



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:21 AM UTC

PDB ID : 6DHG / pdb_00006dhg
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.5 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 : 2.50 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

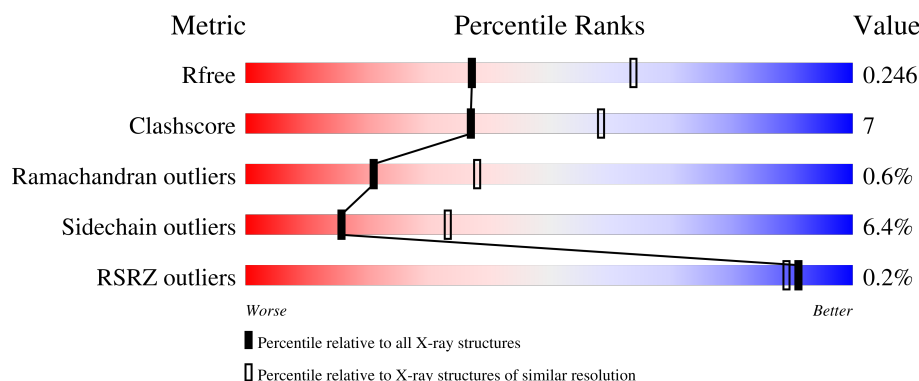
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

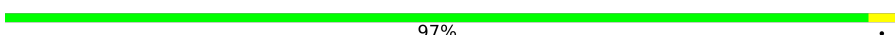
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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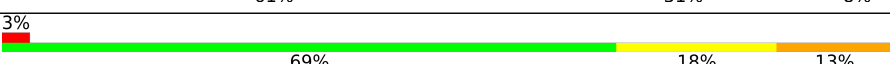
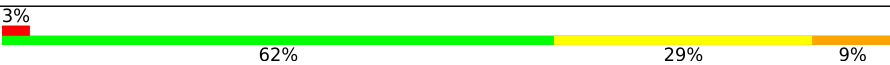
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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

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Mol	Chain	Length	Quality of chain
1	a	334	 78%21%.
2	B	505	 83%15%.
2	b	505	 85%14%.
3	C	451	 83%15%.
3	c	451	 85%13%.
4	D	341	 84%15%.
4	d	341	 83%17%.
5	E	82	 %62%35%..
5	e	82	 %68%29%.
6	F	34	 82%18%.
6	f	34	 65%26%9%.
7	H	65	 2%80%20%.
7	h	65	 66%28%.
8	I	36	 81%17%.
8	i	36	 61%36%.
9	J	36	 78%22%.
9	j	36	 72%25%.
10	K	37	 3%51%38%11%.
10	k	37	 65%32%.
11	L	37	 97%.
11	l	37	 78%16%.
12	M	33	 73%24%.
12	m	33	 79%18%.
13	O	244	 74%24%.
13	o	244	 79%18%.

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	404	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103658 atoms, of which 51467 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42	1		
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42	1		

- 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	2		
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83	2		

- 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	1		
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42	1		
9	j	36	Total	C	H	N	O	0	0	0
			516	172	261	40	42	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	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	S	0	0
			620	202	316	48	53	1		
11	l	36	Total	C	H	N	O		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	S	0	0
			525	171	269	37	47	1		
12	m	32	Total	C	H	N	O	S	0	0
			518	168	267	36	46	1		

- 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	S	0	1
			3730	1174	1850	317	385	4		0
13	o	244	Total	C	H	N	O	S	0	0
			3718	1170	1844	317	383	4		0

- 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	S	0	0
			519	181	261	36	39	2		
14	t	30	Total	C	H	N	O	S	0	0
			512	180	256	36	38	2		

- 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
			450	144	232	35	36	3			

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

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

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

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

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

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

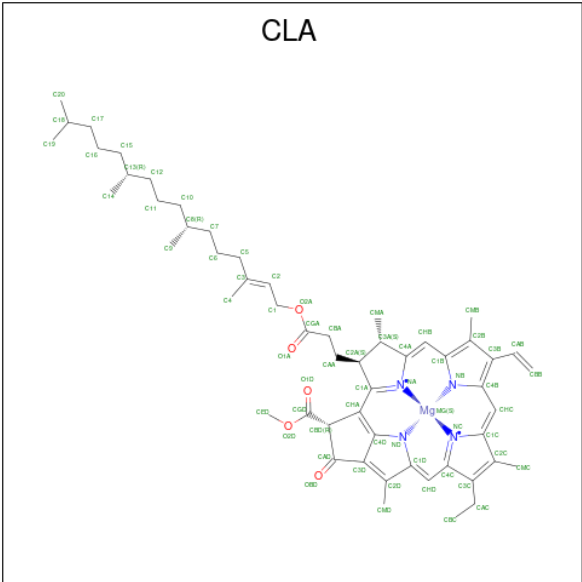
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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

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

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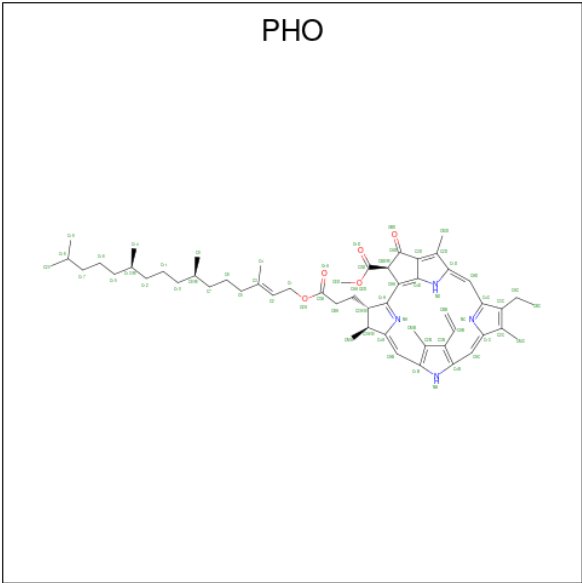
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total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

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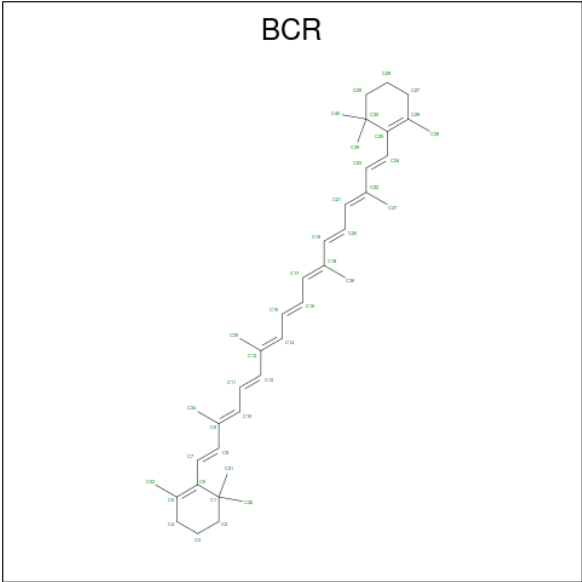
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



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

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



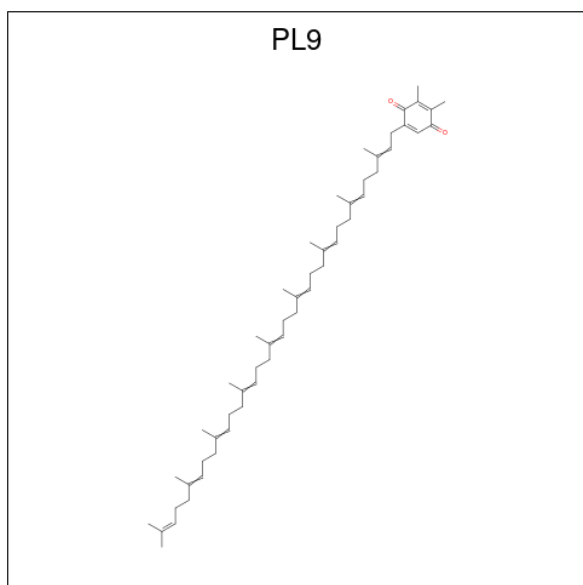
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total	C	H	0	0
			96	40	56		
25	H	1	Total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

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

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



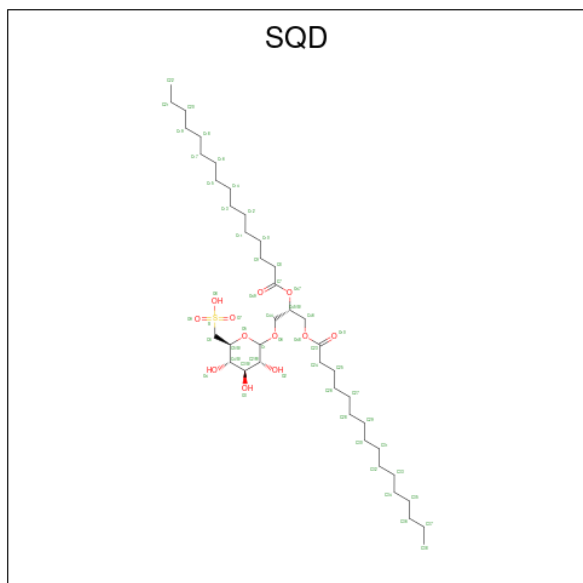
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		

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

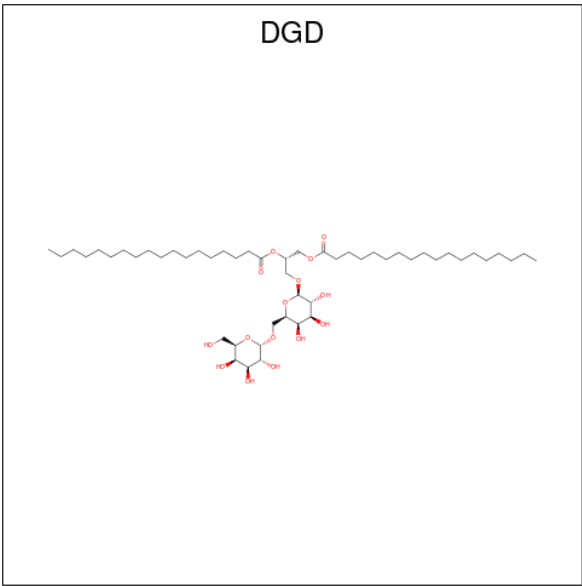
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	a	1	Total	C	H	O		0	0
			92	31	56	5			
27	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

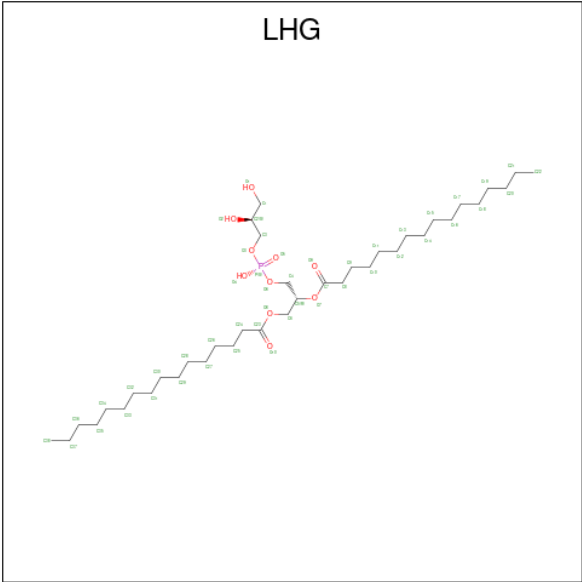
- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

C₅₁H₉₆O₁₅).



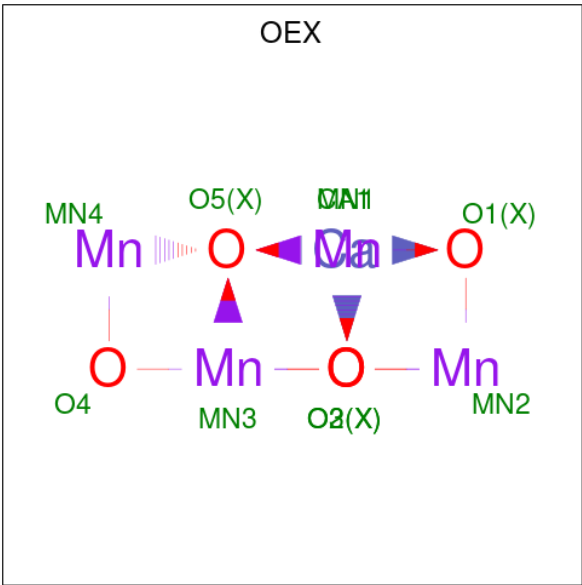
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			162	51	96	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	H	1	Total	C	H	O	0	0
			144	47	82	15		
28	a	1	Total	C	H	O	0	0
			119	39	75	5		
28	c	1	Total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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



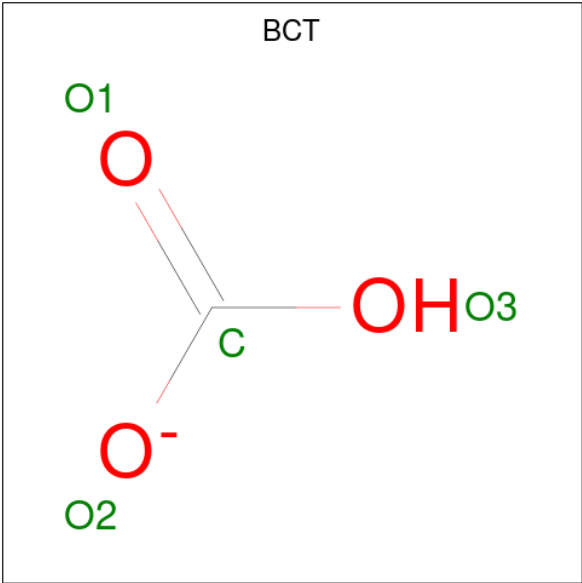
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
29	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



