8
33	e	101	LHG	C18-C19-C20-C21
29	A	413	DGD	C8A-C9A-CAA-CBA
27	D	407	LMG	C18-C19-C20-C21
23	C	506	CLA	CBA-CGA-O2A-C1
23	B	604	CLA	O2A-C1-C2-C3
23	C	512	CLA	O2A-C1-C2-C3
28	f	101	SQD	C46-C45-O47-C7
29	C	516	DGD	C9B-CAB-CBB-CCB
29	c	517	DGD	C6A-C7A-C8A-C9A
27	A	410	LMG	C12-C13-C14-C15
28	f	101	SQD	C24-C25-C26-C27
33	e	101	LHG	C25-C26-C27-C28
23	a	404	CLA	C16-C17-C18-C19
23	c	504	CLA	C11-C12-C13-C14
27	c	522	LMG	C12-C13-C14-C15
27	D	410	LMG	C28-C29-C30-C31
27	d	409	LMG	C34-C35-C36-C37
28	A	411	SQD	C26-C27-C28-C29
23	C	511	CLA	O1D-CGD-O2D-CED
25	y	101	BCR	C11-C10-C9-C8
27	a	414	LMG	C11-C12-C13-C14
29	c	517	DGD	CAB-CBB-CCB-CDB
23	B	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C19-C20-C21-C22
29	c	518	DGD	C7A-C8A-C9A-CAA
27	b	623	LMG	C38-C39-C40-C41
27	d	409	LMG	C39-C40-C41-C42
28	F	101	SQD	C33-C34-C35-C36
33	L	101	LHG	C15-C16-C17-C18
23	B	615	CLA	C2-C3-C5-C6
26	d	406	PL9	C13-C14-C16-C17
26	d	406	PL9	C28-C29-C31-C32
27	C	519	LMG	C19-C20-C21-C22
33	D	408	LHG	C35-C36-C37-C38
33	a	410	LHG	C19-C20-C21-C22
27	c	519	LMG	C35-C36-C37-C38
28	F	101	SQD	C30-C31-C32-C33
28	a	412	SQD	C24-C25-C26-C27
29	A	413	DGD	CEB-CFB-CGB-CHB
33	B	622	LHG	C18-C19-C20-C21
33	D	409	LHG	C11-C12-C13-C14
33	d	407	LHG	C14-C15-C16-C17
23	B	611	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C20
28	b	601	SQD	C25-C26-C27-C28
29	C	516	DGD	CCB-CDB-CEB-CFB
29	C	518	DGD	CBB-CCB-CDB-CEB
33	D	409	LHG	C25-C26-C27-C28
33	d	407	LHG	C15-C16-C17-C18
28	a	412	SQD	C31-C32-C33-C34
33	E	101	LHG	C35-C36-C37-C38
26	A	409	PL9	C17-C18-C19-C21
28	A	412	SQD	C10-C11-C12-C13
29	c	517	DGD	CCB-CDB-CEB-CFB
33	d	408	LHG	C33-C34-C35-C36
27	a	414	LMG	O7-C8-C9-O8
33	e	101	LHG	C28-C29-C30-C31
33	E	101	LHG	C19-C20-C21-C22
29	h	103	DGD	O2G-C1B-C2B-C3B
29	c	518	DGD	C3A-C4A-C5A-C6A
29	c	517	DGD	CDA-CEA-CFA-CGA
27	a	414	LMG	C35-C36-C37-C38
29	h	103	DGD	CCB-CDB-CEB-CFB
33	E	101	LHG	C16-C17-C18-C19
23	c	505	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	D	409	LHG	C17-C18-C19-C20
28	B	623	SQD	C13-C14-C15-C16
28	a	412	SQD	C9-C10-C11-C12
33	d	408	LHG	C25-C26-C27-C28
23	c	511	CLA	C15-C16-C17-C18
27	a	414	LMG	C34-C35-C36-C37
23	c	506	CLA	C8-C10-C11-C12
23	b	608	CLA	O1D-CGD-O2D-CED
23	C	502	CLA	C16-C17-C18-C19
24	A	406	PHO	C16-C17-C18-C19
26	a	409	PL9	C40-C39-C41-C42
27	D	411	LMG	C37-C38-C39-C40
23	C	513	CLA	O1A-CGA-O2A-C1
23	B	616	CLA	CBA-CGA-O2A-C1
23	c	504	CLA	CBA-CGA-O2A-C1
28	B	623	SQD	C24-C23-O48-C46
29	A	413	DGD	C2A-C1A-O1G-C1G
27	D	407	LMG	C40-C41-C42-C43
33	D	409	LHG	C15-C16-C17-C18
23	C	508	CLA	O1D-CGD-O2D-CED
28	A	411	SQD	C10-C11-C12-C13
29	h	103	DGD	C6A-C7A-C8A-C9A
27	B	620	LMG	O9-C10-O7-C8
29	H	102	DGD	O1B-C1B-O2G-C2G
28	F	101	SQD	C45-C44-O6-C1
23	B	613	CLA	C6-C7-C8-C9
23	B	615	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	C	510	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C9
23	a	405	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C14
23	b	608	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	b	615	CLA	C11-C12-C13-C14
23	c	504	CLA	C11-C10-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	510	CLA	C14-C13-C15-C16
23	h	101	CLA	C14-C13-C15-C16
24	D	401	PHO	C6-C7-C8-C9
28	a	412	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	b	607	CLA	C10-C11-C12-C13
27	b	623	LMG	C33-C34-C35-C36
27	b	623	LMG	C36-C37-C38-C39
27	m	101	LMG	C33-C34-C35-C36
29	c	516	DGD	C2A-C3A-C4A-C5A
33	D	409	LHG	C31-C32-C33-C34
33	l	101	LHG	C33-C34-C35-C36
27	c	522	LMG	C4-C5-C6-O5
28	b	601	SQD	C19-C20-C21-C22
27	b	623	LMG	C30-C31-C32-C33
27	D	410	LMG	C15-C16-C17-C18
33	B	622	LHG	C16-C17-C18-C19
33	E	101	LHG	C13-C14-C15-C16
33	E	101	LHG	C26-C27-C28-C29
27	D	407	LMG	C31-C32-C33-C34
28	a	411	SQD	C26-C27-C28-C29
33	D	408	LHG	C29-C30-C31-C32
33	D	409	LHG	C24-C25-C26-C27
27	m	101	LMG	C22-C23-C24-C25
23	B	604	CLA	C12-C13-C15-C16
23	B	606	CLA	C11-C12-C13-C15
23	B	613	CLA	C6-C7-C8-C10
23	B	615	CLA	C6-C7-C8-C10
23	C	507	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
23	C	510	CLA	C11-C10-C8-C7
23	C	510	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	a	405	CLA	C11-C10-C8-C7
23	a	405	CLA	C12-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C12-C13-C15
23	b	617	CLA	C11-C10-C8-C7
23	c	508	CLA	C12-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C10
23	c	510	CLA	C12-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C10
23	h	101	CLA	C12-C13-C15-C16
23	B	616	CLA	O1A-CGA-O2A-C1
29	c	518	DGD	CDB-CEB-CFB-CGB
28	a	412	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	d	404	CLA	C16-C17-C18-C20
33	E	101	LHG	C10-C11-C12-C13
23	B	614	CLA	O1A-CGA-O2A-C1
27	m	101	LMG	C30-C31-C32-C33
23	B	609	CLA	C4-C3-C5-C6
26	D	406	PL9	C30-C29-C31-C32
29	C	516	DGD	O1G-C1A-C2A-C3A
29	C	518	DGD	C7A-C8A-C9A-CAA
33	e	101	LHG	C27-C28-C29-C30
29	A	413	DGD	C3B-C4B-C5B-C6B
23	c	503	CLA	O1A-CGA-O2A-C1
23	b	615	CLA	C8-C10-C11-C12
33	E	101	LHG	C27-C28-C29-C30
23	c	502	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	CBA-CGA-O2A-C1
27	m	101	LMG	C29-C28-O8-C9
33	L	101	LHG	C24-C23-O8-C6
25	C	520	BCR	C15-C16-C17-C18
25	T	101	BCR	C9-C10-C11-C12
23	c	507	CLA	C16-C17-C18-C19
28	A	411	SQD	C24-C25-C26-C27
23	B	613	CLA	C2C-C3C-CAC-CBC
23	b	608	CLA	C8-C10-C11-C12
27	B	620	LMG	C33-C34-C35-C36
27	C	519	LMG	C37-C38-C39-C40
29	A	413	DGD	CCB-CDB-CEB-CFB
27	B	620	LMG	C7-C8-C9-O8
33	d	408	LHG	C4-C5-C6-O8
29	A	413	DGD	CFA-CGA-CHA-CIA
23	B	603	CLA	C16-C17-C18-C19
24	A	406	PHO	C16-C17-C18-C20
23	B	607	CLA	C8-C10-C11-C12
27	B	620	LMG	C39-C40-C41-C42
29	H	102	DGD	CDB-CEB-CFB-CGB
28	F	101	SQD	C26-C27-C28-C29
29	H	102	DGD	CBB-CCB-CDB-CEB
29	C	518	DGD	CDB-CEB-CFB-CGB
26	a	409	PL9	C35-C34-C36-C37
26	d	406	PL9	C15-C14-C16-C17
26	d	406	PL9	C30-C29-C31-C32
28	a	412	SQD	C17-C18-C19-C20
23	c	506	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	d	403	CLA	C16-C17-C18-C19
28	a	412	SQD	C29-C30-C31-C32
25	C	515	BCR	C23-C24-C25-C30
25	h	102	BCR	C23-C24-C25-C30
25	y	101	BCR	C1-C6-C7-C8
28	b	601	SQD	C8-C7-O47-C45
23	c	508	CLA	C15-C16-C17-C18
23	b	613	CLA	C3-C5-C6-C7
28	a	411	SQD	C27-C28-C29-C30
29	H	102	DGD	CCB-CDB-CEB-CFB
23	b	614	CLA	C13-C15-C16-C17
27	D	411	LMG	C11-C12-C13-C14
23	c	508	CLA	C16-C17-C18-C19
27	c	522	LMG	O1-C7-C8-O7
28	a	411	SQD	O6-C44-C45-O47
29	c	517	DGD	C3B-C4B-C5B-C6B
23	C	506	CLA	O1A-CGA-O2A-C1
23	c	507	CLA	CBD-CGD-O2D-CED
26	a	409	PL9	C4-C3-C7-C8
27	D	411	LMG	C13-C14-C15-C16
33	L	101	LHG	C9-C10-C11-C12
23	c	509	CLA	C8-C10-C11-C12
26	a	409	PL9	C38-C39-C41-C42
27	A	410	LMG	C30-C31-C32-C33
23	c	513	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C19
27	A	410	LMG	C17-C18-C19-C20
27	c	522	LMG	C28-C29-C30-C31
23	C	513	CLA	C14-C13-C15-C16
23	c	506	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
25	K	101	BCR	C22-C23-C24-C25
25	d	405	BCR	C22-C23-C24-C25
23	b	604	CLA	O1A-CGA-O2A-C1
33	E	101	LHG	C30-C31-C32-C33
27	c	522	LMG	C32-C33-C34-C35
29	A	413	DGD	CBA-CCA-CDA-CEA
23	C	502	CLA	C16-C17-C18-C20
23	c	505	CLA	O1A-CGA-O2A-C1
28	A	412	SQD	C27-C28-C29-C30
29	C	518	DGD	C3B-C4B-C5B-C6B
29	a	413	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
27	a	414	LMG	C33-C34-C35-C36
33	l	101	LHG	C35-C36-C37-C38
29	C	517	DGD	C6A-C7A-C8A-C9A
23	b	604	CLA	CBA-CGA-O2A-C1
25	T	101	BCR	C13-C14-C15-C16
23	B	611	CLA	C16-C17-C18-C19
33	d	407	LHG	C33-C34-C35-C36
27	D	410	LMG	C36-C37-C38-C39
33	l	101	LHG	C13-C14-C15-C16
33	D	408	LHG	C1-C2-C3-O3
25	A	408	BCR	C20-C21-C22-C37
25	a	408	BCR	C20-C21-C22-C37
25	c	514	BCR	C16-C17-C18-C36
25	d	405	BCR	C20-C21-C22-C37
25	h	102	BCR	C16-C17-C18-C36
28	a	411	SQD	C19-C20-C21-C22
23	C	504	CLA	C3-C5-C6-C7
23	C	506	CLA	C3-C5-C6-C7
28	a	411	SQD	C24-C23-O48-C46
23	b	605	CLA	C13-C15-C16-C17
23	c	507	CLA	C5-C6-C7-C8
33	d	407	LHG	C12-C13-C14-C15
33	l	101	LHG	O6-C4-C5-C6
29	c	516	DGD	O1A-C1A-O1G-C1G
23	h	101	CLA	C10-C11-C12-C13
23	B	611	CLA	C11-C12-C13-C15
23	B	616	CLA	C6-C7-C8-C10
23	C	504	CLA	C11-C10-C8-C7
23	D	404	CLA	C12-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C15
23	c	509	CLA	C11-C12-C13-C15
23	d	403	CLA	C6-C7-C8-C10
27	b	623	LMG	C34-C35-C36-C37
29	C	517	DGD	C7B-C8B-C9B-CAB
33	d	407	LHG	C34-C35-C36-C37
29	C	516	DGD	CDA-CEA-CFA-CGA
29	H	102	DGD	CDA-CEA-CFA-CGA
25	T	101	BCR	C21-C22-C23-C24
25	d	405	BCR	C21-C22-C23-C24
27	m	101	LMG	C15-C16-C17-C18
23	B	607	CLA	O1A-CGA-O2A-C1
29	C	517	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	C5D-C6D-O5D-C1E
29	c	517	DGD	C5D-C6D-O5D-C1E
29	C	518	DGD	CBA-CCA-CDA-CEA
23	c	511	CLA	C16-C17-C18-C20
23	c	510	CLA	C4-C3-C5-C6
26	d	406	PL9	C45-C44-C46-C47
23	c	502	CLA	O1A-CGA-O2A-C1
23	c	504	CLA	O1A-CGA-O2A-C1
27	C	519	LMG	O10-C28-O8-C9
23	C	506	CLA	C13-C15-C16-C17
29	C	517	DGD	CDA-CEA-CFA-CGA
27	B	620	LMG	C28-C29-C30-C31
23	b	608	CLA	C5-C6-C7-C8
23	C	513	CLA	O2A-C1-C2-C3
23	h	101	CLA	O2A-C1-C2-C3
27	A	410	LMG	C9-C8-O7-C10
23	c	508	CLA	O1A-CGA-O2A-C1
29	A	413	DGD	C9B-CAB-CBB-CCB
23	D	404	CLA	C16-C17-C18-C20
23	c	504	CLA	C11-C12-C13-C15
33	D	409	LHG	C11-C10-C9-C8
33	l	101	LHG	O6-C4-C5-O7
27	B	620	LMG	C38-C39-C40-C41
29	c	516	DGD	C3B-C4B-C5B-C6B
29	A	413	DGD	O6D-C1D-O3G-C3G
27	c	522	LMG	O1-C7-C8-C9
27	c	522	LMG	C7-C8-C9-O8
28	a	412	SQD	C44-C45-C46-O48
34	E	102	HEM	C4C-C3C-CAC-CBC
34	e	102	HEM	C4B-C3B-CAB-CBB
24	A	406	PHO	C4-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
27	c	519	LMG	C34-C35-C36-C37
27	d	409	LMG	C12-C13-C14-C15
28	b	601	SQD	O6-C44-C45-O47
28	b	601	SQD	O47-C45-C46-O48
28	f	101	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
23	b	613	CLA	C10-C11-C12-C13
23	B	614	CLA	C14-C13-C15-C16
23	C	504	CLA	C11-C10-C8-C9
23	a	405	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C11-C12-C13-C14
27	d	409	LMG	C35-C36-C37-C38
29	H	102	DGD	O2G-C1B-C2B-C3B
29	c	516	DGD	C6A-C7A-C8A-C9A
29	c	518	DGD	C8B-C9B-CAB-CBB
27	a	414	LMG	C18-C19-C20-C21
28	b	601	SQD	C13-C14-C15-C16
29	A	413	DGD	CDA-CEA-CFA-CGA
29	c	518	DGD	CBA-CCA-CDA-CEA
23	b	612	CLA	C10-C11-C12-C13
28	A	411	SQD	C32-C33-C34-C35
28	A	412	SQD	C16-C17-C18-C19
28	A	412	SQD	C26-C27-C28-C29
28	a	411	SQD	C18-C19-C20-C21
29	c	518	DGD	C6B-C7B-C8B-C9B
29	a	413	DGD	C6B-C7B-C8B-C9B
28	A	411	SQD	C25-C26-C27-C28
33	L	101	LHG	C11-C12-C13-C14
23	c	506	CLA	C2-C1-O2A-CGA
23	A	405	CLA	C16-C17-C18-C20
29	c	518	DGD	C9A-CAA-CBA-CCA
23	c	505	CLA	CBD-CGD-O2D-CED
29	a	413	DGD	CEB-CFB-CGB-CHB
29	c	516	DGD	CBA-CCA-CDA-CEA
25	C	514	BCR	C14-C15-C16-C17
24	D	401	PHO	O1D-CGD-O2D-CED
27	c	519	LMG	C39-C40-C41-C42
27	m	101	LMG	C37-C38-C39-C40
27	c	519	LMG	C29-C28-O8-C9
29	h	103	DGD	C6B-C7B-C8B-C9B
29	a	413	DGD	CFA-CGA-CHA-CIA
23	C	512	CLA	C4B-C3B-CAB-CBB
23	b	605	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	C4B-C3B-CAB-CBB
25	b	618	BCR	C22-C23-C24-C25
25	b	620	BCR	C6-C7-C8-C9
25	C	520	BCR	C13-C14-C15-C16
25	C	520	BCR	C19-C20-C21-C22
23	C	509	CLA	C16-C17-C18-C19
23	c	511	CLA	C16-C17-C18-C19
27	m	101	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
26	a	409	PL9	C12-C13-C14-C15
27	A	410	LMG	C37-C38-C39-C40
33	D	409	LHG	C10-C11-C12-C13
28	B	623	SQD	C25-C26-C27-C28
33	D	408	LHG	C16-C17-C18-C19
23	B	603	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	D	403	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C12-C13-C15
23	b	605	CLA	C12-C13-C15-C16
23	b	610	CLA	C12-C13-C15-C16
23	b	613	CLA	C11-C10-C8-C7
23	b	616	CLA	C11-C10-C8-C7
23	c	503	CLA	C11-C10-C8-C7
23	c	505	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
24	A	406	PHO	C6-C7-C8-C10
23	b	612	CLA	C16-C17-C18-C19
28	F	101	SQD	C29-C30-C31-C32
33	B	622	LHG	C24-C25-C26-C27
33	D	408	LHG	C34-C35-C36-C37
33	d	407	LHG	C26-C27-C28-C29
27	c	522	LMG	C11-C12-C13-C14
29	H	102	DGD	C7A-C8A-C9A-CAA
23	B	603	CLA	O1D-CGD-O2D-CED
23	b	612	CLA	C5-C6-C7-C8
29	C	517	DGD	C5A-C6A-C7A-C8A
33	L	101	LHG	C31-C32-C33-C34
23	c	512	CLA	C4-C3-C5-C6
23	c	505	CLA	C16-C17-C18-C20
29	c	518	DGD	C4A-C5A-C6A-C7A
23	D	404	CLA	C14-C13-C15-C16
23	b	609	CLA	C11-C12-C13-C14
23	b	613	CLA	C11-C10-C8-C9
23	c	503	CLA	C11-C10-C8-C9
27	c	519	LMG	C32-C33-C34-C35
25	C	514	BCR	C15-C16-C17-C18
25	b	619	BCR	C9-C10-C11-C12
25	t	101	BCR	C13-C14-C15-C16
29	c	516	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C11-C10-C9-C8
29	C	516	DGD	C7B-C8B-C9B-CAB
29	c	517	DGD	C8B-C9B-CAB-CBB
27	B	620	LMG	O7-C8-C9-O8
27	b	622	LMG	O1-C7-C8-O7
27	c	522	LMG	O7-C8-C9-O8
28	a	412	SQD	O47-C45-C46-O48
33	d	408	LHG	O7-C5-C6-O8
27	D	410	LMG	C31-C32-C33-C34
27	a	414	LMG	C19-C20-C21-C22
23	D	403	CLA	C2C-C3C-CAC-CBC
23	B	608	CLA	C13-C15-C16-C17
23	c	513	CLA	C5-C6-C7-C8
28	B	623	SQD	C33-C34-C35-C36
23	A	405	CLA	C16-C17-C18-C19
23	C	508	CLA	C16-C17-C18-C19
28	f	101	SQD	C44-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-C3G
23	C	505	CLA	C8-C10-C11-C12
23	c	513	CLA	C3-C5-C6-C7
33	d	407	LHG	C16-C17-C18-C19
23	B	601	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
23	a	404	CLA	O1D-CGD-O2D-CED
23	C	512	CLA	C2A-CAA-CBA-CGA
28	A	412	SQD	O49-C7-O47-C45
33	D	408	LHG	C13-C14-C15-C16
28	B	623	SQD	C26-C27-C28-C29
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	CHA-CBD-CGD-O2D
25	C	514	BCR	C9-C10-C11-C12
25	b	620	BCR	C35-C13-C14-C15
25	c	521	BCR	C9-C10-C11-C12
33	D	408	LHG	C4-O6-P-O3
33	E	101	LHG	C4-O6-P-O5
33	d	407	LHG	C4-O6-P-O5
33	e	101	LHG	C3-O3-P-O6
29	C	518	DGD	CCA-CDA-CEA-CFA
23	C	509	CLA	C16-C17-C18-C20
23	B	606	CLA	C8-C10-C11-C12
23	B	606	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C2B-C3B-CAB-CBB
29	a	413	DGD	C4B-C5B-C6B-C7B
26	D	406	PL9	C28-C29-C31-C32
25	A	408	BCR	C7-C8-C9-C34
25	c	514	BCR	C7-C8-C9-C34
33	E	101	LHG	C2-C3-O3-P
23	c	506	CLA	C16-C17-C18-C20
23	C	513	CLA	C2C-C3C-CAC-CBC
23	c	509	CLA	CAA-CBA-CGA-O2A
29	a	413	DGD	C3A-C4A-C5A-C6A
26	A	409	PL9	C4-C3-C7-C8
23	B	605	CLA	C16-C17-C18-C20
23	B	606	CLA	C2C-C3C-CAC-CBC
27	D	410	LMG	C9-C8-O7-C10
28	b	601	SQD	C46-C45-O47-C7
29	a	413	DGD	C3G-C2G-O2G-C1B
29	C	516	DGD	C6A-C7A-C8A-C9A
29	A	413	DGD	O6D-C5D-C6D-O5D
24	A	406	PHO	C2-C3-C5-C6
33	a	410	LHG	C31-C32-C33-C34
23	C	509	CLA	C5-C6-C7-C8
23	B	604	CLA	C14-C13-C15-C16
23	B	606	CLA	C11-C12-C13-C14
23	B	616	CLA	C6-C7-C8-C9
23	C	506	CLA	C11-C12-C13-C14
23	b	605	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C10-C8-C9
29	C	518	DGD	CDA-CEA-CFA-CGA
23	B	607	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	b	607	CLA	C11-C12-C13-C15
23	c	509	CLA	C12-C13-C15-C16
33	D	408	LHG	C10-C11-C12-C13
33	a	410	LHG	C11-C10-C9-C8
24	A	406	PHO	C2C-C3C-CAC-CBC
33	B	622	LHG	C30-C31-C32-C33
23	B	605	CLA	C10-C11-C12-C13
23	c	510	CLA	C10-C11-C12-C13
26	d	406	PL9	C18-C19-C21-C22
23	B	608	CLA	C10-C11-C12-C13
33	l	101	LHG	O2-C2-C3-O3
29	C	516	DGD	C5B-C6B-C7B-C8B
23	b	612	CLA	C16-C17-C18-C20
23	C	502	CLA	C15-C16-C17-C18
29	C	517	DGD	C8B-C9B-CAB-CBB
29	H	102	DGD	CCA-CDA-CEA-CFA
23	B	601	CLA	C2-C1-O2A-CGA
27	D	407	LMG	C28-C29-C30-C31
27	D	410	LMG	C12-C13-C14-C15
27	m	101	LMG	C17-C18-C19-C20
29	C	517	DGD	C8A-C9A-CAA-CBA
29	h	103	DGD	CDA-CEA-CFA-CGA
27	A	410	LMG	O1-C7-C8-C9
27	b	622	LMG	O1-C7-C8-C9
29	C	516	DGD	C1G-C2G-C3G-O3G
33	E	101	LHG	C18-C19-C20-C21
33	D	409	LHG	C12-C13-C14-C15
27	C	519	LMG	C39-C40-C41-C42
27	b	622	LMG	C35-C36-C37-C38
29	C	516	DGD	C5D-C6D-O5D-C1E
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
25	C	515	BCR	C13-C14-C15-C16
25	C	515	BCR	C15-C16-C17-C18
25	D	405	BCR	C19-C20-C21-C22
23	B	610	CLA	C2C-C3C-CAC-CBC
27	m	101	LMG	C11-C12-C13-C14
23	c	505	CLA	C4-C3-C5-C6
26	A	409	PL9	C20-C19-C21-C22
33	E	101	LHG	C29-C30-C31-C32
29	C	516	DGD	C4B-C5B-C6B-C7B
23	b	604	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C14-C13-C15-C16
23	C	502	CLA	C6-C7-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	b	610	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
28	a	412	SQD	C13-C14-C15-C16
23	c	507	CLA	O1D-CGD-O2D-CED
33	a	410	LHG	C24-C23-O8-C6
27	C	519	LMG	C33-C34-C35-C36
27	a	414	LMG	C30-C31-C32-C33
23	c	501	CLA	CBD-CGD-O2D-CED
27	D	407	LMG	C13-C14-C15-C16
23	B	613	CLA	C4C-C3C-CAC-CBC
33	L	101	LHG	C10-C11-C12-C13
28	F	101	SQD	C32-C33-C34-C35
29	a	413	DGD	C6A-C7A-C8A-C9A
23	B	612	CLA	O1A-CGA-O2A-C1
25	c	521	BCR	C15-C16-C17-C18
23	B	603	CLA	C13-C15-C16-C17
27	m	101	LMG	C40-C41-C42-C43
23	B	609	CLA	O1D-CGD-O2D-CED
23	a	404	CLA	C11-C10-C8-C7
23	b	605	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C10-C8-C7
29	a	413	DGD	O2G-C1B-C2B-C3B
27	d	409	LMG	C36-C37-C38-C39
29	C	518	DGD	C2A-C3A-C4A-C5A
27	A	410	LMG	C31-C32-C33-C34
23	d	404	CLA	C3A-C2A-CAA-CBA
27	D	410	LMG	C16-C17-C18-C19
25	A	408	BCR	C16-C17-C18-C36
25	D	405	BCR	C11-C10-C9-C34
25	b	620	BCR	C11-C10-C9-C34
23	C	502	CLA	C3-C5-C6-C7
27	b	623	LMG	C35-C36-C37-C38
23	B	601	CLA	C8-C10-C11-C12
23	c	503	CLA	C5-C6-C7-C8
29	A	413	DGD	CEA-CFA-CGA-CHA
28	A	412	SQD	C44-C45-O47-C7
27	c	522	LMG	C35-C36-C37-C38
23	b	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	c	516	DGD	C7B-C8B-C9B-CAB
23	c	512	CLA	C2-C1-O2A-CGA
25	c	514	BCR	C15-C16-C17-C18
25	c	515	BCR	C9-C10-C11-C12
35	v	201	HEC	CAD-CBD-CGD-O2D
23	C	503	CLA	C15-C16-C17-C18
27	C	519	LMG	C40-C41-C42-C43
23	c	512	CLA	C2-C3-C5-C6
26	D	406	PL9	C14-C16-C17-C18
27	b	622	LMG	C7-C8-C9-O8
33	D	408	LHG	C9-C10-C11-C12
23	d	403	CLA	C3-C5-C6-C7
23	B	607	CLA	C11-C10-C8-C9
23	a	404	CLA	C11-C10-C8-C9
23	a	405	CLA	C6-C7-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	b	608	CLA	C11-C10-C8-C9
23	b	613	CLA	C6-C7-C8-C9
23	b	613	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C14
24	a	406	PHO	C11-C10-C8-C9
27	A	410	LMG	C32-C33-C34-C35
27	b	622	LMG	C10-C11-C12-C13
23	a	404	CLA	CBD-CGD-O2D-CED
29	h	103	DGD	C9A-CAA-CBA-CCA
27	d	409	LMG	C38-C39-C40-C41
28	f	101	SQD	C29-C30-C31-C32
27	a	414	LMG	C9-C8-O7-C10
23	c	503	CLA	C8-C10-C11-C12
23	B	603	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	C2C-C3C-CAC-CBC
23	B	604	CLA	C3-C5-C6-C7
27	D	411	LMG	O10-C28-C29-C30
35	V	201	HEC	CAD-CBD-CGD-O1D
35	v	201	HEC	CAD-CBD-CGD-O1D
33	L	101	LHG	C33-C34-C35-C36
23	B	602	CLA	C1A-C2A-CAA-CBA
23	D	403	CLA	C1A-C2A-CAA-CBA
23	c	503	CLA	C1A-C2A-CAA-CBA
23	b	617	CLA	C11-C12-C13-C15
23	c	505	CLA	C16-C17-C18-C19
33	e	101	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
27	C	519	LMG	C14-C15-C16-C17
23	d	402	CLA	C2C-C3C-CAC-CBC
23	c	504	CLA	C5-C6-C7-C8
23	C	504	CLA	C2B-C3B-CAB-CBB
23	d	403	CLA	C2B-C3B-CAB-CBB
23	h	101	CLA	C2B-C3B-CAB-CBB
25	C	515	BCR	C23-C24-C25-C26
25	C	520	BCR	C23-C24-C25-C30
25	h	102	BCR	C23-C24-C25-C26
34	e	102	HEM	CAD-CBD-CGD-O2D
27	a	414	LMG	C40-C41-C42-C43
23	a	405	CLA	C10-C11-C12-C13
29	c	518	DGD	C2A-C3A-C4A-C5A
33	d	408	LHG	C2-C3-O3-P
23	c	512	CLA	C8-C10-C11-C12
23	h	101	CLA	C8-C10-C11-C12
34	e	102	HEM	CAD-CBD-CGD-O1D
23	B	601	CLA	C4-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
27	D	411	LMG	O9-C10-C11-C12
23	B	603	CLA	C6-C7-C8-C10
23	C	506	CLA	C11-C12-C13-C15
23	C	512	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C10-C8-C7
23	b	611	CLA	C12-C13-C15-C16
23	b	613	CLA	C6-C7-C8-C10
23	b	613	CLA	C12-C13-C15-C16
23	c	507	CLA	C12-C13-C15-C16
23	c	512	CLA	C11-C10-C8-C7
23	B	607	CLA	C16-C17-C18-C19
27	D	407	LMG	C32-C33-C34-C35
28	F	101	SQD	C31-C32-C33-C34
29	C	516	DGD	CAA-CBA-CCA-CDA
26	d	406	PL9	C4-C3-C7-C8
29	c	517	DGD	C9A-CAA-CBA-CCA
35	V	201	HEC	CAD-CBD-CGD-O2D
29	H	102	DGD	C5A-C6A-C7A-C8A
23	c	513	CLA	C13-C15-C16-C17
29	C	518	DGD	C4B-C5B-C6B-C7B
33	d	407	LHG	C17-C18-C19-C20
33	l	101	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
29	C	518	DGD	O1A-C1A-O1G-C1G
23	c	512	CLA	C2A-CAA-CBA-CGA
23	B	606	CLA	C14-C13-C15-C16
29	h	103	DGD	C7B-C8B-C9B-CAB
27	m	101	LMG	C18-C19-C20-C21
27	D	411	LMG	O7-C10-C11-C12
29	H	102	DGD	C9B-CAB-CBB-CCB
23	b	616	CLA	C8-C10-C11-C12
23	c	504	CLA	C8-C10-C11-C12
27	D	407	LMG	C39-C40-C41-C42
33	a	410	LHG	C33-C34-C35-C36
23	b	611	CLA	C8-C10-C11-C12
23	c	512	CLA	C15-C16-C17-C18
27	b	623	LMG	C39-C40-C41-C42
27	D	411	LMG	O8-C28-C29-C30
33	d	408	LHG	C30-C31-C32-C33
26	d	406	PL9	C9-C11-C12-C13
26	d	406	PL9	C39-C41-C42-C43
28	B	623	SQD	C45-C46-O48-C23
28	A	411	SQD	O49-C7-O47-C45
33	L	101	LHG	C29-C30-C31-C32
33	l	101	LHG	C32-C33-C34-C35
27	D	407	LMG	C15-C16-C17-C18
27	b	622	LMG	C14-C15-C16-C17
23	B	611	CLA	O1A-CGA-O2A-C1
28	F	101	SQD	O10-C23-C24-C25
25	C	514	BCR	C11-C10-C9-C34
25	b	619	BCR	C11-C10-C9-C34
23	B	613	CLA	C10-C11-C12-C13
23	B	612	CLA	C2C-C3C-CAC-CBC
27	m	101	LMG	C36-C37-C38-C39
33	l	101	LHG	C29-C30-C31-C32
23	B	610	CLA	C16-C17-C18-C19
29	C	517	DGD	O6D-C1D-O3G-C3G
29	c	516	DGD	O6E-C1E-O5D-C6D
23	C	513	CLA	C8-C10-C11-C12
33	D	409	LHG	C2-C3-O3-P
27	B	620	LMG	C30-C31-C32-C33
23	B	606	CLA	C12-C13-C15-C16
23	b	607	CLA	C12-C13-C15-C16
33	D	408	LHG	C19-C20-C21-C22
28	A	412	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	A	408	BCR	C15-C16-C17-C18
23	B	610	CLA	C4C-C3C-CAC-CBC
23	C	505	CLA	C11-C12-C13-C14
23	a	404	CLA	C14-C13-C15-C16
33	E	101	LHG	C32-C33-C34-C35
27	B	620	LMG	C8-C7-O1-C1
23	c	505	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	C2A-CAA-CBA-CGA
23	C	507	CLA	C2-C1-O2A-CGA
23	d	403	CLA	C2-C1-O2A-CGA
29	c	517	DGD	C5B-C6B-C7B-C8B
23	D	403	CLA	C3A-C2A-CAA-CBA
23	D	404	CLA	C3A-C2A-CAA-CBA
28	A	412	SQD	C34-C35-C36-C37
23	a	404	CLA	C3-C5-C6-C7
29	A	413	DGD	C3A-C4A-C5A-C6A
23	B	611	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	CBA-CGA-O2A-C1
33	D	409	LHG	C24-C23-O8-C6
28	F	101	SQD	O48-C23-C24-C25
27	B	620	LMG	C9-C8-O7-C10
28	B	623	SQD	C46-C45-O47-C7
25	c	521	BCR	C18-C19-C20-C21
27	C	519	LMG	C32-C33-C34-C35
33	D	408	LHG	C25-C26-C27-C28
28	a	411	SQD	C17-C18-C19-C20
29	C	516	DGD	O6D-C5D-C6D-O5D
25	C	514	BCR	C20-C21-C22-C23
25	y	101	BCR	C20-C21-C22-C23
23	A	404	CLA	C2C-C3C-CAC-CBC
28	A	411	SQD	C35-C36-C37-C38
28	a	411	SQD	C13-C14-C15-C16
27	C	519	LMG	O1-C7-C8-C9
28	b	601	SQD	O6-C44-C45-C46
24	A	406	PHO	O1A-CGA-O2A-C1
23	C	501	CLA	C3-C5-C6-C7
27	D	410	LMG	C37-C38-C39-C40
26	A	409	PL9	C40-C39-C41-C42
26	a	409	PL9	C12-C11-C9-C8
25	C	514	BCR	C13-C14-C15-C16
29	c	516	DGD	CAB-CBB-CCB-CDB
23	B	608	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	b	622	LMG	C38-C39-C40-C41
27	b	622	LMG	O7-C8-C9-O8
29	C	516	DGD	O2G-C2G-C3G-O3G
23	B	614	CLA	C11-C12-C13-C14
23	b	604	CLA	C11-C12-C13-C14
23	d	403	CLA	C11-C10-C8-C9
24	A	406	PHO	C6-C7-C8-C9
33	l	101	LHG	C15-C16-C17-C18
28	a	411	SQD	C34-C35-C36-C37
23	b	609	CLA	C4C-C3C-CAC-CBC
28	b	601	SQD	C30-C31-C32-C33
23	B	612	CLA	CAA-CBA-CGA-O2A
26	A	409	PL9	C33-C34-C36-C37
26	a	409	PL9	C13-C14-C16-C17
23	B	611	CLA	C6-C7-C8-C10
23	C	503	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C12-C13-C15
23	C	508	CLA	C12-C13-C15-C16
23	a	405	CLA	C6-C7-C8-C10
23	a	407	CLA	C11-C10-C8-C7
23	d	404	CLA	C11-C12-C13-C15
23	d	404	CLA	C10-C11-C12-C13
23	d	402	CLA	C2B-C3B-CAB-CBB
25	B	618	BCR	C23-C24-C25-C26
25	B	618	BCR	C23-C24-C25-C30
25	B	619	BCR	C5-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
27	a	414	LMG	C13-C14-C15-C16
28	a	411	SQD	O47-C7-C8-C9
23	A	404	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
29	c	518	DGD	C6A-C7A-C8A-C9A
27	B	620	LMG	C16-C17-C18-C19
27	b	622	LMG	O7-C10-C11-C12
27	b	622	LMG	O8-C28-C29-C30
23	B	601	CLA	C2-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
28	B	623	SQD	C30-C31-C32-C33
23	C	509	CLA	C2A-CAA-CBA-CGA
33	a	410	LHG	C28-C29-C30-C31
28	b	601	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	d	409	LMG	C11-C12-C13-C14
29	h	103	DGD	C4A-C5A-C6A-C7A
23	b	613	CLA	CAA-CBA-CGA-O2A
29	C	516	DGD	O2G-C1B-C2B-C3B
27	b	623	LMG	C29-C30-C31-C32
33	a	410	LHG	C15-C16-C17-C18
27	B	620	LMG	C11-C12-C13-C14
23	C	511	CLA	C8-C10-C11-C12
23	B	603	CLA	C2A-CAA-CBA-CGA
29	c	518	DGD	CCB-CDB-CEB-CFB
33	B	622	LHG	C19-C20-C21-C22
33	D	408	LHG	O9-C7-O7-C5
23	B	603	CLA	C6-C7-C8-C9
23	D	403	CLA	C6-C7-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	b	609	CLA	C11-C10-C8-C9
23	c	501	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
27	m	101	LMG	O7-C10-C11-C12
29	H	102	DGD	C8B-C9B-CAB-CBB
29	a	413	DGD	CDB-CEB-CFB-CGB
27	a	414	LMG	C7-C8-C9-O8
29	c	516	DGD	C1G-C2G-C3G-O3G
23	d	404	CLA	C8-C10-C11-C12
23	C	504	CLA	C4B-C3B-CAB-CBB
23	d	402	CLA	C4B-C3B-CAB-CBB
26	A	409	PL9	C30-C29-C31-C32
28	a	411	SQD	O48-C23-C24-C25
25	K	101	BCR	C7-C8-C9-C10
25	T	101	BCR	C11-C12-C13-C14
25	d	405	BCR	C13-C14-C15-C16
23	b	617	CLA	C11-C12-C13-C14
26	a	409	PL9	C17-C18-C19-C21
27	B	620	LMG	C32-C33-C34-C35
28	A	411	SQD	C31-C32-C33-C34
29	c	516	DGD	C2B-C3B-C4B-C5B
23	b	614	CLA	CAA-CBA-CGA-O2A
23	A	404	CLA	C4C-C3C-CAC-CBC
27	D	410	LMG	C34-C35-C36-C37
23	C	512	CLA	C5-C6-C7-C8
29	A	413	DGD	C1B-C2B-C3B-C4B
23	a	407	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	O7-C7-C8-C9
23	a	407	CLA	C15-C16-C17-C18
23	d	402	CLA	C4C-C3C-CAC-CBC
26	A	409	PL9	C11-C12-C13-C14
23	D	403	CLA	C2-C1-O2A-CGA
23	B	603	CLA	C11-C10-C8-C7
23	C	505	CLA	C11-C12-C13-C15
23	b	609	CLA	C6-C7-C8-C10
23	c	513	CLA	C12-C13-C15-C16
23	C	506	CLA	C10-C11-C12-C13
23	B	603	CLA	O1A-CGA-O2A-C1
27	a	414	LMG	C15-C16-C17-C18
27	b	622	LMG	C12-C13-C14-C15
29	a	413	DGD	C1G-C2G-O2G-C1B
29	C	517	DGD	C6B-C7B-C8B-C9B
29	c	517	DGD	C4A-C5A-C6A-C7A
23	C	507	CLA	C15-C16-C17-C18
23	C	501	CLA	C16-C17-C18-C20
27	b	622	LMG	C32-C33-C34-C35
29	c	516	DGD	CDB-CEB-CFB-CGB
23	B	602	CLA	C3A-C2A-CAA-CBA
23	c	501	CLA	CAA-CBA-CGA-O2A
29	C	517	DGD	C3A-C4A-C5A-C6A
29	a	413	DGD	C9B-CAB-CBB-CCB
33	L	101	LHG	C24-C25-C26-C27
24	A	406	PHO	CBA-CGA-O2A-C1
23	B	611	CLA	C6-C7-C8-C9
23	B	612	CLA	C11-C10-C8-C9
23	B	615	CLA	C11-C10-C8-C9
23	C	507	CLA	C6-C7-C8-C9
23	c	507	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C10-C8-C9
23	d	403	CLA	C6-C7-C8-C9
25	c	515	BCR	C19-C20-C21-C22
23	C	513	CLA	C4C-C3C-CAC-CBC
26	D	406	PL9	C22-C23-C24-C25
23	a	407	CLA	CAA-CBA-CGA-O1A
23	b	613	CLA	CAA-CBA-CGA-O1A
27	m	101	LMG	O9-C10-C11-C12
29	c	516	DGD	O1B-C1B-C2B-C3B
33	D	409	LHG	O10-C23-C24-C25
23	c	508	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	C	519	LMG	O9-C10-C11-C12
28	b	601	SQD	C45-C44-O6-C1
29	A	413	DGD	C2E-C1E-O5D-C6D
23	B	612	CLA	CAA-CBA-CGA-O1A
33	e	101	LHG	O10-C23-C24-C25
24	D	401	PHO	C8-C10-C11-C12
26	a	409	PL9	C47-C48-C49-C51
26	D	406	PL9	C11-C12-C13-C14
23	B	607	CLA	C15-C16-C17-C18
23	b	606	CLA	C10-C11-C12-C13
27	D	407	LMG	O7-C10-C11-C12
27	A	410	LMG	C8-C9-O8-C28
34	E	102	HEM	CAD-CBD-CGD-O2D
27	b	623	LMG	C28-C29-C30-C31
23	B	612	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAA-CBA-CGA-O2A
29	c	518	DGD	O1B-C1B-C2B-C3B
33	l	101	LHG	C12-C13-C14-C15
26	D	406	PL9	C41-C42-C43-C44
23	c	510	CLA	CAA-CBA-CGA-O1A
27	a	414	LMG	O8-C28-C29-C30
29	c	516	DGD	O2G-C1B-C2B-C3B
23	B	603	CLA	C5-C6-C7-C8
27	a	414	LMG	C31-C32-C33-C34
29	A	413	DGD	O2G-C1B-C2B-C3B
33	e	101	LHG	O8-C23-C24-C25
29	C	516	DGD	O1B-C1B-C2B-C3B
29	c	517	DGD	C2B-C3B-C4B-C5B

There are no ring outliers.

96 monomers are involved in 151 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	601	CLA	3	0
23	B	605	CLA	2	0
23	b	616	CLA	5	0
23	h	101	CLA	5	0
33	L	101	LHG	2	0
25	K	101	BCR	3	0
23	b	614	CLA	2	0
33	E	101	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	412	SQD	2	0
24	d	401	PHO	1	0
23	b	606	CLA	2	0
28	A	412	SQD	1	0
23	a	404	CLA	1	0
23	c	511	CLA	1	0
25	B	619	BCR	1	0
23	A	405	CLA	2	0
23	B	607	CLA	1	0
25	a	408	BCR	2	0
23	b	613	CLA	1	0
23	D	403	CLA	3	0
23	B	608	CLA	1	0
25	d	405	BCR	2	0
28	f	101	SQD	2	0
23	b	617	CLA	2	0
23	B	613	CLA	1	0
23	D	402	CLA	1	0
33	d	407	LHG	1	0
27	m	101	LMG	1	0
26	A	409	PL9	3	0
25	b	618	BCR	1	0
33	D	408	LHG	4	0
25	y	101	BCR	1	0
27	D	407	LMG	3	0
23	B	602	CLA	1	0
23	c	505	CLA	3	0
25	c	514	BCR	2	0
25	D	405	BCR	2	0
25	b	620	BCR	2	0
28	B	623	SQD	2	0
29	a	413	DGD	2	0
23	c	504	CLA	1	0
27	a	414	LMG	2	0
23	C	505	CLA	2	0
23	c	512	CLA	2	0
23	c	508	CLA	1	0
23	c	510	CLA	1	0
28	a	411	SQD	1	0
23	c	503	CLA	1	0
27	B	620	LMG	3	0
33	l	101	LHG	1	0

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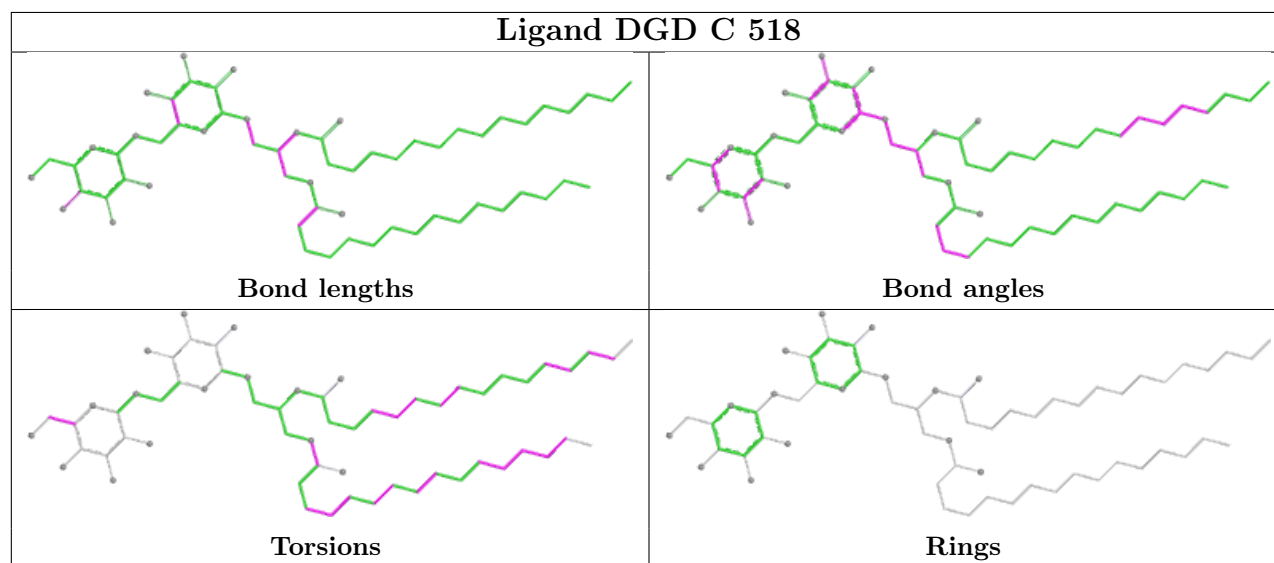
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	513	CLA	1	0
25	A	408	BCR	1	0
25	H	101	BCR	2	0
34	e	102	HEM	3	0
23	b	615	CLA	4	0
27	c	519	LMG	1	0
33	B	622	LHG	1	0
23	B	614	CLA	1	0
33	d	408	LHG	1	0
33	a	410	LHG	3	0
23	B	606	CLA	2	0
23	C	511	CLA	1	0
23	c	502	CLA	1	0
25	C	520	BCR	1	0
27	A	410	LMG	1	0
23	c	506	CLA	2	0
30	a	416	OEY	1	0
29	H	102	DGD	1	0
25	b	619	BCR	5	0
25	t	101	BCR	4	0
23	B	611	CLA	1	0
25	c	521	BCR	4	0
23	b	610	CLA	2	0
23	c	509	CLA	1	0
23	C	509	CLA	3	0
25	c	515	BCR	2	0
24	D	401	PHO	1	0
25	B	617	BCR	4	0
25	C	515	BCR	3	0
35	V	201	HEC	1	0
23	b	607	CLA	2	0
25	T	101	BCR	2	0
33	e	101	LHG	1	0
26	D	406	PL9	1	0
25	B	618	BCR	1	0
23	d	404	CLA	1	0
26	d	406	PL9	1	0
25	h	102	BCR	3	0
29	A	413	DGD	2	0
23	A	407	CLA	1	0
30	A	414	OEY	1	0
23	b	604	CLA	3	0

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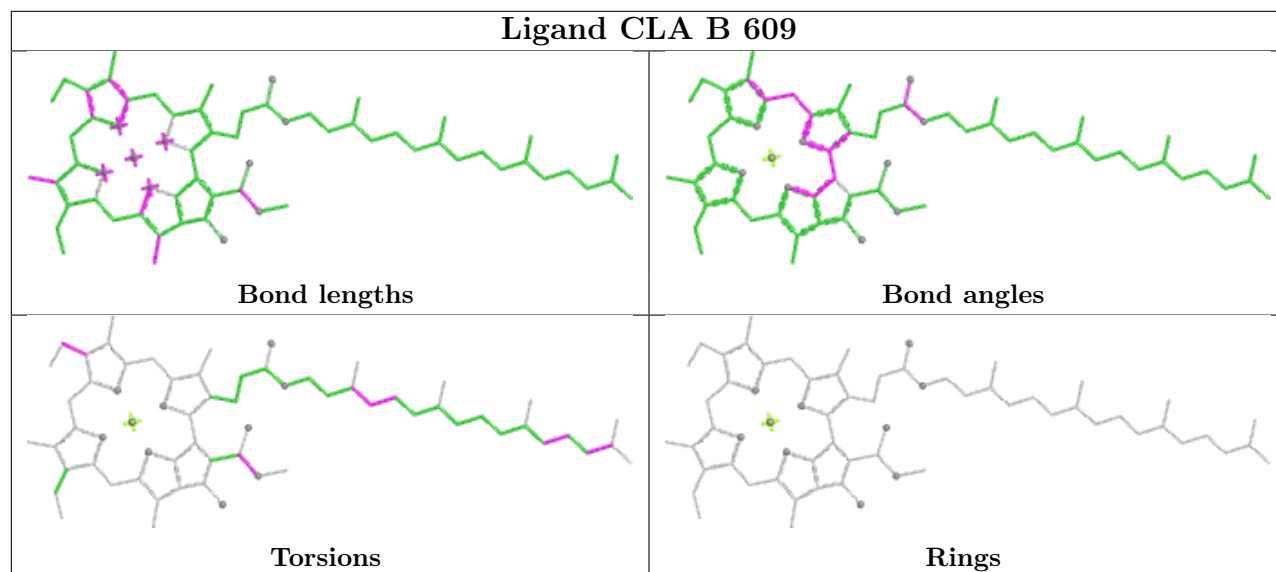
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	612	CLA	1	0
24	A	406	PHO	1	0
26	a	409	PL9	2	0
34	E	102	HEM	2	0

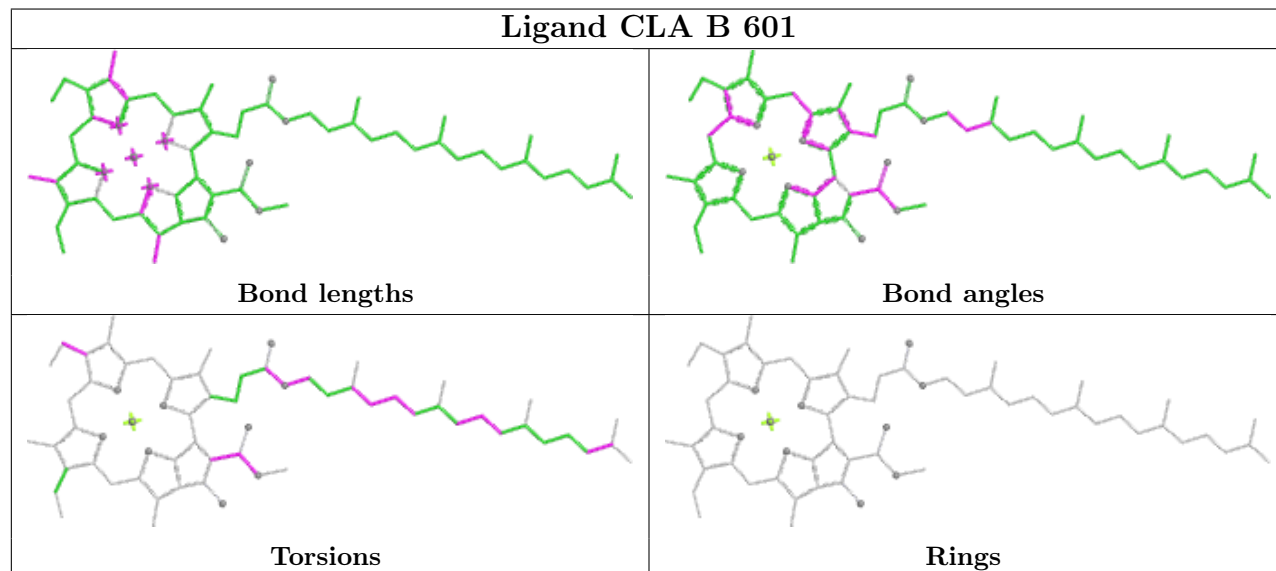
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



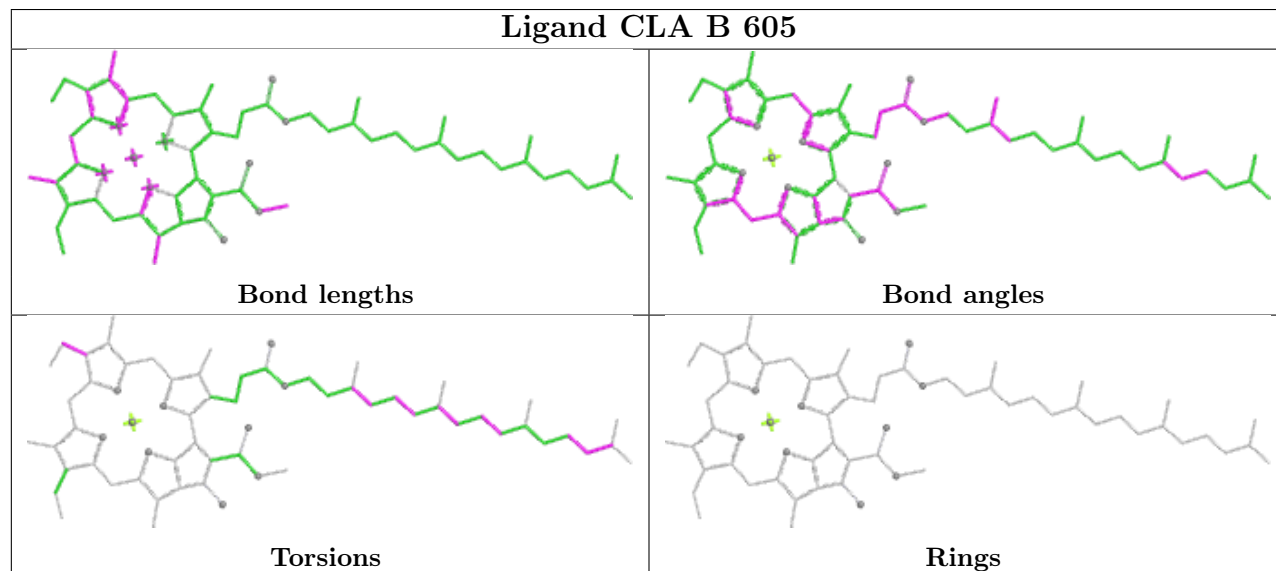
Ligand CLA B 609



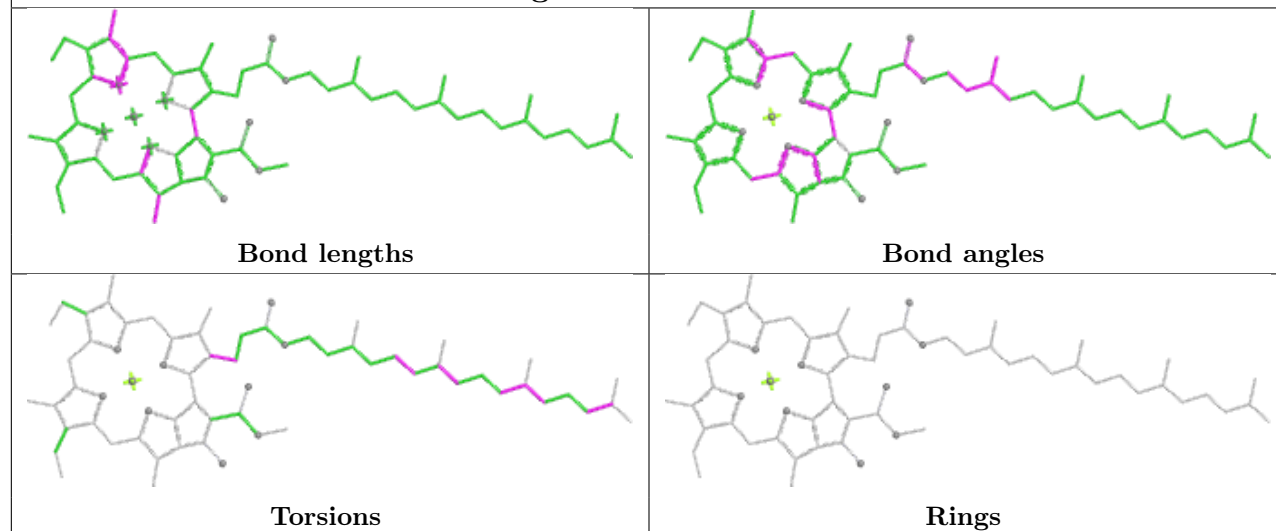
Ligand CLA B 601



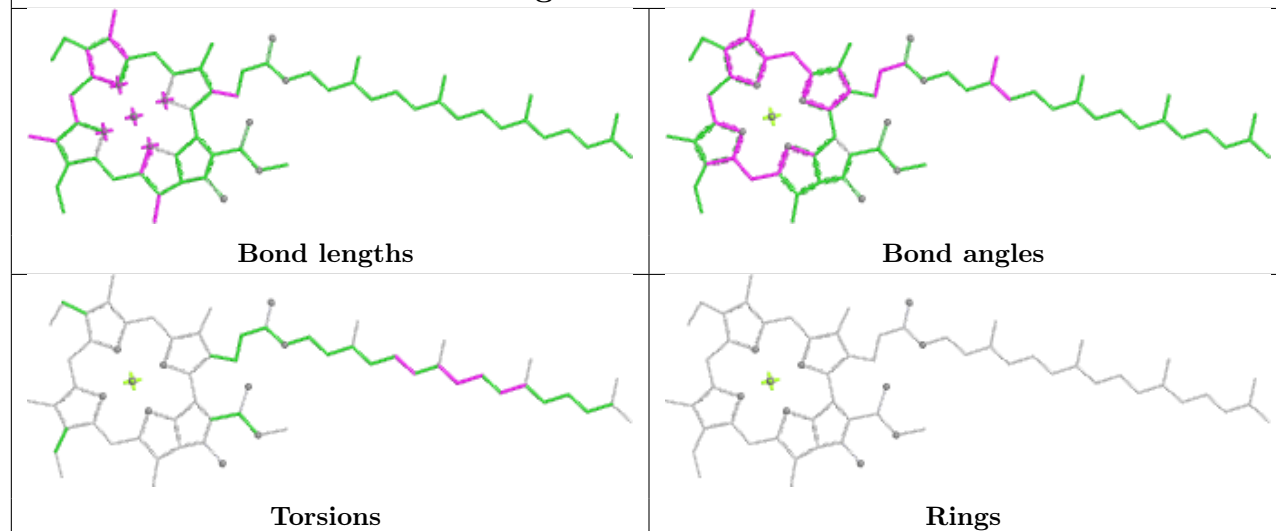
Ligand CLA B 605



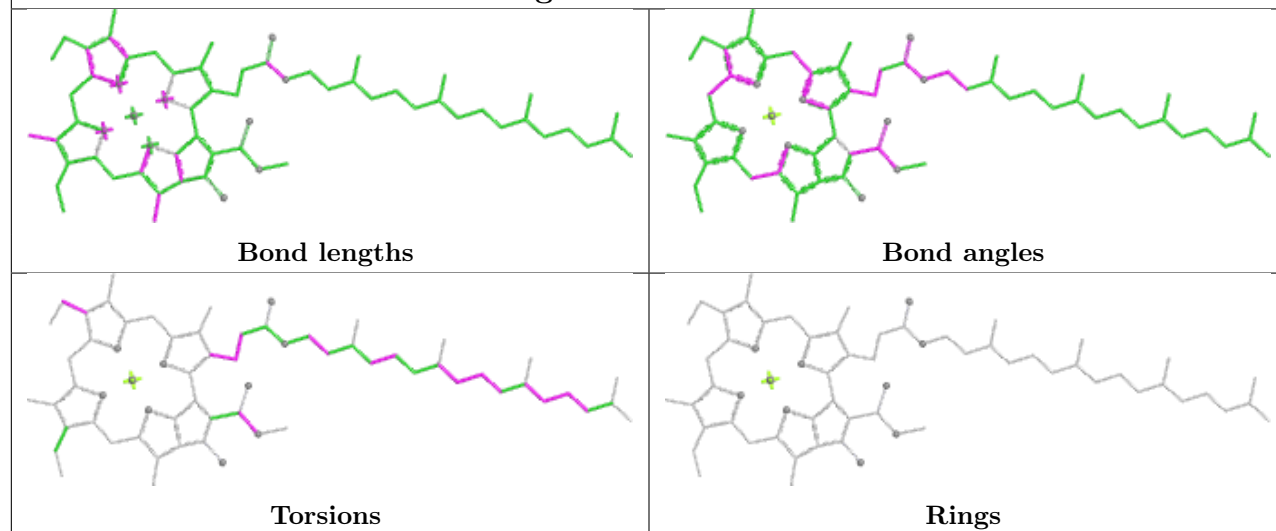
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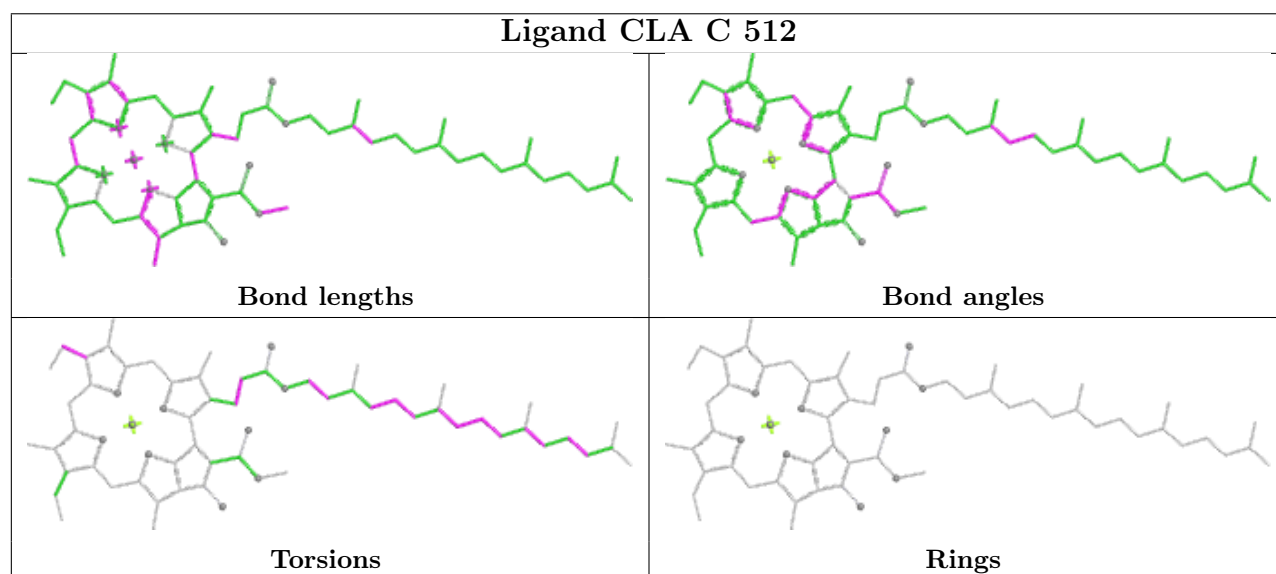
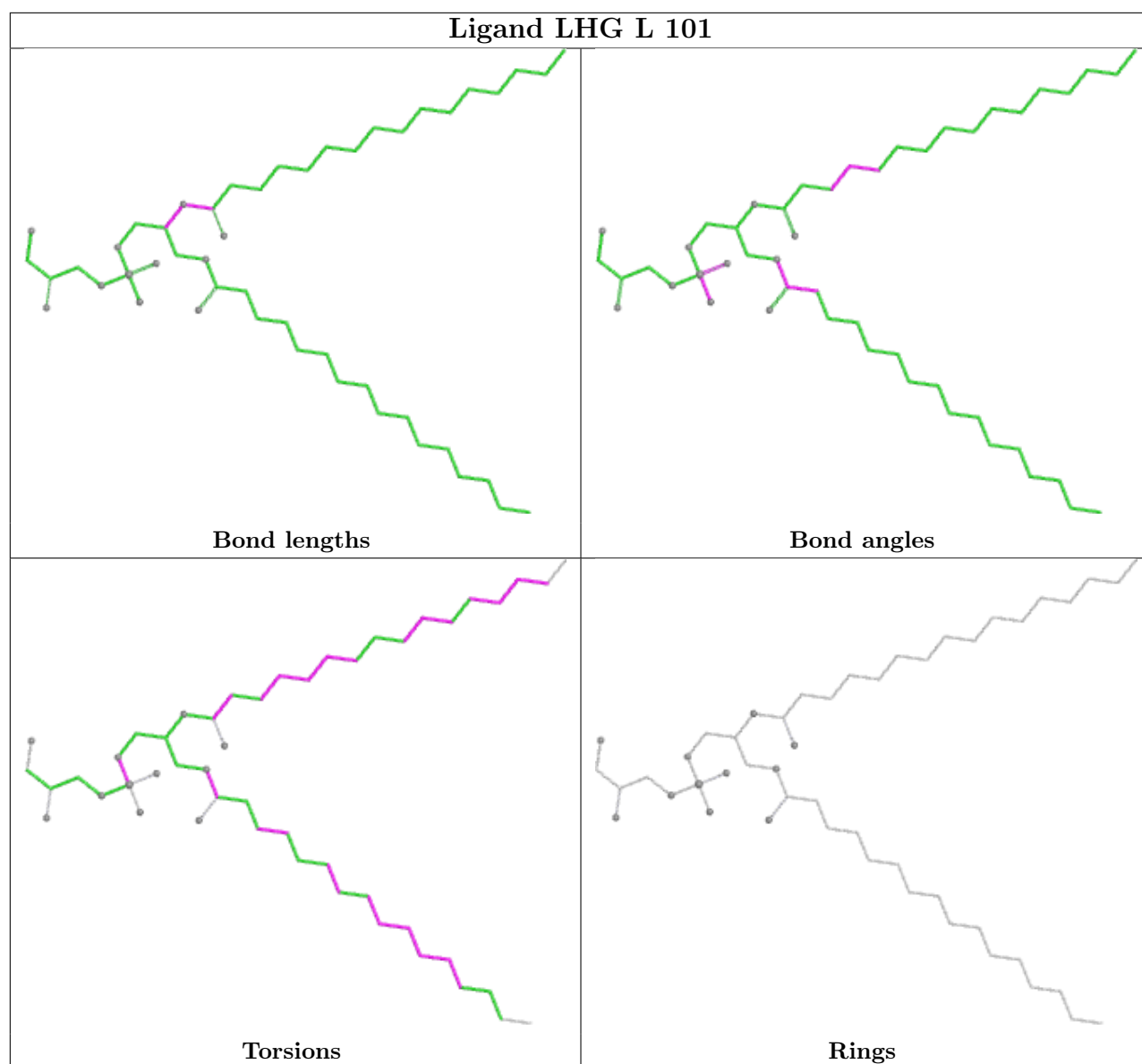


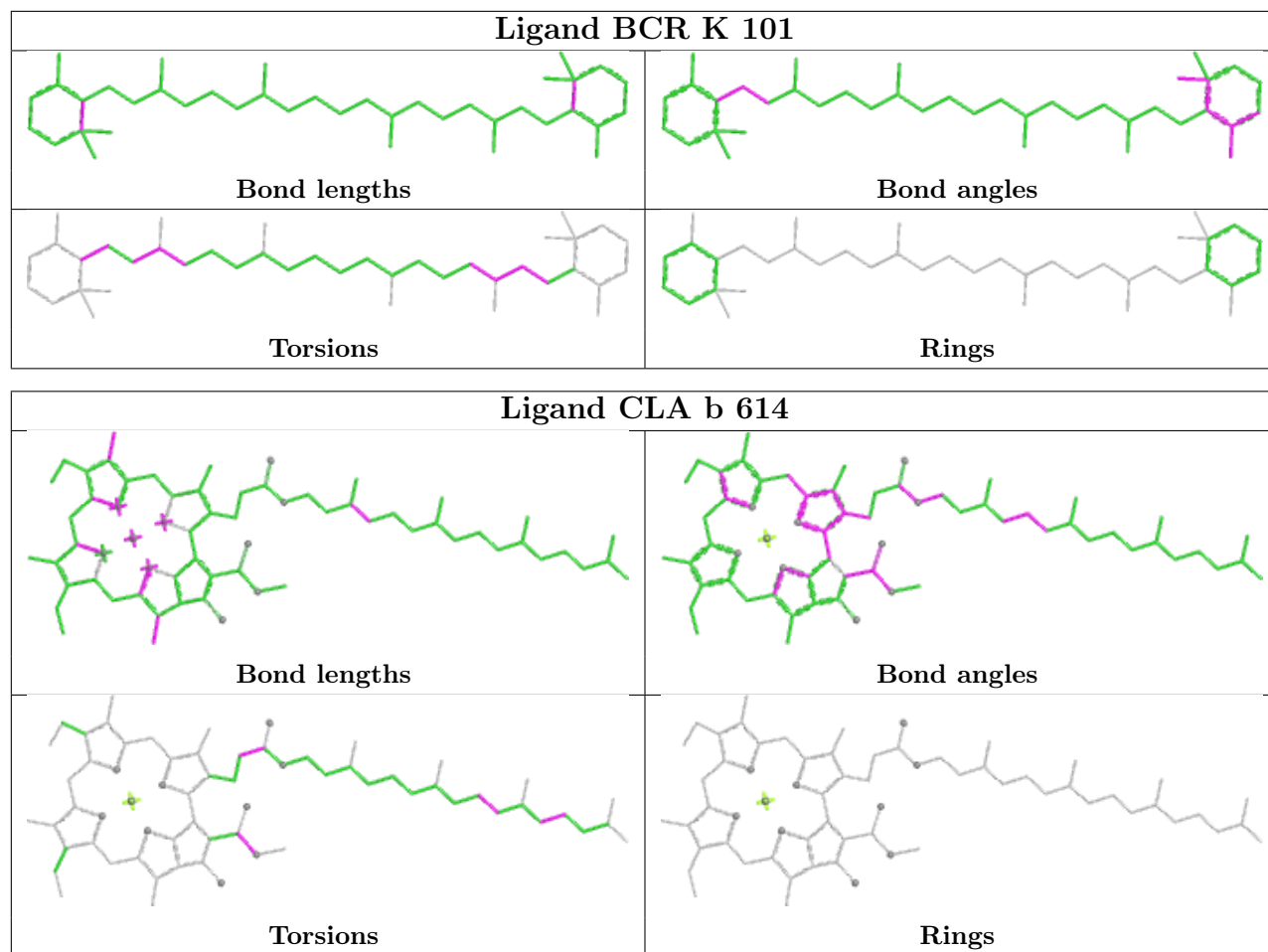
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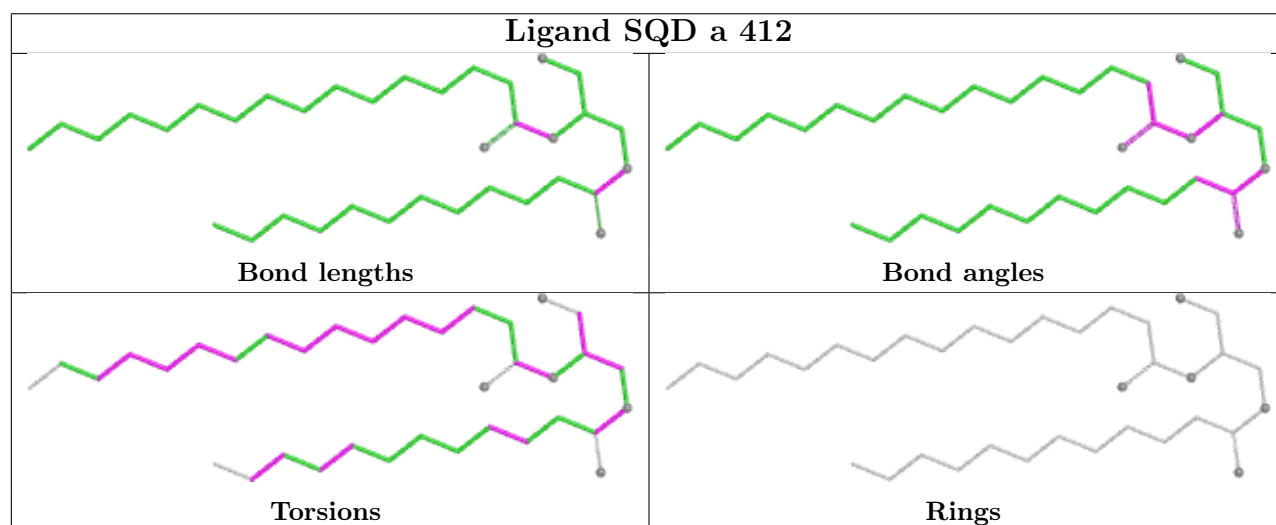
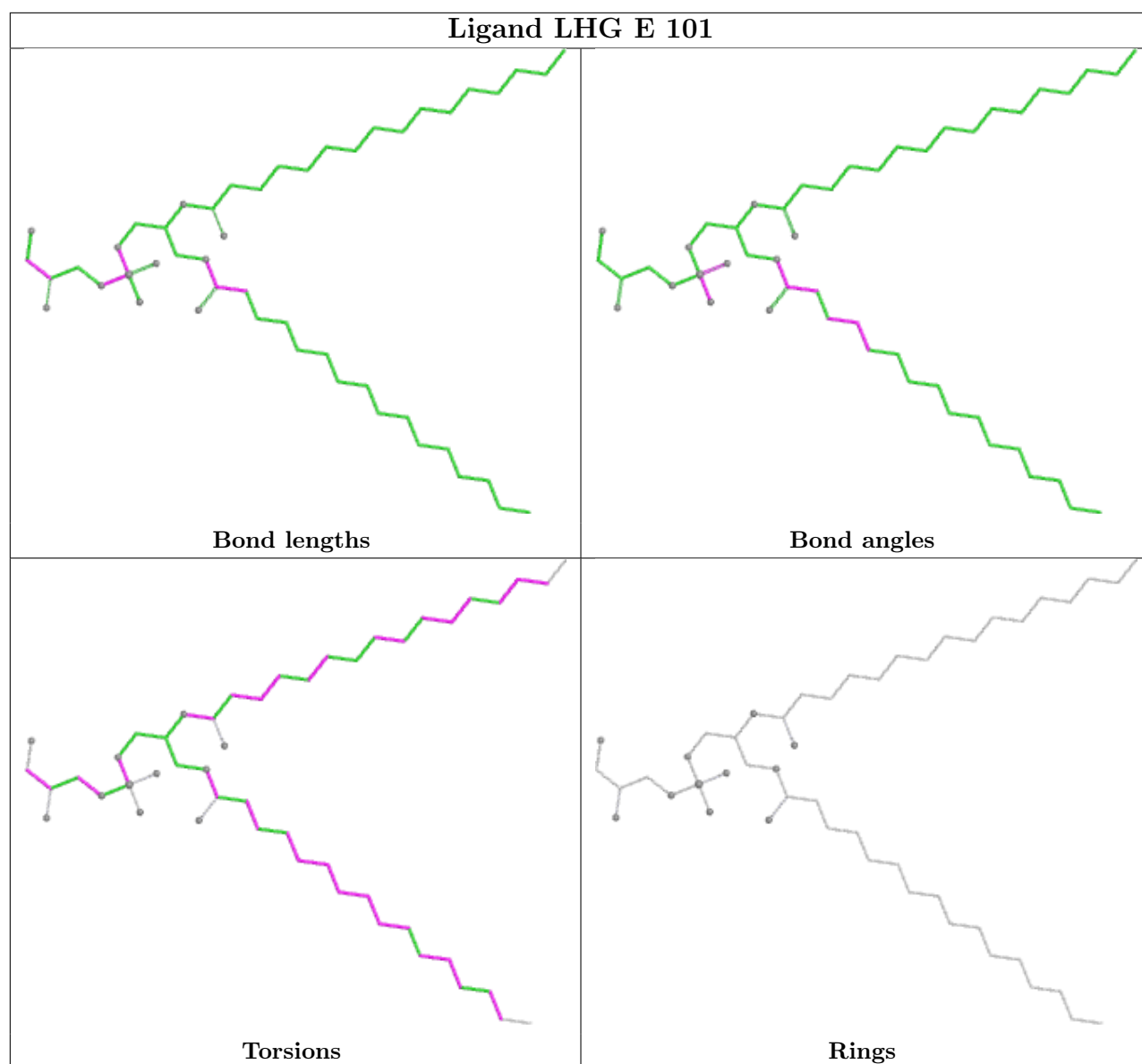


