



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:41 PM UTC

PDB ID : 6DHF / pdb_00006dhf
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.08 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 : 2.08 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

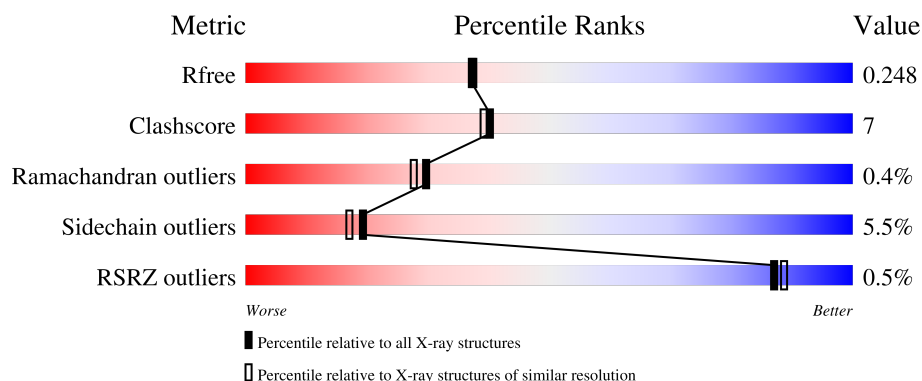
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

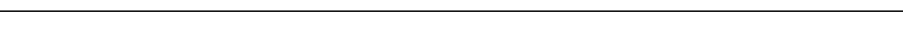
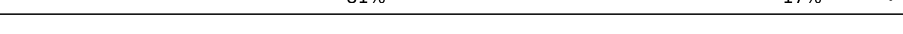
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 90% 10%

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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	 82% 17% .
2	B	505	 82% 16% .
2	b	505	 84% 15% .
3	C	451	 84% 14% .
3	c	451	 84% 16% .
4	D	341	 85% 15% .
4	d	341	 86% 13% .
5	E	82	 60% 35% . .
5	e	82	 79% 20% .
6	F	34	 3% 76% 24%
6	f	34	 59% 32% 9%
7	H	65	 2% 85% 14% .
7	h	65	 75% 20% . .
8	I	36	 83% 14% .
8	i	36	 81% 17% .
9	J	36	 69% 28% .
9	j	36	 3% 72% 25% .
10	K	37	 3% 68% 24% 8%
10	k	37	 3% 65% 30% 5%
11	L	37	 86% 14%
11	l	37	 76% 22% .
12	M	33	 76% 21% .
12	m	33	 79% 18% .
13	O	244	 81% 17% .
13	o	244	 84% 14% . .

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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
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	408	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	404	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	h	101	X	-	-	-
31	UNL	x	101	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103698 atoms, of which 51491 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	1	0
			6768	2249	3346	570	590	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6911	2290	3411	587	610	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				

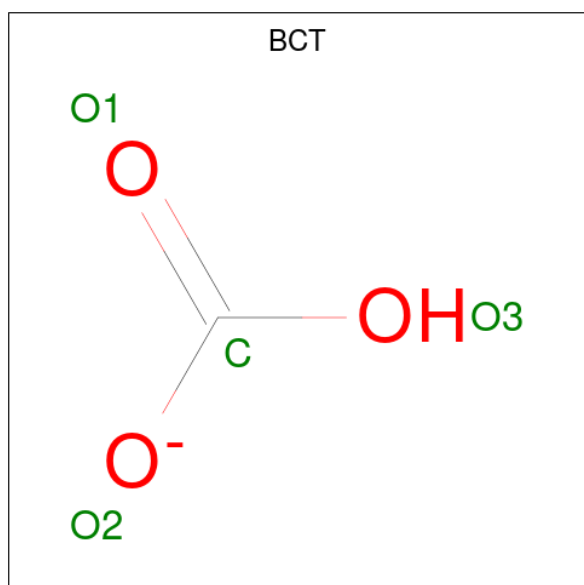
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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).

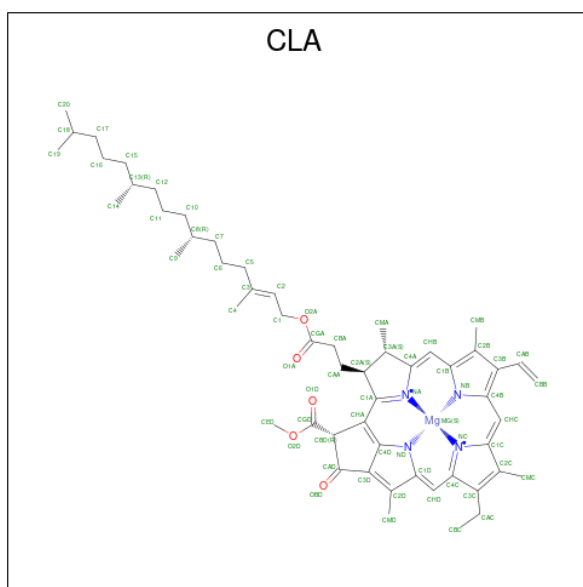
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).

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

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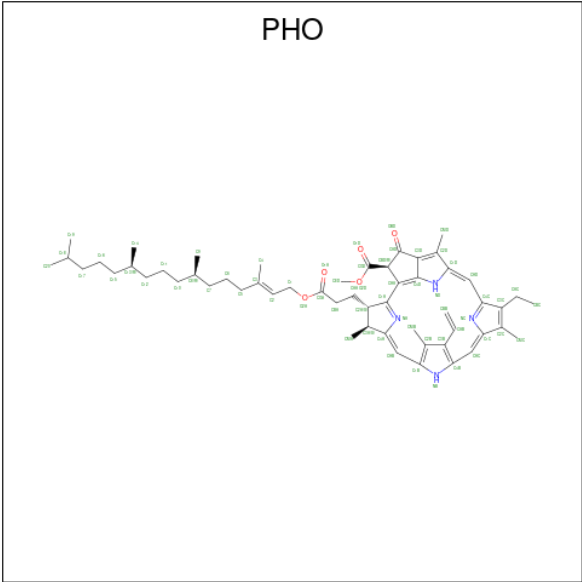
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4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

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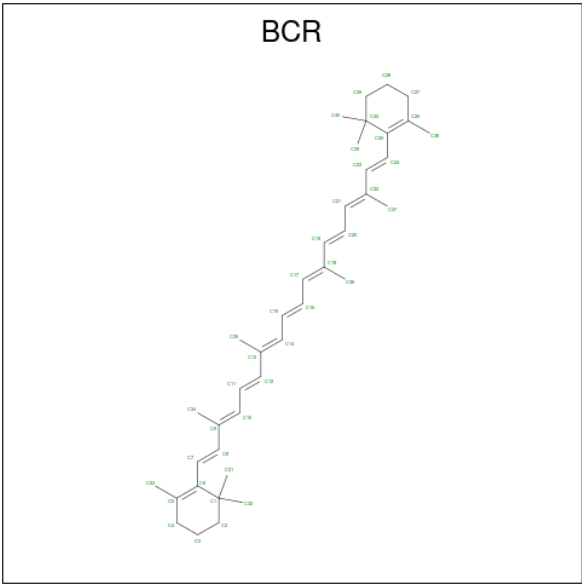
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	c	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 132	C 54	H 68	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



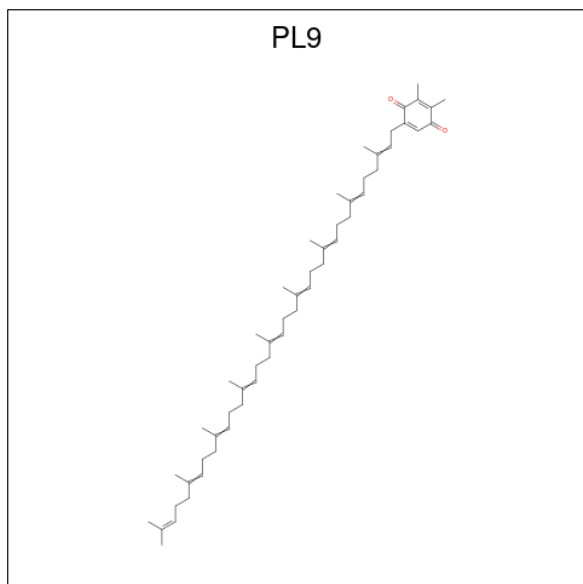
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



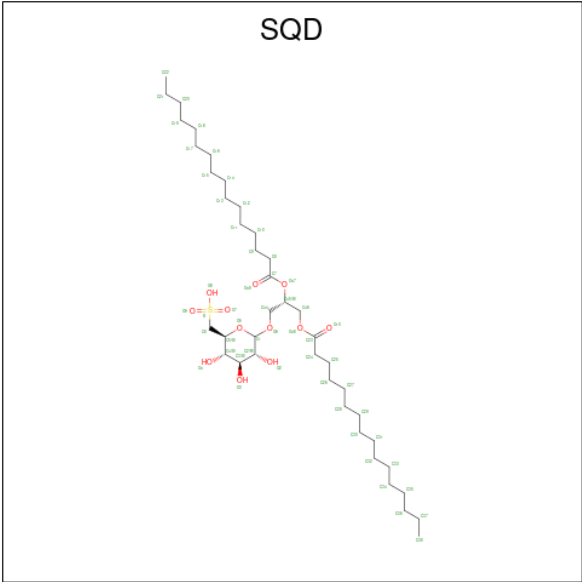
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	D	1	Total	C	H	0	0
			96	40	56		
26	H	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	Y	1	Total	C	H	0	0
			96	40	56		
26	a	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	h	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	t	1	Total	C	H	0	0
			96	40	56		

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



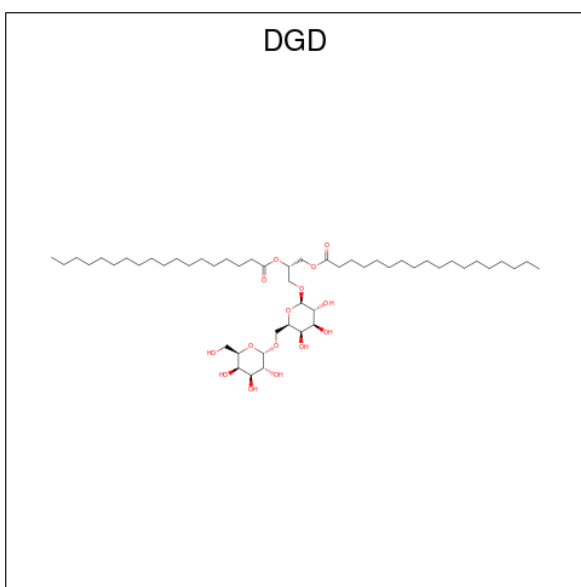
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			135	53	80	2		
27	D	1	Total	C	H	O	0	0
			135	53	80	2		
27	a	1	Total	C	H	O	0	0
			135	53	80	2		
27	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



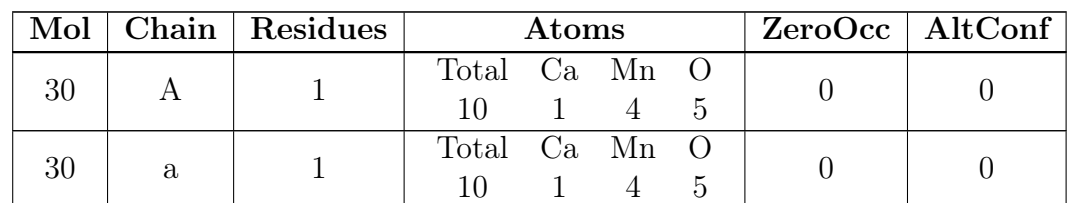
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
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: C₅₁H₉₆O₁₅).



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-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



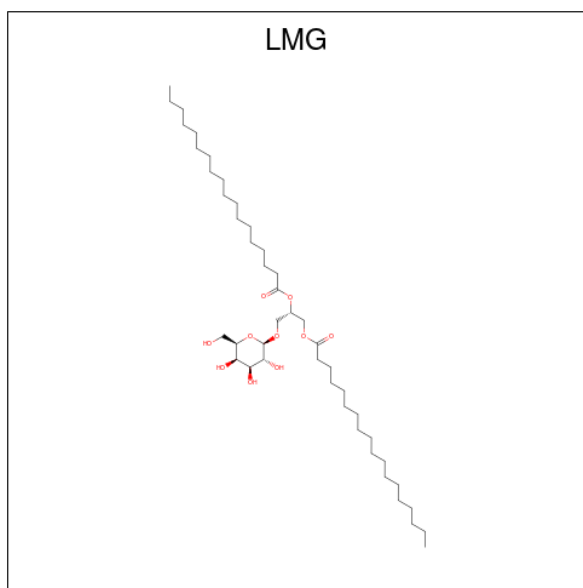
- | Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|---------|----------|--------|---------|---------|
| 31 | B | 5 | Total
192 | C
67 | H
117 | O
8 | 0 | 0 |
| 31 | C | 3 | Total
103 | C
36 | H
63 | O
4 | 0 | 0 |
| 31 | E | 1 | Total
28 | C
10 | H
16 | O
2 | 0 | 0 |
| 31 | H | 1 | Total
53 | C
18 | H
35 | | 0 | 0 |
| 31 | I | 1 | Total
41 | C
15 | H
26 | | 0 | 0 |
| 31 | J | 1 | Total
28 | C
10 | H
16 | O
2 | 0 | 0 |
| 31 | M | 3 | Total
116 | C
41 | H
73 | O
2 | 0 | 0 |
| 31 | T | 2 | Total
91 | C
31 | H
60 | | 0 | 0 |
| 31 | X | 1 | Total
55 | C
18 | H
35 | O
2 | 0 | 0 |
| 31 | a | 1 | Total
28 | C
10 | H
16 | O
2 | 0 | 0 |



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	4	Total	C	H	O	0	0
			176	60	110	6		
31	c	2	Total	C	H	O	0	0
			83	28	51	4		
31	d	1	Total	C	H	O	0	0
			43	15	26	2		
31	j	1	Total	C	H	O	0	0
			28	10	16	2		
31	m	1	Total	C	H	O	0	0
			28	10	16	2		
31	t	2	Total	C	H	O	0	0
			60	22	36	2		
31	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



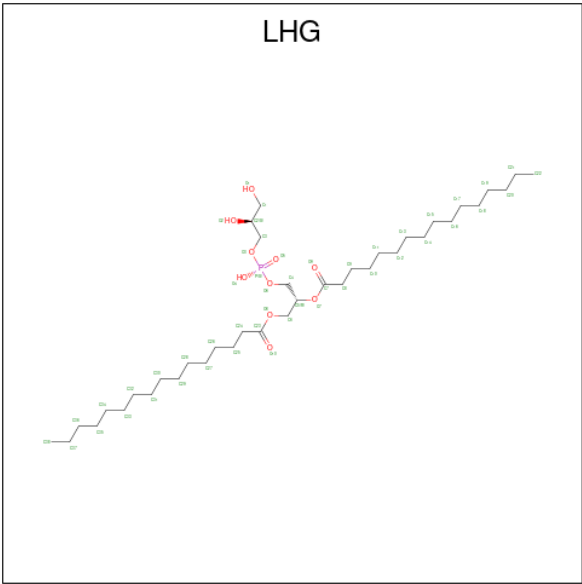
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			68	24	40	4		
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	D	1	Total	C	H	O	0	0
			123	41	72	10		
32	D	1	Total	C	H	O	0	0
			78	27	45	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	K	1	Total	C	H	O	0	0
			114	38	66	10		
32	M	1	Total	C	H	O	0	0
			123	41	72	10		
32	b	1	Total	C	H	O	0	0
			123	41	72	10		
32	b	1	Total	C	H	O	0	0
			141	45	86	10		
32	c	1	Total	C	H	O	0	0
			81	27	44	10		
32	c	1	Total	C	H	O	0	0
			117	38	69	10		
32	c	1	Total	C	H	O	0	0
			117	39	68	10		
32	d	1	Total	C	H	O	0	0
			102	34	58	10		
32	h	1	Total	C	H	O	0	0
			57	21	34	2		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



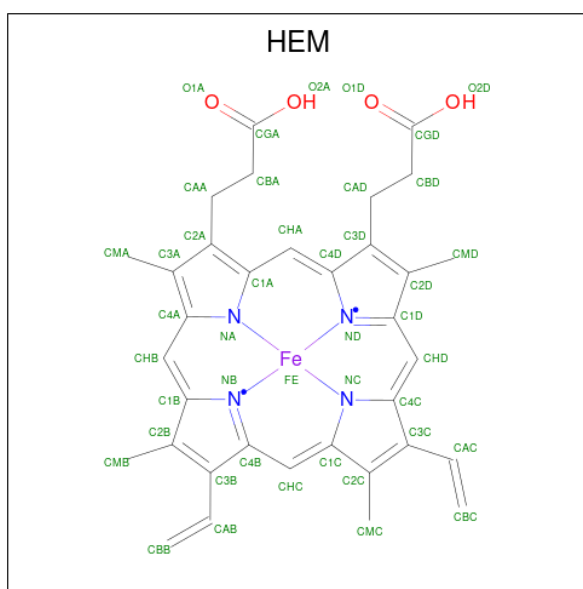
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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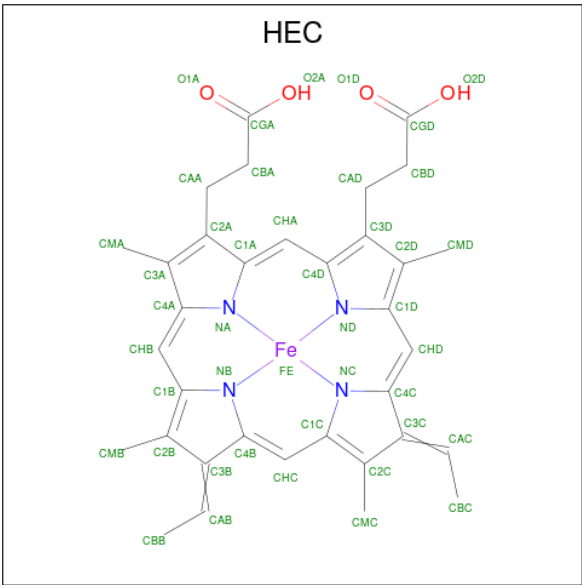
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	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	F	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	141	Total	O	0	0
			141	141		
36	B	218	Total	O	0	0
			218	218		
36	C	197	Total	O	0	0
			197	197		
36	D	138	Total	O	0	0
			138	138		
36	E	29	Total	O	0	0
			29	29		
36	F	14	Total	O	0	0
			14	14		
36	H	26	Total	O	0	0
			26	26		
36	I	16	Total	O	0	0
			16	16		
36	J	12	Total	O	0	0
			12	12		
36	K	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	L	9	Total O 9 9	0	0
36	M	5	Total O 5 5	0	0
36	O	125	Total O 125 125	0	0
36	T	11	Total O 11 11	0	0
36	U	52	Total O 52 52	0	0
36	V	68	Total O 68 68	0	0
36	Y	5	Total O 5 5	0	0
36	X	6	Total O 6 6	0	0
36	Z	3	Total O 3 3	0	0
36	R	4	Total O 4 4	0	0
36	a	121	Total O 121 121	0	0
36	b	187	Total O 187 187	0	0
36	c	156	Total O 156 156	0	0
36	d	123	Total O 123 123	0	0
36	e	22	Total O 22 22	0	0
36	f	2	Total O 2 2	0	0
36	h	19	Total O 19 19	0	0
36	i	10	Total O 10 10	0	0
36	j	10	Total O 10 10	0	0
36	k	5	Total O 5 5	0	0
36	l	9	Total O 9 9	0	0

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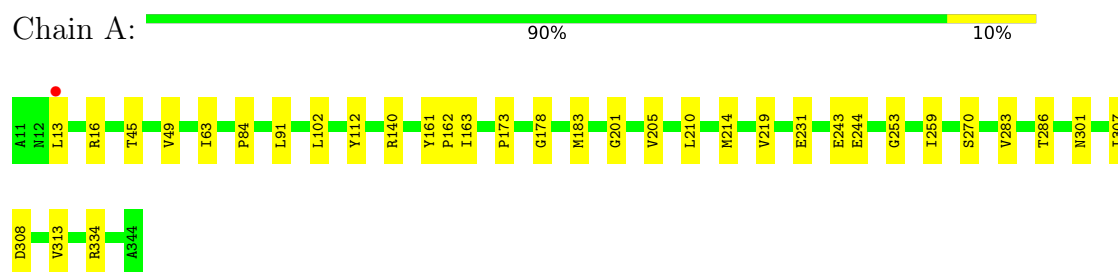
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	m	7	Total 7	O 7	0	0
36	o	113	Total 113	O 113	0	0
36	t	11	Total 11	O 11	0	0
36	u	57	Total 57	O 57	0	0
36	v	62	Total 62	O 62	0	0
36	y	4	Total 4	O 4	0	0
36	x	12	Total 12	O 12	0	0
36	z	1	Total 1	O 1	0	0
36	r	5	Total 5	O 5	0	0

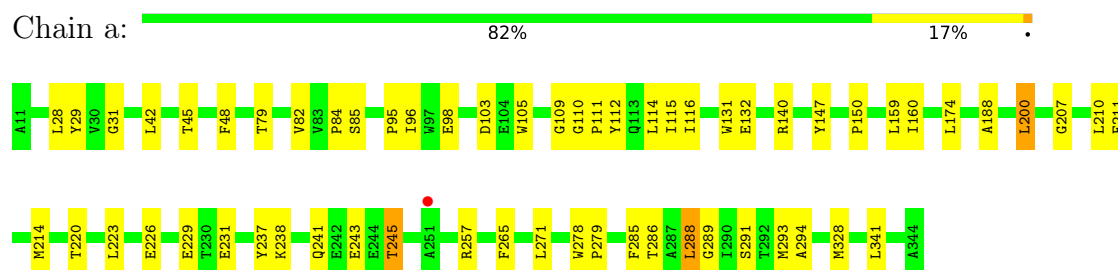
3 Residue-property plots

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

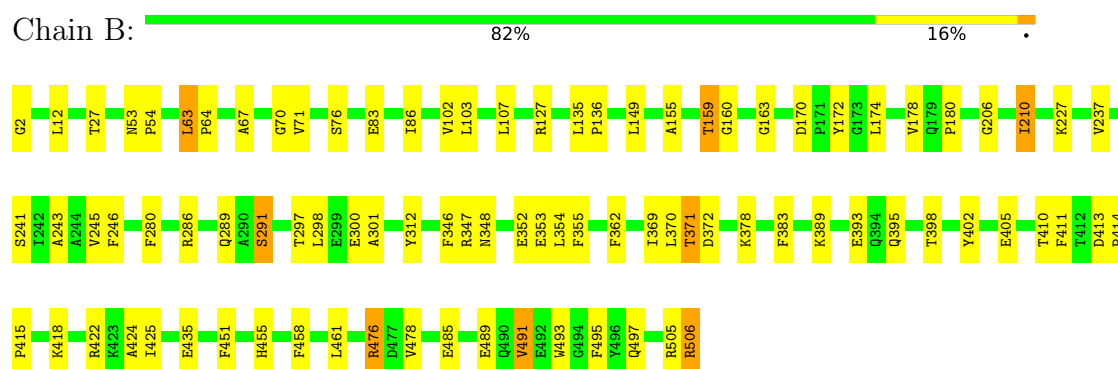
• Molecule 1: Photosystem II protein D1 1



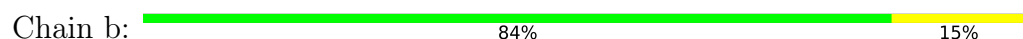
• Molecule 1: Photosystem II protein D1 1

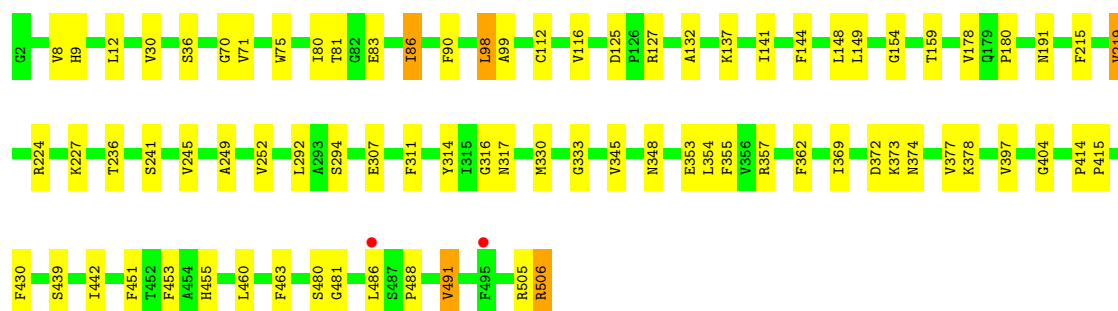


• Molecule 2: Photosystem II CP47 reaction center protein

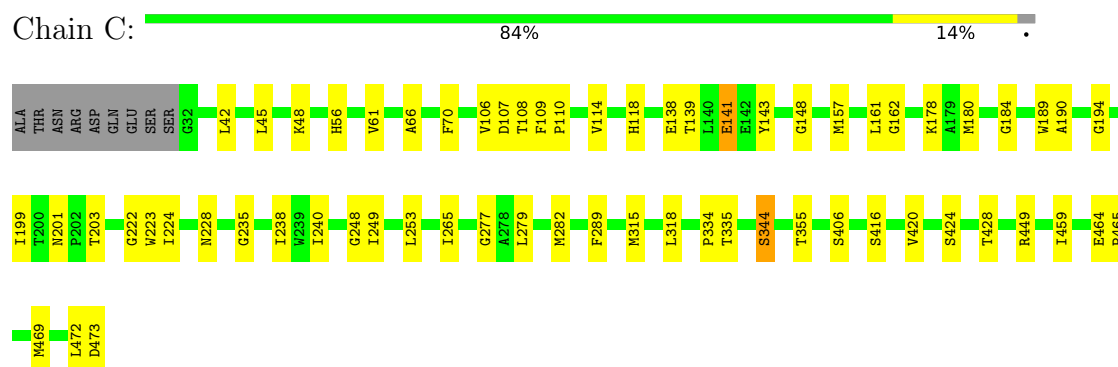


• Molecule 2: Photosystem II CP47 reaction center protein

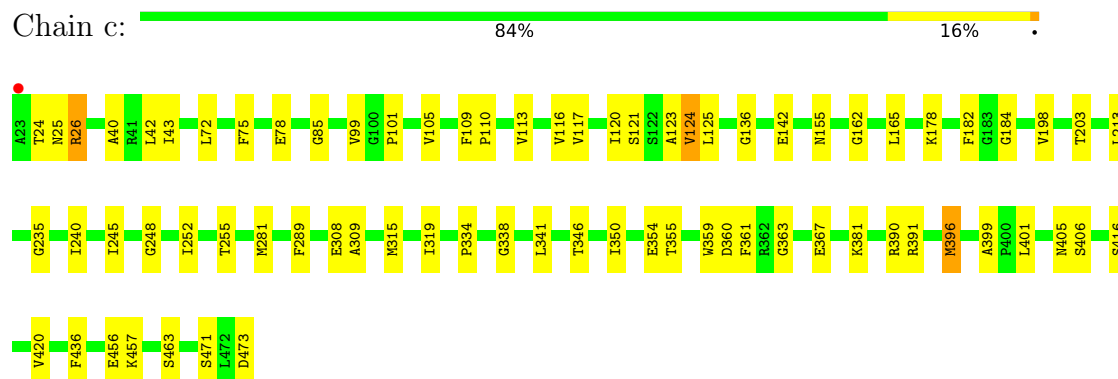




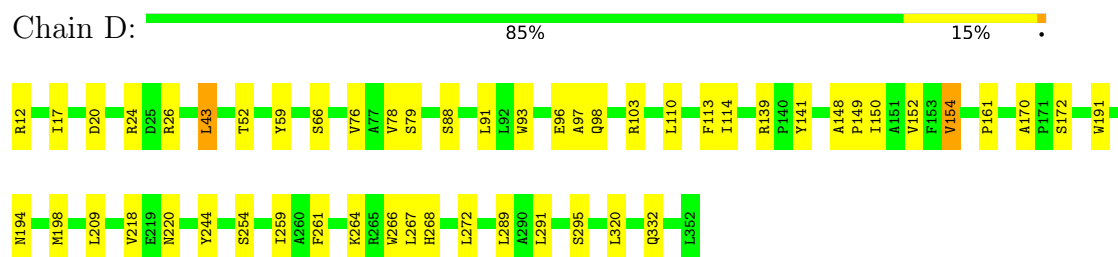
- Molecule 3: Photosystem II CP43 reaction center protein



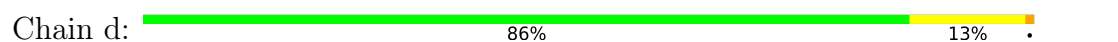
- Molecule 3: Photosystem II CP43 reaction center protein

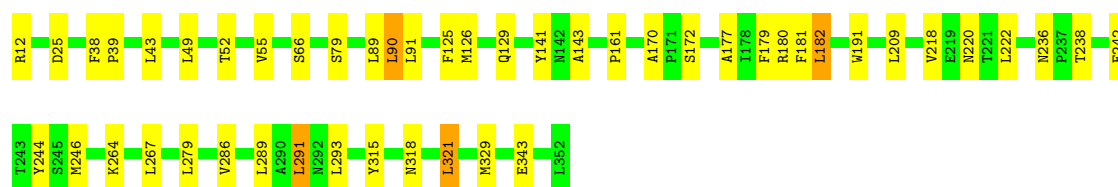


- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein





- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 60% 35% . .



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 79% 20% .



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 3% 76% 24%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 59% 32% 9%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 2% 85% 14% .



- Molecule 7: Photosystem II reaction center protein H

Chain h: 75% 20% . .



- Molecule 8: Photosystem II reaction center protein I

Chain I:  83% 14% .



- Molecule 8: Photosystem II reaction center protein I

Chain i:  81% 17% .



- Molecule 9: Photosystem II reaction center protein J

Chain J:  69% 28% .



- Molecule 9: Photosystem II reaction center protein J

Chain j:  3% 72% 25% .



- Molecule 10: Photosystem II reaction center protein K

Chain K:  3% 68% 24% 8% .



- Molecule 10: Photosystem II reaction center protein K

Chain k:  3% 65% 30% 5% .



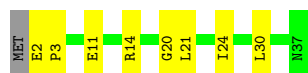
- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14% .



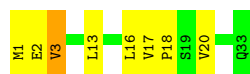
- Molecule 11: Photosystem II reaction center protein L

Chain l:  76% 22% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  76% 21% .



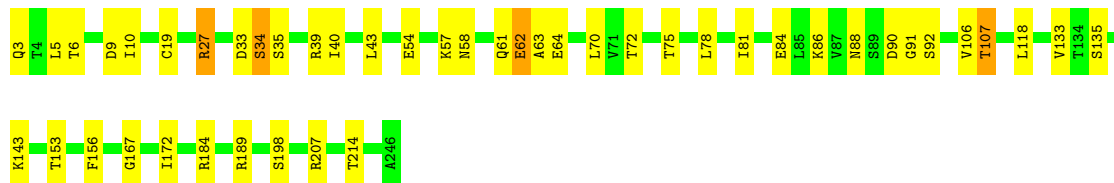
- Molecule 12: Photosystem II reaction center protein M

Chain m:  79% 18% .



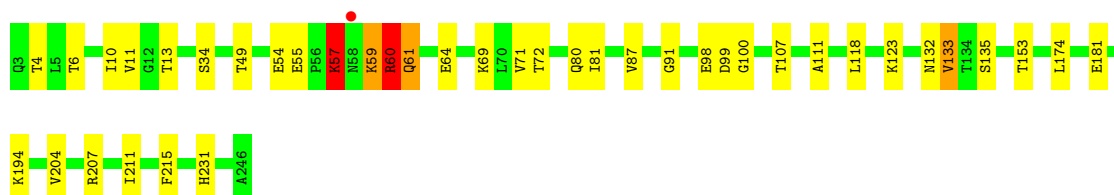
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  81% 17% .



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  84% 14% ..



- Molecule 14: Photosystem II reaction center protein T

Chain T:  83% 13% .



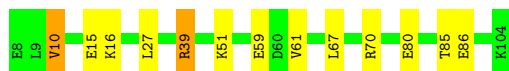
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 83% 17%



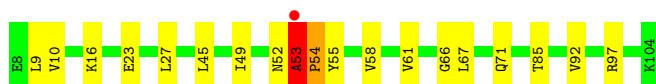
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 87% 11% .



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 80% 18% ..



- Molecule 16: Cytochrome c-550

Chain V: 79% 19% .



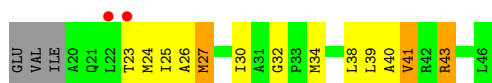
- Molecule 16: Cytochrome c-550

Chain v: 77% 22% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 7% 47% 33% 10% 10%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 60% 37% .



- Molecule 18: Photosystem II reaction center X protein

Chain X: 3% 84% 16%



- Molecule 18: Photosystem II reaction center X protein

Chain x: 82% 18%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 3% 61% 35% .



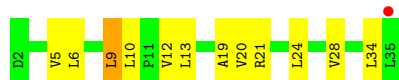
- Molecule 19: Photosystem II reaction center protein Z

Chain z: 3% 66% 24% 10%



- Molecule 20: Photosystem II protein Y

Chain R: 3% 65% 32% .



- Molecule 20: Photosystem II protein Y

Chain r: 9% 47% 26% 18% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.82Å 220.89Å 307.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.43 – 2.08 30.43 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.43-2.08) 86.9 (30.43-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 2.08Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.189 , 0.247 0.189 , 0.248	Depositor DCC
R_{free} test set	4194 reflections (0.71%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103698	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.64	0/2707	0.73	0/3692
1	a	0.63	0/2704	0.73	1/3688 (0.0%)
2	B	0.60	0/4160	0.68	0/5668
2	b	0.57	0/4118	0.67	0/5611
3	C	0.59	0/3538	0.66	0/4818
3	c	0.53	0/3619	0.65	0/4926
4	D	0.63	0/2812	0.71	0/3832
4	d	0.57	0/2821	0.67	0/3844
5	E	0.43	0/684	0.61	0/935
5	e	0.41	0/683	0.57	0/932
6	F	0.47	0/284	0.59	0/387
6	f	0.42	0/284	0.63	0/387
7	H	0.58	0/520	0.70	0/709
7	h	0.51	0/511	0.61	0/697
8	I	0.60	0/293	0.74	0/396
8	i	0.67	0/293	0.72	0/396
9	J	0.45	0/263	0.65	0/356
9	j	0.40	0/261	0.54	0/353
10	K	0.44	0/314	0.58	0/427
10	k	0.38	0/303	0.50	0/416
11	L	0.65	0/311	0.67	0/422
11	l	0.66	0/303	0.68	0/412
12	M	0.57	0/249	0.69	0/341
12	m	0.64	0/244	0.67	0/334
13	O	0.56	0/1914	0.69	0/2596
13	o	0.55	0/1905	0.70	0/2583
14	T	0.63	0/257	0.76	0/349
14	t	0.63	0/255	0.67	0/346
15	U	0.51	0/785	0.63	0/1064
15	u	0.58	0/785	0.69	0/1064
16	V	0.54	0/1085	0.64	0/1473
16	v	0.49	0/1085	0.62	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.40	0/197	0.60	0/264
17	y	0.29	0/219	0.47	0/294
18	X	0.46	0/284	0.59	0/384
18	x	0.35	0/284	0.48	0/384
19	Z	0.43	0/490	0.55	0/669
19	z	0.32	0/488	0.48	0/666
20	R	0.37	0/277	0.53	0/380
20	r	0.32	0/233	0.51	0/323
All	All	0.56	0/42822	0.67	1/58291 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	110	GLY	O-C-N	9.17	124.37	121.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	53	ALA	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	22	0
1	a	2619	2499	2510	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4004	3845	3864	56	0
2	b	3978	3811	3836	52	0
3	C	3422	3346	3359	38	0
3	c	3500	3411	3426	42	0
4	D	2717	2613	2621	37	0
4	d	2723	2619	2627	35	0
5	E	662	647	648	24	0
5	e	664	647	648	14	0
6	F	275	281	282	7	0
6	f	275	281	282	12	0
7	H	507	523	523	5	0
7	h	498	518	518	9	0
8	I	296	311	311	2	0
8	i	296	311	311	4	0
9	J	257	268	268	10	0
9	j	255	261	261	10	0
10	K	302	318	318	12	0
10	k	293	305	305	10	0
11	L	304	316	316	5	0
11	l	296	304	304	3	0
12	M	256	269	269	6	0
12	m	251	267	267	5	0
13	O	1880	1850	1852	30	0
13	o	1874	1844	1846	23	0
14	T	258	261	261	3	0
14	t	256	256	256	4	0
15	U	774	772	773	6	0
15	u	774	772	773	11	0
16	V	1064	1070	1073	15	0
16	v	1064	1070	1073	17	0
17	Y	196	208	217	9	0
17	y	218	241	241	5	0
18	X	281	312	312	4	0
18	x	281	312	312	5	0
19	Z	479	509	516	12	0
19	z	477	509	509	10	0
20	R	271	298	298	6	0
20	r	227	234	224	11	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	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
23	A	4	1	1	0	0
23	d	4	1	1	0	0
24	A	184	192	192	1	0
24	B	1035	1139	1139	18	0
24	C	839	922	922	12	0
24	D	195	216	216	3	0
24	a	195	216	216	2	0
24	b	970	1067	1067	26	0
24	c	839	919	919	7	0
24	d	195	216	216	3	0
24	h	65	72	72	4	0
25	A	64	74	74	0	0
25	D	64	74	74	1	0
25	a	64	74	74	1	0
25	d	64	74	74	1	0
26	A	40	56	56	1	0
26	B	120	168	168	8	0
26	C	80	112	112	3	0
26	D	40	56	56	5	0
26	H	40	56	56	1	0
26	K	40	56	56	4	0
26	Y	40	56	56	3	0
26	a	40	56	56	1	0
26	b	160	224	224	11	0
26	c	120	168	168	4	0
26	d	40	56	56	2	0
26	h	40	56	56	4	0
26	k	40	56	56	0	0
26	t	40	56	56	6	0
27	A	55	80	80	0	0
27	D	55	80	80	1	0
27	a	55	80	80	3	0
27	d	55	80	80	0	0
28	A	91	135	135	2	0
28	B	54	78	78	3	0
28	F	36	45	46	1	0
28	a	90	134	133	3	0
28	b	49	65	65	0	0
28	f	41	49	48	4	0
29	A	66	96	96	2	0
29	C	186	246	245	0	0
29	H	62	82	82	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	44	75	75	1	0
29	c	186	246	244	1	0
29	h	62	82	82	1	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	B	75	117	0	2	0
31	C	40	63	0	0	0
31	E	12	16	0	0	0
31	H	18	35	0	0	0
31	I	15	26	0	0	0
31	J	12	16	0	0	0
31	M	43	73	0	0	0
31	T	31	60	0	0	0
31	X	20	35	0	0	0
31	a	12	16	0	0	0
31	b	66	110	0	0	0
31	c	32	51	0	1	0
31	d	17	26	0	1	0
31	j	12	16	0	0	0
31	m	12	16	0	0	0
31	t	24	36	0	0	0
31	x	20	35	0	2	0
32	B	28	40	40	0	0
32	C	48	66	66	0	0
32	D	84	117	116	0	0
32	K	48	66	66	0	0
32	M	51	72	72	1	0
32	b	106	158	158	2	0
32	c	134	181	181	4	0
32	d	44	58	58	0	0
32	h	23	34	34	0	0
33	D	145	215	215	5	0
33	E	49	74	74	2	0
33	L	49	74	74	1	0
33	d	137	199	199	5	0
33	e	42	57	57	0	0
33	l	49	74	74	1	0
34	F	43	30	30	4	0
34	e	43	30	30	5	0
35	V	43	30	30	1	0
35	v	43	30	30	2	0
36	A	141	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	B	218	0	0	9	0
36	C	197	0	0	4	0
36	D	138	0	0	6	0
36	E	29	0	0	0	0
36	F	14	0	0	1	0
36	H	26	0	0	0	0
36	I	16	0	0	0	0
36	J	12	0	0	2	0
36	K	2	0	0	0	0
36	L	9	0	0	2	0
36	M	5	0	0	0	0
36	O	125	0	0	11	0
36	R	4	0	0	0	0
36	T	11	0	0	0	0
36	U	52	0	0	2	0
36	V	68	0	0	2	0
36	X	6	0	0	0	0
36	Y	5	0	0	0	0
36	Z	3	0	0	0	0
36	a	121	0	0	1	0
36	b	187	0	0	10	0
36	c	156	0	0	7	0
36	d	123	0	0	5	0
36	e	22	0	0	1	0
36	f	2	0	0	1	0
36	h	19	0	0	0	0
36	i	10	0	0	1	0
36	j	10	0	0	1	0
36	k	5	0	0	2	0
36	l	9	0	0	0	0
36	m	7	0	0	1	0
36	o	113	0	0	5	0
36	r	5	0	0	2	0
36	t	11	0	0	1	0
36	u	57	0	0	1	0
36	v	62	0	0	1	0
36	x	12	0	0	0	0
36	y	4	0	0	0	0
36	z	1	0	0	0	0
All	All	52207	51491	50871	668	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (668) 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)
2:B:497:GLN:OE1	36:B:701:HOH:O	1.85	0.94
2:B:2:GLY:N	36:L:201:HOH:O	2.01	0.94
4:D:332:GLN:NE2	36:D:501:HOH:O	2.04	0.90
4:d:12:ARG:N	36:d:501:HOH:O	2.04	0.90
2:B:410:THR:O	36:B:702:HOH:O	1.91	0.89
12:m:5:GLN:O	36:m:201:HOH:O	1.90	0.88
1:a:103:ASP:OD2	13:o:69:LYS:NZ	2.08	0.87
11:L:11:GLU:OE2	36:L:201:HOH:O	1.94	0.84
13:O:19:CYS:O	36:O:301:HOH:O	1.96	0.83
34:F:102:HEM:O2A	36:F:201:HOH:O	1.96	0.83
7:H:56:ASP:OD1	18:X:2:THR:N	2.12	0.83
32:b:621:LMG:O10	12:m:4:ASN:ND2	2.11	0.83
2:B:241:SER:O	2:B:245:VAL:HG23	1.78	0.82
15:U:80:GLU:O	36:U:201:HOH:O	1.99	0.81
4:d:141:TYR:OH	33:d:408:LHG:O4	1.97	0.81
13:o:98:GLU:OE2	36:o:301:HOH:O	1.98	0.80
2:b:506:ARG:HD3	2:b:506:ARG:C	2.06	0.80
1:a:243:GLU:OE1	36:a:501:HOH:O	2.01	0.79
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.67	0.77
19:z:32:ASP:N	19:z:32:ASP:OD1	2.17	0.77
31:B:623:UNL:O1	36:B:703:HOH:O	2.03	0.76
5:e:61:ARG:NH2	16:v:125:ILE:O	2.19	0.76
2:B:413:ASP:OD1	36:B:704:HOH:O	2.04	0.75
13:O:34:SER:O	36:O:302:HOH:O	2.02	0.75
2:B:155:ALA:O	2:B:159:THR:OG1	2.05	0.74
24:b:609:CLA:HMB1	24:b:609:CLA:HBB1	1.72	0.72
6:F:45:ARG:NH1	9:J:40:LEU:OXT	2.23	0.72
8:i:5:LYS:NZ	36:i:101:HOH:O	2.19	0.72
13:O:84:GLU:OE1	13:O:86:LYS:NZ	2.22	0.71
34:e:102:HEM:HMC2	34:e:102:HEM:HBC2	1.71	0.71
3:C:277:GLY:C	24:C:506:CLA:HBC2	2.15	0.71
4:d:25:ASP:OD1	36:d:502:HOH:O	2.09	0.70
35:v:201:HEC:HBC3	35:v:201:HEC:HMC3	1.72	0.70
2:b:372:ASP:OD2	36:b:701:HOH:O	2.09	0.69
4:d:246:MET:HE3	4:d:264:LYS:CG	2.23	0.68
9:j:36:LEU:O	36:j:201:HOH:O	2.11	0.68
34:F:102:HEM:HBC2	34:F:102:HEM:HHD	1.74	0.68
34:e:102:HEM:HHC	34:e:102:HEM:HBB2	1.75	0.68
4:D:254:SER:OG	14:T:24:ARG:NH2	2.27	0.68
2:b:506:ARG:O	36:b:702:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:GLY:O	36:C:601:HOH:O	2.11	0.68
13:O:184:ARG:NH1	36:O:307:HOH:O	2.27	0.68
28:f:101:SQD:H312	18:x:27:VAL:HG11	1.76	0.67
13:o:98:GLU:OE1	36:o:302:HOH:O	2.12	0.67
2:b:307:GLU:OE1	36:b:703:HOH:O	2.13	0.67
4:d:242:GLU:OE2	36:d:503:HOH:O	2.11	0.67
13:o:194:LYS:NZ	36:o:304:HOH:O	2.23	0.67
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.78	0.66
31:c:520:UNL:O2	36:c:601:HOH:O	2.12	0.66
6:f:12:SER:O	36:f:201:HOH:O	2.14	0.65
4:D:291:LEU:HD21	29:H:102:DGD:CGB	2.26	0.65
14:t:2:GLU:OE1	36:t:201:HOH:O	2.14	0.65
15:U:10:VAL:HG11	15:U:15:GLU:OE2	1.97	0.65
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.79	0.64
6:f:24:HIS:O	6:f:28:VAL:HG13	1.96	0.64
9:J:5:GLY:N	36:J:202:HOH:O	2.30	0.64
26:D:405:BCR:H23C	26:D:405:BCR:H392	1.78	0.64
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.78	0.64
20:r:2:ASP:N	36:r:101:HOH:O	2.29	0.64
3:C:406:SER:HA	3:C:420:VAL:HG23	1.79	0.64
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.80	0.64
4:D:141:TYR:OH	33:D:411:LHG:O4	2.11	0.64
10:K:22:VAL:HA	10:K:25:LEU:HD22	1.80	0.64
13:O:88:ASN:ND2	13:O:92:SER:OG	2.31	0.63
3:C:42:LEU:HD21	24:C:512:CLA:H2A	1.79	0.63
3:C:157:MET:HE2	3:C:157:MET:HA	1.81	0.63
16:V:28:GLU:OE2	16:V:31:ARG:NH2	2.24	0.63
20:r:2:ASP:N	20:r:5:VAL:HG23	2.14	0.63
1:a:220:THR:HA	1:a:223:LEU:HD13	1.81	0.62
9:J:15:THR:HG22	9:J:19:MET:HE2	1.80	0.62
4:D:26:ARG:NH1	36:D:504:HOH:O	2.33	0.61
19:z:31:GLN:NE2	19:z:32:ASP:OD1	2.32	0.61
13:O:143:LYS:NZ	36:O:309:HOH:O	2.33	0.61
24:B:606:CLA:H91	28:a:411:SQD:H211	1.84	0.60
10:K:17:ILE:HD12	10:K:17:ILE:H	1.65	0.60
29:a:412:DGD:O1G	29:a:412:DGD:O1B	2.19	0.60
24:B:606:CLA:H191	31:B:620:UNL:O1	2.00	0.60
3:c:473:ASP:OXT	14:t:28:ARG:NH1	2.34	0.60
2:b:249:ALA:HB2	24:b:605:CLA:HBC3	1.83	0.60
3:c:40:ALA:O	3:c:43:ILE:HD12	2.01	0.60
25:a:406:PHO:H141	24:d:403:CLA:HBB1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.82	0.60
17:Y:40:ALA:O	17:Y:41:VAL:HB	2.00	0.59
3:C:66:ALA:HB1	10:K:25:LEU:HB3	1.84	0.59
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.35	0.59
15:u:53:ALA:HB3	15:u:54:PRO:HD3	1.84	0.59
3:c:315:MET:HE3	3:c:319:ILE:HD11	1.85	0.59
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.66	0.59
24:a:404:CLA:HBB1	24:a:404:CLA:HMB3	1.85	0.59
10:k:46:ARG:O	36:k:201:HOH:O	2.17	0.59
17:y:23:THR:O	17:y:27:MET:HE2	2.03	0.58
4:D:272:LEU:C	4:D:272:LEU:HD23	2.28	0.58
5:e:30:LEU:HD11	34:e:102:HEM:CBB	2.34	0.58
9:j:19:MET:O	9:j:23:VAL:HG23	2.03	0.58
2:B:12:LEU:HB2	24:B:612:CLA:HMC2	1.85	0.57
13:O:92:SER:N	36:O:304:HOH:O	2.20	0.57
13:O:156:PHE:O	36:O:303:HOH:O	2.17	0.57
5:E:53:ASP:O	16:V:1:ALA:N	2.38	0.57
26:b:602:BCR:H321	26:b:602:BCR:HC8	1.86	0.57
20:r:29:LYS:O	20:r:31:VAL:N	2.38	0.57
28:A:412:SQD:H312	26:b:620:BCR:H363	1.85	0.57
20:R:9:LEU:O	20:R:12:VAL:HG22	2.04	0.57
1:A:16:ARG:NH1	36:A:503:HOH:O	2.33	0.57
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.39	0.57
3:C:178:LYS:NZ	3:C:184:GLY:O	2.36	0.57
3:c:155:ASN:OD1	3:c:255:THR:HG22	2.05	0.57
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.86	0.57
2:b:480:SER:N	36:b:715:HOH:O	2.38	0.56
16:V:99:ASP:OD1	16:V:99:ASP:N	2.37	0.56
1:a:45:THR:HG23	24:d:403:CLA:H201	1.88	0.56
3:c:113:VAL:O	3:c:117:VAL:HG23	2.05	0.56
3:c:406:SER:HA	3:c:420:VAL:HG23	1.88	0.56
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.87	0.56
3:c:42:LEU:HD21	24:c:511:CLA:H2A	1.87	0.56
2:B:506:ARG:HH11	2:B:506:ARG:CB	2.18	0.56
5:E:14:ILE:O	5:E:20:TRP:NE1	2.38	0.56
4:d:79:SER:HA	4:d:172:SER:HB3	1.88	0.56
2:B:206:GLY:O	2:B:210:ILE:HD12	2.06	0.56
2:b:292:LEU:O	36:b:704:HOH:O	2.18	0.56
26:C:515:BCR:H331	26:C:515:BCR:C8	2.36	0.56
3:c:456:GLU:OE1	3:c:457:LYS:NZ	2.33	0.56
4:d:209:LEU:HD23	4:d:209:LEU:C	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:317:ASN:HA	2:b:330:MET:HE1	1.88	0.55
26:b:619:BCR:H331	26:b:619:BCR:C8	2.37	0.55
11:l:20:GLY:O	11:l:24:ILE:HG12	2.07	0.55
5:E:68:ASP:O	5:E:72:ALA:HB2	2.05	0.55
1:A:334:ARG:NH2	36:A:507:HOH:O	2.40	0.55
28:B:622:SQD:H3	11:l:14:ARG:HH22	1.71	0.55
16:V:102:PRO:HA	16:V:105:ARG:HD3	1.89	0.55
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.89	0.55
5:E:30:LEU:HD23	20:R:12:VAL:HG12	1.89	0.54
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.07	0.54
9:J:15:THR:HG22	9:J:19:MET:CE	2.37	0.54
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.90	0.54
24:B:606:CLA:H72	26:B:619:BCR:H311	1.90	0.54
1:a:29:TYR:CE2	1:a:31:GLY:HA3	2.42	0.54
8:i:14:PHE:CZ	8:i:18:LEU:HD11	2.43	0.54
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.43	0.54
19:Z:5:PHE:CE2	19:Z:54:VAL:HG13	2.43	0.54
24:c:506:CLA:O1A	24:c:506:CLA:C2	2.54	0.54
15:u:53:ALA:O	15:u:54:PRO:C	2.50	0.54
5:E:17:VAL:HG23	9:J:7:ARG:HG3	1.90	0.54
4:d:291:LEU:HD11	29:h:104:DGD:CGB	2.37	0.54
3:c:178:LYS:NZ	3:c:184:GLY:O	2.40	0.54
3:c:78:GLU:OE1	16:v:106:ASN:ND2	2.41	0.54
2:B:347:ARG:HA	2:B:352:GLU:O	2.08	0.53
26:d:406:BCR:H331	26:d:406:BCR:C8	2.36	0.53
15:u:27:LEU:HD22	15:u:49:ILE:HG21	1.91	0.53
16:v:100:ILE:C	16:v:102:PRO:HD3	2.34	0.53
5:e:68:ASP:O	5:e:72:ALA:HB2	2.07	0.53
28:A:412:SQD:C44	36:A:627:HOH:O	2.56	0.53
33:D:409:LHG:H141	33:D:409:LHG:H341	1.88	0.53
2:B:346:PHE:HA	2:B:398:THR:O	2.09	0.52
2:b:30:VAL:HG12	24:b:606:CLA:HHD	1.91	0.52
1:A:334:ARG:HD3	4:D:320:LEU:HD13	1.91	0.52
32:c:524:LMG:C30	32:c:524:LMG:HC91	2.40	0.52
3:C:473:ASP:OD2	14:T:24:ARG:HD3	2.08	0.52
26:D:405:BCR:H331	26:D:405:BCR:C8	2.38	0.52
10:k:40:GLN:HA	10:k:43:VAL:HG22	1.92	0.52
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.92	0.52
4:D:209:LEU:HD23	4:D:209:LEU:C	2.35	0.52
4:d:236:ASN:OD1	4:d:238:THR:OG1	2.28	0.52
3:C:61:VAL:HG12	3:C:118:HIS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:70:ARG:NH2	16:V:85:GLU:OE1	2.43	0.52
11:L:36:PHE:HB3	12:M:3:VAL:HG22	1.90	0.51
3:c:391[A]:ARG:NH1	36:c:609:HOH:O	2.42	0.51
24:c:501:CLA:H192	24:c:507:CLA:HBB1	1.92	0.51
2:B:347:ARG:HB2	36:B:801:HOH:O	2.09	0.51
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.92	0.51
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.91	0.51
2:b:378:LYS:HE3	36:b:701:HOH:O	2.10	0.51
3:c:245:ILE:HD13	32:c:522:LMG:H371	1.92	0.51
4:d:286:VAL:HG21	24:d:404:CLA:HED2	1.91	0.51
20:r:2:ASP:N	36:r:102:HOH:O	2.42	0.51
2:B:170:ASP:OD2	36:B:705:HOH:O	2.19	0.51
36:D:588:HOH:O	18:X:6:SER:HA	2.11	0.51
36:A:569:HOH:O	13:O:107:THR:HG21	2.11	0.51
2:B:160:GLY:HA2	2:B:163:GLY:O	2.10	0.51
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.44	0.51
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.93	0.51
19:Z:27:TYR:HE2	19:Z:33:TRP:CH2	2.28	0.51
19:Z:55:GLY:HA2	19:Z:58:ASN:HB3	1.93	0.51
1:a:95:PRO:HG2	1:a:98:GLU:HG2	1.91	0.51
13:o:123:LYS:NZ	36:o:303:HOH:O	2.21	0.51
19:z:14:ILE:N	19:z:14:ILE:HD12	2.26	0.51
1:A:63:ILE:HB	3:C:335:THR:HG21	1.93	0.51
3:C:318:LEU:C	3:C:318:LEU:HD23	2.36	0.51
1:a:147:TYR:O	1:a:150:PRO:HG2	2.11	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.46	0.50
19:z:19:MET:HE1	19:z:44:SER:HA	1.92	0.50
2:B:102:VAL:HA	26:B:618:BCR:C40	2.41	0.50
26:B:618:BCR:H331	26:B:618:BCR:C8	2.40	0.50
1:a:114:LEU:C	1:a:114:LEU:HD23	2.36	0.50
3:c:308:GLU:HG3	3:c:361:PHE:CZ	2.45	0.50
24:B:602:CLA:HBB1	24:B:602:CLA:HMB1	1.93	0.50
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.47	0.50
29:A:413:DGD:HD5	2:b:75:TRP:HB3	1.92	0.50
13:O:58:ASN:HB3	36:b:703:HOH:O	2.11	0.50
6:f:19:ARG:O	6:f:23:VAL:HG13	2.11	0.50
20:r:3:TRP:CD1	20:r:3:TRP:C	2.90	0.50
24:C:514:CLA:CMC	26:K:101:BCR:H372	2.42	0.50
3:C:334:PRO:HA	13:O:153:THR:OG1	2.12	0.50
3:c:391[B]:ARG:NE	36:c:610:HOH:O	2.44	0.50
4:D:198:MET:SD	24:D:402:CLA:HED2	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:623:LMG:C10	32:b:623:LMG:O8	2.59	0.50
4:d:52:THR:O	4:d:66:SER:HA	2.11	0.50
1:A:45:THR:O	1:A:49:VAL:HG23	2.12	0.50
6:f:26:LEU:O	6:f:29:PRO:HD2	2.11	0.50
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.11	0.50
4:d:126:MET:HE3	4:d:143:ALA:O	2.12	0.49
4:d:246:MET:HE3	4:d:264:LYS:HG3	1.92	0.49
24:b:611:CLA:H202	24:b:613:CLA:HMD2	1.93	0.49
2:B:506:ARG:HH11	2:B:506:ARG:HB2	1.76	0.49
16:V:87:GLU:HB3	36:V:338:HOH:O	2.12	0.49
16:V:95:LEU:HD11	16:V:112:LEU:HD11	1.93	0.49
17:Y:27:MET:HA	17:Y:30:ILE:HG22	1.94	0.49
1:a:220:THR:HA	1:a:223:LEU:CD1	2.42	0.49
3:c:350:ILE:HG21	3:c:359:TRP:HB2	1.95	0.49
28:B:622:SQD:H442	14:t:23:PHE:HB3	1.95	0.49
26:D:405:BCR:H392	26:D:405:BCR:C23	2.42	0.49
9:J:36:LEU:O	36:J:201:HOH:O	2.19	0.49
16:v:41:HIS:HA	16:v:45:ILE:O	2.12	0.49
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.94	0.49
4:D:52:THR:O	4:D:66:SER:HA	2.12	0.49
5:E:36:LEU:O	5:E:40:THR:HG23	2.13	0.49
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.95	0.49
2:b:414:PRO:N	2:b:415:PRO:HD2	2.27	0.49
28:a:410:SQD:C38	9:j:22:ILE:HD11	2.42	0.49
8:i:33:LYS:O	8:i:35:LYS:NZ	2.45	0.49
13:o:80:GLN:NE2	36:o:309:HOH:O	2.46	0.49
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.95	0.49
4:D:96:GLU:HB2	36:D:505:HOH:O	2.12	0.49
1:a:210:LEU:C	1:a:210:LEU:HD23	2.38	0.49
3:c:350:ILE:CG2	3:c:359:TRP:HB2	2.43	0.49
18:x:37:VAL:HG12	18:x:38:GLN:N	2.27	0.49
4:D:194:ASN:HA	4:D:295:SER:OG	2.12	0.49
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.49
26:t:101:BCR:C8	26:t:101:BCR:H311	2.43	0.49
26:t:101:BCR:H23C	26:t:101:BCR:H382	1.95	0.49
2:B:371:THR:HG23	2:B:372:ASP:O	2.12	0.48
1:a:207:GLY:O	1:a:211:PHE:CD2	2.66	0.48
5:e:81:GLU:HA	5:e:84:LYS:HE3	1.95	0.48
26:h:103:BCR:H331	26:h:103:BCR:C8	2.43	0.48
2:B:424:ALA:O	36:B:706:HOH:O	2.20	0.48
15:U:39:ARG:HG2	36:U:241:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:9:LEU:HA	36:u:237:HOH:O	2.12	0.48
2:b:453:PHE:HB2	4:d:291:LEU:HD23	1.96	0.48
3:c:116:VAL:O	3:c:120:ILE:HG12	2.13	0.48
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.95	0.48
24:B:605:CLA:HMC3	24:B:615:CLA:H43	1.94	0.48
13:O:90:ASP:CG	36:O:304:HOH:O	2.57	0.48
13:O:107:THR:HG22	36:O:346:HOH:O	2.13	0.48
4:d:49:LEU:HD13	26:d:406:BCR:C15	2.44	0.48
24:B:604:CLA:H172	24:B:604:CLA:H141	1.95	0.48
3:c:334:PRO:HA	13:o:153:THR:OG1	2.14	0.48
2:b:442:ILE:HD11	13:o:174:LEU:HD23	1.96	0.48
32:c:524:LMG:HC5	36:c:683:HOH:O	2.12	0.48
4:d:55:VAL:O	4:d:66:SER:HB3	2.13	0.48
3:C:110:PRO:O	3:C:114:VAL:HG23	2.13	0.48
2:b:36:SER:OG	26:b:619:BCR:H362	2.14	0.48
5:e:17:VAL:HG23	9:j:7:ARG:HB2	1.96	0.48
5:E:37:PHE:CD2	5:E:42:LEU:HD23	2.49	0.48
36:d:585:HOH:O	18:x:29:ILE:HG23	2.13	0.48
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.96	0.48
5:E:15:THR:HB	9:J:8:ILE:O	2.14	0.48
2:b:154:GLY:O	2:b:159:THR:HG23	2.14	0.48
24:c:513:CLA:HBB1	24:c:513:CLA:HMB1	1.94	0.48
19:Z:46:LEU:O	19:Z:50:LEU:HB2	2.14	0.48
24:b:604:CLA:H2	24:b:606:CLA:H91	1.95	0.48
3:c:309:ALA:HB1	3:c:399:ALA:HB2	1.95	0.47
3:C:143:TYR:CE1	24:C:514:CLA:HED3	2.50	0.47
5:E:17:VAL:O	5:E:21:VAL:HG23	2.14	0.47
8:I:35:LYS:HD2	8:I:35:LYS:H	1.78	0.47
24:b:603:CLA:H43	7:h:45:ILE:HG22	1.96	0.47
27:D:406:PL9:H412	11:L:29:LEU:HD23	1.95	0.47
7:h:39:LEU:C	7:h:39:LEU:HD23	2.39	0.47
1:A:210:LEU:HD23	1:A:214:MET:HG2	1.96	0.47
2:b:481:GLY:N	36:b:715:HOH:O	2.46	0.47
2:b:355:PHE:HE2	2:b:373:LYS:HG2	1.79	0.47
3:c:363:GLY:O	3:c:367:GLU:HG2	2.15	0.47
3:C:228:ASN:ND2	36:C:618:HOH:O	2.42	0.47
4:D:150:ILE:O	4:D:154:VAL:HG13	2.14	0.47
1:a:84:PRO:HA	1:a:112:TYR:CG	2.50	0.47
26:c:521:BCR:C21	10:k:32:PHE:CE2	2.97	0.47
2:B:76:SER:O	13:o:111:ALA:HA	2.15	0.47
24:B:601:CLA:CBA	24:B:601:CLA:HBD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:604:CLA:H43	24:B:605:CLA:H2	1.95	0.47
3:C:472:LEU:HD12	36:D:623:HOH:O	2.14	0.47
4:D:264:LYS:CE	36:D:502:HOH:O	2.62	0.47
13:O:54:GLU:O	13:O:63:ALA:HB3	2.14	0.47
13:O:189:ARG:NH2	36:O:310:HOH:O	2.35	0.47
14:T:14:ILE:HG22	26:b:602:BCR:H10C	1.97	0.47
24:b:610:CLA:C2B	26:h:103:BCR:H323	2.45	0.47
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.97	0.47
24:C:512:CLA:H41	17:Y:39:LEU:CD1	2.45	0.47
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.49	0.47
2:b:374:ASN:ND2	36:b:714:HOH:O	2.37	0.47
19:z:14:ILE:O	19:z:15:LEU:CB	2.62	0.47
20:r:7:VAL:O	20:r:11:PRO:HD2	2.14	0.47
33:D:411:LHG:H222	12:M:18:PRO:HG3	1.96	0.47
2:b:86:ILE:HD13	2:b:86:ILE:O	2.15	0.47
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.03	0.47
2:b:99:ALA:HB1	24:b:607:CLA:H72	1.97	0.47
13:o:57:LYS:O	13:o:60:ARG:N	2.44	0.47
4:D:261:PHE:CZ	33:D:408:LHG:HC81	2.50	0.46
10:K:27:VAL:HG12	10:K:27:VAL:O	2.15	0.46
17:Y:32:GLY:HA3	26:Y:101:BCR:C15	2.45	0.46
19:Z:29:SER:HB3	19:Z:31:GLN:HG3	1.98	0.46
6:f:29:PRO:O	6:f:33:PHE:HD2	1.99	0.46
17:y:39:LEU:O	17:y:44:GLY:N	2.46	0.46
1:A:301:ASN:OD1	1:A:301:ASN:C	2.58	0.46
24:b:615:CLA:H141	24:b:615:CLA:C17	2.46	0.46
3:c:381:LYS:NZ	13:o:99:ASP:OD2	2.34	0.46
5:e:22:ILE:HG23	20:r:19:ALA:HB2	1.97	0.46
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.96	0.46
16:V:13:ASN:OD1	16:V:15:GLU:HB2	2.15	0.46
16:V:29:GLY:HA3	16:V:114:ALA:O	2.15	0.46
1:a:265:PHE:O	27:a:409:PL9:H532	2.15	0.46
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.96	0.46
2:B:369:ILE:C	2:B:370:LEU:HD12	2.40	0.46
3:c:121:SER:O	3:c:124:VAL:HG13	2.16	0.46
26:t:101:BCR:H321	26:t:101:BCR:C8	2.43	0.46
5:E:30:LEU:HD11	34:F:102:HEM:HAB	1.98	0.46
10:k:26:PRO:O	10:k:29:PRO:HD2	2.15	0.46
26:a:408:BCR:C8	26:a:408:BCR:H331	2.44	0.46
5:E:10:PHE:HB2	33:E:101:LHG:O4	2.15	0.46
5:E:65:LEU:O	5:E:67:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:43:ILE:CD1	6:f:43:ILE:N	2.79	0.46
13:O:5:LEU:HD12	13:O:10:ILE:HD11	1.97	0.46
2:b:159:THR:O	2:b:180:PRO:HB3	2.16	0.46
4:d:267:LEU:C	4:d:267:LEU:HD23	2.40	0.46
31:d:412:UNL:C4	31:d:412:UNL:O2	2.64	0.46
24:C:510:CLA:H91	24:C:513:CLA:HAA2	1.98	0.45
2:B:476:ARG:NH1	36:B:727:HOH:O	2.47	0.45
15:U:16:LYS:HE3	15:U:85:THR:OG1	2.16	0.45
2:B:297:THR:HG23	2:B:300:GLU:OE1	2.16	0.45
7:H:12:ARG:NH1	7:H:15:ASN:O	2.45	0.45
13:O:61:GLN:O	13:O:62:GLU:O	2.34	0.45
4:d:39:PRO:O	4:d:43:LEU:HG	2.16	0.45
33:d:408:LHG:H101	33:d:408:LHG:H351	1.97	0.45
7:h:12:ARG:NH2	7:h:15:ASN:O	2.49	0.45
26:D:405:BCR:H23C	26:D:405:BCR:C39	2.46	0.45
16:V:4:THR:O	16:V:7:VAL:HG13	2.16	0.45
15:u:58:VAL:O	15:u:61:VAL:HG12	2.15	0.45
4:d:89:LEU:HB3	4:d:91:LEU:HD21	1.99	0.45
7:h:25:TRP:O	7:h:26:GLY:C	2.60	0.45
2:B:280:PHE:CD2	2:B:312:TYR:HB3	2.51	0.45
3:C:70:PHE:CD1	10:K:23:ASP:HA	2.52	0.45
16:V:6:GLU:CD	16:V:6:GLU:H	2.25	0.45
24:b:606:CLA:HHC	24:b:606:CLA:HBB1	1.99	0.45
13:o:133:VAL:HG12	13:o:133:VAL:O	2.17	0.45
16:v:122:GLU:N	16:v:123:PRO:HD2	2.31	0.45
7:H:50:ASN:OD1	7:H:52:THR:CG2	2.65	0.45
9:J:21:VAL:O	9:J:22:ILE:C	2.58	0.45
24:b:615:CLA:H92	26:b:618:BCR:H362	1.98	0.45
3:c:399:ALA:O	3:c:401:LEU:N	2.48	0.45
5:e:30:LEU:HD23	5:e:30:LEU:HA	1.82	0.45
16:v:104:MET:HA	16:v:107:LEU:HD22	1.98	0.45
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.98	0.45
17:Y:25:ILE:O	17:Y:26:ALA:C	2.59	0.45
24:c:508:CLA:HBB1	24:c:508:CLA:HMB1	1.98	0.45
9:j:18:GLY:C	9:j:22:ILE:HD12	2.41	0.45
12:M:17:VAL:HB	12:M:18:PRO:HD3	1.98	0.45
20:R:24:LEU:O	20:R:28:VAL:HG23	2.16	0.45
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.97	0.45
1:a:289:GLY:O	1:a:293:MET:HE3	2.16	0.45
5:e:30:LEU:HD11	34:e:102:HEM:HBB1	1.98	0.45
2:B:353:GLU:HG2	2:B:355:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:GLU:HA	3:C:148:GLY:HA3	1.99	0.45
4:D:152:VAL:HG22	24:D:403:CLA:HED3	1.98	0.45
5:E:34:GLY:HA2	6:F:32:PHE:CE1	2.52	0.45
1:a:271:LEU:HD13	1:a:271:LEU:C	2.43	0.45
2:b:125:ASP:OD2	2:b:127:ARG:HB2	2.17	0.45
24:b:608:CLA:HAA1	24:b:608:CLA:HBD	1.99	0.45
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.99	0.45
10:K:15:TYR:O	10:K:16:ALA:C	2.60	0.44
13:O:27:ARG:HG3	13:O:27:ARG:HH11	1.81	0.44
2:b:70:GLY:HA2	2:b:178:VAL:HG11	1.98	0.44
3:c:338:GLY:HA3	3:c:341:LEU:O	2.17	0.44
16:v:41:HIS:CD2	35:v:201:HEC:NB	2.84	0.44
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.99	0.44
2:B:243:ALA:HA	2:B:246:PHE:CE1	2.53	0.44
3:C:465:PRO:O	3:C:469:MET:HG3	2.18	0.44
2:b:191:ASN:HB2	7:h:58:VAL:HG13	1.99	0.44
2:b:249:ALA:CB	24:b:605:CLA:HBC3	2.47	0.44
33:d:409:LHG:H321	14:t:21:ILE:HD11	1.99	0.44
2:B:149[A]:LEU:HD21	24:B:606:CLA:HBB2	1.99	0.44
7:h:43:LEU:O	7:h:47:GLU:HG3	2.18	0.44
4:D:266:TRP:CD1	33:D:408:LHG:HC31	2.52	0.44
10:K:15:TYR:O	10:K:17:ILE:N	2.50	0.44
5:e:13:ILE:HG22	5:e:19:TYR:CD2	2.53	0.44
24:b:609:CLA:H141	24:b:609:CLA:H161	1.85	0.44
24:c:501:CLA:C3D	24:c:503:CLA:H2	2.47	0.44
4:d:125:PHE:O	4:d:129:GLN:HG3	2.17	0.44
20:r:18:TRP:O	20:r:22:ASN:HB2	2.18	0.44
24:C:503:CLA:H61	24:C:513:CLA:H42	2.00	0.44
1:a:112:TYR:CE2	1:a:116:ILE:HD13	2.53	0.44
2:b:311:PHE:HA	2:b:430:PHE:CZ	2.53	0.44
1:A:253:GLY:HA2	2:B:493:TRP:CH2	2.52	0.44
4:D:97:ALA:O	4:D:98:GLN:C	2.61	0.44
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.06	0.44
24:b:606:CLA:HMA1	24:b:607:CLA:H3A	1.99	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.99	0.44
24:a:404:CLA:HBB1	24:a:404:CLA:CMB	2.48	0.44
2:b:98:LEU:HD11	24:b:607:CLA:H151	2.00	0.44
2:b:112:CYS:O	2:b:116:VAL:HG23	2.18	0.44
2:B:291:SER:HB3	2:B:301:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:622:SQD:H45	28:B:622:SQD:O10	2.17	0.44
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.78	0.44
4:D:43:LEU:HG	4:D:113:PHE:HZ	1.83	0.44
26:H:101:BCR:H331	26:H:101:BCR:C8	2.48	0.44
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.78	0.44
1:a:85:SER:HA	1:a:109:GLY:HA3	2.00	0.44
1:a:257:ARG:NH1	2:b:491:VAL:O	2.51	0.44
1:a:278:TRP:HB3	1:a:279:PRO:HD3	1.99	0.44
26:c:521:BCR:H24C	26:c:521:BCR:H371	1.85	0.44
5:e:17:VAL:H	9:j:7:ARG:HD2	1.82	0.44
26:h:103:BCR:H15C	26:h:103:BCR:H351	1.81	0.44
8:i:31:ASN:HB2	8:i:32:PRO:HD2	1.99	0.44
11:l:2:GLU:N	11:l:3:PRO:CD	2.81	0.44
15:u:52:ASN:O	15:u:53:ALA:C	2.61	0.44
2:B:378:LYS:O	2:B:395:GLN:HG3	2.17	0.43
24:B:606:CLA:H91	24:B:606:CLA:H112	1.80	0.43
33:L:101:LHG:H102	33:L:101:LHG:O8	2.19	0.43
2:b:12:LEU:HB2	24:b:613:CLA:HMC2	2.00	0.43
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.99	0.43
24:C:512:CLA:H142	26:Y:101:BCR:H353	2.00	0.43
10:K:15:TYR:C	10:K:17:ILE:N	2.76	0.43
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.18	0.43
2:b:125:ASP:HB2	2:b:132:ALA:HB3	2.00	0.43
26:c:521:BCR:H21C	10:k:32:PHE:CE2	2.53	0.43
3:C:249:ILE:O	3:C:253:LEU:HG	2.18	0.43
4:D:17:ILE:O	4:D:20:ASP:HB2	2.18	0.43
7:H:12:ARG:HB3	7:H:13:PRO:HD3	1.99	0.43
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.00	0.43
19:Z:55:GLY:HA2	19:Z:58:ASN:CB	2.48	0.43
1:a:105:TRP:CZ3	1:a:111:PRO:HG3	2.54	0.43
1:a:291:SER:O	1:a:294:ALA:HB3	2.17	0.43
26:b:620:BCR:C8	26:b:620:BCR:H331	2.48	0.43
3:c:26:ARG:O	10:k:46:ARG:HD2	2.16	0.43
5:e:25:ILE:O	5:e:28:PRO:HD2	2.17	0.43
13:o:71:VAL:HG22	13:o:107:THR:O	2.18	0.43
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.49	0.43
5:E:22[A]:ILE:HD12	20:R:19:ALA:CB	2.49	0.43
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.53	0.43
16:v:3:LEU:HD23	16:v:23:GLU:HG3	2.00	0.43
2:b:357:ARG:NE	36:b:705:HOH:O	2.21	0.43
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:144:PHE:CE2	2:b:148:LEU:HD11	2.53	0.43
26:b:618:BCR:H24C	26:b:618:BCR:H371	1.84	0.43
16:v:10:VAL:HG23	16:v:69:ILE:HD11	2.00	0.43
16:v:110:LYS:HA	16:v:113:VAL:HG22	2.00	0.43
3:C:424:SER:O	3:C:428:THR:HG23	2.19	0.43
4:D:24:ARG:NH2	28:F:101:SQD:O4	2.52	0.43
4:D:59:TYR:O	5:E:65:LEU:HD22	2.18	0.43
24:D:403:CLA:HBC3	24:D:403:CLA:HHD	2.00	0.43
1:a:237:TYR:CD2	1:a:237:TYR:C	2.97	0.43
24:b:605:CLA:HMB3	24:b:605:CLA:HBB1	2.01	0.43
6:f:16:PHE:HZ	20:r:23:ILE:HG21	1.84	0.43
15:u:16:LYS:HE3	15:u:85:THR:OG1	2.19	0.43
2:B:298:LEU:HD23	2:B:402:TYR:CE1	2.54	0.43
3:C:459:ILE:HG21	3:C:464:GLU:HG3	2.00	0.43
10:K:26:PRO:O	10:K:29:PRO:HD2	2.19	0.43
3:c:85:GLY:O	24:c:504:CLA:HED2	2.18	0.43
24:B:608:CLA:H172	24:B:609:CLA:H193	2.00	0.43
26:D:405:BCR:H352	6:F:29:PRO:HG2	2.01	0.43
10:K:25:LEU:N	10:K:26:PRO:HD2	2.34	0.43
28:a:410:SQD:H381	9:j:22:ILE:HD11	2.00	0.43
2:B:63:LEU:N	2:B:64:PRO:HD2	2.34	0.43
2:B:458:PHE:HB3	24:B:604:CLA:HBC2	2.01	0.43
3:C:344:SER:O	13:O:75:THR:HG22	2.18	0.43
5:E:22[A]:ILE:HD11	34:F:102:HEM:CHB	2.49	0.43
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.51	0.43
3:c:109:PHE:N	3:c:110:PRO:CD	2.82	0.43
3:c:123:ALA:HB2	26:c:521:BCR:H14C	2.01	0.43
3:c:391[B]:ARG:CZ	36:c:610:HOH:O	2.66	0.43
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.75	0.43
13:o:10:ILE:O	13:o:13:THR:HG23	2.19	0.43
3:C:222:GLY:O	3:C:223:TRP:C	2.62	0.42
10:K:43:VAL:O	10:K:43:VAL:HG13	2.19	0.42
2:B:411:PHE:N	2:B:411:PHE:CD2	2.86	0.42
24:B:601:CLA:HBD	24:B:601:CLA:HBA1	2.01	0.42
26:B:618:BCR:H20C	26:B:618:BCR:H361	1.80	0.42
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.01	0.42
13:O:189:ARG:NE	36:O:310:HOH:O	2.34	0.42
19:Z:37:LYS:O	19:Z:41:PHE:HB2	2.20	0.42
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.54	0.42
20:r:6:LEU:O	20:r:10:LEU:HG	2.19	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.00	0.42
13:O:143:LYS:HD2	13:O:198:SER:HB3	2.00	0.42
2:b:141:ILE:HD11	7:h:14:LEU:HD22	2.01	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.20	0.42
10:k:19:ASP:OD1	36:k:202:HOH:O	2.22	0.42
17:y:19:ILE:O	17:y:23:THR:N	2.44	0.42
2:B:159:THR:O	2:B:180:PRO:HB2	2.19	0.42
2:B:476:ARG:HD3	36:B:727:HOH:O	2.19	0.42
2:b:81:THR:OG1	2:b:83:GLU:HG3	2.18	0.42
2:b:90:PHE:HZ	2:b:98:LEU:HD12	1.83	0.42
2:b:245:VAL:CG1	24:b:605:CLA:HAC1	2.49	0.42
33:l:101:LHG:H271	12:m:22:LEU:HD21	2.02	0.42
24:C:514:CLA:HMC3	26:K:101:BCR:H372	2.02	0.42
8:I:6:ILE:HG22	8:I:10:ILE:HD12	2.02	0.42
16:V:41:HIS:HA	16:V:45:ILE:O	2.19	0.42
2:b:241:SER:HB3	24:b:613:CLA:HED3	2.01	0.42
4:d:180:ARG:HD3	4:d:180:ARG:C	2.44	0.42
2:B:172:TYR:O	2:B:174:LEU:HG	2.19	0.42
33:d:408:LHG:HC32	36:d:562:HOH:O	2.19	0.42
5:e:36:LEU:O	5:e:40:THR:HG23	2.19	0.42
10:k:28:ILE:HA	10:k:31:LEU:HD12	2.02	0.42
20:r:29:LYS:O	20:r:30:GLN:C	2.62	0.42
1:A:308:ASP:O	6:F:45:ARG:HD2	2.20	0.42
3:C:109:PHE:N	3:C:110:PRO:CD	2.83	0.42
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.50	0.42
1:a:48:PHE:HA	1:a:115:ILE:HD11	2.01	0.42
4:d:318:ASN:HA	4:d:321:LEU:HD22	2.01	0.42
2:B:102:VAL:HA	26:B:618:BCR:H401	2.02	0.42
3:C:190:ALA:HB3	3:C:194:GLY:HA2	2.01	0.42
26:C:515:BCR:H20C	26:C:515:BCR:H361	1.91	0.42
5:E:74:GLN:N	5:E:74:GLN:CD	2.78	0.42
2:b:369:ILE:HG23	2:b:377:VAL:HG13	2.02	0.42
24:b:616:CLA:HHC	24:b:616:CLA:HBB1	2.00	0.42
5:e:84:LYS:NZ	36:e:205:HOH:O	2.40	0.42
24:h:101:CLA:CHA	24:h:101:CLA:HBA2	2.50	0.42
24:h:101:CLA:H193	24:h:101:CLA:HMB2	2.02	0.42
15:u:66:GLY:O	15:u:67:LEU:C	2.63	0.42
2:B:237:VAL:CG2	24:B:610:CLA:HBC2	2.50	0.42
2:B:478:VAL:O	4:D:139:ARG:HG2	2.19	0.42
26:B:619:BCR:C23	26:B:619:BCR:H383	2.49	0.42
4:D:79:SER:HA	4:D:172:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:100:ILE:HG13	16:V:101:PHE:CD2	2.54	0.42
19:Z:49:ALA:O	19:Z:53:VAL:HG23	2.20	0.42
6:f:43:ILE:CG2	9:j:36:LEU:HD22	2.50	0.42
13:o:91:GLY:HA3	13:o:132:ASN:HA	2.01	0.42
15:u:45:LEU:HD21	15:u:71:GLN:HB3	2.01	0.42
2:B:414:PRO:N	2:B:415:PRO:HD2	2.34	0.42
18:X:34:ILE:HG22	20:R:34:LEU:HD22	2.01	0.42
13:O:33:ASP:CG	13:O:35:SER:HG	2.27	0.41
1:a:82:VAL:HB	1:a:174:LEU:HB2	2.02	0.41
1:a:214:MET:HB3	27:a:409:PL9:HC8	2.01	0.41
27:a:409:PL9:H33	4:d:38:PHE:HD1	1.85	0.41
2:b:215:PHE:O	2:b:219:VAL:HG13	2.20	0.41
3:c:162:GLY:HA3	3:c:252:ILE:HG13	2.00	0.41
4:d:179:PHE:HA	4:d:182:LEU:HD22	2.02	0.41
4:d:279:LEU:HD22	25:d:402:PHO:HBC3	2.02	0.41
19:z:42:LEU:N	19:z:42:LEU:CD1	2.82	0.41
26:A:409:BCR:H24C	26:A:409:BCR:H371	1.84	0.41
17:Y:23:THR:O	17:Y:23:THR:HG22	2.20	0.41
19:z:36:SER:O	19:z:37:LYS:C	2.63	0.41
24:B:613:CLA:H143	32:M:101:LMG:H232	2.01	0.41
26:B:619:BCR:C23	26:B:619:BCR:C38	2.98	0.41
25:D:401:PHO:HBC2	25:D:401:PHO:HHD	2.02	0.41
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.55	0.41
16:v:120:LEU:O	36:v:301:HOH:O	2.22	0.41
29:A:413:DGD:HB42	29:A:413:DGD:HB91	2.02	0.41
2:B:67:ALA:HA	2:B:71:VAL:O	2.20	0.41
6:F:19:ARG:O	6:F:20:TRP:C	2.61	0.41
3:c:26:ARG:O	10:k:46:ARG:CD	2.69	0.41
4:d:218:VAL:O	4:d:222:LEU:HD23	2.20	0.41
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.38	0.41
1:A:161:TYR:N	1:A:162:PRO:CD	2.84	0.41
26:B:618:BCR:H363	26:t:101:BCR:H19C	2.02	0.41
3:C:48:LYS:HD2	3:C:138:GLU:HG2	2.02	0.41
3:C:56:HIS:CE1	24:C:510:CLA:HMA2	2.55	0.41
13:O:91:GLY:N	36:O:304:HOH:O	2.53	0.41
19:Z:32:ASP:CG	19:Z:35:ARG:HB3	2.45	0.41
19:Z:61:VAL:O	19:Z:62:VAL:C	2.62	0.41
1:a:288:LEU:HD21	3:c:436:PHE:CE1	2.56	0.41
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.85	0.41
3:c:360:ASP:HB2	36:c:638:HOH:O	2.20	0.41
6:f:18:VAL:HG23	28:f:101:SQD:O8	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:t:101:BCR:H371	26:t:101:BCR:H24C	1.79	0.41
15:u:53:ALA:O	15:u:55:TYR:CD2	2.73	0.41
1:A:201:GLY:HA3	1:A:286:THR:HB	2.03	0.41
1:A:283:VAL:HA	1:A:286:THR:HG22	2.02	0.41
2:B:422:ARG:O	2:B:425:ILE:HG12	2.19	0.41
3:C:107:ASP:OD2	36:C:602:HOH:O	2.22	0.41
4:D:218:VAL:HG22	4:D:244:TYR:CE2	2.56	0.41
5:E:60:GLN:NE2	5:E:62:SER:O	2.54	0.41
10:K:28:ILE:N	10:K:29:PRO:CD	2.84	0.41
35:V:201:HEC:HMC1	35:V:201:HEC:HBC3	2.02	0.41
2:b:333:GLY:O	2:b:439:SER:HB3	2.21	0.41
28:f:101:SQD:H442	28:f:101:SQD:O2	2.21	0.41
7:h:30:LEU:HG	7:h:34:PHE:CE2	2.56	0.41
16:v:99:ASP:OD1	16:v:99:ASP:N	2.53	0.41
19:z:48:ILE:O	19:z:52:LEU:HG	2.20	0.41
2:B:53:ASN:N	2:B:54:PRO:CD	2.83	0.41
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.86	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.03	0.41
18:X:2:THR:OG1	18:X:3:ILE:N	2.54	0.41
20:R:5:VAL:HG12	20:R:9:LEU:HD22	2.02	0.41
2:b:98:LEU:HD11	24:b:607:CLA:C15	2.50	0.41
13:o:59:LYS:O	13:o:60:ARG:O	2.39	0.41
16:v:22:THR:HG23	16:v:25:GLN:OE1	2.20	0.41
2:B:393:GLU:OE2	2:B:418:LYS:NZ	2.49	0.41
24:B:603:CLA:CMD	24:B:606:CLA:HMB2	2.49	0.41
24:B:614:CLA:H141	24:B:614:CLA:H161	1.90	0.41
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.81	0.41
5:E:17:VAL:HG23	9:J:7:ARG:CG	2.51	0.41
13:O:27:ARG:HG2	13:O:27:ARG:O	2.21	0.41
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.55	0.41
3:c:101:PRO:HD2	36:c:696:HOH:O	2.21	0.41
31:x:101:UNL:C4	31:x:101:UNL:O2	2.67	0.41
5:E:36:LEU:O	5:E:37:PHE:C	2.64	0.41
16:V:89:ALA:HB2	36:V:338:HOH:O	2.19	0.41
26:Y:101:BCR:H322	19:Z:17:PHE:CE1	2.56	0.41
1:a:341:LEU:HD12	3:c:396:MET:HE3	2.03	0.41
24:b:614:CLA:H51	33:d:408:LHG:H361	2.03	0.41
26:b:618:BCR:H15C	26:b:618:BCR:H351	1.93	0.41
4:d:180:ARG:HD3	4:d:181:PHE:N	2.36	0.41
2:B:103:LEU:O	2:B:107:LEU:HG	2.20	0.41
3:C:201:ASN:HB3	36:C:743:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:E:101:LHG:H311	33:E:101:LHG:H271	2.02	0.41
13:O:70:LEU:CD1	13:O:106:VAL:HG13	2.51	0.41
2:b:451:PHE:CE1	2:b:455:HIS:CE1	3.09	0.41
26:b:619:BCR:H15C	26:b:619:BCR:H351	1.76	0.41
34:e:102:HEM:O1D	6:f:19:ARG:NE	2.53	0.41
13:o:10:ILE:O	13:o:11:VAL:C	2.64	0.41
17:y:41:VAL:C	17:y:43:ARG:H	2.28	0.41
1:A:173:PRO:HB2	1:A:178:GLY:HA3	2.04	0.40
1:A:253:GLY:HA3	2:B:491:VAL:HG13	2.02	0.40
3:C:180:MET:HG2	3:C:199:ILE:O	2.21	0.40
4:D:91:LEU:HD13	4:D:93:TRP:CE2	2.56	0.40
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.56	0.40
2:b:345:VAL:HG13	2:b:353:GLU:OE2	2.21	0.40
24:b:609:CLA:H92	24:b:609:CLA:H62	1.94	0.40
3:c:405:ASN:HB3	29:c:518:DGD:O1B	2.20	0.40
9:j:21:VAL:HG23	9:j:22:ILE:N	2.35	0.40
2:B:135:LEU:N	2:B:136:PRO:CD	2.84	0.40
2:B:451:PHE:CD2	2:B:451:PHE:C	2.98	0.40
3:C:45:LEU:HA	3:C:139:THR:HG22	2.03	0.40
4:D:267:LEU:C	4:D:267:LEU:HD23	2.45	0.40
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.56	0.40
11:L:25:LEU:HD23	11:L:25:LEU:HA	1.90	0.40
11:L:36:PHE:HB3	12:M:3:VAL:CG2	2.50	0.40
17:Y:34:MET:O	17:Y:38:LEU:HD13	2.21	0.40
2:b:460:LEU:O	2:b:463:PHE:HB3	2.21	0.40
3:c:281:MET:HG3	32:c:524:LMG:H401	2.03	0.40
13:o:54:GLU:HG2	13:o:64:GLU:O	2.21	0.40
13:o:55:GLU:OE1	13:o:231:HIS:CD2	2.74	0.40
13:o:60:ARG:O	13:o:61:GLN:HB2	2.21	0.40
3:C:223:TRP:CG	3:C:224:ILE:H	2.40	0.40
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.03	0.40
17:Y:27:MET:HB2	19:Z:17:PHE:CZ	2.56	0.40
2:b:71:VAL:HG23	24:b:607:CLA:HMA2	2.03	0.40
28:f:101:SQD:C31	18:x:27:VAL:HG11	2.48	0.40
13:o:215:PHE:CD1	13:o:215:PHE:C	3.00	0.40
18:x:16:SER:HB3	31:x:101:UNL:C7	2.51	0.40
1:A:91:LEU:HD11	1:A:163:ILE:HA	2.03	0.40
1:A:244:GLU:OE2	4:D:264:LYS:NZ	2.55	0.40
2:B:461:LEU:HD23	2:B:461:LEU:HA	1.94	0.40
24:C:506:CLA:HAA1	24:C:506:CLA:HBD	2.03	0.40
13:O:72:THR:HG21	13:O:107:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:27:LEU:HD13	15:U:61:VAL:CG1	2.52	0.40
2:b:488:PRO:HA	2:b:491:VAL:HG22	2.04	0.40
24:b:615:CLA:H141	24:b:615:CLA:H171	2.02	0.40
26:b:620:BCR:H20C	26:b:620:BCR:H361	1.88	0.40
24:h:101:CLA:C9	26:h:103:BCR:H23C	2.51	0.40
13:o:81:ILE:HA	13:o:100:GLY:HA3	2.03	0.40
16:v:55:ARG:HH11	16:v:132:GLY:HA2	1.86	0.40
3:C:189:TRP:O	3:C:190:ALA:C	2.63	0.40
24:C:514:CLA:HMC2	26:K:101:BCR:H372	2.03	0.40
17:Y:30:ILE:O	17:Y:30:ILE:HG13	2.21	0.40
1:a:200:LEU:HD23	1:a:285:PHE:CG	2.56	0.40
24:h:101:CLA:H91	24:h:101:CLA:H111	1.79	0.40
19:z:40:ILE:HG13	19:z:41:PHE:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	325 (98%)	6 (2%)	1 (0%)	36	36
1	a	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
2	B	508/505 (101%)	494 (97%)	14 (3%)	0	100	100
2	b	503/505 (100%)	491 (98%)	10 (2%)	2 (0%)	30	28
3	C	441/451 (98%)	428 (97%)	12 (3%)	1 (0%)	43	44
3	c	451/451 (100%)	433 (96%)	15 (3%)	3 (1%)	18	14
4	D	339/341 (99%)	328 (97%)	11 (3%)	0	100	100
4	d	340/341 (100%)	325 (96%)	15 (4%)	0	100	100
5	E	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
5	e	80/82 (98%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	55 (90%)	5 (8%)	1 (2%)	7	4
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
10	K	35/37 (95%)	34 (97%)	0	1 (3%)	3	1
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%)	228 (94%)	13 (5%)	2 (1%)	16	12
13	o	242/244 (99%)	228 (94%)	11 (4%)	3 (1%)	10	6
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
15	u	95/97 (98%)	89 (94%)	4 (4%)	2 (2%)	5	2
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
17	Y	25/30 (83%)	20 (80%)	3 (12%)	2 (8%)	1	0
17	y	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	7	3
20	R	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
20	r	29/34 (85%)	23 (79%)	5 (17%)	1 (3%)	3	1
All	All	5237/5326 (98%)	5019 (96%)	197 (4%)	21 (0%)	30	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	62	GLU
17	Y	41	VAL
3	c	416	SER
3	c	463	SER
13	o	60	ARG
15	u	53	ALA
20	r	30	GLN
17	Y	43	ARG
13	o	57	LYS
13	o	61	GLN
19	z	15	LEU
2	b	505	ARG
15	u	54	PRO
2	b	404	GLY
13	O	133	VAL
7	h	60	VAL
9	J	6	GLY
1	A	259	ILE
3	c	136	GLY

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%)	264 (98%)	6 (2%)	45	51
1	a	269/270 (100%)	257 (96%)	12 (4%)	24	24
2	B	407/403 (101%)	385 (95%)	22 (5%)	20	17
2	b	402/403 (100%)	387 (96%)	15 (4%)	30	31
3	C	345/352 (98%)	335 (97%)	10 (3%)	37	40
3	c	354/352 (101%)	336 (95%)	18 (5%)	21	20
4	D	276/276 (100%)	271 (98%)	5 (2%)	51	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	277/276 (100%)	270 (98%)	7 (2%)	42	46
5	E	72/72 (100%)	63 (88%)	9 (12%)	4	2
5	e	71/72 (99%)	68 (96%)	3 (4%)	26	26
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	32
6	f	28/28 (100%)	23 (82%)	5 (18%)	2	1
7	H	53/54 (98%)	50 (94%)	3 (6%)	18	16
7	h	53/54 (98%)	51 (96%)	2 (4%)	29	30
8	I	32/32 (100%)	29 (91%)	3 (9%)	8	5
8	i	32/32 (100%)	31 (97%)	1 (3%)	35	38
9	J	24/24 (100%)	23 (96%)	1 (4%)	26	26
9	j	23/24 (96%)	20 (87%)	3 (13%)	4	2
10	K	31/30 (103%)	28 (90%)	3 (10%)	8	5
10	k	30/30 (100%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	40
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	6
12	M	28/29 (97%)	24 (86%)	4 (14%)	3	1
12	m	28/29 (97%)	27 (96%)	1 (4%)	31	32
13	O	208/207 (100%)	194 (93%)	14 (7%)	15	11
13	o	207/207 (100%)	193 (93%)	14 (7%)	14	11
14	T	26/26 (100%)	23 (88%)	3 (12%)	5	3
14	t	25/26 (96%)	25 (100%)	0	100	100
15	U	84/84 (100%)	78 (93%)	6 (7%)	13	10
15	u	84/84 (100%)	82 (98%)	2 (2%)	43	47
16	V	117/117 (100%)	109 (93%)	8 (7%)	14	11
16	v	117/117 (100%)	109 (93%)	8 (7%)	14	11
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2	1
17	y	22/23 (96%)	18 (82%)	4 (18%)	2	1
18	X	31/31 (100%)	29 (94%)	2 (6%)	15	12
18	x	31/31 (100%)	29 (94%)	2 (6%)	15	12
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
19	z	51/52 (98%)	39 (76%)	12 (24%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	28/29 (97%)	22 (79%)	6 (21%)	1	0
20	r	19/29 (66%)	13 (68%)	6 (32%)	0	0
All	All	4323/4348 (99%)	4083 (94%)	240 (6%)	19	16

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	102	LEU
1	A	205	VAL
1	A	231	GLU
1	A	243	GLU
1	A	270	SER
2	B	63	LEU
2	B	83	GLU
2	B	86	ILE
2	B	127	ARG
2	B	159	THR
2	B	210	ILE
2	B	227	LYS
2	B	286	ARG
2	B	289	GLN
2	B	291	SER
2	B	362	PHE
2	B	371	THR
2	B	389	LYS
2	B	405	GLU
2	B	435	GLU
2	B	476	ARG
2	B	485	GLU
2	B	489	GLU
2	B	491	VAL
2	B	495	PHE
2	B	505	ARG
2	B	506	ARG
3	C	106	VAL
3	C	108	THR
3	C	141	GLU
3	C	161	LEU
3	C	238	ILE
3	C	240	ILE

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Mol	Chain	Res	Type
3	C	289	PHE
3	C	315	MET
3	C	344	SER
3	C	355	THR
4	D	12	ARG
4	D	43	LEU
4	D	76	VAL
4	D	154	VAL
4	D	259	ILE
5	E	4	THR
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	65	LEU
5	E	71	GLU
5	E	76	VAL
5	E	77	GLU
5	E	83	LEU
6	F	25	THR
7	H	20	LYS
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	33	LYS
8	I	35	LYS
9	J	8	ILE
10	K	10	LYS
10	K	25	LEU
10	K	43	VAL
11	L	2	GLU
12	M	2	GLU
12	M	3	VAL
12	M	13	LEU
12	M	16	LEU
13	O	3	GLN
13	O	27	ARG
13	O	34	SER
13	O	39	ARG
13	O	40	ILE
13	O	57	LYS
13	O	64	GLU
13	O	78	LEU

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Mol	Chain	Res	Type
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	172	ILE
13	O	207	ARG
13	O	214	THR
14	T	2	GLU
14	T	24	ARG
14	T	25	GLU
15	U	10	VAL
15	U	39	ARG
15	U	51	LYS
15	U	59	GLU
15	U	67	LEU
15	U	86	GLU
16	V	3	LEU
16	V	7	VAL
16	V	14	SER
16	V	19	ILE
16	V	23	GLU
16	V	31	ARG
16	V	90	GLU
16	V	105	ARG
17	Y	24	MET
17	Y	27	MET
17	Y	43	ARG
18	X	28	LEU
18	X	29	ILE
19	Z	3	ILE
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	29	SER
19	Z	40	ILE
19	Z	52	LEU
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	13	LEU
20	R	20	VAL
20	R	21	ARG
1	a	28	LEU

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Mol	Chain	Res	Type
1	a	42	LEU
1	a	159	LEU
1	a	160	ILE
1	a	200	LEU
1	a	226	GLU
1	a	229	GLU
1	a	231	GLU
1	a	238	LYS
1	a	245	THR
1	a	286	THR
1	a	288	LEU
2	b	80	ILE
2	b	86	ILE
2	b	98	LEU
2	b	137	LYS
2	b	149	LEU
2	b	219	VAL
2	b	227	LYS
2	b	236	THR
2	b	252	VAL
2	b	294	SER
2	b	362	PHE
2	b	397	VAL
2	b	486	LEU
2	b	491	VAL
2	b	506	ARG
3	c	24	THR
3	c	25	ASN
3	c	26	ARG
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	142	GLU
3	c	165	LEU
3	c	198	VAL
3	c	213	LEU
3	c	240	ILE
3	c	289	PHE
3	c	346	THR
3	c	354	GLU
3	c	355	THR

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Mol	Chain	Res	Type
3	c	396	MET
3	c	471	SER
4	d	90	LEU
4	d	182	LEU
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
4	d	329	MET
4	d	343	GLU
5	e	8	ARG
5	e	83	LEU
5	e	84	LYS
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
6	f	43	ILE
6	f	44	GLN
7	h	7	LEU
7	h	43	LEU
8	i	33	LYS
9	j	13	VAL
9	j	15	THR
9	j	36	LEU
10	k	10	LYS
10	k	19	ASP
10	k	22	VAL
10	k	30	VAL
10	k	46	ARG
11	l	11	GLU
11	l	21	LEU
11	l	30	LEU
12	m	9	ILE
13	o	4	THR
13	o	6	THR
13	o	34	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

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Mol	Chain	Res	Type
13	o	133	VAL
13	o	135	SER
13	o	181	GLU
13	o	207	ARG
15	u	10	VAL
15	u	23	GLU
16	v	6	GLU
16	v	10	VAL
16	v	15	GLU
16	v	24	LYS
16	v	52	LEU
16	v	69	ILE
16	v	90	GLU
16	v	109	GLU
17	y	22	LEU
17	y	30	ILE
17	y	38	LEU
17	y	45	ASN
18	x	8	LYS
18	x	15	LEU
19	z	1	MET
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	19	MET
19	z	20	VAL
19	z	31	GLN
19	z	32	ASP
19	z	37	LYS
19	z	38	GLN
19	z	42	LEU
19	z	46	LEU
20	r	3	TRP
20	r	6	LEU
20	r	7	VAL
20	r	13	LEU
20	r	22	ASN
20	r	23	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
2	B	289	GLN
3	C	201	ASN
4	D	186	GLN
4	D	334	GLN
4	D	350	ASN
13	O	82	GLN
13	O	88	ASN
13	O	124	ASN
13	O	155	ASN
13	O	231	HIS
15	U	81	HIS
16	V	86	GLN
16	V	106	ASN
18	X	38	GLN
1	a	165	GLN
1	a	296	ASN
2	b	282	GLN
2	b	338	GLN
2	b	409	GLN
3	c	25	ASN
3	c	28	GLN
3	c	201	ASN
3	c	322	GLN
3	c	378	ASN
3	c	415	ASN
4	d	83	ASN
13	o	58	ASN
13	o	124	ASN
13	o	200	ASN
18	x	33	GLN
19	z	38	GLN

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	$\# Z > 2$
8	FME	i	1	8	8,9,10	1.12	0	8,9,11	0.93	0
12	FME	m	1	12	8,9,10	1.22	1 (12%)	8,9,11	1.00	1 (12%)
14	FME	T	1	14	8,9,10	1.08	1 (12%)	8,9,11	1.56	2 (25%)
14	FME	t	1	14	8,9,10	1.43	1 (12%)	8,9,11	1.32	1 (12%)
12	FME	M	1	12	8,9,10	1.27	1 (12%)	8,9,11	1.01	0
8	FME	I	1	8	8,9,10	1.00	0	8,9,11	1.54	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-3.62	1.41	1.46
12	M	1	FME	CA-N	-2.93	1.42	1.46
12	m	1	FME	CA-N	-2.65	1.42	1.46
14	T	1	FME	CA-N	-2.37	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	C-CA-N	3.83	116.89	109.50
14	T	1	FME	CA-N-CN	-2.56	118.89	122.82
14	t	1	FME	C-CA-N	2.43	114.18	109.50
14	T	1	FME	O1-CN-N	-2.29	119.39	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CB-CA-N	2.00	114.16	110.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	H	102	-	63,63,67	1.29	8 (12%)	77,77,81	1.45	9 (11%)
30	OEX	A	414	3,36,1	0,15,15	-	-	-		
32	LMG	C	501	-	48,48,55	0.91	2 (4%)	56,56,63	1.39	9 (16%)
23	BCT	A	404	21	3,3,3	1.06	0	2,3,3	3.25	1 (50%)
24	CLA	B	612	-	69,73,73	0.96	4 (5%)	82,113,113	1.32	10 (12%)
32	LMG	c	522	-	48,48,55	1.19	6 (12%)	56,56,63	1.34	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	a	411	-	35,35,54	1.12	2 (5%)	37,37,65	1.36	4 (10%)
24	CLA	C	512	3	69,73,73	1.35	10 (14%)	82,113,113	1.48	8 (9%)
24	CLA	b	603	-	69,73,73	1.21	9 (13%)	82,113,113	1.52	12 (14%)
33	LHG	l	101	-	48,48,48	0.86	2 (4%)	51,54,54	1.28	7 (13%)
32	LMG	c	519	-	37,37,55	1.10	3 (8%)	45,45,63	1.25	5 (11%)
24	CLA	B	613	-	69,73,73	1.37	11 (15%)	82,113,113	1.58	11 (13%)
25	PHO	A	407	-	58,69,69	1.81	11 (18%)	55,99,99	1.37	7 (12%)
24	CLA	c	512	-	69,73,73	1.20	9 (13%)	82,113,113	1.31	8 (9%)
24	CLA	B	615	-	69,73,73	1.29	8 (11%)	82,113,113	1.41	9 (10%)
24	CLA	b	616	-	69,73,73	1.52	10 (14%)	82,113,113	1.56	10 (12%)
29	DGD	h	104	-	63,63,67	1.07	5 (7%)	77,77,81	1.40	8 (10%)
24	CLA	b	612	-	69,73,73	1.57	8 (11%)	82,113,113	1.25	10 (12%)
24	CLA	b	604	-	69,73,73	1.22	8 (11%)	82,113,113	1.48	11 (13%)
26	BCR	B	619	-	41,41,41	1.30	3 (7%)	56,56,56	1.52	12 (21%)
32	LMG	h	102	-	21,21,55	0.84	1 (4%)	20,20,63	1.01	1 (5%)
24	CLA	b	614	-	69,73,73	1.56	11 (15%)	82,113,113	1.37	13 (15%)
32	LMG	b	621	-	51,51,55	0.83	0	59,59,63	1.53	9 (15%)
35	HEC	V	201	16	46,50,50	1.88	7 (15%)	58,82,82	1.35	3 (5%)
24	CLA	a	407	-	69,73,73	1.66	13 (18%)	82,113,113	1.31	10 (12%)
24	CLA	c	510	-	69,73,73	1.31	7 (10%)	82,113,113	1.44	7 (8%)
24	CLA	d	405	-	69,73,73	1.59	8 (11%)	82,113,113	1.42	17 (20%)
24	CLA	C	506	-	69,73,73	1.28	9 (13%)	82,113,113	1.27	10 (12%)
24	CLA	c	504	36	64,68,73	1.29	10 (15%)	76,107,113	1.33	8 (10%)
26	BCR	b	618	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
32	LMG	K	102	-	48,48,55	1.06	4 (8%)	56,56,63	1.33	5 (8%)
24	CLA	B	607	36	69,73,73	1.59	6 (8%)	82,113,113	1.34	8 (9%)
24	CLA	B	614	-	69,73,73	1.44	9 (13%)	82,113,113	1.16	5 (6%)
26	BCR	c	521	-	41,41,41	0.98	3 (7%)	56,56,56	1.27	6 (10%)
26	BCR	B	618	-	41,41,41	1.18	2 (4%)	56,56,56	1.35	8 (14%)
24	CLA	B	605	-	69,73,73	1.48	9 (13%)	82,113,113	1.50	12 (14%)
26	BCR	C	519	-	41,41,41	1.05	2 (4%)	56,56,56	1.39	8 (14%)
29	DGD	c	516	-	63,63,67	1.12	3 (4%)	77,77,81	1.39	9 (11%)
24	CLA	c	501	-	69,73,73	1.35	13 (18%)	82,113,113	1.56	10 (12%)
25	PHO	d	402	-	58,69,69	2.09	9 (15%)	55,99,99	1.74	12 (21%)
33	LHG	d	409	-	48,48,48	0.72	0	51,54,54	1.26	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	602	-	69,73,73	1.42	9 (13%)	82,113,113	1.30	12 (14%)
24	CLA	c	505	-	69,73,73	1.18	7 (10%)	82,113,113	1.39	10 (12%)
24	CLA	A	408	-	58,62,73	1.46	12 (20%)	68,99,113	1.50	11 (16%)
24	CLA	D	402	36	69,73,73	1.27	10 (14%)	82,113,113	1.35	8 (9%)
32	LMG	b	623	-	55,55,55	0.96	5 (9%)	63,63,63	1.43	7 (11%)
33	LHG	D	411	-	48,48,48	1.07	6 (12%)	51,54,54	1.44	8 (15%)
24	CLA	B	604	-	69,73,73	1.31	6 (8%)	82,113,113	1.54	8 (9%)
26	BCR	a	408	-	41,41,41	1.19	4 (9%)	56,56,56	1.43	8 (14%)
33	LHG	D	408	-	48,48,48	1.08	5 (10%)	51,54,54	1.27	5 (9%)
26	BCR	d	406	-	41,41,41	1.17	2 (4%)	56,56,56	1.25	6 (10%)
26	BCR	b	602	-	41,41,41	1.20	3 (7%)	56,56,56	1.33	7 (12%)
33	LHG	L	101	-	48,48,48	0.71	1 (2%)	51,54,54	1.18	4 (7%)
26	BCR	h	103	-	41,41,41	1.16	1 (2%)	56,56,56	1.48	13 (23%)
24	CLA	c	507	36	69,73,73	1.16	8 (11%)	82,113,113	1.47	13 (15%)
24	CLA	b	606	-	69,73,73	1.28	9 (13%)	82,113,113	1.49	16 (19%)
24	CLA	b	617	-	64,68,73	1.30	9 (14%)	76,107,113	1.52	9 (11%)
28	SQD	b	601	-	47,49,54	0.95	2 (4%)	57,60,65	1.97	14 (24%)
26	BCR	c	515	-	41,41,41	1.41	4 (9%)	56,56,56	1.42	10 (17%)
26	BCR	Y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	6 (10%)
33	LHG	e	101	-	41,41,48	0.76	0	44,47,54	1.32	3 (6%)
27	PL9	D	406	-	55,55,55	1.92	9 (16%)	68,69,69	1.45	13 (19%)
24	CLA	C	502	-	69,73,73	1.59	11 (15%)	82,113,113	1.32	9 (10%)
33	LHG	d	408	-	48,48,48	0.73	0	51,54,54	1.24	5 (9%)
26	BCR	b	619	-	41,41,41	1.29	2 (4%)	56,56,56	1.46	10 (17%)
30	OEX	a	414	3,36,1	0,15,15	-	-	-	-	-
33	LHG	d	410	-	38,38,48	0.80	2 (5%)	41,44,54	1.17	3 (7%)
24	CLA	C	510	-	69,73,73	1.20	7 (10%)	82,113,113	1.20	6 (7%)
33	LHG	E	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.14	2 (3%)
24	CLA	c	502	-	69,73,73	1.28	7 (10%)	82,113,113	1.24	11 (13%)
24	CLA	c	503	-	69,73,73	1.28	4 (5%)	82,113,113	1.41	7 (8%)
25	PHO	a	406	-	58,69,69	2.07	9 (15%)	55,99,99	1.49	8 (14%)
29	DGD	c	517	-	63,63,67	1.23	9 (14%)	77,77,81	1.42	11 (14%)
24	CLA	C	509	-	69,73,73	1.46	8 (11%)	82,113,113	1.47	13 (15%)
24	CLA	h	101	36	69,73,73	1.50	10 (14%)	82,113,113	1.43	11 (13%)
24	CLA	b	607	-	69,73,73	1.70	7 (10%)	82,113,113	1.58	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HEC	v	201	16	46,50,50	1.85	8 (17%)	58,82,82	1.32	9 (15%)
24	CLA	b	608	36	69,73,73	1.26	6 (8%)	82,113,113	1.26	5 (6%)
34	HEM	F	102	5,6	50,50,50	1.42	7 (14%)	67,82,82	1.02	3 (4%)
32	LMG	M	101	-	51,51,55	1.13	6 (11%)	59,59,63	1.59	14 (23%)
26	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
26	BCR	D	405	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
29	DGD	a	412	-	43,43,67	1.24	3 (6%)	45,45,81	1.34	8 (17%)
24	CLA	C	503	-	69,73,73	1.31	7 (10%)	82,113,113	1.50	11 (13%)
24	CLA	B	606	-	69,73,73	1.51	9 (13%)	82,113,113	1.37	11 (13%)
24	CLA	d	404	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	8 (9%)
32	LMG	D	410	-	31,31,55	1.17	3 (9%)	33,33,63	1.10	0
33	LHG	D	409	-	46,46,48	1.13	3 (6%)	49,52,54	1.43	7 (14%)
24	CLA	C	511	-	69,73,73	1.37	11 (15%)	82,113,113	1.28	5 (6%)
24	CLA	a	405	36	69,73,73	1.10	7 (10%)	82,113,113	1.29	8 (9%)
24	CLA	D	404	-	69,73,73	1.60	11 (15%)	82,113,113	1.07	6 (7%)
24	CLA	A	406	36	69,73,73	1.21	9 (13%)	82,113,113	1.32	10 (12%)
27	PL9	a	409	-	55,55,55	1.15	4 (7%)	68,69,69	1.46	11 (16%)
24	CLA	C	513	-	69,73,73	1.20	9 (13%)	82,113,113	1.36	10 (12%)
26	BCR	H	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.30	8 (14%)
24	CLA	b	611	36	69,73,73	1.22	9 (13%)	82,113,113	1.36	12 (14%)
24	CLA	d	403	36	69,73,73	1.44	9 (13%)	82,113,113	1.41	12 (14%)
24	CLA	C	508	36	69,73,73	1.74	5 (7%)	82,113,113	1.36	8 (9%)
24	CLA	b	610	-	69,73,73	1.14	5 (7%)	82,113,113	1.30	9 (10%)
24	CLA	B	601	36	69,73,73	1.96	9 (13%)	82,113,113	1.46	9 (10%)
24	CLA	c	508	-	68,72,73	1.28	11 (16%)	80,111,113	1.09	4 (5%)
29	DGD	A	413	-	67,67,67	1.24	7 (10%)	81,81,81	1.47	11 (13%)
28	SQD	F	101	-	34,36,54	1.01	1 (2%)	42,45,65	1.71	12 (28%)
24	CLA	B	608	-	69,73,73	1.22	8 (11%)	82,113,113	1.21	7 (8%)
29	DGD	C	517	-	63,63,67	1.16	6 (9%)	77,77,81	1.46	13 (16%)
24	CLA	C	505	36	63,67,73	1.15	5 (7%)	74,105,113	1.43	15 (20%)
24	CLA	C	504	-	69,73,73	1.42	12 (17%)	82,113,113	1.48	11 (13%)
24	CLA	b	613	-	69,73,73	1.37	6 (8%)	82,113,113	1.31	11 (13%)
24	CLA	c	506	-	69,73,73	2.02	10 (14%)	82,113,113	1.33	10 (12%)
28	SQD	f	101	-	39,41,54	1.13	5 (12%)	49,52,65	1.57	7 (14%)
32	LMG	D	407	-	51,51,55	1.13	4 (7%)	59,59,63	1.24	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	609	-	69,73,73	1.20	7 (10%)	82,113,113	1.35	12 (14%)
23	BCT	d	401	21	3,3,3	1.22	0	2,3,3	3.08	2 (100%)
24	CLA	b	605	-	69,73,73	1.28	10 (14%)	82,113,113	1.53	13 (15%)
24	CLA	C	514	-	69,73,73	1.21	7 (10%)	82,113,113	1.37	10 (12%)
24	CLA	B	603	-	69,73,73	1.15	6 (8%)	82,113,113	1.39	11 (13%)
34	HEM	e	102	5,6	50,50,50	1.56	8 (16%)	67,82,82	1.09	3 (4%)
32	LMG	d	411	-	44,44,55	1.09	3 (6%)	52,52,63	1.35	5 (9%)
28	SQD	A	412	-	38,38,54	1.09	3 (7%)	40,40,65	1.33	4 (10%)
24	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.48	11 (13%)
28	SQD	B	622	-	52,54,54	0.94	2 (3%)	62,65,65	1.79	14 (22%)
28	SQD	A	411	-	50,52,54	1.01	4 (8%)	60,63,65	2.31	14 (23%)
26	BCR	C	515	-	41,41,41	1.48	4 (9%)	56,56,56	1.37	10 (17%)
24	CLA	A	405	-	69,73,73	1.37	10 (14%)	82,113,113	1.24	7 (8%)
24	CLA	C	507	-	69,73,73	1.52	10 (14%)	82,113,113	1.15	8 (9%)
32	LMG	c	524	-	49,49,55	0.83	2 (4%)	57,57,63	1.37	4 (7%)
24	CLA	B	616	-	64,68,73	1.53	10 (15%)	76,107,113	1.39	11 (14%)
28	SQD	a	410	-	52,54,54	1.01	5 (9%)	62,65,65	1.97	12 (19%)
26	BCR	A	409	-	41,41,41	1.09	3 (7%)	56,56,56	1.33	8 (14%)
26	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.57	12 (21%)
24	CLA	B	609	-	69,73,73	1.43	9 (13%)	82,113,113	1.31	11 (13%)
26	BCR	b	620	-	41,41,41	1.14	2 (4%)	56,56,56	1.29	9 (16%)
24	CLA	a	404	-	69,73,73	1.35	12 (17%)	82,113,113	1.50	9 (10%)
24	CLA	c	511	3	69,73,73	1.63	7 (10%)	82,113,113	1.25	7 (8%)
26	BCR	B	617	-	41,41,41	1.25	3 (7%)	56,56,56	1.47	7 (12%)
29	DGD	C	518	-	63,63,67	1.09	6 (9%)	77,77,81	1.47	13 (16%)
24	CLA	B	610	36	69,73,73	1.43	10 (14%)	82,113,113	1.45	12 (14%)
24	CLA	D	403	-	69,73,73	1.30	10 (14%)	82,113,113	1.25	9 (10%)
24	CLA	b	615	-	69,73,73	1.42	9 (13%)	82,113,113	1.50	12 (14%)
32	LMG	B	621	-	26,26,55	0.83	1 (3%)	26,26,63	1.17	2 (7%)
27	PL9	A	410	-	55,55,55	1.37	5 (9%)	68,69,69	1.43	11 (16%)
26	BCR	t	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.40	8 (14%)
27	PL9	d	407	-	55,55,55	1.43	5 (9%)	68,69,69	1.77	20 (29%)
24	CLA	c	513	-	69,73,73	1.31	10 (14%)	82,113,113	1.09	6 (7%)
24	CLA	c	509	-	69,73,73	1.38	9 (13%)	82,113,113	1.46	10 (12%)
25	PHO	D	401	-	58,69,69	2.03	11 (18%)	55,99,99	1.54	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DGD	c	518	-	63,63,67	1.10	4 (6%)	77,77,81	1.42	10 (12%)
29	DGD	C	516	-	63,63,67	1.20	6 (9%)	77,77,81	1.32	12 (15%)
26	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.15	3 (5%)