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

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

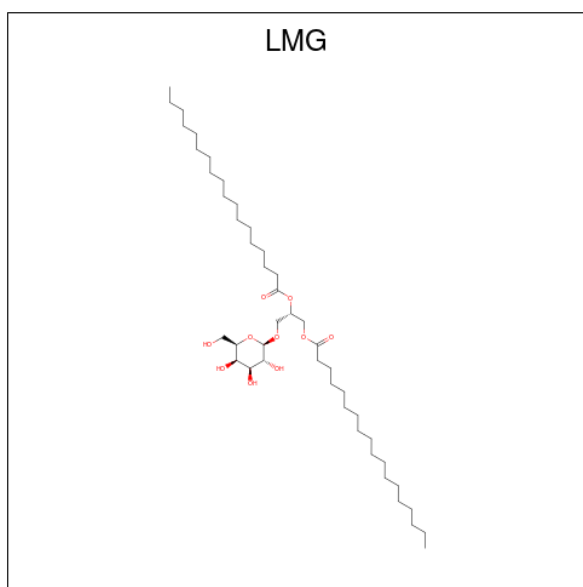


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			5	1	1	3		
31	a	1	Total	C	H	O	0	0
			5	1	1	3		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	6	Total	C	H	O	0	0
			226	79	137	10		
32	C	3	Total	C	H	O	0	0
			103	36	63	4		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	E	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			
32	I	1	Total	C	H		0	0
			41	15	26			
32	J	1	Total	C	H	O	0	0
			28	10	16	2		
32	M	2	Total	C	H	O	0	0
			63	23	38	2		
32	T	1	Total	C	H		0	0
			47	16	31			
32	a	1	Total	C	H	O	0	0
			28	10	16	2		
32	b	5	Total	C	H	O	0	0
			220	75	139	6		
32	c	2	Total	C	H	O	0	0
			83	28	51	4		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H		0	0
			26	10	16			
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

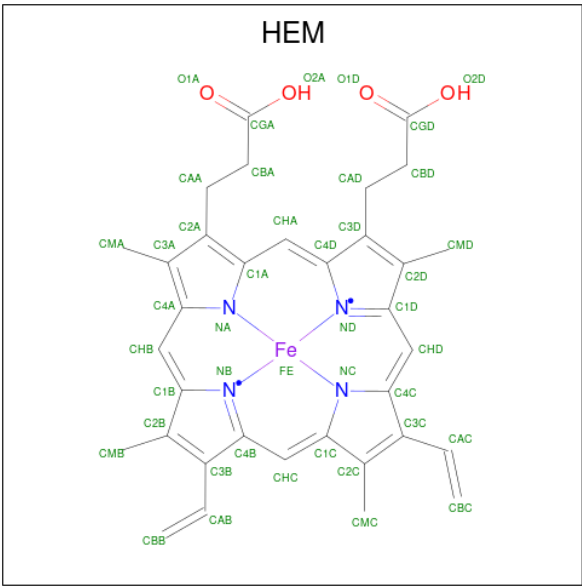
- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			123	41	72	10		
33	D	1	Total	C	H	O	0	0
			78	27	45	6		
33	D	1	Total	C	H	O	0	0
			68	24	40	4		
33	M	1	Total	C	H	O	0	0
			123	41	72	10		
33	b	1	Total	C	H	O	0	0
			141	45	86	10		
33	c	1	Total	C	H	O	0	0
			81	27	44	10		
33	c	1	Total	C	H	O	0	0
			117	38	69	10		
33	c	1	Total	C	H	O	0	0
			117	39	68	10		
33	d	1	Total	C	H	O	0	0
			57	21	34	2		
33	d	1	Total	C	H	O	0	0
			102	34	58	10		
33	m	1	Total	C	H	O	0	0
			123	41	72	10		

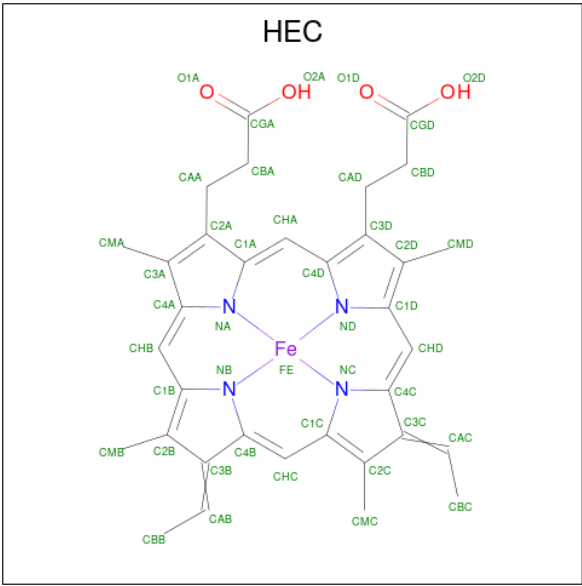
- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

C₃₄H₃₂FeN₄O₄).



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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	136	Total	O	0	0
			136	136		
36	B	216	Total	O	0	0
			216	216		
36	C	192	Total	O	0	0
			192	192		
36	D	138	Total	O	0	0
			138	138		
36	E	30	Total	O	0	0
			30	30		
36	F	10	Total	O	0	0
			10	10		
36	H	25	Total	O	0	0
			25	25		
36	I	16	Total	O	0	0
			16	16		
36	J	13	Total	O	0	0
			13	13		
36	L	7	Total	O	0	0
			7	7		
36	M	7	Total	O	0	0
			7	7		
36	O	128	Total	O	0	0
			128	128		
36	T	11	Total	O	0	0
			11	11		
36	U	47	Total	O	0	0
			47	47		
36	V	73	Total	O	0	0
			73	73		
36	Y	6	Total	O	0	0
			6	6		
36	X	8	Total	O	0	0
			8	8		
36	Z	5	Total	O	0	0
			5	5		

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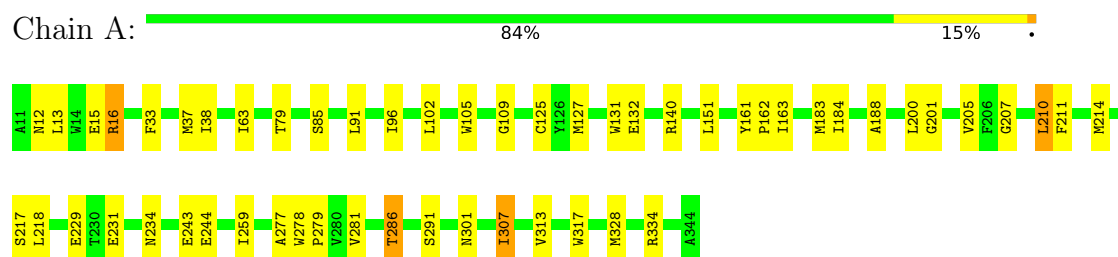
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	R	4	Total 4	O 4	0	0
36	a	119	Total 119	O 119	0	0
36	b	190	Total 190	O 190	0	0
36	c	162	Total 162	O 162	0	0
36	d	120	Total 120	O 120	0	0
36	e	22	Total 22	O 22	0	0
36	f	4	Total 4	O 4	0	0
36	h	19	Total 19	O 19	0	0
36	i	10	Total 10	O 10	0	0
36	j	8	Total 8	O 8	0	0
36	k	5	Total 5	O 5	0	0
36	l	11	Total 11	O 11	0	0
36	m	5	Total 5	O 5	0	0
36	o	113	Total 113	O 113	0	0
36	t	11	Total 11	O 11	0	0
36	u	54	Total 54	O 54	0	0
36	v	64	Total 64	O 64	0	0
36	y	4	Total 4	O 4	0	0
36	x	13	Total 13	O 13	0	0
36	z	1	Total 1	O 1	0	0
36	r	5	Total 5	O 5	0	0

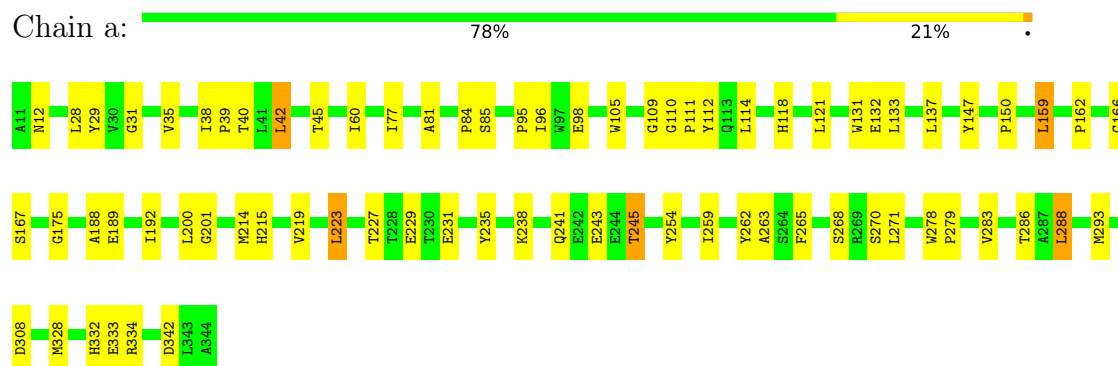
3 Residue-property plots

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.

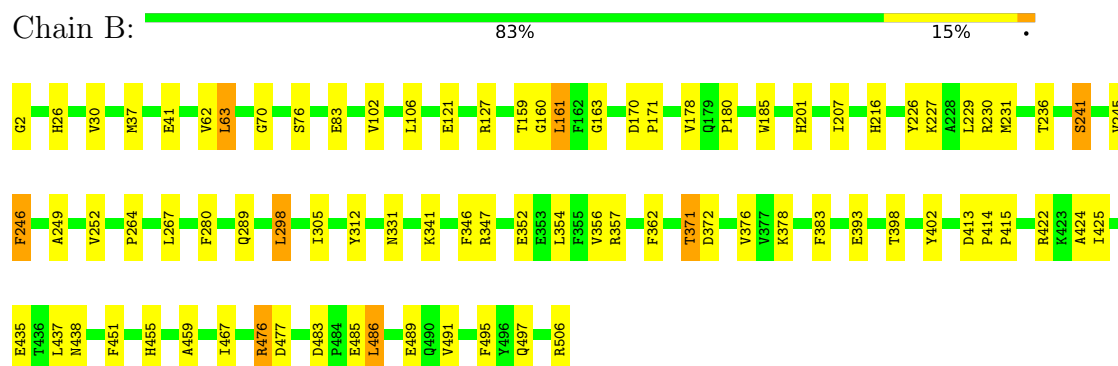
- Molecule 1: Photosystem II protein D1 1



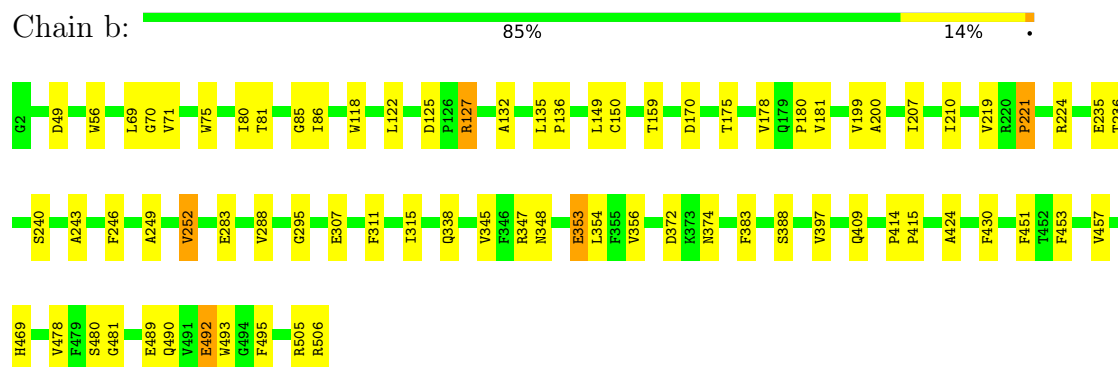
- Molecule 1: Photosystem II protein D1 1



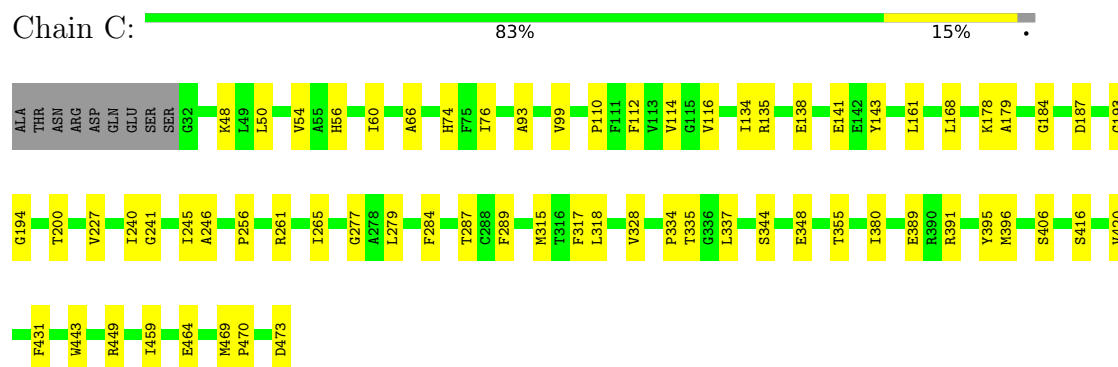
- Molecule 2: Photosystem II CP47 reaction center protein



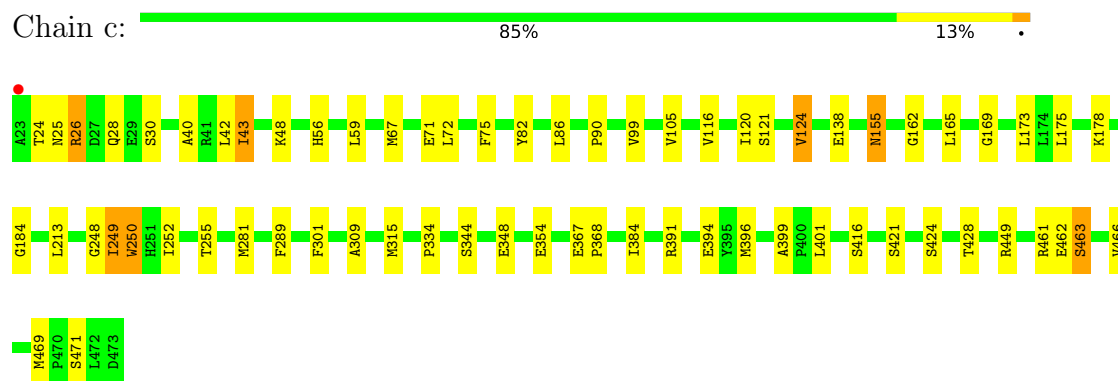
- Molecule 2: Photosystem II CP47 reaction center protein



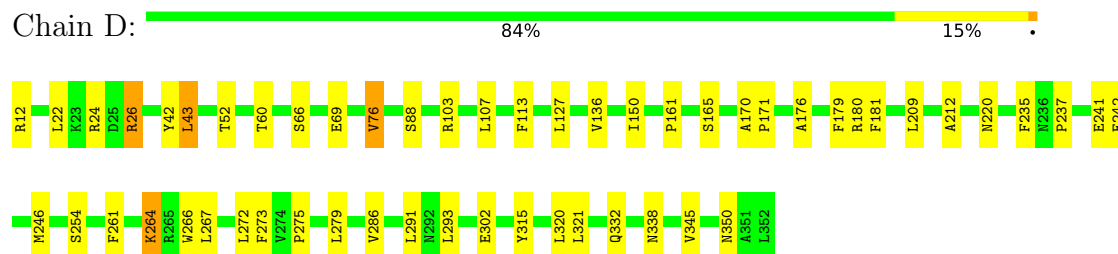
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

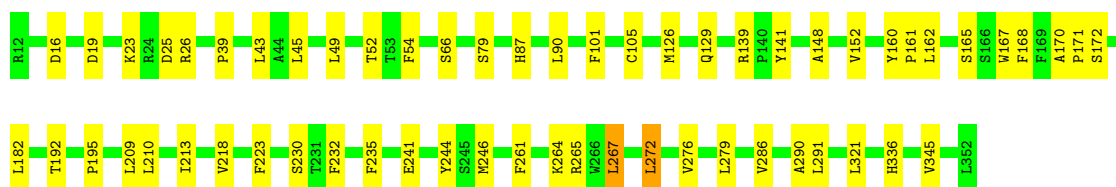


• Molecule 4: Photosystem II D2 protein



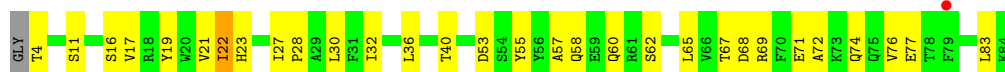
• Molecule 4: Photosystem II D2 protein

Chain d:  83% 17% .