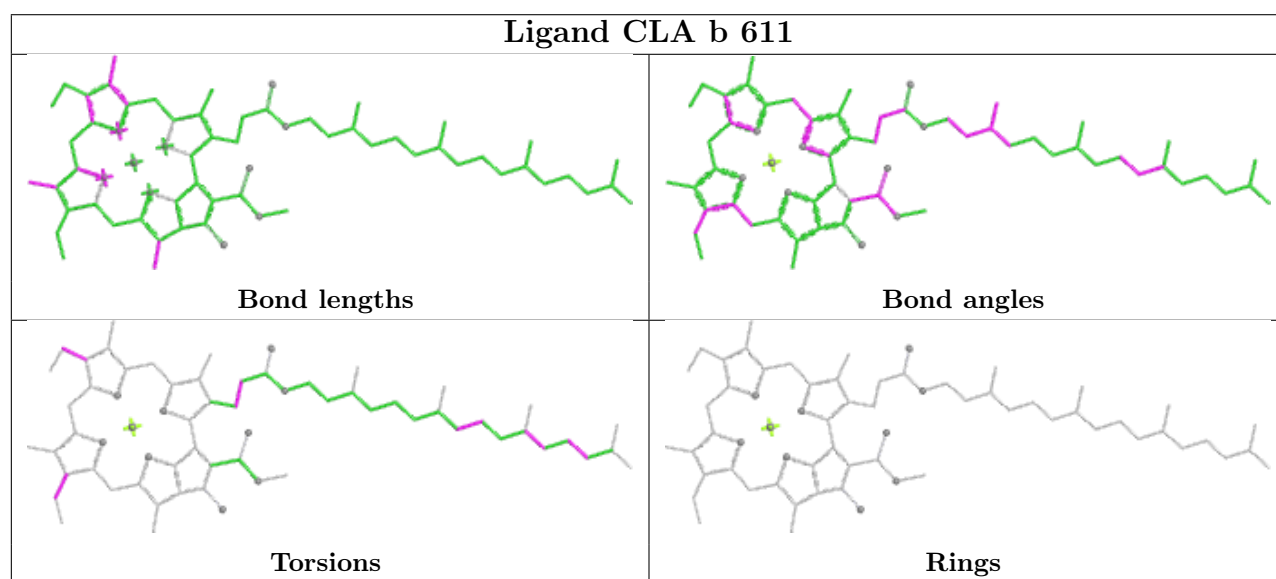
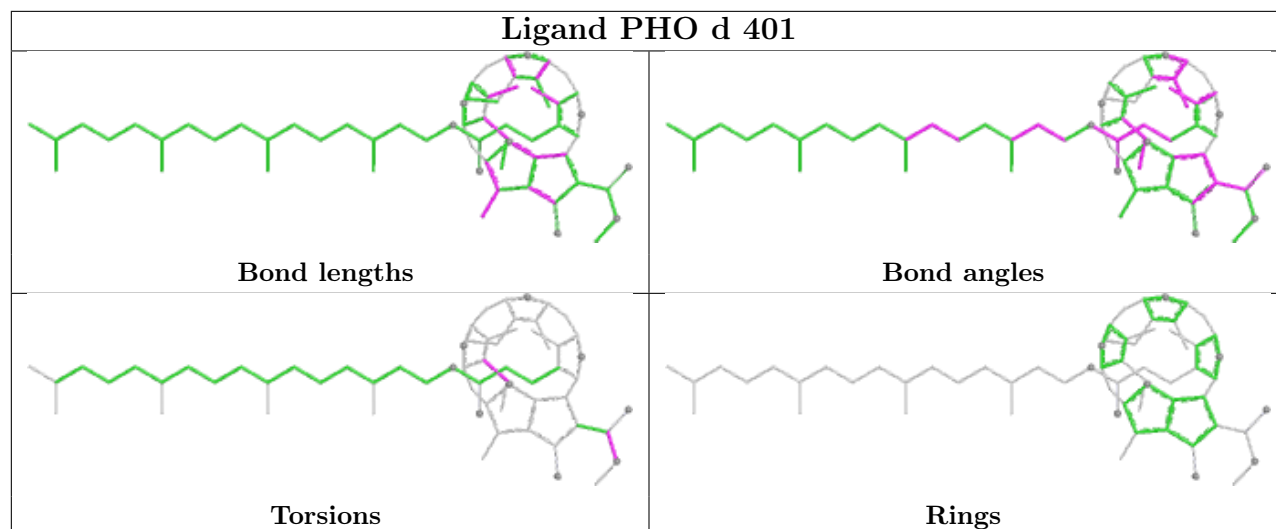
Ligand CLA h 101

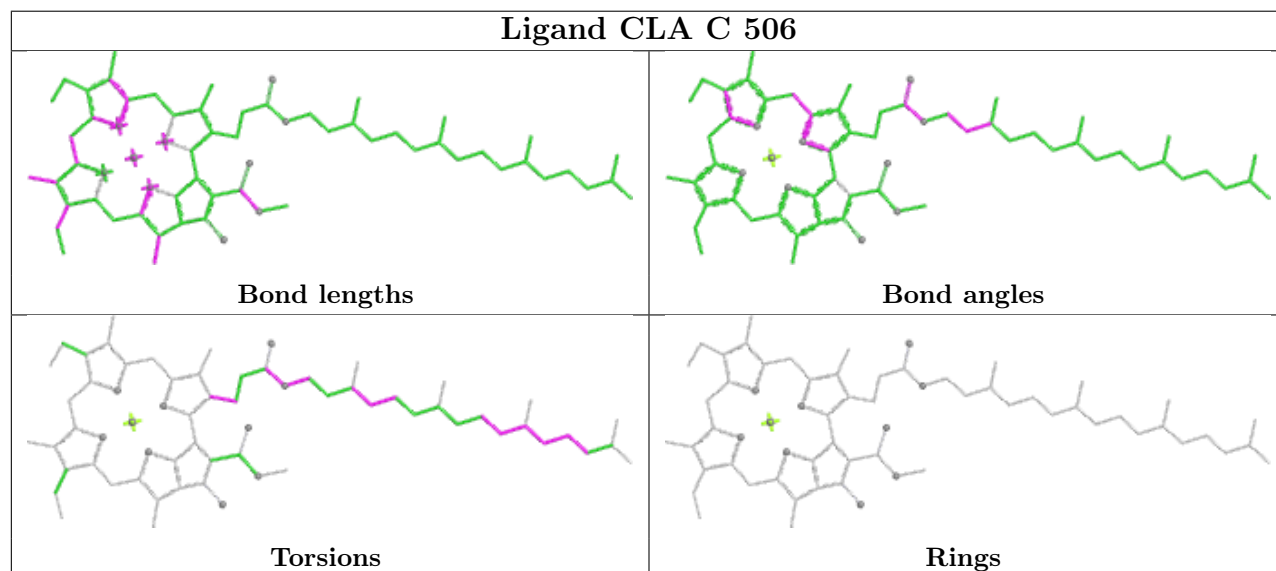
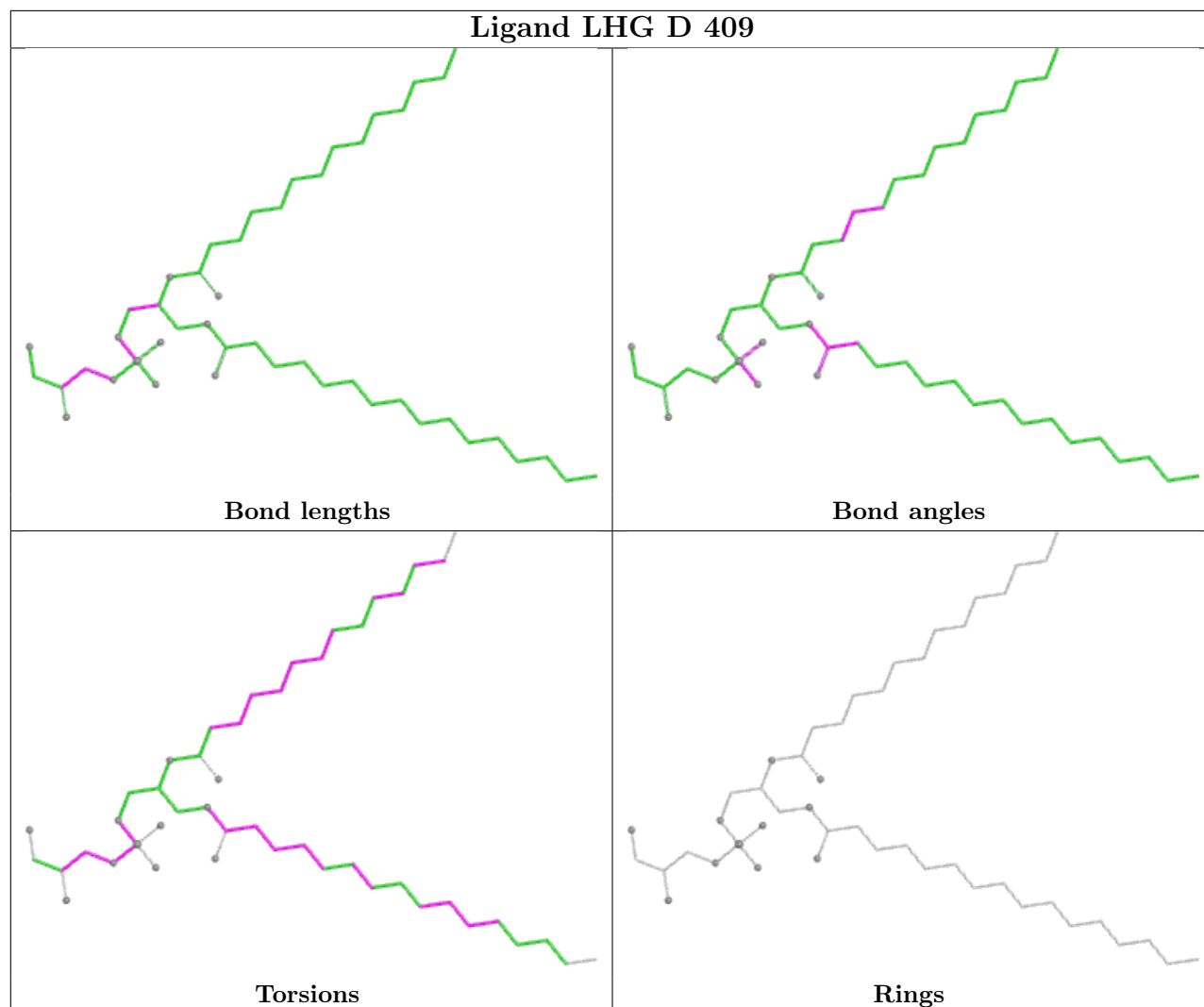




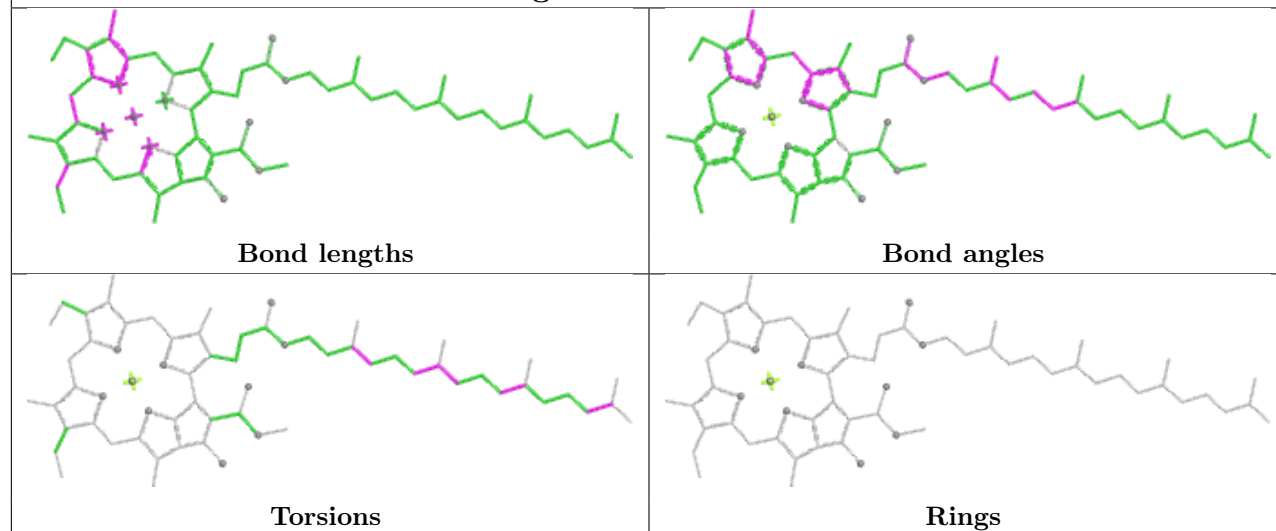




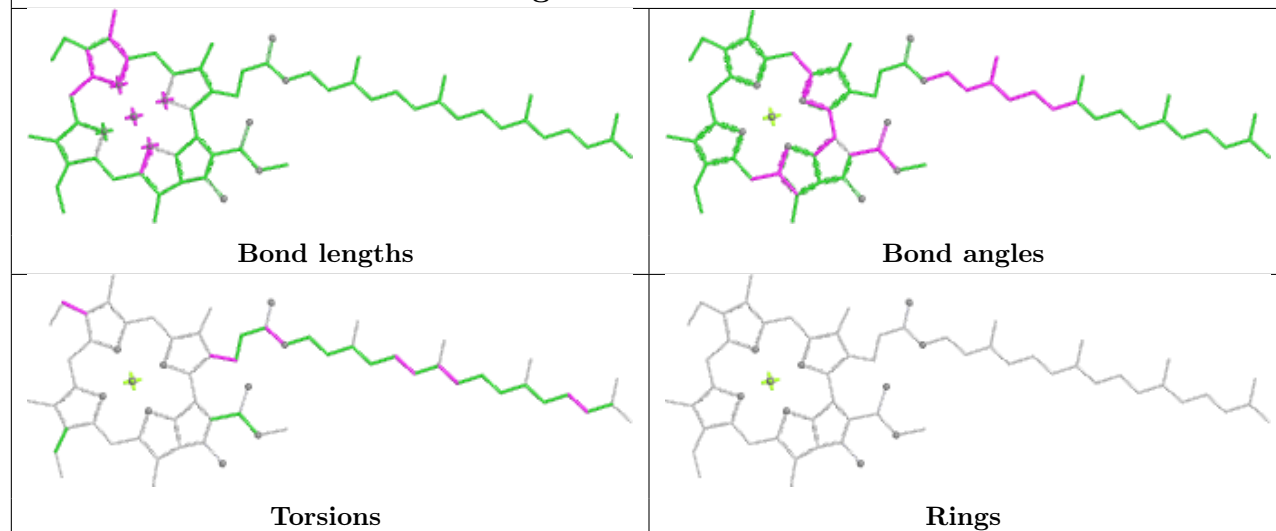




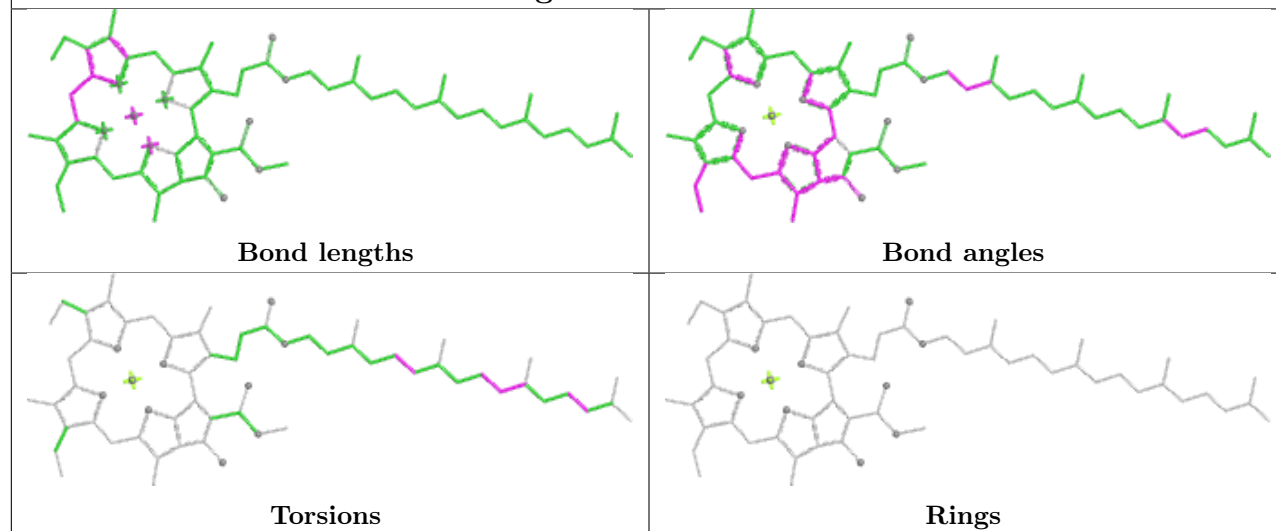
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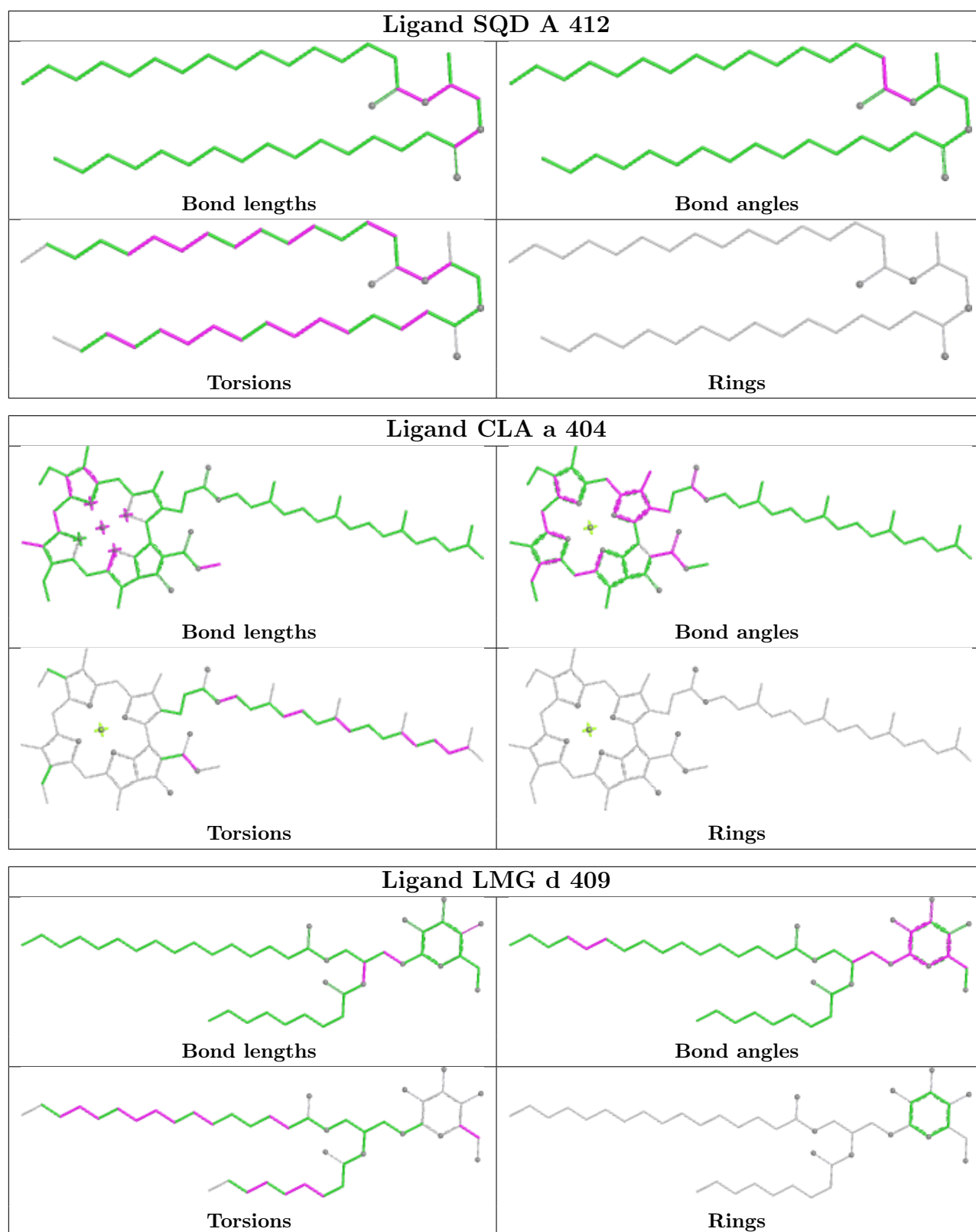


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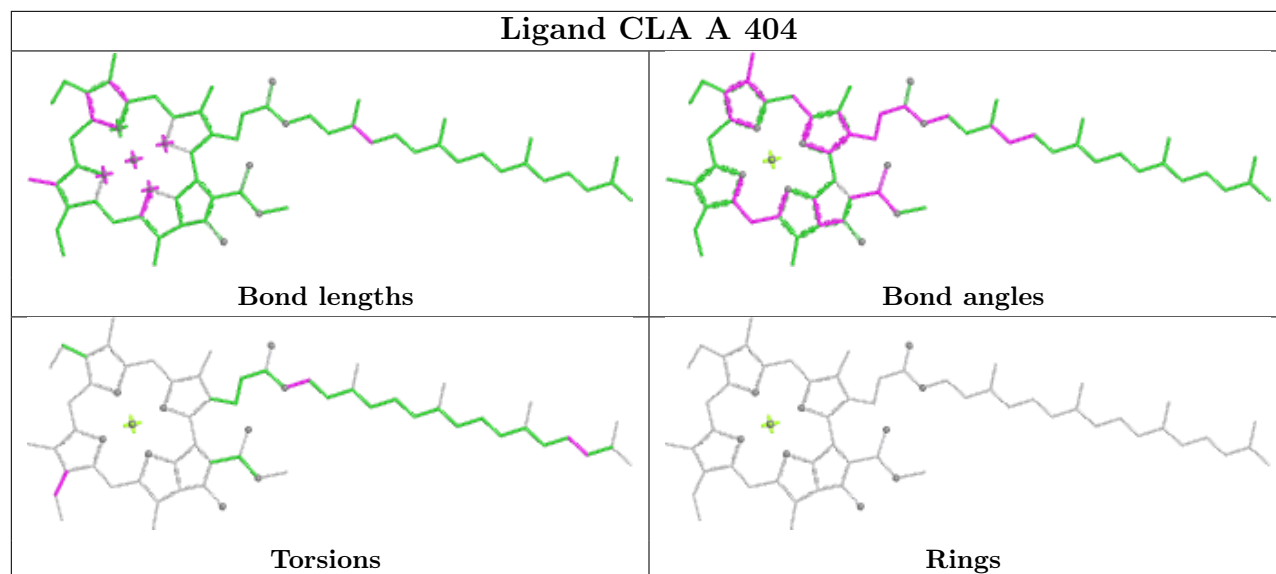


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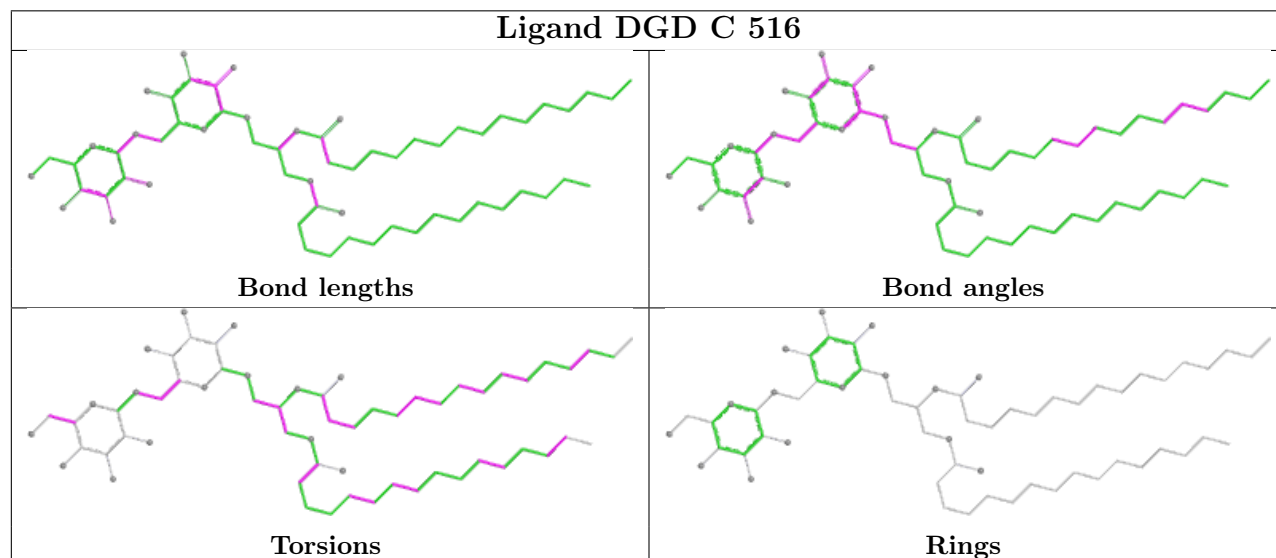




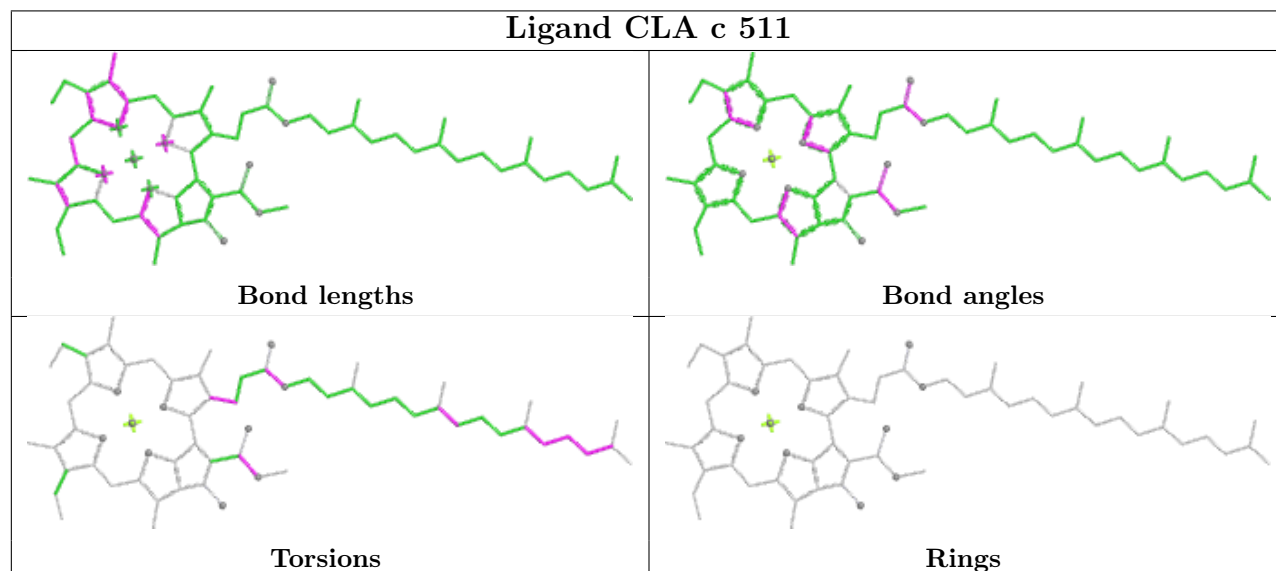
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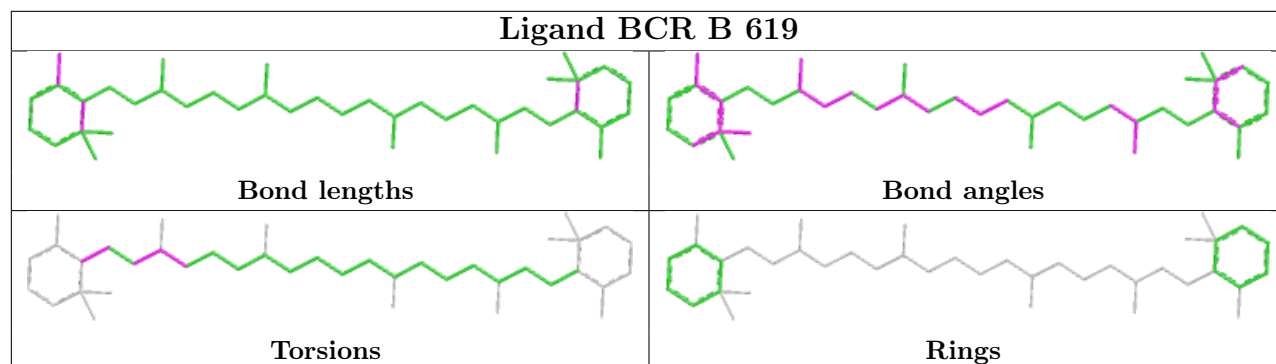
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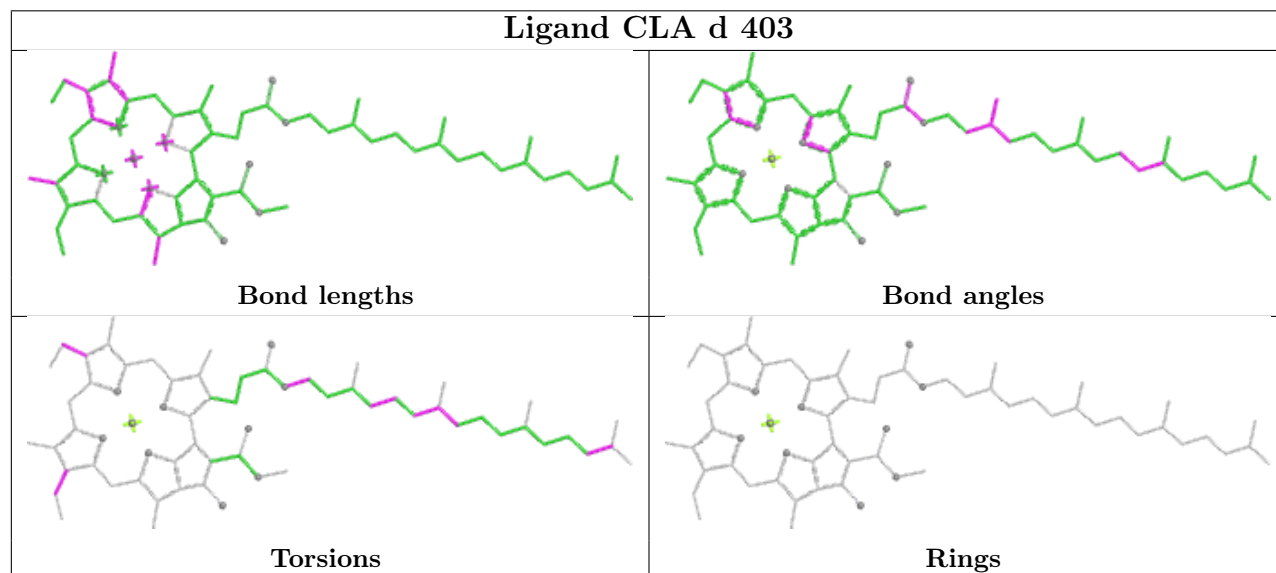
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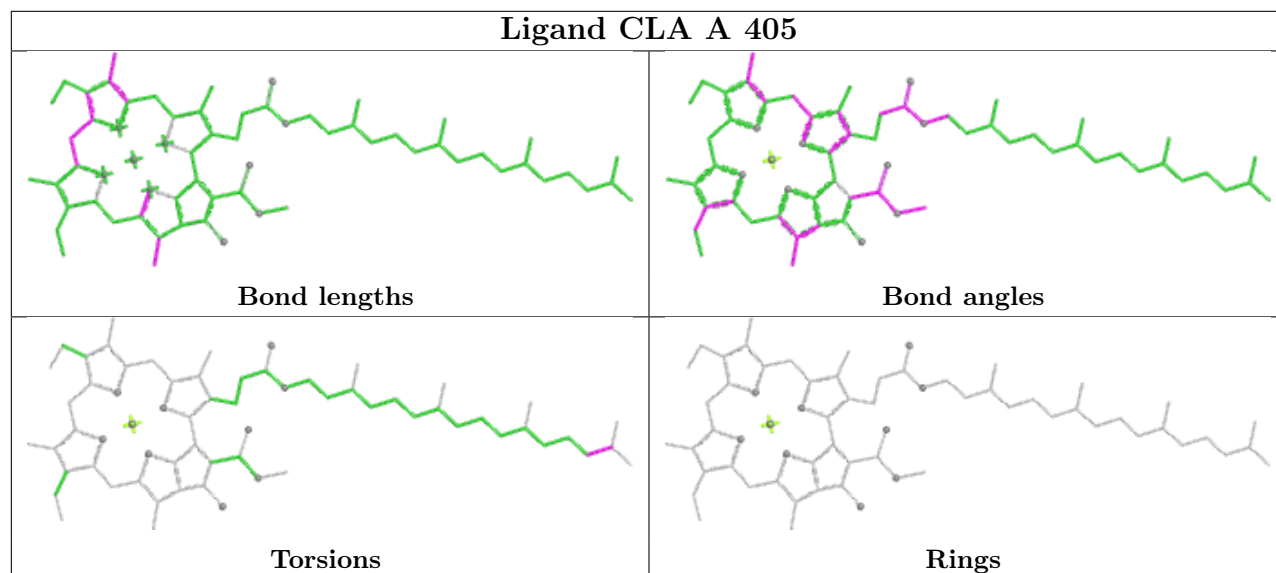
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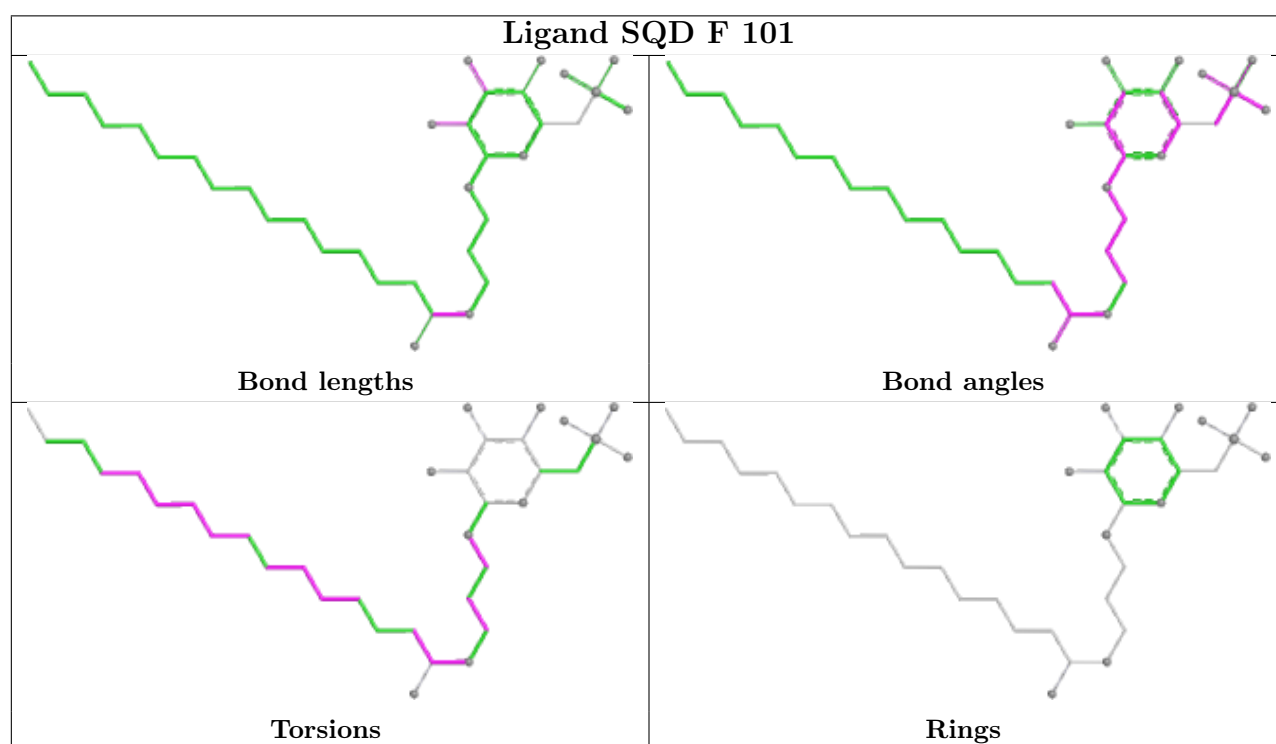
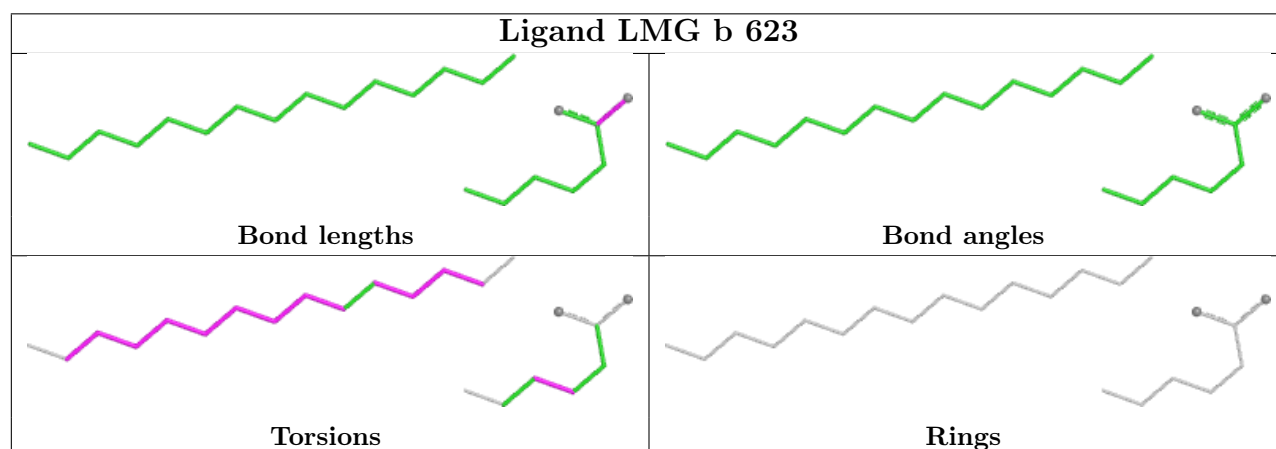
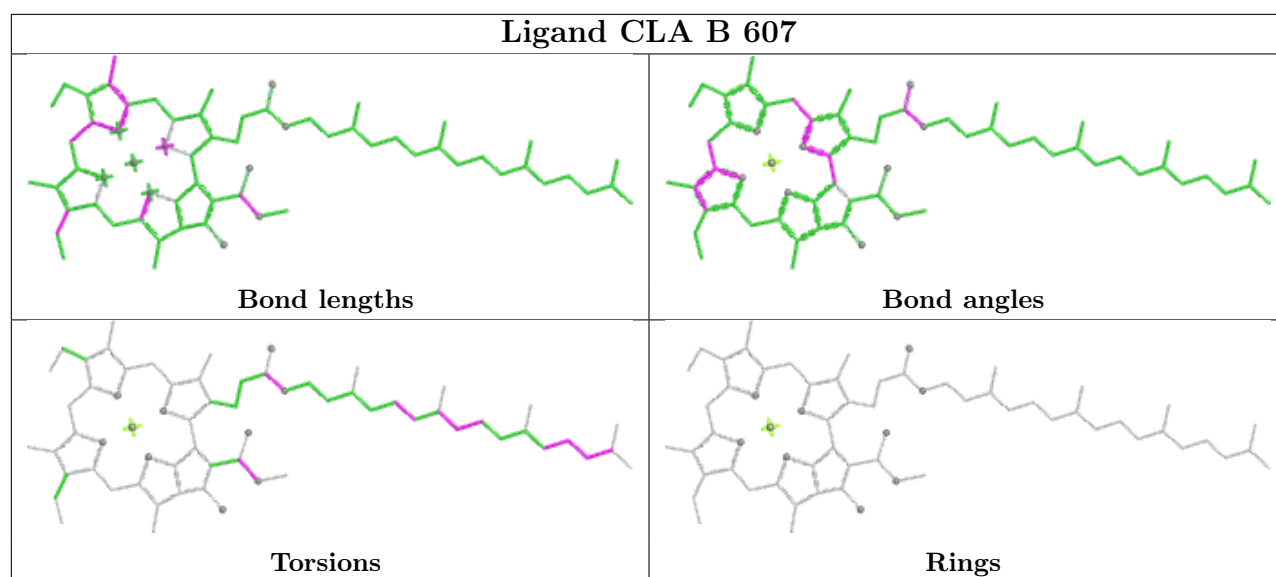


Ligand CLA d 403

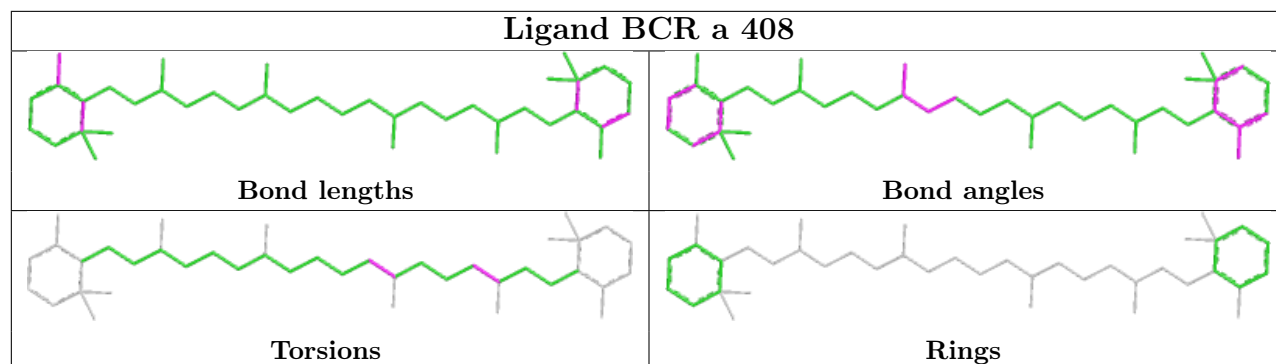


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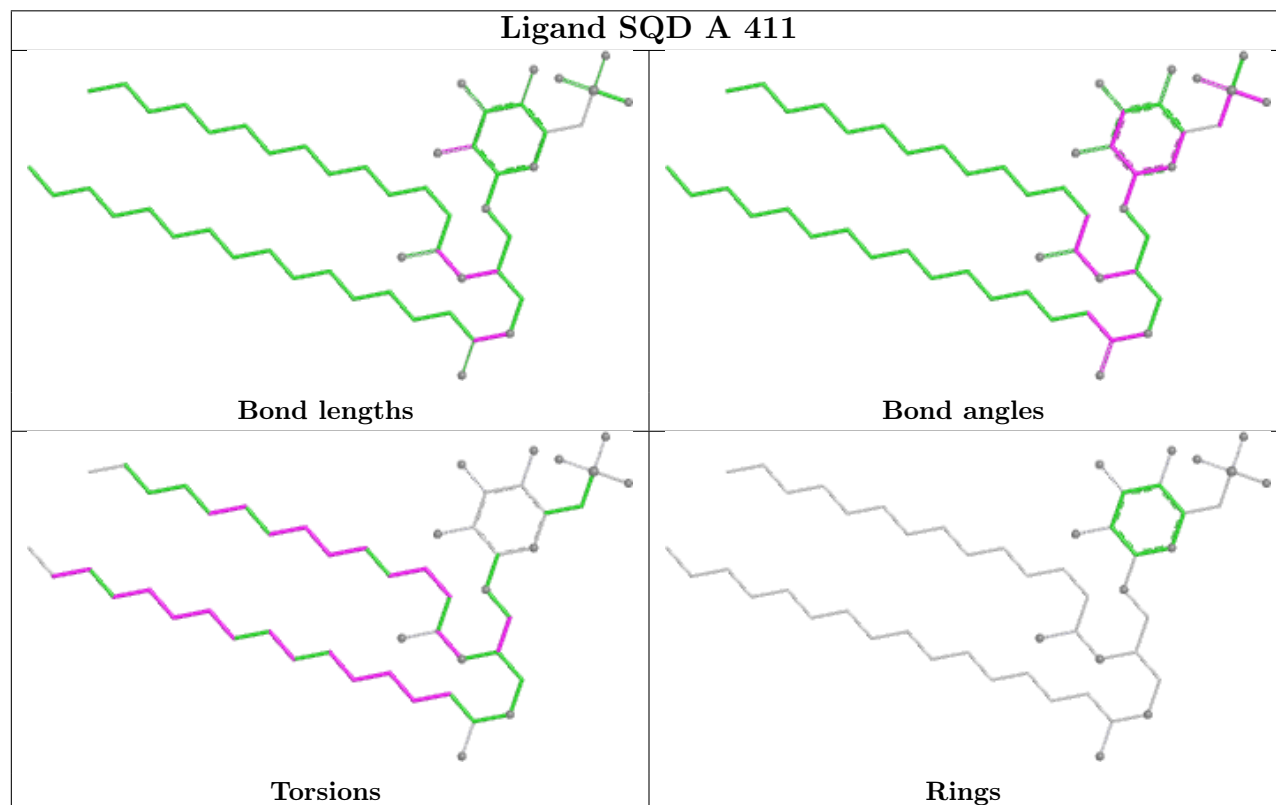




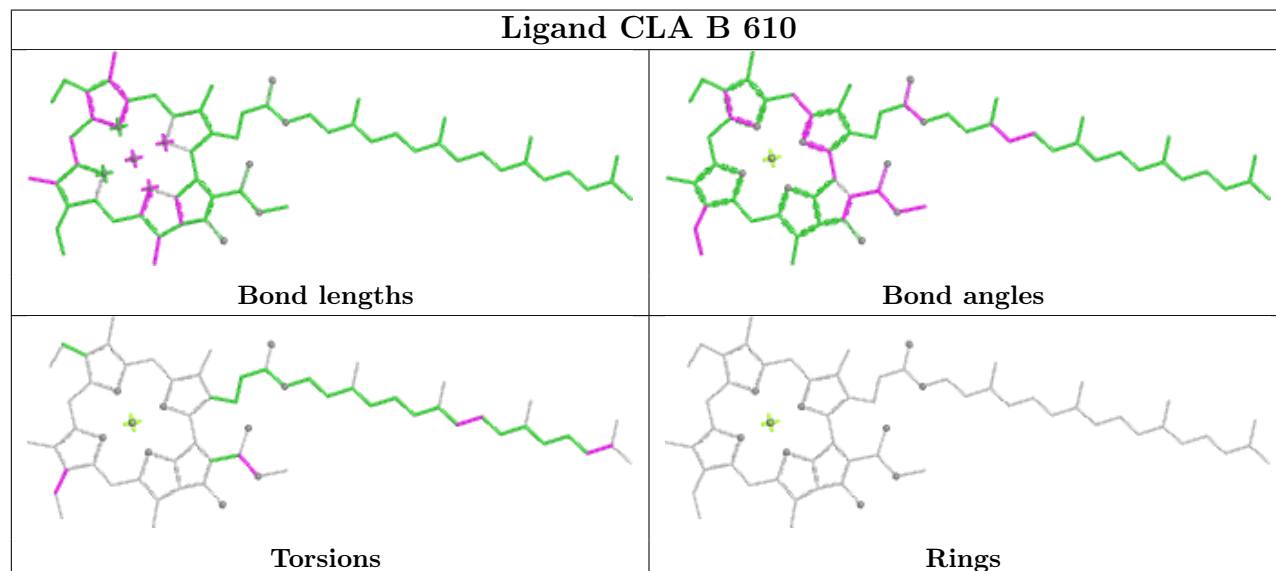
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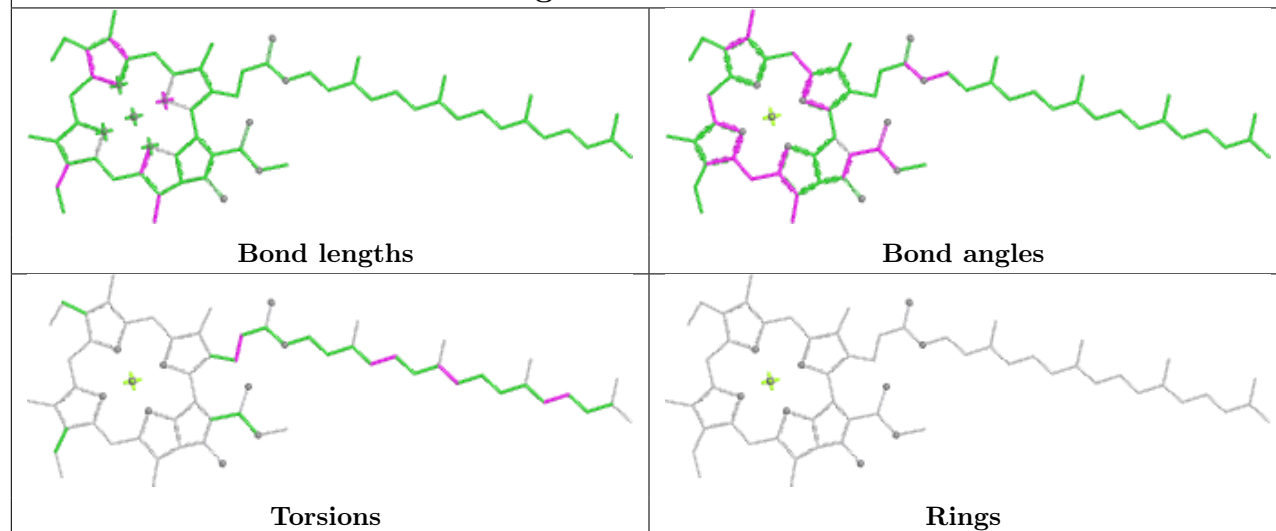
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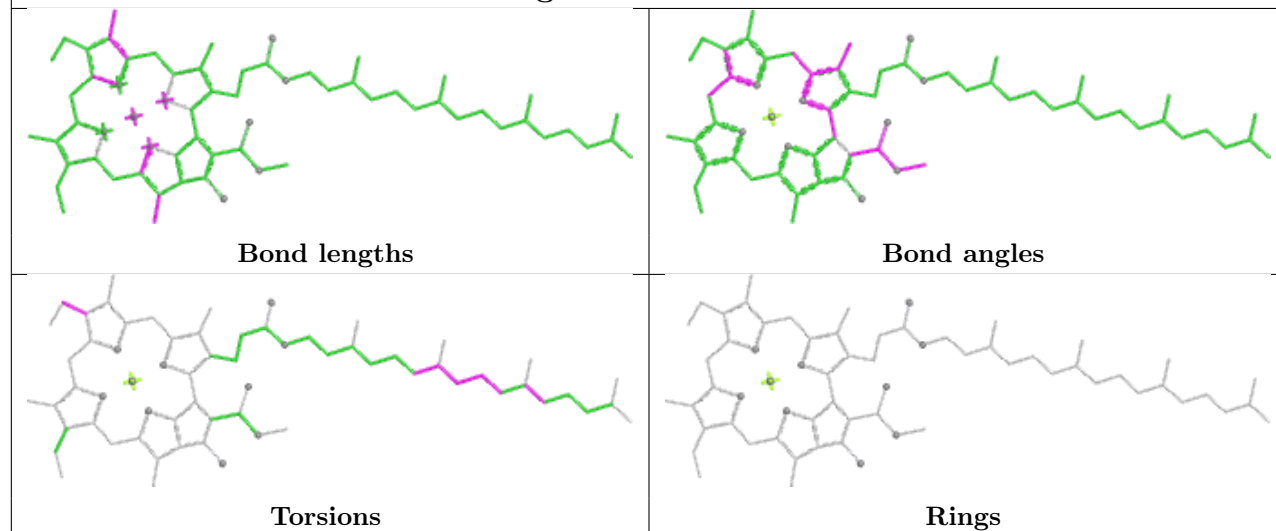
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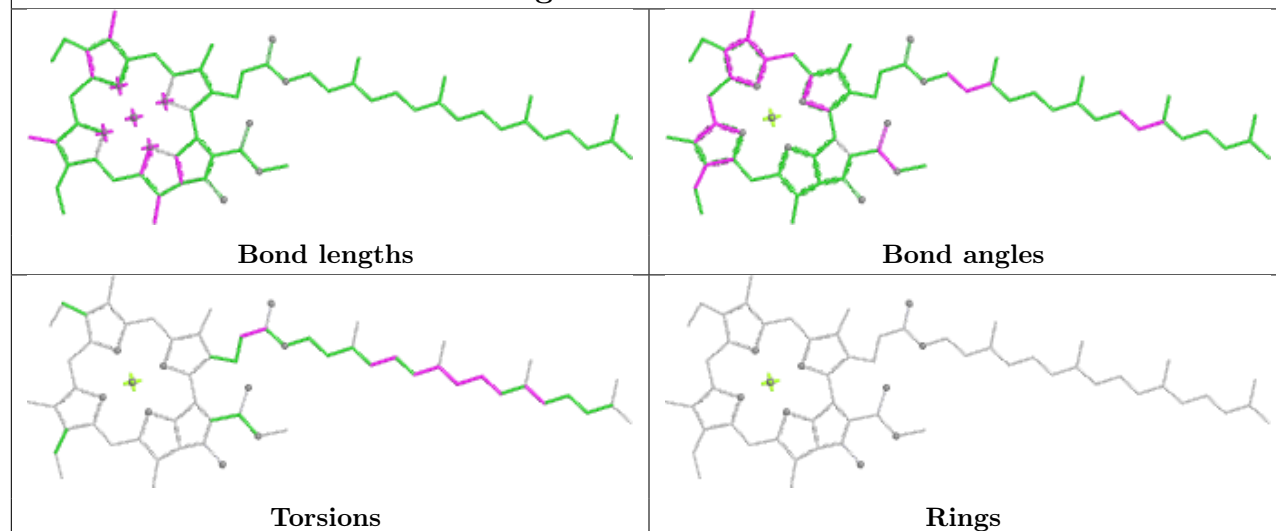
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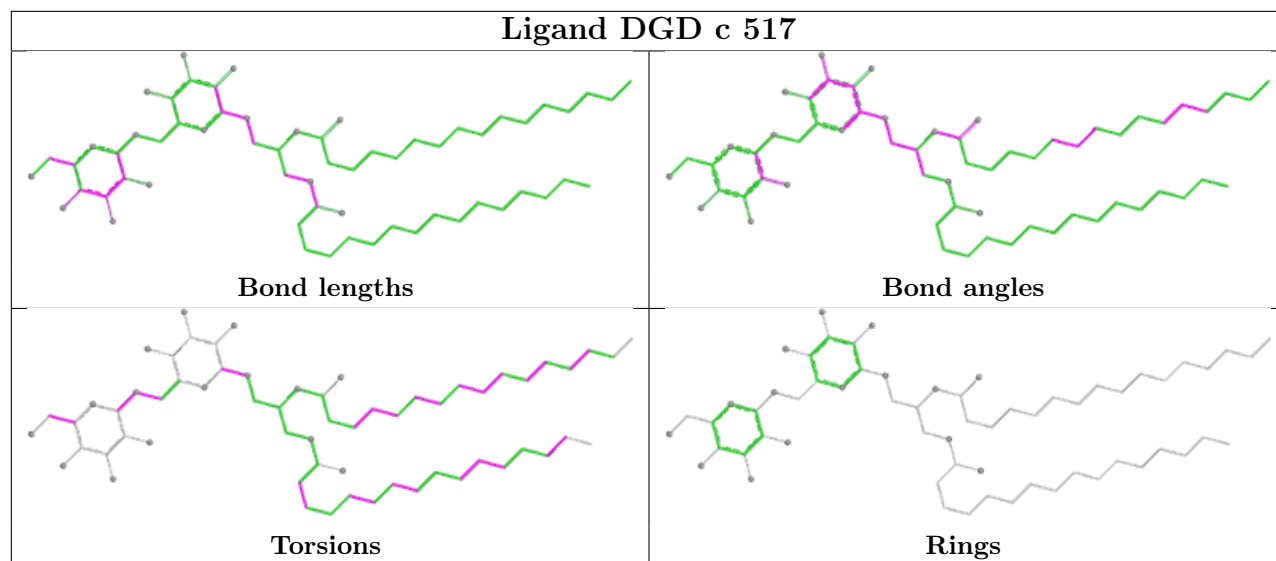
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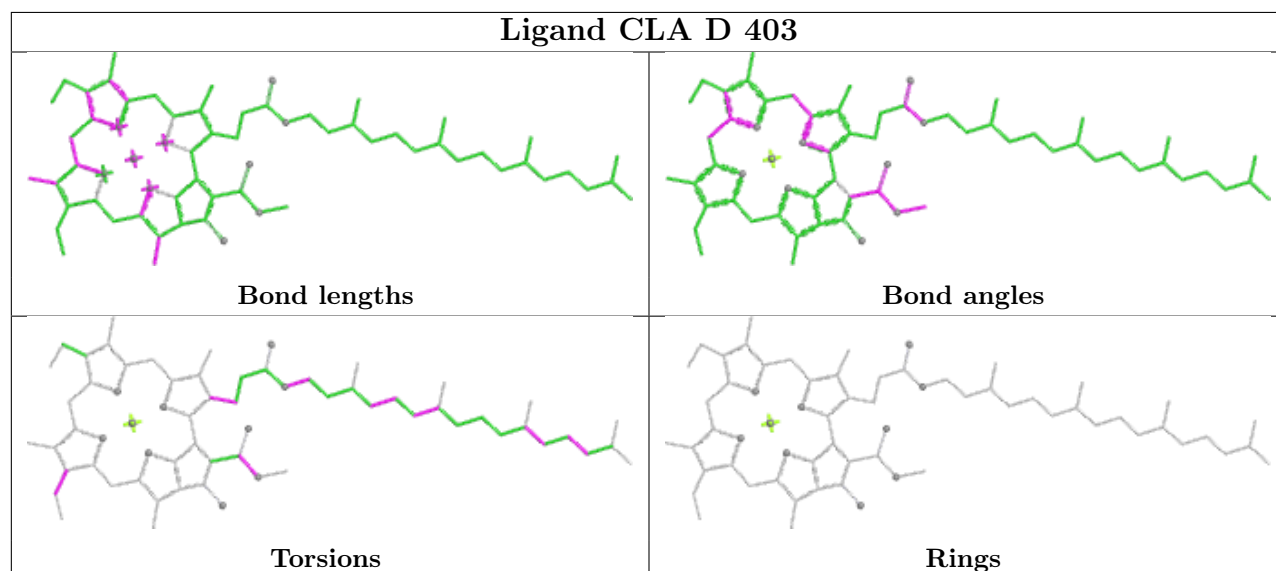
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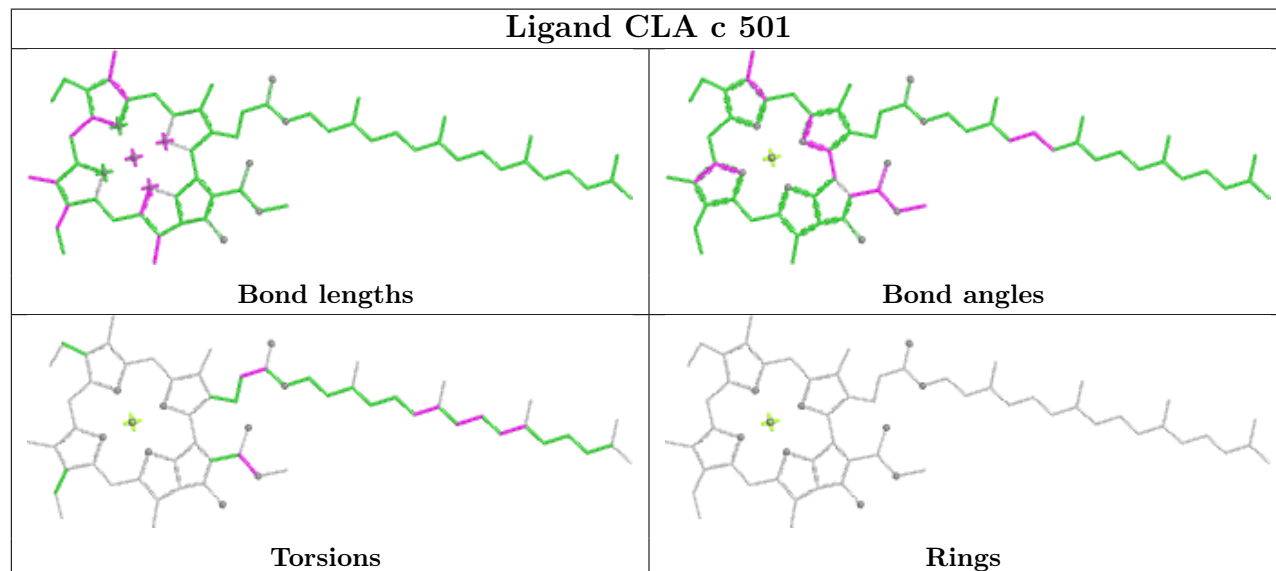
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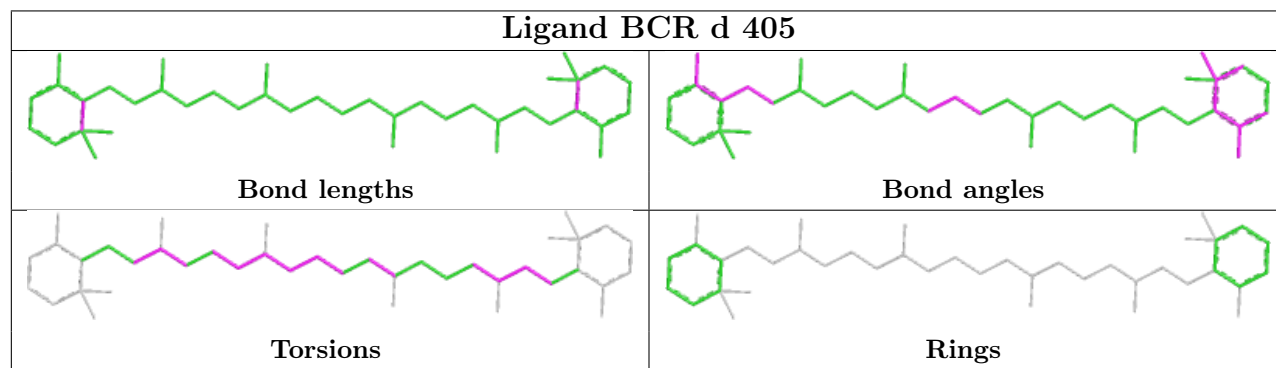
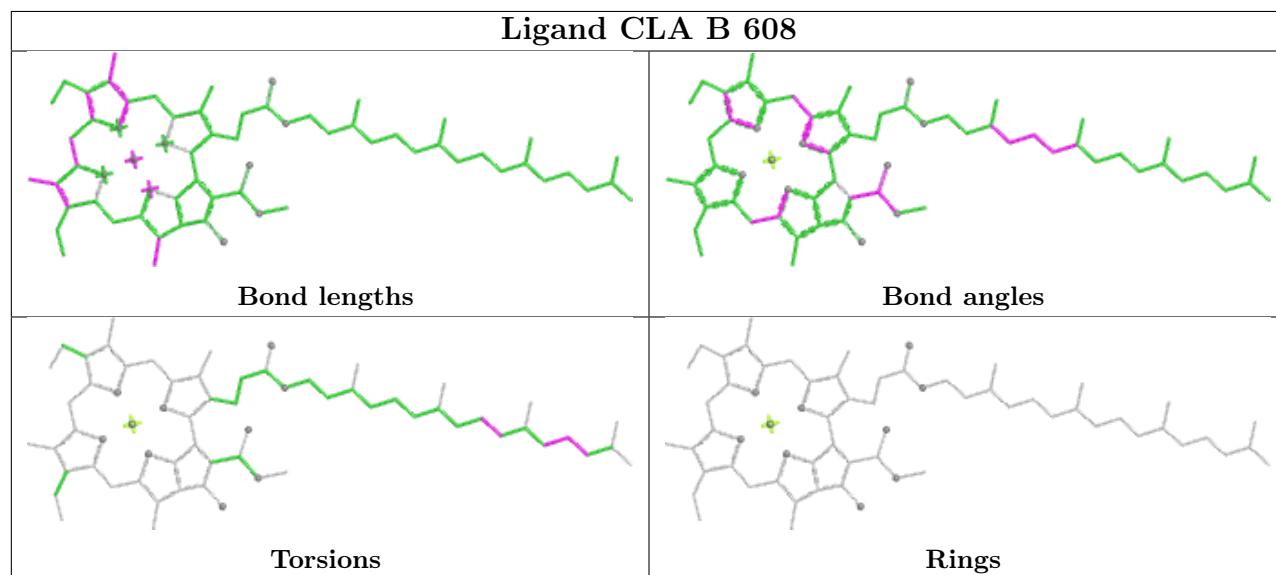
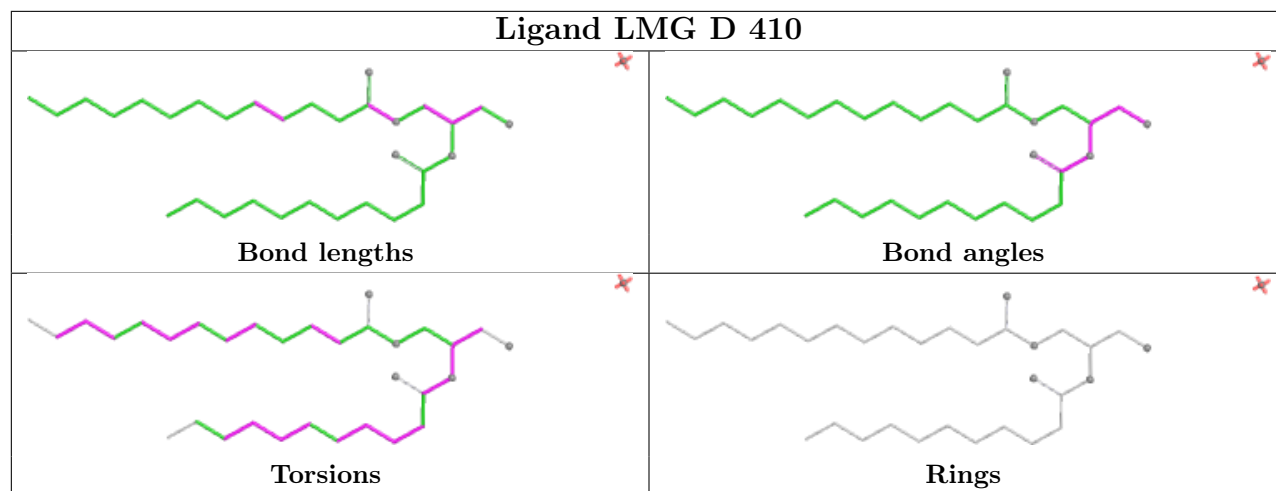