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	H	102	-	-	17/51/91/95	0/2/2/2
32	LMG	C	501	-	-	23/43/63/70	0/1/1/1
24	CLA	B	612	-	1/1/20/20	11/39/115/115	-
32	LMG	c	522	-	-	24/43/63/70	0/1/1/1
28	SQD	a	411	-	-	23/37/37/69	-
24	CLA	C	512	3	1/1/20/20	5/39/115/115	-
24	CLA	b	603	-	1/1/20/20	9/39/115/115	-
33	LHG	l	101	-	-	17/53/53/53	-
32	LMG	c	519	-	-	13/31/51/70	0/1/1/1
24	CLA	B	613	-	1/1/20/20	10/39/115/115	-
25	PHO	A	407	-	-	6/37/103/103	0/5/6/6
24	CLA	c	512	-	1/1/20/20	22/39/115/115	-
24	CLA	B	615	-	1/1/20/20	13/39/115/115	-
24	CLA	b	616	-	1/1/20/20	9/39/115/115	-
29	DGD	h	104	-	-	18/51/91/95	0/2/2/2
24	CLA	b	612	-	1/1/20/20	7/39/115/115	-
24	CLA	b	604	-	1/1/20/20	6/39/115/115	-
26	BCR	B	619	-	-	7/29/63/63	0/2/2/2
32	LMG	h	102	-	-	13/17/17/70	-
24	CLA	b	614	-	1/1/20/20	6/39/115/115	-
32	LMG	b	621	-	-	20/46/66/70	0/1/1/1
35	HEC	V	201	16	-	6/14/54/54	-
24	CLA	a	407	-	1/1/20/20	8/39/115/115	-
24	CLA	c	510	-	1/1/20/20	15/39/115/115	-
24	CLA	d	405	-	1/1/20/20	4/39/115/115	-
24	CLA	C	506	-	1/1/20/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	504	36	1/1/19/20	7/33/109/115	-
26	BCR	b	618	-	-	6/29/63/63	0/2/2/2
32	LMG	K	102	-	-	11/43/63/70	0/1/1/1
24	CLA	B	607	36	1/1/20/20	10/39/115/115	-
24	CLA	B	614	-	1/1/20/20	10/39/115/115	-
26	BCR	c	521	-	-	14/29/63/63	0/2/2/2
26	BCR	B	618	-	-	1/29/63/63	0/2/2/2
24	CLA	B	605	-	1/1/20/20	11/39/115/115	-
26	BCR	C	519	-	-	11/29/63/63	0/2/2/2
29	DGD	c	516	-	-	27/51/91/95	0/2/2/2
24	CLA	c	501	-	1/1/20/20	6/39/115/115	-
25	PHO	d	402	-	-	5/37/103/103	0/5/6/6
33	LHG	d	409	-	-	16/53/53/53	-
24	CLA	B	602	-	1/1/20/20	4/39/115/115	-
24	CLA	c	505	-	1/1/20/20	9/39/115/115	-
24	CLA	A	408	-	1/1/17/20	4/26/102/115	-
24	CLA	D	402	36	1/1/20/20	1/39/115/115	-
32	LMG	b	623	-	-	18/50/70/70	0/1/1/1
33	LHG	D	411	-	-	16/53/53/53	-
24	CLA	B	604	-	1/1/20/20	12/39/115/115	-
26	BCR	a	408	-	-	3/29/63/63	0/2/2/2
33	LHG	D	408	-	-	20/53/53/53	-
26	BCR	d	406	-	-	11/29/63/63	0/2/2/2
26	BCR	b	602	-	-	11/29/63/63	0/2/2/2
33	LHG	L	101	-	-	21/53/53/53	-
26	BCR	h	103	-	-	10/29/63/63	0/2/2/2
24	CLA	c	507	36	1/1/20/20	11/39/115/115	-
24	CLA	b	606	-	1/1/20/20	10/39/115/115	-
24	CLA	b	617	-	1/1/19/20	7/33/109/115	-
28	SQD	b	601	-	-	21/44/64/69	0/1/1/1
26	BCR	c	515	-	-	8/29/63/63	0/2/2/2
26	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
33	LHG	e	101	-	-	29/46/46/53	-
27	PL9	D	406	-	-	10/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	502	-	1/1/20/20	4/39/115/115	-
33	LHG	d	408	-	-	20/53/53/53	-
26	BCR	b	619	-	-	5/29/63/63	0/2/2/2
33	LHG	d	410	-	-	11/43/43/53	-
24	CLA	C	510	-	1/1/20/20	10/39/115/115	-
33	LHG	E	101	-	-	25/53/53/53	-
24	CLA	c	502	-	1/1/20/20	3/39/115/115	-
24	CLA	c	503	-	1/1/20/20	7/39/115/115	-
25	PHO	a	406	-	-	2/37/103/103	0/5/6/6
29	DGD	c	517	-	-	15/51/91/95	0/2/2/2
24	CLA	C	509	-	-	9/39/115/115	-
24	CLA	h	101	36	1/1/20/20	20/39/115/115	-
24	CLA	b	607	-	1/1/20/20	8/39/115/115	-
35	HEC	v	201	16	-	6/14/54/54	-
24	CLA	b	608	36	1/1/20/20	12/39/115/115	-
34	HEM	F	102	5,6	-	3/14/54/54	-
32	LMG	M	101	-	-	21/46/66/70	0/1/1/1
26	BCR	c	514	-	-	9/29/63/63	0/2/2/2
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
29	DGD	a	412	-	-	21/45/45/95	-
24	CLA	C	503	-	1/1/20/20	11/39/115/115	-
24	CLA	B	606	-	1/1/20/20	6/39/115/115	-
24	CLA	d	404	-	1/1/20/20	6/39/115/115	-
32	LMG	D	410	-	-	19/33/33/70	-
33	LHG	D	409	-	-	25/51/51/53	-
24	CLA	C	511	-	1/1/20/20	13/39/115/115	-
24	CLA	a	405	36	-	13/39/115/115	-
24	CLA	D	404	-	-	11/39/115/115	-
24	CLA	A	406	36	1/1/20/20	5/39/115/115	-
27	PL9	a	409	-	-	22/53/73/73	0/1/1/1
24	CLA	C	513	-	1/1/20/20	11/39/115/115	-
26	BCR	H	101	-	-	6/29/63/63	0/2/2/2
24	CLA	b	611	36	1/1/20/20	9/39/115/115	-
24	CLA	d	403	36	1/1/20/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	508	36	1/1/20/20	7/39/115/115	-
24	CLA	b	610	-	1/1/20/20	11/39/115/115	-
24	CLA	B	601	36	1/1/20/20	15/39/115/115	-
24	CLA	c	508	-	-	7/38/114/115	-
29	DGD	A	413	-	-	25/55/95/95	0/2/2/2
28	SQD	F	101	-	-	13/28/48/69	0/1/1/1
24	CLA	B	608	-	-	5/39/115/115	-
29	DGD	C	517	-	-	19/51/91/95	0/2/2/2
24	CLA	C	505	36	1/1/18/20	8/32/108/115	-
24	CLA	C	504	-	1/1/20/20	4/39/115/115	-
24	CLA	b	613	-	1/1/20/20	5/39/115/115	-
24	CLA	c	506	-	1/1/20/20	15/39/115/115	-
28	SQD	f	101	-	-	18/36/56/69	0/1/1/1
32	LMG	D	407	-	-	17/46/66/70	0/1/1/1
24	CLA	b	609	-	1/1/20/20	5/39/115/115	-
24	CLA	b	605	-	1/1/20/20	10/39/115/115	-
24	CLA	C	514	-	1/1/20/20	11/39/115/115	-
24	CLA	B	603	-	-	11/39/115/115	-
34	HEM	e	102	5,6	-	4/14/54/54	-
32	LMG	d	411	-	-	11/39/59/70	0/1/1/1
28	SQD	A	412	-	-	17/39/39/69	-
24	CLA	B	611	-	-	9/39/115/115	-
28	SQD	B	622	-	-	21/49/69/69	0/1/1/1
28	SQD	A	411	-	-	23/47/67/69	0/1/1/1
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	A	405	-	1/1/20/20	3/39/115/115	-
24	CLA	C	507	-	-	9/39/115/115	-
32	LMG	c	524	-	-	25/44/64/70	0/1/1/1
24	CLA	B	616	-	1/1/19/20	9/33/109/115	-
28	SQD	a	410	-	-	22/49/69/69	0/1/1/1
26	BCR	A	409	-	-	6/29/63/63	0/2/2/2
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2
24	CLA	B	609	-	-	5/39/115/115	-
26	BCR	b	620	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	404	-	1/1/20/20	6/39/115/115	-
24	CLA	c	511	3	1/1/20/20	6/39/115/115	-
26	BCR	B	617	-	-	5/29/63/63	0/2/2/2
29	DGD	C	518	-	-	13/51/91/95	0/2/2/2
24	CLA	B	610	36	1/1/20/20	5/39/115/115	-
24	CLA	D	403	-	1/1/20/20	7/39/115/115	-
24	CLA	b	615	-	1/1/20/20	13/39/115/115	-
32	LMG	B	621	-	-	8/22/22/70	-
27	PL9	A	410	-	-	24/53/73/73	0/1/1/1
26	BCR	t	101	-	-	12/29/63/63	0/2/2/2
27	PL9	d	407	-	-	18/53/73/73	0/1/1/1
24	CLA	c	513	-	1/1/20/20	11/39/115/115	-
24	CLA	c	509	-	1/1/20/20	14/39/115/115	-
25	PHO	D	401	-	-	2/37/103/103	0/5/6/6
29	DGD	c	518	-	-	14/51/91/95	0/2/2/2
29	DGD	C	516	-	-	17/51/91/95	0/2/2/2
26	BCR	k	101	-	-	9/29/63/63	0/2/2/2

All (899) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	MG-ND	-12.77	1.80	2.05
24	C	508	CLA	MG-NA	10.07	2.30	2.06
24	b	607	CLA	MG-NA	9.96	2.29	2.06
25	d	402	PHO	C1B-C2B	9.78	1.50	1.39
25	a	406	PHO	C1B-C2B	9.34	1.49	1.39
24	B	607	CLA	MG-NB	-9.24	1.87	2.05
24	B	601	CLA	MG-NA	9.03	2.27	2.06
24	B	601	CLA	MG-NB	-8.94	1.88	2.05
25	D	401	PHO	C1B-C2B	8.77	1.49	1.39
24	c	511	CLA	MG-NA	8.19	2.25	2.06
25	D	401	PHO	C3B-C4B	8.03	1.49	1.41
25	A	407	PHO	C1B-C2B	7.95	1.48	1.39
25	d	402	PHO	C3B-C4B	7.42	1.49	1.41
24	C	502	CLA	MG-ND	-7.13	1.91	2.05
27	D	406	PL9	C6-C1	-7.12	1.36	1.48
24	B	616	CLA	MG-NA	6.84	2.22	2.06
24	d	405	CLA	MG-NA	6.78	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	MG-NA	6.66	2.22	2.06
25	a	406	PHO	C3B-C4B	6.50	1.48	1.41
24	b	612	CLA	MG-NC	-6.47	1.90	2.06
24	C	507	CLA	MG-ND	-6.44	1.93	2.05
24	b	614	CLA	MG-NB	-6.43	1.93	2.05
35	v	201	HEC	CAB-C3B	6.40	1.55	1.35
35	V	201	HEC	CAC-C3C	6.38	1.55	1.35
27	D	406	PL9	C3-C4	-6.34	1.39	1.49
24	b	616	CLA	MG-NA	6.26	2.21	2.06
24	B	605	CLA	MG-NB	6.24	2.18	2.05
24	a	407	CLA	MG-NB	-6.18	1.93	2.05
24	D	404	CLA	MG-ND	-6.13	1.93	2.05
24	C	509	CLA	MG-ND	6.11	2.17	2.05
24	h	101	CLA	MG-NA	6.06	2.20	2.06
24	b	613	CLA	MG-ND	-6.02	1.93	2.05
24	b	612	CLA	MG-NA	5.94	2.20	2.06
26	C	515	BCR	C1-C6	-5.94	1.46	1.53
34	e	102	HEM	FE-NA	5.90	2.14	1.95
35	v	201	HEC	CAC-C3C	5.88	1.54	1.35
24	C	506	CLA	MG-NB	-5.79	1.94	2.05
24	c	509	CLA	MG-ND	5.73	2.17	2.05
24	B	613	CLA	MG-NA	5.71	2.19	2.06
24	a	407	CLA	MG-ND	-5.71	1.94	2.05
35	V	201	HEC	CAB-C3B	5.69	1.53	1.35
24	d	403	CLA	MG-ND	5.69	2.17	2.05
24	C	512	CLA	MG-NA	5.68	2.19	2.06
24	B	614	CLA	MG-NC	-5.65	1.92	2.06
24	B	614	CLA	MG-ND	-5.62	1.94	2.05
24	b	615	CLA	MG-NB	-5.52	1.94	2.05
24	c	503	CLA	MG-NC	5.39	2.19	2.06
24	b	608	CLA	MG-NB	-5.34	1.95	2.05
27	D	406	PL9	C11-C9	-5.30	1.40	1.51
24	D	404	CLA	MG-NC	5.30	2.18	2.06
24	c	510	CLA	MG-ND	-5.27	1.95	2.05
24	b	614	CLA	MG-NA	5.24	2.18	2.06
24	c	501	CLA	MG-NA	5.23	2.18	2.06
27	d	407	PL9	C3-C4	-5.19	1.41	1.49
24	C	504	CLA	MG-NA	5.15	2.18	2.06
24	B	606	CLA	MG-NC	-5.11	1.94	2.06
24	c	502	CLA	MG-NC	-5.11	1.94	2.06
25	A	407	PHO	C3B-C4B	5.06	1.46	1.41
29	A	413	DGD	C4D-C5D	5.06	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	515	BCR	C30-C25	-5.01	1.47	1.53
27	A	410	PL9	C3-C4	-4.95	1.41	1.49
24	d	405	CLA	MG-NC	-4.94	1.94	2.06
24	B	609	CLA	MG-NB	-4.92	1.96	2.05
24	C	509	CLA	MG-NA	4.83	2.17	2.06
26	B	619	BCR	C1-C6	-4.79	1.47	1.53
26	h	103	BCR	C30-C25	-4.71	1.47	1.53
27	a	409	PL9	C6-C1	-4.55	1.40	1.48
26	B	617	BCR	C1-C6	-4.55	1.48	1.53
33	D	409	LHG	P-O6	4.48	1.76	1.59
24	B	604	CLA	MG-NA	4.44	2.16	2.06
24	b	607	CLA	C1D-ND	4.44	1.43	1.37
24	B	607	CLA	C1D-ND	4.44	1.43	1.37
24	c	506	CLA	MG-NB	4.43	2.14	2.05
24	B	602	CLA	C4B-NB	4.41	1.43	1.37
29	H	102	DGD	O5D-C1E	4.37	1.47	1.40
24	B	602	CLA	MG-NA	4.34	2.16	2.06
24	C	502	CLA	MG-NA	4.34	2.16	2.06
26	B	618	BCR	C30-C25	-4.33	1.48	1.53
26	c	514	BCR	C1-C6	-4.31	1.48	1.53
24	C	508	CLA	MG-NC	-4.31	1.96	2.06
24	B	610	CLA	C1D-ND	4.31	1.43	1.37
24	b	606	CLA	MG-NB	-4.29	1.97	2.05
24	c	511	CLA	C4B-NB	4.26	1.43	1.37
24	A	408	CLA	MG-ND	-4.26	1.97	2.05
24	C	503	CLA	MG-ND	4.24	2.14	2.05
26	b	619	BCR	C30-C25	-4.23	1.48	1.53
24	b	616	CLA	MG-ND	-4.23	1.97	2.05
24	B	609	CLA	MG-ND	-4.21	1.97	2.05
24	D	403	CLA	MG-ND	-4.21	1.97	2.05
24	a	407	CLA	MG-NC	-4.20	1.96	2.06
24	b	611	CLA	MG-NB	-4.19	1.97	2.05
24	c	504	CLA	MG-ND	-4.19	1.97	2.05
26	H	101	BCR	C30-C25	-4.17	1.48	1.53
26	d	406	BCR	C1-C6	-4.17	1.48	1.53
24	B	610	CLA	C4B-NB	4.16	1.43	1.37
25	D	401	PHO	C4D-ND	-4.15	1.32	1.38
25	a	406	PHO	C1D-C2D	4.15	1.44	1.39
24	c	502	CLA	MG-NA	4.15	2.16	2.06
24	A	405	CLA	MG-NB	4.12	2.14	2.05
24	c	513	CLA	MG-ND	-4.08	1.97	2.05
29	C	518	DGD	O3G-C3G	-4.05	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	MG-NC	-4.01	1.96	2.06
24	B	601	CLA	C4B-NB	4.01	1.43	1.37
26	Y	101	BCR	C30-C25	-4.00	1.48	1.53
26	Y	101	BCR	C1-C6	-3.96	1.48	1.53
24	B	602	CLA	C1D-ND	3.94	1.43	1.37
24	C	507	CLA	MG-NB	3.94	2.13	2.05
25	d	402	PHO	C1D-C2D	3.93	1.43	1.39
26	a	408	BCR	C1-C6	-3.93	1.48	1.53
26	C	515	BCR	C30-C25	-3.91	1.48	1.53
26	K	101	BCR	C30-C25	-3.91	1.48	1.53
26	c	515	BCR	C1-C6	-3.90	1.48	1.53
24	B	609	CLA	C1D-ND	3.90	1.43	1.37
24	A	406	CLA	C1D-ND	3.87	1.42	1.37
29	c	517	DGD	O2G-C2G	-3.82	1.37	1.46
24	b	614	CLA	C4B-NB	3.82	1.42	1.37
26	D	405	BCR	C30-C25	-3.81	1.48	1.53
24	D	404	CLA	MG-NB	-3.80	1.98	2.05
28	a	410	SQD	O48-C23	3.80	1.44	1.33
24	D	404	CLA	C1D-ND	3.80	1.42	1.37
24	C	511	CLA	MG-NB	3.79	2.13	2.05
26	k	101	BCR	C1-C6	-3.78	1.48	1.53
35	v	201	HEC	CBB-CAB	-3.78	1.35	1.49
32	K	102	LMG	O7-C8	-3.78	1.37	1.46
26	b	618	BCR	C1-C6	-3.77	1.49	1.53
24	C	511	CLA	C1D-ND	3.76	1.42	1.37
32	d	411	LMG	O7-C8	-3.76	1.37	1.46
24	B	610	CLA	MG-ND	-3.76	1.98	2.05
24	c	506	CLA	C1D-ND	3.76	1.42	1.37
24	b	604	CLA	MG-NA	3.74	2.15	2.06
24	d	403	CLA	MG-NB	3.73	2.13	2.05
24	B	616	CLA	C1D-ND	3.73	1.42	1.37
24	C	503	CLA	MG-NB	-3.72	1.98	2.05
24	B	605	CLA	C1D-ND	3.70	1.42	1.37
24	C	512	CLA	C1D-ND	3.69	1.42	1.37
24	B	613	CLA	C4B-NB	3.69	1.42	1.37
35	V	201	HEC	CBC-CAC	-3.68	1.35	1.49
26	b	619	BCR	C1-C6	-3.67	1.49	1.53
24	c	513	CLA	MG-NA	3.67	2.15	2.06
32	c	522	LMG	O1-C1	3.66	1.46	1.40
33	D	408	LHG	O8-C6	-3.65	1.37	1.45
24	B	608	CLA	CMD-C2D	-3.64	1.43	1.50
24	c	501	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	MG-NB	-3.61	1.98	2.05
28	A	412	SQD	O47-C7	3.61	1.44	1.34
24	D	402	CLA	C1D-ND	3.61	1.42	1.37
28	A	412	SQD	O48-C23	3.60	1.43	1.33
28	a	411	SQD	O48-C23	3.60	1.43	1.33
29	a	412	DGD	O2G-C1B	3.57	1.44	1.34
29	C	516	DGD	C4E-C3E	3.57	1.61	1.52
24	a	404	CLA	MG-NC	3.56	2.14	2.06
24	C	502	CLA	C4B-NB	3.56	1.42	1.37
26	A	409	BCR	C1-C6	-3.55	1.49	1.53
26	b	620	BCR	C1-C6	-3.55	1.49	1.53
24	C	502	CLA	C1D-ND	3.55	1.42	1.37
24	B	605	CLA	C3B-C4B	3.54	1.53	1.42
35	V	201	HEC	CBB-CAB	-3.52	1.36	1.49
24	a	407	CLA	CHC-C4B	-3.51	1.31	1.39
35	v	201	HEC	CBC-CAC	-3.51	1.36	1.49
24	C	508	CLA	C1B-C2B	3.51	1.51	1.43
24	C	513	CLA	MG-NB	3.49	2.12	2.05
24	C	514	CLA	MG-ND	3.49	2.12	2.05
24	B	605	CLA	CHC-C1C	3.49	1.45	1.38
24	c	503	CLA	C1D-ND	3.48	1.42	1.37
26	b	602	BCR	C30-C25	-3.48	1.49	1.53
24	C	514	CLA	C1D-ND	3.47	1.42	1.37
26	K	101	BCR	C1-C6	-3.47	1.49	1.53
24	C	507	CLA	C1D-ND	3.47	1.42	1.37
24	C	511	CLA	MG-NC	3.46	2.14	2.06
27	d	407	PL9	C7-C8	-3.46	1.45	1.50
28	a	411	SQD	O47-C7	3.46	1.44	1.34
24	h	101	CLA	C4B-NB	3.45	1.42	1.37
32	M	101	LMG	C1-C2	3.42	1.62	1.52
24	b	605	CLA	MG-NB	3.42	2.12	2.05
28	F	101	SQD	O48-C23	3.41	1.43	1.33
33	D	411	LHG	O7-C5	-3.41	1.38	1.46
24	c	512	CLA	MG-NA	3.41	2.14	2.06
24	B	604	CLA	MG-ND	-3.40	1.99	2.05
25	a	406	PHO	C3D-C4D	3.40	1.45	1.41
29	C	517	DGD	O2G-C2G	-3.39	1.38	1.46
28	B	622	SQD	O47-C7	3.39	1.43	1.34
25	a	406	PHO	CBD-CGD	-3.38	1.48	1.52
26	k	101	BCR	C30-C25	-3.38	1.49	1.53
24	B	603	CLA	MG-NB	-3.38	1.99	2.05
24	h	101	CLA	C1D-ND	3.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	PHO	CMC-C2C	-3.38	1.45	1.50
25	A	407	PHO	CMC-C2C	-3.37	1.45	1.50
26	b	602	BCR	C1-C6	-3.37	1.49	1.53
24	D	403	CLA	C1D-ND	3.36	1.42	1.37
29	a	412	DGD	C1G-C2G	3.35	1.61	1.50
26	B	618	BCR	C1-C6	-3.35	1.49	1.53
32	M	101	LMG	C9-C8	3.35	1.61	1.50
24	C	511	CLA	C1B-C2B	3.34	1.51	1.43
28	b	601	SQD	O48-C23	3.33	1.43	1.33
26	b	620	BCR	C30-C25	-3.32	1.49	1.53
24	b	610	CLA	C4B-NB	3.32	1.42	1.37
29	c	516	DGD	O2E-C2E	-3.31	1.34	1.43
26	B	617	BCR	C30-C25	-3.31	1.49	1.53
24	b	616	CLA	C1D-ND	3.31	1.42	1.37
24	b	617	CLA	C4B-NB	3.31	1.42	1.37
24	a	404	CLA	C1D-ND	3.30	1.42	1.37
24	b	615	CLA	MG-ND	3.30	2.12	2.05
26	B	619	BCR	C30-C25	-3.30	1.49	1.53
24	d	404	CLA	MG-ND	3.29	2.12	2.05
24	B	601	CLA	C1D-ND	3.29	1.42	1.37
26	t	101	BCR	C30-C25	-3.28	1.49	1.53
24	b	612	CLA	C1B-C2B	3.28	1.50	1.43
24	b	614	CLA	MG-ND	-3.28	1.99	2.05
29	c	518	DGD	O1G-C1G	-3.27	1.37	1.45
28	B	622	SQD	O48-C23	3.27	1.42	1.33
24	b	608	CLA	CMD-C2D	-3.26	1.44	1.50
24	d	403	CLA	CHC-C1C	3.26	1.45	1.38
24	C	507	CLA	C1B-NB	-3.25	1.33	1.37
24	A	405	CLA	MG-NC	-3.25	1.98	2.06
24	a	404	CLA	C1B-C2B	3.25	1.50	1.43
29	C	517	DGD	C4D-C3D	3.25	1.60	1.52
29	H	102	DGD	O1G-C1G	-3.23	1.37	1.45
24	B	614	CLA	C4B-NB	3.23	1.42	1.37
24	b	615	CLA	C1D-ND	3.23	1.42	1.37
24	b	605	CLA	C1D-ND	3.21	1.42	1.37
24	C	510	CLA	MG-NB	-3.21	1.99	2.05
29	c	518	DGD	C4D-C5D	3.21	1.59	1.53
24	A	405	CLA	C1B-C2B	3.21	1.50	1.43
24	c	509	CLA	MG-NA	-3.21	1.98	2.06
24	C	510	CLA	C1D-ND	3.20	1.42	1.37
24	C	503	CLA	MG-NC	3.20	2.13	2.06
24	c	509	CLA	C1D-ND	3.20	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	PHO	C4D-ND	-3.20	1.33	1.38
24	C	508	CLA	C1D-ND	3.19	1.42	1.37
24	c	513	CLA	C1B-C2B	3.18	1.50	1.43
24	b	611	CLA	C1D-ND	3.18	1.42	1.37
29	H	102	DGD	C4D-C5D	3.18	1.59	1.53
24	D	403	CLA	MG-NC	3.18	2.13	2.06
24	C	504	CLA	C1B-C2B	3.18	1.50	1.43
24	B	602	CLA	C1B-C2B	3.17	1.50	1.43
24	B	604	CLA	C1D-ND	3.17	1.42	1.37
32	c	522	LMG	C4-C5	3.17	1.59	1.53
27	A	410	PL9	C7-C8	-3.16	1.45	1.50
24	C	512	CLA	C1B-C2B	3.16	1.50	1.43
24	B	601	CLA	MG-NC	-3.16	1.98	2.06
24	B	611	CLA	MG-NB	3.15	2.12	2.05
24	a	407	CLA	C1B-C2B	3.15	1.50	1.43
24	B	611	CLA	C1B-C2B	3.15	1.50	1.43
29	c	516	DGD	O2G-C2G	-3.14	1.39	1.46
24	D	402	CLA	C1B-C2B	3.14	1.50	1.43
24	c	508	CLA	CHC-C1C	3.14	1.44	1.38
24	B	605	CLA	C1B-C2B	3.13	1.50	1.43
28	f	101	SQD	O47-C7	3.13	1.43	1.34
24	c	510	CLA	C4B-NB	3.13	1.42	1.37
24	b	612	CLA	CMD-C2D	-3.13	1.44	1.50
24	b	607	CLA	C4B-NB	3.11	1.42	1.37
24	A	408	CLA	C1D-ND	3.11	1.41	1.37
24	b	607	CLA	C1B-C2B	3.11	1.50	1.43
24	a	407	CLA	C1D-ND	3.11	1.41	1.37
24	c	512	CLA	C1D-ND	3.11	1.41	1.37
24	c	511	CLA	C1D-ND	3.10	1.41	1.37
24	c	505	CLA	CHC-C1C	3.10	1.44	1.38
24	b	609	CLA	CHC-C1C	3.10	1.44	1.38
25	a	406	PHO	C4D-ND	-3.10	1.33	1.38
24	A	408	CLA	C1B-C2B	3.09	1.50	1.43
28	A	411	SQD	O47-C7	3.09	1.43	1.34
27	A	410	PL9	C7-C3	-3.08	1.47	1.51
24	b	615	CLA	C4B-NB	3.08	1.41	1.37
32	D	407	LMG	C4-C3	3.07	1.60	1.52
24	h	101	CLA	MG-NB	-3.07	1.99	2.05
24	d	405	CLA	C4B-NB	3.06	1.41	1.37
32	D	410	LMG	C7-C8	3.06	1.58	1.51
24	C	508	CLA	C4B-NB	3.06	1.41	1.37
28	b	601	SQD	O47-C7	3.06	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	C1D-ND	3.05	1.41	1.37
24	c	512	CLA	C1B-C2B	3.05	1.50	1.43
24	c	504	CLA	C1B-C2B	3.05	1.50	1.43
29	c	517	DGD	O3G-C1D	-3.04	1.35	1.40
24	c	511	CLA	CHC-C1C	3.04	1.44	1.38
32	D	410	LMG	C9-C8	3.04	1.60	1.50
24	B	616	CLA	MG-NB	-3.03	1.99	2.05
34	F	102	HEM	FE-NB	3.02	2.04	1.94
24	B	615	CLA	MG-NA	3.02	2.13	2.06
24	c	511	CLA	MG-NC	3.02	2.13	2.06
24	B	605	CLA	MG-ND	-3.01	1.99	2.05
29	a	412	DGD	O1G-C1A	3.00	1.42	1.33
24	c	511	CLA	C1B-C2B	3.00	1.50	1.43
24	c	504	CLA	C4B-NB	2.99	1.41	1.37
24	D	402	CLA	C4B-NB	2.99	1.41	1.37
24	c	510	CLA	C1D-ND	2.99	1.41	1.37
25	A	407	PHO	C1D-C2D	2.99	1.42	1.39
25	A	407	PHO	C3B-C2B	-2.98	1.36	1.40
24	b	603	CLA	C1B-C2B	2.98	1.50	1.43
24	a	405	CLA	C1D-ND	2.98	1.41	1.37
27	d	407	PL9	C26-C24	-2.98	1.45	1.51
24	B	615	CLA	C1B-NB	-2.97	1.34	1.37
24	b	606	CLA	C1D-ND	2.97	1.41	1.37
24	c	507	CLA	C1B-C2B	2.97	1.50	1.43
26	t	101	BCR	C1-C6	-2.97	1.50	1.53
24	B	615	CLA	CMB-C2B	-2.97	1.44	1.50
24	B	609	CLA	C1B-C2B	2.96	1.50	1.43
24	b	617	CLA	MG-ND	-2.96	1.99	2.05
24	c	512	CLA	C4B-NB	2.96	1.41	1.37
24	c	513	CLA	MG-NC	-2.96	1.99	2.06
24	c	505	CLA	C3B-C4B	2.95	1.51	1.42
24	b	606	CLA	C4B-NB	2.95	1.41	1.37
24	B	608	CLA	MG-ND	-2.95	1.99	2.05
24	B	610	CLA	CMB-C2B	-2.95	1.44	1.50
33	D	408	LHG	O7-C5	-2.95	1.39	1.46
24	B	603	CLA	C1D-ND	2.94	1.41	1.37
24	C	509	CLA	C1B-C2B	2.94	1.50	1.43
24	B	615	CLA	C4B-NB	2.94	1.41	1.37
26	d	406	BCR	C30-C25	-2.94	1.50	1.53
24	b	615	CLA	MG-NC	2.93	2.13	2.06
25	a	406	PHO	CMB-C2B	-2.93	1.45	1.51
29	H	102	DGD	C3E-C2E	2.93	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	517	DGD	O3D-C3D	-2.93	1.35	1.43
24	D	402	CLA	MG-NB	-2.92	2.00	2.05
24	b	613	CLA	CMC-C2C	-2.92	1.44	1.50
24	a	405	CLA	C1B-NB	-2.92	1.34	1.37
24	c	503	CLA	C4B-NB	2.92	1.41	1.37
24	A	405	CLA	C1D-ND	2.92	1.41	1.37
26	D	405	BCR	C1-C6	-2.91	1.50	1.53
26	b	618	BCR	C30-C25	-2.91	1.50	1.53
24	d	404	CLA	MG-NA	2.91	2.13	2.06
25	A	407	PHO	C4D-ND	-2.91	1.34	1.38
32	b	623	LMG	O1-C7	-2.90	1.38	1.43
24	c	508	CLA	C3B-C4B	2.90	1.51	1.42
24	C	502	CLA	CMD-C2D	-2.89	1.44	1.50
24	B	609	CLA	CMD-C2D	-2.89	1.44	1.50
24	C	505	CLA	C3B-C4B	2.89	1.51	1.42
27	D	406	PL9	C41-C39	-2.88	1.45	1.51
24	b	606	CLA	MG-NA	2.88	2.13	2.06
28	f	101	SQD	O48-C23	2.87	1.41	1.33
32	c	519	LMG	C1-C2	2.86	1.60	1.52
24	B	607	CLA	CAC-C3C	-2.85	1.43	1.51
25	D	401	PHO	CMD-C2D	-2.85	1.45	1.51
24	D	404	CLA	C1B-C2B	2.84	1.49	1.43
24	b	603	CLA	CMC-C2C	-2.84	1.44	1.50
26	c	515	BCR	C33-C5	-2.84	1.46	1.50
24	D	404	CLA	CMD-C2D	-2.84	1.45	1.50
24	B	609	CLA	C4B-NB	2.83	1.41	1.37
24	C	510	CLA	C1B-C2B	2.82	1.49	1.43
24	b	605	CLA	C4B-NB	2.82	1.41	1.37
24	a	407	CLA	CMD-C2D	-2.81	1.45	1.50
24	b	612	CLA	CHC-C4B	-2.81	1.33	1.39
29	C	518	DGD	O1G-C1G	-2.81	1.38	1.45
33	l	101	LHG	O8-C23	2.81	1.41	1.33
24	b	616	CLA	CMB-C2B	-2.81	1.45	1.50
24	B	602	CLA	MG-ND	-2.80	2.00	2.05
24	d	403	CLA	CMD-C2D	-2.80	1.45	1.50
24	c	508	CLA	MG-NA	2.80	2.12	2.06
32	D	407	LMG	O2-C2	-2.79	1.36	1.43
24	A	405	CLA	MG-ND	-2.79	2.00	2.05
32	d	411	LMG	O6-C5	-2.79	1.37	1.44
24	c	511	CLA	C3B-C4B	2.78	1.50	1.42
26	C	519	BCR	C30-C25	-2.78	1.50	1.53
27	A	410	PL9	C6-C1	-2.78	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	409	BCR	C33-C5	-2.77	1.46	1.50
24	a	407	CLA	CMB-C2B	-2.77	1.45	1.50
33	E	101	LHG	O8-C23	2.77	1.41	1.33
24	B	614	CLA	MG-NA	2.77	2.12	2.06
29	c	518	DGD	C2A-C1A	-2.77	1.42	1.50
34	e	102	HEM	CAC-C3C	2.76	1.54	1.47
24	B	610	CLA	CHC-C1C	2.76	1.44	1.38
24	c	508	CLA	C1B-C2B	2.76	1.49	1.43
29	H	102	DGD	O2G-C2G	-2.76	1.40	1.46
24	d	404	CLA	C1B-C2B	2.75	1.49	1.43
24	C	514	CLA	MG-NB	-2.75	2.00	2.05
24	c	508	CLA	C4B-NB	2.75	1.41	1.37
24	C	511	CLA	MG-ND	-2.75	2.00	2.05
25	A	407	PHO	C3D-C4D	2.74	1.45	1.41
24	b	604	CLA	C1D-ND	2.74	1.41	1.37
24	b	615	CLA	CMC-C2C	-2.74	1.45	1.50
24	b	617	CLA	C1D-ND	2.74	1.41	1.37
24	c	510	CLA	CMB-C2B	-2.74	1.45	1.50
24	C	504	CLA	C1D-ND	2.73	1.41	1.37
24	b	616	CLA	C3B-C4B	2.73	1.50	1.42
24	A	408	CLA	C4B-NB	2.73	1.41	1.37
24	c	501	CLA	C4B-NB	2.72	1.41	1.37
24	C	507	CLA	MG-NA	2.72	2.12	2.06
24	a	404	CLA	C3B-C4B	2.72	1.50	1.42
24	b	610	CLA	C1D-ND	2.71	1.41	1.37
24	B	608	CLA	C1B-NB	-2.71	1.34	1.37
24	B	608	CLA	CHC-C1C	2.71	1.43	1.38
24	b	605	CLA	MG-ND	-2.71	2.00	2.05
24	B	613	CLA	C1B-C2B	2.71	1.49	1.43
35	V	201	HEC	CMB-C2B	2.70	1.56	1.50
24	B	611	CLA	C1B-NB	-2.70	1.34	1.37
26	b	602	BCR	C27-C26	-2.70	1.46	1.51
24	a	404	CLA	MG-ND	2.70	2.11	2.05
26	C	519	BCR	C1-C6	-2.70	1.50	1.53
29	C	516	DGD	O3G-C3G	-2.69	1.39	1.43
24	b	611	CLA	C1C-NC	-2.69	1.33	1.37
25	A	407	PHO	CMD-C2D	-2.69	1.46	1.51
27	d	407	PL9	C46-C44	-2.69	1.45	1.51
24	c	505	CLA	C1B-C2B	2.69	1.49	1.43
24	b	616	CLA	CMD-C2D	-2.69	1.45	1.50
24	d	403	CLA	C1B-C2B	2.69	1.49	1.43
24	D	404	CLA	C3B-C4B	2.69	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	CMC-C2C	-2.68	1.45	1.50
24	A	406	CLA	CMB-C2B	-2.68	1.45	1.50
24	c	513	CLA	C4B-NB	2.68	1.41	1.37
24	B	616	CLA	CMB-C2B	-2.68	1.45	1.50
32	c	524	LMG	C4-C5	2.68	1.58	1.53
24	c	507	CLA	MG-NC	-2.68	1.99	2.06
27	D	406	PL9	C52-C5	-2.68	1.45	1.50
35	V	201	HEC	C3D-C2D	-2.68	1.31	1.38
24	B	610	CLA	CMC-C2C	-2.68	1.45	1.50
32	K	102	LMG	C4-C3	2.68	1.59	1.52
27	a	409	PL9	C53-C6	-2.67	1.45	1.50
28	A	411	SQD	O48-C23	2.67	1.41	1.33
24	b	603	CLA	CMD-C2D	-2.67	1.45	1.50
24	D	404	CLA	C4B-NB	2.67	1.41	1.37
24	C	509	CLA	C3B-C4B	2.66	1.50	1.42
24	b	617	CLA	C1B-C2B	2.66	1.49	1.43
24	b	617	CLA	CAA-C2A	-2.66	1.49	1.54
27	a	409	PL9	C25-C24	-2.66	1.44	1.50
24	C	505	CLA	C1B-NB	-2.66	1.34	1.37
24	C	506	CLA	CHC-C1C	2.65	1.43	1.38
25	D	401	PHO	CAC-C3C	-2.65	1.47	1.51
24	h	101	CLA	O2A-CGA	2.65	1.41	1.33
24	d	405	CLA	O1D-CGD	2.65	1.27	1.21
29	C	518	DGD	O2G-C2G	-2.65	1.40	1.46
24	d	404	CLA	C3B-C4B	2.64	1.50	1.42
24	C	509	CLA	CMD-C2D	-2.64	1.45	1.50
24	B	610	CLA	MG-NC	-2.64	2.00	2.06
29	A	413	DGD	C1E-C2E	2.64	1.60	1.52
24	b	617	CLA	CMD-C2D	-2.64	1.45	1.50
24	D	403	CLA	CMD-C2D	-2.63	1.45	1.50
29	A	413	DGD	C4D-C3D	2.63	1.59	1.52
24	d	404	CLA	CMB-C2B	-2.63	1.45	1.50
24	B	615	CLA	C5-C3	-2.63	1.45	1.51
24	B	610	CLA	C1B-C2B	2.63	1.49	1.43
24	b	607	CLA	MG-ND	-2.63	2.00	2.05
34	F	102	HEM	CAC-C3C	2.63	1.54	1.47
24	B	607	CLA	MG-NA	2.62	2.12	2.06
24	B	606	CLA	C1D-ND	2.62	1.41	1.37
28	a	410	SQD	O47-C7	2.62	1.41	1.34
24	c	509	CLA	MG-NC	2.62	2.12	2.06
24	c	502	CLA	C1D-ND	2.62	1.41	1.37
24	b	616	CLA	C4B-NB	2.62	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	C1B-C2B	2.61	1.49	1.43
33	d	410	LHG	O8-C6	-2.61	1.39	1.45
24	B	616	CLA	C4B-NB	2.61	1.41	1.37
24	c	501	CLA	C1B-NB	-2.61	1.34	1.37
24	b	617	CLA	MG-NA	2.61	2.12	2.06
24	A	408	CLA	CMD-C2D	-2.61	1.45	1.50
24	c	506	CLA	CAC-C3C	-2.60	1.44	1.51
24	d	404	CLA	MG-NB	-2.60	2.00	2.05
24	C	511	CLA	C3B-C4B	2.60	1.50	1.42
24	B	611	CLA	C4B-NB	2.59	1.41	1.37
29	A	413	DGD	C3E-C2E	2.59	1.59	1.52
24	b	611	CLA	C3D-C4D	2.59	1.50	1.44
24	h	101	CLA	C1B-C2B	2.59	1.49	1.43
24	B	601	CLA	C1B-C2B	2.59	1.49	1.43
29	C	517	DGD	O3D-C3D	-2.58	1.36	1.43
24	A	406	CLA	CHC-C4B	-2.58	1.33	1.39
34	e	102	HEM	CAB-C3B	2.58	1.54	1.47
29	h	104	DGD	C4D-C5D	2.58	1.58	1.53
24	a	404	CLA	CMC-C2C	-2.58	1.45	1.50
34	F	102	HEM	C2A-C3A	-2.58	1.32	1.38
24	c	513	CLA	C3B-C4B	2.57	1.50	1.42
24	a	407	CLA	CMC-C2C	-2.57	1.45	1.50
24	a	407	CLA	C1B-NB	-2.57	1.34	1.37
24	c	505	CLA	CMB-C2B	-2.57	1.45	1.50
24	b	605	CLA	C1B-C2B	2.57	1.49	1.43
24	C	513	CLA	MG-NC	-2.57	2.00	2.06
24	b	603	CLA	CAC-C3C	-2.57	1.44	1.51
24	C	513	CLA	C1B-C2B	2.57	1.49	1.43
25	a	406	PHO	O2D-CGD	2.57	1.39	1.33
24	B	606	CLA	C1B-C2B	2.57	1.49	1.43
24	b	610	CLA	CMD-C2D	-2.57	1.45	1.50
24	c	506	CLA	MG-NC	2.57	2.12	2.06
26	c	514	BCR	C30-C25	-2.57	1.50	1.53
24	b	614	CLA	C1D-ND	2.56	1.41	1.37
26	B	617	BCR	C33-C5	-2.56	1.46	1.50
24	h	101	CLA	CMC-C2C	-2.56	1.45	1.50
24	b	609	CLA	C3B-C4B	2.56	1.50	1.42
24	b	617	CLA	CMB-C2B	-2.55	1.45	1.50
24	c	509	CLA	MG-NB	-2.55	2.00	2.05
24	B	613	CLA	MG-ND	-2.55	2.00	2.05
24	C	513	CLA	CMD-C2D	-2.55	1.45	1.50
24	c	513	CLA	C1D-ND	2.55	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	CBD-CGD	-2.55	1.49	1.52
24	b	603	CLA	C4B-NB	2.54	1.41	1.37
24	B	614	CLA	CMB-C2B	-2.54	1.45	1.50
26	H	101	BCR	C1-C6	-2.54	1.50	1.53
29	c	517	DGD	C4E-C3E	2.54	1.58	1.52
24	d	403	CLA	C3B-C4B	2.54	1.50	1.42
34	F	102	HEM	CAB-C3B	2.54	1.54	1.47
35	v	201	HEC	CMD-C2D	2.53	1.56	1.50
25	a	406	PHO	CMD-C2D	-2.53	1.46	1.51
24	c	509	CLA	CHC-C1C	2.53	1.43	1.38
25	d	402	PHO	CMA-C3A	-2.53	1.49	1.53
24	c	507	CLA	CMC-C2C	-2.53	1.45	1.50
24	C	512	CLA	CMB-C2B	-2.52	1.45	1.50
24	C	505	CLA	CMB-C2B	-2.52	1.45	1.50
24	b	614	CLA	CMC-C2C	-2.52	1.45	1.50
24	b	606	CLA	C3B-C4B	2.52	1.50	1.42
24	c	508	CLA	MG-ND	2.52	2.10	2.05
29	C	516	DGD	C3E-C2E	2.51	1.58	1.52
24	A	406	CLA	MG-ND	-2.51	2.00	2.05
25	d	402	PHO	CMD-C2D	-2.51	1.46	1.51
24	C	503	CLA	C3B-C4B	2.51	1.50	1.42
27	D	406	PL9	C7-C8	-2.50	1.46	1.50
24	B	602	CLA	CMB-C2B	-2.50	1.45	1.50
24	D	402	CLA	CMC-C2C	-2.50	1.45	1.50
29	c	517	DGD	C4E-C5E	2.50	1.58	1.53
24	C	502	CLA	C3D-C4D	2.50	1.49	1.44
24	B	611	CLA	CHC-C1C	2.49	1.43	1.38
29	C	517	DGD	C1G-C2G	2.49	1.58	1.50
24	b	604	CLA	CHC-C1C	2.49	1.43	1.38
35	v	201	HEC	C3B-C2B	-2.49	1.32	1.41
24	B	609	CLA	C3B-C4B	2.49	1.50	1.42
24	C	507	CLA	CHC-C1C	2.48	1.43	1.38
24	B	606	CLA	C4B-NB	2.48	1.41	1.37
29	c	517	DGD	C4D-C3D	2.48	1.58	1.52
24	D	403	CLA	C1C-NC	-2.48	1.34	1.37
24	D	403	CLA	MG-NA	-2.48	2.00	2.06
24	C	504	CLA	MG-NB	2.48	2.10	2.05
24	c	508	CLA	C1D-ND	2.47	1.41	1.37
24	B	603	CLA	C1A-CHA	-2.47	1.32	1.43
29	h	104	DGD	C1E-C2E	2.47	1.59	1.52
24	b	610	CLA	C1B-C2B	2.47	1.48	1.43
24	a	404	CLA	C4B-NB	2.47	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C1B-C2B	2.46	1.48	1.43
24	B	608	CLA	C1B-C2B	2.46	1.48	1.43
24	D	403	CLA	CMB-C2B	-2.46	1.45	1.50
24	D	402	CLA	CHC-C4B	-2.46	1.33	1.39
24	b	604	CLA	MG-ND	-2.46	2.00	2.05
24	b	605	CLA	C3B-C4B	2.46	1.49	1.42
24	C	503	CLA	C1D-ND	2.46	1.41	1.37
24	C	507	CLA	CMC-C2C	-2.45	1.45	1.50
32	c	522	LMG	C7-C8	2.45	1.58	1.50
26	a	408	BCR	C38-C26	-2.45	1.47	1.50
27	a	409	PL9	C46-C44	-2.45	1.46	1.51
24	c	507	CLA	MG-NB	-2.45	2.00	2.05
24	C	512	CLA	CMC-C2C	-2.45	1.45	1.50
24	B	613	CLA	C1D-ND	2.45	1.41	1.37
24	D	402	CLA	C1B-NB	-2.44	1.34	1.37
24	B	613	CLA	CMB-C2B	-2.44	1.45	1.50
24	c	508	CLA	CMC-C2C	-2.44	1.45	1.50
24	B	614	CLA	CHC-C4B	-2.44	1.33	1.39
24	c	504	CLA	C3B-C4B	2.44	1.49	1.42
33	E	101	LHG	P-O6	2.44	1.68	1.59
24	B	609	CLA	CMC-C2C	-2.44	1.45	1.50
24	B	615	CLA	C1B-C2B	2.44	1.48	1.43
24	B	604	CLA	MG-NB	2.44	2.10	2.05
26	b	618	BCR	C33-C5	-2.44	1.47	1.50
24	c	505	CLA	MG-NA	-2.44	2.00	2.06
24	c	506	CLA	C1B-NB	-2.43	1.34	1.37
24	d	403	CLA	O1D-CGD	2.43	1.27	1.21
24	D	402	CLA	CMB-C2B	-2.43	1.45	1.50
24	B	610	CLA	MG-NB	-2.43	2.01	2.05
32	M	101	LMG	O3-C3	-2.43	1.36	1.43
24	b	603	CLA	C3B-C4B	2.43	1.49	1.42
24	c	502	CLA	CMD-C2D	-2.43	1.45	1.50
35	V	201	HEC	C3B-C2B	-2.43	1.33	1.41
24	C	502	CLA	C1B-C2B	2.43	1.48	1.43
24	A	406	CLA	MG-NC	2.43	2.12	2.06
24	c	506	CLA	C1B-C2B	2.42	1.48	1.43
32	c	522	LMG	C4-C3	2.42	1.58	1.52
24	b	615	CLA	CHC-C1C	2.42	1.43	1.38
24	C	506	CLA	CMC-C2C	-2.42	1.45	1.50
24	b	614	CLA	C5-C3	-2.42	1.46	1.51
24	C	502	CLA	CMB-C2B	-2.42	1.45	1.50
28	f	101	SQD	O3-C3	-2.41	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	623	LMG	O6-C1	2.41	1.48	1.41
24	a	407	CLA	C3B-C4B	2.41	1.49	1.42
24	b	608	CLA	C3B-C4B	2.41	1.49	1.42
24	c	513	CLA	CHC-C1C	2.41	1.43	1.38
24	C	511	CLA	CMD-C2D	-2.41	1.45	1.50
24	h	101	CLA	CHC-C1C	2.41	1.43	1.38
24	B	602	CLA	C3B-C4B	2.41	1.49	1.42
24	b	605	CLA	CMC-C2C	-2.41	1.45	1.50
25	A	407	PHO	C4D-CHA	2.40	1.43	1.39
24	b	606	CLA	CMD-C2D	-2.40	1.45	1.50
32	D	410	LMG	O8-C28	2.40	1.40	1.33
25	D	401	PHO	CMB-C2B	-2.40	1.46	1.51
33	D	408	LHG	C24-C23	2.40	1.57	1.50
33	D	411	LHG	O8-C6	2.40	1.50	1.45
29	H	102	DGD	C4E-C5E	2.40	1.58	1.53
24	D	404	CLA	C3B-C2B	-2.40	1.33	1.41
24	B	605	CLA	C3D-C4D	2.40	1.49	1.44
24	b	613	CLA	C3B-C4B	2.40	1.49	1.42
29	c	518	DGD	O2G-C1B	2.40	1.41	1.34
24	c	508	CLA	CMD-C2D	-2.39	1.45	1.50
24	D	404	CLA	CMB-C2B	-2.39	1.45	1.50
28	a	410	SQD	O3-C3	-2.39	1.37	1.43
24	C	504	CLA	CHC-C1C	2.39	1.43	1.38
27	D	406	PL9	C5-C4	-2.38	1.39	1.47
24	b	609	CLA	C1D-ND	2.38	1.41	1.37
26	a	408	BCR	C27-C26	-2.38	1.46	1.51
32	K	102	LMG	C1-C2	2.38	1.59	1.52
24	A	406	CLA	C3B-C4B	2.38	1.49	1.42
33	D	409	LHG	O3-C3	-2.38	1.35	1.44
27	D	406	PL9	C15-C14	-2.37	1.44	1.50
24	b	612	CLA	C1B-NB	-2.37	1.34	1.37
24	c	507	CLA	C1D-ND	2.37	1.41	1.37
24	a	405	CLA	C3B-C4B	2.37	1.49	1.42
24	C	514	CLA	CHC-C4B	-2.36	1.34	1.39
24	d	405	CLA	CMD-C2D	-2.36	1.45	1.50
24	a	405	CLA	C1B-C2B	2.36	1.48	1.43
24	A	408	CLA	CMC-C2C	-2.36	1.45	1.50
24	C	511	CLA	C4B-NB	2.36	1.41	1.37
24	b	611	CLA	CMA-C3A	-2.36	1.48	1.53
29	c	516	DGD	O5D-C1E	-2.36	1.36	1.40
33	D	411	LHG	C24-C23	2.36	1.57	1.50
24	B	606	CLA	CMB-C2B	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C1B-NB	-2.35	1.34	1.37
24	B	614	CLA	CMC-C2C	-2.35	1.45	1.50
24	a	404	CLA	O2D-CED	-2.35	1.40	1.45
24	B	606	CLA	CMC-C2C	-2.35	1.46	1.50
25	A	407	PHO	C1C-NC	-2.35	1.30	1.37
25	D	401	PHO	CMC-C2C	-2.35	1.47	1.50
32	d	411	LMG	O1-C7	-2.35	1.39	1.43
24	b	616	CLA	CMC-C2C	-2.35	1.46	1.50
29	h	104	DGD	C3G-C2G	2.35	1.58	1.50
28	A	411	SQD	O2-C2	-2.34	1.37	1.43
24	B	610	CLA	C3D-C4D	2.34	1.49	1.44
24	C	504	CLA	C4B-NB	2.34	1.40	1.37
24	B	615	CLA	MG-NC	2.34	2.11	2.06
29	A	413	DGD	O2G-C1B	2.34	1.40	1.34
24	B	603	CLA	C3B-C4B	2.34	1.49	1.42
24	B	606	CLA	CHC-C1C	2.34	1.43	1.38
26	A	409	BCR	C30-C25	-2.34	1.50	1.53
26	t	101	BCR	C27-C26	-2.34	1.46	1.51
26	c	521	BCR	C30-C25	-2.33	1.50	1.53
24	C	507	CLA	C1B-C2B	2.33	1.48	1.43
24	c	508	CLA	CMB-C2B	-2.33	1.46	1.50
29	H	102	DGD	O6E-C1E	2.33	1.47	1.41
24	c	504	CLA	CMD-C2D	-2.33	1.46	1.50
24	b	610	CLA	MG-NB	-2.33	2.01	2.05
24	C	506	CLA	C4B-NB	2.33	1.40	1.37
29	c	517	DGD	O5D-C1E	2.33	1.44	1.40
24	B	604	CLA	C4B-NB	2.32	1.40	1.37
29	C	518	DGD	C4D-C5D	2.32	1.58	1.53
24	b	604	CLA	C4B-NB	2.32	1.40	1.37
24	C	502	CLA	MG-NC	-2.32	2.00	2.06
24	b	606	CLA	CHC-C4B	-2.32	1.34	1.39
24	b	616	CLA	CHC-C1C	2.32	1.43	1.38
24	a	407	CLA	C1C-NC	-2.32	1.34	1.37
24	C	504	CLA	MG-NC	2.32	2.11	2.06
25	d	402	PHO	CAC-C3C	-2.31	1.47	1.51
24	b	616	CLA	C1B-C2B	2.31	1.48	1.43
24	h	101	CLA	C3B-C4B	2.31	1.49	1.42
24	c	501	CLA	CMB-C2B	-2.30	1.46	1.50
24	C	514	CLA	C1B-C2B	2.30	1.48	1.43
28	f	101	SQD	O2-C2	-2.30	1.37	1.43
24	C	514	CLA	CMB-C2B	-2.30	1.46	1.50
24	c	501	CLA	MG-NC	-2.30	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	C3B-C4B	2.30	1.49	1.42
24	C	510	CLA	CMC-C2C	-2.30	1.46	1.50
24	b	605	CLA	CMD-C2D	-2.30	1.46	1.50
29	C	517	DGD	O5D-C6D	-2.30	1.39	1.43
27	D	406	PL9	C10-C9	-2.30	1.45	1.50
24	C	513	CLA	CAA-C2A	-2.29	1.49	1.54
24	c	512	CLA	CMD-C2D	-2.29	1.46	1.50
27	d	407	PL9	C6-C1	-2.29	1.44	1.48
24	C	507	CLA	C4B-NB	2.29	1.40	1.37
24	b	606	CLA	C1B-C2B	2.29	1.48	1.43
24	b	603	CLA	CMB-C2B	-2.28	1.46	1.50
25	D	401	PHO	C3B-C2B	-2.28	1.37	1.40
24	b	607	CLA	C3B-C4B	2.28	1.49	1.42
32	h	102	LMG	O7-C10	2.28	1.38	1.30
25	D	401	PHO	C1D-C2D	2.28	1.42	1.39
24	C	510	CLA	O2D-CGD	2.28	1.38	1.33
24	B	611	CLA	CMB-C2B	-2.28	1.46	1.50
34	F	102	HEM	FE-NC	2.27	2.02	1.95
24	B	614	CLA	C1B-NB	-2.27	1.34	1.37
24	b	609	CLA	MG-ND	-2.27	2.01	2.05
24	b	607	CLA	CAC-C3C	-2.27	1.45	1.51
32	b	623	LMG	C7-C8	2.26	1.57	1.50
24	B	616	CLA	C1B-C2B	2.26	1.48	1.43
24	C	512	CLA	CHC-C4B	-2.26	1.34	1.39
24	D	402	CLA	CHC-C1C	2.25	1.43	1.38
24	a	405	CLA	CHC-C1C	2.25	1.43	1.38
32	c	522	LMG	C1-C2	2.25	1.59	1.52
24	c	510	CLA	C1B-C2B	2.25	1.48	1.43
24	C	511	CLA	CMB-C2B	-2.25	1.46	1.50
29	c	517	DGD	C3E-C2E	2.25	1.58	1.52
24	C	502	CLA	C3B-C4B	2.25	1.49	1.42
24	d	405	CLA	CMB-C2B	-2.25	1.46	1.50
24	b	613	CLA	MG-NB	2.25	2.10	2.05
24	c	510	CLA	CHC-C1C	2.25	1.43	1.38
32	b	623	LMG	C3-C2	2.24	1.58	1.52
29	C	517	DGD	C4E-C3E	2.24	1.58	1.52
24	a	407	CLA	C4B-NB	2.24	1.40	1.37
32	M	101	LMG	O1-C7	-2.24	1.39	1.43
29	H	102	DGD	C6E-C5E	2.24	1.59	1.51
24	D	403	CLA	CHC-C4B	-2.24	1.34	1.39
24	d	403	CLA	C1B-NB	-2.24	1.34	1.37
24	b	608	CLA	C1B-C2B	2.24	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	101	LMG	O8-C28	2.24	1.39	1.33
24	B	614	CLA	C1A-CHA	-2.23	1.33	1.43
24	c	509	CLA	C3B-C4B	2.23	1.49	1.42
32	C	501	LMG	C4-C3	2.23	1.58	1.52
24	b	608	CLA	CMC-C2C	-2.23	1.46	1.50
24	h	101	CLA	CMD-C2D	-2.23	1.46	1.50
24	a	404	CLA	CMB-C2B	-2.23	1.46	1.50
24	d	405	CLA	C1B-C2B	2.23	1.48	1.43
24	B	608	CLA	CMC-C2C	-2.23	1.46	1.50
26	c	515	BCR	C36-C18	-2.23	1.46	1.50
24	d	403	CLA	C1D-C2D	2.23	1.49	1.45
24	C	510	CLA	C4B-NB	2.23	1.40	1.37
24	B	605	CLA	O2D-CED	-2.22	1.40	1.45
24	B	601	CLA	CMD-C2D	-2.22	1.46	1.50
24	b	611	CLA	CMB-C2B	-2.22	1.46	1.50
24	d	404	CLA	CHC-C1C	2.22	1.42	1.38
35	v	201	HEC	CMB-C2B	2.21	1.55	1.50
24	B	609	CLA	CHC-C4B	-2.21	1.34	1.39
24	C	509	CLA	C1D-C2D	2.21	1.49	1.45
24	b	604	CLA	C1A-CHA	-2.20	1.34	1.43
24	b	608	CLA	C4B-NB	2.20	1.40	1.37
25	A	407	PHO	CAC-C3C	-2.20	1.47	1.51
24	c	510	CLA	C1B-NB	-2.20	1.35	1.37
34	e	102	HEM	C2A-C3A	-2.19	1.33	1.38
24	c	504	CLA	O2D-CGD	2.19	1.38	1.33
24	A	405	CLA	O2D-CED	-2.19	1.40	1.45
24	a	404	CLA	C1D-C2D	2.19	1.49	1.45
24	c	513	CLA	CMB-C2B	-2.19	1.46	1.50
24	b	613	CLA	C1D-ND	2.19	1.40	1.37
24	C	513	CLA	MG-ND	-2.18	2.01	2.05
24	d	404	CLA	C1D-ND	2.18	1.40	1.37
24	C	505	CLA	C4B-NB	2.18	1.40	1.37
24	B	602	CLA	CHC-C1C	2.18	1.42	1.38
24	c	506	CLA	CMD-C2D	-2.18	1.46	1.50
33	L	101	LHG	O7-C5	-2.18	1.41	1.46
24	B	616	CLA	O2D-CED	-2.18	1.40	1.45
24	B	616	CLA	CMD-C2D	-2.18	1.46	1.50
26	k	101	BCR	C38-C26	-2.18	1.47	1.50
24	c	506	CLA	C4B-NB	2.18	1.40	1.37
24	A	405	CLA	CMC-C2C	-2.17	1.46	1.50
24	b	611	CLA	C1A-CHA	-2.17	1.34	1.43
24	c	512	CLA	C3B-C4B	2.17	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C4B-NB	2.17	1.40	1.37
29	C	516	DGD	C2B-C1B	-2.17	1.44	1.50
25	d	402	PHO	CHA-CBD	-2.17	1.49	1.51
32	M	101	LMG	O7-C10	2.17	1.40	1.34
24	b	609	CLA	MG-NA	2.17	2.11	2.06
24	c	513	CLA	CMD-C2D	-2.17	1.46	1.50
24	B	613	CLA	CMC-C2C	-2.17	1.46	1.50
33	D	411	LHG	O6-C4	-2.17	1.36	1.44
24	c	501	CLA	CAC-C3C	-2.17	1.45	1.51
24	A	408	CLA	C3D-C4D	2.16	1.49	1.44
24	b	614	CLA	CMB-C2B	-2.16	1.46	1.50
24	D	403	CLA	CMC-C2C	-2.16	1.46	1.50
24	B	613	CLA	C1B-NB	-2.16	1.35	1.37
24	A	405	CLA	C3B-C4B	2.16	1.49	1.42
24	B	604	CLA	O2D-CGD	2.16	1.38	1.33
24	B	607	CLA	CHC-C4B	-2.15	1.34	1.39
24	a	404	CLA	O2D-CGD	2.15	1.38	1.33
24	D	403	CLA	C1A-CHA	-2.15	1.34	1.43
26	C	515	BCR	C33-C5	-2.15	1.47	1.50
24	B	616	CLA	C1B-NB	-2.15	1.35	1.37
24	b	614	CLA	CMD-C2D	-2.15	1.46	1.50
29	A	413	DGD	C6E-C5E	2.15	1.59	1.51
24	B	605	CLA	CMC-C2C	-2.15	1.46	1.50
24	C	502	CLA	C1D-C2D	2.15	1.49	1.45
32	c	522	LMG	C3-C2	2.15	1.57	1.52
26	c	521	BCR	C38-C26	-2.15	1.47	1.50
24	C	507	CLA	C3B-C4B	2.14	1.49	1.42
24	B	612	CLA	C1B-NB	-2.14	1.35	1.37
28	A	412	SQD	O47-C45	-2.14	1.43	1.47
24	B	603	CLA	C4B-NB	2.14	1.40	1.37
24	A	408	CLA	C1C-NC	-2.14	1.34	1.37
24	C	514	CLA	C4B-NB	2.14	1.40	1.37
24	B	602	CLA	C1A-CHA	-2.14	1.34	1.43
29	C	516	DGD	C2A-C1A	-2.14	1.44	1.50
24	A	406	CLA	CMD-C2D	-2.14	1.46	1.50
24	C	509	CLA	C1B-NB	-2.14	1.35	1.37
24	B	613	CLA	CMD-C2D	-2.14	1.46	1.50
24	C	504	CLA	C3B-C4B	2.14	1.49	1.42
32	c	519	LMG	C3-C2	2.13	1.57	1.52
24	C	506	CLA	CHC-C4B	-2.13	1.34	1.39
24	B	613	CLA	CHC-C1C	2.13	1.42	1.38
24	b	614	CLA	C1B-C2B	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	408	CLA	CMB-C2B	-2.13	1.46	1.50
24	C	509	CLA	C1D-ND	2.13	1.40	1.37
24	b	609	CLA	C3D-C4D	2.13	1.49	1.44
24	b	604	CLA	CMD-C2D	-2.13	1.46	1.50
24	C	512	CLA	C3B-C4B	2.13	1.48	1.42
24	c	504	CLA	CMC-C2C	-2.13	1.46	1.50
24	B	611	CLA	MG-NC	-2.13	2.01	2.06
24	c	505	CLA	MG-ND	2.12	2.10	2.05
24	b	611	CLA	C1B-NB	-2.12	1.35	1.37
32	b	623	LMG	O8-C28	2.12	1.39	1.33
24	C	504	CLA	CMB-C2B	-2.12	1.46	1.50
24	C	503	CLA	C3D-C4D	2.12	1.49	1.44
24	A	406	CLA	C1B-C2B	2.12	1.48	1.43
24	c	503	CLA	C1B-C2B	2.12	1.48	1.43
32	B	621	LMG	O8-C28	2.12	1.37	1.30
24	c	501	CLA	CHC-C4B	-2.12	1.34	1.39
33	D	408	LHG	O6-C4	-2.11	1.36	1.44
24	a	404	CLA	C1B-NB	-2.11	1.35	1.37
24	D	404	CLA	CHC-C1C	2.11	1.42	1.38
24	B	601	CLA	CMB-C2B	-2.11	1.46	1.50
24	A	405	CLA	C5-C3	-2.11	1.46	1.51
32	D	407	LMG	C7-C8	2.11	1.57	1.50
24	C	504	CLA	C1B-NB	-2.11	1.35	1.37
24	D	402	CLA	CAC-C3C	-2.11	1.45	1.51
33	D	411	LHG	O7-C7	2.11	1.40	1.34
24	A	408	CLA	C3B-C4B	2.11	1.48	1.42
24	A	408	CLA	CHC-C4B	-2.11	1.34	1.39
24	C	506	CLA	C1B-C2B	2.11	1.48	1.43
34	e	102	HEM	CMA-C3A	2.11	1.55	1.50
28	A	411	SQD	O4-C4	-2.11	1.37	1.43
26	c	521	BCR	C1-C6	-2.10	1.51	1.53
24	A	406	CLA	CMC-C2C	-2.10	1.46	1.50
24	B	606	CLA	C3B-C4B	2.10	1.48	1.42
24	c	504	CLA	C1B-NB	-2.10	1.35	1.37
24	b	611	CLA	C3B-C4B	2.10	1.48	1.42
32	c	519	LMG	C7-C8	2.10	1.57	1.50
34	F	102	HEM	CMD-C2D	2.10	1.55	1.50
24	c	507	CLA	CMB-C2B	-2.10	1.46	1.50
33	D	408	LHG	P-O3	2.10	1.67	1.59
33	d	410	LHG	P-O6	2.10	1.67	1.59
29	C	516	DGD	O1G-C1A	2.10	1.39	1.33
24	b	617	CLA	MG-NC	-2.10	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	CMB-C2B	-2.09	1.46	1.50
24	b	614	CLA	CHC-C4B	-2.09	1.34	1.39
29	h	104	DGD	O2D-C2D	-2.09	1.37	1.43
24	B	608	CLA	C1D-ND	2.09	1.40	1.37
24	c	501	CLA	C1B-C2B	2.09	1.48	1.43
33	D	411	LHG	P-O4	-2.09	1.45	1.55
29	h	104	DGD	C4E-C5E	2.08	1.57	1.53
28	a	410	SQD	O4-C4	-2.08	1.37	1.43
24	C	511	CLA	CHC-C1C	2.08	1.42	1.38
24	a	405	CLA	CMD-C2D	-2.08	1.46	1.50
24	B	612	CLA	C1A-CHA	-2.08	1.34	1.43
24	b	609	CLA	CMB-C2B	-2.08	1.46	1.50
34	e	102	HEM	FE-NB	2.08	2.01	1.94
24	B	612	CLA	CMD-C2D	-2.08	1.46	1.50
24	c	501	CLA	CMC-C2C	-2.08	1.46	1.50
24	c	508	CLA	C1B-NB	-2.08	1.35	1.37
24	C	512	CLA	C4D-CHA	2.08	1.45	1.38
24	b	612	CLA	C1D-C2D	2.08	1.49	1.45
24	C	513	CLA	C3D-C4D	2.07	1.48	1.44
24	C	504	CLA	CMC-C2C	-2.07	1.46	1.50
24	C	505	CLA	CMC-C2C	-2.07	1.46	1.50
29	C	518	DGD	C6D-C5D	2.07	1.57	1.51
24	B	603	CLA	CMC-C2C	-2.07	1.46	1.50
24	c	504	CLA	C1D-ND	2.06	1.40	1.37
24	b	603	CLA	CHC-C1C	2.06	1.42	1.38
24	c	502	CLA	CHC-C1C	2.06	1.42	1.38
28	f	101	SQD	O4-C4	-2.06	1.37	1.43
24	b	615	CLA	C5-C3	-2.06	1.47	1.51
24	c	502	CLA	C1B-C2B	2.06	1.48	1.43
24	B	615	CLA	CAC-C3C	-2.06	1.45	1.51
24	C	513	CLA	CHC-C1C	2.06	1.42	1.38
24	B	613	CLA	CHD-C1D	-2.06	1.34	1.38
34	e	102	HEM	C3B-C2B	-2.05	1.33	1.37
26	C	515	BCR	C36-C18	-2.05	1.46	1.50
33	E	101	LHG	P-O3	2.05	1.67	1.59
24	C	513	CLA	C3B-C4B	2.05	1.48	1.42
24	c	501	CLA	CMD-C2D	-2.05	1.46	1.50
26	H	101	BCR	C33-C5	-2.05	1.47	1.50
34	F	102	HEM	CMC-C2C	2.05	1.55	1.50
32	C	501	LMG	O1-C7	-2.05	1.40	1.43
24	c	501	CLA	MG-NB	-2.05	2.01	2.05
24	b	606	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C3D-C4D	2.05	1.48	1.44
24	A	405	CLA	CMD-C2D	-2.05	1.46	1.50
27	A	410	PL9	C25-C24	-2.04	1.45	1.50
32	D	407	LMG	C6-C5	2.04	1.58	1.51
24	c	512	CLA	C3C-C2C	2.04	1.41	1.36
29	C	518	DGD	O5D-C1E	-2.04	1.36	1.40
24	a	405	CLA	CAC-C3C	-2.04	1.45	1.51
35	v	201	HEC	C3D-C2D	-2.04	1.33	1.38
24	b	604	CLA	MG-NC	-2.04	2.01	2.06
24	C	506	CLA	O1D-CGD	2.04	1.26	1.21
24	C	510	CLA	C3B-C4B	2.04	1.48	1.42
24	c	509	CLA	C4B-NB	2.04	1.40	1.37
24	b	605	CLA	O2D-CED	-2.04	1.40	1.45
34	e	102	HEM	CMC-C2C	2.04	1.54	1.50
29	c	517	DGD	O2E-C2E	-2.04	1.37	1.43
29	A	413	DGD	C3G-C2G	2.03	1.57	1.50
24	b	612	CLA	CHC-C1C	2.03	1.42	1.38
24	c	502	CLA	O2D-CGD	2.03	1.38	1.33
24	B	608	CLA	CAC-C3C	-2.03	1.45	1.51
32	K	102	LMG	O8-C9	-2.03	1.40	1.45
24	c	501	CLA	CHC-C1C	2.03	1.42	1.38
24	C	511	CLA	C3D-C4D	2.03	1.48	1.44
24	A	408	CLA	MG-NB	-2.03	2.01	2.05
24	B	612	CLA	CMB-C2B	-2.03	1.46	1.50
26	a	408	BCR	C39-C30	-2.03	1.49	1.53
33	D	409	LHG	O8-C6	2.02	1.49	1.45
24	C	506	CLA	MG-NA	2.02	2.11	2.06
24	C	504	CLA	C5-C3	-2.02	1.47	1.51
26	B	619	BCR	C38-C26	-2.02	1.47	1.50
33	l	101	LHG	P-O6	2.01	1.67	1.59
24	b	605	CLA	C3D-C4D	2.01	1.48	1.44
24	C	506	CLA	CMB-C2B	-2.01	1.46	1.50
24	c	512	CLA	C1B-NB	-2.01	1.35	1.37
24	c	512	CLA	C3D-C4D	2.01	1.48	1.44
24	c	504	CLA	C3D-C4D	2.01	1.48	1.44
32	c	524	LMG	C4-C3	2.01	1.57	1.52
25	D	401	PHO	C3D-CAD	-2.01	1.43	1.47
28	a	410	SQD	O2-C2	-2.00	1.38	1.43
24	B	601	CLA	CMC-C2C	-2.00	1.46	1.50
24	c	505	CLA	MG-NB	2.00	2.09	2.05
24	c	506	CLA	CHC-C4B	-2.00	1.34	1.39
24	C	512	CLA	C3D-C4D	2.00	1.48	1.44