• Molecule 5: Cytochrome b559 subunit alpha

Chain E:  62% 35% ..



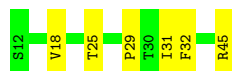
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:  68% 29% .



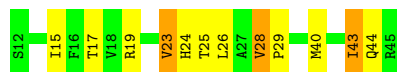
• Molecule 6: Cytochrome b559 subunit beta

Chain F:  82% 18%



• Molecule 6: Cytochrome b559 subunit beta

Chain f:  65% 26% 9%



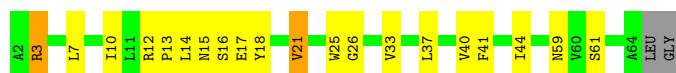
• Molecule 7: Photosystem II reaction center protein H

Chain H:  80% 20%



• Molecule 7: Photosystem II reaction center protein H

Chain h:  66% 28% . .



- Molecule 8: Photosystem II reaction center protein I

Chain I: 81% 17% .



- Molecule 8: Photosystem II reaction center protein I

Chain i: 61% 36% .



- Molecule 9: Photosystem II reaction center protein J

Chain J: 78% 22% .



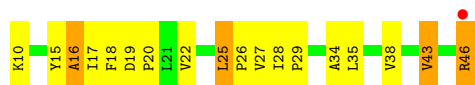
- Molecule 9: Photosystem II reaction center protein J

Chain j: 72% 25% .



- Molecule 10: Photosystem II reaction center protein K

Chain K: 3% 51% 38% 11% .



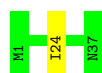
- Molecule 10: Photosystem II reaction center protein K

Chain k: 65% 32% .



- Molecule 11: Photosystem II reaction center protein L

Chain L: 97% .



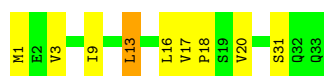
- Molecule 11: Photosystem II reaction center protein L

Chain l: 78% 16% . .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 73% 24% .



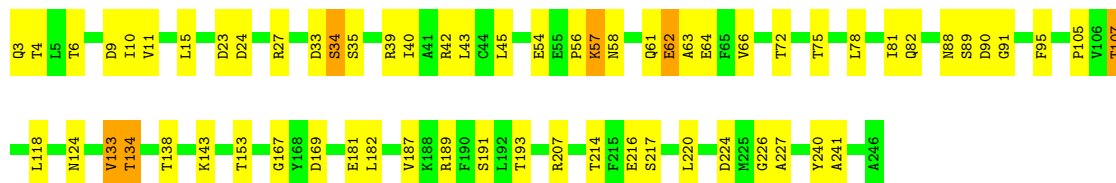
- Molecule 12: Photosystem II reaction center protein M

Chain m: 79% 18% .



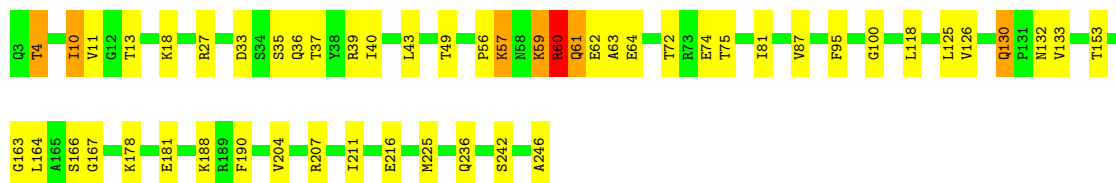
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 74% 24% .



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

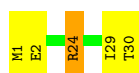
Chain o: 79% 18% .



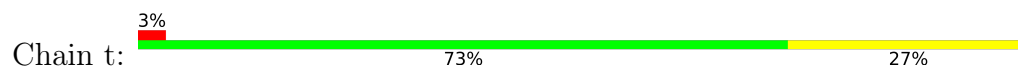
- Molecule 14: Photosystem II reaction center protein T

Chain T: 83% 13% .

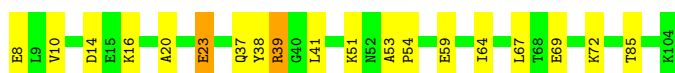
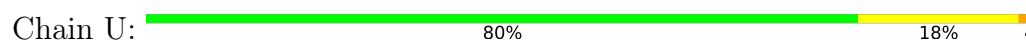




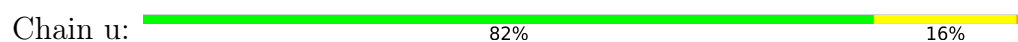
- Molecule 14: Photosystem II reaction center protein T



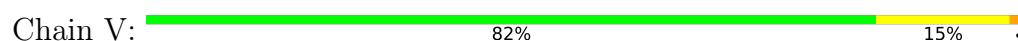
- Molecule 15: Photosystem II 12 kDa extrinsic protein



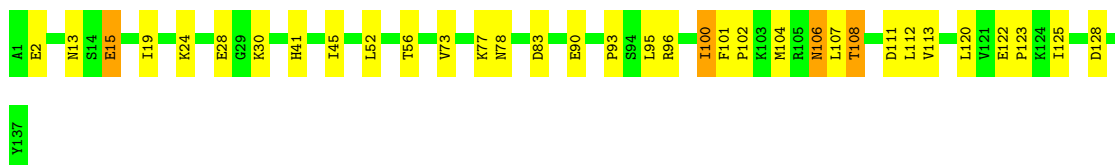
- Molecule 15: Photosystem II 12 kDa extrinsic protein



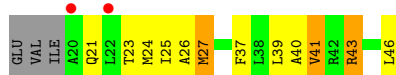
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  53% 43% .



- Molecule 18: Photosystem II reaction center X protein

Chain X:  74% 24% .



- Molecule 18: Photosystem II reaction center X protein

Chain x:  58% 39% .



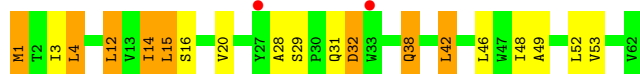
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  61% 31% 8% .



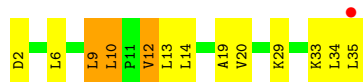
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  3% 69% 18% 13% .



- Molecule 20: Photosystem II protein Y

Chain R:  3% 62% 29% 9% .