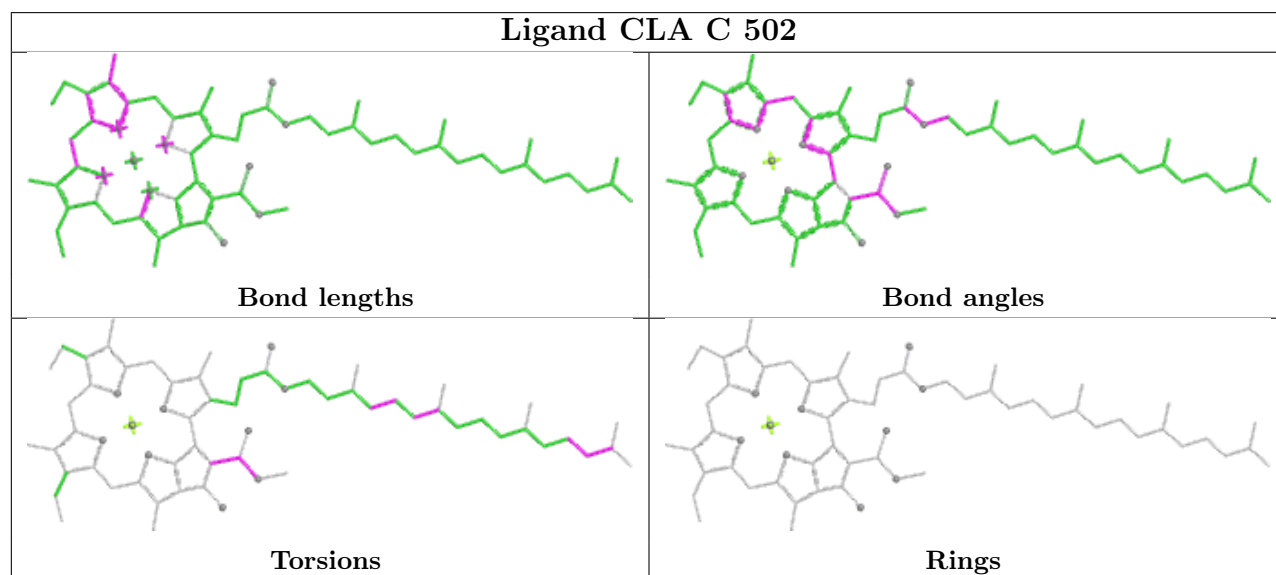
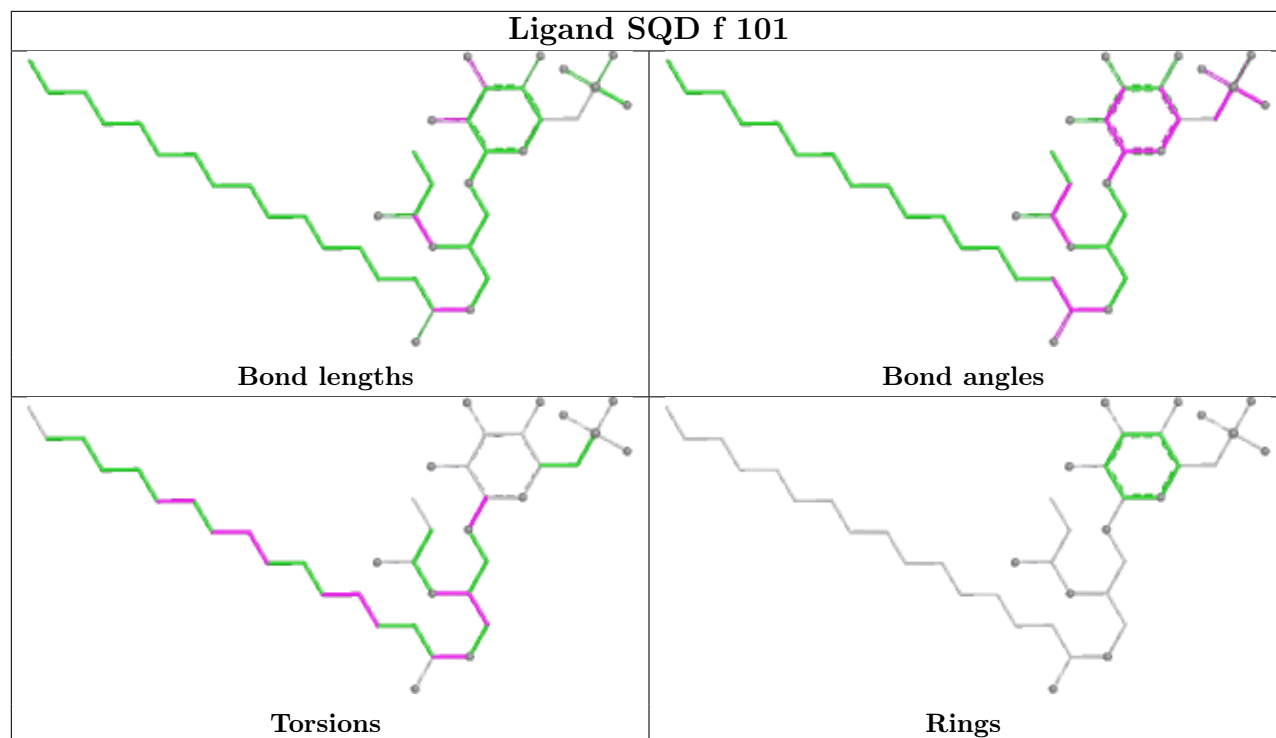
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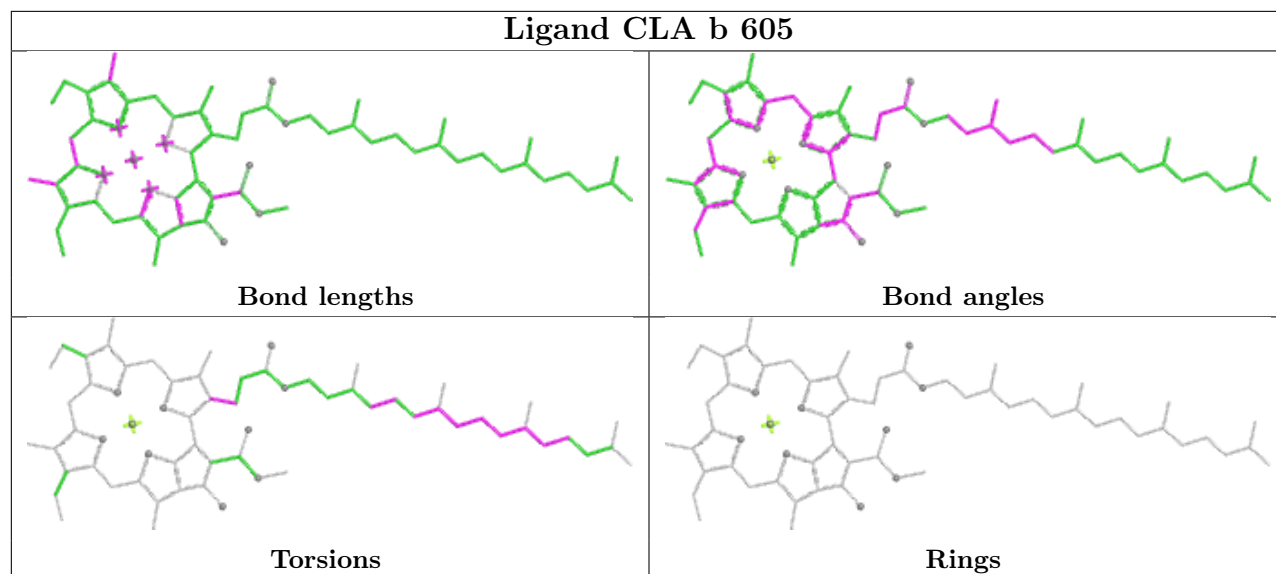
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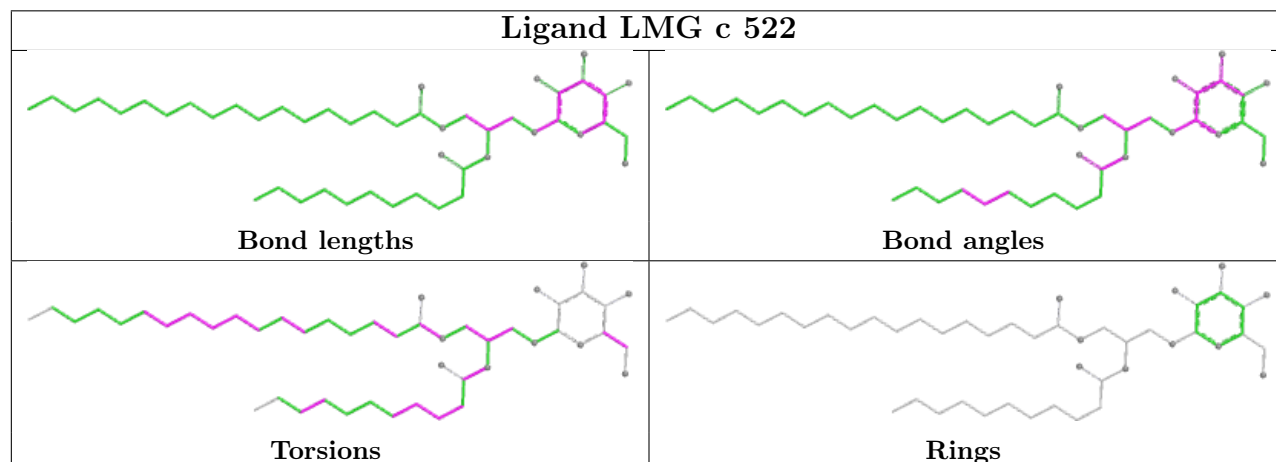




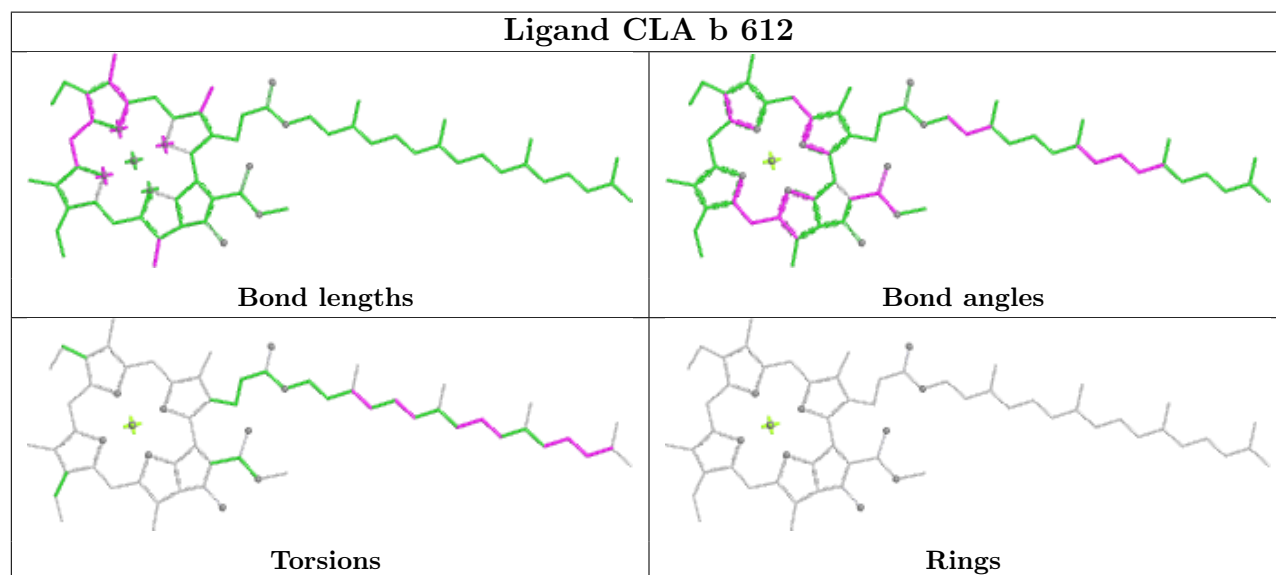
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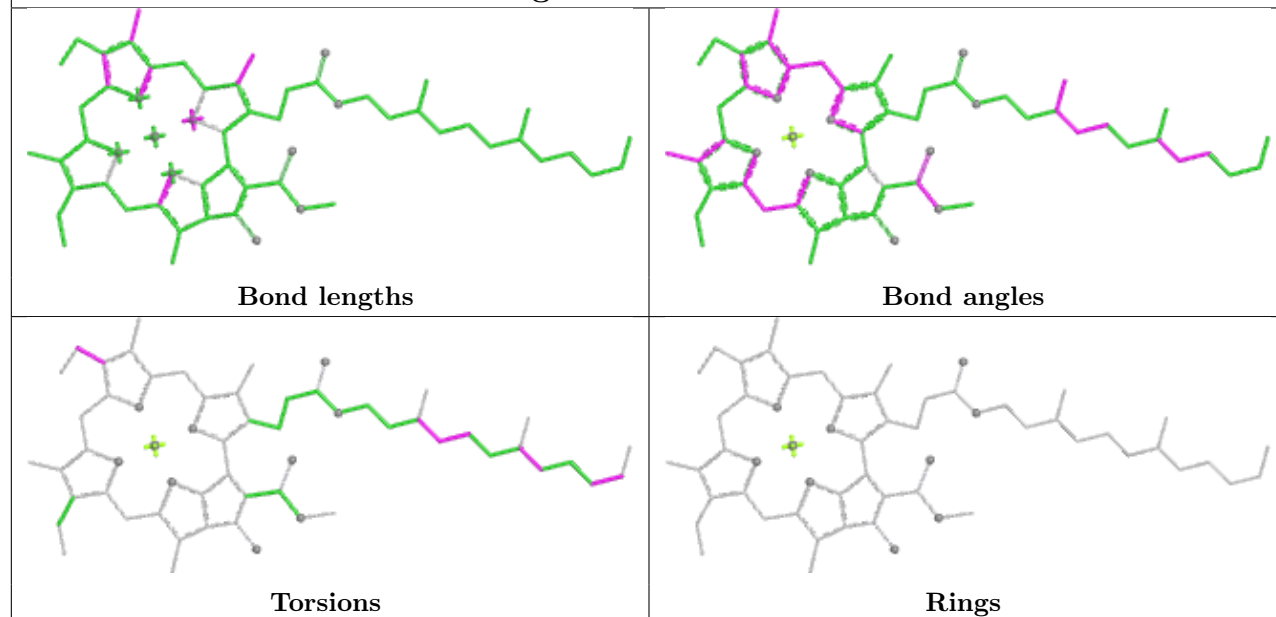
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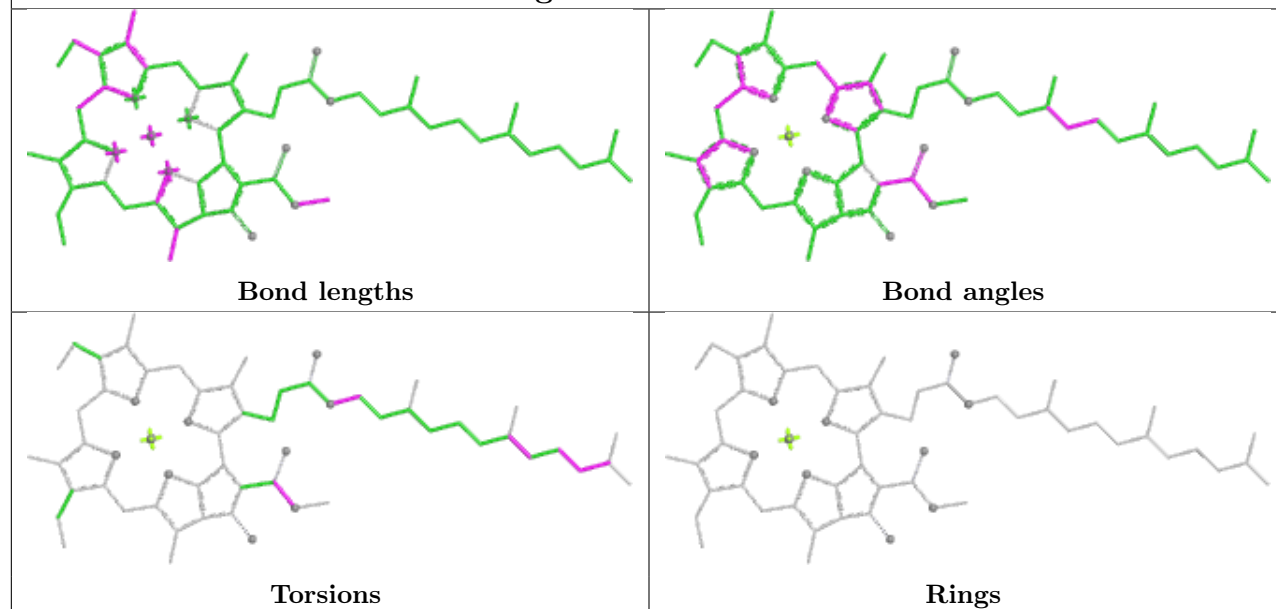
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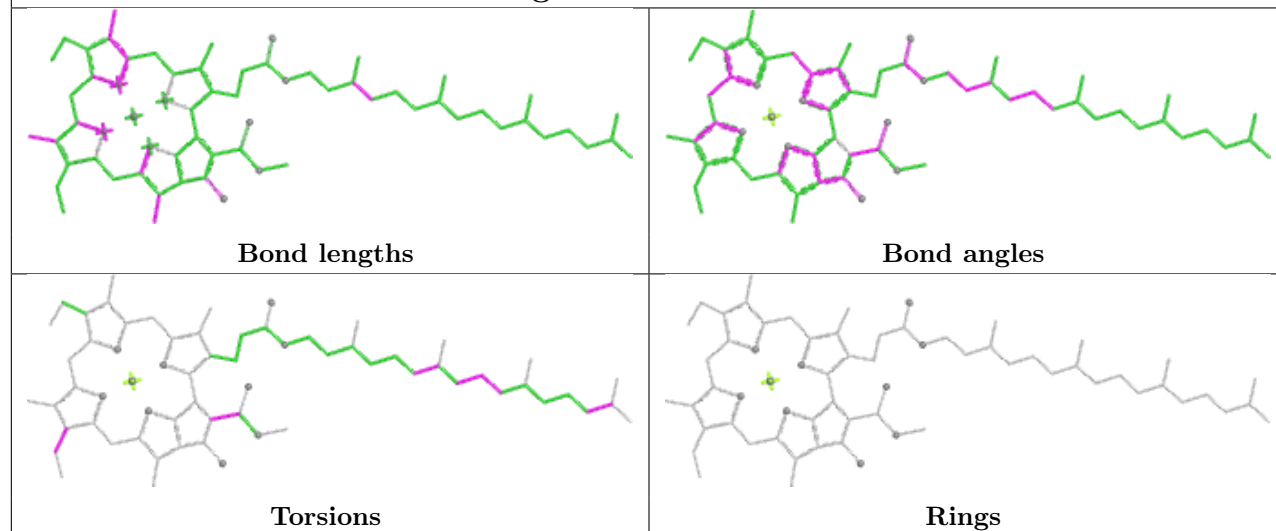
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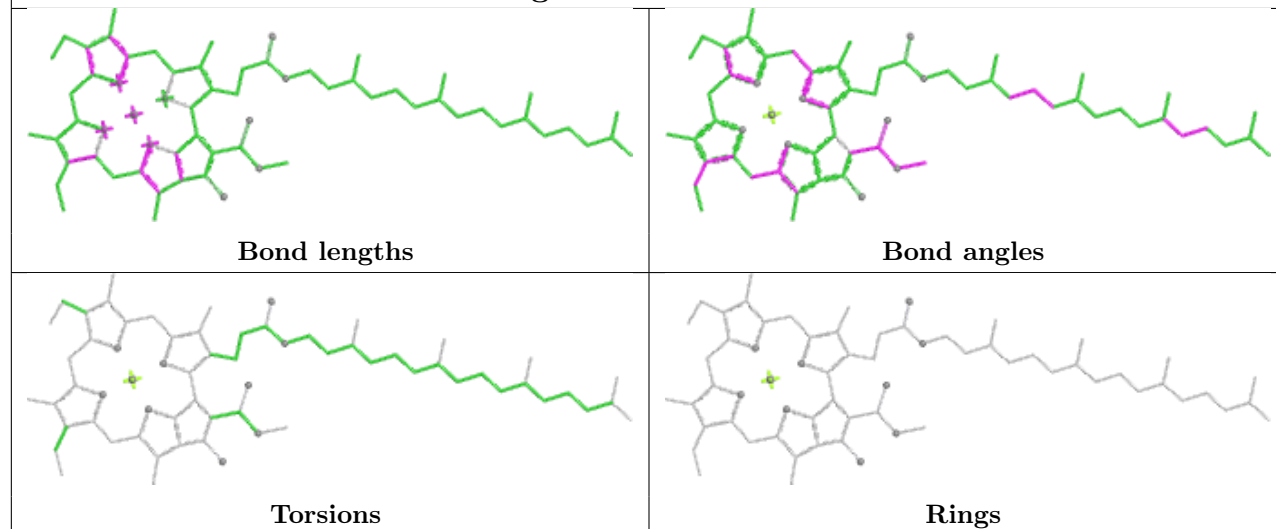
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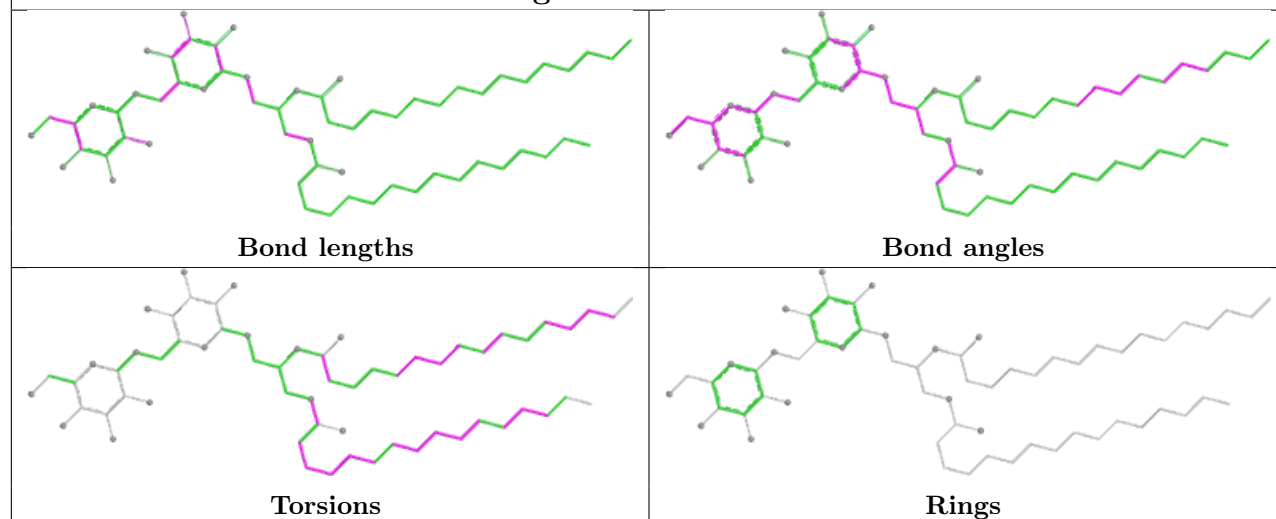
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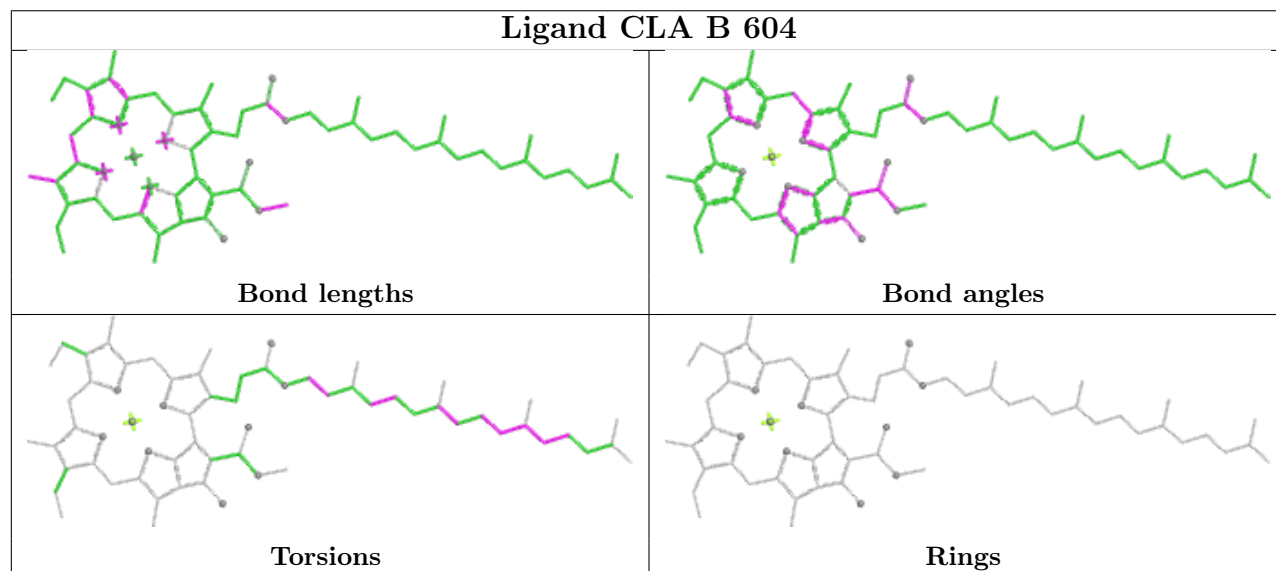
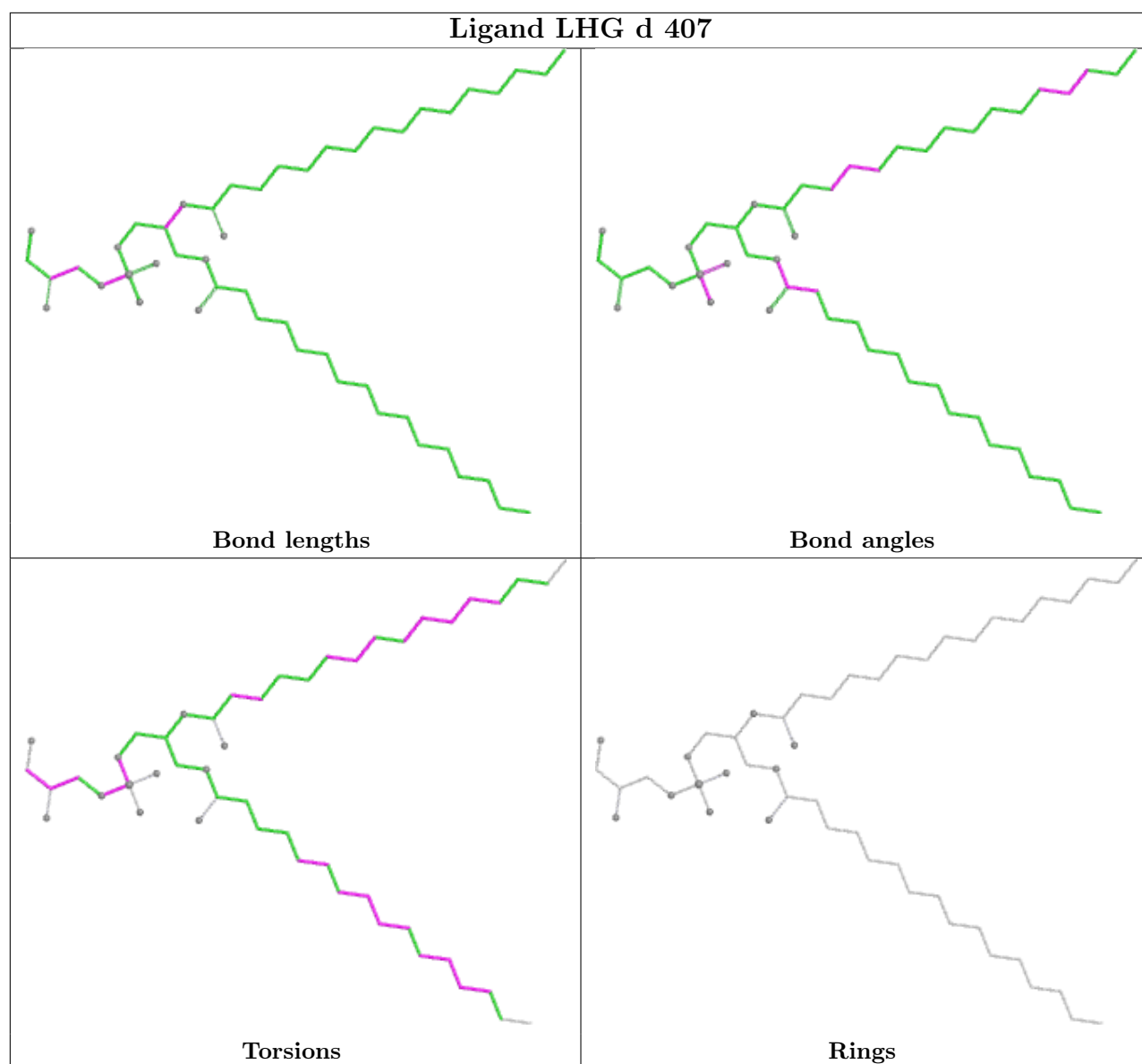


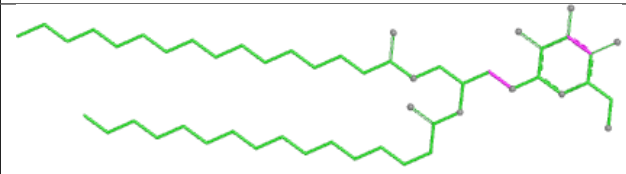
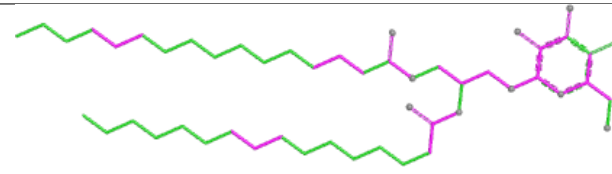
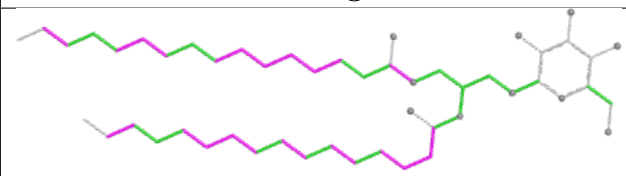
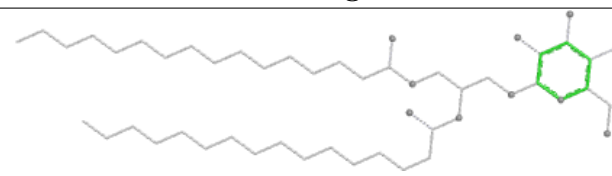
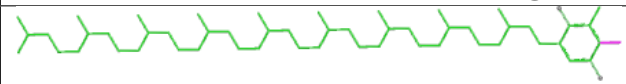
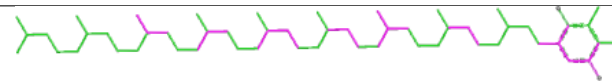
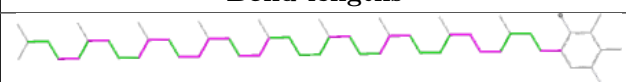
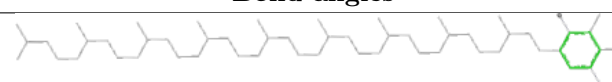
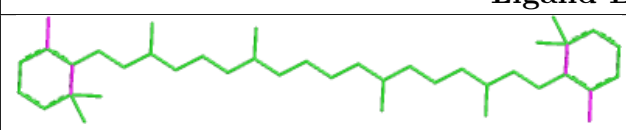
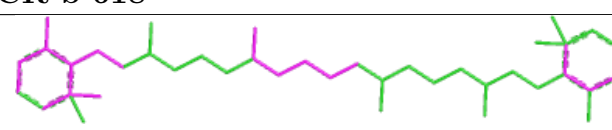
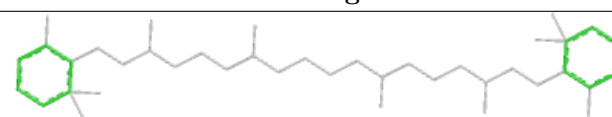
Ligand CLA D 402

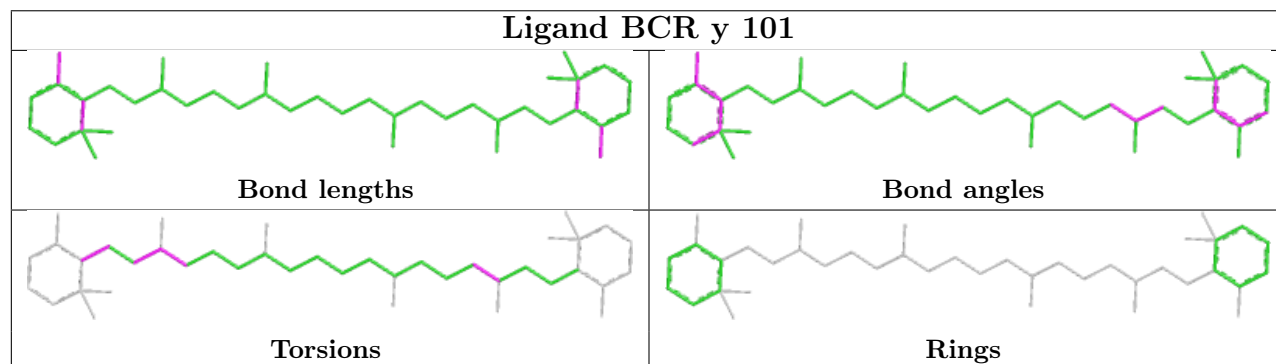
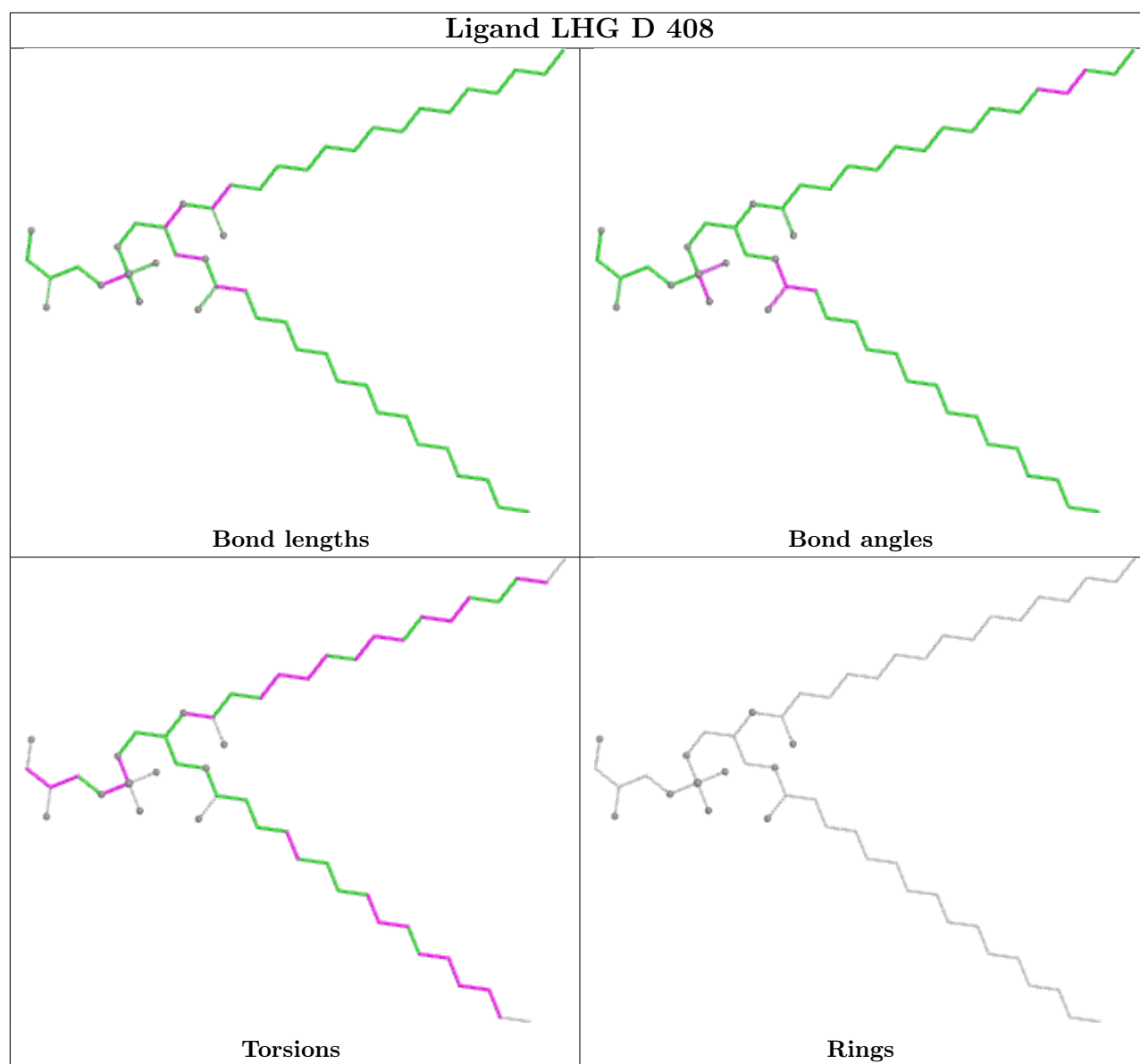


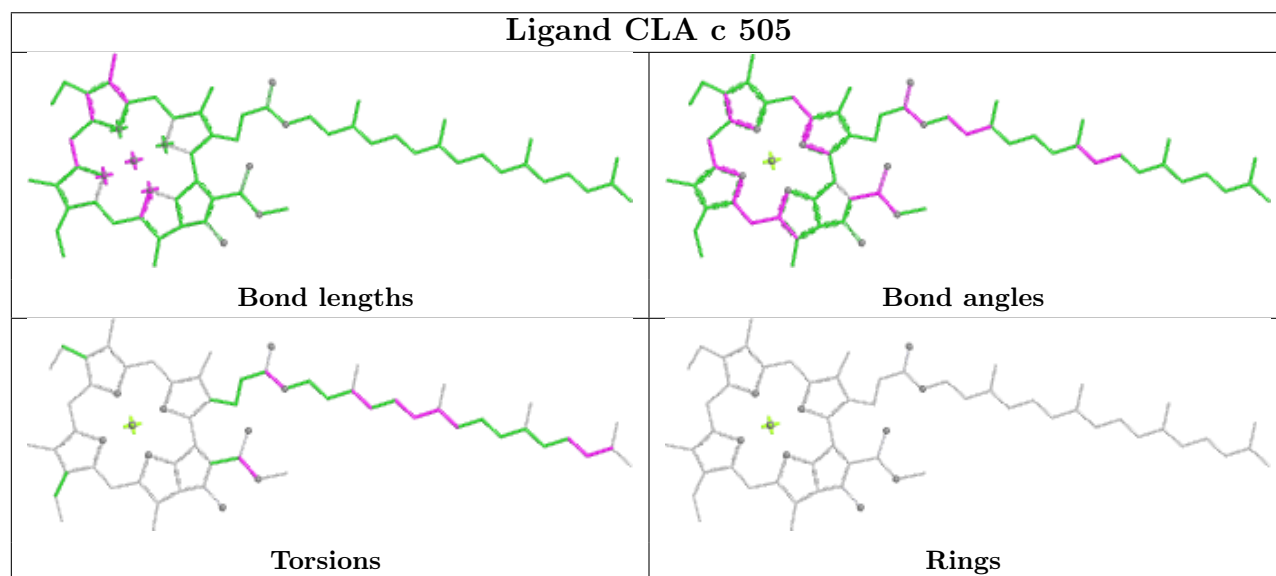
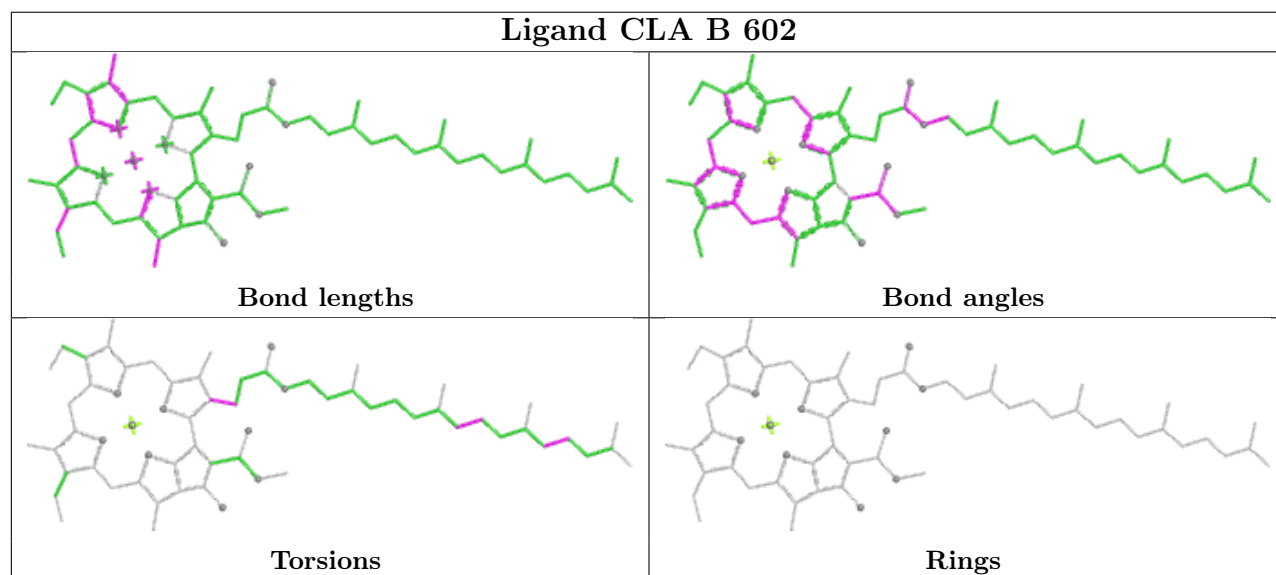
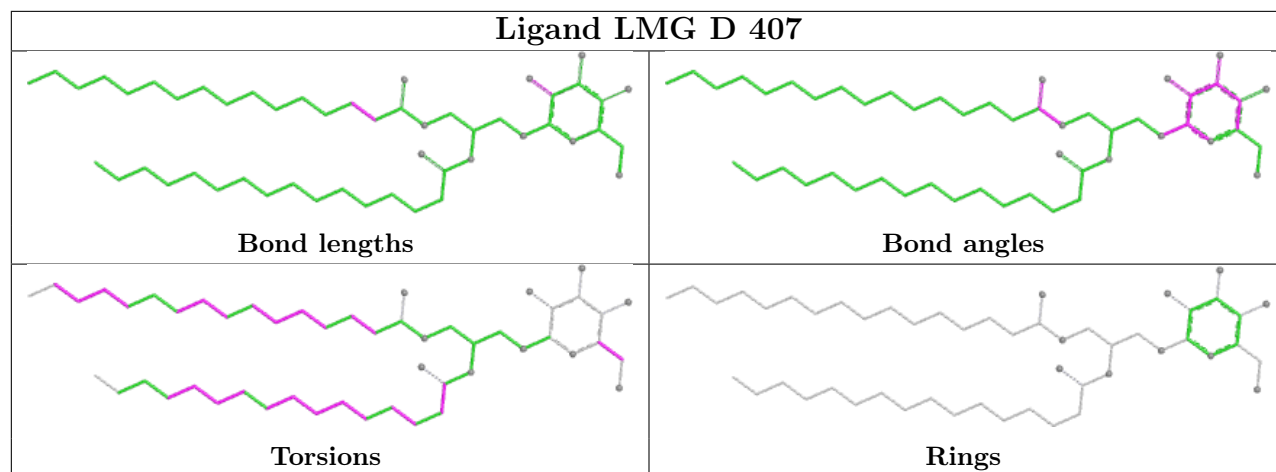
Ligand DGD c 518

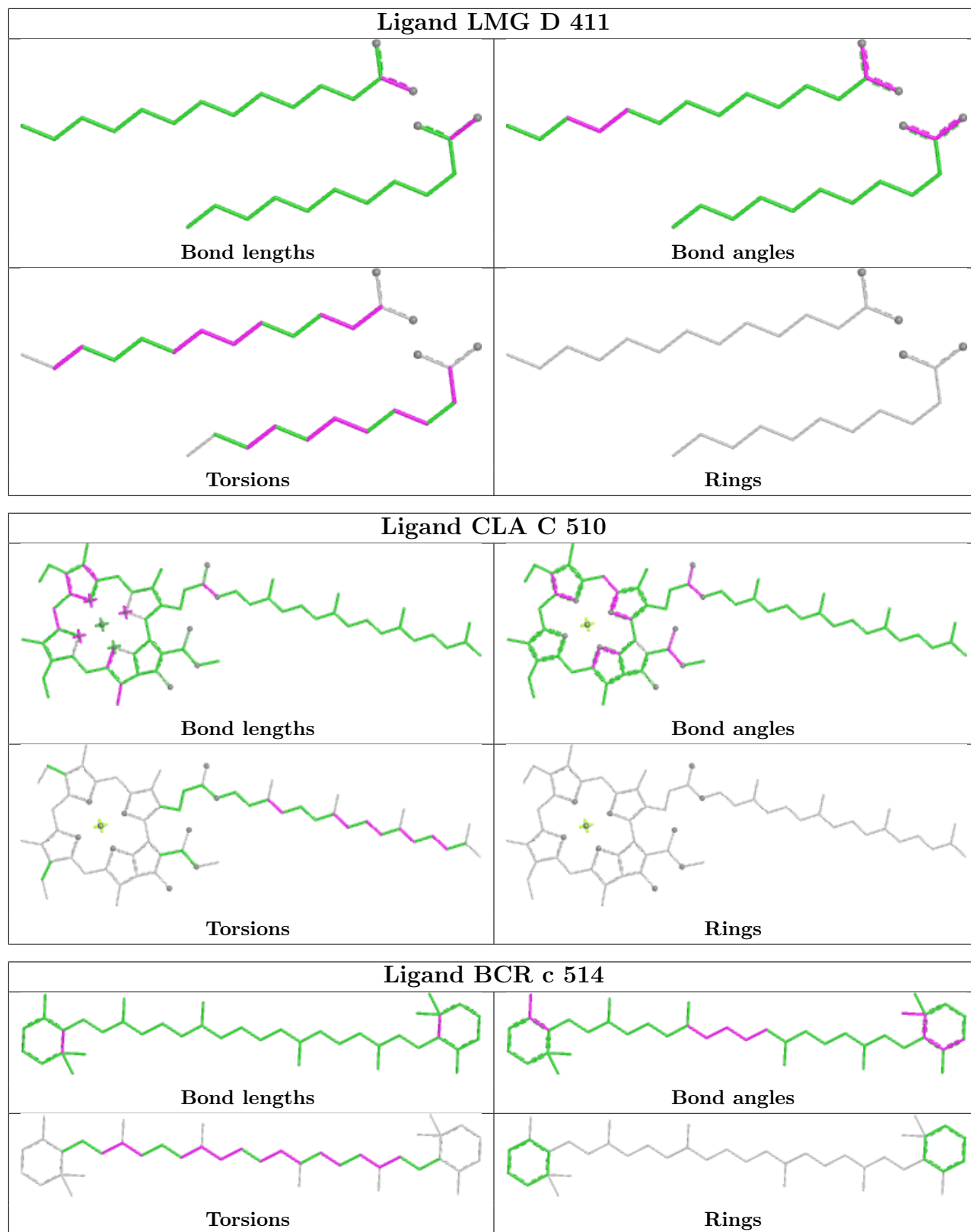




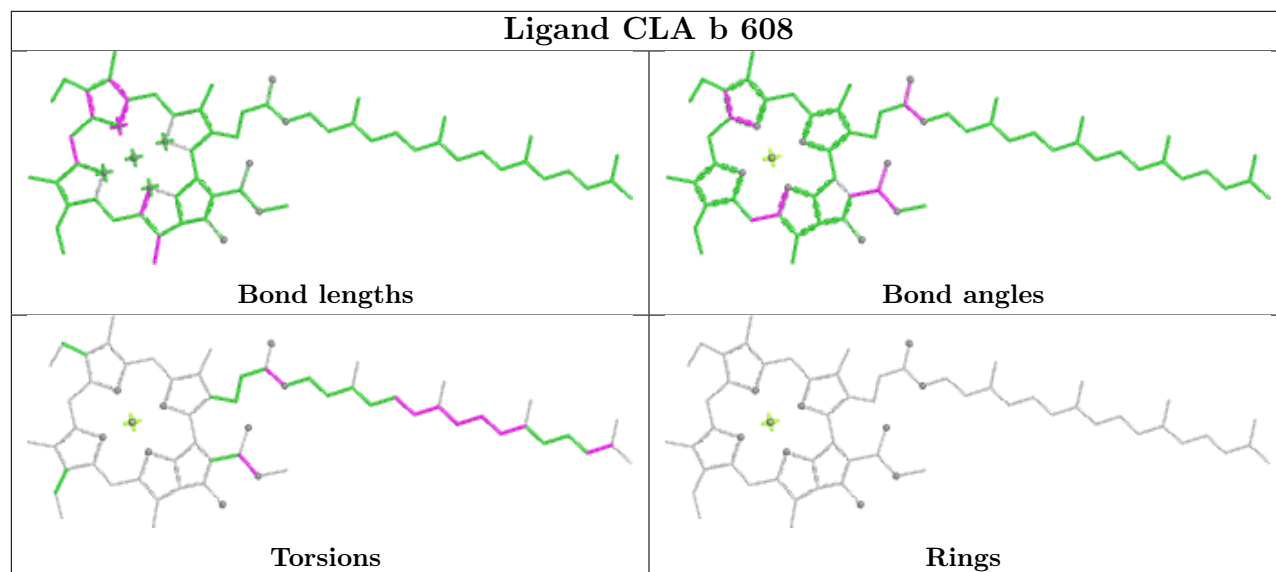
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings



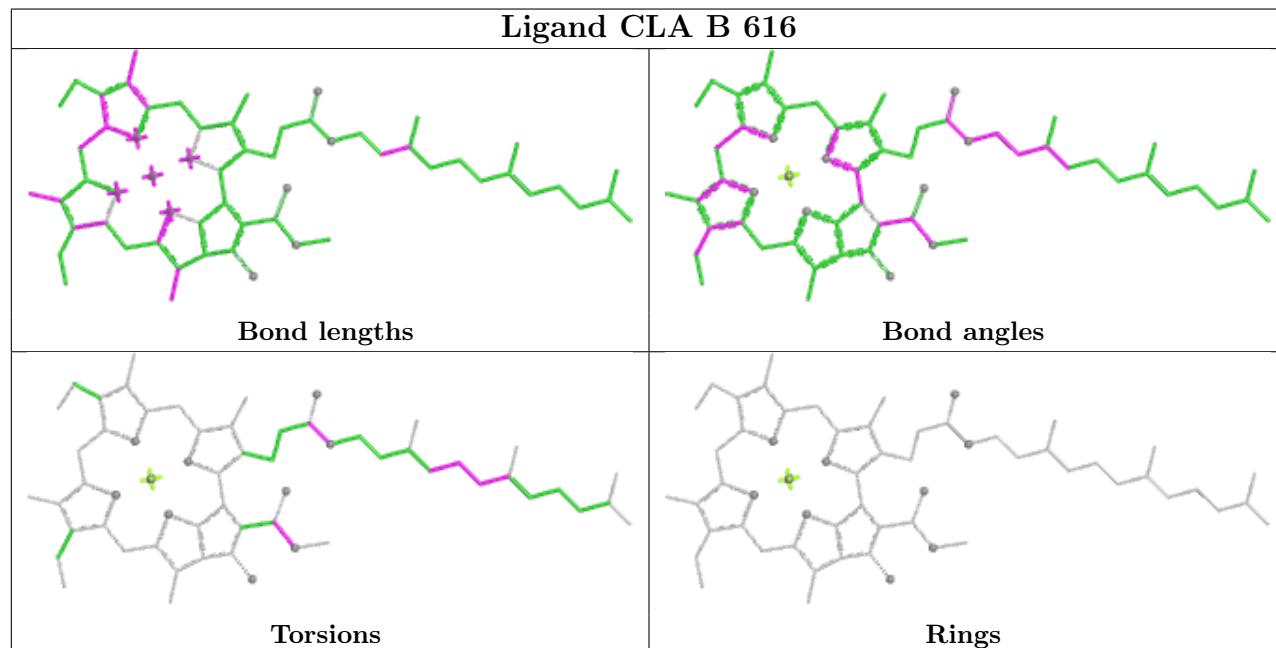




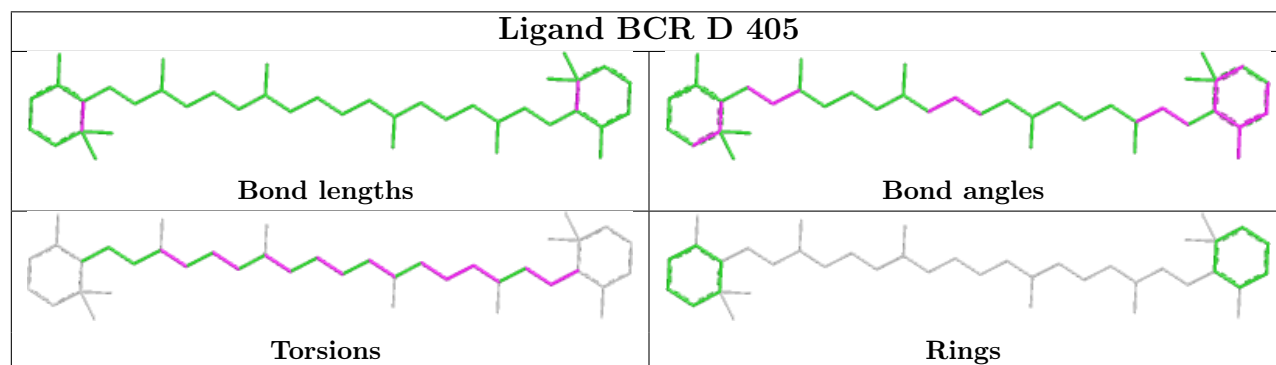
Ligand CLA b 608



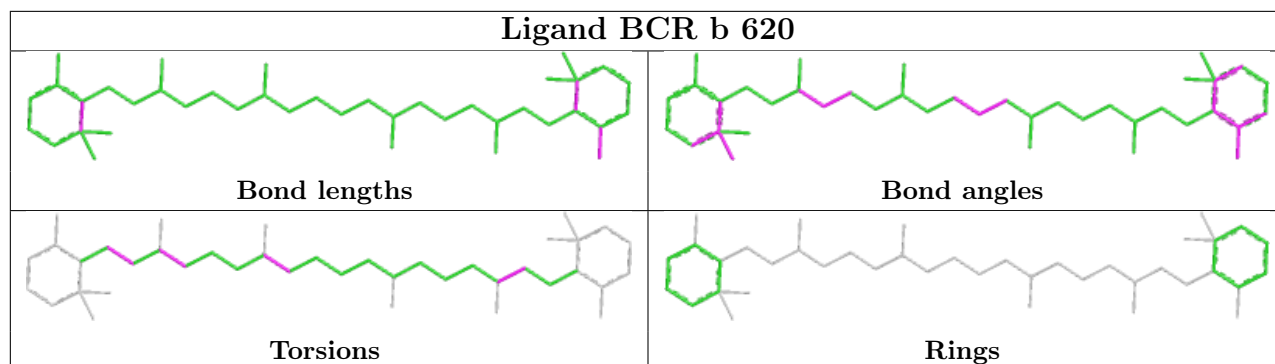
Ligand CLA B 616



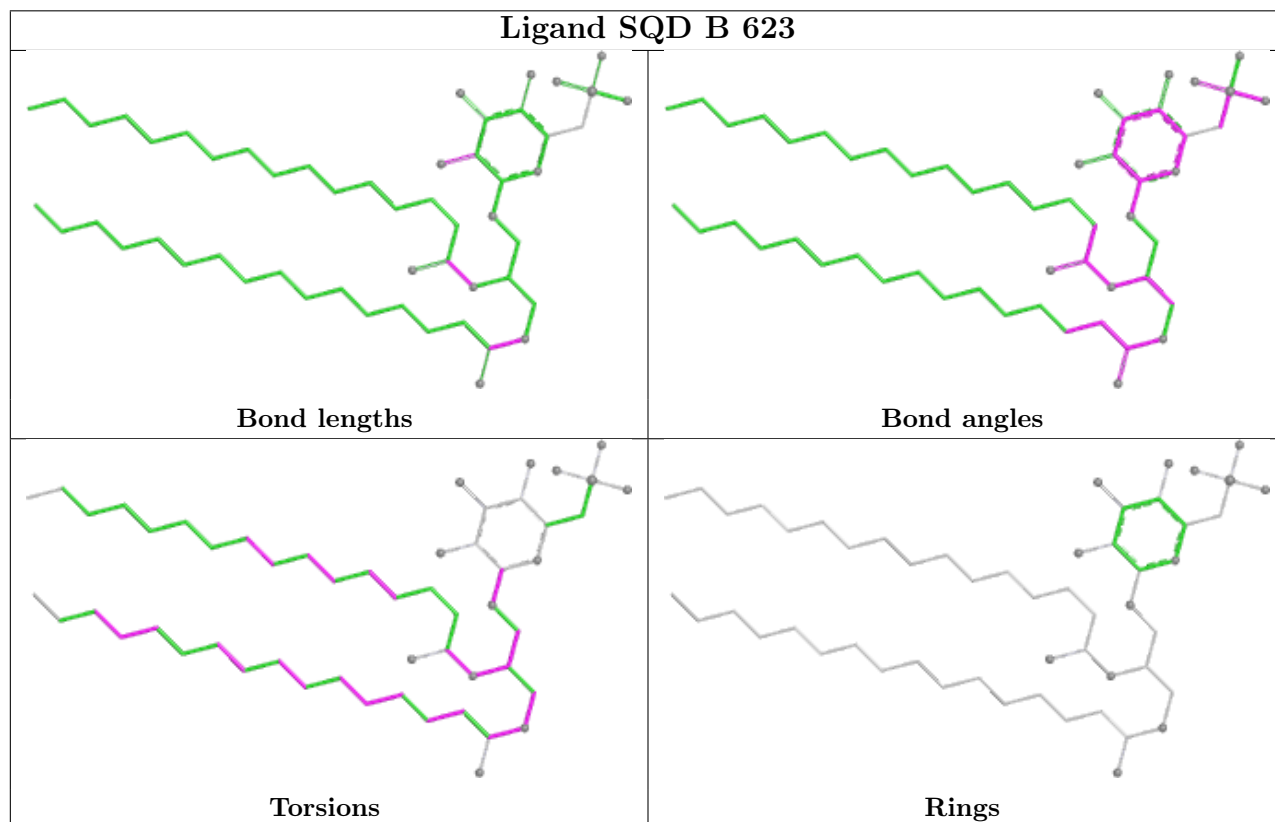
Ligand BCR D 405



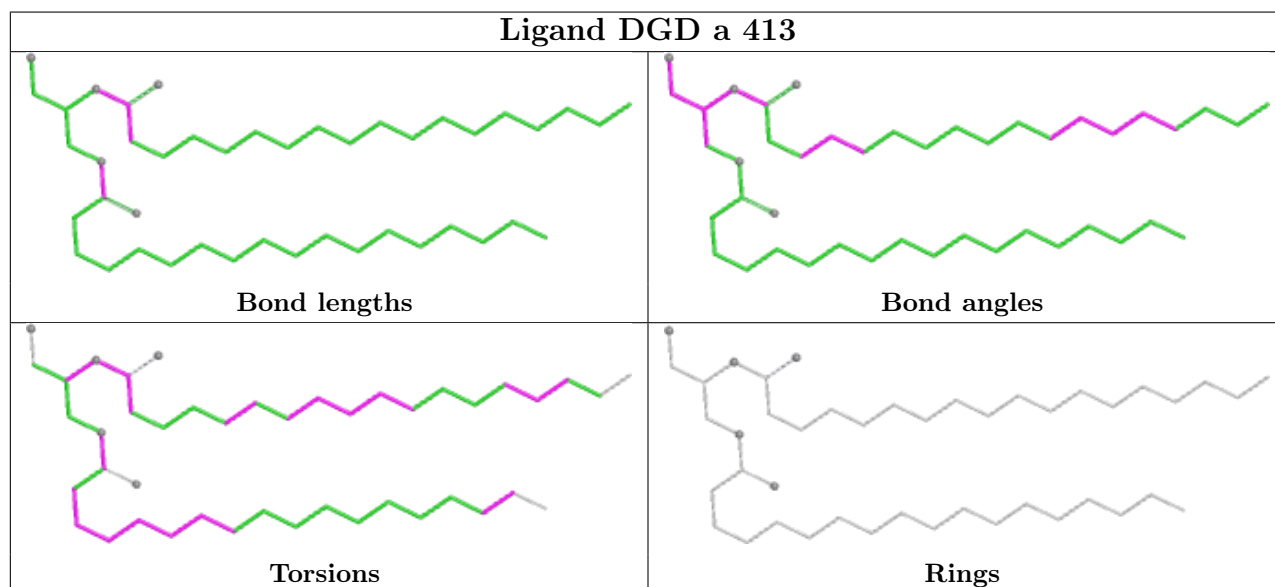
Ligand BCR b 620



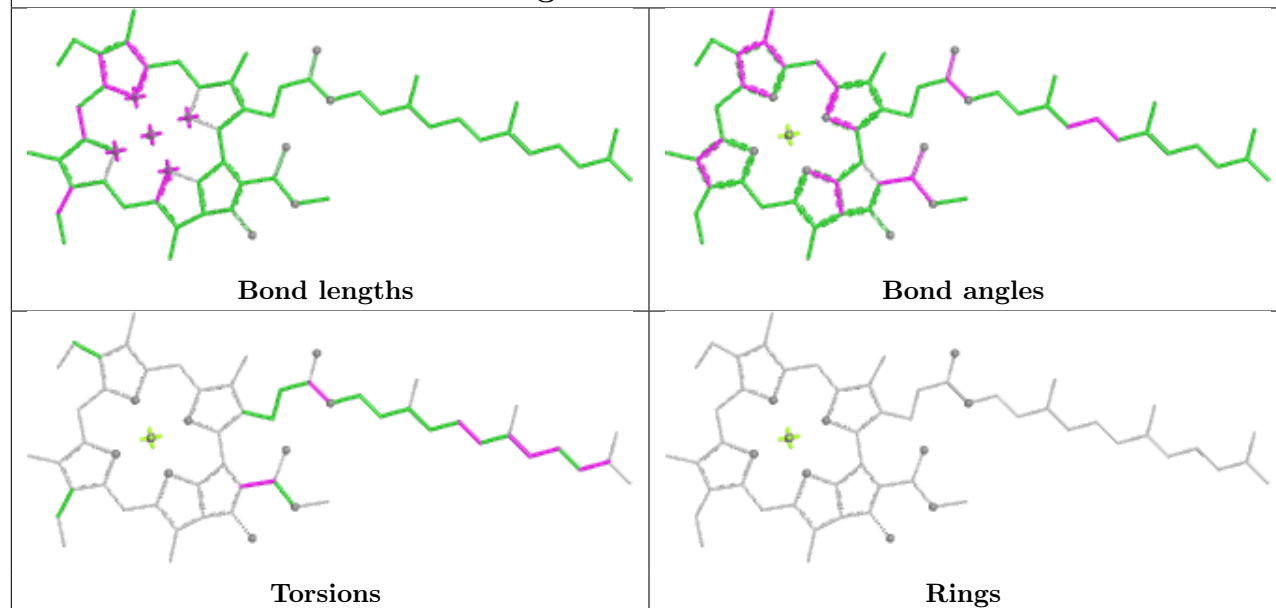
Ligand SQD B 623



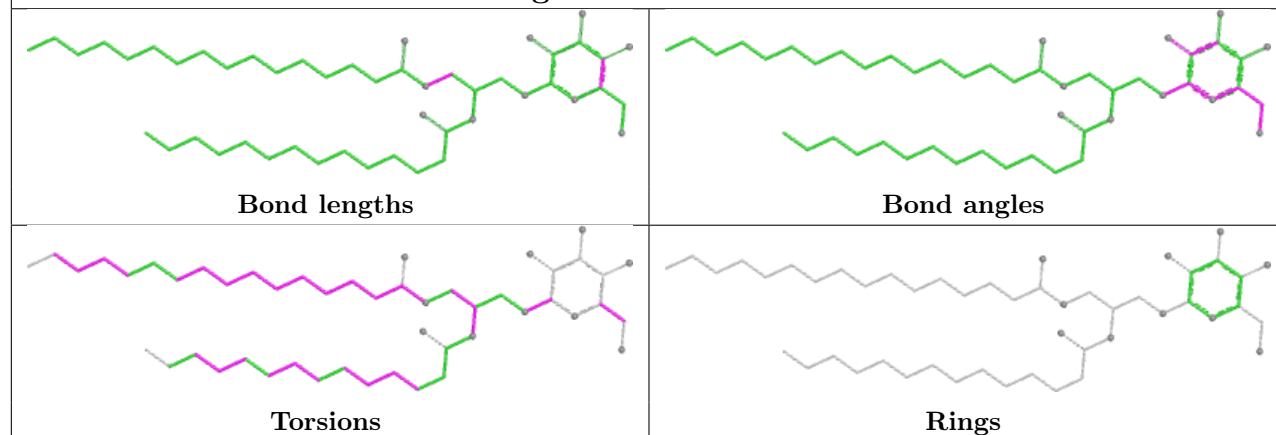
Ligand DGD a 413



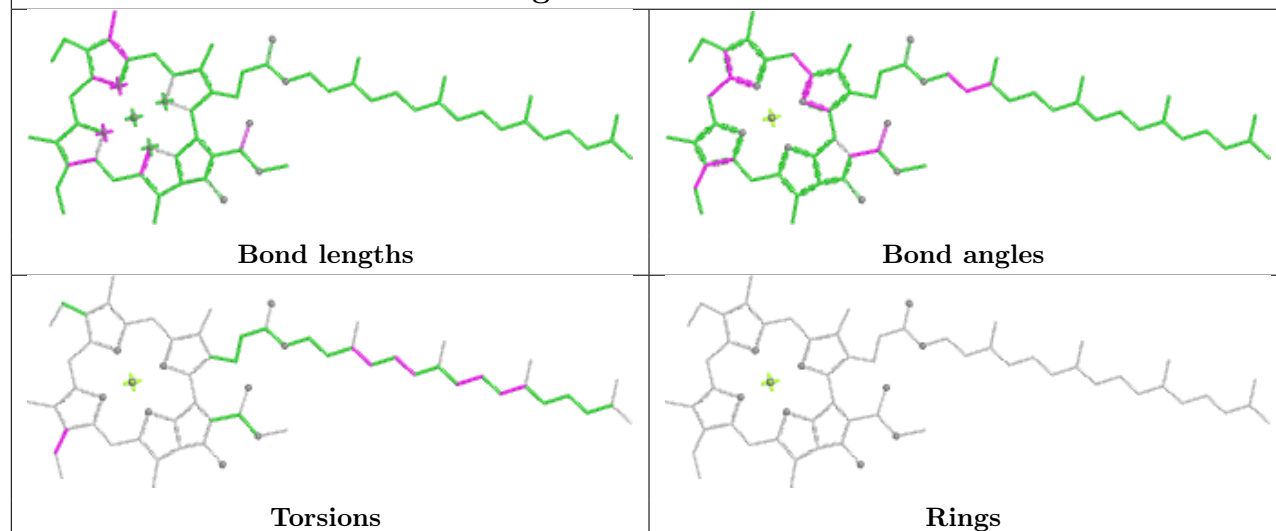
Ligand CLA c 504



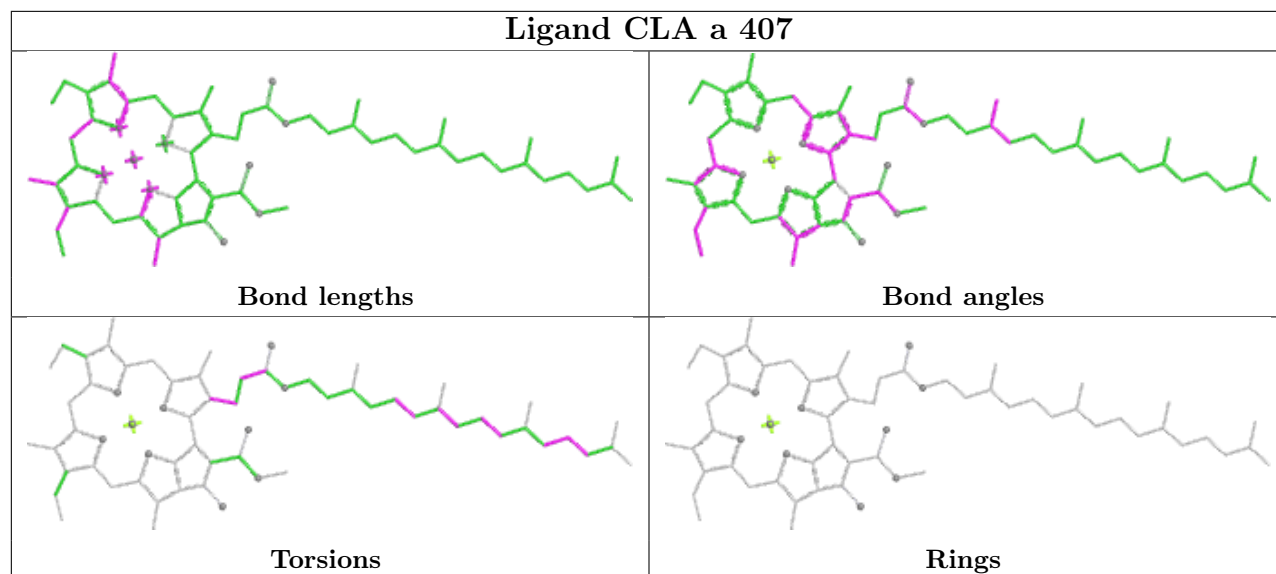
Ligand LMG a 414



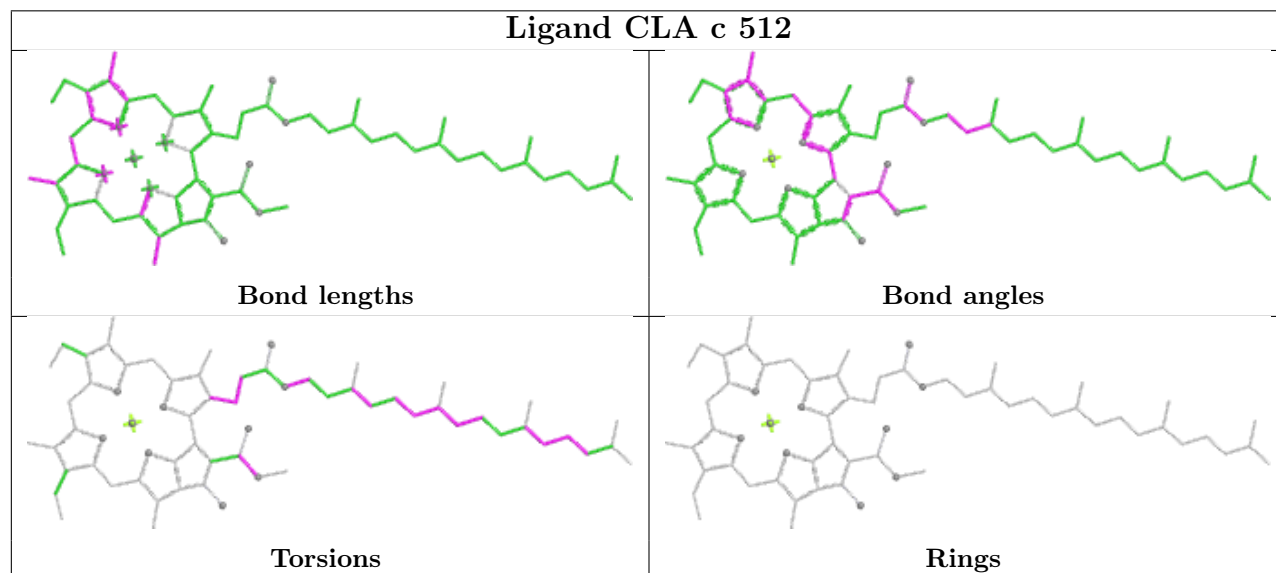
Ligand CLA C 505



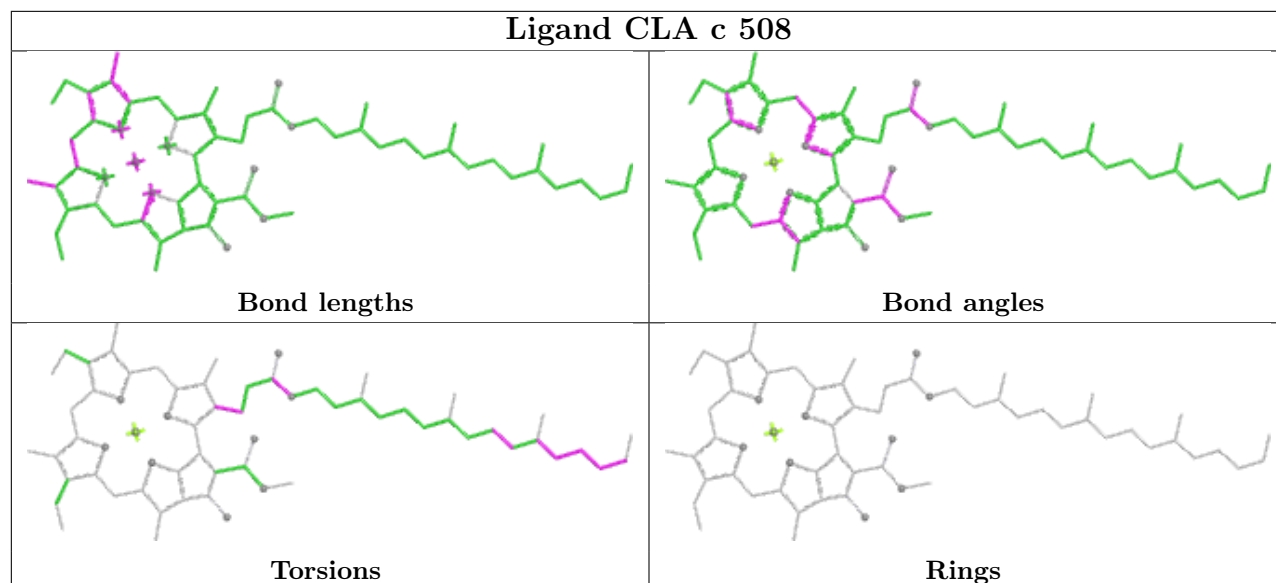
Ligand CLA a 407



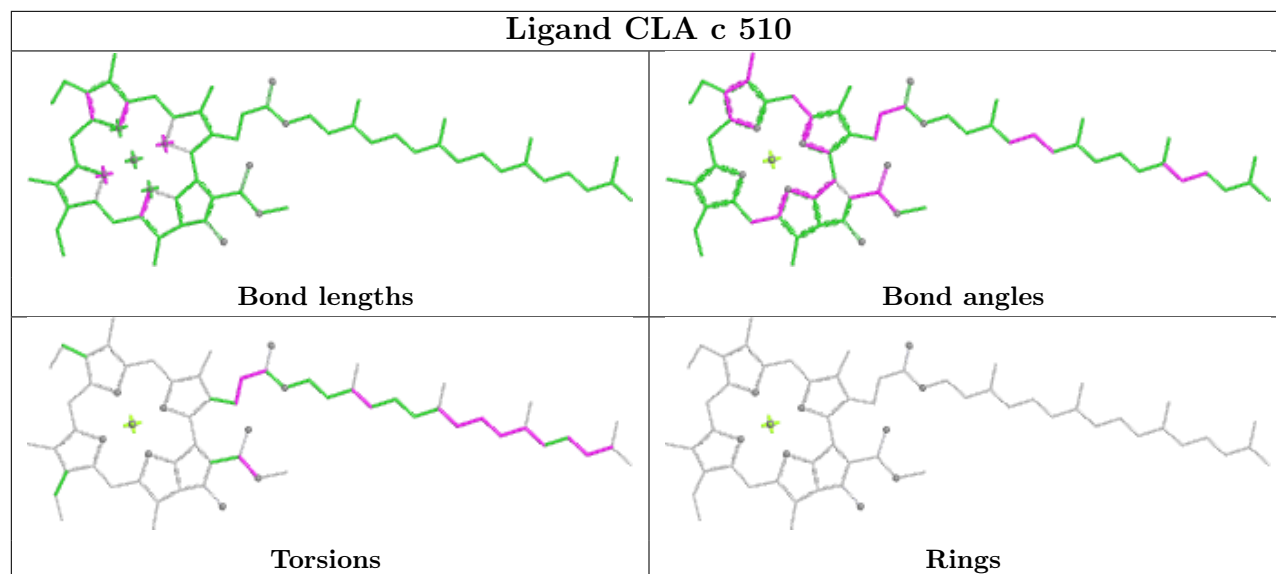
Ligand CLA c 512



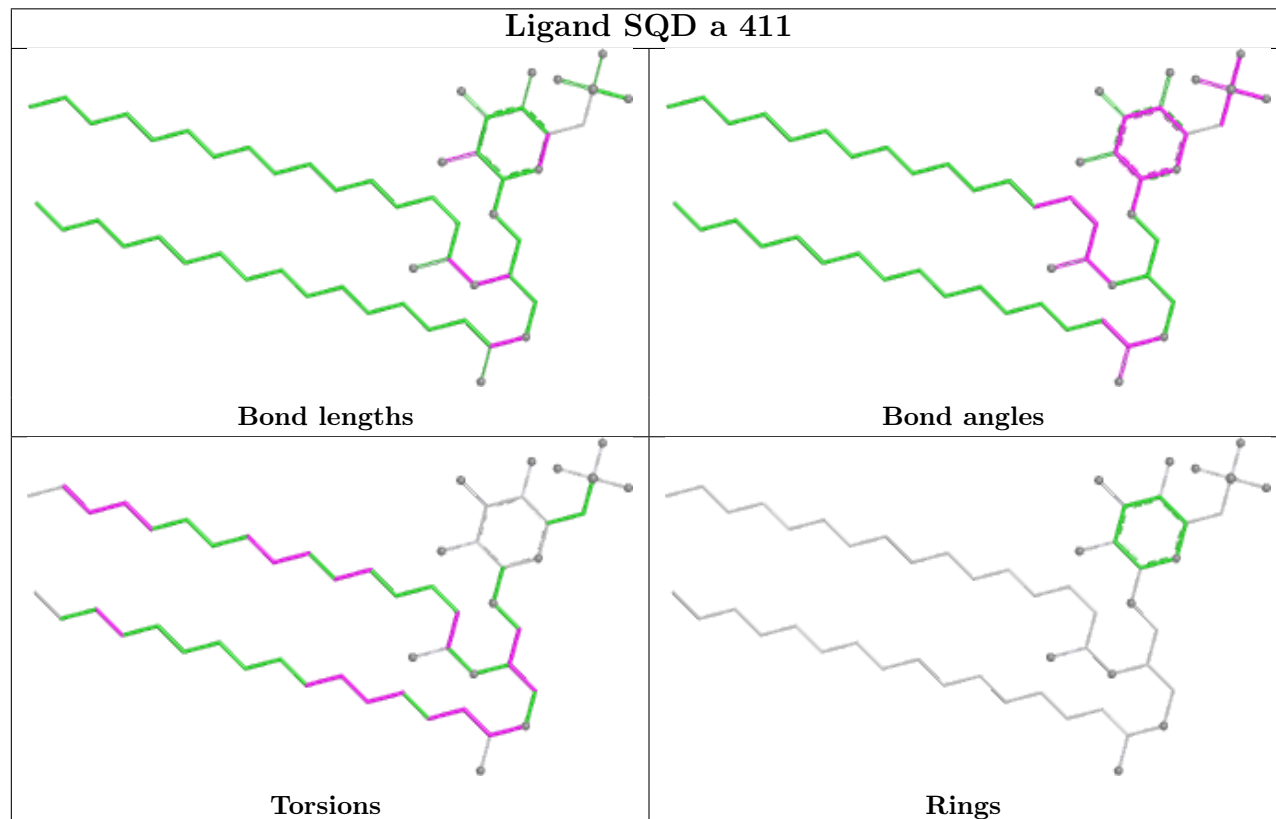
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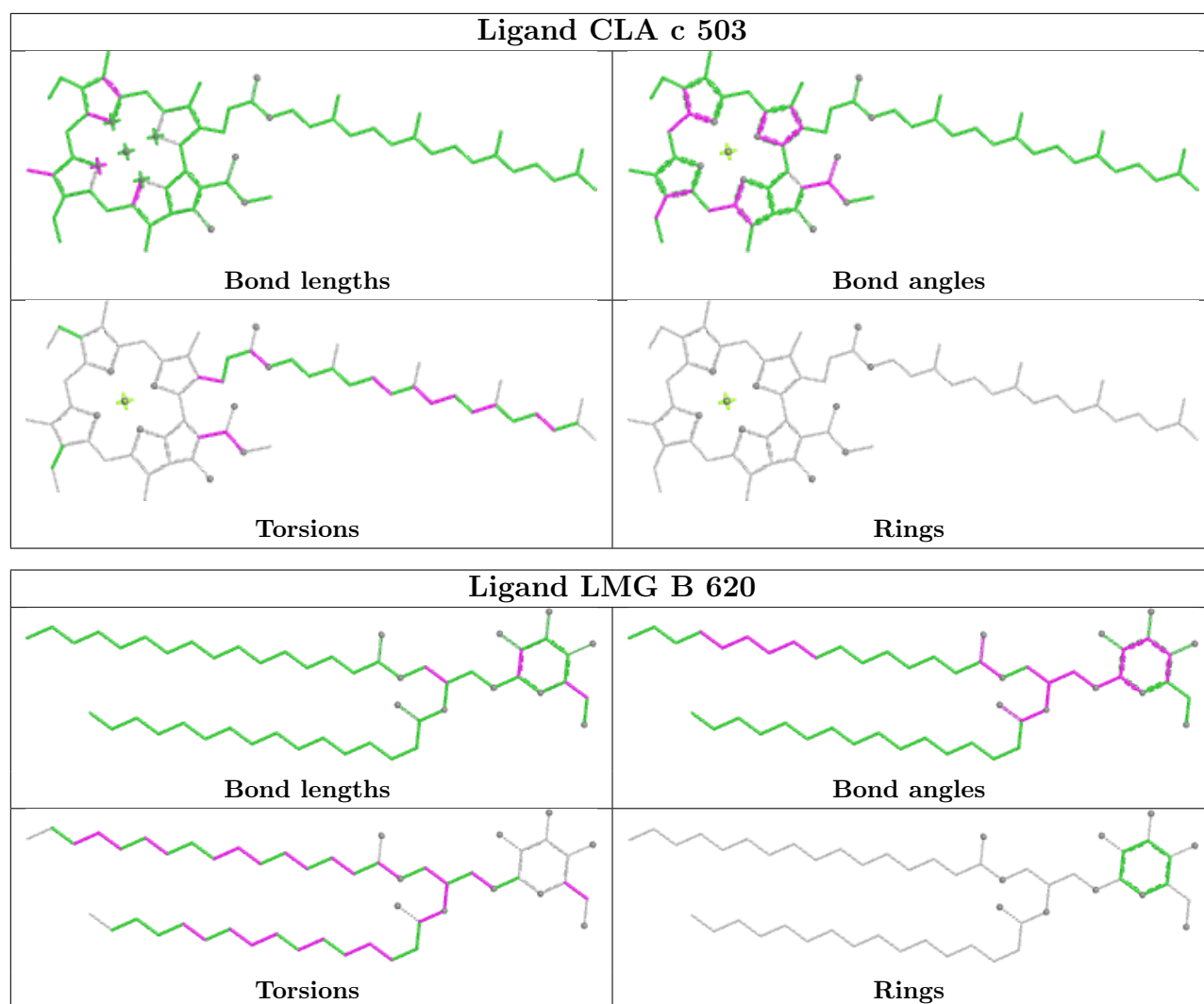