All (1286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	411	SQD	O6-C1-C2	9.81	123.17	108.27
28	a	410	SQD	O6-C1-C2	9.43	122.59	108.27
24	b	607	CLA	C4A-NA-C1A	8.39	110.51	106.68
24	a	404	CLA	C4A-NA-C1A	8.36	110.49	106.68
28	b	601	SQD	O6-C1-C2	8.22	120.75	108.27
24	C	512	CLA	C4A-NA-C1A	8.11	110.38	106.68
24	B	604	CLA	C4A-NA-C1A	7.98	110.32	106.68
24	B	613	CLA	C4A-NA-C1A	7.93	110.30	106.68
28	A	411	SQD	O7-S-C6	7.69	118.24	106.76
24	B	601	CLA	C4A-NA-C1A	7.58	110.14	106.68
24	C	508	CLA	C4A-NA-C1A	7.29	110.00	106.68
24	C	511	CLA	C4A-NA-C1A	6.83	109.80	106.68
24	b	616	CLA	C4A-NA-C1A	6.78	109.77	106.68
24	C	504	CLA	C4A-NA-C1A	6.77	109.77	106.68
24	c	509	CLA	C4A-NA-C1A	6.73	109.75	106.68
24	c	507	CLA	C4A-NA-C1A	6.58	109.68	106.68
24	D	402	CLA	C4A-NA-C1A	6.34	109.57	106.68
24	b	615	CLA	C4A-NA-C1A	6.33	109.57	106.68
24	C	514	CLA	C4A-NA-C1A	6.25	109.53	106.68
35	V	201	HEC	CBB-CAB-C3B	-6.18	115.07	127.43
24	b	605	CLA	C4A-NA-C1A	6.10	109.46	106.68
24	C	503	CLA	C4A-NA-C1A	6.03	109.43	106.68
24	c	504	CLA	C4A-NA-C1A	5.85	109.35	106.68
24	c	503	CLA	C4A-NA-C1A	5.77	109.31	106.68
24	c	501	CLA	O2D-CGD-O1D	-5.76	112.64	123.85
24	B	615	CLA	C4A-NA-C1A	5.74	109.30	106.68
24	B	607	CLA	C4A-NA-C1A	5.62	109.25	106.68
24	d	404	CLA	C4A-NA-C1A	5.62	109.25	106.68
27	a	409	PL9	C7-C3-C4	5.54	121.47	116.91
24	b	616	CLA	C3B-C4B-NB	-5.47	105.64	110.53
28	F	101	SQD	O9-S-C6	5.41	114.83	106.76
24	c	505	CLA	C4A-NA-C1A	5.39	109.14	106.68
24	B	610	CLA	O2D-CGD-O1D	-5.32	113.49	123.85
24	b	603	CLA	C4A-NA-C1A	5.28	109.09	106.68
29	H	102	DGD	O3G-C3G-C2G	-5.28	97.98	110.82
24	b	617	CLA	O2D-CGD-O1D	-5.27	113.59	123.85
24	b	617	CLA	C4A-NA-C1A	5.19	109.05	106.68
25	d	402	PHO	CBC-CAC-C3C	5.14	120.23	112.87
24	b	608	CLA	C4A-NA-C1A	5.14	109.02	106.68
24	c	502	CLA	C4A-NA-C1A	5.13	109.02	106.68
28	a	411	SQD	O47-C7-C8	5.12	122.55	111.48
24	B	616	CLA	C4A-NA-C1A	5.11	109.01	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	411	SQD	O9-S-O7	-5.05	97.40	113.82
24	c	510	CLA	C4A-NA-C1A	4.98	108.95	106.68
24	c	501	CLA	C4A-NA-C1A	4.97	108.95	106.68
24	b	604	CLA	O2D-CGD-O1D	-4.97	114.17	123.85
24	a	405	CLA	C4A-NA-C1A	4.92	108.92	106.68
35	V	201	HEC	CBC-CAC-C3C	-4.89	117.65	127.43
24	c	510	CLA	O2D-CGD-CBD	4.89	119.77	111.23
24	h	101	CLA	C3B-C4B-NB	-4.88	106.17	110.53
28	f	101	SQD	O6-C1-C2	4.88	115.68	108.27
25	d	402	PHO	O1D-CGD-CBD	4.86	132.10	124.72
32	b	623	LMG	O1-C1-C2	-4.83	100.94	108.27
35	v	201	HEC	CBC-CAC-C3C	-4.80	117.83	127.43
24	d	403	CLA	C4A-NA-C1A	4.77	108.86	106.68
24	b	603	CLA	O2D-CGD-O1D	-4.73	114.64	123.85
24	C	510	CLA	C4A-NA-C1A	4.66	108.80	106.68
33	D	408	LHG	O4-P-O5	4.65	134.05	112.44
24	C	509	CLA	C4A-NA-C1A	4.63	108.79	106.68
25	D	401	PHO	O1D-CGD-CBD	4.63	131.74	124.72
24	c	512	CLA	C1-C2-C3	-4.63	118.61	126.20
24	c	510	CLA	O2D-CGD-O1D	-4.55	114.98	123.85
28	B	622	SQD	O7-S-C6	4.54	113.54	106.76
24	b	604	CLA	O2D-CGD-CBD	4.54	119.16	111.23
25	a	406	PHO	C4D-CHA-CBD	-4.54	106.28	108.45
29	C	517	DGD	O3G-C3G-C2G	-4.52	99.82	110.82
33	e	101	LHG	O4-P-O5	4.48	133.30	112.44
27	d	407	PL9	C40-C39-C41	4.48	123.00	115.23
28	f	101	SQD	O9-S-C6	4.46	113.42	106.76
25	D	401	PHO	C4D-CHA-CBD	-4.46	106.32	108.45
24	C	509	CLA	O2D-CGD-O1D	-4.44	115.20	123.85
24	c	511	CLA	C4A-NA-C1A	4.44	108.70	106.68
24	b	609	CLA	C3B-C4B-NB	-4.44	106.57	110.53
24	B	612	CLA	C4A-NA-C1A	4.43	108.70	106.68
28	A	412	SQD	O47-C7-C8	4.42	121.05	111.48
23	A	404	BCT	O2-C-O1	4.42	130.97	119.68
24	c	501	CLA	O2D-CGD-CBD	4.41	118.93	111.23
33	D	409	LHG	O4-P-O5	4.40	132.92	112.44
33	d	409	LHG	O4-P-O5	4.38	132.82	112.44
26	B	617	BCR	C2-C1-C6	4.36	116.77	110.44
24	C	513	CLA	C3B-C4B-NB	-4.31	106.68	110.53
24	B	602	CLA	O2D-CGD-CBD	4.31	118.76	111.23
24	d	405	CLA	CHD-C1D-ND	-4.30	118.75	124.80
33	d	408	LHG	O4-P-O5	4.30	132.44	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C4A-NA-C1A	4.29	108.64	106.68
24	B	611	CLA	O2D-CGD-CBD	4.28	118.72	111.23
33	d	410	LHG	O4-P-O5	4.27	132.31	112.44
24	B	609	CLA	C4A-NA-C1A	4.25	108.62	106.68
28	A	411	SQD	C1-C2-C3	-4.23	101.11	110.01
33	E	101	LHG	O4-P-O5	4.23	132.10	112.44
24	c	506	CLA	C4A-NA-C1A	4.19	108.59	106.68
24	B	611	CLA	O2D-CGD-O1D	-4.19	115.70	123.85
28	a	410	SQD	O8-S-C6	4.19	114.05	105.97
24	b	617	CLA	O2D-CGD-CBD	4.18	118.53	111.23
29	A	413	DGD	C3G-C2G-C1G	-4.16	102.09	111.78
25	D	401	PHO	O2D-CGD-CBD	-4.13	106.41	110.95
24	A	405	CLA	C4A-NA-C1A	4.13	108.56	106.68
24	b	603	CLA	O2D-CGD-CBD	4.11	118.42	111.23
24	B	601	CLA	O2D-CGD-O1D	-4.11	115.85	123.85
33	l	101	LHG	O4-P-O5	4.10	131.54	112.44
24	c	512	CLA	C4A-NA-C1A	4.09	108.55	106.68
28	B	622	SQD	O6-C1-C2	4.09	114.48	108.27
33	D	411	LHG	O4-P-O5	4.08	131.41	112.44
28	B	622	SQD	C3-C4-C5	4.07	117.61	110.23
24	C	502	CLA	O2D-CGD-O1D	-4.05	115.95	123.85
28	a	410	SQD	O9-S-C6	4.05	112.81	106.76
24	b	605	CLA	C3B-C4B-NB	-4.04	106.92	110.53
24	c	505	CLA	C3B-C4B-NB	-4.04	106.92	110.53
24	A	408	CLA	O2D-CGD-O1D	-4.03	115.99	123.85
27	a	409	PL9	C7-C3-C2	-4.03	118.64	123.39
24	C	504	CLA	C7-C6-C5	-4.02	102.54	113.26
24	A	406	CLA	C4A-NA-C1A	4.02	108.51	106.68
24	B	614	CLA	O2D-CGD-O1D	-4.01	116.03	123.85
29	A	413	DGD	O5D-C6D-C5D	-4.01	100.39	109.42
24	b	607	CLA	O2D-CGD-O1D	-4.00	116.05	123.85
25	d	402	PHO	C2B-C1B-NB	-4.00	106.54	109.43
24	C	502	CLA	C4A-NA-C1A	3.99	108.50	106.68
24	c	511	CLA	C3B-C4B-NB	-3.97	106.98	110.53
24	a	405	CLA	CHB-C4A-NA	3.97	130.13	124.40
24	b	604	CLA	C4-C3-C5	3.97	122.12	115.23
24	d	404	CLA	C3B-C4B-NB	-3.96	106.99	110.53
28	B	622	SQD	O47-C7-C8	3.96	120.05	111.48
24	B	605	CLA	O1D-CGD-CBD	3.94	132.30	124.52
28	B	622	SQD	O9-S-O7	-3.93	101.03	113.82
24	D	403	CLA	C3B-C4B-NB	-3.93	107.02	110.53
24	h	101	CLA	O2D-CGD-O1D	-3.92	116.21	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	515	BCR	C27-C26-C25	3.92	128.00	122.70
28	A	411	SQD	O47-C7-C8	3.91	119.94	111.48
29	C	518	DGD	O3G-C3G-C2G	-3.87	101.40	110.82
24	B	610	CLA	C4A-NA-C1A	3.86	108.44	106.68
24	a	405	CLA	CED-O2D-CGD	-3.86	107.16	115.92
24	b	611	CLA	O2D-CGD-O1D	-3.85	116.35	123.85
24	c	503	CLA	C3B-C4B-NB	-3.84	107.11	110.53
27	d	407	PL9	C20-C19-C21	3.83	121.87	115.23
24	C	505	CLA	CMB-C2B-C1B	-3.82	119.60	125.42
23	d	401	BCT	O2-C-O1	3.82	129.45	119.68
24	C	502	CLA	O2D-CGD-CBD	3.81	117.89	111.23
28	A	412	SQD	O47-C45-C44	3.81	116.49	107.96
33	L	101	LHG	O4-P-O5	3.79	130.07	112.44
25	A	407	PHO	O2D-CGD-O1D	-3.79	116.47	123.85
24	C	503	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
33	D	411	LHG	O8-C23-O10	-3.78	114.18	123.63
24	b	603	CLA	CHB-C4A-NA	3.76	129.83	124.40
24	B	616	CLA	O2D-CGD-O1D	-3.76	116.54	123.85
24	c	505	CLA	CHB-C4A-NA	3.76	129.82	124.40
34	e	102	HEM	CBD-CAD-C3D	-3.75	102.16	112.53
24	b	606	CLA	C4-C3-C5	3.75	121.73	115.23
24	A	408	CLA	O2D-CGD-CBD	3.74	117.78	111.23
24	B	606	CLA	CHD-C1D-ND	-3.73	119.55	124.80
24	B	606	CLA	C4A-NA-C1A	3.73	108.38	106.68
24	b	615	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
33	d	409	LHG	O8-C23-C24	3.72	123.17	111.83
25	a	406	PHO	C2B-C1B-NB	-3.71	106.75	109.43
24	B	603	CLA	C3B-C4B-NB	-3.70	107.23	110.53
26	K	101	BCR	C34-C9-C10	-3.70	116.83	122.82
24	C	512	CLA	CAC-C3C-C4C	3.69	129.60	124.79
24	a	404	CLA	C3B-C4B-NB	-3.68	107.24	110.53
25	d	402	PHO	C4D-CHA-CBD	-3.68	106.69	108.45
32	c	524	LMG	C1-O6-C5	-3.67	106.55	113.72
24	b	606	CLA	C1-C2-C3	-3.67	120.18	126.20
24	B	602	CLA	CHB-C4A-NA	3.67	129.70	124.40
24	a	407	CLA	O2D-CGD-O1D	-3.65	116.73	123.85
26	b	620	BCR	C29-C30-C25	3.65	115.74	110.44
24	b	616	CLA	CHB-C1B-NB	3.65	129.52	124.05
29	C	516	DGD	O1G-C1A-C2A	-3.65	100.72	111.83
26	B	619	BCR	C33-C5-C6	-3.64	120.51	124.48
26	b	619	BCR	C15-C14-C13	-3.64	122.17	127.28
24	B	605	CLA	C3B-C4B-NB	-3.64	107.28	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C4A-NA-C1A	3.63	108.34	106.68
24	A	408	CLA	C1D-ND-C4D	-3.61	103.78	106.31
24	b	613	CLA	CMB-C2B-C1B	-3.60	119.93	125.42
24	d	403	CLA	C3B-C4B-NB	-3.60	107.31	110.53
27	d	407	PL9	C7-C3-C4	3.60	119.88	116.91
24	b	616	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
24	a	407	CLA	O2D-CGD-CBD	3.60	117.52	111.23
24	c	509	CLA	O2A-CGA-O1A	-3.59	114.64	123.63
32	c	522	LMG	O6-C1-O1	-3.59	101.57	110.04
24	B	612	CLA	C3B-C4B-NB	-3.58	107.33	110.53
24	B	615	CLA	CHC-C4B-NB	3.58	129.42	124.05
24	c	501	CLA	CMB-C2B-C1B	-3.57	119.98	125.42
24	B	615	CLA	C3B-C4B-NB	-3.57	107.35	110.53
24	b	610	CLA	C3B-C4B-NB	-3.56	107.35	110.53
26	b	618	BCR	C15-C14-C13	-3.56	122.28	127.28
33	D	409	LHG	O8-C23-O10	-3.56	114.72	123.63
24	B	606	CLA	C3B-C4B-NB	-3.56	107.36	110.53
26	t	101	BCR	C15-C16-C17	-3.56	116.24	123.52
24	B	604	CLA	CHB-C4A-NA	3.55	129.52	124.40
24	c	507	CLA	CHB-C4A-NA	3.55	129.52	124.40
28	A	411	SQD	O9-S-C6	3.53	112.03	106.76
24	b	612	CLA	O2D-CGD-CBD	3.52	117.39	111.23
24	B	610	CLA	CHB-C4A-NA	3.51	129.47	124.40
24	c	508	CLA	C3B-C4B-NB	-3.51	107.40	110.53
24	b	610	CLA	O1D-CGD-CBD	3.51	131.43	124.52
27	d	407	PL9	C22-C23-C24	-3.50	119.61	127.62
24	c	509	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
26	c	521	BCR	C27-C26-C25	3.49	127.42	122.70
28	b	601	SQD	C1-C2-C3	-3.49	102.67	110.01
25	A	407	PHO	O2D-CGD-CBD	3.49	114.78	110.95
29	H	102	DGD	C1D-O6D-C5D	-3.49	106.91	113.72
28	F	101	SQD	O9-S-O7	-3.48	102.51	113.82
28	A	411	SQD	C1-O5-C5	-3.48	106.93	113.72
24	b	605	CLA	C1-C2-C3	-3.48	120.50	126.20
24	h	101	CLA	C4A-NA-C1A	3.46	108.26	106.68
24	a	405	CLA	C3B-C4B-NB	-3.46	107.44	110.53
29	C	518	DGD	O3G-C1D-C2D	-3.46	103.02	108.27
24	b	606	CLA	O1D-CGD-CBD	3.45	131.32	124.52
28	B	622	SQD	C1-C2-C3	-3.44	102.77	110.01
26	C	519	BCR	C15-C16-C17	-3.44	116.47	123.52
28	B	622	SQD	O5-C5-C4	3.44	115.89	109.70
24	b	606	CLA	O2D-CGD-O1D	-3.43	117.17	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	C3B-C4B-NB	-3.43	107.47	110.53
24	c	509	CLA	O1D-CGD-CBD	3.42	131.27	124.52
26	D	405	BCR	C2-C1-C6	3.42	115.41	110.44
24	C	506	CLA	CAC-C3C-C4C	3.42	129.24	124.79
29	c	517	DGD	O3G-C1D-C2D	-3.42	103.09	108.27
27	D	406	PL9	C37-C38-C39	-3.41	119.82	127.62
24	C	513	CLA	CHB-C4A-NA	3.40	129.31	124.40
26	b	602	BCR	C27-C26-C25	3.40	127.30	122.70
24	B	613	CLA	C4-C3-C5	3.39	121.12	115.23
24	B	603	CLA	O2A-CGA-O1A	-3.39	115.14	123.63
24	B	610	CLA	O2A-CGA-O1A	-3.38	115.16	123.63
26	K	101	BCR	C33-C5-C6	-3.38	120.79	124.48
26	K	101	BCR	C11-C10-C9	-3.38	122.54	127.28
24	b	609	CLA	O2D-CGD-CBD	3.38	117.14	111.23
24	b	611	CLA	CHB-C4A-NA	3.37	129.27	124.40
25	D	401	PHO	CMB-C2B-C3B	3.37	131.43	124.68
26	h	103	BCR	C30-C25-C26	-3.37	118.03	122.64
28	b	601	SQD	O7-S-C6	3.37	111.78	106.76
24	B	605	CLA	C16-C15-C13	-3.37	104.78	115.97
28	b	601	SQD	O5-C5-C4	3.36	115.76	109.70
27	D	406	PL9	C22-C23-C24	-3.36	119.94	127.62
28	A	411	SQD	O47-C7-O49	-3.35	115.86	123.70
24	B	605	CLA	CHB-C4A-NA	3.34	129.23	124.40
24	b	615	CLA	CHD-C1D-ND	-3.34	120.10	124.80
26	b	618	BCR	C2-C1-C6	3.34	115.29	110.44
26	b	602	BCR	C38-C26-C27	-3.34	106.48	113.60
24	b	613	CLA	CMB-C2B-C3B	3.34	134.40	126.55
24	D	403	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
24	B	613	CLA	C3B-C4B-NB	-3.33	107.56	110.53
32	d	411	LMG	O2-C2-C1	-3.33	102.15	110.08
28	a	410	SQD	O8-S-O9	-3.33	103.08	111.40
28	b	601	SQD	C3-C4-C5	3.32	116.26	110.23
26	b	618	BCR	C33-C5-C6	-3.32	120.86	124.48
24	b	609	CLA	CHB-C4A-NA	3.32	129.19	124.40
24	b	605	CLA	O2A-CGA-O1A	-3.32	115.33	123.63
28	b	601	SQD	O9-S-O7	-3.31	103.06	113.82
24	B	616	CLA	C1-O2A-CGA	3.31	124.66	116.65
27	A	410	PL9	C7-C3-C4	3.30	119.63	116.91
26	c	514	BCR	C27-C26-C25	3.30	127.16	122.70
24	b	606	CLA	C4A-NA-C1A	3.29	108.18	106.68
24	b	614	CLA	CMB-C2B-C1B	-3.29	120.42	125.42
29	c	518	DGD	O6D-C1D-O3G	-3.28	102.30	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	516	DGD	O3G-C3G-C2G	-3.28	102.85	110.82
24	b	617	CLA	CHB-C4A-NA	3.26	129.11	124.40
24	c	507	CLA	CHD-C1D-ND	-3.26	120.21	124.80
24	C	512	CLA	CHB-C4A-NA	3.26	129.11	124.40
24	B	607	CLA	C2C-C1C-NC	3.25	113.40	109.98
24	b	616	CLA	C6-C5-C3	-3.25	105.56	113.47
24	B	612	CLA	C11-C12-C13	-3.24	105.18	115.97
24	C	506	CLA	O1D-CGD-CBD	3.23	130.88	124.52
32	C	501	LMG	O6-C1-O1	-3.22	102.42	110.04
24	B	606	CLA	CHD-C4C-NC	3.22	129.23	124.23
26	C	515	BCR	C27-C26-C25	3.22	127.06	122.70
28	B	622	SQD	O8-S-C6	3.22	112.19	105.97
29	c	518	DGD	O3G-C3G-C2G	-3.22	103.00	110.82
24	c	504	CLA	O2D-CGD-CBD	3.21	116.85	111.23
26	b	619	BCR	C30-C25-C26	-3.21	118.25	122.64
24	B	602	CLA	C4A-NA-C1A	3.21	108.14	106.68
26	k	101	BCR	C27-C26-C25	3.20	127.03	122.70
24	A	408	CLA	CED-O2D-CGD	-3.20	108.66	115.92
29	A	413	DGD	C4E-C3E-C2E	-3.19	105.23	110.83
24	B	605	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
26	c	514	BCR	C15-C16-C17	-3.18	117.00	123.52
26	B	618	BCR	C27-C26-C25	3.18	127.00	122.70
24	A	406	CLA	CED-O2D-CGD	-3.18	108.70	115.92
24	C	509	CLA	CHD-C1D-ND	-3.18	120.33	124.80
24	c	510	CLA	CHB-C4A-NA	3.17	128.98	124.40
24	B	607	CLA	O2A-CGA-O1A	-3.17	115.69	123.63
24	C	509	CLA	C1D-ND-C4D	3.17	108.53	106.31
24	d	405	CLA	C3B-C4B-NB	-3.17	107.70	110.53
24	b	613	CLA	O1D-CGD-CBD	3.16	130.75	124.52
24	C	514	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
29	c	516	DGD	O3E-C3E-C2E	-3.15	102.94	110.38
27	A	410	PL9	O1-C4-C3	-3.15	117.40	120.73
26	h	103	BCR	C27-C26-C25	3.15	126.97	122.70
26	c	515	BCR	C33-C5-C6	-3.15	121.04	124.48
24	c	512	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
33	D	411	LHG	O8-C23-C24	3.15	121.44	111.83
24	D	402	CLA	CHC-C4B-NB	3.15	128.77	124.05
28	b	601	SQD	O48-C23-C24	3.15	121.44	111.83
27	d	407	PL9	O1-C4-C3	-3.15	117.41	120.73
28	A	411	SQD	O2-C2-C1	3.15	117.58	110.08
32	b	621	LMG	O7-C10-O9	-3.15	116.35	123.70
32	M	101	LMG	O1-C1-C2	-3.15	103.50	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	515	BCR	C33-C5-C6	-3.13	121.07	124.48
24	D	403	CLA	O2D-CGD-CBD	3.13	116.71	111.23
24	c	510	CLA	CAA-CBA-CGA	-3.13	104.32	113.21
26	A	409	BCR	C29-C30-C25	3.13	114.98	110.44
24	C	513	CLA	C1-C2-C3	-3.13	121.08	126.20
24	C	509	CLA	CHD-C1D-C2D	3.13	131.99	125.49
24	a	405	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
26	b	619	BCR	C8-C7-C6	-3.12	118.67	127.00
24	b	615	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
25	D	401	PHO	C1-C2-C3	-3.12	121.09	126.20
28	F	101	SQD	C3-C4-C5	3.11	115.88	110.23
26	c	515	BCR	C15-C14-C13	-3.11	122.92	127.28
24	D	402	CLA	C3B-C4B-NB	-3.11	107.76	110.53
29	c	518	DGD	O3E-C3E-C2E	-3.09	103.08	110.38
32	c	519	LMG	O6-C1-O1	-3.09	102.74	110.04
24	B	601	CLA	O1D-CGD-CBD	3.09	130.61	124.52
26	B	617	BCR	C15-C14-C13	-3.09	122.95	127.28
24	C	506	CLA	C3B-C4B-NB	-3.09	107.78	110.53
24	c	503	CLA	C4-C3-C5	3.09	120.58	115.23
32	D	407	LMG	C3-C4-C5	-3.08	104.64	110.23
24	b	611	CLA	CAA-C2A-C3A	-3.08	104.68	113.00
24	D	404	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
33	E	101	LHG	O8-C23-C24	3.08	121.22	111.83
29	h	104	DGD	O3G-C3G-C2G	-3.07	103.34	110.82
29	c	517	DGD	O3G-C3G-C2G	-3.07	103.34	110.82
27	A	410	PL9	C22-C23-C24	-3.07	120.59	127.62
24	C	505	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	d	403	CLA	CHD-C1D-ND	-3.07	120.48	124.80
24	b	605	CLA	CHB-C4A-NA	3.07	128.83	124.40
24	b	605	CLA	CHC-C1C-NC	3.07	128.93	124.31
24	b	610	CLA	CHC-C4B-NB	3.06	128.64	124.05
24	D	404	CLA	C3B-C4B-NB	-3.06	107.80	110.53
24	d	403	CLA	C1D-ND-C4D	3.06	108.46	106.31
26	K	101	BCR	C38-C26-C25	-3.06	121.15	124.48
27	a	409	PL9	C22-C23-C24	-3.05	120.63	127.62
33	e	101	LHG	O8-C23-O10	-3.04	116.03	123.63
29	C	518	DGD	O3E-C3E-C2E	-3.03	103.22	110.38
28	b	601	SQD	C45-O47-C7	3.03	125.04	117.80
24	C	505	CLA	C4A-NA-C1A	3.03	108.06	106.68
24	b	611	CLA	C3B-C4B-NB	-3.03	107.83	110.53
26	B	619	BCR	C38-C26-C25	-3.03	121.18	124.48
32	M	101	LMG	C8-O7-C10	3.02	125.03	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	407	PL9	C42-C43-C44	-3.02	120.71	127.62
24	C	505	CLA	CHB-C1B-NB	3.02	128.58	124.05
24	A	405	CLA	CHB-C4A-NA	3.02	128.76	124.40
24	B	605	CLA	C1-O2A-CGA	-3.02	109.35	116.65
26	A	409	BCR	C27-C26-C25	3.02	126.78	122.70
24	b	603	CLA	CHC-C1C-NC	3.01	128.85	124.31
26	K	101	BCR	C2-C1-C6	3.01	114.81	110.44
26	B	619	BCR	C2-C1-C6	3.00	114.80	110.44
28	B	622	SQD	C1-O5-C5	-3.00	107.86	113.72
28	a	410	SQD	C1-C2-C3	-3.00	103.70	110.01
29	c	517	DGD	O2E-C2E-C1E	-2.99	102.94	110.08
24	b	614	CLA	O1D-CGD-CBD	2.99	130.42	124.52
26	B	617	BCR	C15-C16-C17	-2.99	117.40	123.52
32	d	411	LMG	O6-C1-O1	-2.99	102.99	110.04
29	a	412	DGD	C2G-O2G-C1B	2.98	124.94	117.80
24	c	503	CLA	CHC-C4B-NB	2.98	128.53	124.05
24	B	610	CLA	O2D-CGD-CBD	2.98	116.44	111.23
26	B	618	BCR	C2-C1-C6	2.98	114.77	110.44
28	a	410	SQD	O47-C7-C8	2.98	117.92	111.48
26	b	602	BCR	C7-C8-C9	-2.97	121.84	126.23
28	a	411	SQD	O48-C23-C24	2.97	120.89	111.83
24	D	402	CLA	O2D-CGD-CBD	2.97	116.42	111.23
29	C	517	DGD	O6D-C1D-O3G	-2.96	103.04	110.04
24	b	615	CLA	C3B-C4B-NB	-2.96	107.88	110.53
24	B	605	CLA	CHD-C1D-ND	-2.96	120.64	124.80
24	B	604	CLA	C3B-C4B-NB	-2.96	107.89	110.53
24	c	507	CLA	C4-C3-C5	2.95	120.36	115.23
24	B	611	CLA	CHD-C4C-NC	2.95	128.81	124.23
26	B	618	BCR	C3-C4-C5	-2.95	108.79	114.06
24	C	502	CLA	C1D-ND-C4D	-2.95	104.24	106.31
28	b	601	SQD	O2-C2-C1	2.95	117.10	110.08
24	h	101	CLA	CBA-CAA-C2A	2.95	122.56	113.79
29	c	516	DGD	O6D-C1D-O3G	-2.95	103.08	110.04
24	b	615	CLA	C1-C2-C3	-2.94	121.37	126.20
26	H	101	BCR	C16-C15-C14	-2.94	117.50	123.52
24	c	501	CLA	CED-O2D-CGD	-2.94	109.24	115.92
32	b	621	LMG	O1-C7-C8	-2.94	103.67	110.82
24	B	606	CLA	CHD-C4C-C3C	-2.94	120.49	124.77
24	b	611	CLA	CHD-C1D-ND	-2.93	120.67	124.80
24	a	407	CLA	O2A-CGA-O1A	-2.93	116.29	123.63
24	b	607	CLA	C1C-C2C-C3C	-2.93	103.89	106.98
26	c	515	BCR	C35-C13-C14	-2.93	118.06	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C3B-C4B-NB	-2.93	107.91	110.53
24	C	507	CLA	C3B-C4B-NB	-2.93	107.91	110.53
24	B	614	CLA	O1D-CGD-CBD	2.93	130.30	124.52
24	B	605	CLA	C4-C3-C5	2.93	120.31	115.23
32	K	102	LMG	O1-C7-C8	-2.92	103.71	110.82
24	B	608	CLA	C4A-NA-C1A	2.92	108.01	106.68
32	D	407	LMG	O6-C1-O1	-2.92	103.15	110.04
26	h	103	BCR	C15-C16-C17	-2.92	117.55	123.52
26	b	618	BCR	C15-C16-C17	-2.91	117.56	123.52
24	c	501	CLA	O2A-CGA-O1A	-2.91	116.34	123.63
24	d	404	CLA	O2A-CGA-O1A	-2.91	116.34	123.63
25	d	402	PHO	CMA-C3A-C4A	-2.91	108.34	114.61
26	a	408	BCR	C30-C25-C26	-2.91	118.66	122.64
24	b	614	CLA	C4A-NA-C1A	2.91	108.01	106.68
26	C	519	BCR	C29-C30-C25	2.91	114.67	110.44
29	A	413	DGD	C1D-C2D-C3D	-2.91	103.89	110.01
24	b	604	CLA	C3B-C4B-NB	-2.91	107.93	110.53
24	b	605	CLA	C7-C6-C5	-2.91	105.51	113.26
33	D	411	LHG	C11-C10-C9	-2.90	99.68	114.37
24	b	609	CLA	CMA-C3A-C4A	-2.90	103.97	111.77
24	B	603	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	c	506	CLA	CGD-CBD-CAD	-2.90	101.46	110.85
24	c	510	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	h	104	DGD	C4D-C3D-C2D	-2.89	105.75	110.83
28	F	101	SQD	C46-C45-C44	-2.89	104.33	113.67
24	D	402	CLA	CHB-C4A-NA	2.89	128.57	124.40
28	b	601	SQD	O9-S-C6	2.88	111.06	106.76
33	D	411	LHG	O3-P-O5	-2.88	97.50	108.94
24	B	611	CLA	CHD-C1D-ND	-2.88	120.75	124.80
29	c	518	DGD	C3G-C2G-C1G	-2.88	105.08	111.78
27	D	406	PL9	C42-C43-C44	-2.88	121.04	127.62
28	a	410	SQD	C1-O5-C5	-2.88	108.10	113.72
24	d	403	CLA	CHD-C1D-C2D	2.88	131.47	125.49
24	C	507	CLA	C4A-NA-C1A	2.87	107.99	106.68
32	c	522	LMG	O3-C3-C2	-2.87	103.60	110.38
28	b	601	SQD	O8-S-C6	2.87	111.51	105.97
24	B	602	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
24	A	408	CLA	O2A-CGA-O1A	-2.86	116.46	123.63
24	b	614	CLA	CHA-C1A-NA	-2.86	119.91	126.39
24	C	509	CLA	O2D-CGD-CBD	2.86	116.23	111.23
26	B	619	BCR	C29-C30-C25	2.86	114.59	110.44
24	B	612	CLA	O2A-CGA-O1A	-2.85	116.49	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	408	BCR	C33-C5-C6	-2.85	121.37	124.48
26	K	101	BCR	C27-C26-C25	2.85	126.56	122.70
24	C	504	CLA	C3B-C4B-NB	-2.85	107.99	110.53
32	M	101	LMG	C40-C39-C38	-2.85	99.98	114.37
26	K	101	BCR	C7-C8-C9	-2.85	122.03	126.23
24	C	505	CLA	C7-C6-C5	-2.84	105.69	113.26
24	C	503	CLA	CHD-C1D-ND	-2.84	120.81	124.80
29	C	517	DGD	O6E-C1E-O5D	-2.84	103.33	110.04
26	k	101	BCR	C33-C5-C6	-2.84	121.39	124.48
29	A	413	DGD	O6E-C1E-O5D	-2.84	103.34	110.04
24	B	602	CLA	C11-C12-C13	-2.84	106.54	115.97
24	C	507	CLA	CHB-C4A-NA	2.83	128.49	124.40
26	B	617	BCR	C29-C30-C25	2.83	114.55	110.44
24	b	614	CLA	CHB-C1B-NB	2.83	128.29	124.05
26	K	101	BCR	C34-C9-C8	-2.83	113.77	118.09
24	c	504	CLA	O2A-CGA-O1A	-2.83	116.55	123.63
24	b	611	CLA	CAA-CBA-CGA	-2.83	105.17	113.21
34	F	102	HEM	CBD-CAD-C3D	-2.83	104.72	112.53
24	B	607	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
24	B	616	CLA	CHB-C1B-NB	2.83	128.29	124.05
27	d	407	PL9	C37-C38-C39	-2.82	121.16	127.62
24	B	608	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
28	B	622	SQD	O48-C23-C24	2.82	120.43	111.83
28	F	101	SQD	O8-S-C6	2.82	111.41	105.97
26	Y	101	BCR	C27-C26-C25	2.82	126.51	122.70
35	v	201	HEC	CBB-CAB-C3B	-2.81	121.81	127.43
26	C	519	BCR	C2-C1-C6	2.81	114.52	110.44
24	C	510	CLA	CHB-C4A-NA	2.81	128.46	124.40
24	C	514	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
24	h	101	CLA	CHB-C4A-NA	2.80	128.44	124.40
24	c	512	CLA	CHB-C4A-NA	2.80	128.44	124.40
24	c	505	CLA	O2A-CGA-O1A	-2.80	116.63	123.63
24	b	604	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
24	C	511	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
24	d	405	CLA	C4D-CHA-C1A	2.79	124.57	121.24
26	h	103	BCR	C39-C30-C25	-2.79	105.87	110.24
32	M	101	LMG	O1-C7-C8	-2.79	104.03	110.82
27	d	407	PL9	C7-C3-C2	-2.79	120.10	123.39
24	C	513	CLA	C4A-NA-C1A	2.79	107.95	106.68
24	C	511	CLA	CHB-C4A-NA	2.78	128.42	124.40
26	a	408	BCR	C27-C26-C25	2.78	126.47	122.70
24	C	503	CLA	C3B-C4B-NB	-2.78	108.05	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	O1D-CGD-CBD	2.78	130.00	124.52
24	d	405	CLA	C1D-ND-C4D	-2.77	104.36	106.31
26	B	619	BCR	C37-C22-C21	-2.77	118.32	122.82
28	a	411	SQD	O48-C23-O10	-2.77	116.69	123.63
24	A	405	CLA	O1D-CGD-CBD	2.77	129.99	124.52
24	c	508	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	b	606	CLA	CHB-C1B-NB	2.77	128.20	124.05
26	b	620	BCR	C2-C1-C6	2.77	114.46	110.44
32	C	501	LMG	O8-C28-O10	-2.77	116.70	123.63
33	d	410	LHG	O8-C6-C5	-2.77	100.42	108.40
29	h	104	DGD	C3D-C4D-C5D	-2.76	105.22	110.23
24	B	611	CLA	C3B-C4B-NB	-2.76	108.06	110.53
27	D	406	PL9	C12-C13-C14	-2.76	121.30	127.62
24	B	614	CLA	C4-C3-C5	2.76	120.02	115.23
24	A	408	CLA	C4-C3-C5	2.76	120.02	115.23
32	M	101	LMG	O6-C1-O1	-2.76	103.52	110.04
24	B	615	CLA	C4-C3-C5	-2.76	110.44	115.23
24	C	503	CLA	O2D-CGD-CBD	2.76	116.05	111.23
26	t	101	BCR	C24-C23-C22	-2.76	122.16	126.23
24	B	616	CLA	O1D-CGD-CBD	2.75	129.95	124.52
24	b	613	CLA	CHB-C4A-NA	2.75	128.37	124.40
24	C	510	CLA	C1-C2-C3	-2.75	121.69	126.20
24	b	606	CLA	C3B-C4B-NB	-2.75	108.08	110.53
29	a	412	DGD	O3G-C3G-C2G	-2.75	104.71	111.77
32	M	101	LMG	C9-C8-C7	-2.75	105.38	111.78
28	a	410	SQD	O10-C23-C24	-2.74	113.05	123.78
24	d	403	CLA	C4D-CHA-C1A	2.74	124.52	121.24
24	d	404	CLA	C6-C5-C3	2.74	120.15	113.47
29	H	102	DGD	CDB-CCB-CBB	-2.74	100.51	114.37
24	c	506	CLA	CHA-C1A-NA	-2.74	120.19	126.39
26	C	515	BCR	C15-C14-C13	-2.74	123.44	127.28
27	D	406	PL9	C50-C49-C48	-2.74	114.44	122.66
33	e	101	LHG	O8-C23-C24	2.74	120.18	111.83
24	b	614	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
24	C	507	CLA	C1-C2-C3	-2.73	121.72	126.20
24	b	608	CLA	O1D-CGD-CBD	2.73	129.90	124.52
28	a	410	SQD	O9-S-O7	-2.73	104.96	113.82
27	d	407	PL9	C41-C39-C38	-2.73	115.05	121.17
24	C	505	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
24	b	614	CLA	C2C-C1C-NC	2.72	112.84	109.98
32	M	101	LMG	O3-C3-C2	-2.72	103.96	110.38
32	d	411	LMG	C6-C5-C4	-2.72	106.33	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	103	BCR	C35-C13-C12	2.72	122.25	118.09
33	D	409	LHG	O8-C23-C24	2.72	120.13	111.83
26	H	101	BCR	C27-C26-C25	2.72	126.38	122.70
32	c	524	LMG	O8-C28-O10	-2.72	116.83	123.63
24	C	505	CLA	CHB-C4A-NA	2.72	128.32	124.40
24	b	612	CLA	CHD-C1D-C2D	2.72	131.13	125.49
24	c	501	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	C	513	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
24	d	403	CLA	CHB-C4A-NA	2.71	128.31	124.40
24	c	506	CLA	C4-C3-C5	2.70	119.92	115.23
32	M	101	LMG	C37-C36-C35	-2.70	100.70	114.37
24	b	612	CLA	CHD-C1D-ND	-2.70	121.00	124.80
24	c	507	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	a	404	CLA	CHB-C4A-NA	2.70	128.29	124.40
32	b	621	LMG	O8-C28-O10	-2.69	116.89	123.63
24	B	609	CLA	CHA-C1A-NA	-2.69	120.29	126.39
25	A	407	PHO	C1-O2A-CGA	2.69	123.16	116.65
29	C	518	DGD	CDB-CCB-CBB	-2.69	100.78	114.37
32	D	407	LMG	O3-C3-C2	-2.69	104.04	110.38
25	A	407	PHO	OBD-CAD-CBD	-2.69	121.88	125.82
26	b	619	BCR	C11-C10-C9	-2.69	123.51	127.28
26	A	409	BCR	C29-C28-C27	2.69	117.18	111.28
27	A	410	PL9	C27-C28-C29	-2.69	121.47	127.62
26	b	619	BCR	C27-C26-C25	2.69	126.33	122.70
32	D	407	LMG	O2-C2-C1	-2.68	103.69	110.08
26	A	409	BCR	C2-C1-C6	2.68	114.33	110.44
24	C	514	CLA	C1-O2A-CGA	-2.67	110.18	116.65
24	b	610	CLA	CHB-C4A-NA	2.67	128.26	124.40
29	a	412	DGD	O1G-C1A-O1A	-2.67	116.94	123.63
28	B	622	SQD	O47-C45-C46	2.67	117.92	108.34
24	B	603	CLA	CHD-C4C-NC	2.67	128.37	124.23
24	C	502	CLA	O2A-CGA-O1A	-2.66	116.96	123.63
24	a	407	CLA	CHB-C4A-NA	2.66	128.24	124.40
32	b	621	LMG	C40-C39-C38	-2.66	100.91	114.37
24	b	604	CLA	CHD-C1D-ND	-2.66	121.06	124.80
26	d	406	BCR	C27-C26-C25	2.66	126.30	122.70
24	C	507	CLA	O2A-CGA-O1A	-2.66	116.99	123.63
24	b	613	CLA	CHD-C1D-ND	-2.65	121.07	124.80
25	A	407	PHO	O1D-CGD-CBD	2.65	128.75	124.72
24	B	608	CLA	CAA-CBA-CGA	-2.65	105.67	113.21
29	c	518	DGD	C3D-C4D-C5D	-2.65	105.42	110.23
28	A	411	SQD	O48-C23-O10	-2.65	116.99	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
24	B	608	CLA	CHB-C4A-NA	2.65	128.23	124.40
24	C	508	CLA	CHD-C1D-ND	-2.65	121.07	124.80
26	H	101	BCR	C29-C30-C25	2.65	114.29	110.44
24	C	509	CLA	C3B-C4B-NB	-2.65	108.17	110.53
32	c	524	LMG	O6-C1-O1	-2.65	103.79	110.04
34	F	102	HEM	CBA-CAA-C2A	-2.65	105.22	112.53
32	b	621	LMG	O6-C1-O1	-2.64	103.81	110.04
27	d	407	PL9	C36-C34-C33	-2.64	115.25	121.17
27	A	410	PL9	C36-C34-C33	-2.64	115.25	121.17
26	c	514	BCR	C33-C5-C6	-2.63	121.61	124.48
33	D	408	LHG	O8-C23-O10	-2.63	117.04	123.63
25	d	402	PHO	CMB-C2B-C3B	2.63	129.94	124.68
34	e	102	HEM	C3B-C2B-C1B	2.63	108.39	106.41
28	f	101	SQD	O9-S-O7	-2.63	105.27	113.82
29	c	517	DGD	C8B-C7B-C6B	-2.63	101.08	114.37
32	C	501	LMG	C38-C37-C36	-2.63	101.08	114.37
24	c	509	CLA	CHB-C4A-NA	2.63	128.19	124.40
24	h	101	CLA	O2D-CGD-CBD	2.62	115.81	111.23
24	C	513	CLA	C7-C6-C5	-2.62	106.28	113.26
24	a	407	CLA	CAA-CBA-CGA	-2.61	105.79	113.21
25	a	406	PHO	OBD-CAD-C3D	2.61	131.97	127.89
24	c	511	CLA	CHB-C1B-NB	2.61	127.97	124.05
27	A	410	PL9	C20-C19-C21	2.61	119.76	115.23
24	b	608	CLA	C2D-C1D-ND	-2.61	107.54	110.13
24	C	502	CLA	CHD-C1D-ND	-2.61	121.13	124.80
26	C	515	BCR	C35-C13-C14	-2.61	118.59	122.82
26	a	408	BCR	C38-C26-C27	-2.60	108.04	113.60
24	b	604	CLA	C5-C3-C2	-2.60	115.32	121.17
24	c	502	CLA	C3B-C4B-NB	-2.60	108.21	110.53
26	H	101	BCR	C38-C26-C25	-2.60	121.64	124.48
24	B	614	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	d	405	CLA	O1D-CGD-CBD	2.60	129.64	124.52
24	d	405	CLA	C4A-NA-C1A	2.60	107.86	106.68
24	B	602	CLA	C3B-C4B-NB	-2.60	108.21	110.53
24	c	509	CLA	O2A-CGA-CBA	2.60	119.75	111.83
29	C	516	DGD	C3D-C4D-C5D	-2.60	105.53	110.23
24	b	606	CLA	O1A-CGA-CBA	2.60	133.93	123.78
26	B	619	BCR	C12-C13-C14	-2.59	114.93	119.01
24	c	506	CLA	CHC-C4B-NB	2.59	127.94	124.05
33	D	409	LHG	O8-C6-C5	-2.59	100.92	108.40
24	c	508	CLA	O2D-CGD-O1D	-2.59	118.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C24-C23-C22	-2.59	122.41	126.23
24	B	603	CLA	CHD-C4C-C3C	-2.59	121.00	124.77
24	h	101	CLA	C6-C5-C3	-2.59	107.17	113.47
25	d	402	PHO	C1-C2-C3	-2.59	121.96	126.20
24	B	608	CLA	CHA-C1A-NA	-2.59	120.53	126.39
29	c	517	DGD	O2D-C2D-C1D	-2.58	103.92	110.08
24	B	610	CLA	C1D-ND-C4D	-2.58	104.50	106.31
24	c	507	CLA	CHC-C4B-NB	2.58	127.92	124.05
29	H	102	DGD	C3G-C2G-C1G	-2.58	105.78	111.78
33	l	101	LHG	O8-C23-O10	-2.58	117.18	123.63
24	b	610	CLA	CHD-C1D-ND	-2.58	121.18	124.80
27	d	407	PL9	C40-C39-C38	-2.58	117.01	123.63
24	h	101	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
24	C	503	CLA	CAA-C2A-C3A	-2.57	106.04	113.00
24	A	405	CLA	CHD-C1D-ND	-2.57	121.18	124.80
24	b	615	CLA	CMB-C2B-C3B	2.57	132.60	126.55
24	c	503	CLA	C7-C6-C5	-2.57	106.41	113.26
26	C	515	BCR	C15-C16-C17	-2.57	118.26	123.52
24	B	609	CLA	CED-O2D-CGD	2.57	121.74	115.92
26	c	515	BCR	C15-C16-C17	-2.56	118.27	123.52
24	C	508	CLA	CAA-CBA-CGA	-2.56	105.93	113.21
27	D	406	PL9	O1-C4-C3	-2.56	118.03	120.73
26	b	618	BCR	C24-C23-C22	-2.56	122.45	126.23
32	K	102	LMG	O2-C2-C1	-2.56	103.98	110.08
26	B	618	BCR	C16-C15-C14	-2.56	118.28	123.52
33	l	101	LHG	O8-C23-C24	2.55	119.62	111.83
33	d	410	LHG	C25-C24-C23	2.55	123.05	113.69
24	a	405	CLA	O2D-CGD-CBD	2.55	115.69	111.23
29	C	517	DGD	C1D-C2D-C3D	-2.55	104.65	110.01
29	h	104	DGD	O2D-C2D-C1D	-2.55	104.00	110.08
24	B	603	CLA	C6-C5-C3	2.55	119.67	113.47
24	B	601	CLA	CAA-C2A-C3A	-2.55	106.12	113.00
24	d	405	CLA	C1-C2-C3	-2.55	122.03	126.20
29	C	516	DGD	O6D-C1D-O3G	-2.55	104.03	110.04
29	c	516	DGD	C3G-C2G-C1G	-2.54	105.85	111.78
26	B	618	BCR	C11-C10-C9	-2.54	123.71	127.28
26	b	619	BCR	C33-C5-C6	-2.54	121.71	124.48
29	C	517	DGD	O2D-C2D-C1D	-2.54	104.02	110.08
25	a	406	PHO	OBD-CAD-CBD	-2.54	122.09	125.82
24	B	610	CLA	CHD-C1D-ND	-2.54	121.22	124.80
24	C	506	CLA	C4A-NA-C1A	2.54	107.84	106.68
24	C	504	CLA	C4D-CHA-C1A	2.54	124.27	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	C4-C3-C2	-2.54	117.11	123.63
27	A	410	PL9	C30-C29-C28	-2.54	117.11	123.63
24	B	606	CLA	CGD-CBD-CAD	-2.54	102.64	110.85
25	d	402	PHO	C3D-C4D-ND	2.53	110.95	107.71
33	d	408	LHG	C11-C10-C9	-2.53	101.56	114.37
26	b	620	BCR	C38-C26-C25	-2.53	121.72	124.48
24	C	505	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
26	C	515	BCR	C38-C26-C25	-2.53	121.73	124.48
24	b	616	CLA	CED-O2D-CGD	2.53	121.65	115.92
26	b	619	BCR	C35-C13-C12	2.53	121.95	118.09
29	C	516	DGD	O5D-C6D-C5D	-2.53	103.73	109.42
32	K	102	LMG	C38-C37-C36	-2.52	101.61	114.37
24	D	402	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	a	407	CLA	C4A-NA-C1A	2.52	107.83	106.68
24	C	514	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
24	b	607	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
29	C	517	DGD	O5D-C1E-C2E	2.51	112.09	108.27
24	b	615	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
27	D	406	PL9	C20-C19-C21	2.51	119.59	115.23
32	b	621	LMG	C9-C8-C7	-2.51	105.93	111.78
24	c	503	CLA	C5-C3-C2	-2.51	115.53	121.17
24	B	609	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
24	B	606	CLA	C6-C5-C3	-2.51	107.36	113.47
24	c	513	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
28	f	101	SQD	O48-C23-O10	-2.50	117.37	123.63
29	C	518	DGD	O2D-C2D-C1D	-2.50	104.12	110.08
24	C	512	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
24	B	611	CLA	C4A-NA-C1A	2.50	107.82	106.68
24	c	513	CLA	C3B-C4B-NB	-2.50	108.30	110.53
29	c	516	DGD	CDB-CCB-CBB	-2.50	101.75	114.37
32	c	522	LMG	O7-C10-O9	-2.50	117.87	123.70
24	B	613	CLA	C1-C2-C3	-2.50	122.11	126.20
26	b	619	BCR	C16-C15-C14	-2.49	118.42	123.52
24	C	514	CLA	CHB-C4A-NA	2.49	128.00	124.40
24	B	609	CLA	C1D-CHD-C4C	-2.49	120.73	126.02
24	b	613	CLA	C11-C12-C13	-2.49	107.69	115.97
24	b	609	CLA	C11-C10-C8	-2.49	107.69	115.97
24	b	615	CLA	O1D-CGD-CBD	2.49	129.43	124.52
26	c	515	BCR	C2-C1-C6	2.49	114.05	110.44
24	C	506	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
24	b	616	CLA	C2B-C1B-NB	-2.48	107.75	110.33
24	b	609	CLA	O2D-CGD-O1D	-2.48	119.02	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
28	f	101	SQD	O47-C7-C8	2.48	120.03	110.93
28	A	411	SQD	C3-C4-C5	2.48	114.72	110.23
29	H	102	DGD	C1D-C2D-C3D	-2.48	104.80	110.01
24	C	509	CLA	C2D-C1D-ND	-2.48	107.68	110.13
24	b	612	CLA	C4A-NA-C1A	2.47	107.81	106.68
29	C	518	DGD	O6D-C1D-O3G	-2.47	104.20	110.04
24	B	602	CLA	CHA-C1A-NA	-2.47	120.79	126.39
29	H	102	DGD	C1E-O6E-C5E	2.47	118.54	113.72
24	c	506	CLA	C2A-C1A-CHA	2.47	128.15	123.87
32	b	623	LMG	C1-O6-C5	-2.47	108.91	113.72
29	C	517	DGD	O5D-C6D-C5D	-2.46	103.87	109.42
29	C	518	DGD	O1G-C1A-C2A	-2.46	104.33	111.83
24	c	513	CLA	CHB-C4A-NA	2.46	127.95	124.40
32	b	623	LMG	O2-C2-C1	-2.46	104.21	110.08
24	d	405	CLA	CHD-C1D-C2D	2.46	130.61	125.49
29	C	518	DGD	C3G-C2G-C1G	-2.46	106.05	111.78
26	c	514	BCR	C24-C23-C22	-2.46	122.59	126.23
27	d	407	PL9	C50-C49-C48	-2.46	115.27	122.66
28	a	411	SQD	O49-C7-C8	-2.46	114.17	123.78
32	C	501	LMG	C1-O6-C5	-2.46	108.92	113.72
33	d	408	LHG	O8-C23-C24	2.46	119.33	111.83
26	b	619	BCR	C35-C13-C14	-2.46	118.84	122.82
24	B	613	CLA	CAC-C3C-C4C	2.46	127.98	124.79
35	v	201	HEC	C3D-C4D-ND	-2.46	107.43	110.15
26	c	514	BCR	C11-C10-C9	-2.45	123.84	127.28
24	b	615	CLA	CMD-C2D-C1D	2.45	129.05	124.73
26	D	405	BCR	C16-C15-C14	-2.45	118.50	123.52
33	d	408	LHG	O8-C6-C5	-2.45	101.33	108.40
24	c	507	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
24	B	615	CLA	CHB-C4A-NA	2.45	127.94	124.40
26	C	519	BCR	C11-C10-C9	-2.45	123.85	127.28
24	A	408	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	A	405	CLA	C4D-C3D-CAD	-2.44	105.45	108.11
24	C	511	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	C	513	CLA	CAA-CBA-CGA	-2.44	106.28	113.21
29	c	517	DGD	CDB-CCB-CBB	-2.44	102.03	114.37
24	C	508	CLA	CHC-C4B-NB	2.44	127.71	124.05
24	b	607	CLA	CHB-C1B-NB	2.44	127.71	124.05
26	c	515	BCR	C1-C6-C5	-2.44	119.30	122.64
24	c	504	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	h	101	CLA	CHD-C1D-ND	-2.44	121.37	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	C1-C2-C3	-2.44	122.21	126.20
24	B	609	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
28	a	410	SQD	O48-C23-C24	2.43	119.26	111.83
24	c	505	CLA	O2D-CGD-CBD	2.43	115.48	111.23
24	A	406	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
24	A	406	CLA	CAC-C3C-C4C	2.43	127.95	124.79
24	C	503	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
26	t	101	BCR	C19-C18-C17	-2.43	115.19	119.01
24	B	609	CLA	O1D-CGD-CBD	2.43	129.30	124.52
32	c	522	LMG	C9-C8-C7	-2.42	106.14	111.78
24	c	509	CLA	C3A-C2A-C1A	2.42	104.97	101.34
24	C	504	CLA	O2A-C1-C2	-2.42	98.79	108.11
28	A	412	SQD	O48-C23-C24	2.42	119.22	111.83
24	D	402	CLA	CHD-C1D-ND	-2.42	121.40	124.80
29	A	413	DGD	CDB-CCB-CBB	-2.42	102.15	114.37
24	B	612	CLA	C9-C8-C10	-2.42	102.66	111.27
24	B	610	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	c	504	CLA	C7-C6-C5	-2.41	106.83	113.26
24	B	604	CLA	C11-C12-C13	-2.41	107.95	115.97
29	h	104	DGD	O6D-C1D-O3G	-2.41	104.34	110.04
24	B	604	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
25	D	401	PHO	CBC-CAC-C3C	2.41	116.32	112.87
32	b	623	LMG	C8-O7-C10	2.41	123.56	117.80
24	b	611	CLA	CHA-C1A-NA	-2.41	120.94	126.39
24	B	604	CLA	C1-C2-C3	2.41	130.14	126.20
26	h	103	BCR	C2-C1-C6	2.41	113.94	110.44
28	F	101	SQD	C44-O6-C1	2.41	117.79	113.68
24	b	613	CLA	C1-C2-C3	-2.41	122.25	126.20
24	C	506	CLA	CMD-C2D-C1D	-2.41	120.49	124.73
25	a	406	PHO	C1-C2-C3	-2.40	122.26	126.20
24	b	605	CLA	C4-C3-C5	2.40	119.40	115.23
28	f	101	SQD	O8-S-C6	2.40	110.61	105.97
29	c	516	DGD	CBB-CAB-C9B	-2.40	102.22	114.37
24	D	404	CLA	CMB-C2B-C1B	2.40	129.08	125.42
27	d	407	PL9	C8-C7-C3	2.40	118.24	112.03
29	c	517	DGD	O5D-C6D-C5D	-2.40	104.01	109.42
24	c	505	CLA	C6-C7-C8	-2.40	107.98	115.97
24	C	505	CLA	CHD-C4C-C3C	-2.40	121.28	124.77
24	D	403	CLA	CHC-C4B-NB	2.40	127.65	124.05
24	B	615	CLA	C4-C3-C2	2.40	129.79	123.63
24	C	504	CLA	C5-C3-C2	-2.40	115.78	121.17
26	h	103	BCR	C7-C8-C9	-2.40	122.69	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	CHA-C1A-NA	-2.40	120.97	126.39
33	d	408	LHG	O8-C23-O10	-2.39	117.64	123.63
26	B	619	BCR	C15-C16-C17	-2.39	118.62	123.52
29	h	104	DGD	CDB-CCB-CBB	-2.39	102.28	114.37
29	c	516	DGD	O6E-C5E-C4E	2.39	114.01	109.70
24	c	504	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
26	c	521	BCR	C24-C23-C22	-2.39	122.70	126.23
26	Y	101	BCR	C39-C30-C25	-2.39	106.50	110.24
24	C	503	CLA	C4D-CHA-C1A	2.39	124.09	121.24
24	b	614	CLA	CHB-C4A-NA	2.39	127.84	124.40
33	D	408	LHG	C11-C10-C9	-2.39	102.30	114.37
24	B	601	CLA	C2A-C1A-CHA	2.38	128.01	123.87
29	c	518	DGD	O1G-C1A-C2A	-2.38	104.56	111.83
24	B	606	CLA	CHB-C1B-NB	2.38	127.63	124.05
24	c	512	CLA	C3B-C4B-NB	-2.38	108.40	110.53
24	c	501	CLA	CMB-C2B-C3B	2.38	132.15	126.55
24	b	605	CLA	CHC-C1C-C2C	-2.38	120.18	126.95
29	C	516	DGD	CCB-CBB-CAB	-2.38	102.34	114.37
24	b	606	CLA	CHD-C1D-ND	-2.38	121.46	124.80
26	t	101	BCR	C7-C8-C9	-2.38	122.72	126.23
29	H	102	DGD	C8B-C7B-C6B	-2.38	102.36	114.37
26	t	101	BCR	C27-C26-C25	2.37	125.91	122.70
24	c	509	CLA	CHD-C1D-ND	-2.37	121.46	124.80
24	b	613	CLA	CAC-C3C-C4C	2.37	127.88	124.79
24	a	404	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
26	b	620	BCR	C8-C7-C6	-2.37	120.66	127.00
24	d	405	CLA	CHA-C1A-NA	-2.37	121.02	126.39
24	b	614	CLA	CAC-C3C-C4C	2.37	127.88	124.79
26	t	101	BCR	C11-C10-C9	-2.37	123.95	127.28
32	b	621	LMG	C38-C37-C36	-2.37	102.39	114.37
24	B	611	CLA	C14-C13-C15	-2.37	102.83	111.27
27	d	407	PL9	C7-C8-C9	-2.37	122.75	126.83
26	b	618	BCR	C32-C1-C6	-2.37	106.53	110.24
26	B	617	BCR	C35-C13-C14	-2.36	118.98	122.82
24	b	604	CLA	C7-C6-C5	-2.36	106.96	113.26
24	B	609	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
24	B	603	CLA	C4D-C3D-CAD	-2.36	105.54	108.11
24	C	514	CLA	CMB-C2B-C3B	2.36	132.11	126.55
24	B	602	CLA	CHA-C4D-ND	2.36	137.42	132.55
28	F	101	SQD	C1-O5-C5	-2.36	109.11	113.72
24	B	611	CLA	CHC-C4B-NB	2.36	127.59	124.05
24	B	602	CLA	C4D-CHA-C1A	-2.36	118.43	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	CDB-CCB-CBB	-2.36	102.45	114.37
29	a	412	DGD	O2G-C2G-C1G	2.36	116.80	108.34
24	B	610	CLA	CHD-C4C-NC	2.36	127.88	124.23
26	b	602	BCR	C33-C5-C6	-2.35	121.92	124.48
24	B	612	CLA	CHB-C4A-NA	2.35	127.80	124.40
24	B	613	CLA	CHC-C4B-NB	2.35	127.58	124.05
24	C	513	CLA	CHD-C1D-ND	-2.35	121.49	124.80
24	d	403	CLA	CAC-C3C-C4C	2.35	127.84	124.79
24	B	613	CLA	CHA-C1A-NA	-2.35	121.08	126.39
24	a	407	CLA	CMD-C2D-C3D	2.35	133.07	127.69
32	M	101	LMG	C35-C34-C33	-2.34	102.52	114.37
26	h	103	BCR	C3-C4-C5	-2.34	109.88	114.06
27	d	407	PL9	C45-C44-C46	-2.34	111.16	115.23
24	A	408	CLA	C4A-NA-C1A	2.34	107.75	106.68
29	a	412	DGD	C1G-O1G-C1A	2.34	125.68	117.12
24	c	507	CLA	O1D-CGD-CBD	2.34	129.14	124.52
28	a	410	SQD	O5-C5-C4	2.34	113.92	109.70
27	D	406	PL9	C7-C8-C9	-2.34	122.80	126.83
24	B	611	CLA	CHD-C1D-C2D	2.34	130.36	125.49
28	F	101	SQD	C4-C3-C2	2.34	114.94	110.83
24	B	604	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
28	B	622	SQD	O10-C23-C24	-2.34	114.63	123.78
26	t	101	BCR	C36-C18-C19	2.34	121.66	118.09
24	C	513	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
24	B	612	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
24	B	614	CLA	CHD-C1D-ND	-2.34	121.52	124.80
24	C	505	CLA	CMB-C2B-C3B	2.33	132.04	126.55
24	B	610	CLA	C11-C10-C8	-2.33	108.20	115.97
24	c	506	CLA	C1-C2-C3	-2.33	122.37	126.20
24	b	609	CLA	C6-C7-C8	-2.33	108.21	115.97
24	B	606	CLA	C1-C2-C3	-2.33	122.38	126.20
29	c	517	DGD	CBB-CAB-C9B	-2.33	102.58	114.37
26	c	514	BCR	C15-C14-C13	-2.33	124.01	127.28
24	d	405	CLA	OBD-CAD-C3D	2.33	133.86	128.42
27	A	410	PL9	C7-C3-C2	-2.33	120.64	123.39
24	a	407	CLA	C2C-C1C-NC	2.33	112.42	109.98
24	B	611	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
33	l	101	LHG	O10-C23-C24	-2.32	114.70	123.78
24	b	617	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	b	612	CLA	C2D-C1D-ND	-2.32	107.83	110.13
26	h	103	BCR	C15-C14-C13	-2.32	124.03	127.28
24	b	613	CLA	C3B-C4B-NB	-2.32	108.46	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	621	LMG	O7-C10-C11	2.32	116.49	111.48
24	b	608	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	b	606	CLA	C16-C15-C13	-2.31	108.27	115.97
24	h	101	CLA	CHB-C1B-NB	2.31	127.52	124.05
26	K	101	BCR	C24-C23-C22	-2.31	122.81	126.23
26	c	515	BCR	C4-C5-C6	2.31	125.83	122.70
32	c	524	LMG	O5-C6-C5	-2.31	103.47	111.33
24	a	407	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
24	B	613	CLA	C2A-C1A-CHA	2.31	127.87	123.87
24	d	405	CLA	CHB-C1B-NB	2.31	127.51	124.05
24	d	404	CLA	CMB-C2B-C3B	2.30	131.97	126.55
24	C	504	CLA	C6-C5-C3	2.30	119.08	113.47
27	a	409	PL9	C36-C34-C33	-2.30	116.00	121.17
24	B	613	CLA	C1D-ND-C4D	-2.30	104.70	106.31
25	d	402	PHO	O2D-CGD-O1D	-2.30	119.37	123.85
28	F	101	SQD	O6-C1-C2	2.30	111.77	108.27
27	D	406	PL9	C11-C9-C8	-2.30	116.00	121.17
27	A	410	PL9	C25-C24-C26	2.30	119.22	115.23
24	c	501	CLA	CHA-C1A-NA	-2.30	121.19	126.39
24	A	405	CLA	C3A-C2A-C1A	2.30	104.78	101.34
24	c	504	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
26	C	519	BCR	C15-C14-C13	-2.30	124.06	127.28
25	A	407	PHO	C3D-C4D-ND	2.30	110.65	107.71
26	H	101	BCR	C16-C17-C18	-2.29	124.06	127.28
24	b	614	CLA	C7-C6-C5	-2.29	107.15	113.26
24	b	612	CLA	C1-C2-C3	-2.29	122.44	126.20
24	b	604	CLA	C4A-NA-C1A	2.29	107.72	106.68
26	c	521	BCR	C40-C30-C25	2.29	113.84	110.24
29	C	518	DGD	CBB-CAB-C9B	-2.29	102.79	114.37
24	a	407	CLA	CMD-C2D-C1D	-2.29	120.69	124.73
24	c	505	CLA	CED-O2D-CGD	-2.29	110.72	115.92
35	V	201	HEC	CHD-C4C-NC	2.29	126.95	124.45
24	b	609	CLA	CHA-C1A-NA	-2.29	121.21	126.39
24	b	606	CLA	CHD-C4C-NC	2.29	127.78	124.23
26	b	618	BCR	C8-C7-C6	-2.29	120.89	127.00
24	C	506	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
25	D	401	PHO	C3D-C4D-ND	2.29	110.64	107.71
24	b	606	CLA	CHA-C1A-NA	-2.29	121.22	126.39
33	D	408	LHG	C20-C19-C18	-2.28	102.83	114.37
24	b	604	CLA	CGD-CBD-CAD	-2.28	103.46	110.85
26	t	101	BCR	C38-C26-C27	-2.28	108.73	113.60
27	a	409	PL9	C40-C39-C38	-2.28	117.77	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	101	LMG	C1-O6-C5	-2.28	109.27	113.72
29	a	412	DGD	C5B-C4B-C3B	-2.28	102.86	114.37
24	b	607	CLA	O2D-CGD-CBD	2.27	115.21	111.23
24	c	502	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
24	C	502	CLA	C3D-C4D-ND	2.27	113.68	109.99
24	b	609	CLA	CMB-C2B-C3B	2.27	131.89	126.55
24	C	510	CLA	CHA-C1A-NA	-2.27	121.25	126.39
24	c	507	CLA	CHD-C4C-C3C	-2.27	121.46	124.77
24	D	403	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
24	b	610	CLA	C4A-NA-C1A	2.27	107.71	106.68
29	a	412	DGD	CDB-CCB-CBB	-2.27	102.90	114.37
26	a	408	BCR	C24-C23-C22	-2.27	122.88	126.23
26	c	515	BCR	C30-C25-C26	-2.27	119.54	122.64
24	c	512	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
32	C	501	LMG	C1-C2-C3	-2.27	105.24	110.01
26	D	405	BCR	C24-C23-C22	-2.27	122.88	126.23
24	b	610	CLA	CHD-C4C-NC	2.26	127.74	124.23
24	A	406	CLA	CHB-C4A-NA	2.26	127.67	124.40
24	A	406	CLA	CMB-C2B-C3B	2.26	131.87	126.55
24	b	617	CLA	C4-C3-C5	2.26	119.15	115.23
25	a	406	PHO	CMB-C2B-C3B	2.26	129.20	124.68
24	b	616	CLA	C1-O2A-CGA	2.26	122.12	116.65
24	d	404	CLA	O1D-CGD-CBD	2.26	128.97	124.52
33	D	411	LHG	C18-C17-C16	-2.26	102.95	114.37
24	B	615	CLA	C6-C7-C8	-2.26	108.46	115.97
33	d	409	LHG	O8-C23-O10	-2.26	117.98	123.63
26	C	515	BCR	C35-C13-C12	2.25	121.53	118.09
24	b	611	CLA	O1D-CGD-CBD	2.25	128.96	124.52
24	C	510	CLA	C3B-C4B-NB	-2.25	108.52	110.53
32	M	101	LMG	O5-C6-C5	-2.25	103.67	111.33
27	d	407	PL9	C27-C28-C29	-2.25	122.47	127.62
24	c	511	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
29	A	413	DGD	O3G-C3G-C2G	-2.25	105.35	110.82
25	a	406	PHO	C3D-C4D-ND	2.25	110.59	107.71
26	b	618	BCR	C27-C26-C25	2.25	125.74	122.70
24	C	504	CLA	CHA-C1A-NA	-2.25	121.30	126.39
29	A	413	DGD	C5B-C4B-C3B	-2.25	103.01	114.37
24	B	616	CLA	C3B-C4B-NB	-2.25	108.52	110.53
24	b	615	CLA	CHC-C4B-NB	2.25	127.42	124.05
24	B	605	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
26	B	618	BCR	C35-C13-C14	-2.24	119.18	122.82
24	c	502	CLA	C1-O2A-CGA	2.24	122.08	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C4-C3-C5	2.24	119.12	115.23
26	h	103	BCR	C34-C9-C8	-2.24	114.66	118.09
24	A	406	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
26	a	408	BCR	C20-C21-C22	-2.24	124.14	127.28
24	B	613	CLA	CHB-C4A-NA	2.24	127.63	124.40
24	c	502	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
24	C	505	CLA	CHD-C1D-ND	-2.24	121.65	124.80
24	C	506	CLA	CHB-C1B-NB	2.23	127.40	124.05
24	b	606	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
27	D	406	PL9	C40-C39-C38	-2.23	117.89	123.63
24	b	609	CLA	C6-C5-C3	-2.23	108.03	113.47
24	D	403	CLA	C4A-NA-C1A	2.23	107.70	106.68
29	h	104	DGD	CBB-CAB-C9B	-2.23	103.08	114.37
26	b	620	BCR	C16-C15-C14	-2.23	118.95	123.52
26	B	617	BCR	C33-C5-C6	-2.23	122.05	124.48
24	c	502	CLA	CHB-C4A-NA	2.23	127.62	124.40
32	M	101	LMG	C22-C21-C20	-2.23	103.08	114.37
24	C	510	CLA	CHD-C1D-ND	-2.23	121.66	124.80
26	b	619	BCR	C15-C16-C17	-2.23	118.95	123.52
32	h	102	LMG	O7-C10-O9	-2.23	117.59	123.33
27	a	409	PL9	C32-C33-C34	-2.23	122.53	127.62
26	c	514	BCR	C38-C26-C25	-2.23	122.05	124.48
29	C	516	DGD	C7B-C6B-C5B	-2.23	103.12	114.37
27	a	409	PL9	C12-C13-C14	-2.22	122.53	127.62
32	c	519	LMG	C40-C39-C38	-2.22	103.12	114.37
32	C	501	LMG	O7-C10-O9	-2.22	118.50	123.70
26	B	619	BCR	C27-C26-C25	2.22	125.71	122.70
32	c	519	LMG	O7-C10-O9	-2.22	118.70	122.99
27	A	410	PL9	C40-C39-C38	-2.22	117.92	123.63
24	c	512	CLA	CHA-C1A-NA	-2.22	121.36	126.39
24	C	512	CLA	C4-C3-C5	2.22	119.08	115.23
29	C	516	DGD	CDB-CCB-CBB	-2.22	103.15	114.37
24	B	601	CLA	CHA-C4D-ND	2.22	137.13	132.55
26	h	103	BCR	C35-C13-C14	-2.22	119.22	122.82
32	M	101	LMG	C38-C37-C36	-2.22	103.15	114.37
24	C	508	CLA	CGD-CBD-CAD	-2.22	103.67	110.85
26	a	408	BCR	C11-C10-C9	-2.22	124.17	127.28
29	C	517	DGD	O3E-C3E-C2E	-2.22	105.15	110.38
24	c	508	CLA	C4A-NA-C1A	2.22	107.69	106.68
35	v	201	HEC	CHD-C1D-ND	2.22	127.88	123.86
24	c	506	CLA	CED-O2D-CGD	2.21	120.94	115.92
24	C	507	CLA	CMB-C2B-C1B	-2.21	122.05	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	104	DGD	C1E-O6E-C5E	2.21	118.04	113.72
24	B	609	CLA	C7-C6-C5	-2.21	107.36	113.26
24	c	509	CLA	C4D-C3D-CAD	-2.21	105.70	108.11
24	b	603	CLA	CHC-C1C-C2C	-2.21	120.66	126.95
25	A	407	PHO	C6-C7-C8	-2.21	108.61	115.97
24	C	503	CLA	C4D-C3D-CAD	-2.21	105.71	108.11
24	C	502	CLA	CHB-C1B-NB	2.21	127.36	124.05
24	B	602	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
24	a	405	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
26	c	514	BCR	C10-C11-C12	-2.20	116.81	123.20
32	K	102	LMG	O1-C1-C2	-2.20	104.92	108.27
35	v	201	HEC	CAD-CBD-CGD	-2.20	107.82	113.67
24	B	611	CLA	CHB-C4A-NA	2.20	127.58	124.40
28	b	601	SQD	O47-C7-C8	2.20	116.25	111.48
24	B	616	CLA	CHB-C4A-NA	2.20	127.58	124.40
25	d	402	PHO	O2D-CGD-CBD	-2.20	108.53	110.95
29	C	516	DGD	CAB-C9B-C8B	-2.20	103.24	114.37
24	D	402	CLA	C16-C15-C13	-2.20	108.65	115.97
28	F	101	SQD	O5-C5-C4	2.20	113.67	109.70
24	B	603	CLA	CHA-C1A-NA	-2.20	121.41	126.39
26	C	519	BCR	C27-C26-C25	2.20	125.68	122.70
26	c	521	BCR	C16-C15-C14	-2.20	119.02	123.52
29	c	517	DGD	C1D-C2D-C3D	-2.20	105.38	110.01
24	B	607	CLA	O1A-CGA-CBA	2.20	132.38	123.78
24	C	511	CLA	O2D-CGD-CBD	2.20	115.07	111.23
24	b	605	CLA	C11-C10-C8	-2.20	108.66	115.97
27	a	409	PL9	C27-C28-C29	-2.20	122.60	127.62
26	b	620	BCR	C15-C16-C17	-2.19	119.03	123.52
24	d	403	CLA	CHD-C4C-NC	2.19	127.63	124.23
24	b	604	CLA	C6-C5-C3	2.19	118.81	113.47
24	C	509	CLA	C3C-C4C-NC	-2.19	107.62	110.43
24	C	514	CLA	C4-C3-C5	2.19	119.03	115.23
32	b	623	LMG	C6-C5-C4	-2.19	107.64	113.02
26	Y	101	BCR	C33-C5-C6	-2.19	122.09	124.48
24	C	505	CLA	CHD-C4C-NC	2.19	127.63	124.23
24	b	609	CLA	CHB-C1B-NB	2.19	127.33	124.05
26	b	618	BCR	C29-C30-C25	2.19	113.62	110.44
32	c	519	LMG	C9-C8-C7	-2.19	106.68	111.78
33	l	101	LHG	C11-C10-C9	-2.19	103.31	114.37
24	B	615	CLA	CHB-C1B-NB	2.19	127.33	124.05
24	c	506	CLA	O1D-CGD-CBD	2.18	128.83	124.52
24	b	612	CLA	C11-C10-C8	-2.18	108.70	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	PL9	C8-C7-C3	2.18	117.68	112.03
24	B	616	CLA	CHA-C1A-NA	-2.18	121.44	126.39
24	d	404	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
26	Y	101	BCR	C23-C24-C25	-2.18	121.17	127.00
26	b	620	BCR	C11-C10-C9	-2.18	124.22	127.28
24	C	505	CLA	C6-C5-C3	2.18	118.78	113.47
28	b	601	SQD	O47-C45-C46	2.18	116.17	108.34
24	B	616	CLA	CHC-C4B-NB	2.18	127.32	124.05
26	B	619	BCR	C32-C1-C6	-2.18	106.82	110.24
26	b	618	BCR	C3-C4-C5	-2.18	110.17	114.06
35	v	201	HEC	CHB-C1B-NB	2.18	127.81	123.86
34	e	102	HEM	CHB-C1B-NB	2.18	127.06	124.37
29	C	516	DGD	O2D-C2D-C1D	-2.18	104.88	110.08
24	B	607	CLA	C4-C3-C5	2.18	119.00	115.23
26	C	515	BCR	C11-C10-C9	-2.18	124.23	127.28
26	B	618	BCR	C8-C7-C6	-2.18	121.19	127.00
24	b	603	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
32	C	501	LMG	C36-C35-C34	-2.17	103.38	114.37
29	C	516	DGD	C6B-C5B-C4B	-2.17	103.38	114.37
24	b	608	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
26	B	619	BCR	C15-C14-C13	-2.17	124.23	127.28
32	K	102	LMG	C3-C4-C5	-2.17	106.29	110.23
24	d	404	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
24	C	508	CLA	CHB-C4A-NA	2.17	127.53	124.40
24	D	404	CLA	C3D-C4D-ND	2.17	113.52	109.99
24	B	603	CLA	CMD-C2D-C3D	2.17	132.67	127.69
24	C	503	CLA	CHA-C1A-NA	-2.17	121.48	126.39
24	A	406	CLA	C3B-C4B-NB	-2.17	108.59	110.53
24	D	403	CLA	CBA-CAA-C2A	-2.17	107.34	113.79
25	a	406	PHO	O2A-CGA-O1A	-2.17	118.21	123.63
24	C	508	CLA	C3B-C4B-NB	-2.17	108.59	110.53
24	b	607	CLA	C2C-C1C-NC	2.17	112.26	109.98
24	B	608	CLA	C6-C5-C3	-2.16	108.19	113.47
32	d	411	LMG	C40-C39-C38	-2.16	103.43	114.37
33	D	409	LHG	C11-C10-C9	-2.16	103.43	114.37
24	b	612	CLA	C2C-C1C-NC	2.16	112.25	109.98
26	h	103	BCR	C38-C26-C25	-2.16	122.12	124.48
32	B	621	LMG	C38-C37-C36	-2.16	103.44	114.37
24	c	504	CLA	C1D-ND-C4D	-2.16	104.80	106.31
26	C	515	BCR	C29-C30-C25	2.16	113.57	110.44
27	d	407	PL9	O2-C1-C2	-2.16	116.92	121.83
27	d	407	PL9	C11-C9-C8	-2.16	116.33	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	621	LMG	O1-C1-C2	-2.16	105.00	108.27
24	c	501	CLA	C1-O2A-CGA	-2.15	111.43	116.65
26	A	409	BCR	C8-C7-C6	-2.15	121.24	127.00
26	H	101	BCR	C11-C10-C9	-2.15	124.26	127.28
24	c	511	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
24	b	606	CLA	C4D-CHA-C1A	2.15	123.81	121.24
24	C	507	CLA	CMB-C2B-C3B	2.15	131.61	126.55
24	c	502	CLA	CMB-C2B-C3B	2.15	131.61	126.55
24	B	603	CLA	CHB-C4A-NA	2.15	127.50	124.40
26	d	406	BCR	C38-C26-C25	-2.15	122.14	124.48
26	K	101	BCR	C15-C16-C17	-2.15	119.12	123.52
24	B	605	CLA	C3A-C2A-C1A	2.15	104.56	101.34
24	d	405	CLA	C3D-C4D-ND	2.15	113.48	109.99
29	C	516	DGD	C8B-C7B-C6B	-2.15	103.50	114.37
24	b	613	CLA	C3D-C4D-ND	2.15	113.48	109.99
29	c	517	DGD	C7A-C6A-C5A	-2.15	103.52	114.37
32	B	621	LMG	O7-C10-O9	-2.15	117.81	123.33
24	b	616	CLA	CMB-C2B-C3B	2.14	131.59	126.55
26	c	521	BCR	C30-C25-C26	-2.14	119.70	122.64
28	A	411	SQD	O3-C3-C4	2.14	115.43	110.38
27	a	409	PL9	O1-C4-C3	-2.14	118.47	120.73
29	A	413	DGD	C4A-C3A-C2A	-2.14	105.25	113.13
28	A	411	SQD	O5-C1-C2	-2.14	105.97	110.37
24	d	403	CLA	C11-C12-C13	-2.14	108.85	115.97
24	b	606	CLA	C1-O2A-CGA	-2.14	111.47	116.65
24	C	509	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
32	d	411	LMG	O1-C7-C8	-2.14	105.61	110.82
24	A	408	CLA	C1D-CHD-C4C	-2.14	121.47	126.02
24	b	610	CLA	C5-C3-C2	2.14	125.97	121.17
24	c	502	CLA	CHD-C1D-ND	-2.14	121.79	124.80
24	c	503	CLA	C11-C10-C8	-2.13	108.87	115.97
29	H	102	DGD	CAB-C9B-C8B	-2.13	103.58	114.37
24	c	513	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	b	609	CLA	CHD-C1D-ND	-2.13	121.80	124.80
33	D	409	LHG	C27-C26-C25	-2.13	103.58	114.37
24	b	607	CLA	CHA-C4D-ND	2.13	136.95	132.55
26	C	519	BCR	C8-C7-C6	-2.13	121.31	127.00
24	a	404	CLA	C11-C10-C8	-2.13	108.88	115.97
26	H	101	BCR	C35-C13-C12	2.13	121.34	118.09
24	C	504	CLA	O1D-CGD-CBD	2.13	128.72	124.52
24	b	603	CLA	CHD-C1D-ND	-2.13	121.81	124.80
24	C	504	CLA	CHD-C1D-ND	-2.13	121.81	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	CHD-C1D-C2D	2.13	129.91	125.49
24	c	507	CLA	CHD-C4C-NC	2.13	127.53	124.23
29	C	518	DGD	C5B-C4B-C3B	-2.13	103.62	114.37
26	d	406	BCR	C16-C15-C14	-2.13	119.17	123.52
24	B	603	CLA	CMB-C2B-C3B	2.13	131.55	126.55
27	a	409	PL9	C45-C44-C46	-2.13	111.54	115.23
24	C	502	CLA	C3B-C4B-NB	-2.12	108.64	110.53
33	l	101	LHG	C29-C28-C27	-2.12	103.64	114.37
27	d	407	PL9	C12-C13-C14	-2.12	122.77	127.62
28	A	411	SQD	O4-C4-C3	-2.12	105.38	110.38
24	C	504	CLA	C1-C2-C3	2.12	129.67	126.20
26	k	101	BCR	C1-C6-C5	-2.12	119.74	122.64
29	c	518	DGD	O6E-C1E-O5D	-2.12	105.03	110.04
24	c	507	CLA	C5-C3-C2	-2.12	116.41	121.17
24	B	606	CLA	O1A-CGA-CBA	2.12	132.06	123.78
26	B	617	BCR	C27-C26-C25	2.12	125.56	122.70
24	B	607	CLA	C3B-C4B-NB	-2.12	108.64	110.53
24	B	601	CLA	CHA-C1A-NA	-2.11	121.60	126.39
24	d	403	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
24	c	512	CLA	CGD-CBD-CAD	2.11	117.69	110.85
24	b	605	CLA	CAC-C3C-C4C	2.11	127.54	124.79
24	D	403	CLA	CHB-C4A-NA	2.11	127.45	124.40
33	D	409	LHG	O3-P-O5	-2.11	100.56	108.94
26	h	103	BCR	C11-C10-C9	-2.11	124.31	127.28
26	d	406	BCR	C1-C6-C5	-2.11	119.75	122.64
24	d	405	CLA	C4-C3-C5	2.11	118.89	115.23
24	b	614	CLA	CMB-C2B-C3B	2.11	131.52	126.55
26	d	406	BCR	C8-C7-C6	-2.11	121.36	127.00
25	d	402	PHO	CMC-C2C-C1C	-2.11	120.94	124.73
32	c	519	LMG	O8-C28-O10	-2.11	118.36	123.63
29	C	518	DGD	O6D-C5D-C6D	-2.11	102.52	106.69
32	C	501	LMG	O6-C1-C2	-2.11	106.04	110.37
24	b	611	CLA	C16-C17-C18	-2.11	106.54	115.94
26	B	619	BCR	C40-C30-C29	-2.10	100.87	108.95
32	c	522	LMG	C35-C34-C33	-2.10	103.74	114.37
24	d	403	CLA	C2D-C1D-ND	-2.10	108.05	110.13
24	c	507	CLA	C3B-C4B-NB	-2.10	108.65	110.53
26	A	409	BCR	C38-C26-C25	-2.10	122.19	124.48
24	c	506	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	C	512	CLA	O2D-CGD-CBD	2.10	114.90	111.23
24	B	604	CLA	CED-O2D-CGD	2.10	120.67	115.92
24	b	615	CLA	C6-C5-C3	-2.10	108.36	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	CAC-C3C-C4C	2.10	127.52	124.79
33	d	409	LHG	C20-C19-C18	-2.10	103.77	114.37
24	B	616	CLA	CHA-C4D-ND	2.10	136.87	132.55
26	C	515	BCR	C4-C5-C6	2.10	125.54	122.70
24	c	513	CLA	C11-C12-C13	-2.10	109.00	115.97
29	C	518	DGD	C8B-C7B-C6B	-2.09	103.78	114.37
27	A	410	PL9	C12-C13-C14	-2.09	122.83	127.62
34	F	102	HEM	O2D-CGD-CBD	2.09	120.61	114.00
24	B	602	CLA	C1-C2-C3	-2.09	122.77	126.20
32	c	522	LMG	C42-C41-C40	-2.09	103.80	114.37
26	A	409	BCR	C15-C16-C17	-2.09	119.25	123.52
24	B	601	CLA	CHB-C1B-NB	2.09	127.18	124.05
24	B	609	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
24	b	607	CLA	CHD-C4C-NC	2.09	127.47	124.23
24	C	509	CLA	CMC-C2C-C3C	2.09	131.79	126.15
29	c	518	DGD	C1D-C2D-C3D	-2.09	105.62	110.01
24	a	404	CLA	CAA-C2A-C1A	-2.09	105.14	111.97
24	b	605	CLA	OBD-CAD-C3D	2.09	133.29	128.42
24	B	612	CLA	C16-C15-C13	-2.09	109.03	115.97
33	D	408	LHG	C27-C26-C25	-2.09	103.82	114.37
24	b	611	CLA	C11-C12-C13	-2.09	109.03	115.97
24	C	506	CLA	C11-C10-C8	-2.08	109.03	115.97
24	C	512	CLA	CHC-C1C-NC	2.08	127.45	124.31
26	b	620	BCR	C7-C8-C9	-2.08	123.15	126.23
24	d	405	CLA	CMB-C2B-C3B	2.08	131.45	126.55
24	a	404	CLA	C7-C6-C5	-2.08	107.71	113.26
32	C	501	LMG	C40-C39-C38	-2.08	103.84	114.37
23	d	401	BCT	O3-C-O1	-2.08	114.35	119.68
24	b	614	CLA	C2A-C1A-CHA	2.08	127.48	123.87
24	C	505	CLA	C11-C10-C8	-2.08	109.05	115.97
24	b	611	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	C	518	DGD	C3G-O3G-C1D	-2.08	109.34	113.80
28	B	622	SQD	C4-C3-C2	2.08	114.48	110.83
26	K	101	BCR	C39-C30-C25	-2.08	106.99	110.24
24	A	406	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
24	C	509	CLA	CMB-C2B-C3B	2.07	131.43	126.55
28	F	101	SQD	O48-C23-O10	-2.07	118.44	123.63
24	b	607	CLA	O1D-CGD-CBD	2.07	128.61	124.52
24	c	502	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
24	b	607	CLA	CHA-C1A-NA	-2.07	121.70	126.39
29	C	516	DGD	C9B-C8B-C7B	-2.07	103.90	114.37
24	B	613	CLA	C11-C10-C8	-2.07	109.09	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	CGD-CBD-CAD	-2.07	104.15	110.85
24	b	607	CLA	C2A-C1A-CHA	2.07	127.46	123.87
27	D	406	PL9	C35-C34-C36	2.07	118.81	115.23
33	D	411	LHG	C20-C19-C18	-2.06	103.94	114.37
24	B	612	CLA	CHD-C4C-C3C	-2.06	121.77	124.77
24	A	405	CLA	C7-C6-C5	-2.06	107.76	113.26
29	c	516	DGD	C7A-C6A-C5A	-2.06	103.94	114.37
24	b	617	CLA	CHC-C4B-NB	2.06	127.14	124.05
24	b	611	CLA	CED-O2D-CGD	-2.06	111.24	115.92
26	C	519	BCR	C33-C5-C6	-2.06	122.23	124.48
26	c	521	BCR	C38-C26-C27	-2.06	109.20	113.60
24	b	616	CLA	CHA-C4D-ND	2.06	136.80	132.55
24	a	405	CLA	CHA-C1A-NA	-2.06	121.73	126.39
24	b	617	CLA	CMC-C2C-C1C	2.06	128.25	125.03
27	d	407	PL9	O2-C1-C6	2.06	123.75	120.48
29	C	517	DGD	C5B-C4B-C3B	-2.06	103.97	114.37
24	C	503	CLA	C1-C2-C3	-2.06	122.83	126.20
24	C	507	CLA	CHA-C1A-NA	-2.06	121.73	126.39
29	c	517	DGD	O6D-C1D-O3G	-2.06	105.19	110.04
24	a	404	CLA	C1D-CHD-C4C	-2.06	121.65	126.02
25	D	401	PHO	CBA-CAA-C2A	-2.06	107.72	113.78
27	a	409	PL9	C37-C38-C39	-2.06	122.92	127.62
24	c	511	CLA	O1A-CGA-CBA	2.05	131.82	123.78
26	d	406	BCR	C30-C25-C26	-2.05	119.83	122.64
26	B	619	BCR	C35-C13-C14	-2.05	119.49	122.82
24	C	513	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
24	D	404	CLA	CHA-C1A-NA	-2.05	121.74	126.39
24	B	609	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
35	v	201	HEC	O1D-CGD-CBD	-2.05	116.58	123.09
29	C	517	DGD	O3G-C1D-C2D	-2.05	105.16	108.27
26	b	620	BCR	C27-C26-C25	2.05	125.47	122.70
26	b	602	BCR	C4-C5-C6	2.05	125.47	122.70
29	a	412	DGD	C1G-C2G-C3G	-2.05	107.07	111.80
32	c	522	LMG	C33-C32-C31	-2.05	104.02	114.37
29	A	413	DGD	C2G-O2G-C1B	2.05	122.69	117.80
29	C	517	DGD	CAB-C9B-C8B	-2.05	104.03	114.37
24	b	617	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
24	a	404	CLA	C17-C16-C15	-2.04	104.11	113.28
32	M	101	LMG	C31-C30-C29	-2.04	105.61	113.13
29	c	518	DGD	C9B-C8B-C7B	-2.04	104.03	114.37
24	b	613	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
27	D	406	PL9	C27-C28-C29	-2.04	122.94	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	602	BCR	C15-C16-C17	-2.04	119.34	123.52
25	d	402	PHO	C1A-C2A-C3A	-2.04	100.89	102.84
29	A	413	DGD	C6D-O5D-C1E	2.04	118.17	113.80
24	c	505	CLA	C11-C10-C8	-2.04	109.18	115.97
24	B	605	CLA	CHD-C4C-NC	2.04	127.39	124.23
24	C	508	CLA	CHA-C4D-ND	2.04	136.76	132.55
24	C	509	CLA	O1D-CGD-CBD	2.04	128.54	124.52
24	d	405	CLA	CHD-C4C-NC	2.04	127.39	124.23
24	b	612	CLA	CHA-C1A-NA	-2.04	121.77	126.39
33	d	409	LHG	C29-C28-C27	-2.04	104.06	114.37
26	B	618	BCR	C29-C30-C25	2.04	113.40	110.44
26	A	409	BCR	C40-C30-C39	-2.04	102.80	108.63
29	C	517	DGD	C7B-C6B-C5B	-2.03	104.09	114.37
24	b	605	CLA	CMA-C3A-C4A	2.03	117.24	111.77
28	a	410	SQD	O7-S-C6	2.03	109.79	106.76
24	c	510	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
33	L	101	LHG	C5-O7-C7	-2.03	112.93	117.80
26	b	618	BCR	C11-C10-C9	-2.03	124.43	127.28
24	b	614	CLA	C1-C2-C3	-2.03	122.87	126.20
32	b	623	LMG	C3-C4-C5	-2.03	106.55	110.23
33	l	101	LHG	C20-C19-C18	-2.03	104.11	114.37
24	b	603	CLA	CAA-CBA-CGA	-2.03	107.45	113.21
33	D	411	LHG	O8-C6-C5	-2.03	102.55	108.40
35	v	201	HEC	O2A-CGA-CBA	2.03	120.41	114.00
33	L	101	LHG	C27-C26-C25	-2.03	104.12	114.37
24	c	502	CLA	C3A-C2A-C1A	2.03	104.37	101.34
28	F	101	SQD	O7-S-C6	-2.03	103.73	106.76
33	L	101	LHG	C20-C19-C18	-2.03	104.13	114.37
29	H	102	DGD	C7B-C6B-C5B	-2.02	104.14	114.37
35	v	201	HEC	CHA-C4D-ND	2.02	127.53	123.86
24	B	602	CLA	C6-C5-C3	-2.02	108.54	113.47
24	D	403	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
26	Y	101	BCR	C40-C30-C25	2.02	113.41	110.24
24	d	405	CLA	CGD-CBD-CAD	-2.02	104.30	110.85
24	h	101	CLA	CHD-C4C-NC	2.02	127.36	124.23
28	A	412	SQD	O48-C23-O10	-2.02	118.57	123.63
24	B	612	CLA	CMB-C2B-C3B	2.02	131.30	126.55
24	A	406	CLA	C1-O2A-CGA	2.02	121.54	116.65
26	Y	101	BCR	C8-C7-C6	-2.02	121.60	127.00
29	c	516	DGD	C5B-C4B-C3B	-2.02	104.16	114.37
24	B	607	CLA	CHB-C4A-NA	2.02	127.31	124.40
24	c	505	CLA	O1A-CGA-CBA	2.02	131.67	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	602	BCR	C1-C6-C5	-2.02	119.88	122.64
24	c	502	CLA	CHB-C1B-NB	2.02	127.08	124.05
32	b	623	LMG	C42-C41-C40	-2.02	104.17	114.37
26	c	515	BCR	C36-C18-C17	-2.02	119.55	122.82
24	c	507	CLA	O1A-CGA-CBA	2.02	131.67	123.78
28	f	101	SQD	O8-S-O9	-2.02	106.36	111.40
24	D	404	CLA	C1D-ND-C4D	-2.02	104.90	106.31
24	b	603	CLA	CMB-C2B-C3B	2.01	131.29	126.55
24	A	408	CLA	CHD-C1D-ND	-2.01	121.97	124.80
28	B	622	SQD	C46-C45-C44	-2.01	107.09	111.78
24	C	506	CLA	CMD-C2D-C3D	2.01	132.30	127.69
24	b	603	CLA	CGD-CBD-CAD	-2.01	104.33	110.85
24	C	514	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	C	505	CLA	CHA-C1A-NA	-2.01	121.84	126.39
24	C	512	CLA	CHD-C4C-C3C	2.01	127.70	124.77
24	B	601	CLA	CHD-C1D-ND	-2.01	121.98	124.80
24	d	405	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
24	B	606	CLA	CHA-C1A-NA	-2.01	121.85	126.39
26	K	101	BCR	C15-C14-C13	-2.01	124.46	127.28
29	c	518	DGD	CDB-CCB-CBB	-2.01	104.23	114.37
24	B	610	CLA	CHB-C1B-NB	2.01	127.06	124.05
24	A	408	CLA	C3D-C4D-ND	2.00	113.25	109.99
26	a	408	BCR	C40-C30-C25	2.00	113.39	110.24
24	C	514	CLA	O1D-CGD-CBD	2.00	128.47	124.52
24	b	607	CLA	CMD-C2D-C1D	2.00	128.25	124.73
28	b	601	SQD	O10-C23-C24	-2.00	115.96	123.78

All (61) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	408	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	610	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	508	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	402	CLA	ND
24	D	403	CLA	ND
24	a	404	CLA	ND
24	a	407	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	c	501	CLA	ND
24	c	502	CLA	ND
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND

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Mol	Chain	Res	Type	Atom
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	d	403	CLA	ND
24	d	404	CLA	ND
24	d	405	CLA	ND
24	h	101	CLA	ND

All (1647) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	408	CLA	C4-C3-C5-C6
24	B	606	CLA	C4B-C3B-CAB-CBB
24	B	616	CLA	CBD-CGD-O2D-CED
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	C11-C10-C8-C9
24	b	611	CLA	C4B-C3B-CAB-CBB
24	b	615	CLA	CAD-CBD-CGD-O1D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CBD-CGD-O2D-CED
24	c	505	CLA	C2B-C3B-CAB-CBB
24	c	505	CLA	C4B-C3B-CAB-CBB
24	c	506	CLA	C4-C3-C5-C6
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	C11-C12-C13-C14
24	c	510	CLA	CBD-CGD-O2D-CED
24	h	101	CLA	C4B-C3B-CAB-CBB
26	A	409	BCR	C7-C8-C9-C10
26	A	409	BCR	C7-C8-C9-C34
26	A	409	BCR	C17-C18-C19-C20
26	B	617	BCR	C35-C13-C14-C15
26	C	519	BCR	C7-C8-C9-C10
26	C	519	BCR	C35-C13-C14-C15
26	C	519	BCR	C16-C17-C18-C36
26	D	405	BCR	C21-C22-C23-C24
26	D	405	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	D	405	BCR	C23-C24-C25-C30
26	K	101	BCR	C11-C10-C9-C8
26	K	101	BCR	C11-C12-C13-C14
26	K	101	BCR	C11-C12-C13-C35
26	K	101	BCR	C16-C17-C18-C19
26	K	101	BCR	C16-C17-C18-C36
26	K	101	BCR	C22-C23-C24-C25
26	Y	101	BCR	C5-C6-C7-C8
26	Y	101	BCR	C21-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
26	a	408	BCR	C20-C21-C22-C37
26	b	602	BCR	C1-C6-C7-C8
26	b	602	BCR	C5-C6-C7-C8
26	b	602	BCR	C7-C8-C9-C10
26	b	602	BCR	C11-C12-C13-C14
26	b	619	BCR	C37-C22-C23-C24
26	b	620	BCR	C11-C12-C13-C14
26	b	620	BCR	C11-C12-C13-C35
26	c	514	BCR	C11-C10-C9-C8
26	c	515	BCR	C16-C17-C18-C36
26	c	515	BCR	C18-C19-C20-C21
26	c	515	BCR	C20-C21-C22-C37
26	c	521	BCR	C6-C7-C8-C9
26	c	521	BCR	C35-C13-C14-C15
26	c	521	BCR	C18-C19-C20-C21
26	c	521	BCR	C20-C21-C22-C37
26	d	406	BCR	C18-C19-C20-C21
26	d	406	BCR	C21-C22-C23-C24
26	h	103	BCR	C11-C10-C9-C8
26	h	103	BCR	C16-C17-C18-C36
26	k	101	BCR	C7-C8-C9-C10
26	k	101	BCR	C7-C8-C9-C34
26	k	101	BCR	C17-C18-C19-C20
26	t	101	BCR	C11-C12-C13-C14
26	t	101	BCR	C12-C13-C14-C15
26	t	101	BCR	C16-C17-C18-C36
26	t	101	BCR	C20-C21-C22-C37
27	A	410	PL9	C12-C13-C14-C15
27	A	410	PL9	C12-C13-C14-C16
27	A	410	PL9	C22-C23-C24-C25
27	A	410	PL9	C22-C23-C24-C26
27	A	410	PL9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
27	A	410	PL9	C37-C38-C39-C41
27	D	406	PL9	C32-C33-C34-C35
27	D	406	PL9	C32-C33-C34-C36
27	a	409	PL9	C22-C23-C24-C25
27	a	409	PL9	C22-C23-C24-C26
27	a	409	PL9	C30-C29-C31-C32
27	a	409	PL9	C32-C33-C34-C35
27	a	409	PL9	C37-C38-C39-C40
27	a	409	PL9	C42-C43-C44-C45
27	d	407	PL9	C32-C33-C34-C36
27	d	407	PL9	C37-C38-C39-C41
27	d	407	PL9	C42-C43-C44-C45
27	d	407	PL9	C42-C43-C44-C46
27	d	407	PL9	C47-C48-C49-C50
28	A	412	SQD	C46-C45-O47-C7
28	B	622	SQD	O49-C7-O47-C45
28	B	622	SQD	C8-C7-O47-C45
28	a	410	SQD	O47-C45-C46-O48
28	a	411	SQD	O6-C44-C45-O47
28	a	411	SQD	O49-C7-O47-C45
28	a	411	SQD	C8-C7-O47-C45
28	b	601	SQD	O10-C23-O48-C46
28	f	101	SQD	O5-C1-O6-C44
29	A	413	DGD	O1B-C1B-O2G-C2G
29	A	413	DGD	O2G-C2G-C3G-O3G
32	C	501	LMG	O9-C10-O7-C8
32	C	501	LMG	C11-C10-O7-C8
32	D	410	LMG	C11-C10-O7-C8
32	K	102	LMG	C11-C10-O7-C8
32	b	623	LMG	C11-C10-O7-C8
32	c	522	LMG	O10-C28-O8-C9
32	c	524	LMG	O6-C1-O1-C7
32	c	524	LMG	O10-C28-O8-C9
33	D	408	LHG	O1-C1-C2-O2
33	D	408	LHG	C3-O3-P-O5
33	D	408	LHG	C3-O3-P-O6
33	D	408	LHG	C4-O6-P-O3
33	D	408	LHG	C4-O6-P-O4
33	D	409	LHG	C3-O3-P-O6
33	E	101	LHG	O1-C1-C2-C3
33	E	101	LHG	C4-O6-P-O3
33	E	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	O10-C23-O8-C6
33	L	101	LHG	C3-O3-P-O4
33	L	101	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C3-O3-P-O5
33	d	409	LHG	O1-C1-C2-C3
33	d	409	LHG	C3-O3-P-O5
33	d	409	LHG	C4-O6-P-O3
33	d	409	LHG	C4-O6-P-O4
33	d	410	LHG	O1-C1-C2-C3
33	e	101	LHG	C1-C2-C3-O3
33	e	101	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O5
33	e	101	LHG	O10-C23-O8-C6
33	l	101	LHG	C4-O6-P-O3
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
24	h	101	CLA	O1D-CGD-O2D-CED
24	b	617	CLA	O1D-CGD-O2D-CED
24	c	510	CLA	O1D-CGD-O2D-CED
24	B	601	CLA	CBD-CGD-O2D-CED
24	C	510	CLA	CBD-CGD-O2D-CED
24	c	509	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	CBD-CGD-O2D-CED
24	h	101	CLA	CBD-CGD-O2D-CED
27	d	407	PL9	C47-C48-C49-C51
24	B	601	CLA	O1D-CGD-O2D-CED
24	c	509	CLA	O1D-CGD-O2D-CED
28	a	411	SQD	C24-C23-O48-C46
28	b	601	SQD	C24-C23-O48-C46
32	c	524	LMG	C29-C28-O8-C9
33	E	101	LHG	C24-C23-O8-C6
33	e	101	LHG	C24-C23-O8-C6
28	a	411	SQD	O10-C23-O48-C46
29	a	412	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	O1D-CGD-O2D-CED
24	B	616	CLA	O1D-CGD-O2D-CED
32	c	519	LMG	C11-C10-O7-C8
24	C	502	CLA	CBD-CGD-O2D-CED
24	C	509	CLA	CBD-CGD-O2D-CED
32	D	410	LMG	O9-C10-O7-C8
32	K	102	LMG	O9-C10-O7-C8
32	b	623	LMG	O9-C10-O7-C8
32	c	522	LMG	O9-C10-O7-C8
32	c	522	LMG	C4-C5-C6-O5
24	b	605	CLA	C3-C5-C6-C7
24	D	403	CLA	CBD-CGD-O2D-CED
24	a	405	CLA	CBD-CGD-O2D-CED
24	c	511	CLA	CBD-CGD-O2D-CED
25	d	402	PHO	CBD-CGD-O2D-CED
29	A	413	DGD	C2B-C1B-O2G-C2G
24	B	605	CLA	C4-C3-C5-C6
24	c	507	CLA	C4-C3-C5-C6
24	A	408	CLA	C2-C3-C5-C6
24	c	506	CLA	C2-C3-C5-C6
27	A	410	PL9	C43-C44-C46-C47
27	a	409	PL9	C33-C34-C36-C37
28	F	101	SQD	O10-C23-O48-C46
24	B	601	CLA	CBA-CGA-O2A-C1
28	f	101	SQD	C24-C23-O48-C46
29	a	412	DGD	C2A-C1A-O1G-C1G
32	c	522	LMG	C29-C28-O8-C9
27	A	410	PL9	C32-C33-C34-C36
27	a	409	PL9	C32-C33-C34-C36
28	a	410	SQD	O10-C23-O48-C46
32	C	501	LMG	O10-C28-O8-C9
32	M	101	LMG	O10-C28-O8-C9
27	A	410	PL9	C47-C48-C49-C50
24	b	615	CLA	C3-C5-C6-C7
28	B	622	SQD	C45-C46-O48-C23
33	D	409	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
24	B	601	CLA	O1A-CGA-O2A-C1
26	c	515	BCR	C14-C15-C16-C17
24	D	403	CLA	O1D-CGD-O2D-CED
24	B	614	CLA	C4-C3-C5-C6
24	b	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C4-C3-C5-C6
27	A	410	PL9	C40-C39-C41-C42
24	B	605	CLA	C2-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
24	b	604	CLA	C2-C3-C5-C6
24	b	606	CLA	C2-C3-C5-C6
24	c	507	CLA	C2-C3-C5-C6
24	B	604	CLA	C13-C15-C16-C17
32	c	524	LMG	O6-C5-C6-O5
27	A	410	PL9	C9-C11-C12-C13
27	A	410	PL9	C19-C21-C22-C23
27	A	410	PL9	C29-C31-C32-C33
27	A	410	PL9	C44-C46-C47-C48
27	a	409	PL9	C24-C26-C27-C28
27	a	409	PL9	C44-C46-C47-C48
27	d	407	PL9	C44-C46-C47-C48
24	c	501	CLA	CBD-CGD-O2D-CED
32	C	501	LMG	O6-C5-C6-O5
32	c	519	LMG	O6-C5-C6-O5
29	c	518	DGD	O1A-C1A-O1G-C1G
28	B	622	SQD	O5-C1-O6-C44
25	d	402	PHO	C2C-C3C-CAC-CBC
28	F	101	SQD	C24-C23-O48-C46
24	B	607	CLA	CBD-CGD-O2D-CED
24	B	614	CLA	CBD-CGD-O2D-CED
24	c	504	CLA	CBD-CGD-O2D-CED
24	c	512	CLA	CBD-CGD-O2D-CED
27	D	406	PL9	C37-C38-C39-C40
32	c	522	LMG	O6-C5-C6-O5
27	A	410	PL9	C47-C48-C49-C51
29	C	516	DGD	O6E-C5E-C6E-O5E
29	a	412	DGD	O1B-C1B-O2G-C2G
32	C	501	LMG	C29-C28-O8-C9
32	M	101	LMG	C29-C28-O8-C9
32	c	519	LMG	C29-C28-O8-C9
33	d	408	LHG	C28-C29-C30-C31
24	c	513	CLA	O1D-CGD-O2D-CED
27	A	410	PL9	C18-C19-C21-C22
27	d	407	PL9	C38-C39-C41-C42
24	B	605	CLA	C11-C10-C8-C9
24	B	607	CLA	C14-C13-C15-C16
24	C	503	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	508	CLA	C11-C10-C8-C9
24	C	509	CLA	C11-C12-C13-C14
24	C	513	CLA	C11-C10-C8-C9
24	b	611	CLA	C14-C13-C15-C16
24	b	615	CLA	C6-C7-C8-C9
24	b	617	CLA	C11-C10-C8-C9
24	c	509	CLA	C6-C7-C8-C9
24	c	510	CLA	C11-C10-C8-C9
24	c	511	CLA	C14-C13-C15-C16
24	h	101	CLA	C11-C10-C8-C9
25	A	407	PHO	C14-C13-C15-C16
32	c	524	LMG	C4-C5-C6-O5
24	C	502	CLA	O1D-CGD-O2D-CED
24	C	509	CLA	O1D-CGD-O2D-CED
28	B	622	SQD	C2-C1-O6-C44
33	D	408	LHG	O2-C2-C3-O3
25	d	402	PHO	O1D-CGD-O2D-CED
26	B	619	BCR	C7-C8-C9-C34
26	B	619	BCR	C11-C12-C13-C35
26	C	515	BCR	C37-C22-C23-C24
26	C	519	BCR	C7-C8-C9-C34
26	C	519	BCR	C11-C12-C13-C35
26	K	101	BCR	C7-C8-C9-C34
26	b	602	BCR	C7-C8-C9-C34
26	b	602	BCR	C11-C12-C13-C35
26	b	602	BCR	C37-C22-C23-C24
26	b	620	BCR	C37-C22-C23-C24
26	c	515	BCR	C7-C8-C9-C34
26	c	521	BCR	C36-C18-C19-C20
26	d	406	BCR	C37-C22-C23-C24
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C12-C13-C35
24	a	405	CLA	O1D-CGD-O2D-CED
29	C	518	DGD	O1A-C1A-O1G-C1G
28	B	622	SQD	O6-C44-C45-O47
28	a	410	SQD	O6-C44-C45-O47
32	K	102	LMG	C29-C28-O8-C9
29	c	517	DGD	C1B-C2B-C3B-C4B
24	c	511	CLA	O1D-CGD-O2D-CED
29	H	102	DGD	C4E-C5E-C6E-O5E
24	B	611	CLA	C8-C10-C11-C12
24	B	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	H	102	DGD	O6E-C5E-C6E-O5E
33	E	101	LHG	O1-C1-C2-O2
33	e	101	LHG	C7-C8-C9-C10
24	B	611	CLA	C12-C13-C15-C16
27	a	409	PL9	C14-C16-C17-C18
27	a	409	PL9	C29-C31-C32-C33
24	B	608	CLA	C15-C16-C17-C18
24	b	612	CLA	C8-C10-C11-C12
24	c	503	CLA	C5-C6-C7-C8
24	h	101	CLA	C8-C10-C11-C12
29	C	517	DGD	C1B-C2B-C3B-C4B
29	H	102	DGD	C1A-C2A-C3A-C4A
32	D	410	LMG	C10-C11-C12-C13
32	c	524	LMG	C28-C29-C30-C31
32	d	411	LMG	C28-C29-C30-C31
33	L	101	LHG	C23-C24-C25-C26
33	e	101	LHG	C23-C24-C25-C26
24	a	404	CLA	CBD-CGD-O2D-CED
24	B	612	CLA	C10-C11-C12-C13
24	C	506	CLA	C5-C6-C7-C8
24	D	404	CLA	C5-C6-C7-C8
24	c	506	CLA	C13-C15-C16-C17
24	c	511	CLA	C15-C16-C17-C18
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C2A-CAA-CBA-CGA
24	B	614	CLA	C13-C15-C16-C17
24	C	506	CLA	C8-C10-C11-C12
24	b	610	CLA	C15-C16-C17-C18
24	b	614	CLA	C13-C15-C16-C17
24	c	512	CLA	C13-C15-C16-C17
28	A	411	SQD	C7-C8-C9-C10
28	A	411	SQD	C23-C24-C25-C26
28	B	622	SQD	C23-C24-C25-C26
33	d	408	LHG	C23-C24-C25-C26
26	b	620	BCR	C6-C7-C8-C9
29	c	517	DGD	O6E-C1E-O5D-C6D
32	C	501	LMG	O6-C1-O1-C7
28	F	101	SQD	C45-C46-O48-C23
24	A	405	CLA	C15-C16-C17-C18
24	B	602	CLA	C13-C15-C16-C17
24	C	510	CLA	C10-C11-C12-C13
24	b	608	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	F	101	SQD	O6-C44-C45-C46
28	a	410	SQD	C24-C23-O48-C46
24	b	607	CLA	C15-C16-C17-C18
24	c	504	CLA	O1D-CGD-O2D-CED
24	c	509	CLA	C8-C10-C11-C12
32	b	621	LMG	C10-C11-C12-C13
24	C	513	CLA	C10-C11-C12-C13
24	a	407	CLA	C13-C15-C16-C17
24	b	612	CLA	C13-C15-C16-C17
24	b	615	CLA	C5-C6-C7-C8
24	h	101	CLA	C15-C16-C17-C18
24	c	512	CLA	CBA-CGA-O2A-C1
33	E	101	LHG	C8-C7-O7-C5
24	b	603	CLA	C3-C5-C6-C7
24	c	505	CLA	CBD-CGD-O2D-CED
26	b	602	BCR	C9-C10-C11-C12
26	h	103	BCR	C14-C15-C16-C17
24	B	609	CLA	C13-C15-C16-C17
24	C	508	CLA	C10-C11-C12-C13
24	b	616	CLA	C15-C16-C17-C18
24	c	509	CLA	C15-C16-C17-C18
27	a	409	PL9	C47-C48-C49-C50
32	C	501	LMG	C4-C5-C6-O5
24	B	605	CLA	C5-C6-C7-C8
24	B	611	CLA	C13-C15-C16-C17
24	C	507	CLA	C13-C15-C16-C17
24	a	407	CLA	C5-C6-C7-C8
24	c	503	CLA	C8-C10-C11-C12
24	c	505	CLA	C15-C16-C17-C18
24	c	506	CLA	C5-C6-C7-C8
33	l	101	LHG	C7-C8-C9-C10
27	d	407	PL9	C40-C39-C41-C42
24	B	606	CLA	C15-C16-C17-C18
24	c	509	CLA	C10-C11-C12-C13
28	f	101	SQD	C2-C1-O6-C44
29	C	517	DGD	C2E-C1E-O5D-C6D
29	c	517	DGD	C2E-C1E-O5D-C6D
27	a	409	PL9	C39-C41-C42-C43
29	A	413	DGD	O6D-C5D-C6D-O5D
24	b	616	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C19
26	C	519	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
26	C	519	BCR	C20-C21-C22-C37
26	D	405	BCR	C20-C21-C22-C37
26	H	101	BCR	C16-C17-C18-C36
26	H	101	BCR	C20-C21-C22-C37
26	K	101	BCR	C20-C21-C22-C37
26	b	620	BCR	C20-C21-C22-C37
26	c	514	BCR	C11-C10-C9-C34
26	c	515	BCR	C35-C13-C14-C15
26	d	406	BCR	C16-C17-C18-C36
26	d	406	BCR	C20-C21-C22-C37
26	h	103	BCR	C11-C10-C9-C34
26	k	101	BCR	C16-C17-C18-C36
26	k	101	BCR	C20-C21-C22-C37
26	t	101	BCR	C11-C10-C9-C34
24	d	404	CLA	C3-C5-C6-C7
24	D	403	CLA	C2C-C3C-CAC-CBC
24	b	610	CLA	CBD-CGD-O2D-CED
24	c	512	CLA	O1A-CGA-O2A-C1
28	f	101	SQD	O10-C23-O48-C46
24	B	615	CLA	C13-C15-C16-C17
33	D	408	LHG	O1-C1-C2-C3
33	D	411	LHG	O1-C1-C2-C3
32	D	410	LMG	C28-C29-C30-C31
32	c	519	LMG	C28-C29-C30-C31
24	C	514	CLA	O2A-C1-C2-C3
29	C	518	DGD	C8A-C9A-CAA-CBA
24	c	510	CLA	C16-C17-C18-C19
24	C	503	CLA	C3-C5-C6-C7
24	B	607	CLA	C13-C15-C16-C17
24	B	613	CLA	C5-C6-C7-C8
26	B	617	BCR	C12-C13-C14-C15
26	B	619	BCR	C11-C10-C9-C8
26	B	619	BCR	C16-C17-C18-C19
26	K	101	BCR	C20-C21-C22-C23
26	a	408	BCR	C20-C21-C22-C23
26	b	620	BCR	C12-C13-C14-C15
26	c	514	BCR	C16-C17-C18-C19
26	c	515	BCR	C20-C21-C22-C23
26	d	406	BCR	C16-C17-C18-C19
26	h	103	BCR	C16-C17-C18-C19
26	t	101	BCR	C16-C17-C18-C19
29	C	517	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
28	b	601	SQD	C8-C7-O47-C45
24	c	512	CLA	O1D-CGD-O2D-CED
29	h	104	DGD	O6E-C5E-C6E-O5E
24	c	506	CLA	C2-C1-O2A-CGA
24	A	406	CLA	C16-C17-C18-C19
24	C	503	CLA	C16-C17-C18-C19
24	c	510	CLA	C16-C17-C18-C20
29	c	516	DGD	C4B-C5B-C6B-C7B
32	c	522	LMG	C32-C33-C34-C35
26	A	409	BCR	C14-C15-C16-C17
26	D	405	BCR	C14-C15-C16-C17
26	d	406	BCR	C14-C15-C16-C17
29	A	413	DGD	C4A-C5A-C6A-C7A
29	C	517	DGD	C6A-C7A-C8A-C9A
29	C	518	DGD	CCA-CDA-CEA-CFA
29	H	102	DGD	C4B-C5B-C6B-C7B
29	c	516	DGD	C5B-C6B-C7B-C8B
32	B	621	LMG	C14-C15-C16-C17
32	B	621	LMG	C29-C30-C31-C32
33	D	408	LHG	C12-C13-C14-C15
33	D	408	LHG	C15-C16-C17-C18
33	E	101	LHG	C9-C10-C11-C12
33	D	408	LHG	C10-C11-C12-C13
33	L	101	LHG	C27-C28-C29-C30
33	d	408	LHG	C16-C17-C18-C19
33	l	101	LHG	C9-C10-C11-C12
28	f	101	SQD	C32-C33-C34-C35
29	H	102	DGD	C3B-C4B-C5B-C6B
29	c	518	DGD	C8A-C9A-CAA-CBA
29	h	104	DGD	C2B-C3B-C4B-C5B
32	K	102	LMG	C32-C33-C34-C35
32	b	621	LMG	C32-C33-C34-C35
32	c	524	LMG	C12-C13-C14-C15
33	d	408	LHG	C32-C33-C34-C35
33	d	409	LHG	C26-C27-C28-C29
33	d	409	LHG	O1-C1-C2-O2
28	A	412	SQD	C12-C13-C14-C15
28	a	411	SQD	C12-C13-C14-C15
32	b	621	LMG	C31-C32-C33-C34
32	c	522	LMG	C11-C12-C13-C14
32	h	102	LMG	C11-C12-C13-C14
33	d	409	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
33	e	101	LHG	C13-C14-C15-C16
24	c	501	CLA	O1D-CGD-O2D-CED
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	504	CLA	C4B-C3B-CAB-CBB
24	c	507	CLA	C4B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
28	A	412	SQD	C7-C8-C9-C10
28	a	410	SQD	C34-C35-C36-C37
32	h	102	LMG	C36-C37-C38-C39
24	A	406	CLA	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C20
33	D	411	LHG	C25-C26-C27-C28
24	c	513	CLA	C8-C10-C11-C12
32	c	522	LMG	C11-C10-O7-C8
33	E	101	LHG	C33-C34-C35-C36
29	a	412	DGD	C6A-C7A-C8A-C9A
33	D	411	LHG	C12-C13-C14-C15
24	b	607	CLA	C10-C11-C12-C13
32	D	407	LMG	C14-C15-C16-C17
33	d	408	LHG	C10-C11-C12-C13
24	c	512	CLA	C3A-C2A-CAA-CBA
24	h	101	CLA	C3A-C2A-CAA-CBA
29	c	518	DGD	CCA-CDA-CEA-CFA
32	D	407	LMG	C34-C35-C36-C37
33	e	101	LHG	C14-C15-C16-C17
24	a	404	CLA	C15-C16-C17-C18
24	b	609	CLA	C13-C15-C16-C17
32	c	519	LMG	C4-C5-C6-O5
29	C	518	DGD	C6B-C7B-C8B-C9B
24	C	503	CLA	C16-C17-C18-C20
24	D	404	CLA	C16-C17-C18-C19
24	b	608	CLA	C16-C17-C18-C20
24	b	610	CLA	C16-C17-C18-C19
24	b	616	CLA	C16-C17-C18-C19
24	d	404	CLA	C16-C17-C18-C19
27	D	406	PL9	C47-C48-C49-C51
29	c	518	DGD	CCB-CDB-CEB-CFB
28	f	101	SQD	C44-C45-C46-O48
32	c	522	LMG	O1-C7-C8-C9
28	f	101	SQD	C24-C25-C26-C27
29	C	516	DGD	CCB-CDB-CEB-CFB
32	D	410	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	d	410	LHG	C30-C31-C32-C33
33	e	101	LHG	C12-C13-C14-C15
24	C	513	CLA	C3-C5-C6-C7
32	M	101	LMG	C28-C29-C30-C31
32	b	623	LMG	C10-C11-C12-C13
33	D	411	LHG	C23-C24-C25-C26
28	b	601	SQD	C12-C13-C14-C15
29	A	413	DGD	C5B-C6B-C7B-C8B
29	c	518	DGD	C4B-C5B-C6B-C7B
32	d	411	LMG	C34-C35-C36-C37
33	D	409	LHG	C27-C28-C29-C30
33	D	411	LHG	C14-C15-C16-C17
33	L	101	LHG	C30-C31-C32-C33
32	c	519	LMG	O10-C28-O8-C9
28	B	622	SQD	C13-C14-C15-C16
29	c	516	DGD	C9A-CAA-CBA-CCA
29	c	518	DGD	C5B-C6B-C7B-C8B
32	D	407	LMG	C18-C19-C20-C21
33	e	101	LHG	C26-C27-C28-C29
24	B	614	CLA	O1D-CGD-O2D-CED
32	B	621	LMG	C16-C17-C18-C19
28	F	101	SQD	C25-C26-C27-C28
29	A	413	DGD	C2B-C3B-C4B-C5B
29	h	104	DGD	C9A-CAA-CBA-CCA
32	b	621	LMG	C29-C30-C31-C32
32	b	623	LMG	C11-C12-C13-C14
32	b	623	LMG	C18-C19-C20-C21
32	c	519	LMG	C36-C37-C38-C39
32	c	522	LMG	C36-C37-C38-C39
24	c	513	CLA	C16-C17-C18-C20
24	d	404	CLA	C16-C17-C18-C20
24	B	601	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C2B-C3B-CAB-CBB
24	b	611	CLA	C2B-C3B-CAB-CBB
24	h	101	CLA	C2B-C3B-CAB-CBB
26	A	409	BCR	C1-C6-C7-C8
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	Y	101	BCR	C1-C6-C7-C8
26	b	619	BCR	C23-C24-C25-C26
26	b	619	BCR	C23-C24-C25-C30
29	A	413	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
29	a	412	DGD	C2B-C1B-O2G-C2G
24	b	617	CLA	C10-C11-C12-C13
28	B	622	SQD	C33-C34-C35-C36
33	L	101	LHG	C9-C10-C11-C12
29	c	516	DGD	C1A-C2A-C3A-C4A
24	c	508	CLA	C13-C15-C16-C17
32	M	101	LMG	C38-C39-C40-C41
32	b	623	LMG	C16-C17-C18-C19
32	d	411	LMG	C14-C15-C16-C17
33	L	101	LHG	O10-C23-O8-C6
27	d	407	PL9	C4-C3-C7-C8
32	D	407	LMG	C20-C21-C22-C23
33	E	101	LHG	O9-C7-O7-C5
32	C	501	LMG	C30-C31-C32-C33
26	c	514	BCR	C18-C19-C20-C21
26	c	521	BCR	C10-C11-C12-C13
26	d	406	BCR	C10-C11-C12-C13
26	h	103	BCR	C18-C19-C20-C21
24	B	615	CLA	C10-C11-C12-C13
24	C	514	CLA	C13-C15-C16-C17
27	D	406	PL9	C38-C39-C41-C42
27	d	407	PL9	C33-C34-C36-C37
27	a	409	PL9	C47-C48-C49-C51
28	A	412	SQD	C26-C27-C28-C29
32	D	407	LMG	C30-C31-C32-C33
32	M	101	LMG	C36-C37-C38-C39
33	D	409	LHG	C30-C31-C32-C33
33	L	101	LHG	C11-C12-C13-C14
24	B	607	CLA	O1D-CGD-O2D-CED
29	c	518	DGD	C2A-C1A-O1G-C1G
24	c	512	CLA	C6-C7-C8-C9
32	C	501	LMG	C14-C15-C16-C17
32	D	407	LMG	C35-C36-C37-C38
32	M	101	LMG	C32-C33-C34-C35
32	b	623	LMG	C31-C32-C33-C34
24	B	613	CLA	C8-C10-C11-C12
24	b	605	CLA	C10-C11-C12-C13
28	A	412	SQD	C28-C29-C30-C31
28	B	622	SQD	C11-C12-C13-C14
28	B	622	SQD	C17-C18-C19-C20
29	a	412	DGD	C7B-C8B-C9B-CAB
29	h	104	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
32	d	411	LMG	C39-C40-C41-C42
33	d	410	LHG	C27-C28-C29-C30
32	c	519	LMG	C39-C40-C41-C42
33	D	411	LHG	C11-C12-C13-C14
32	c	524	LMG	C2-C1-O1-C7
29	C	518	DGD	C2A-C3A-C4A-C5A
33	D	409	LHG	C11-C12-C13-C14
32	c	522	LMG	C10-C11-C12-C13
32	D	407	LMG	C11-C12-C13-C14
33	d	409	LHG	C34-C35-C36-C37
28	A	411	SQD	C31-C32-C33-C34
29	C	516	DGD	C2B-C3B-C4B-C5B
33	D	408	LHG	C34-C35-C36-C37
24	a	407	CLA	C10-C11-C12-C13
24	b	608	CLA	C16-C17-C18-C19
33	l	101	LHG	C27-C28-C29-C30
33	e	101	LHG	C8-C7-O7-C5
32	B	621	LMG	C28-C29-C30-C31
33	E	101	LHG	C7-C8-C9-C10
33	d	410	LHG	C23-C24-C25-C26
28	F	101	SQD	C27-C28-C29-C30
29	h	104	DGD	CCB-CDB-CEB-CFB
24	C	504	CLA	C5-C6-C7-C8
28	f	101	SQD	O49-C7-O47-C45
28	A	412	SQD	C14-C15-C16-C17
29	c	516	DGD	C4A-C5A-C6A-C7A
29	h	104	DGD	C7B-C8B-C9B-CAB
28	B	622	SQD	C26-C27-C28-C29
29	A	413	DGD	C4B-C5B-C6B-C7B
33	L	101	LHG	C7-C8-C9-C10
29	A	413	DGD	C8B-C9B-CAB-CBB
24	c	506	CLA	C16-C17-C18-C20
28	f	101	SQD	C28-C29-C30-C31
33	d	408	LHG	C29-C30-C31-C32
29	C	517	DGD	C8A-C9A-CAA-CBA
32	b	621	LMG	C17-C18-C19-C20
33	d	410	LHG	C29-C30-C31-C32
29	c	517	DGD	C7B-C8B-C9B-CAB
24	c	507	CLA	C8-C10-C11-C12
24	c	510	CLA	C10-C11-C12-C13
32	b	621	LMG	C28-C29-C30-C31
32	M	101	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	d	408	LHG	C17-C18-C19-C20
28	a	410	SQD	O49-C7-O47-C45
32	b	623	LMG	O6-C5-C6-O5
33	d	408	LHG	C31-C32-C33-C34
27	a	409	PL9	C19-C21-C22-C23
24	B	614	CLA	C8-C10-C11-C12
24	C	507	CLA	C15-C16-C17-C18
24	b	610	CLA	C16-C17-C18-C20
29	C	518	DGD	C5A-C6A-C7A-C8A
32	c	519	LMG	C35-C36-C37-C38
28	A	411	SQD	C28-C29-C30-C31
28	F	101	SQD	C33-C34-C35-C36
29	a	412	DGD	C4A-C5A-C6A-C7A
32	h	102	LMG	C37-C38-C39-C40
24	B	601	CLA	C10-C11-C12-C13
24	C	509	CLA	C13-C15-C16-C17
24	C	513	CLA	C15-C16-C17-C18
33	d	409	LHG	C14-C15-C16-C17
28	A	411	SQD	O6-C44-C45-O47
28	A	411	SQD	C11-C12-C13-C14
29	A	413	DGD	CBB-CCB-CDB-CEB
32	C	501	LMG	C12-C13-C14-C15
29	C	517	DGD	C6B-C7B-C8B-C9B
29	a	412	DGD	C8B-C9B-CAB-CBB
29	h	104	DGD	C5B-C6B-C7B-C8B
24	B	607	CLA	C15-C16-C17-C18
24	c	502	CLA	C15-C16-C17-C18
24	c	513	CLA	C5-C6-C7-C8
28	a	410	SQD	C13-C14-C15-C16
29	C	517	DGD	C5A-C6A-C7A-C8A
33	d	408	LHG	C33-C34-C35-C36
29	C	516	DGD	C5B-C6B-C7B-C8B
29	c	518	DGD	C3A-C4A-C5A-C6A
32	c	524	LMG	C38-C39-C40-C41
24	B	609	CLA	C16-C17-C18-C19
24	B	609	CLA	C16-C17-C18-C20
24	B	605	CLA	C15-C16-C17-C18
28	b	601	SQD	C13-C14-C15-C16
24	C	507	CLA	C3-C5-C6-C7
24	c	506	CLA	C3-C5-C6-C7
28	a	410	SQD	C26-C27-C28-C29
29	a	412	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
32	B	621	LMG	C32-C33-C34-C35
32	b	623	LMG	C23-C24-C25-C26
32	c	524	LMG	C33-C34-C35-C36
32	h	102	LMG	C31-C32-C33-C34
33	L	101	LHG	C31-C32-C33-C34
33	d	409	LHG	C28-C29-C30-C31
24	h	101	CLA	C2A-CAA-CBA-CGA
32	D	407	LMG	O6-C5-C6-O5
28	A	411	SQD	C24-C25-C26-C27
28	a	411	SQD	C18-C19-C20-C21
33	l	101	LHG	C31-C32-C33-C34
28	A	411	SQD	C30-C31-C32-C33
24	b	611	CLA	C15-C16-C17-C18
24	b	616	CLA	C8-C10-C11-C12
24	c	512	CLA	C5-C6-C7-C8
24	C	505	CLA	C11-C12-C13-C14
28	b	601	SQD	C10-C11-C12-C13
33	E	101	LHG	C15-C16-C17-C18
24	C	506	CLA	C10-C11-C12-C13
33	d	408	LHG	O1-C1-C2-O2
29	A	413	DGD	C4D-C5D-C6D-O5D
28	A	411	SQD	C32-C33-C34-C35
32	C	501	LMG	C16-C17-C18-C19
32	D	407	LMG	C19-C20-C21-C22
24	C	509	CLA	C1A-C2A-CAA-CBA
24	C	512	CLA	C1A-C2A-CAA-CBA
24	a	407	CLA	C1A-C2A-CAA-CBA
24	h	101	CLA	C1A-C2A-CAA-CBA
29	a	412	DGD	C5B-C6B-C7B-C8B
32	d	411	LMG	C13-C14-C15-C16
32	c	522	LMG	C34-C35-C36-C37
29	C	517	DGD	C9A-CAA-CBA-CCA
33	D	408	LHG	C11-C12-C13-C14
33	E	101	LHG	O6-C4-C5-C6
33	l	101	LHG	O6-C4-C5-C6
28	a	411	SQD	C10-C11-C12-C13
33	d	408	LHG	C7-C8-C9-C10
24	B	606	CLA	C6-C7-C8-C10
24	B	615	CLA	C6-C7-C8-C10
24	C	507	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	C	511	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	a	405	CLA	C11-C10-C8-C7
24	a	405	CLA	C12-C13-C15-C16
24	a	407	CLA	C11-C10-C8-C7
24	b	605	CLA	C11-C10-C8-C7
24	b	607	CLA	C11-C10-C8-C7
24	b	615	CLA	C11-C12-C13-C15
24	b	616	CLA	C12-C13-C15-C16
24	c	508	CLA	C12-C13-C15-C16
24	c	510	CLA	C11-C10-C8-C7
29	C	517	DGD	C3B-C4B-C5B-C6B
24	B	602	CLA	C8-C10-C11-C12
29	H	102	DGD	CCA-CDA-CEA-CFA
24	b	615	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	C10-C11-C12-C13
27	d	407	PL9	C15-C14-C16-C17
27	a	409	PL9	C13-C14-C16-C17
32	M	101	LMG	C12-C13-C14-C15
24	b	616	CLA	C5-C6-C7-C8
24	B	601	CLA	C3-C5-C6-C7
24	B	611	CLA	C14-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C9
24	C	511	CLA	C11-C10-C8-C9
24	b	603	CLA	C6-C7-C8-C9
24	b	605	CLA	C11-C10-C8-C9
24	b	610	CLA	C14-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C9
24	c	508	CLA	C14-C13-C15-C16
24	d	404	CLA	C6-C7-C8-C9
32	D	407	LMG	C13-C14-C15-C16
24	C	512	CLA	CBA-CGA-O2A-C1
29	h	104	DGD	C7A-C8A-C9A-CAA
24	B	616	CLA	C5-C6-C7-C8
24	b	604	CLA	C8-C10-C11-C12
24	c	510	CLA	C15-C16-C17-C18
32	M	101	LMG	C14-C15-C16-C17
33	L	101	LHG	C18-C19-C20-C21
28	A	411	SQD	O6-C44-C45-C46
28	B	622	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
29	C	516	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
32	c	522	LMG	C7-C8-C9-O8
33	l	101	LHG	C13-C14-C15-C16
29	c	516	DGD	O6E-C5E-C6E-O5E
32	c	519	LMG	C31-C32-C33-C34
24	a	405	CLA	C8-C10-C11-C12
24	b	617	CLA	C5-C6-C7-C8
32	h	102	LMG	C33-C34-C35-C36
33	D	408	LHG	C25-C26-C27-C28
24	B	611	CLA	CBA-CGA-O2A-C1
29	C	517	DGD	O6E-C5E-C6E-O5E
32	d	411	LMG	O6-C5-C6-O5
24	B	601	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C19
28	A	411	SQD	C26-C27-C28-C29
28	B	622	SQD	C31-C32-C33-C34
26	Y	101	BCR	C11-C10-C9-C34
24	c	504	CLA	C5-C6-C7-C8
24	c	510	CLA	C8-C10-C11-C12
33	l	101	LHG	C29-C30-C31-C32
29	C	518	DGD	CBA-CCA-CDA-CEA
24	C	511	CLA	C4-C3-C5-C6
24	C	507	CLA	C2-C3-C5-C6
24	C	511	CLA	C2-C3-C5-C6
29	A	413	DGD	CEA-CFA-CGA-CHA
24	B	603	CLA	C10-C11-C12-C13
24	B	606	CLA	C8-C10-C11-C12
26	h	103	BCR	C36-C18-C19-C20
28	b	601	SQD	O49-C7-O47-C45
33	d	408	LHG	C15-C16-C17-C18
32	c	524	LMG	C30-C31-C32-C33
28	a	411	SQD	C19-C20-C21-C22
24	c	512	CLA	C2A-CAA-CBA-CGA
28	B	622	SQD	C34-C35-C36-C37
24	B	611	CLA	O1A-CGA-O2A-C1
28	F	101	SQD	C26-C27-C28-C29
29	c	516	DGD	C2A-C3A-C4A-C5A
33	E	101	LHG	C11-C10-C9-C8
24	B	604	CLA	O2A-C1-C2-C3
24	C	513	CLA	O2A-C1-C2-C3
24	h	101	CLA	O2A-C1-C2-C3
28	b	601	SQD	C46-C45-O47-C7
32	D	410	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
32	C	501	LMG	C39-C40-C41-C42
32	c	522	LMG	C40-C41-C42-C43
24	B	608	CLA	C5-C6-C7-C8
29	A	413	DGD	CDB-CEB-CFB-CGB
29	C	518	DGD	CAA-CBA-CCA-CDA
33	d	410	LHG	C32-C33-C34-C35
26	c	514	BCR	C13-C14-C15-C16
32	c	522	LMG	C38-C39-C40-C41
33	l	101	LHG	C16-C17-C18-C19
26	C	519	BCR	C12-C13-C14-C15
26	d	406	BCR	C11-C10-C9-C8
28	a	410	SQD	C12-C13-C14-C15
26	B	617	BCR	C6-C7-C8-C9
24	h	101	CLA	C10-C11-C12-C13
28	a	411	SQD	C11-C12-C13-C14
32	b	621	LMG	C37-C38-C39-C40
33	E	101	LHG	C27-C28-C29-C30
33	d	409	LHG	C11-C12-C13-C14
28	B	622	SQD	C24-C23-O48-C46
29	A	413	DGD	C8A-C9A-CAA-CBA
32	h	102	LMG	C32-C33-C34-C35
29	H	102	DGD	C9B-CAB-CBB-CCB
33	D	411	LHG	C10-C11-C12-C13
24	C	505	CLA	C4-C3-C5-C6
28	B	622	SQD	C9-C10-C11-C12
29	h	104	DGD	CAB-CBB-CCB-CDB
33	D	411	LHG	C27-C28-C29-C30
33	L	101	LHG	C32-C33-C34-C35
24	A	408	CLA	C6-C7-C8-C9
29	c	517	DGD	C6A-C7A-C8A-C9A
28	b	601	SQD	O6-C44-C45-O47
32	c	522	LMG	O1-C7-C8-O7
28	a	411	SQD	C15-C16-C17-C18
33	e	101	LHG	C17-C18-C19-C20
32	d	411	LMG	C15-C16-C17-C18
29	a	412	DGD	C3B-C4B-C5B-C6B
33	D	411	LHG	C18-C19-C20-C21
32	h	102	LMG	C29-C30-C31-C32
28	A	411	SQD	C15-C16-C17-C18
24	B	612	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C16-C17-C18-C19
29	A	413	DGD	CFA-CGA-CHA-CIA

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C35-C36-C37-C38
27	d	407	PL9	C34-C36-C37-C38
33	E	101	LHG	C24-C25-C26-C27
33	e	101	LHG	C28-C29-C30-C31
32	h	102	LMG	C39-C40-C41-C42
29	H	102	DGD	CBA-CCA-CDA-CEA
24	B	605	CLA	C10-C11-C12-C13
24	c	511	CLA	C13-C15-C16-C17
29	c	516	DGD	C8B-C9B-CAB-CBB
29	a	412	DGD	CFA-CGA-CHA-CIA
32	h	102	LMG	C28-C29-C30-C31
33	D	409	LHG	C17-C18-C19-C20
24	b	608	CLA	C8-C10-C11-C12
24	C	510	CLA	C16-C17-C18-C20
24	a	404	CLA	C16-C17-C18-C20
24	B	615	CLA	C4-C3-C5-C6
24	C	507	CLA	C4-C3-C5-C6
27	A	410	PL9	C30-C29-C31-C32
29	C	518	DGD	C2A-C1A-O1G-C1G
29	h	104	DGD	CDA-CEA-CFA-CGA
32	d	411	LMG	C35-C36-C37-C38
33	d	410	LHG	C25-C26-C27-C28
28	F	101	SQD	C45-C44-O6-C1
24	B	611	CLA	C11-C12-C13-C14
24	B	614	CLA	C14-C13-C15-C16
24	B	615	CLA	C6-C7-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	C	507	CLA	C14-C13-C15-C16
24	C	508	CLA	C14-C13-C15-C16
24	C	514	CLA	C11-C10-C8-C9
24	a	405	CLA	C11-C10-C8-C9
24	a	405	CLA	C14-C13-C15-C16
24	a	407	CLA	C11-C10-C8-C9
24	b	607	CLA	C11-C10-C8-C9
24	b	609	CLA	C11-C12-C13-C14
24	b	615	CLA	C11-C12-C13-C14
24	b	616	CLA	C14-C13-C15-C16
32	d	411	LMG	C30-C31-C32-C33
33	d	409	LHG	C33-C34-C35-C36
24	B	604	CLA	C10-C11-C12-C13
24	b	606	CLA	C15-C16-C17-C18
24	b	615	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C19-C20-C21-C22
24	B	615	CLA	C4B-C3B-CAB-CBB
24	c	508	CLA	C15-C16-C17-C18
29	h	104	DGD	C3B-C4B-C5B-C6B
24	D	402	CLA	C15-C16-C17-C18
24	d	405	CLA	C8-C10-C11-C12
24	b	603	CLA	C16-C17-C18-C20
24	h	101	CLA	C16-C17-C18-C20
24	a	404	CLA	O1D-CGD-O2D-CED
24	C	512	CLA	O1A-CGA-O2A-C1
28	b	601	SQD	C19-C20-C21-C22
28	A	412	SQD	C30-C31-C32-C33
29	A	413	DGD	CDA-CEA-CFA-CGA
32	D	407	LMG	C33-C34-C35-C36
33	D	409	LHG	C9-C10-C11-C12
29	a	412	DGD	C8A-C9A-CAA-CBA
32	K	102	LMG	C30-C31-C32-C33
32	b	621	LMG	C19-C20-C21-C22
33	l	101	LHG	C24-C25-C26-C27
29	A	413	DGD	C1A-C2A-C3A-C4A
29	C	517	DGD	CDA-CEA-CFA-CGA
33	d	408	LHG	C19-C20-C21-C22
24	C	506	CLA	C11-C12-C13-C15
24	C	513	CLA	C12-C13-C15-C16
24	C	514	CLA	C11-C10-C8-C7
24	C	514	CLA	C12-C13-C15-C16
24	D	404	CLA	C11-C10-C8-C7
24	b	603	CLA	C6-C7-C8-C10
24	b	608	CLA	C11-C12-C13-C15
24	b	609	CLA	C11-C10-C8-C7
24	b	609	CLA	C11-C12-C13-C15
24	b	610	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	c	509	CLA	C11-C12-C13-C15
24	d	404	CLA	C6-C7-C8-C10
25	A	407	PHO	C12-C13-C15-C16
28	a	411	SQD	C31-C32-C33-C34
29	c	517	DGD	CDA-CEA-CFA-CGA
32	D	407	LMG	C40-C41-C42-C43
32	K	102	LMG	O10-C28-O8-C9
27	D	406	PL9	C7-C8-C9-C10
28	A	412	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
32	c	524	LMG	C32-C33-C34-C35
28	A	412	SQD	C44-C45-C46-O48
24	c	506	CLA	CBA-CGA-O2A-C1
28	f	101	SQD	C31-C32-C33-C34
32	c	524	LMG	C16-C17-C18-C19
26	K	101	BCR	C9-C10-C11-C12
26	c	514	BCR	C15-C16-C17-C18
26	k	101	BCR	C19-C20-C21-C22
29	c	518	DGD	C7A-C8A-C9A-CAA
32	D	410	LMG	C37-C38-C39-C40
33	L	101	LHG	C19-C20-C21-C22
28	A	412	SQD	C10-C11-C12-C13
32	b	621	LMG	C13-C14-C15-C16
32	c	524	LMG	C39-C40-C41-C42
26	c	515	BCR	C21-C22-C23-C24
29	C	518	DGD	C3A-C4A-C5A-C6A
33	L	101	LHG	C26-C27-C28-C29
32	c	519	LMG	C38-C39-C40-C41
33	D	408	LHG	C1-C2-C3-O3
24	B	613	CLA	O1D-CGD-O2D-CED
33	D	408	LHG	C33-C34-C35-C36
28	a	410	SQD	O6-C44-C45-C46
28	a	410	SQD	C44-C45-C46-O48
29	C	516	DGD	O6D-C5D-C6D-O5D
33	E	101	LHG	C16-C17-C18-C19
24	c	508	CLA	C16-C17-C18-C19
24	B	601	CLA	C16-C17-C18-C19
24	B	610	CLA	C16-C17-C18-C20
24	B	616	CLA	C11-C12-C13-C14
24	a	404	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C20
24	b	611	CLA	C8-C10-C11-C12
29	H	102	DGD	C7A-C8A-C9A-CAA
24	b	610	CLA	O1D-CGD-O2D-CED
28	a	411	SQD	O6-C44-C45-C46
27	D	406	PL9	C30-C29-C31-C32
27	a	409	PL9	C15-C14-C16-C17
28	F	101	SQD	C23-C24-C25-C26
32	M	101	LMG	C15-C16-C17-C18
27	a	409	PL9	C38-C39-C41-C42
27	d	407	PL9	C28-C29-C31-C32
28	A	412	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
24	B	610	CLA	C16-C17-C18-C19
32	M	101	LMG	O9-C10-O7-C8
33	D	409	LHG	C23-C24-C25-C26
33	e	101	LHG	O6-C4-C5-O7
26	h	103	BCR	C23-C24-C25-C26
26	h	103	BCR	C23-C24-C25-C30
29	c	516	DGD	C3A-C4A-C5A-C6A
29	c	517	DGD	CAB-CBB-CCB-CDB
32	b	621	LMG	C4-C5-C6-O5
24	b	606	CLA	C10-C11-C12-C13
32	C	501	LMG	C10-C11-C12-C13
33	d	410	LHG	C26-C27-C28-C29
24	B	613	CLA	CBD-CGD-O2D-CED
32	D	410	LMG	C33-C34-C35-C36
29	A	413	DGD	CEB-CFB-CGB-CHB
29	c	516	DGD	CAB-CBB-CCB-CDB
33	E	101	LHG	C30-C31-C32-C33
24	c	513	CLA	C16-C17-C18-C19
28	a	411	SQD	O47-C45-C46-O48
32	M	101	LMG	O7-C8-C9-O8
32	c	522	LMG	O7-C8-C9-O8
28	a	410	SQD	C10-C11-C12-C13
27	D	406	PL9	C4-C3-C7-C8
27	a	409	PL9	C4-C3-C7-C8
28	f	101	SQD	C25-C26-C27-C28
24	b	610	CLA	C4-C3-C5-C6
24	b	612	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
27	a	409	PL9	C40-C39-C41-C42
33	D	409	LHG	C25-C26-C27-C28
32	c	519	LMG	O9-C10-O7-C8
24	b	612	CLA	C2-C3-C5-C6
27	D	406	PL9	C28-C29-C31-C32
32	M	101	LMG	C40-C41-C42-C43
28	A	411	SQD	C11-C10-C9-C8
28	A	411	SQD	C13-C14-C15-C16
28	B	622	SQD	C25-C26-C27-C28
32	c	524	LMG	C14-C15-C16-C17
33	e	101	LHG	C27-C28-C29-C30
24	B	616	CLA	C11-C12-C13-C15
29	C	517	DGD	C7A-C8A-C9A-CAA
32	B	621	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	C	501	LMG	C32-C33-C34-C35
32	D	410	LMG	C12-C13-C14-C15
32	D	410	LMG	C14-C15-C16-C17
24	C	513	CLA	C14-C13-C15-C16
24	C	514	CLA	C14-C13-C15-C16
24	D	404	CLA	C11-C10-C8-C9
24	b	604	CLA	C11-C12-C13-C14
24	b	608	CLA	C6-C7-C8-C9
29	C	516	DGD	CDA-CEA-CFA-CGA
25	D	401	PHO	C2C-C3C-CAC-CBC
28	A	411	SQD	C14-C15-C16-C17
26	C	519	BCR	C6-C7-C8-C9
26	c	514	BCR	C22-C23-C24-C25
32	b	623	LMG	C19-C20-C21-C22
33	D	408	LHG	C29-C30-C31-C32
28	f	101	SQD	C33-C34-C35-C36
29	C	517	DGD	C3A-C4A-C5A-C6A
32	c	522	LMG	C12-C13-C14-C15
33	D	409	LHG	C24-C25-C26-C27
33	E	101	LHG	C23-C24-C25-C26
33	d	410	LHG	O1-C1-C2-O2
24	C	503	CLA	CBA-CGA-O2A-C1
28	F	101	SQD	O48-C23-C24-C25
24	B	615	CLA	C2-C3-C5-C6
24	b	610	CLA	C2-C3-C5-C6
24	D	404	CLA	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C19
29	c	516	DGD	O6D-C5D-C6D-O5D
29	c	516	DGD	O1B-C1B-O2G-C2G
33	D	409	LHG	C1-C2-C3-O3
29	c	516	DGD	CCB-CDB-CEB-CFB
32	D	410	LMG	C34-C35-C36-C37
26	B	617	BCR	C16-C17-C18-C36
26	K	101	BCR	C11-C10-C9-C34
26	b	618	BCR	C35-C13-C14-C15
26	b	620	BCR	C35-C13-C14-C15
26	c	514	BCR	C16-C17-C18-C36
32	M	101	LMG	O6-C5-C6-O5
24	B	612	CLA	C16-C17-C18-C19
24	B	615	CLA	C16-C17-C18-C19
28	a	411	SQD	C13-C14-C15-C16
24	B	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	D	411	LHG	C11-C10-C9-C8
24	B	603	CLA	C6-C7-C8-C10
24	B	605	CLA	C11-C10-C8-C7
24	B	616	CLA	C6-C7-C8-C10
24	C	505	CLA	C11-C10-C8-C7
24	D	404	CLA	C12-C13-C15-C16
24	b	604	CLA	C11-C12-C13-C15
24	b	605	CLA	C12-C13-C15-C16
24	c	501	CLA	C11-C12-C13-C15
24	c	505	CLA	C6-C7-C8-C10
24	h	101	CLA	C11-C12-C13-C15
32	d	411	LMG	C38-C39-C40-C41
24	B	608	CLA	C13-C15-C16-C17
26	a	408	BCR	C21-C22-C23-C24
26	b	619	BCR	C21-C22-C23-C24
26	h	103	BCR	C17-C18-C19-C20
28	b	601	SQD	C16-C17-C18-C19
32	b	621	LMG	O10-C28-O8-C9
29	C	517	DGD	C2G-C3G-O3G-C1D
29	C	517	DGD	C5D-C6D-O5D-C1E
29	c	517	DGD	C2G-C3G-O3G-C1D
29	c	517	DGD	C5D-C6D-O5D-C1E
24	c	507	CLA	C5-C6-C7-C8
32	c	522	LMG	C31-C32-C33-C34
29	H	102	DGD	O2G-C1B-C2B-C3B
24	C	513	CLA	C8-C10-C11-C12
32	c	524	LMG	C35-C36-C37-C38
24	c	506	CLA	O1A-CGA-O2A-C1
32	b	623	LMG	C15-C16-C17-C18
26	b	620	BCR	C9-C10-C11-C12
33	D	409	LHG	C31-C32-C33-C34
24	b	608	CLA	C5-C6-C7-C8
26	H	101	BCR	C11-C10-C9-C8
26	b	602	BCR	C20-C21-C22-C23
24	b	615	CLA	C8-C10-C11-C12
33	D	409	LHG	O6-C4-C5-O7
33	E	101	LHG	O6-C4-C5-O7
29	C	518	DGD	C4B-C5B-C6B-C7B
32	D	410	LMG	C7-C8-C9-O8
32	M	101	LMG	C7-C8-C9-O8
34	F	102	HEM	C4C-C3C-CAC-CBC
34	e	102	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	b	603	CLA	C16-C17-C18-C19
24	C	511	CLA	C15-C16-C17-C18
32	c	524	LMG	C11-C12-C13-C14
33	D	409	LHG	C35-C36-C37-C38
29	a	412	DGD	O1G-C1G-C2G-O2G
32	D	410	LMG	O7-C8-C9-O8
24	b	605	CLA	C14-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C9
24	b	614	CLA	C11-C12-C13-C14
24	c	505	CLA	C11-C10-C8-C9
24	c	506	CLA	C6-C7-C8-C9
24	d	405	CLA	C11-C12-C13-C14
32	b	621	LMG	C11-C12-C13-C14
28	a	410	SQD	C9-C10-C11-C12
32	C	501	LMG	C35-C36-C37-C38
32	C	501	LMG	C38-C39-C40-C41
28	B	622	SQD	C24-C25-C26-C27
24	b	612	CLA	C10-C11-C12-C13
24	c	506	CLA	C15-C16-C17-C18
33	e	101	LHG	C16-C17-C18-C19
24	B	601	CLA	C2-C1-O2A-CGA
24	B	615	CLA	C16-C17-C18-C20
29	h	104	DGD	C6A-C7A-C8A-C9A
24	B	603	CLA	C13-C15-C16-C17
29	h	104	DGD	C8B-C9B-CAB-CBB
29	C	516	DGD	O1G-C1A-C2A-C3A
24	c	510	CLA	C2-C3-C5-C6
32	D	410	LMG	C36-C37-C38-C39
24	B	607	CLA	C10-C11-C12-C13
29	C	516	DGD	C2A-C3A-C4A-C5A
29	h	104	DGD	CCA-CDA-CEA-CFA
24	a	405	CLA	C16-C17-C18-C20
29	C	516	DGD	C4D-C5D-C6D-O5D
29	c	516	DGD	C4D-C5D-C6D-O5D
32	K	102	LMG	C28-C29-C30-C31
24	b	608	CLA	O1A-CGA-O2A-C1
28	A	412	SQD	C11-C12-C13-C14
24	B	616	CLA	C3-C5-C6-C7
24	B	601	CLA	C4B-C3B-CAB-CBB
24	a	405	CLA	C4B-C3B-CAB-CBB
24	c	512	CLA	C1A-C2A-CAA-CBA
28	A	412	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C4-C3-C5-C6
26	b	618	BCR	C6-C7-C8-C9
33	D	409	LHG	C29-C30-C31-C32
29	C	516	DGD	C4E-C5E-C6E-O5E
28	b	601	SQD	C24-C25-C26-C27
29	A	413	DGD	CBA-CCA-CDA-CEA
32	D	410	LMG	C15-C16-C17-C18
28	a	410	SQD	C30-C31-C32-C33
33	l	101	LHG	C34-C35-C36-C37
24	B	604	CLA	C12-C13-C15-C16
24	B	605	CLA	C11-C12-C13-C15
24	B	611	CLA	C6-C7-C8-C10
24	C	503	CLA	C6-C7-C8-C10
24	C	506	CLA	C6-C7-C8-C10
24	C	511	CLA	C11-C12-C13-C15
24	C	513	CLA	C11-C10-C8-C7
24	b	605	CLA	C11-C12-C13-C15
24	b	607	CLA	C11-C12-C13-C15
24	c	509	CLA	C6-C7-C8-C10
24	c	512	CLA	C12-C13-C15-C16
29	C	517	DGD	C5B-C6B-C7B-C8B
24	C	511	CLA	C16-C17-C18-C20
24	h	101	CLA	C16-C17-C18-C19
32	h	102	LMG	C35-C36-C37-C38
29	a	412	DGD	C5A-C6A-C7A-C8A
24	C	503	CLA	O1A-CGA-O2A-C1
29	c	518	DGD	C1A-C2A-C3A-C4A
33	d	410	LHG	C2-C3-O3-P
32	M	101	LMG	C19-C20-C21-C22
24	B	602	CLA	C3A-C2A-CAA-CBA
24	c	512	CLA	C4-C3-C5-C6
24	B	612	CLA	C16-C17-C18-C20
29	H	102	DGD	C3A-C4A-C5A-C6A
24	C	505	CLA	C2-C3-C5-C6
29	H	102	DGD	O1A-C1A-O1G-C1G
33	l	101	LHG	O6-C4-C5-O7
32	c	524	LMG	C40-C41-C42-C43
24	b	608	CLA	CBD-CGD-O2D-CED
24	C	509	CLA	C2C-C3C-CAC-CBC
24	B	611	CLA	C6-C7-C8-C9
24	B	616	CLA	C6-C7-C8-C9
24	C	505	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	511	CLA	C11-C12-C13-C14
24	D	404	CLA	C14-C13-C15-C16
24	b	607	CLA	C14-C13-C15-C16
24	b	608	CLA	C11-C12-C13-C14
24	c	505	CLA	C6-C7-C8-C9
33	E	101	LHG	C28-C29-C30-C31
26	b	618	BCR	C15-C16-C17-C18
28	A	411	SQD	C25-C26-C27-C28
32	b	623	LMG	C35-C36-C37-C38
33	D	409	LHG	C11-C10-C9-C8
28	b	601	SQD	O47-C45-C46-O48
28	f	101	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
24	C	512	CLA	C8-C10-C11-C12
29	a	412	DGD	O1G-C1G-C2G-C3G
32	d	411	LMG	C33-C34-C35-C36
24	h	101	CLA	C3-C5-C6-C7
32	h	102	LMG	C38-C39-C40-C41
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	505	CLA	CAD-CBD-CGD-O2D
24	C	514	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	h	101	CLA	CAD-CBD-CGD-O2D
24	B	612	CLA	CBA-CGA-O2A-C1
24	b	608	CLA	CBA-CGA-O2A-C1
29	c	517	DGD	C1A-C2A-C3A-C4A
24	B	603	CLA	C5-C6-C7-C8
24	b	614	CLA	C8-C10-C11-C12
28	a	411	SQD	C9-C10-C11-C12
32	M	101	LMG	C39-C40-C41-C42
32	C	501	LMG	C19-C20-C21-C22
29	c	518	DGD	C8B-C9B-CAB-CBB
28	A	411	SQD	C33-C34-C35-C36
33	l	101	LHG	C33-C34-C35-C36
25	A	407	PHO	C2C-C3C-CAC-CBC
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	C	514	CLA	CAD-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	h	101	CLA	CAD-CBD-CGD-O1D
26	t	101	BCR	C13-C14-C15-C16
33	D	408	LHG	C3-O3-P-O4
33	D	409	LHG	C3-O3-P-O5
33	e	101	LHG	C3-O3-P-O6
33	e	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
33	D	409	LHG	C15-C16-C17-C18
29	A	413	DGD	CCA-CDA-CEA-CFA
24	C	506	CLA	C4-C3-C5-C6
24	C	514	CLA	C4-C3-C5-C6
24	B	606	CLA	C2B-C3B-CAB-CBB
24	C	504	CLA	C2B-C3B-CAB-CBB
24	C	513	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C2B-C3B-CAB-CBB
26	b	618	BCR	C11-C12-C13-C35
26	b	619	BCR	C7-C8-C9-C34
32	c	524	LMG	C13-C14-C15-C16
29	C	517	DGD	O1B-C1B-O2G-C2G
33	L	101	LHG	C24-C25-C26-C27
27	A	410	PL9	C4-C3-C7-C8
24	B	604	CLA	C2C-C3C-CAC-CBC
32	D	407	LMG	C28-C29-C30-C31
33	d	409	LHG	O9-C7-O7-C5
28	f	101	SQD	C46-C45-O47-C7
29	a	412	DGD	C1G-C2G-O2G-C1B
32	b	623	LMG	C9-C8-O7-C10
32	K	102	LMG	C14-C15-C16-C17
28	B	622	SQD	C28-C29-C30-C31
29	C	516	DGD	CCA-CDA-CEA-CFA
24	a	405	CLA	C16-C17-C18-C19
24	d	405	CLA	C16-C17-C18-C19
29	C	517	DGD	CCB-CDB-CEB-CFB
29	H	102	DGD	CAB-CBB-CCB-CDB
29	c	517	DGD	C8A-C9A-CAA-CBA
24	B	604	CLA	C11-C10-C8-C9
24	C	509	CLA	C6-C7-C8-C9
24	b	603	CLA	C11-C10-C8-C9
24	b	609	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	501	CLA	C11-C12-C13-C14
24	c	506	CLA	C11-C10-C8-C9
24	b	608	CLA	C6-C7-C8-C10
24	b	613	CLA	C12-C13-C15-C16
24	b	617	CLA	C11-C10-C8-C7
24	c	505	CLA	C11-C10-C8-C7
26	B	617	BCR	C20-C21-C22-C23
26	c	514	BCR	C12-C13-C14-C15
33	d	408	LHG	C9-C10-C11-C12
28	F	101	SQD	O5-C1-O6-C44
32	b	621	LMG	C15-C16-C17-C18
29	A	413	DGD	C2E-C1E-O5D-C6D
27	a	409	PL9	C28-C29-C31-C32
33	l	101	LHG	C12-C13-C14-C15
24	c	503	CLA	CBD-CGD-O2D-CED
27	A	410	PL9	C17-C18-C19-C21
29	c	516	DGD	O1G-C1G-C2G-O2G
32	D	410	LMG	C31-C32-C33-C34
26	k	101	BCR	C13-C14-C15-C16
28	a	411	SQD	C11-C10-C9-C8
28	b	601	SQD	C18-C19-C20-C21
32	D	407	LMG	C38-C39-C40-C41
33	D	408	LHG	C13-C14-C15-C16
24	D	403	CLA	C15-C16-C17-C18
33	L	101	LHG	C10-C11-C12-C13
28	b	601	SQD	C30-C31-C32-C33
24	B	613	CLA	C4-C3-C5-C6
29	c	518	DGD	CBB-CCB-CDB-CEB
29	h	104	DGD	O2G-C1B-C2B-C3B
24	b	604	CLA	C13-C15-C16-C17
32	c	524	LMG	C34-C35-C36-C37
28	b	601	SQD	C26-C27-C28-C29
33	D	408	LHG	C18-C19-C20-C21
28	A	412	SQD	C44-C45-O47-C7
29	a	412	DGD	O2G-C1B-C2B-C3B
24	c	503	CLA	C15-C16-C17-C18
32	c	524	LMG	C17-C18-C19-C20
29	A	413	DGD	C6B-C7B-C8B-C9B
29	c	516	DGD	C6B-C7B-C8B-C9B
32	b	623	LMG	C38-C39-C40-C41
33	d	409	LHG	C25-C26-C27-C28
28	B	622	SQD	C45-C44-O6-C1