- Molecule 20: Photosystem II protein Y

Chain r:  3% 56% 21% 15% 9% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.55Å 222.69Å 309.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.78 – 2.50 30.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.78-2.50) 87.5 (30.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.167 , 0.246 0.168 , 0.246	Depositor DCC
R_{free} test set	2481 reflections (0.42%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103658	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.68	1/2707 (0.0%)	0.75	0/3692
1	a	0.61	1/2704 (0.0%)	0.72	0/3688
2	B	0.62	0/4160	0.69	0/5668
2	b	0.58	1/4118 (0.0%)	0.69	1/5611 (0.0%)
3	C	0.58	0/3530	0.69	0/4807
3	c	0.55	0/3610	0.68	0/4914
4	D	0.63	0/2812	0.72	0/3832
4	d	0.59	0/2821	0.70	0/3844
5	E	0.50	0/684	0.64	0/935
5	e	0.48	0/683	0.64	0/932
6	F	0.50	0/284	0.60	0/387
6	f	0.47	0/284	0.61	0/387
7	H	0.60	0/520	0.72	0/709
7	h	0.54	0/511	0.71	0/697
8	I	0.63	0/293	0.75	0/396
8	i	0.70	0/293	0.73	0/396
9	J	0.51	0/263	0.73	0/356
9	j	0.46	0/261	0.62	0/353
10	K	0.43	0/314	0.56	0/427
10	k	0.43	0/303	0.58	0/416
11	L	0.62	0/311	0.70	0/422
11	l	0.61	0/303	0.69	0/412
12	M	0.64	0/249	0.72	0/341
12	m	0.66	0/244	0.70	0/334
13	O	0.59	0/1914	0.72	0/2596
13	o	0.56	0/1905	0.70	0/2583
14	T	0.68	0/257	0.77	0/349
14	t	0.60	0/255	0.65	0/346
15	U	0.56	0/785	0.67	0/1064
15	u	0.59	0/785	0.72	0/1064
16	V	0.56	0/1085	0.68	0/1473
16	v	0.57	0/1085	0.68	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.48	0/197	0.68	0/264
17	y	0.36	0/219	0.46	0/294
18	X	0.51	0/284	0.67	0/384
18	x	0.39	0/284	0.57	0/384
19	Z	0.47	0/490	0.61	0/669
19	z	0.39	0/488	0.54	0/666
20	R	0.35	0/277	0.55	0/380
20	r	0.34	0/233	0.52	0/323
All	All	0.58	3/42805 (0.0%)	0.69	1/58268 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	Y	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	6.85	1.58	1.54
2	b	221	PRO	CA-C	5.77	1.56	1.52
1	a	263	ALA	CA-C	-5.01	1.44	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	221	PRO	O-C-N	5.84	123.89	121.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	Y	21	GLN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2508	2519	32	0
1	a	2619	2499	2510	44	0
2	B	4004	3845	3864	48	0
2	b	3978	3811	3836	44	0
3	C	3417	3335	3348	42	0
3	c	3494	3407	3420	37	0
4	D	2717	2613	2621	50	0
4	d	2723	2619	2627	44	0
5	E	662	647	648	17	0
5	e	664	647	648	20	0
6	F	275	281	282	7	0
6	f	275	281	282	9	0
7	H	507	523	523	7	0
7	h	498	518	518	12	0
8	I	296	311	311	2	0
8	i	296	311	311	10	0
9	J	257	268	268	6	0
9	j	255	261	261	7	0
10	K	302	318	318	17	0
10	k	293	305	305	6	0
11	L	304	316	316	1	0
11	l	296	304	304	3	0
12	M	256	269	269	10	0
12	m	251	267	267	7	0
13	O	1880	1850	1852	39	0
13	o	1874	1844	1846	31	0
14	T	258	261	261	4	0
14	t	256	256	256	5	0
15	U	774	772	773	7	0
15	u	774	772	773	12	0
16	V	1064	1070	1073	15	0
16	v	1064	1070	1073	21	0
17	Y	196	208	217	9	0
17	y	218	232	241	9	0
18	X	281	312	312	5	0
18	x	281	312	312	11	0
19	Z	479	509	516	15	0
19	z	477	509	509	9	0
20	R	271	298	298	8	0
20	r	227	234	224	9	0
21	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	184	192	192	2	0
23	B	1035	1139	1139	12	0
23	C	839	922	922	16	0
23	D	195	216	216	3	0
23	a	195	216	216	2	0
23	b	1035	1139	1139	23	0
23	c	839	919	919	10	0
23	d	195	216	216	4	0
24	A	64	74	74	1	0
24	D	64	74	74	3	0
24	a	64	74	74	1	0
24	d	64	74	74	3	0
25	A	40	56	56	0	0
25	B	120	168	168	6	0
25	C	80	112	112	5	0
25	D	40	56	56	6	0
25	H	40	56	56	4	0
25	K	40	56	56	4	0
25	T	40	56	56	2	0
25	Z	40	56	56	1	0
25	a	40	56	56	1	0
25	b	120	168	168	7	0
25	c	120	168	168	7	0
25	d	40	56	56	3	0
25	k	40	56	56	1	0
25	t	40	56	56	7	0
25	x	40	56	56	0	0
26	A	55	80	80	1	0
26	D	55	80	80	1	0
26	a	55	80	80	3	0
26	d	55	80	80	0	0
27	A	91	135	134	2	0
27	B	54	78	78	1	0
27	F	36	45	45	2	0
27	a	90	134	133	4	0
27	b	49	65	64	1	0
27	f	41	49	48	2	0
28	A	66	96	96	5	0
28	C	186	246	246	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	H	62	82	80	1	0
28	a	44	75	75	2	0
28	c	186	246	245	0	0
28	h	62	82	81	0	0
29	A	49	74	74	4	0
29	D	96	141	141	2	0
29	E	49	74	74	0	0
29	L	49	74	74	3	0
29	d	137	199	199	4	0
29	e	42	57	57	1	0
29	l	49	74	74	0	0
30	A	10	0	0	0	0
30	a	10	0	0	1	0
31	A	4	1	1	0	0
31	a	4	1	1	0	0
32	B	89	137	0	0	0
32	C	40	63	0	0	0
32	D	20	35	0	0	0
32	E	12	16	0	0	0
32	H	18	35	0	0	0
32	I	15	26	0	0	0
32	J	12	16	0	0	0
32	M	25	38	0	0	0
32	T	16	31	0	0	0
32	a	12	16	0	0	0
32	b	81	139	0	0	0
32	c	32	51	0	1	0
32	d	17	26	0	0	0
32	j	12	16	0	0	0
32	l	18	35	0	0	0
32	m	12	16	0	0	0
32	t	10	16	0	0	0
32	x	20	35	0	1	0
33	C	96	132	132	0	0
33	D	112	157	157	4	0
33	M	51	72	72	1	0
33	b	55	86	86	0	0
33	c	134	181	181	3	0
33	d	67	92	91	1	0
33	m	51	72	72	1	0
34	E	43	30	30	4	0
34	e	43	30	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	V	43	30	30	0	0
35	v	43	30	30	0	0
36	A	136	0	0	6	0
36	B	216	0	0	10	0
36	C	192	0	0	3	0
36	D	138	0	0	8	0
36	E	30	0	0	0	0
36	F	10	0	0	0	0
36	H	25	0	0	2	0
36	I	16	0	0	0	0
36	J	13	0	0	2	0
36	L	7	0	0	0	0
36	M	7	0	0	0	0
36	O	128	0	0	10	0
36	R	4	0	0	1	0
36	T	11	0	0	1	0
36	U	47	0	0	1	0
36	V	73	0	0	3	0
36	X	8	0	0	0	0
36	Y	6	0	0	0	0
36	Z	5	0	0	0	0
36	a	119	0	0	3	0
36	b	190	0	0	11	0
36	c	162	0	0	4	0
36	d	120	0	0	8	0
36	e	22	0	0	0	0
36	f	4	0	0	1	0
36	h	19	0	0	2	0
36	i	10	0	0	1	0
36	j	8	0	0	0	0
36	k	5	0	0	0	0
36	l	11	0	0	0	0
36	m	5	0	0	1	0
36	o	113	0	0	2	0
36	r	5	0	0	1	0
36	t	11	0	0	0	0
36	u	54	0	0	2	0
36	v	64	0	0	5	0
36	x	13	0	0	1	0
36	y	4	0	0	0	0
36	z	1	0	0	0	0
All	All	52191	51467	50850	715	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 (715) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:90:ASP:OD1	36:O:301:HOH:O	1.76	1.02
13:O:169:ASP:O	36:O:302:HOH:O	1.79	0.99
2:B:497:GLN:OE1	36:B:701:HOH:O	1.87	0.93
7:H:56:ASP:OD1	18:X:2:THR:N	2.07	0.87
13:O:216:GLU:OE2	36:O:303:HOH:O	1.92	0.86
3:C:389:GLU:OE1	36:C:601:HOH:O	1.91	0.86
2:b:489:GLU:OE2	2:b:505:ARG:NH1	2.09	0.86
2:B:413:ASP:OD1	36:B:702:HOH:O	1.94	0.84
18:x:39:ARG:O	36:x:201:HOH:O	1.96	0.83
32:c:520:UNL:O2	36:c:601:HOH:O	1.98	0.81
4:d:25:ASP:OD1	36:d:501:HOH:O	1.96	0.81
12:m:5:GLN:O	36:m:201:HOH:O	1.99	0.81
5:e:61:ARG:NH2	16:v:125:ILE:O	2.15	0.80
28:A:412:DGD:O2D	36:A:501:HOH:O	1.99	0.79
2:B:2:GLY:N	36:B:704:HOH:O	2.14	0.79
1:a:235:TYR:OH	11:l:11:GLU:OE2	2.01	0.77
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.19	0.76
13:O:89:SER:O	36:O:304:HOH:O	2.05	0.74
2:b:307:GLU:OE1	36:b:701:HOH:O	2.06	0.74
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.69	0.74
15:U:69:GLU:OE1	15:U:72:LYS:NZ	2.21	0.73
3:c:391[B]:ARG:NE	36:c:602:HOH:O	2.22	0.73
6:f:17:THR:OG1	36:f:201:HOH:O	2.07	0.73
13:o:27:ARG:NH1	36:o:301:HOH:O	2.22	0.71
4:d:241:GLU:OE1	36:d:502:HOH:O	2.07	0.71
13:o:57:LYS:O	13:o:60:ARG:N	2.22	0.71
25:C:515:BCR:H331	25:C:515:BCR:C8	2.19	0.71
3:c:178:LYS:NZ	3:c:184:GLY:O	2.23	0.71
9:J:36:LEU:O	36:J:201:HOH:O	2.08	0.70
1:A:334:ARG:NH2	36:A:503:HOH:O	2.25	0.70
34:e:102:HEM:HHC	34:e:102:HEM:HBB2	1.73	0.70
23:D:402:CLA:HBB1	23:D:402:CLA:HMB3	1.73	0.70
16:V:28:GLU:OE2	16:V:31:ARG:NH2	2.25	0.69
4:D:241:GLU:OE2	36:D:501:HOH:O	2.09	0.69
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.73	0.69
16:v:120:LEU:O	36:v:302:HOH:O	2.11	0.68
33:D:407:LMG:O4	36:J:201:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:78:ASN:O	36:v:301:HOH:O	2.11	0.68
10:K:46[A]:ARG:NH1	17:Y:46:LEU:O	2.26	0.68
15:u:53:ALA:O	15:u:55:TYR:CD2	2.46	0.68
1:a:342:ASP:O	36:a:501:HOH:O	2.12	0.67
2:b:235:GLU:OE1	2:b:469:HIS:ND1	2.23	0.67
2:b:283:GLU:OE1	36:b:702:HOH:O	2.13	0.67
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.76	0.67
25:D:405:BCR:H331	25:D:405:BCR:C8	2.24	0.67
4:D:261:PHE:CD2	4:D:267:LEU:HD12	2.29	0.67
4:d:336:HIS:NE2	36:d:505:HOH:O	2.28	0.66
3:C:380:ILE:O	36:C:602:HOH:O	2.11	0.66
2:B:354:LEU:O	36:B:703:HOH:O	2.13	0.66
25:t:101:BCR:HC8	25:t:101:BCR:H311	1.75	0.66
25:c:514:BCR:H382	25:c:514:BCR:H23C	1.76	0.66
23:d:404:CLA:H92	18:x:18:ALA:HB2	1.78	0.65
2:b:372:ASP:OD2	36:b:703:HOH:O	2.14	0.65
23:c:505:CLA:HBB1	23:c:505:CLA:HMB3	1.80	0.64
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.26	0.64
28:A:412:DGD:O1B	36:A:502:HOH:O	2.15	0.63
28:a:413:DGD:O1B	28:a:413:DGD:O1G	2.16	0.63
2:B:483:ASP:HB3	2:B:486:LEU:HD13	1.81	0.62
7:h:14:LEU:O	36:h:201:HOH:O	2.15	0.62
2:B:476:ARG:NH1	36:B:705:HOH:O	2.16	0.62
24:d:401:PHO:HBB1	24:d:401:PHO:HMB1	1.82	0.62
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.00	0.62
13:O:181:GLU:N	13:O:181:GLU:OE1	2.32	0.62
20:r:2:ASP:N	36:r:101:HOH:O	2.33	0.62
19:Z:32:ASP:OD1	19:Z:35:ARG:N	2.32	0.62
7:h:13:PRO:O	7:h:16:SER:OG	2.16	0.62
2:B:241:SER:O	2:B:245:VAL:HG23	2.01	0.61
4:D:165:SER:O	36:D:502:HOH:O	2.16	0.61
1:a:189:GLU:OE2	30:a:415:OEX:MN1	1.56	0.61
4:d:286:VAL:HG21	23:d:403:CLA:HED2	1.83	0.61
4:D:272:LEU:C	4:D:272:LEU:HD23	2.26	0.61
19:z:14:ILE:HG22	19:z:14:ILE:O	2.01	0.60
13:o:18:LYS:NZ	13:o:74:GLU:OE1	2.34	0.60
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.37	0.60
2:B:371:THR:HG23	2:B:372:ASP:O	2.01	0.59
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.84	0.59
7:h:3:ARG:NH1	36:h:202:HOH:O	2.30	0.59
23:b:608:CLA:HMB1	23:b:608:CLA:HBB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:82:TYR:OH	3:c:394:GLU:OE2	2.09	0.59
1:A:16:ARG:NH1	36:A:508:HOH:O	2.36	0.59
3:C:279:LEU:HD12	23:C:510:CLA:HED2	1.84	0.59
17:Y:23:THR:O	17:Y:27:MET:HE1	2.03	0.59
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.85	0.59
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.83	0.58
3:c:40:ALA:O	3:c:43:ILE:HD12	2.04	0.58
2:B:264:PRO:HG2	2:B:267:LEU:HD12	1.85	0.58
3:C:277:GLY:C	23:C:506:CLA:HBC2	2.29	0.58
27:A:411:SQD:H383	23:b:607:CLA:H93	1.86	0.58
17:Y:40:ALA:O	17:Y:41:VAL:HB	2.03	0.58
26:A:409:PL9:H361	6:F:25:THR:HG21	1.86	0.58
3:C:334:PRO:HA	13:O:153:THR:OG1	2.03	0.58
23:a:405:CLA:HMB3	23:a:405:CLA:HBB1	1.85	0.58
2:B:506:ARG:HB3	36:B:709:HOH:O	2.03	0.58
3:C:110:PRO:O	3:C:114:VAL:HG23	2.04	0.58
20:r:29:LYS:O	20:r:31:VAL:N	2.37	0.58
25:D:405:BCR:H352	6:F:29:PRO:HG2	1.85	0.57
23:C:512:CLA:H143	19:Z:20:VAL:HG13	1.86	0.57
14:T:30:THR:O	36:T:201:HOH:O	2.17	0.57
7:H:47:GLU:OE2	36:H:201:HOH:O	2.16	0.57
4:D:279:LEU:HD22	24:D:401:PHO:HBC3	1.87	0.57
13:O:56:PRO:O	13:O:58:ASN:N	2.36	0.57
4:d:54:PHE:O	5:e:49:THR:OG1	2.22	0.57
4:D:254:SER:OG	14:T:24:ARG:NH2	2.37	0.56
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.39	0.56
5:e:81:GLU:O	5:e:84:LYS:NZ	2.38	0.56
4:D:291:LEU:HD21	28:H:102:DGD:CGB	2.35	0.56
16:V:41:HIS:HA	16:V:45:ILE:O	2.05	0.56
34:E:103:HEM:HBC2	34:E:103:HEM:HHD	1.86	0.56
20:R:33:LYS:O	20:R:35:LEU:N	2.38	0.56
2:b:71:VAL:HG23	23:b:607:CLA:HMA2	1.88	0.56
17:y:39:LEU:HB3	17:y:46:LEU:HD21	1.88	0.56
1:A:63:ILE:HB	3:C:335:THR:HG21	1.88	0.56
27:b:601:SQD:H112	25:b:618:BCR:H383	1.88	0.56
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.88	0.56
5:E:17:VAL:O	5:E:21:VAL:HG23	2.06	0.56
13:O:34:SER:O	36:O:305:HOH:O	2.17	0.56
17:Y:41:VAL:HG12	17:Y:41:VAL:O	2.05	0.56
4:d:267:LEU:C	4:d:267:LEU:HD23	2.31	0.56
3:C:66:ALA:HB1	10:K:25:LEU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:15:GLU:O	36:u:201:HOH:O	2.17	0.55
25:D:405:BCR:H331	25:D:405:BCR:HC8	1.88	0.55
13:O:27:ARG:O	13:O:27:ARG:HG2	2.06	0.55
5:e:17:VAL:HG23	9:j:7:ARG:HD2	1.88	0.55
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.37	0.55
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.55
2:b:125:ASP:HB2	2:b:132:ALA:HB3	1.87	0.55
6:F:45:ARG:NH1	9:J:40:LEU:OXT	2.39	0.54
23:A:405:CLA:H92	33:D:407:LMG:C25	2.38	0.54
23:c:506:CLA:O1A	23:c:506:CLA:C2	2.55	0.54
15:u:36:ILE:O	36:u:202:HOH:O	2.18	0.54
9:J:15:THR:HG22	9:J:19:MET:HE2	1.89	0.54
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.90	0.54
13:O:33:ASP:OD2	13:O:35:SER:OG	2.10	0.54
23:A:404:CLA:HBB1	23:A:404:CLA:HMB3	1.90	0.54
2:B:26:HIS:O	2:B:30:VAL:HG23	2.07	0.54
3:C:143:TYR:CE1	23:C:514:CLA:HED3	2.43	0.53
11:l:2:GLU:N	11:l:3:PRO:CD	2.71	0.53
1:A:217:SER:HA	4:D:272:LEU:HD12	1.89	0.53
29:A:413:LHG:H222	12:M:18:PRO:HG3	1.91	0.53
3:c:26:ARG:O	10:k:46:ARG:HD2	2.08	0.53
2:B:160:GLY:HA2	2:B:163:GLY:O	2.09	0.53
4:d:52:THR:O	4:d:66:SER:HA	2.09	0.53
5:e:30:LEU:HD11	34:e:102:HEM:HBB1	1.91	0.53
8:i:14:PHE:CZ	8:i:18:LEU:HD11	2.43	0.53
14:t:15:ALA:HB2	25:t:101:BCR:H14C	1.91	0.53
15:u:53:ALA:O	15:u:55:TYR:CE2	2.61	0.53
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.91	0.53
12:M:20:VAL:HG13	12:m:20:VAL:HG13	1.91	0.53
27:f:101:SQD:H312	18:x:27:VAL:HG11	1.90	0.53
17:y:39:LEU:O	17:y:44:GLY:N	2.37	0.52
15:u:8:GLU:HG3	15:u:9:LEU:HG	1.92	0.52
5:e:30:LEU:HD11	34:e:102:HEM:CBB	2.39	0.52
27:f:101:SQD:H351	18:x:27:VAL:HG21	1.91	0.52
1:A:277:ALA:O	1:A:281:VAL:HG23	2.09	0.52
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.44	0.52
2:B:393:GLU:OE2	15:U:14:ASP:HB3	2.09	0.52
16:v:73:VAL:HG21	16:v:113:VAL:HG12	1.90	0.52
2:B:347:ARG:HA	2:B:352:GLU:O	2.10	0.52
25:a:409:BCR:H331	25:a:409:BCR:C8	2.40	0.52
8:i:8:VAL:O	8:i:12:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:59:LYS:O	13:o:60:ARG:NH1	2.43	0.52
3:C:318:LEU:HD21	3:C:328:VAL:HG21	1.92	0.52
29:D:408:LHG:O1	29:L:101:LHG:O4	2.27	0.52
16:V:102:PRO:HA	16:V:105:ARG:HD3	1.92	0.52
3:c:334:PRO:HA	13:o:153:THR:OG1	2.10	0.52
3:c:449:ARG:NH1	8:i:27:ASP:OD1	2.35	0.52
4:d:49:LEU:HD13	25:d:405:BCR:C15	2.40	0.52
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.40	0.51