Ligand CLA c 510

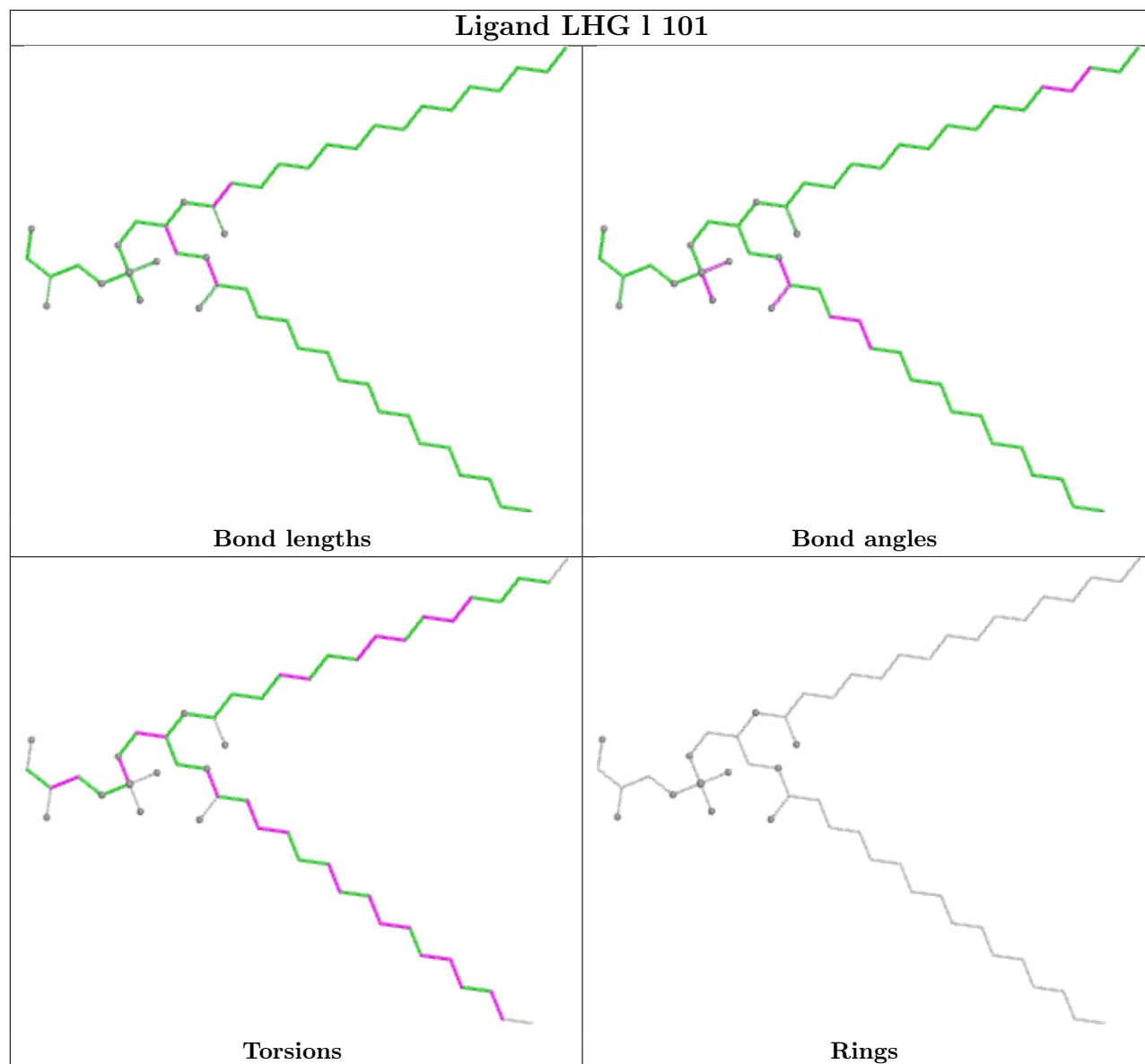


Ligand SQD a 411

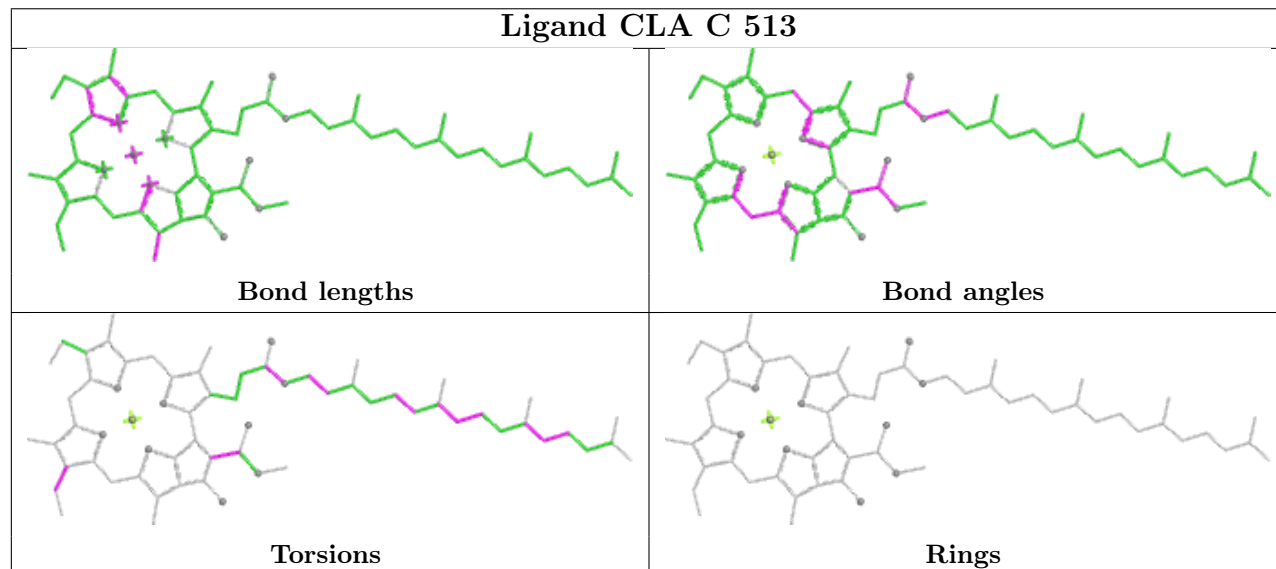


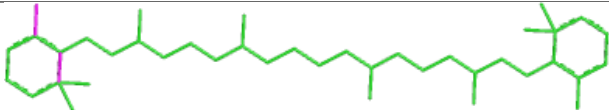
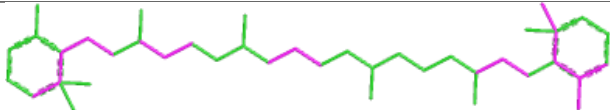
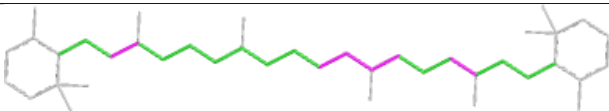
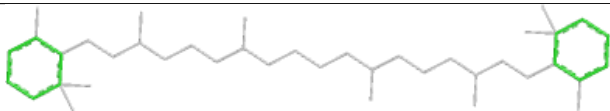


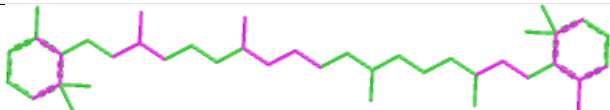
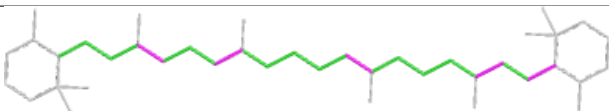
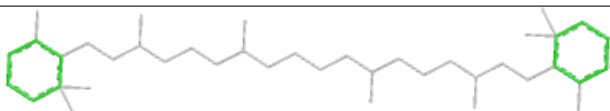
Ligand LHG 1 101

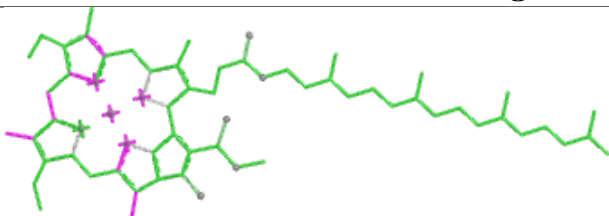
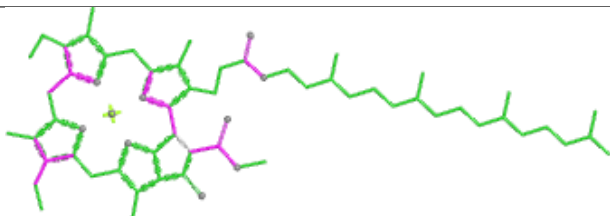
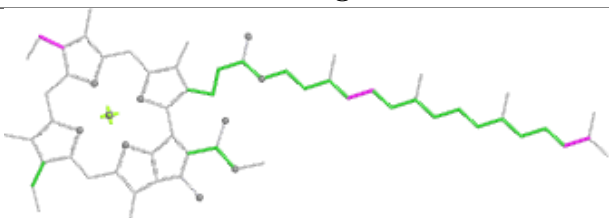
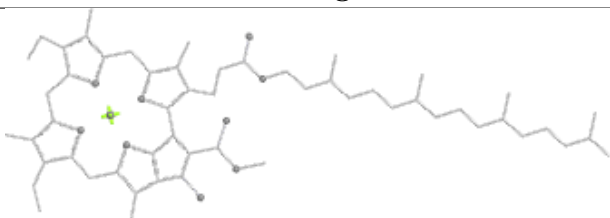


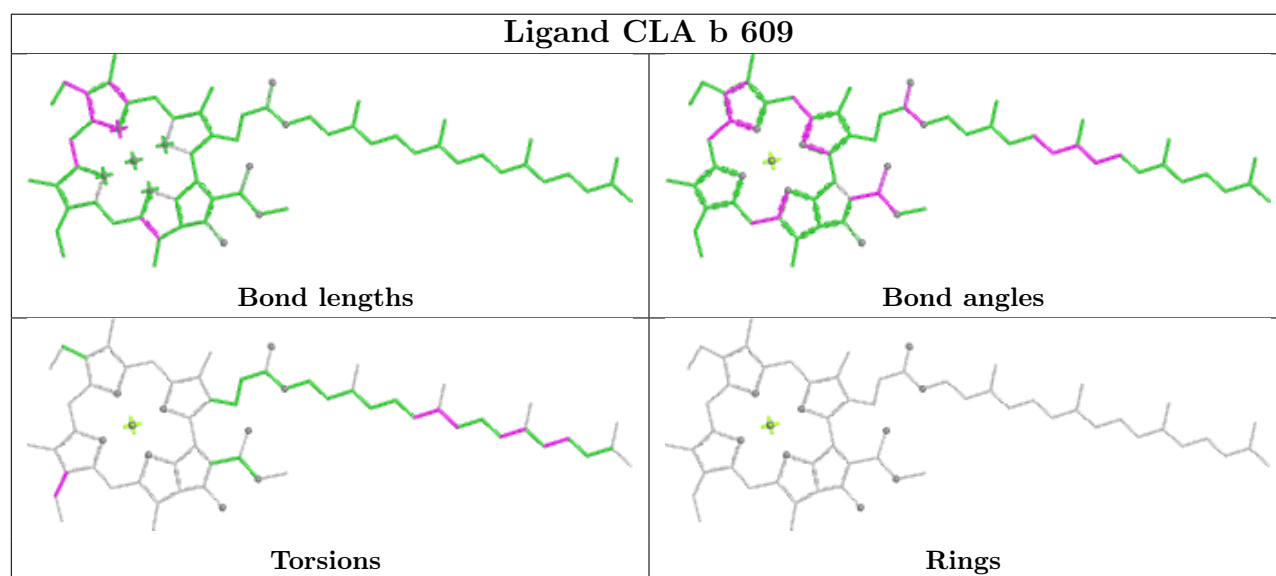
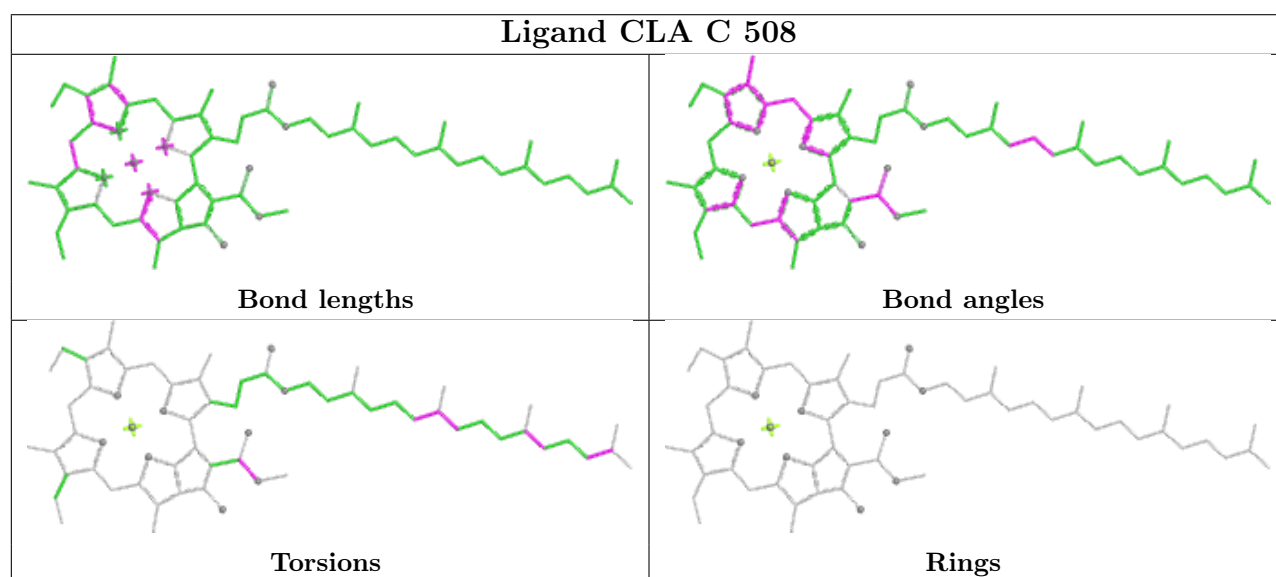
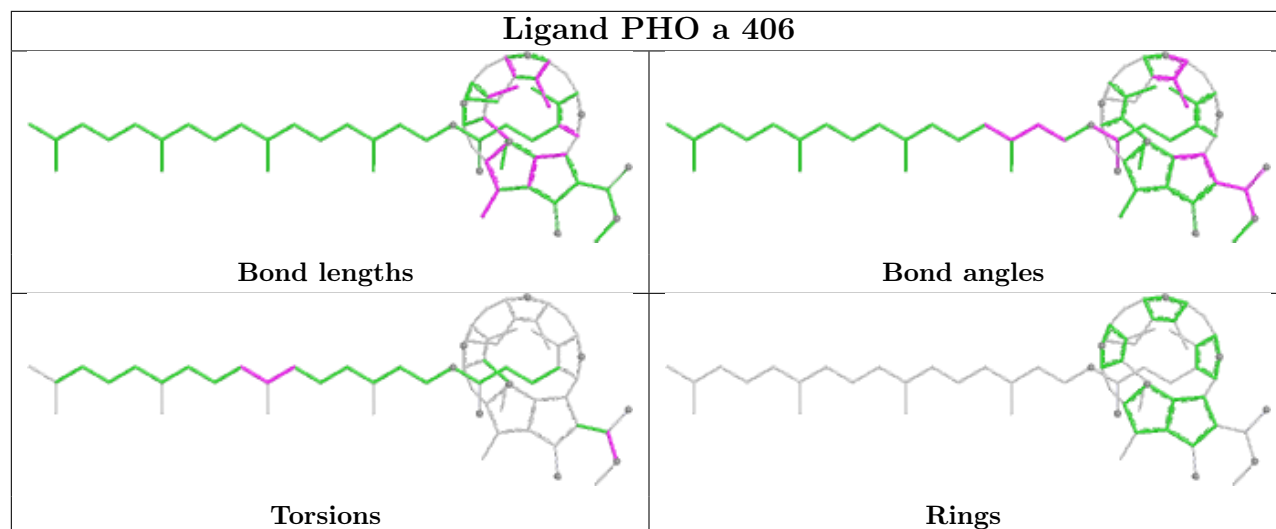
Ligand CLA C 513

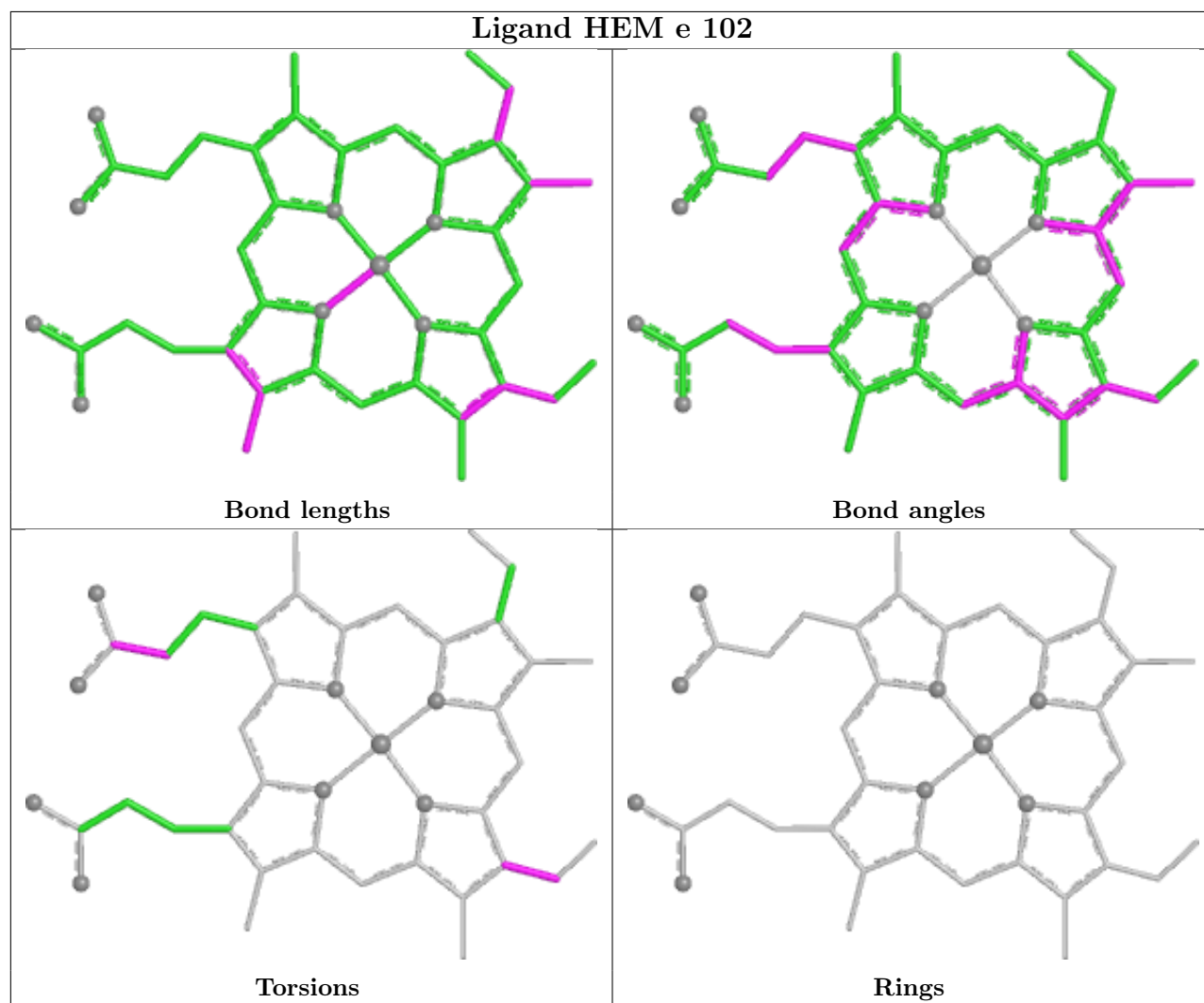
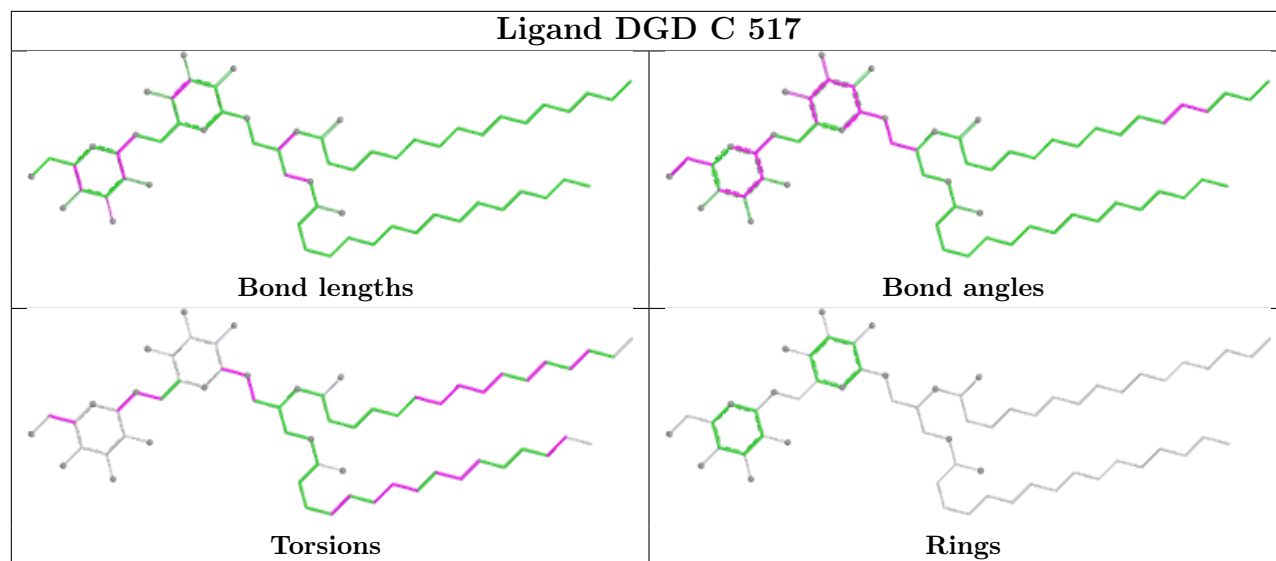


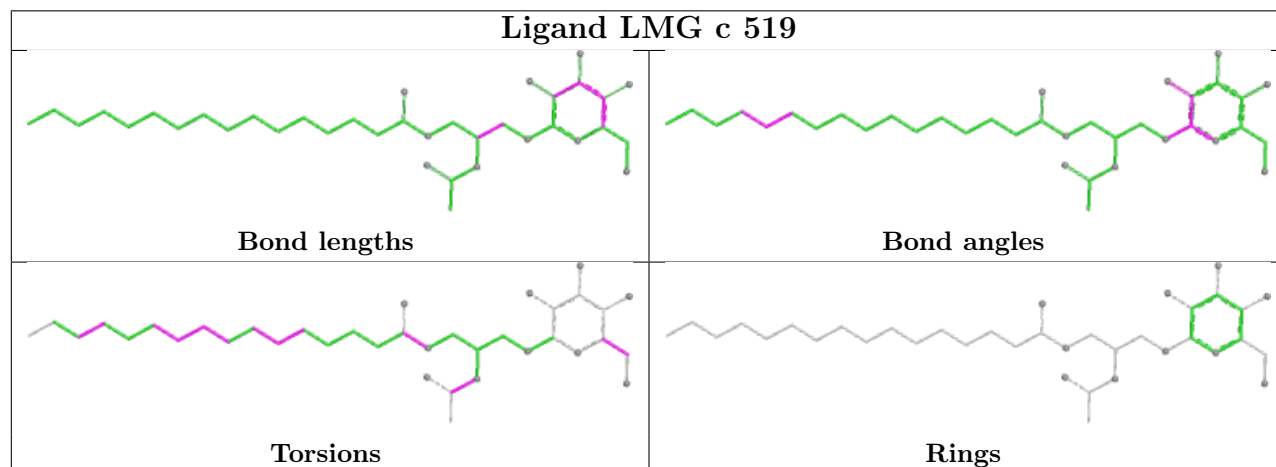
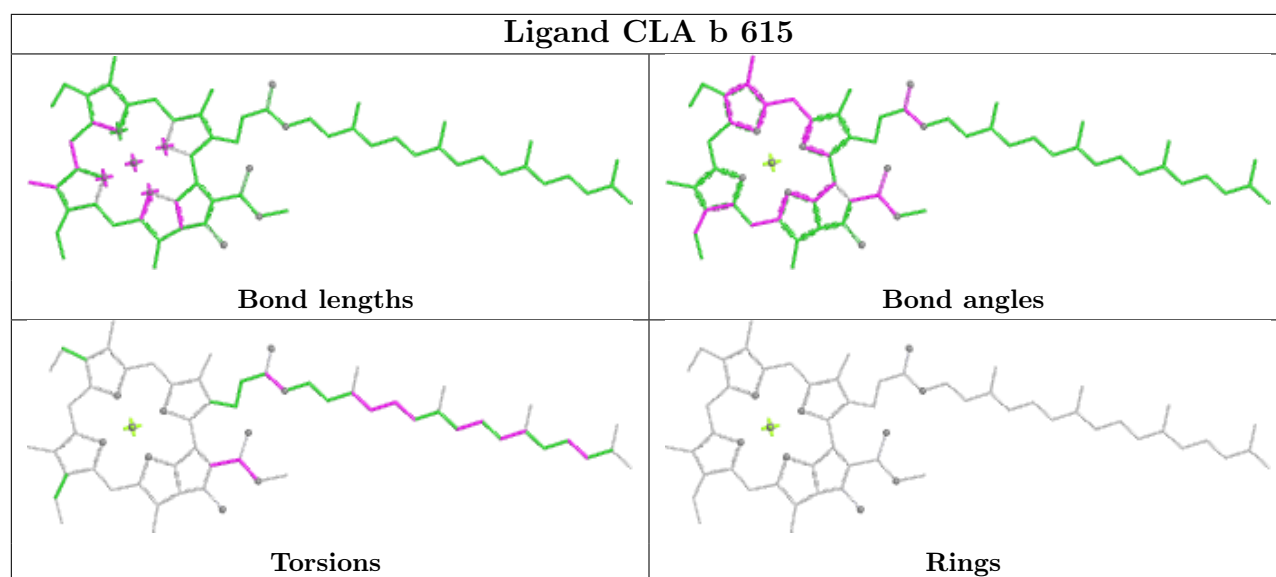
Ligand BCR A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

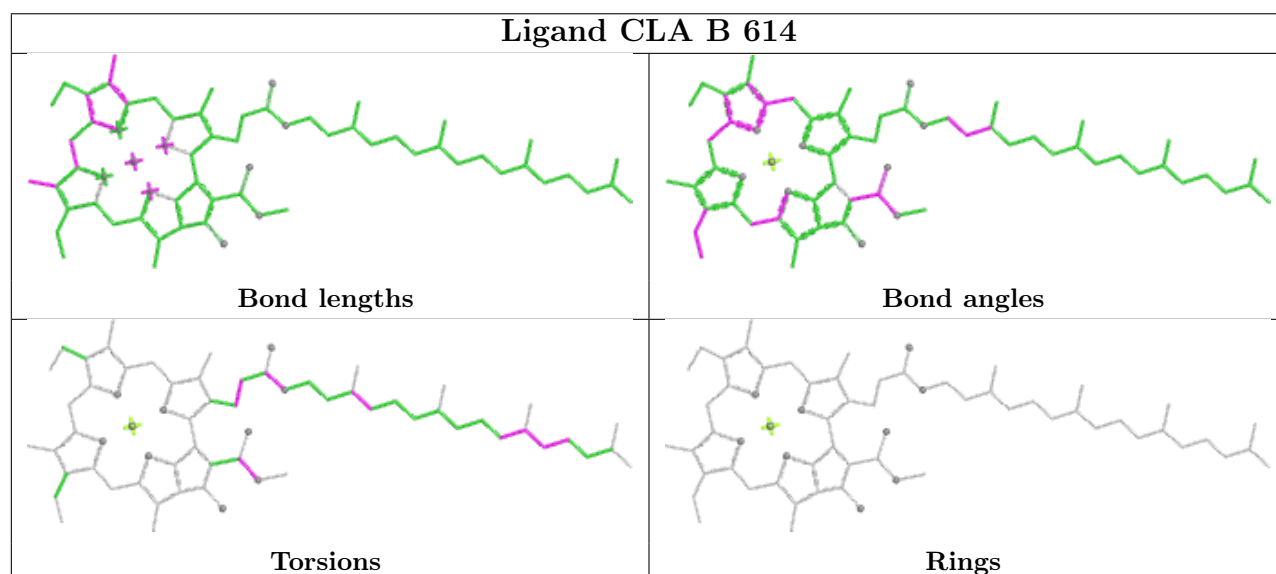
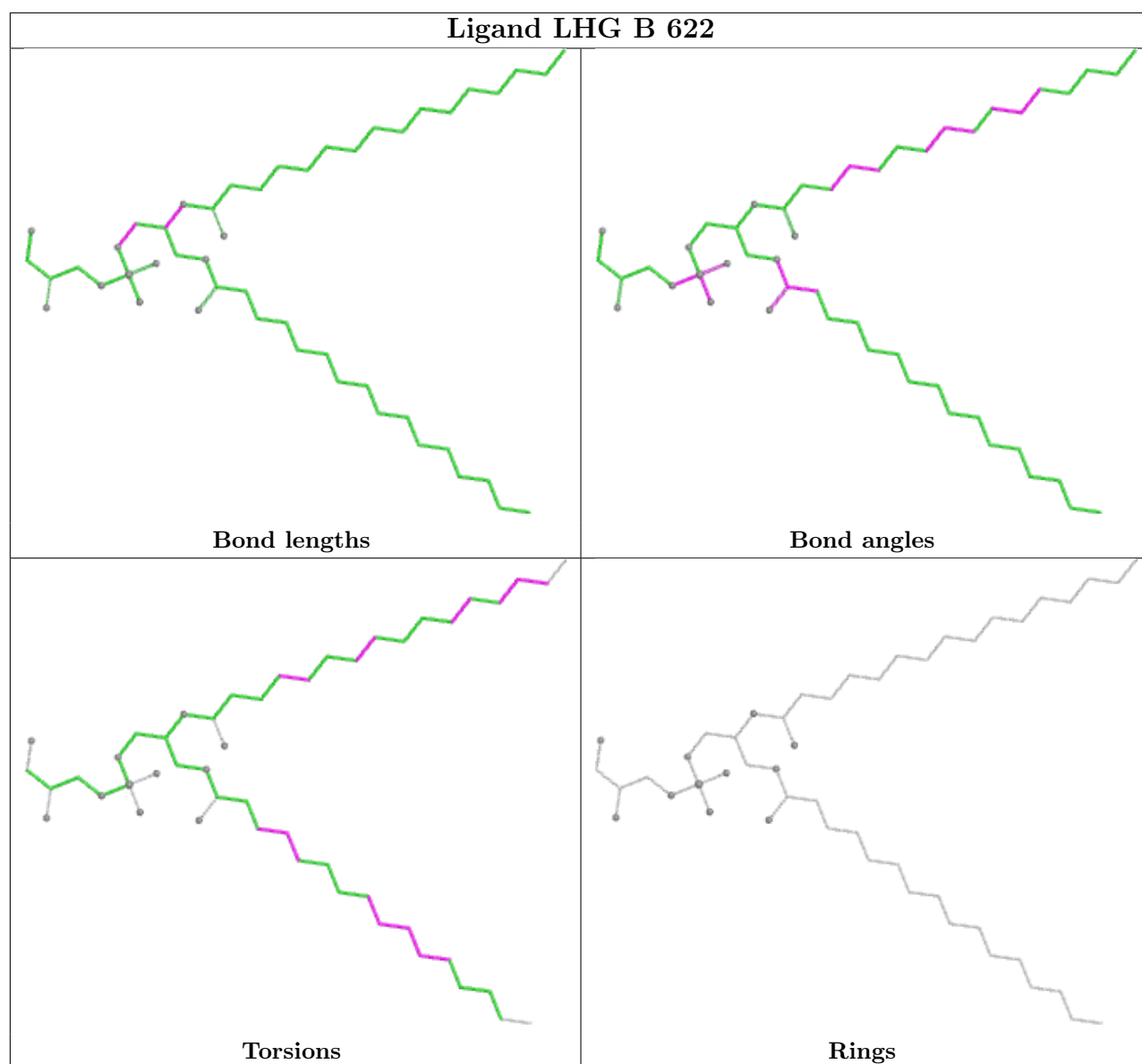
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

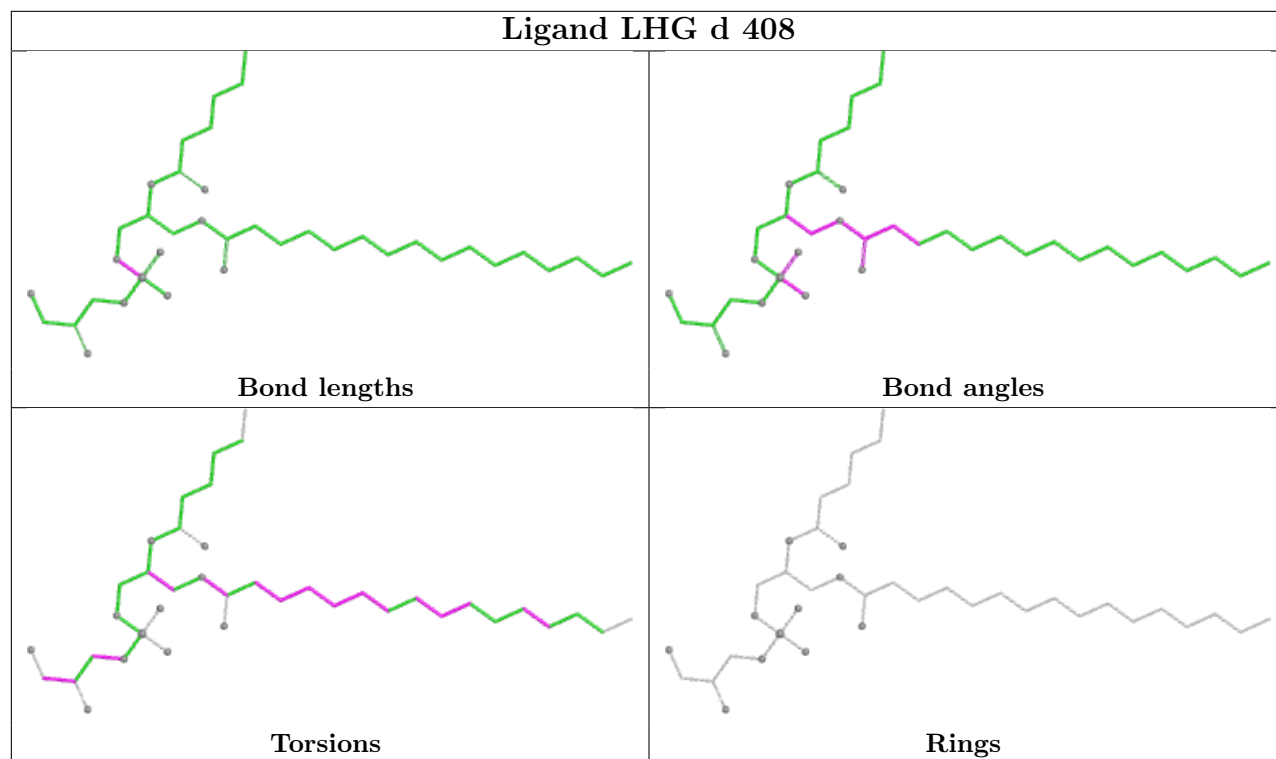
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

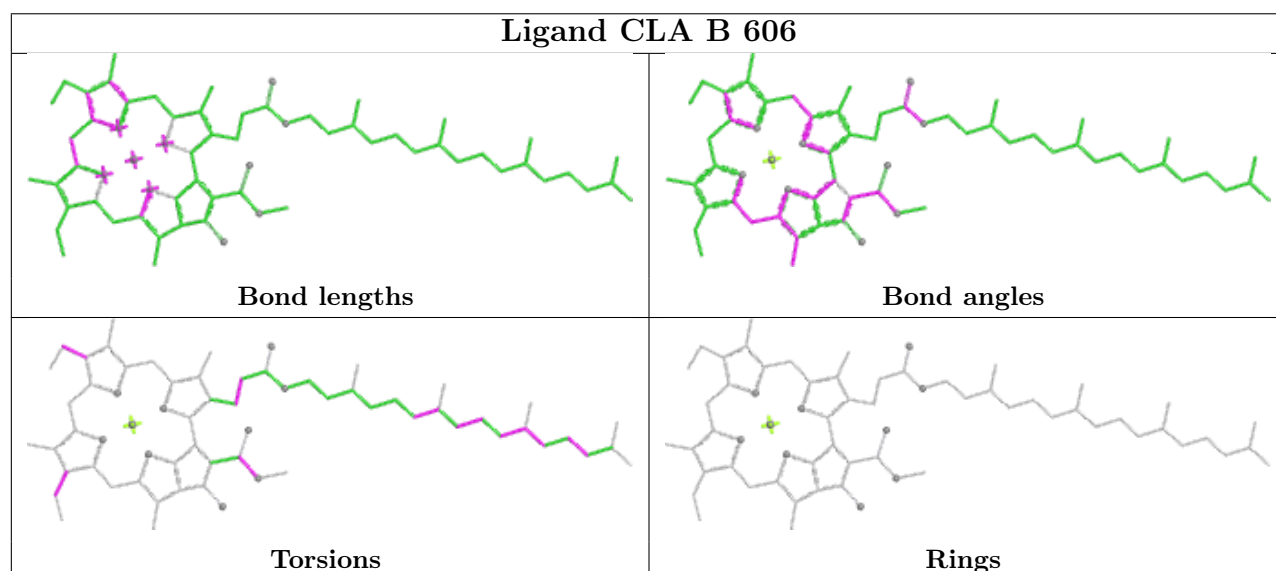
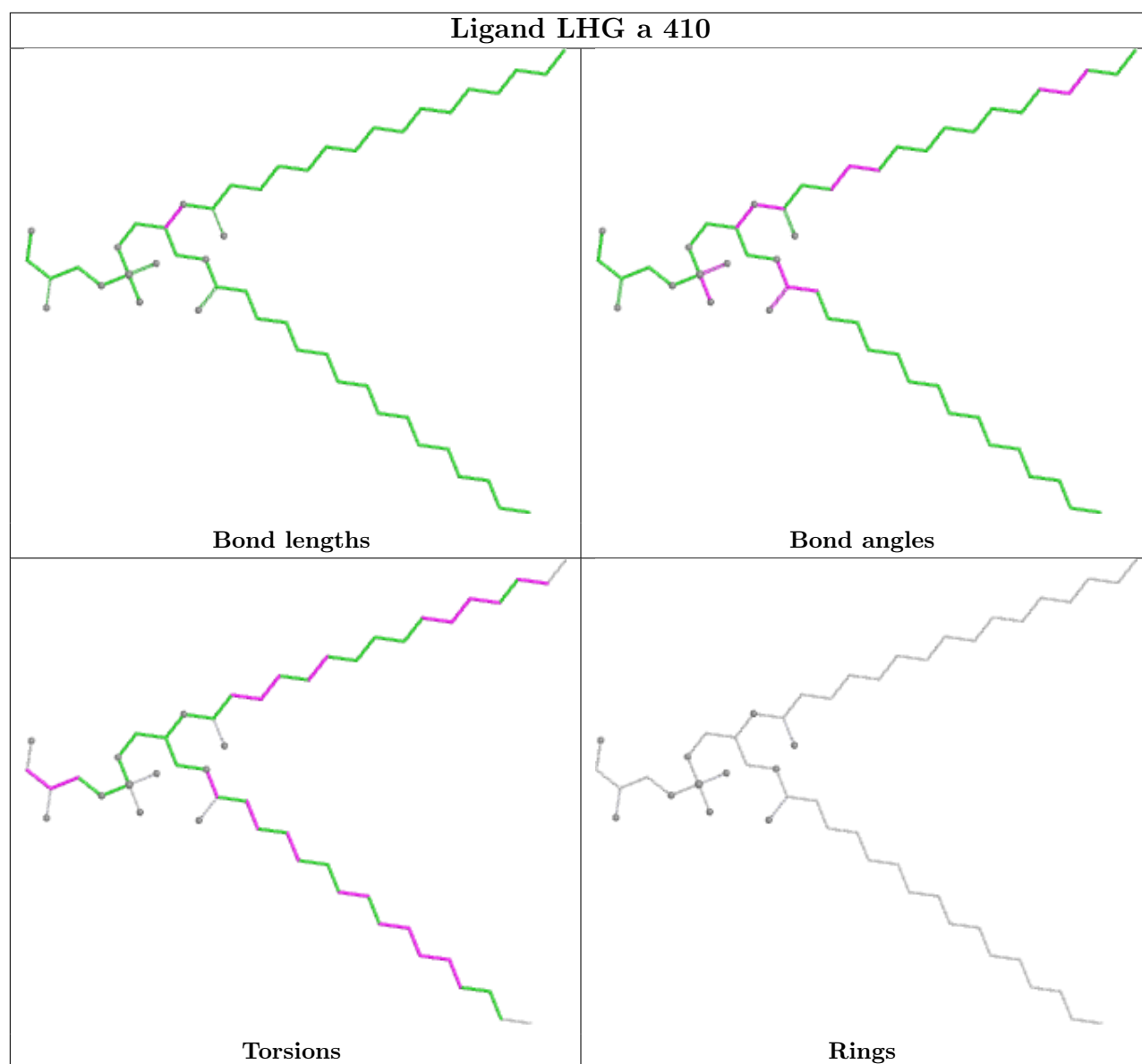


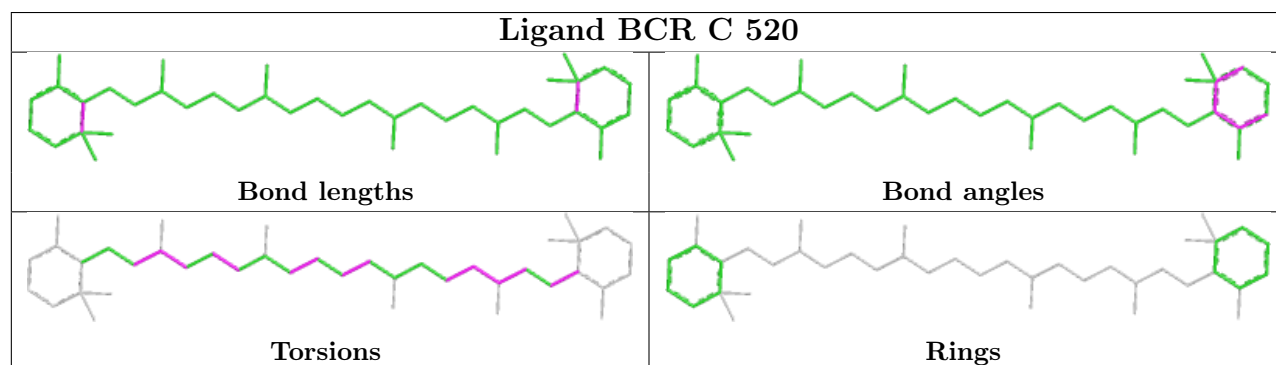
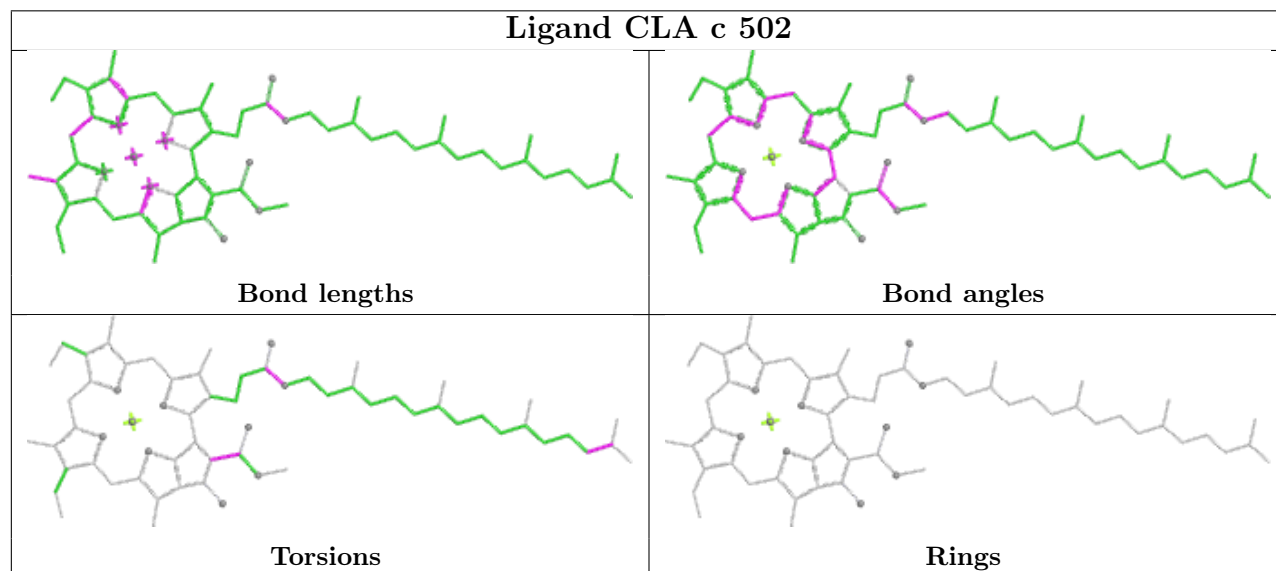
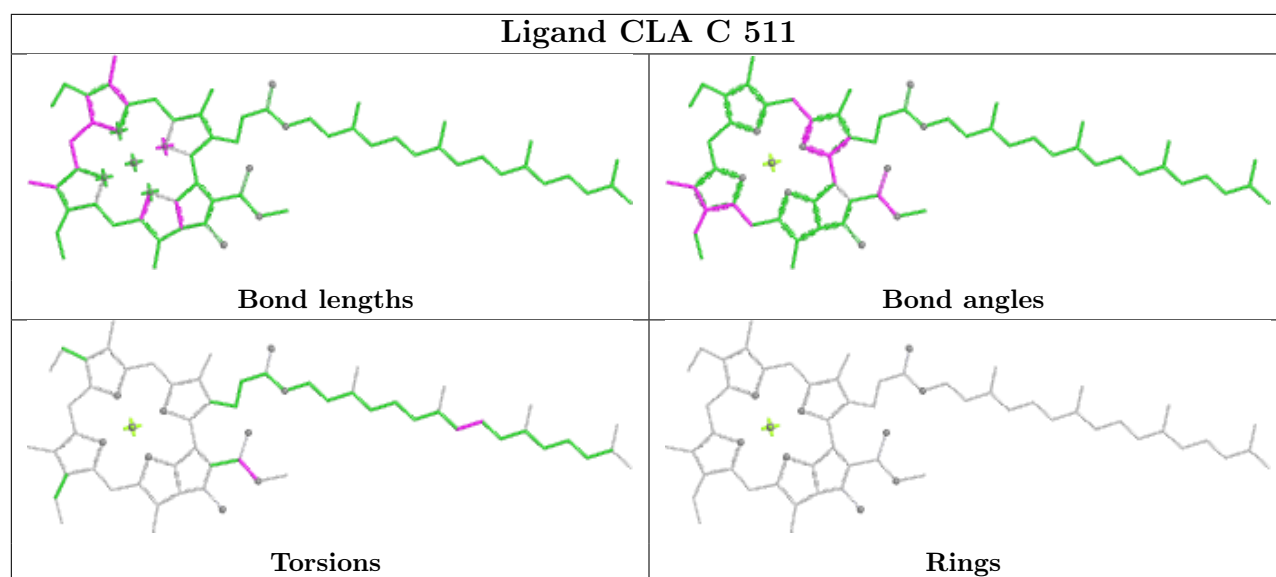


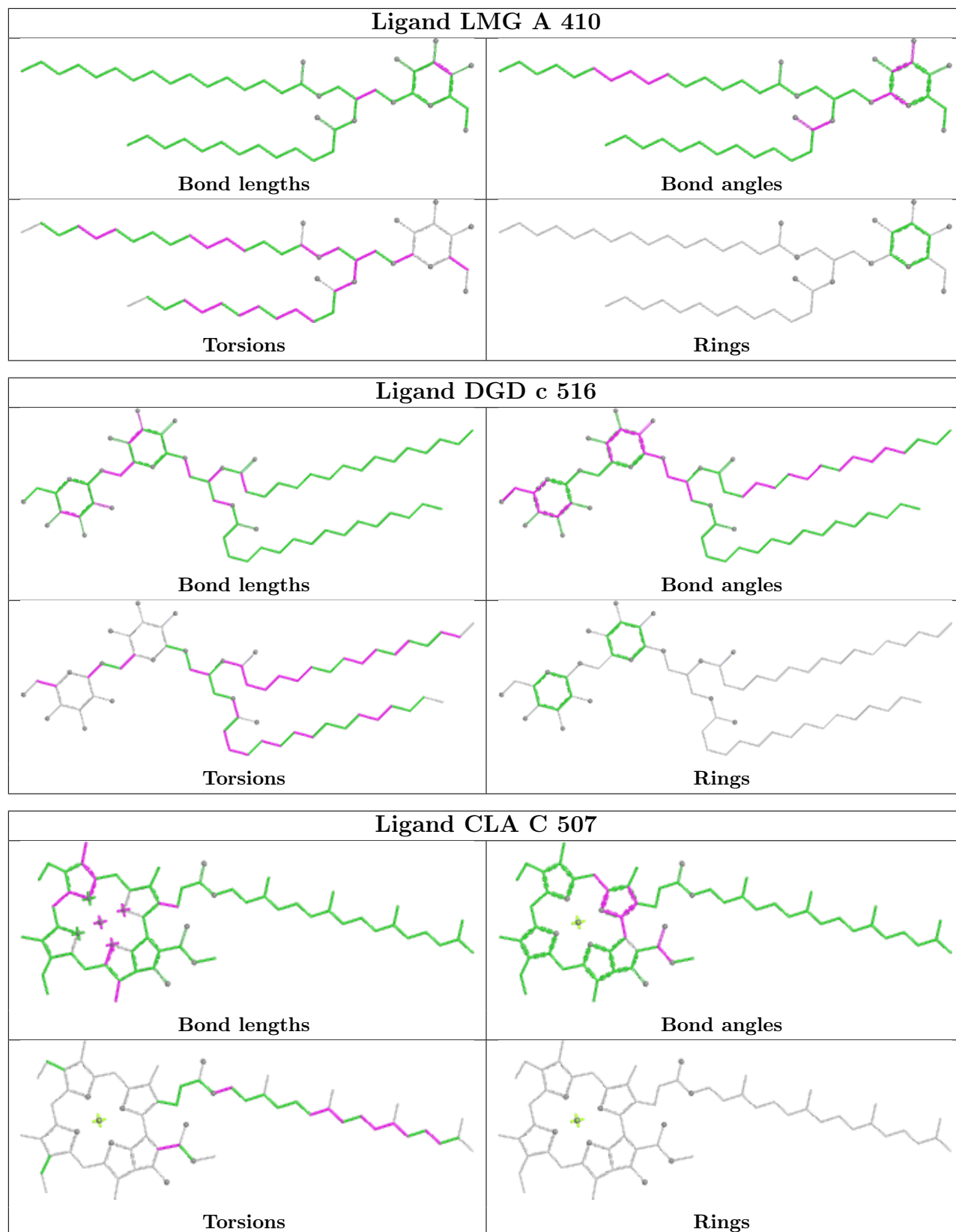


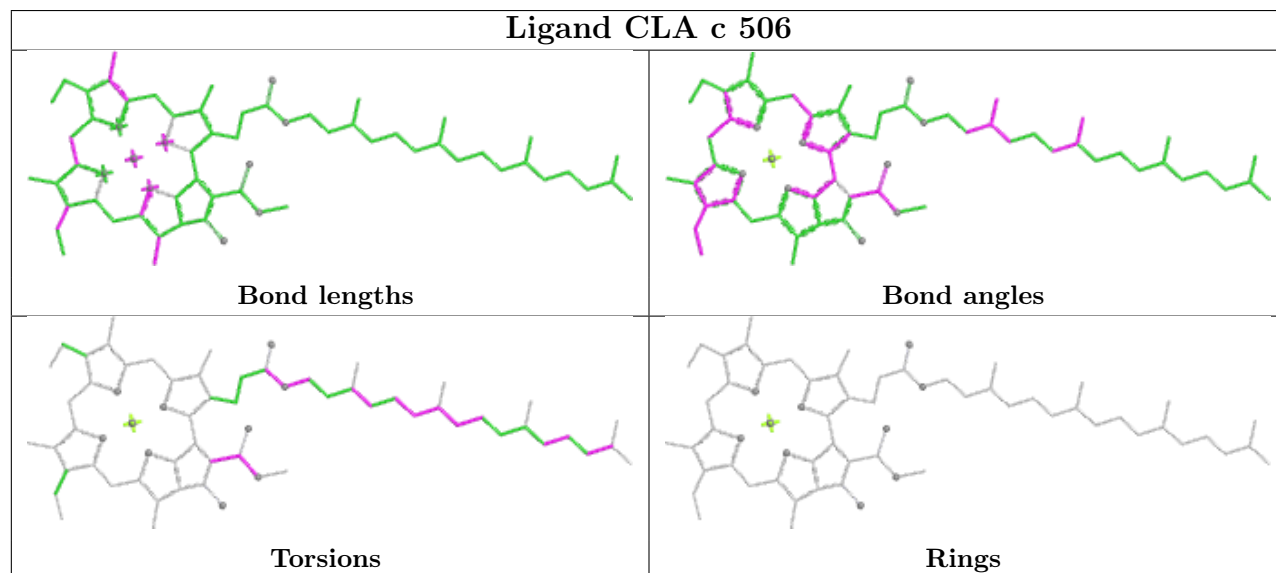
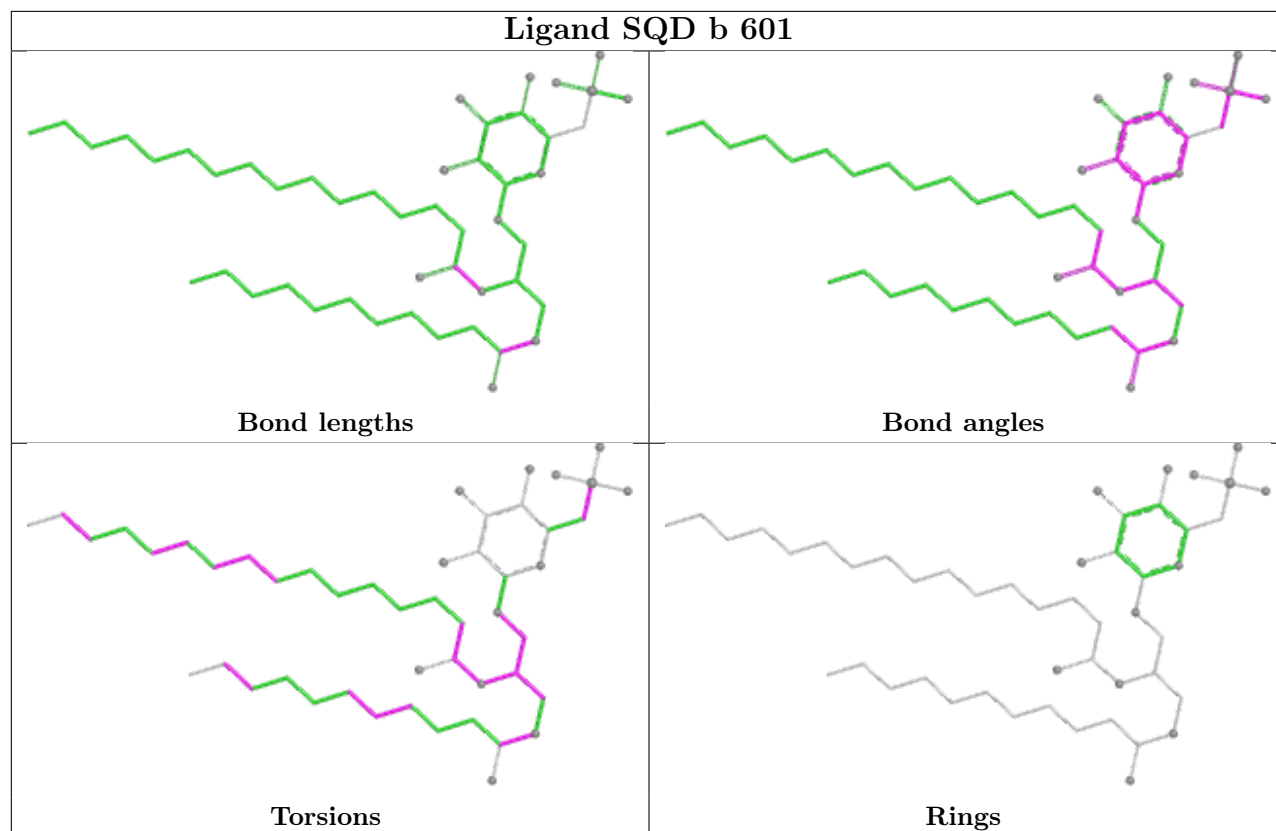


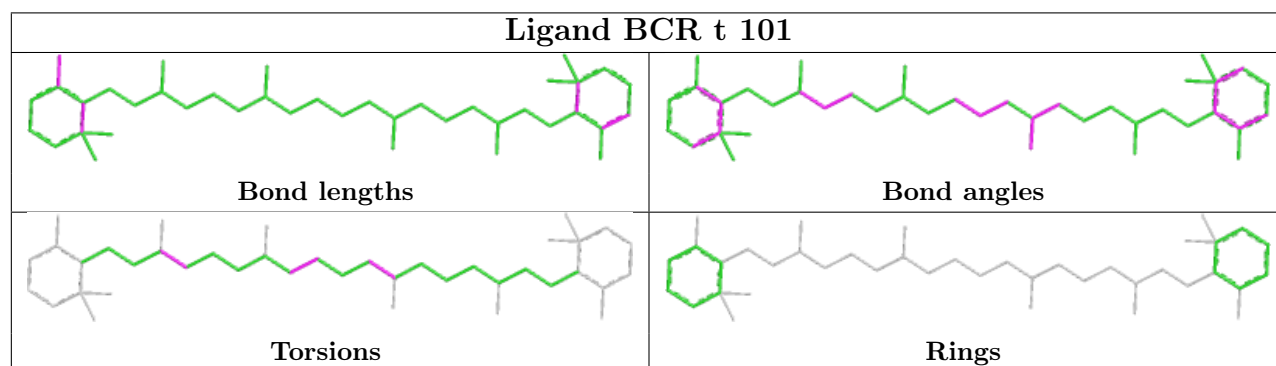
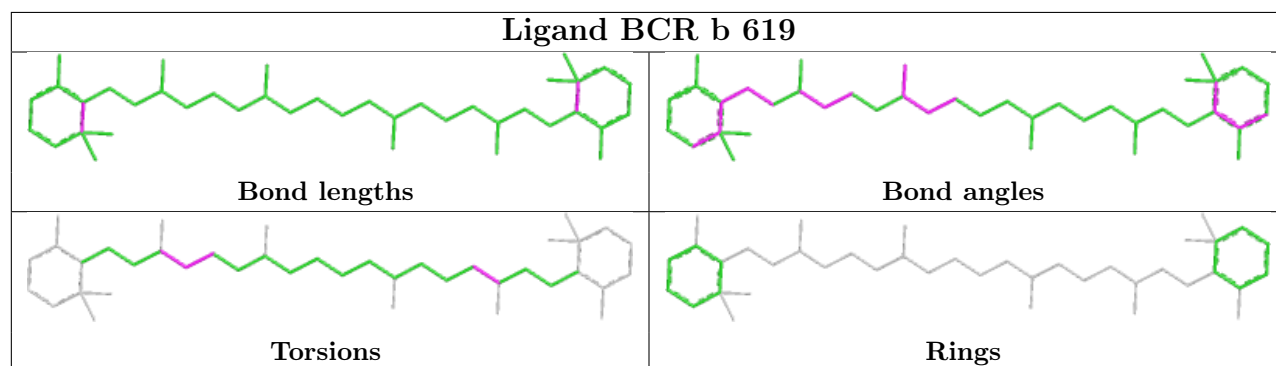
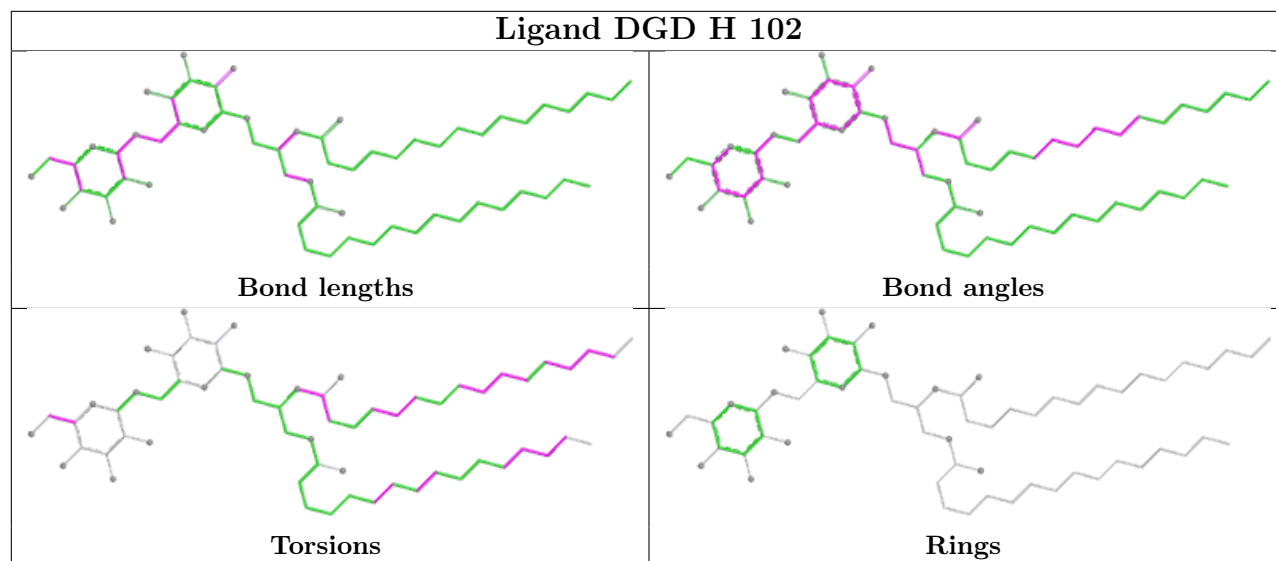