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Mol	Chain	Res	Type	Atoms
24	b	615	CLA	C13-C15-C16-C17
28	A	412	SQD	C27-C28-C29-C30
24	B	603	CLA	C2A-CAA-CBA-CGA
33	D	411	LHG	C7-C8-C9-C10
25	A	407	PHO	C15-C16-C17-C18
24	c	503	CLA	O1D-CGD-O2D-CED
29	a	412	DGD	CEB-CFB-CGB-CHB
24	B	612	CLA	C11-C10-C8-C9
24	B	613	CLA	C6-C7-C8-C9
24	a	405	CLA	C6-C7-C8-C9
24	b	613	CLA	C14-C13-C15-C16
33	E	101	LHG	C2-C3-O3-P
24	D	404	CLA	C4B-C3B-CAB-CBB
24	b	610	CLA	C4B-C3B-CAB-CBB
28	a	411	SQD	C17-C18-C19-C20
33	d	409	LHG	C32-C33-C34-C35
27	A	410	PL9	C32-C33-C34-C35
32	b	621	LMG	C33-C34-C35-C36
24	B	601	CLA	C2-C3-C5-C6
24	C	506	CLA	C2-C3-C5-C6
29	c	516	DGD	CBB-CCB-CDB-CEB
24	b	612	CLA	C15-C16-C17-C18
32	c	522	LMG	C16-C17-C18-C19
24	b	612	CLA	C16-C17-C18-C20
24	D	403	CLA	C4C-C3C-CAC-CBC
24	a	405	CLA	C6-C7-C8-C10
24	b	611	CLA	C12-C13-C15-C16
29	c	516	DGD	C8A-C9A-CAA-CBA
33	l	101	LHG	C10-C11-C12-C13
32	M	101	LMG	C17-C18-C19-C20
32	c	522	LMG	C29-C30-C31-C32
24	a	407	CLA	O1A-CGA-O2A-C1
25	A	407	PHO	O1A-CGA-O2A-C1
24	B	607	CLA	C3A-C2A-CAA-CBA
24	C	507	CLA	C3A-C2A-CAA-CBA
32	C	501	LMG	C17-C18-C19-C20
33	D	411	LHG	C24-C25-C26-C27
24	B	603	CLA	C8-C10-C11-C12
26	B	619	BCR	C35-C13-C14-C15
26	b	602	BCR	C16-C17-C18-C36
26	d	406	BCR	C22-C23-C24-C25
29	A	413	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
29	C	518	DGD	C8B-C9B-CAB-CBB
33	e	101	LHG	O9-C7-O7-C5
35	v	201	HEC	CAD-CBD-CGD-O2D
24	C	507	CLA	C2-C1-O2A-CGA
24	c	510	CLA	C2-C1-O2A-CGA
32	b	621	LMG	C39-C40-C41-C42
28	a	410	SQD	C16-C17-C18-C19
26	C	515	BCR	C21-C22-C23-C24
24	c	512	CLA	C2-C3-C5-C6
33	L	101	LHG	C17-C18-C19-C20
32	D	407	LMG	C17-C18-C19-C20
24	c	511	CLA	C3-C5-C6-C7
24	B	610	CLA	C15-C16-C17-C18
33	d	408	LHG	C24-C25-C26-C27
24	B	612	CLA	O1A-CGA-O2A-C1
24	B	604	CLA	C11-C12-C13-C14
24	B	605	CLA	C11-C12-C13-C14
24	B	615	CLA	C11-C12-C13-C14
24	C	510	CLA	C11-C10-C8-C9
24	C	511	CLA	C6-C7-C8-C9
24	b	605	CLA	C6-C7-C8-C9
28	A	411	SQD	C10-C11-C12-C13
28	f	101	SQD	C44-C45-O47-C7
32	C	501	LMG	C7-C8-O7-C10
29	H	102	DGD	C7B-C8B-C9B-CAB
33	d	408	LHG	C18-C19-C20-C21
24	c	513	CLA	C3-C5-C6-C7
32	D	410	LMG	O1-C7-C8-C9
24	c	513	CLA	CBA-CGA-O2A-C1
32	b	621	LMG	O6-C5-C6-O5
33	D	411	LHG	O1-C1-C2-O2
32	b	621	LMG	C22-C23-C24-C25
34	e	102	HEM	CAD-CBD-CGD-O1D
35	v	201	HEC	CAD-CBD-CGD-O1D
25	D	401	PHO	C5-C6-C7-C8
24	B	602	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
26	c	521	BCR	C20-C21-C22-C23
34	F	102	HEM	CAD-CBD-CGD-O1D
35	V	201	HEC	CAD-CBD-CGD-O2D
24	B	615	CLA	C2B-C3B-CAB-CBB
24	D	404	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	a	405	CLA	C2B-C3B-CAB-CBB
24	c	507	CLA	C2B-C3B-CAB-CBB
26	A	409	BCR	C5-C6-C7-C8
26	C	519	BCR	C23-C24-C25-C30
26	Y	101	BCR	C23-C24-C25-C30
26	c	521	BCR	C1-C6-C7-C8
26	k	101	BCR	C1-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
29	H	102	DGD	C2B-C3B-C4B-C5B
33	D	409	LHG	C2-C3-O3-P
28	a	411	SQD	C25-C26-C27-C28
24	B	603	CLA	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
33	D	409	LHG	O6-C4-C5-C6
32	c	524	LMG	C29-C30-C31-C32
28	f	101	SQD	C34-C35-C36-C37
26	c	521	BCR	C15-C16-C17-C18
24	A	406	CLA	C11-C12-C13-C15
24	B	603	CLA	C12-C13-C15-C16
24	B	604	CLA	C11-C10-C8-C7
24	B	613	CLA	C6-C7-C8-C10
24	C	508	CLA	C11-C10-C8-C7
24	C	510	CLA	C12-C13-C15-C16
24	C	511	CLA	C12-C13-C15-C16
24	D	403	CLA	C12-C13-C15-C16
24	b	606	CLA	C11-C10-C8-C7
24	c	503	CLA	C11-C10-C8-C7
24	c	513	CLA	C12-C13-C15-C16
24	d	404	CLA	C11-C12-C13-C15
35	V	201	HEC	CAD-CBD-CGD-O1D
28	a	410	SQD	C27-C28-C29-C30
32	D	407	LMG	C16-C17-C18-C19
26	b	602	BCR	C36-C18-C19-C20
27	A	410	PL9	C28-C29-C31-C32
27	D	406	PL9	C43-C44-C46-C47
27	d	407	PL9	C13-C14-C16-C17
32	M	101	LMG	C35-C36-C37-C38
33	e	101	LHG	C25-C26-C27-C28
24	d	405	CLA	O1D-CGD-O2D-CED
24	c	509	CLA	C3-C5-C6-C7
29	c	516	DGD	C7B-C8B-C9B-CAB
24	b	606	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	c	512	CLA	C11-C12-C13-C14
28	b	601	SQD	C25-C26-C27-C28
24	C	505	CLA	C8-C10-C11-C12
26	k	101	BCR	C22-C23-C24-C25
24	C	508	CLA	O1D-CGD-O2D-CED
27	d	407	PL9	C45-C44-C46-C47
24	B	615	CLA	C5-C6-C7-C8
24	b	603	CLA	C8-C10-C11-C12
27	A	410	PL9	C13-C14-C16-C17
24	B	613	CLA	C13-C15-C16-C17
33	e	101	LHG	C18-C19-C20-C21
32	b	621	LMG	C14-C15-C16-C17
27	A	410	PL9	C34-C36-C37-C38
27	A	410	PL9	C39-C41-C42-C43
29	c	516	DGD	O1G-C1G-C2G-C3G
34	e	102	HEM	CAD-CBD-CGD-O2D
32	D	410	LMG	O1-C7-C8-O7
24	c	513	CLA	O1A-CGA-O2A-C1
24	B	608	CLA	C16-C17-C18-C20
29	c	518	DGD	C2A-C3A-C4A-C5A
32	c	524	LMG	C19-C20-C21-C22
24	C	513	CLA	C4B-C3B-CAB-CBB
24	A	408	CLA	C5-C6-C7-C8
24	c	509	CLA	CAA-CBA-CGA-O2A
29	c	516	DGD	O1G-C1A-C2A-C3A
29	H	102	DGD	CAA-CBA-CCA-CDA
33	D	409	LHG	C13-C14-C15-C16
24	c	505	CLA	O1D-CGD-O2D-CED
25	d	402	PHO	CHA-CBD-CGD-O1D
25	d	402	PHO	CHA-CBD-CGD-O2D
34	F	102	HEM	CAD-CBD-CGD-O2D
33	e	101	LHG	O6-C4-C5-C6
24	C	504	CLA	C8-C10-C11-C12
24	b	603	CLA	C13-C15-C16-C17
24	b	605	CLA	C8-C10-C11-C12
33	L	101	LHG	C14-C15-C16-C17
28	a	411	SQD	C24-C25-C26-C27
24	B	612	CLA	C11-C10-C8-C7
24	B	615	CLA	C11-C12-C13-C15
24	C	511	CLA	C6-C7-C8-C10
24	b	606	CLA	C11-C12-C13-C15
26	t	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	a	412	DGD	C9A-CAA-CBA-CCA
24	B	603	CLA	C6-C7-C8-C9
24	C	506	CLA	C6-C7-C8-C9
24	C	512	CLA	C11-C10-C8-C9
32	c	522	LMG	C35-C36-C37-C38
28	A	411	SQD	C12-C13-C14-C15
32	B	621	LMG	C37-C38-C39-C40
32	c	522	LMG	C28-C29-C30-C31
32	c	519	LMG	C32-C33-C34-C35
32	h	102	LMG	O9-C10-C11-C12
29	c	516	DGD	CBA-CCA-CDA-CEA
29	C	516	DGD	CBA-CCA-CDA-CEA
24	D	404	CLA	C13-C15-C16-C17
25	a	406	PHO	O2A-C1-C2-C3
29	c	518	DGD	C9A-CAA-CBA-CCA
32	b	623	LMG	C40-C41-C42-C43
33	D	409	LHG	C16-C17-C18-C19
25	A	407	PHO	CBA-CGA-O2A-C1
29	c	517	DGD	C3A-C4A-C5A-C6A
26	c	521	BCR	C12-C13-C14-C15
29	c	516	DGD	C1B-C2B-C3B-C4B
29	c	517	DGD	C9A-CAA-CBA-CCA
33	l	101	LHG	C30-C31-C32-C33
28	a	411	SQD	C30-C31-C32-C33
29	h	104	DGD	C5A-C6A-C7A-C8A
33	L	101	LHG	O9-C7-O7-C5
24	C	514	CLA	C2-C3-C5-C6
28	a	411	SQD	C26-C27-C28-C29
28	b	601	SQD	C15-C16-C17-C18
24	B	616	CLA	O1A-CGA-O2A-C1
24	b	613	CLA	CAA-CBA-CGA-O2A
28	a	410	SQD	O47-C7-C8-C9
32	C	501	LMG	C34-C35-C36-C37
33	E	101	LHG	C10-C11-C12-C13
33	D	411	LHG	C16-C17-C18-C19
24	A	406	CLA	C15-C16-C17-C18
24	B	604	CLA	C14-C13-C15-C16
24	C	503	CLA	C14-C13-C15-C16
24	C	511	CLA	C14-C13-C15-C16
24	b	605	CLA	C11-C12-C13-C14
24	c	503	CLA	C11-C10-C8-C9
24	c	509	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	512	CLA	C14-C13-C15-C16
33	e	101	LHG	C10-C11-C12-C13
33	d	409	LHG	C12-C13-C14-C15
26	c	521	BCR	C17-C18-C19-C20
24	A	405	CLA	C13-C15-C16-C17
29	h	104	DGD	CAA-CBA-CCA-CDA
24	B	604	CLA	C11-C12-C13-C15
24	B	605	CLA	C12-C13-C15-C16
24	b	606	CLA	C12-C13-C15-C16
24	b	615	CLA	C6-C7-C8-C10
24	c	506	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C12-C13-C15
24	b	610	CLA	C2B-C3B-CAB-CBB
26	B	619	BCR	C1-C6-C7-C8
26	B	619	BCR	C5-C6-C7-C8
26	C	519	BCR	C23-C24-C25-C26
26	b	618	BCR	C1-C6-C7-C8
26	b	618	BCR	C5-C6-C7-C8
26	c	521	BCR	C5-C6-C7-C8
26	c	521	BCR	C23-C24-C25-C26
26	c	521	BCR	C23-C24-C25-C30
26	t	101	BCR	C1-C6-C7-C8
28	a	410	SQD	C24-C25-C26-C27
29	a	412	DGD	CDB-CEB-CFB-CGB
32	M	101	LMG	C11-C12-C13-C14
33	d	408	LHG	C27-C28-C29-C30
33	D	409	LHG	C32-C33-C34-C35
24	B	612	CLA	CAA-CBA-CGA-O2A
28	a	410	SQD	C19-C20-C21-C22
33	d	410	LHG	C24-C23-O8-C6
24	b	603	CLA	C2A-CAA-CBA-CGA
28	A	412	SQD	C8-C7-O47-C45
28	a	410	SQD	C8-C7-O47-C45
24	B	607	CLA	C5-C6-C7-C8
28	A	411	SQD	O47-C7-C8-C9
29	C	518	DGD	CBB-CCB-CDB-CEB
29	c	517	DGD	CCA-CDA-CEA-CFA
33	D	408	LHG	C16-C17-C18-C19
29	c	516	DGD	C3B-C4B-C5B-C6B
32	b	623	LMG	C32-C33-C34-C35
29	h	104	DGD	CBB-CCB-CDB-CEB
28	a	410	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
24	c	501	CLA	C2A-CAA-CBA-CGA
32	M	101	LMG	C30-C31-C32-C33
32	h	102	LMG	C34-C35-C36-C37
24	B	605	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C14
24	c	513	CLA	C14-C13-C15-C16
25	a	406	PHO	C14-C13-C15-C16
26	d	406	BCR	C7-C8-C9-C34
24	B	613	CLA	CAA-CBA-CGA-O2A
28	b	601	SQD	O6-C44-C45-C46
32	c	524	LMG	O1-C7-C8-C9
28	f	101	SQD	C29-C30-C31-C32
24	B	604	CLA	C1A-C2A-CAA-CBA
24	B	610	CLA	C4B-C3B-CAB-CBB
24	B	604	CLA	C4-C3-C5-C6
24	B	609	CLA	C4-C3-C5-C6
29	C	516	DGD	O6E-C1E-O5D-C6D
32	c	524	LMG	O8-C28-C29-C30
32	K	102	LMG	C18-C19-C20-C21
32	C	501	LMG	O1-C7-C8-O7
26	B	618	BCR	C11-C12-C13-C14
26	H	101	BCR	C21-C22-C23-C24
32	C	501	LMG	C8-C9-O8-C28
24	b	613	CLA	C3-C5-C6-C7
32	b	621	LMG	C40-C41-C42-C43
24	c	510	CLA	CAA-CBA-CGA-O2A
24	B	614	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C2A-CAA-CBA-CGA
32	D	410	LMG	C16-C17-C18-C19
28	b	601	SQD	O47-C7-C8-C9
33	L	101	LHG	O7-C7-C8-C9
24	c	506	CLA	C8-C10-C11-C12
33	L	101	LHG	C15-C16-C17-C18
28	a	410	SQD	C5-C6-S-O7
29	C	516	DGD	C6A-C7A-C8A-C9A
29	H	102	DGD	C8B-C9B-CAB-CBB
24	b	617	CLA	C4-C3-C5-C6
33	e	101	LHG	C19-C20-C21-C22
28	f	101	SQD	O48-C23-C24-C25
24	B	607	CLA	C12-C13-C15-C16
24	b	611	CLA	C11-C12-C13-C15
24	c	512	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	h	101	CLA	C11-C10-C8-C7
33	D	411	LHG	C24-C23-O8-C6
24	c	512	CLA	C8-C10-C11-C12
29	c	517	DGD	CAA-CBA-CCA-CDA
32	C	501	LMG	C9-C8-O7-C10
33	D	409	LHG	C4-C5-O7-C7
24	b	614	CLA	CAA-CBA-CGA-O2A
32	D	407	LMG	C15-C16-C17-C18
24	C	514	CLA	C5-C6-C7-C8
28	A	411	SQD	C9-C10-C11-C12
32	b	621	LMG	O9-C10-C11-C12
28	A	411	SQD	C17-C18-C19-C20
33	d	408	LHG	O8-C23-C24-C25
27	d	407	PL9	C12-C11-C9-C8
28	A	411	SQD	C27-C28-C29-C30
32	c	522	LMG	C39-C40-C41-C42
29	C	516	DGD	O2G-C1B-C2B-C3B
32	b	623	LMG	O7-C10-C11-C12
32	K	102	LMG	C38-C39-C40-C41
24	B	612	CLA	CAA-CBA-CGA-O1A
24	b	614	CLA	CAA-CBA-CGA-O1A
24	c	504	CLA	C11-C12-C13-C15
24	b	615	CLA	C2A-CAA-CBA-CGA
28	F	101	SQD	C34-C35-C36-C37
24	A	406	CLA	C11-C12-C13-C14
24	B	603	CLA	C14-C13-C15-C16
24	C	510	CLA	C14-C13-C15-C16
24	b	606	CLA	C14-C13-C15-C16
24	h	101	CLA	C11-C12-C13-C14
32	b	623	LMG	O9-C10-C11-C12
24	b	611	CLA	C13-C15-C16-C17
33	e	101	LHG	C11-C10-C9-C8
24	c	504	CLA	C8-C10-C11-C12
24	b	613	CLA	CAA-CBA-CGA-O1A
33	e	101	LHG	O10-C23-C24-C25
32	B	621	LMG	O8-C28-C29-C30
24	B	603	CLA	CBD-CGD-O2D-CED
24	c	510	CLA	CAA-CBA-CGA-O1A
33	D	409	LHG	O10-C23-C24-C25
29	c	516	DGD	O2G-C1B-C2B-C3B
29	C	517	DGD	CAA-CBA-CCA-CDA
24	B	608	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	c	516	DGD	C1G-C2G-C3G-O3G
32	K	102	LMG	O1-C7-C8-C9
24	C	503	CLA	C15-C16-C17-C18
24	A	405	CLA	CAD-CBD-CGD-O2D
24	B	607	CLA	CAD-CBD-CGD-O2D
24	D	404	CLA	CAD-CBD-CGD-O2D
24	a	404	CLA	CAD-CBD-CGD-O2D
24	c	501	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
27	d	407	PL9	C37-C38-C39-C40
29	c	516	DGD	O1B-C1B-C2B-C3B
24	D	403	CLA	C2-C1-O2A-CGA
28	A	412	SQD	C19-C20-C21-C22
24	B	613	CLA	CAA-CBA-CGA-O1A
24	a	407	CLA	CAA-CBA-CGA-O2A
24	B	609	CLA	C2-C3-C5-C6
34	e	102	HEM	CAA-CBA-CGA-O2A
24	c	507	CLA	C3-C5-C6-C7
33	D	411	LHG	C19-C20-C21-C22
24	d	403	CLA	C4C-C3C-CAC-CBC

There are no ring outliers.

97 monomers are involved in 174 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	H	102	DGD	1	0
24	B	612	CLA	1	0
32	c	522	LMG	1	0
28	a	411	SQD	1	0
24	C	512	CLA	3	0
24	b	603	CLA	1	0
33	l	101	LHG	1	0
24	B	613	CLA	1	0
24	B	615	CLA	1	0
24	b	616	CLA	1	0
29	h	104	DGD	1	0
24	b	604	CLA	1	0
26	B	619	BCR	3	0
24	b	614	CLA	1	0
32	b	621	LMG	1	0
35	V	201	HEC	1	0
24	C	506	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	504	CLA	1	0
26	b	618	BCR	3	0
24	B	614	CLA	1	0
26	c	521	BCR	4	0
26	B	618	BCR	5	0
24	B	605	CLA	2	0
24	c	501	CLA	2	0
25	d	402	PHO	1	0
33	d	409	LHG	1	0
24	B	602	CLA	1	0
24	D	402	CLA	1	0
32	b	623	LMG	1	0
33	D	411	LHG	2	0
24	B	604	CLA	3	0
26	a	408	BCR	1	0
33	D	408	LHG	2	0
26	d	406	BCR	2	0
26	b	602	BCR	2	0
33	L	101	LHG	1	0
26	h	103	BCR	4	0
24	c	507	CLA	1	0
24	b	606	CLA	4	0
26	Y	101	BCR	3	0
27	D	406	PL9	1	0
33	d	408	LHG	4	0
26	b	619	BCR	3	0
24	C	510	CLA	2	0
33	E	101	LHG	2	0
24	c	503	CLA	1	0
25	a	406	PHO	1	0
24	h	101	CLA	4	0
24	b	607	CLA	5	0
35	v	201	HEC	2	0
24	b	608	CLA	1	0
34	F	102	HEM	4	0
32	M	101	LMG	1	0
26	D	405	BCR	5	0
29	a	412	DGD	1	0
24	C	503	CLA	1	0
24	B	606	CLA	6	0
24	d	404	CLA	1	0
33	D	409	LHG	1	0

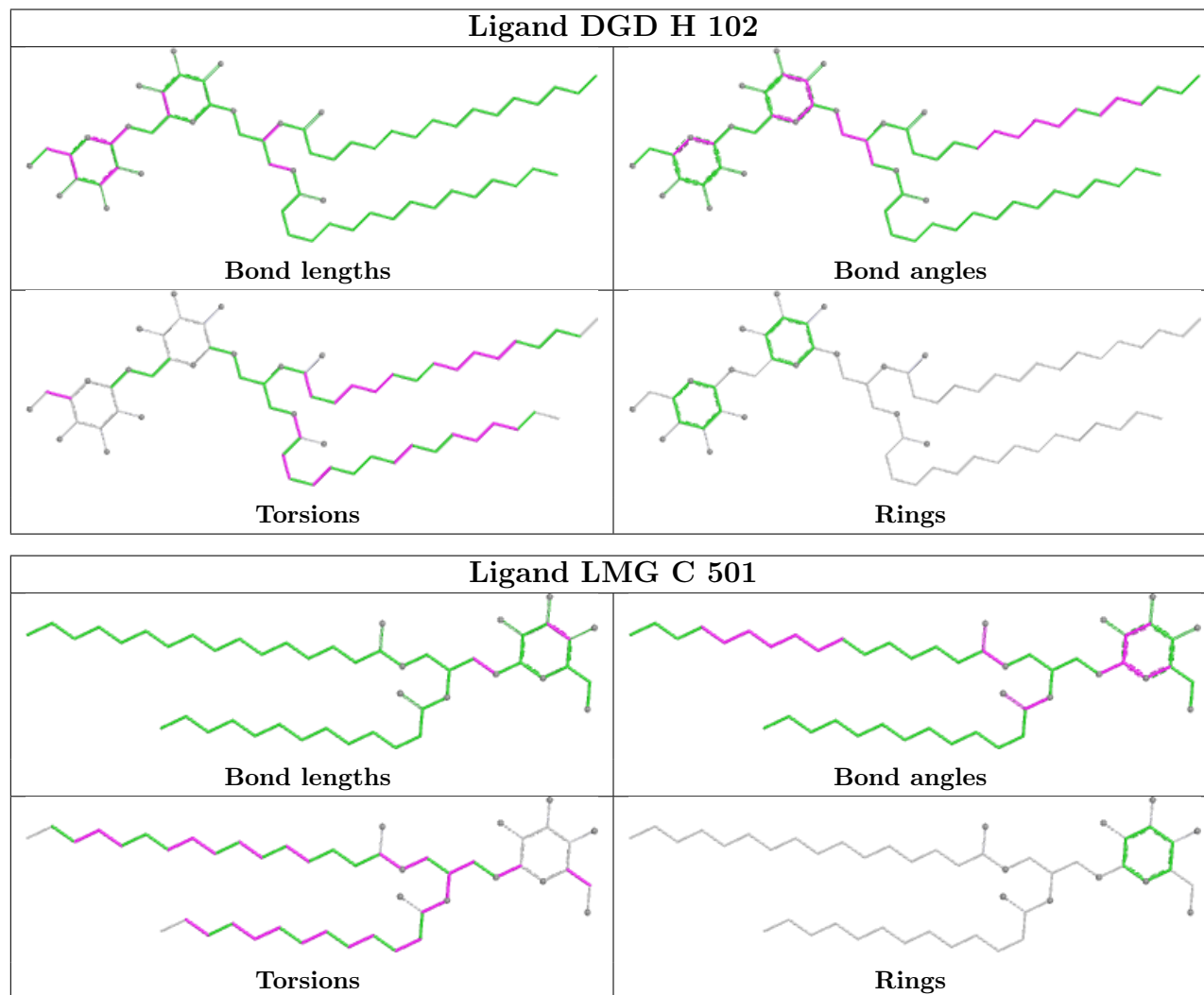
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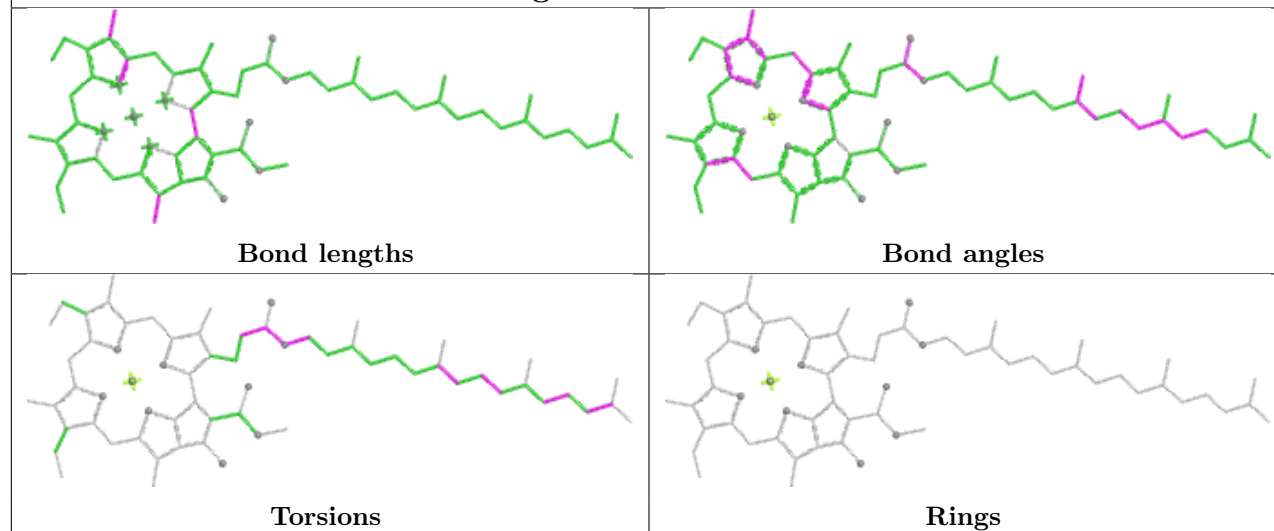
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	409	PL9	3	0
24	C	513	CLA	2	0
26	H	101	BCR	1	0
24	b	611	CLA	1	0
24	d	403	CLA	2	0
24	b	610	CLA	1	0
24	B	601	CLA	2	0
24	c	508	CLA	1	0
29	A	413	DGD	2	0
28	F	101	SQD	1	0
24	B	608	CLA	1	0
24	b	613	CLA	3	0
24	c	506	CLA	1	0
28	f	101	SQD	4	0
24	b	609	CLA	3	0
24	b	605	CLA	4	0
24	C	514	CLA	4	0
24	B	603	CLA	1	0
34	e	102	HEM	5	0
28	A	412	SQD	2	0
28	B	622	SQD	3	0
26	C	515	BCR	3	0
24	A	405	CLA	1	0
32	c	524	LMG	3	0
28	a	410	SQD	2	0
26	A	409	BCR	1	0
26	K	101	BCR	4	0
24	B	609	CLA	1	0
26	b	620	BCR	3	0
24	a	404	CLA	2	0
24	c	511	CLA	1	0
24	B	610	CLA	1	0
24	D	403	CLA	2	0
24	b	615	CLA	3	0
26	t	101	BCR	6	0
24	c	513	CLA	1	0
25	D	401	PHO	1	0
29	c	518	DGD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

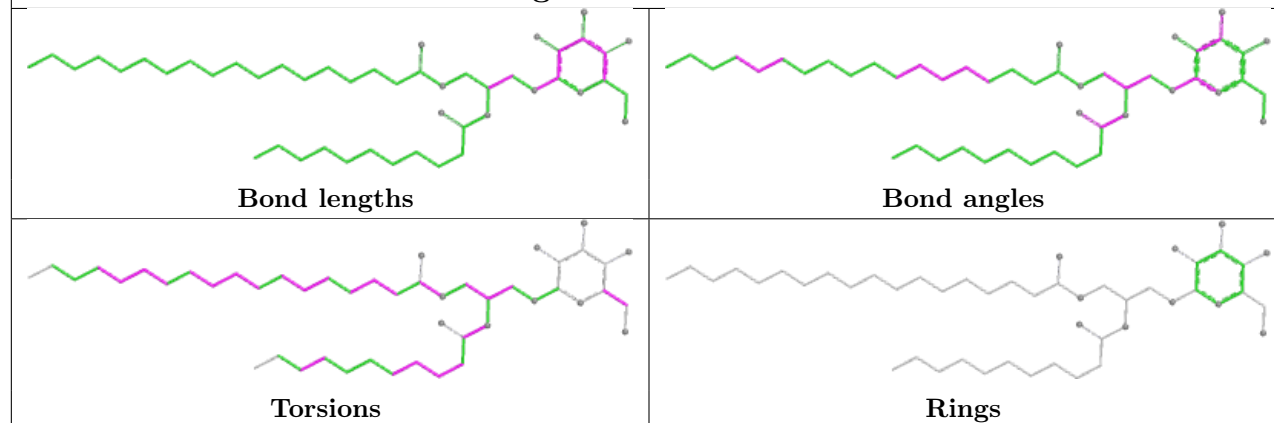
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



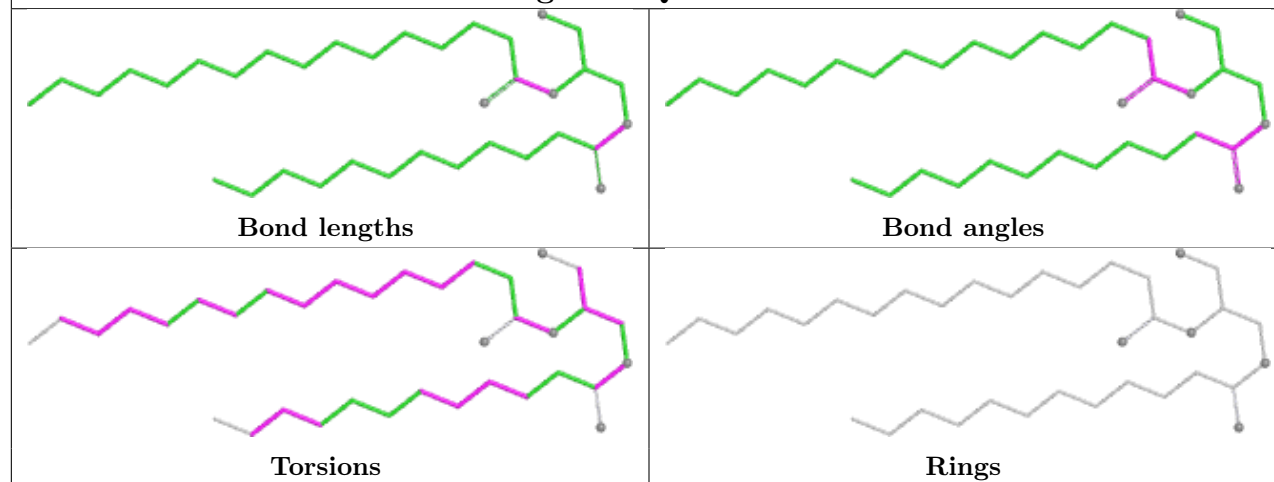
Ligand CLA B 612

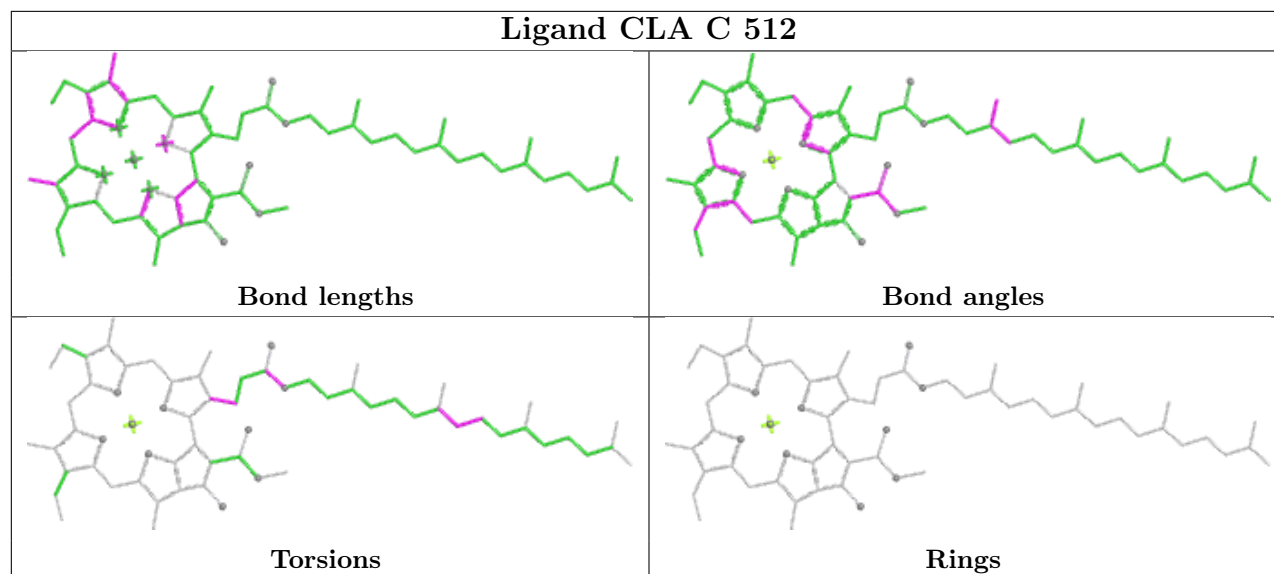
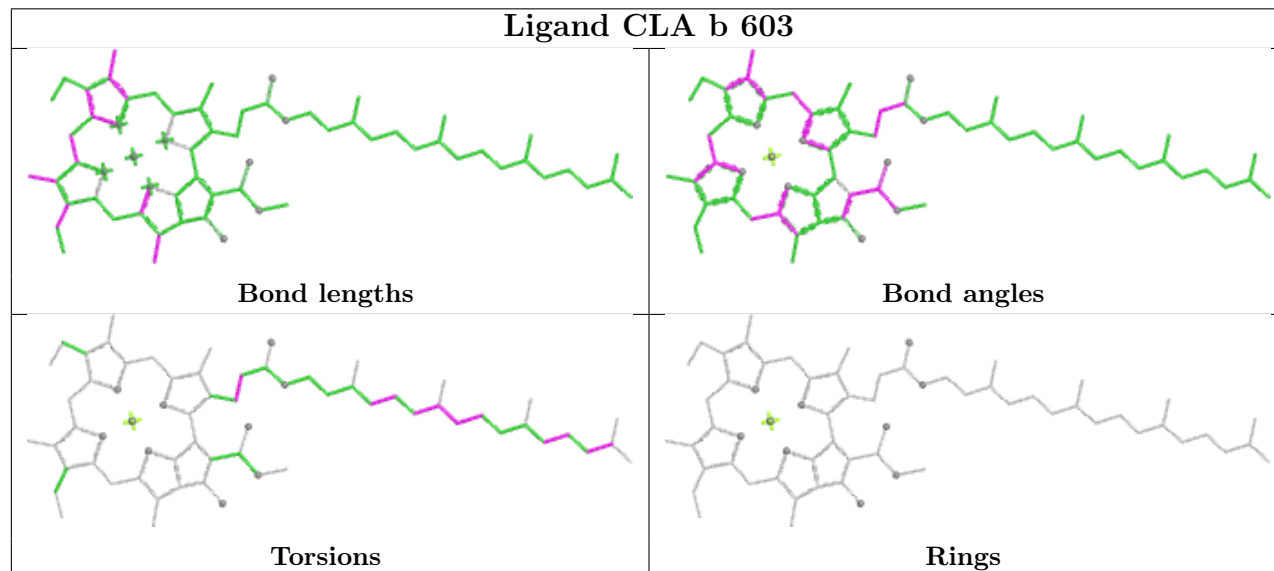


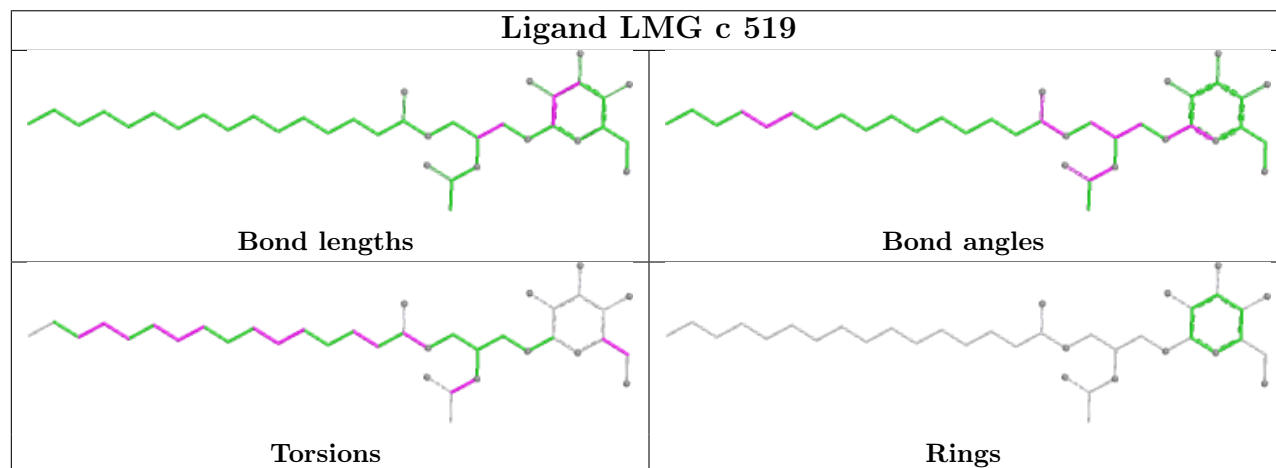
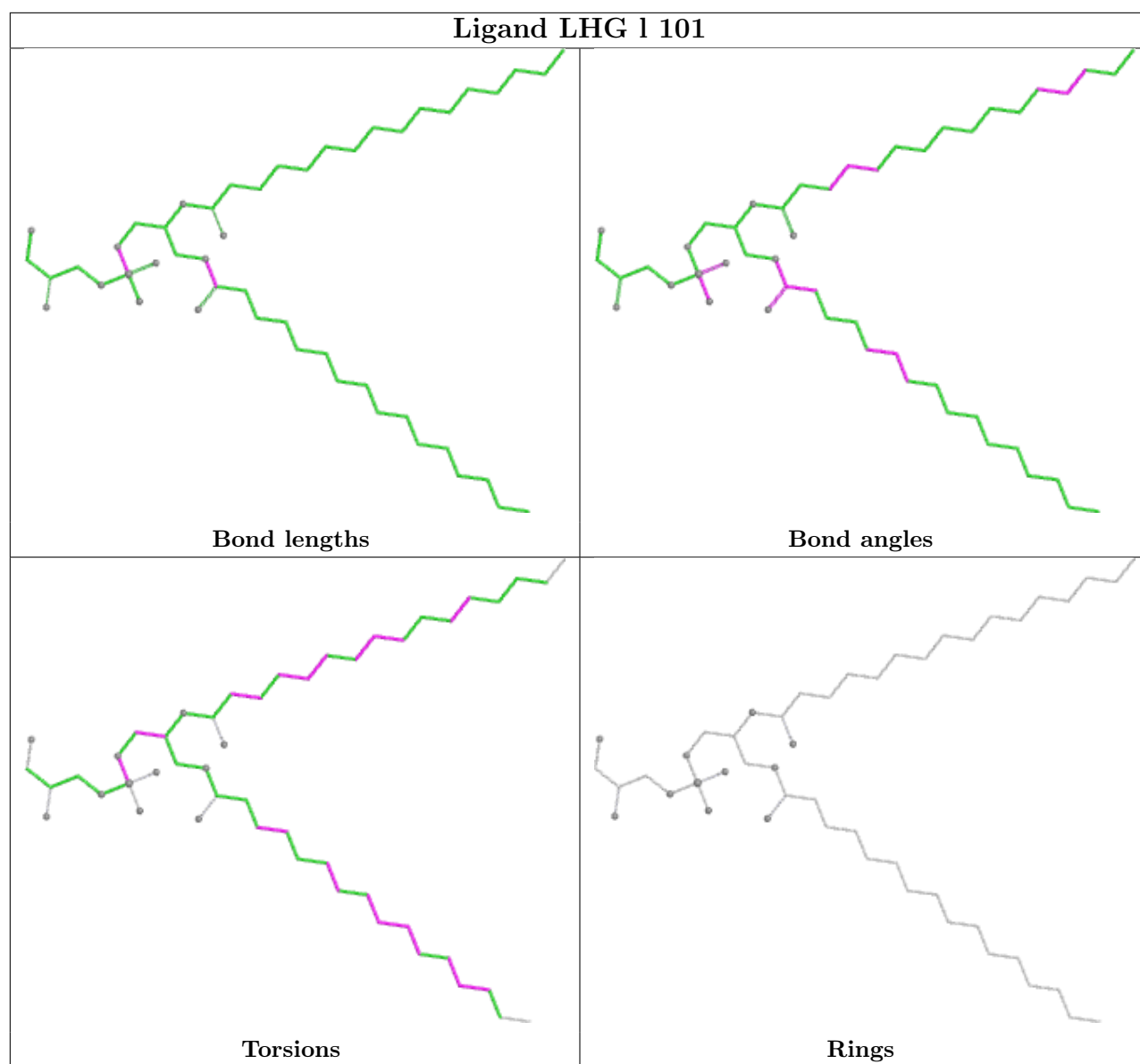
Ligand LMG c 522



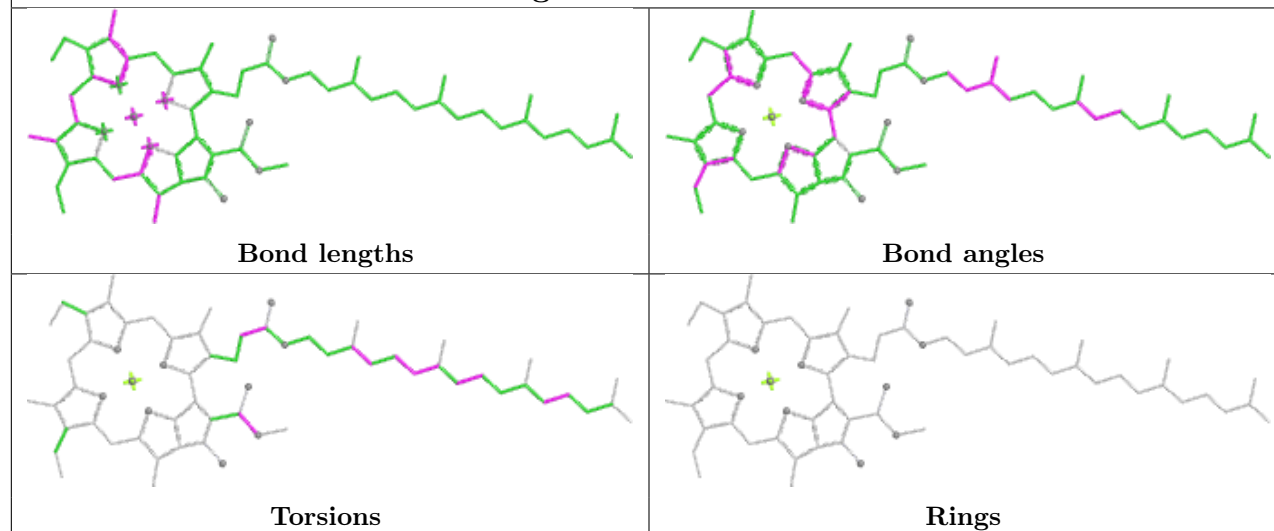
Ligand SQD a 411



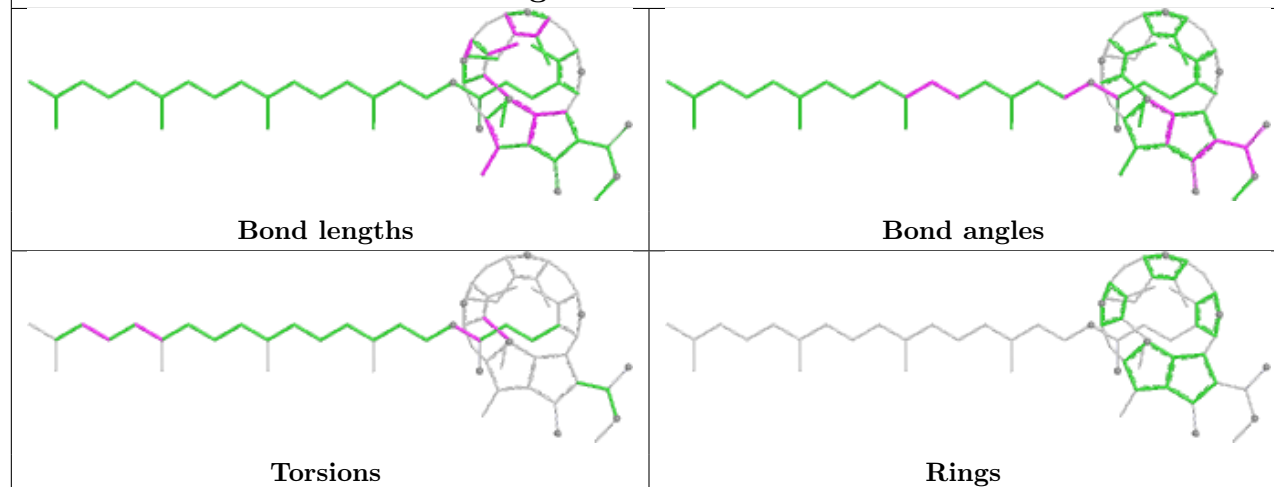
Ligand CLA C 512**Ligand CLA b 603**



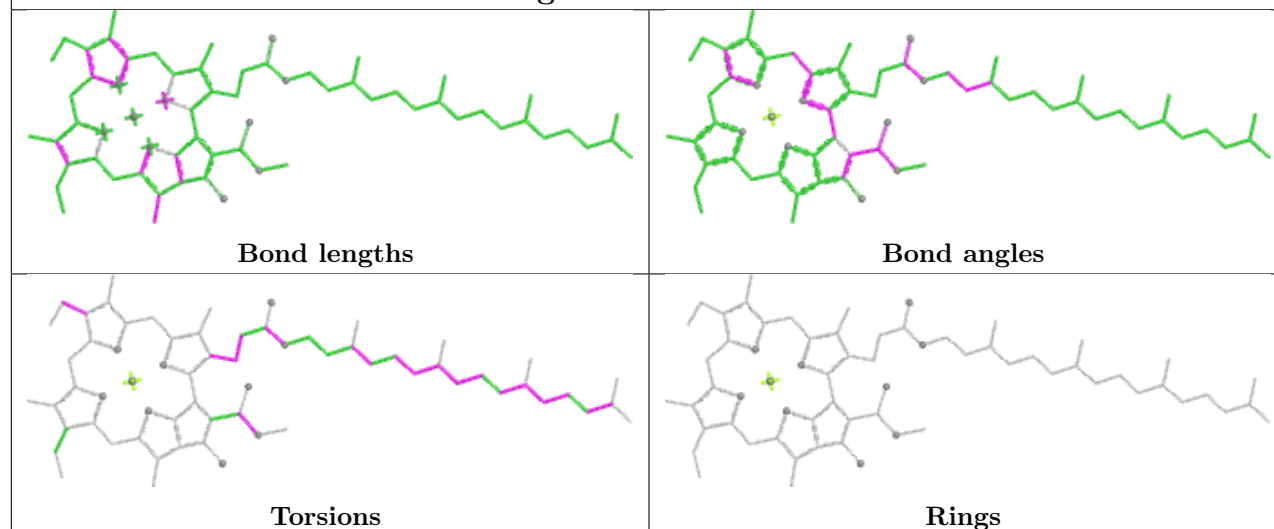
Ligand CLA B 613



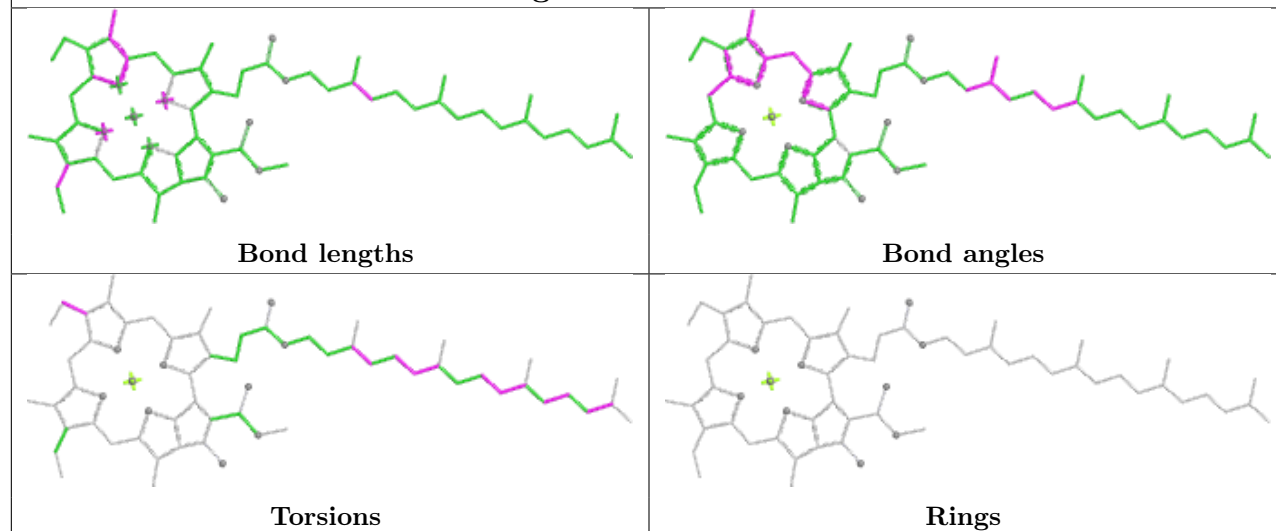
Ligand PHO A 407



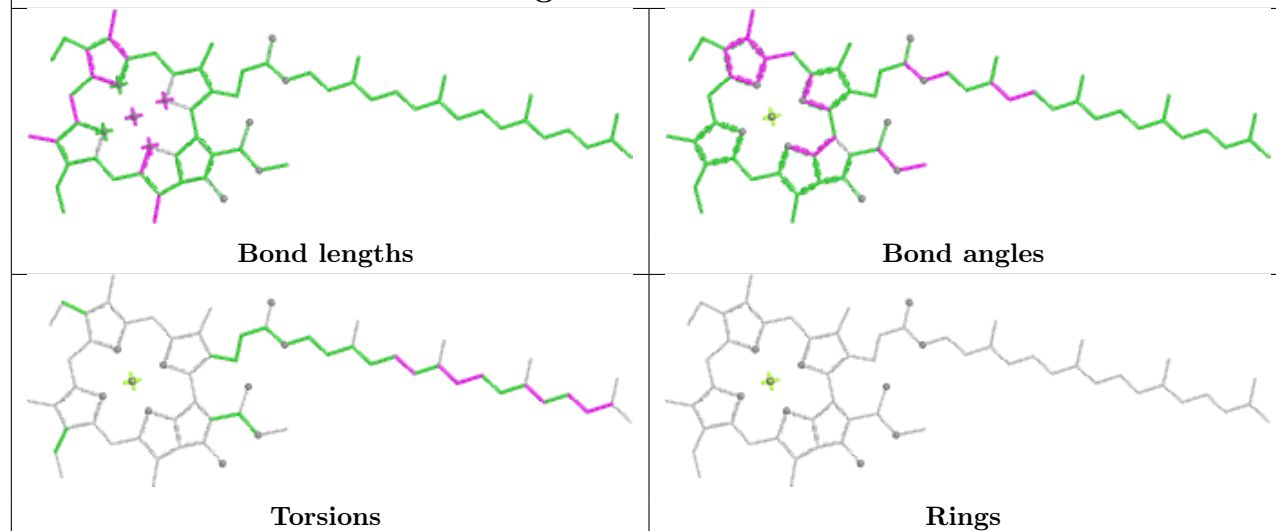
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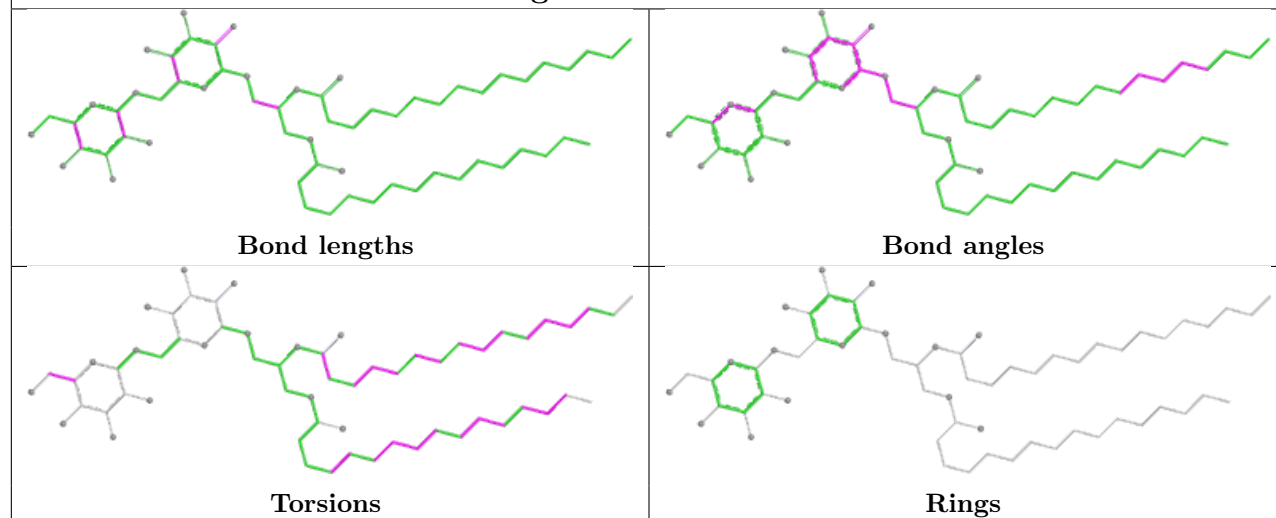
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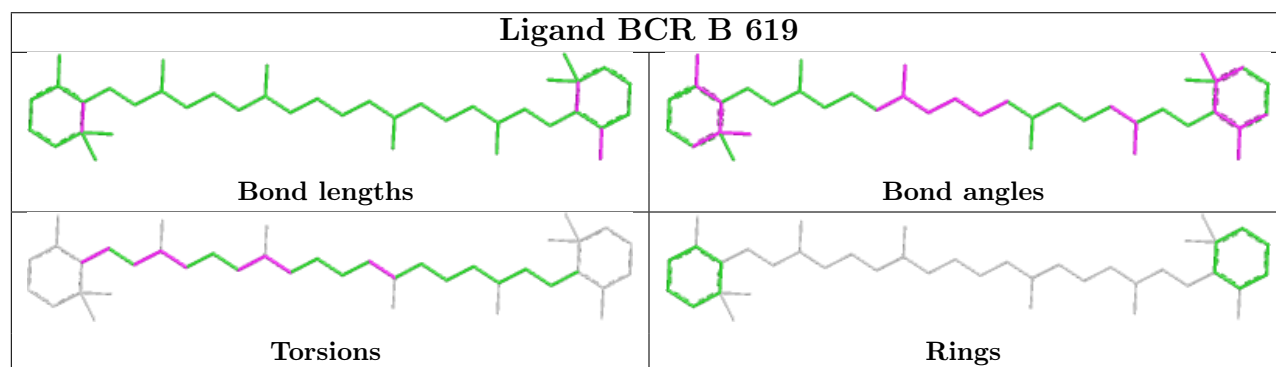
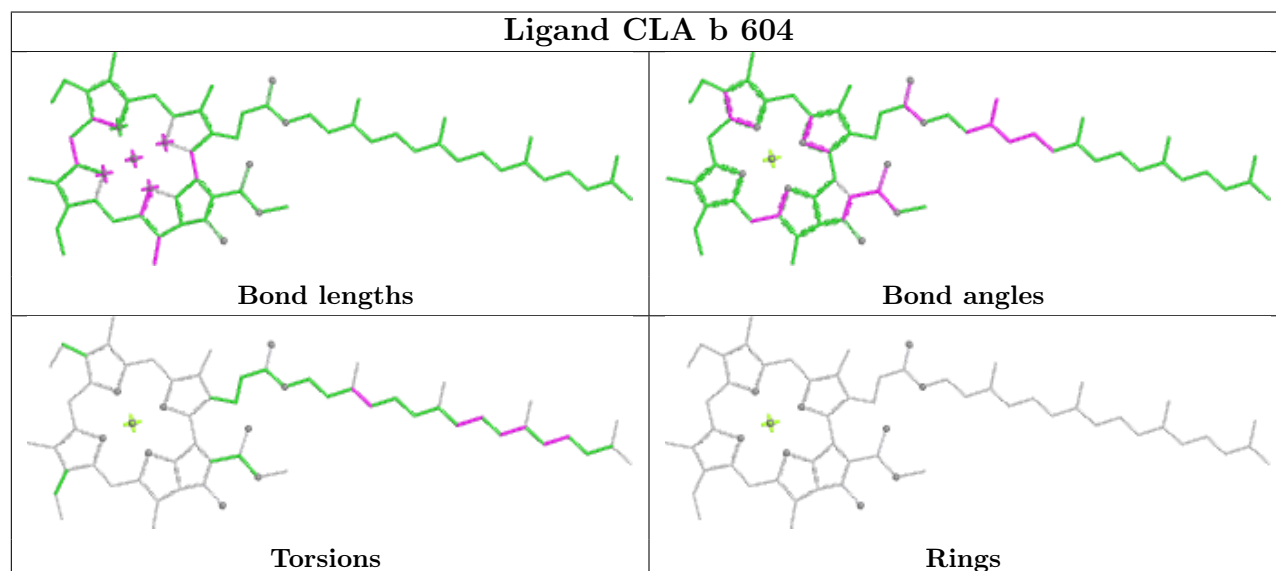
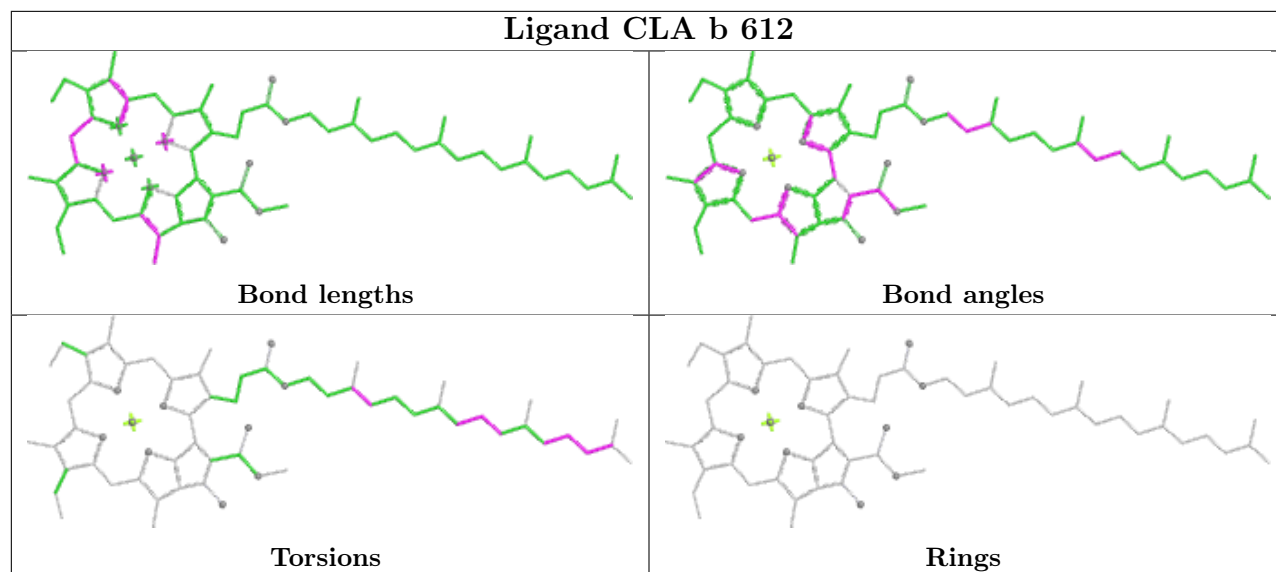


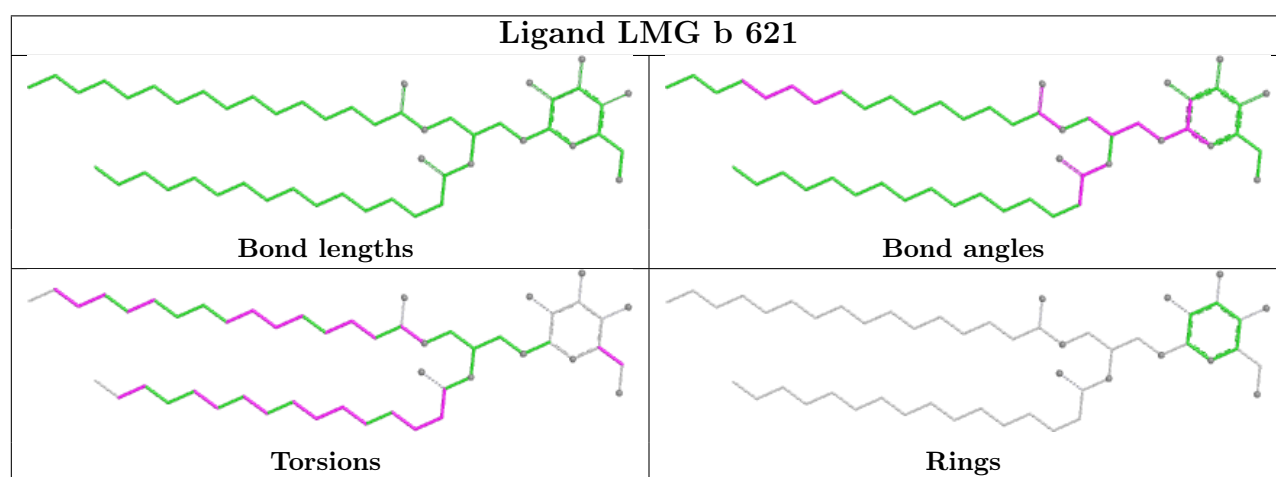
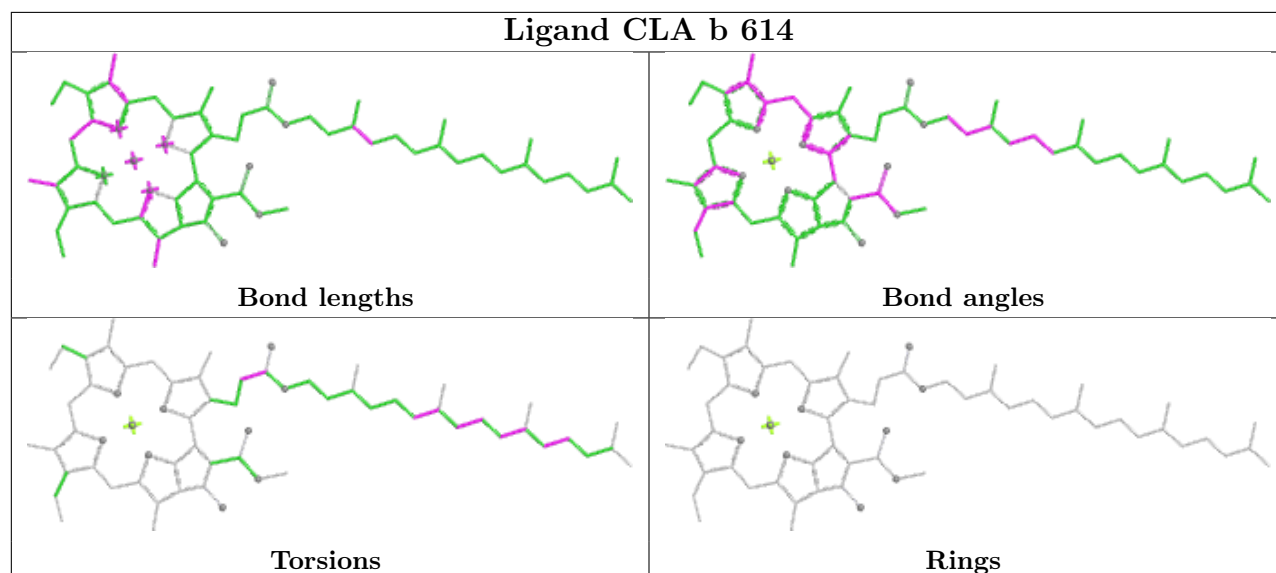
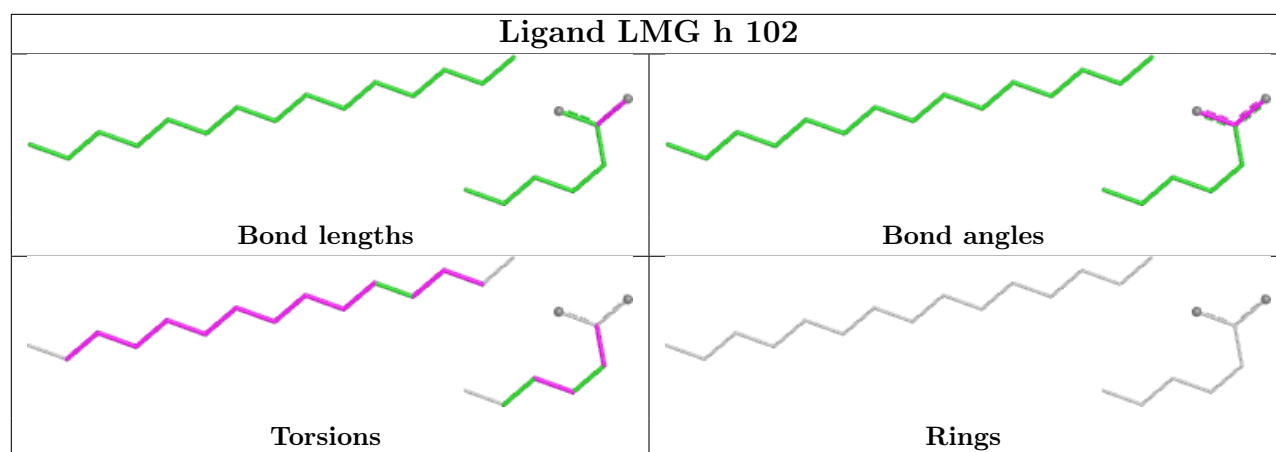
Ligand CLA b 616



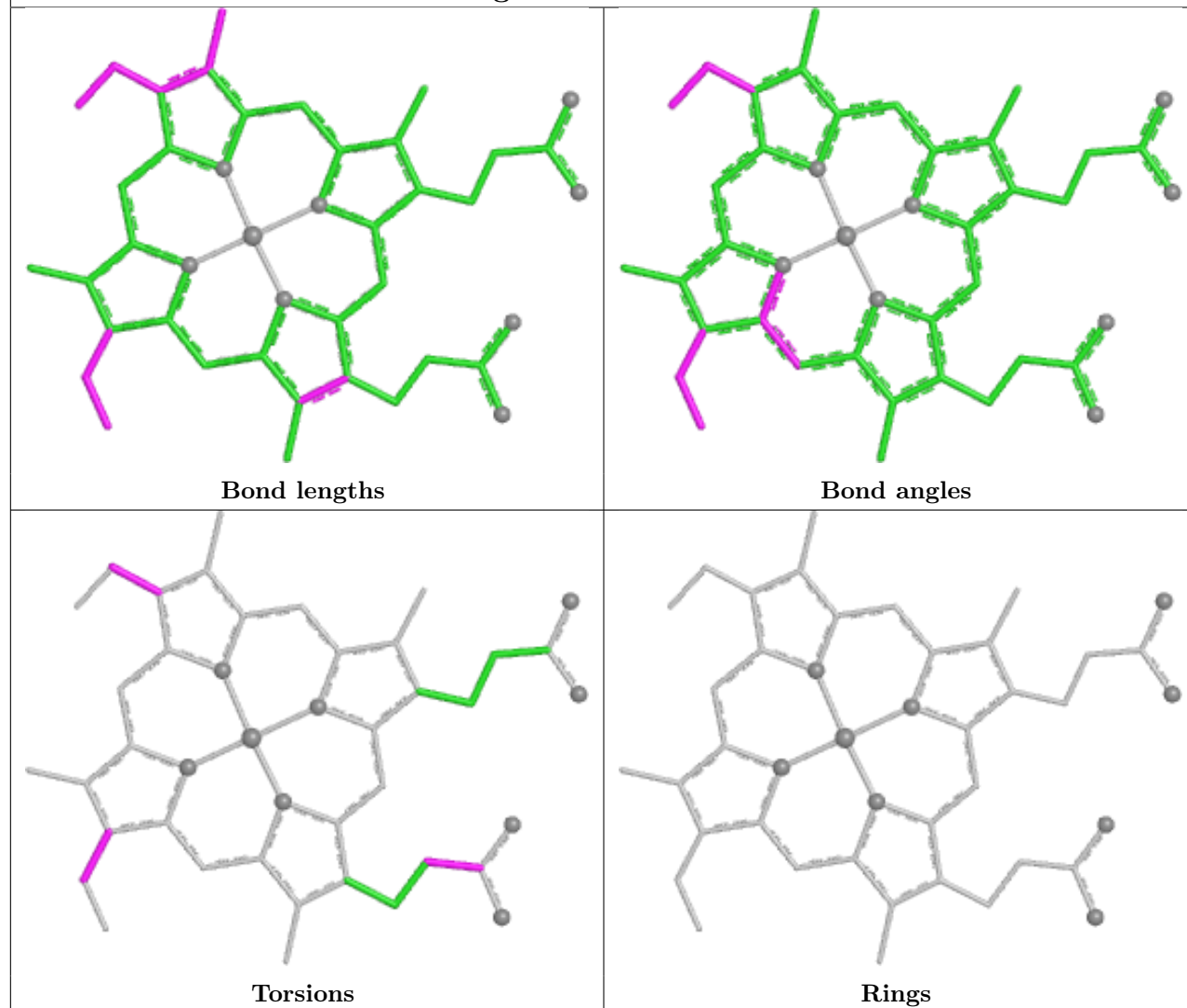
Ligand DGD h 104



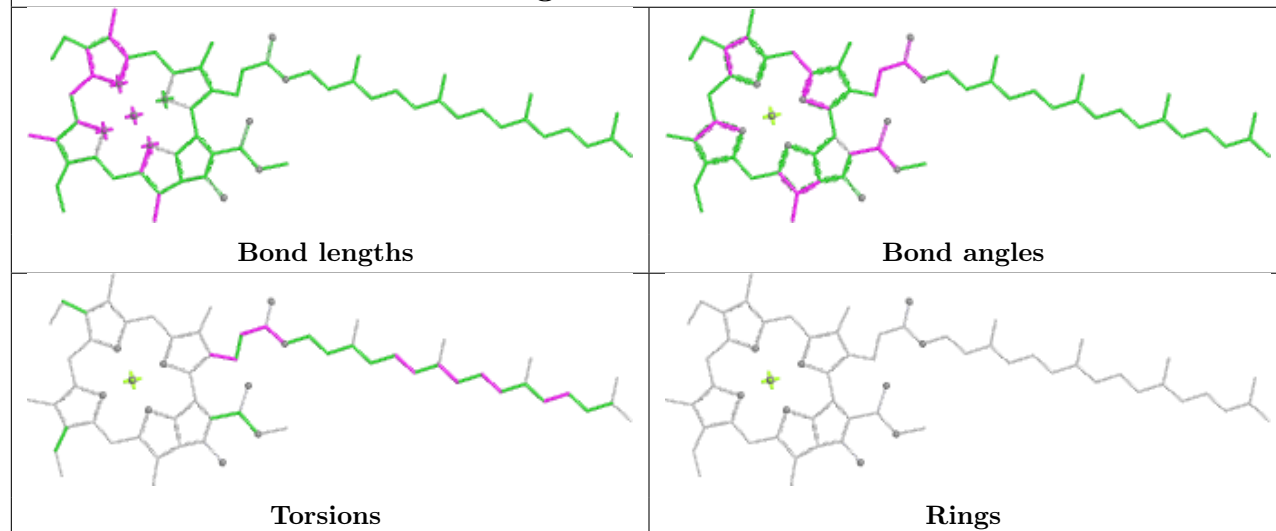




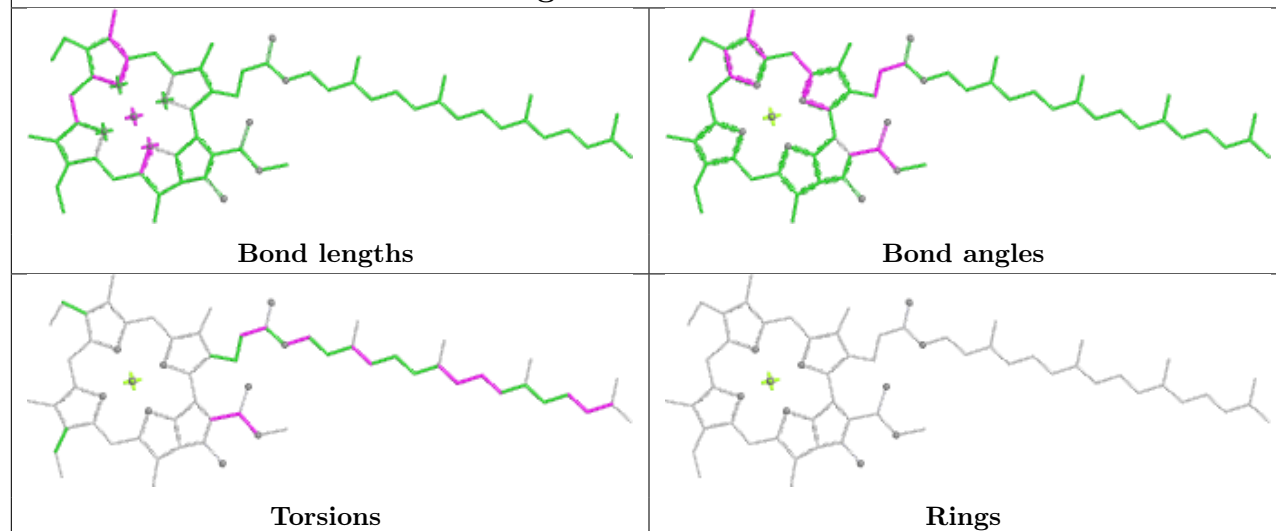
Ligand HEC V 201



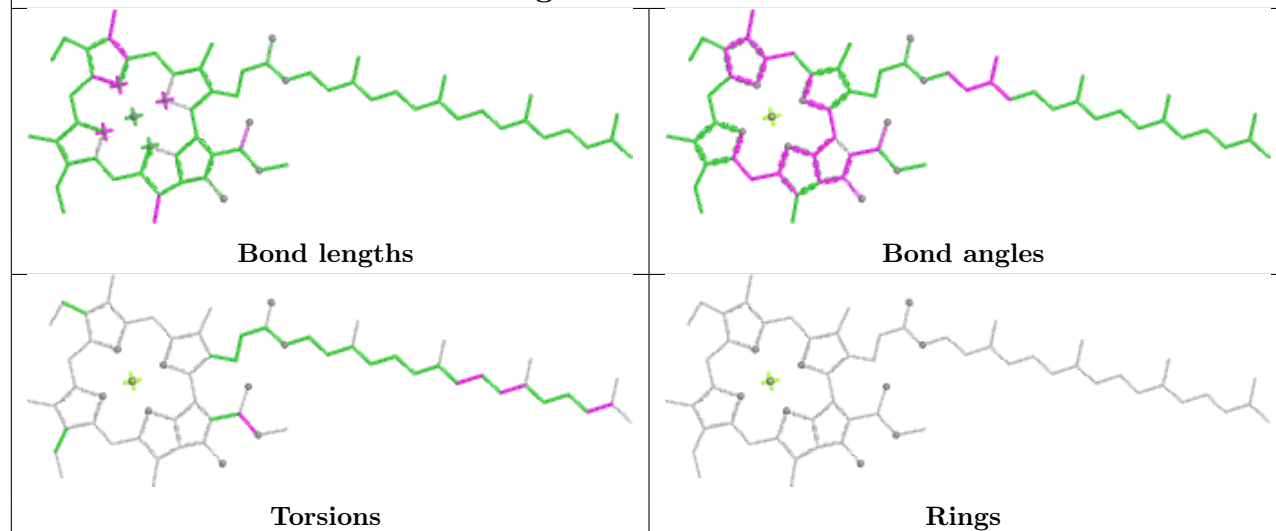
Ligand CLA a 407



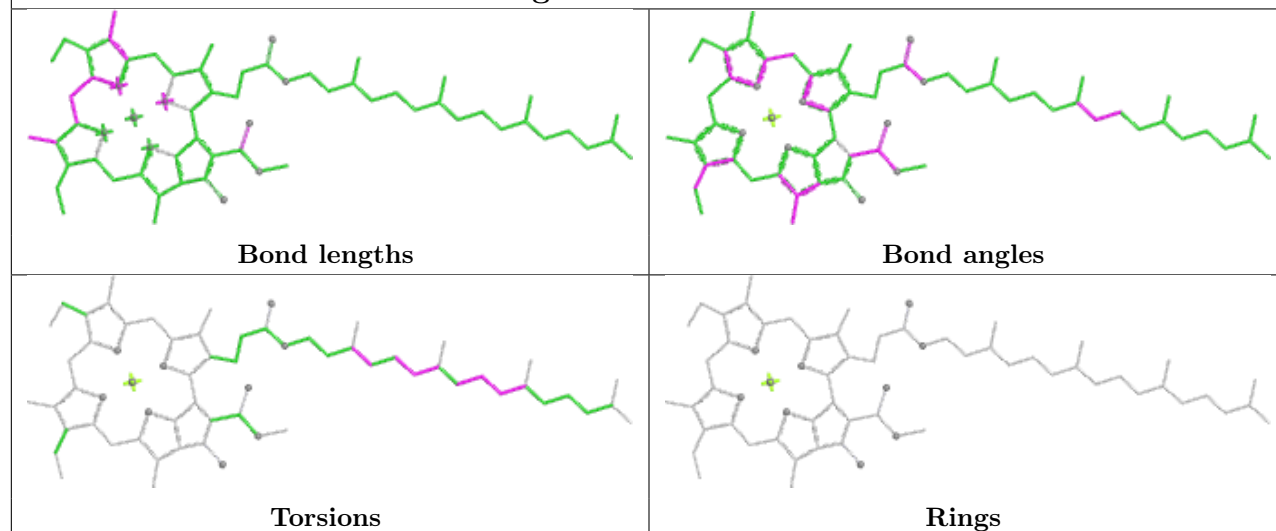
Ligand CLA c 510



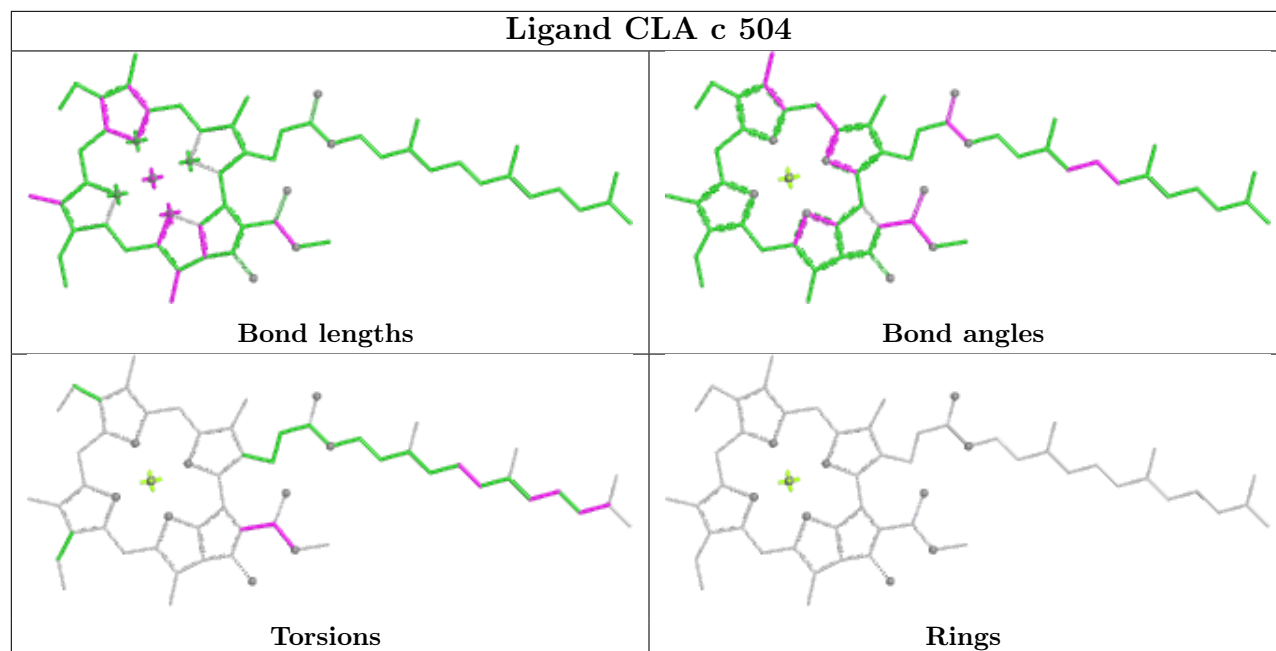
Ligand CLA d 405



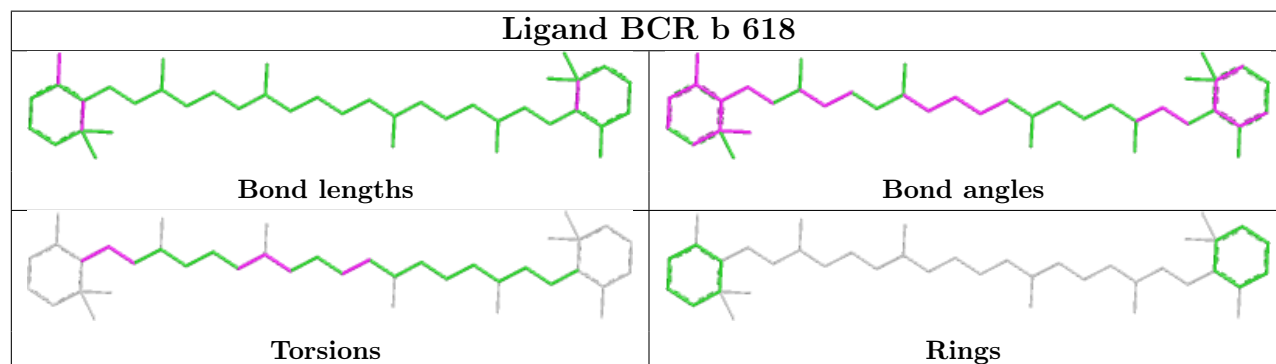
Ligand CLA C 506



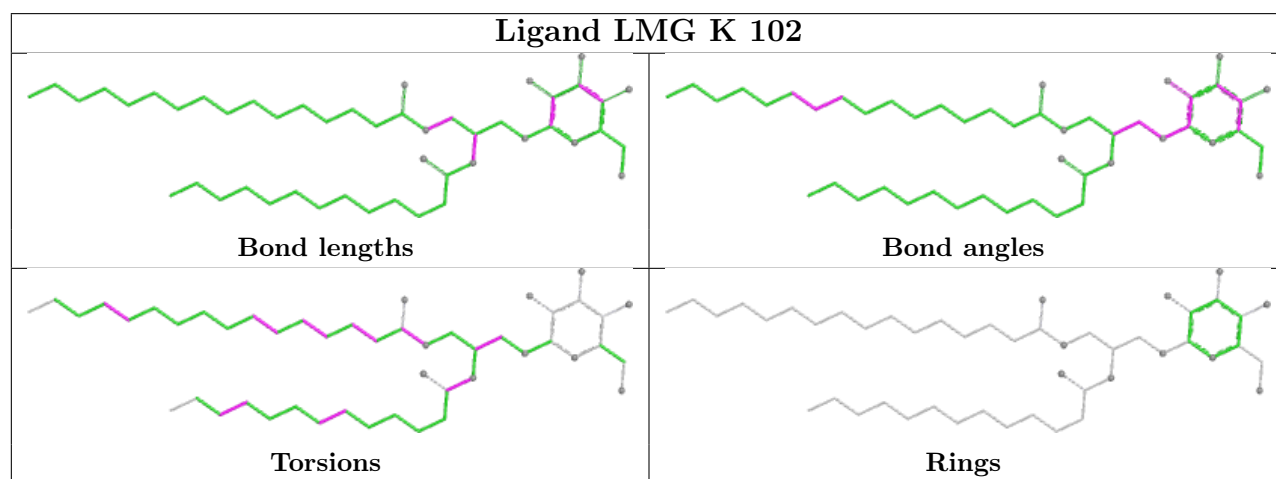
Ligand CLA c 504



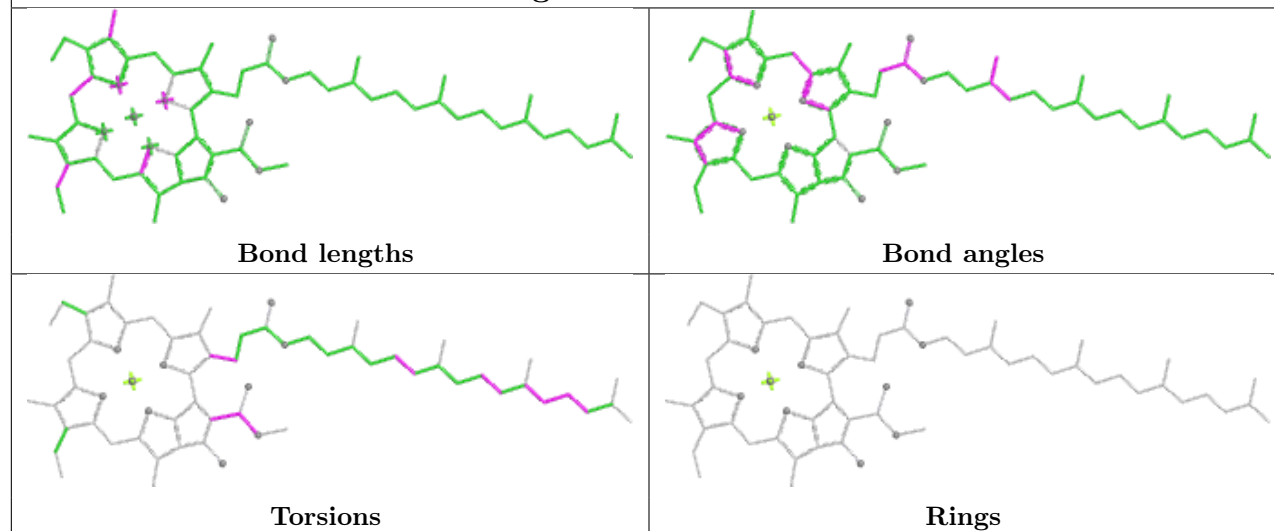
Ligand BCR b 618



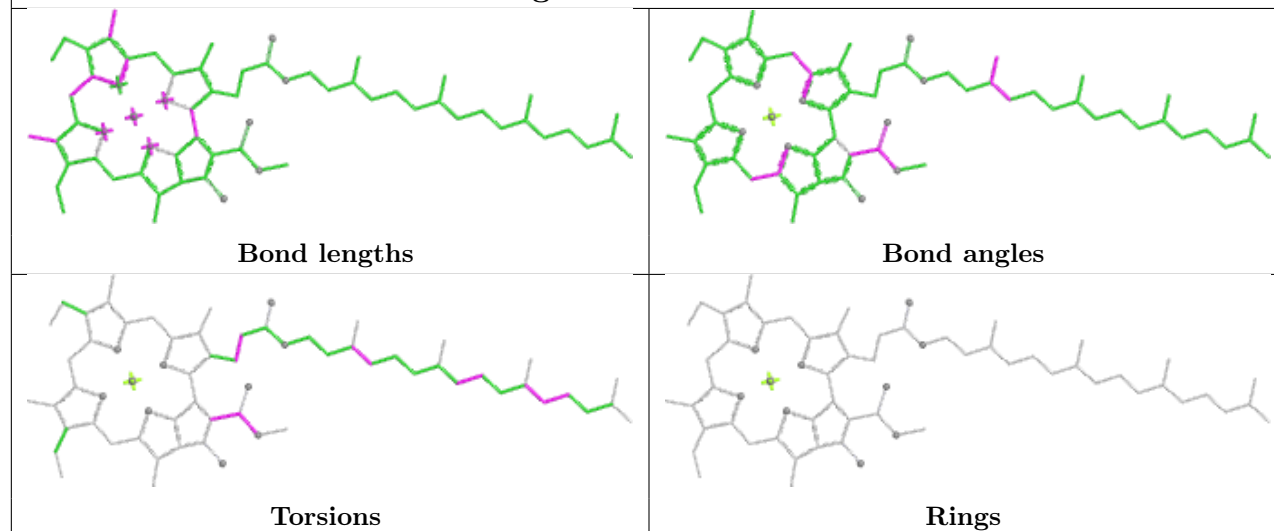
Ligand LMG K 102



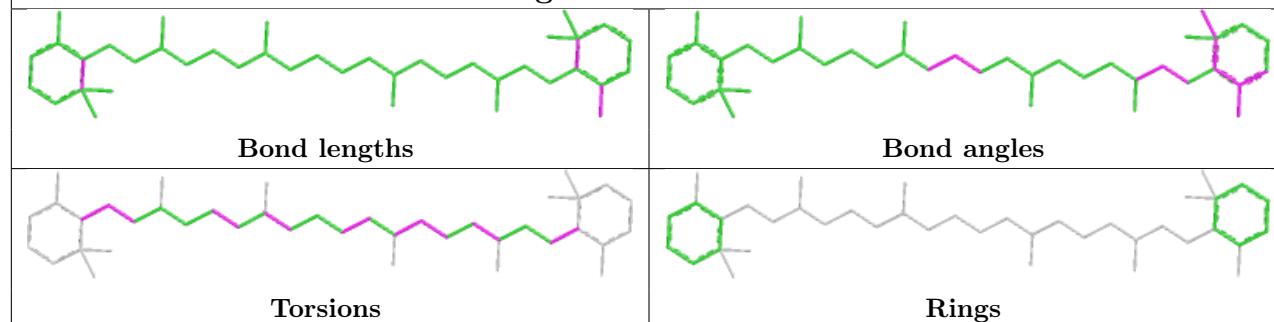
Ligand CLA B 607



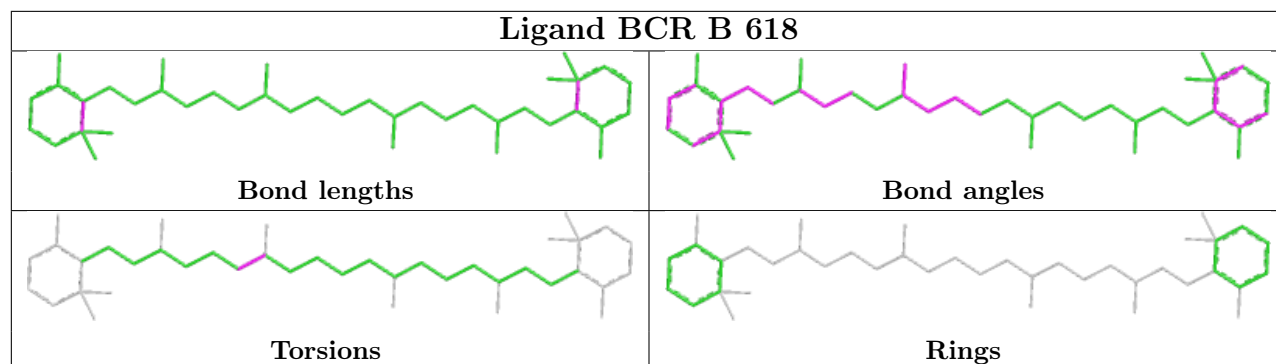
Ligand CLA B 614



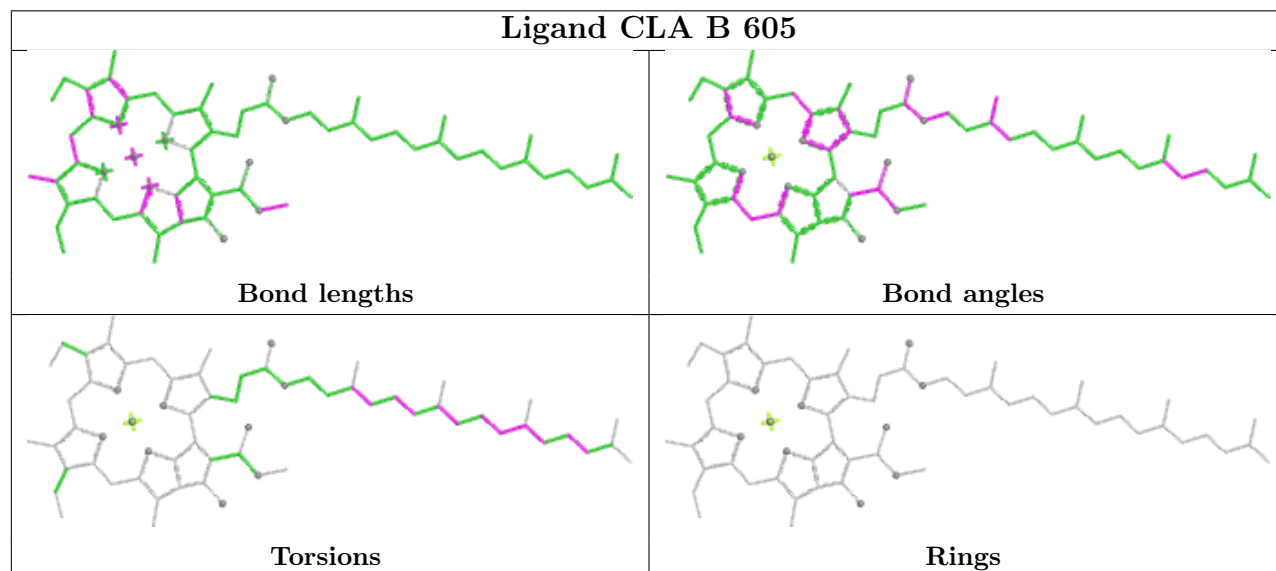
Ligand BCR c 521



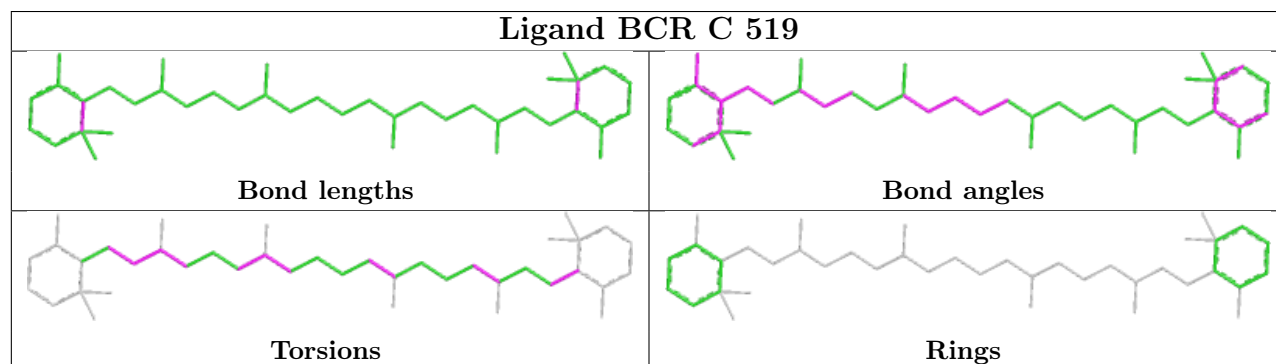
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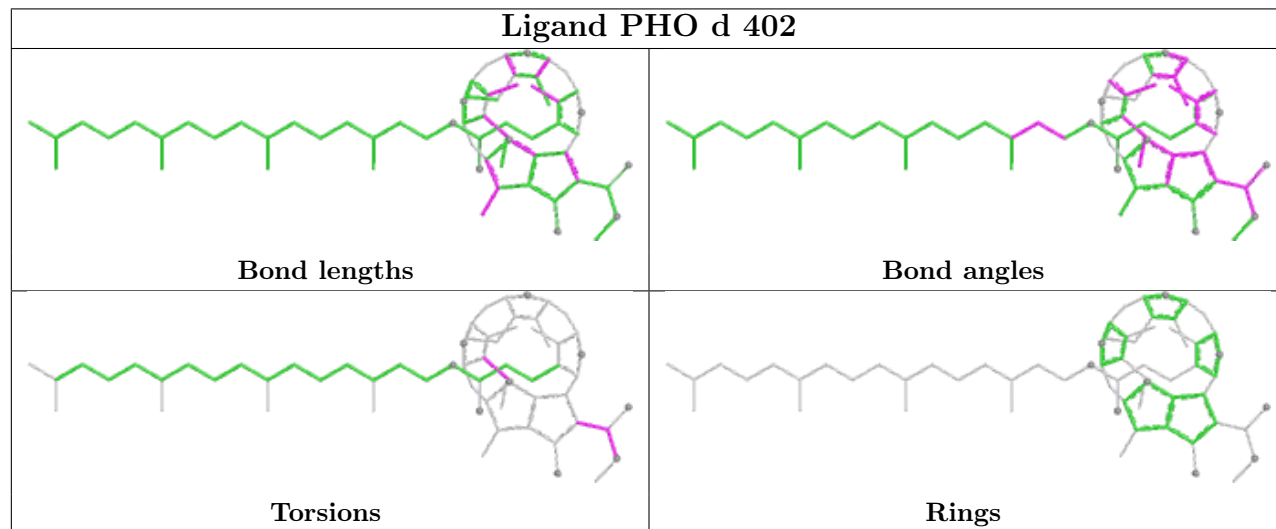
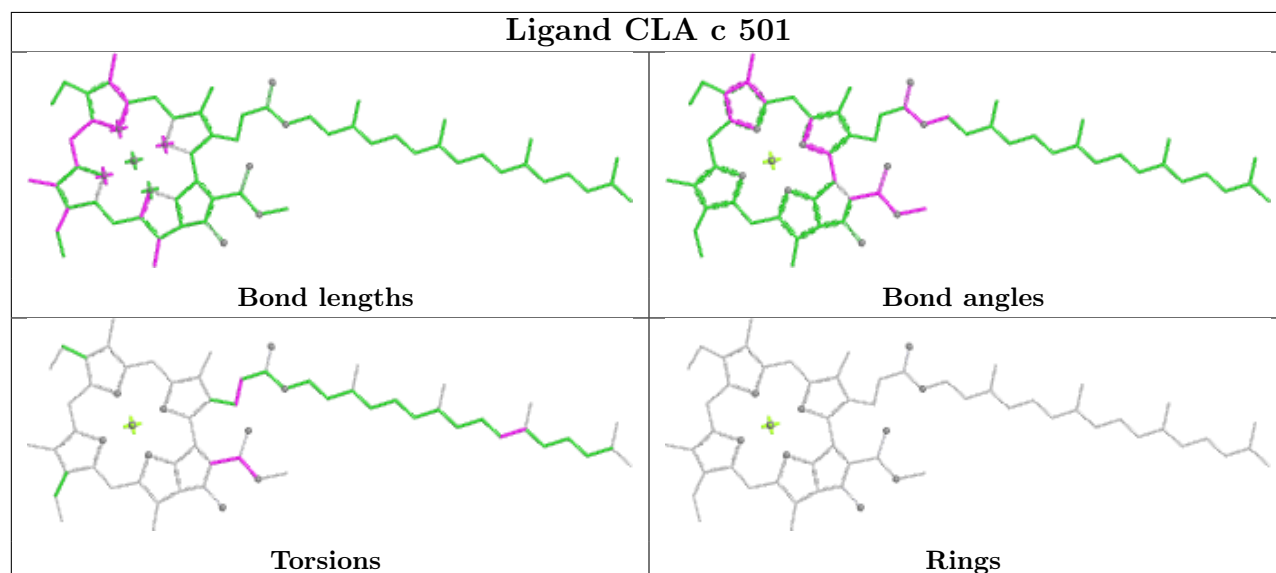
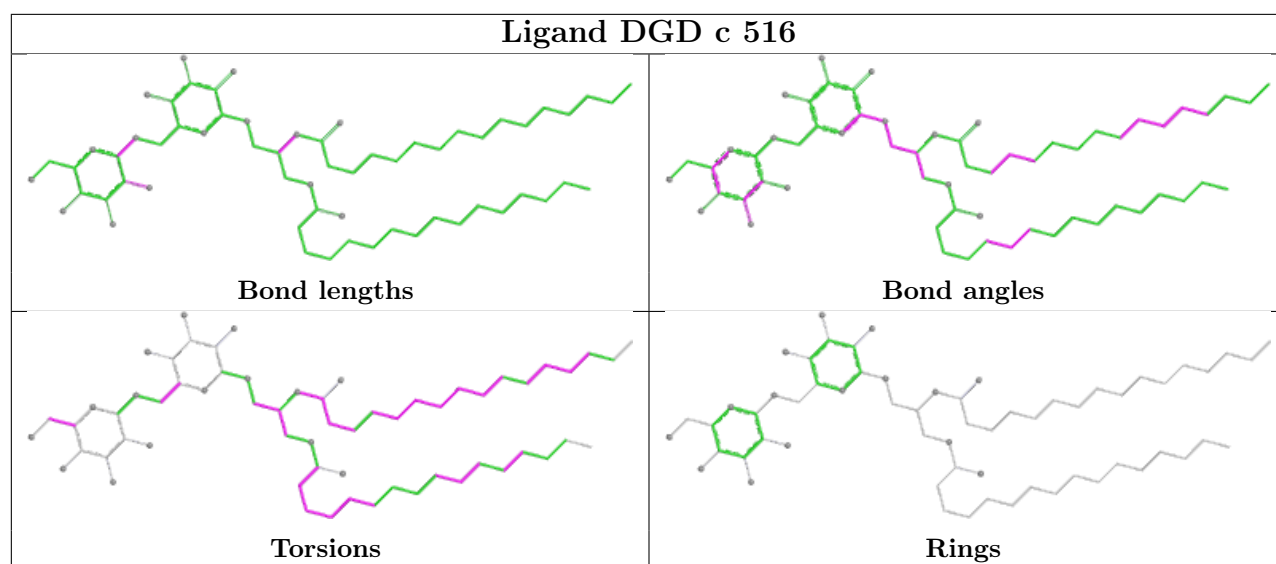


Ligand CLA B 605

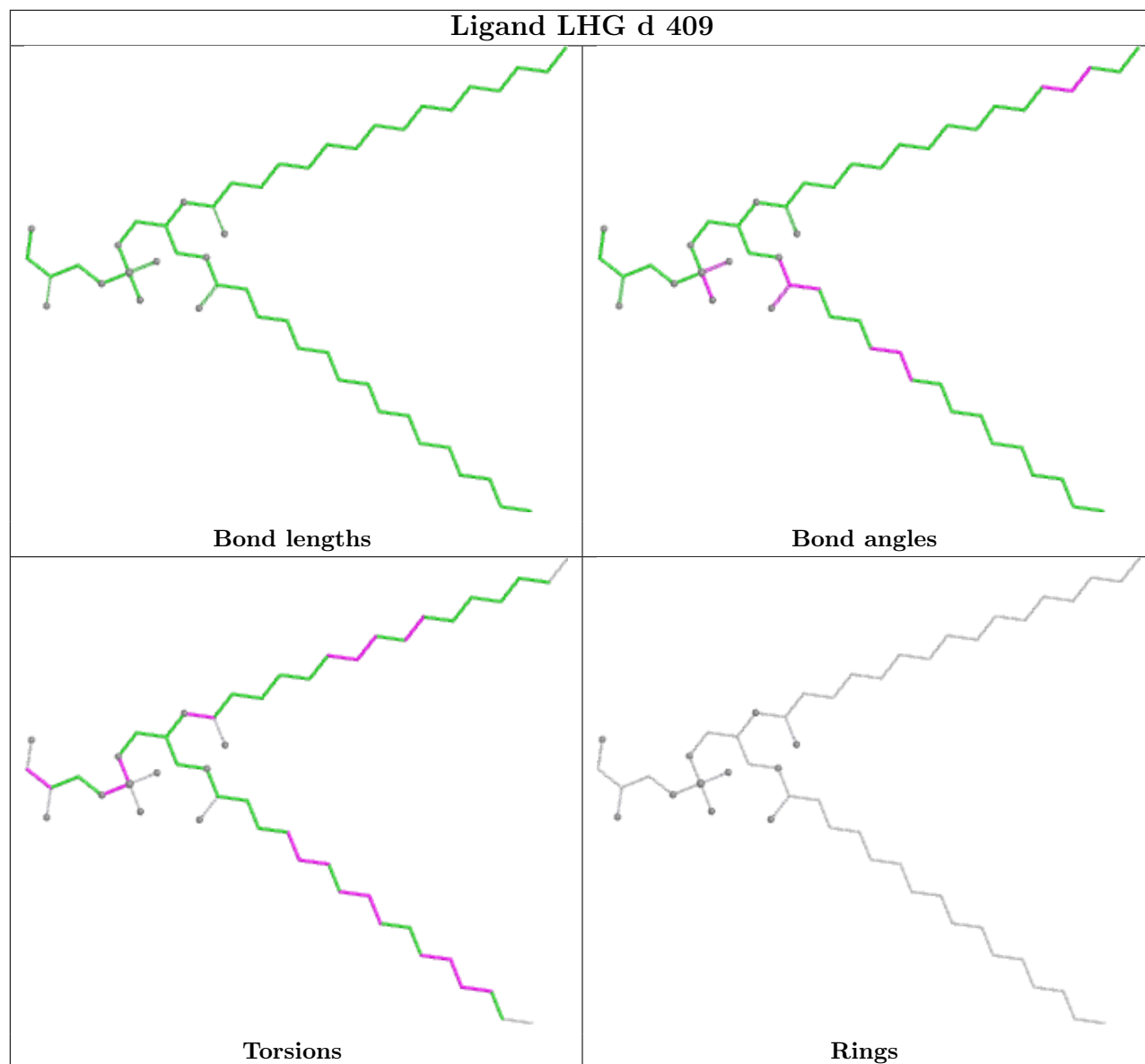


Ligand BCR C 519

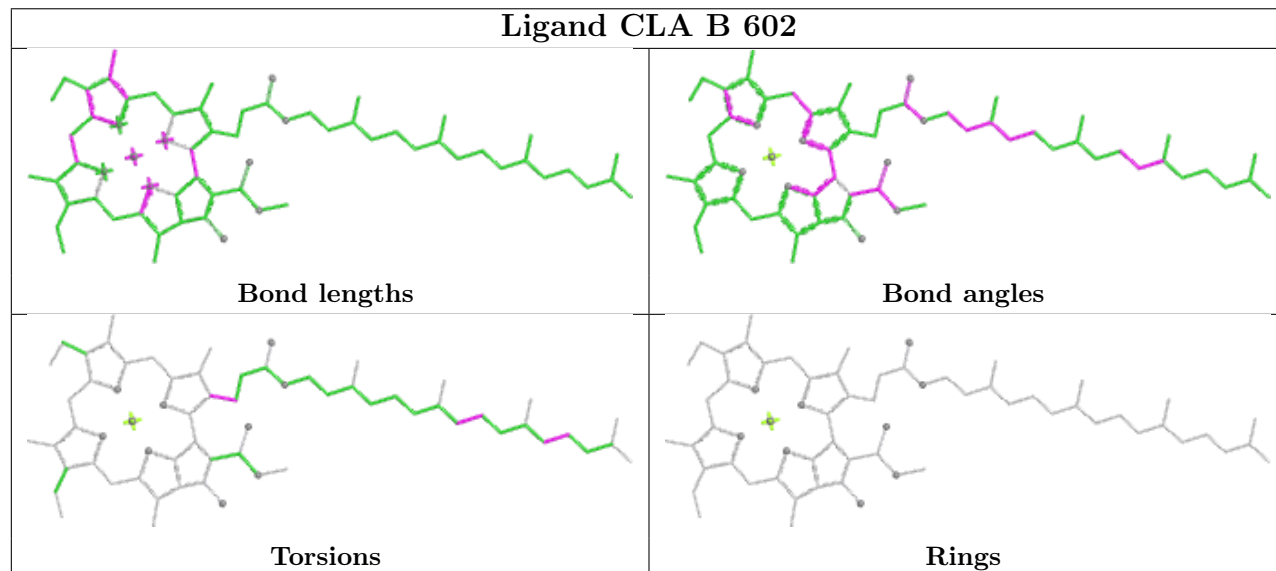




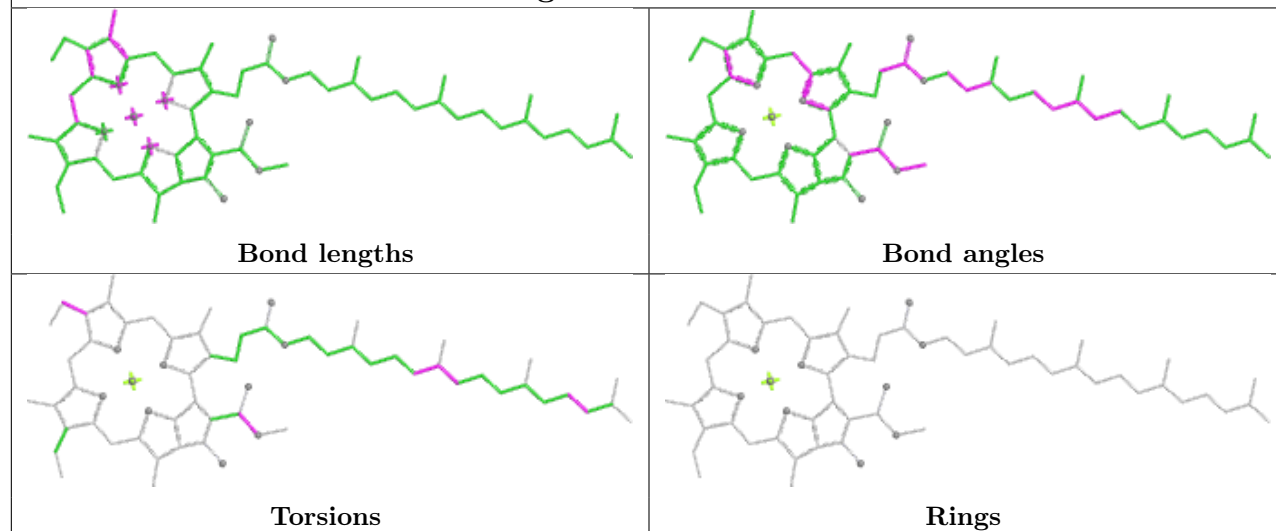
Ligand LHG d 409



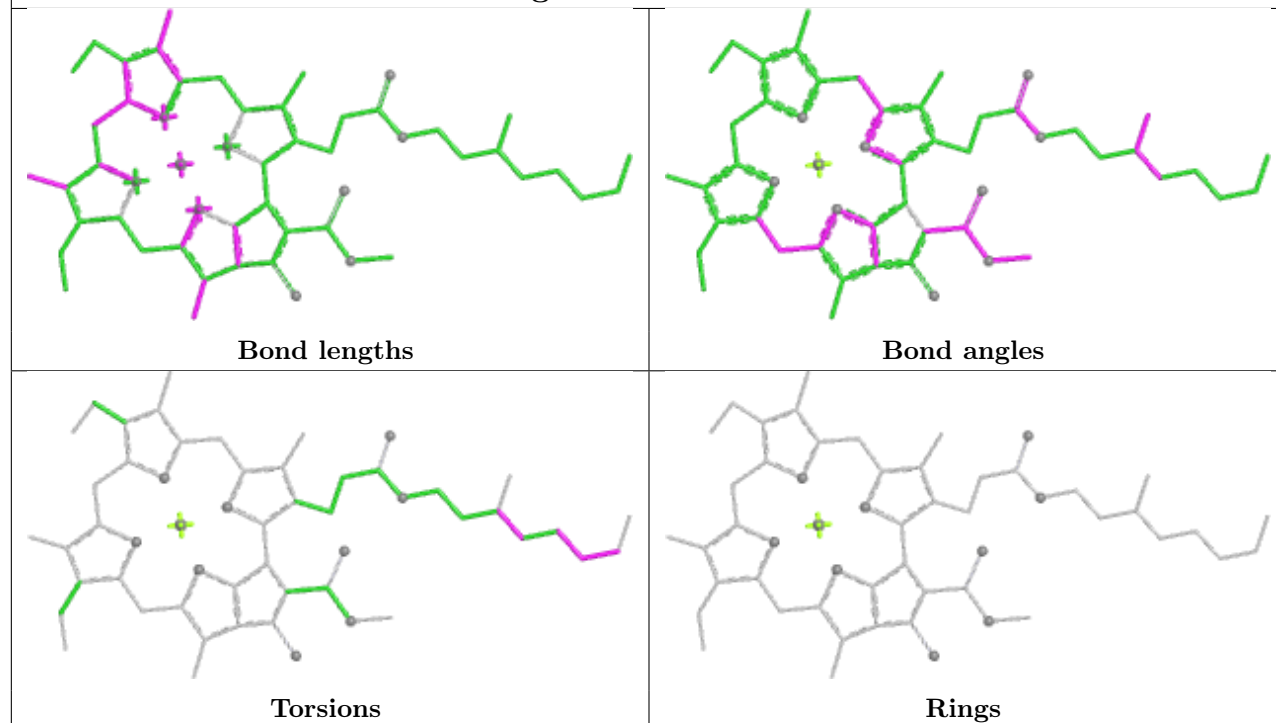
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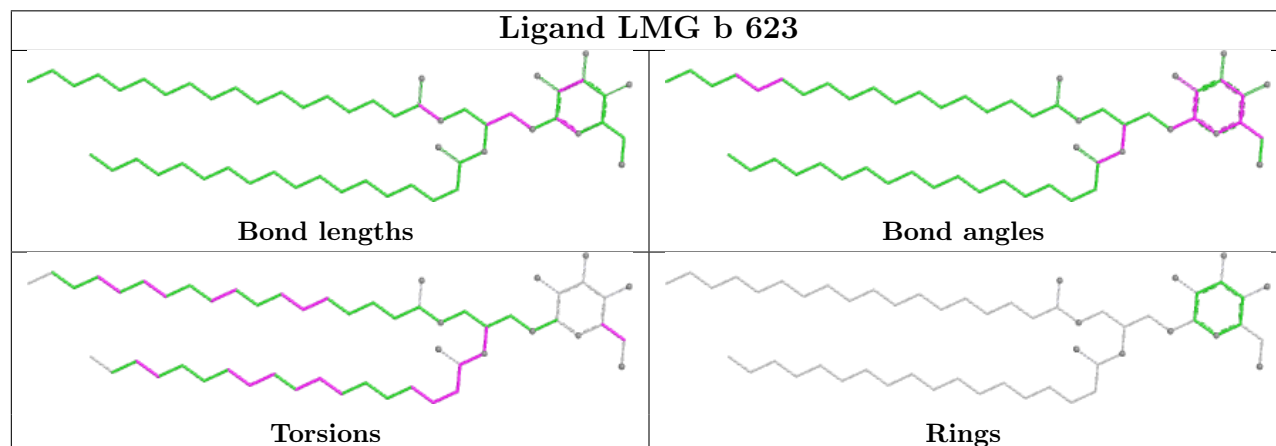
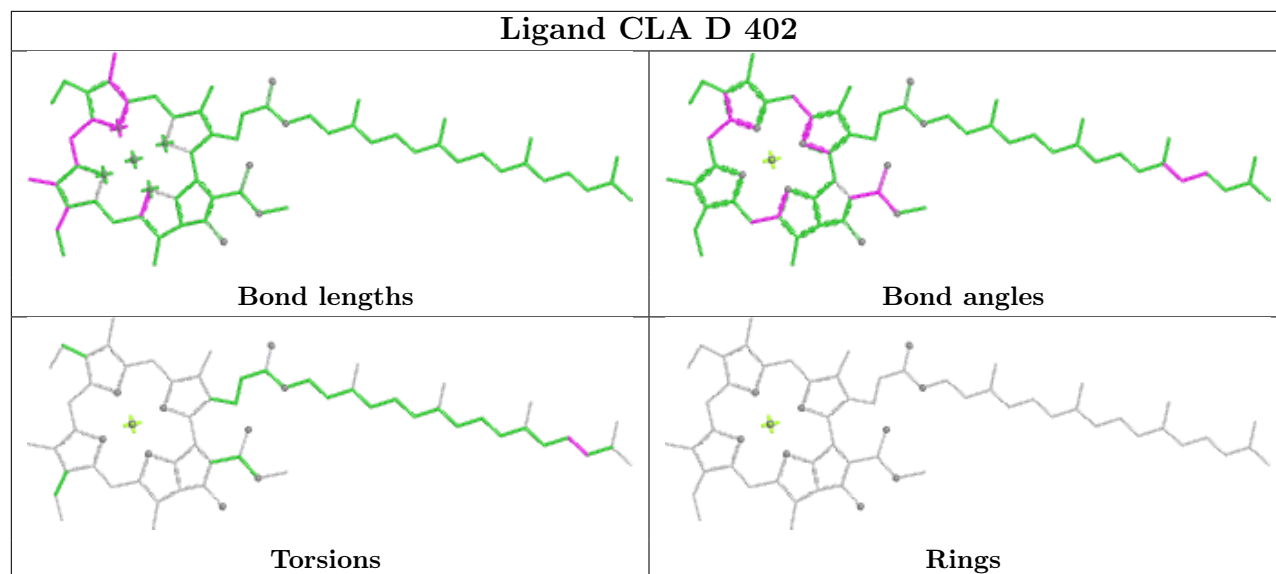