5:E:53:ASP:O	16:V:1:ALA:N	2.43	0.51
8:i:35:LYS:N	36:i:101:HOH:O	2.43	0.51
25:t:101:BCR:H23C	25:t:101:BCR:H382	1.92	0.51
3:c:90:PRO:HB3	3:c:301:PHE:HB3	1.91	0.51
3:c:344:SER:O	13:o:75:THR:HG22	2.10	0.51
4:d:246:MET:HE3	4:d:264:LYS:CG	2.41	0.51
6:f:43:ILE:HD12	6:f:43:ILE:N	2.24	0.51
17:y:29:GLY:O	17:y:33:PRO:HD2	2.09	0.51
2:b:506:ARG:HG2	36:b:866:HOH:O	2.08	0.51
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.91	0.51
4:d:79:SER:HA	4:d:172:SER:HB3	1.92	0.51
5:e:12:ASP:OD1	5:e:12:ASP:O	2.28	0.51
13:o:33:ASP:O	13:o:36:GLN:N	2.42	0.51
19:z:49:ALA:O	19:z:53:VAL:HG23	2.10	0.51
24:D:401:PHO:HMB3	24:D:401:PHO:HBB1	1.92	0.51
13:o:40:ILE:HG21	13:o:43:LEU:HB2	1.92	0.51
2:B:341:LYS:NZ	36:B:720:HOH:O	2.42	0.51
4:D:242:GLU:OE1	36:D:503:HOH:O	2.19	0.51
16:v:41:HIS:HA	16:v:45:ILE:O	2.11	0.51
19:Z:27:TYR:HE2	19:Z:33:TRP:CH2	2.29	0.51
3:C:193:GLY:C	36:C:627:HOH:O	2.54	0.51
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.93	0.51
5:E:22[A]:ILE:HD11	34:E:103:HEM:CHB	2.41	0.51
4:d:39:PRO:O	4:d:43:LEU:HG	2.10	0.51
20:R:9:LEU:O	20:R:12:VAL:HG22	2.10	0.51
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.93	0.50
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.93	0.50
25:B:617:BCR:C8	25:B:617:BCR:H311	2.41	0.50
15:u:53:ALA:O	15:u:54:PRO:C	2.52	0.50
5:E:19:TYR:CE1	5:E:23:HIS:CE1	2.99	0.50
1:a:81:ALA:HB2	1:a:175:GLY:HA3	1.93	0.50
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.94	0.50
6:f:40:MET:HA	6:f:43:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:207:ILE:HA	2:b:210:ILE:HD12	1.94	0.50
16:v:128:ASP:HA	36:v:311:HOH:O	2.11	0.50
1:a:12:ASN:C	1:a:12:ASN:OD1	2.54	0.50
9:j:18:GLY:O	9:j:21:VAL:HG22	2.12	0.50
19:Z:49:ALA:O	19:Z:53:VAL:HG23	2.11	0.50
2:b:505:ARG:O	2:b:506:ARG:HB2	2.10	0.50
13:O:187:VAL:O	13:O:189:ARG:NH1	2.41	0.49
2:b:118:TRP:NE1	36:b:710:HOH:O	2.29	0.49
17:y:39:LEU:HD21	19:z:28:ALA:HB3	1.94	0.49
23:B:613:CLA:H143	33:M:101:LMG:H232	1.94	0.49
3:C:93:ALA:HB1	3:C:99:VAL:HG11	1.94	0.49
2:b:311:PHE:HA	2:b:430:PHE:CZ	2.47	0.49
5:E:22[A]:ILE:HD12	20:R:19:ALA:HB1	1.95	0.49
3:c:162:GLY:HA3	3:c:252:ILE:HG13	1.94	0.49
3:c:213:LEU:HD21	25:c:515:BCR:C20	2.42	0.49
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.12	0.49
8:I:6:ILE:HG22	8:I:10:ILE:HD11	1.94	0.49
16:v:108:THR:HG23	16:v:111:ASP:OD1	2.11	0.49
25:B:618:BCR:H331	25:B:618:BCR:C8	2.42	0.49
4:d:218:VAL:HG22	4:d:244:TYR:CE1	2.47	0.49
16:v:112:LEU:N	16:v:112:LEU:HD23	2.27	0.49
3:C:227:VAL:HG13	3:C:227:VAL:O	2.13	0.49
17:Y:39:LEU:CD2	19:Z:28:ALA:HB3	2.42	0.49
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.95	0.49
3:c:56:HIS:HA	3:c:59:LEU:HD12	1.95	0.49
10:k:28:ILE:HA	10:k:31:LEU:HD12	1.95	0.49
5:E:60:GLN:HE21	5:E:62:SER:HB2	1.76	0.49
25:d:405:BCR:H331	25:d:405:BCR:C8	2.43	0.49
23:B:606:CLA:H91	27:a:412:SQD:H223	1.95	0.48
28:a:413:DGD:O1G	28:a:413:DGD:C1B	2.61	0.48
4:d:170:ALA:HB1	4:d:171:PRO:CD	2.43	0.48
8:i:33:LYS:O	8:i:35:LYS:NZ	2.46	0.48
2:B:106:LEU:HD11	27:a:412:SQD:H201	1.95	0.48
2:B:331:ASN:HB3	2:B:437:LEU:CD1	2.43	0.48
19:Z:46:LEU:O	19:Z:50:LEU:HB2	2.13	0.48
23:c:508:CLA:H92	23:c:510:CLA:H52	1.95	0.48
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.96	0.48
10:K:17:ILE:N	10:K:17:ILE:HD12	2.28	0.48
2:b:414:PRO:N	2:b:415:PRO:HD2	2.28	0.48
4:D:43:LEU:HG	4:D:113:PHE:HZ	1.78	0.48
1:a:278:TRP:HB3	1:a:279:PRO:CD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:90:ASP:N	36:O:301:HOH:O	2.46	0.48
13:o:60:ARG:O	13:o:61:GLN:HB2	2.13	0.48
19:z:32:ASP:OD1	19:z:32:ASP:N	2.37	0.48
27:B:621:SQD:H442	14:t:23:PHE:CD1	2.49	0.48
4:d:26:ARG:NH2	36:d:513:HOH:O	2.45	0.48
3:c:466:VAL:HA	3:c:469:MET:HG3	1.96	0.48
12:m:4:ASN:ND2	33:m:101:LMG:O10	2.40	0.48
16:V:30:LYS:O	16:V:34:GLN:HG3	2.14	0.48
23:b:602:CLA:CHA	23:b:602:CLA:HBA2	2.44	0.48
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.49	0.48
2:B:159:THR:O	2:B:180:PRO:CB	2.62	0.48
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.95	0.48
13:O:189:ARG:CZ	13:O:226:GLY:HA3	2.44	0.48
2:b:345:VAL:HG13	2:b:353:GLU:OE2	2.14	0.48
2:b:481:GLY:N	36:b:725:HOH:O	2.47	0.48
4:d:141:TYR:OH	29:d:407:LHG:O4	2.18	0.48
25:t:101:BCR:H311	25:t:101:BCR:C8	2.42	0.48
16:v:28:GLU:HA	16:v:28:GLU:OE1	2.14	0.48
3:C:135:ARG:O	3:C:135:ARG:HD3	2.15	0.47
16:V:87:GLU:HB3	36:V:339:HOH:O	2.13	0.47
6:f:43:ILE:N	6:f:43:ILE:CD1	2.77	0.47
8:i:7:THR:O	8:i:11:VAL:HG23	2.14	0.47
19:z:14:ILE:O	19:z:15:LEU:HB2	2.14	0.47
4:D:275:PRO:HB2	24:D:401:PHO:HBC1	1.97	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.96	0.47
10:K:22:VAL:HA	10:K:25:LEU:HD22	1.97	0.47
16:v:122:GLU:N	16:v:123:PRO:HD2	2.29	0.47
3:C:178:LYS:NZ	3:C:184:GLY:O	2.47	0.47
3:C:318:LEU:C	3:C:318:LEU:HD23	2.39	0.47
5:E:74:GLN:N	5:E:74:GLN:CD	2.73	0.47
18:X:9:GLY:HA2	18:X:12:ILE:HD12	1.95	0.47
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.49	0.47
13:o:57:LYS:HB3	13:o:59:LYS:HD3	1.96	0.47
1:A:127:MET:HE2	1:A:151:LEU:CD2	2.44	0.47
10:K:35:LEU:HD22	25:K:101:BCR:H351	1.96	0.47
13:O:133:VAL:C	13:O:134:THR:HG23	2.39	0.47
3:c:48:LYS:HG3	3:c:138:GLU:HA	1.95	0.47
13:o:130:GLN:HB2	36:o:369:HOH:O	2.14	0.47
2:B:305:ILE:O	36:B:706:HOH:O	2.20	0.47
25:c:515:BCR:C8	25:c:515:BCR:H331	2.45	0.47
4:d:209:LEU:HD23	4:d:209:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:25:TRP:O	7:h:26:GLY:C	2.57	0.47
1:A:301:ASN:OD1	1:A:301:ASN:C	2.58	0.47
2:B:121:GLU:OE1	7:H:12:ARG:NH2	2.40	0.47
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.48	0.47
3:C:48:LYS:HD2	3:C:138:GLU:HG2	1.97	0.47
5:E:36:LEU:O	5:E:40:THR:HG23	2.15	0.47
11:L:24:ILE:HD13	12:M:18:PRO:HB2	1.97	0.47
25:T:101:BCR:H19C	25:b:619:BCR:H363	1.97	0.47
20:R:29:LYS:NZ	36:R:101:HOH:O	2.45	0.47
3:c:424:SER:O	3:c:428:THR:HG23	2.14	0.47
5:e:14:ILE:O	5:e:20:TRP:NE1	2.46	0.47
23:B:614:CLA:H62	23:B:614:CLA:H41	1.78	0.47
1:a:147:TYR:O	1:a:150:PRO:HG2	2.15	0.47
23:b:610:CLA:HBB1	23:b:610:CLA:HMB3	1.97	0.47
25:c:521:BCR:C12	25:k:101:BCR:H333	2.44	0.47
4:d:105:CYS:HA	36:d:549:HOH:O	2.15	0.47
6:f:24:HIS:O	6:f:28:VAL:HG13	2.15	0.47
1:A:184:ILE:HG21	4:D:321:LEU:HD13	1.97	0.47
29:A:413:LHG:C22	12:M:18:PRO:HG3	2.44	0.47
23:C:508:CLA:HAA2	23:C:508:CLA:HBD	1.97	0.47
13:O:124:ASN:ND2	36:O:315:HOH:O	2.46	0.47
36:c:621:HOH:O	8:i:27:ASP:HB3	2.15	0.47
20:r:7:VAL:HA	20:r:10:LEU:HD12	1.96	0.47
2:B:414:PRO:N	2:B:415:PRO:HD2	2.29	0.47
4:D:52:THR:CG2	4:D:76:VAL:HG13	2.45	0.47
13:O:91:GLY:N	36:O:301:HOH:O	2.48	0.47
1:a:42:LEU:CD1	27:a:412:SQD:H321	2.44	0.47
23:b:615:CLA:H92	25:b:618:BCR:H362	1.96	0.47
13:o:59:LYS:C	13:o:60:ARG:HG3	2.40	0.47
1:A:291:SER:HB3	3:C:431:PHE:CE2	2.50	0.46
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.97	0.46
4:D:170:ALA:HB1	4:D:171:PRO:HD2	1.97	0.46
28:A:412:DGD:HB91	28:A:412:DGD:HB42	1.97	0.46
1:a:215:HIS:HA	26:a:410:PL9:O1	2.14	0.46
2:b:356:VAL:HG21	2:b:424:ALA:HB3	1.98	0.46
34:e:102:HEM:HMC1	34:e:102:HEM:HBC2	1.97	0.46
7:h:17:GLU:O	7:h:18:TYR:C	2.57	0.46
2:B:346:PHE:HA	2:B:398:THR:O	2.15	0.46
13:O:57:LYS:HD2	36:b:774:HOH:O	2.16	0.46
16:V:28:GLU:HG2	36:V:350:HOH:O	2.15	0.46
23:c:506:CLA:C14	23:c:507:CLA:H141	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:216:GLU:HG3	13:o:236:GLN:HG2	1.97	0.46
17:y:23:THR:HG23	17:y:24:MET:HE2	1.98	0.46
4:D:127:LEU:HD13	33:D:411:LMG:H341	1.97	0.46
16:v:106:ASN:OD1	16:v:106:ASN:N	2.47	0.46
18:x:33:GLN:O	18:x:36:LYS:HD2	2.15	0.46
4:D:266:TRP:CD1	29:D:408:LHG:HC31	2.50	0.46
27:F:101:SQD:H301	18:X:27:VAL:HG11	1.96	0.46
5:e:76:VAL:O	5:e:80:LEU:HG	2.16	0.46
10:k:39:TRP:O	10:k:42:ALA:HB3	2.16	0.46
14:t:20:ALA:O	14:t:24:ARG:HB3	2.16	0.46
4:D:302:GLU:OE1	4:D:302:GLU:HA	2.14	0.46
5:E:22[B]:ILE:HG23	20:R:19:ALA:HB2	1.97	0.46
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.98	0.46
5:e:18:ARG:HD2	20:r:23:ILE:HD12	1.98	0.46
1:a:85:SER:HA	1:a:109:GLY:HA3	1.98	0.46
3:c:463:SER:O	3:c:463:SER:OG	2.27	0.46
1:A:200:LEU:HD21	28:C:518:DGD:HAW2	1.96	0.46
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.97	0.46
10:K:28:ILE:N	10:K:29:PRO:CD	2.79	0.46
2:b:493:TRP:HD1	5:e:5:THR:CG2	2.29	0.46
4:D:103:ARG:O	4:D:107:LEU:HG	2.16	0.46
3:c:169:GLY:O	3:c:173:LEU:HG	2.16	0.46
13:o:4:THR:O	13:o:4:THR:OG1	2.32	0.46
3:c:309:ALA:HB1	3:c:399:ALA:HB2	1.98	0.45
3:c:391[A]:ARG:NH1	36:c:615:HOH:O	2.48	0.45
3:c:391[B]:ARG:HG2	3:c:391[B]:ARG:HH21	1.81	0.45
2:B:357:ARG:NH1	36:B:719:HOH:O	2.41	0.45
2:B:422:ARG:O	2:B:425:ILE:HG12	2.15	0.45
3:C:406:SER:HA	3:C:420:VAL:HG23	1.98	0.45
12:M:20:VAL:HG21	12:m:20:VAL:HG21	1.98	0.45
3:c:213:LEU:HD21	25:c:515:BCR:H20C	1.96	0.45
25:d:405:BCR:H381	33:d:411:LMG:H162	1.97	0.45
8:I:35:LYS:HD2	8:I:35:LYS:N	2.30	0.45
13:o:33:ASP:OD1	13:o:33:ASP:C	2.59	0.45
16:v:77:LYS:HG2	16:v:95:LEU:HD12	1.97	0.45
4:D:136:VAL:O	4:D:136:VAL:HG12	2.14	0.45
4:D:286:VAL:HG21	23:D:403:CLA:HED2	1.99	0.45
17:Y:37:PHE:O	17:Y:40:ALA:O	2.33	0.45
1:a:265:PHE:CD2	1:a:271:LEU:HD23	2.52	0.45
3:c:348:GLU:OE2	13:o:11:VAL:HA	2.16	0.45
19:z:1:MET:HB2	19:z:4:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.98	0.45
23:B:615:CLA:H93	23:B:616:CLA:H13	1.97	0.45
16:V:22:THR:HG21	36:V:330:HOH:O	2.16	0.45
23:b:614:CLA:H192	29:d:407:LHG:H222	1.98	0.45
4:d:167:TRP:O	4:d:168:PHE:C	2.60	0.45
3:C:50:LEU:O	3:C:54:VAL:HG23	2.17	0.45
4:D:209:LEU:HD23	4:D:209:LEU:C	2.41	0.45
23:b:606:CLA:HHC	23:b:606:CLA:HBB1	1.99	0.45
6:f:26:LEU:O	6:f:29:PRO:HD2	2.15	0.45
13:o:40:ILE:HG12	13:o:95:PHE:CD2	2.52	0.45
13:o:62:GLU:OE2	13:o:63:ALA:N	2.50	0.45
1:A:207:GLY:O	1:A:211:PHE:CD2	2.70	0.45
25:C:515:BCR:C8	25:C:515:BCR:C33	2.92	0.45
4:D:43:LEU:HG	4:D:113:PHE:CZ	2.52	0.45
13:O:240:TYR:C	13:O:240:TYR:CD2	2.94	0.45
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.97	0.45
25:c:514:BCR:H23C	25:c:514:BCR:C38	2.45	0.45
18:x:16:SER:HB3	32:x:101:UNL:C7	2.47	0.45
23:C:502:CLA:HHC	23:C:502:CLA:HBB1	1.98	0.45
4:D:26:ARG:NH1	36:D:504:HOH:O	2.50	0.45
17:Y:25:ILE:O	17:Y:26:ALA:C	2.59	0.45
36:A:541:HOH:O	13:O:107:THR:HG21	2.16	0.45
2:B:356:VAL:HG21	2:B:424:ALA:HB3	1.99	0.45
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.99	0.45
3:c:399:ALA:O	3:c:401:LEU:N	2.48	0.45
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.52	0.45
16:v:104:MET:HA	16:v:107:LEU:HD22	1.98	0.45
2:B:378:LYS:HD3	36:B:743:HOH:O	2.16	0.45
26:D:406:PL9:H201	29:L:101:LHG:H211	1.98	0.45
3:c:249:ILE:O	3:c:250:TRP:C	2.60	0.45
2:B:37:MET:O	2:B:41:GLU:HG3	2.16	0.44
3:C:256:PRO:O	3:C:261:ARG:NH1	2.50	0.44
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.99	0.44
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.99	0.44
13:o:56:PRO:HD3	13:o:63:ALA:HB2	1.98	0.44
18:x:34:ILE:HG22	18:x:35:ASP:N	2.31	0.44
4:D:246:MET:HE2	4:D:246:MET:HA	1.99	0.44
10:K:15:TYR:O	10:K:17:ILE:N	2.50	0.44
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.53	0.44
3:c:461:ARG:HG2	4:d:223:PHE:CD1	2.52	0.44
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:12:LEU:O	19:z:16:SER:OG	2.30	0.44
3:C:74:HIS:O	3:C:76:ILE:HD12	2.17	0.44
3:C:179:ALA:O	3:C:184:GLY:HA2	2.16	0.44
1:a:95:PRO:HG2	1:a:98:GLU:HG2	1.99	0.44
2:b:221:PRO:HB3	23:b:610:CLA:O1D	2.17	0.44
14:t:11:ALA:HB3	25:t:101:BCR:H363	2.00	0.44
18:x:23:LEU:O	18:x:26:ALA:HB3	2.17	0.44
3:C:112:PHE:O	3:C:116:VAL:HG23	2.16	0.44
23:C:507:CLA:HHD	23:C:507:CLA:HBC2	2.00	0.44
4:D:22:LEU:O	36:D:504:HOH:O	2.21	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.51	0.44
2:b:122:LEU:O	7:h:15:ASN:ND2	2.45	0.44
5:e:13:ILE:HG22	5:e:19:TYR:CD2	2.53	0.44
25:b:619:BCR:C8	25:b:619:BCR:H331	2.47	0.44
4:d:16:ASP:OD1	36:d:503:HOH:O	2.21	0.44
13:o:10:ILE:O	13:o:13:THR:HG23	2.17	0.44
13:o:178:LYS:HA	13:o:178:LYS:HD3	1.83	0.44
3:C:279:LEU:CD1	23:C:510:CLA:HED2	2.48	0.44
4:D:69:GLU:HG2	5:E:55:TYR:OH	2.18	0.44
10:K:25:LEU:N	10:K:26:PRO:HD2	2.32	0.44
16:V:99:ASP:OD1	16:V:100:ILE:N	2.45	0.44
2:b:49:ASP:C	2:b:49:ASP:OD1	2.61	0.44
2:b:383:PHE:O	13:o:166:SER:HA	2.18	0.44
4:d:19:ASP:OD1	4:d:23:LYS:HE3	2.17	0.44
2:B:331:ASN:HB3	2:B:437:LEU:HD12	2.00	0.44
3:C:443:TRP:CZ2	23:C:509:CLA:HMD1	2.52	0.44
3:C:473:ASP:OD2	14:T:24:ARG:HD3	2.17	0.44
10:K:43:VAL:O	10:K:43:VAL:HG13	2.17	0.44
19:Z:5:PHE:C	19:Z:7:LEU:H	2.26	0.44
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.44
6:F:31:ILE:O	6:F:32:PHE:C	2.61	0.44
10:K:15:TYR:O	10:K:16:ALA:C	2.60	0.44
1:a:201:GLY:HA3	1:a:286:THR:HB	1.99	0.44
1:a:262:TYR:HB3	29:e:101:LHG:O10	2.17	0.44
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.83	0.44
25:D:405:BCR:H372	33:D:407:LMG:H292	2.00	0.44
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.99	0.44
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.44
25:Z:101:BCR:H15C	25:Z:101:BCR:H351	1.88	0.44
2:b:135:LEU:N	2:b:136:PRO:CD	2.80	0.44
2:b:372:ASP:O	2:b:374:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:195:PRO:HG3	11:l:34:TYR:CE2	2.53	0.44
24:d:401:PHO:HBB1	24:d:401:PHO:CMB	2.48	0.44
1:a:243:GLU:HB2	36:a:579:HOH:O	2.18	0.43
1:a:332:HIS:O	1:a:333:GLU:C	2.61	0.43
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.00	0.43
23:B:601:CLA:HBA2	23:B:601:CLA:HBD	2.01	0.43
10:K:19:ASP:N	10:K:20:PRO:CD	2.81	0.43
17:Y:39:LEU:HD21	19:Z:28:ALA:HB3	2.00	0.43
1:a:159:LEU:C	1:a:162:PRO:HD2	2.43	0.43
3:c:121:SER:O	3:c:124:VAL:HG13	2.18	0.43
5:e:30:LEU:HD23	5:e:30:LEU:HA	1.80	0.43
7:h:59:ASN:O	7:h:61:SER:N	2.50	0.43
15:u:66:GLY:O	15:u:67:LEU:C	2.58	0.43
1:A:244:GLU:OE2	4:D:264:LYS:NZ	2.50	0.43