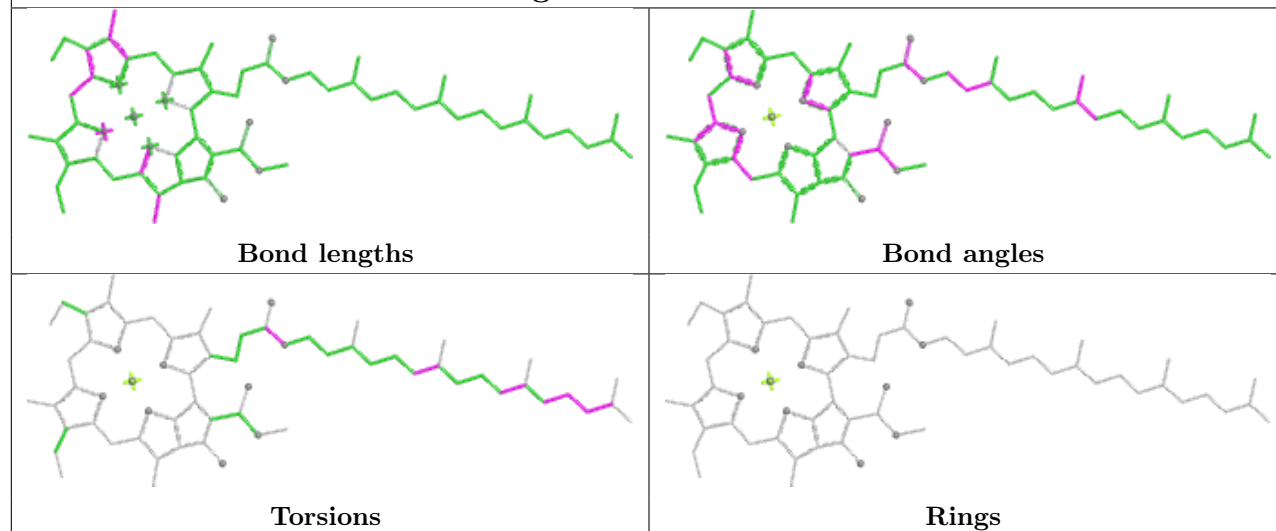




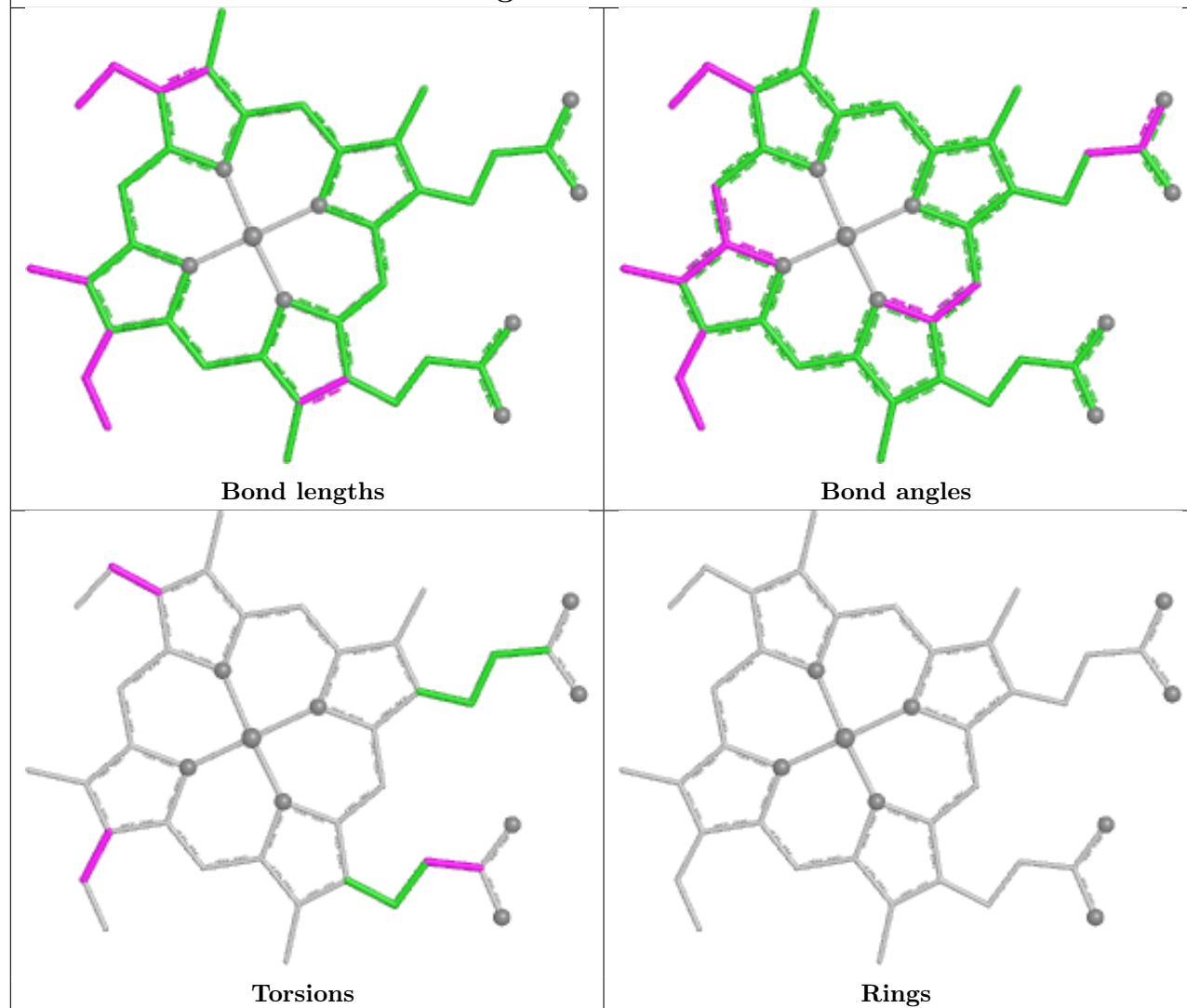


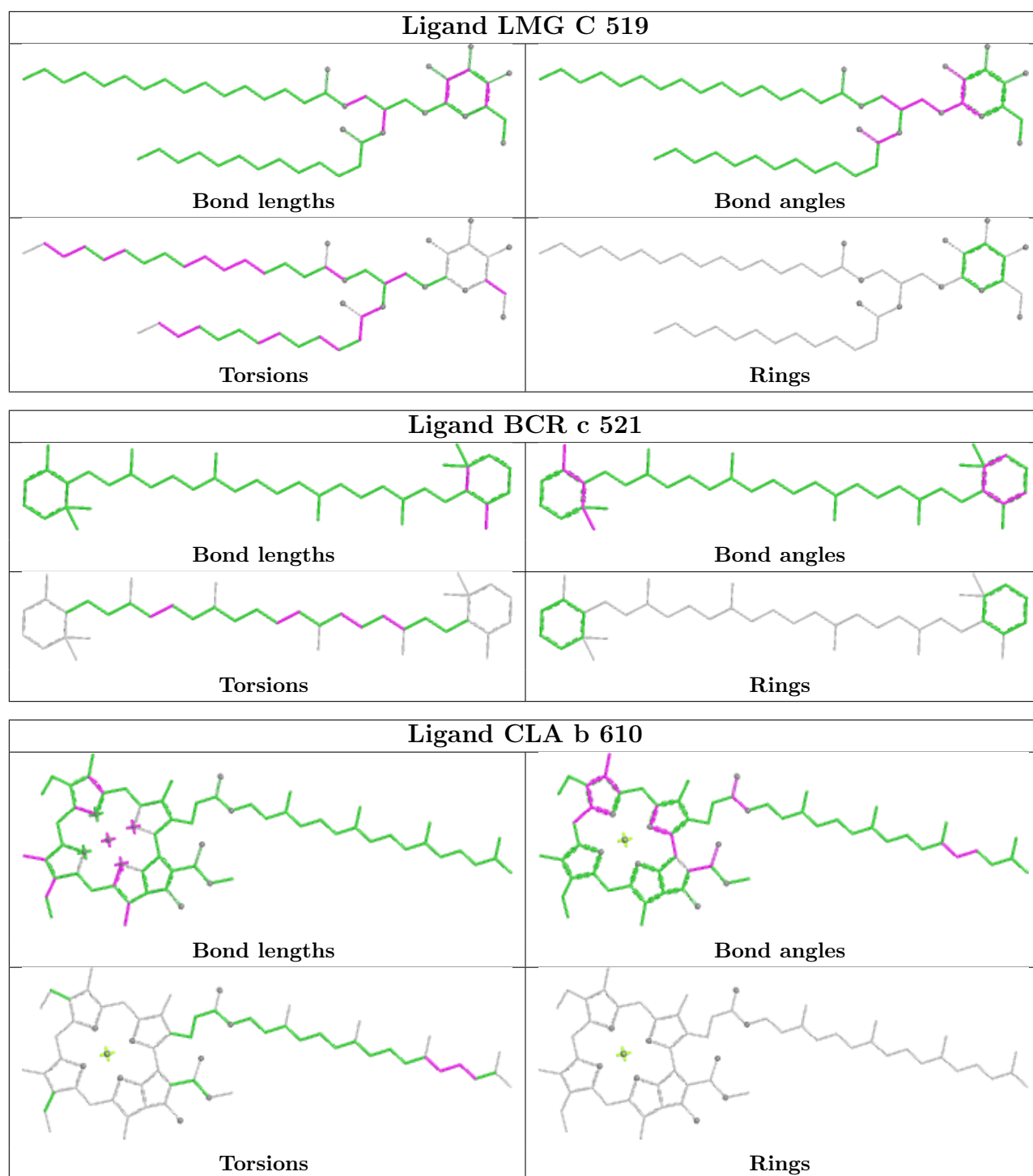


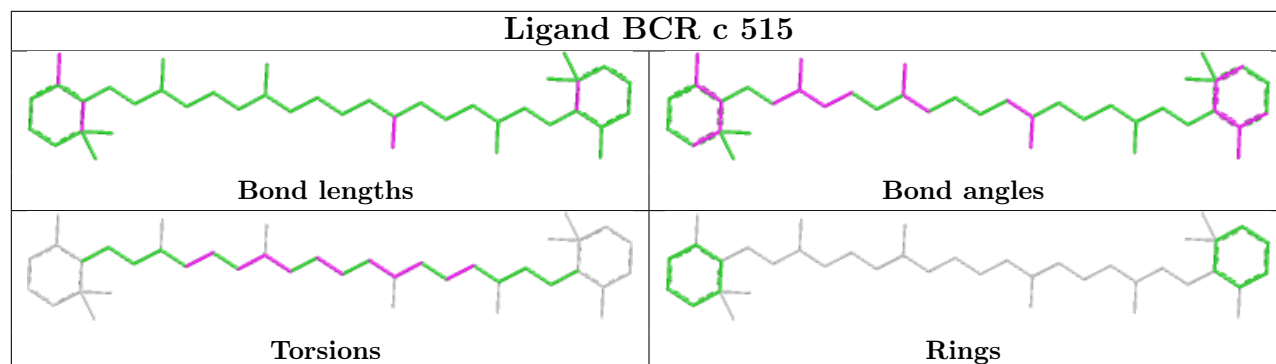
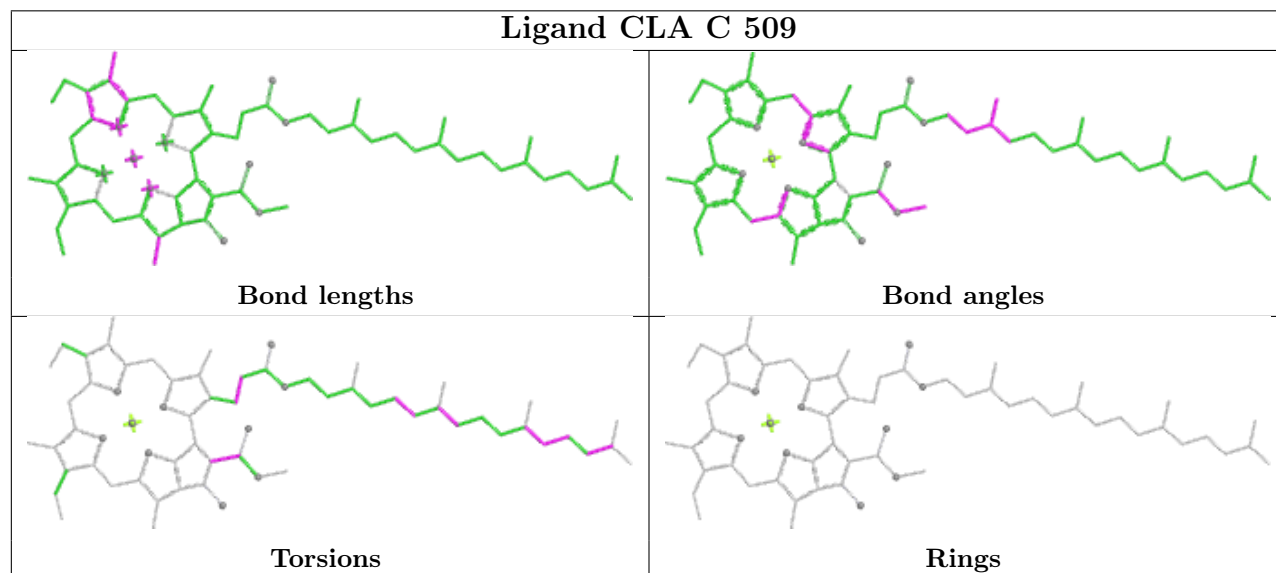
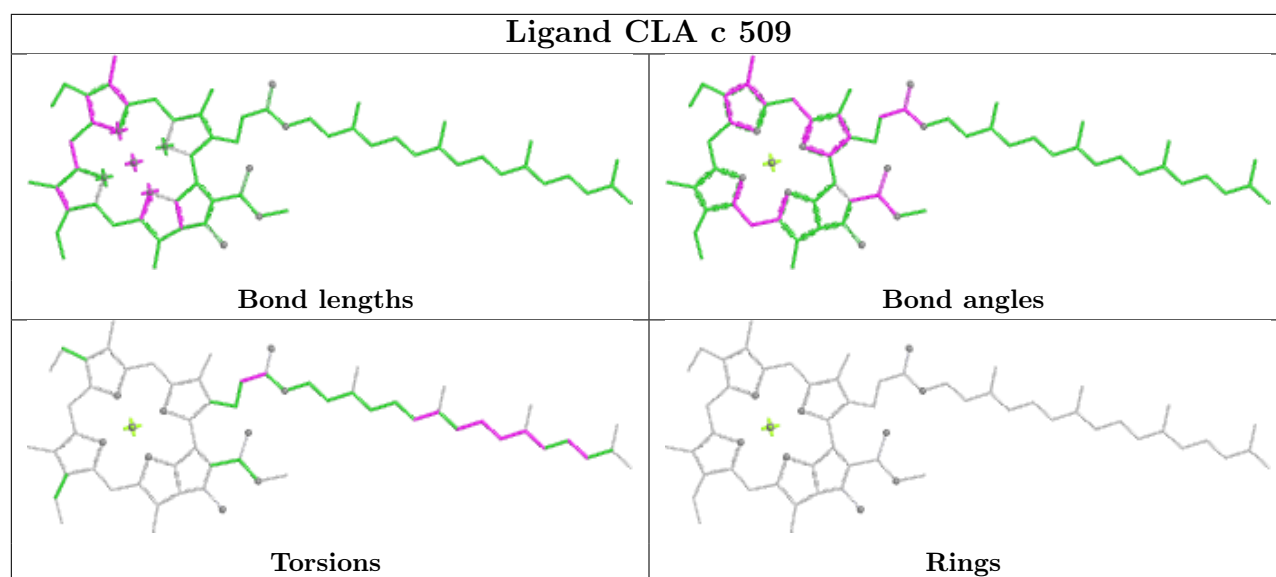
Ligand CLA B 611

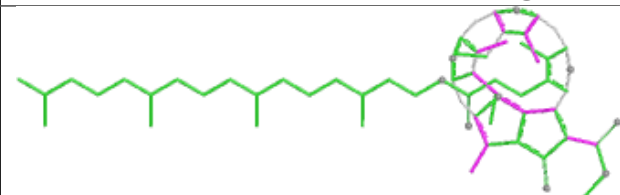
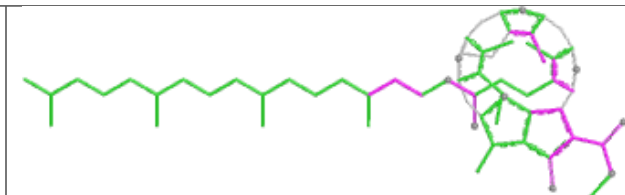
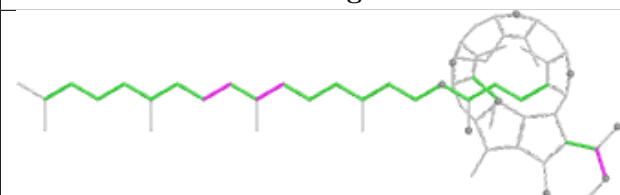
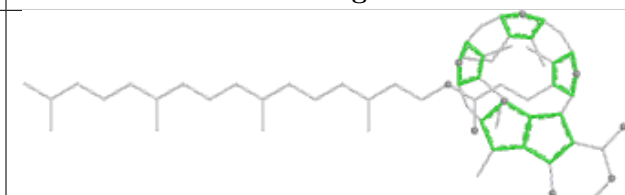
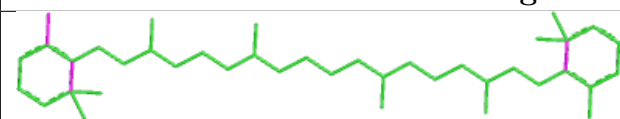
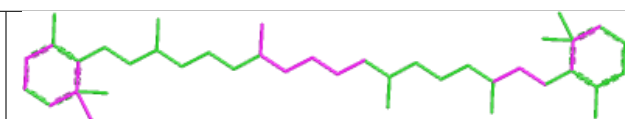
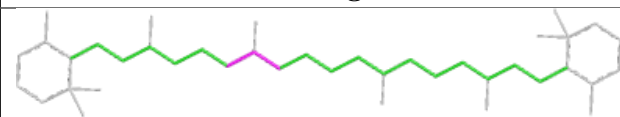
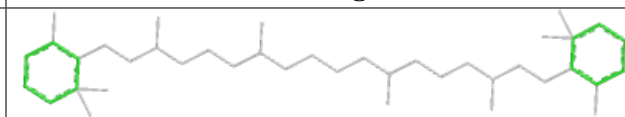
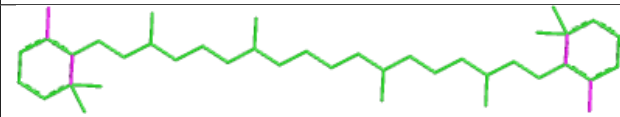
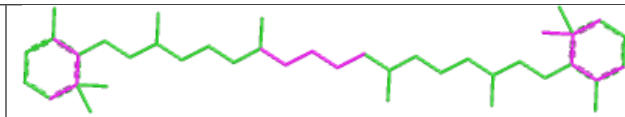
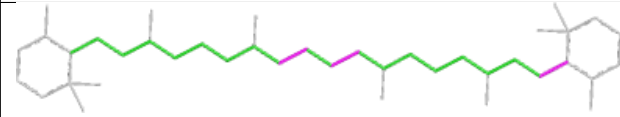
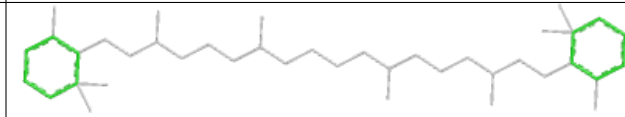


Ligand HEC v 201

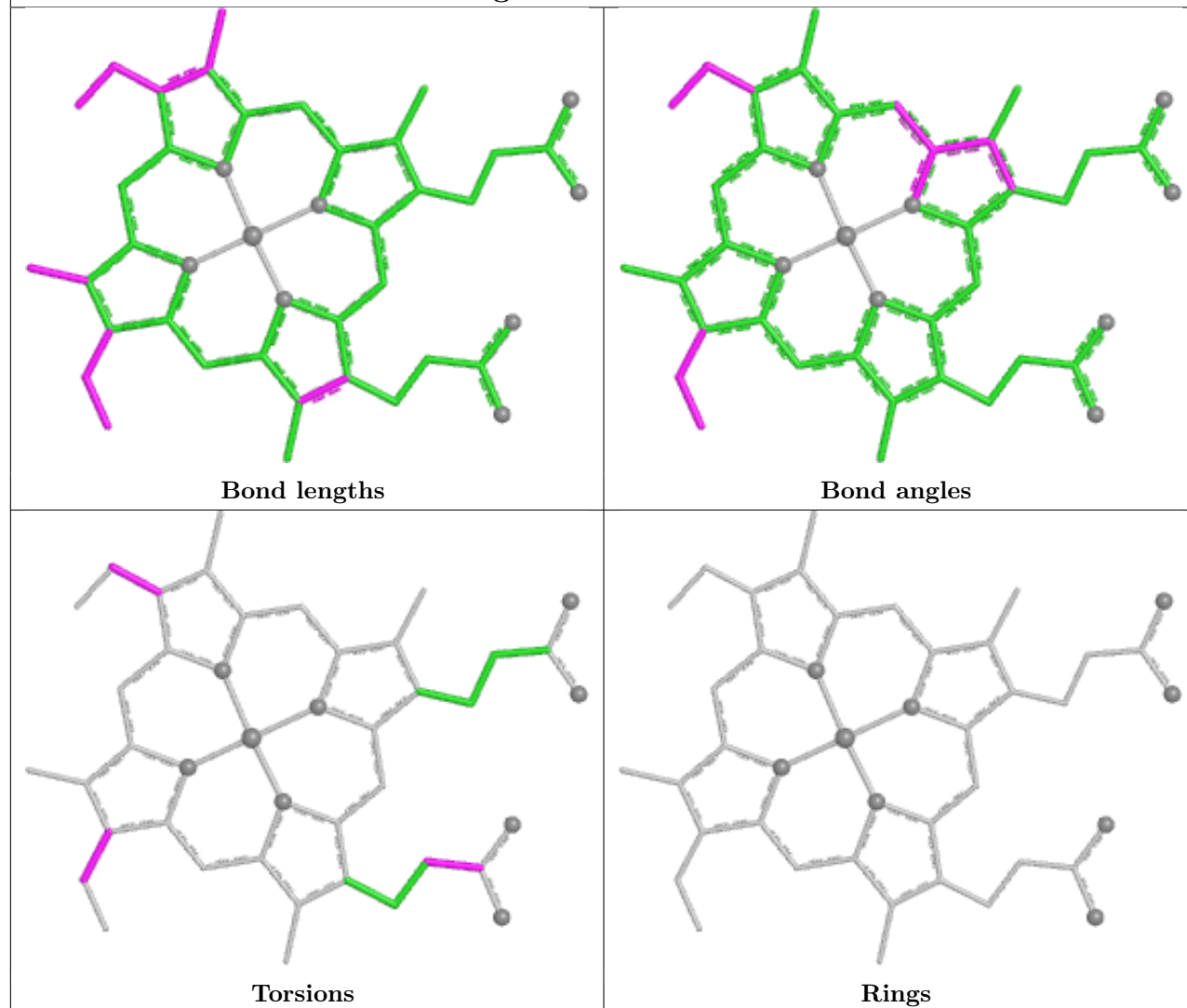




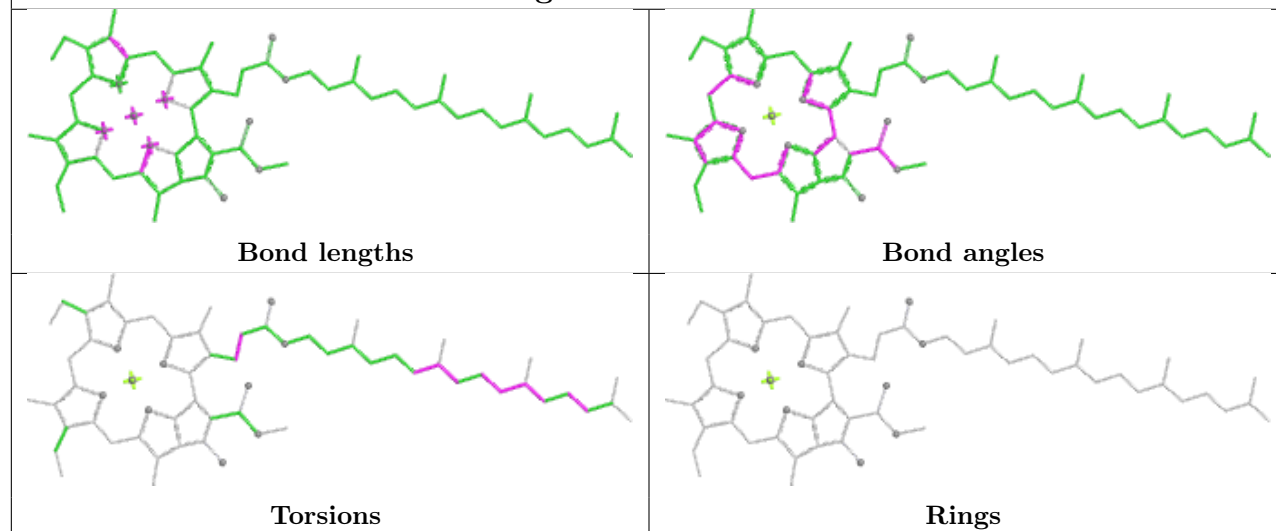


Ligand PHO D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

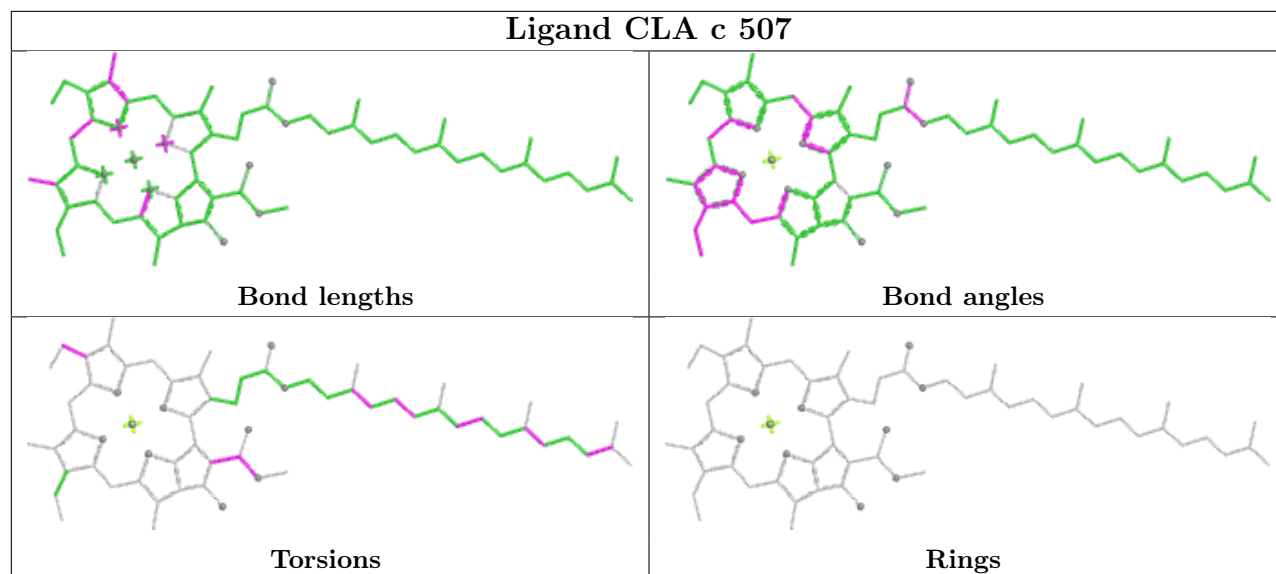
Ligand HEC V 201



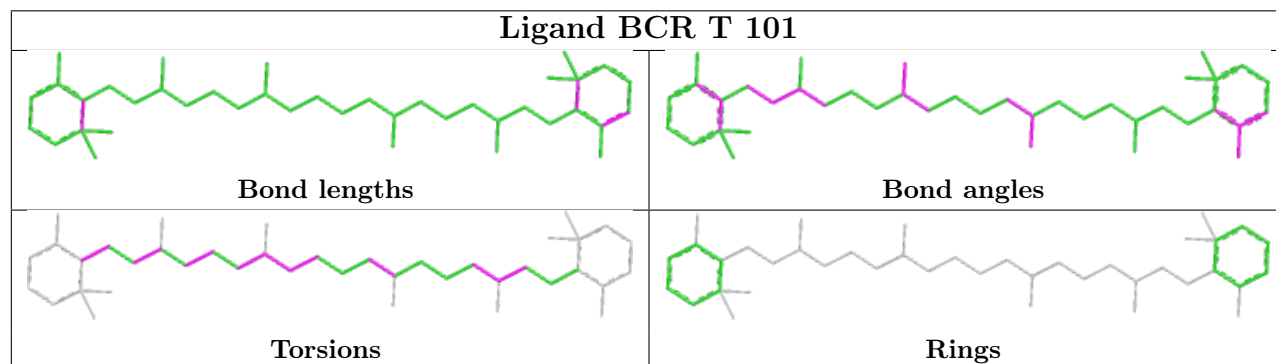
Ligand CLA b 607



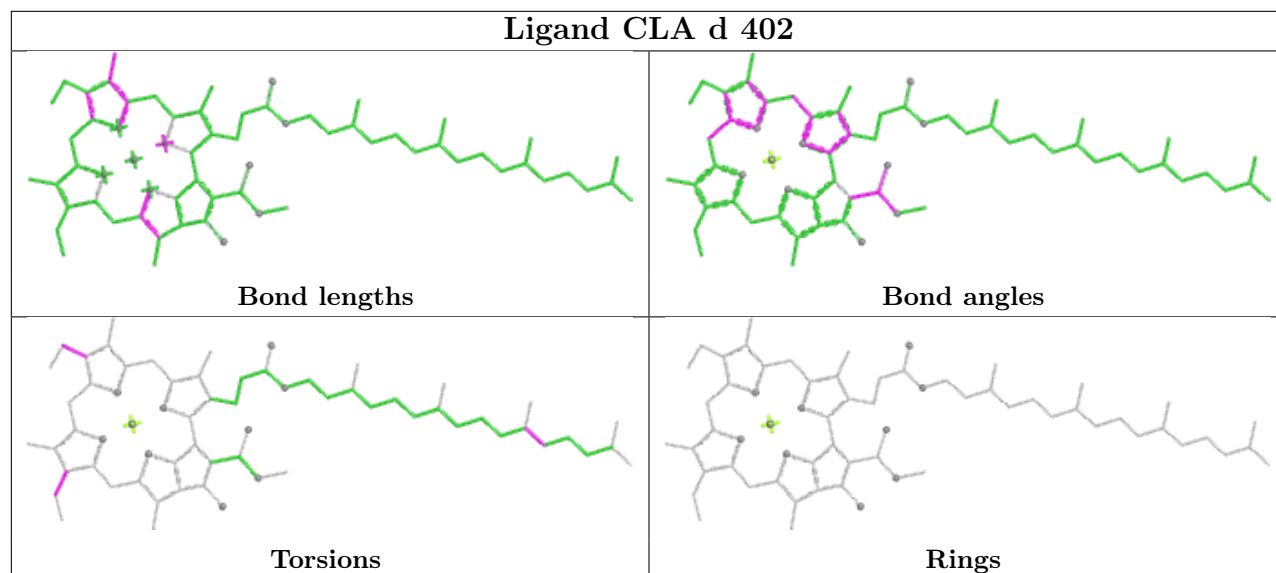
Ligand CLA c 507

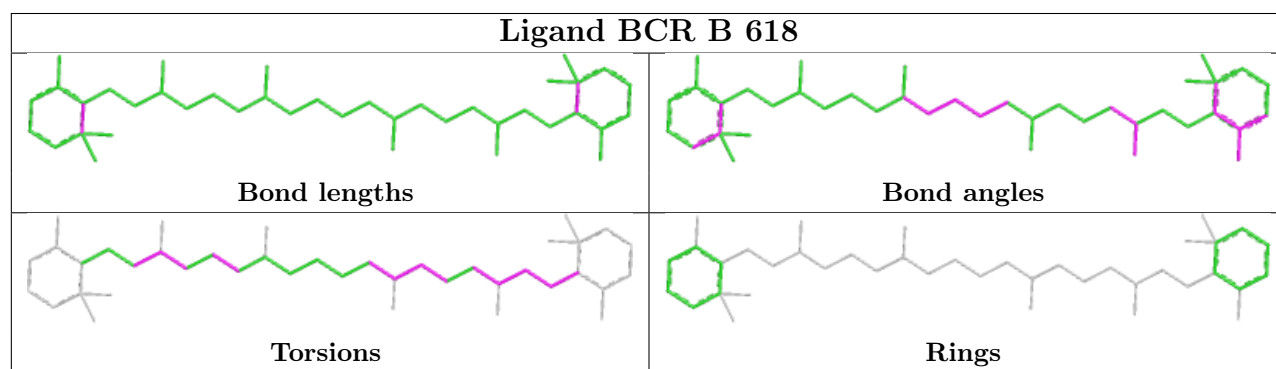
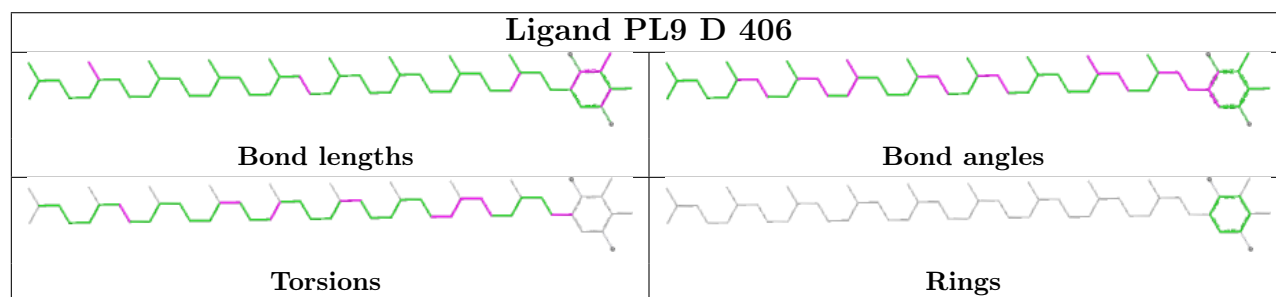
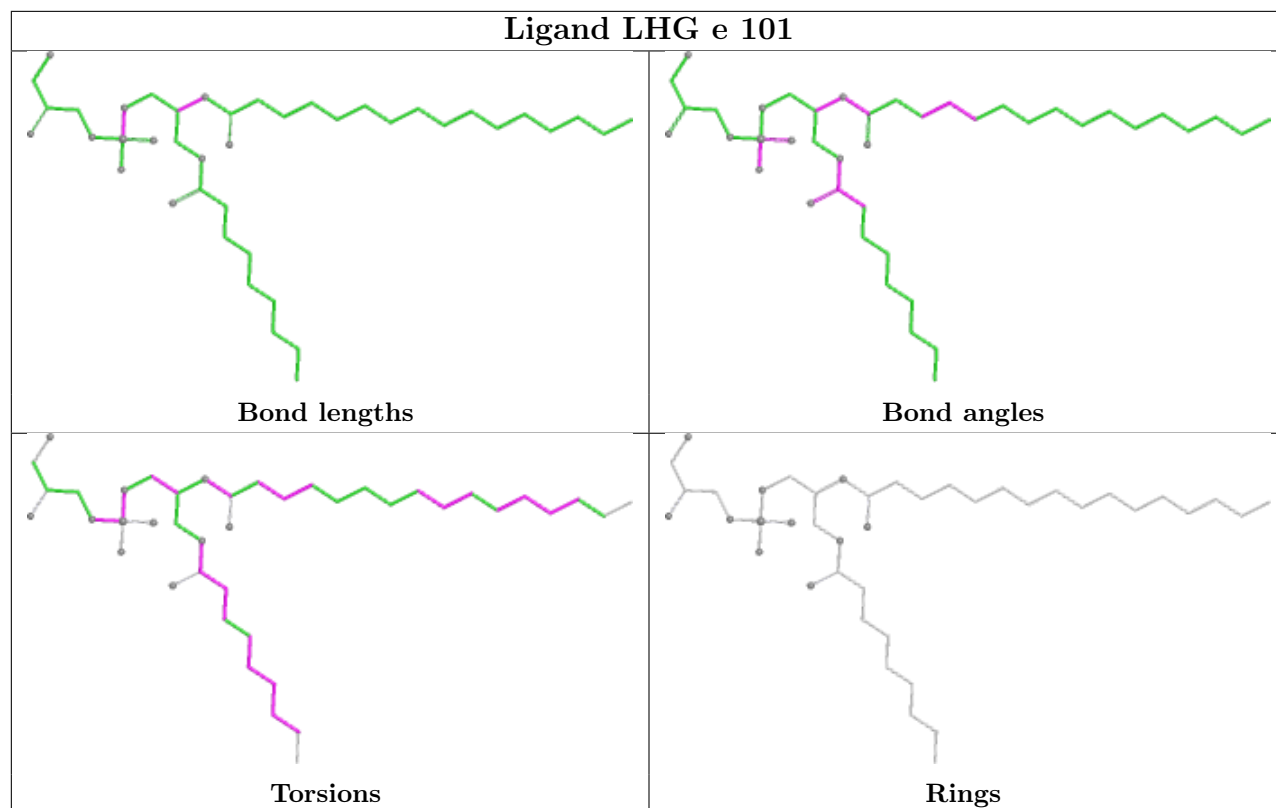


Ligand BCR T 101

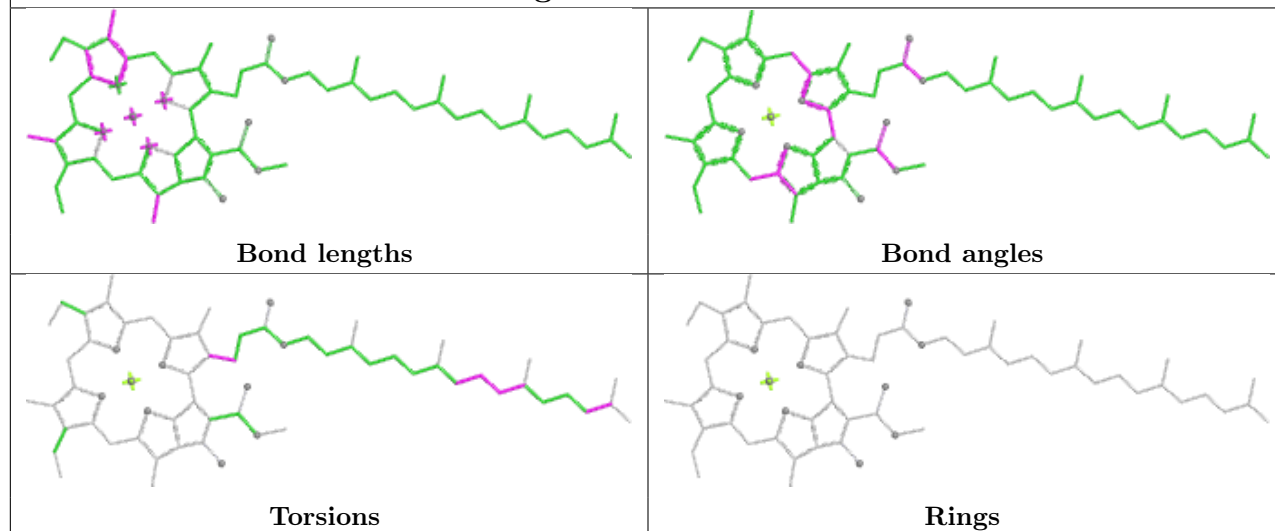


Ligand CLA d 402

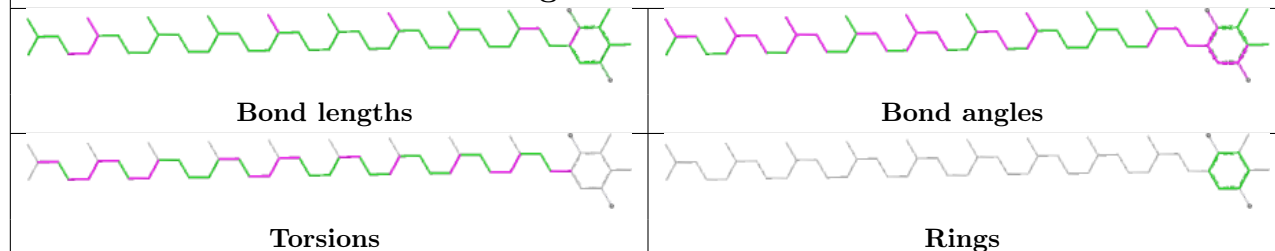




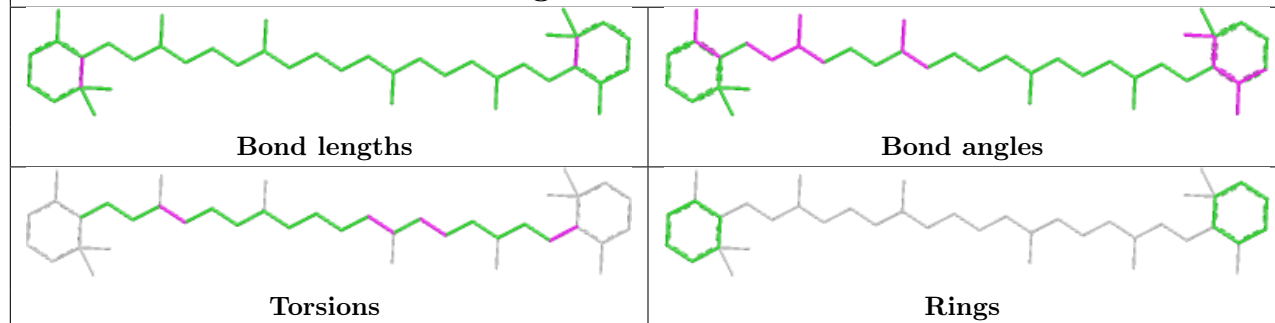
Ligand CLA d 404

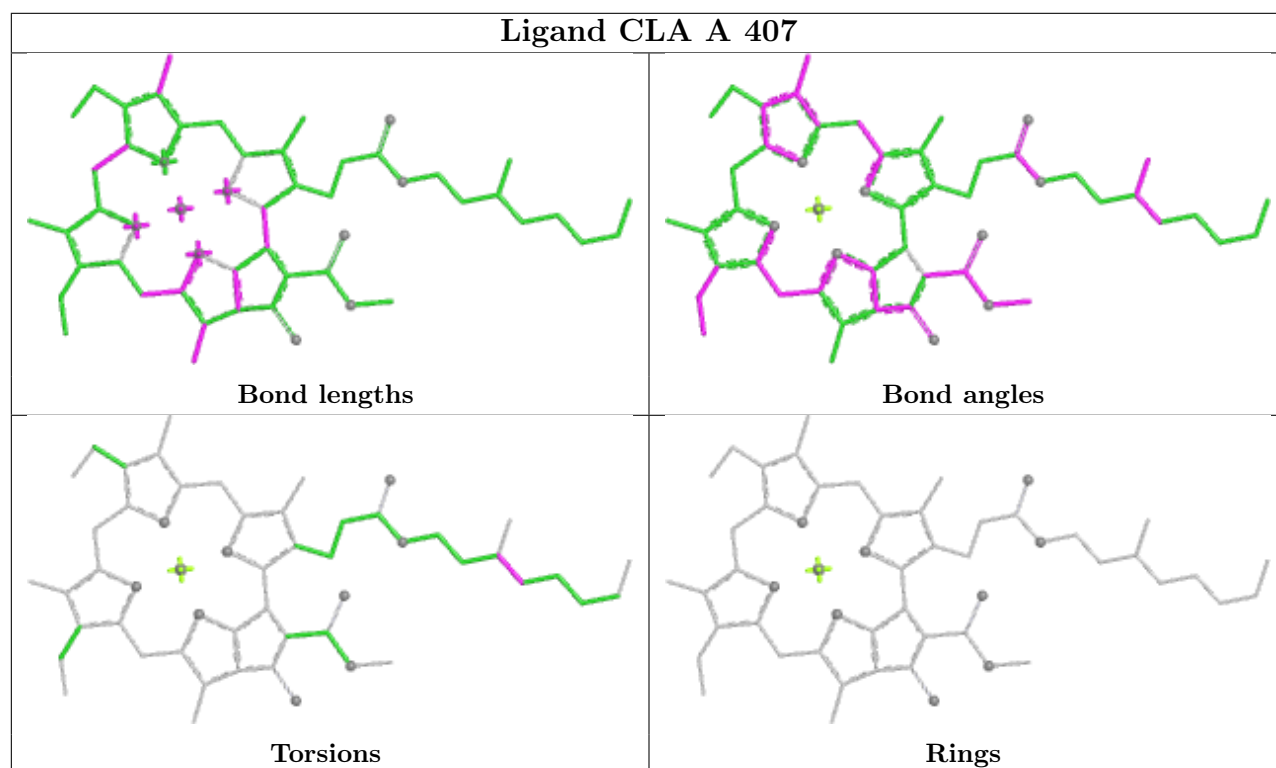
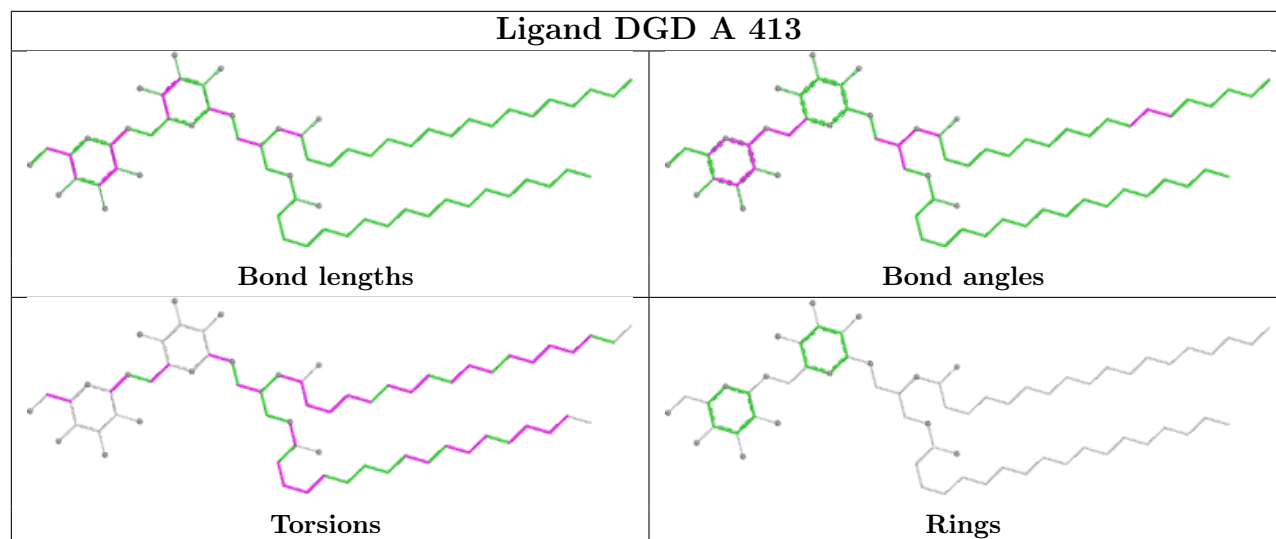


Ligand PL9 d 406

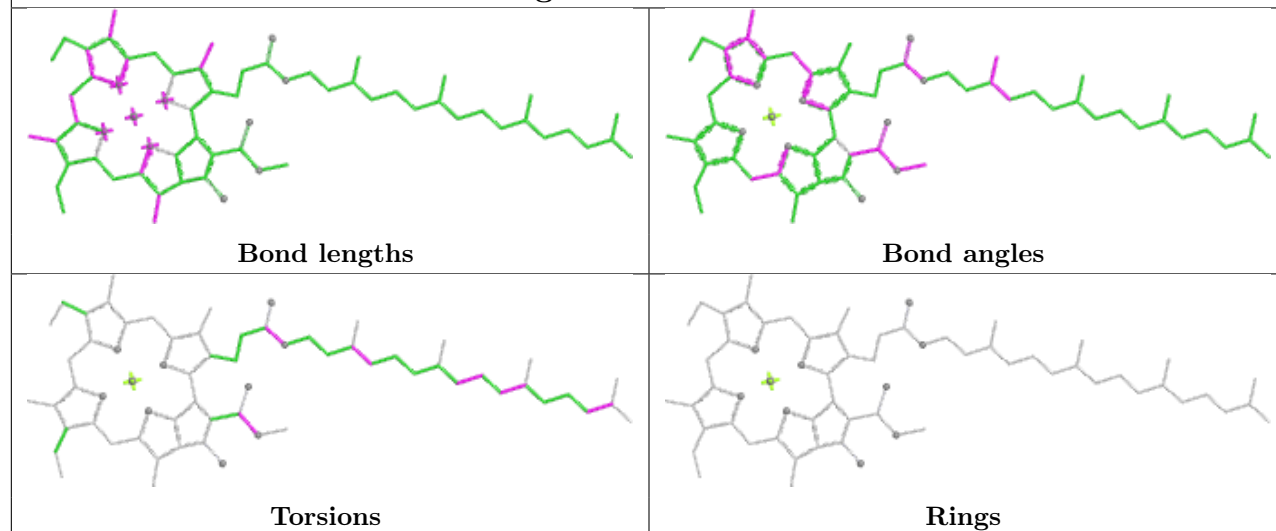


Ligand BCR h 102

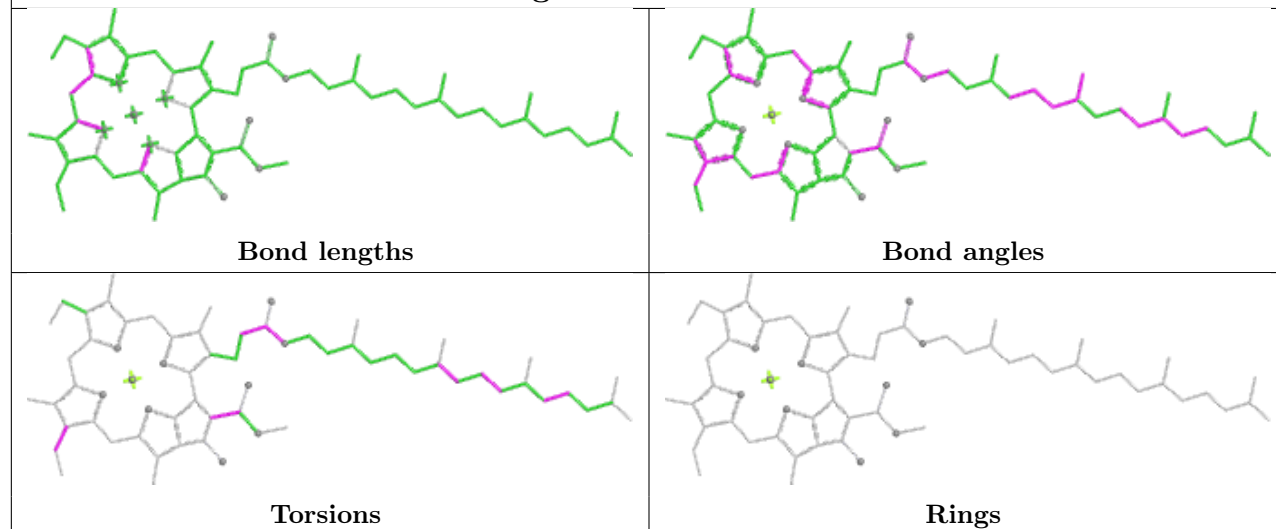




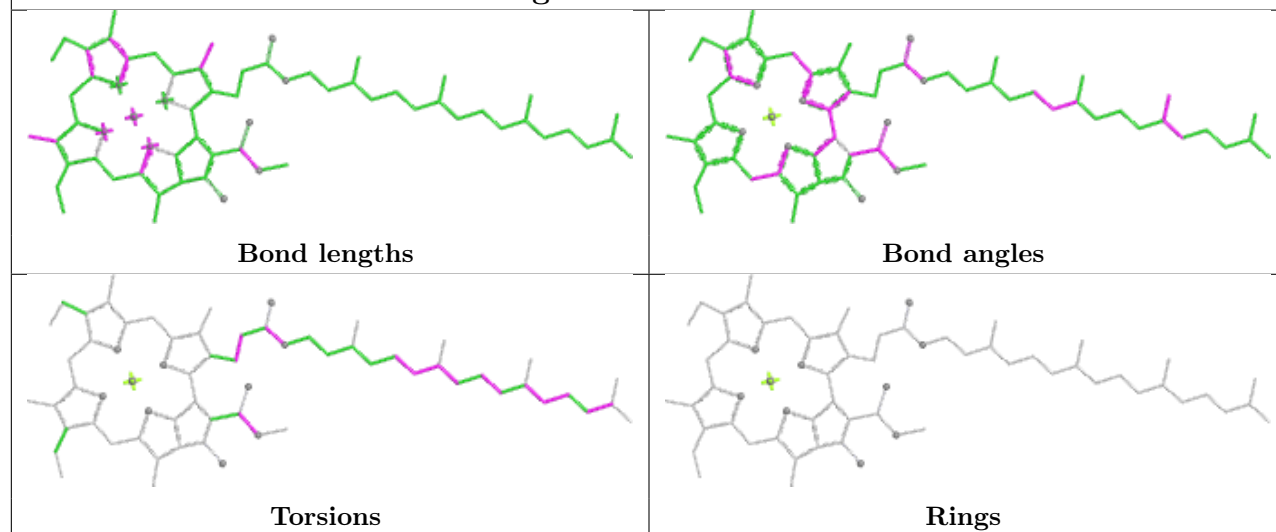
Ligand CLA b 604

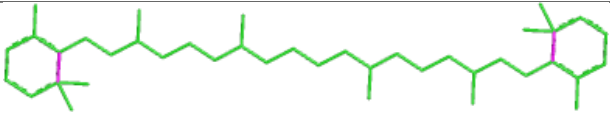
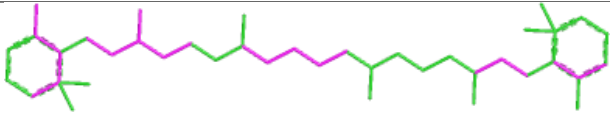
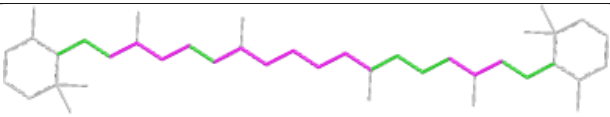
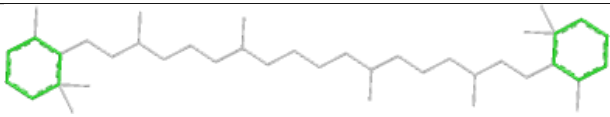
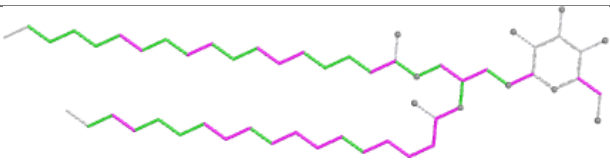
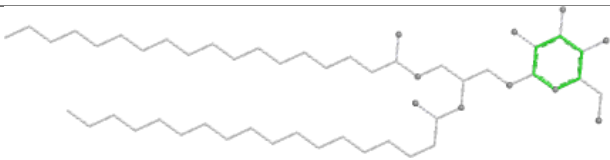
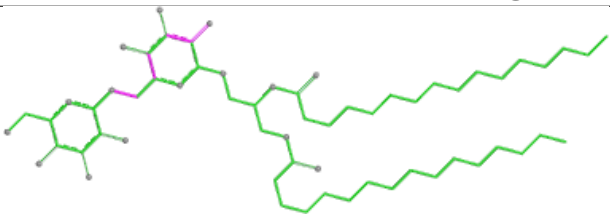
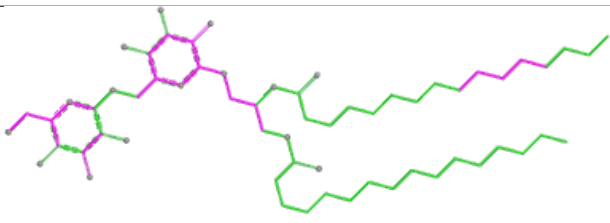
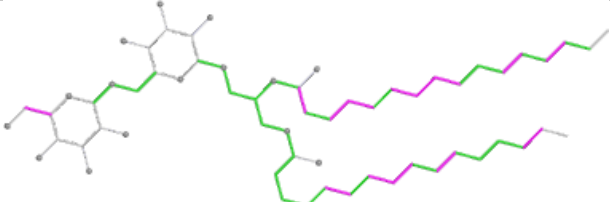
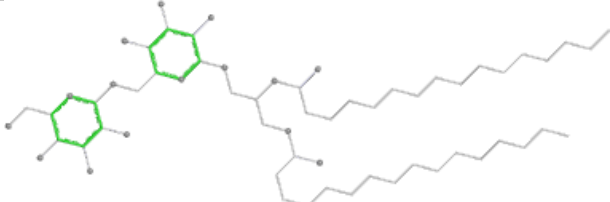


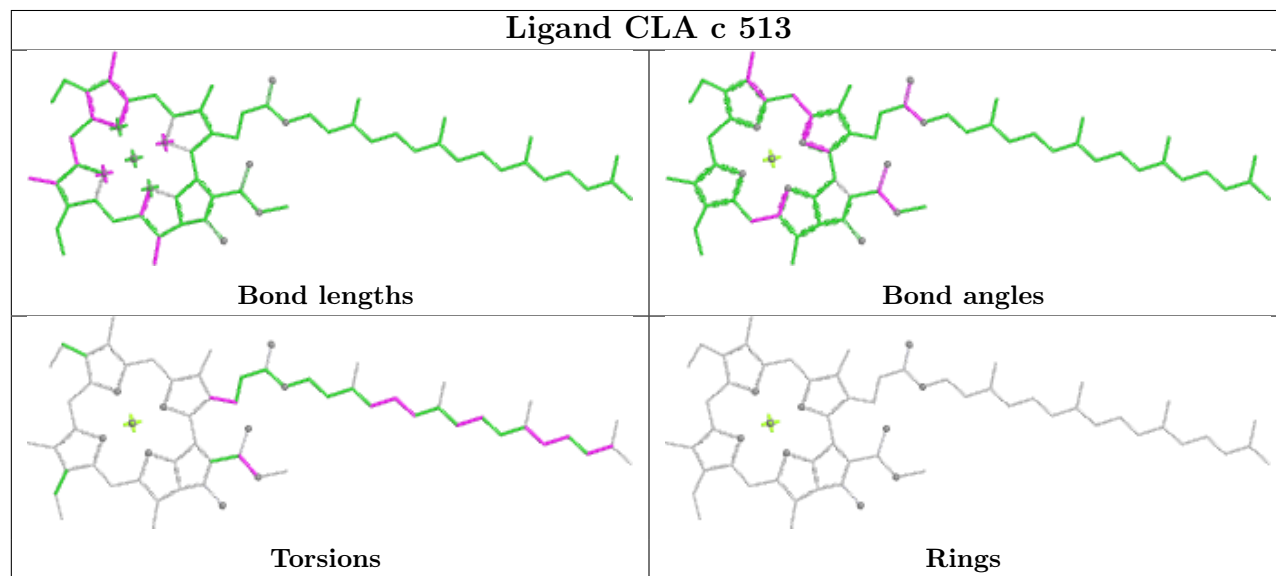
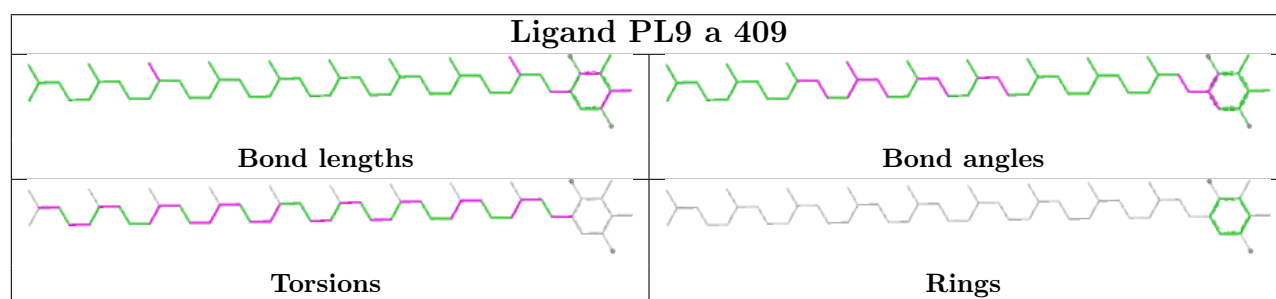
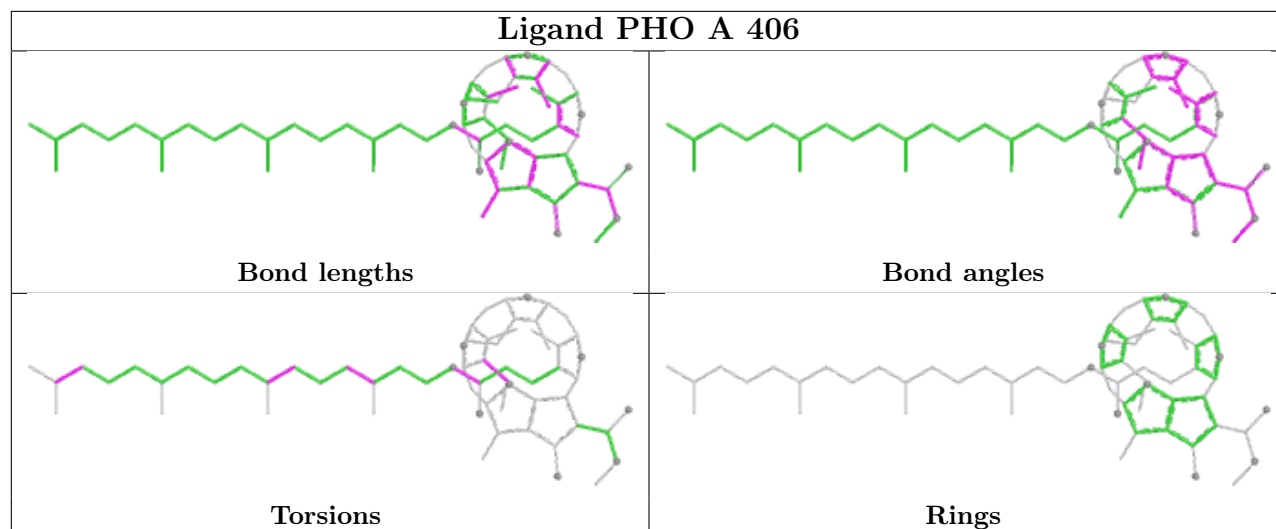
Ligand CLA B 612

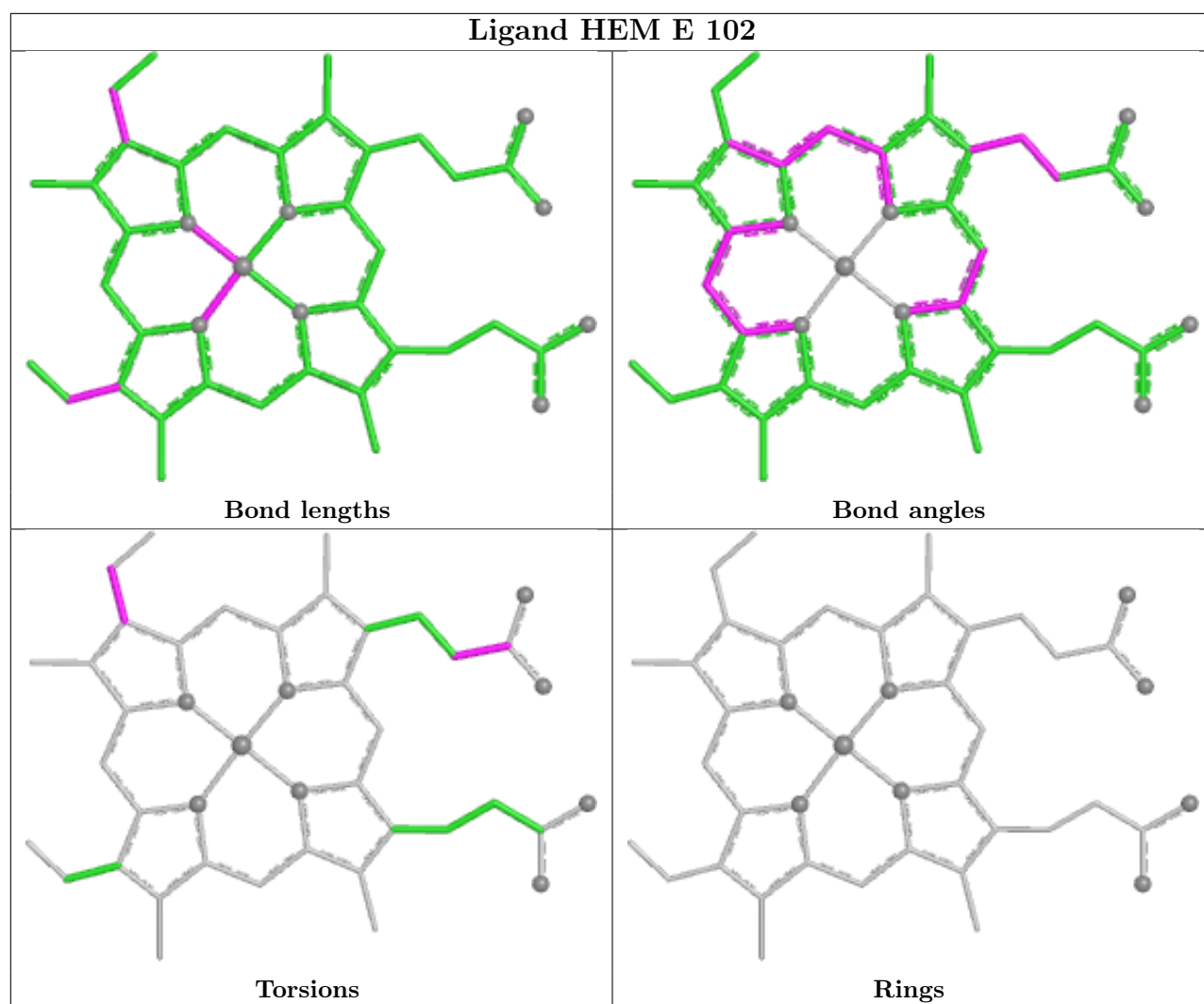


Ligand CLA B 603



Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD h 103	
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.52	0 100 100	23, 33, 56, 83	0
1	a	334/334 (100%)	-0.41	2 (0%) 85 83	23, 36, 67, 90	0
2	B	505/505 (100%)	-0.40	1 (0%) 91 90	18, 38, 71, 113	4 (0%)
2	b	505/505 (100%)	-0.27	3 (0%) 85 83	27, 42, 80, 121	0
3	C	442/451 (98%)	-0.38	0 100 100	25, 42, 61, 86	0
3	c	451/451 (100%)	-0.25	2 (0%) 88 87	23, 46, 69, 116	1 (0%)
4	D	341/341 (100%)	-0.53	0 100 100	24, 35, 55, 97	0
4	d	341/341 (100%)	-0.36	0 100 100	25, 39, 64, 95	1 (0%)
5	E	81/82 (98%)	0.06	0 100 100	32, 55, 75, 81	1 (1%)
5	e	82/82 (100%)	0.30	0 100 100	44, 66, 87, 100	0
6	F	34/34 (100%)	-0.06	1 (2%) 53 50	39, 50, 75, 99	0
6	f	34/34 (100%)	0.26	0 100 100	46, 56, 90, 94	0
7	H	65/65 (100%)	-0.22	0 100 100	35, 45, 66, 74	0
7	h	63/65 (96%)	0.03	1 (1%) 70 67	42, 56, 68, 84	0
8	I	35/36 (97%)	-0.23	0 100 100	34, 44, 78, 88	0
8	i	35/36 (97%)	-0.08	0 100 100	35, 47, 79, 93	0
9	J	36/36 (100%)	-0.06	0 100 100	38, 56, 81, 107	0
9	j	36/36 (100%)	0.17	0 100 100	40, 59, 86, 98	0
10	K	37/37 (100%)	0.15	0 100 100	35, 59, 77, 81	1 (2%)
10	k	37/37 (100%)	0.24	0 100 100	48, 66, 83, 99	0
11	L	37/37 (100%)	-0.52	0 100 100	27, 36, 75, 82	0
11	l	36/37 (97%)	-0.52	0 100 100	29, 37, 82, 86	0
12	M	32/33 (96%)	-0.39	0 100 100	31, 39, 67, 84	0
12	m	31/33 (93%)	-0.45	0 100 100	28, 40, 55, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.20	1 (0%) 88 87	23, 48, 85, 154	1 (0%)
13	o	244/244 (100%)	-0.23	1 (0%) 88 87	26, 46, 90, 131	0
14	T	29/30 (96%)	-0.55	0 100 100	28, 36, 69, 85	0
14	t	29/30 (96%)	-0.34	1 (3%) 48 45	31, 37, 89, 100	0
15	U	97/97 (100%)	-0.23	0 100 100	32, 49, 74, 102	0
15	u	97/97 (100%)	-0.27	1 (1%) 79 77	32, 47, 62, 95	0
16	V	137/137 (100%)	-0.38	0 100 100	31, 45, 62, 87	0
16	v	137/137 (100%)	-0.12	0 100 100	35, 55, 77, 87	0
17	Y	27/30 (90%)	0.90	2 (7%) 20 18	60, 85, 117, 125	0
17	y	30/30 (100%)	0.50	0 100 100	65, 77, 95, 115	0
18	X	38/38 (100%)	-0.02	0 100 100	40, 55, 87, 96	0
18	x	38/38 (100%)	0.03	0 100 100	48, 64, 82, 112	0
19	Z	62/62 (100%)	0.53	2 (3%) 50 47	51, 71, 119, 138	0
19	z	62/62 (100%)	0.70	2 (3%) 50 47	60, 78, 118, 134	0
20	R	34/34 (100%)	0.66	1 (2%) 53 50	60, 78, 102, 106	0
20	r	31/34 (91%)	1.05	3 (9%) 13 10	69, 92, 109, 119	0
All	All	5300/5326 (99%)	-0.25	24 (0%) 87 85	18, 43, 82, 154	9 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	t	30	THR	3.2
19	z	33	TRP	3.2
13	o	58	ASN	2.8
20	R	35	LEU	2.8
3	c	23	ALA	2.6
19	Z	62	VAL	2.6
1	a	11	ALA	2.5
20	r	26	TYR	2.5
20	r	32	GLN	2.5
1	a	248	ILE	2.4
13	O	59	LYS	2.4
17	Y	22	LEU	2.3
6	F	12	SER	2.3
2	b	499	VAL	2.3
2	B	502	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
15	u	53	ALA	2.2
19	Z	33	TRP	2.2
7	h	64	ALA	2.1
20	r	27	ALA	2.1
17	Y	20	ALA	2.1
2	b	495	PHE	2.1
3	c	24	THR	2.1
19	z	30	PRO	2.0
2	b	85	GLY	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
12	FME	M	1	10/11	0.91	0.12	40,50,73,76	0
14	FME	T	1	10/11	0.94	0.09	32,46,75,75	0
14	FME	t	1	10/11	0.94	0.09	33,48,73,78	0
8	FME	i	1	10/11	0.95	0.07	37,52,72,72	0
12	FME	m	1	10/11	0.95	0.10	34,58,78,84	0
8	FME	I	1	10/11	0.95	0.08	39,53,74,74	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
32	UNL	a	415	28/-	0.79	0.13	43,71,87,94	0
32	UNL	T	102	44/-	0.80	0.14	41,55,68,72	0
32	UNL	d	410	43/-	0.80	0.16	33,57,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	UNL	H	103	53/-	0.81	0.14	35,77,97,101	0
32	UNL	b	626	26/-	0.81	0.13	33,59,66,67	0
27	LMG	c	522	48/55	0.81	0.14	50,82,110,114	0
32	UNL	c	523	28/-	0.82	0.12	43,69,80,82	0
27	LMG	b	622	55/55	0.82	0.15	41,78,99,111	0
33	LHG	E	101	49/49	0.82	0.14	51,82,112,120	0
33	LHG	e	101	42/49	0.82	0.13	63,88,113,120	0
27	LMG	b	623	23/55	0.83	0.16	35,66,90,91	0
32	UNL	b	625	55/-	0.84	0.13	44,66,86,91	0
32	UNL	B	627	47/-	0.84	0.15	41,65,89,89	0
26	PL9	A	409	55/55	0.85	0.15	37,62,89,101	0
32	UNL	J	101	28/-	0.85	0.13	49,62,72,75	0
32	UNL	b	624	40/-	0.86	0.12	38,64,80,83	0
32	UNL	C	522	28/-	0.86	0.13	42,59,72,78	0
27	LMG	C	519	48/55	0.86	0.11	43,68,88,96	0
32	UNL	I	101	41/-	0.86	0.14	40,55,77,82	0
28	SQD	A	412	39/54	0.86	0.13	40,69,102,121	0
32	UNL	x	101	55/-	0.86	0.11	47,62,78,78	0
29	DGD	A	413	66/66	0.86	0.12	43,68,93,121	0
27	LMG	D	410	33/55	0.86	0.12	29,57,87,90	0
28	SQD	a	412	36/54	0.87	0.12	29,68,100,110	0
32	UNL	E	103	28/-	0.87	0.14	58,81,95,97	0
23	CLA	h	101	65/65	0.87	0.11	44,72,93,100	0
32	UNL	c	520	55/-	0.87	0.12	42,61,79,90	0
29	DGD	a	413	44/66	0.87	0.13	33,59,88,94	0
32	UNL	B	626	28/-	0.87	0.15	50,75,87,89	0
26	PL9	a	409	55/55	0.87	0.15	34,67,89,101	0
32	UNL	C	521	28/-	0.87	0.13	36,50,61,62	0
32	UNL	b	621	55/-	0.87	0.13	40,62,91,109	0
27	LMG	a	414	49/55	0.88	0.11	36,60,94,101	0
27	LMG	A	410	48/55	0.88	0.10	30,61,81,105	0
32	UNL	m	102	28/-	0.88	0.12	40,55,69,77	0
27	LMG	D	411	28/55	0.88	0.12	30,51,68,74	0
28	SQD	b	601	49/54	0.88	0.10	44,64,103,114	0
32	UNL	b	602	47/-	0.88	0.12	36,59,74,79	0
27	LMG	c	519	37/55	0.89	0.11	34,70,93,96	0
23	CLA	B	601	65/65	0.89	0.11	31,63,100,113	0
32	UNL	l	102	53/-	0.89	0.14	30,48,99,103	0
23	CLA	c	512	65/65	0.89	0.11	39,60,93,109	0
32	UNL	t	103	46/-	0.89	0.12	38,61,81,82	0
32	UNL	M	102	26/-	0.89	0.12	30,53,63,67	0
28	SQD	a	411	54/54	0.89	0.10	36,71,94,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	UNL	B	624	34/-	0.89	0.11	39,55,71,72	0
25	BCR	y	101	40/40	0.90	0.11	41,63,77,84	0
25	BCR	C	514	40/40	0.90	0.10	34,59,76,77	0
25	BCR	D	405	40/40	0.90	0.10	29,46,100,116	0
25	BCR	c	514	40/40	0.90	0.10	37,58,73,75	0
27	LMG	B	620	51/55	0.90	0.09	29,51,72,81	0
32	UNL	j	101	28/-	0.90	0.11	42,60,71,74	0
32	UNL	B	621	43/-	0.90	0.10	38,54,69,73	0
25	BCR	d	405	40/40	0.90	0.10	36,57,95,108	0
32	UNL	t	102	26/-	0.90	0.11	42,56,67,68	0
32	UNL	B	625	28/-	0.90	0.10	29,46,67,72	0
27	LMG	m	101	51/55	0.90	0.10	29,52,83,98	0
25	BCR	h	102	40/40	0.90	0.10	33,56,73,81	0
28	SQD	B	623	54/54	0.90	0.10	37,62,88,98	0
25	BCR	c	521	40/40	0.91	0.11	34,57,70,77	0
32	UNL	C	523	47/-	0.91	0.10	39,52,63,69	0
32	UNL	D	412	55/-	0.91	0.11	32,51,79,101	0
23	CLA	c	513	65/65	0.91	0.10	42,75,107,123	0
28	SQD	f	101	41/54	0.91	0.12	49,85,120,123	0
25	BCR	K	101	40/40	0.91	0.09	41,56,68,75	0
25	BCR	C	520	40/40	0.91	0.12	38,55,67,74	0
32	UNL	M	101	37/-	0.91	0.11	30,49,71,75	0
29	DGD	h	103	62/66	0.91	0.10	35,54,73,79	0
29	DGD	C	517	62/66	0.92	0.10	31,56,95,117	0
23	CLA	C	513	65/65	0.92	0.10	40,70,102,114	0
27	LMG	d	409	44/55	0.92	0.09	31,53,84,107	0
25	BCR	B	617	40/40	0.92	0.09	26,43,57,60	0
25	BCR	T	101	40/40	0.92	0.08	29,43,58,68	0
25	BCR	b	619	40/40	0.92	0.07	25,42,59,66	0
29	DGD	c	517	62/66	0.93	0.08	32,52,81,95	0
29	DGD	c	518	62/66	0.93	0.09	26,54,77,93	0
23	CLA	c	511	65/65	0.93	0.10	34,62,79,87	0
23	CLA	C	511	65/65	0.93	0.09	33,57,78,85	0
23	CLA	C	512	65/65	0.93	0.10	36,61,111,127	0
25	BCR	H	101	40/40	0.93	0.07	32,46,59,66	0
28	SQD	A	411	52/54	0.93	0.09	30,64,88,97	0
23	CLA	C	510	65/65	0.93	0.08	31,51,78,88	0
24	PHO	d	401	64/64	0.93	0.08	27,42,52,57	0
28	SQD	F	101	36/54	0.93	0.10	43,66,89,96	0
25	BCR	a	408	40/40	0.93	0.07	25,35,50,55	0
25	BCR	b	618	40/40	0.93	0.07	25,46,57,65	0
23	CLA	c	503	65/65	0.93	0.08	31,48,61,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	b	620	40/40	0.93	0.08	30,50,66,69	0
25	BCR	B	618	40/40	0.93	0.07	25,43,58,64	0
25	BCR	c	515	40/40	0.93	0.10	32,49,69,77	0
29	DGD	H	102	62/66	0.93	0.09	28,49,67,77	0
33	LHG	a	410	49/49	0.93	0.10	38,53,87,104	0
25	BCR	B	619	40/40	0.93	0.08	33,47,58,62	0
33	LHG	l	101	49/49	0.93	0.09	31,49,66,78	0
27	LMG	D	407	51/55	0.94	0.10	27,59,79,87	0
23	CLA	B	606	65/65	0.94	0.08	21,41,75,98	0
23	CLA	B	615	65/65	0.94	0.08	20,41,67,95	0
23	CLA	B	616	60/65	0.94	0.09	27,44,87,103	0
23	CLA	C	503	65/65	0.94	0.07	27,44,56,69	0
25	BCR	A	408	40/40	0.94	0.07	24,34,42,56	0
31	BCT	A	415	4/4	0.94	0.07	31,36,37,44	0
23	CLA	b	610	65/65	0.94	0.08	28,46,65,77	0
23	CLA	b	615	65/65	0.94	0.08	23,44,73,79	0
23	CLA	b	616	65/65	0.94	0.08	20,40,63,68	0
23	CLA	C	505	65/65	0.94	0.09	24,42,75,88	0
25	BCR	t	101	40/40	0.94	0.07	27,42,57,61	0
25	BCR	C	515	40/40	0.94	0.08	21,38,53,67	0
23	CLA	c	505	65/65	0.94	0.08	26,44,62,69	0
26	PL9	D	406	55/55	0.94	0.07	22,36,51,54	0
23	CLA	c	506	65/65	0.94	0.10	32,53,112,129	0
26	PL9	d	406	55/55	0.94	0.07	23,37,48,48	0
33	LHG	B	622	49/49	0.94	0.09	26,46,73,77	0
33	LHG	D	409	47/49	0.94	0.09	25,51,82,101	0
23	CLA	c	508	64/65	0.94	0.08	32,51,98,118	0
23	CLA	c	509	65/65	0.94	0.09	28,49,74,79	0
33	LHG	d	408	39/49	0.94	0.09	36,50,75,78	0
23	CLA	C	508	65/65	0.94	0.08	27,46,102,120	0
29	DGD	C	516	62/66	0.94	0.09	21,40,76,98	0
29	DGD	C	518	62/66	0.95	0.07	28,47,84,98	0
23	CLA	C	507	65/65	0.95	0.07	22,39,51,59	0
23	CLA	D	403	65/65	0.95	0.07	15,34,60,62	0
29	DGD	c	516	62/66	0.95	0.08	20,45,71,80	0
23	CLA	a	405	65/65	0.95	0.08	25,42,98,111	0
23	CLA	c	510	65/65	0.95	0.08	30,51,72,79	0
23	CLA	b	603	65/65	0.95	0.08	29,47,74,80	0
23	CLA	b	604	65/65	0.95	0.07	24,41,67,69	0
23	CLA	b	607	65/65	0.95	0.08	25,46,80,86	0
23	CLA	d	402	65/65	0.95	0.07	22,34,43,51	0
23	CLA	d	403	65/65	0.95	0.07	20,38,63,75	0

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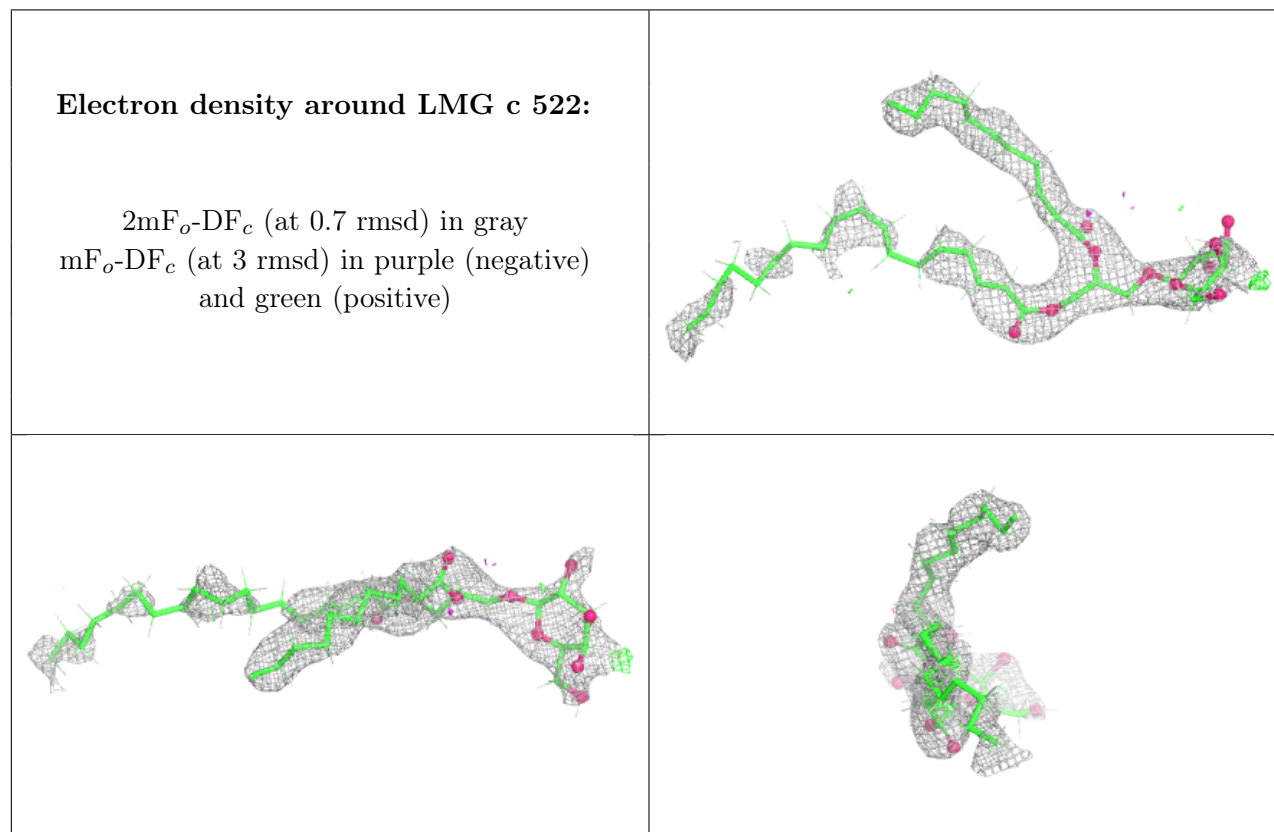
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	d	404	65/65	0.95	0.08	25,53,100,107	0
23	CLA	b	609	65/65	0.95	0.07	26,43,65,70	0
24	PHO	a	406	64/64	0.95	0.07	22,34,46,48	0
23	CLA	C	502	65/65	0.95	0.07	25,42,62,68	0
23	CLA	b	613	65/65	0.95	0.07	17,35,49,56	0
23	CLA	C	509	65/65	0.95	0.08	27,46,61,74	0
23	CLA	B	609	65/65	0.95	0.07	23,37,52,63	0
23	CLA	c	501	65/65	0.95	0.07	25,42,59,68	0
33	LHG	L	101	49/49	0.95	0.07	28,45,61,67	0
23	CLA	c	502	65/65	0.95	0.08	24,46,76,85	0
33	LHG	d	407	49/49	0.95	0.08	26,45,64,80	0
23	CLA	B	613	65/65	0.95	0.07	17,34,63,74	0
23	CLA	c	504	60/65	0.95	0.07	24,47,79,81	0
23	CLA	C	506	65/65	0.95	0.09	28,45,95,114	0
23	CLA	A	404	65/65	0.96	0.06	16,29,43,51	0
23	CLA	B	610	65/65	0.96	0.07	18,33,48,50	0
24	PHO	A	406	64/64	0.96	0.06	17,30,42,53	0
24	PHO	D	401	64/64	0.96	0.06	23,35,46,51	0
23	CLA	b	611	65/65	0.96	0.08	25,39,59,60	0
23	CLA	b	612	65/65	0.96	0.06	18,36,51,56	0
23	CLA	B	611	65/65	0.96	0.06	19,32,49,53	0
23	CLA	b	614	65/65	0.96	0.07	19,33,86,94	0
23	CLA	B	612	65/65	0.96	0.07	17,32,57,69	0
23	CLA	B	602	65/65	0.96	0.07	24,39,68,80	0
23	CLA	b	617	60/65	0.96	0.08	26,49,99,106	0
23	CLA	B	614	65/65	0.96	0.08	22,41,85,96	0
23	CLA	B	603	65/65	0.96	0.07	18,34,60,70	0
23	CLA	B	604	65/65	0.96	0.08	21,36,84,94	0
23	CLA	D	402	65/65	0.96	0.06	17,29,54,61	0
23	CLA	C	501	65/65	0.96	0.07	24,37,54,64	0
23	CLA	D	404	65/65	0.96	0.08	19,42,114,122	0
23	CLA	c	507	65/65	0.96	0.07	28,45,63,74	0
33	LHG	D	408	49/49	0.96	0.07	22,43,59,74	0
23	CLA	a	404	65/65	0.96	0.06	20,32,45,53	0
23	CLA	B	605	65/65	0.96	0.07	18,33,47,57	0
23	CLA	a	407	65/65	0.96	0.08	15,37,99,110	0
23	CLA	A	405	65/65	0.96	0.08	23,36,106,121	0
23	CLA	C	504	59/65	0.96	0.08	22,44,81,96	0
23	CLA	b	605	65/65	0.96	0.08	20,39,87,103	0
23	CLA	b	606	65/65	0.96	0.07	21,36,53,59	0
23	CLA	B	607	65/65	0.96	0.08	18,35,71,85	0
23	CLA	b	608	65/65	0.97	0.07	19,37,78,96	0

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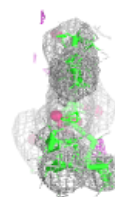
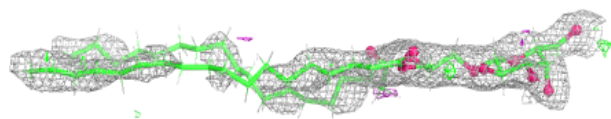
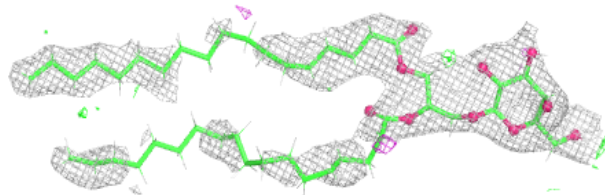
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	A	407	54/65	0.97	0.06	12,31,68,79	0
31	BCT	a	417	4/4	0.97	0.05	30,37,42,45	0
23	CLA	B	608	65/65	0.97	0.06	19,37,56,61	0
34	HEM	E	102	43/43	0.97	0.08	33,52,67,72	0
34	HEM	e	102	43/43	0.97	0.09	39,56,79,91	0
22	CL	A	402	1/1	0.98	0.04	26,26,26,26	0
22	CL	a	403	1/1	0.98	0.09	29,29,29,29	0
35	HEC	V	201	43/43	0.98	0.06	25,34,45,49	0
35	HEC	v	201	43/43	0.98	0.07	26,38,52,54	0
30	OEY	a	416	11/11	0.99	0.03	24,30,34,35	0
21	FE2	a	401	1/1	0.99	0.02	37,37,37,37	0
21	FE2	A	401	1/1	0.99	0.01	33,33,33,33	0
22	CL	A	403	1/1	1.00	0.04	25,25,25,25	0
22	CL	a	402	1/1	1.00	0.04	31,31,31,31	0
30	OEY	A	414	11/11	1.00	0.02	28,31,39,43	1

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.