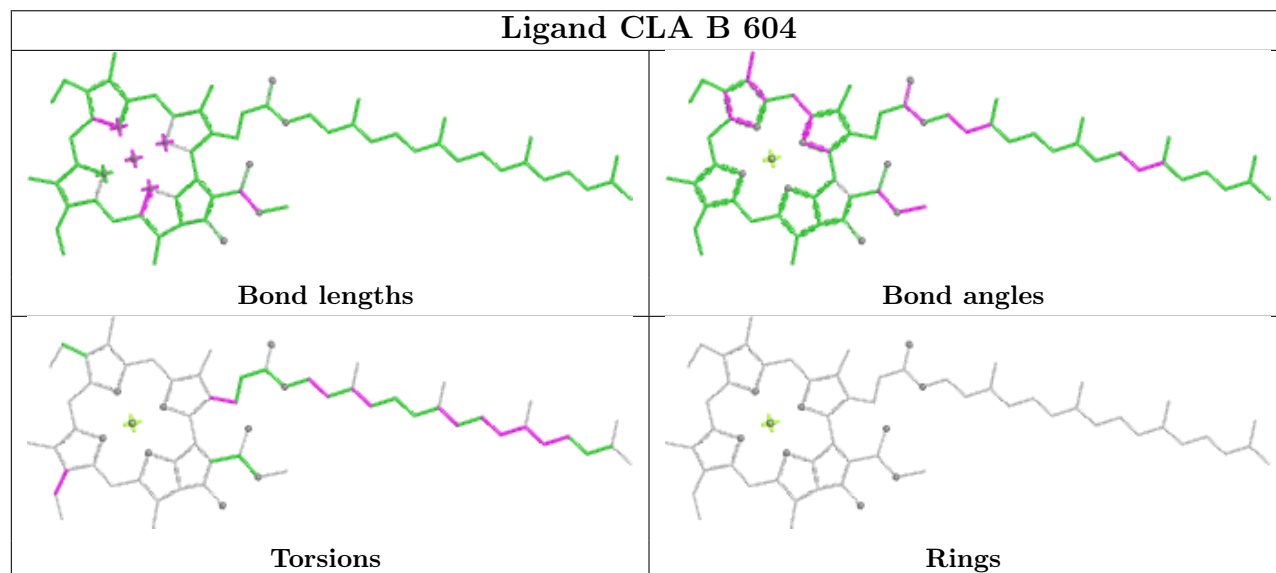
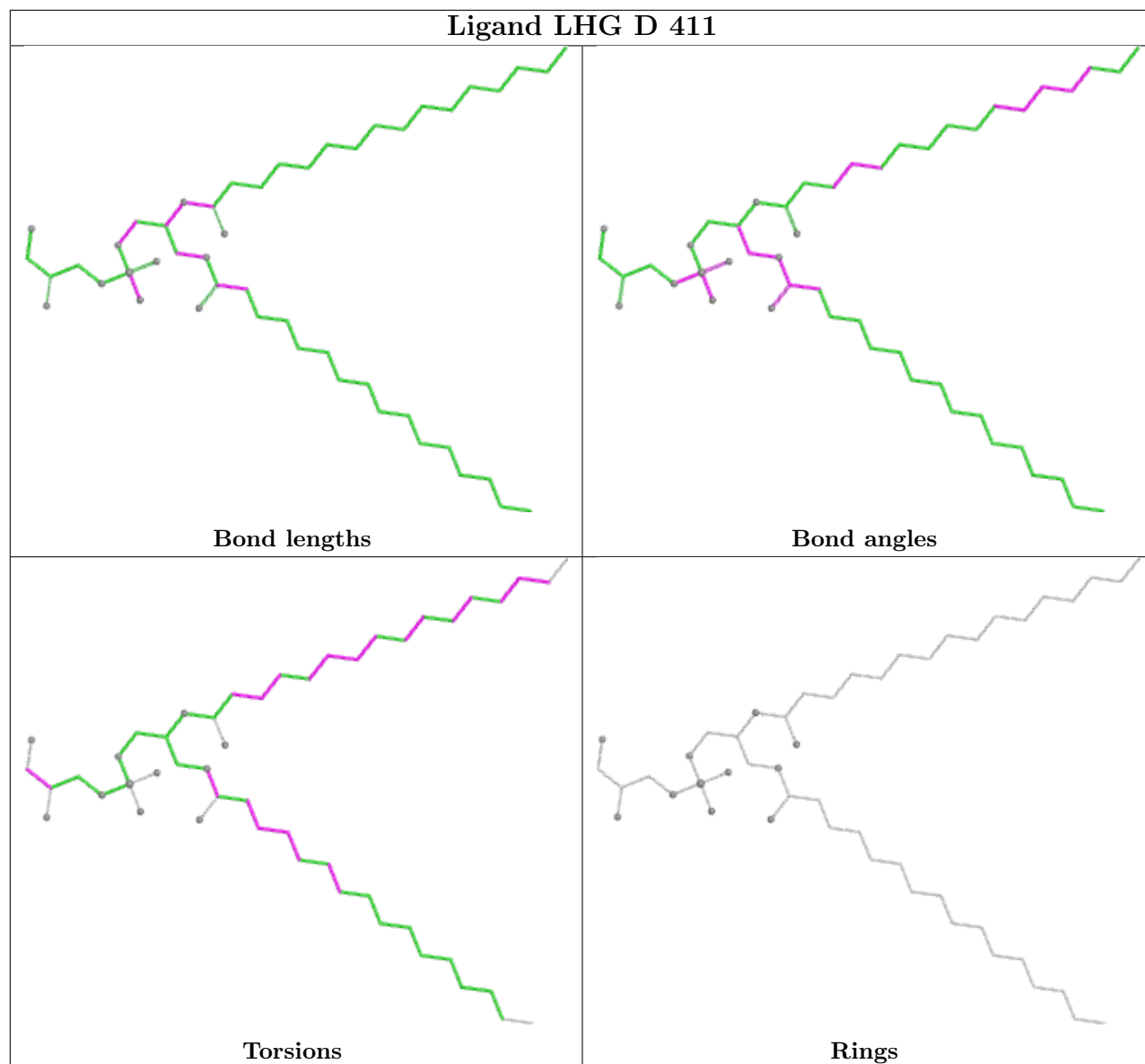
Ligand CLA c 505

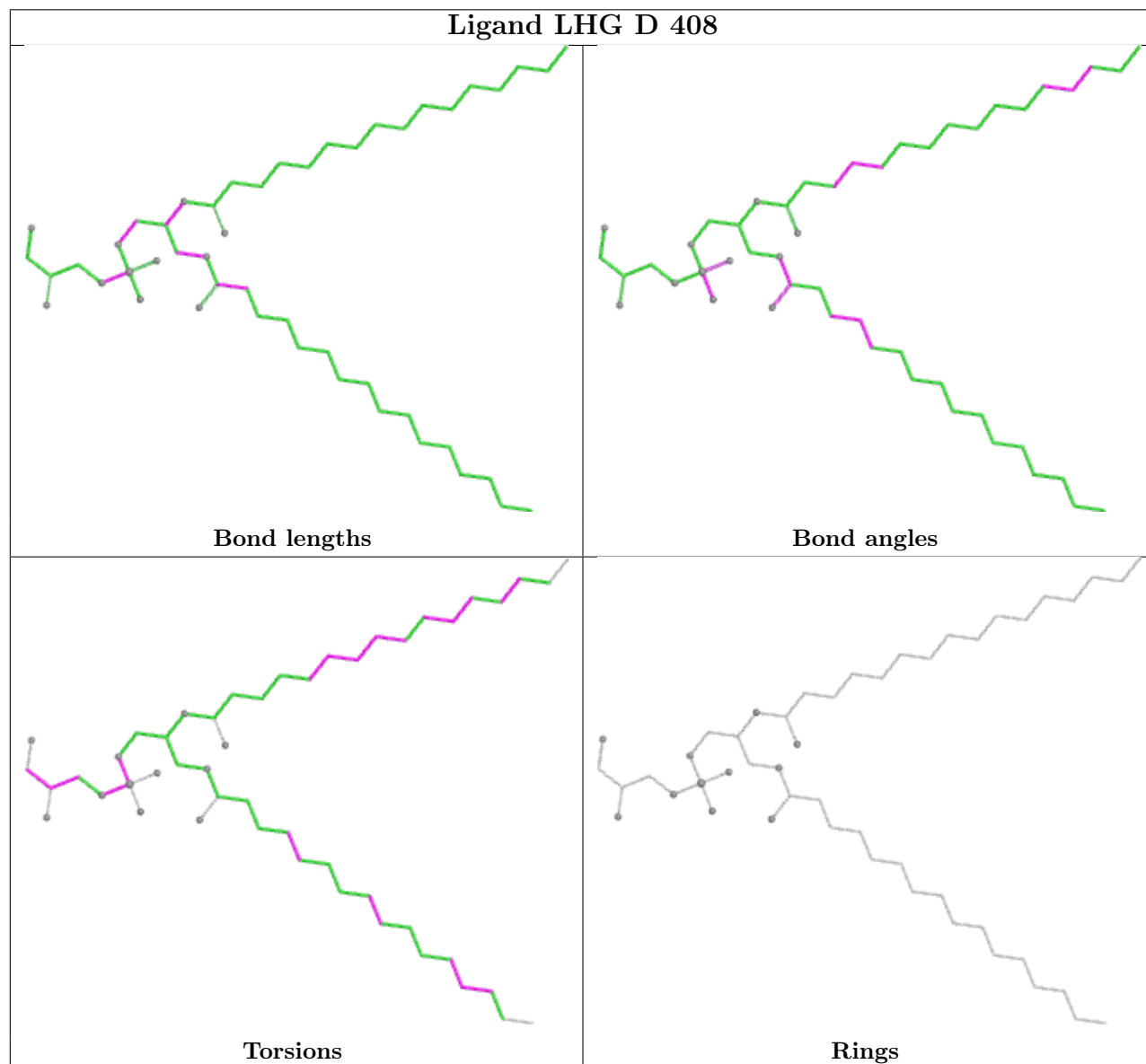
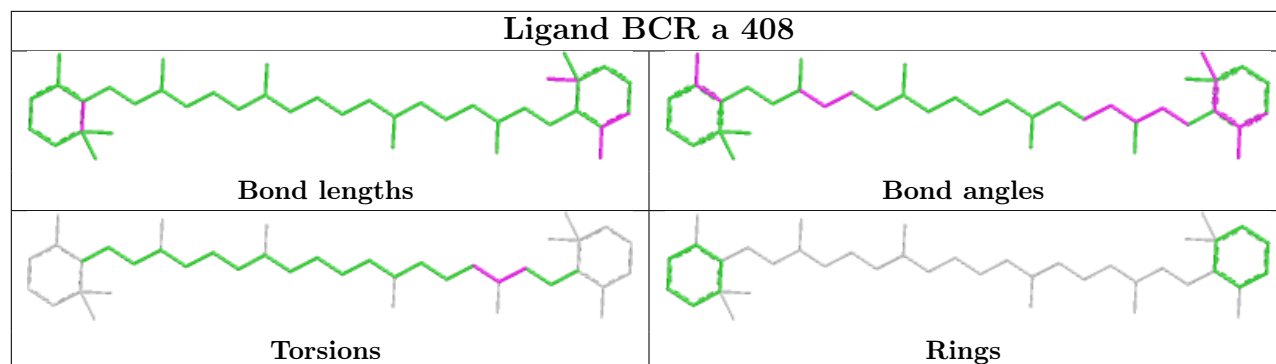


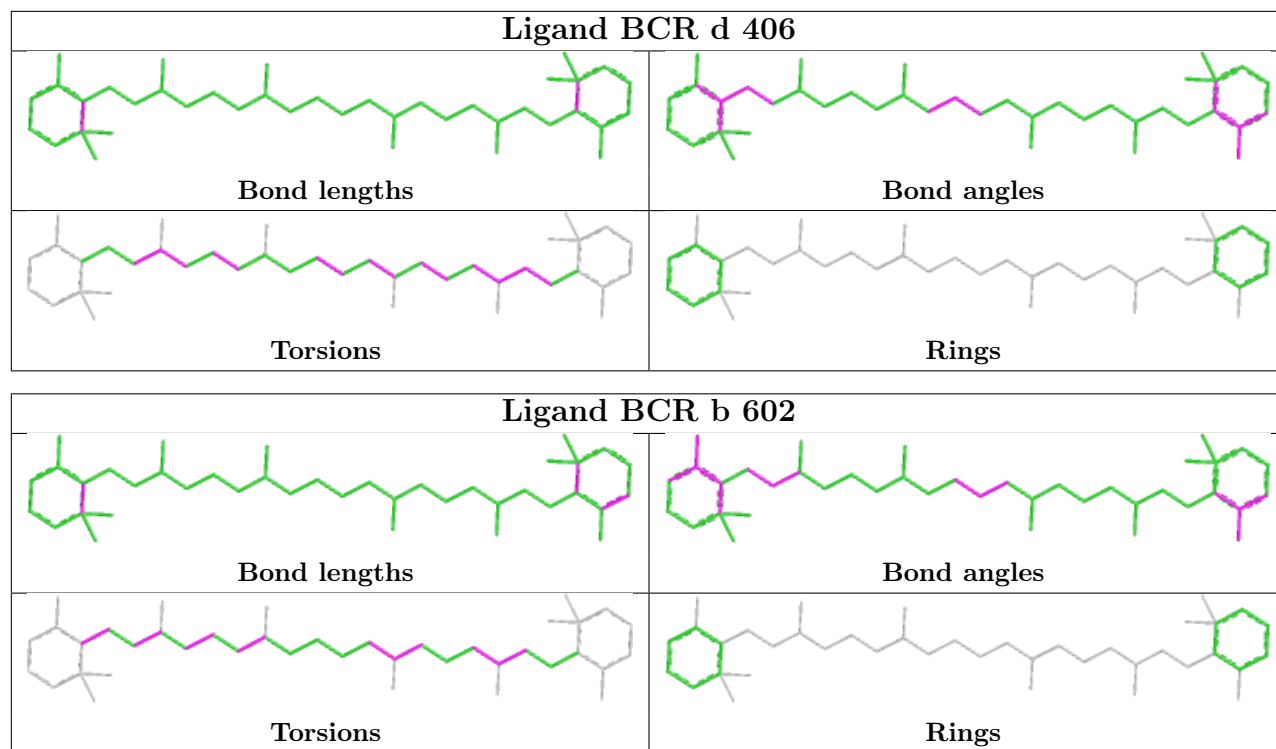
Ligand CLA A 408



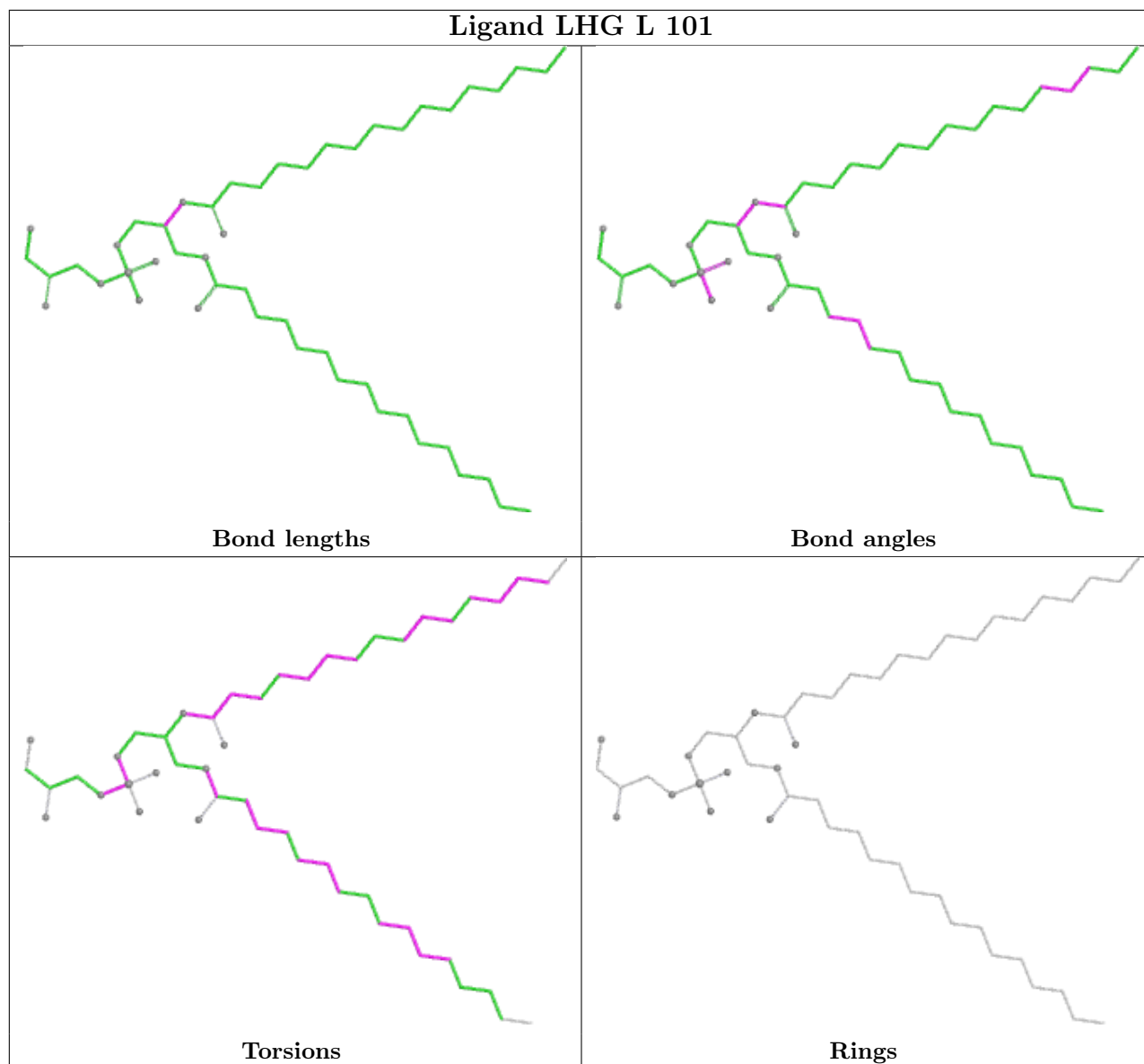




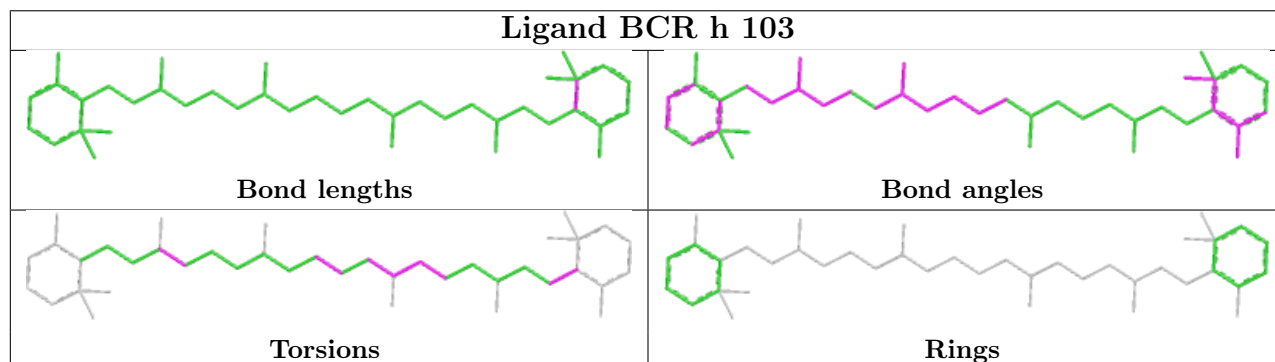




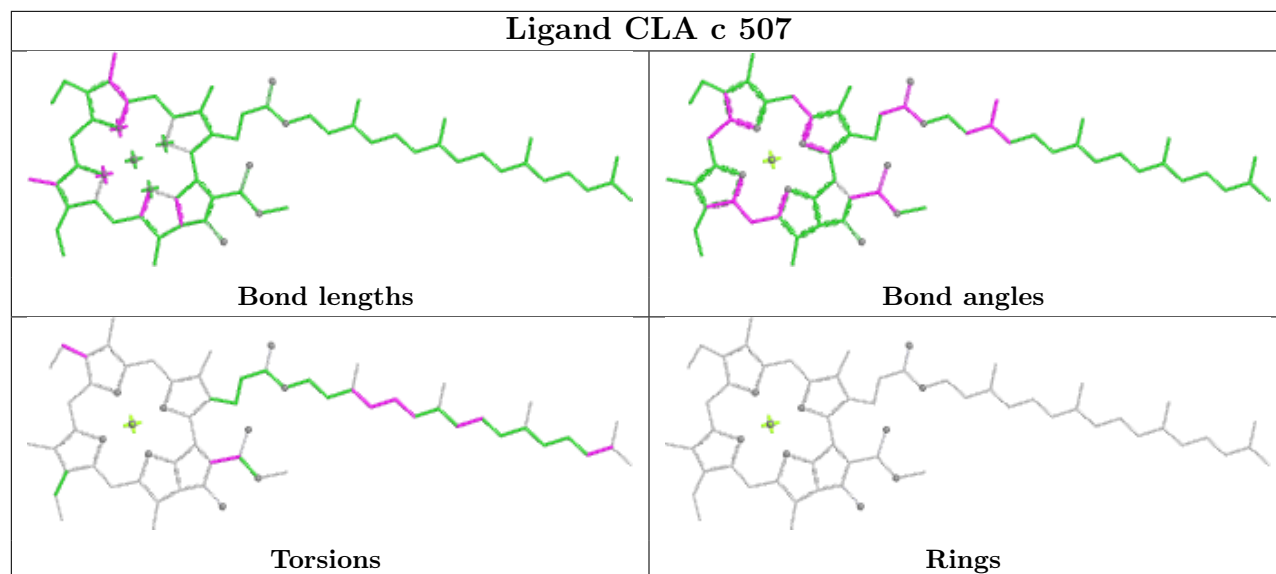
Ligand LHG L 101



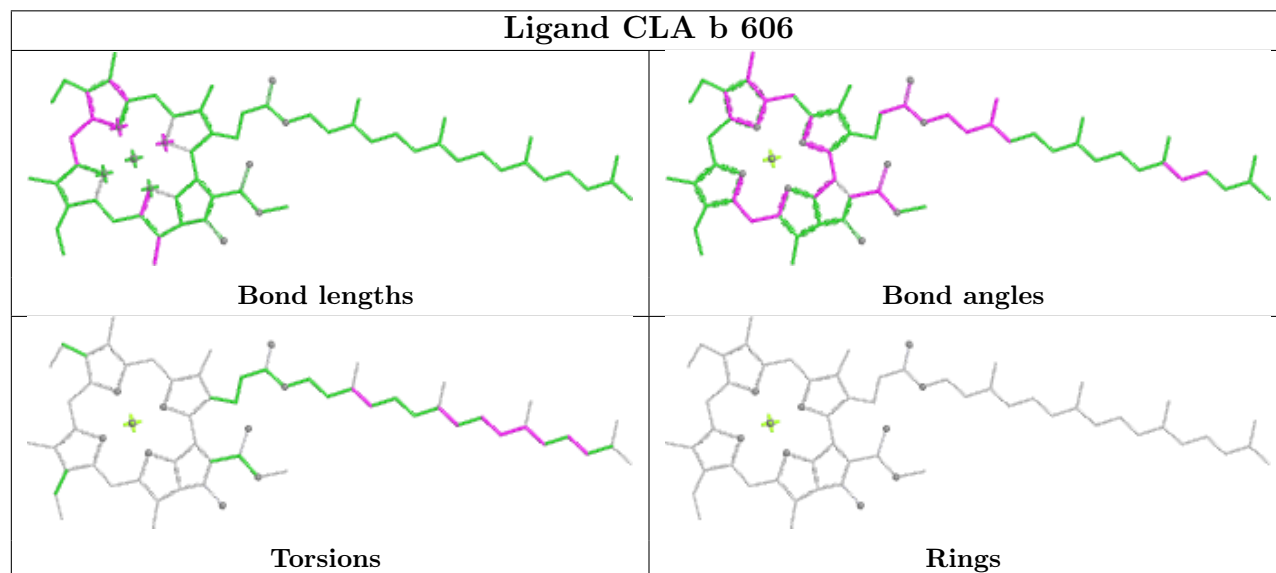
Ligand BCR h 103



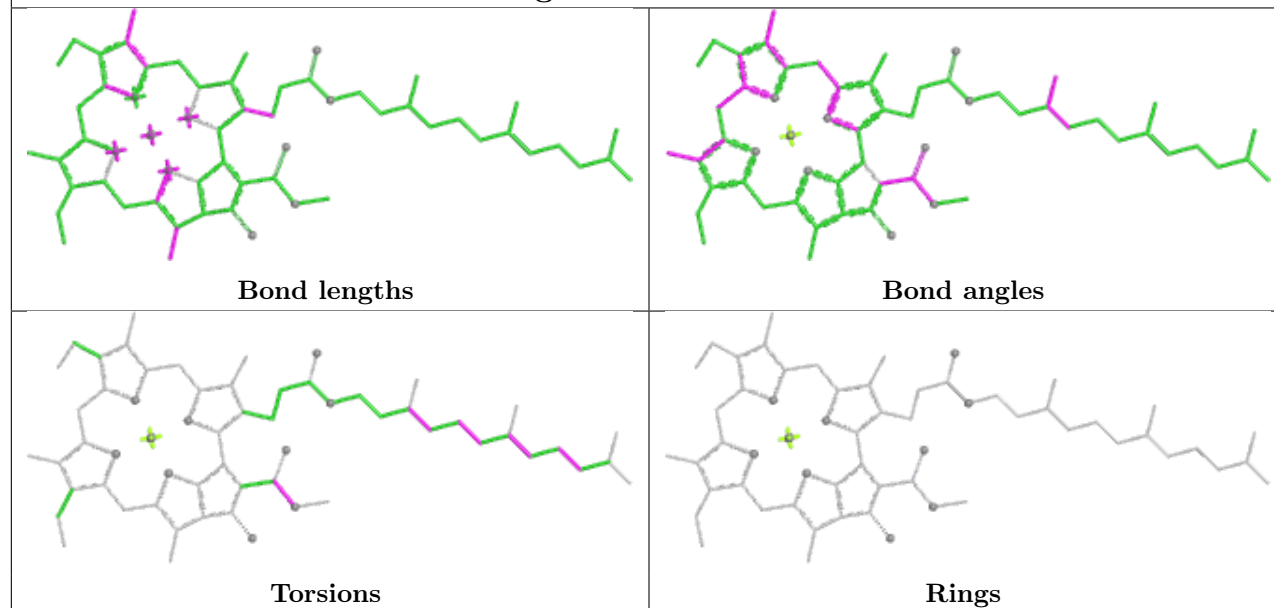
Ligand CLA c 507



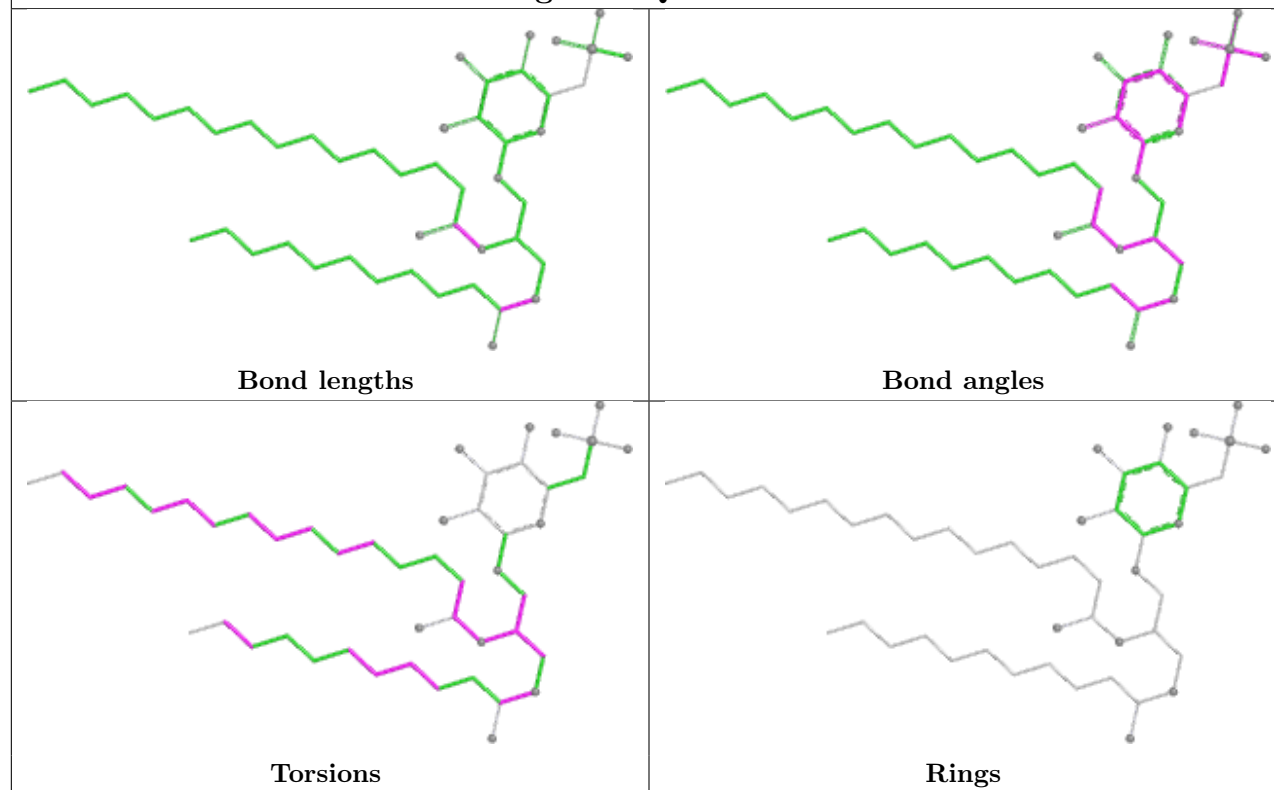
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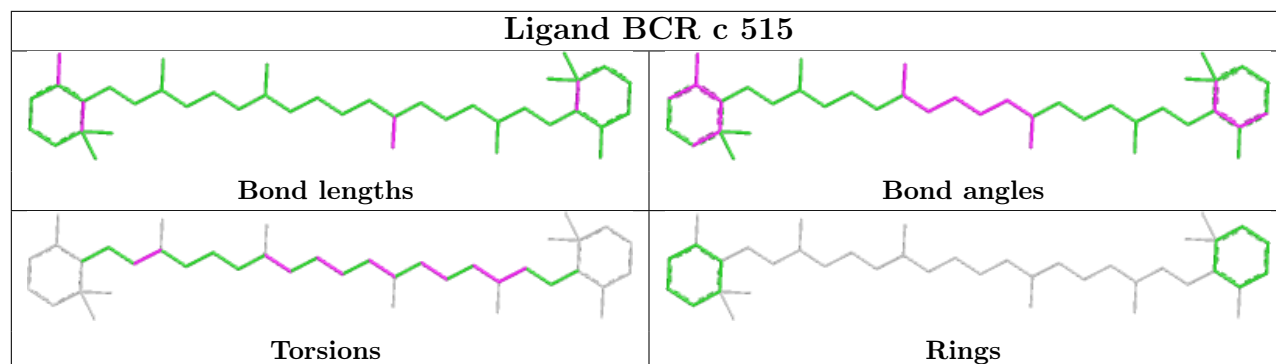
Ligand CLA b 617



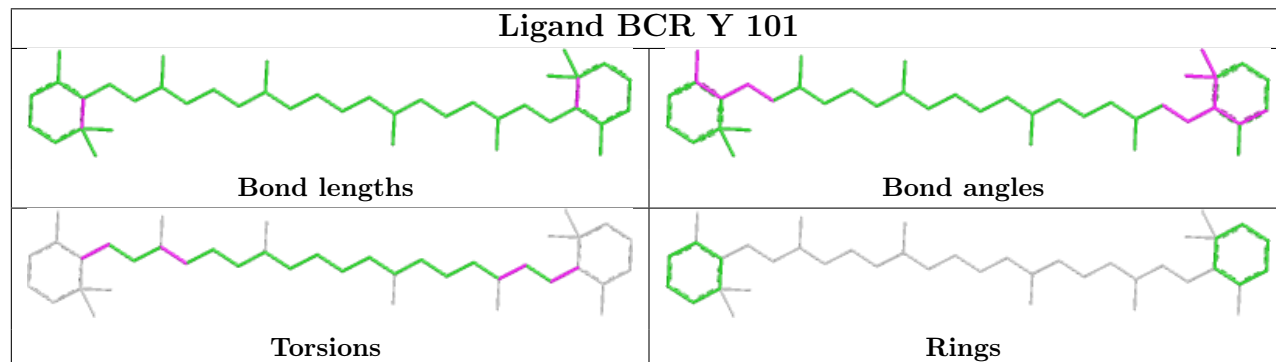
Ligand SQD b 601



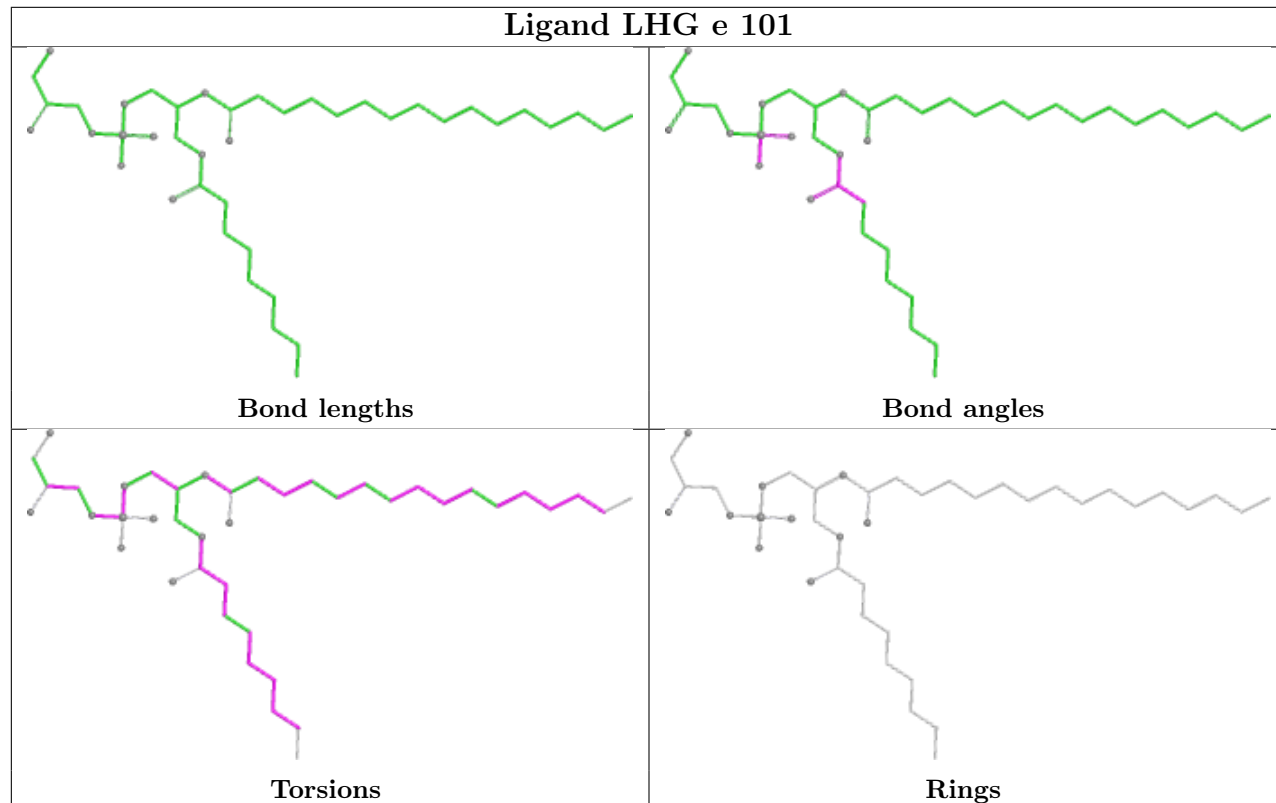
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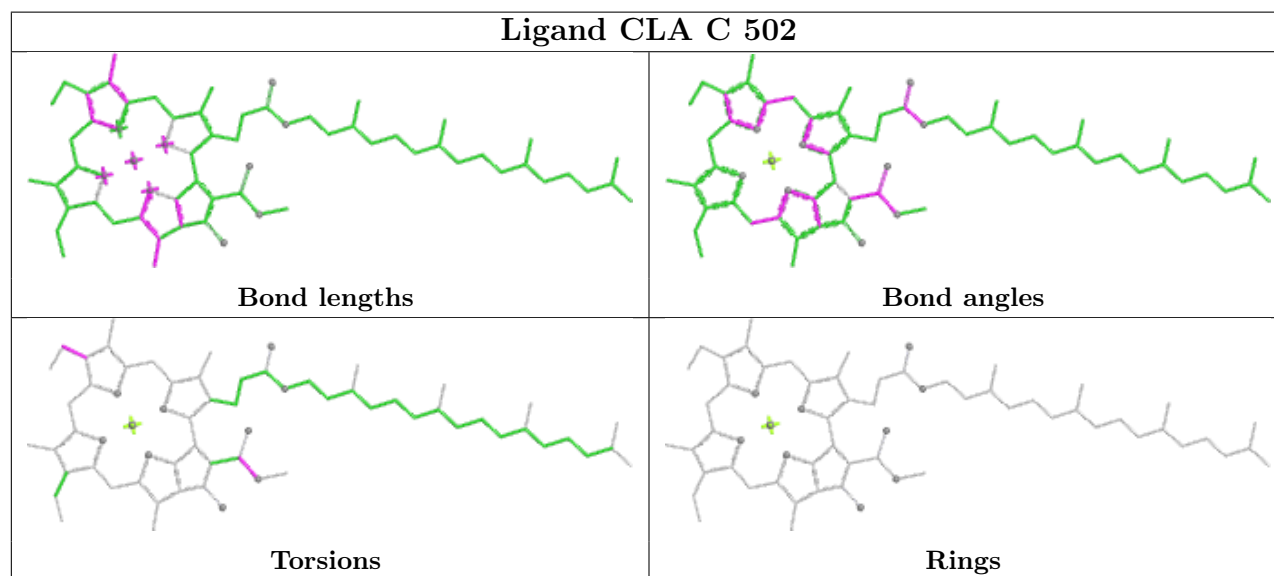
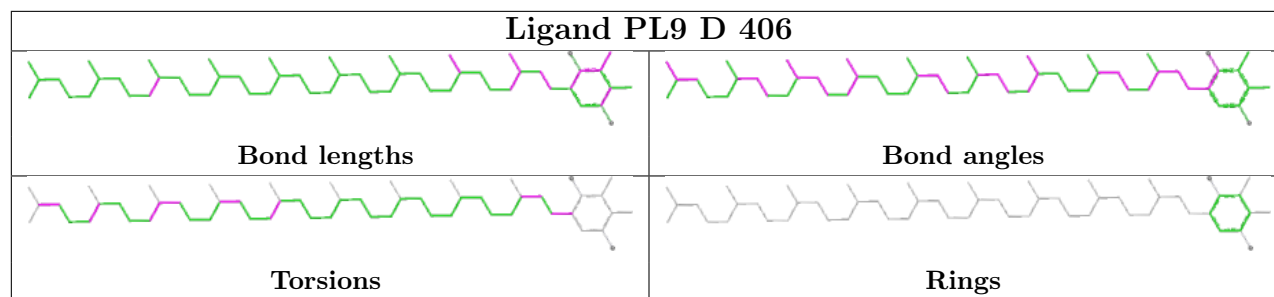


Ligand BCR Y 101

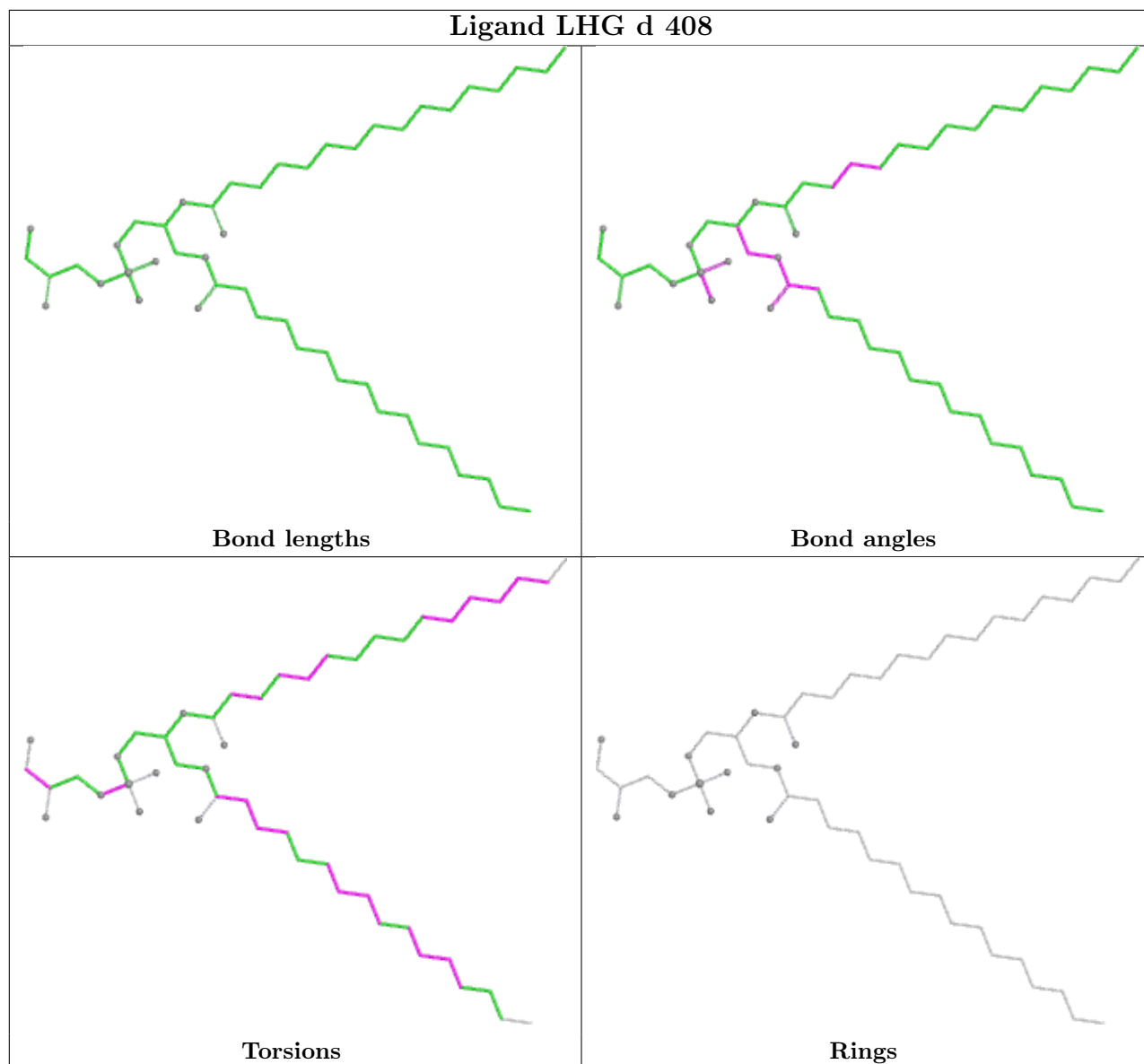


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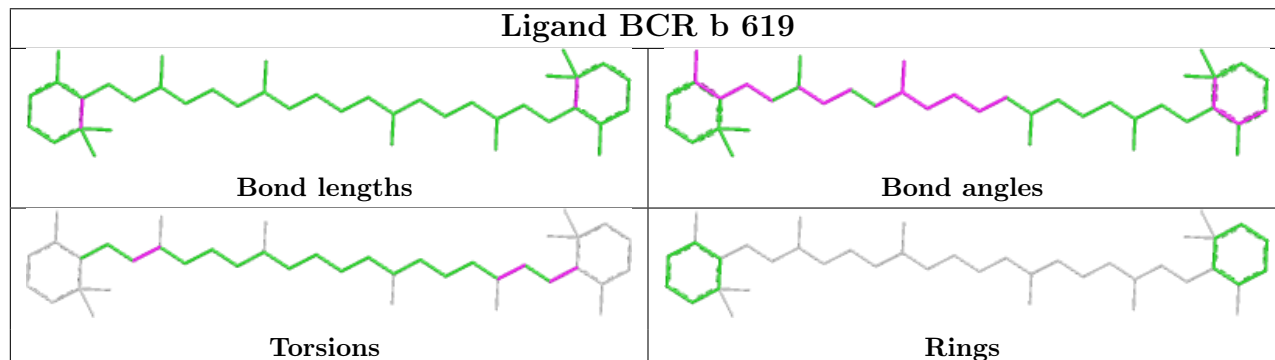




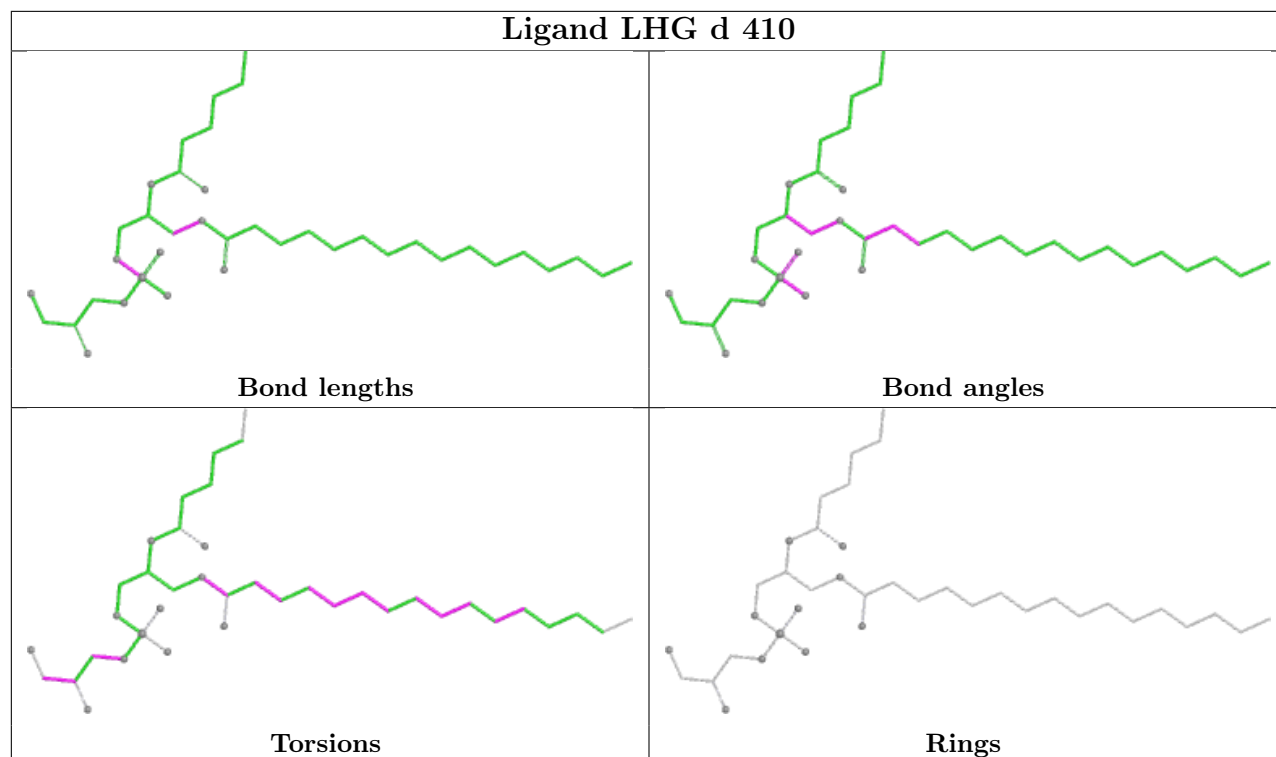
Ligand LHG d 408



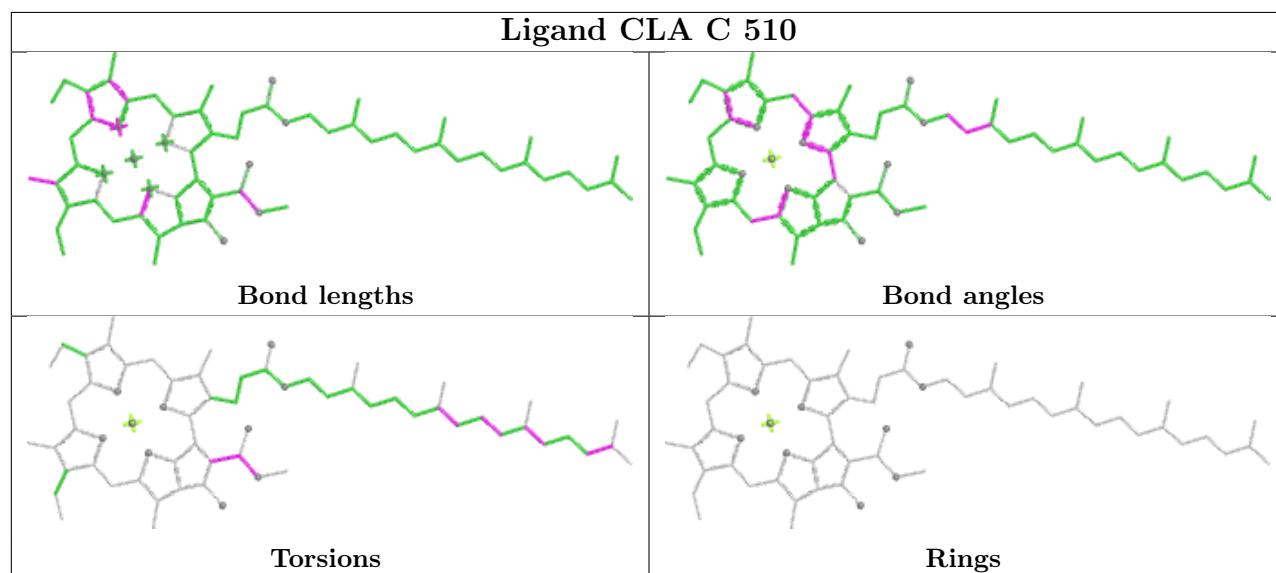
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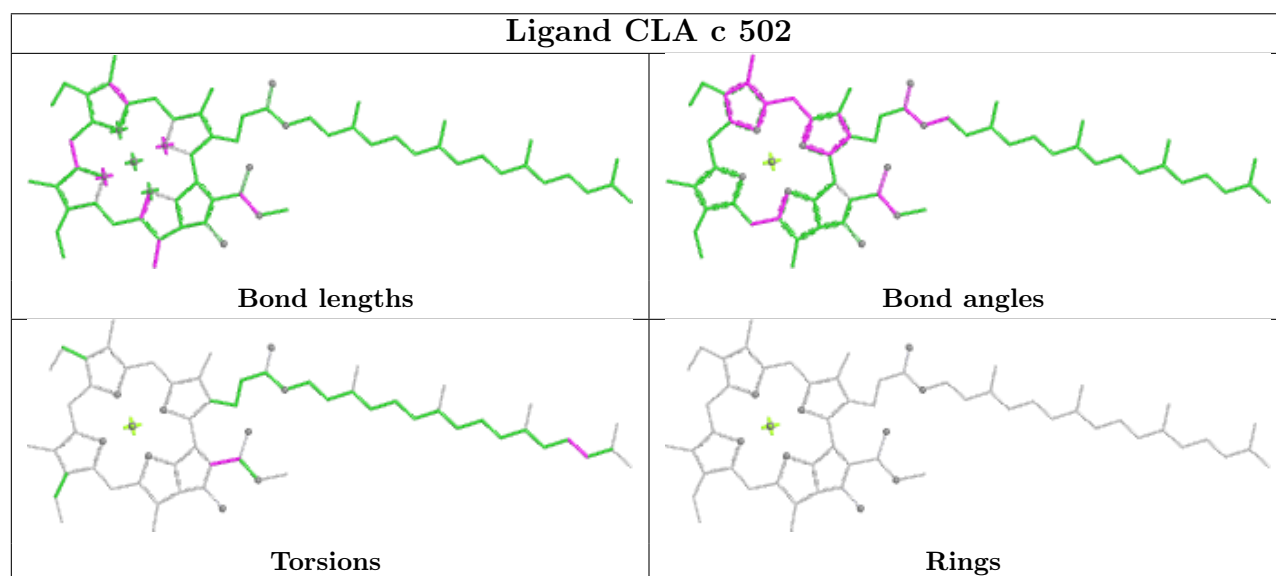
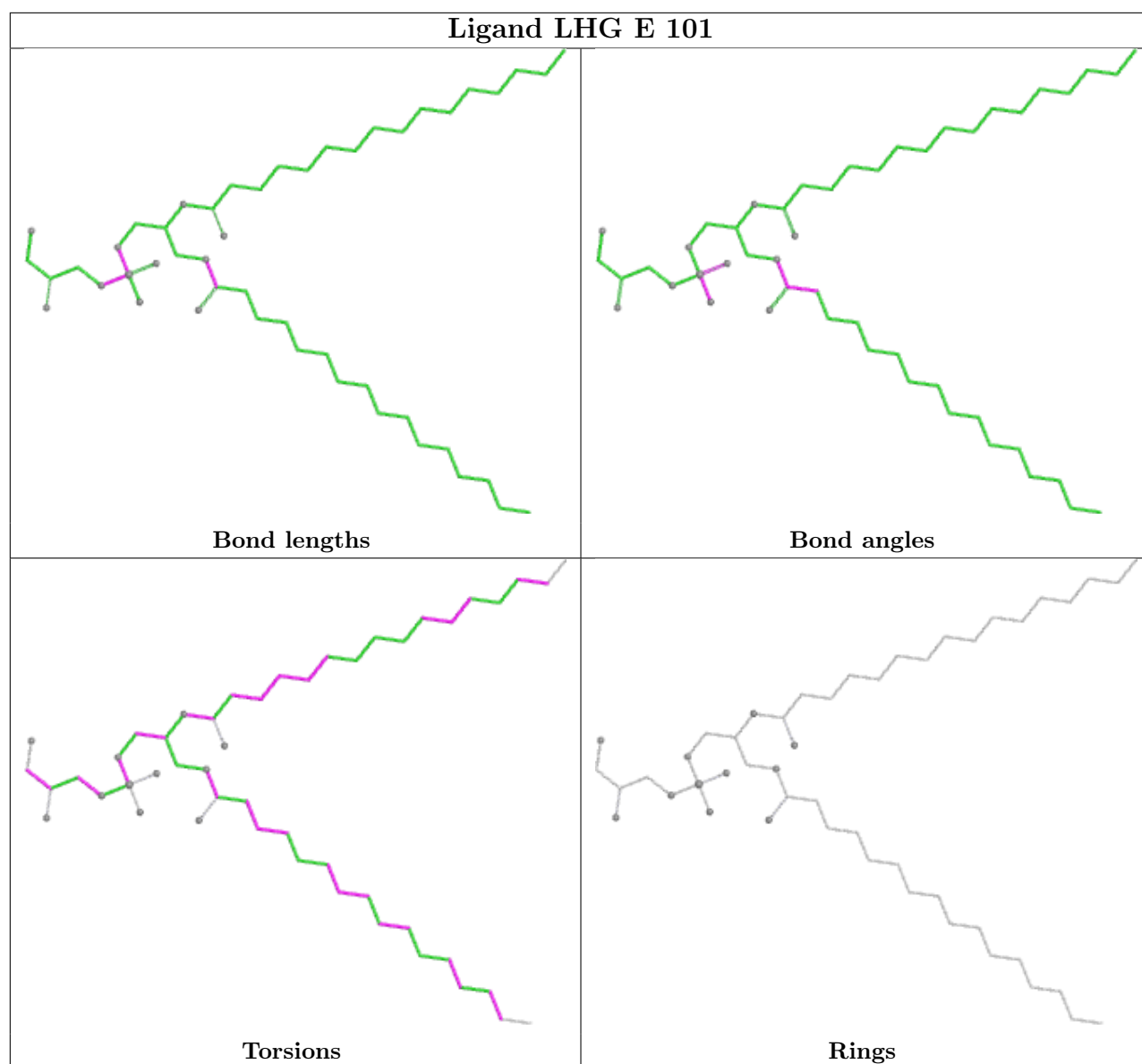


Ligand LHG d 410

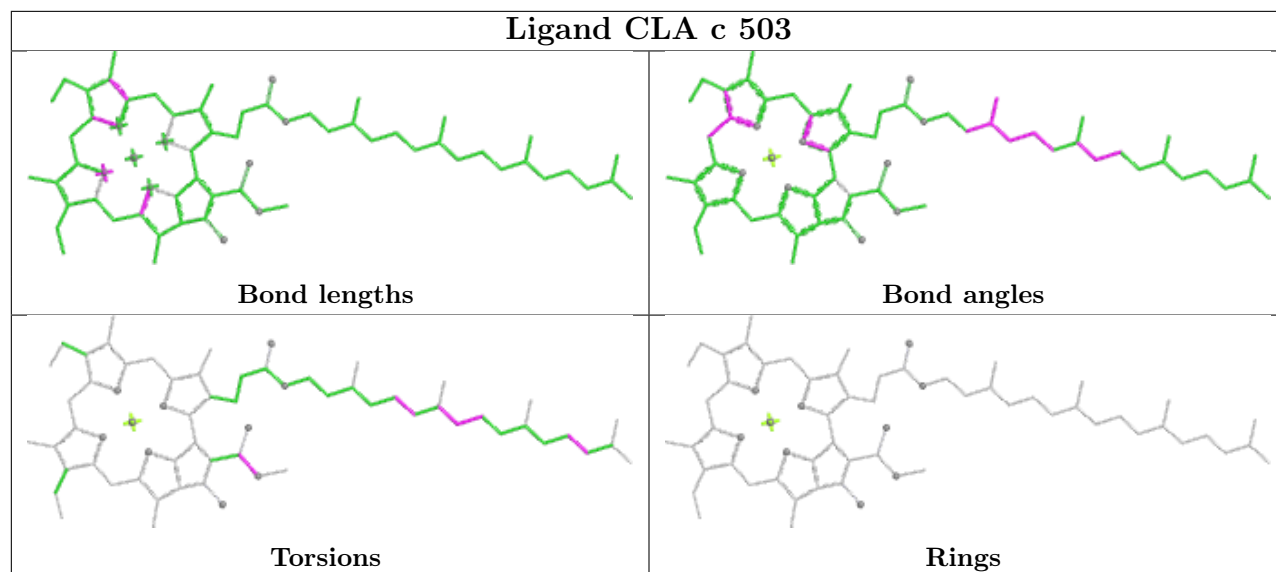


Ligand CLA C 510

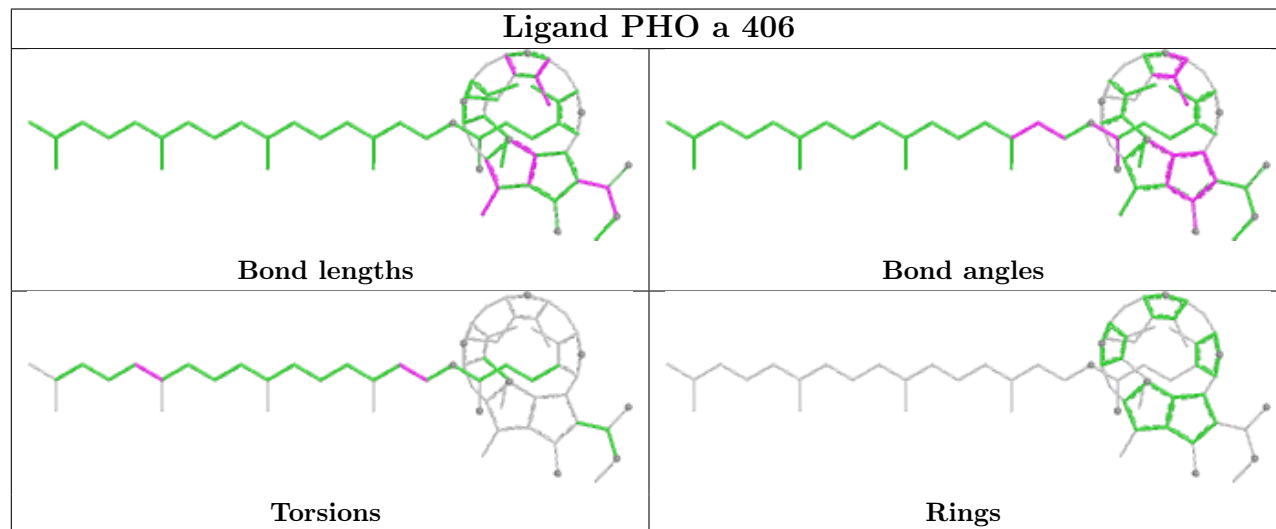




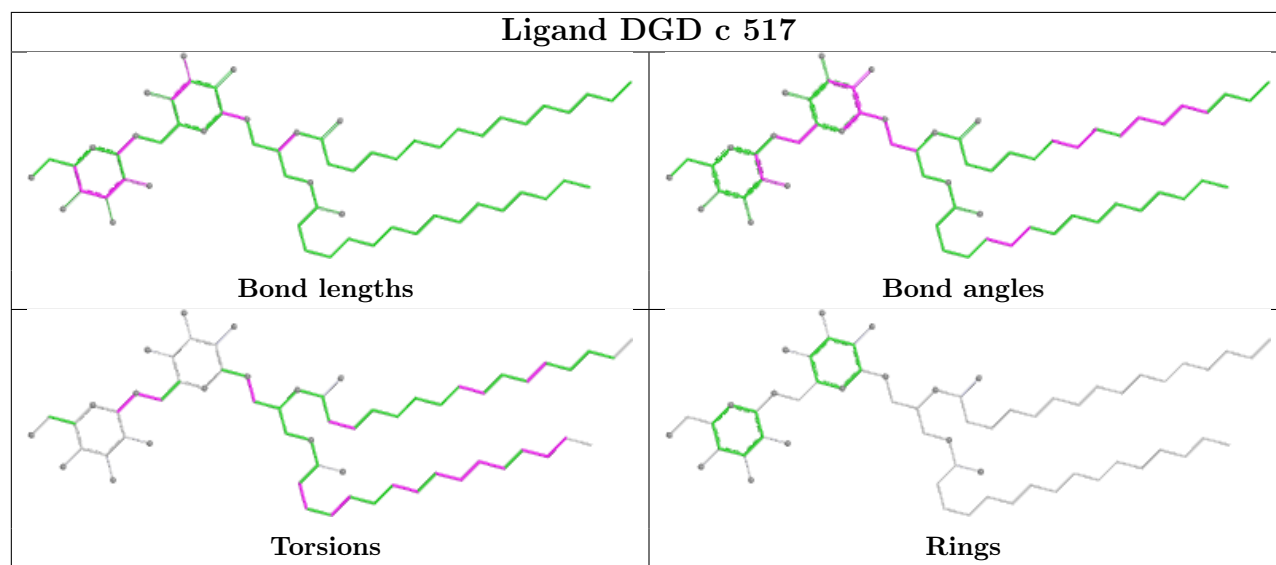
Ligand CLA c 503



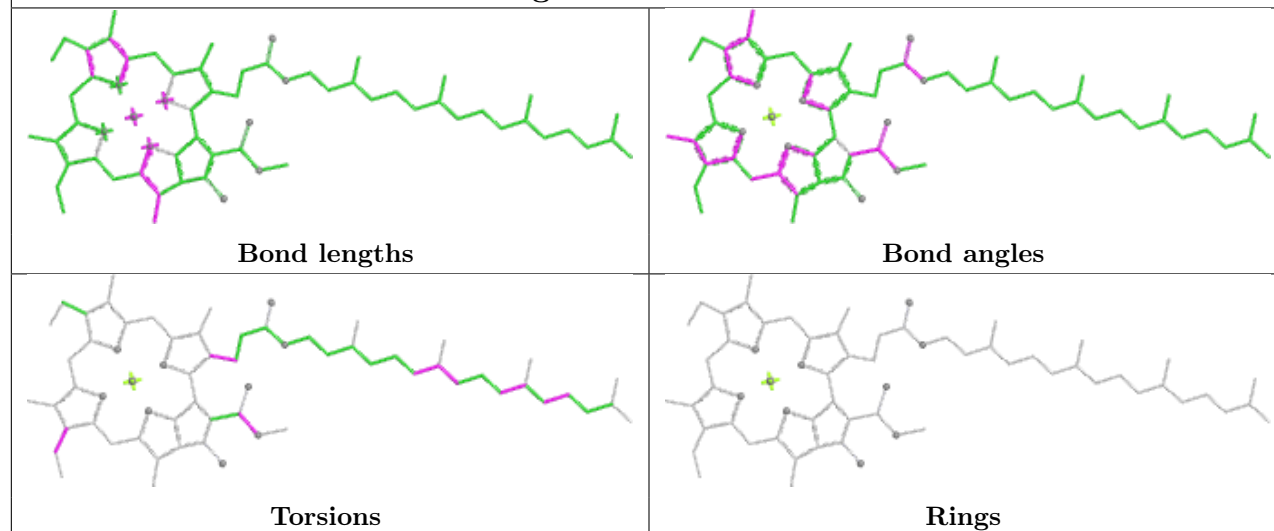
Ligand PHO a 406



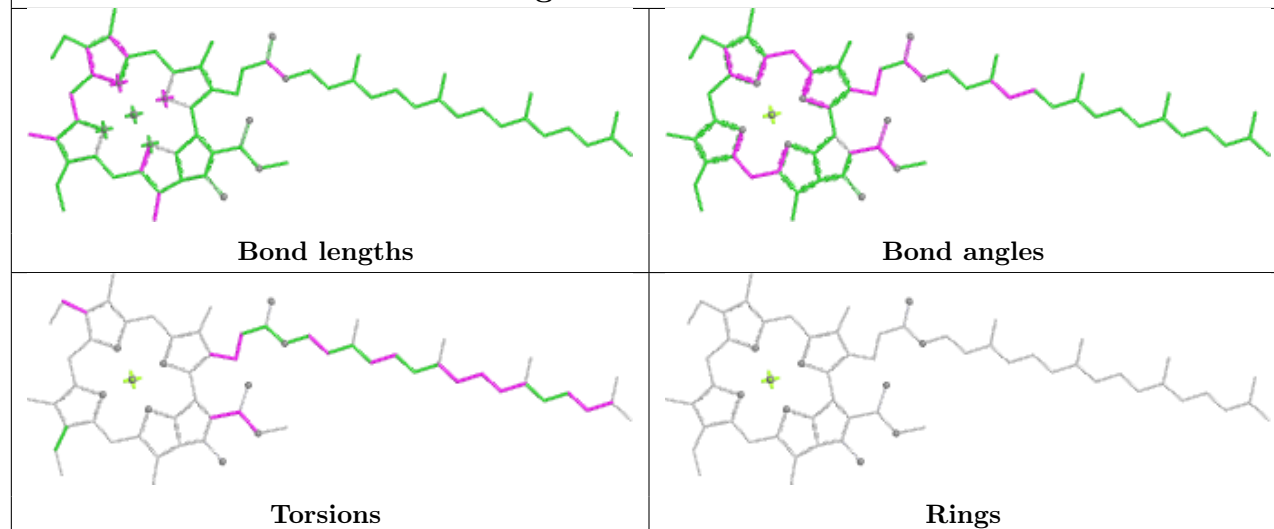
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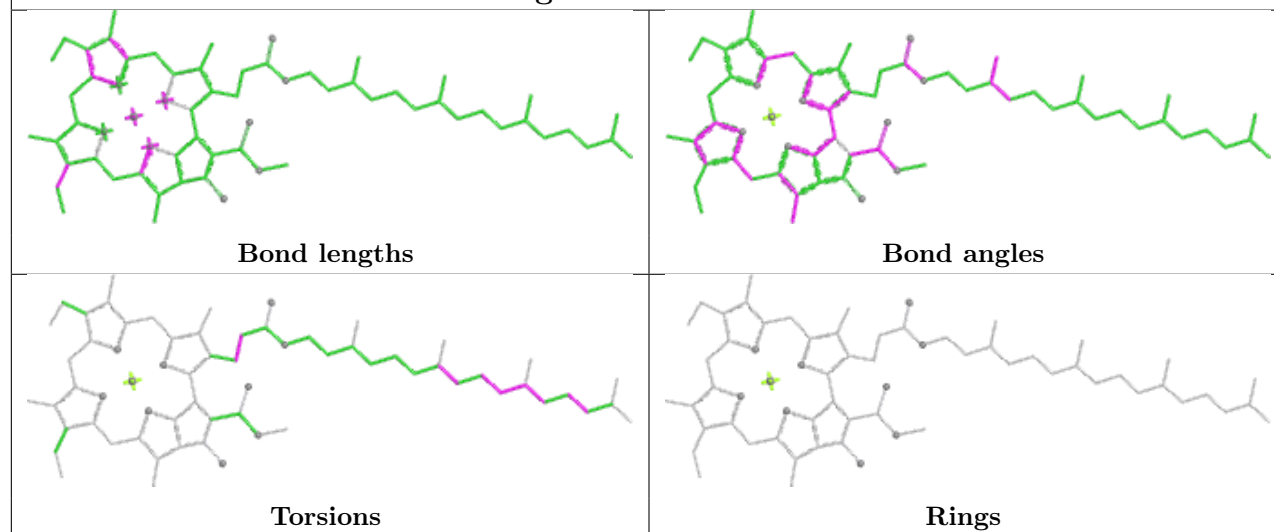
Ligand CLA C 509



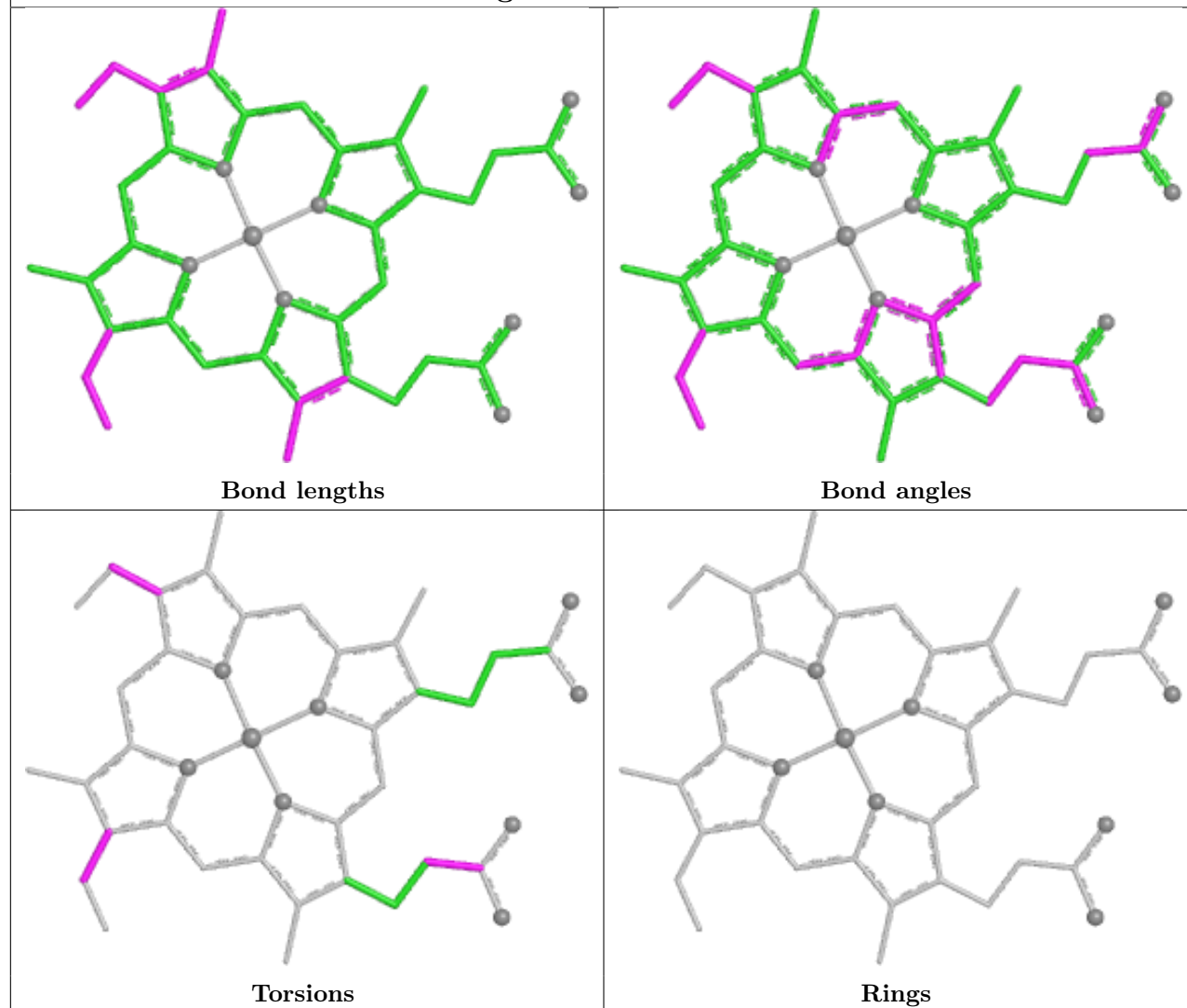
Ligand CLA h 101



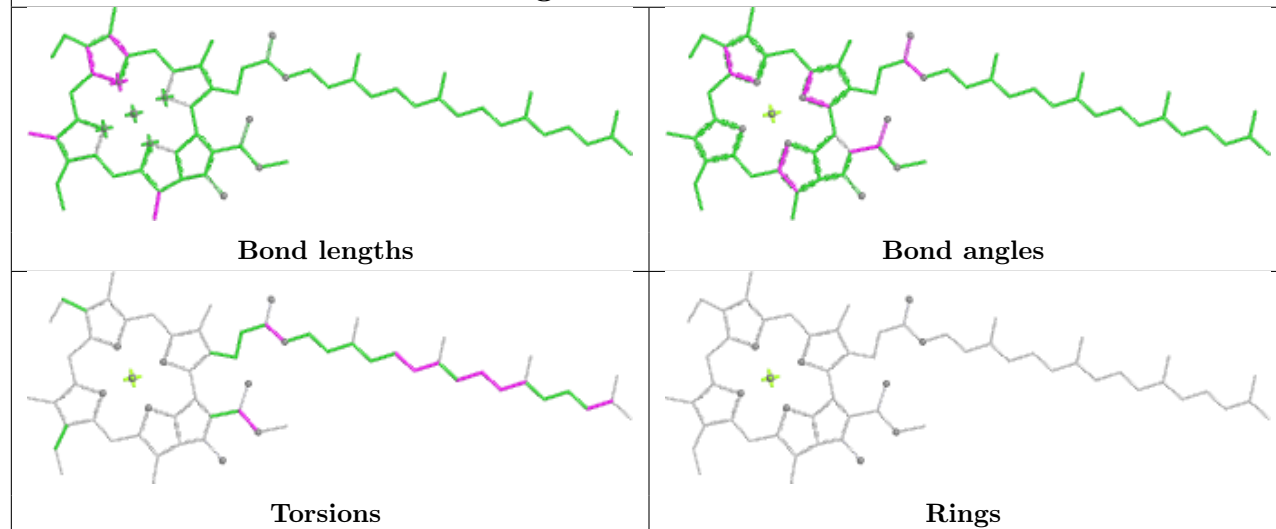
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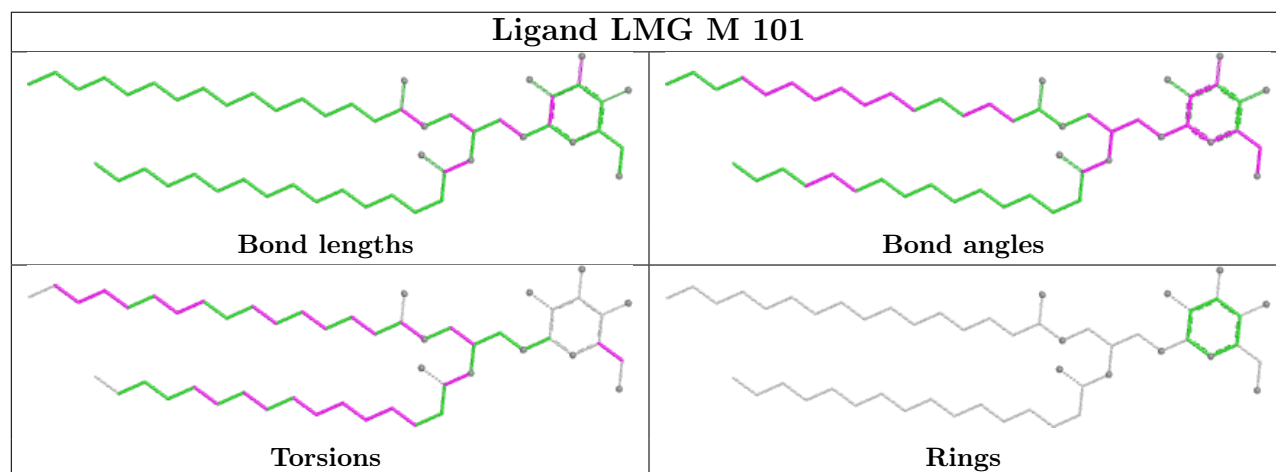
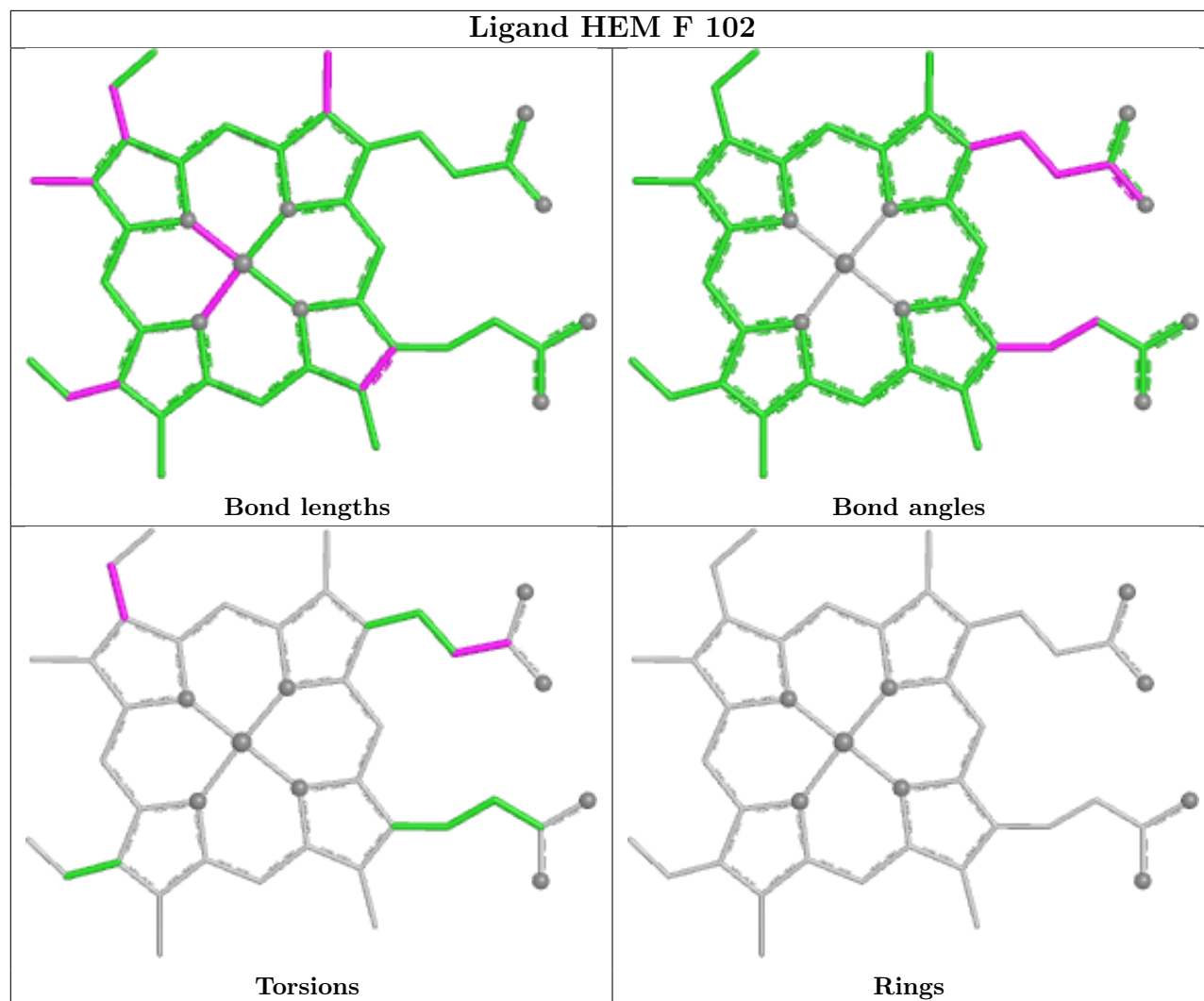


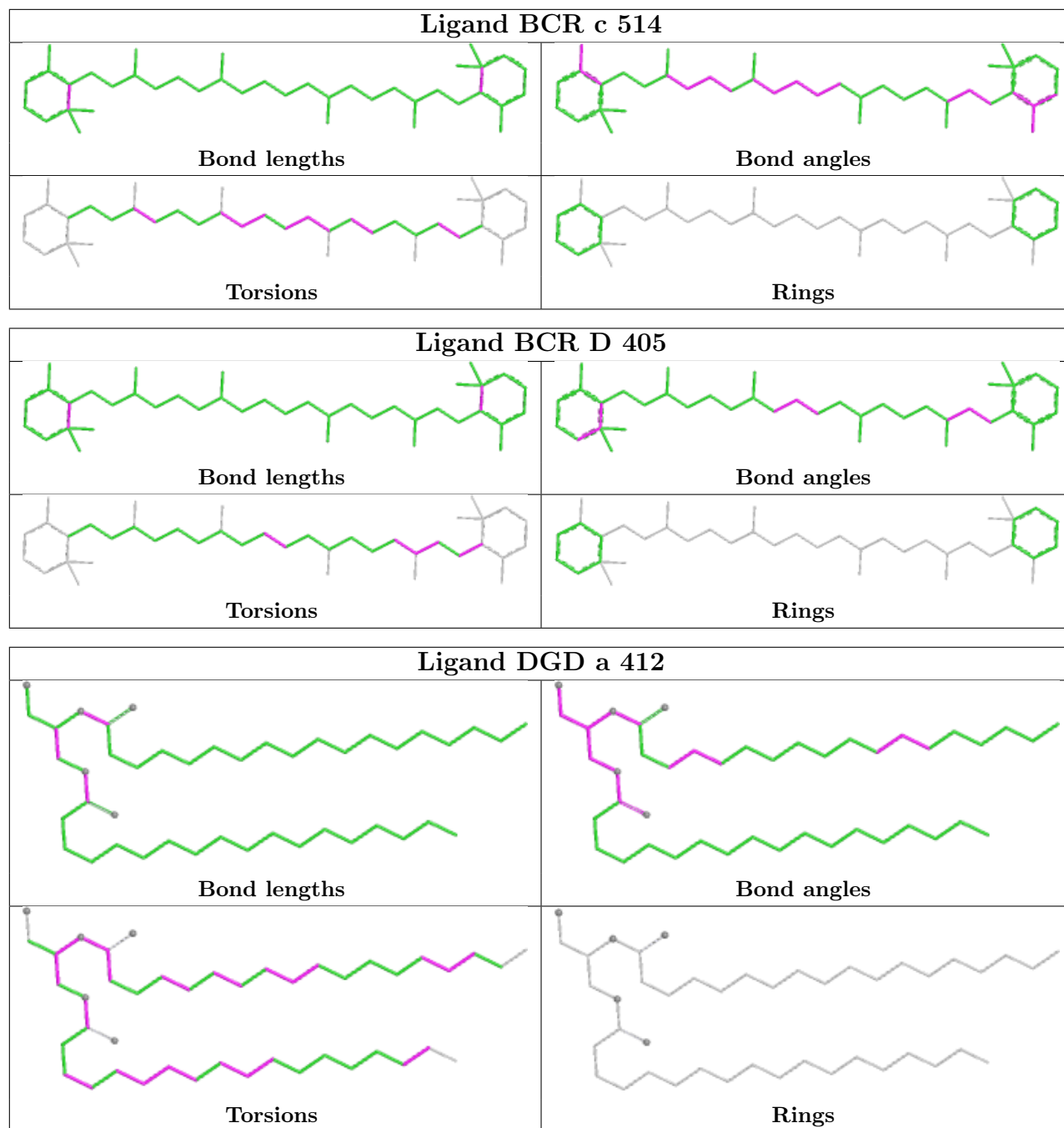
Ligand HEC v 201



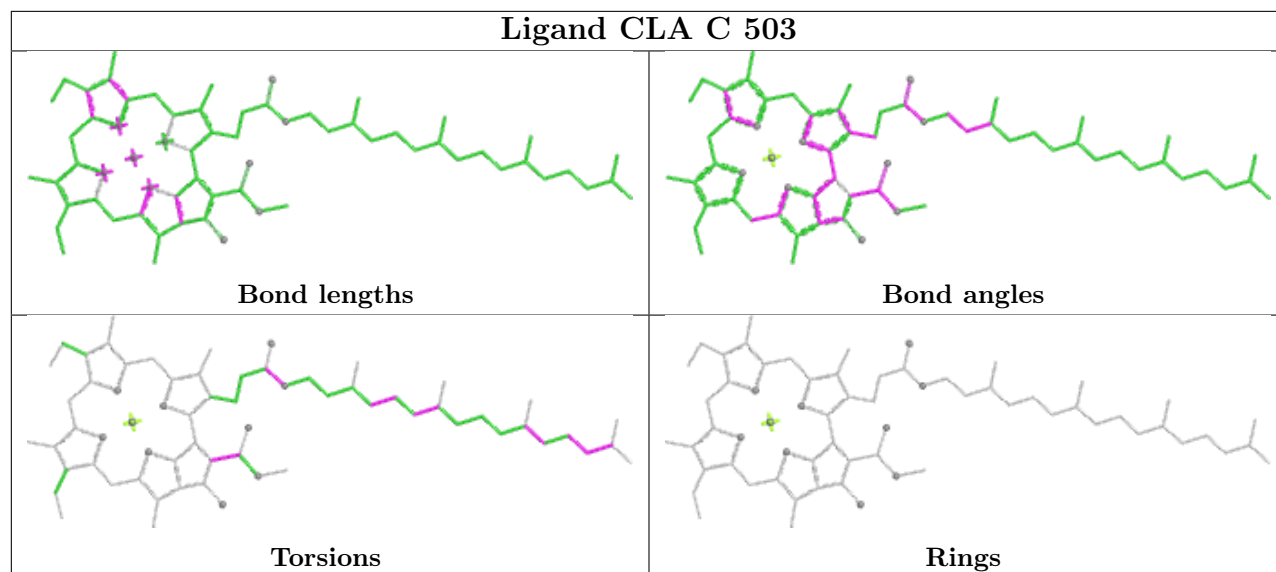
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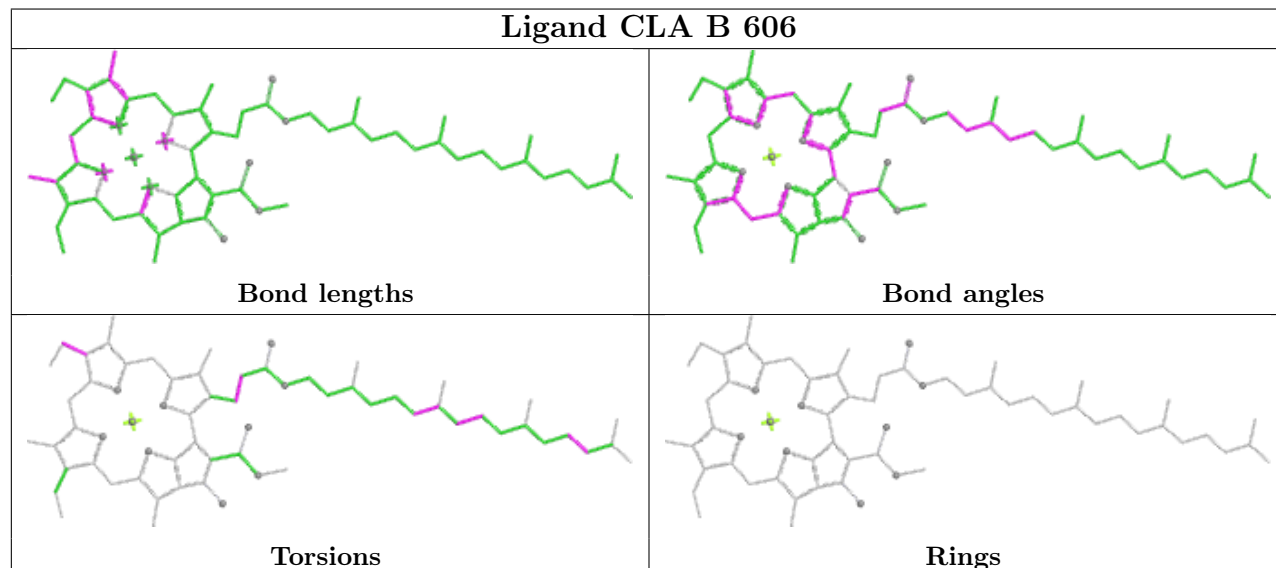




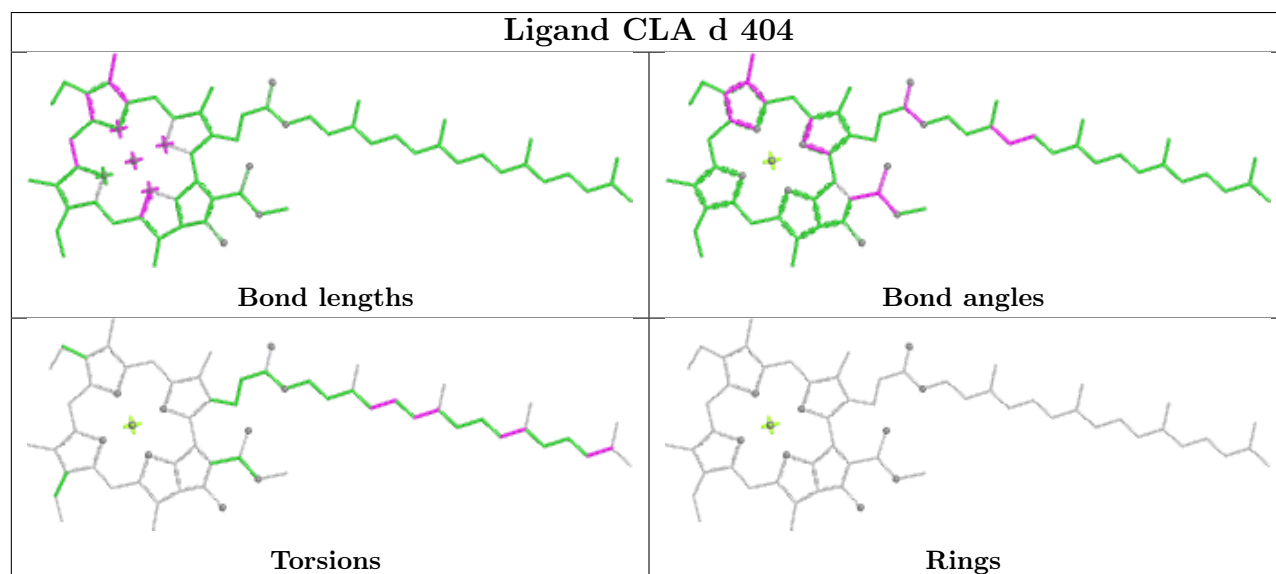
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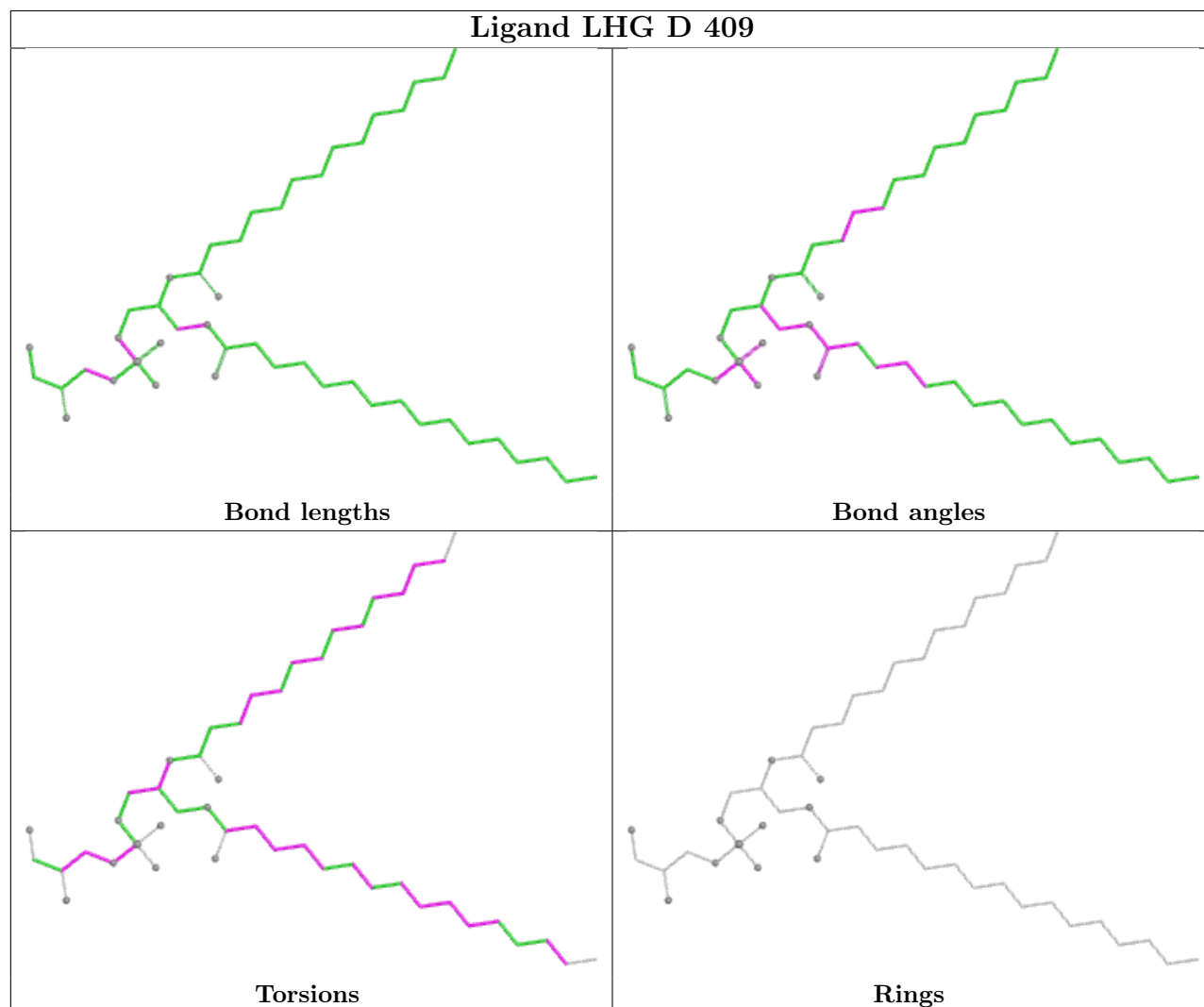
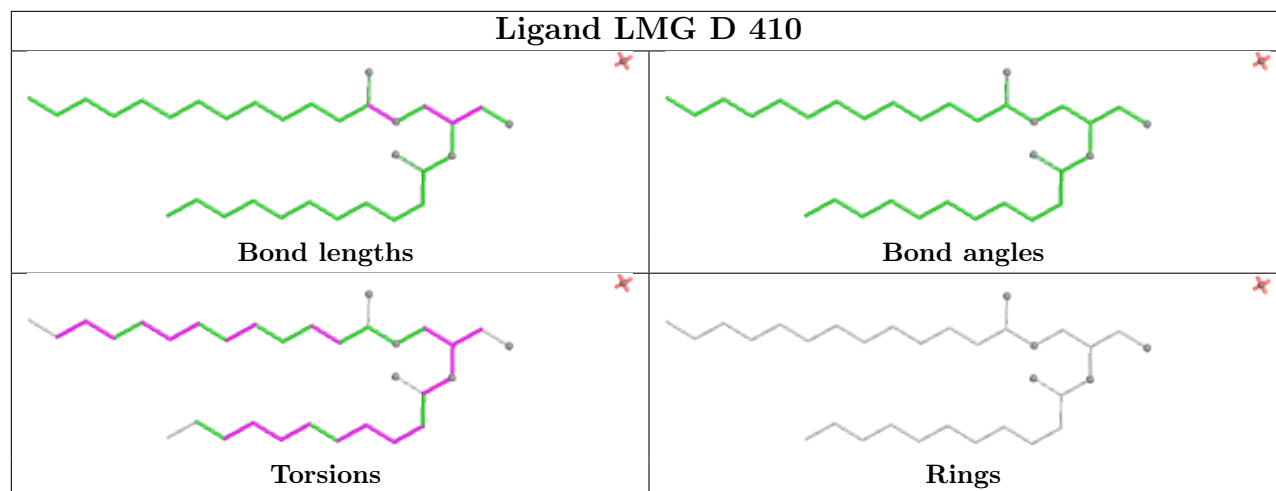


Ligand CLA B 606

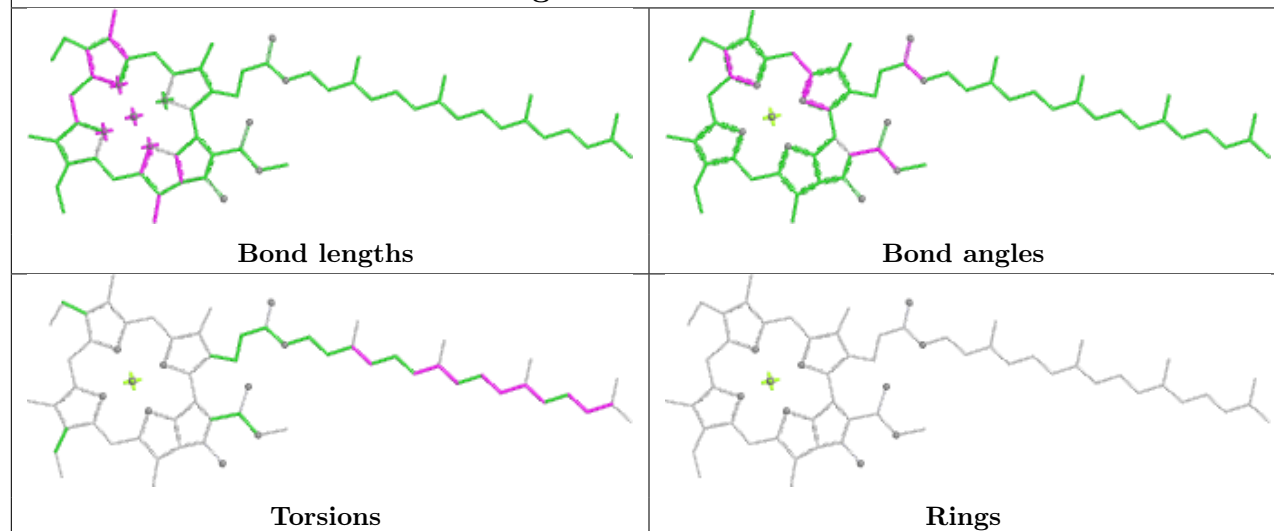


Ligand CLA d 404

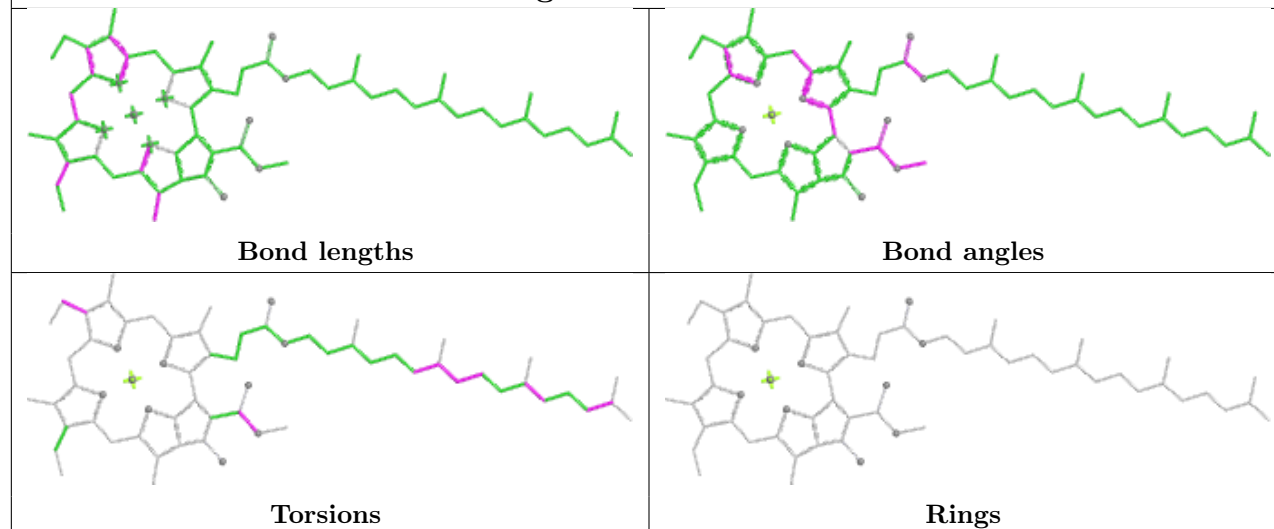




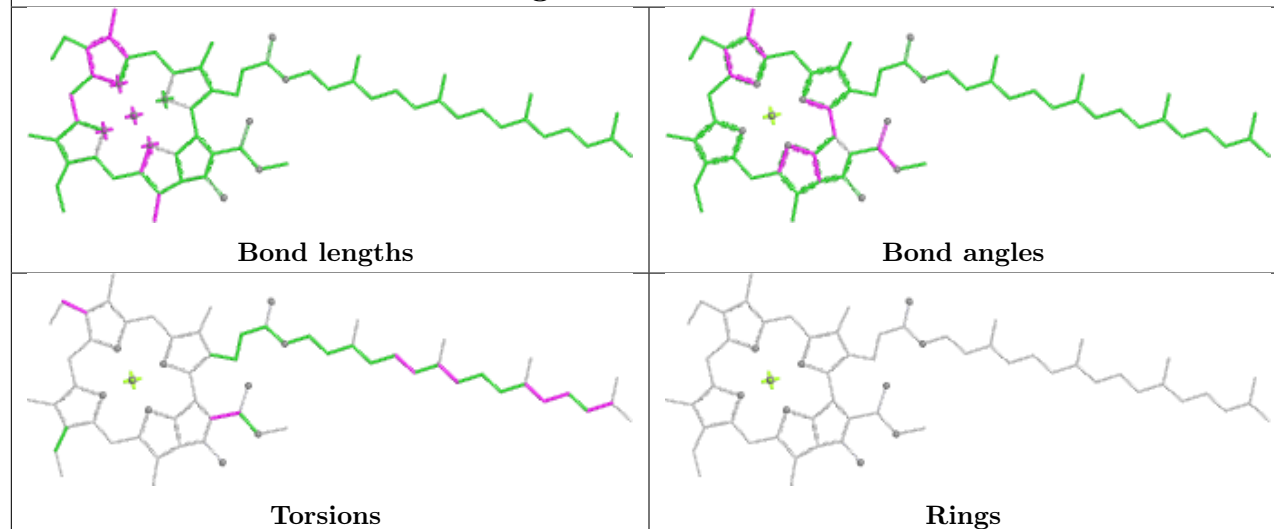
Ligand CLA C 511

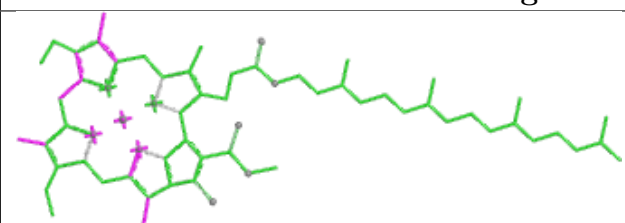
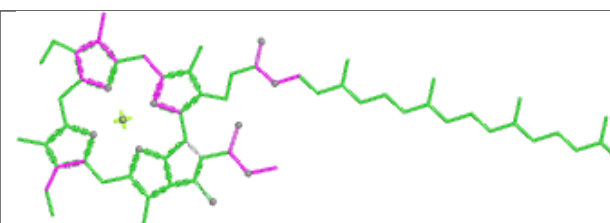
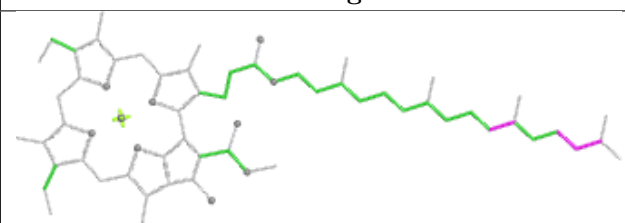
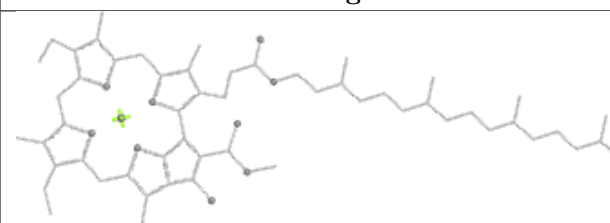


Ligand CLA a 405

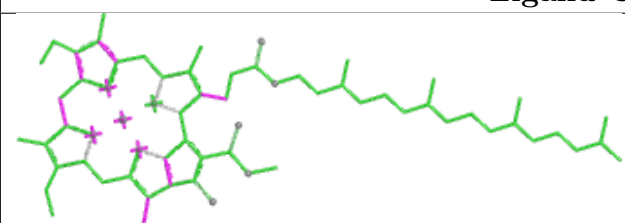
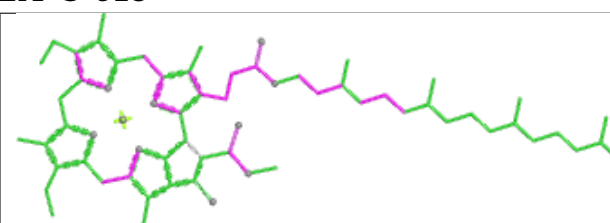
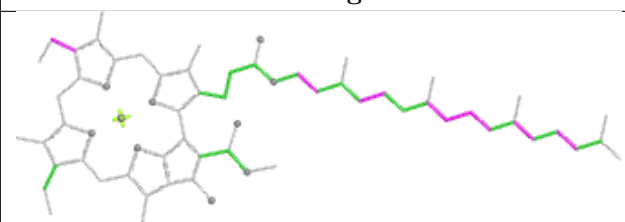
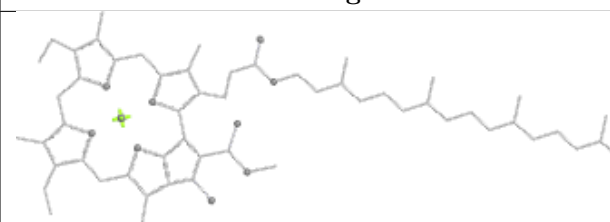


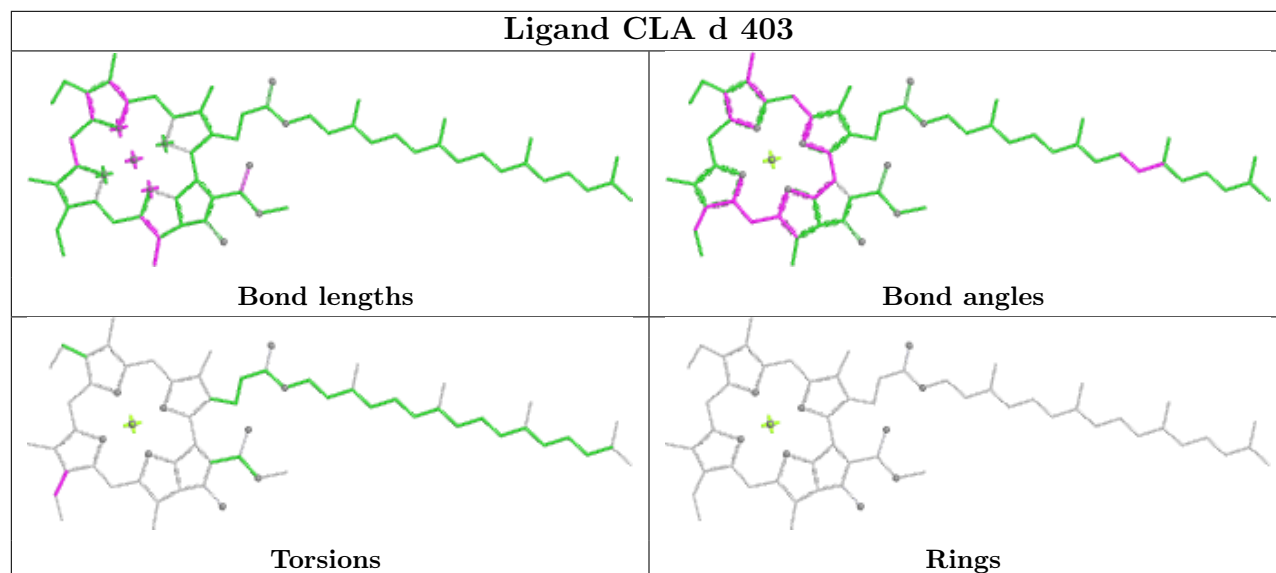
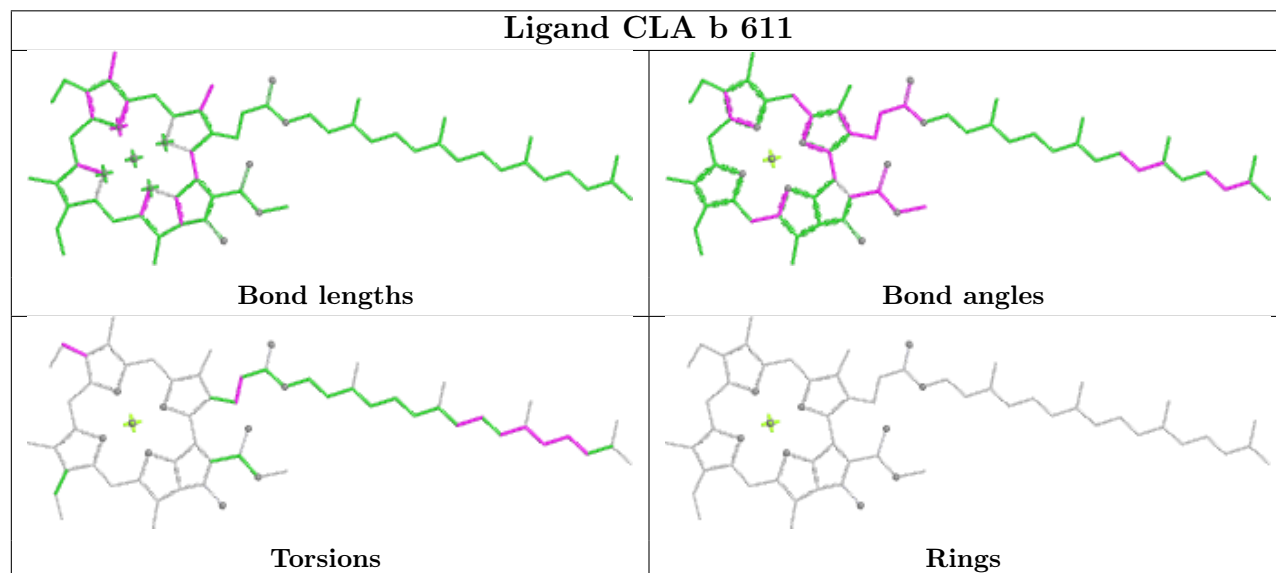
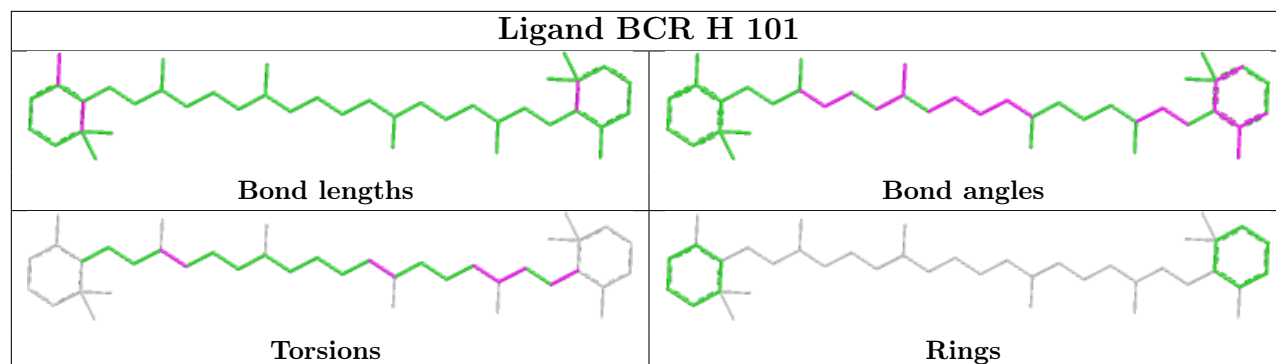
Ligand CLA D 404