2:B:280:PHE:CD2	2:B:312:TYR:HB3	2.53	0.43
25:B:619:BCR:C8	25:B:619:BCR:H331	2.47	0.43
3:C:187:ASP:O	3:C:194:GLY:HA2	2.17	0.43
23:C:507:CLA:H122	25:C:515:BCR:H352	2.00	0.43
4:D:272:LEU:HD23	4:D:272:LEU:O	2.19	0.43
4:d:210:LEU:HA	4:d:213:ILE:HG22	1.99	0.43
5:e:17:VAL:HG23	9:j:7:ARG:HB2	1.99	0.43
10:k:26:PRO:O	10:k:29:PRO:HD2	2.18	0.43
13:o:125:LEU:HG	13:o:126:VAL:N	2.34	0.43
25:B:619:BCR:H20C	25:B:619:BCR:H361	1.88	0.43
3:C:337:LEU:HD23	13:O:105:PRO:HG2	2.00	0.43
12:M:9:ILE:HG13	12:M:13:LEU:HD22	2.01	0.43
12:M:20:VAL:CG1	12:m:20:VAL:HG13	2.49	0.43
3:c:71:GLU:HB3	3:c:86:LEU:HD22	2.01	0.43
4:d:152:VAL:HG21	4:d:279:LEU:HG	2.01	0.43
6:f:19:ARG:O	6:f:23:VAL:HG13	2.17	0.43
13:o:37:THR:OG1	13:o:246:ALA:HB3	2.18	0.43
1:A:33:PHE:HE1	23:C:506:CLA:H92	1.83	0.43
1:A:91:LEU:HD11	1:A:163:ILE:HA	2.01	0.43
25:D:405:BCR:H392	25:D:405:BCR:C23	2.48	0.43
3:c:116:VAL:O	3:c:120:ILE:HG12	2.18	0.43
16:v:100:ILE:C	16:v:102:PRO:HD3	2.44	0.43
24:A:406:PHO:HBC2	24:A:406:PHO:HHD	2.00	0.43
4:D:332:GLN:NE2	36:D:515:HOH:O	2.44	0.43
13:O:58:ASN:HB3	36:b:701:HOH:O	2.19	0.43
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	2.01	0.43
23:b:604:CLA:HMB3	23:b:604:CLA:H51	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:20:ALA:O	17:y:23:THR:HG22	2.19	0.43
28:A:412:DGD:HB21	28:A:412:DGD:HG12	2.01	0.43
4:D:42:TYR:CE1	6:F:25:THR:CG2	3.00	0.43
20:R:10:LEU:CD1	20:R:14:LEU:HD21	2.48	0.43
1:a:308:ASP:OD1	1:a:308:ASP:C	2.61	0.43
25:c:514:BCR:C8	25:c:514:BCR:H331	2.49	0.43
13:o:204:VAL:HG22	13:o:211:ILE:HG22	2.01	0.43
15:u:53:ALA:HB3	15:u:54:PRO:HD3	2.01	0.43
2:B:376:VAL:HG12	2:B:378:LYS:HD3	2.00	0.43
3:C:56:HIS:CE1	3:C:60:ILE:HD11	2.53	0.43
23:C:511:CLA:H202	23:C:511:CLA:H161	1.91	0.43
25:C:515:BCR:H24C	25:C:515:BCR:H371	1.86	0.43
25:K:101:BCR:H322	19:Z:17:PHE:CE1	2.53	0.43
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.54	0.43
34:e:102:HEM:HBC2	34:e:102:HEM:CMC	2.49	0.43
20:r:3:TRP:CD1	20:r:3:TRP:C	2.96	0.43
1:A:307:ILE:HG22	1:A:313:VAL:HA	2.00	0.43
3:C:279:LEU:HD12	23:C:510:CLA:CED	2.48	0.43
4:D:273:PHE:CE1	29:L:101:LHG:H121	2.54	0.43
5:E:68:ASP:O	5:E:72:ALA:HB2	2.19	0.43
9:J:38:SER:O	9:J:39:SER:OG	2.32	0.43
15:U:16:LYS:NZ	36:U:201:HOH:O	2.29	0.43
1:a:29:TYR:CE2	1:a:31:GLY:HA3	2.54	0.43
23:b:602:CLA:CBB	7:h:41:PHE:CZ	3.02	0.43
7:h:40:VAL:O	7:h:44:ILE:HG13	2.19	0.43
18:x:23:LEU:O	18:x:24:THR:C	2.62	0.43
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.07	0.43
13:O:61:GLN:O	13:O:62:GLU:O	2.37	0.43
1:a:270:SER:OG	27:a:411:SQD:H3	2.19	0.43
26:a:410:PL9:C30	4:d:45:LEU:HD22	2.48	0.43
33:c:524:LMG:HC91	33:c:524:LMG:O9	2.18	0.43
9:j:40:LEU:OXT	16:v:30:LYS:NZ	2.50	0.43
5:E:22[A]:ILE:HD12	20:R:19:ALA:CB	2.48	0.42
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.01	0.42
4:d:101:PHE:CD2	4:d:101:PHE:C	2.97	0.42
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.54	0.42
3:C:245:ILE:O	3:C:246:ALA:C	2.60	0.42
3:C:317:PHE:HE2	3:C:396:MET:HE1	1.84	0.42
4:D:60:THR:HG22	36:D:509:HOH:O	2.18	0.42
10:K:38:VAL:HG23	25:K:101:BCR:H21C	2.00	0.42
16:V:95:LEU:HD11	16:V:112:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:604:CLA:H2	23:b:606:CLA:H91	2.01	0.42
23:b:616:CLA:HHC	23:b:616:CLA:CBB	2.50	0.42
13:o:62:GLU:OE2	13:o:63:ALA:O	2.37	0.42
13:o:190:PHE:CD1	13:o:190:PHE:C	2.97	0.42
3:C:168:LEU:HD21	23:C:510:CLA:H61	2.01	0.42
13:O:24:ASP:OD1	13:O:24:ASP:N	2.52	0.42
9:j:19:MET:HA	9:j:22:ILE:HD12	2.01	0.42
1:A:201:GLY:HA3	1:A:286:THR:HB	2.00	0.42
10:K:17:ILE:HD12	10:K:17:ILE:H	1.84	0.42
13:O:10:ILE:HD12	13:O:15:LEU:HD12	2.00	0.42
23:b:615:CLA:H41	23:b:615:CLA:C7	2.49	0.42
3:c:67:MET:O	3:c:71:GLU:HG3	2.19	0.42
3:C:344:SER:O	13:O:75:THR:HG22	2.19	0.42
10:K:18:PHE:CE2	19:Z:9:LEU:HD21	2.55	0.42
1:a:114:LEU:C	1:a:114:LEU:HD23	2.45	0.42
1:a:288:LEU:HD12	1:a:288:LEU:HA	1.92	0.42
2:b:240:SER:HB3	36:b:800:HOH:O	2.19	0.42
23:c:501:CLA:HHC	23:c:501:CLA:HAB	1.86	0.42
4:d:218:VAL:HG22	4:d:244:TYR:CZ	2.55	0.42
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.55	0.42
4:D:235:PHE:CE2	4:D:237:PRO:HA	2.55	0.42
10:K:15:TYR:C	10:K:17:ILE:N	2.77	0.42
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.00	0.42
23:c:510:CLA:HMB1	23:c:510:CLA:HBB1	2.00	0.42
7:H:38:PHE:HB2	25:H:101:BCR:C10	2.50	0.42
7:H:58:VAL:HB	36:H:204:HOH:O	2.19	0.42
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.79	0.42
9:J:15:THR:HG22	9:J:19:MET:CE	2.50	0.42
13:O:27:ARG:HG3	13:O:27:ARG:HH11	1.84	0.42
13:O:57:LYS:HE2	2:b:338:GLN:O	2.20	0.42
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.01	0.42
16:V:3:LEU:HD23	16:V:3:LEU:HA	1.83	0.42
19:Z:15:LEU:HD22	19:Z:19:MET:SD	2.60	0.42
2:b:249:ALA:HB2	23:b:605:CLA:HBC3	2.02	0.42
13:o:81:ILE:HA	13:o:100:GLY:HA3	2.01	0.42
16:v:13:ASN:ND2	16:v:15:GLU:HB2	2.35	0.42
27:A:411:SQD:H341	23:b:617:CLA:C9	2.49	0.42
2:B:201:HIS:HB2	23:B:602:CLA:CHB	2.50	0.42
3:C:284:PHE:O	3:C:287:THR:HB	2.20	0.42
4:D:52:THR:O	4:D:66:SER:HA	2.20	0.42
13:O:107:THR:HG22	36:O:357:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:45:THR:HG23	23:d:402:CLA:H201	2.02	0.42
2:b:221:PRO:O	7:h:21:VAL:HG12	2.19	0.42
4:d:261:PHE:CZ	29:d:408:LHG:HC81	2.55	0.42
20:r:24:LEU:N	20:r:25:PRO:HD2	2.35	0.42
1:A:85:SER:HA	1:A:109:GLY:HA3	2.01	0.42
4:D:264:LYS:HE2	36:D:503:HOH:O	2.19	0.42
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.99	0.42
12:M:20:VAL:HG11	12:m:20:VAL:HG22	2.02	0.42
13:O:88:ASN:HB2	36:O:301:HOH:O	2.20	0.42
18:X:3:ILE:HG23	18:X:3:ILE:O	2.19	0.42
1:a:214:MET:SD	24:d:401:PHO:CAD	3.08	0.42
4:d:192:THR:HG23	23:d:403:CLA:HBC2	2.01	0.42
7:h:33:VAL:O	7:h:37:LEU:HD12	2.20	0.42
16:v:56:THR:OG1	36:v:303:HOH:O	2.22	0.42
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.55	0.42
1:A:214:MET:O	1:A:218:LEU:HG	2.19	0.42
2:B:185:TRP:HB3	23:B:601:CLA:HMA3	2.02	0.42
2:B:249:ALA:HB3	2:B:459:ALA:HB2	2.02	0.42
25:H:101:BCR:H20C	25:H:101:BCR:H361	1.84	0.42
19:Z:57:LEU:N	19:Z:57:LEU:HD23	2.34	0.42
2:b:150:CYS:HB2	23:b:604:CLA:CMC	2.50	0.42
3:c:281:MET:HG3	33:c:524:LMG:H401	2.02	0.42
8:i:16:VAL:O	8:i:20:VAL:HG23	2.20	0.42
4:D:42:TYR:CZ	6:F:25:THR:HG23	2.55	0.41
1:a:133:LEU:O	1:a:137:LEU:HG	2.19	0.41
2:b:453:PHE:O	2:b:457:VAL:HG23	2.20	0.41
23:b:614:CLA:HMB1	23:b:614:CLA:HBB1	2.01	0.41
3:c:175:LEU:HD22	23:c:501:CLA:C3D	2.50	0.41
5:e:22:ILE:HG23	20:r:19:ALA:HB2	2.02	0.41
29:A:413:LHG:H223	23:B:613:CLA:H192	2.02	0.41
10:K:27:VAL:HG12	10:K:27:VAL:O	2.20	0.41
13:O:224:ASP:HB3	13:O:227:ALA:HB3	2.01	0.41
1:a:283:VAL:HG21	24:a:407:PHO:HBC3	2.02	0.41
2:b:125:ASP:OD2	2:b:127:ARG:HB2	2.20	0.41
13:o:163:GLY:HA2	13:o:188:LYS:HG3	2.01	0.41
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.54	0.41
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.02	0.41
2:B:102:VAL:HA	25:B:618:BCR:C40	2.50	0.41
3:C:391:ARG:HD3	3:C:395:TYR:CZ	2.56	0.41
7:H:59:ASN:O	7:H:64:ALA:HB2	2.20	0.41
2:b:56:TRP:HA	36:b:788:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:28:GLN:NE2	4:d:230:SER:HB3	2.36	0.41
18:x:3:ILE:N	18:x:3:ILE:HD12	2.36	0.41
20:r:20:VAL:O	20:r:24:LEU:HB2	2.20	0.41
28:A:412:DGD:HD5	2:b:75:TRP:HB3	2.03	0.41
2:B:159:THR:O	2:B:180:PRO:HB3	2.20	0.41
6:F:18:VAL:HG23	27:F:101:SQD:O8	2.19	0.41
14:T:29:ILE:CG2	14:T:30:THR:N	2.82	0.41
3:c:155:ASN:OD1	3:c:255:THR:HG22	2.20	0.41
4:d:165:SER:HB2	36:d:565:HOH:O	2.21	0.41
15:u:44:THR:OG1	16:v:83:ASP:OD1	2.33	0.41
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.01	0.41
1:A:183:MET:HE2	23:D:403:CLA:CMC	2.49	0.41
1:a:110:GLY:N	1:a:111:PRO:CD	2.83	0.41
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.55	0.41
33:c:524:LMG:HC2	8:i:9:TYR:OH	2.21	0.41
4:d:126:MET:HA	4:d:129:GLN:OE1	2.20	0.41
4:d:232:PHE:HZ	29:d:409:LHG:O9	2.03	0.41
5:e:17:VAL:O	5:e:21:VAL:HG23	2.20	0.41
2:B:252:VAL:HG11	23:B:604:CLA:OBD	2.20	0.41
1:a:40:THR:O	1:a:118:HIS:HB3	2.21	0.41
1:a:219:VAL:O	1:a:223:LEU:HD13	2.21	0.41
1:a:268:SER:HB2	4:d:235:PHE:CZ	2.56	0.41
2:b:159:THR:O	2:b:180:PRO:HB3	2.20	0.41
25:b:618:BCR:H382	25:b:618:BCR:H23C	2.02	0.41
5:e:57:ALA:O	5:e:58:GLN:C	2.64	0.41
25:t:101:BCR:HC8	25:t:101:BCR:H321	2.02	0.41
3:C:241:GLY:O	3:C:245:ILE:HG13	2.20	0.41
23:C:512:CLA:C14	19:Z:20:VAL:HG13	2.51	0.41
13:O:54:GLU:O	13:O:63:ALA:HB3	2.20	0.41
16:V:61:LEU:HD23	16:V:61:LEU:HA	1.89	0.41
23:c:505:CLA:C1A	23:c:505:CLA:CGA	2.98	0.41
10:k:25:LEU:N	10:k:26:PRO:CD	2.84	0.41
13:o:164:LEU:HD13	13:o:188:LYS:O	2.21	0.41
17:y:41:VAL:C	17:y:43:ARG:H	2.29	0.41
2:B:246:PHE:CD2	2:B:246:PHE:C	2.98	0.41
19:Z:29:SER:HB3	19:Z:31:GLN:CG	2.51	0.41
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.86	0.41
4:d:272:LEU:C	4:d:272:LEU:HD23	2.46	0.41
10:k:16:ALA:C	10:k:18:PHE:H	2.29	0.41
1:A:234:ASN:HD21	29:A:413:LHG:HC11	1.86	0.41
36:A:591:HOH:O	4:D:350:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.34	0.41
2:B:229:LEU:O	2:B:230:ARG:C	2.64	0.41
23:B:601:CLA:H2	23:B:601:CLA:HAA2	2.03	0.41
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.88	0.41
5:E:30:LEU:HD12	34:E:103:HEM:HMC2	2.03	0.41
34:E:103:HEM:HBC2	34:E:103:HEM:CHD	2.50	0.41
2:b:199:VAL:O	2:b:200:ALA:C	2.64	0.41
23:b:616:CLA:H2	23:b:617:CLA:HBB2	2.03	0.41
25:t:101:BCR:HC7	25:t:101:BCR:H331	1.82	0.41
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.51	0.41
25:C:515:BCR:H331	25:C:515:BCR:HC8	2.00	0.41
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.56	0.41
25:D:405:BCR:H361	25:D:405:BCR:H20C	1.72	0.41
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.02	0.41
1:a:254:TYR:OH	4:d:129:GLN:HB3	2.21	0.41
2:b:69:LEU:HD21	23:b:604:CLA:HED3	2.03	0.41
2:b:478:VAL:O	4:d:139:ARG:HG2	2.21	0.41
2:b:492:GLU:HB3	2:b:495:PHE:CE2	2.55	0.41
15:u:16:LYS:HE3	15:u:85:THR:OG1	2.21	0.41
16:v:2:GLU:HB2	36:v:332:HOH:O	2.20	0.41
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.03	0.40
2:B:161:LEU:HD12	2:B:161:LEU:HA	1.88	0.40
3:C:469:MET:HB3	3:C:470:PRO:HD2	2.02	0.40
25:H:101:BCR:H15C	25:H:101:BCR:H351	1.97	0.40
15:U:39:ARG:NH2	16:V:60:ALA:O	2.54	0.40
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.02	0.40
25:b:619:BCR:H20C	25:b:619:BCR:H361	1.96	0.40
23:c:505:CLA:HBB1	23:c:505:CLA:CMB	2.49	0.40
19:z:38:GLN:O	19:z:42:LEU:HD13	2.21	0.40
1:A:210:LEU:HD23	1:A:214:MET:HG2	2.03	0.40
15:U:20:ALA:HA	15:U:23:GLU:HG3	2.02	0.40
20:R:29:LYS:O	20:R:33:LYS:HG3	2.21	0.40
1:a:245:THR:HG22	4:d:265:ARG:NH2	2.36	0.40
23:a:408:CLA:H42	8:i:9:TYR:CE2	2.56	0.40
3:c:367:GLU:N	3:c:368:PRO:HD2	2.36	0.40
5:e:17:VAL:H	9:j:7:ARG:HD2	1.86	0.40
9:j:25:VAL:O	9:j:26:GLY:C	2.64	0.40
1:A:37:MET:HB2	1:A:125:CYS:HB2	2.03	0.40
2:B:476:ARG:HE	2:B:477:ASP:N	2.19	0.40
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.56	0.40
4:D:176:ALA:O	4:D:179:PHE:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:VAL:HG23	9:J:7:ARG:CG	2.51	0.40
1:a:166:GLY:O	1:a:167:SER:HB2	2.21	0.40
17:y:43:ARG:HB3	17:y:43:ARG:NH1	2.36	0.40
2:B:62:VAL:O	2:B:63:LEU:C	2.63	0.40
23:C:502:CLA:HHC	23:C:502:CLA:CBB	2.52	0.40
10:K:34:ALA:HB1	25:K:101:BCR:H19C	2.03	0.40
12:M:17:VAL:N	12:M:18:PRO:CD	2.84	0.40
1:a:334:ARG:NH2	36:a:507:HOH:O	2.50	0.40
26:a:410:PL9:H351	6:f:25:THR:OG1	2.21	0.40
23:b:612:CLA:HED2	36:d:534:HOH:O	2.22	0.40
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.04	0.40
19:z:48:ILE:O	19:z:52:LEU:HG	2.21	0.40
20:r:29:LYS:O	20:r:30:GLN:C	2.64	0.40
5:E:57:ALA:O	5:E:58:GLN:C	2.64	0.40
16:V:69:ILE:O	16:V:73:VAL:HG23	2.20	0.40
16:V:87:GLU:OE1	16:V:96:ARG:NH1	2.55	0.40
1:a:278:TRP:HB3	1:a:279:PRO:HD3	2.03	0.40
2:b:181:VAL:HA	36:b:784:HOH:O	2.21	0.40
2:b:252:VAL:HG13	2:b:451:PHE:CE2	2.57	0.40
23:b:615:CLA:H191	25:b:618:BCR:H331	2.04	0.40
5:e:68:ASP:O	5:e:72:ALA:HB2	2.21	0.40
17:y:40:ALA:O	17:y:43:ARG:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	332/334 (99%)	322 (97%)	9 (3%)	1 (0%)	36 55
1	a	332/334 (99%)	320 (96%)	11 (3%)	1 (0%)	36 55
2	B	508/505 (101%)	488 (96%)	19 (4%)	1 (0%)	43 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	503/505 (100%)	480 (95%)	20 (4%)	3 (1%)	21	38
3	C	440/451 (98%)	420 (96%)	19 (4%)	1 (0%)	43	63
3	c	450/451 (100%)	433 (96%)	15 (3%)	2 (0%)	30	49
4	D	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	36	55
4	d	340/341 (100%)	323 (95%)	17 (5%)	0	100	100
5	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	j	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
10	K	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	5
10	k	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	33 (97%)	0	1 (3%)	3	5
12	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	m	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
13	O	243/244 (100%)	225 (93%)	14 (6%)	4 (2%)	7	14
13	o	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	10	20
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
15	u	95/97 (98%)	91 (96%)	3 (3%)	1 (1%)	11	22
16	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	v	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
17	Y	25/30 (83%)	18 (72%)	5 (20%)	2 (8%)	1	0
17	y	28/30 (93%)	23 (82%)	4 (14%)	1 (4%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	X	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	6
18	x	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	47 (78%)	11 (18%)	2 (3%)	3	4
20	R	32/34 (94%)	30 (94%)	1 (3%)	1 (3%)	3	5
20	r	29/34 (85%)	24 (83%)	3 (10%)	2 (7%)	1	1
All	All	5235/5326 (98%)	4963 (95%)	243 (5%)	29 (1%)	21	38