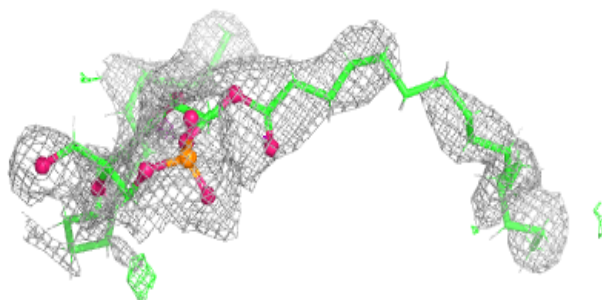
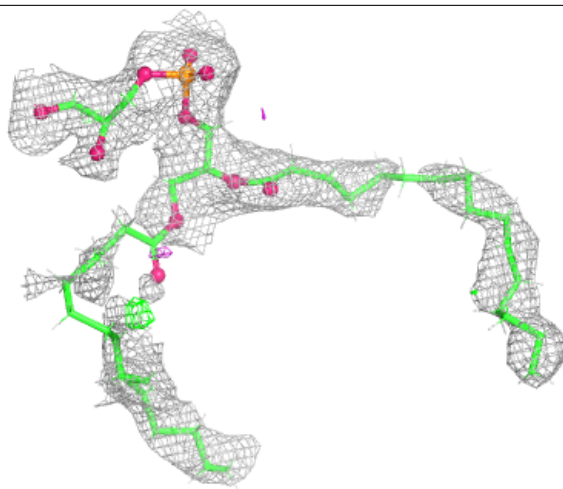
Electron density around LMG b 622:

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



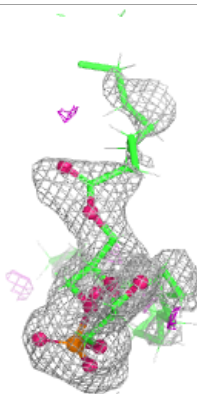
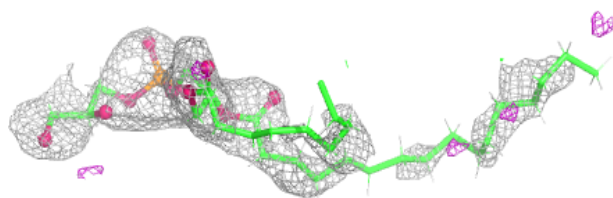
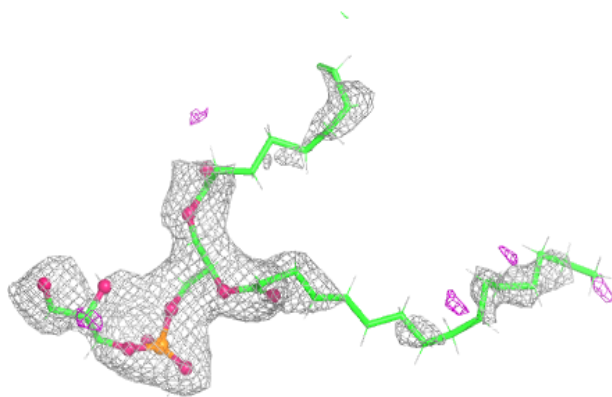
Electron density around LHG E 101:

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

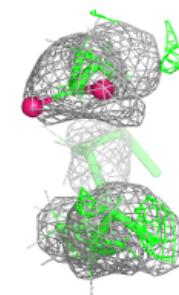
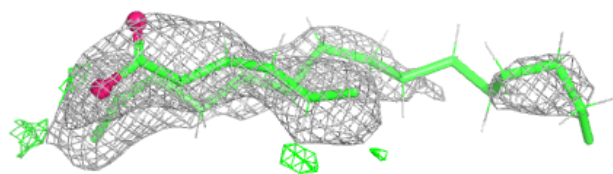
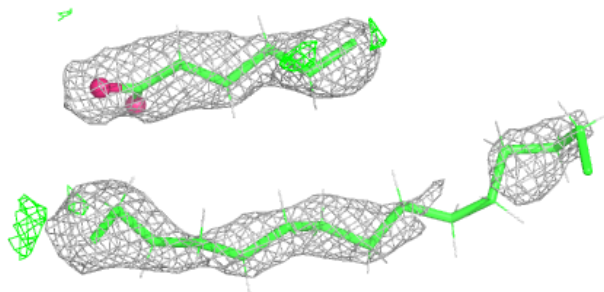


Electron density around LHG e 101:

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

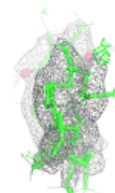
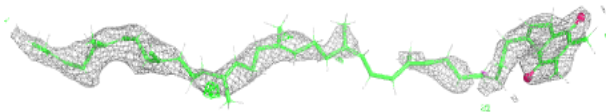
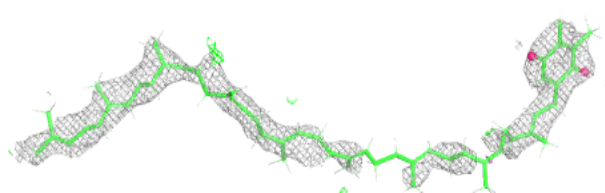
**Electron density around LMG b 623:**

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



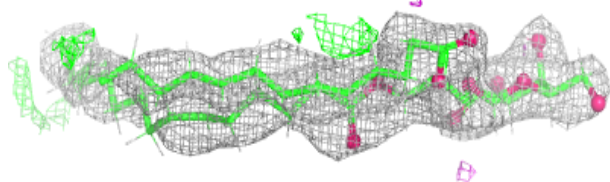
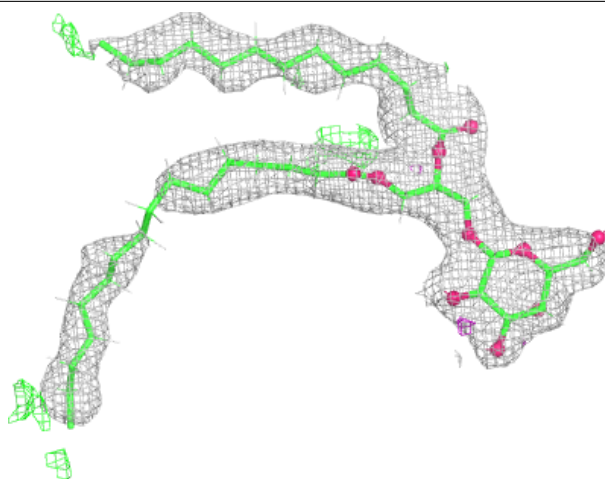
Electron density around PL9 A 409:

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



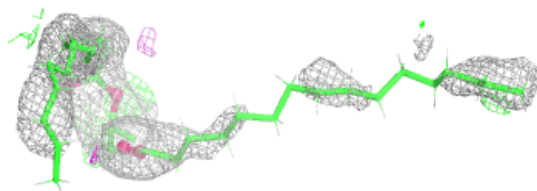
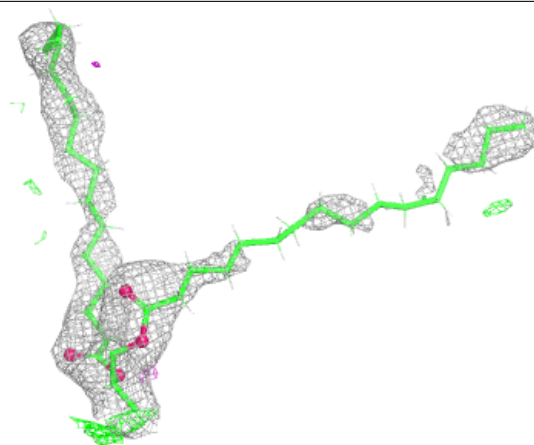
Electron density around LMG C 519:

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

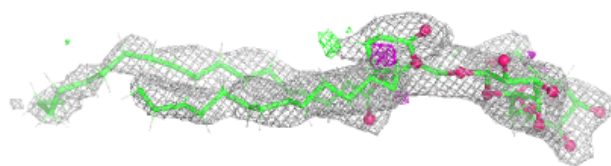
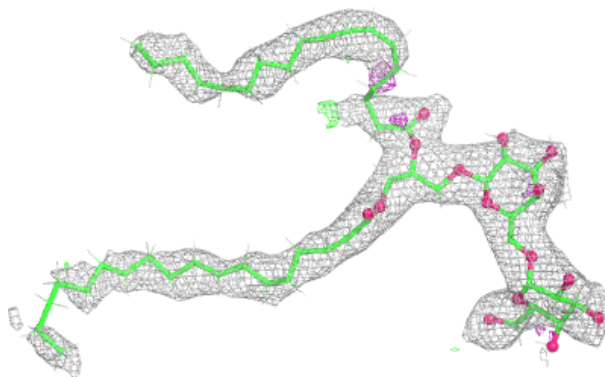


Electron density around SQD A 412:

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

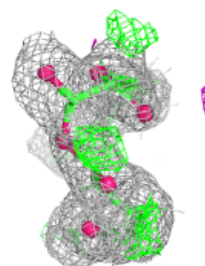
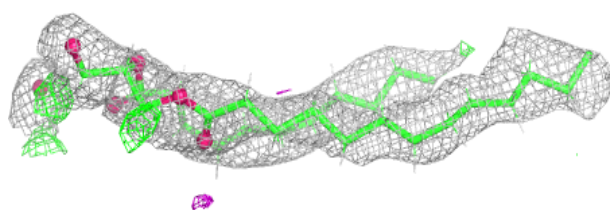
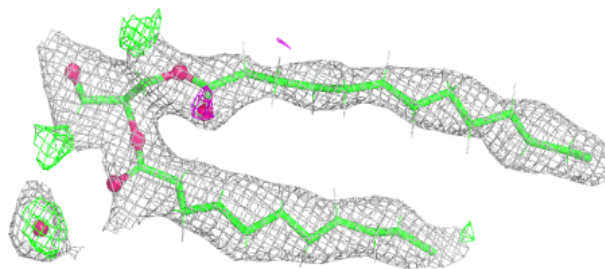
**Electron density around DGD A 413:**

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



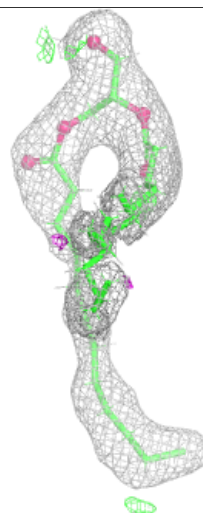
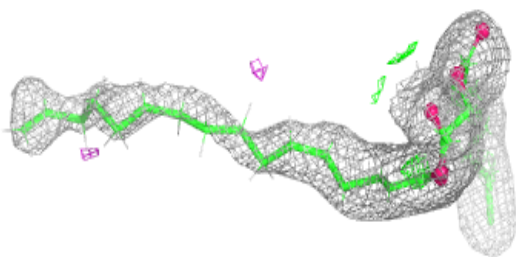
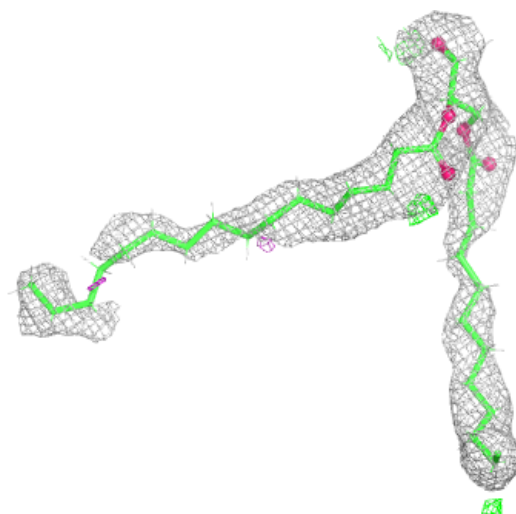
Electron density around LMG D 410:

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



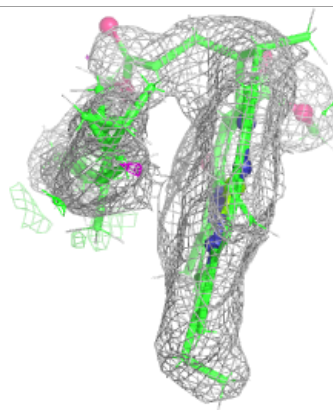
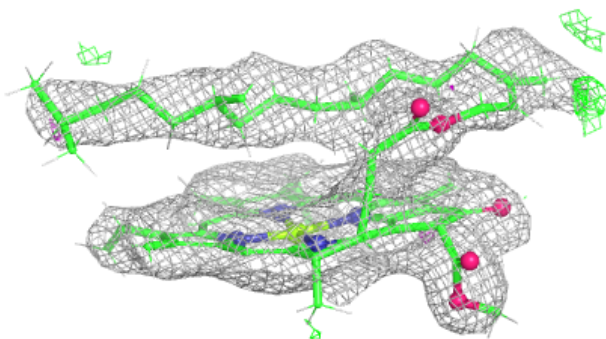
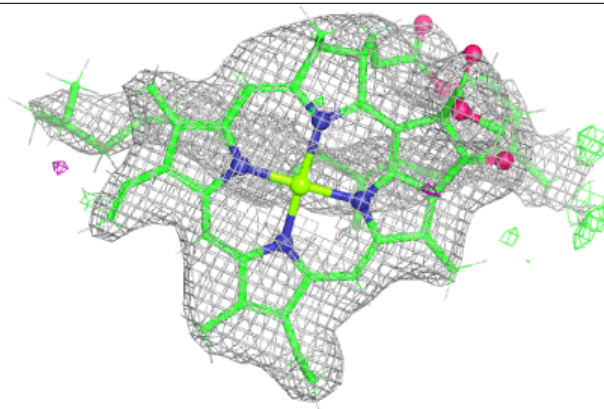
Electron density around SQD a 412:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

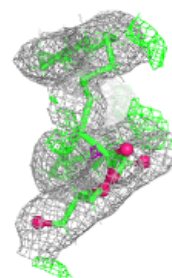
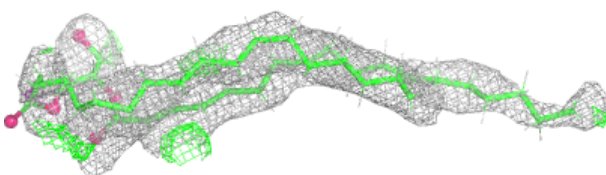
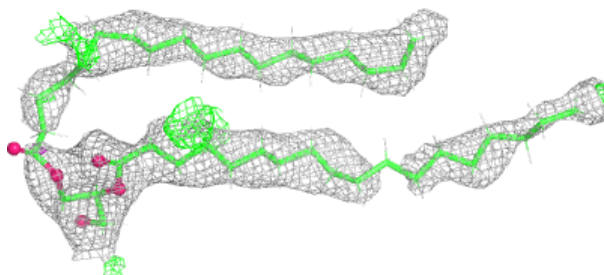


Electron density around CLA h 101:

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

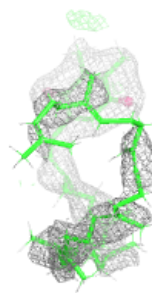
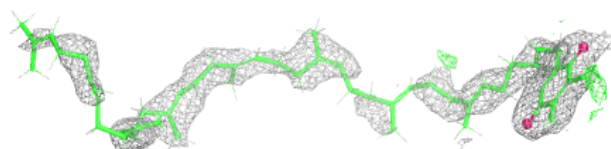
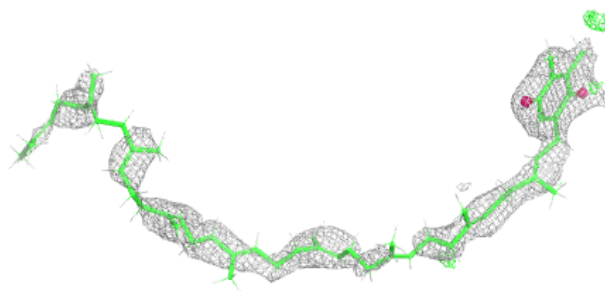
**Electron density around DGD a 413:**

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and green (positive)

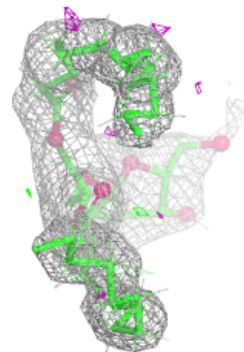
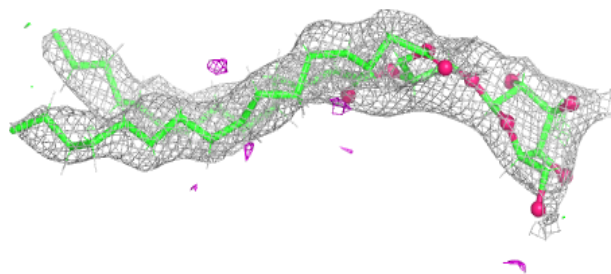
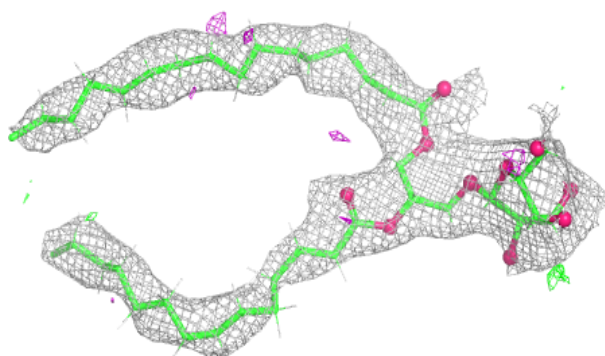


Electron density around PL9 a 409:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

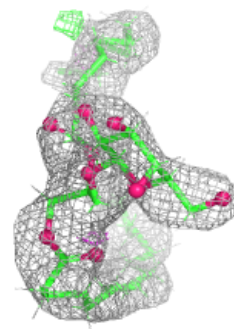
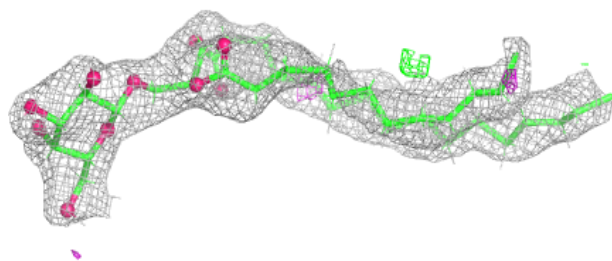
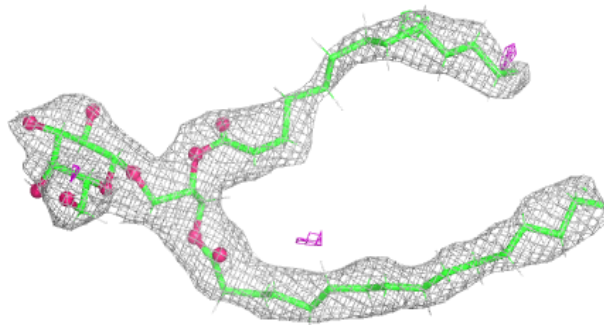
**Electron density around LMG a 414:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

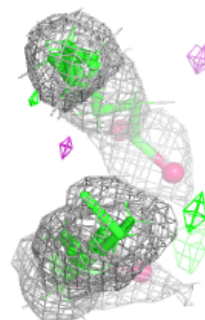
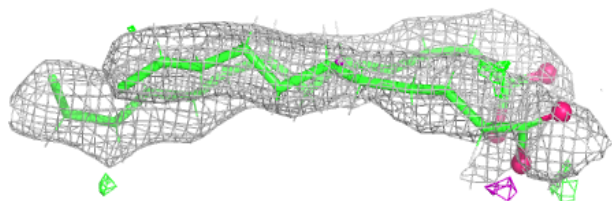
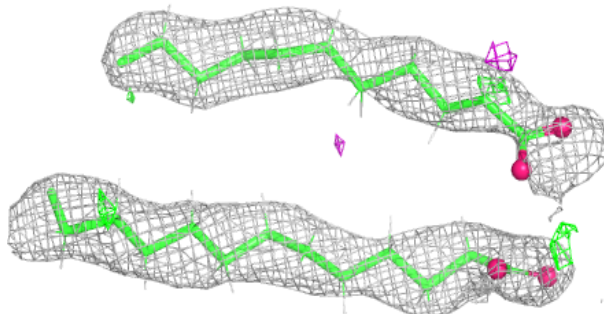


Electron density around LMG A 410:

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

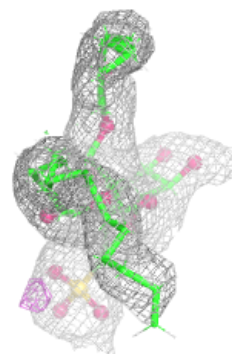
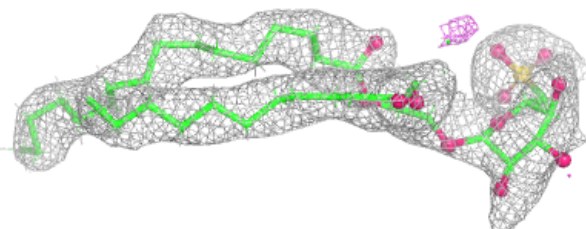
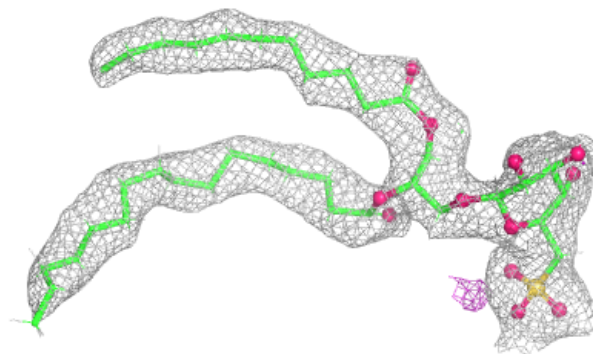
**Electron density around LMG D 411:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

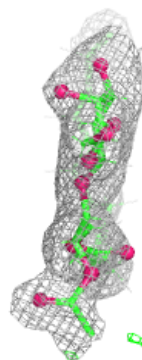
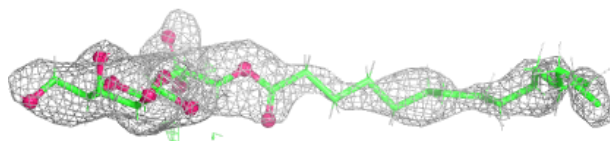
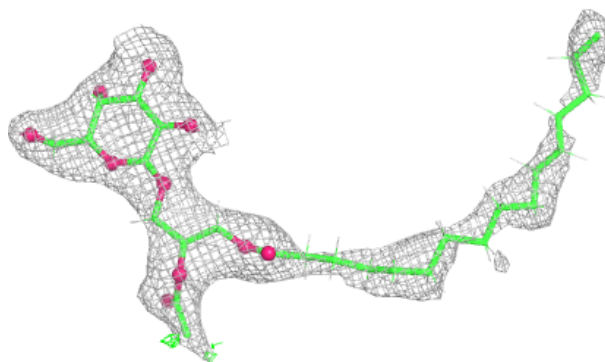


Electron density around SQD b 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

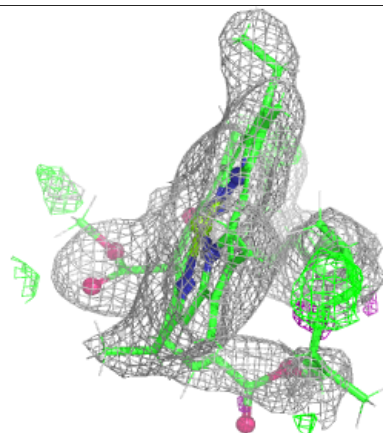
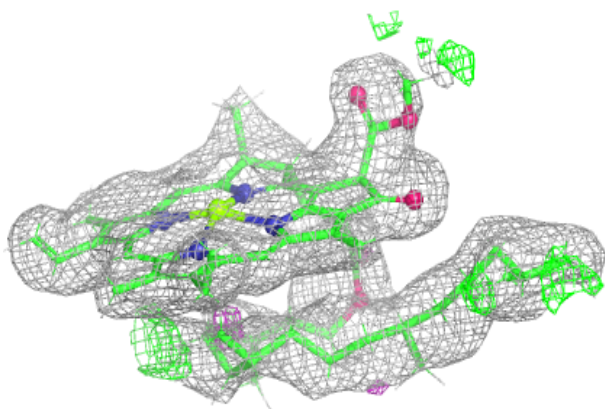
**Electron density around LMG c 519:**

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



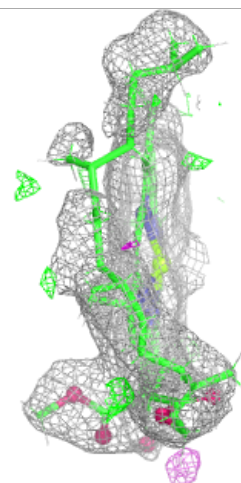
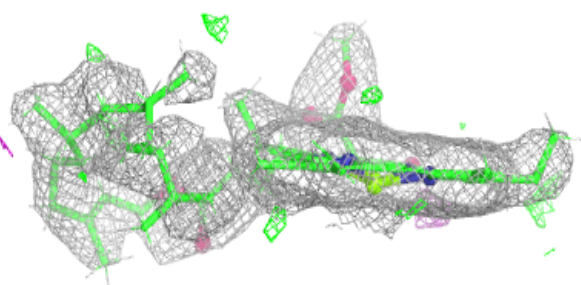
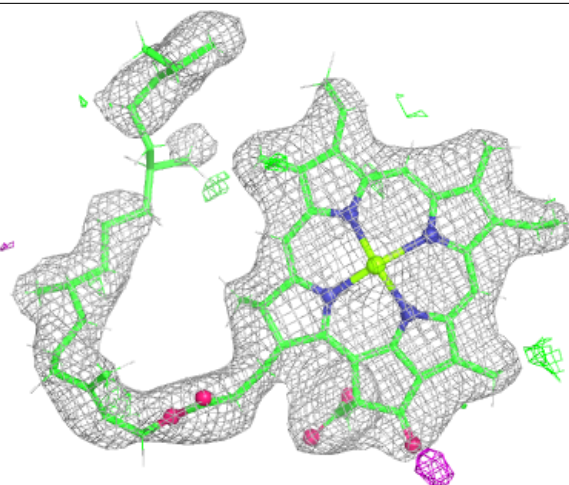
Electron density around CLA B 601:

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



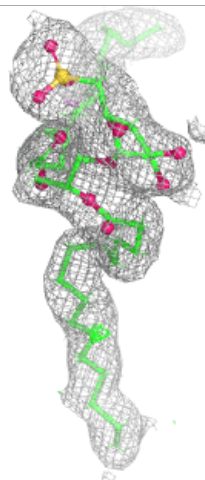
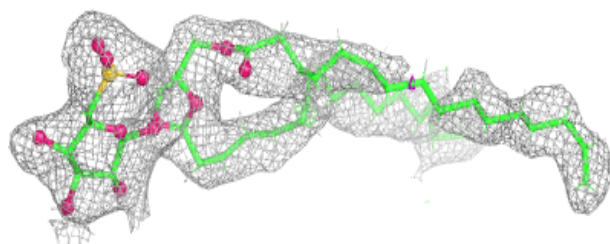
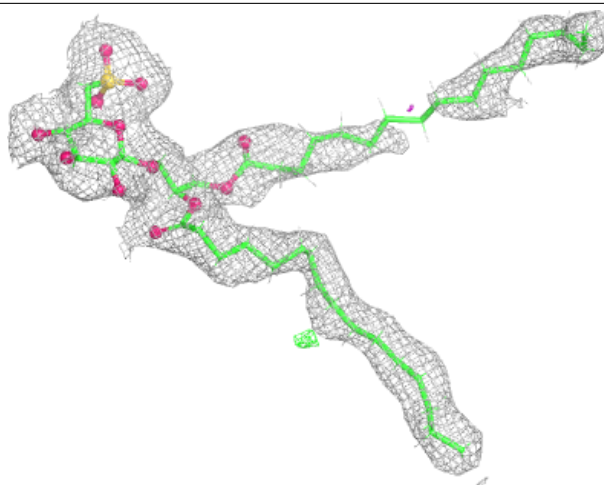
Electron density around CLA c 512:

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



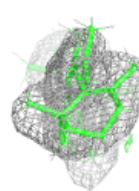
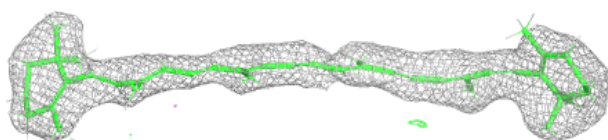
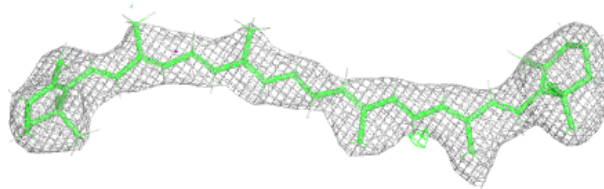
Electron density around SQD a 411:

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

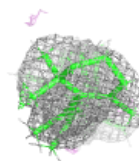
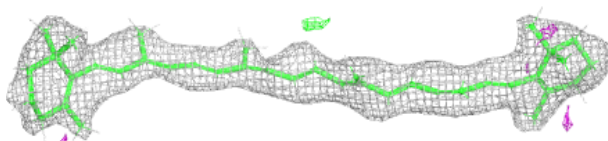
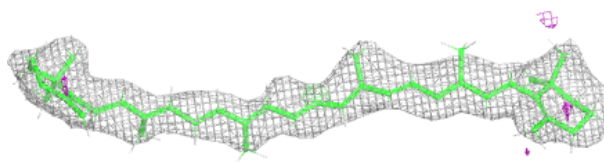


Electron density around BCR y 101:

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

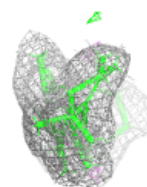
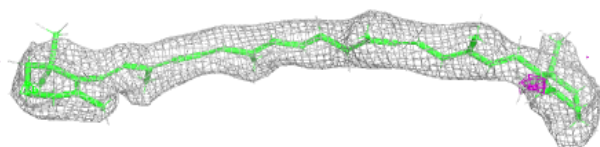
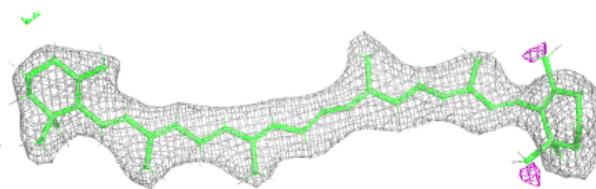
**Electron density around BCR C 514:**

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

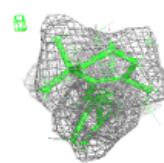
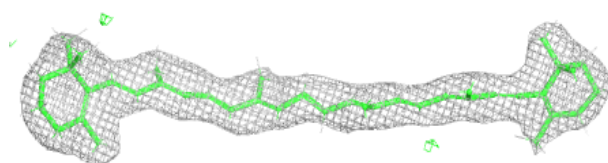


Electron density around BCR D 405:

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

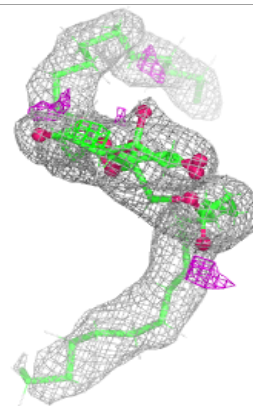
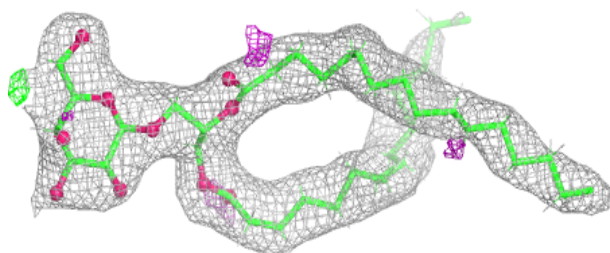
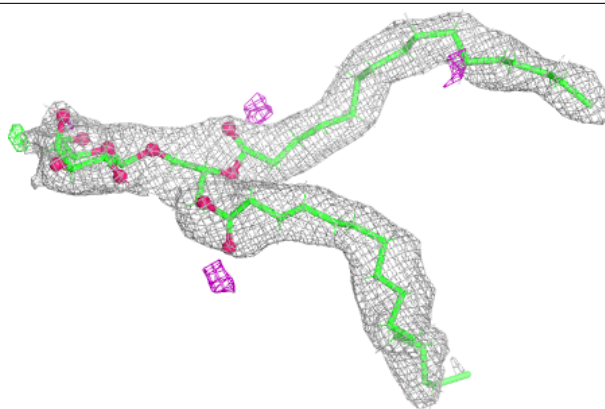
**Electron density around BCR c 514:**

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

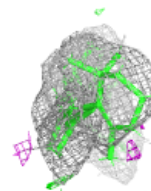
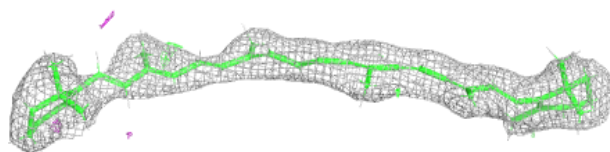
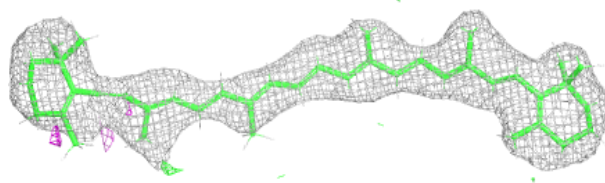


Electron density around LMG B 620:

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

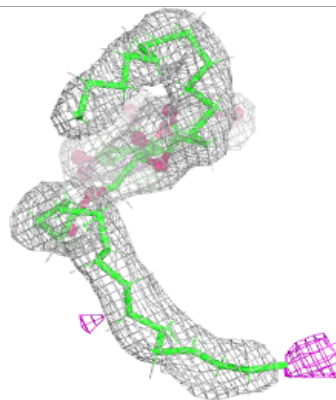
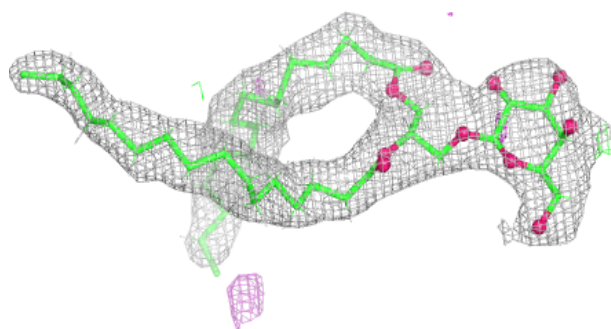
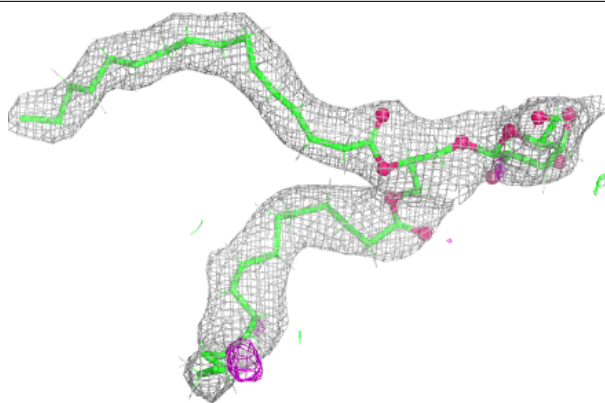
**Electron density around BCR d 405:**

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

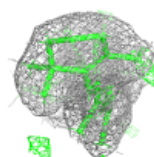
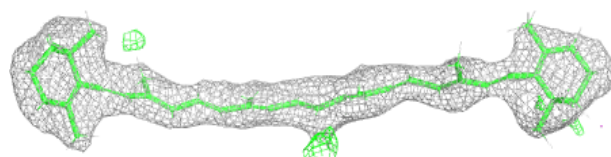
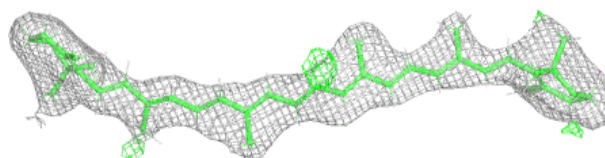


Electron density around LMG m 101:

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

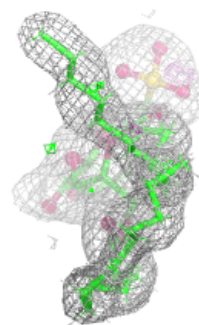
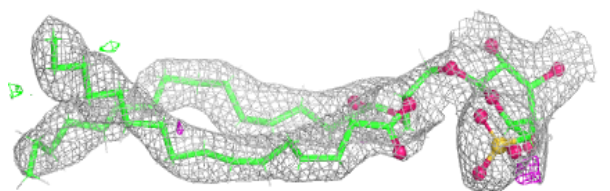
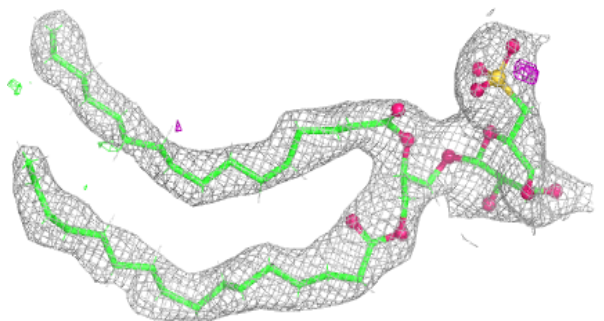
**Electron density around BCR h 102:**

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

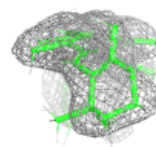
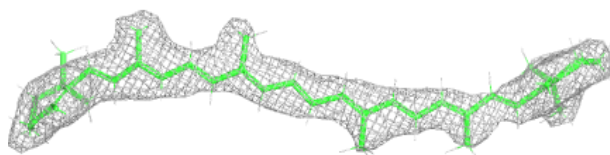
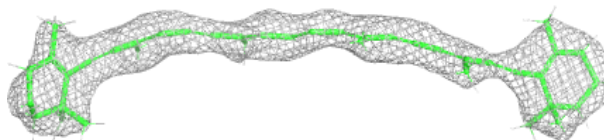


Electron density around SQD B 623:

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

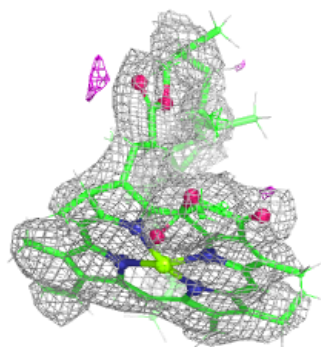
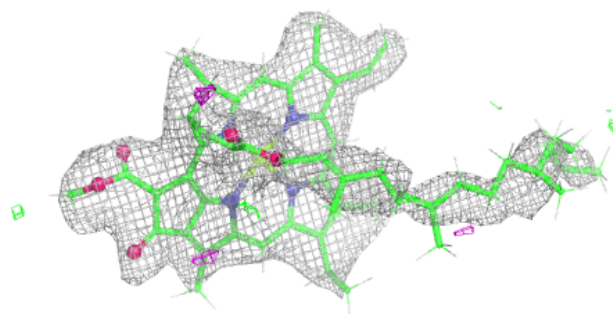
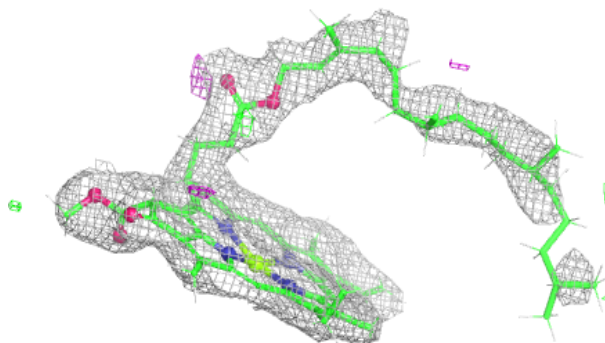
**Electron density around BCR c 521:**

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

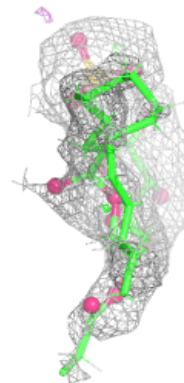
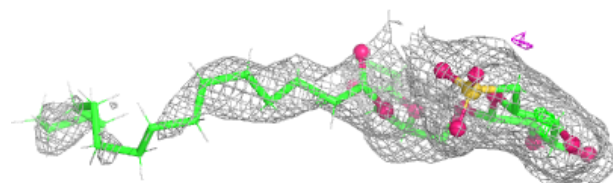
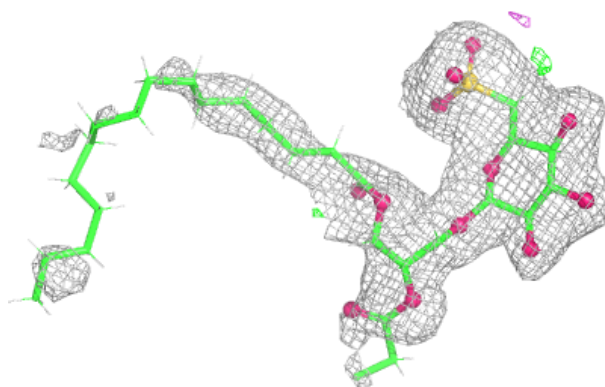


Electron density around CLA c 513:

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

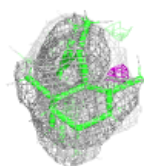
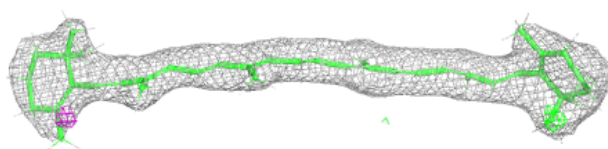
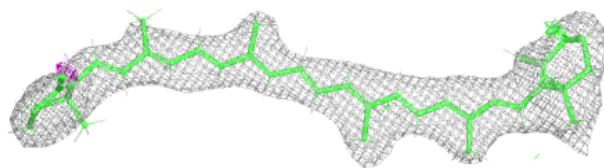
**Electron density around SQD f 101:**

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

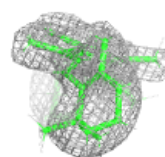
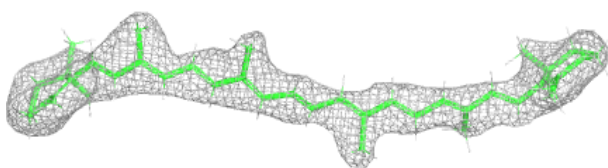
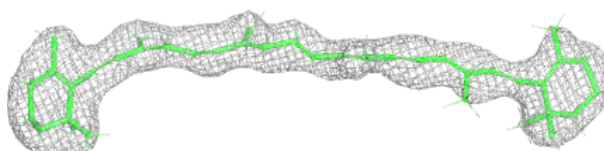


Electron density around BCR K 101:

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

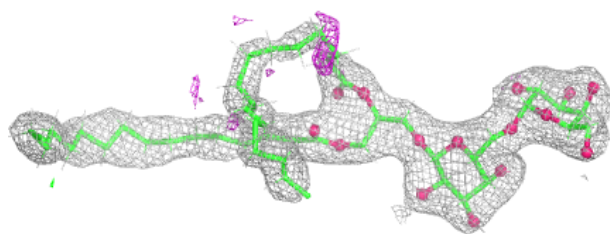
**Electron density around BCR C 520:**

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

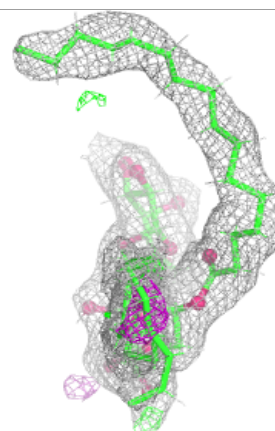
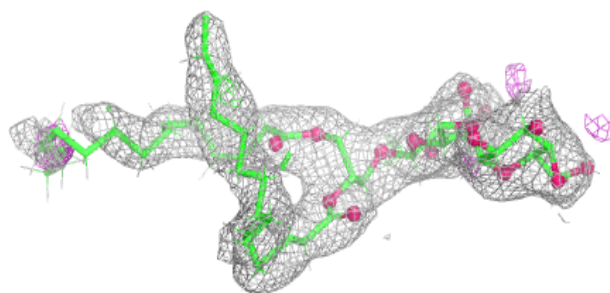
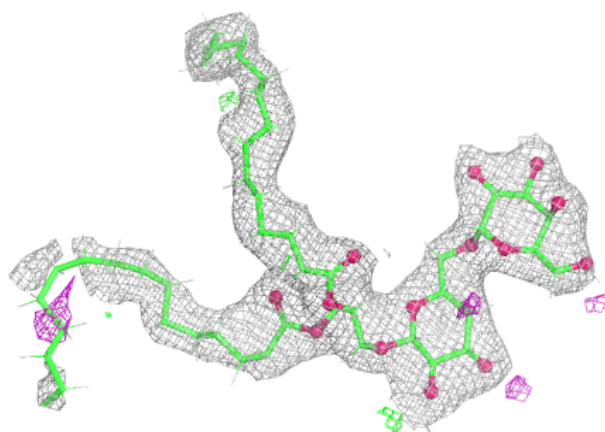


Electron density around DGD h 103:

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

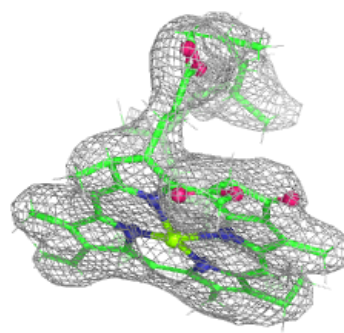
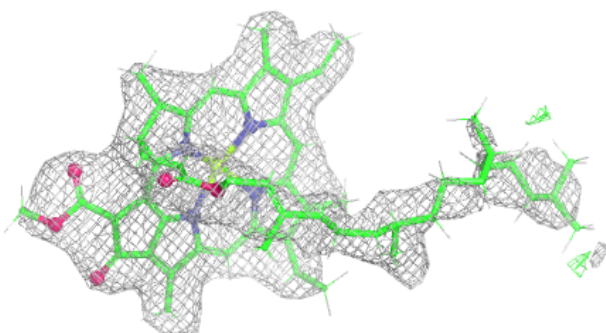
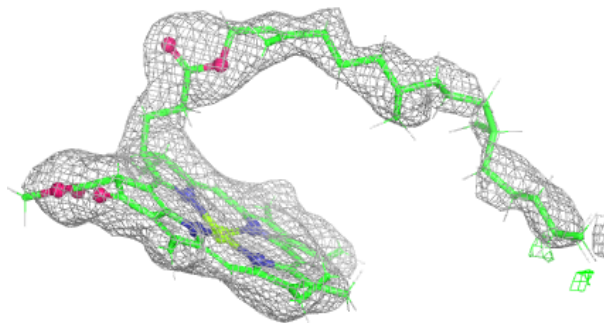
**Electron density around DGD C 517:**

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

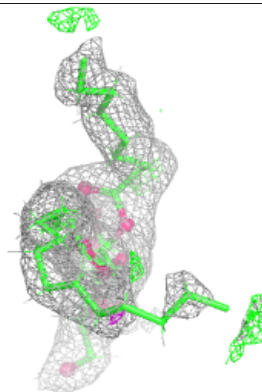
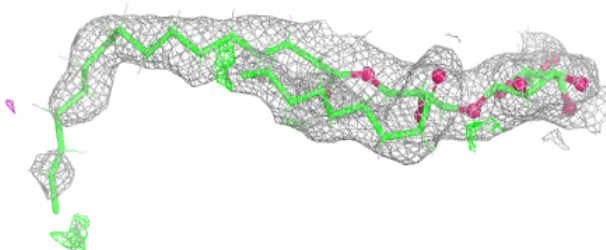
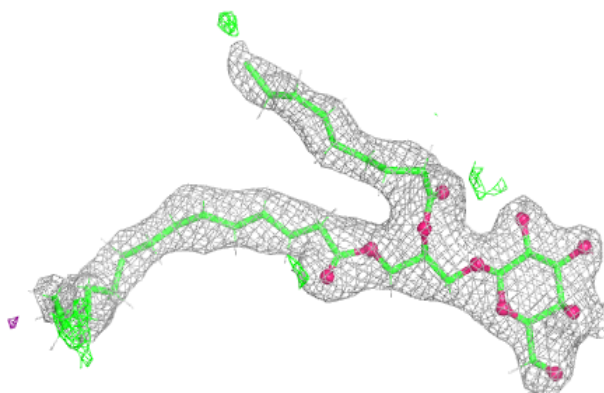


Electron density around CLA C 513:

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

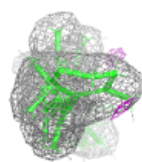
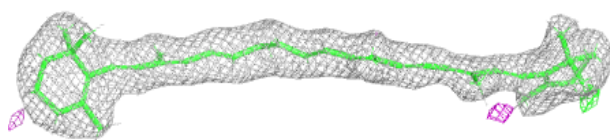
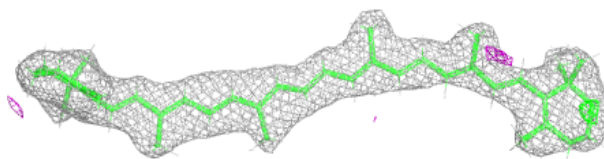
**Electron density around LMG d 409:**

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

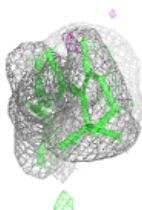
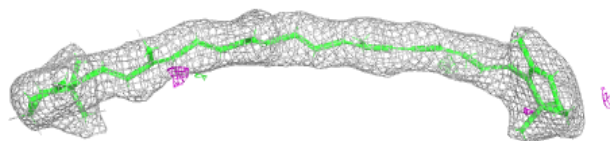
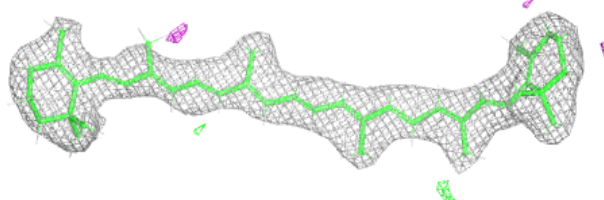


Electron density around BCR B 617:

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

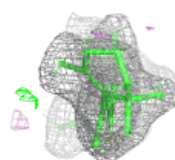
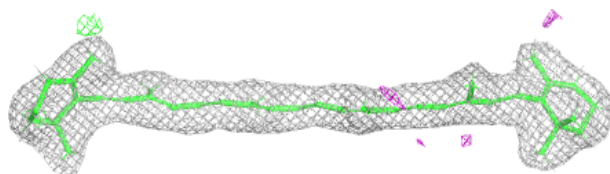
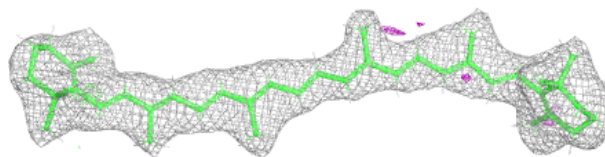
**Electron density around BCR T 101:**

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

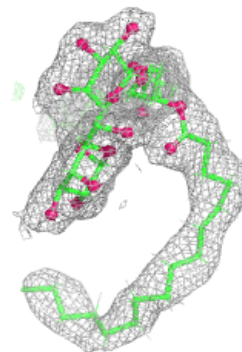
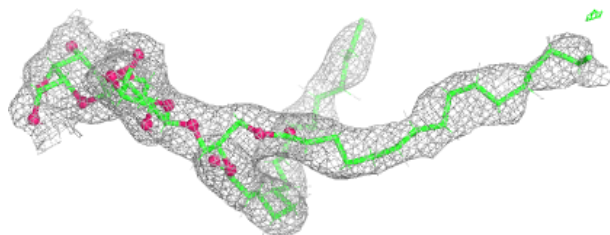
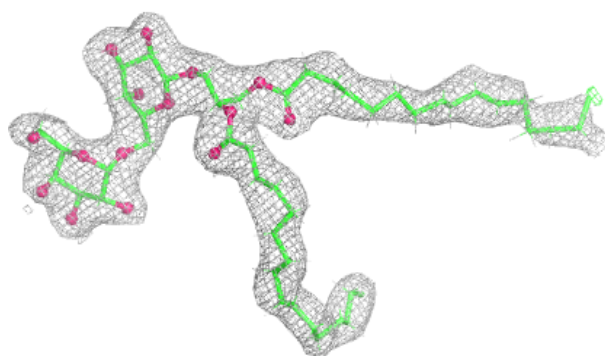


Electron density around BCR b 619:

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

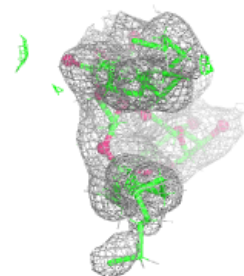
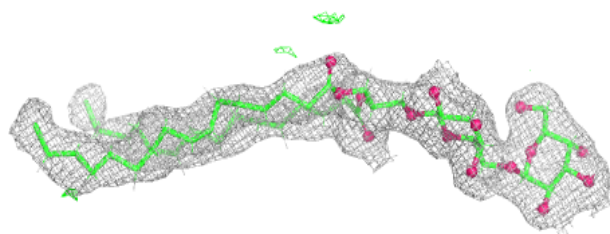
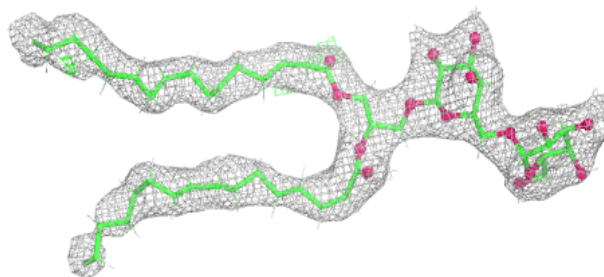
**Electron density around DGD c 517:**

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

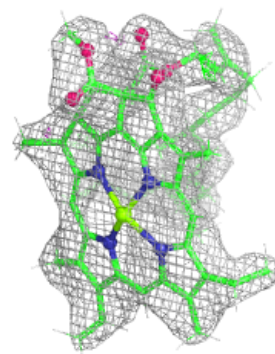
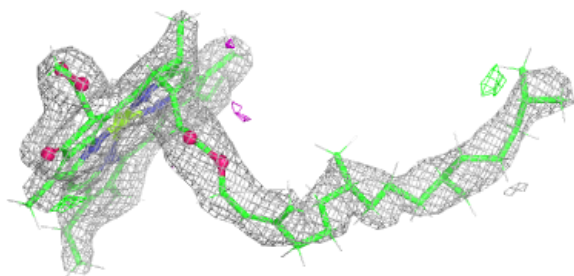
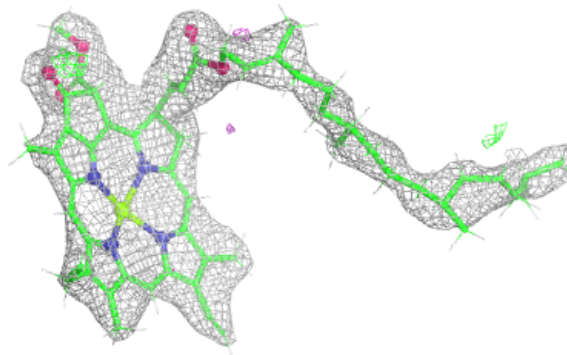


Electron density around DGD c 518:

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

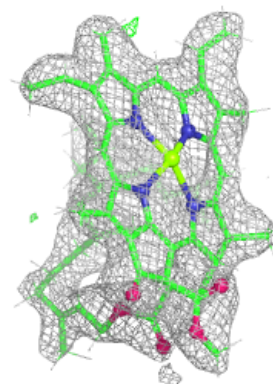
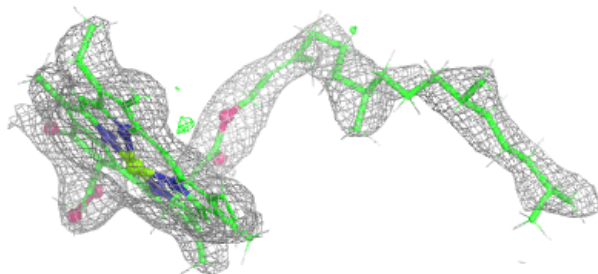
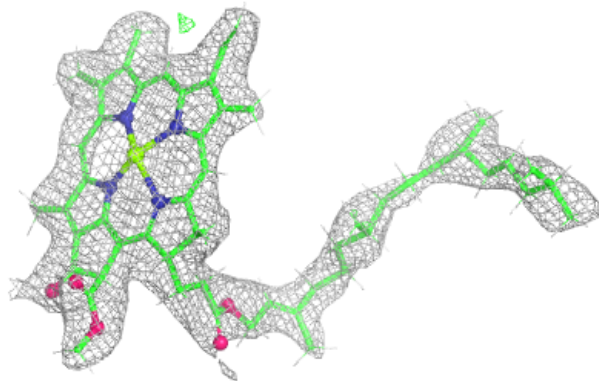
**Electron density around CLA c 511:**

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



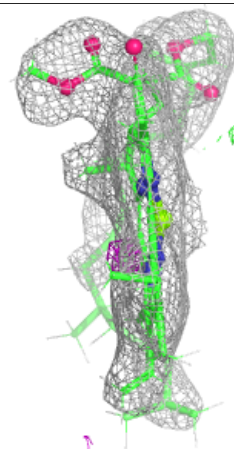
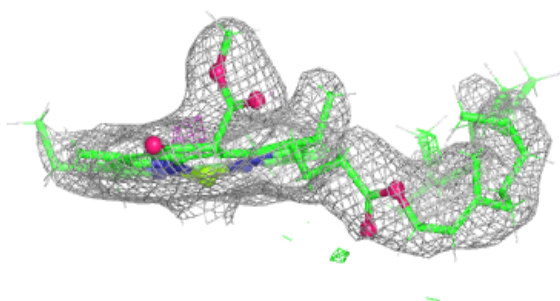
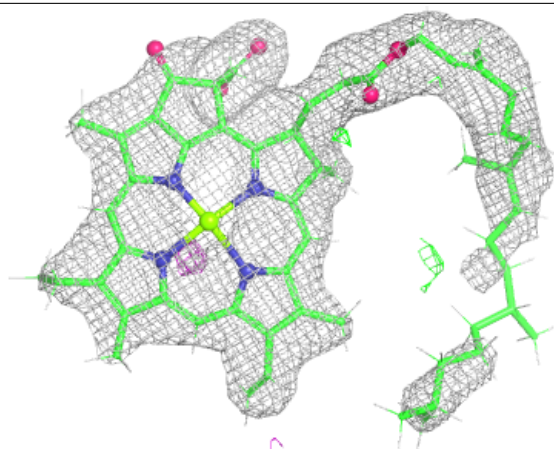
Electron density around CLA C 511:

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

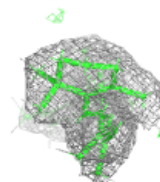
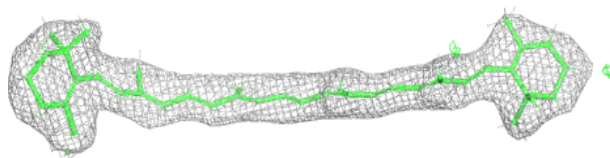
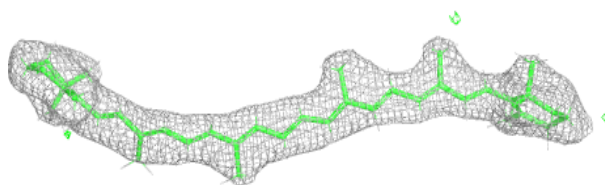


Electron density around CLA C 512:

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

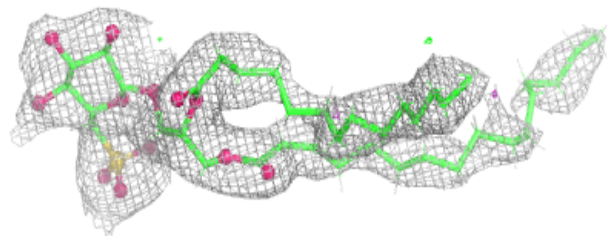
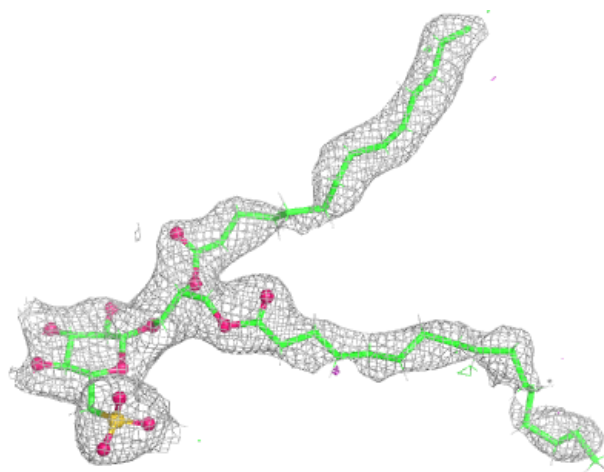
**Electron density around BCR H 101:**

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



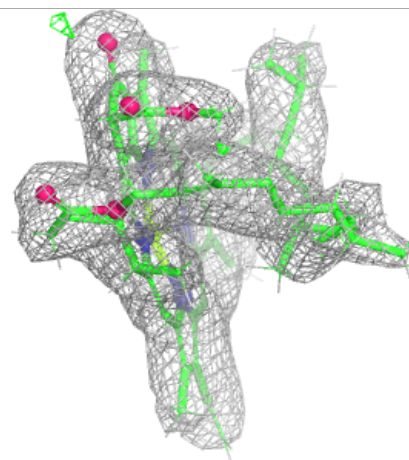
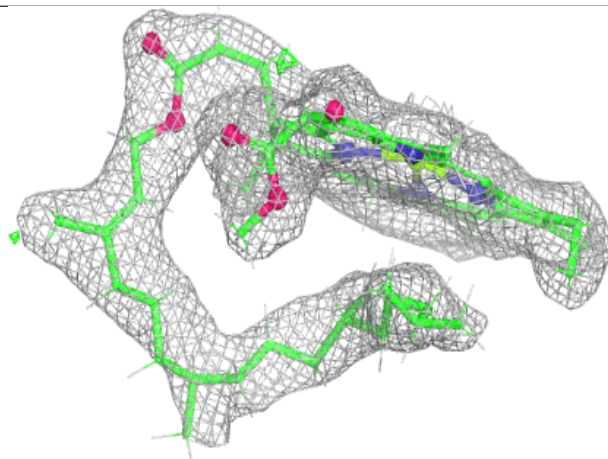
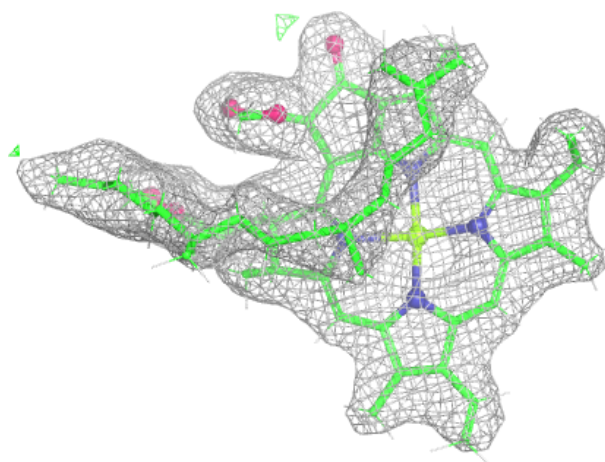
Electron density around SQD A 411:

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



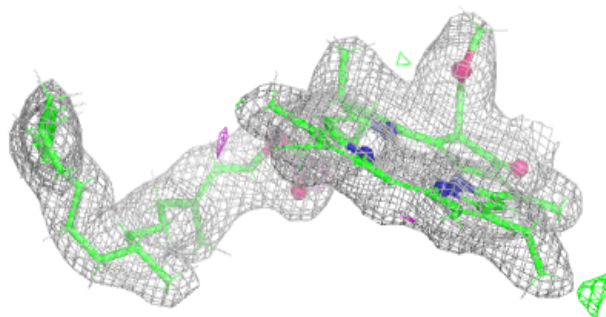
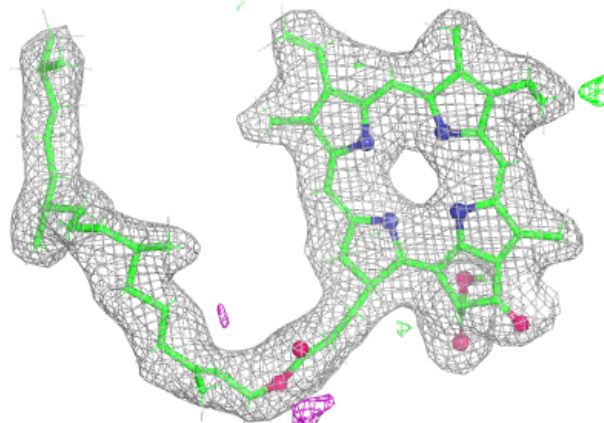
Electron density around CLA C 510:

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



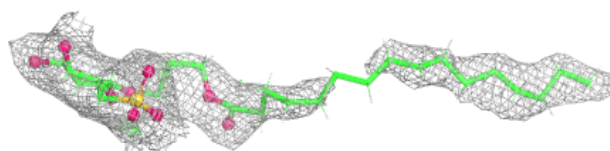
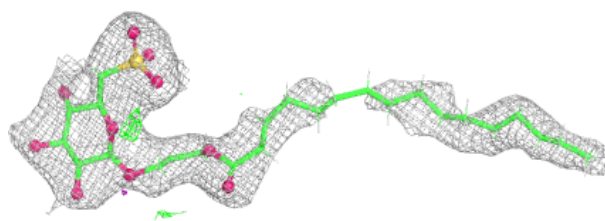
Electron density around PHO d 401:

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

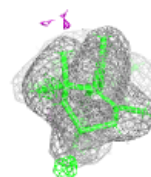
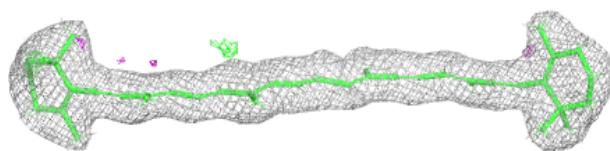
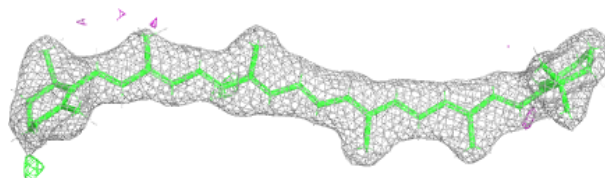


Electron density around SQD F 101:

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

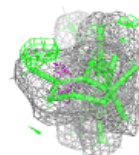
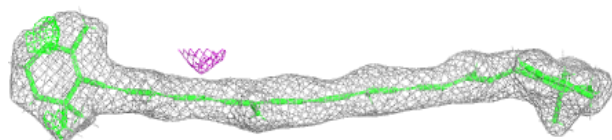
**Electron density around BCR a 408:**

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

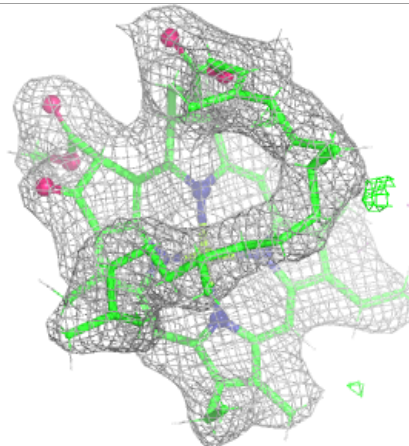
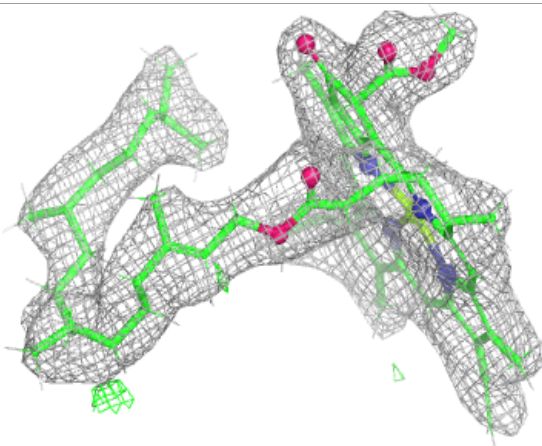
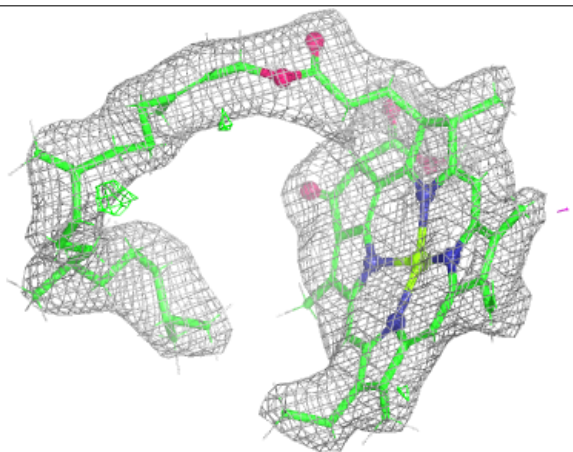


Electron density around BCR b 618:

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

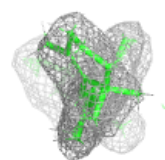
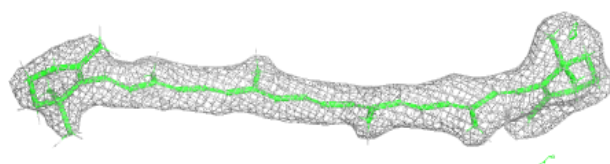
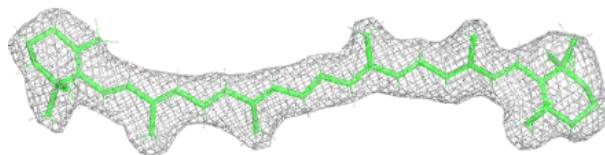
**Electron density around CLA c 503:**

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

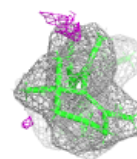
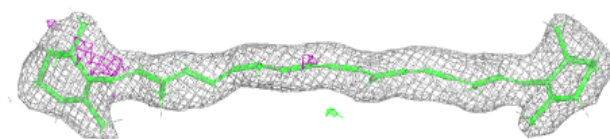
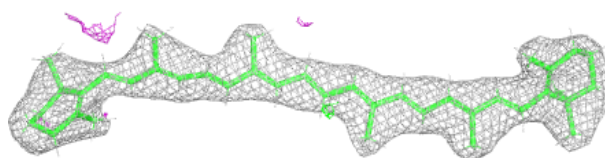


Electron density around BCR b 620:

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

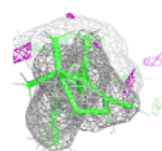
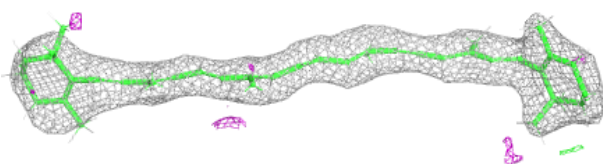
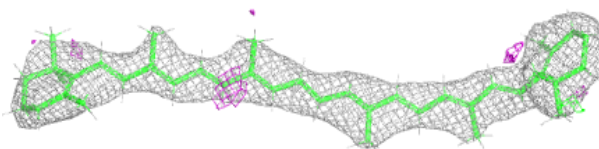
**Electron density around BCR B 618:**

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

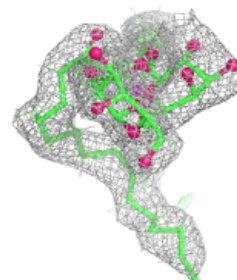
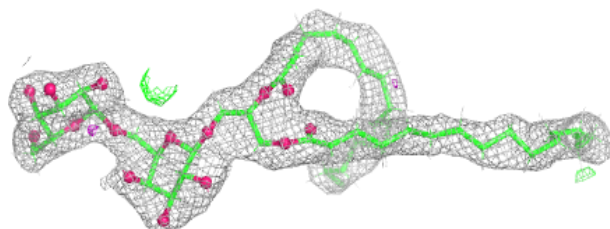
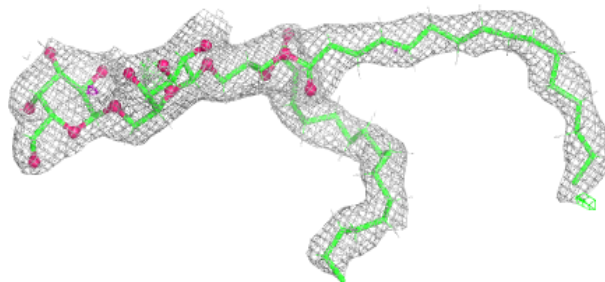


Electron density around BCR c 515:

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

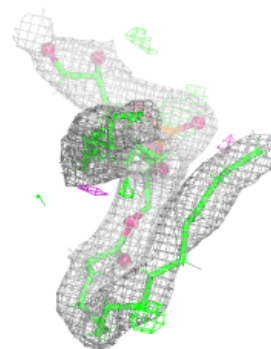
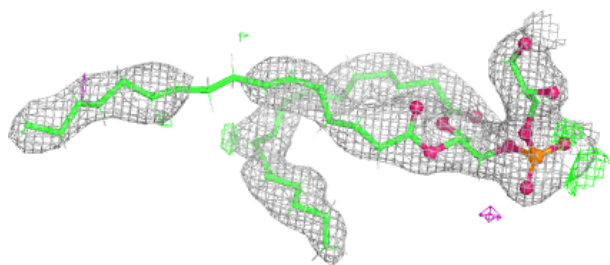
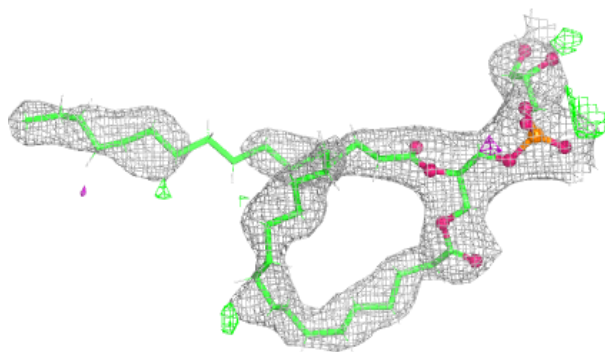
**Electron density around DGD H 102:**

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

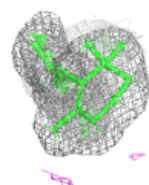
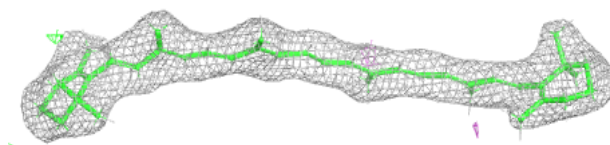
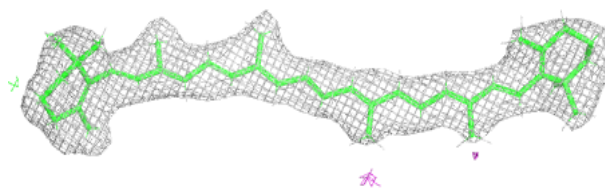


Electron density around LHG a 410:

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

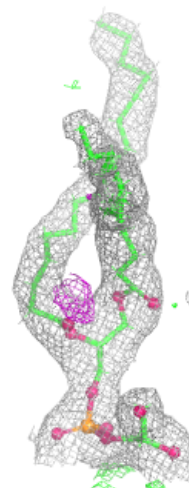
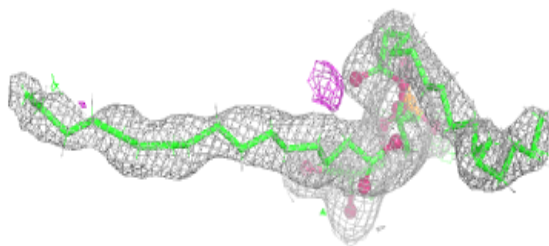
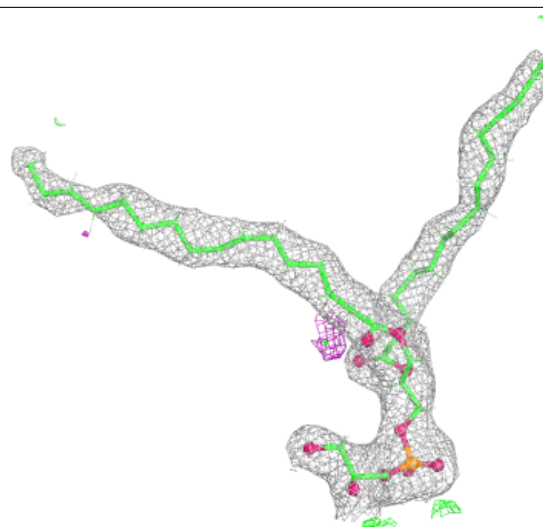
**Electron density around BCR B 619:**

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



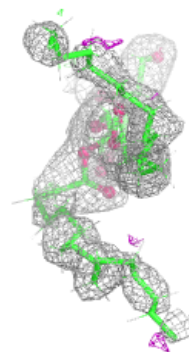
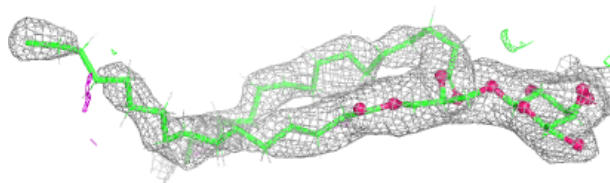
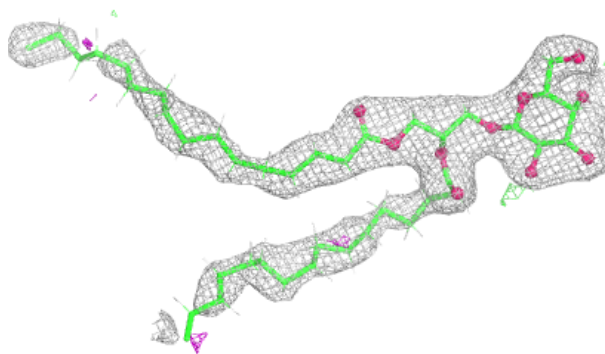
Electron density around LHG 1 101:

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



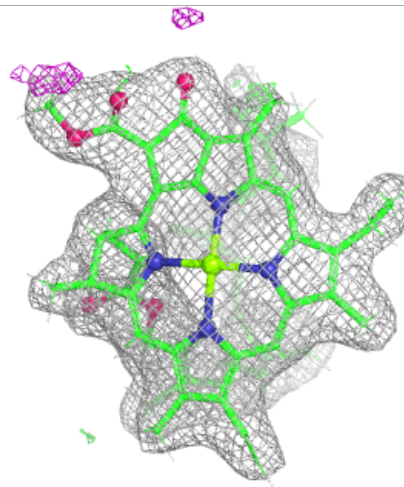
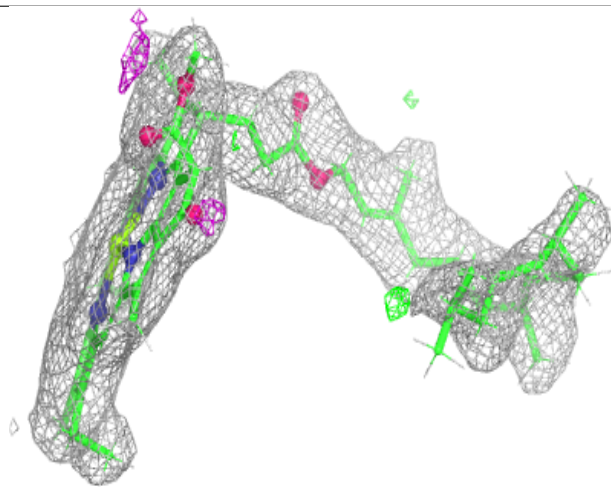
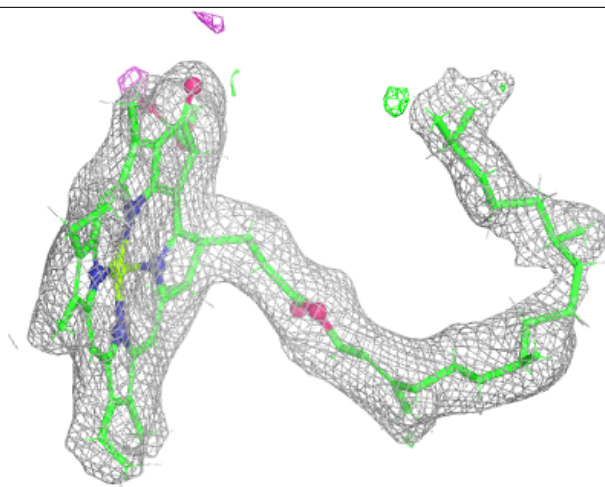
Electron density around LMG D 407:

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



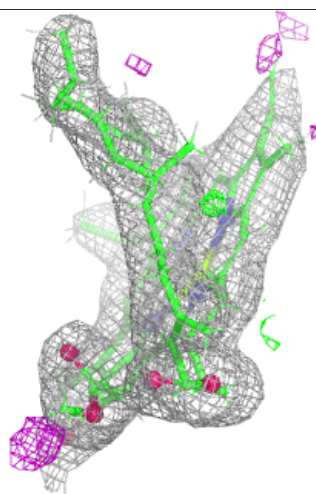
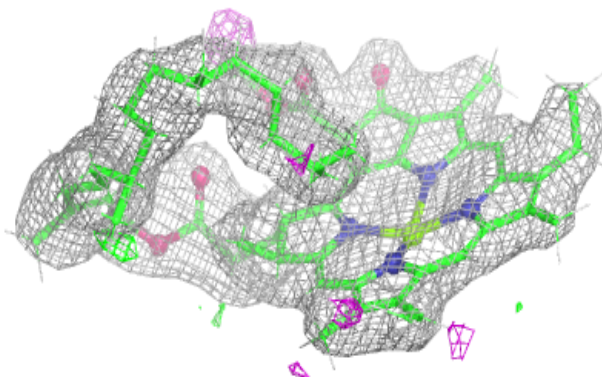
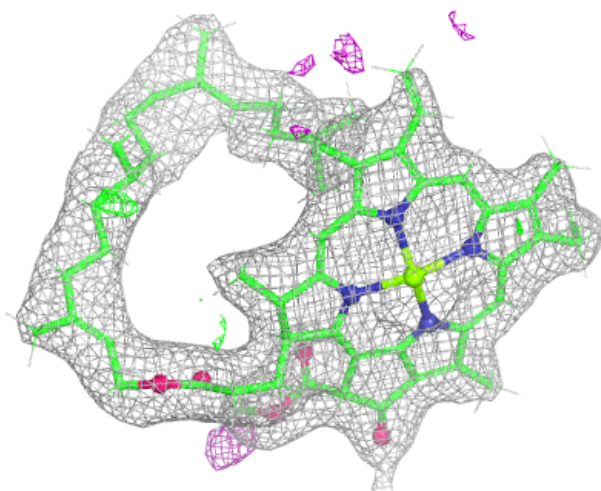
Electron density around CLA B 606:

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



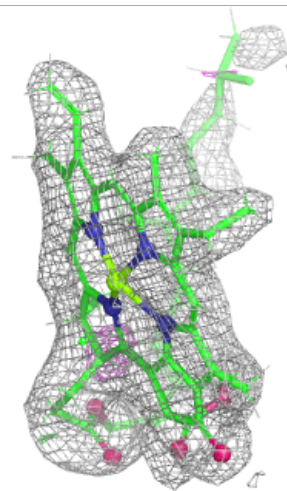
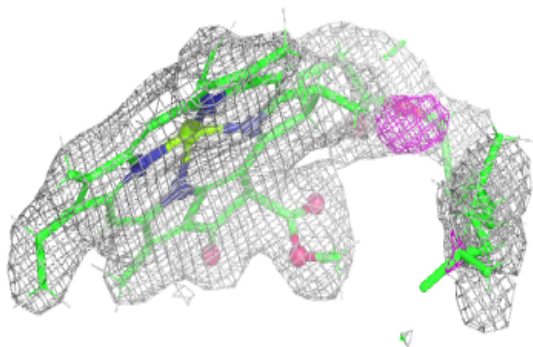
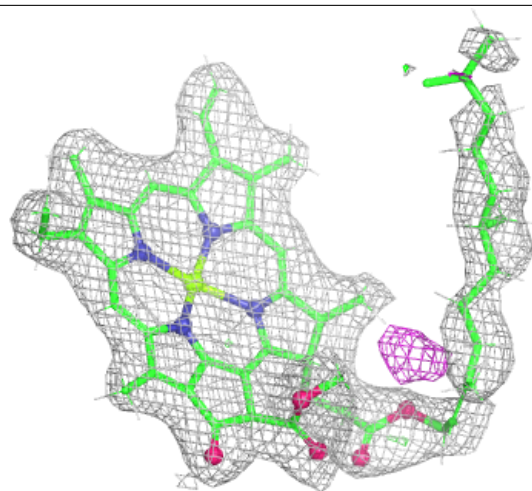
Electron density around CLA B 615:

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



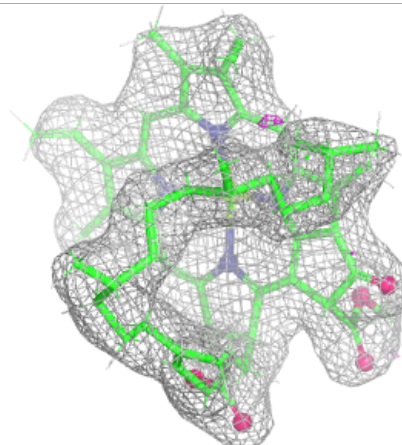
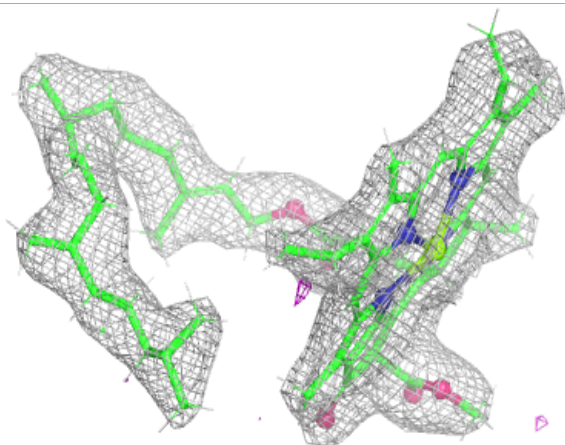
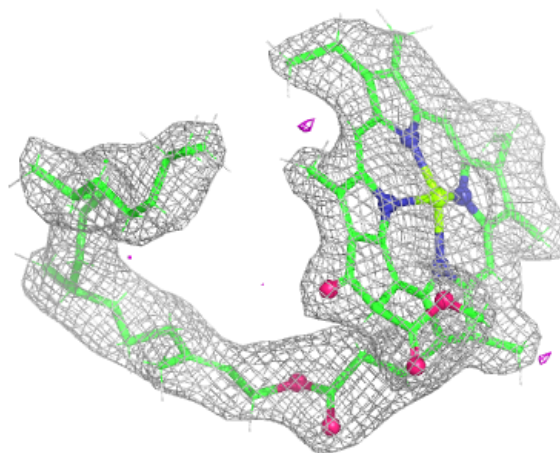
Electron density around CLA B 616:

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



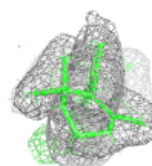
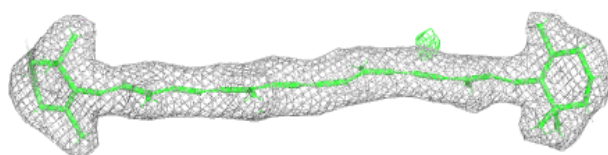
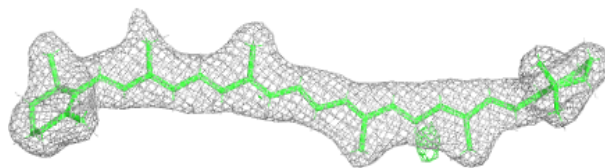
Electron density around CLA C 503:

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

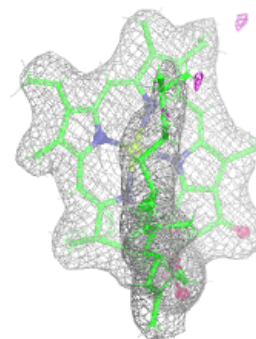
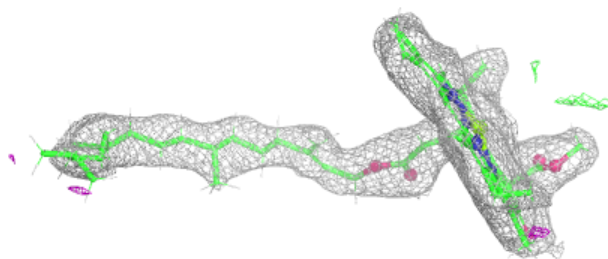
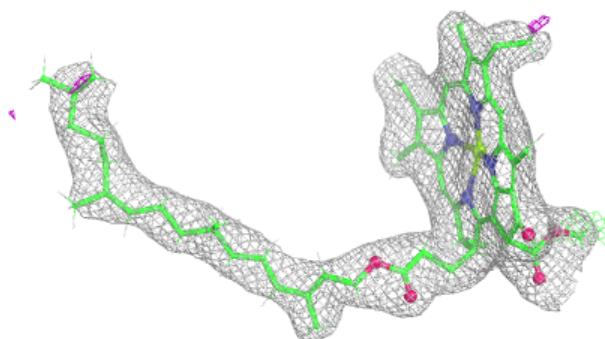


Electron density around BCR A 408:

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

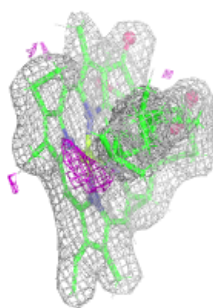
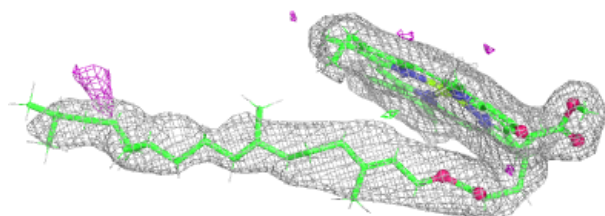
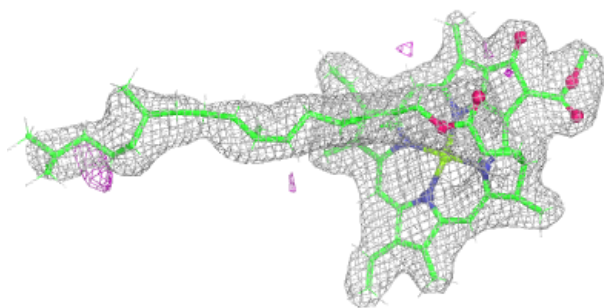
**Electron density around CLA b 610:**

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



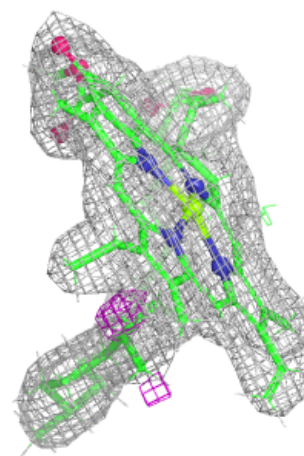
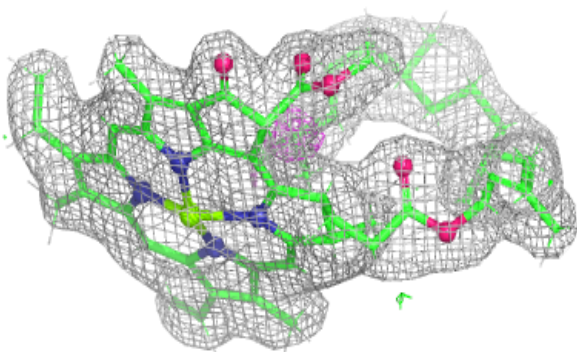
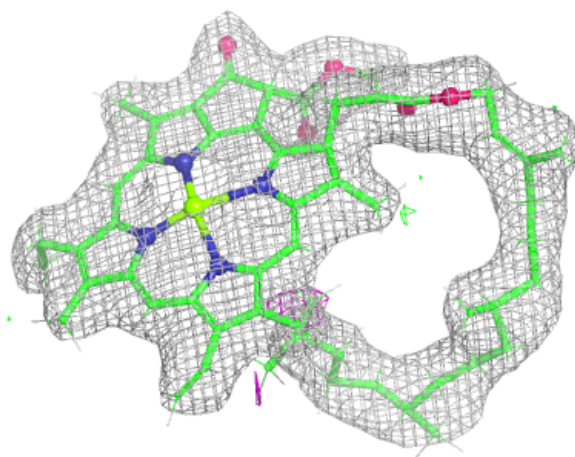
Electron density around CLA b 615:

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



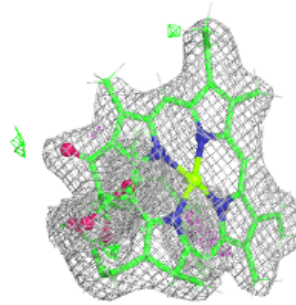
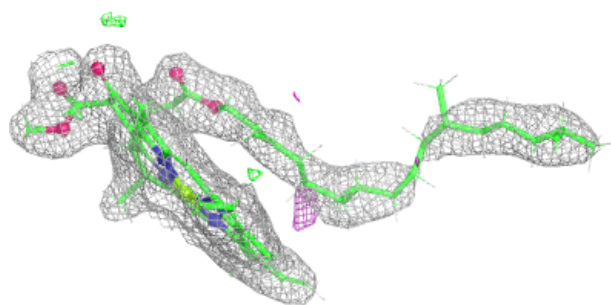
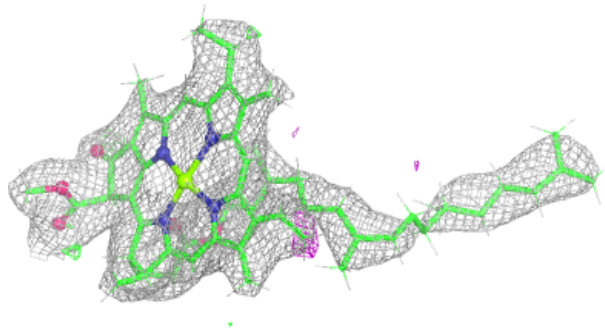
Electron density around CLA b 616:

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

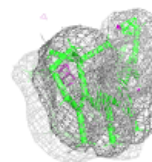
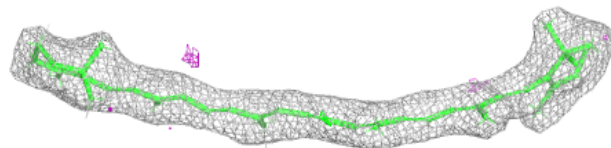
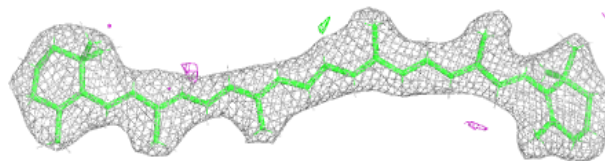


Electron density around CLA C 505:

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

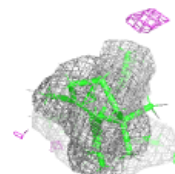
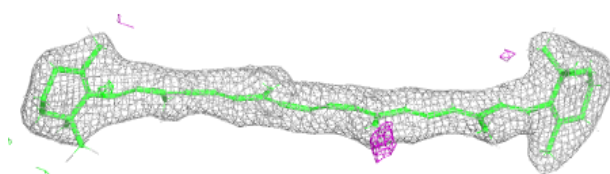
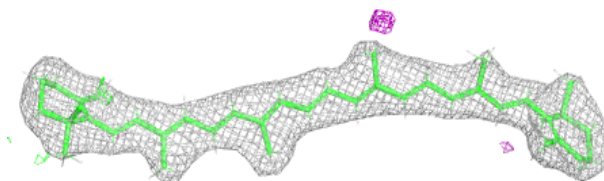
**Electron density around BCR t 101:**

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

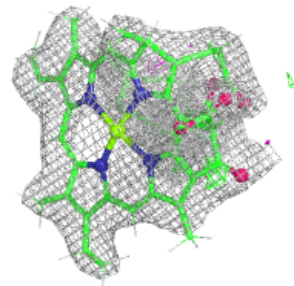
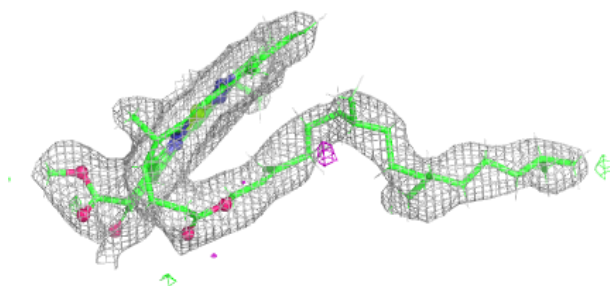
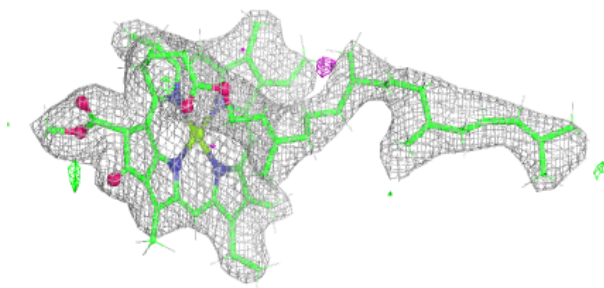


Electron density around BCR C 515:

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

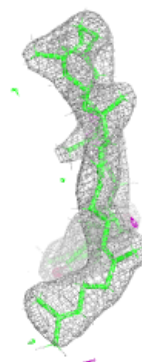
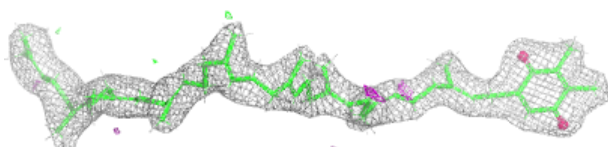
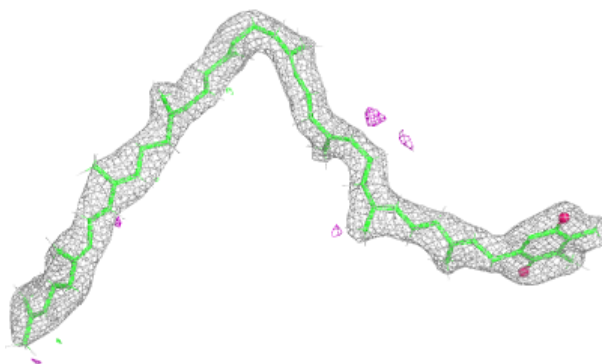
**Electron density around CLA c 505:**

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

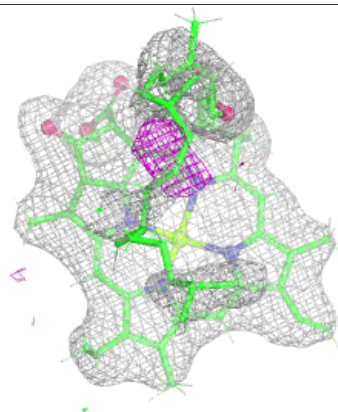
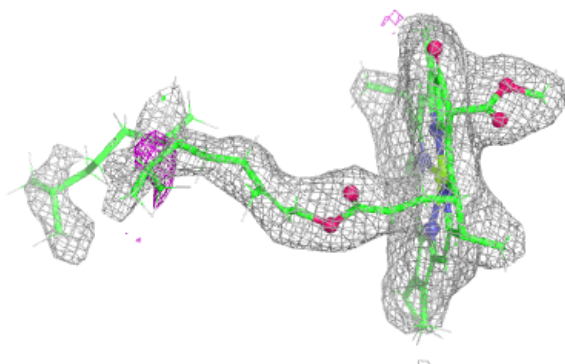
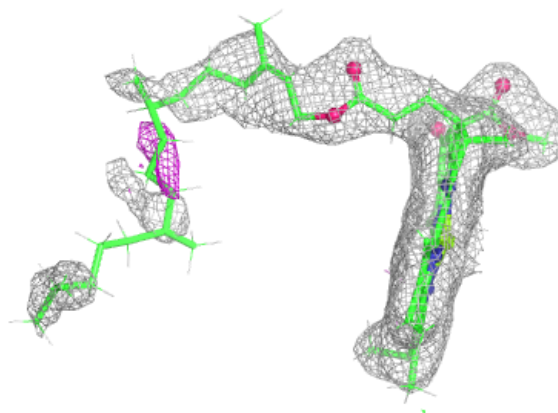


Electron density around PL9 D 406:

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

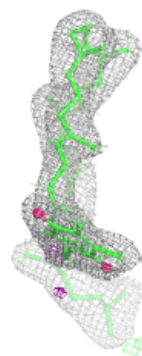
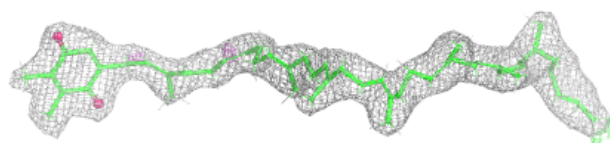
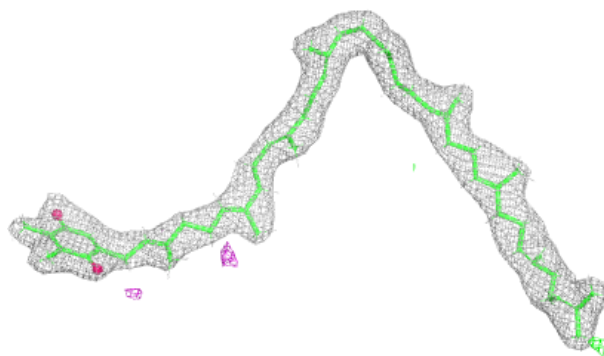
**Electron density around CLA c 506:**

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

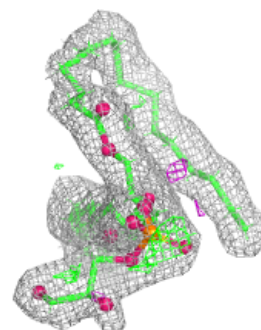
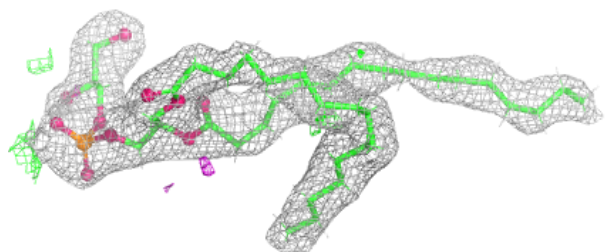
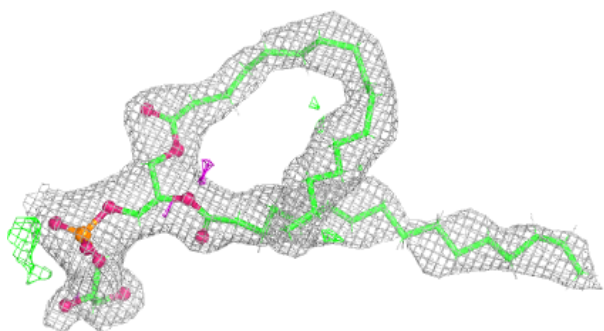


Electron density around PL9 d 406:

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

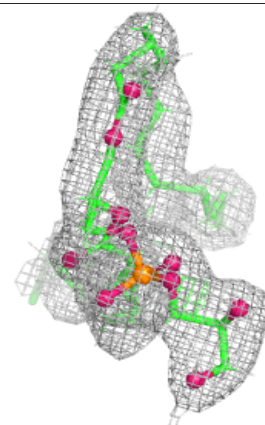
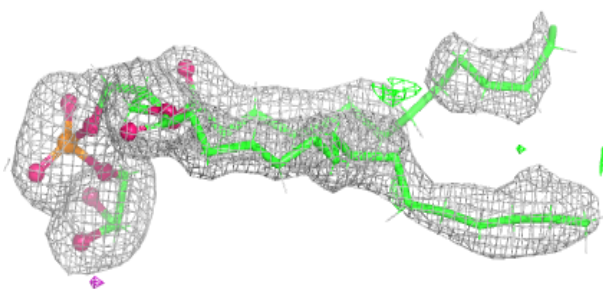
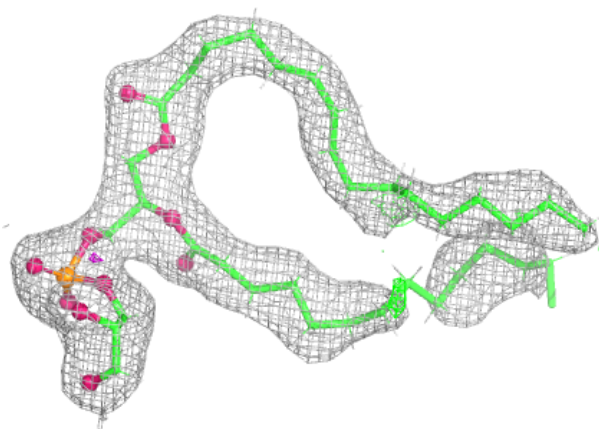
**Electron density around LHG B 622:**

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

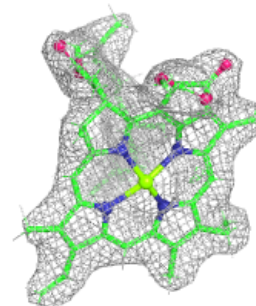
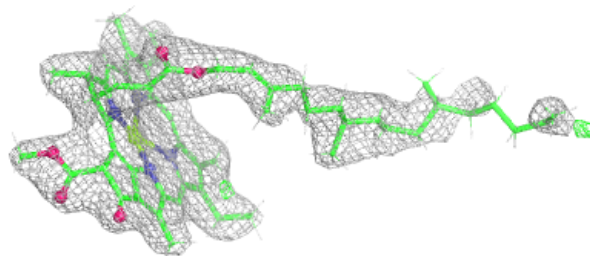
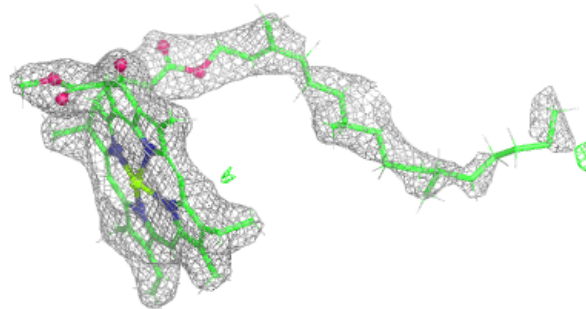


Electron density around LHG D 409:

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

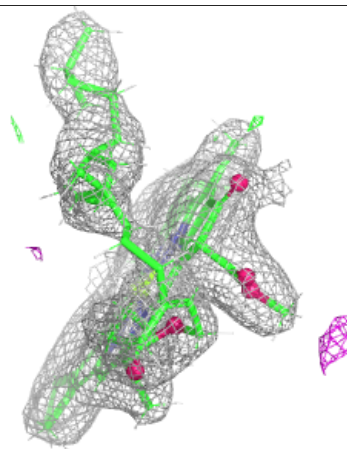
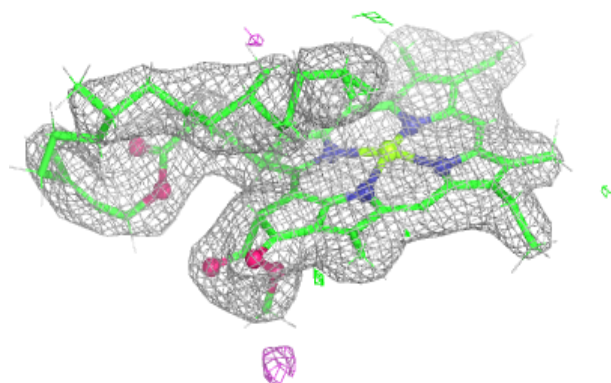
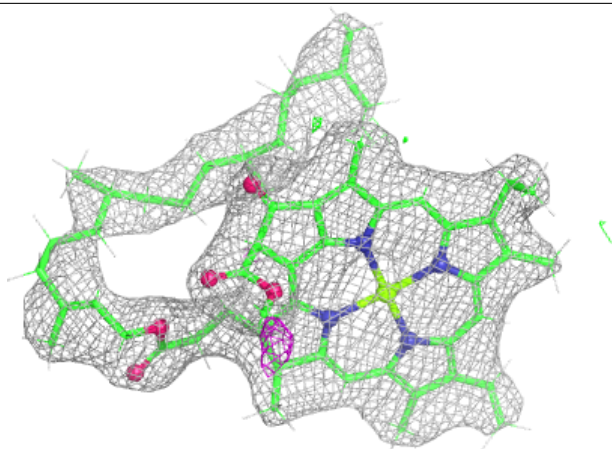
**Electron density around CLA c 508:**

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



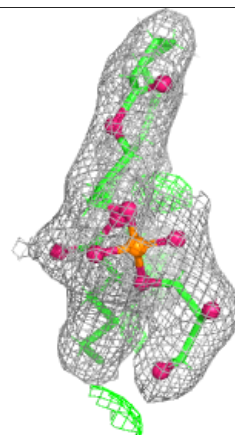
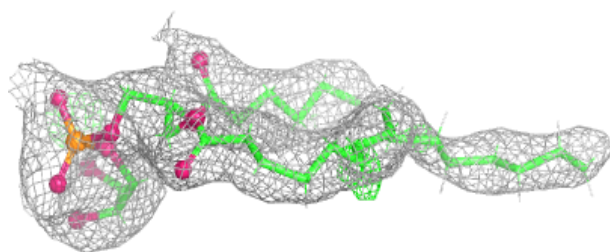
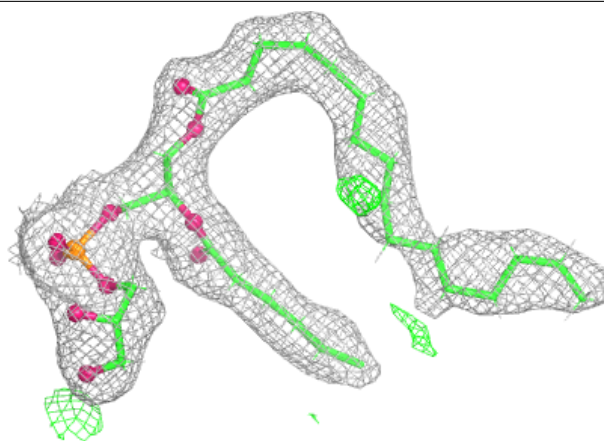
Electron density around CLA c 509:

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



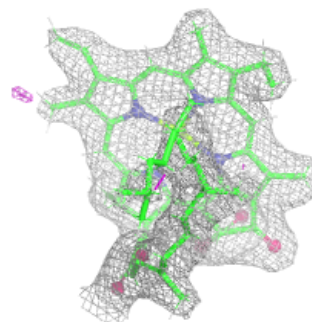
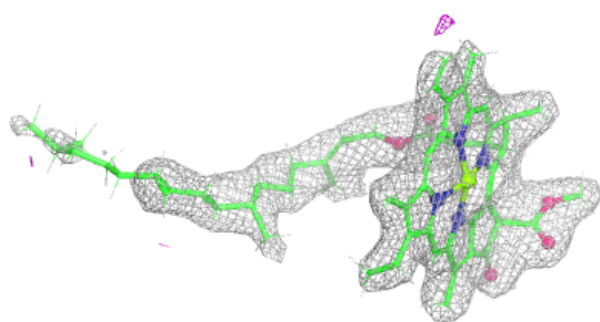
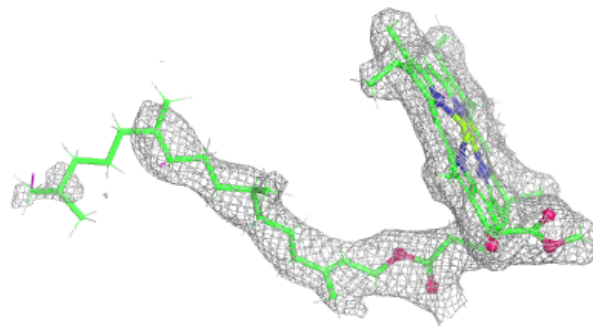
Electron density around LHG d 408:

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

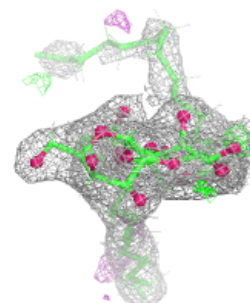
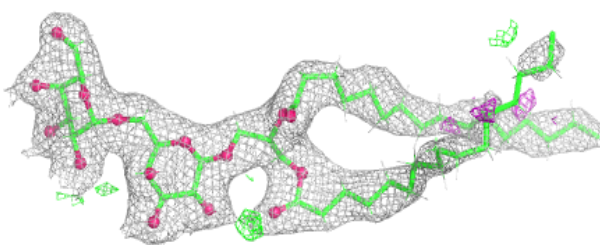
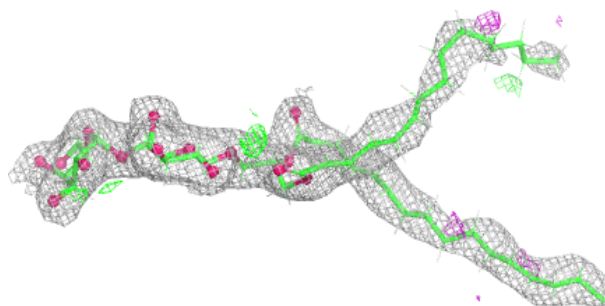


Electron density around CLA C 508:

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

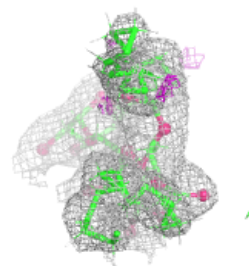
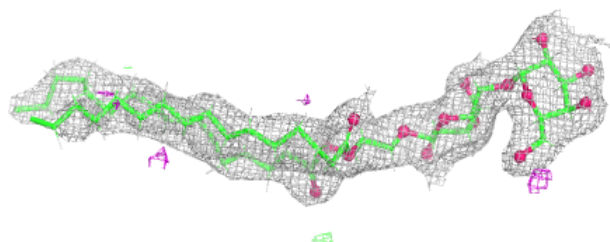
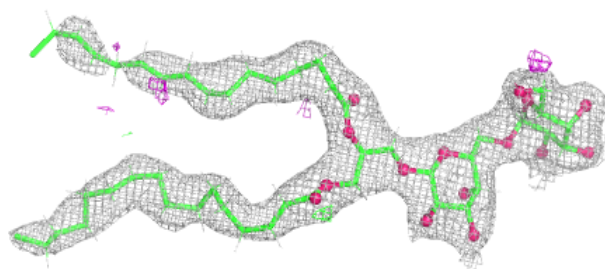
**Electron density around DGD C 516:**

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



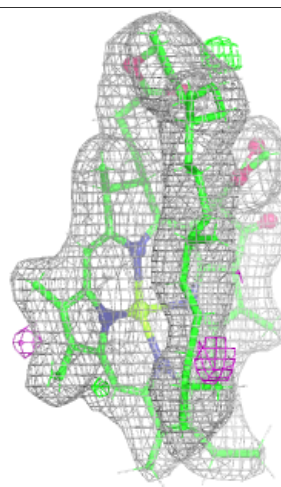
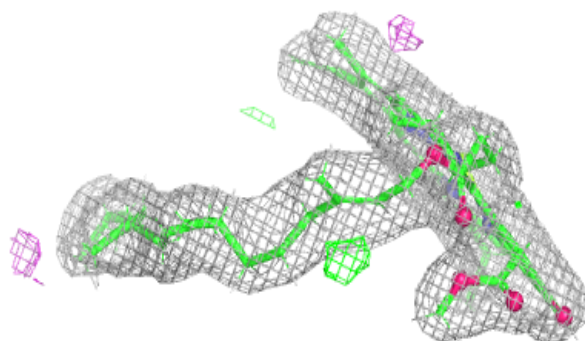
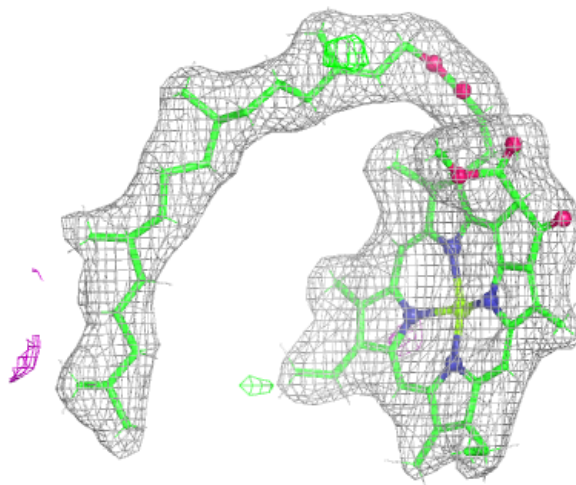
Electron density around DGD C 518:

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



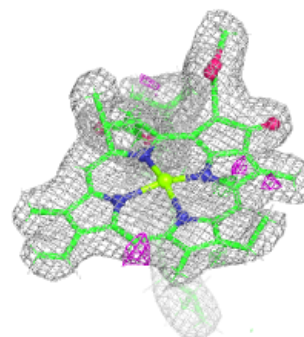
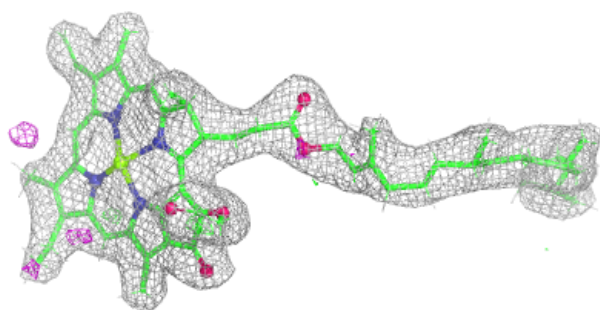
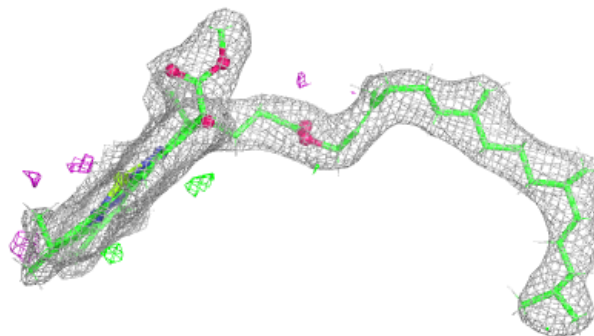
Electron density around CLA C 507:

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

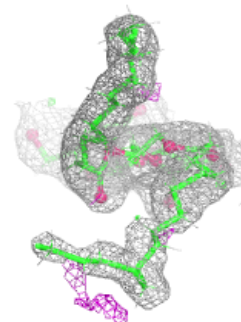
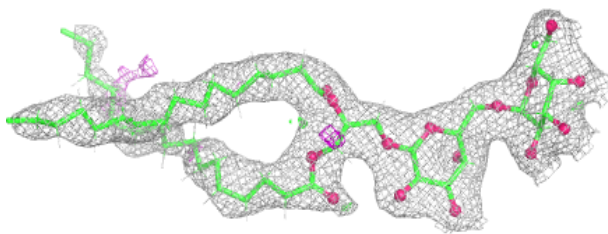
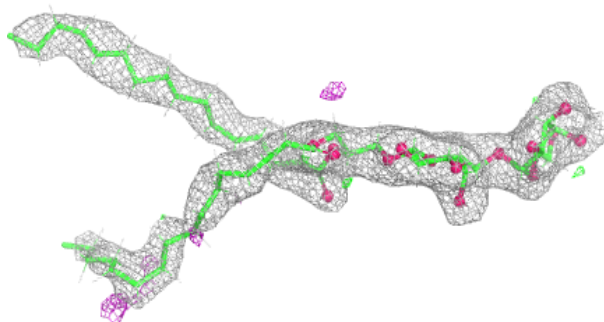


Electron density around CLA D 403:

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

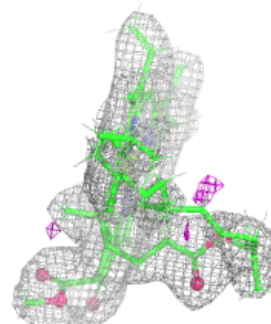
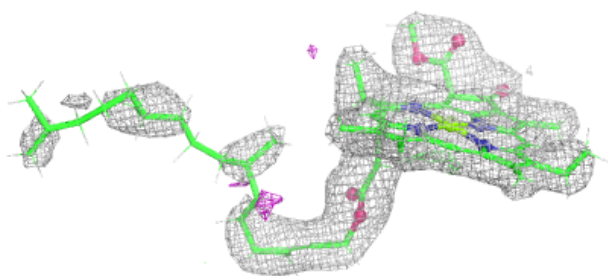
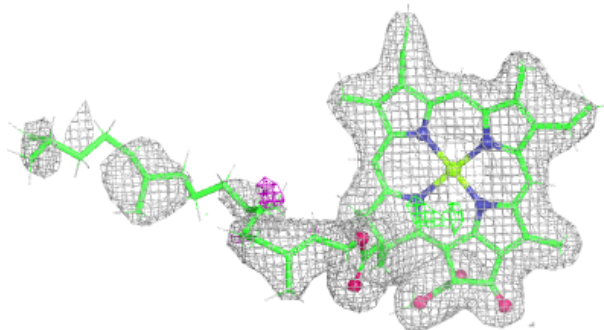
**Electron density around DGD c 516:**

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



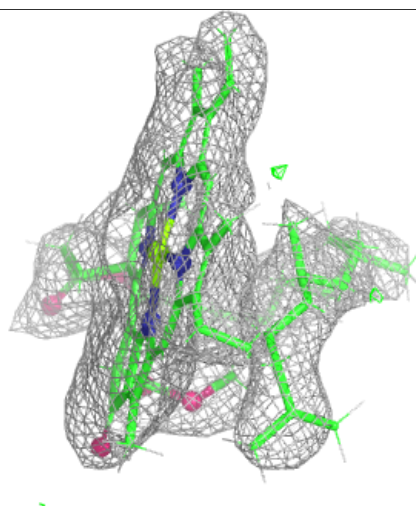
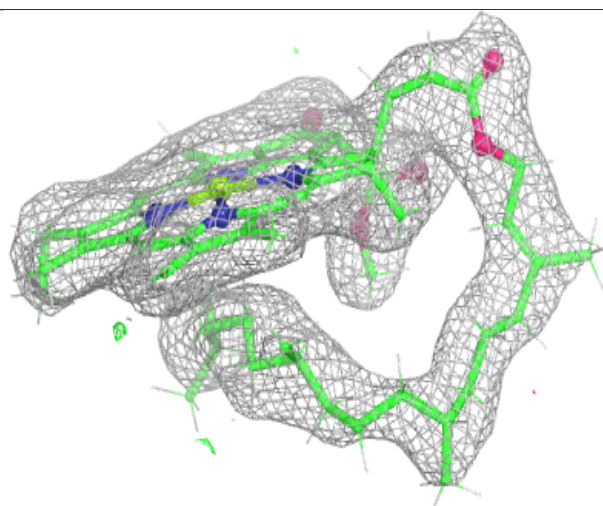
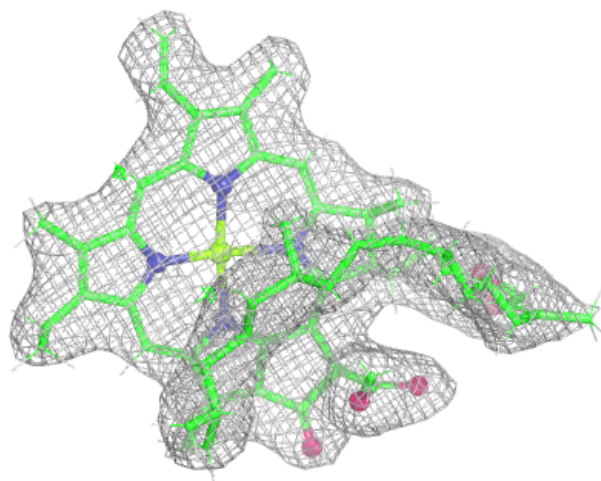
Electron density around CLA a 405:

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



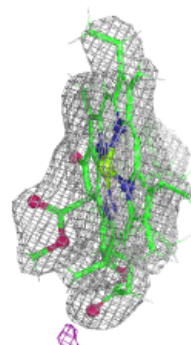
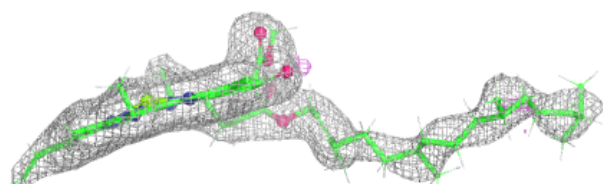
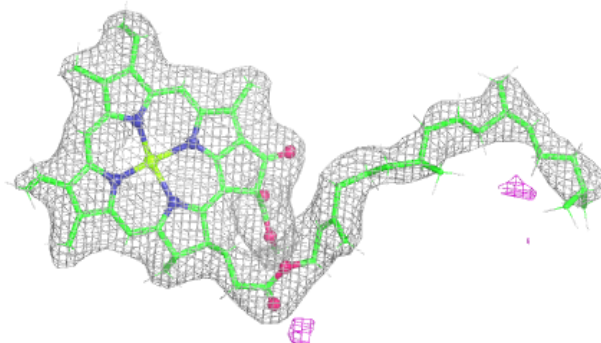
Electron density around CLA c 510:

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

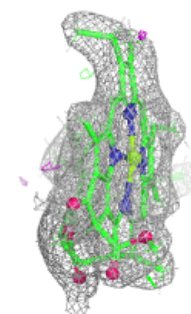
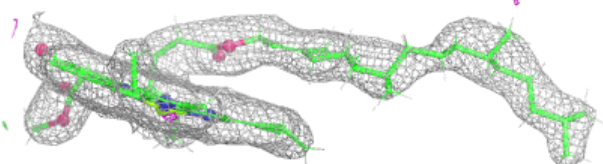
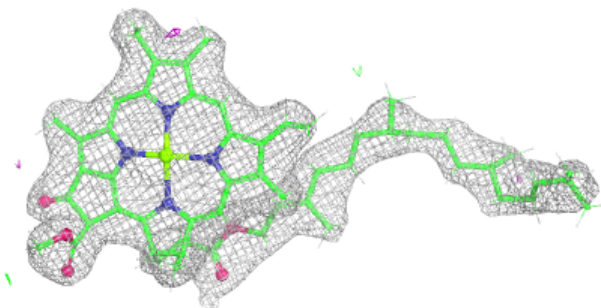


Electron density around CLA b 603:

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

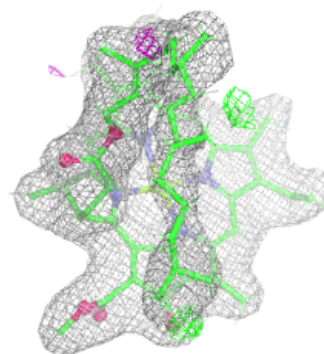
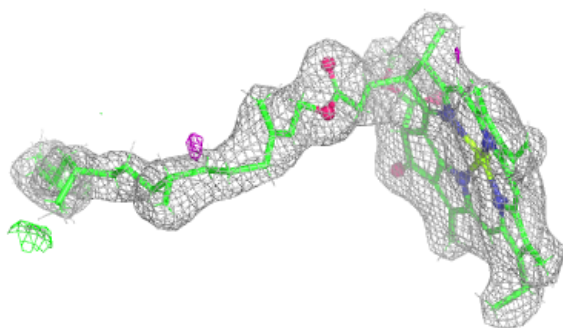
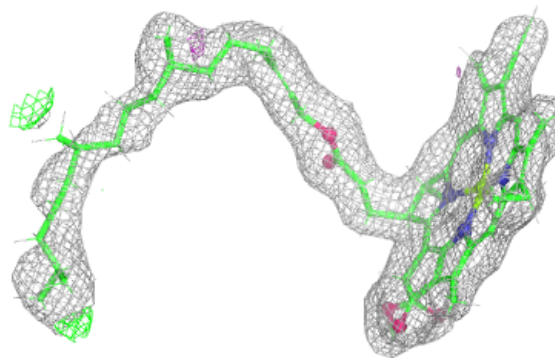
**Electron density around CLA b 604:**

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

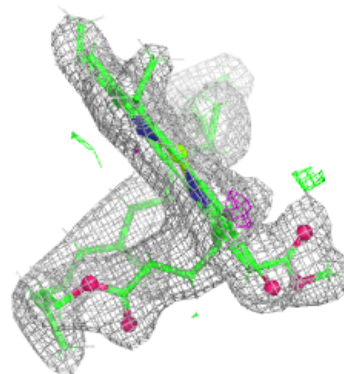
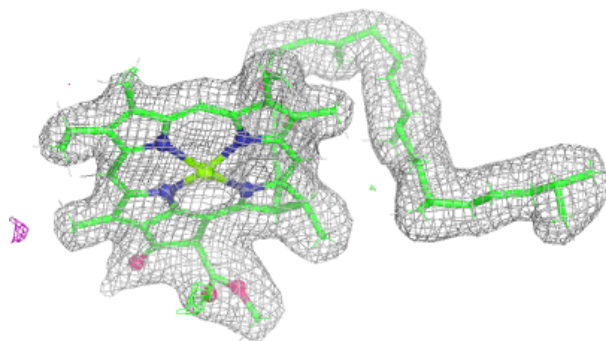
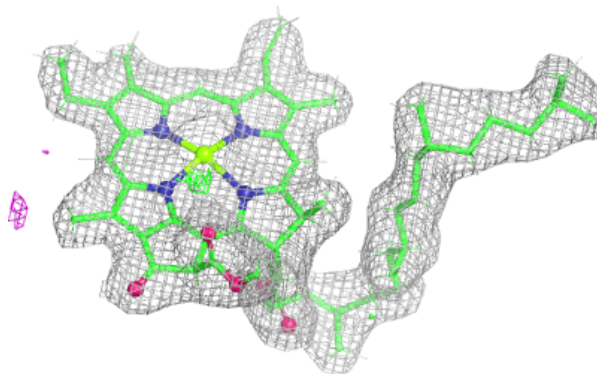


Electron density around CLA b 607:

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

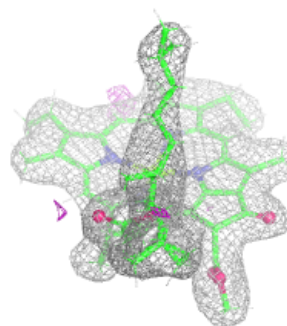
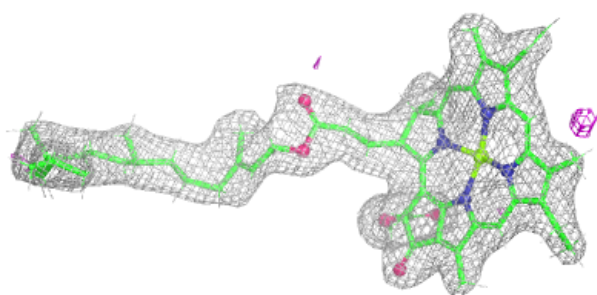
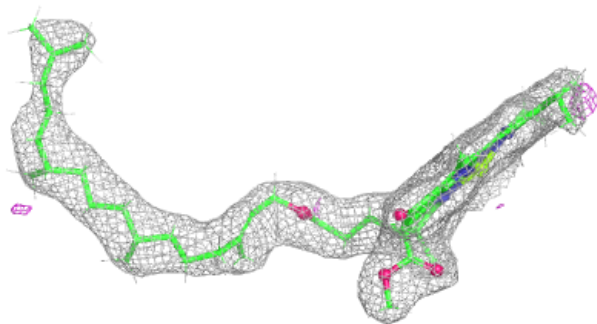
**Electron density around CLA d 402:**

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

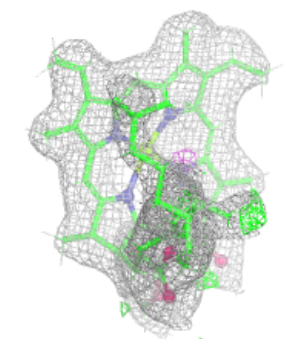
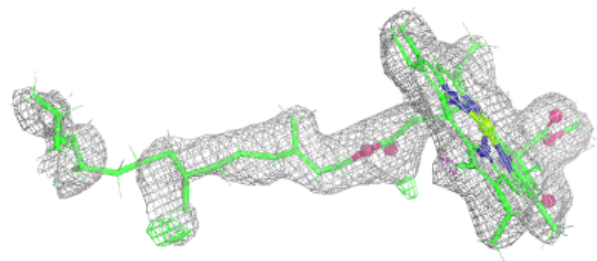
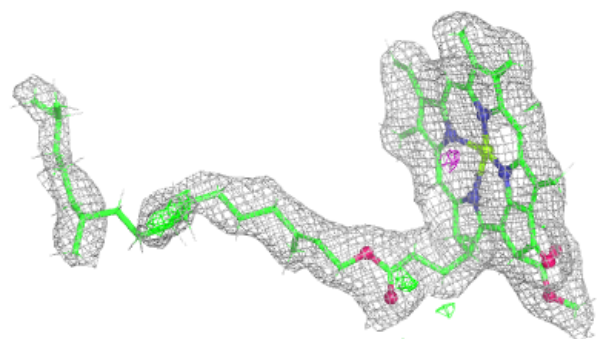


Electron density around CLA d 403:

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

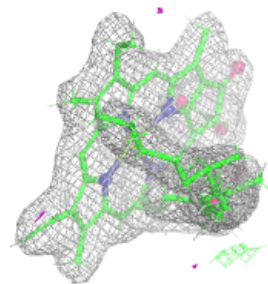
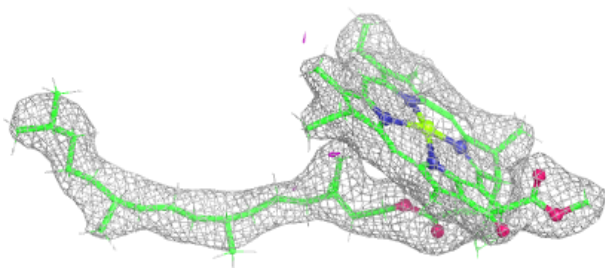
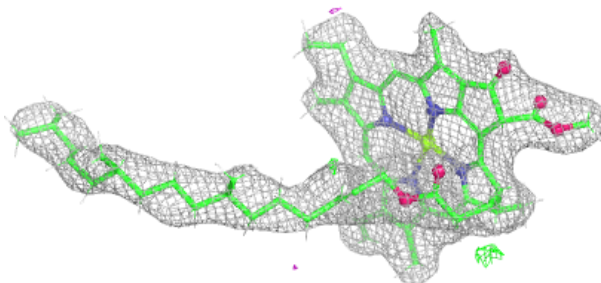
**Electron density around CLA d 404:**

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

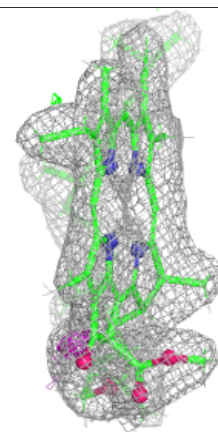
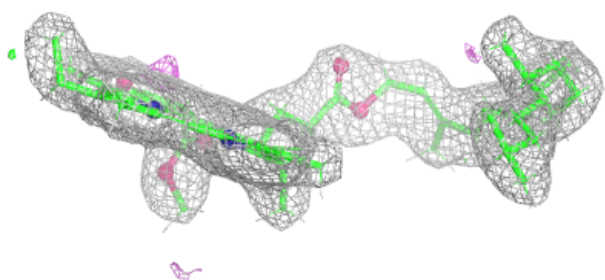
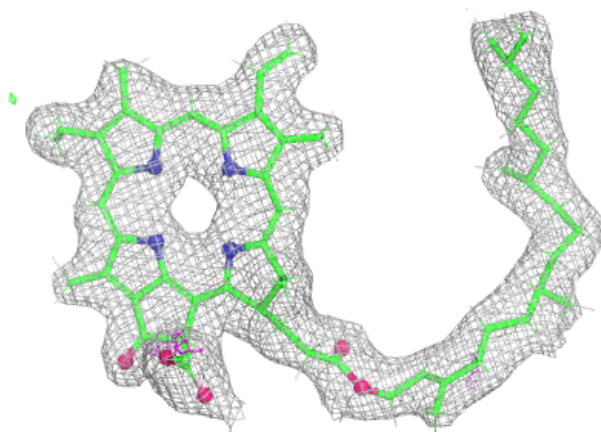


Electron density around CLA b 609:

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

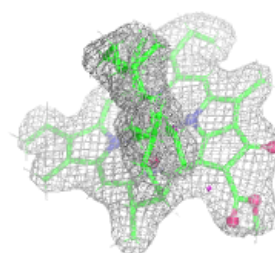
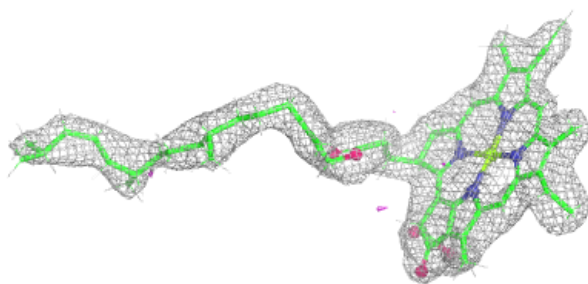
**Electron density around PHO a 406:**

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

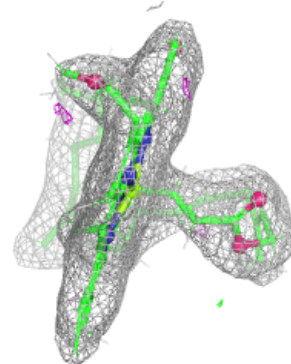
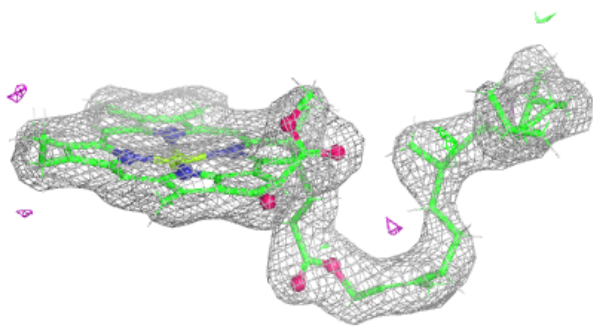
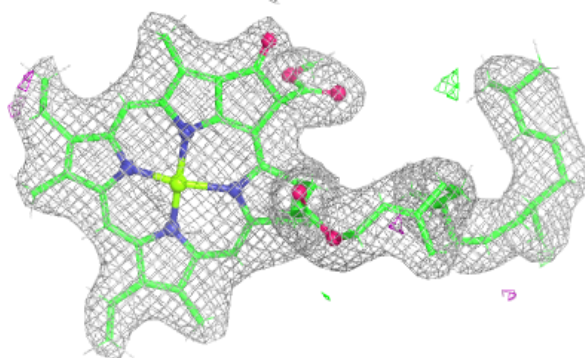


Electron density around CLA C 502:

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

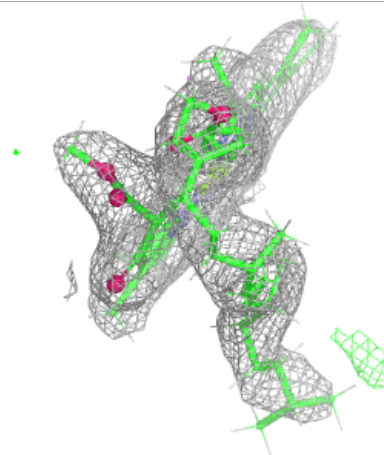
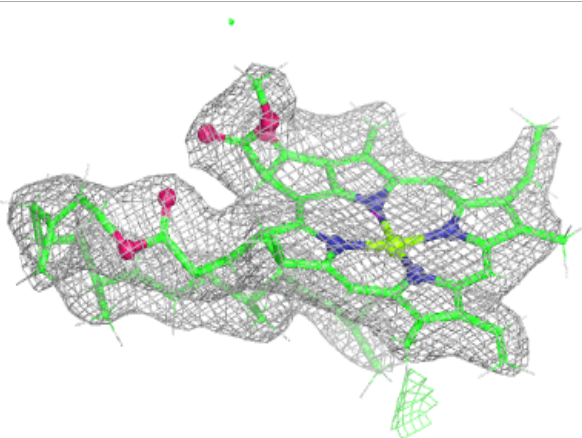
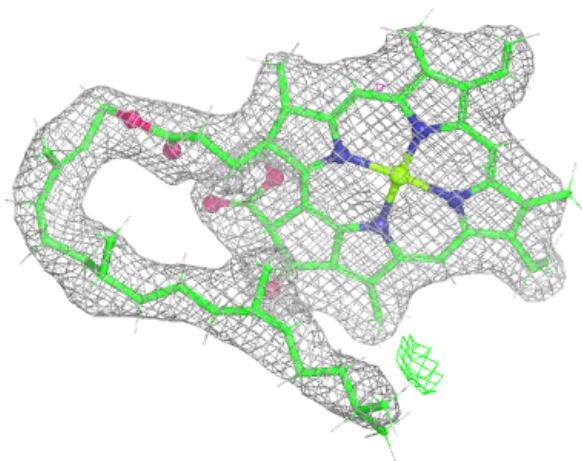
**Electron density around CLA b 613:**

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



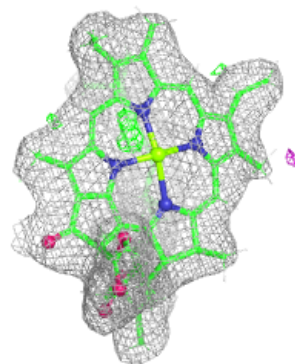
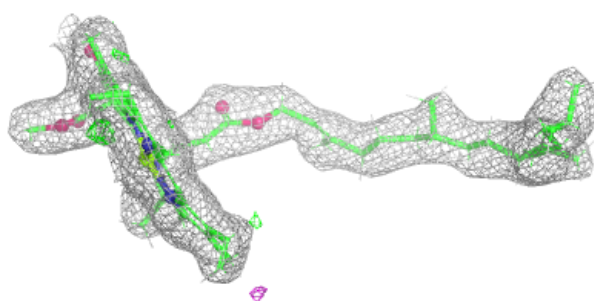
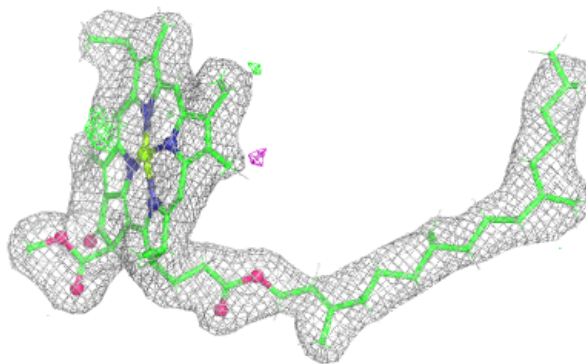
Electron density around CLA C 509:

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

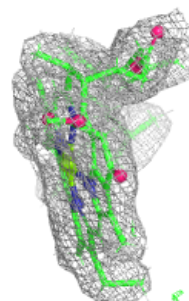
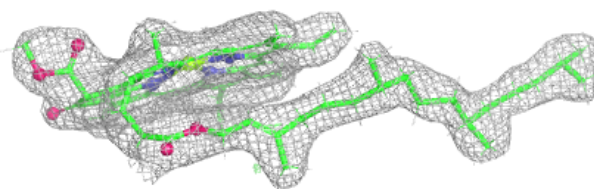
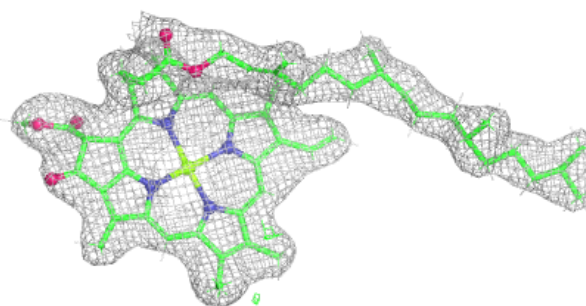


Electron density around CLA B 609:

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

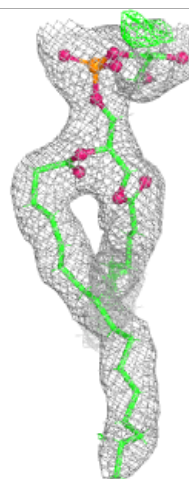
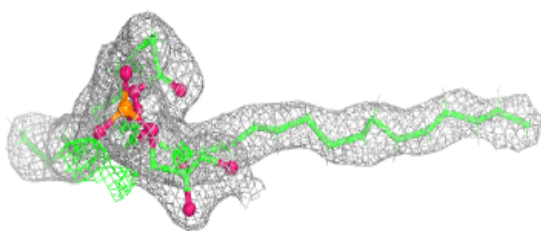
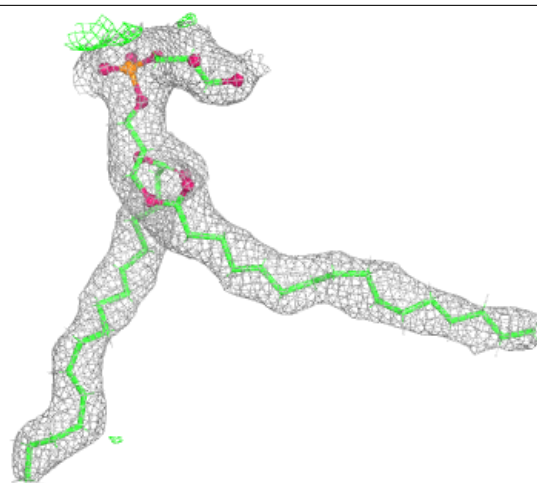
**Electron density around CLA c 501:**

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



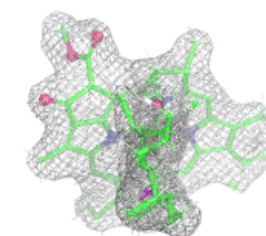
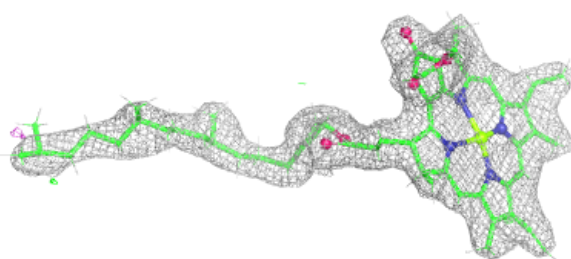
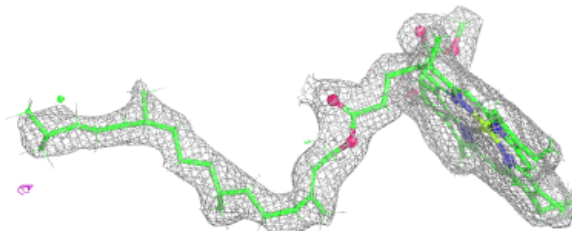
Electron density around LHG L 101:

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



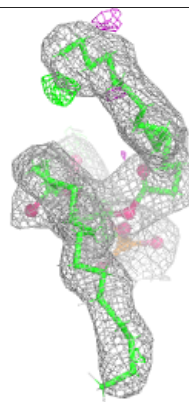
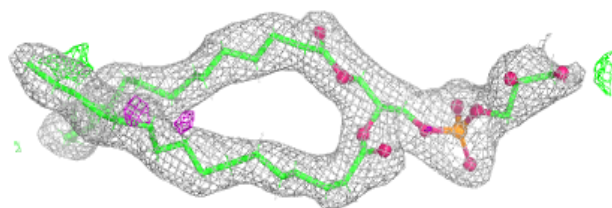
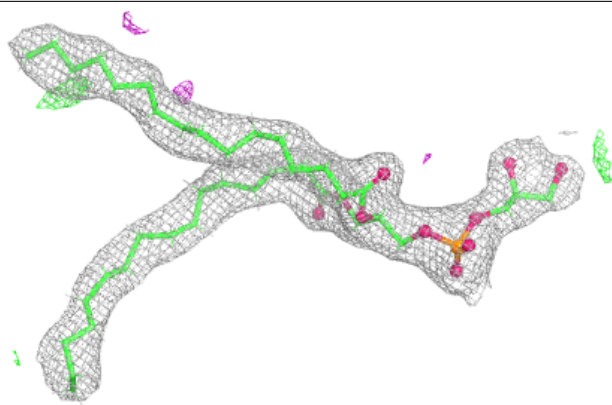
Electron density around CLA c 502:

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



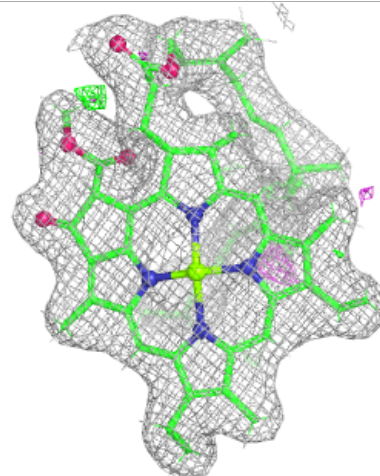
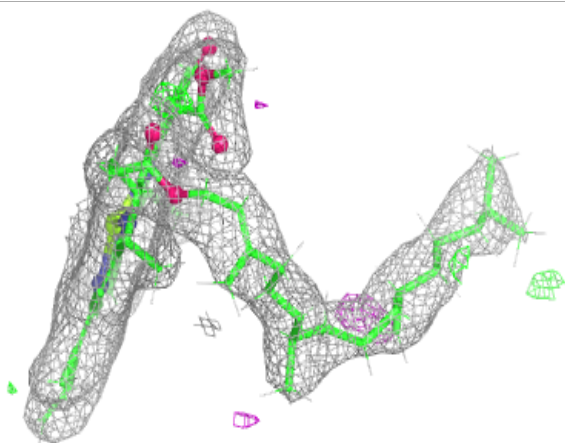
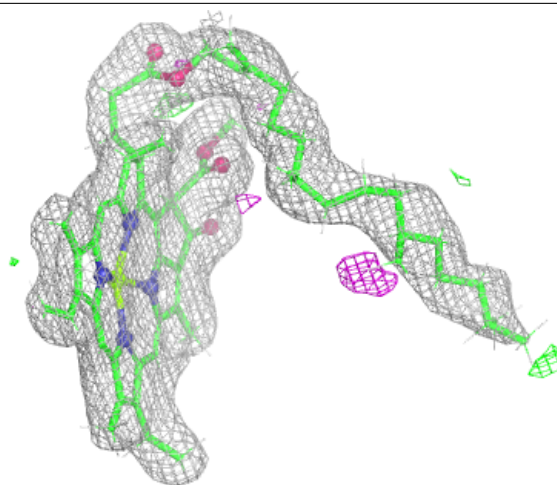
Electron density around LHG d 407:

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



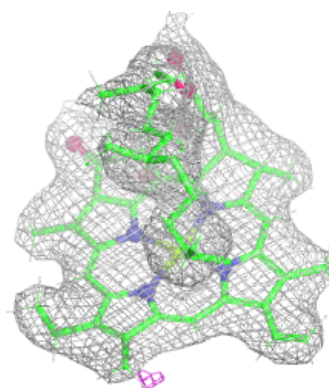
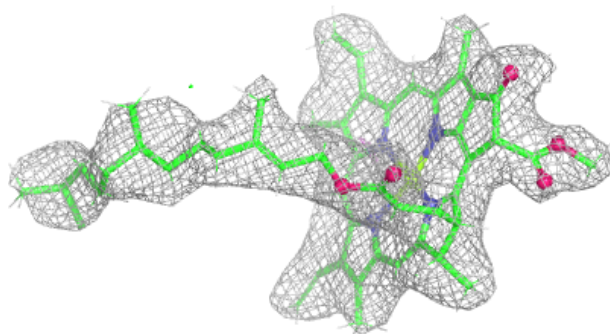
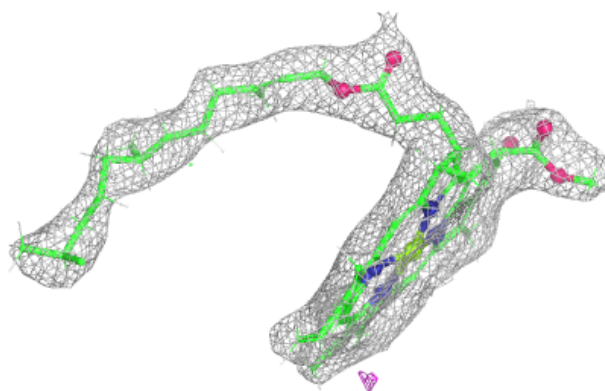
Electron density around CLA B 613:

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

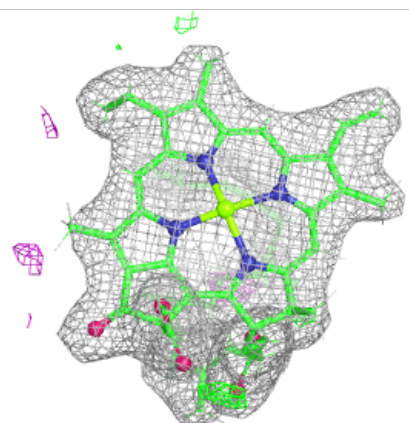
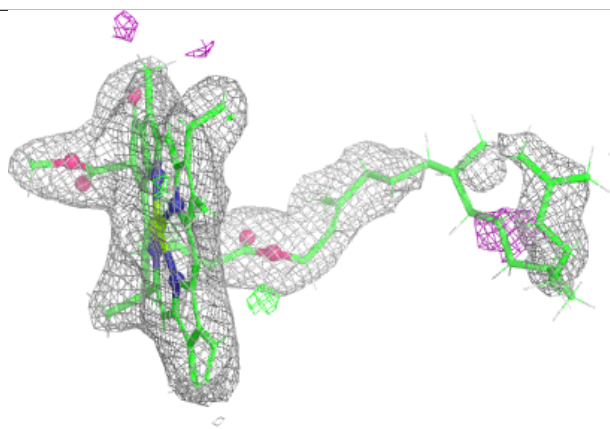
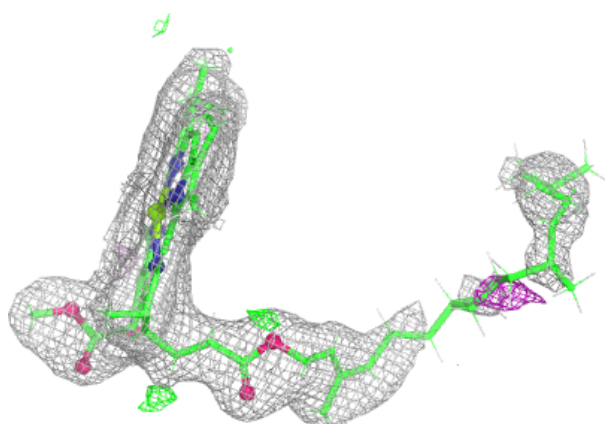


Electron density around CLA c 504:

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

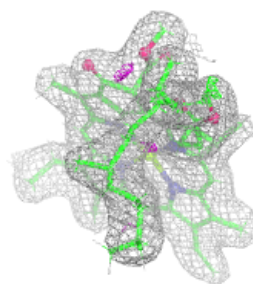
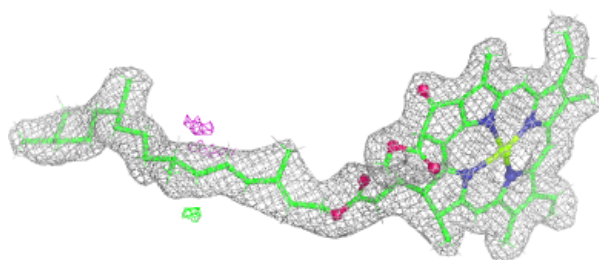
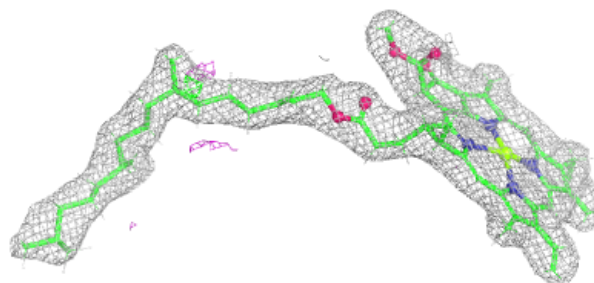
**Electron density around CLA C 506:**

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

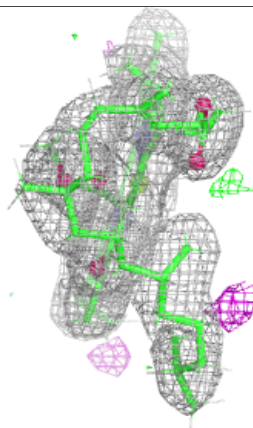
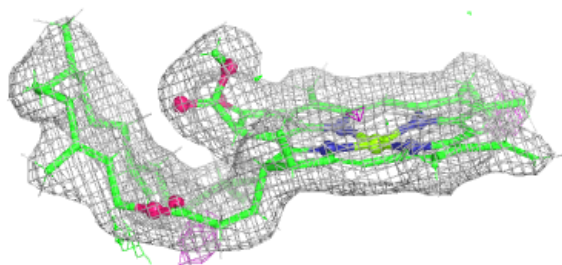
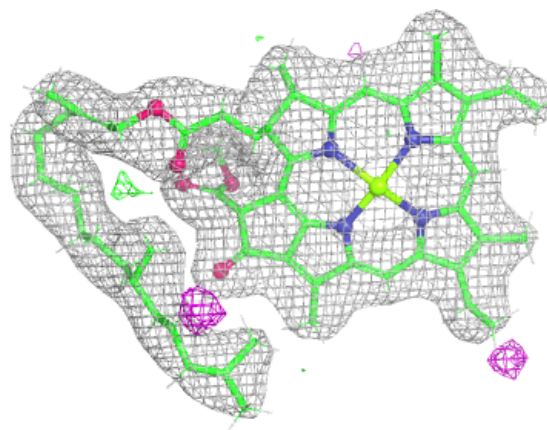


Electron density around CLA A 404:

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

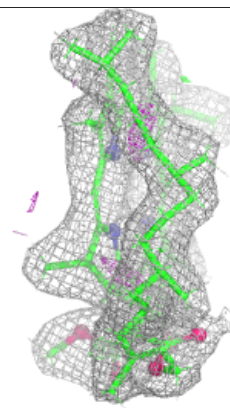
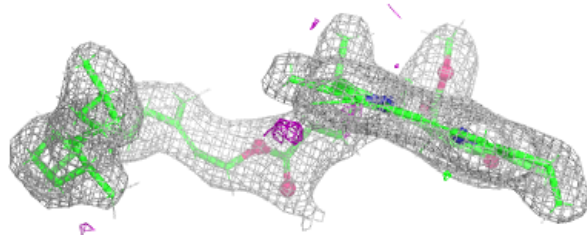
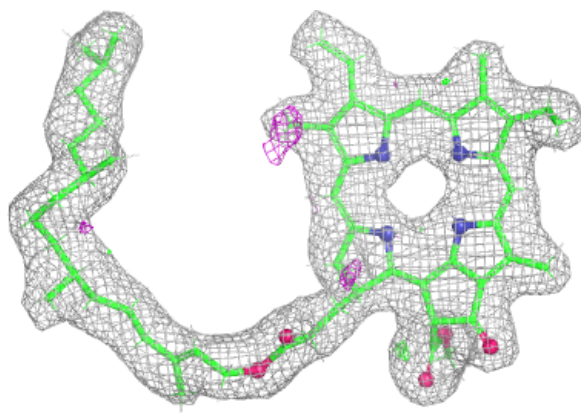
**Electron density around CLA B 610:**

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



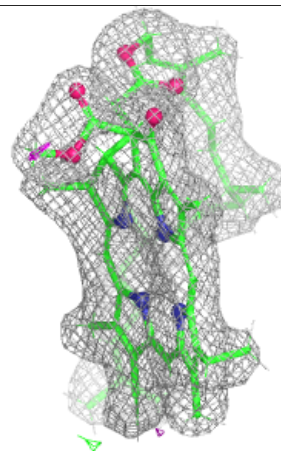
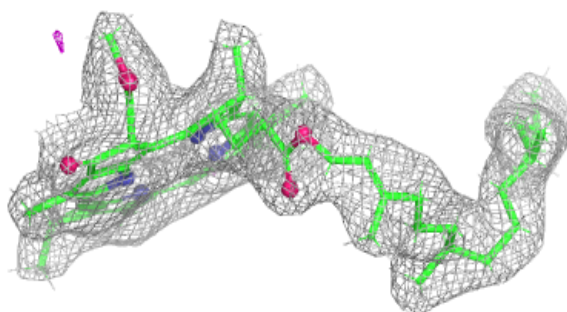
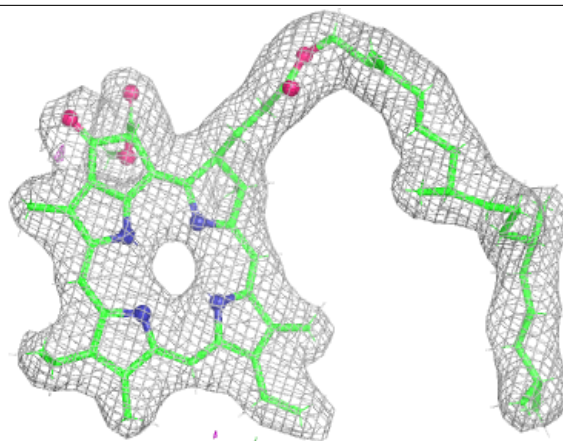
Electron density around PHO A 406:

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



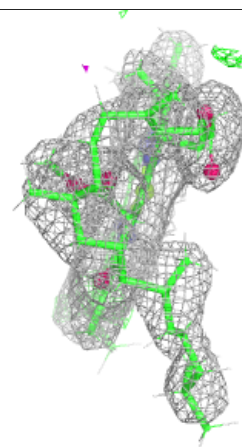
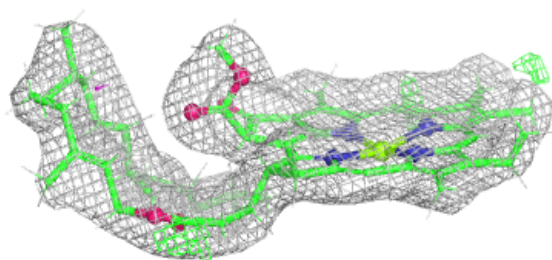
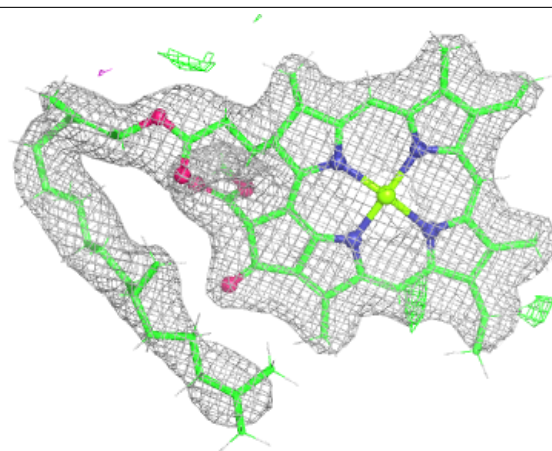
Electron density around PHO D 401:

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



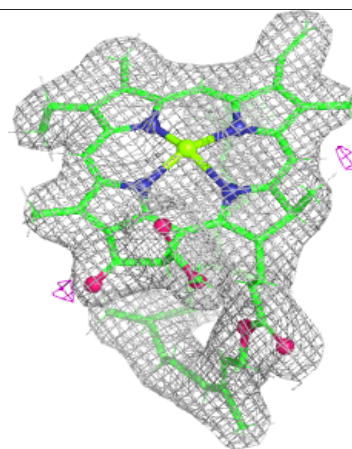
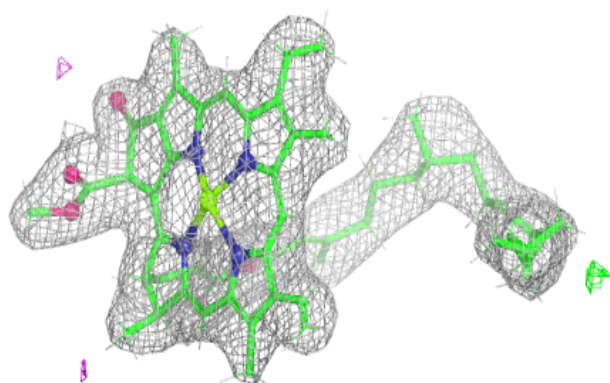
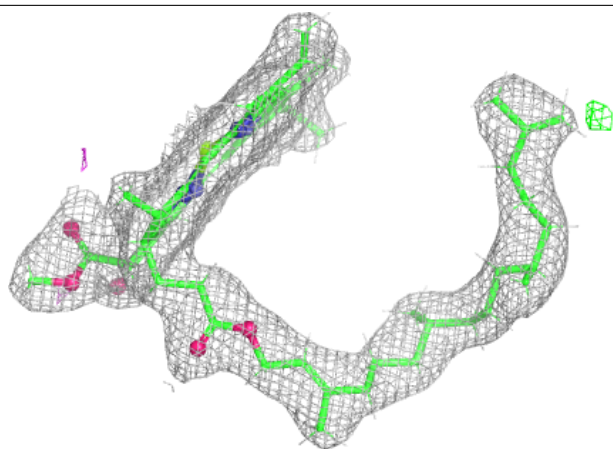
Electron density around CLA b 611:

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



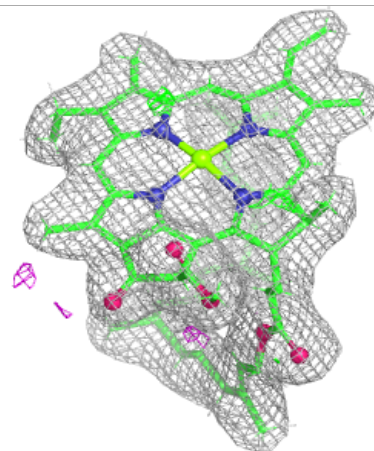
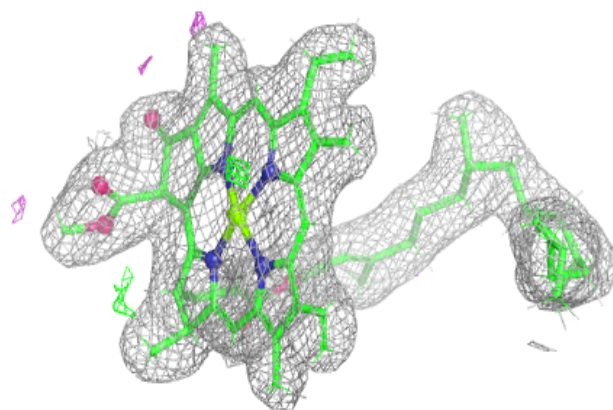
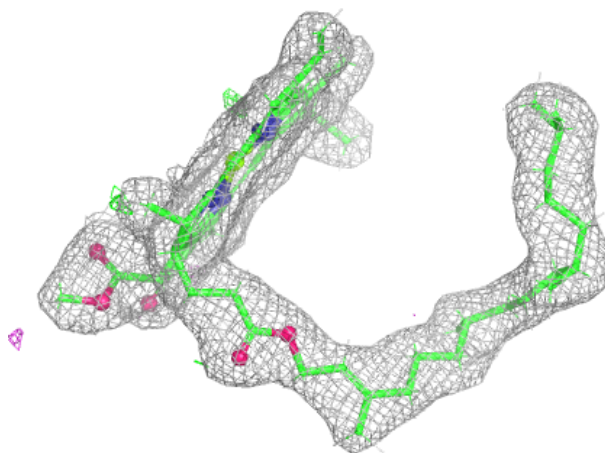
Electron density around CLA b 612:

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



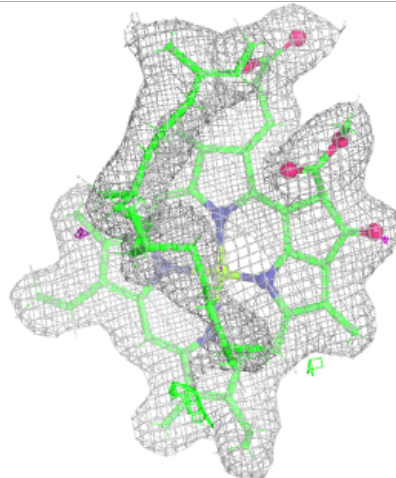
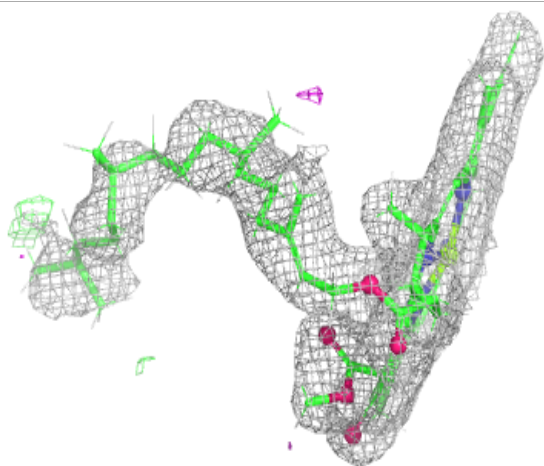
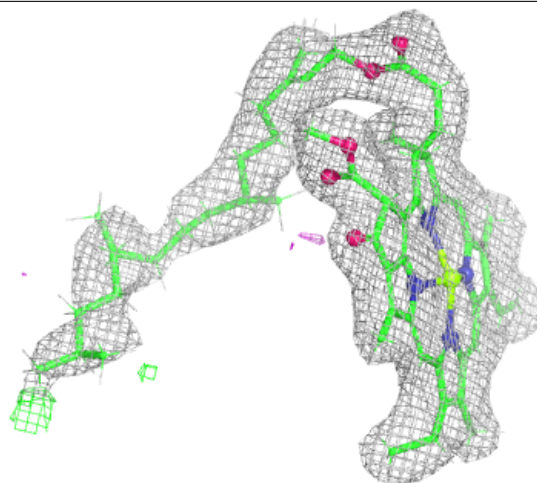
Electron density around CLA B 611:

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



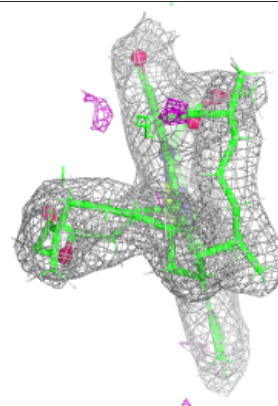
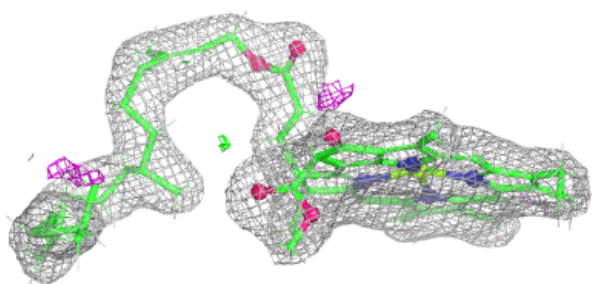
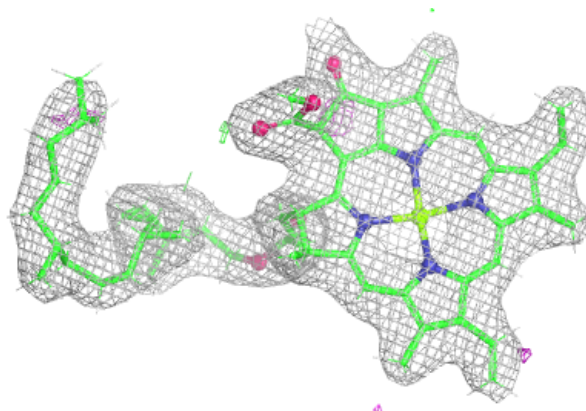
Electron density around CLA b 614:

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

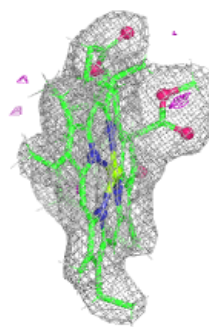
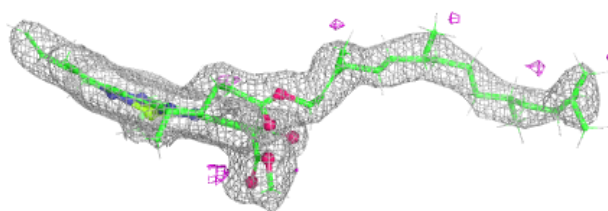
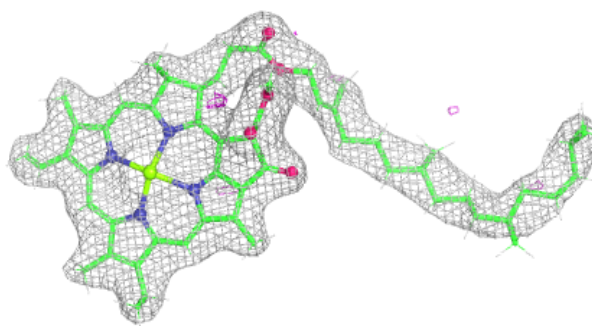


Electron density around CLA B 612:

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

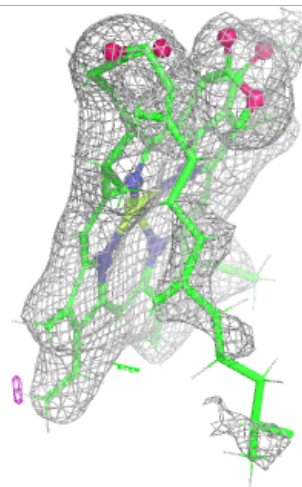
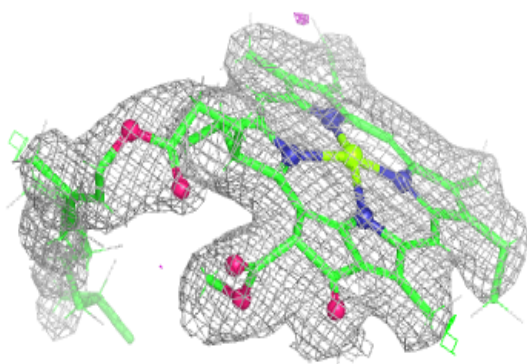
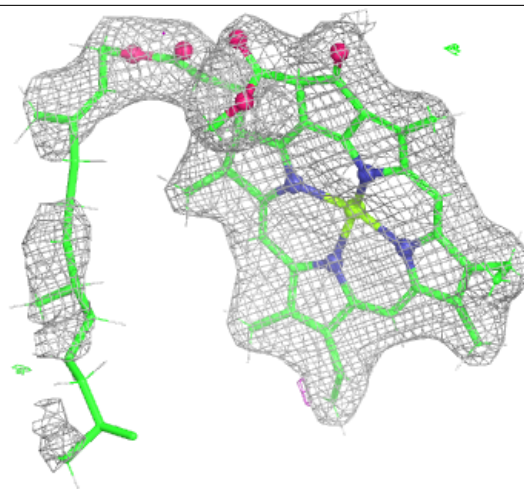
**Electron density around CLA B 602:**

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



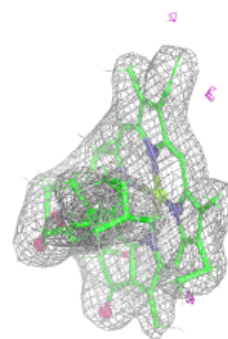
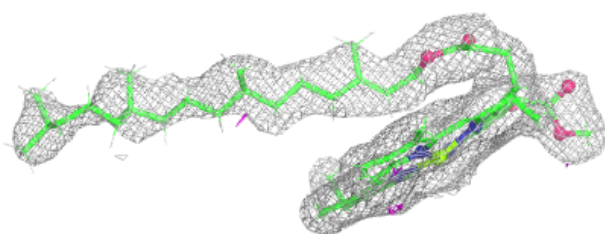
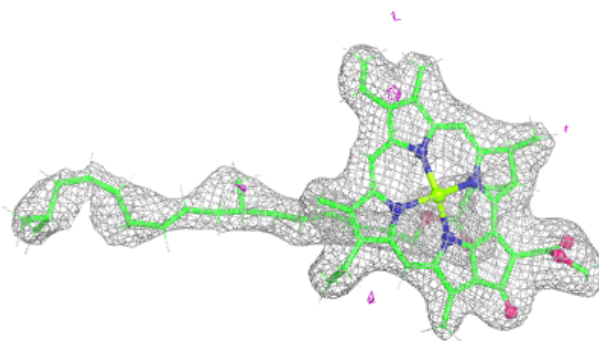
Electron density around CLA b 617:

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

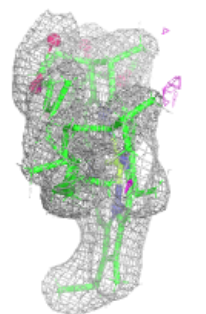
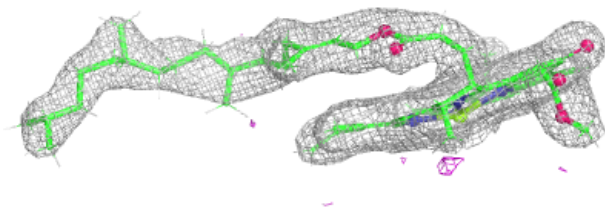
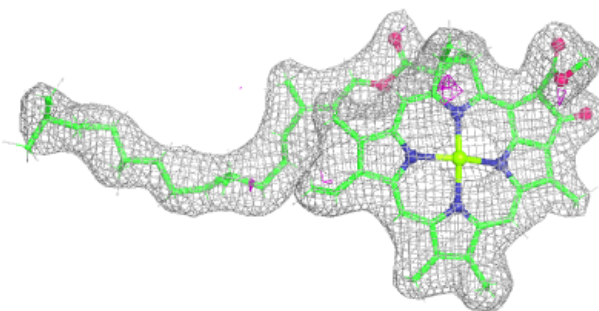


Electron density around CLA B 614:

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

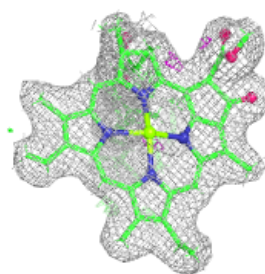
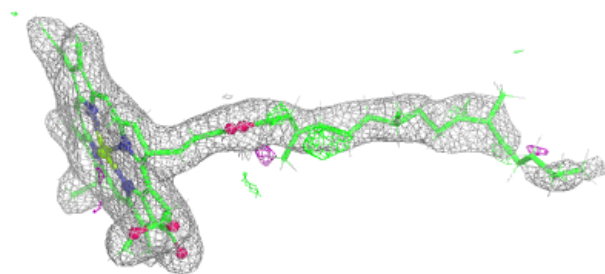
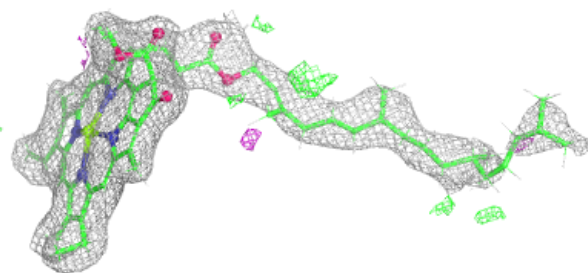
**Electron density around CLA B 603:**

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

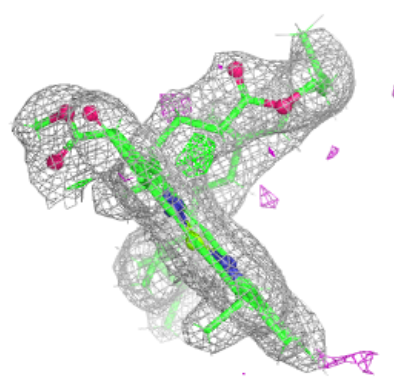
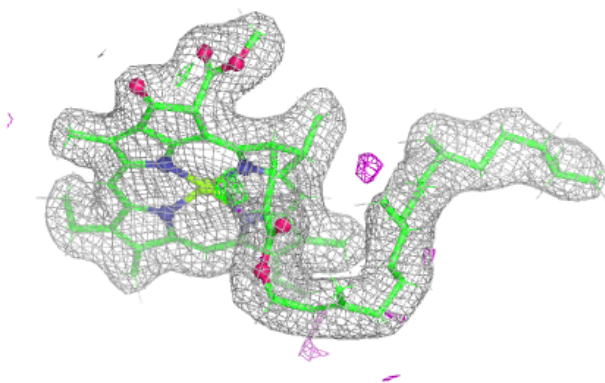
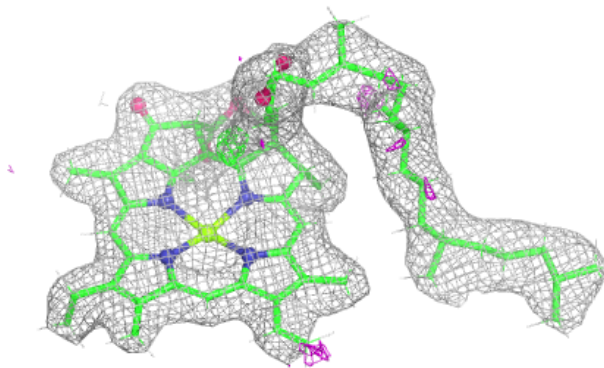


Electron density around CLA B 604:

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

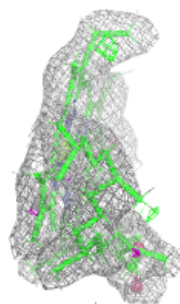
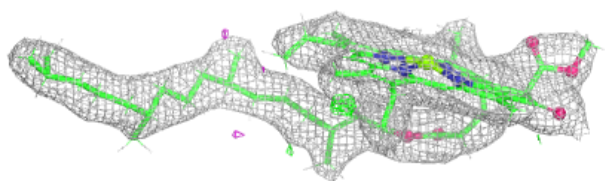
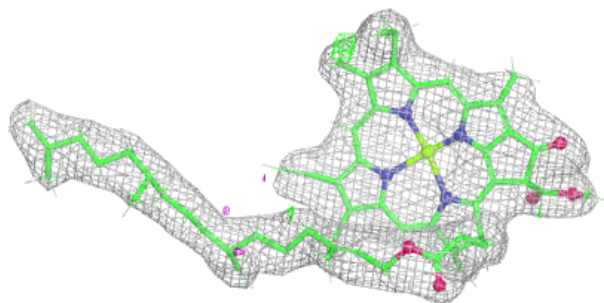
**Electron density around CLA D 402:**

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

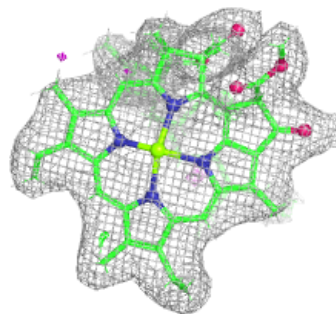
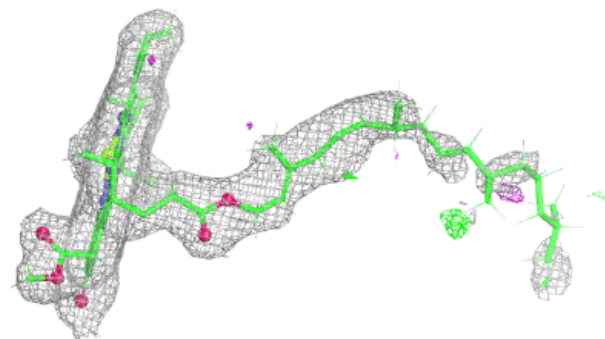
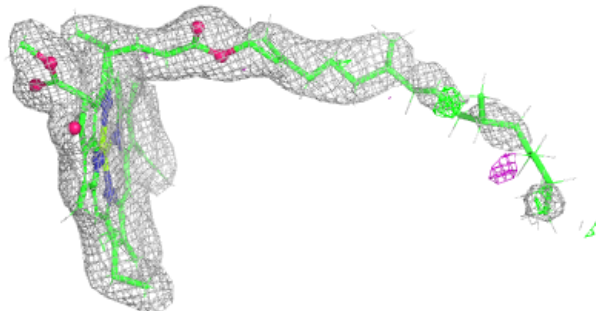


Electron density around CLA C 501:

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

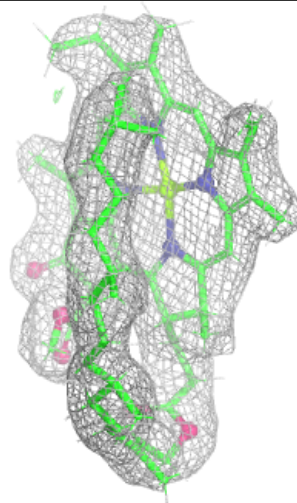
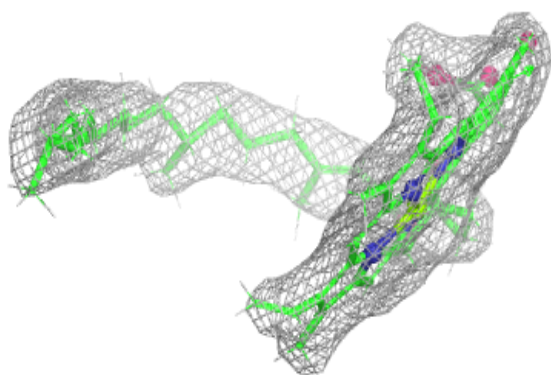
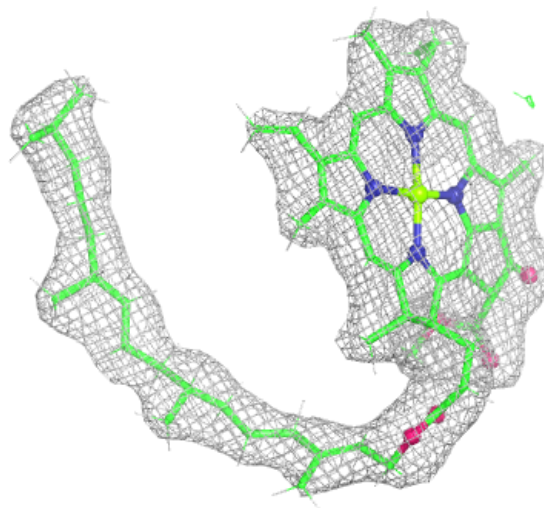
**Electron density around CLA D 404:**

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



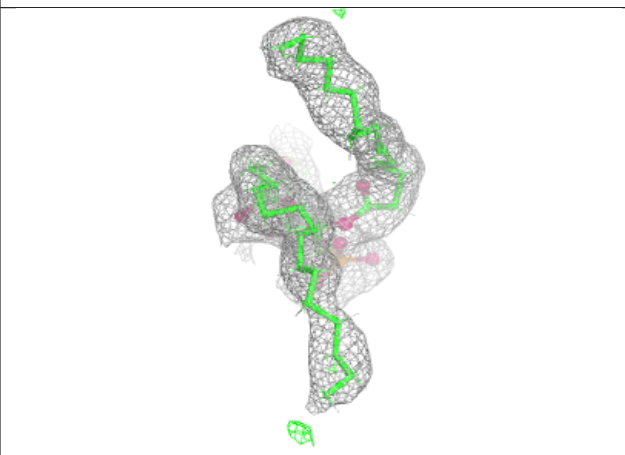
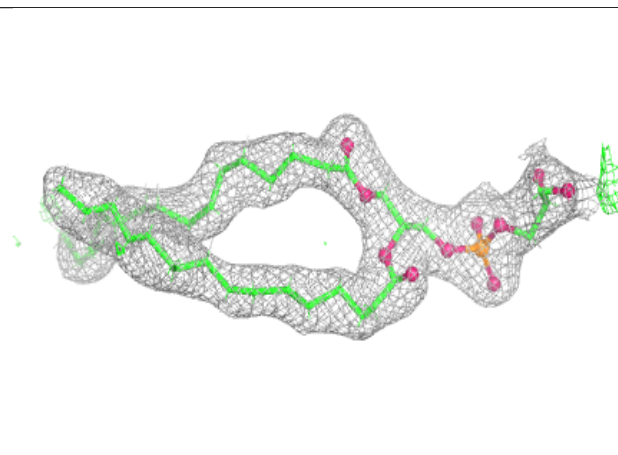
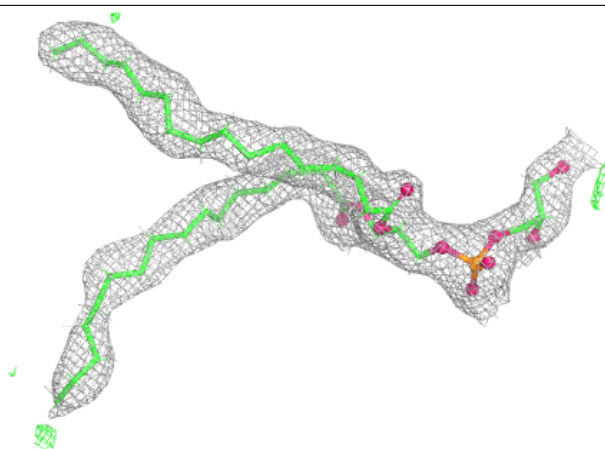
Electron density around CLA c 507:

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



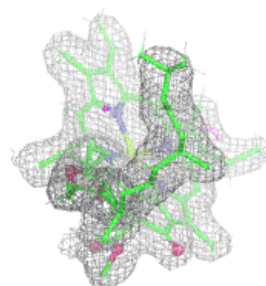
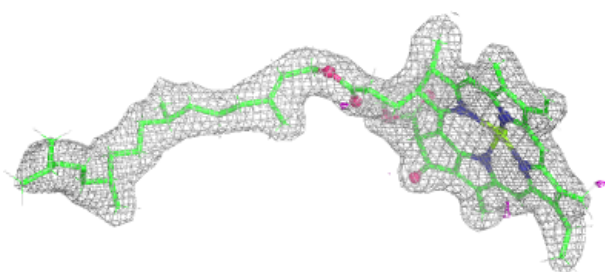
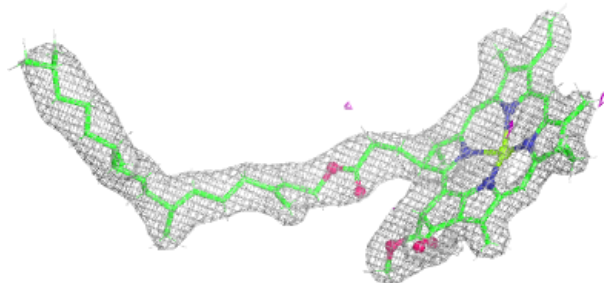
Electron density around LHG D 408:

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

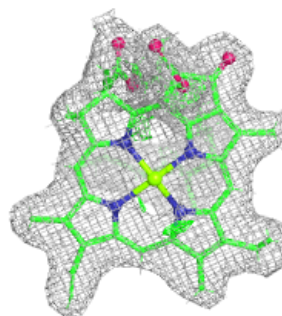
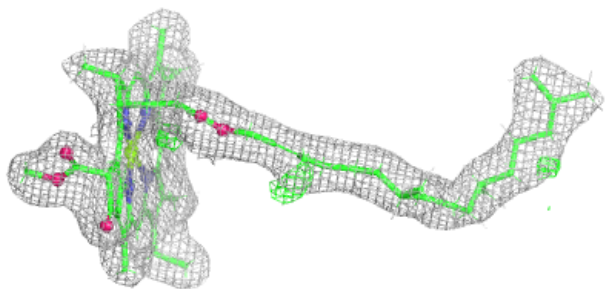
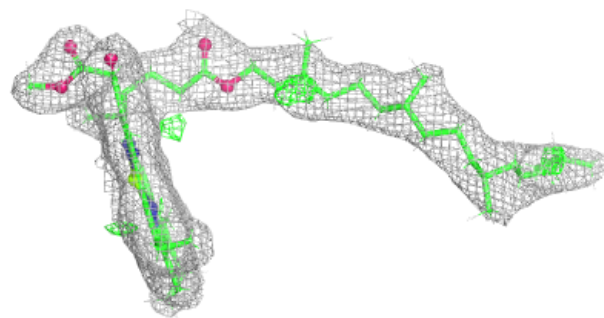


Electron density around CLA a 404:

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

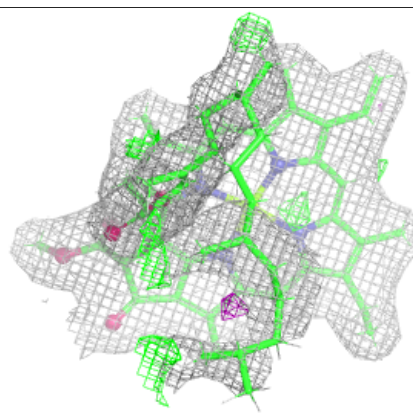
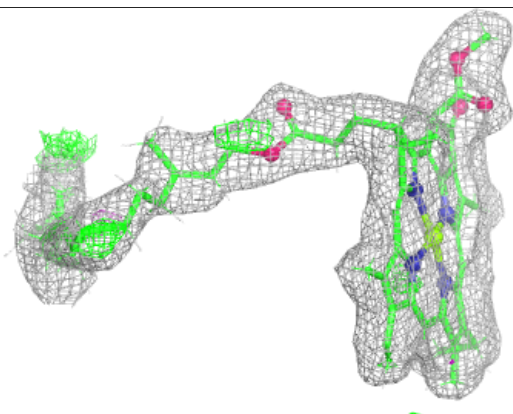
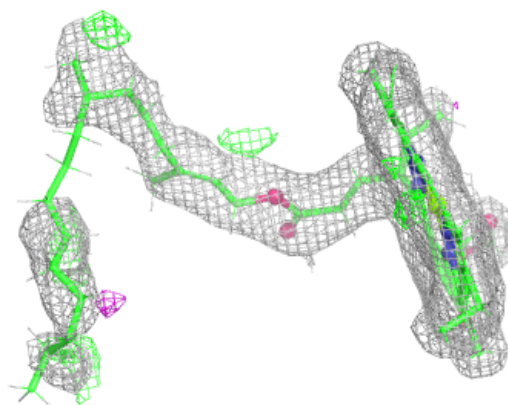
**Electron density around CLA B 605:**

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

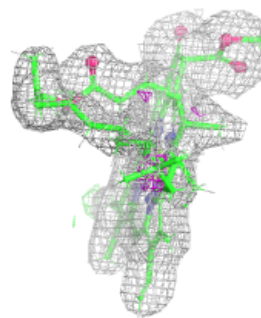
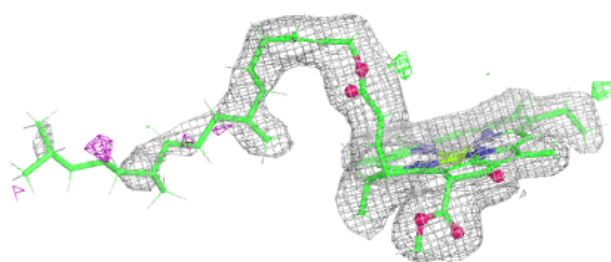
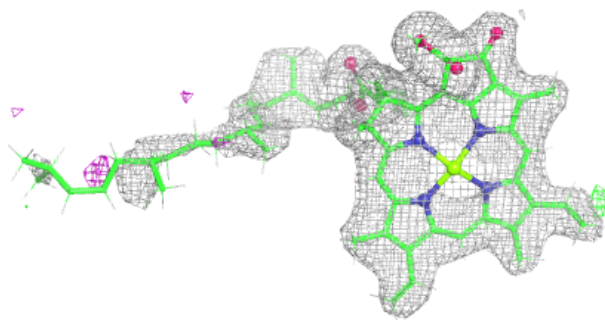


Electron density around CLA a 407:

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

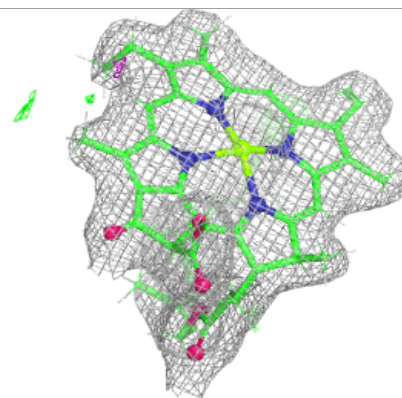
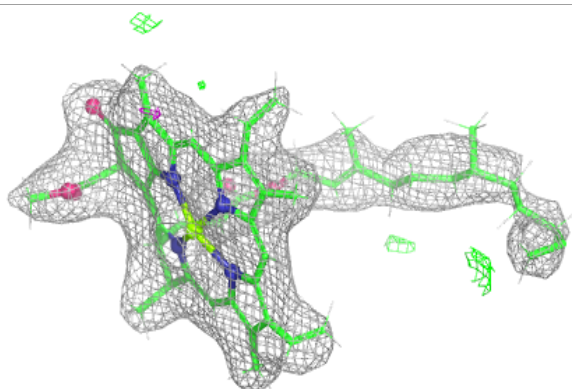
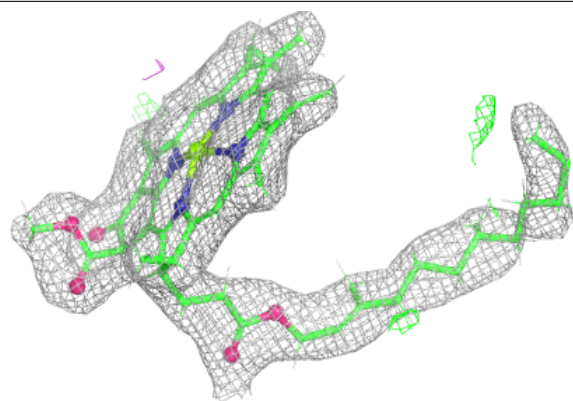
**Electron density around CLA A 405:**

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

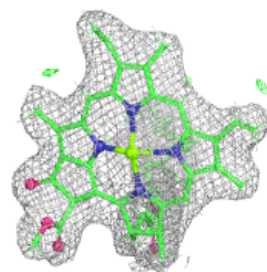
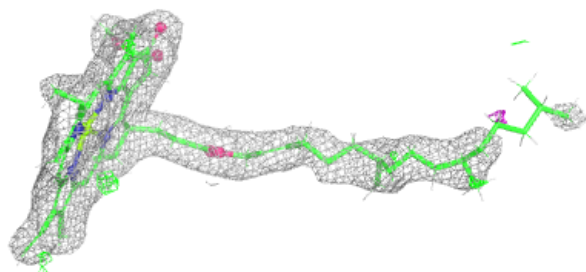


Electron density around CLA C 504:

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

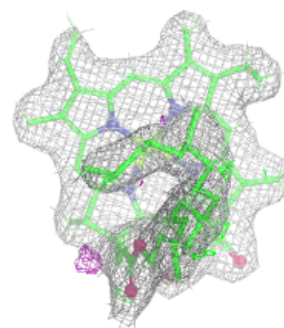
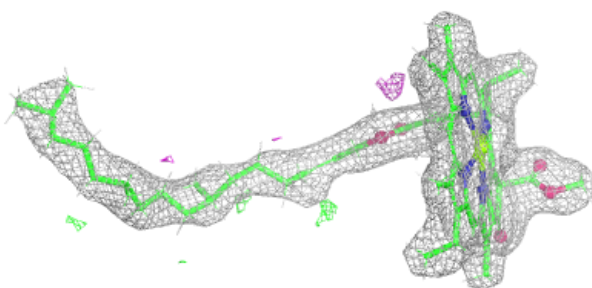
**Electron density around CLA b 605:**

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

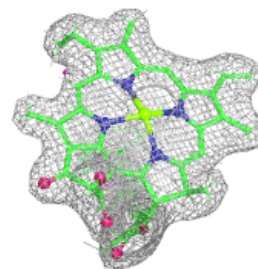
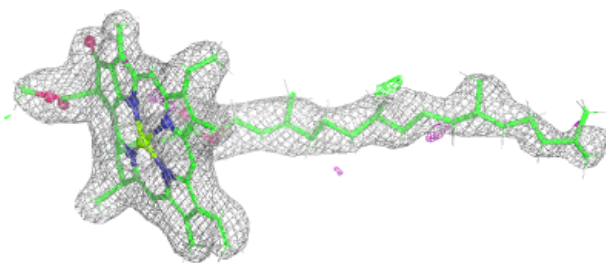
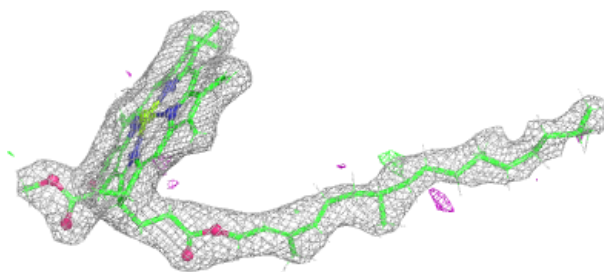


Electron density around CLA b 606:

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

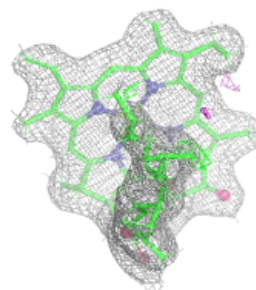
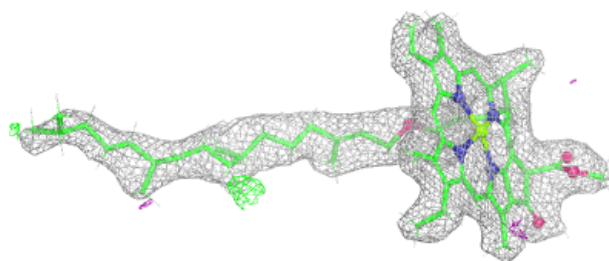
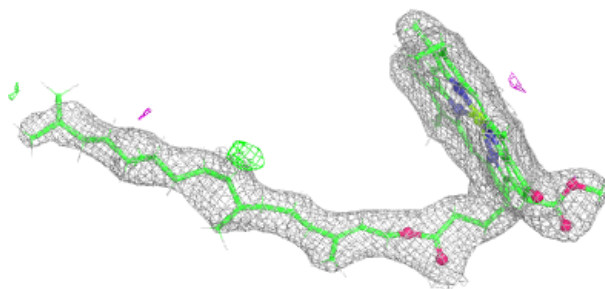
**Electron density around CLA B 607:**

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

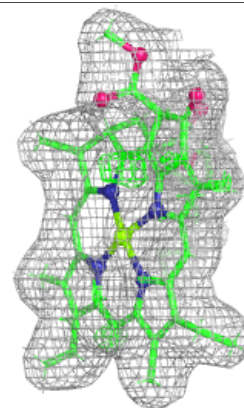
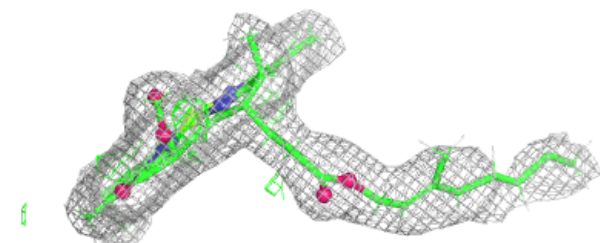
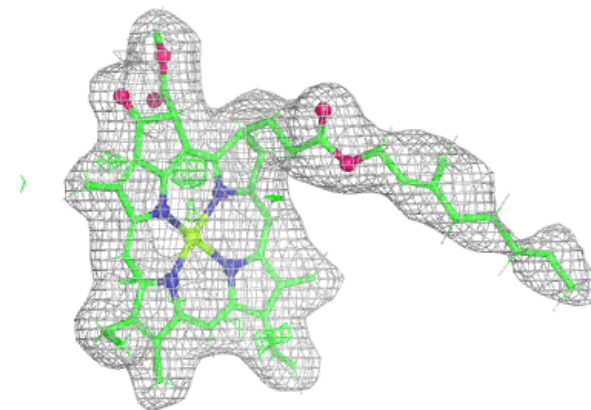


Electron density around CLA b 608:

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

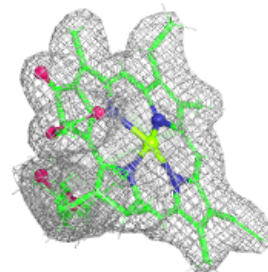
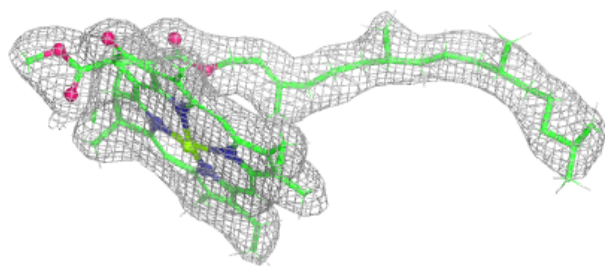
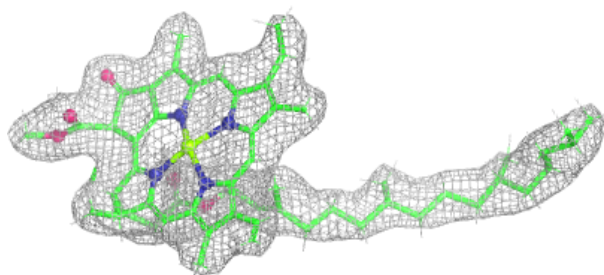
**Electron density around CLA A 407:**

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



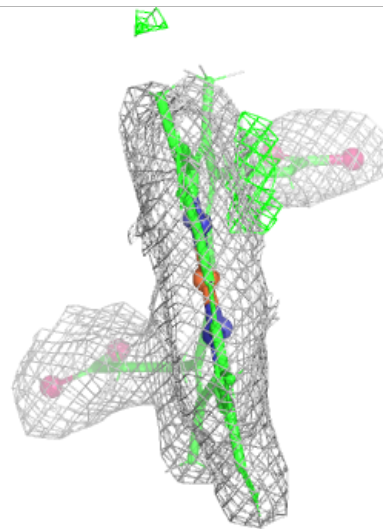
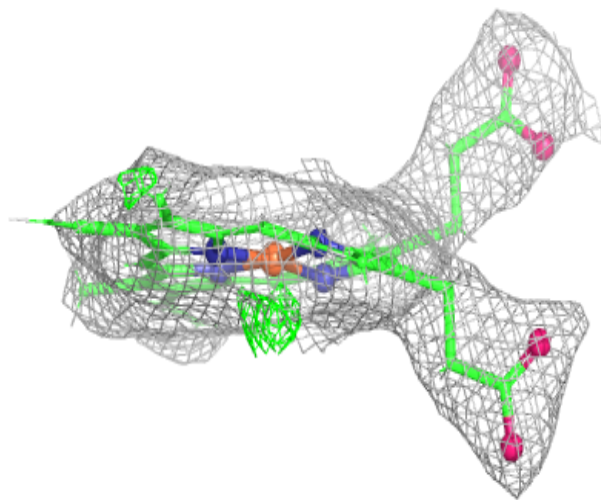
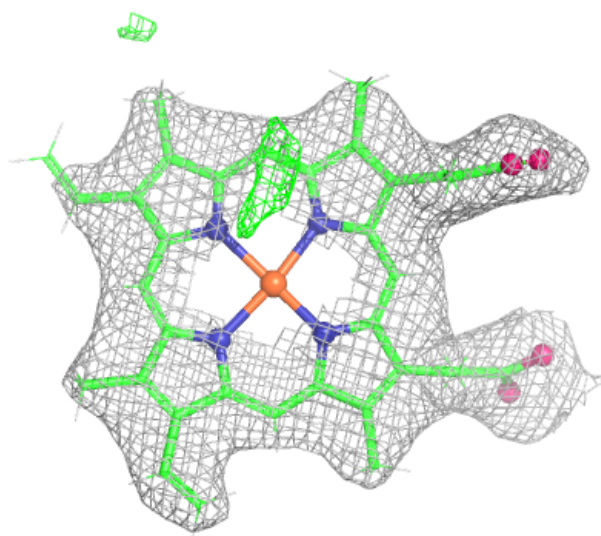
Electron density around CLA B 608:

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



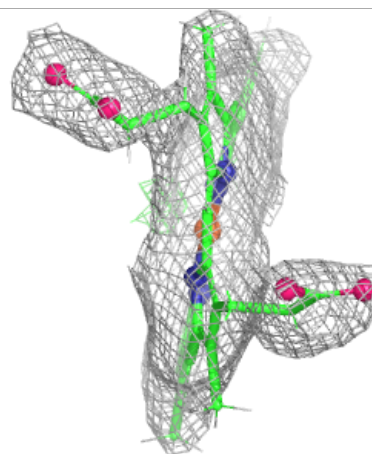
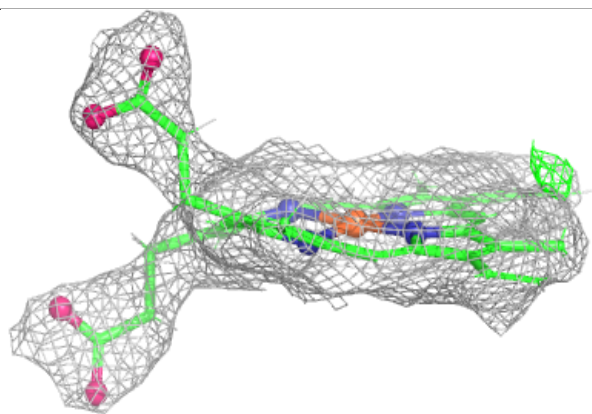
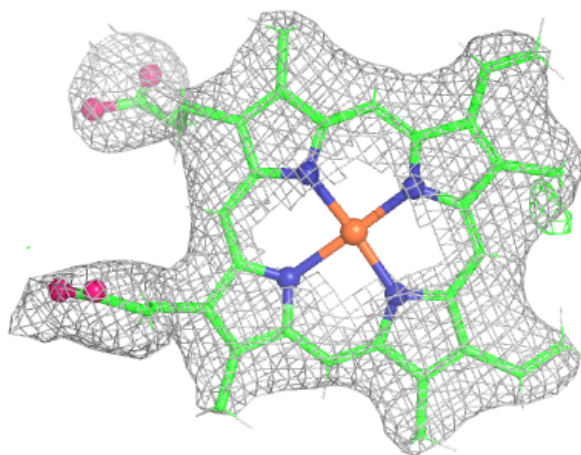
Electron density around HEM E 102:

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



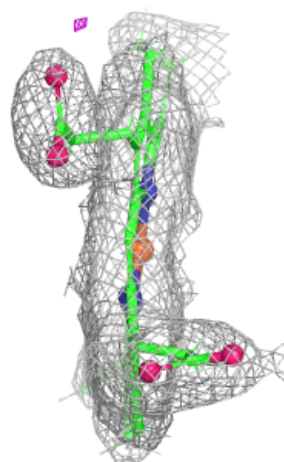
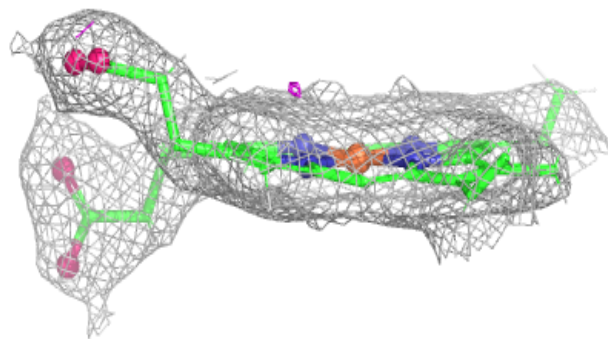
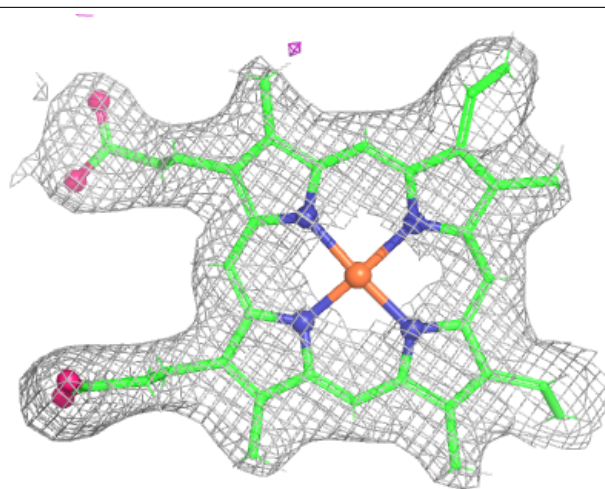
Electron density around HEM e 102:

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



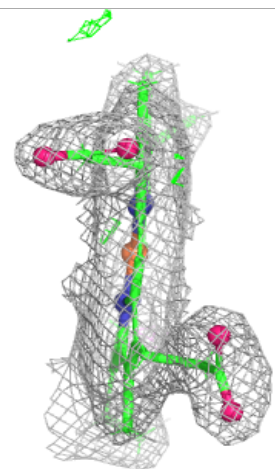
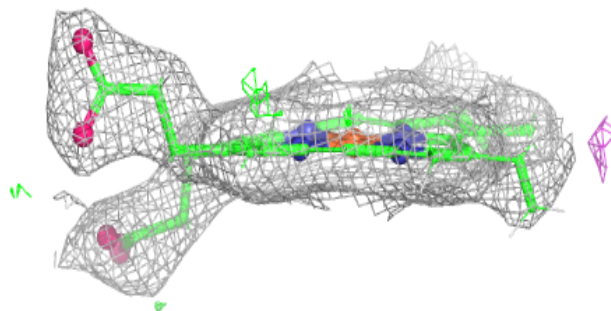
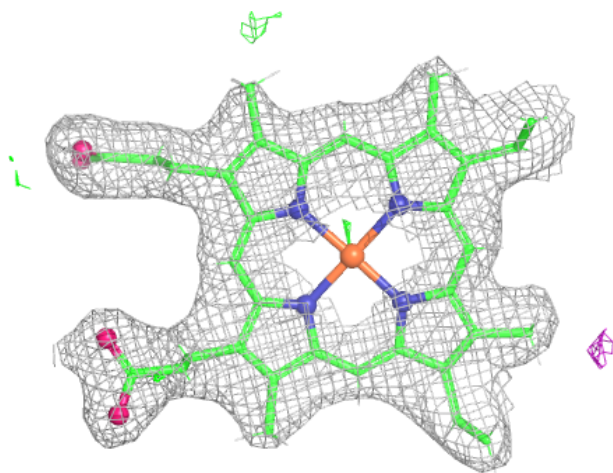
Electron density around HEC V 201:

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



Electron density around HEC v 201:

$2mF_o-DF_c$ (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.