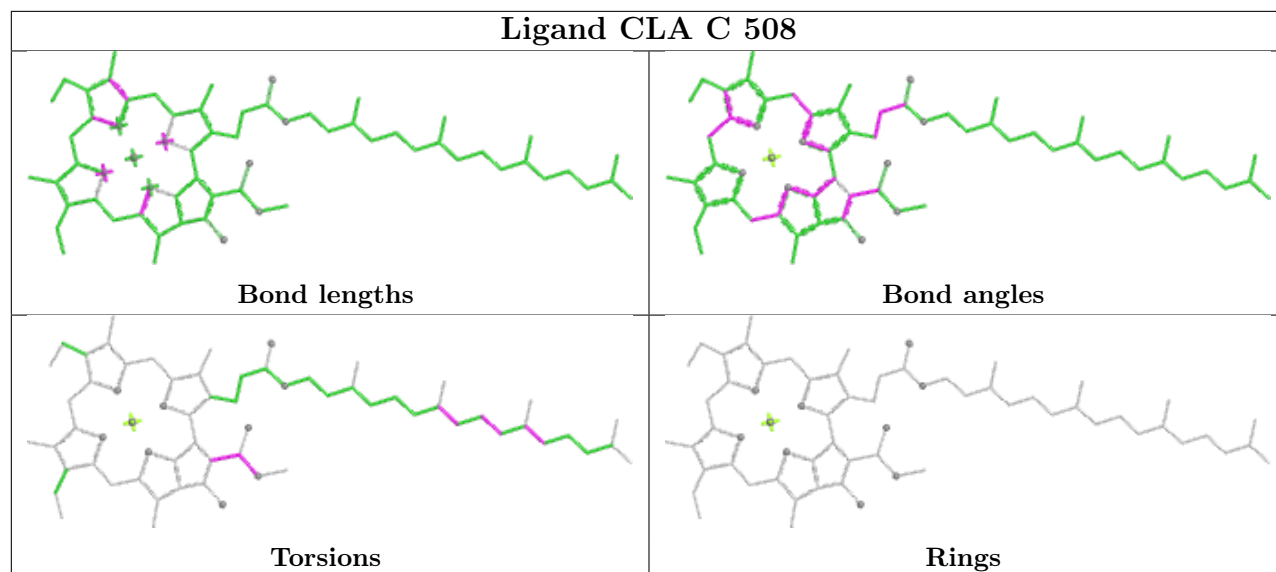
Ligand CLA A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

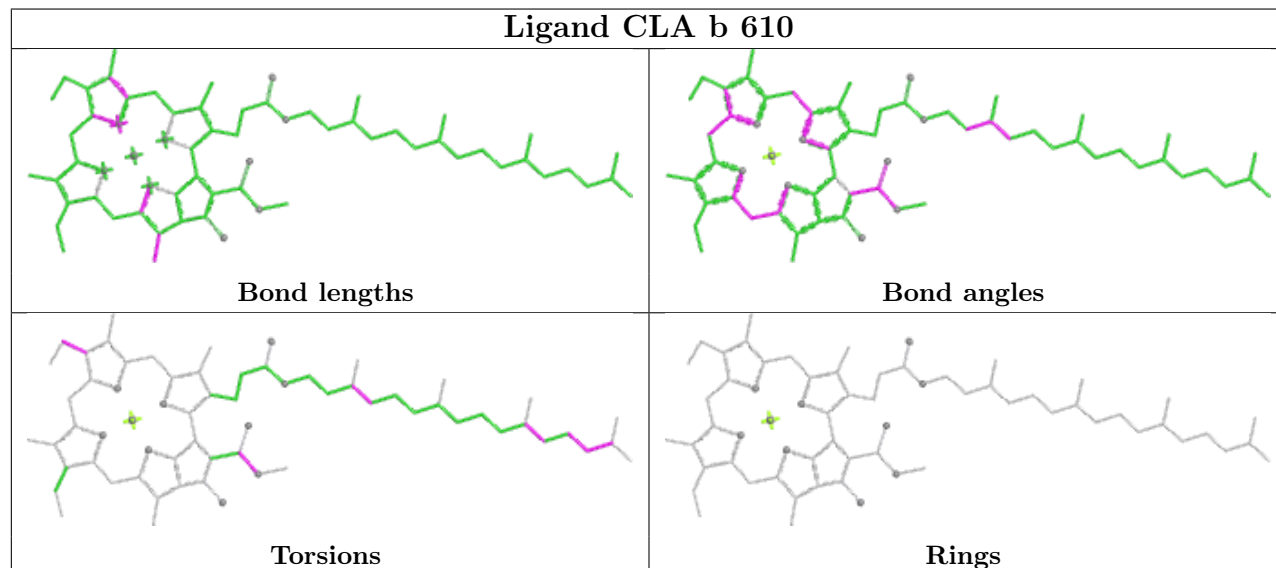
Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings



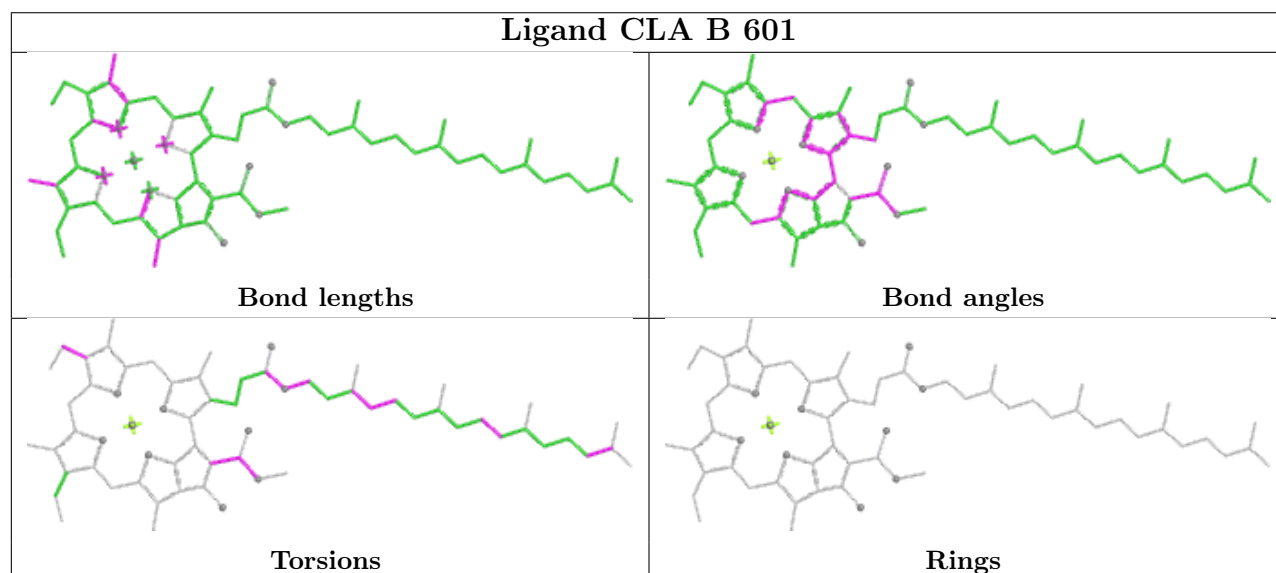
Ligand CLA C 508

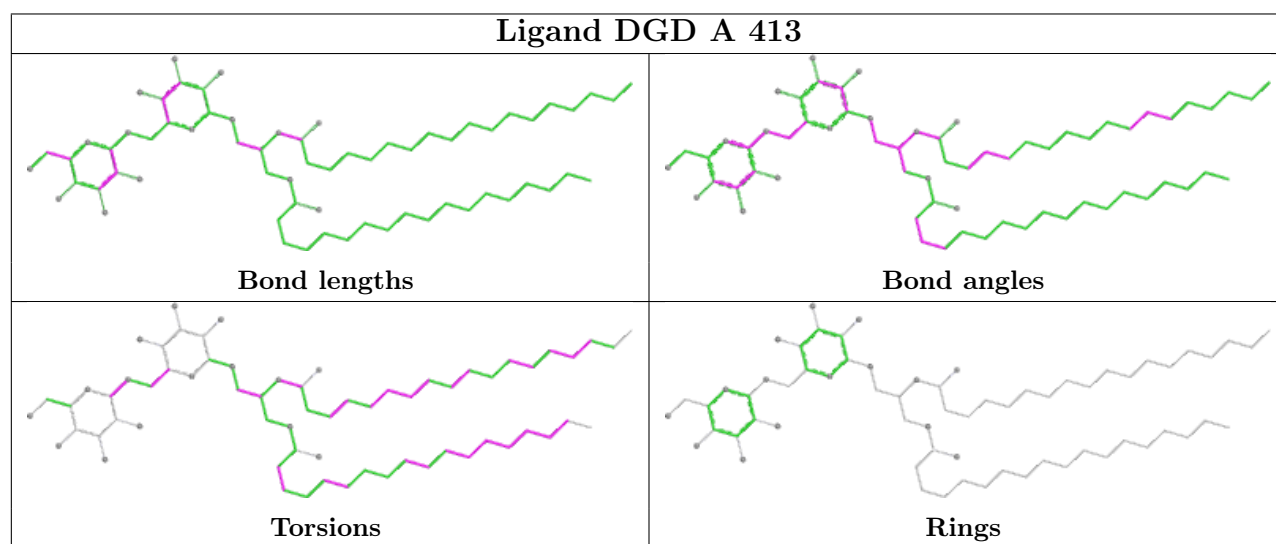
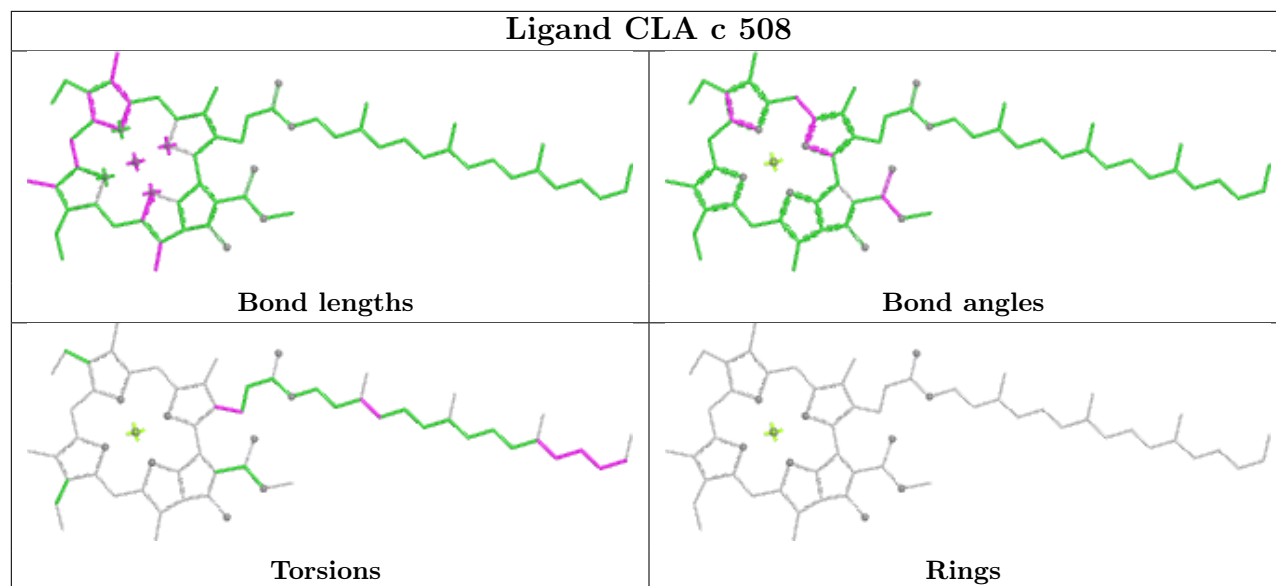


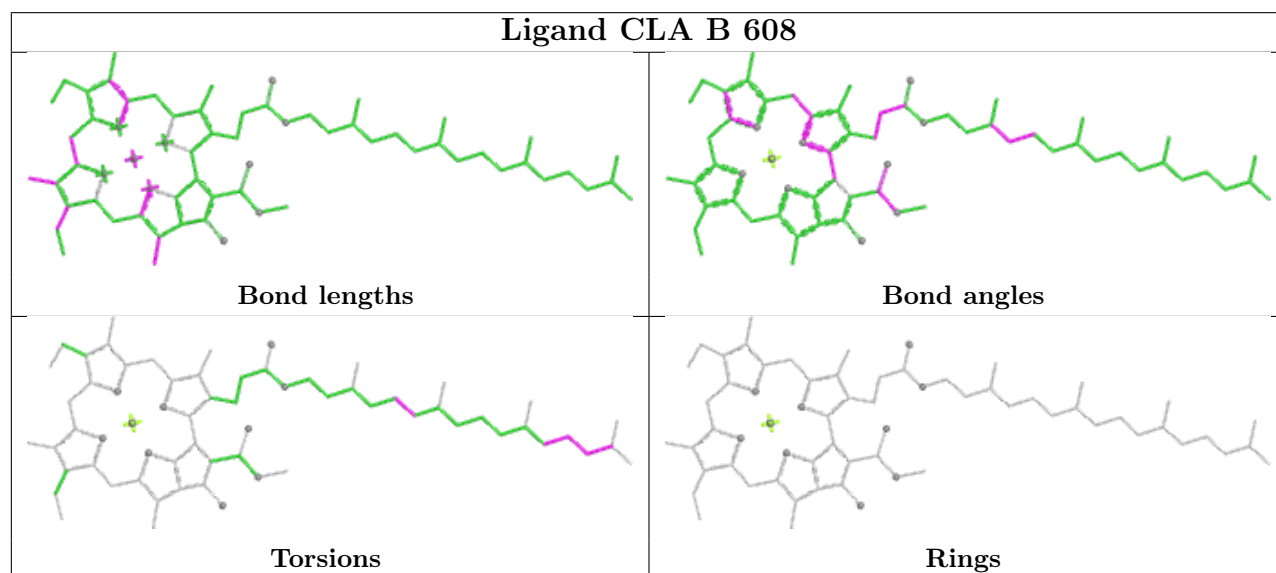
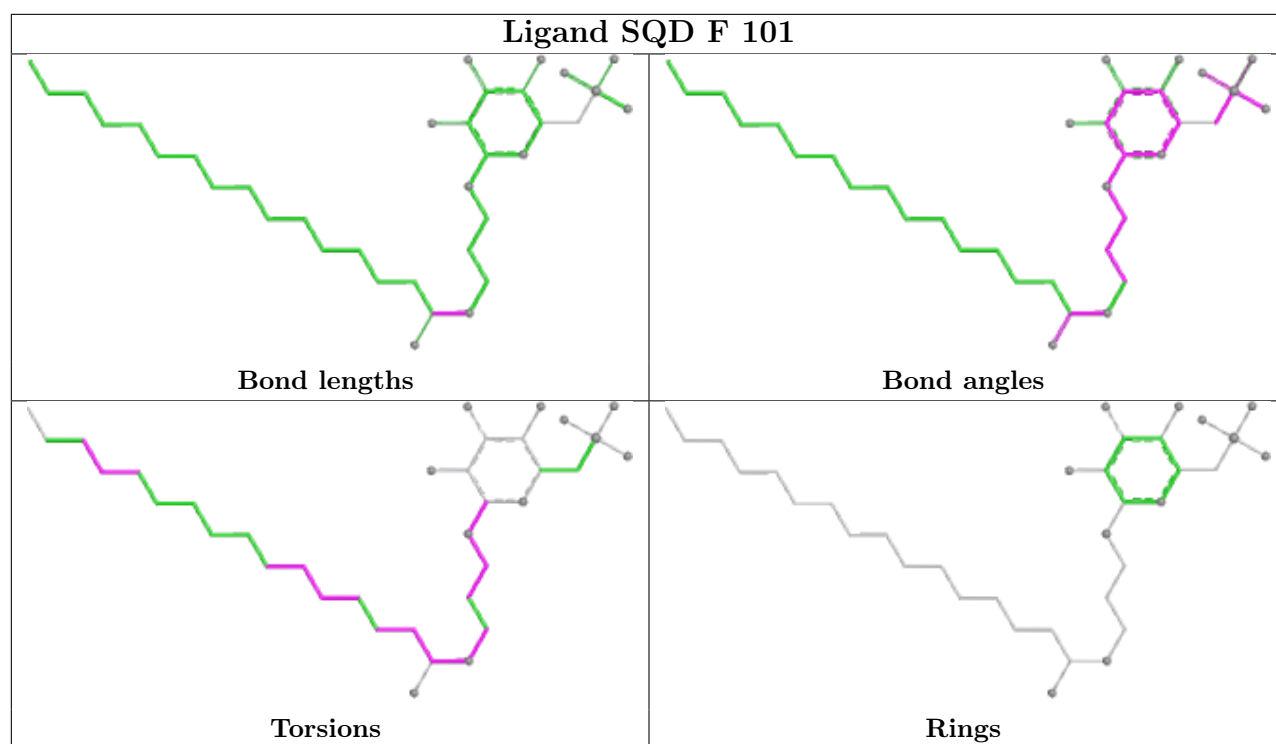
Ligand CLA b 610

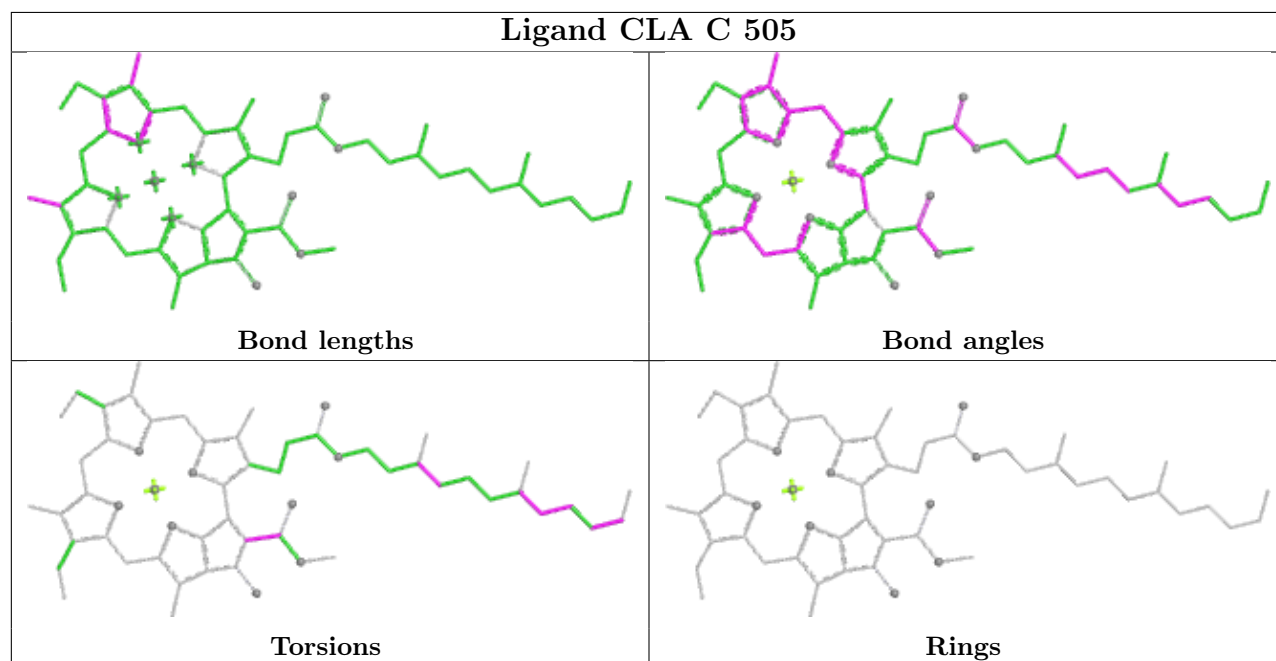
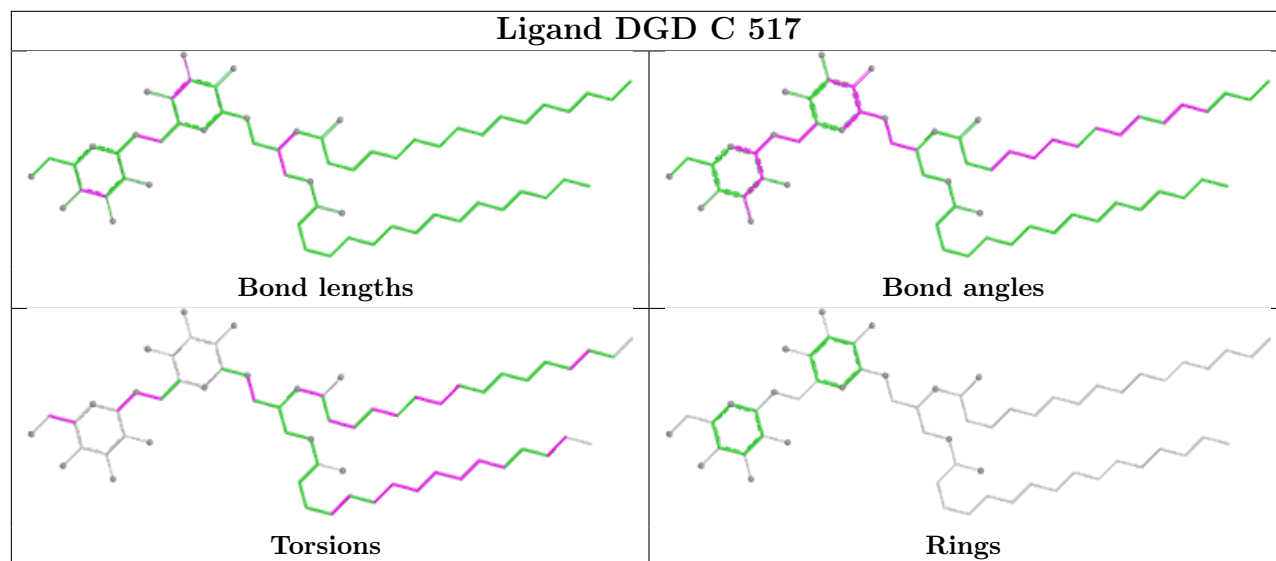


Ligand CLA B 601

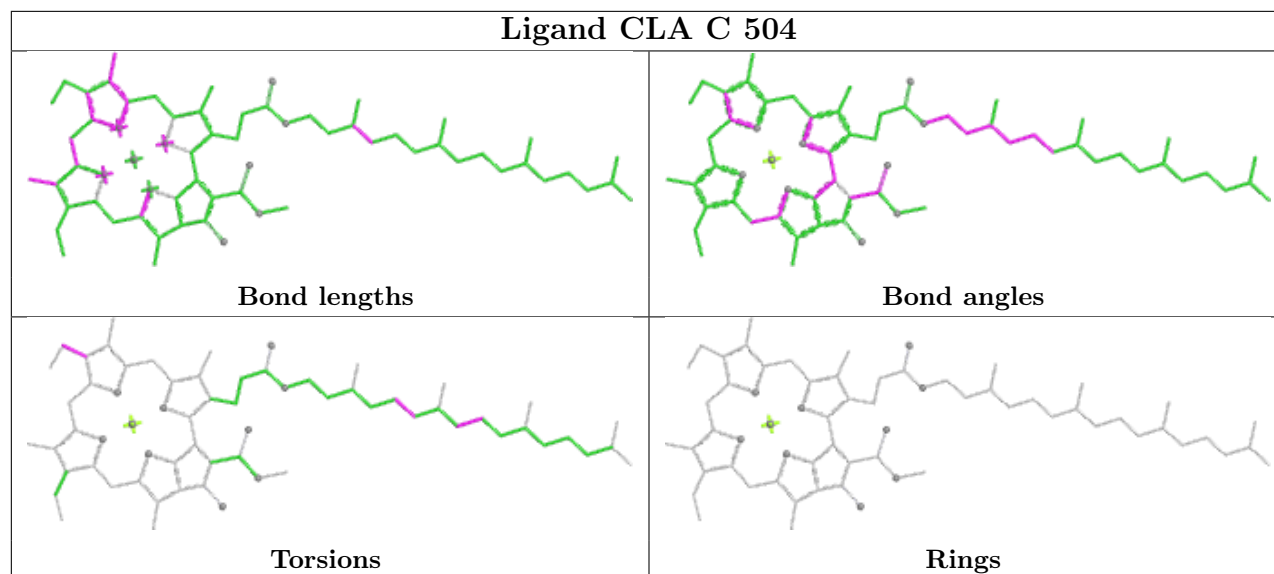




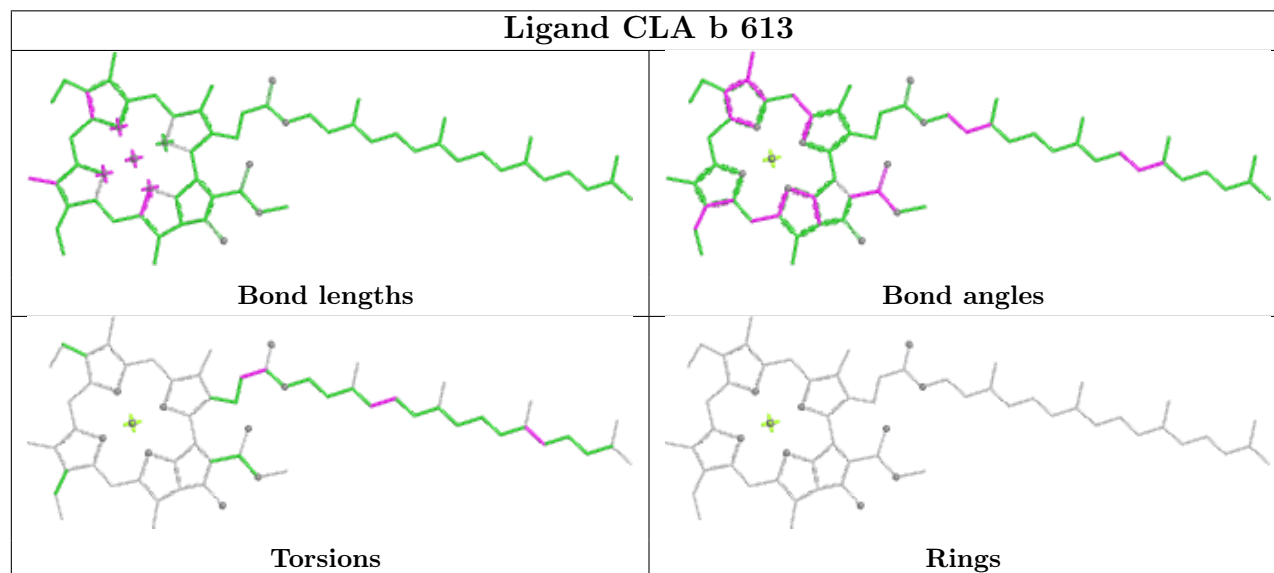




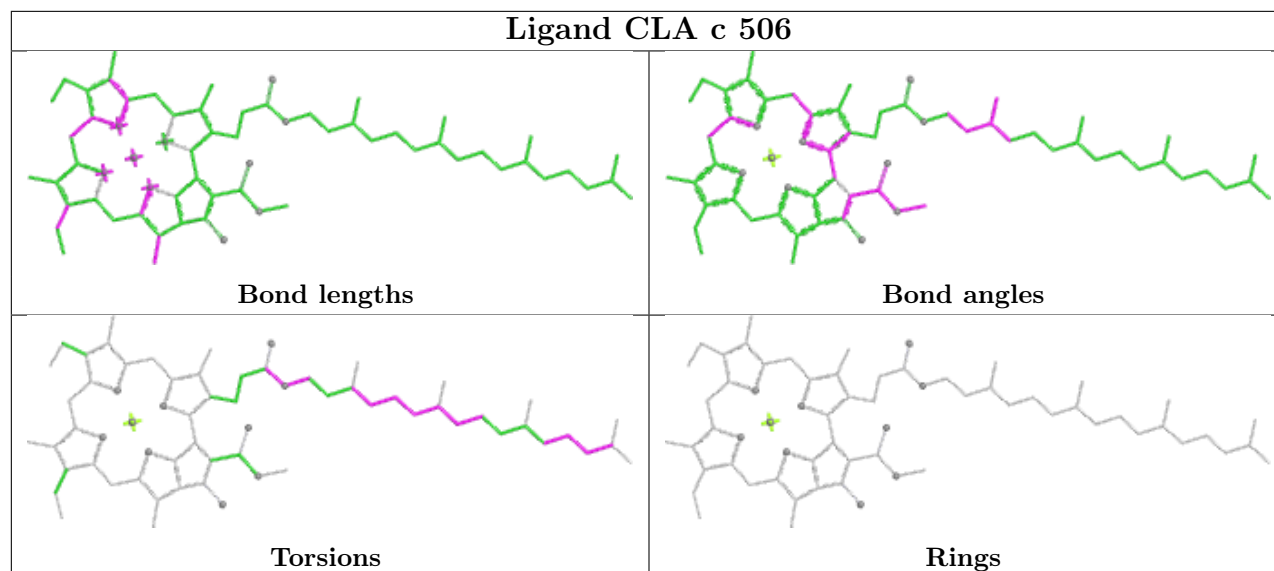
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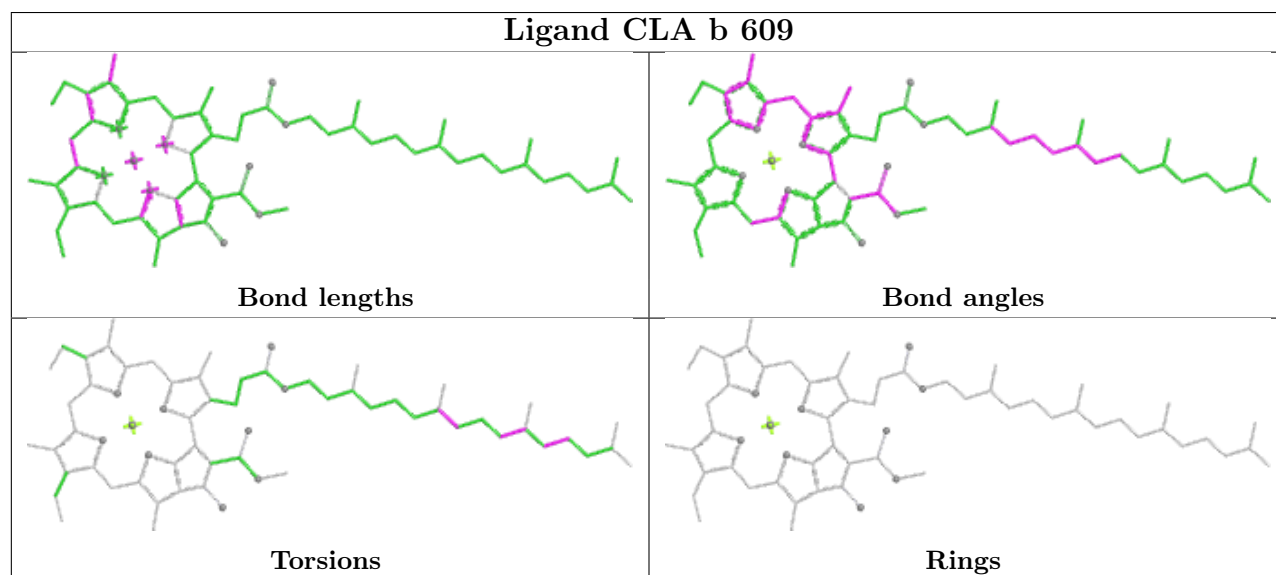
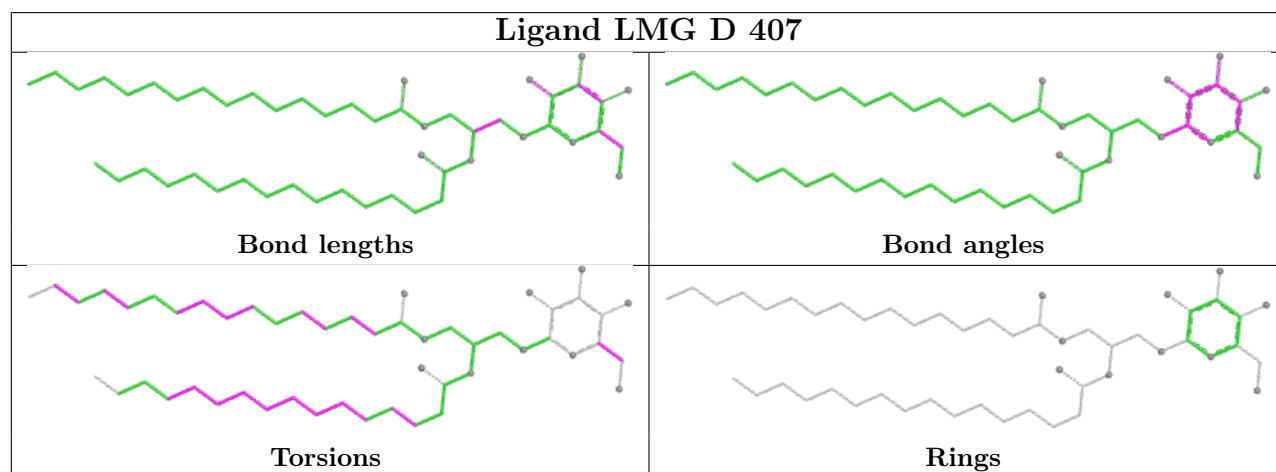
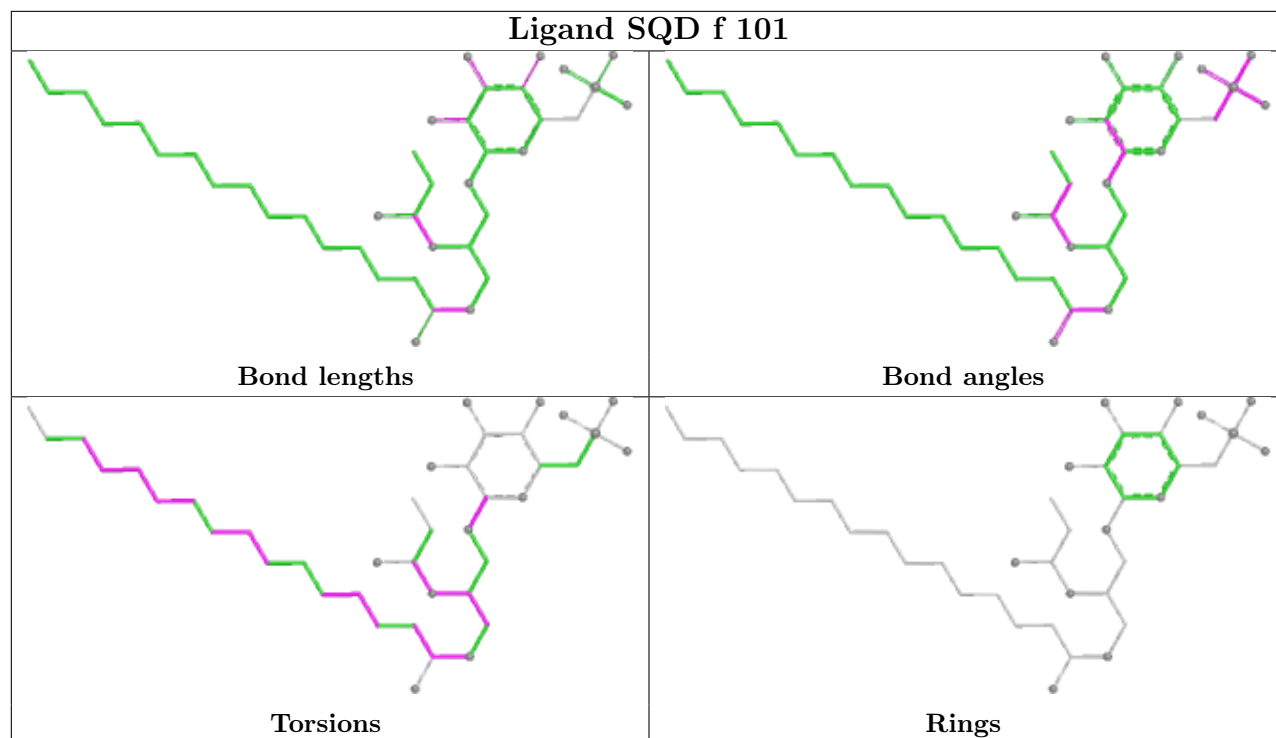


Ligand CLA b 613

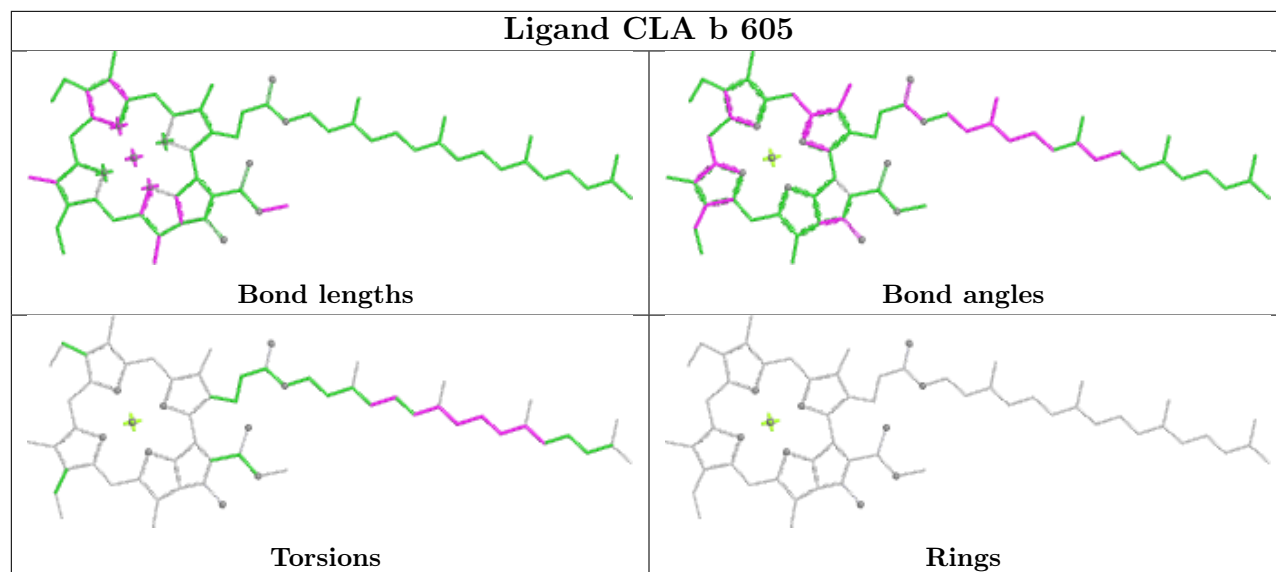


Ligand CLA c 506

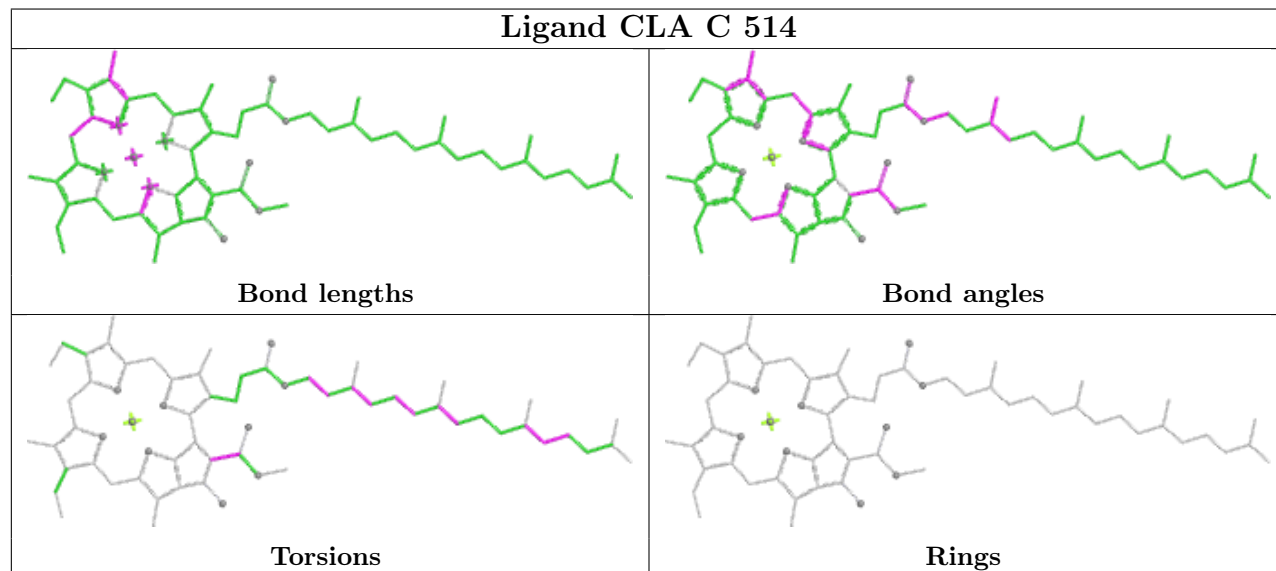




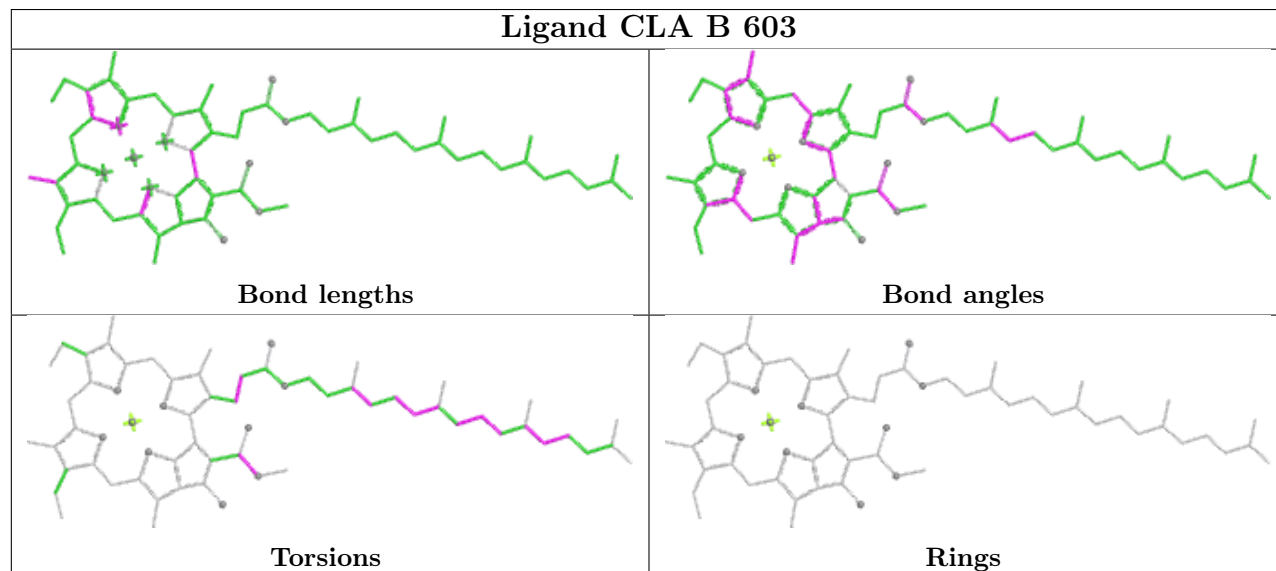
Ligand CLA b 605



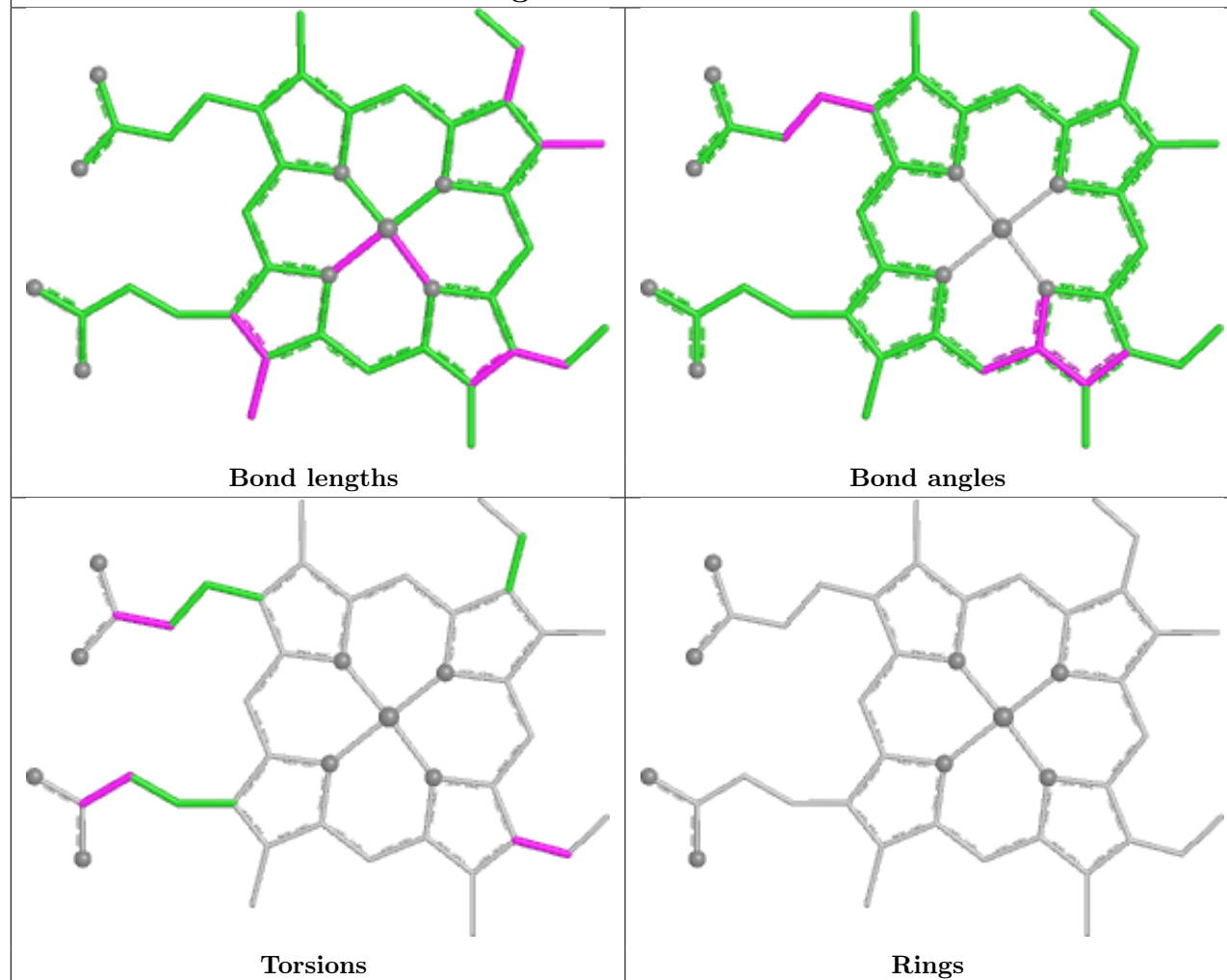
Ligand CLA C 514



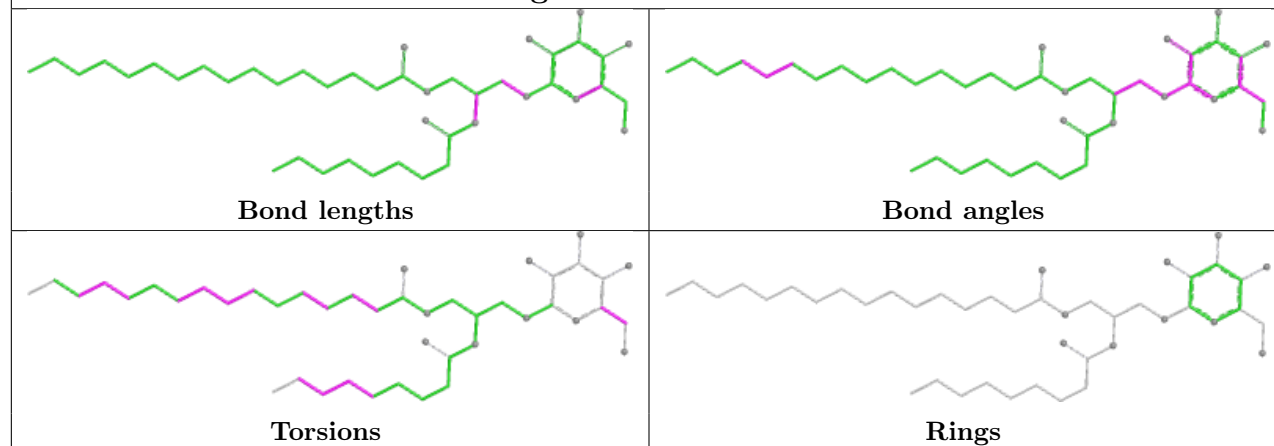
Ligand CLA B 603

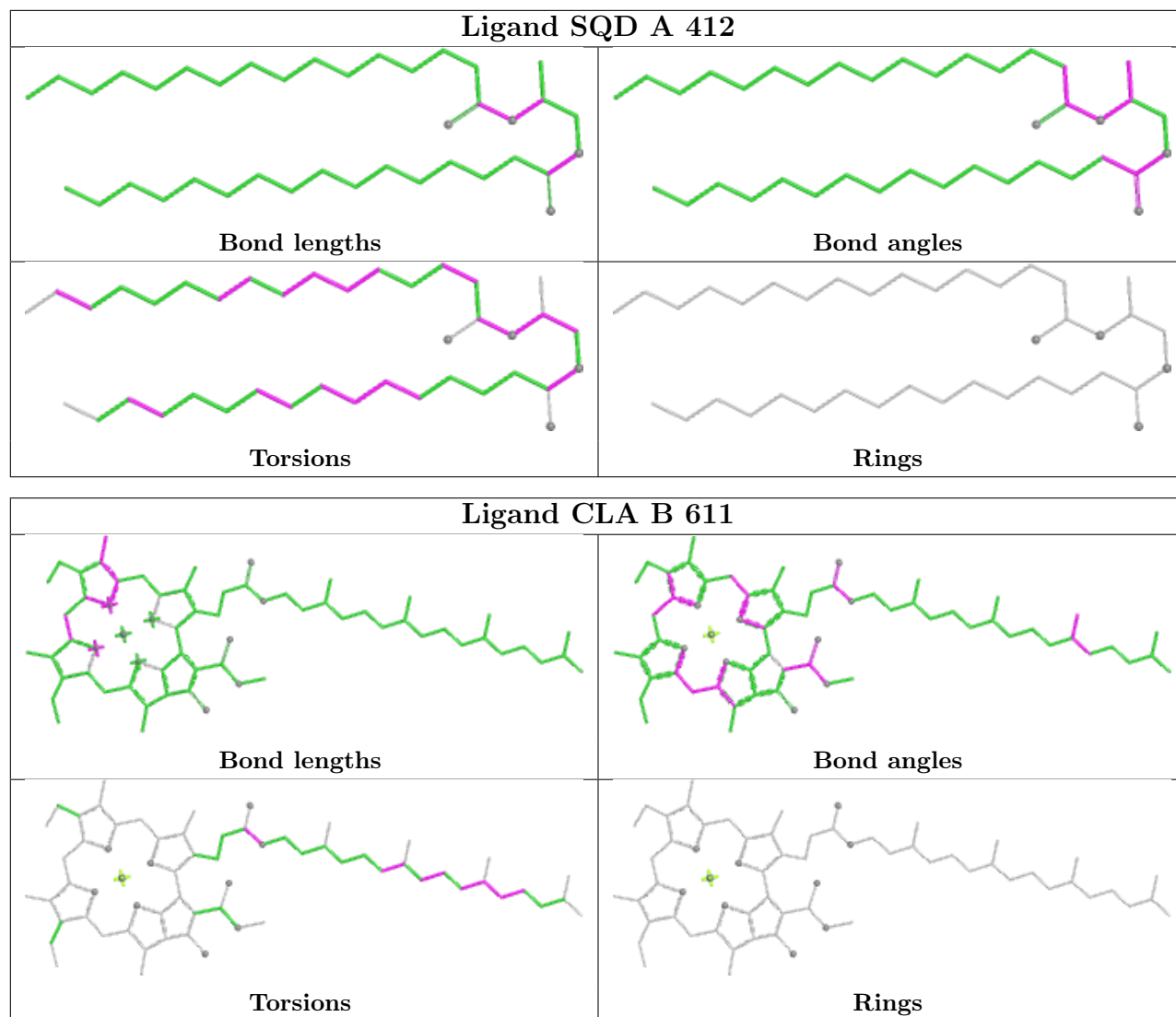


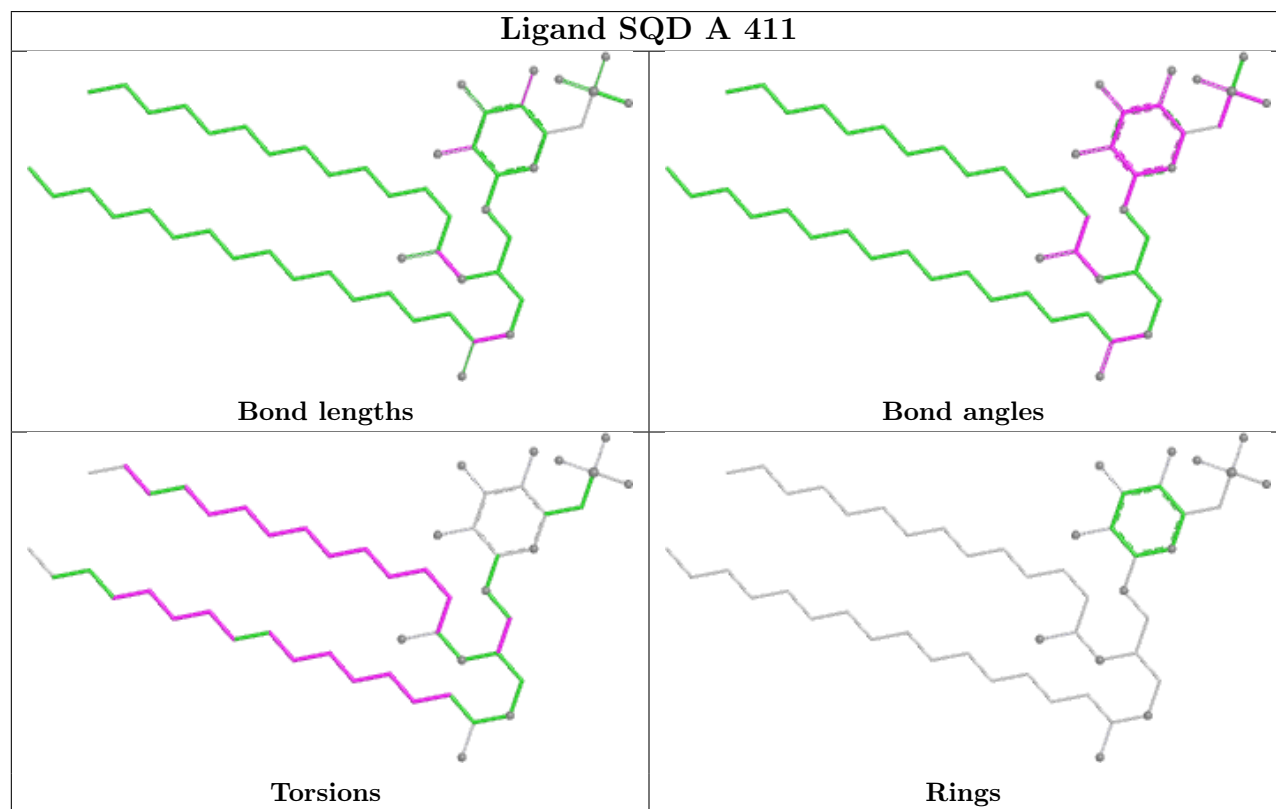
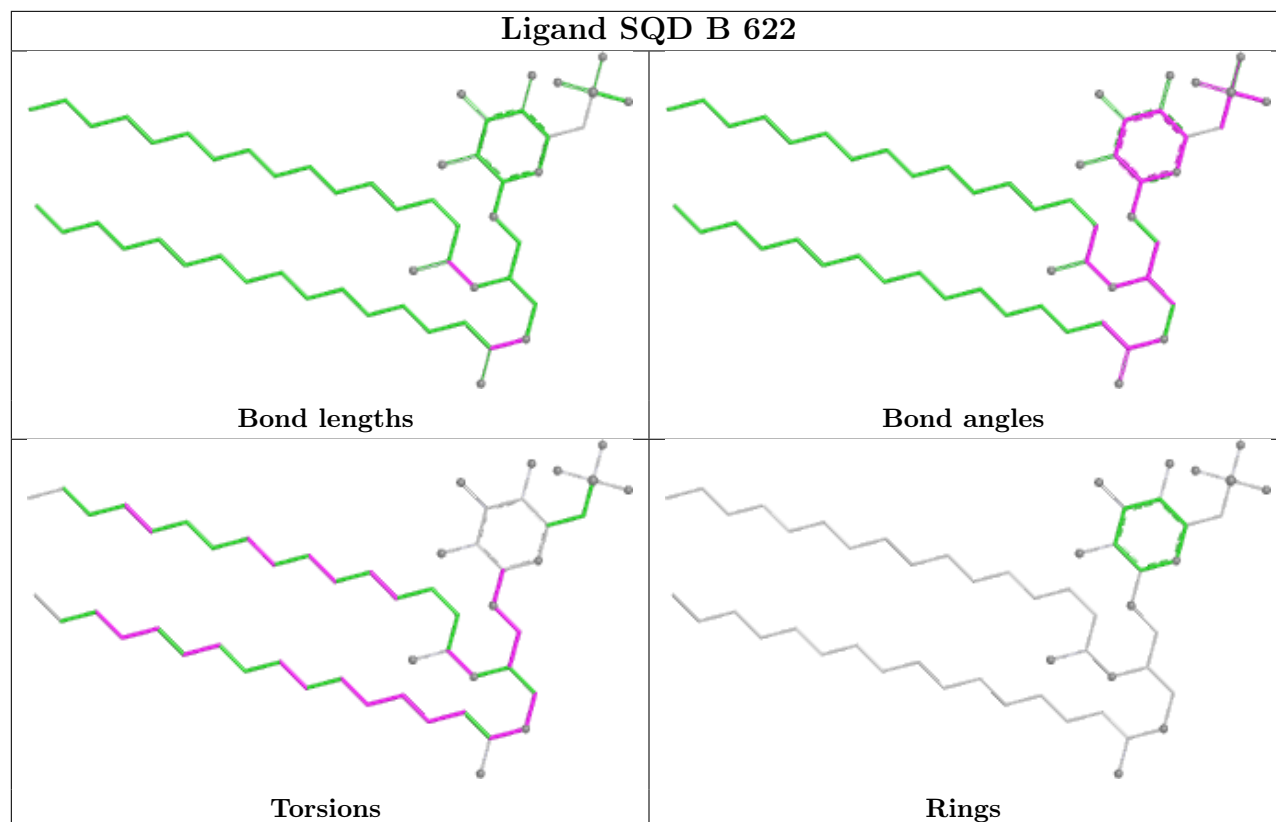
Ligand HEM e 102

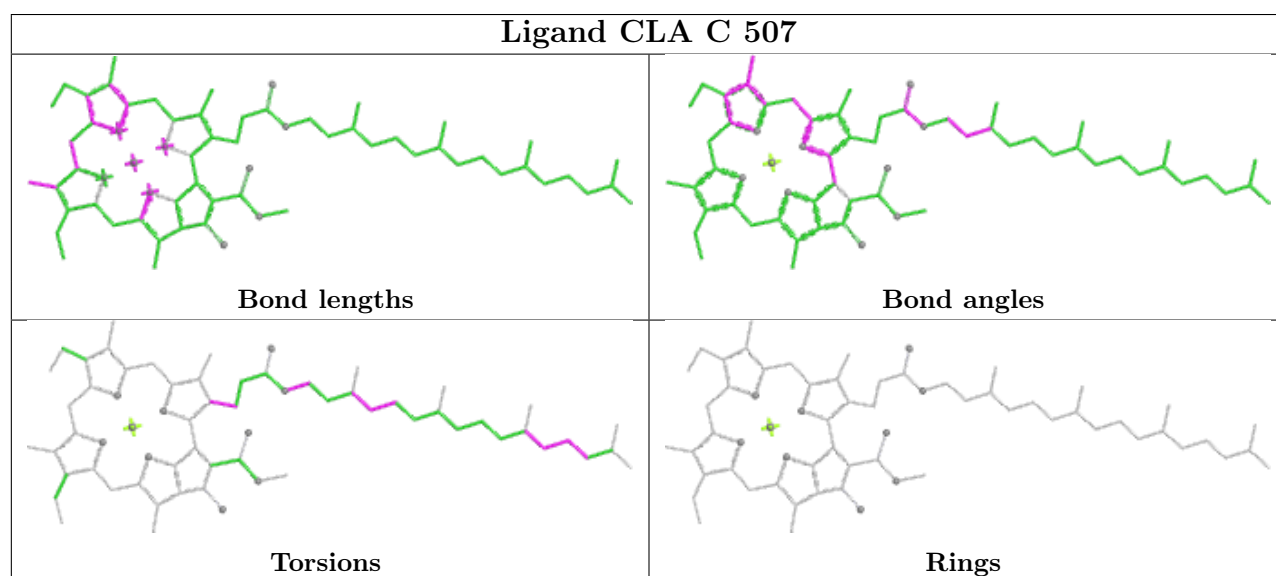
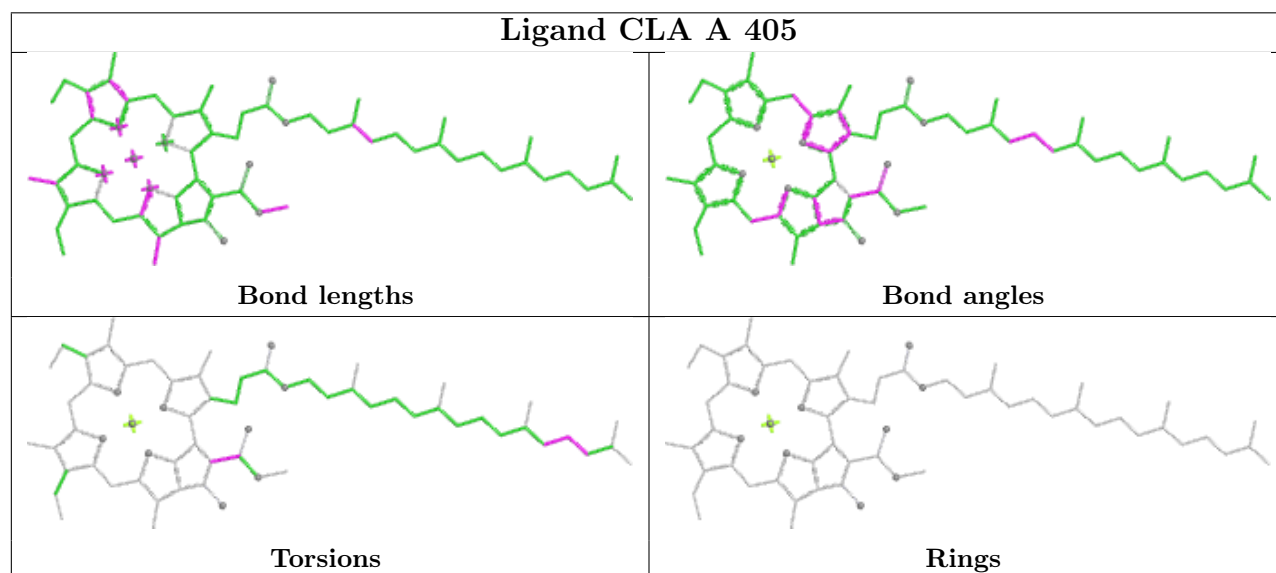
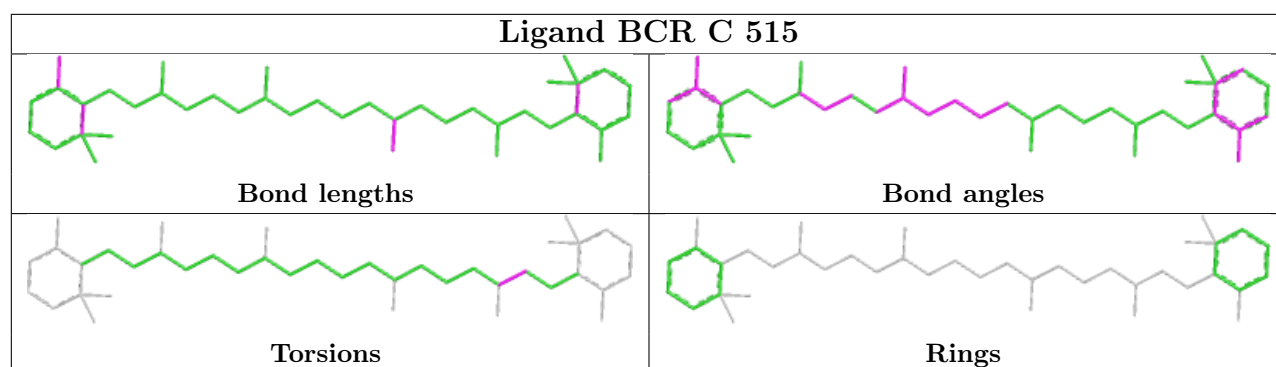


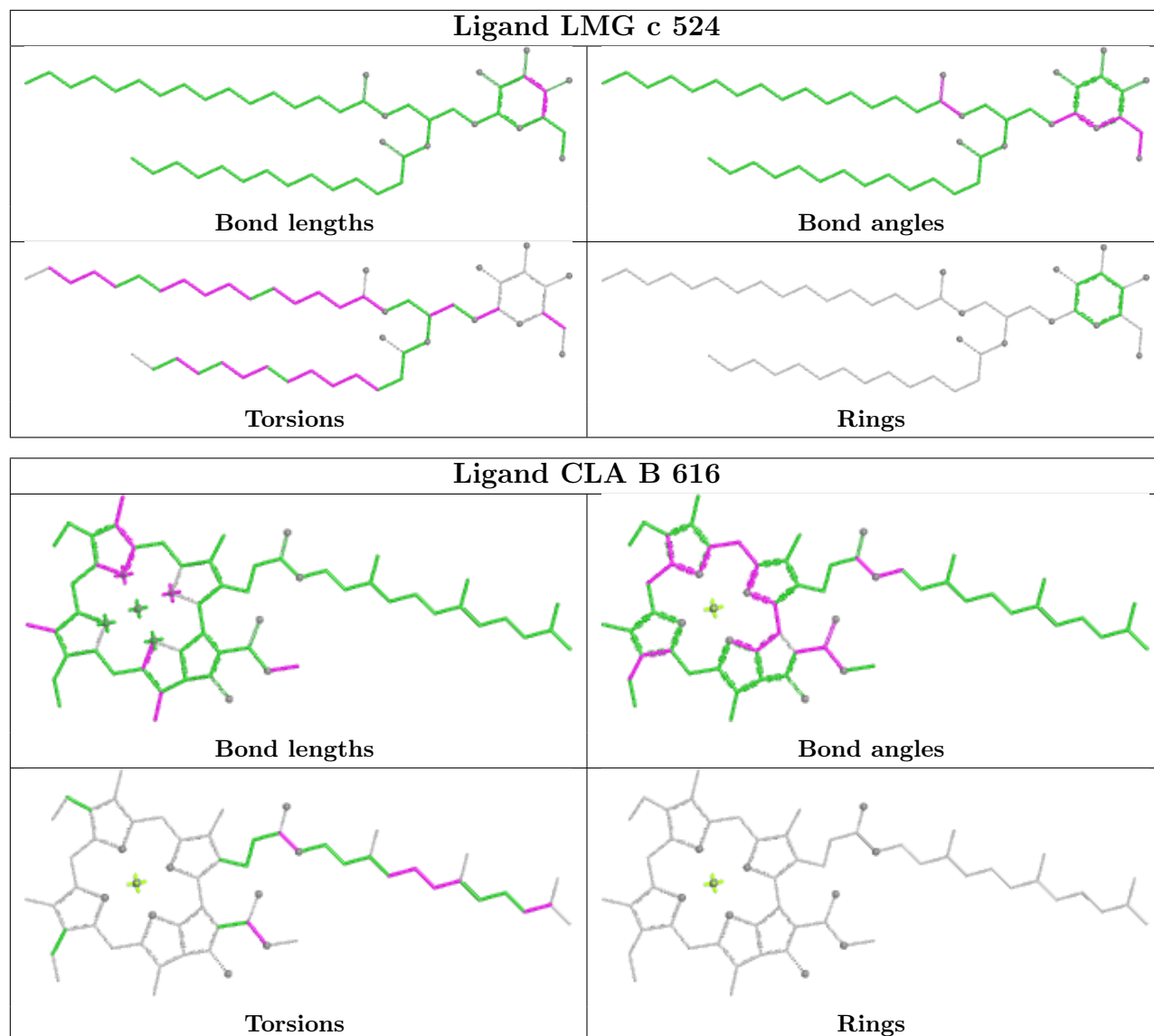
Ligand LMG d 411

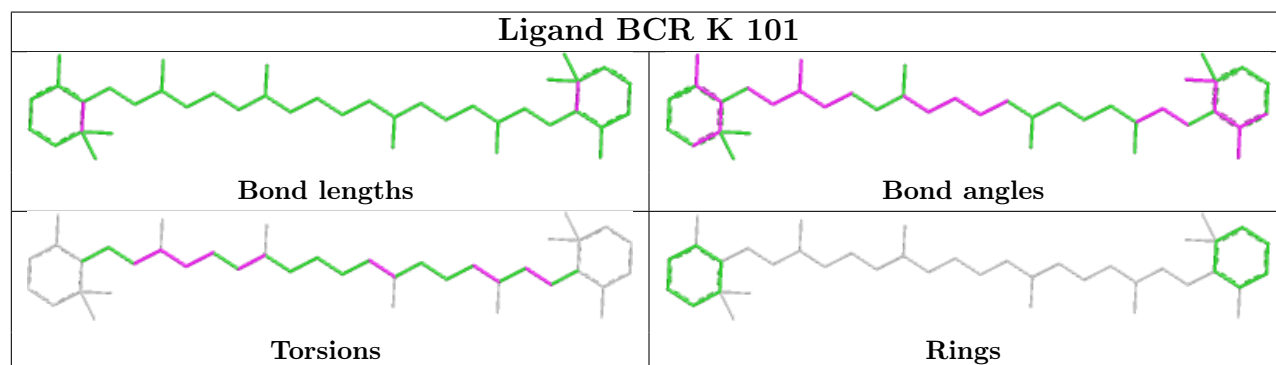
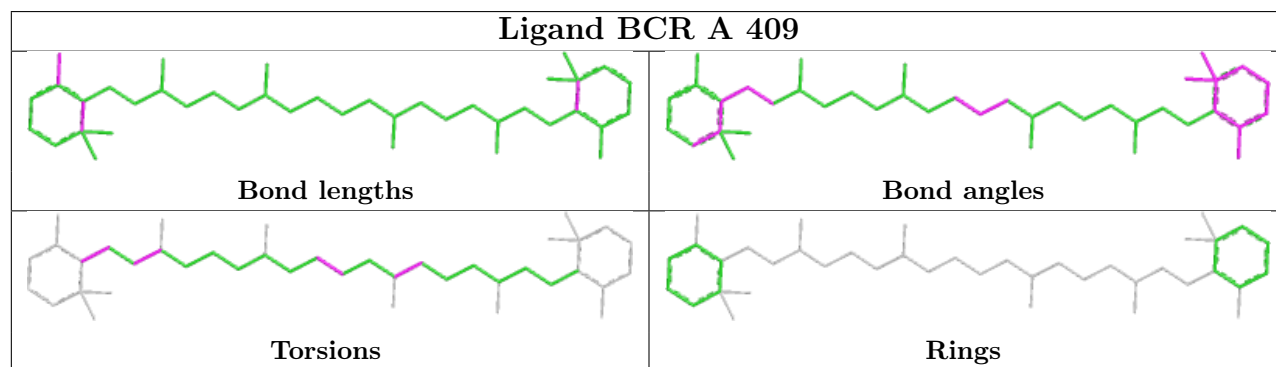
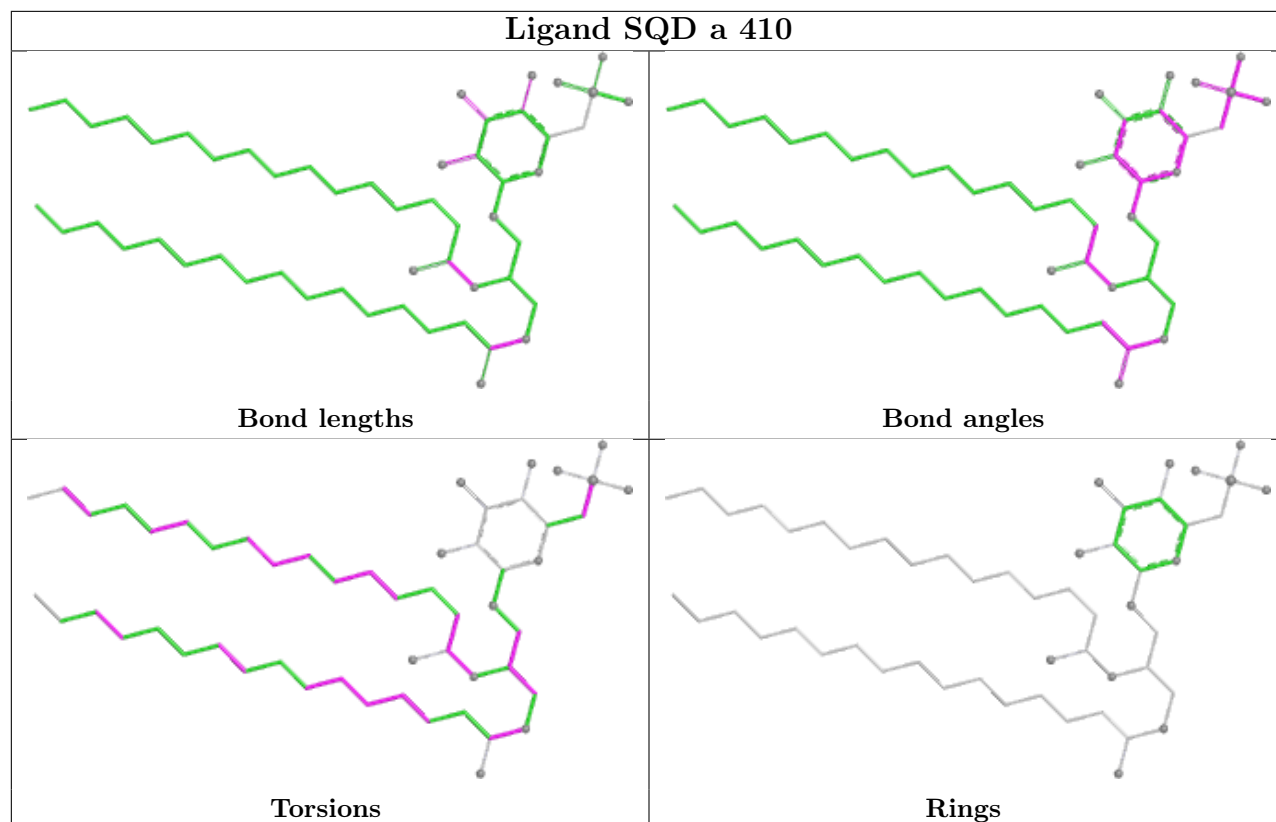


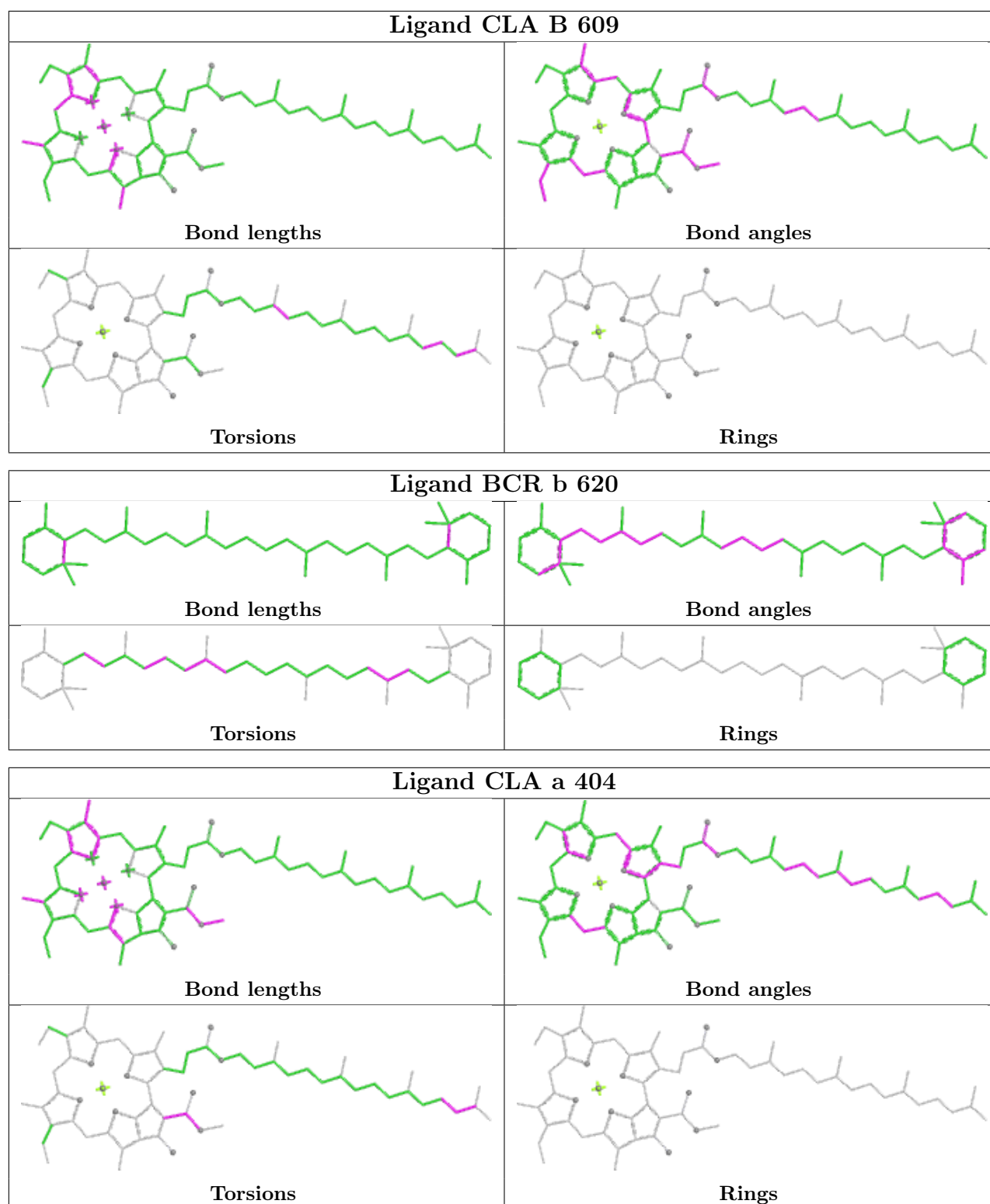


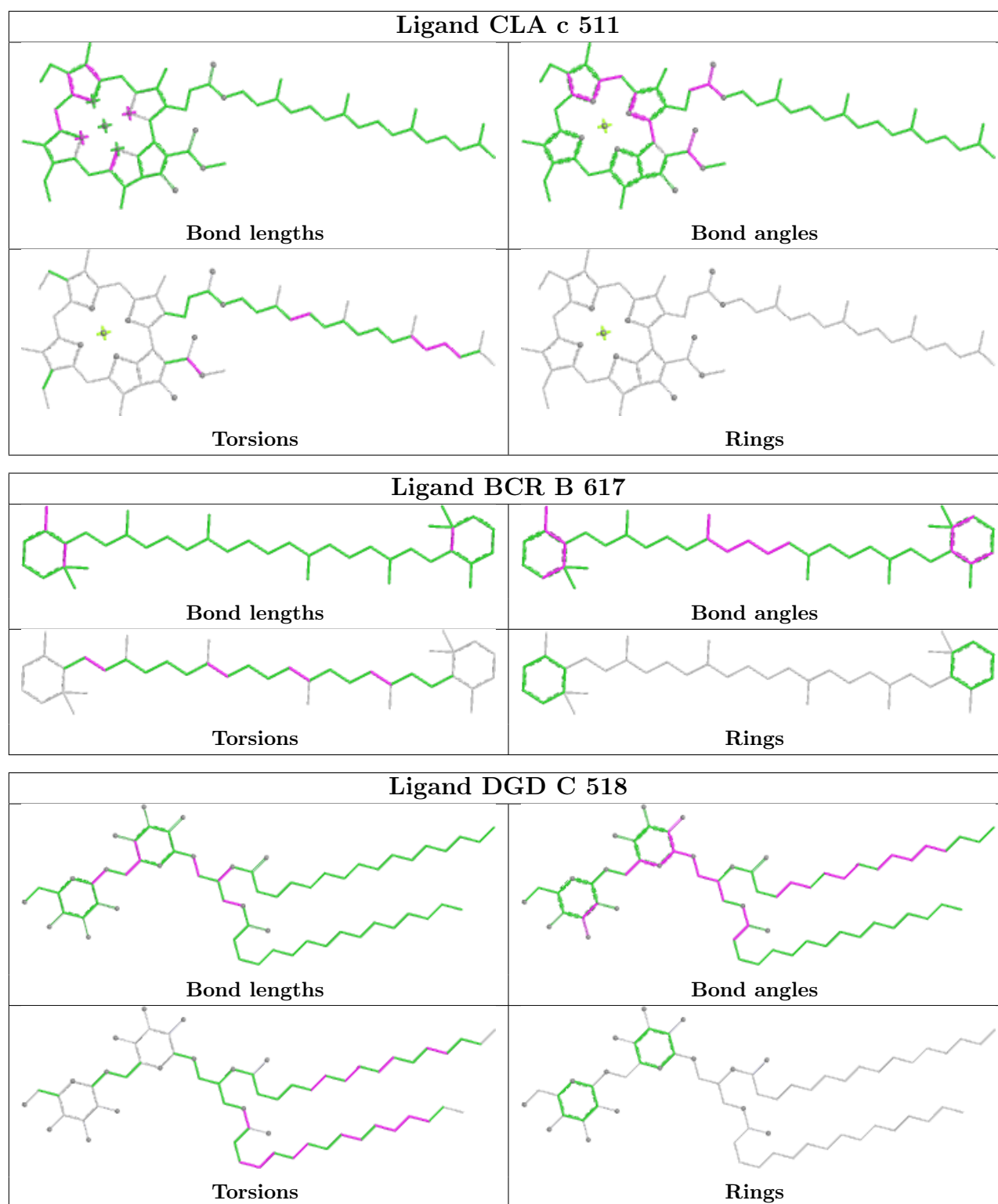




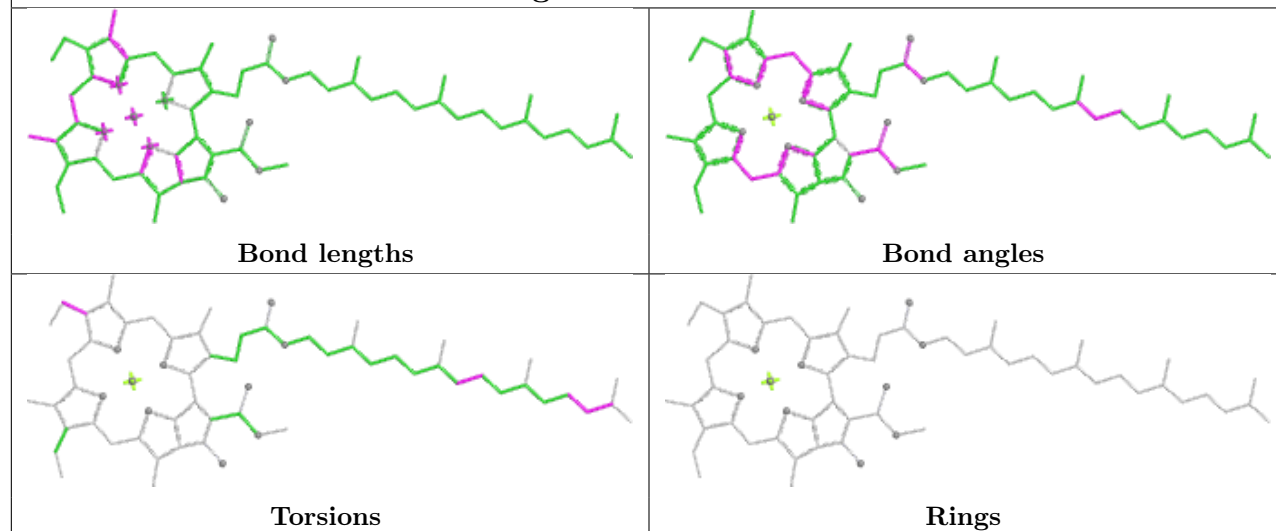




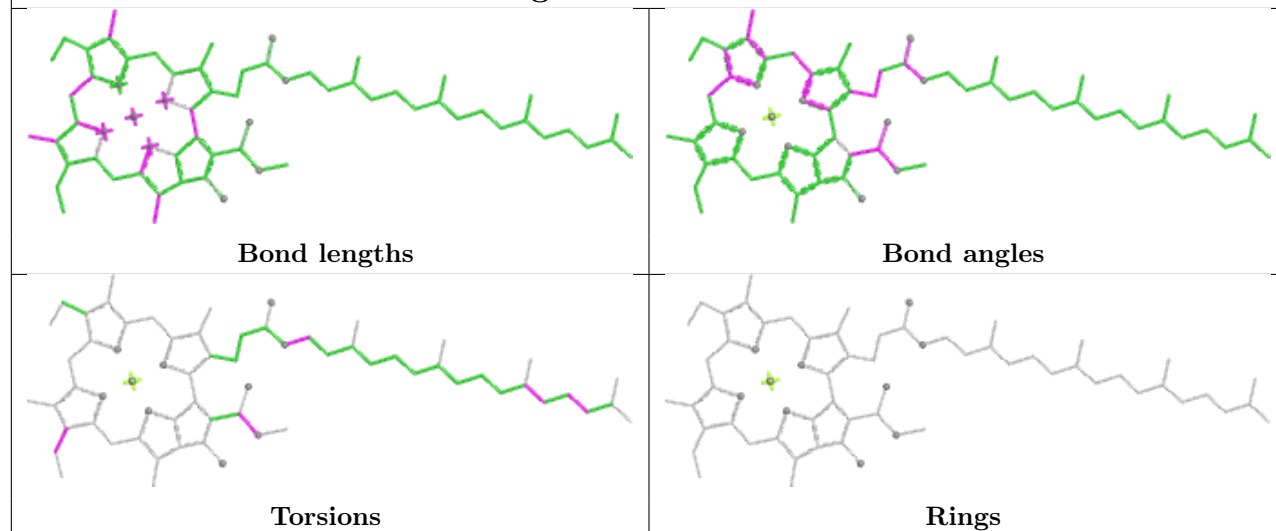




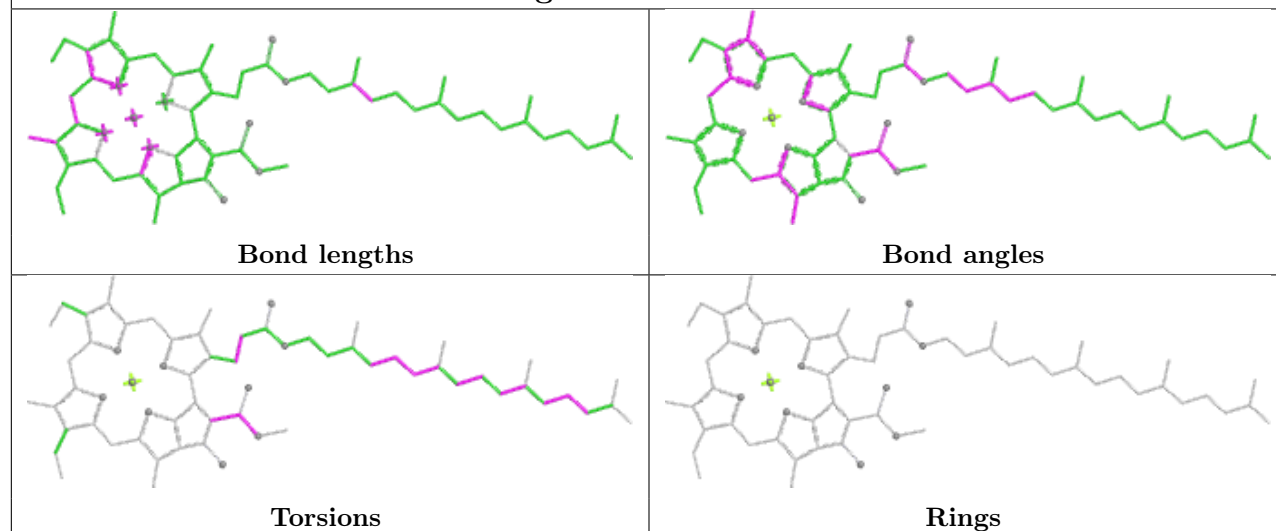
Ligand CLA B 610

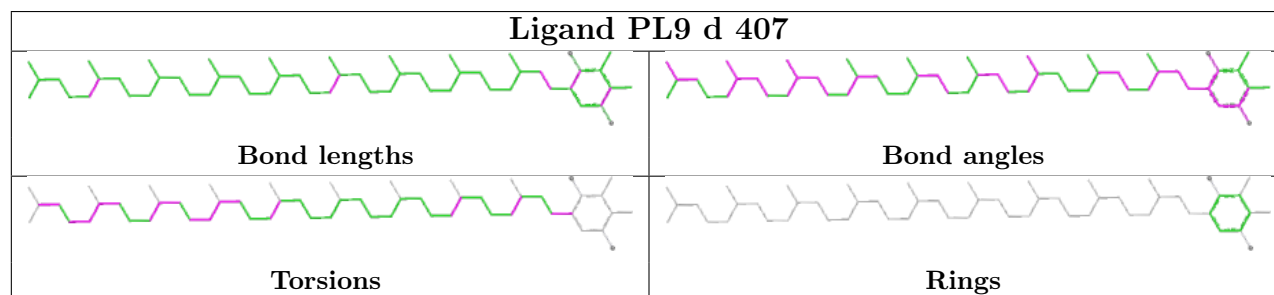
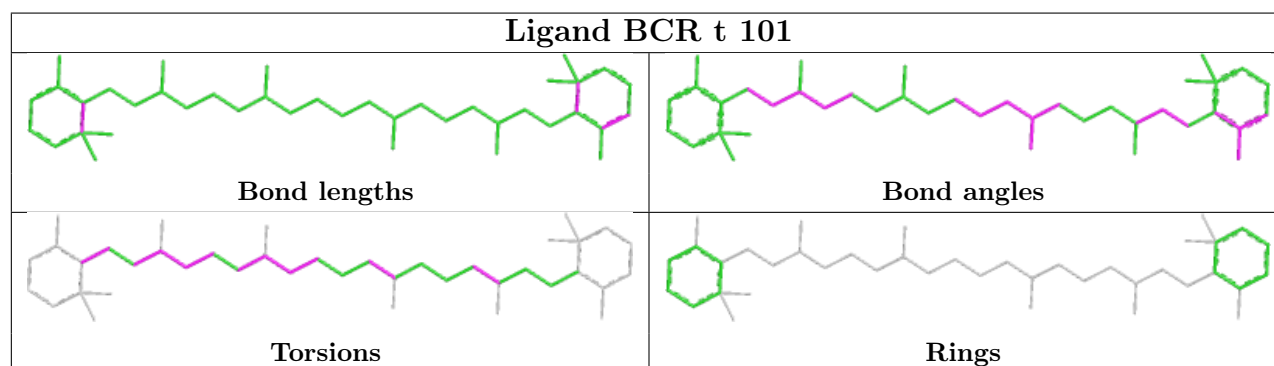
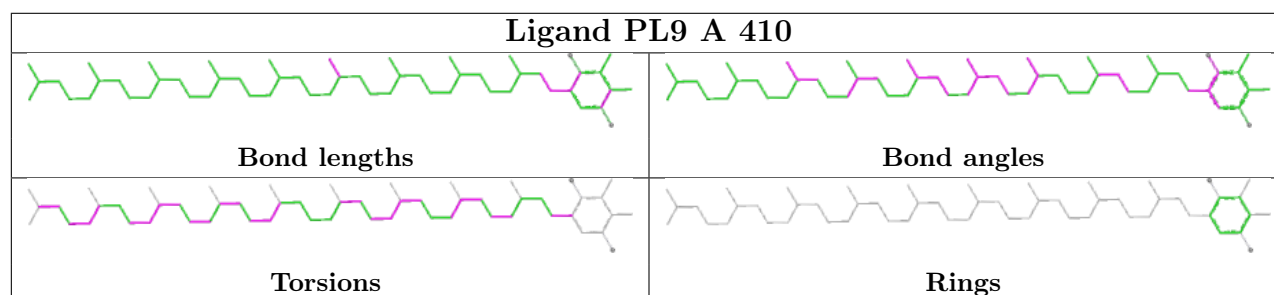
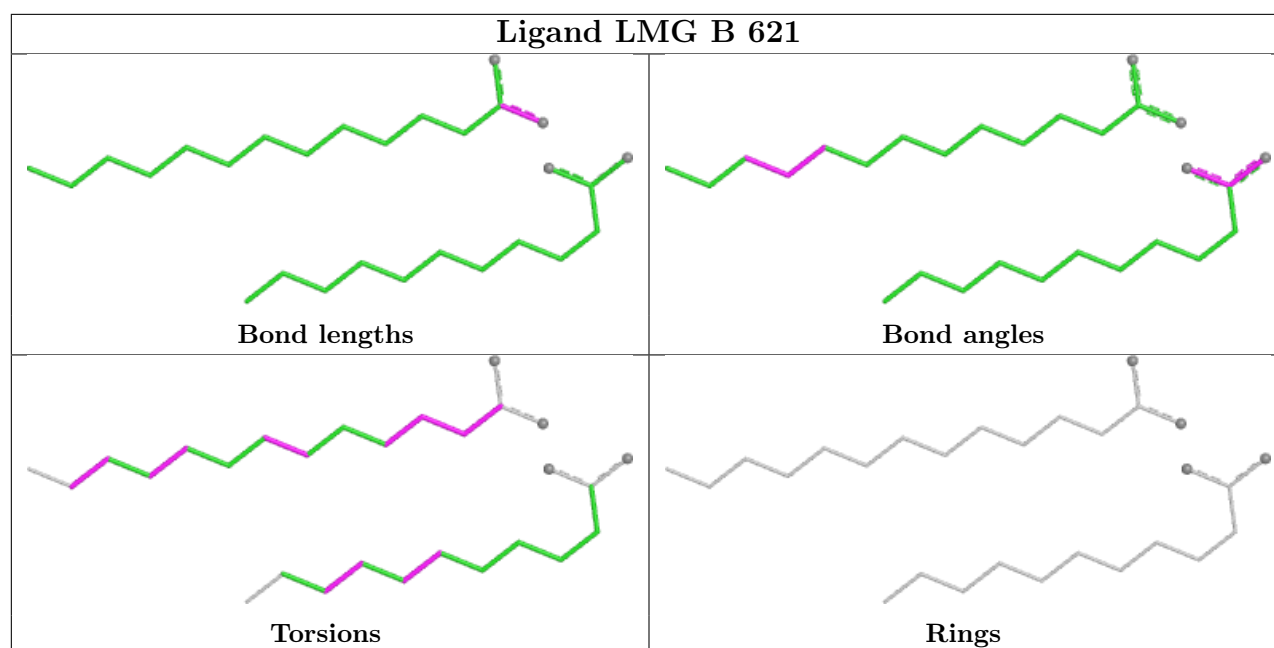


Ligand CLA D 403

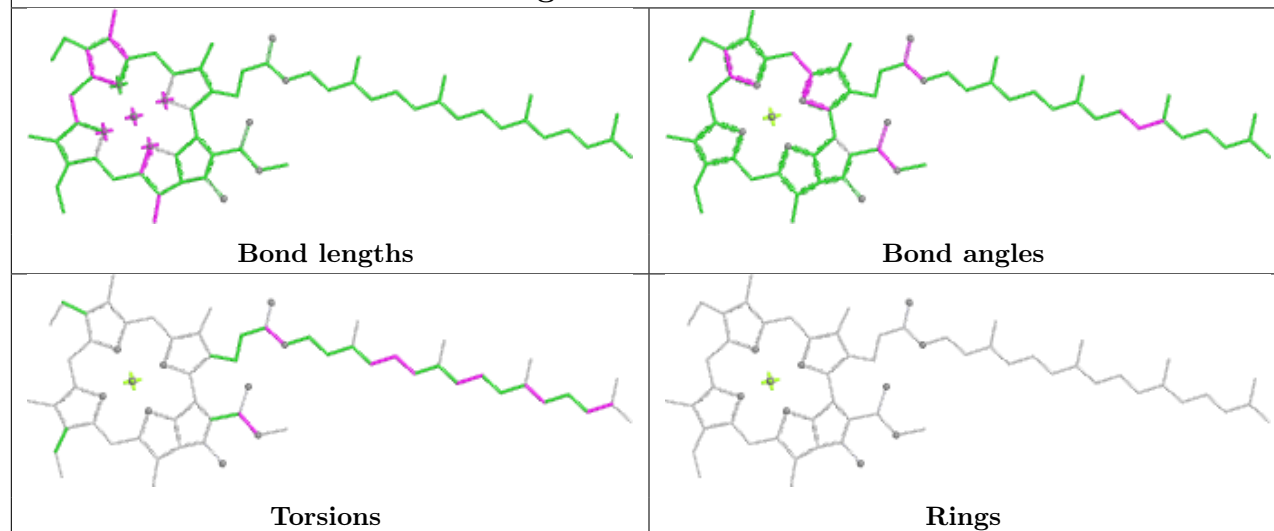


Ligand CLA b 615

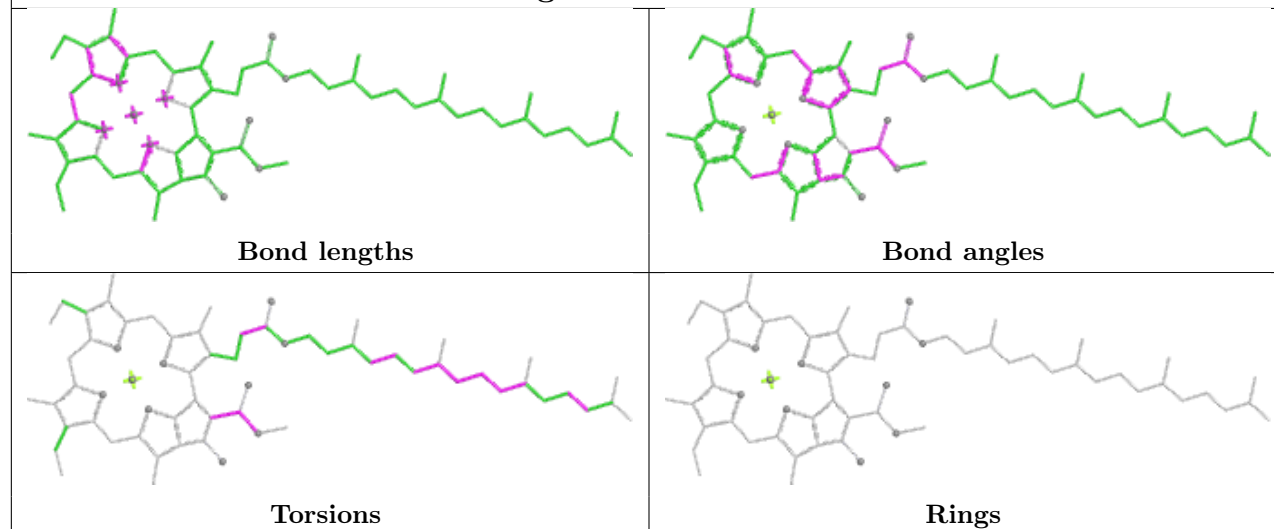




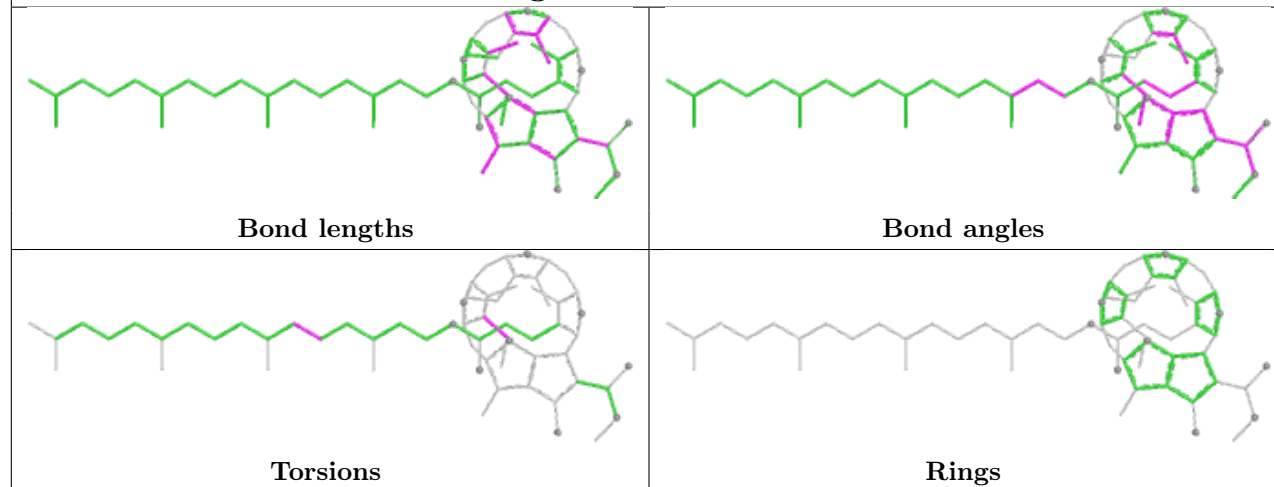
Ligand CLA c 513

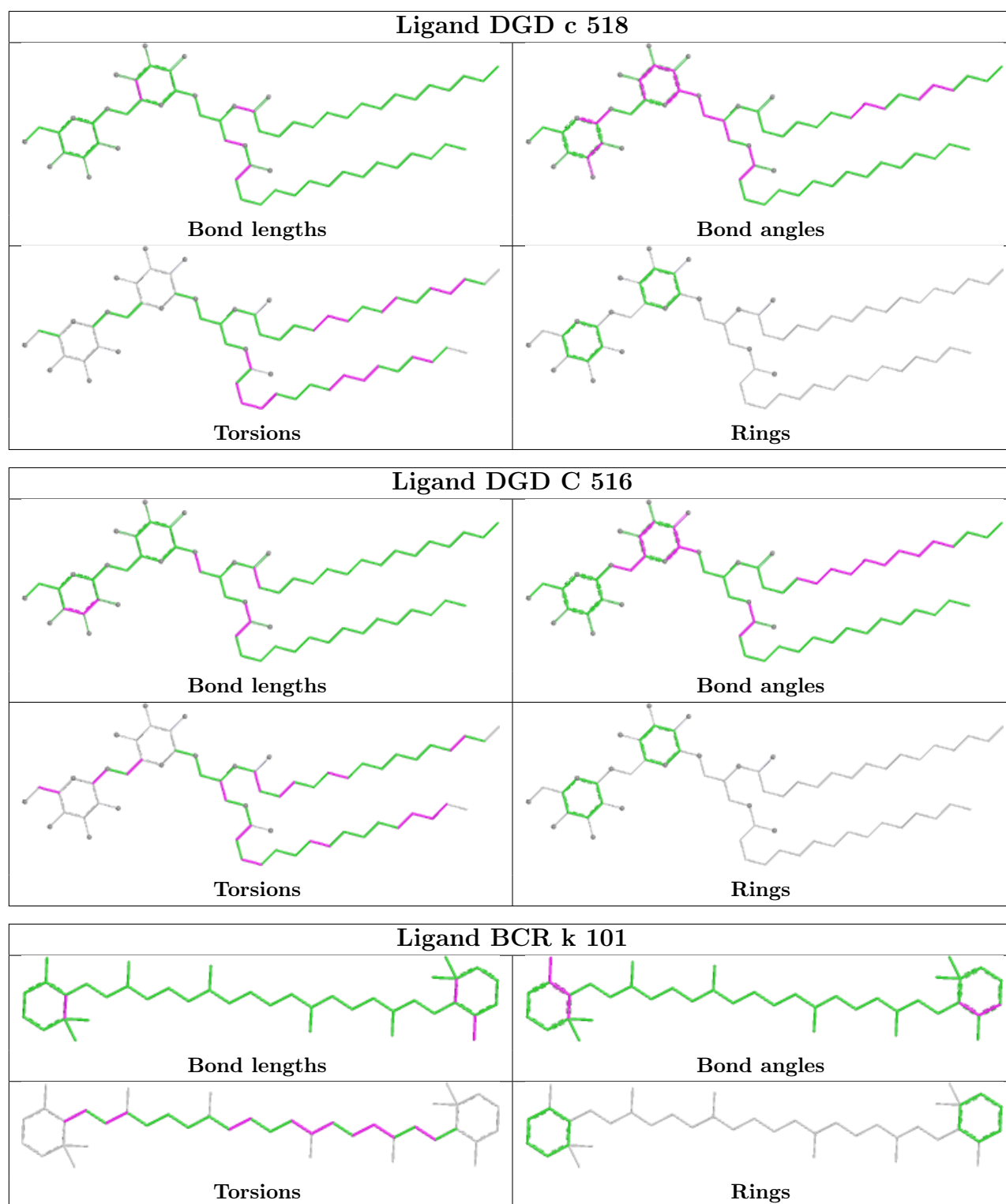


Ligand CLA c 509



Ligand PHO D 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.17

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.65	1 (0%) 90 91	22, 31, 52, 84	0
1	a	334/334 (100%)	-0.54	1 (0%) 90 91	23, 33, 65, 89	0
2	B	505/505 (100%)	-0.51	0 100 100	18, 35, 66, 98	4 (0%)
2	b	505/505 (100%)	-0.38	2 (0%) 88 90	26, 39, 76, 117	0
3	C	442/451 (98%)	-0.45	0 100 100	24, 39, 59, 85	1 (0%)
3	c	451/451 (100%)	-0.38	1 (0%) 91 92	22, 43, 67, 115	2 (0%)
4	D	341/341 (100%)	-0.64	0 100 100	22, 33, 51, 84	0
4	d	341/341 (100%)	-0.48	0 100 100	21, 37, 65, 94	1 (0%)
5	E	81/82 (98%)	0.10	0 100 100	32, 55, 76, 84	1 (1%)
5	e	82/82 (100%)	0.19	0 100 100	42, 66, 87, 98	0
6	F	34/34 (100%)	-0.23	1 (2%) 53 56	38, 47, 71, 88	0
6	f	34/34 (100%)	0.18	0 100 100	44, 54, 82, 101	0
7	H	65/65 (100%)	-0.27	1 (1%) 72 74	36, 45, 65, 81	0
7	h	63/65 (96%)	-0.08	0 100 100	42, 54, 69, 75	0
8	I	35/36 (97%)	-0.41	0 100 100	34, 40, 73, 84	0
8	i	35/36 (97%)	-0.29	0 100 100	33, 44, 75, 83	0
9	J	36/36 (100%)	-0.14	0 100 100	38, 52, 81, 105	0
9	j	36/36 (100%)	0.10	1 (2%) 55 57	44, 56, 90, 92	0
10	K	37/37 (100%)	0.06	1 (2%) 56 58	34, 56, 76, 78	1 (2%)
10	k	37/37 (100%)	0.23	1 (2%) 56 58	49, 63, 81, 90	0
11	L	37/37 (100%)	-0.76	0 100 100	23, 32, 65, 72	0
11	l	36/37 (97%)	-0.58	0 100 100	26, 33, 75, 86	0
12	M	32/33 (96%)	-0.55	0 100 100	28, 36, 65, 82	0
12	m	31/33 (93%)	-0.52	0 100 100	28, 37, 50, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.32	0 100 100	26, 44, 88, 146	1 (0%)
13	o	244/244 (100%)	-0.32	1 (0%) 88 90	24, 44, 84, 138	0
14	T	29/30 (96%)	-0.60	0 100 100	27, 35, 66, 74	0
14	t	29/30 (96%)	-0.42	1 (3%) 48 50	26, 34, 84, 102	0
15	U	97/97 (100%)	-0.31	0 100 100	33, 46, 74, 98	0
15	u	97/97 (100%)	-0.32	1 (1%) 79 82	32, 44, 60, 93	0
16	V	137/137 (100%)	-0.45	0 100 100	26, 44, 59, 88	0
16	v	137/137 (100%)	-0.19	0 100 100	34, 51, 75, 91	0
17	Y	27/30 (90%)	0.95	2 (7%) 20 22	57, 83, 119, 133	0
17	y	30/30 (100%)	0.65	0 100 100	66, 78, 108, 114	0
18	X	38/38 (100%)	-0.04	1 (2%) 57 60	40, 54, 83, 95	0
18	x	38/38 (100%)	0.16	0 100 100	52, 66, 95, 114	0
19	Z	62/62 (100%)	0.55	2 (3%) 50 52	56, 72, 119, 136	0
19	z	62/62 (100%)	0.74	2 (3%) 50 52	59, 79, 121, 134	0
20	R	34/34 (100%)	0.57	1 (2%) 53 56	64, 75, 96, 102	0
20	r	31/34 (91%)	1.17	3 (9%) 13 14	73, 95, 107, 116	0
All	All	5300/5326 (99%)	-0.35	24 (0%) 87 89	18, 41, 80, 146	11 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	t	30	THR	3.7
19	z	33	TRP	3.4
20	r	32	GLN	3.1
2	b	495	PHE	3.0
20	R	35	LEU	2.9
1	A	13	LEU	2.7
17	Y	22	LEU	2.6
19	z	27	TYR	2.5
20	r	26	TYR	2.5
13	o	58	ASN	2.5
3	c	23	ALA	2.5
15	u	53	ALA	2.5
10	K	46[A]	ARG	2.5
1	a	251	ALA	2.4
19	Z	62	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
19	Z	3	ILE	2.3
17	Y	23	THR	2.3
2	b	486	LEU	2.2
18	X	2	THR	2.1
7	H	66	GLY	2.1
9	j	6	GLY	2.1
20	r	30	GLN	2.0
10	k	41	ALA	2.0
6	F	13	TYR	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
8	FME	I	1	10/11	0.95	0.07	33,53,72,72	0
14	FME	T	1	10/11	0.95	0.08	30,49,70,70	0
14	FME	t	1	10/11	0.95	0.07	26,38,64,65	0
8	FME	i	1	10/11	0.96	0.07	38,52,64,68	0
12	FME	m	1	10/11	0.96	0.08	29,50,66,80	0
12	FME	M	1	10/11	0.96	0.08	33,47,76,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	UNL	b	626	26/-	0.78	0.15	39,52,61,63	0
31	UNL	H	103	53/-	0.80	0.14	51,73,94,97	0
31	UNL	c	523	28/-	0.80	0.12	49,72,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LMG	c	522	48/55	0.82	0.14	42,80,114,117	0
33	LHG	E	101	49/49	0.82	0.13	48,83,108,119	0
33	LHG	e	101	42/49	0.82	0.13	58,87,114,129	0
32	LMG	b	623	55/55	0.83	0.14	44,76,98,109	0
31	UNL	B	625	28/-	0.84	0.16	52,73,90,103	0
32	LMG	h	102	23/55	0.84	0.17	41,77,102,105	0
31	UNL	B	626	47/-	0.84	0.15	48,66,91,94	0
29	DGD	a	412	44/66	0.84	0.12	32,57,76,84	0
31	UNL	a	413	28/-	0.85	0.11	31,63,70,81	0
31	UNL	b	624	40/-	0.85	0.13	52,69,88,88	0
31	UNL	b	625	55/-	0.85	0.12	40,60,80,81	0
31	UNL	T	101	47/-	0.85	0.13	38,49,65,71	0
31	UNL	T	102	44/-	0.85	0.14	41,57,76,77	0
29	DGD	A	413	66/66	0.86	0.11	36,68,84,102	0
27	PL9	A	410	55/55	0.86	0.13	31,58,79,91	0
27	PL9	a	409	55/55	0.86	0.13	36,66,86,99	0
31	UNL	c	520	55/-	0.86	0.11	34,61,83,90	0
28	SQD	a	411	36/54	0.86	0.12	38,65,87,97	0
31	UNL	t	103	26/-	0.87	0.12	38,64,77,81	0
32	LMG	K	102	48/55	0.87	0.11	48,71,92,101	0
24	CLA	h	101	65/65	0.87	0.11	45,67,92,104	0
32	LMG	c	519	37/55	0.87	0.11	41,70,83,88	0
31	UNL	I	101	41/-	0.87	0.13	40,51,76,78	0
31	UNL	b	622	55/-	0.87	0.12	39,60,84,89	0
31	UNL	C	522	47/-	0.87	0.12	44,56,66,67	0
31	UNL	d	412	43/-	0.87	0.13	43,58,70,77	0
31	UNL	x	101	55/-	0.88	0.11	39,58,75,78	0
32	LMG	D	410	33/55	0.88	0.11	35,54,89,98	0
28	SQD	b	601	49/54	0.88	0.10	39,58,97,111	0
28	SQD	f	101	41/54	0.89	0.13	55,90,116,124	0
31	UNL	B	620	43/-	0.89	0.09	35,49,60,70	0
31	UNL	X	101	55/-	0.89	0.11	33,54,76,78	0
31	UNL	E	102	28/-	0.89	0.11	53,74,84,86	0
32	LMG	c	524	49/55	0.89	0.10	37,54,88,107	0
31	UNL	B	623	28/-	0.89	0.10	35,51,67,77	0
28	SQD	A	412	39/54	0.89	0.12	41,68,96,103	0
31	UNL	J	101	28/-	0.89	0.11	50,63,71,81	0
31	UNL	m	101	28/-	0.90	0.12	38,53,74,82	0
26	BCR	h	103	40/40	0.90	0.10	31,54,78,88	0
31	UNL	C	521	28/-	0.90	0.10	44,54,60,67	0
32	LMG	B	621	28/55	0.90	0.11	33,50,62,66	0
32	LMG	C	501	48/55	0.90	0.09	34,57,72,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	SQD	B	622	54/54	0.90	0.09	33,60,88,102	0
31	UNL	j	101	28/-	0.90	0.10	44,56,67,68	0
26	BCR	k	101	40/40	0.91	0.10	41,64,77,79	0
31	UNL	B	624	46/-	0.91	0.09	39,54,66,72	0
24	CLA	B	601	65/65	0.91	0.10	32,65,102,107	0
31	UNL	M	103	26/-	0.91	0.11	39,51,59,64	0
31	UNL	M	104	53/-	0.91	0.12	36,48,88,90	0
26	BCR	K	101	40/40	0.91	0.10	33,56,69,76	0
31	UNL	C	520	28/-	0.91	0.09	33,46,50,62	0
26	BCR	c	514	40/40	0.91	0.09	35,60,72,74	0
31	UNL	t	102	34/-	0.91	0.09	38,51,64,77	0
24	CLA	C	514	65/65	0.91	0.10	45,65,91,105	0
28	SQD	a	410	54/54	0.91	0.10	41,68,93,95	0
32	LMG	M	101	51/55	0.92	0.08	25,47,71,81	0
32	LMG	b	621	51/55	0.92	0.09	32,51,76,91	0
26	BCR	d	406	40/40	0.92	0.09	32,56,100,106	0
26	BCR	D	405	40/40	0.92	0.09	29,46,90,104	0
24	CLA	c	513	65/65	0.92	0.10	40,74,109,115	0
26	BCR	Y	101	40/40	0.92	0.08	37,54,73,75	0
24	CLA	c	512	65/65	0.92	0.10	42,60,99,125	0
26	BCR	c	521	40/40	0.92	0.10	40,56,70,75	0
29	DGD	C	517	62/66	0.92	0.09	32,56,96,109	0
24	CLA	c	511	65/65	0.93	0.10	43,56,76,80	0
31	UNL	M	102	37/-	0.93	0.08	33,47,65,67	0
24	CLA	C	513	65/65	0.93	0.09	33,56,93,103	0
28	SQD	A	411	52/54	0.93	0.09	33,59,89,94	0
26	BCR	C	519	40/40	0.93	0.10	29,56,68,74	0
26	BCR	b	619	40/40	0.93	0.07	27,41,54,56	0
29	DGD	H	102	62/66	0.93	0.08	27,48,63,78	0
28	SQD	F	101	36/54	0.93	0.10	41,74,93,99	0
29	DGD	c	517	62/66	0.93	0.08	31,55,92,107	0
29	DGD	h	104	62/66	0.93	0.08	30,51,68,76	0
26	BCR	b	620	40/40	0.93	0.07	29,50,62,66	0
26	BCR	B	619	40/40	0.94	0.07	21,40,62,72	0
26	BCR	t	101	40/40	0.94	0.07	25,40,56,60	0
26	BCR	C	515	40/40	0.94	0.08	28,39,49,64	0
29	DGD	c	518	62/66	0.94	0.08	26,53,78,88	0
26	BCR	c	515	40/40	0.94	0.09	25,45,64,78	0
26	BCR	b	602	40/40	0.94	0.07	23,41,66,72	0
32	LMG	d	411	44/55	0.94	0.09	31,55,91,97	0
32	LMG	D	407	51/55	0.94	0.10	24,58,93,98	0
26	BCR	b	618	40/40	0.94	0.07	25,43,56,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LHG	d	408	49/49	0.94	0.09	31,51,85,94	0
26	BCR	H	101	40/40	0.94	0.07	30,47,67,71	0
24	CLA	B	606	65/65	0.95	0.07	24,38,76,83	0
29	DGD	C	516	62/66	0.95	0.08	21,40,79,95	0
24	CLA	b	613	65/65	0.95	0.07	20,35,45,61	0
29	DGD	C	518	62/66	0.95	0.07	26,48,79,89	0
24	CLA	b	616	65/65	0.95	0.07	26,41,60,72	0
26	BCR	a	408	40/40	0.95	0.06	17,32,48,53	0
24	CLA	b	617	60/65	0.95	0.08	24,44,89,98	0
24	CLA	c	503	65/65	0.95	0.07	24,44,55,60	0
24	CLA	c	504	60/65	0.95	0.08	26,46,87,91	0
24	CLA	c	505	65/65	0.95	0.07	24,42,66,70	0
24	CLA	c	506	65/65	0.95	0.09	25,53,110,118	0
24	CLA	c	508	64/65	0.95	0.08	29,48,80,108	0
24	CLA	c	509	65/65	0.95	0.08	29,48,64,68	0
24	CLA	c	510	65/65	0.95	0.07	32,49,73,84	0
24	CLA	B	609	65/65	0.95	0.07	22,40,57,64	0
24	CLA	C	503	65/65	0.95	0.07	27,42,60,69	0
24	CLA	C	504	65/65	0.95	0.07	22,42,54,57	0
24	CLA	d	405	65/65	0.95	0.08	25,49,107,114	0
24	CLA	C	507	65/65	0.95	0.08	25,42,99,113	0
27	PL9	d	407	55/55	0.95	0.06	19,35,43,50	0
25	PHO	d	402	64/64	0.95	0.07	25,39,53,62	0
26	BCR	A	409	40/40	0.95	0.06	21,34,44,48	0
26	BCR	B	617	40/40	0.95	0.07	24,42,54,55	0
26	BCR	B	618	40/40	0.95	0.06	22,39,51,56	0
24	CLA	C	509	65/65	0.95	0.08	24,42,96,114	0
33	LHG	D	409	47/49	0.95	0.09	20,45,83,99	0
33	LHG	D	411	49/49	0.95	0.08	26,44,69,81	0
24	CLA	C	511	65/65	0.95	0.07	28,47,67,72	0
24	CLA	C	512	65/65	0.95	0.08	34,53,69,75	0
33	LHG	d	410	39/49	0.95	0.08	32,48,71,76	0
23	BCT	d	401	4/4	0.95	0.08	29,29,38,46	0
33	LHG	l	101	49/49	0.95	0.07	28,46,61,67	0
24	CLA	C	505	59/65	0.96	0.07	26,46,75,87	0
24	CLA	c	501	65/65	0.96	0.06	28,39,53,55	0
24	CLA	c	502	65/65	0.96	0.07	27,42,63,71	0
24	CLA	C	506	65/65	0.96	0.08	23,39,65,76	0
24	CLA	A	405	65/65	0.96	0.06	15,28,41,49	0
29	DGD	c	516	62/66	0.96	0.08	22,41,77,90	0
24	CLA	C	508	65/65	0.96	0.06	23,40,61,67	0
24	CLA	B	602	65/65	0.96	0.06	22,36,63,74	0

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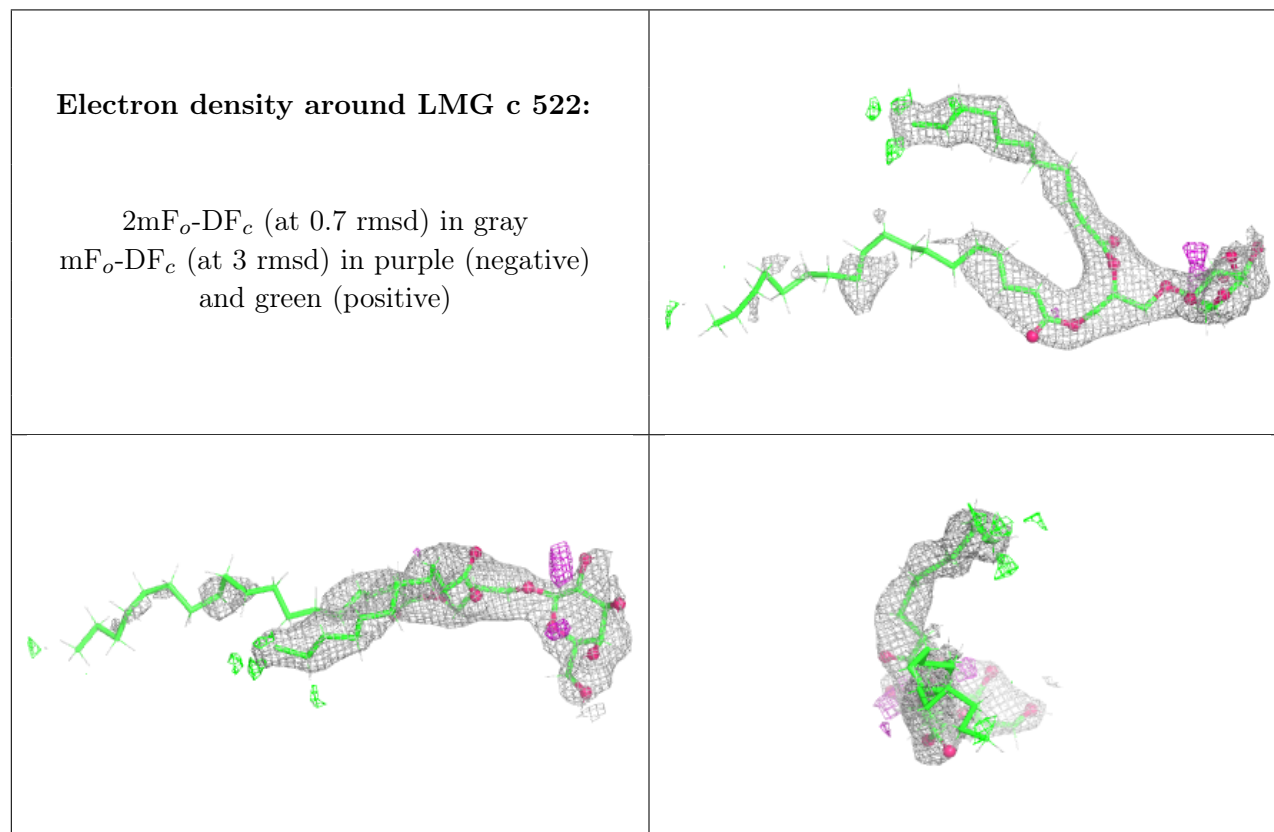
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	507	65/65	0.96	0.07	28,45,64,65	0
24	CLA	C	510	65/65	0.96	0.07	22,46,61,72	0
24	CLA	B	612	65/65	0.96	0.06	17,32,49,59	0
24	CLA	B	614	65/65	0.96	0.08	16,37,88,97	0
24	CLA	B	615	65/65	0.96	0.07	20,38,64,87	0
24	CLA	B	616	60/65	0.96	0.08	23,42,93,98	0
24	CLA	a	404	65/65	0.96	0.06	16,29,44,59	0
24	CLA	d	403	65/65	0.96	0.06	16,30,44,47	0
24	CLA	d	404	65/65	0.96	0.07	19,33,63,70	0
24	CLA	a	405	65/65	0.96	0.08	22,40,97,115	0
27	PL9	D	406	55/55	0.96	0.06	18,34,46,50	0
24	CLA	a	407	65/65	0.96	0.08	17,36,89,116	0
25	PHO	A	407	64/64	0.96	0.05	16,28,39,44	0
25	PHO	D	401	64/64	0.96	0.05	21,33,48,50	0
25	PHO	a	406	64/64	0.96	0.06	22,32,41,45	0
33	LHG	D	408	49/49	0.96	0.07	19,42,59,63	0
24	CLA	b	603	65/65	0.96	0.08	24,44,69,80	0
24	CLA	b	607	65/65	0.96	0.07	22,41,77,84	0
24	CLA	b	609	65/65	0.96	0.07	25,42,58,69	0
24	CLA	b	610	65/65	0.96	0.08	26,46,64,79	0
33	LHG	d	409	49/49	0.96	0.07	22,39,62,67	0
24	CLA	B	604	65/65	0.96	0.07	18,33,77,84	0
24	CLA	b	615	65/65	0.96	0.07	24,42,81,97	0
24	CLA	B	605	65/65	0.96	0.06	15,30,44,61	0
24	CLA	A	406	65/65	0.97	0.08	21,37,99,112	0
24	CLA	b	611	65/65	0.97	0.07	19,38,53,61	0
24	CLA	b	612	65/65	0.97	0.05	19,32,48,58	0
24	CLA	B	613	65/65	0.97	0.06	17,30,65,73	0
24	CLA	b	614	65/65	0.97	0.06	15,33,74,88	0
24	CLA	D	402	65/65	0.97	0.05	17,28,50,57	0
24	CLA	D	403	65/65	0.97	0.06	16,29,61,74	0
24	CLA	D	404	65/65	0.97	0.07	21,42,123,126	0
24	CLA	B	607	65/65	0.97	0.06	15,34,62,70	0
24	CLA	B	608	65/65	0.97	0.05	17,34,59,63	0
24	CLA	B	603	65/65	0.97	0.06	17,34,66,68	0
24	CLA	C	502	65/65	0.97	0.06	22,36,50,60	0
24	CLA	b	604	65/65	0.97	0.06	21,35,67,77	0
33	LHG	L	101	49/49	0.97	0.06	25,41,56,66	0
24	CLA	b	605	65/65	0.97	0.06	18,33,82,98	0
24	CLA	b	606	65/65	0.97	0.06	20,35,50,52	0
24	CLA	B	610	65/65	0.97	0.06	18,32,43,48	0
24	CLA	b	608	65/65	0.97	0.07	16,36,69,79	0

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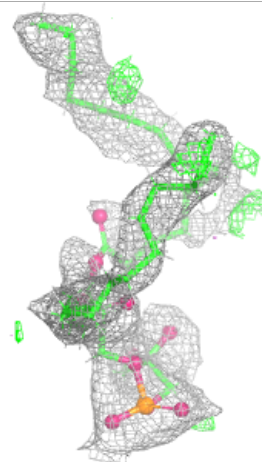
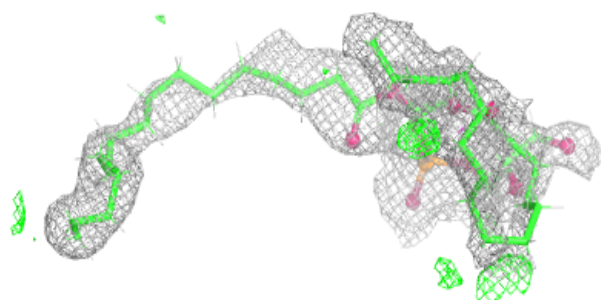
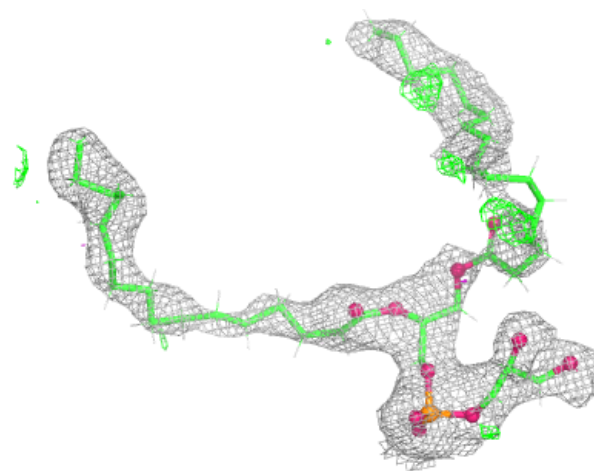
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	611	65/65	0.97	0.05	18,32,46,54	0
34	HEM	F	102	43/43	0.97	0.08	35,49,65,69	0
34	HEM	e	102	43/43	0.97	0.08	43,55,79,79	0
23	BCT	A	404	4/4	0.98	0.04	28,28,30,36	0
22	CL	a	402	1/1	0.98	0.04	28,28,28,28	0
24	CLA	A	408	54/65	0.98	0.06	16,32,62,73	0
35	HEC	v	201	43/43	0.98	0.06	27,36,47,54	0
21	FE2	A	401	1/1	0.99	0.01	28,28,28,28	0
22	CL	a	403	1/1	0.99	0.08	25,25,25,25	0
30	OEX	A	414	10/10	0.99	0.03	19,29,33,33	0
22	CL	A	402	1/1	0.99	0.02	25,25,25,25	0
35	HEC	V	201	43/43	0.99	0.05	22,33,42,48	0
22	CL	A	403	1/1	0.99	0.02	29,29,29,29	0
21	FE2	a	401	1/1	1.00	0.02	33,33,33,33	0
30	OEX	a	414	10/10	1.00	0.02	23,29,33,34	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.