All (29) 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
13	o	60	ARG
13	o	61	GLN
15	u	53	ALA
19	z	15	LEU
20	r	30	GLN
17	Y	43	ARG
20	R	34	LEU
2	b	85	GLY
20	r	31	VAL
2	B	438	ASN
18	X	38	GLN
19	z	14	ILE
4	D	338	ASN
2	b	127	ARG
13	O	138	THR
3	c	250	TRP
11	l	7	ARG
13	o	132	ASN
17	y	41	VAL
13	O	57	LYS
2	b	295	GLY
13	O	133	VAL
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/270 (100%)	258 (96%)	12 (4%)	25	50
1	a	269/270 (100%)	255 (95%)	14 (5%)	21	42
2	B	407/403 (101%)	385 (95%)	22 (5%)	20	41
2	b	402/403 (100%)	383 (95%)	19 (5%)	23	47
3	C	344/352 (98%)	336 (98%)	8 (2%)	44	72
3	c	353/352 (100%)	333 (94%)	20 (6%)	18	39
4	D	276/276 (100%)	269 (98%)	7 (2%)	42	69
4	d	277/276 (100%)	270 (98%)	7 (2%)	42	69
5	E	72/72 (100%)	60 (83%)	12 (17%)	2	4
5	e	71/72 (99%)	65 (92%)	6 (8%)	10	22
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	28/28 (100%)	23 (82%)	5 (18%)	2	3
7	H	53/54 (98%)	48 (91%)	5 (9%)	8	18
7	h	53/54 (98%)	48 (91%)	5 (9%)	8	18
8	I	32/32 (100%)	28 (88%)	4 (12%)	4	9
8	i	32/32 (100%)	30 (94%)	2 (6%)	16	34
9	J	24/24 (100%)	23 (96%)	1 (4%)	26	52
9	j	23/24 (96%)	20 (87%)	3 (13%)	4	8
10	K	31/30 (103%)	26 (84%)	5 (16%)	2	4
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	8
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	20
12	M	28/29 (97%)	24 (86%)	4 (14%)	3	6
12	m	28/29 (97%)	26 (93%)	2 (7%)	13	29
13	O	208/207 (100%)	188 (90%)	20 (10%)	8	17
13	o	207/207 (100%)	189 (91%)	18 (9%)	9	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	26/26 (100%)	24 (92%)	2 (8%)	12	25
14	t	25/26 (96%)	24 (96%)	1 (4%)	28	54
15	U	84/84 (100%)	74 (88%)	10 (12%)	5	11
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	83
16	V	117/117 (100%)	111 (95%)	6 (5%)	21	43
16	v	117/117 (100%)	109 (93%)	8 (7%)	14	31
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2	5
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	8
18	X	31/31 (100%)	27 (87%)	4 (13%)	4	9
18	x	31/31 (100%)	28 (90%)	3 (10%)	8	17
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	4
19	z	51/52 (98%)	40 (78%)	11 (22%)	1	2
20	R	28/29 (97%)	21 (75%)	7 (25%)	0	1
20	r	19/29 (66%)	16 (84%)	3 (16%)	2	5
All	All	4321/4348 (99%)	4042 (94%)	279 (6%)	16	32