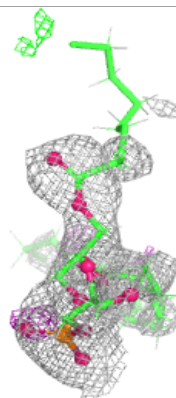
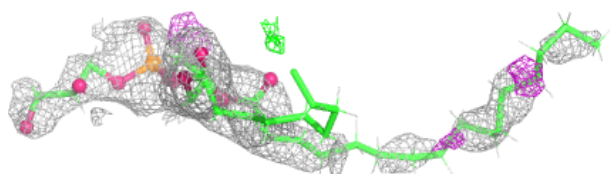
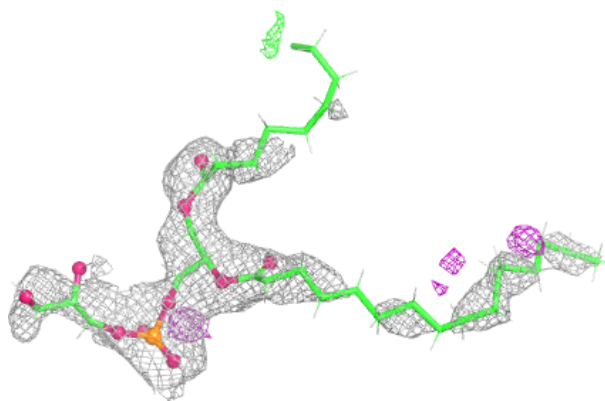
Electron density around LHG E 101:

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

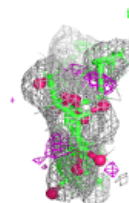
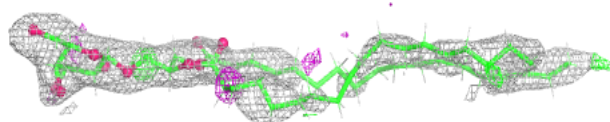
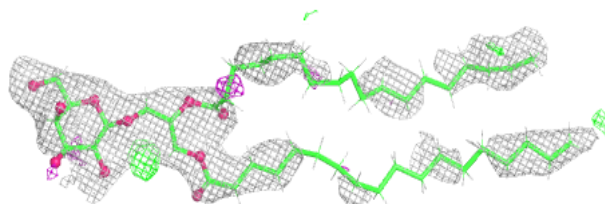


Electron density around LHG e 101:

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

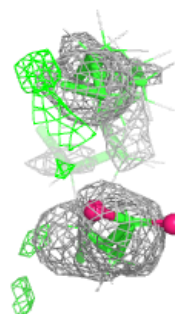
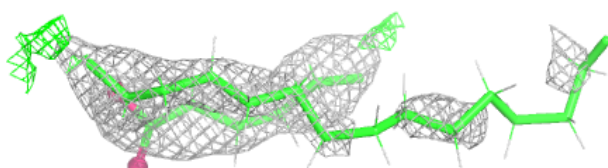
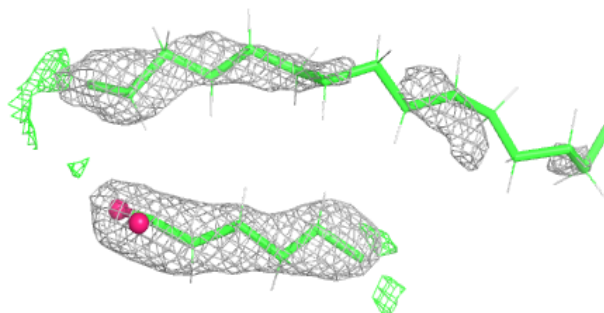
**Electron density around LMG b 623:**

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

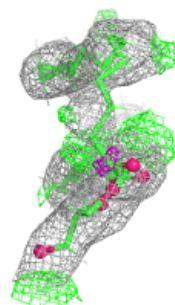
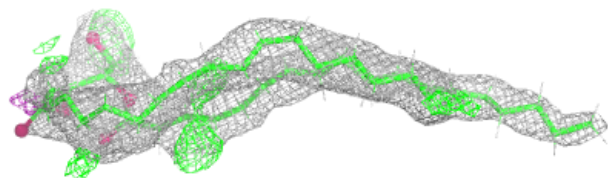
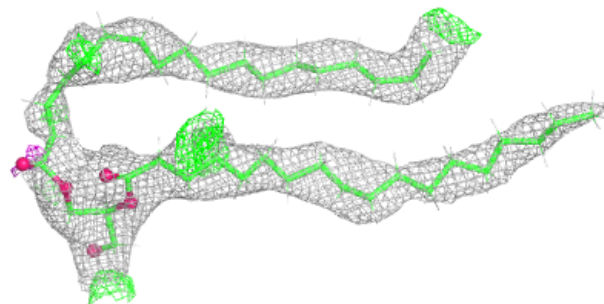


Electron density around LMG h 102:

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

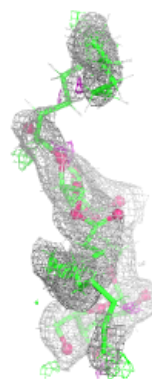
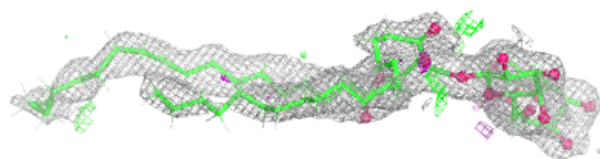
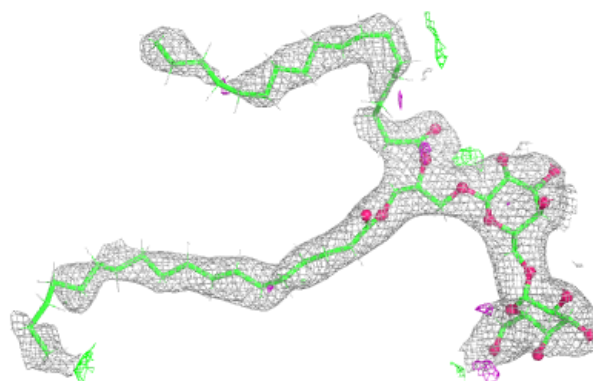
**Electron density around DGD a 412:**

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

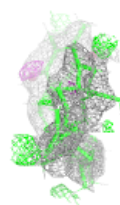
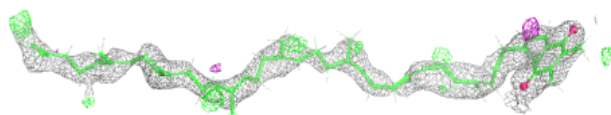
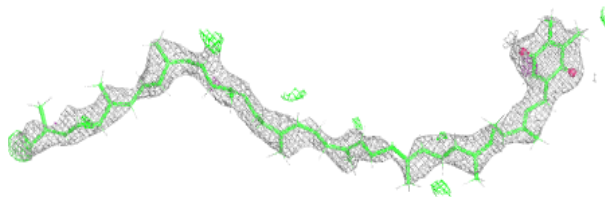


Electron density around DGD A 413:

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

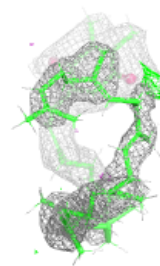
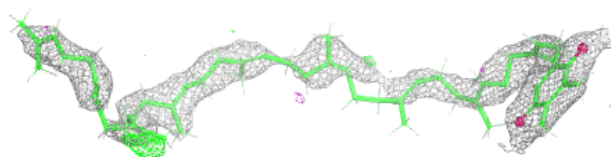
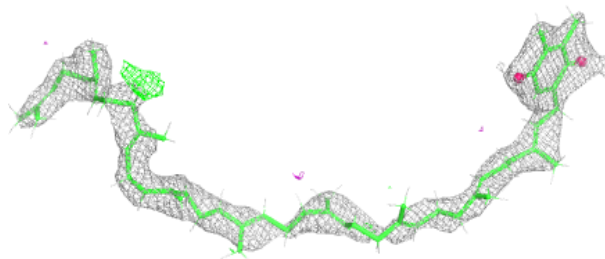
**Electron density around PL9 A 410:**

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



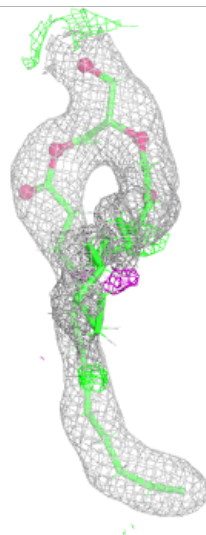
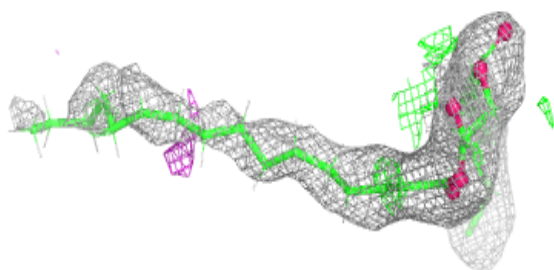
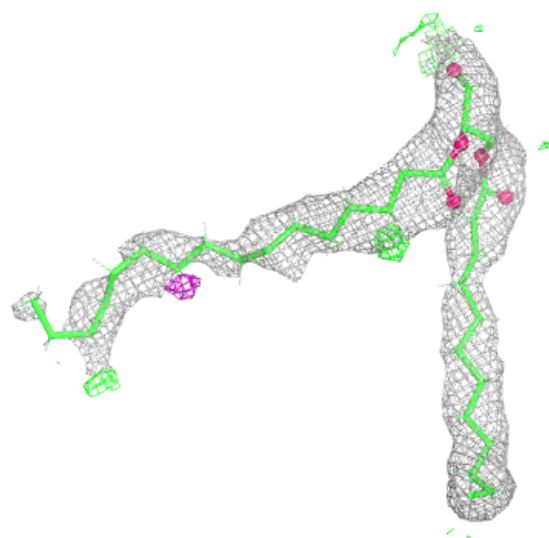
Electron density around PL9 a 409:

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



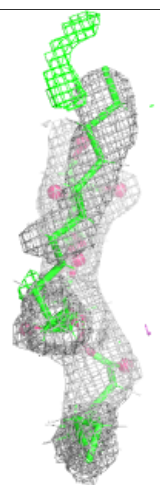
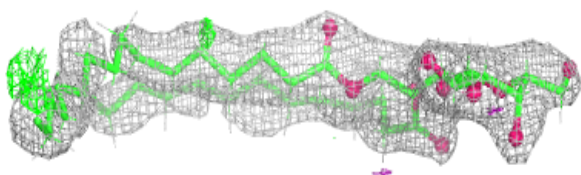
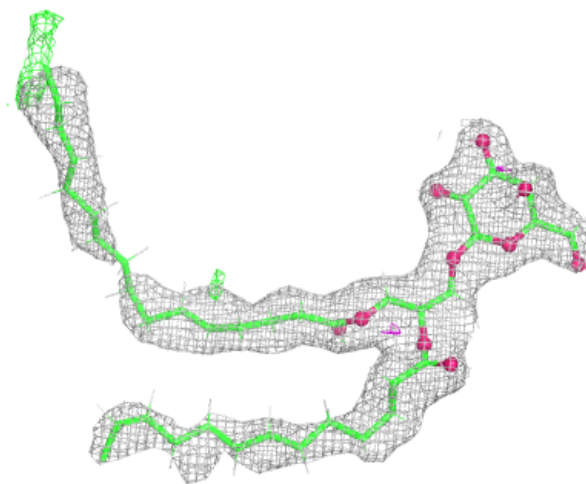
Electron density around SQD a 411:

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



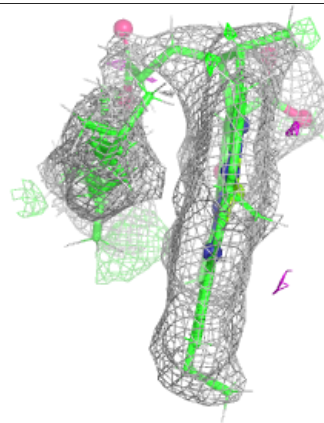
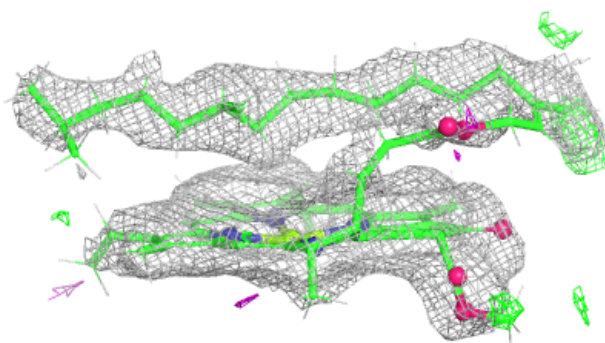
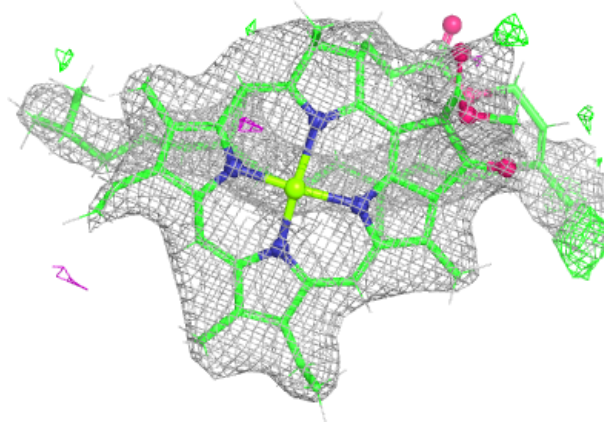
Electron density around LMG K 102:

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

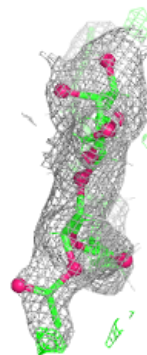
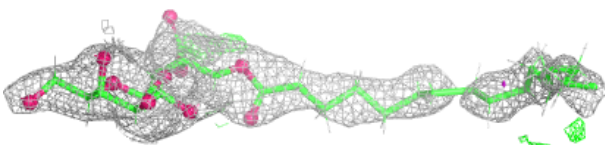
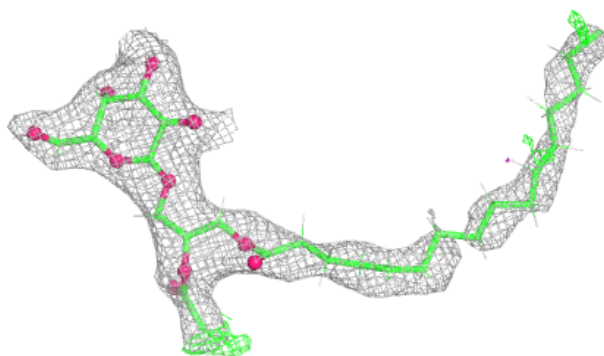


Electron density around CLA h 101:

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

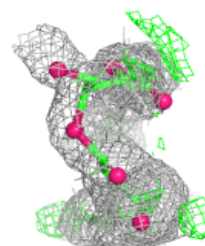
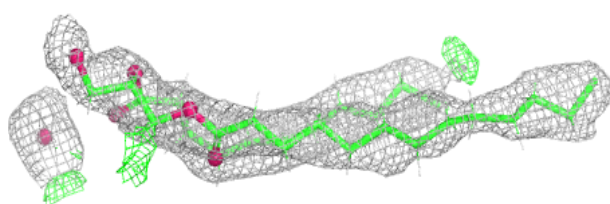
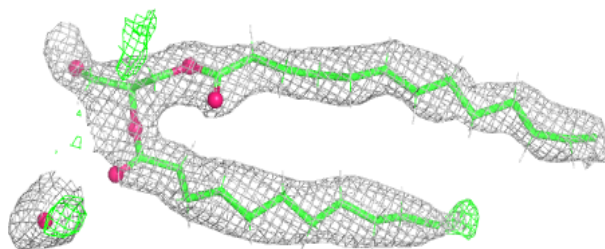
**Electron density around LMG c 519:**

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

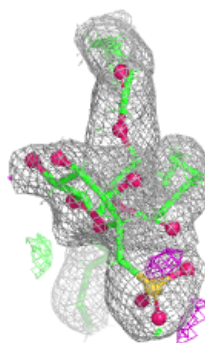
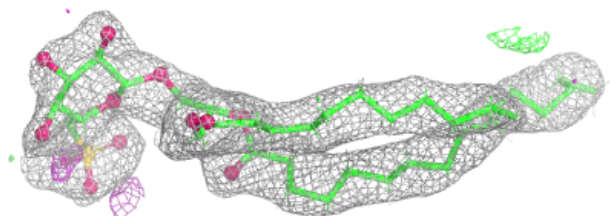
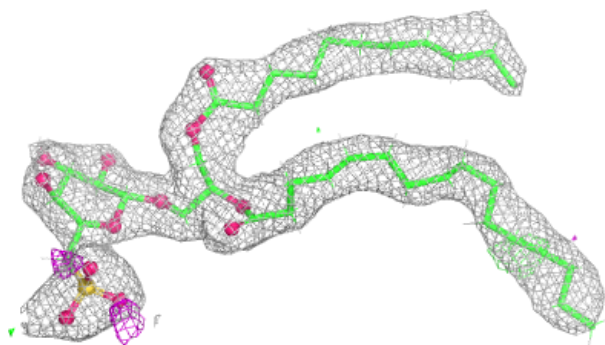


Electron density around LMG D 410:

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

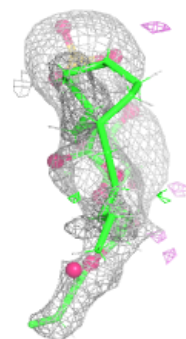
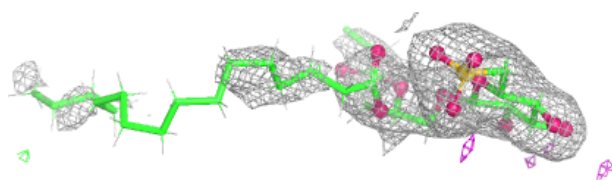
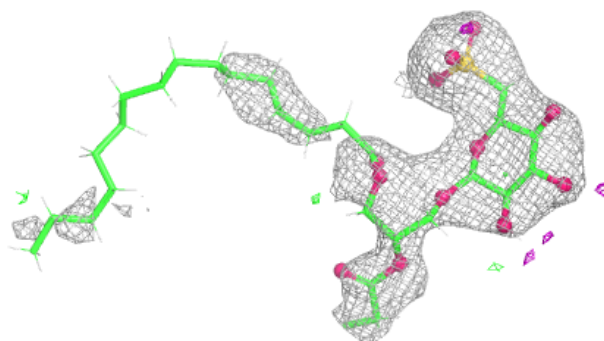
**Electron density around SQD b 601:**

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

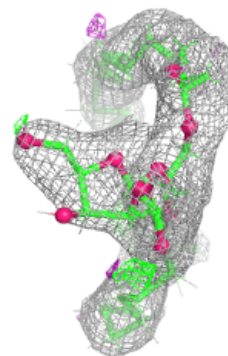
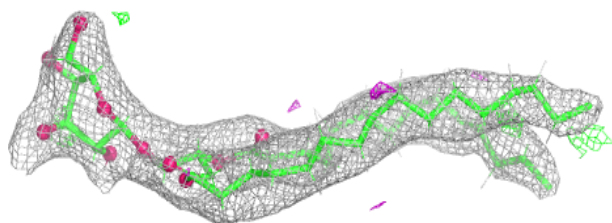
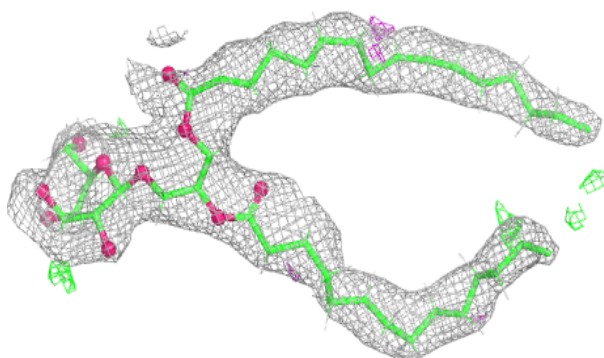


Electron density around SQD f 101:

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and green (positive)

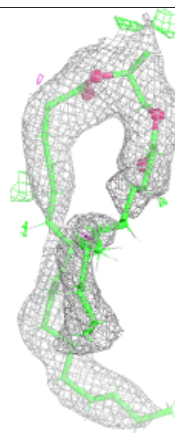
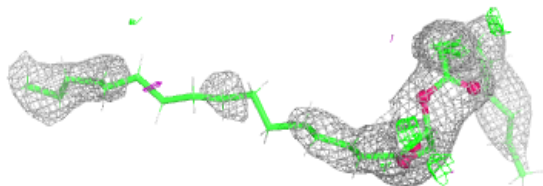
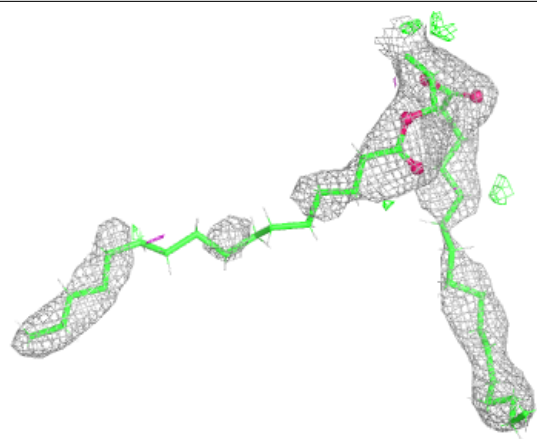
**Electron density around LMG c 524:**

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

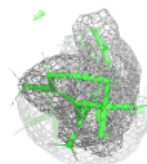
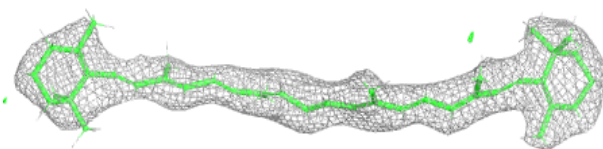
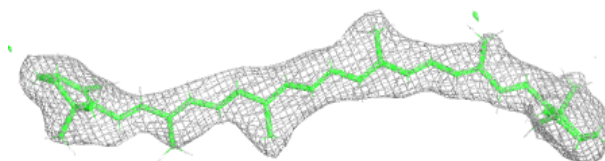


Electron density around SQD A 412:

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

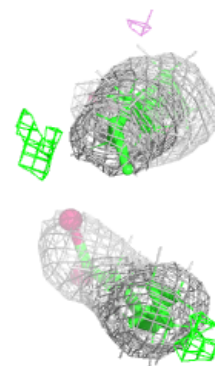
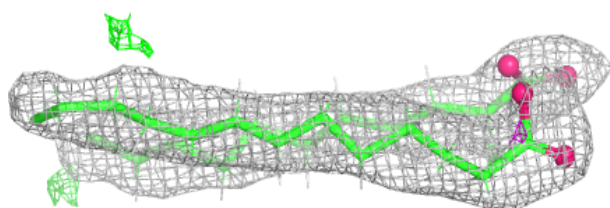
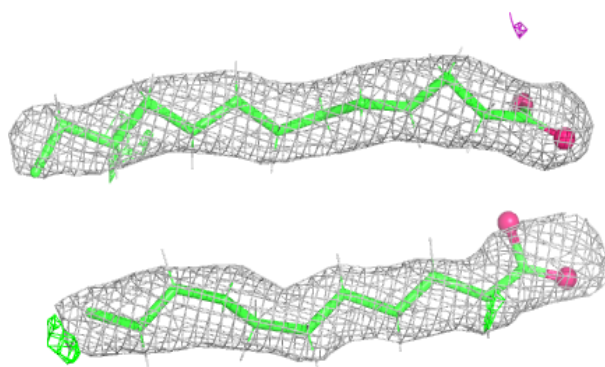
**Electron density around BCR h 103:**

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

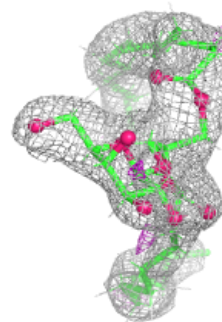
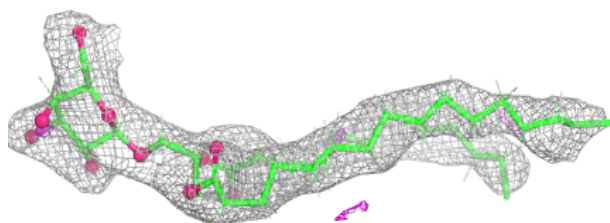
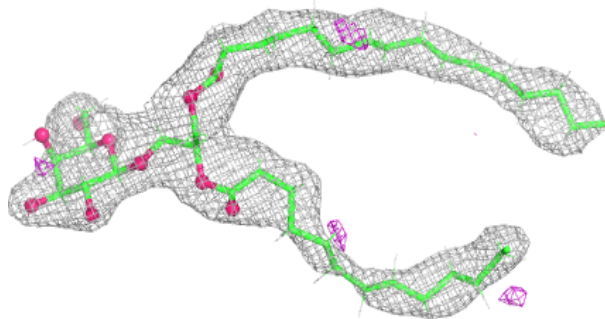


Electron density around LMG B 621:

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

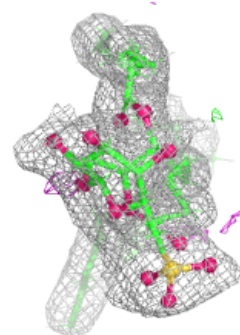
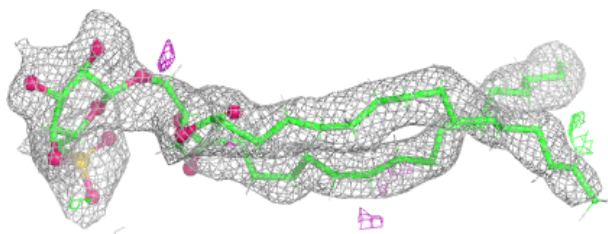
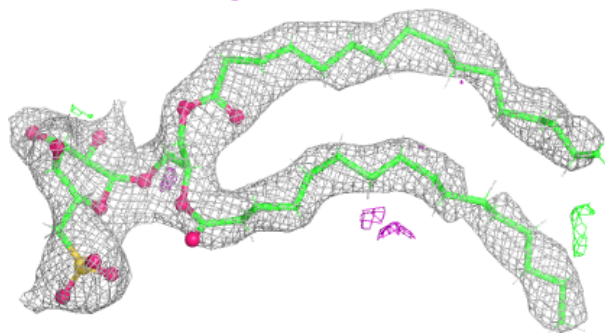
**Electron density around LMG C 501:**

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

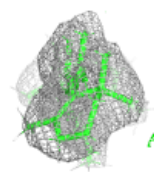
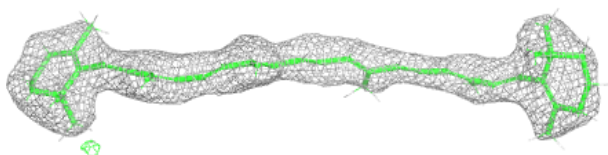
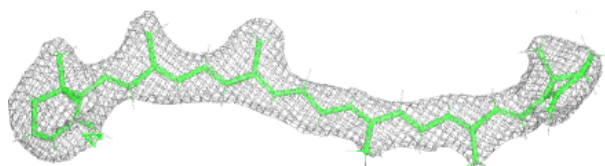


Electron density around SQD B 622:

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

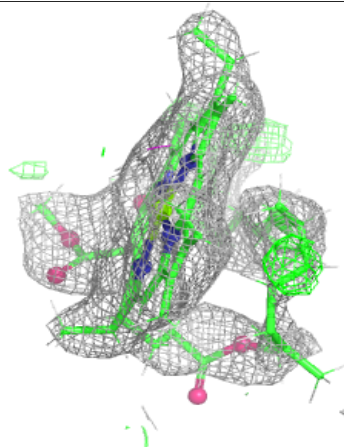
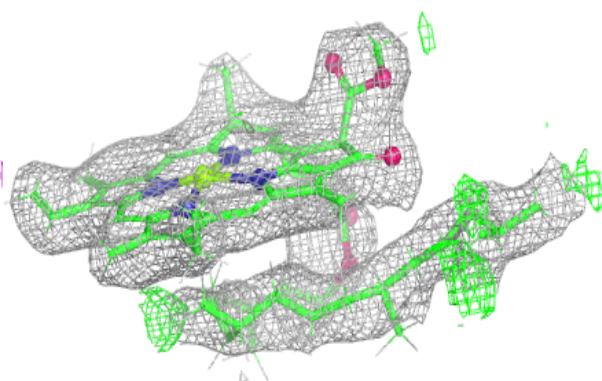
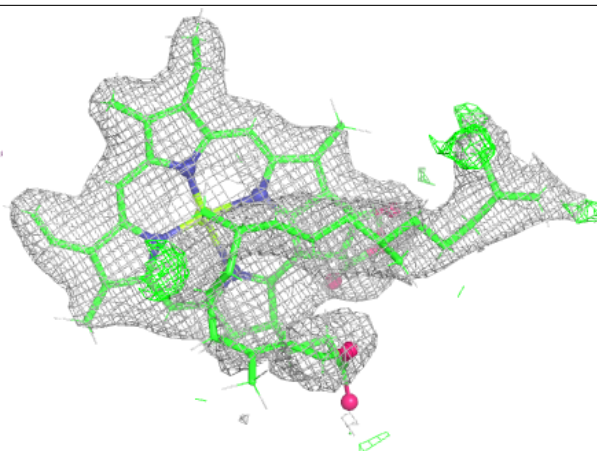
**Electron density around BCR k 101:**

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

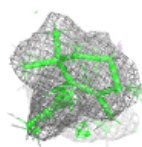
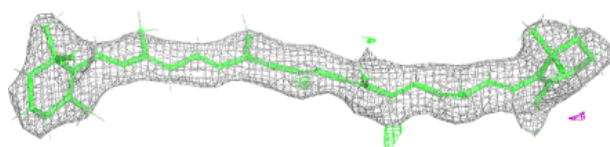


Electron density around CLA B 601:

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

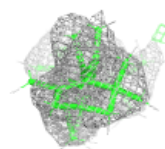
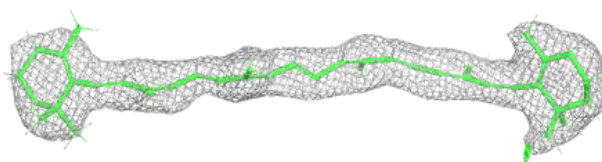
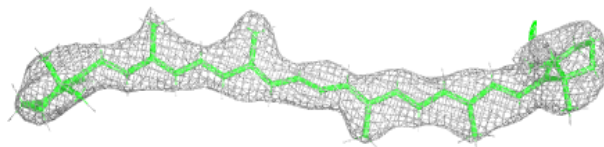
**Electron density around BCR K 101:**

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

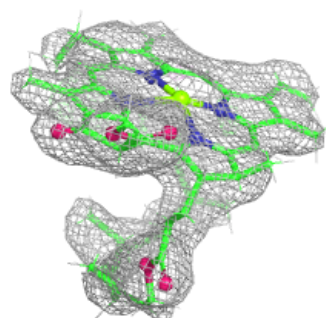
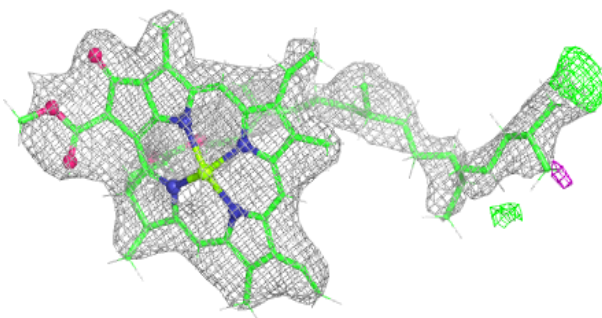
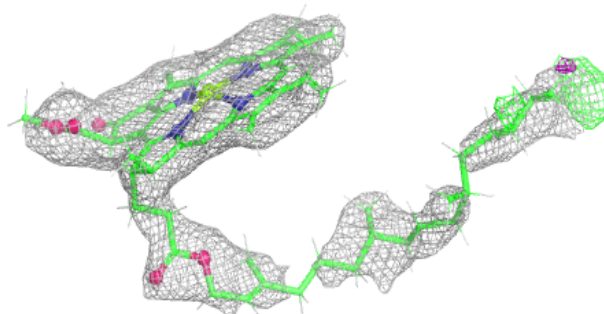


Electron density around BCR c 514:

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

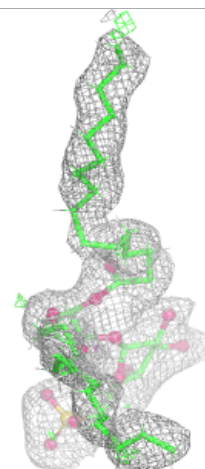
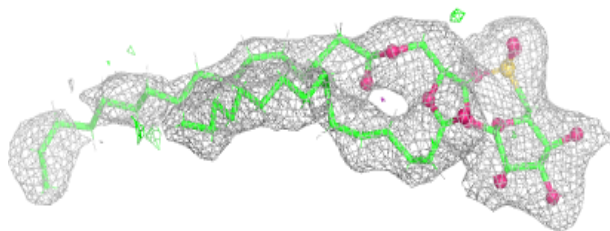
**Electron density around CLA C 514:**

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



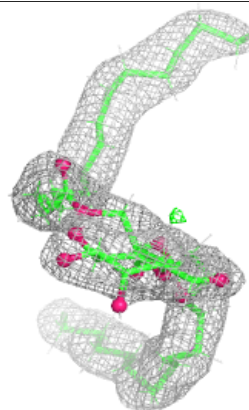
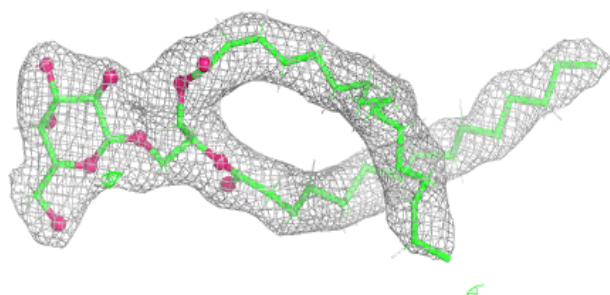
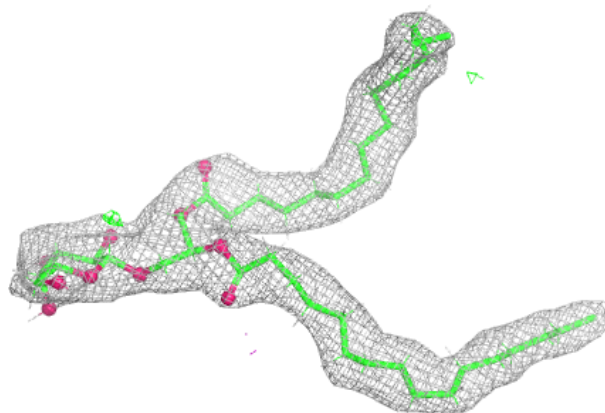
Electron density around SQD a 410:

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

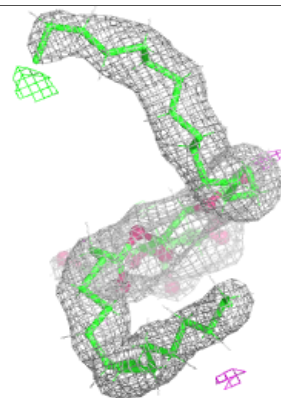
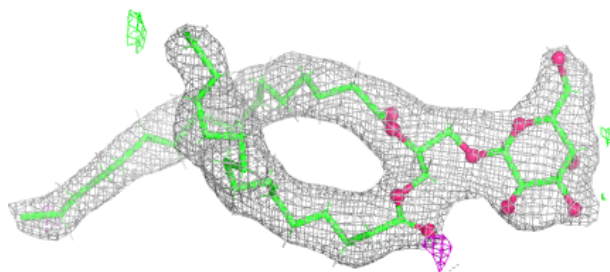
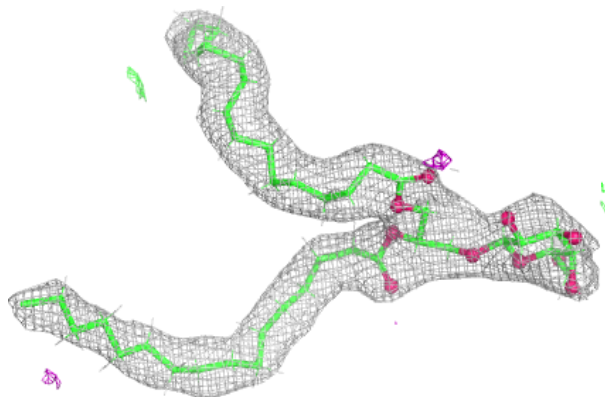


Electron density around LMG M 101:

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

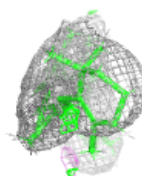
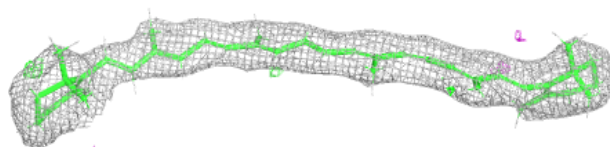
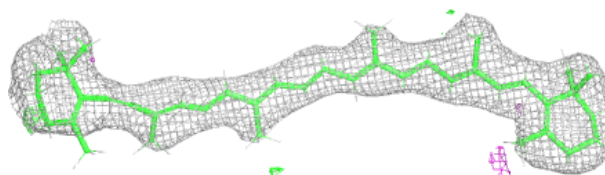
**Electron density around LMG b 621:**

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

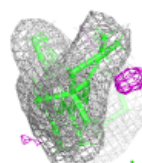
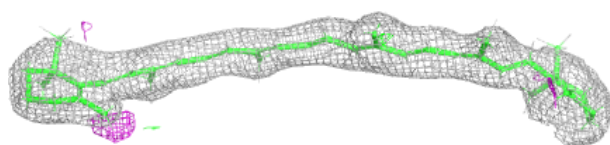
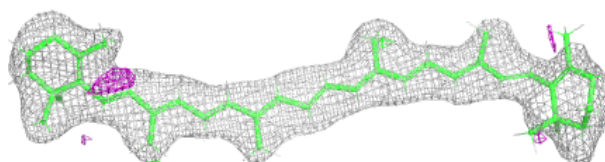


Electron density around BCR d 406:

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

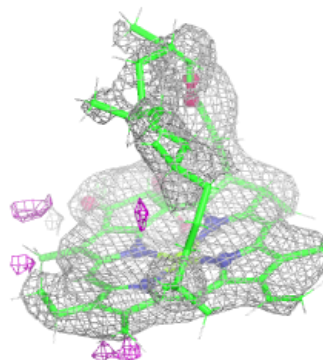
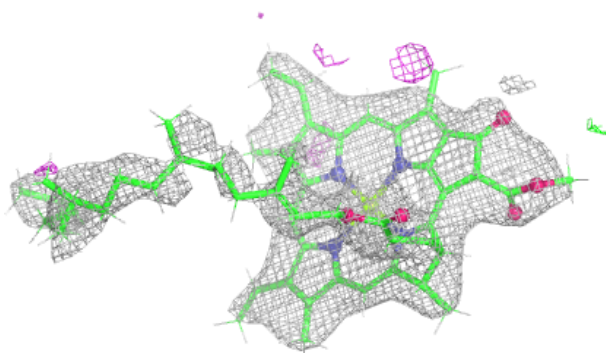
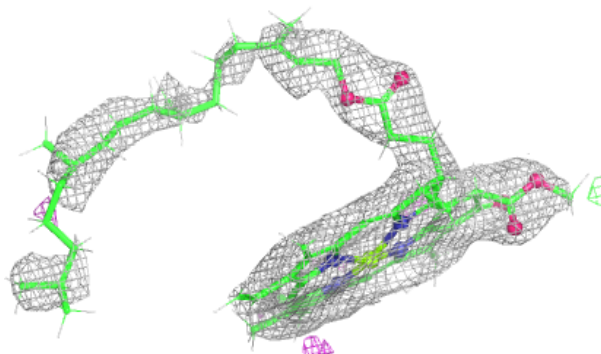
**Electron density around BCR D 405:**

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

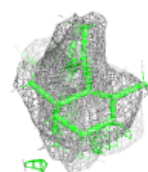
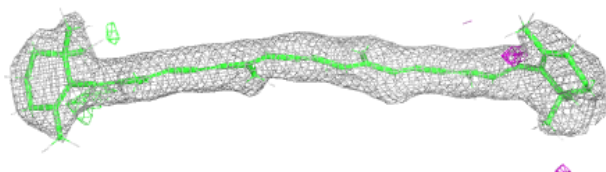
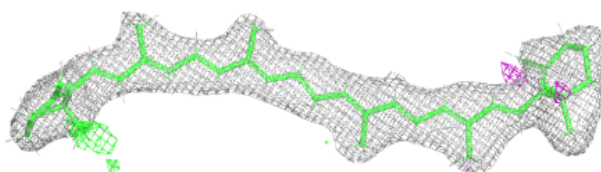


Electron density around CLA c 513:

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

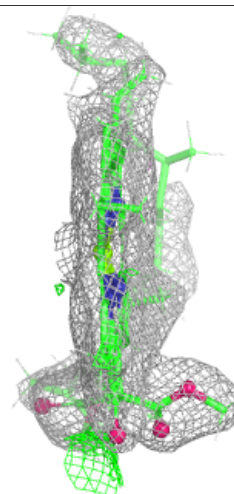
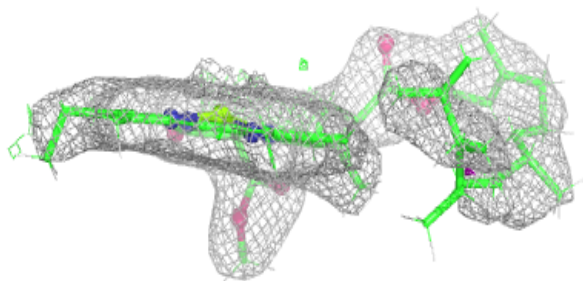
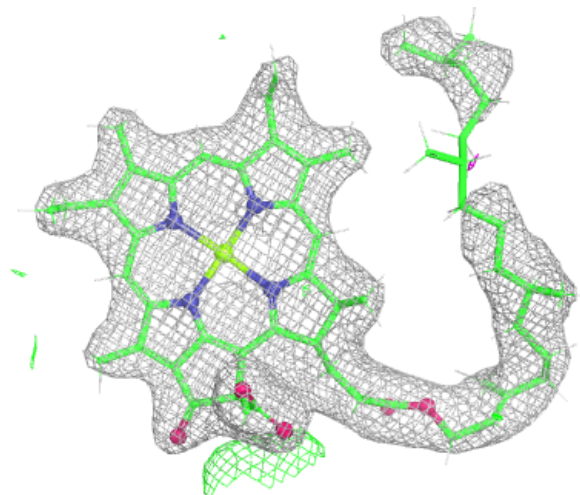
**Electron density around BCR Y 101:**

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



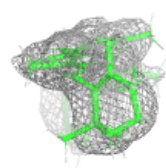
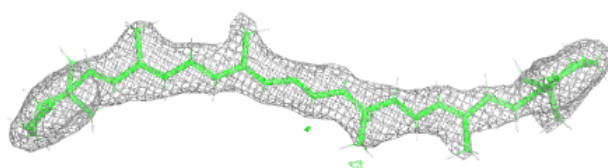
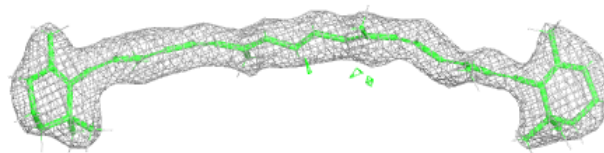
Electron density around CLA c 512:

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

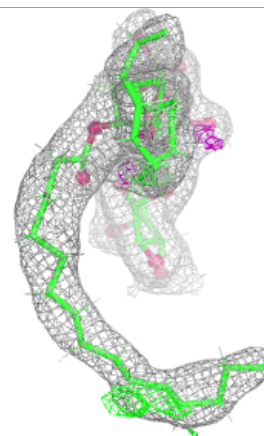
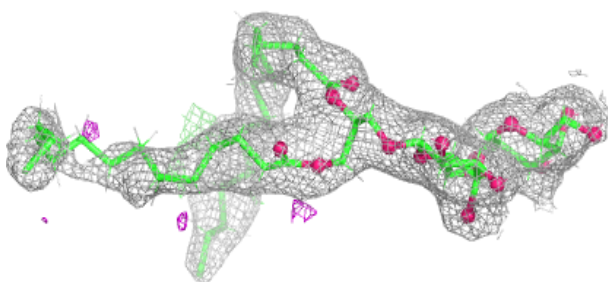
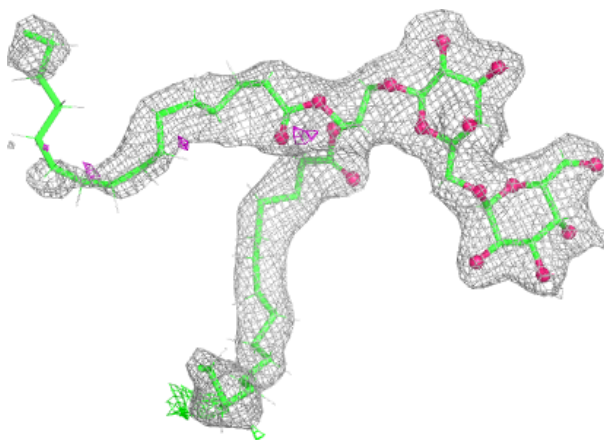


Electron density around BCR c 521:

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

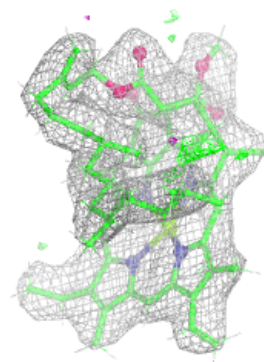
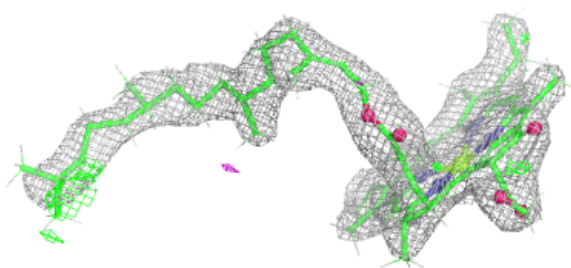
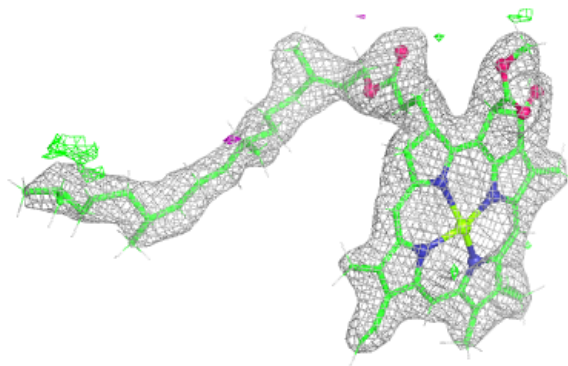
**Electron density around DGD C 517:**

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



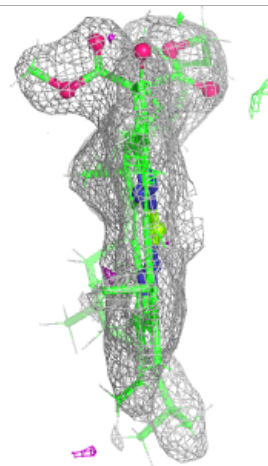
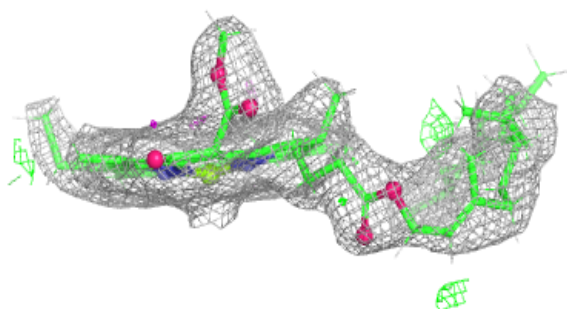
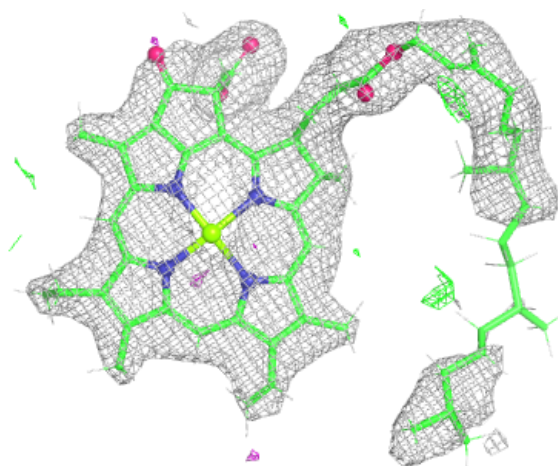
Electron density around CLA c 511:

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



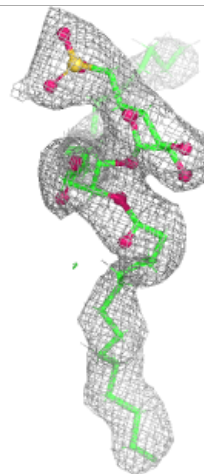
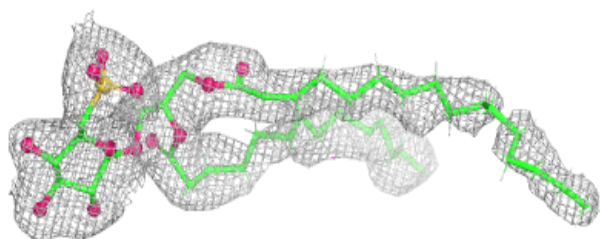
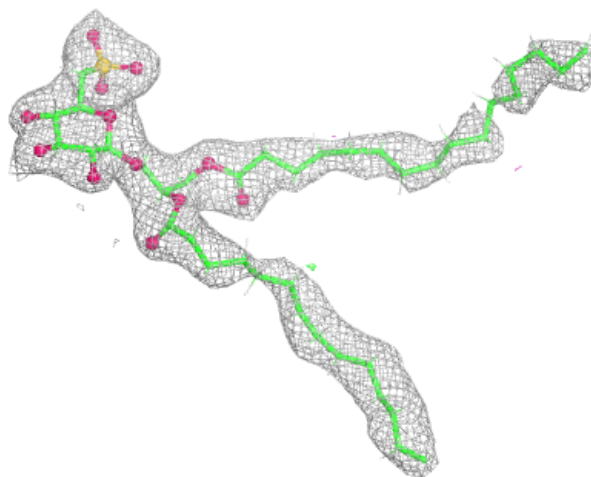
Electron density around CLA C 513:

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



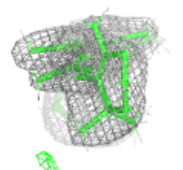
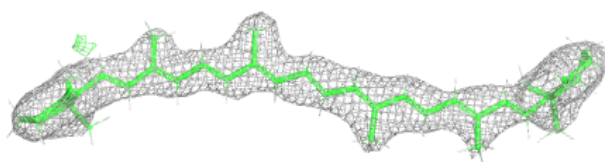
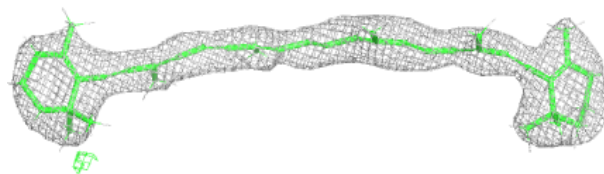
Electron density around SQD A 411:

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

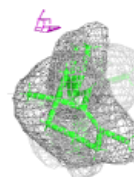
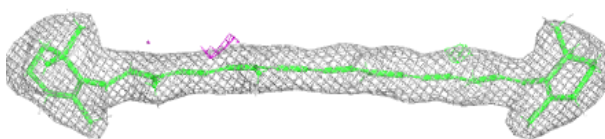
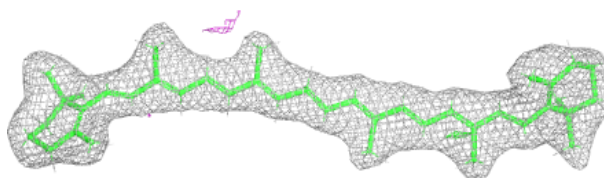


Electron density around BCR C 519:

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

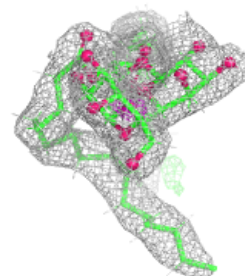
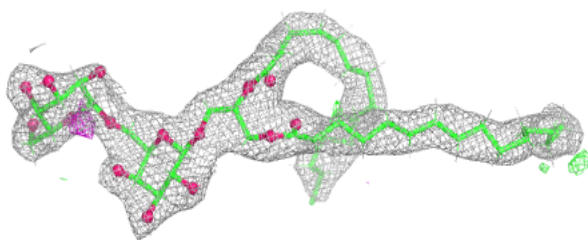
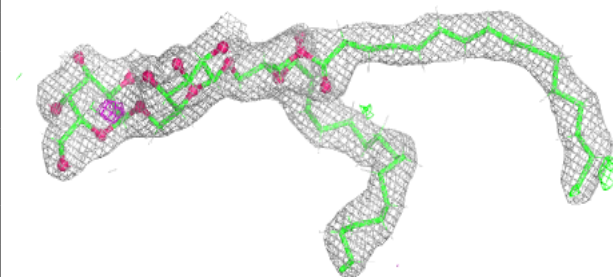
**Electron density around BCR b 619:**

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

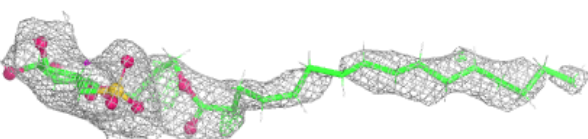
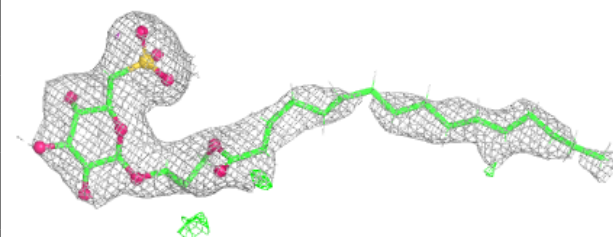


Electron density around DGD H 102:

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

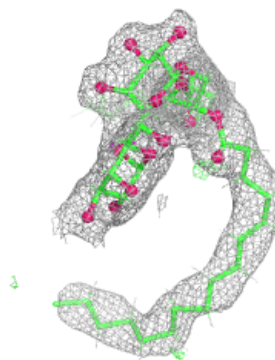
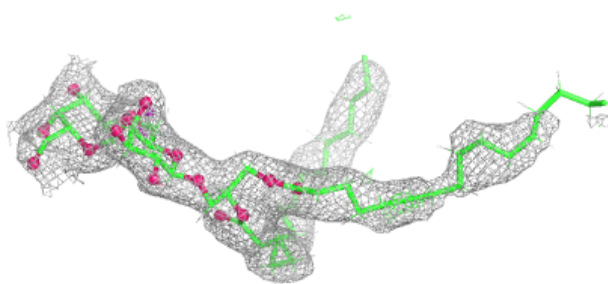
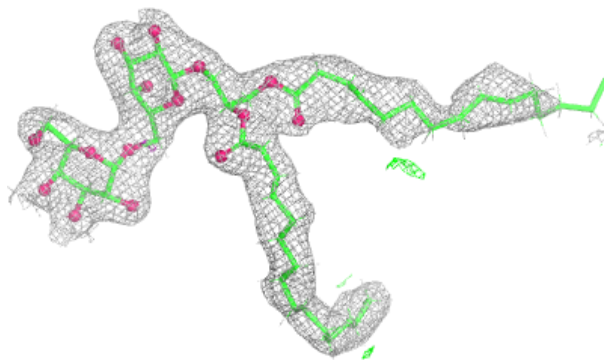
**Electron density around SQD F 101:**

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

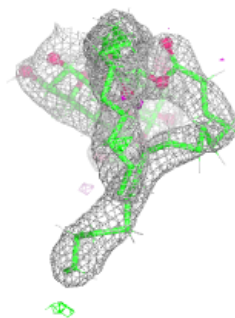
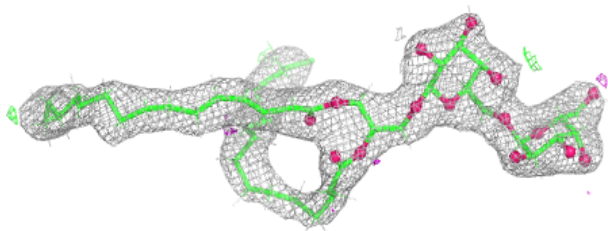
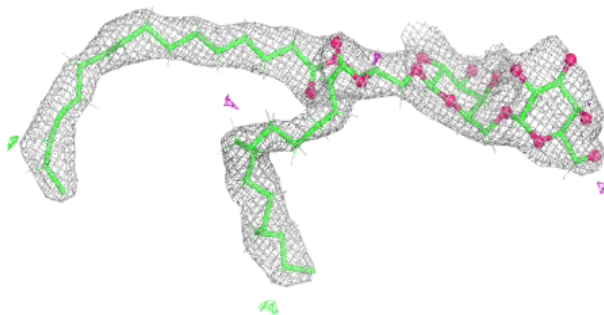


Electron density around DGD c 517:

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

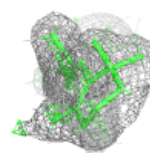
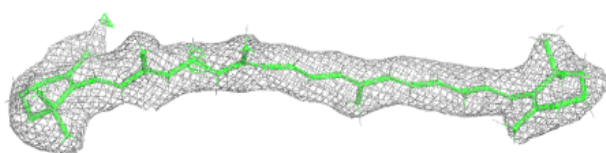
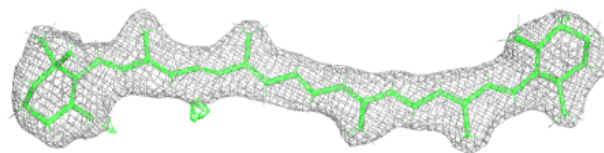
**Electron density around DGD h 104:**

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

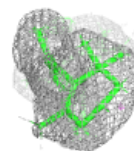
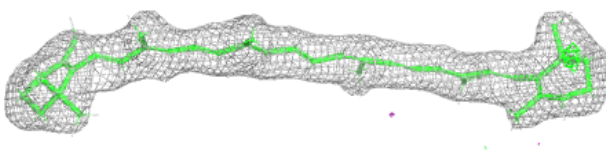
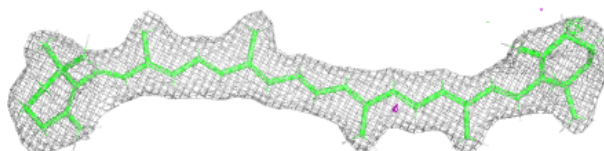


Electron density around BCR b 620:

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

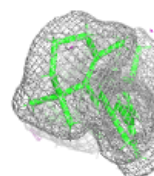
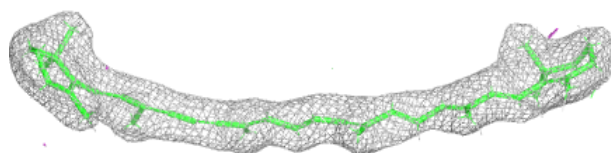
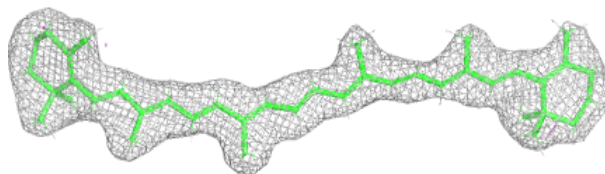
**Electron density around BCR B 619:**

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

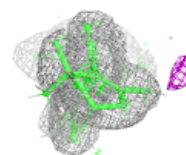
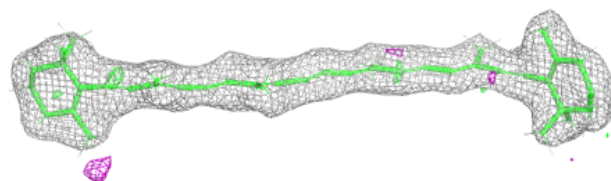
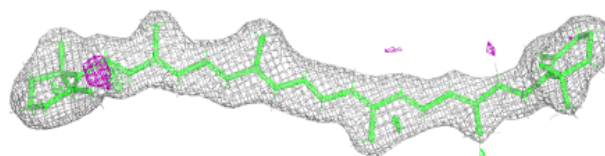


Electron density around BCR t 101:

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

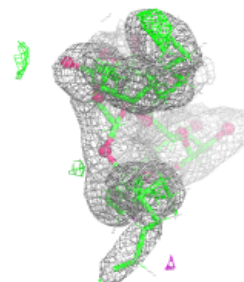
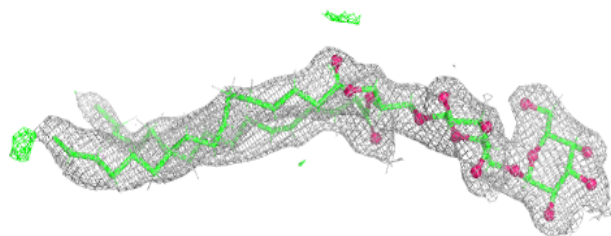
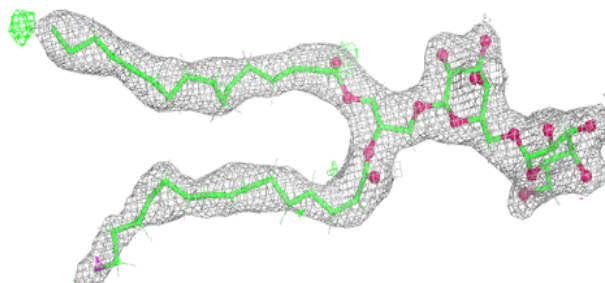
**Electron density around BCR C 515:**

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

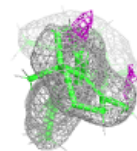
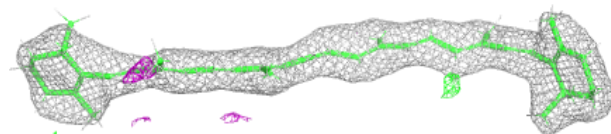
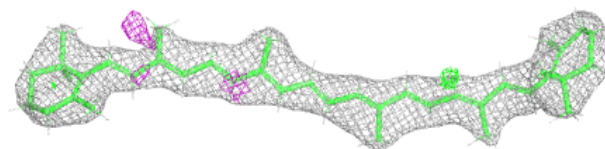


Electron density around DGD c 518:

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

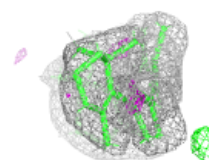
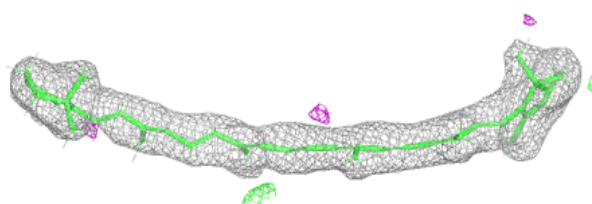
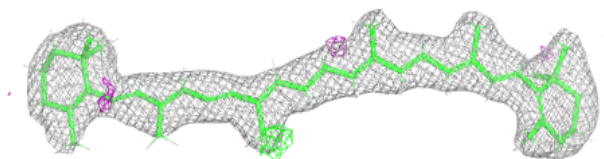
**Electron density around BCR c 515:**

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

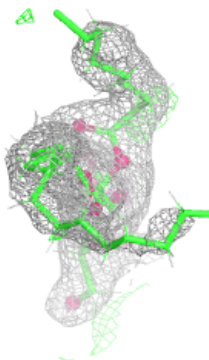
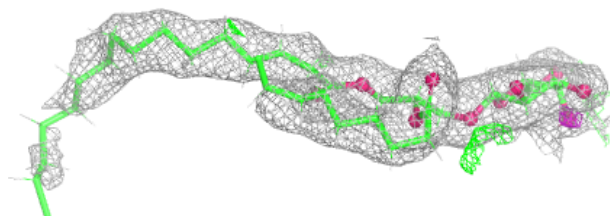
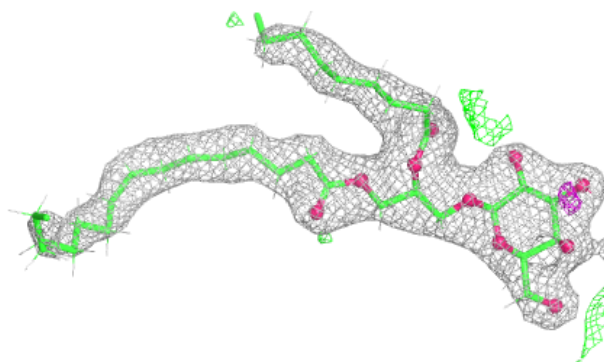


Electron density around BCR b 602:

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

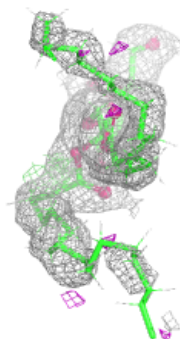
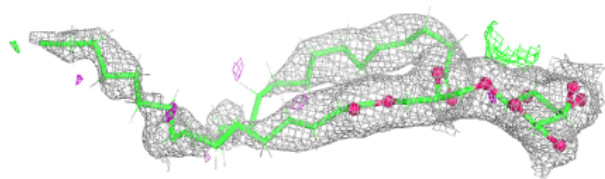
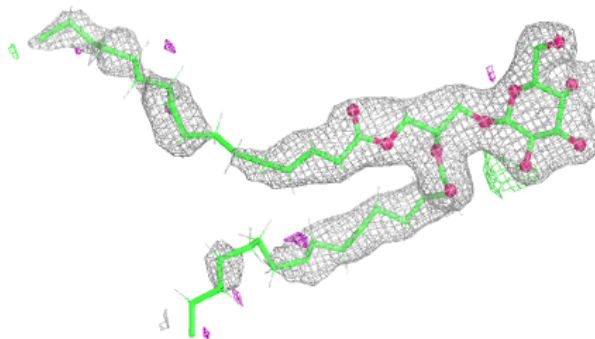
**Electron density around LMG d 411:**

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

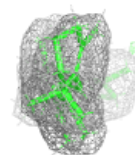
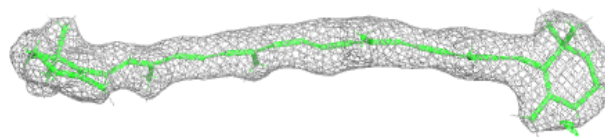
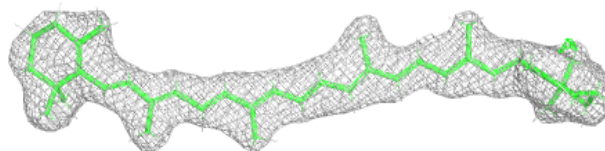


Electron density around LMG D 407:

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

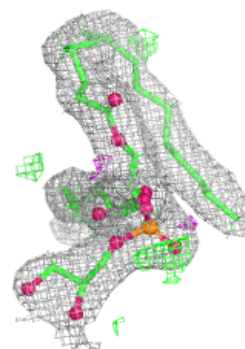
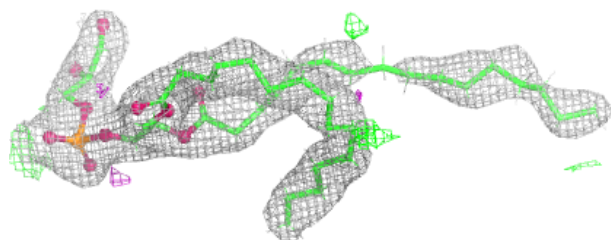
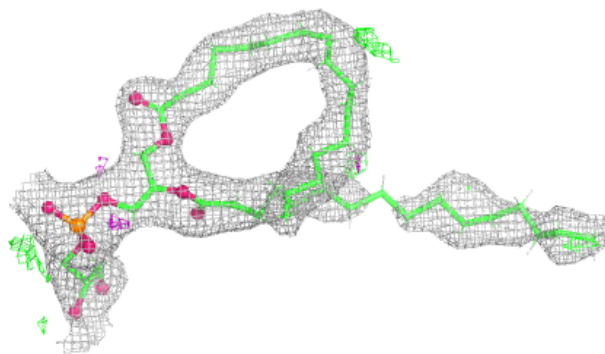
**Electron density around BCR b 618:**

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

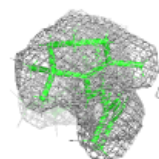
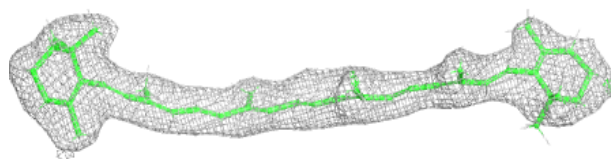
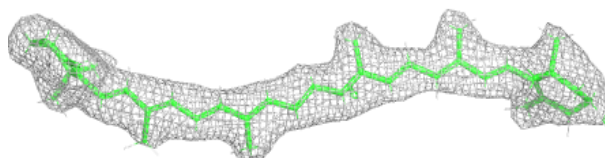


Electron density around LHG d 408:

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

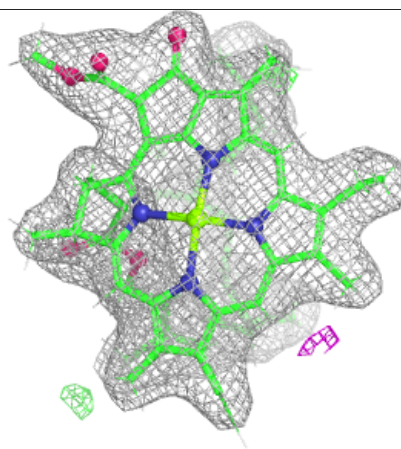
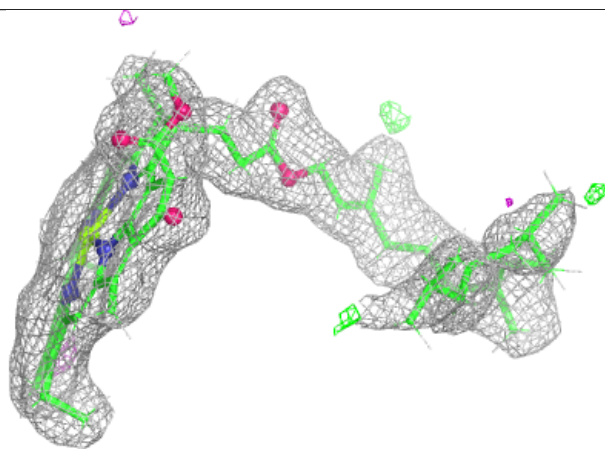
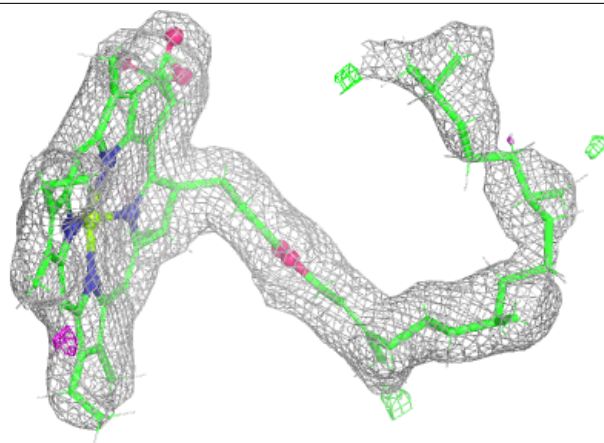
**Electron density around BCR H 101:**

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

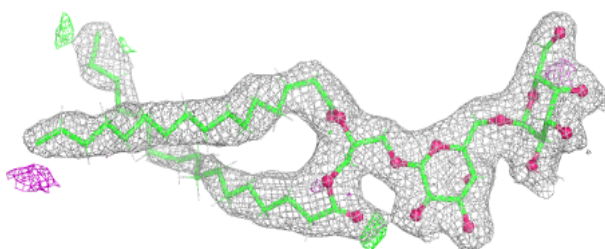
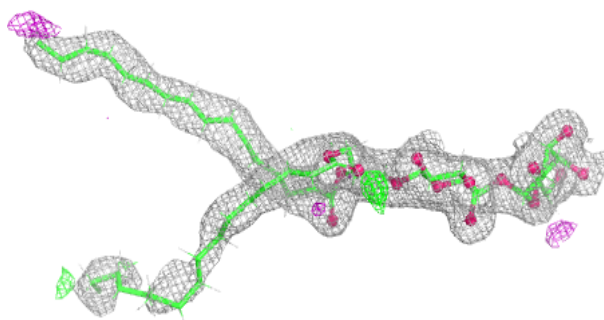


Electron density around CLA B 606:

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

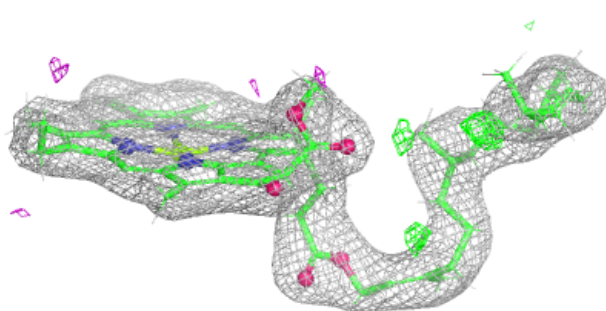
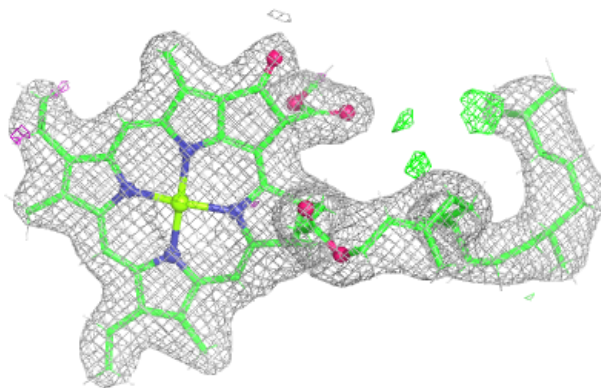
**Electron density around DGD C 516:**

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

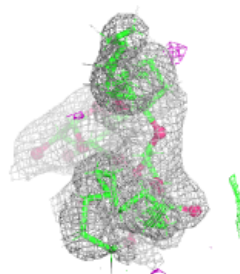
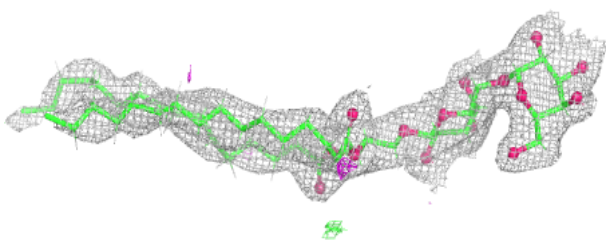
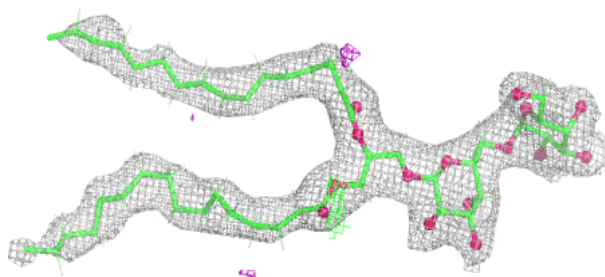


Electron density around CLA b 613:

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

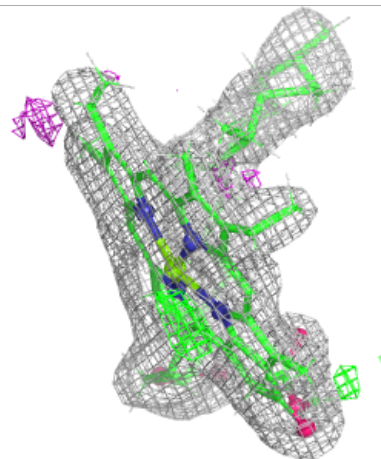
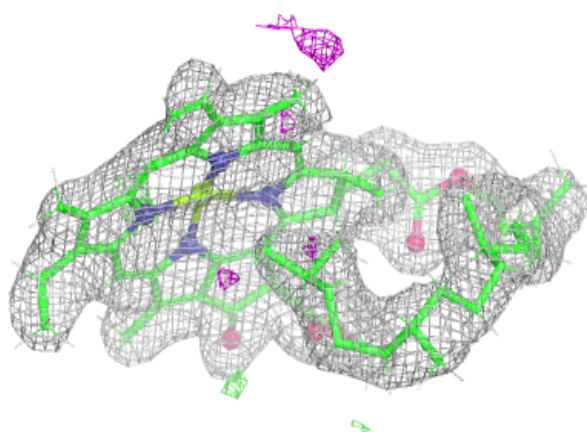
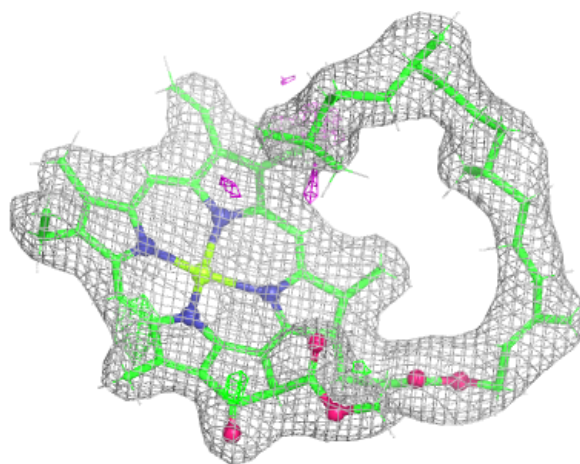
**Electron density around DGD C 518:**

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



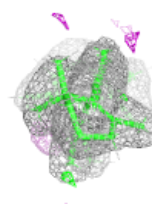
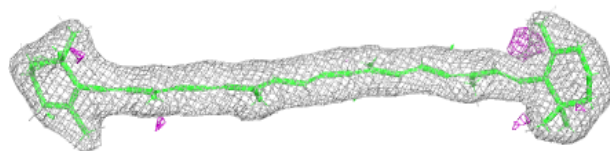
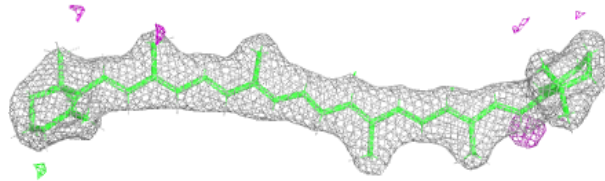
Electron density around CLA b 616:

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



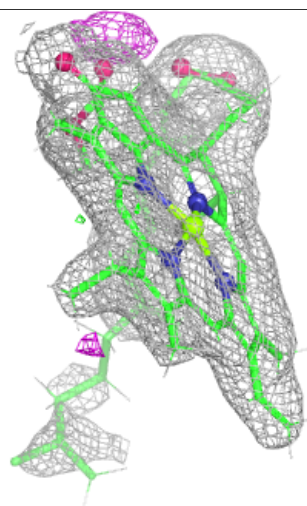
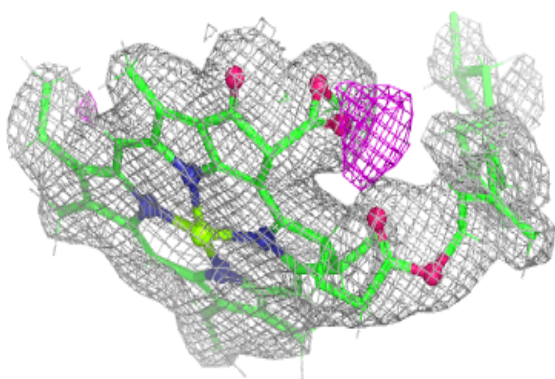
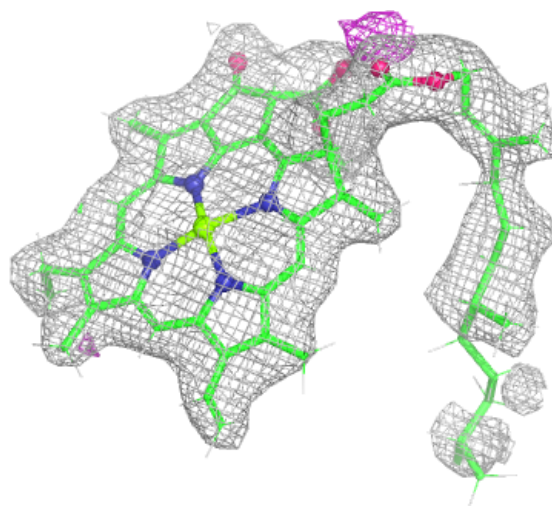
Electron density around BCR a 408:

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



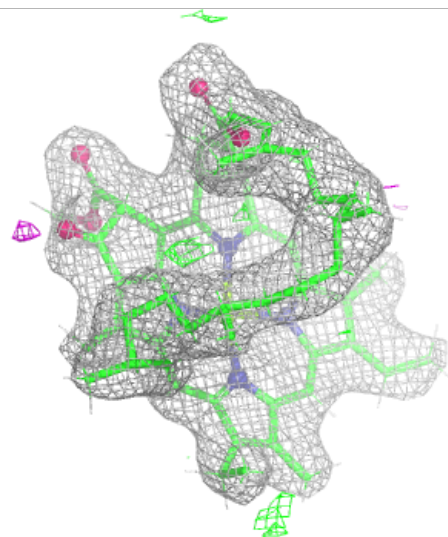
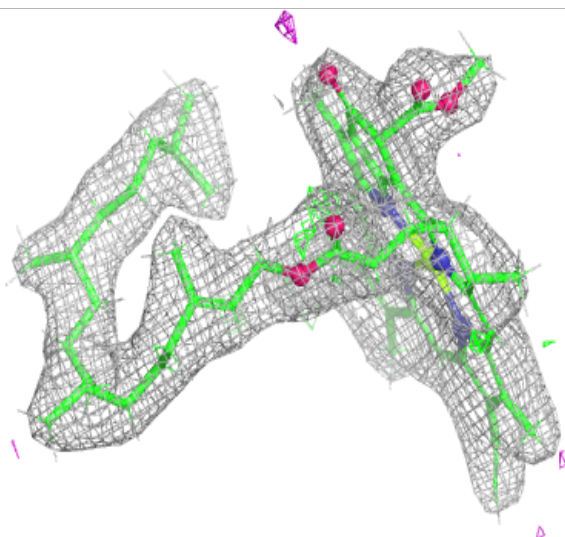
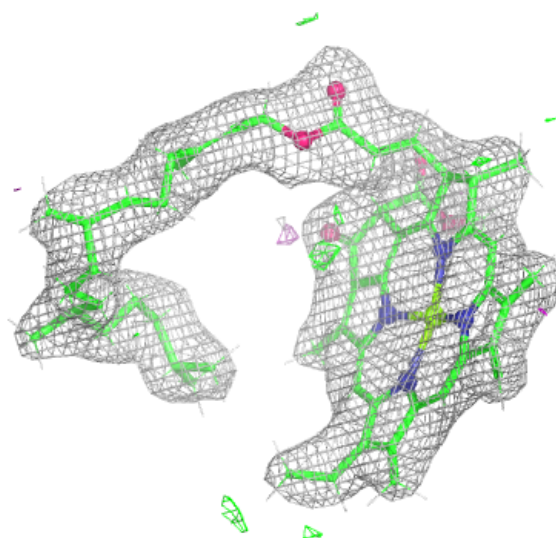
Electron density around CLA b 617:

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



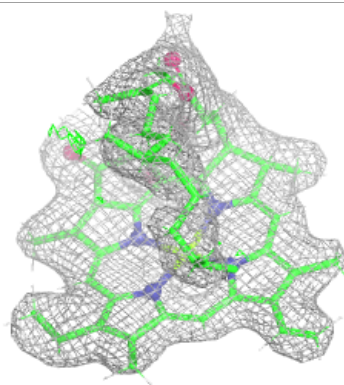
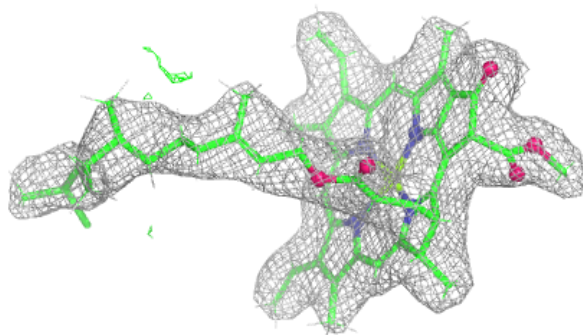
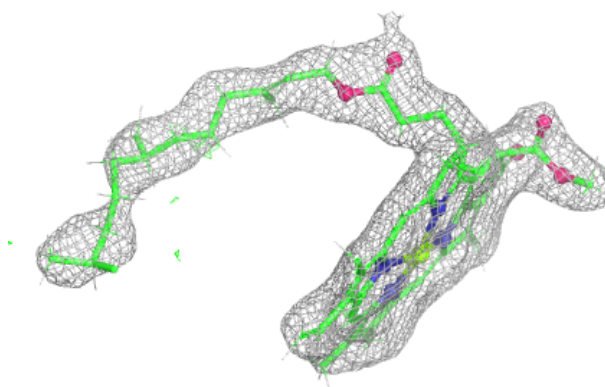
Electron density around CLA c 503:

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

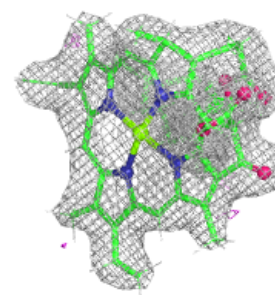
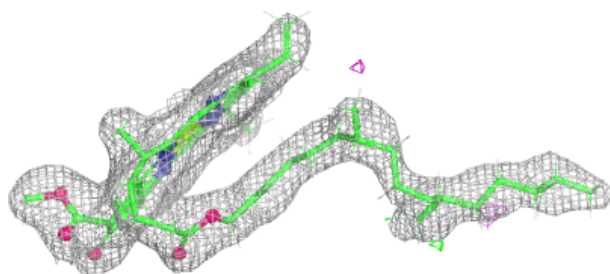
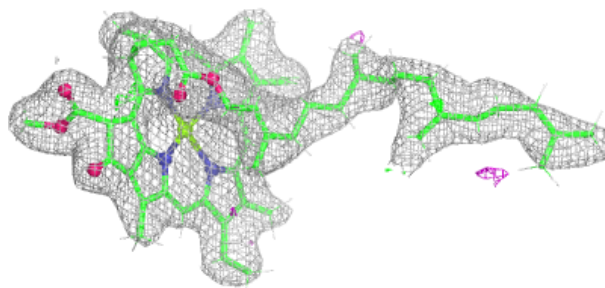


Electron density around CLA c 504:

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

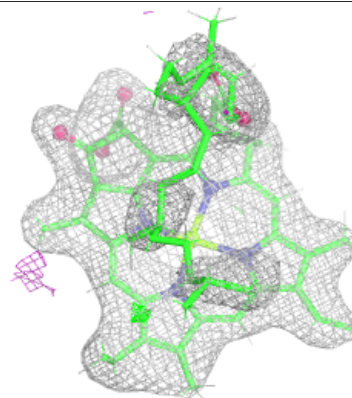
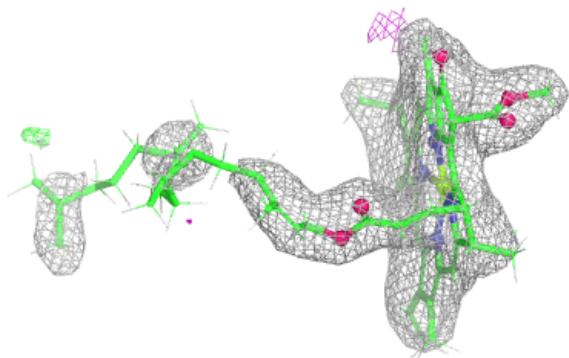
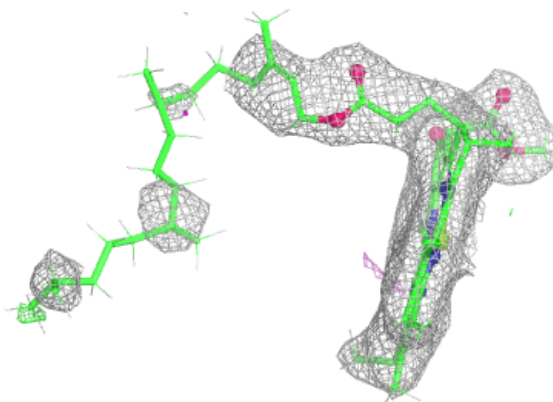
**Electron density around CLA c 505:**

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

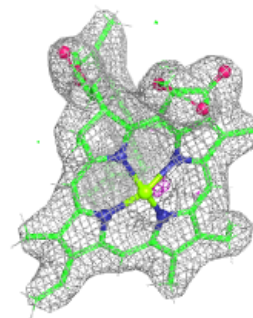
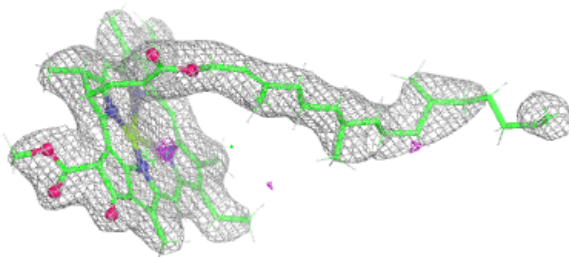
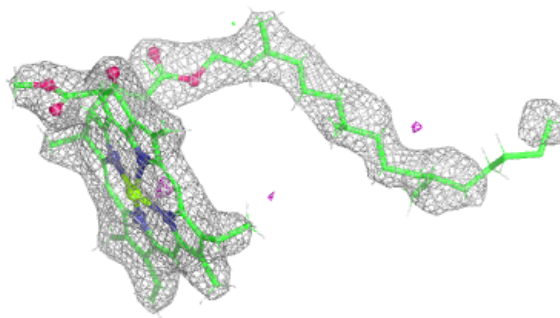


Electron density around CLA c 506:

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

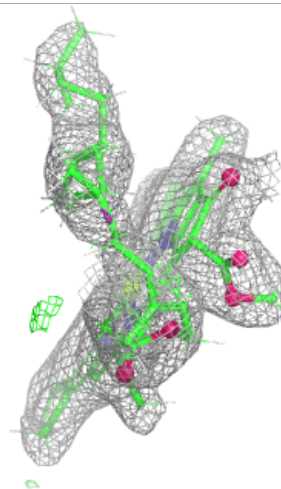
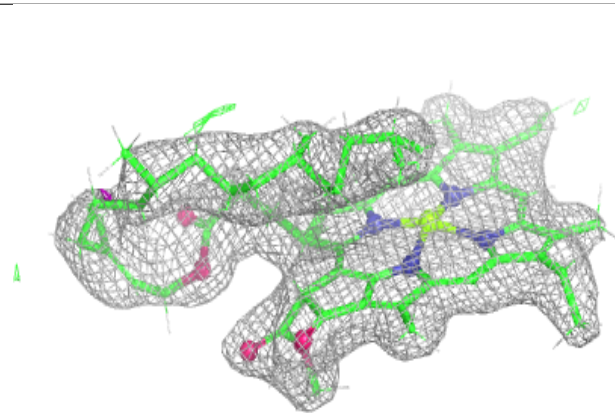
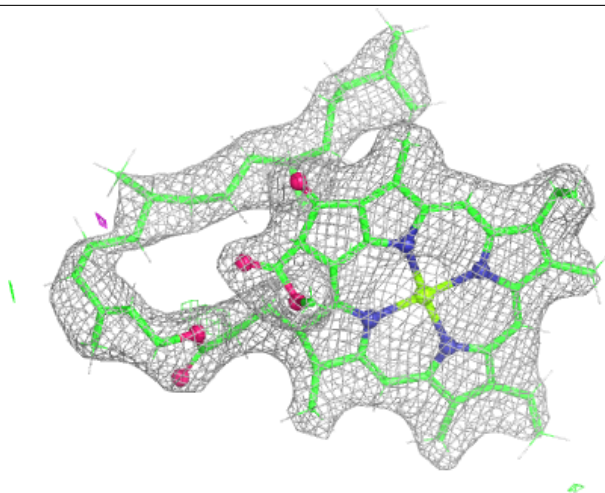
**Electron density around CLA c 508:**

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



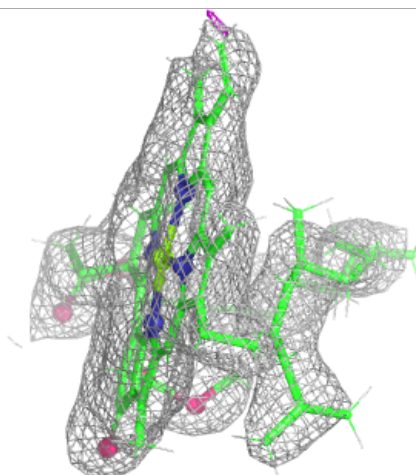
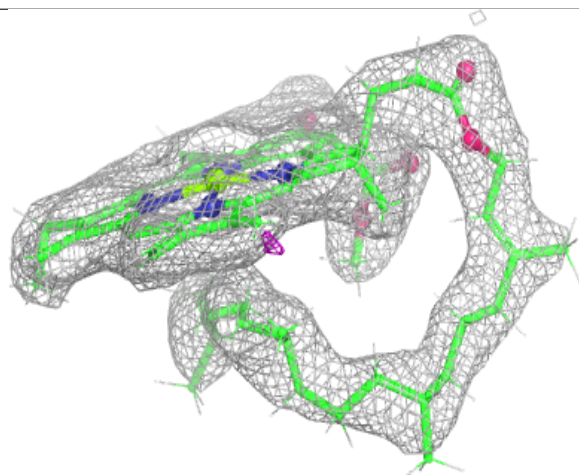
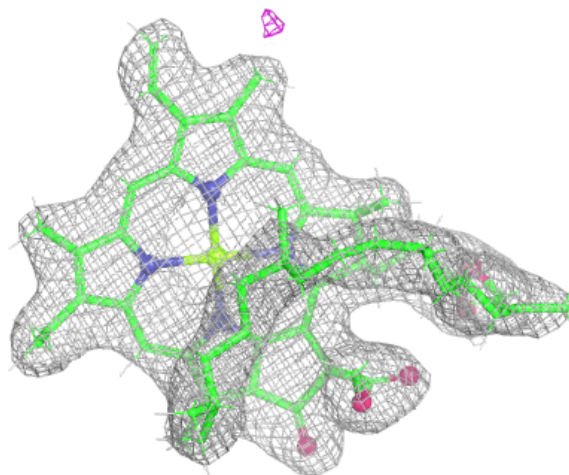
Electron density around CLA c 509:

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



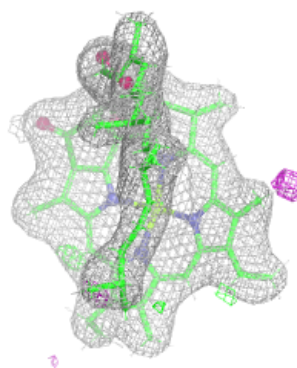
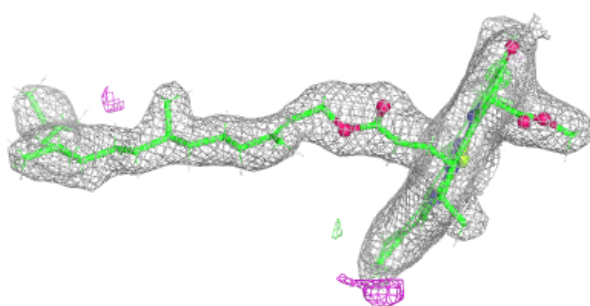
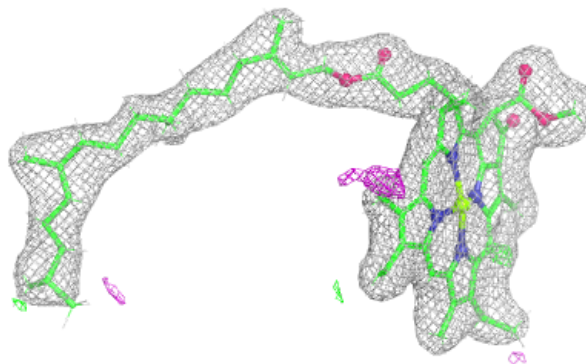
Electron density around CLA c 510:

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

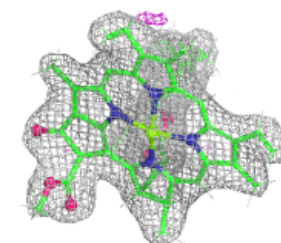
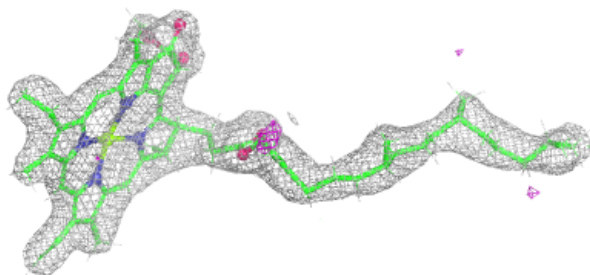
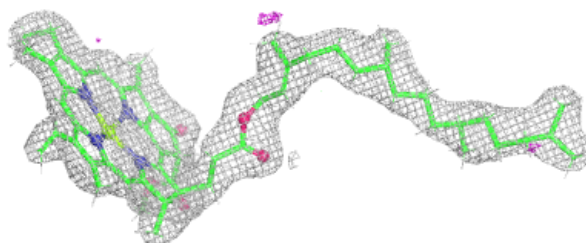


Electron density around CLA B 609:

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

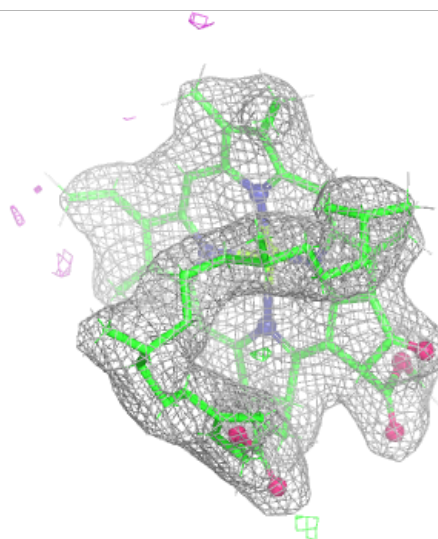
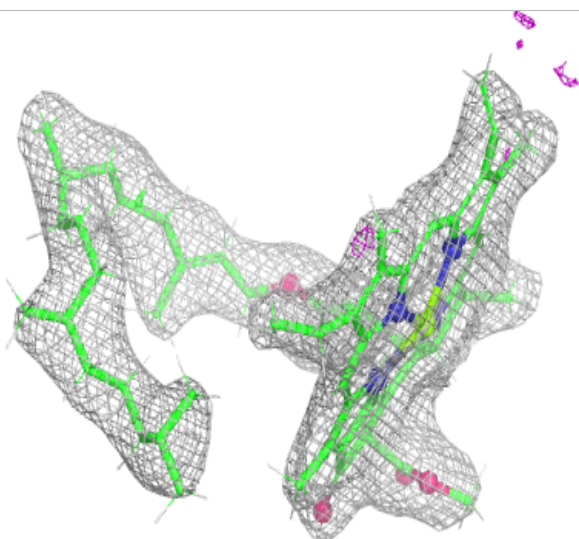
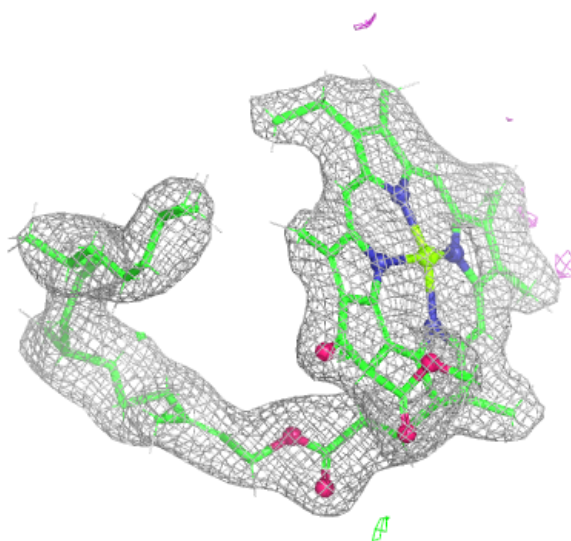
**Electron density around CLA C 503:**

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



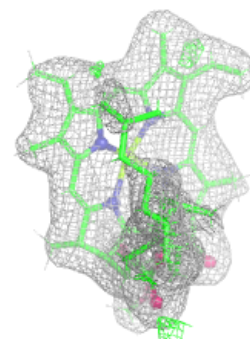
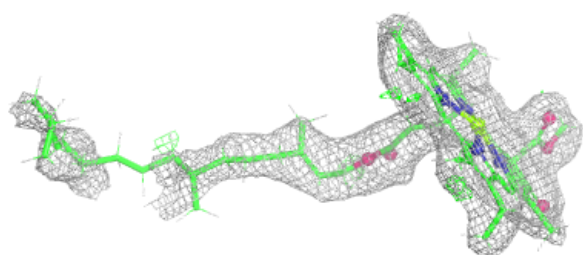
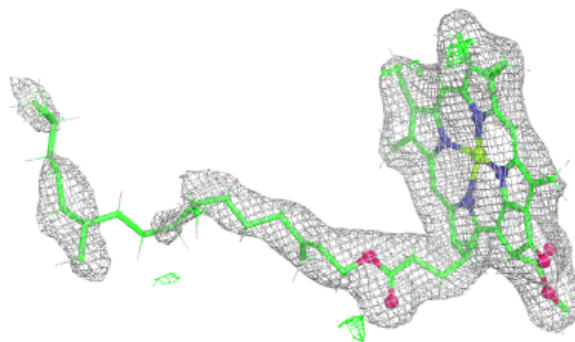
Electron density around CLA C 504:

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

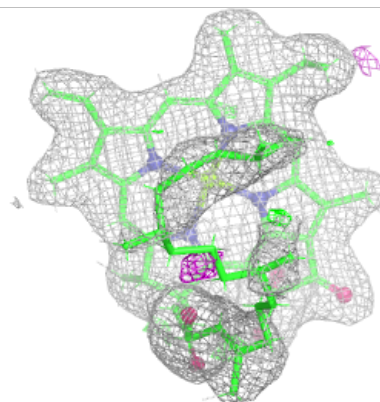
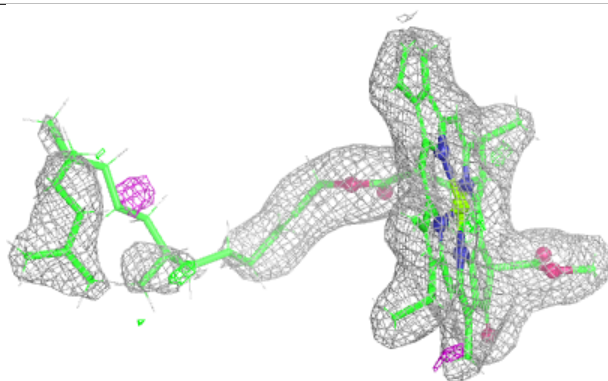
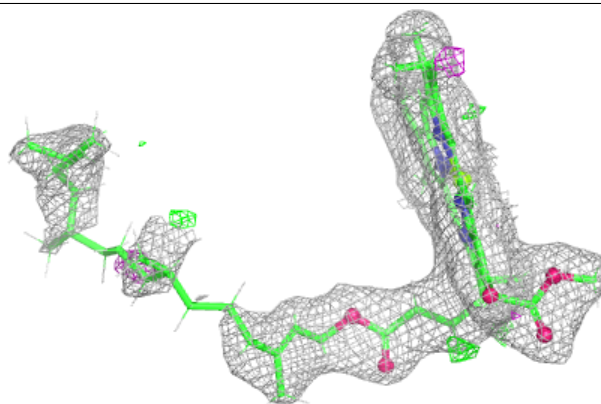


Electron density around CLA d 405:

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

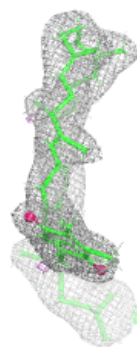
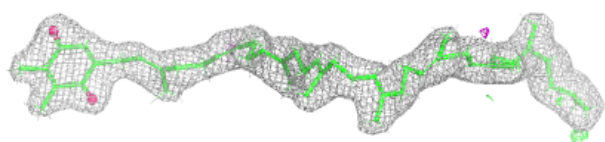
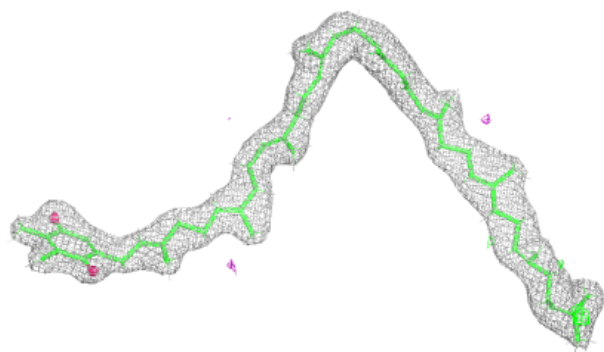
**Electron density around CLA C 507:**

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

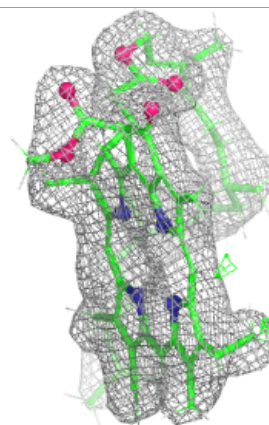
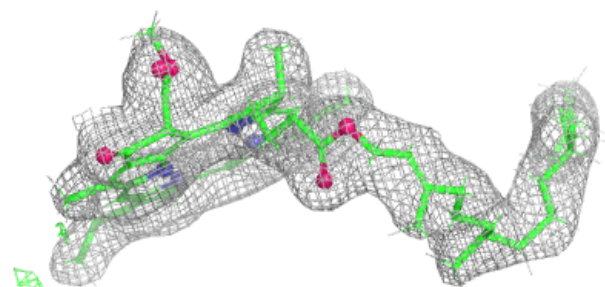
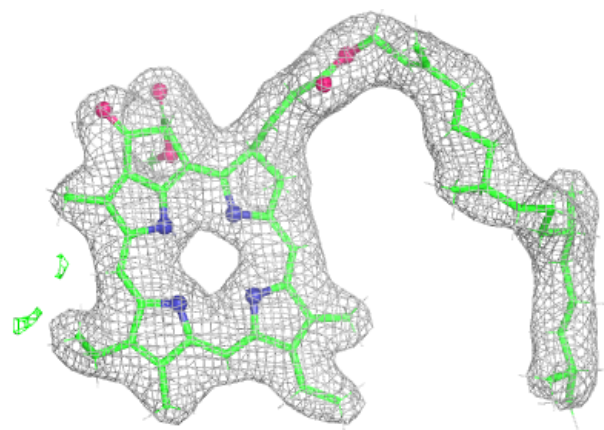


Electron density around PL9 d 407:

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

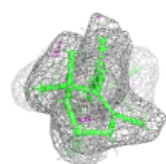
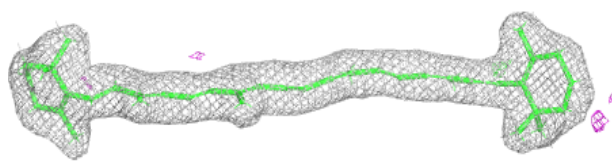
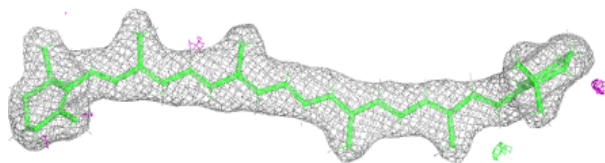
**Electron density around PHO d 402:**

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

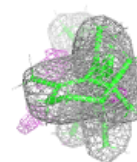
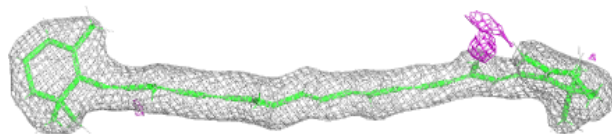
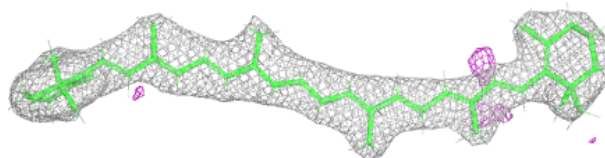


Electron density around BCR A 409:

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

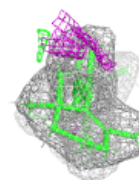
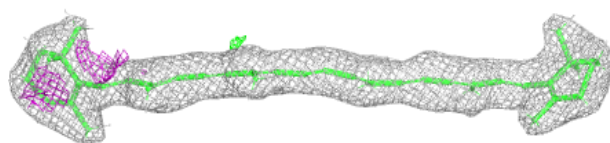
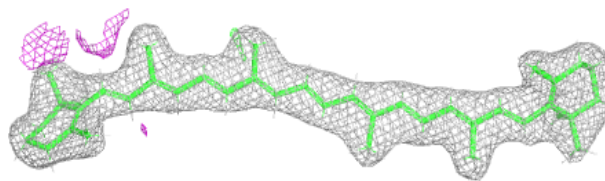
**Electron density around BCR B 617:**

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

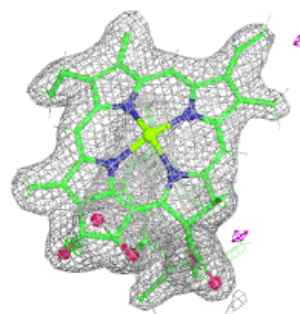
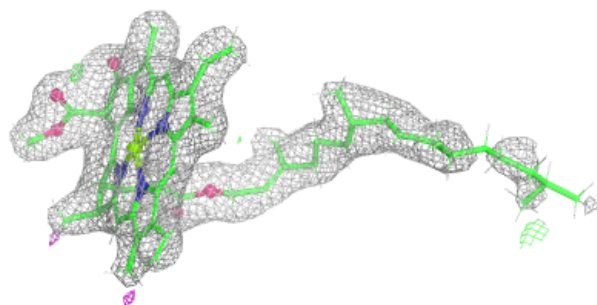
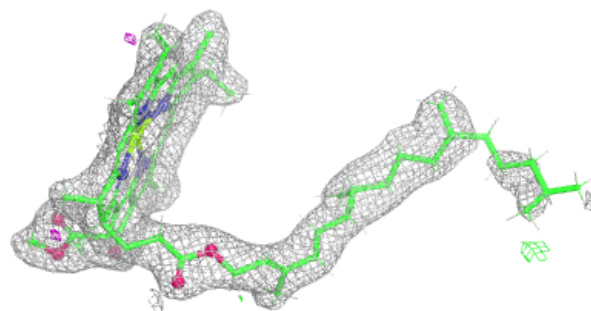


Electron density around BCR B 618:

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

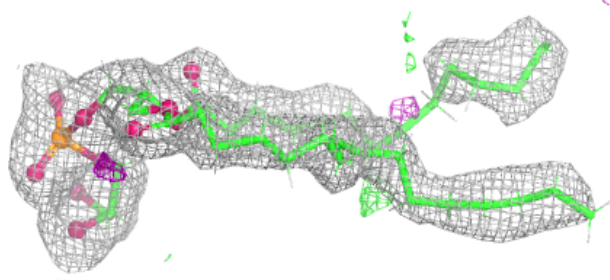
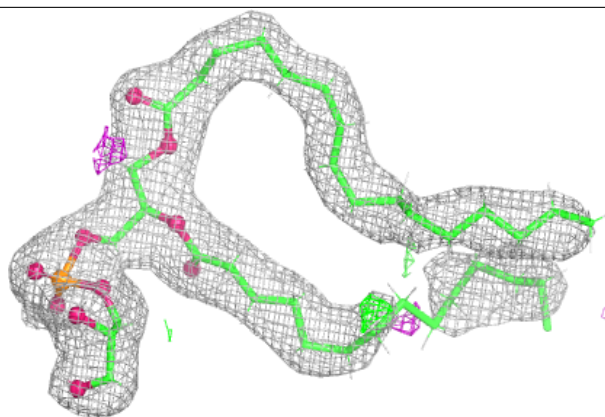
**Electron density around CLA C 509:**

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

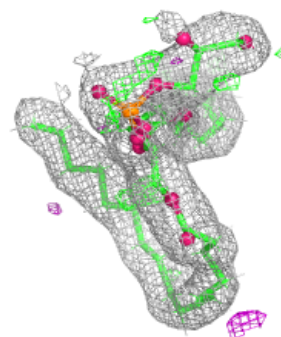
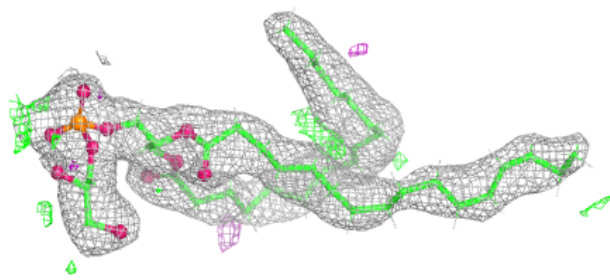
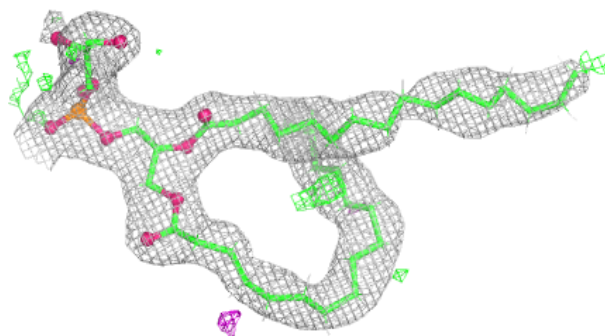


Electron density around LHG D 409:

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

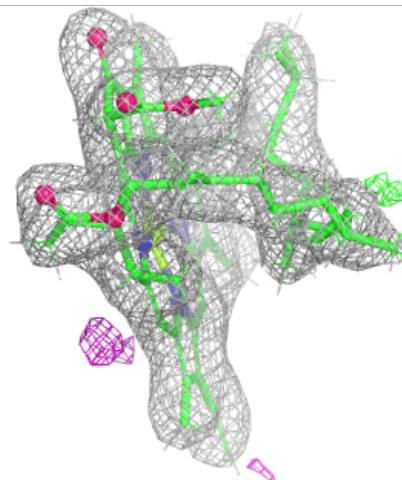
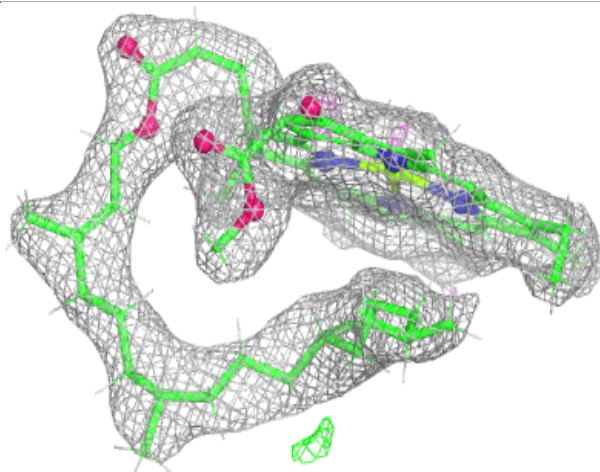
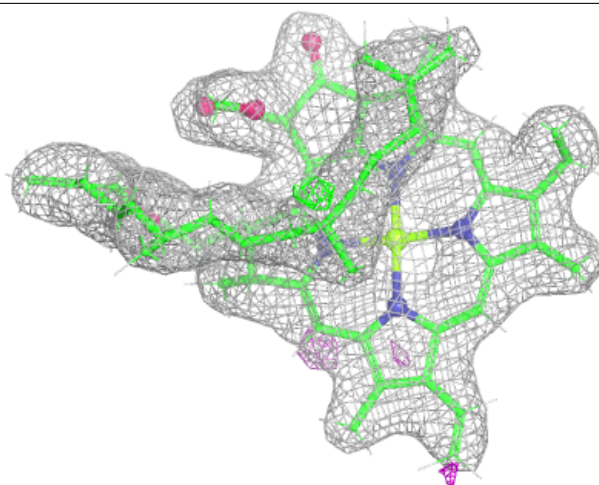
**Electron density around LHG D 411:**

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



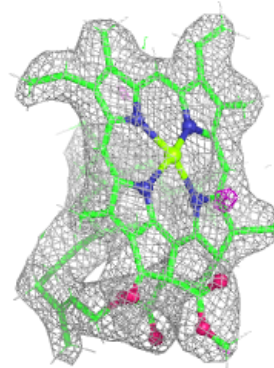
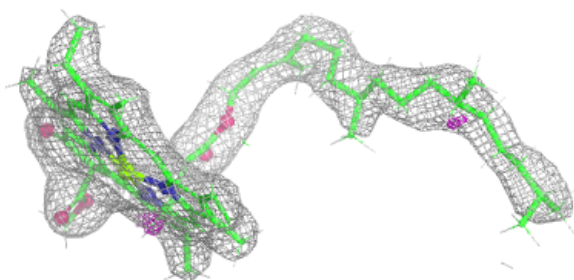
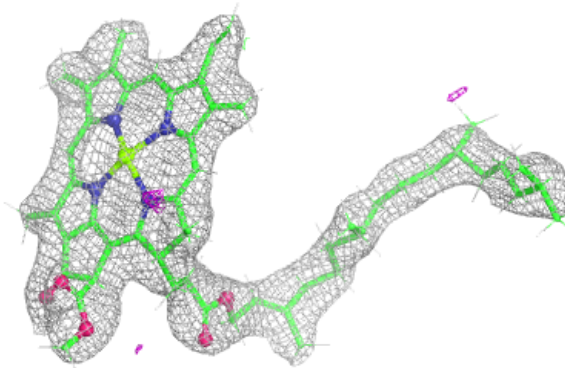
Electron density around CLA C 511:

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

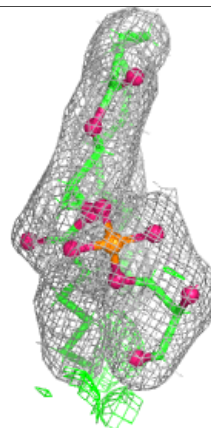
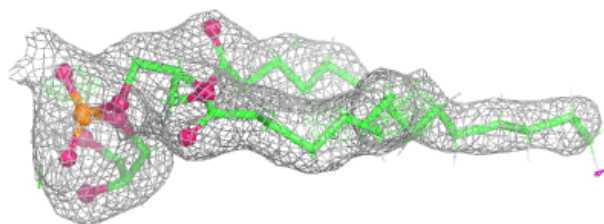
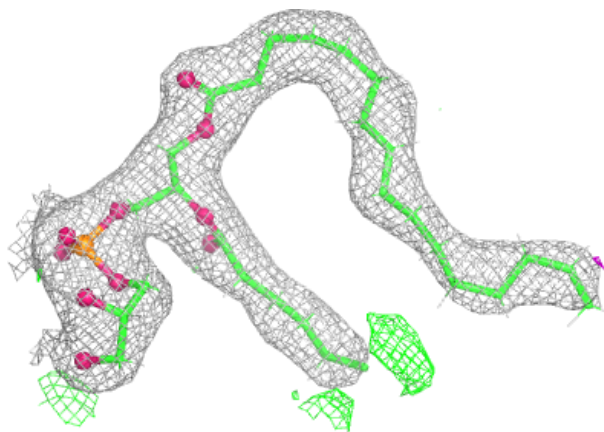


Electron density around CLA C 512:

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

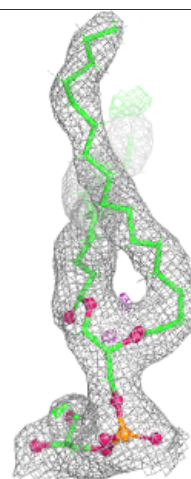
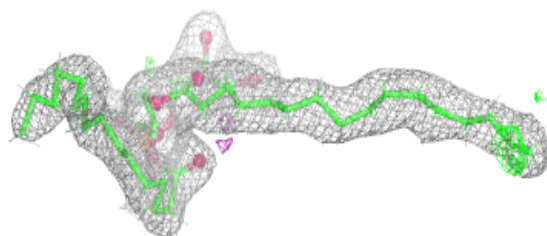
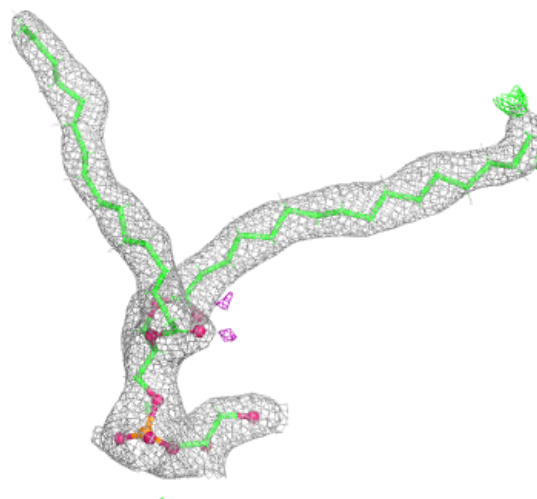
**Electron density around LHG d 410:**

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



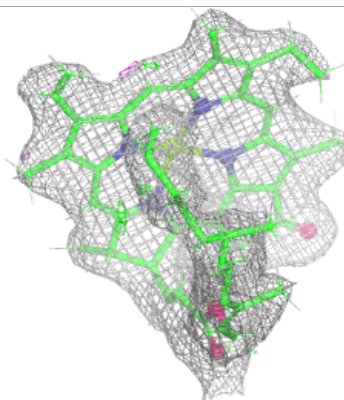
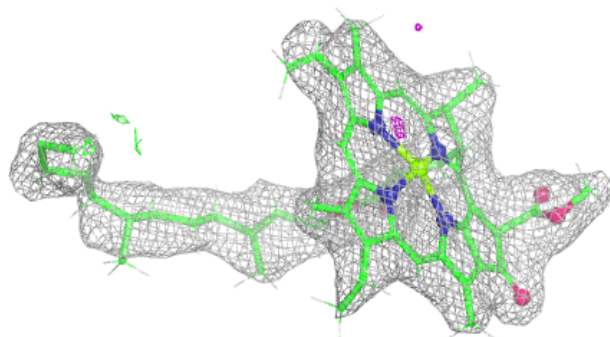
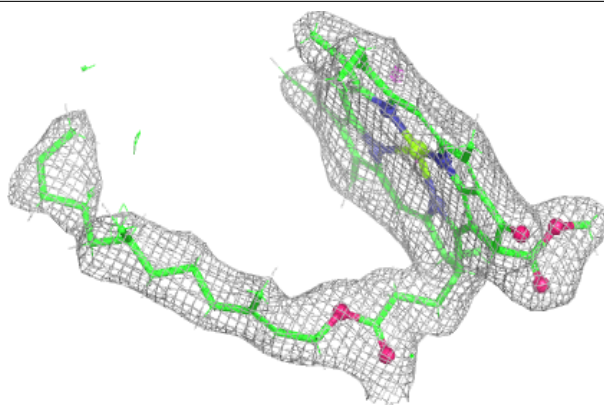
Electron density around LHG 1 101:

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

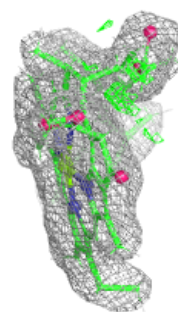
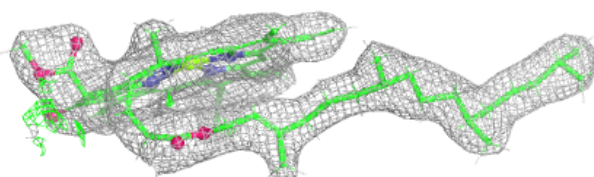
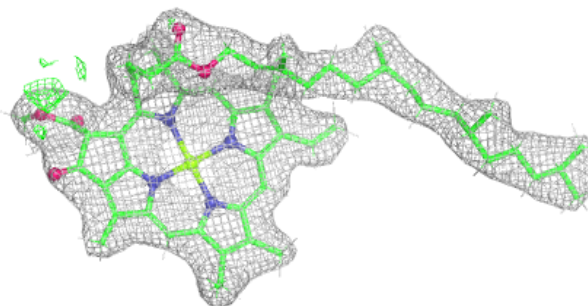


Electron density around CLA C 505:

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

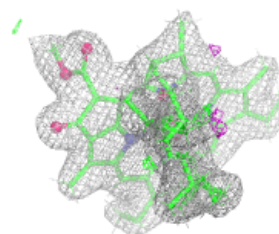
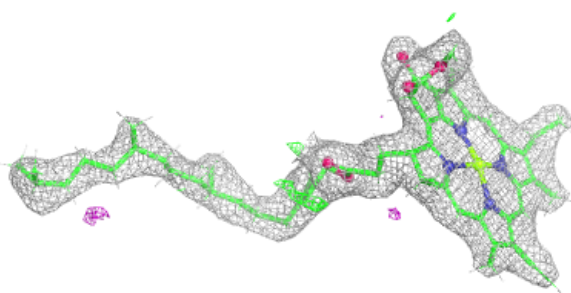
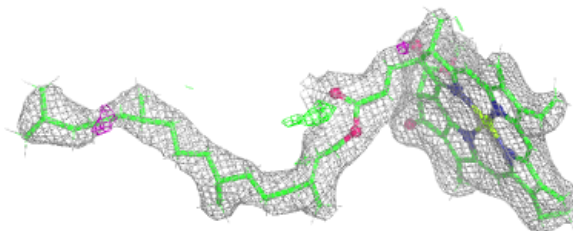
**Electron density around CLA c 501:**

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

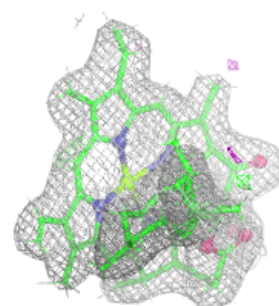
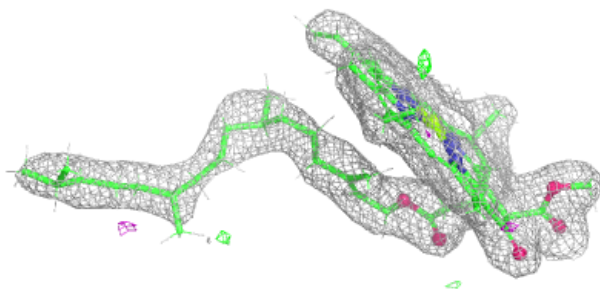
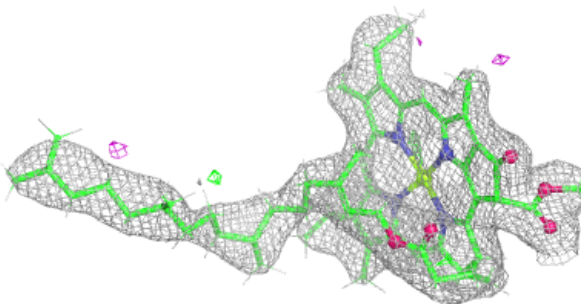


Electron density around CLA c 502:

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

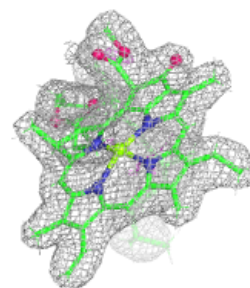
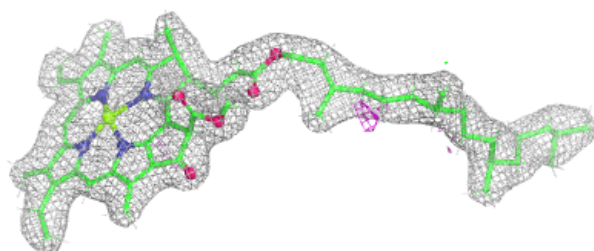
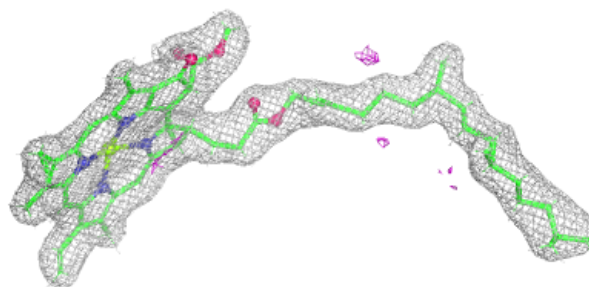
**Electron density around CLA C 506:**

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

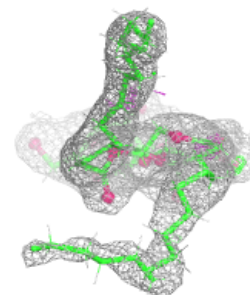
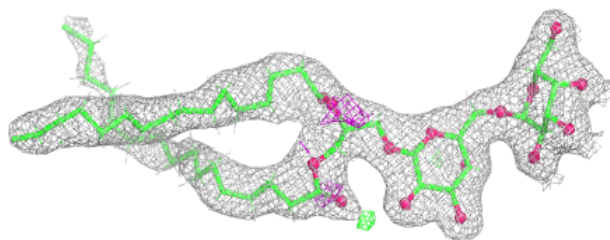
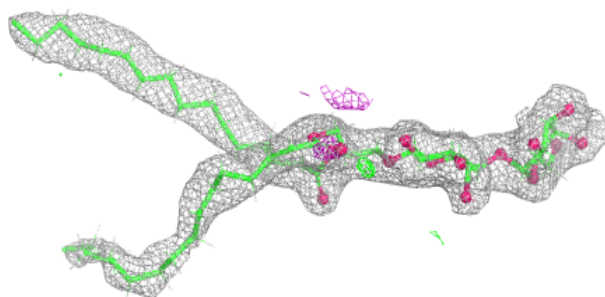


Electron density around CLA A 405:

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

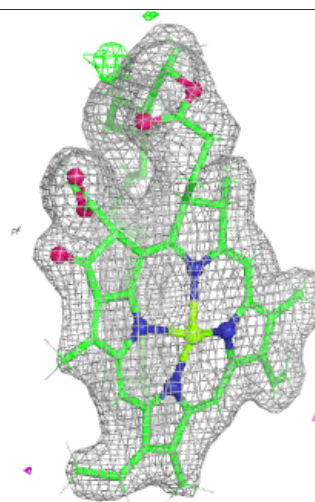
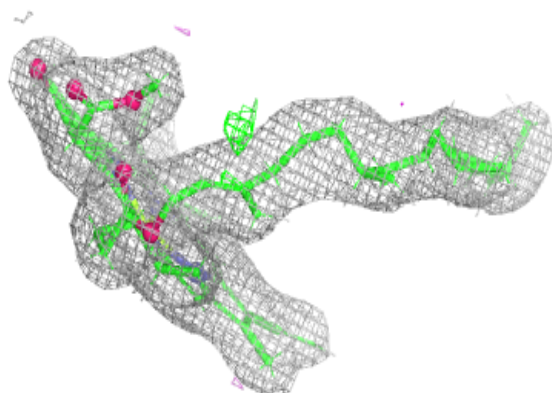
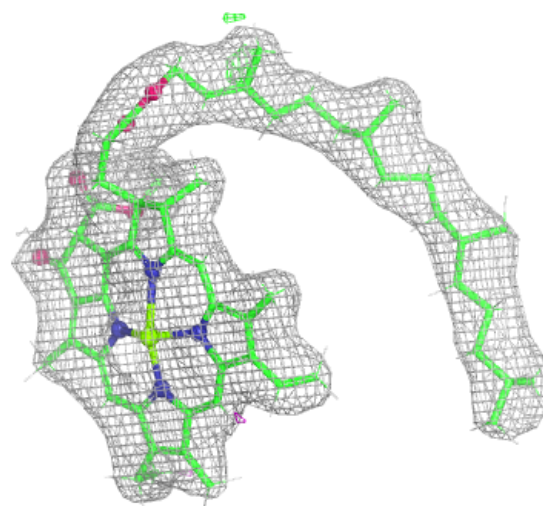
**Electron density around DGD c 516:**

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



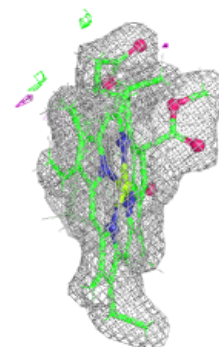
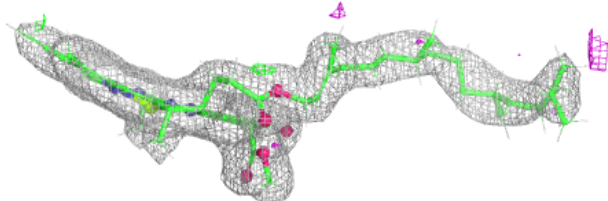
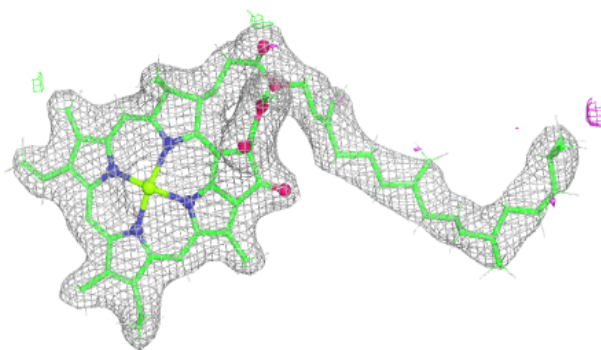
Electron density around CLA C 508:

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



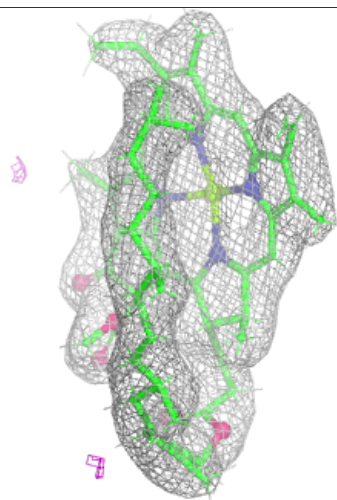
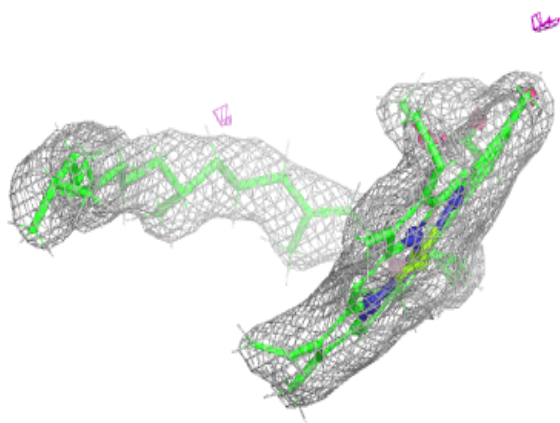
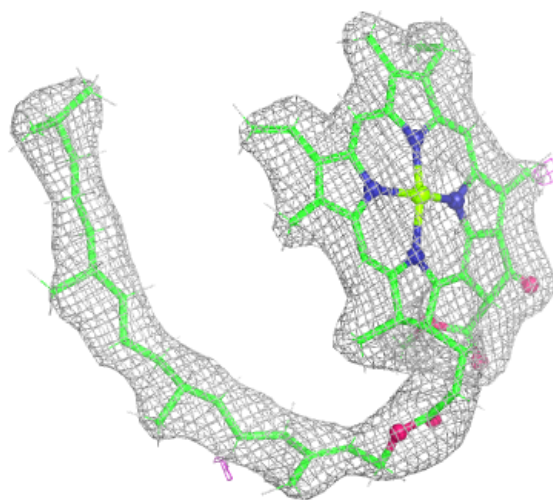
Electron density around CLA B 602:

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



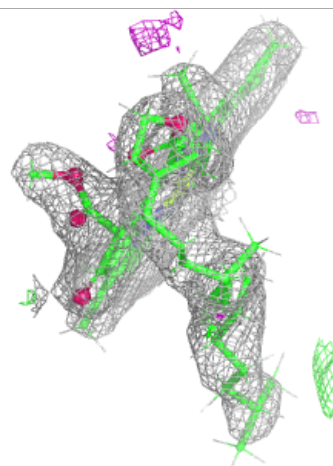
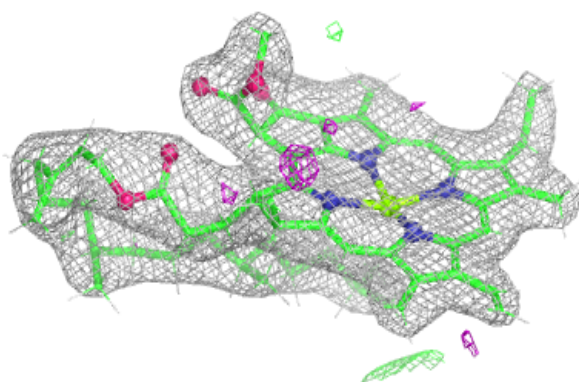
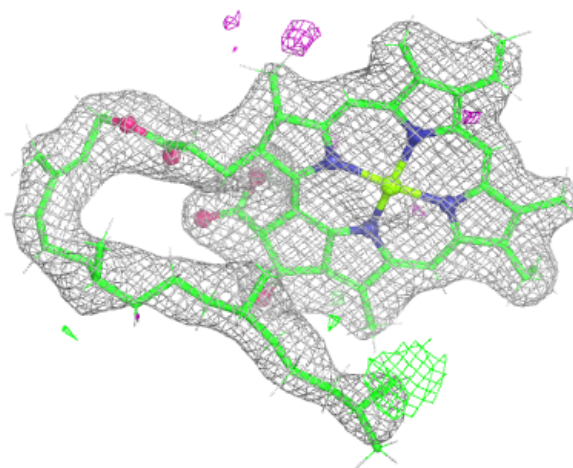
Electron density around CLA c 507:

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



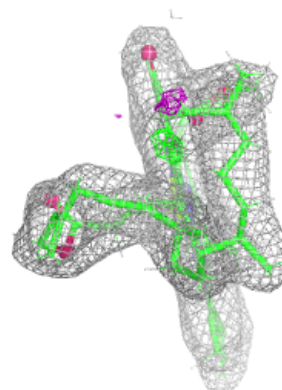
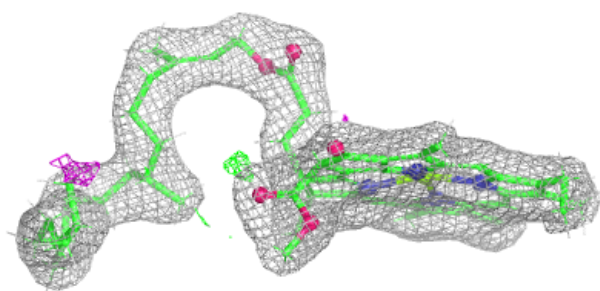
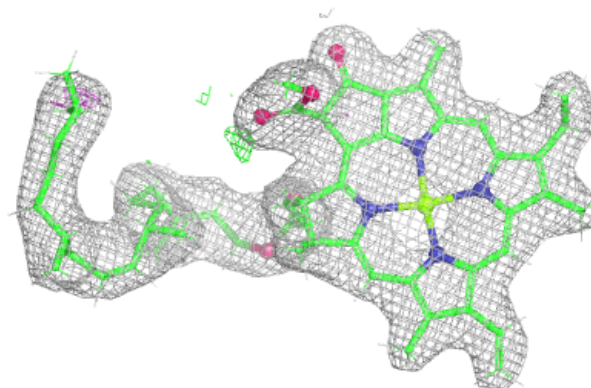
Electron density around CLA C 510:

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

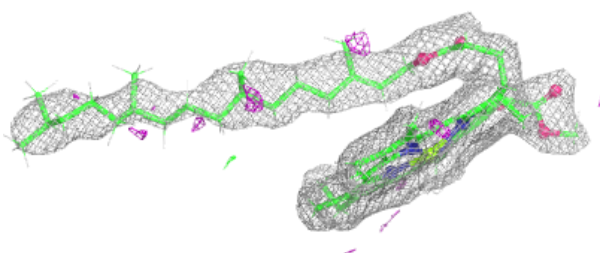
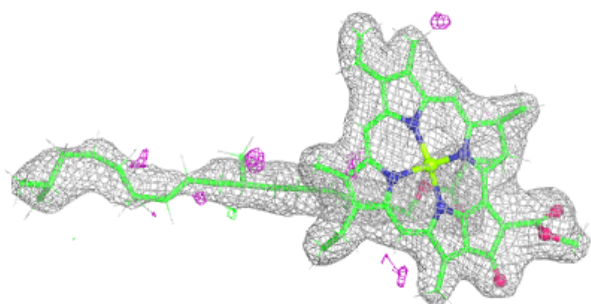


Electron density around CLA B 612:

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

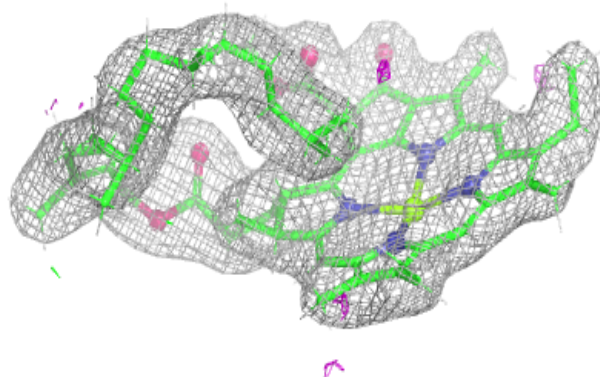
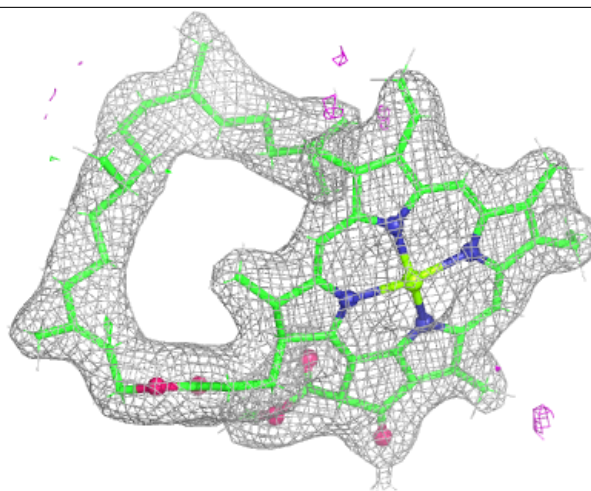
**Electron density around CLA B 614:**

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



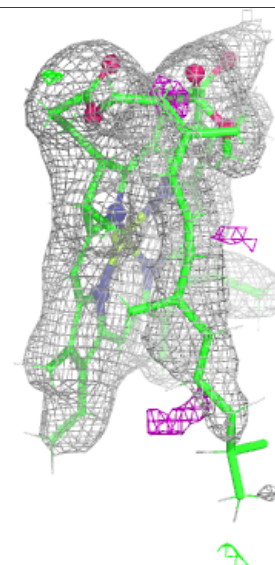
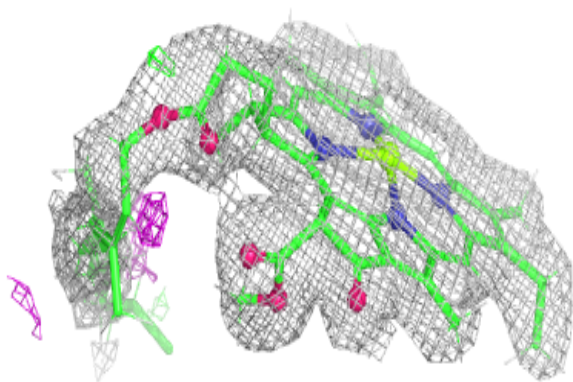
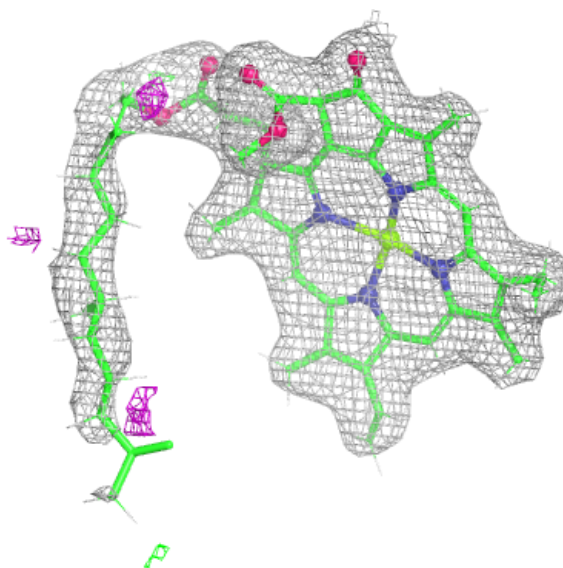
Electron density around CLA B 615:

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



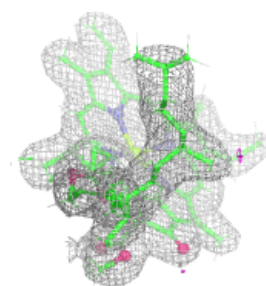
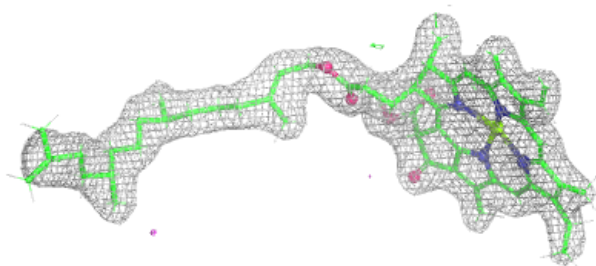
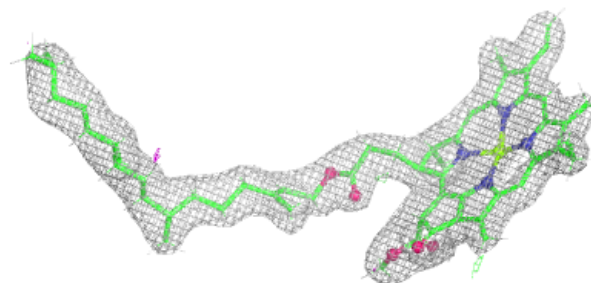
Electron density around CLA B 616:

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

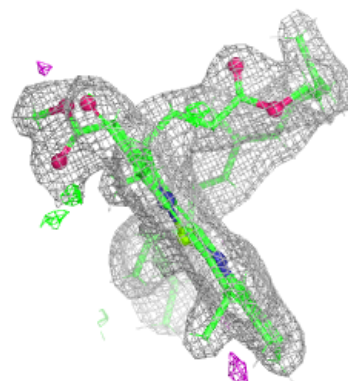
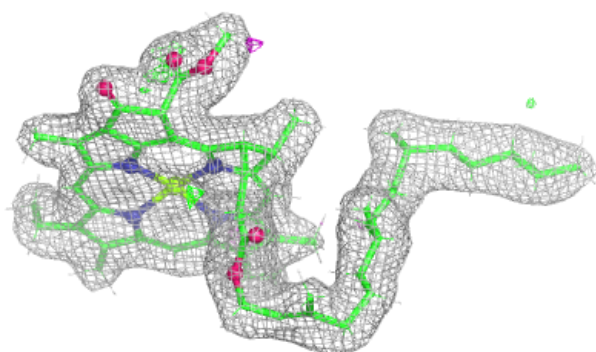
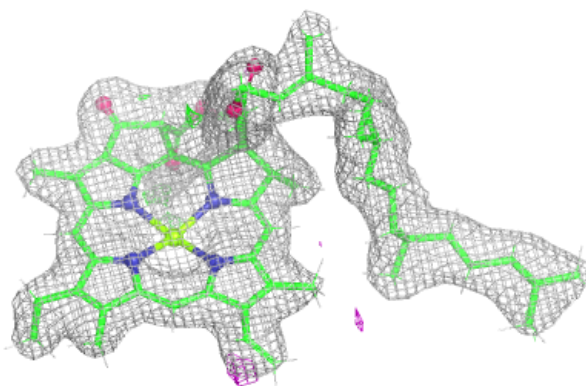


Electron density around CLA a 404:

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

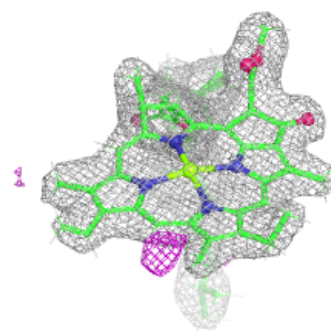
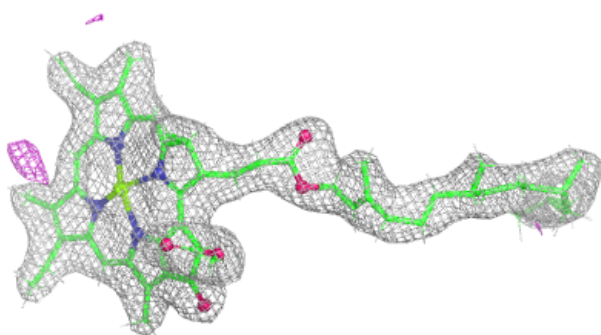
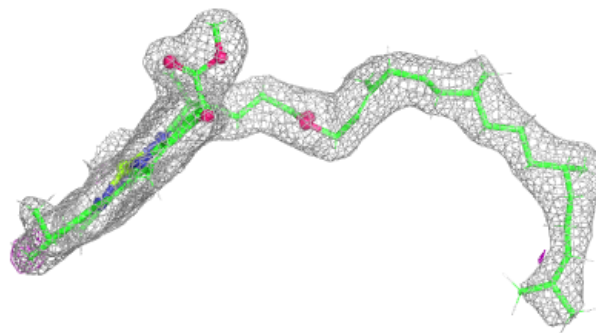
**Electron density around CLA d 403:**

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

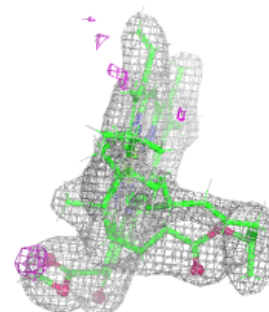
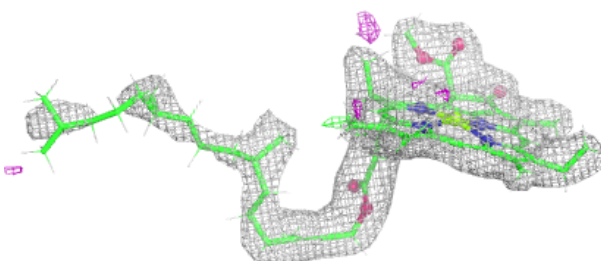
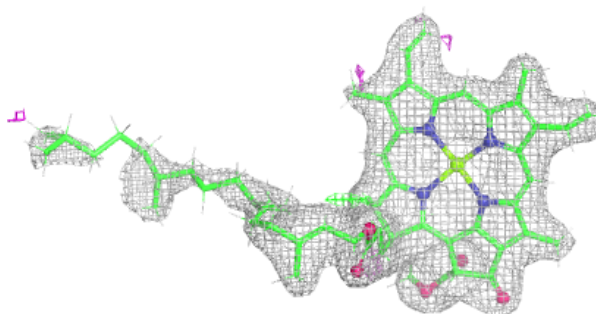


Electron density around CLA d 404:

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

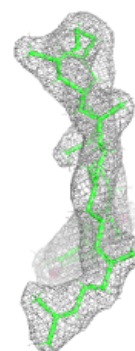
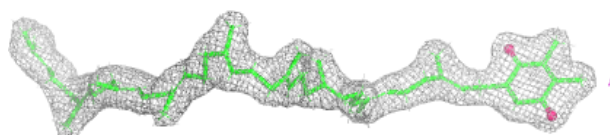
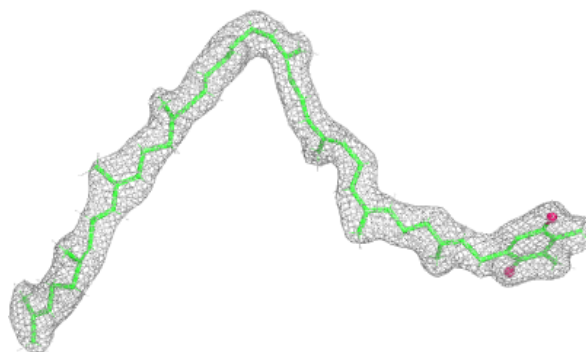
**Electron density around CLA a 405:**

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

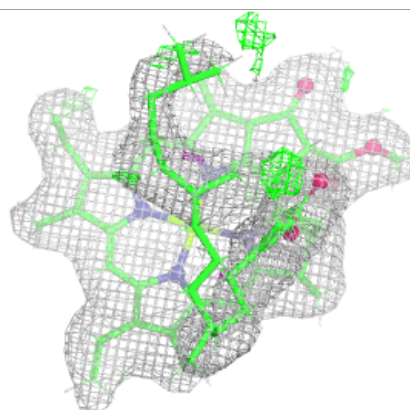
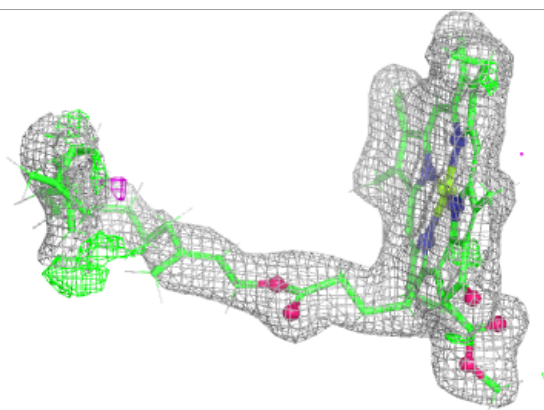
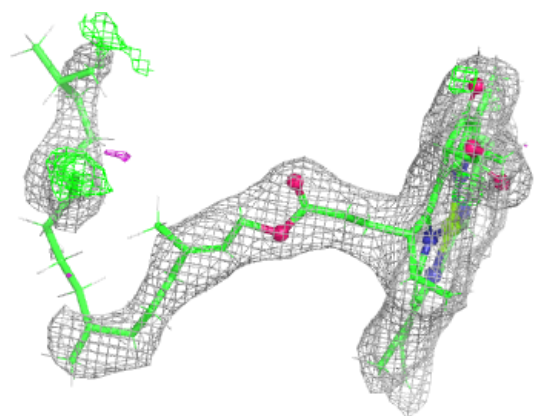


Electron density around PL9 D 406:

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

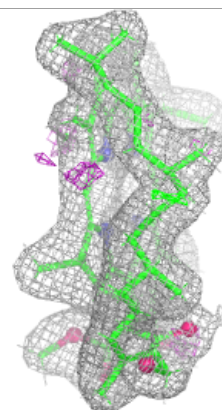
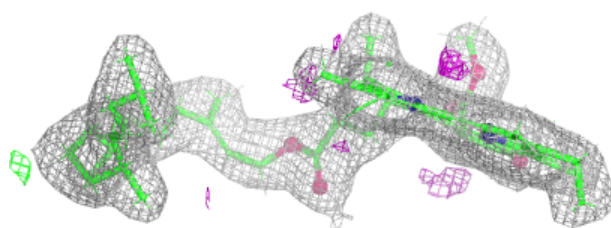
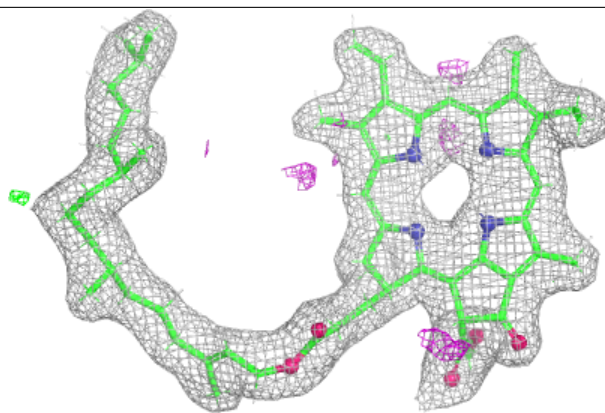
**Electron density around CLA a 407:**

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

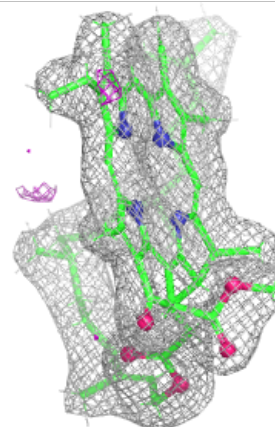
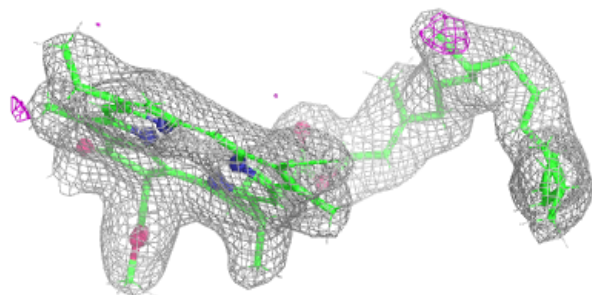
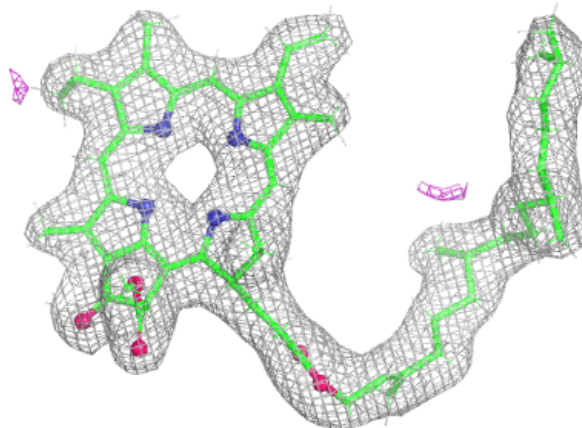


Electron density around PHO A 407:

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

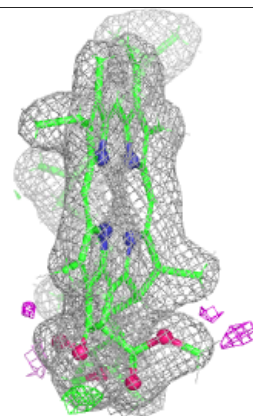
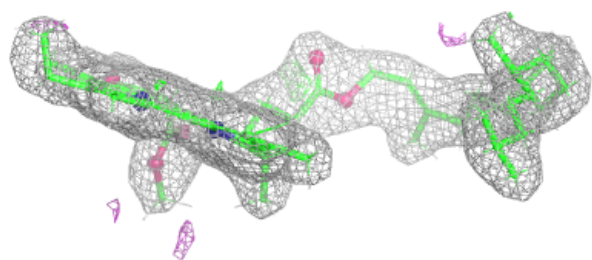
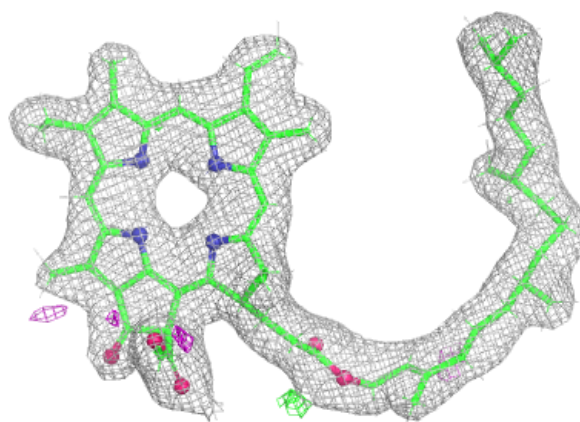
**Electron density around PHO D 401:**

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



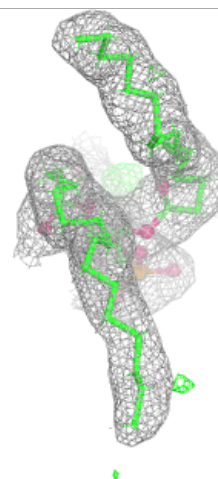
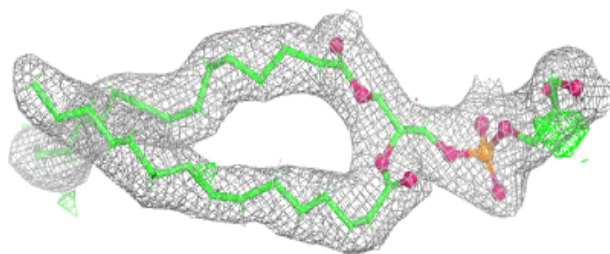
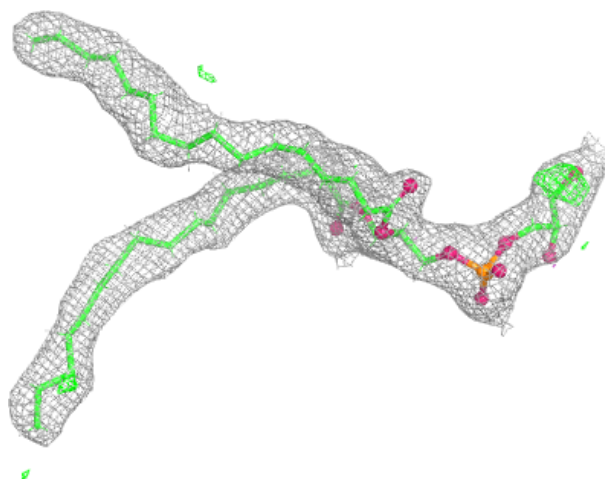
Electron density around PHO a 406:

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



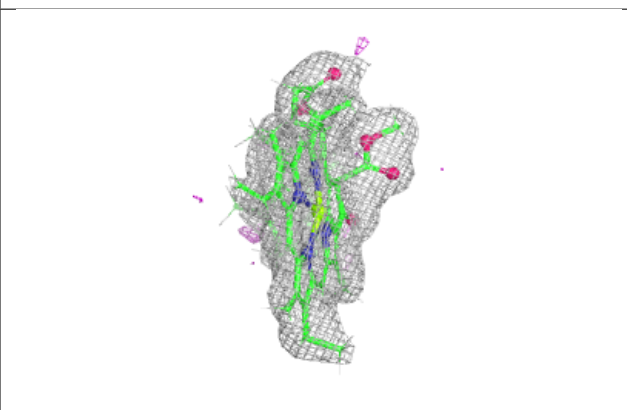
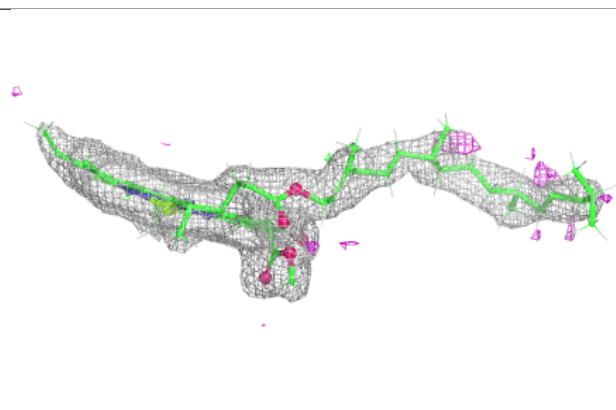
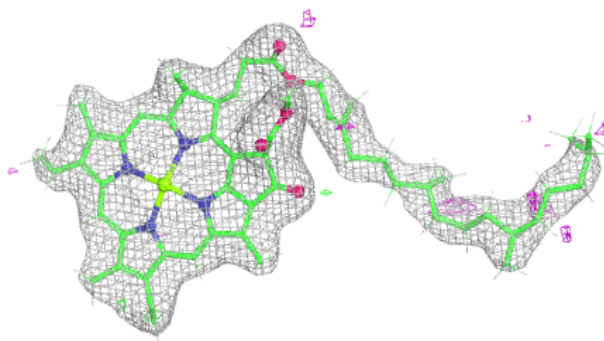
Electron density around LHG D 408:

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

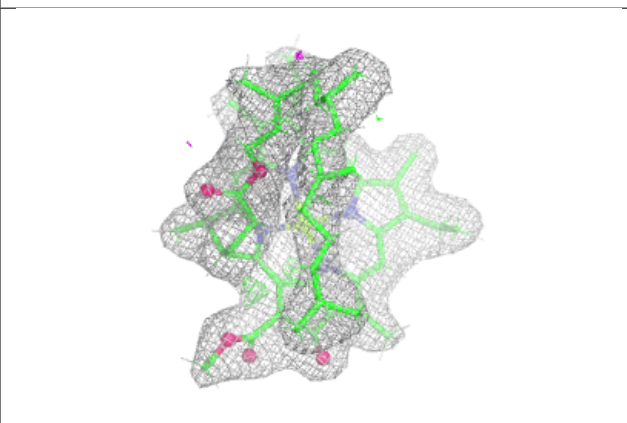
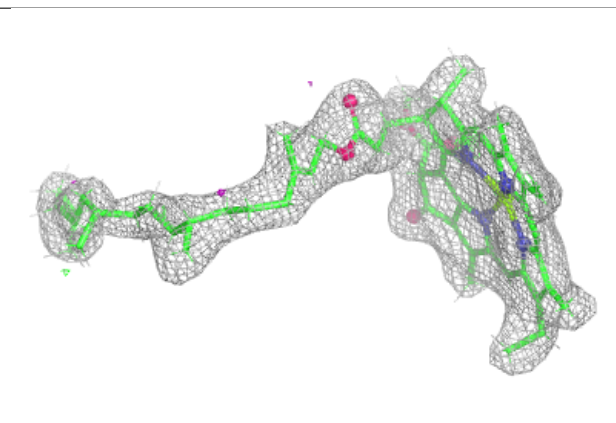
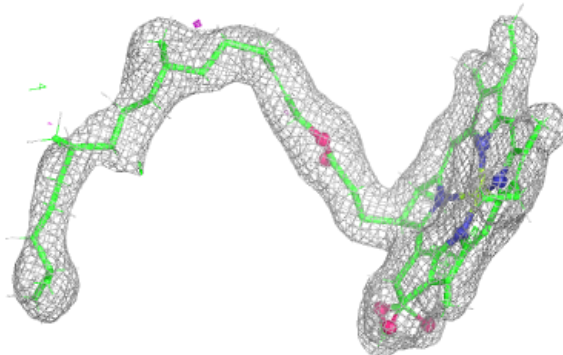


Electron density around CLA b 603:

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

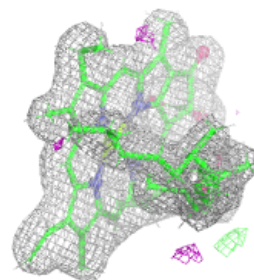
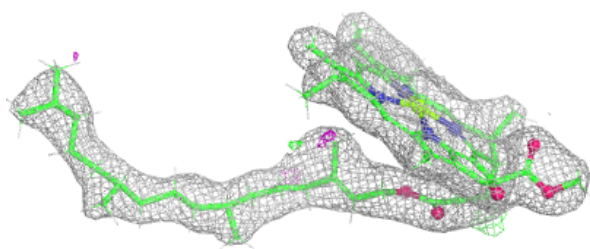
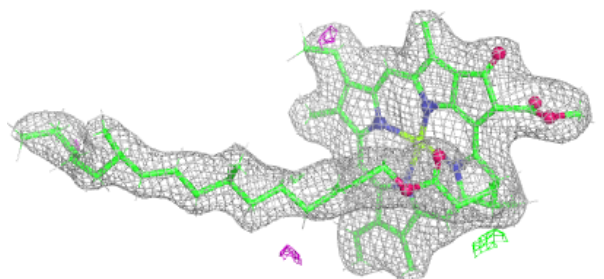
**Electron density around CLA b 607:**

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

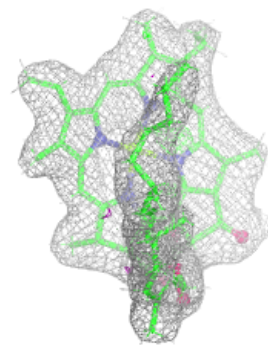
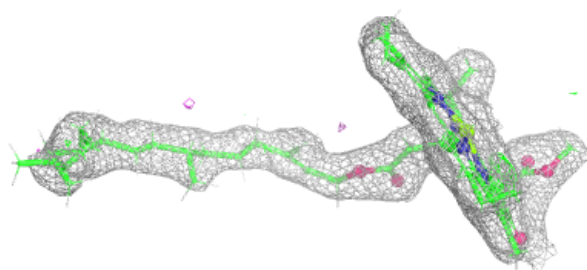
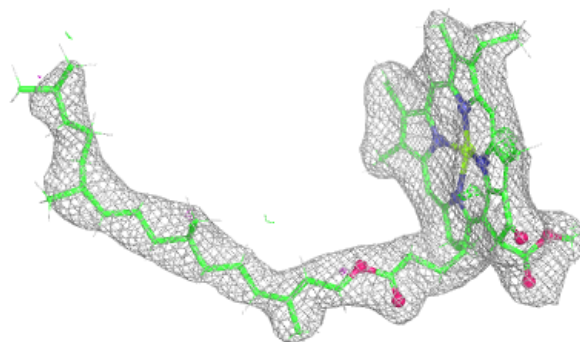


Electron density around CLA b 609:

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

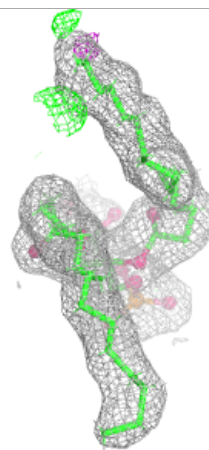
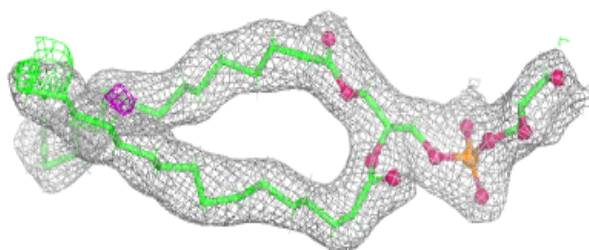
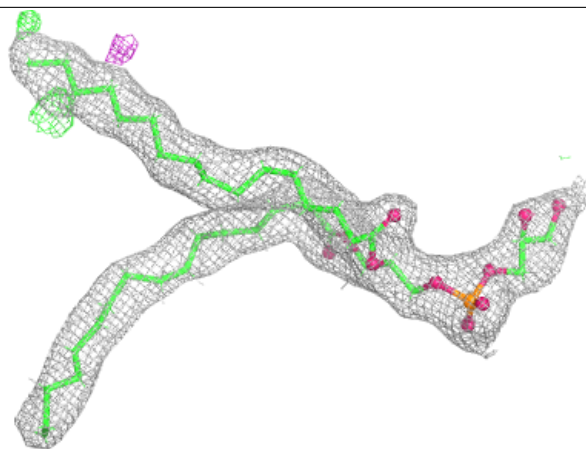
**Electron density around CLA b 610:**

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



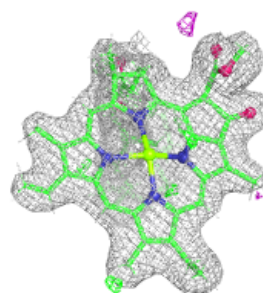
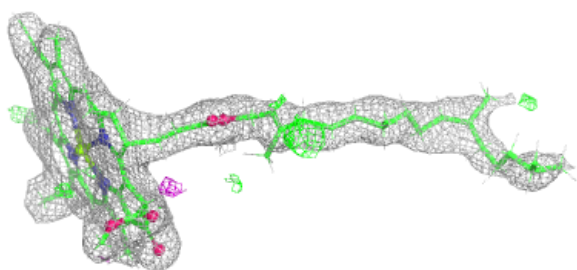
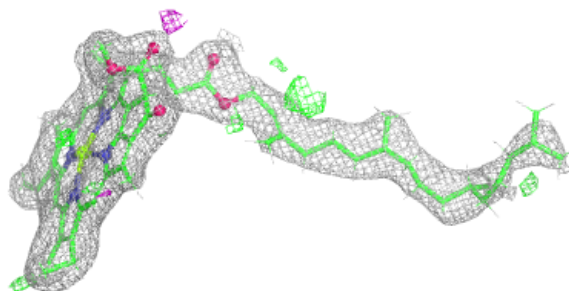
Electron density around LHG d 409:

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

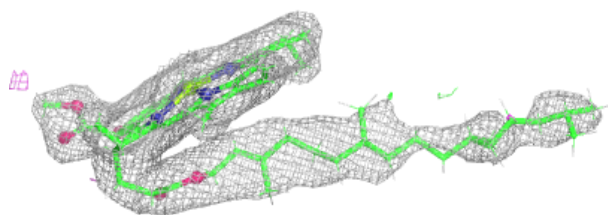
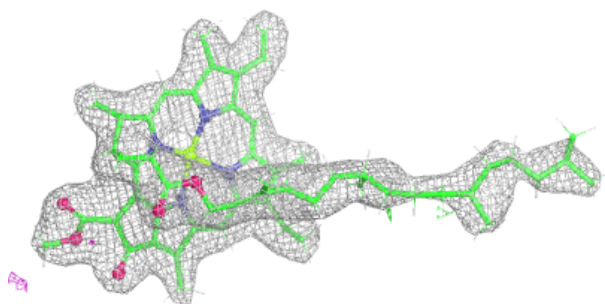


Electron density around CLA B 604:

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

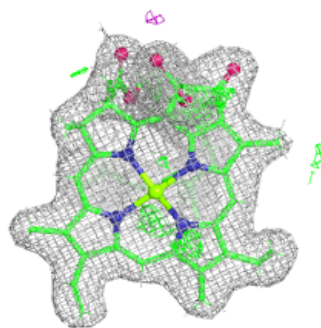
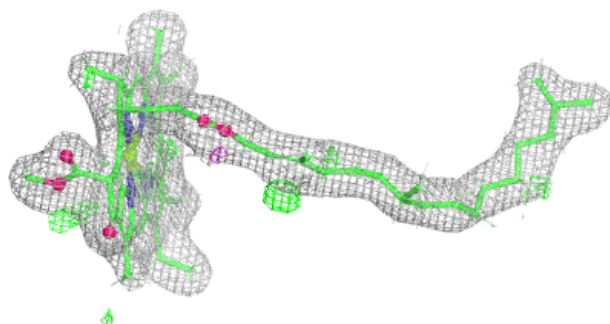
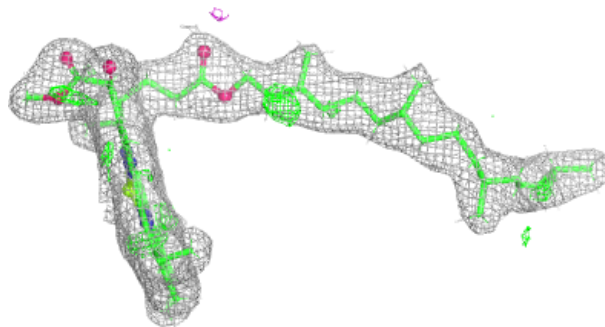
**Electron density around CLA b 615:**

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

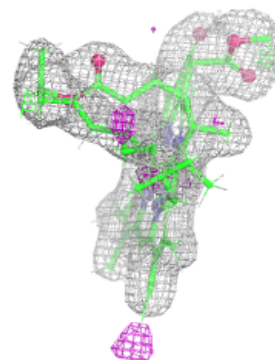
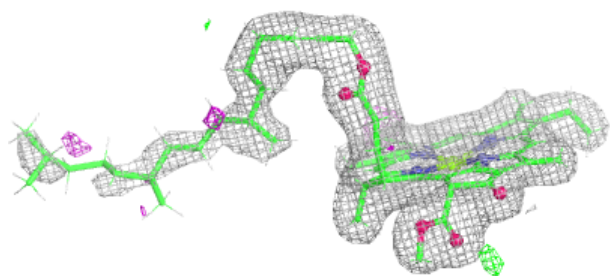
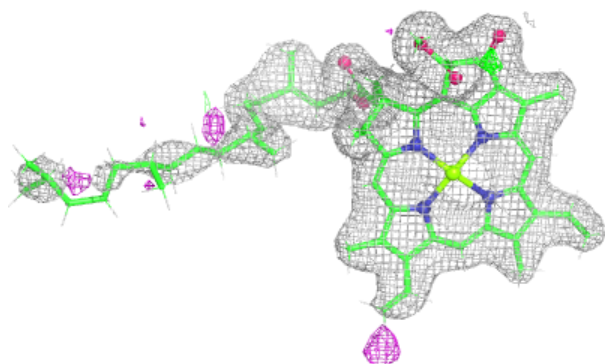


Electron density around CLA B 605:

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

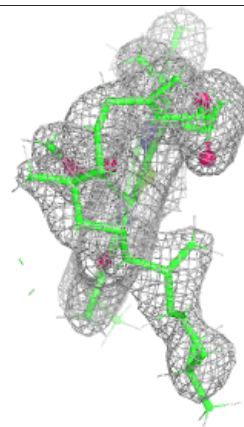
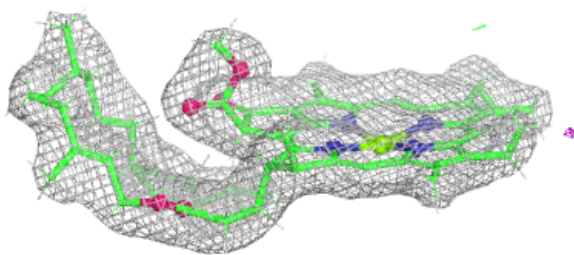
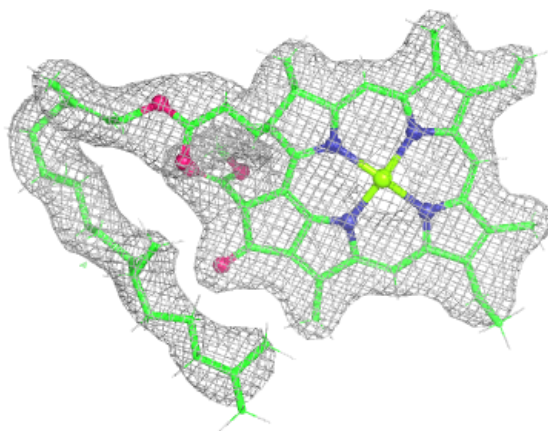
**Electron density around CLA A 406:**

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



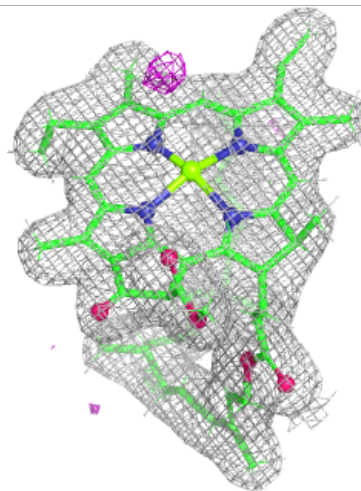
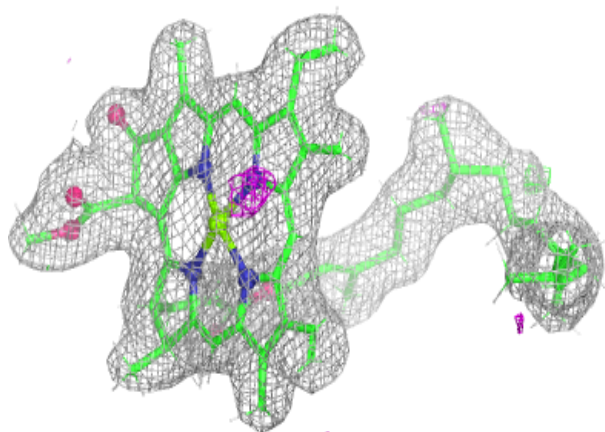
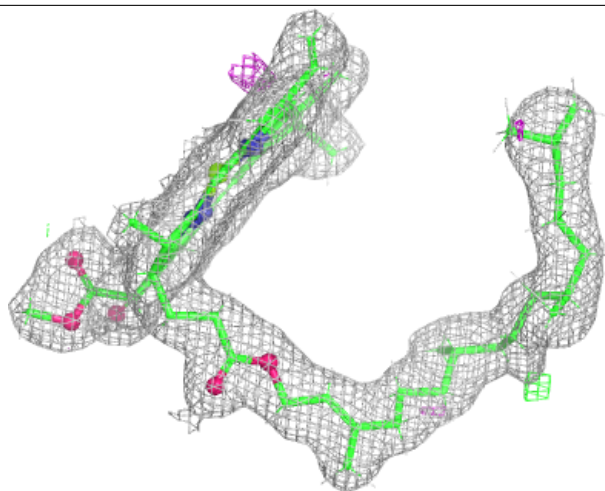
Electron density around CLA b 611:

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



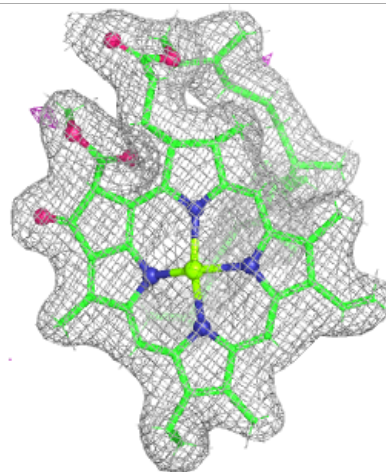
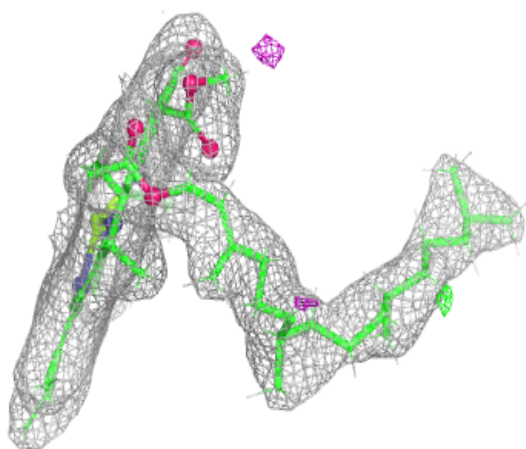
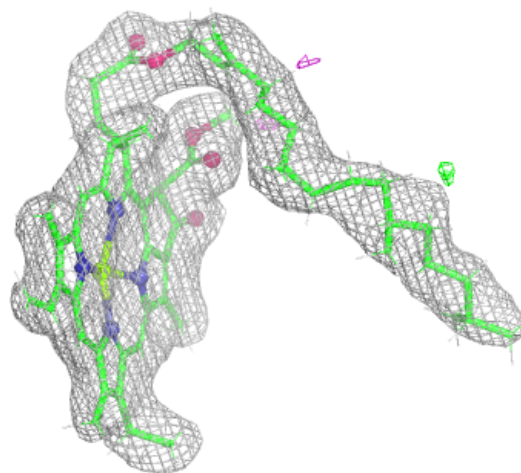
Electron density around CLA b 612:

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



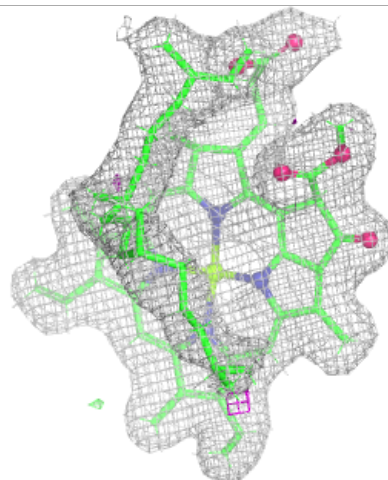
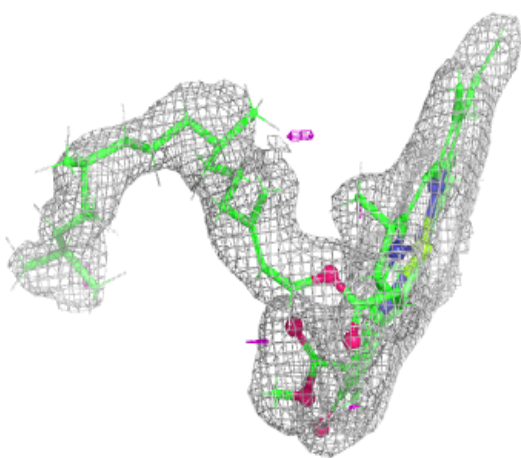
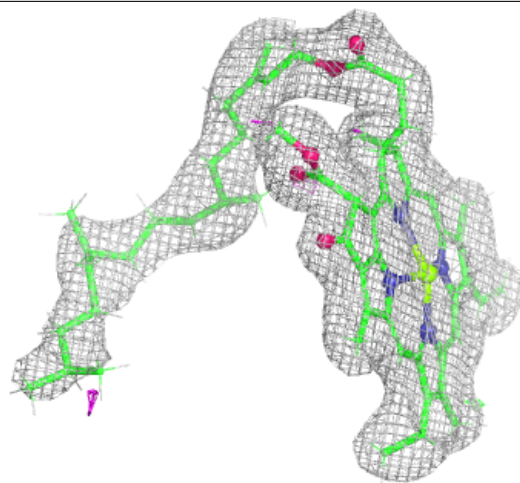
Electron density around CLA B 613:

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



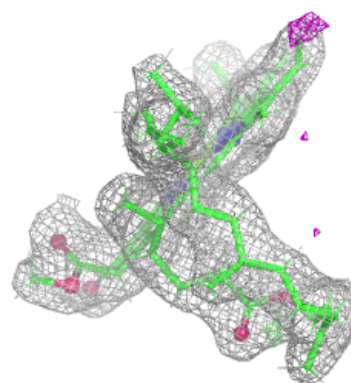
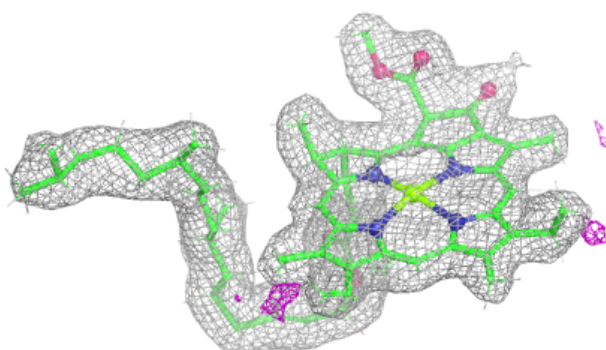
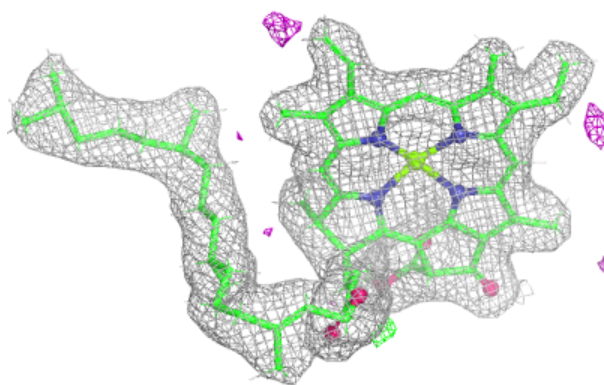
Electron density around CLA b 614:

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

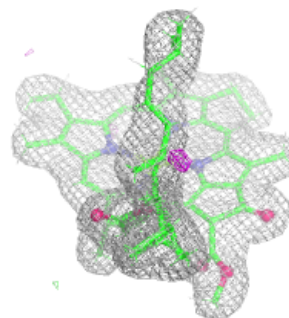
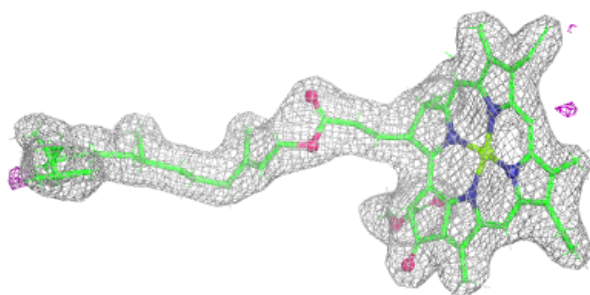
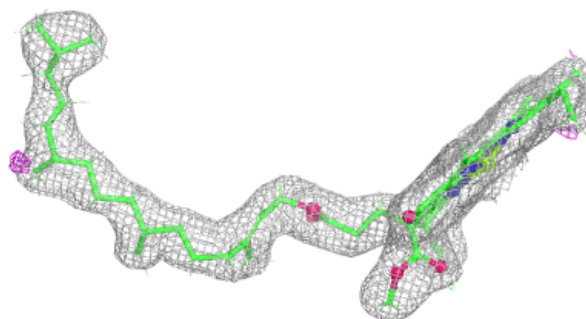


Electron density around CLA D 402:

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

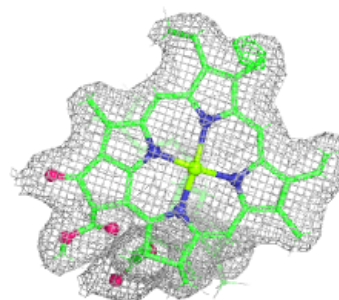
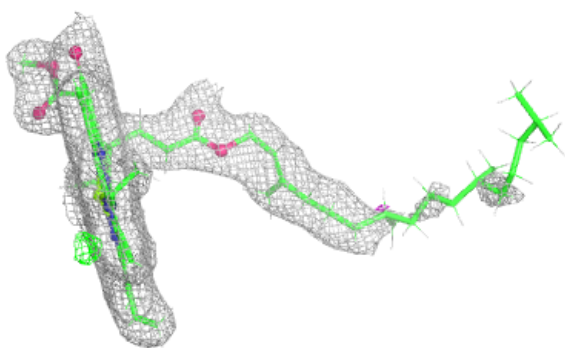
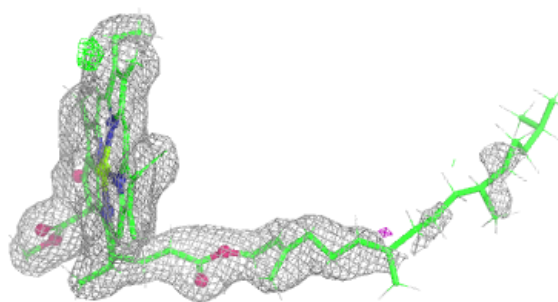
**Electron density around CLA D 403:**

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

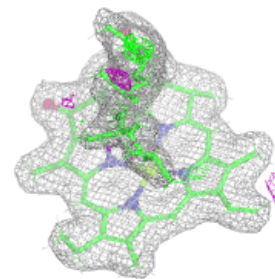
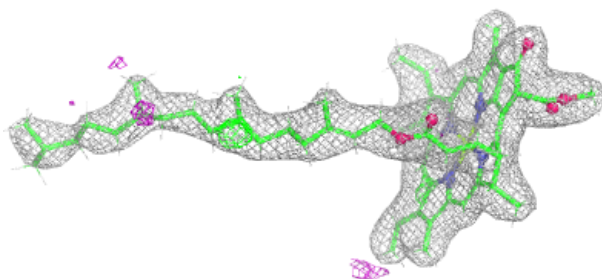
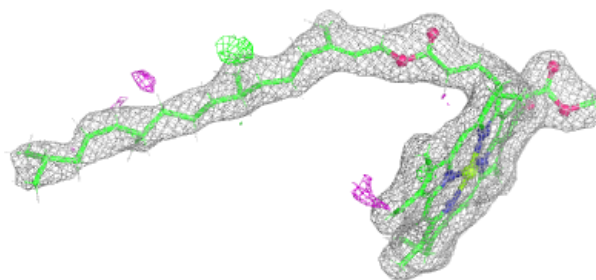


Electron density around CLA D 404:

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

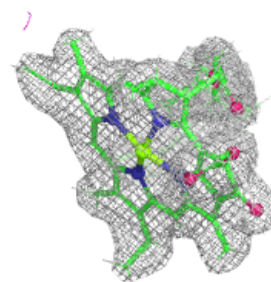
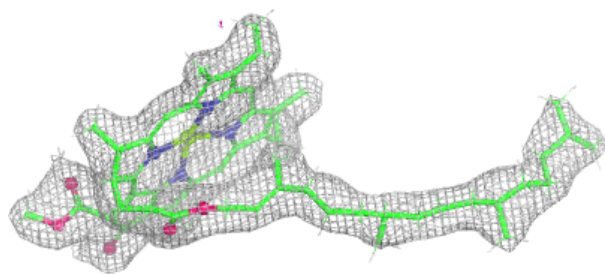
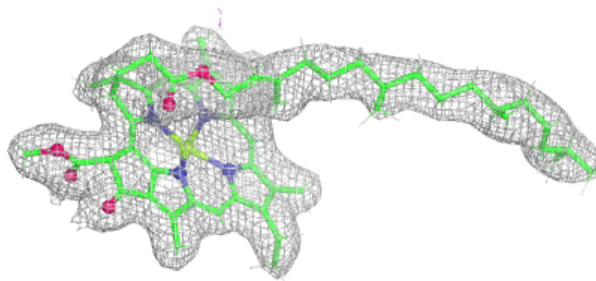
**Electron density around CLA B 607:**

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

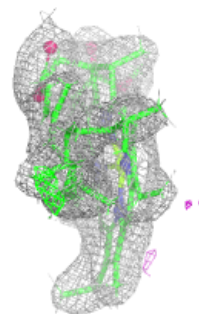
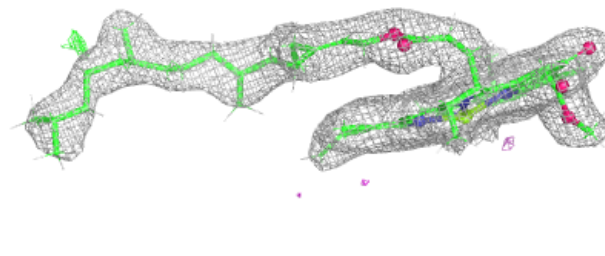
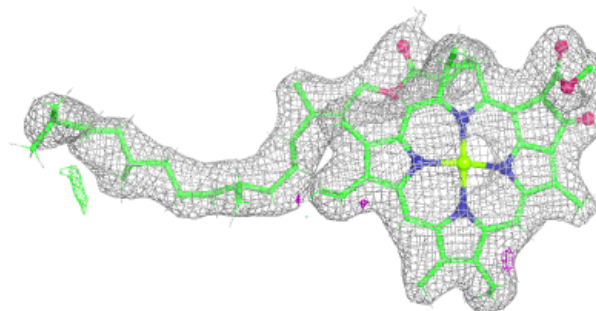


Electron density around CLA B 608:

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

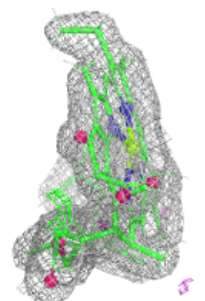
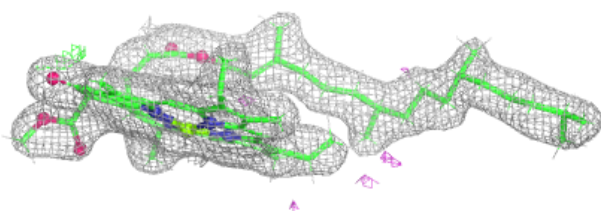
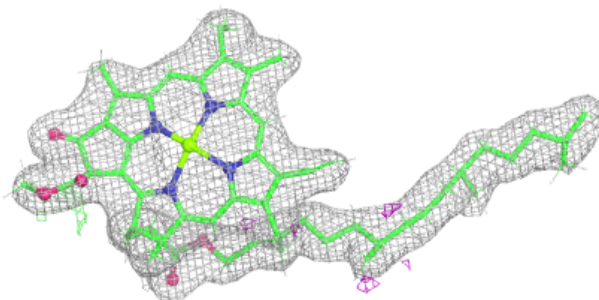
**Electron density around CLA B 603:**

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

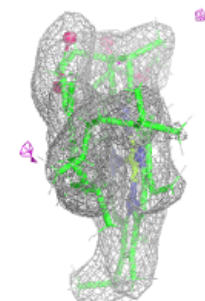
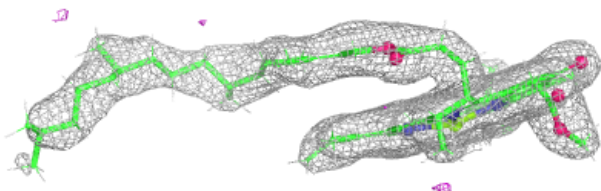
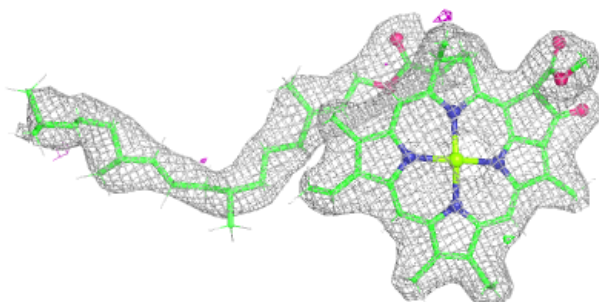


Electron density around CLA C 502:

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

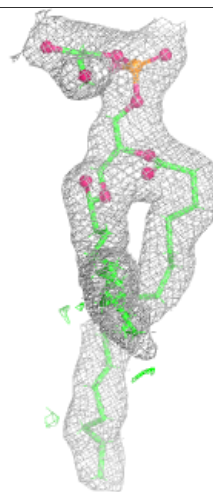
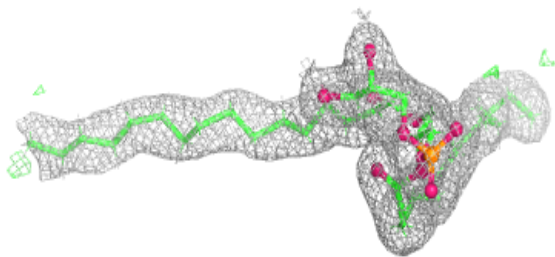
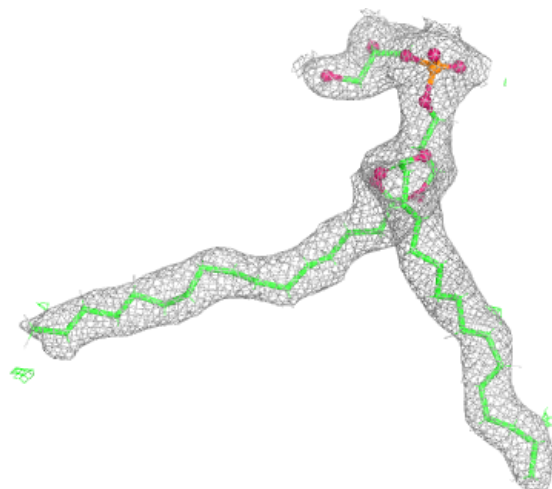
**Electron density around CLA b 604:**

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



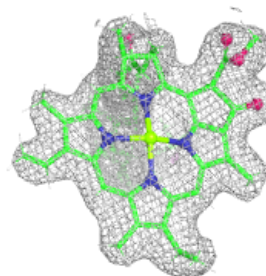
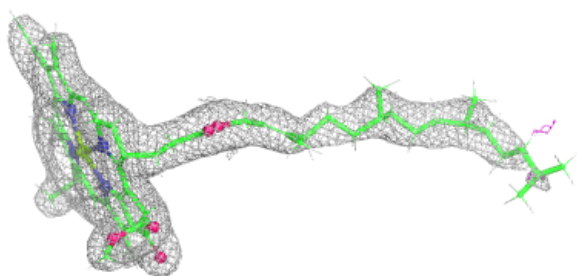
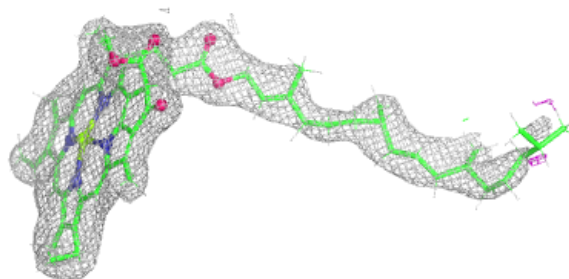
Electron density around LHG L 101:

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

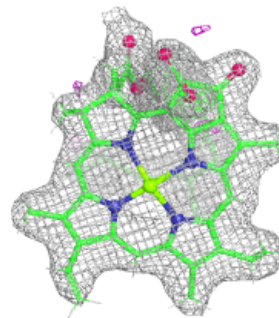
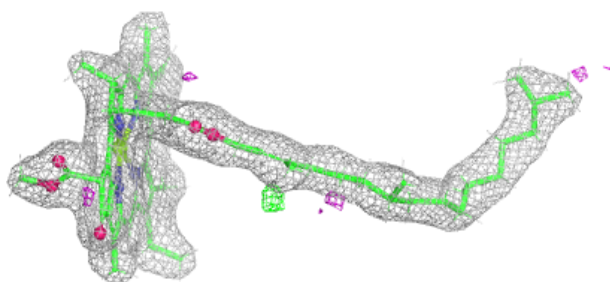
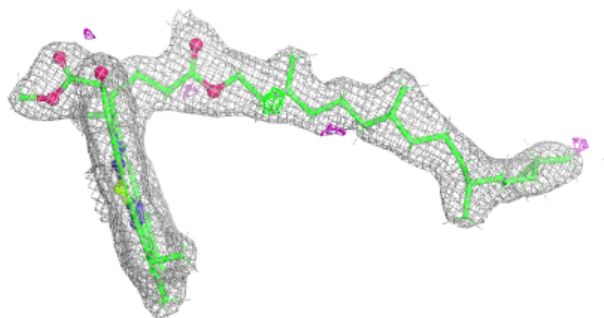


Electron density around CLA b 605:

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

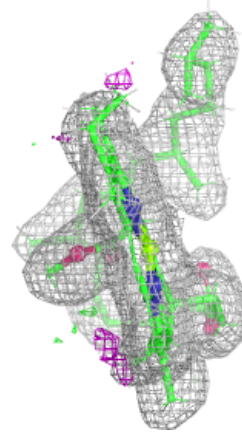
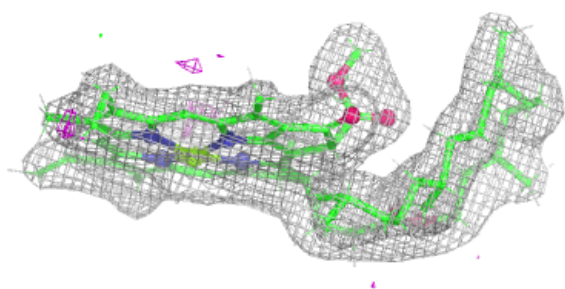
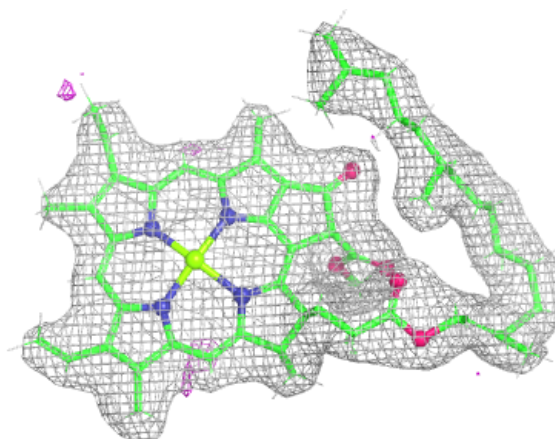
**Electron density around CLA b 606:**

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



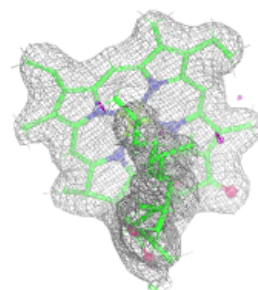
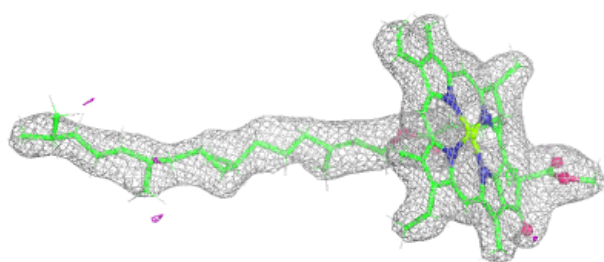
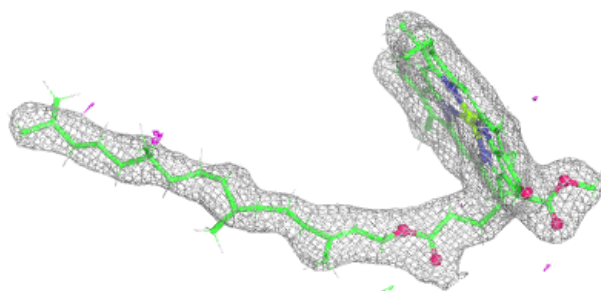
Electron density around CLA B 610:

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



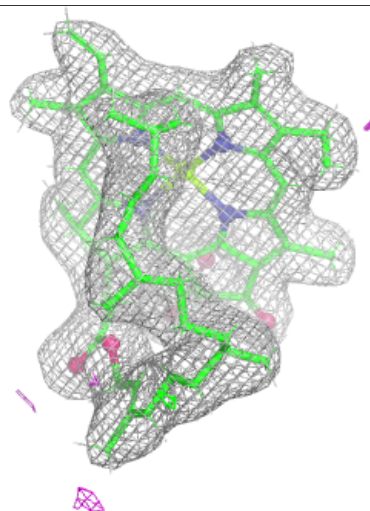
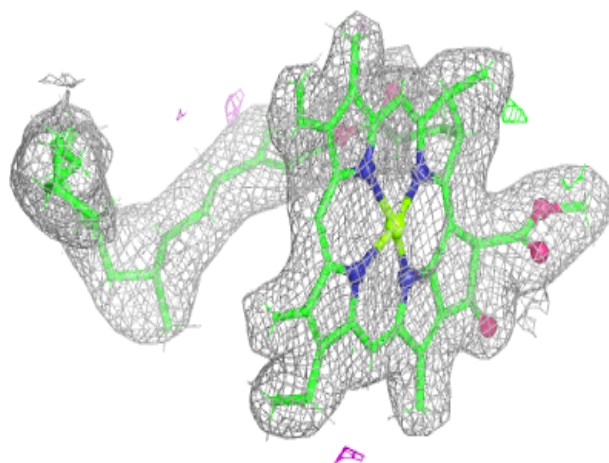
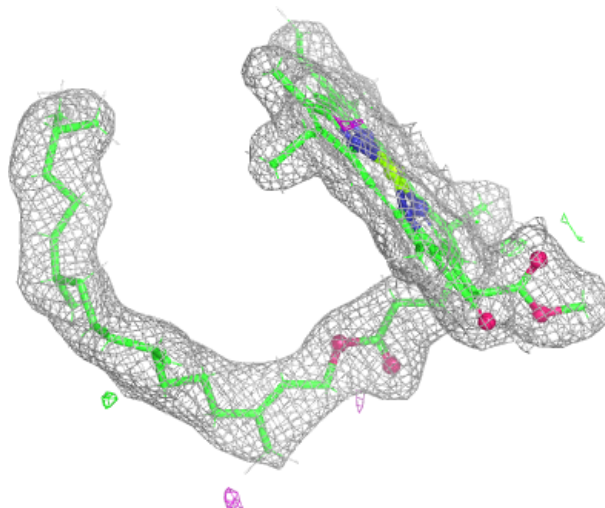
Electron density around CLA b 608:

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



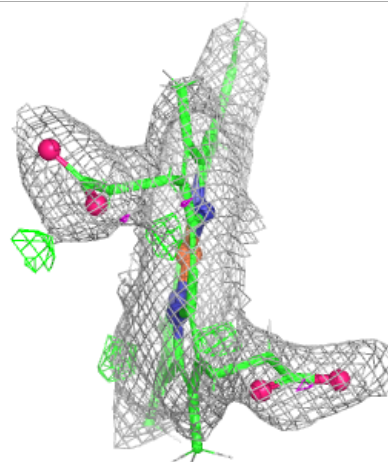
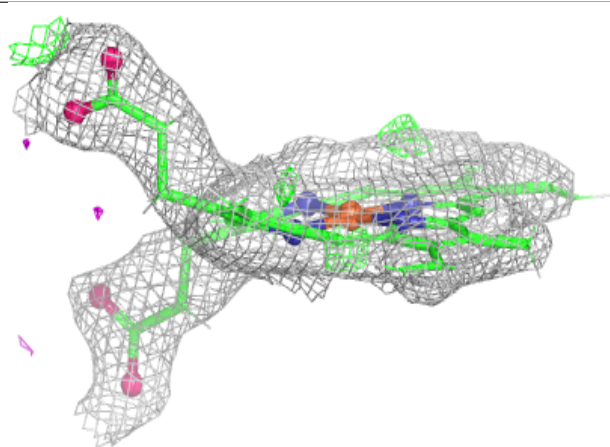
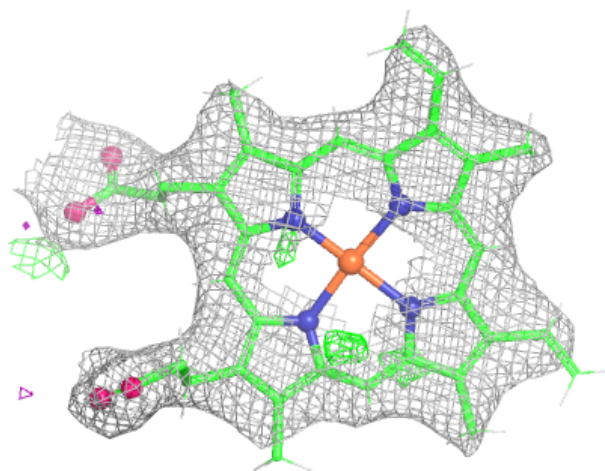
Electron density around CLA B 611:

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



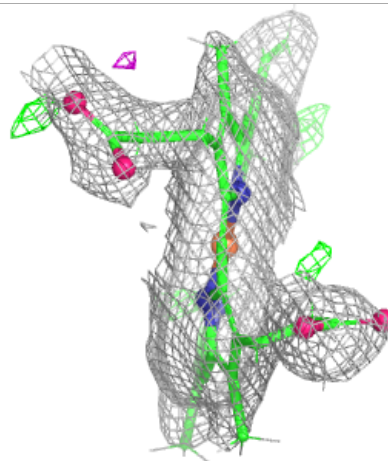
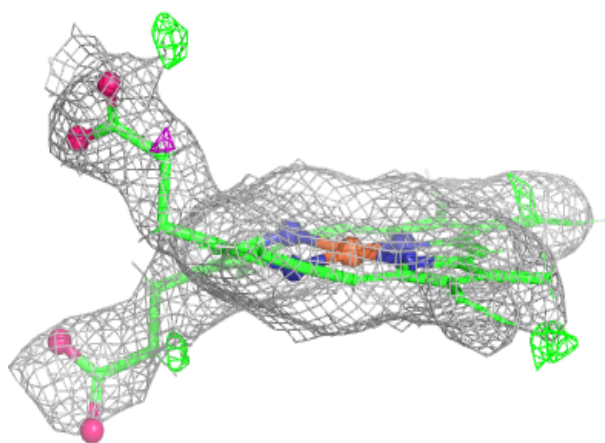
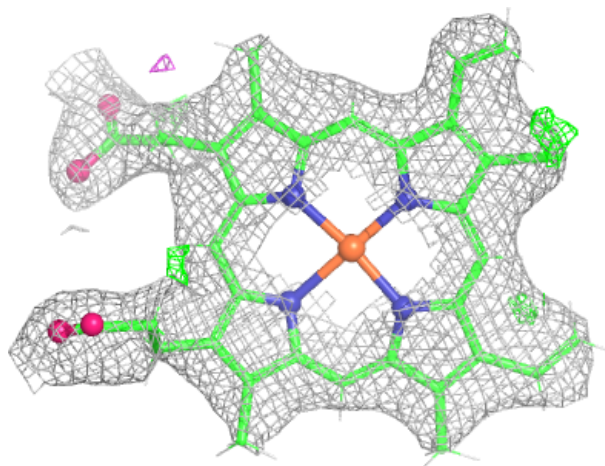
Electron density around HEM F 102:

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



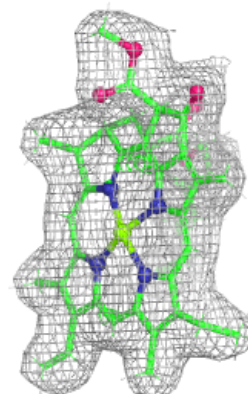
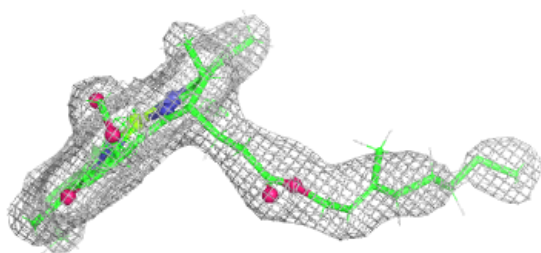
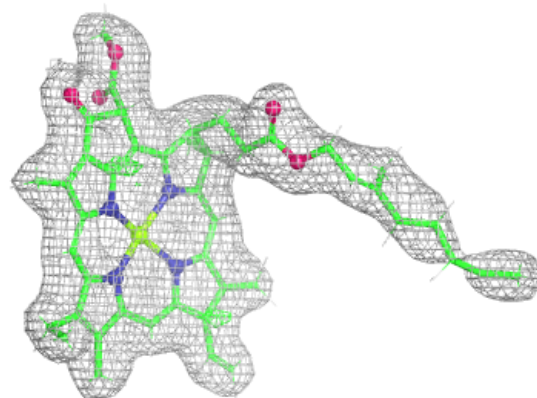
Electron density around HEM e 102:

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



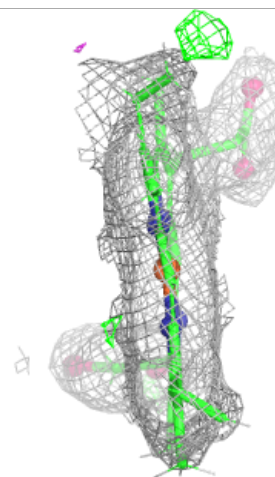
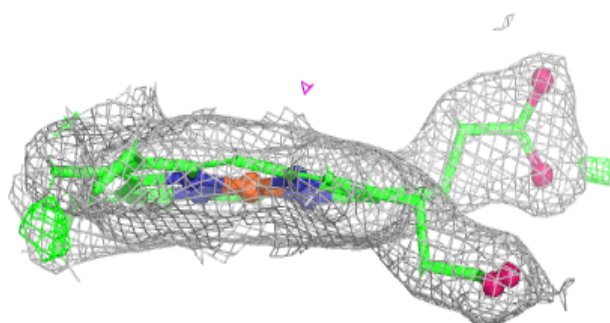
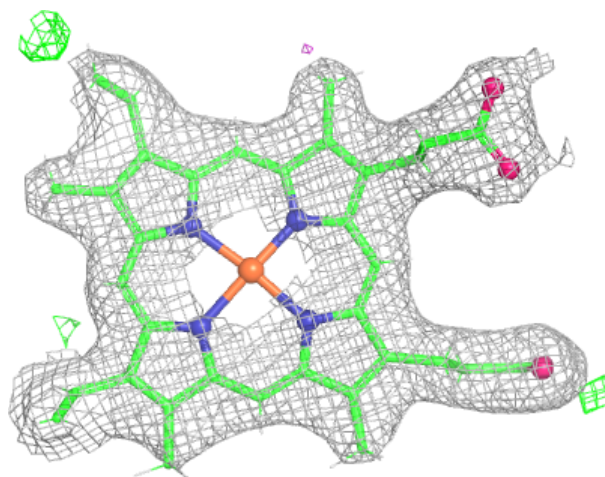
Electron density around CLA A 408:

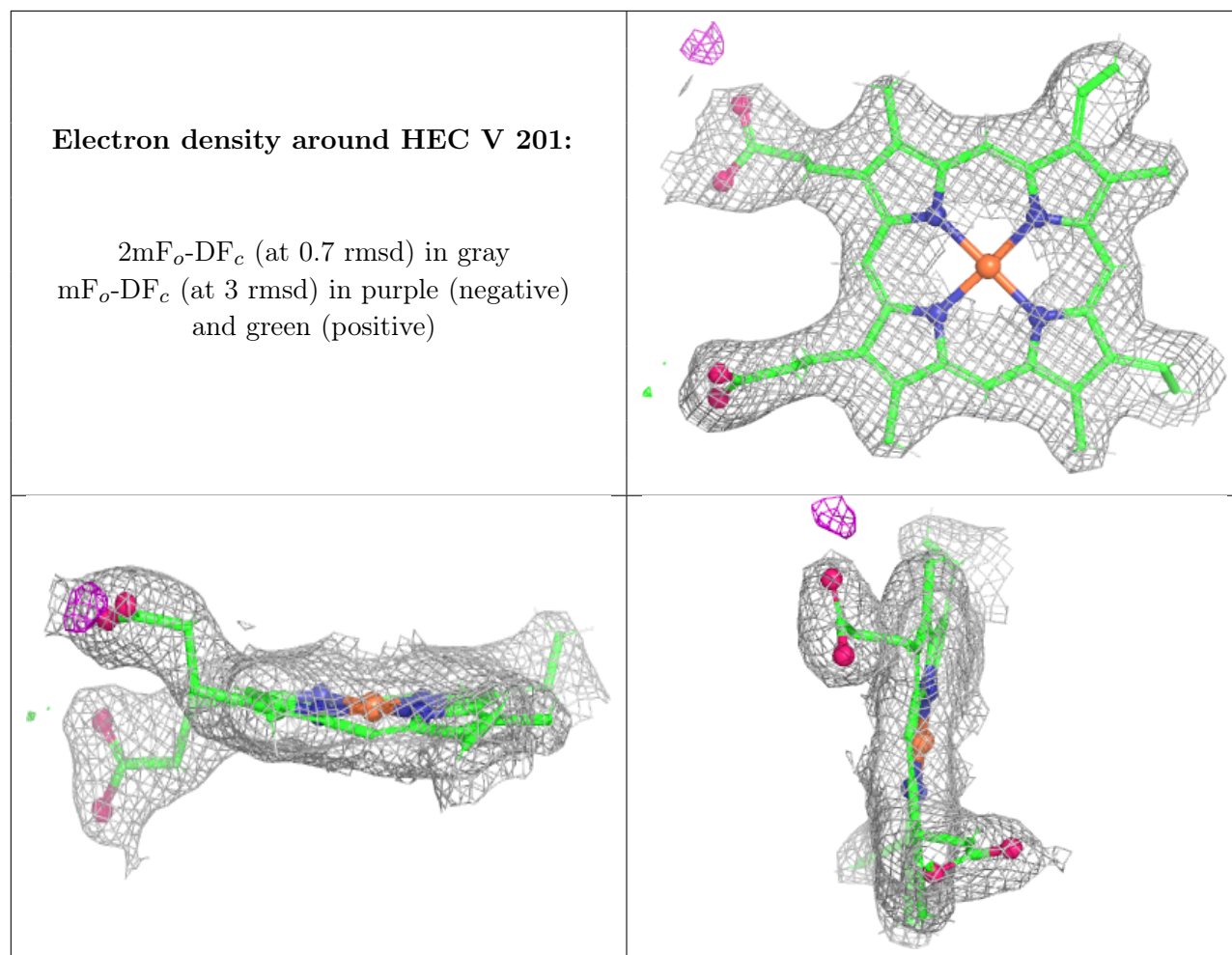
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.