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	15	GLU
1	A	16	ARG
1	A	102	LEU
1	A	205	VAL
1	A	210	LEU
1	A	229	GLU
1	A	231	GLU
1	A	243	GLU
1	A	286	THR
1	A	307	ILE
2	B	63	LEU
2	B	76	SER
2	B	83	GLU
2	B	127	ARG
2	B	161	LEU
2	B	207	ILE

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Mol	Chain	Res	Type
2	B	227	LYS
2	B	236	THR
2	B	241	SER
2	B	246	PHE
2	B	289	GLN
2	B	298	LEU
2	B	362	PHE
2	B	371	THR
2	B	435	GLU
2	B	467	ILE
2	B	476	ARG
2	B	485	GLU
2	B	486	LEU
2	B	489	GLU
2	B	491	VAL
2	B	495	PHE
3	C	134	ILE
3	C	141	GLU
3	C	161	LEU
3	C	200	THR
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	12	ARG
4	D	26	ARG
4	D	43	LEU
4	D	76	VAL
4	D	150	ILE
4	D	264	LYS
4	D	345	VAL
5	E	4	THR
5	E	11	SER
5	E	16	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	32	ILE
5	E	65	LEU
5	E	67	THR
5	E	71	GLU
5	E	76	VAL
5	E	77	GLU

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Mol	Chain	Res	Type
5	E	83	LEU
7	H	5	THR
7	H	20	LYS
7	H	27	THR
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	33	LYS
8	I	34	ARG
8	I	35	LYS
9	J	8	ILE
10	K	10	LYS
10	K	25	LEU
10	K	43	VAL
10	K	46[A]	ARG
10	K	46[B]	ARG
12	M	3	VAL
12	M	13	LEU
12	M	16	LEU
12	M	31	SER
13	O	3	GLN
13	O	4	THR
13	O	23	ASP
13	O	34	SER
13	O	39	ARG
13	O	45	LEU
13	O	64	GLU
13	O	66	VAL
13	O	72	THR
13	O	78	LEU
13	O	82	GLN
13	O	107	THR
13	O	118	LEU
13	O	134	THR
13	O	143	LYS
13	O	182	LEU
13	O	191	SER
13	O	207	ARG
13	O	214	THR
13	O	217	SER
14	T	2	GLU
14	T	24	ARG

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Mol	Chain	Res	Type
15	U	8	GLU
15	U	10	VAL
15	U	23	GLU
15	U	37	GLN
15	U	39	ARG
15	U	51	LYS
15	U	59	GLU
15	U	64	ILE
15	U	67	LEU
15	U	85	THR
16	V	2	GLU
16	V	3	LEU
16	V	7	VAL
16	V	21	LEU
16	V	31	ARG
16	V	105	ARG
17	Y	24	MET
17	Y	27	MET
17	Y	43	ARG
18	X	29	ILE
18	X	36	LYS
18	X	37	VAL
18	X	39	ARG
19	Z	2	THR
19	Z	3	ILE
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	40	ILE
19	Z	46	LEU
19	Z	50	LEU
19	Z	61	VAL
20	R	2	ASP
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	12	VAL
20	R	13	LEU
20	R	20	VAL
1	a	28	LEU
1	a	35	VAL
1	a	42	LEU

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Mol	Chain	Res	Type
1	a	60	ILE
1	a	121	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	227	THR
1	a	229	GLU
1	a	231	GLU
1	a	238	LYS
1	a	245	THR
1	a	288	LEU
2	b	80	ILE
2	b	81	THR
2	b	86	ILE
2	b	149	LEU
2	b	170	ASP
2	b	175	THR
2	b	219	VAL
2	b	236	THR
2	b	252	VAL
2	b	288	VAL
2	b	315	ILE
2	b	347	ARG
2	b	353	GLU
2	b	388	SER
2	b	397	VAL
2	b	409	GLN
2	b	480	SER
2	b	490	GLN
2	b	492	GLU
3	c	24	THR
3	c	25	ASN
3	c	26	ARG
3	c	30	SER
3	c	43	ILE
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	155	ASN
3	c	165	LEU
3	c	249	ILE
3	c	289	PHE

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Mol	Chain	Res	Type
3	c	315	MET
3	c	354	GLU
3	c	384	ILE
3	c	396	MET
3	c	421	SER
3	c	462	GLU
3	c	463	SER
3	c	471	SER
4	d	90	LEU
4	d	182	LEU
4	d	267	LEU
4	d	272	LEU
4	d	291	LEU
4	d	321	LEU
4	d	345	VAL
5	e	8	ARG
5	e	12	ASP
5	e	60	GLN
5	e	67	THR
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	3	ARG
7	h	7	LEU
7	h	10	ILE
7	h	12	ARG
7	h	21	VAL
8	i	32	PRO
8	i	33	LYS
9	j	7	ARG
9	j	13	VAL
9	j	36	LEU
10	k	10	LYS
10	k	21	LEU
10	k	30	VAL
10	k	46	ARG
11	l	7	ARG
11	l	21	LEU

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Mol	Chain	Res	Type
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	4	THR
13	o	10	ILE
13	o	35	SER
13	o	39	ARG
13	o	49	THR
13	o	57	LYS
13	o	59	LYS
13	o	60	ARG
13	o	64	GLU
13	o	72	THR
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	133	VAL
13	o	181	GLU
13	o	207	ARG
13	o	225	MET
13	o	242	SER
14	t	21	ILE
15	u	10	VAL
16	v	15	GLU
16	v	19	ILE
16	v	24	LYS
16	v	52	LEU
16	v	90	GLU
16	v	100	ILE
16	v	106	ASN
16	v	108	THR
17	y	19	ILE
17	y	22	LEU
17	y	38	LEU
18	x	8	LYS
18	x	15	LEU
18	x	34	ILE
19	z	1	MET
19	z	3	ILE
19	z	4	LEU
19	z	12	LEU
19	z	20	VAL

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Mol	Chain	Res	Type
19	z	29	SER
19	z	31	GLN
19	z	32	ASP
19	z	38	GLN
19	z	42	LEU
19	z	46	LEU
20	r	3	TRP
20	r	7	VAL
20	r	23	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	75	ASN
1	A	234	ASN
1	A	261	GLN
2	B	285	ASN
2	B	374	ASN
2	B	497	GLN
3	C	74	HIS
3	C	418	ASN
4	D	186	GLN
4	D	334	GLN
12	M	4	ASN
13	O	82	GLN
13	O	88	ASN
13	O	231	HIS
15	U	37	GLN
15	U	81	HIS
16	V	86	GLN
19	Z	6	GLN
1	a	199	GLN
2	b	14	ASN
2	b	179	GLN
2	b	274	GLN
2	b	281	GLN
2	b	282	GLN
2	b	348	ASN
2	b	497	GLN
3	c	25	ASN
3	c	28	GLN

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Mol	Chain	Res	Type
3	c	201	ASN
3	c	322	GLN
3	c	378	ASN
4	d	334	GLN
5	e	74	GLN
11	l	6	ASN
13	o	36	GLN
13	o	58	ASN
13	o	124	ASN
13	o	147	ASN
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	$\# Z > 2$
14	FME	T	1	14	8,9,10	1.00	1 (12%)	8,9,11	1.41	1 (12%)
8	FME	I	1	8	8,9,10	1.12	1 (12%)	8,9,11	1.44	2 (25%)
12	FME	M	1	12	8,9,10	1.13	1 (12%)	8,9,11	1.00	0
14	FME	t	1	14	8,9,10	1.10	1 (12%)	8,9,11	1.22	1 (12%)
12	FME	m	1	12	8,9,10	1.09	1 (12%)	8,9,11	0.72	0
8	FME	i	1	8	8,9,10	1.27	1 (12%)	8,9,11	1.01	0

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.78	1.42	1.46
14	t	1	FME	CA-N	-2.61	1.42	1.46
14	T	1	FME	CA-N	-2.58	1.42	1.46
12	m	1	FME	CA-N	-2.51	1.42	1.46
8	I	1	FME	CA-N	-2.44	1.43	1.46
12	M	1	FME	CA-N	-2.27	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.37	119.17	122.82
14	T	1	FME	CA-N-CN	-2.36	119.19	122.82
8	I	1	FME	CB-CA-N	2.31	114.72	110.52
14	t	1	FME	CB-CA-N	2.10	114.34	110.52

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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
28	DGD	A	412	-	67,67,67	1.41	12 (17%)	81,81,81	1.37	5 (6%)
23	CLA	c	511	3	69,73,73	1.62	10 (14%)	82,113,113	1.32	4 (4%)
23	CLA	c	507	36	69,73,73	1.32	8 (11%)	82,113,113	1.44	9 (10%)
25	BCR	K	101	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	9 (16%)
23	CLA	C	502	-	69,73,73	1.52	8 (11%)	82,113,113	1.80	11 (13%)
25	BCR	b	619	-	41,41,41	1.32	2 (4%)	56,56,56	1.32	6 (10%)
23	CLA	D	403	-	69,73,73	1.30	7 (10%)	82,113,113	1.53	7 (8%)
30	OEX	a	415	1,3,36	0,15,15	-	-	-	-	-
23	CLA	d	404	-	69,73,73	1.64	8 (11%)	82,113,113	1.35	10 (12%)
23	CLA	B	601	36	69,73,73	1.55	9 (13%)	82,113,113	1.31	9 (10%)
29	LHG	d	409	-	38,38,48	0.89	2 (5%)	41,44,54	1.14	3 (7%)
23	CLA	B	610	36	69,73,73	1.31	9 (13%)	82,113,113	1.56	12 (14%)
26	PL9	a	410	-	55,55,55	1.29	4 (7%)	68,69,69	1.54	15 (22%)
29	LHG	l	101	-	48,48,48	0.80	2 (4%)	51,54,54	1.18	3 (5%)
25	BCR	A	408	-	41,41,41	1.18	5 (12%)	56,56,56	1.51	11 (19%)
28	DGD	a	413	-	43,43,67	1.50	4 (9%)	45,45,81	1.23	5 (11%)
23	CLA	C	513	-	69,73,73	2.10	11 (15%)	82,113,113	1.30	11 (13%)
23	CLA	b	604	-	69,73,73	1.28	9 (13%)	82,113,113	1.45	12 (14%)
25	BCR	t	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.45	13 (23%)
27	SQD	b	601	-	47,49,54	1.00	2 (4%)	57,60,65	2.18	15 (26%)
30	OEX	A	414	1,3,36	0,15,15	-	-	-	-	-
27	SQD	a	411	-	52,54,54	0.98	5 (9%)	62,65,65	1.86	9 (14%)

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	1.84	8 (17%)	58,82,82	1.49	7 (12%)
35	HEC	v	201	16	46,50,50	1.93	8 (17%)	58,82,82	1.35	4 (6%)
23	CLA	c	513	-	69,73,73	1.23	9 (13%)	82,113,113	1.14	7 (8%)
25	BCR	b	620	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	7 (12%)
25	BCR	H	101	-	41,41,41	1.32	3 (7%)	56,56,56	1.35	7 (12%)
23	CLA	B	603	-	69,73,73	1.42	10 (14%)	82,113,113	1.51	10 (12%)
23	CLA	C	508	36	69,73,73	1.38	10 (14%)	82,113,113	1.28	11 (13%)
25	BCR	Z	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.44	9 (16%)
26	PL9	A	409	-	55,55,55	1.29	5 (9%)	68,69,69	1.41	8 (11%)
23	CLA	C	509	-	69,73,73	1.36	10 (14%)	82,113,113	1.66	14 (17%)
23	CLA	C	511	-	69,73,73	1.67	12 (17%)	82,113,113	1.43	9 (10%)
28	DGD	c	518	-	63,63,67	1.27	9 (14%)	77,77,81	1.53	12 (15%)
23	CLA	B	615	-	69,73,73	1.56	10 (14%)	82,113,113	1.38	11 (13%)
23	CLA	b	602	36	69,73,73	1.54	11 (15%)	82,113,113	1.38	13 (15%)
23	CLA	C	504	-	69,73,73	1.51	8 (11%)	82,113,113	1.72	14 (17%)
23	CLA	B	605	-	69,73,73	1.44	12 (17%)	82,113,113	1.40	18 (21%)
23	CLA	c	509	-	69,73,73	1.48	9 (13%)	82,113,113	1.73	8 (9%)
33	LMG	c	524	-	49,49,55	1.17	5 (10%)	57,57,63	1.30	4 (7%)
23	CLA	D	402	36	69,73,73	1.22	7 (10%)	82,113,113	1.16	7 (8%)
23	CLA	b	614	-	69,73,73	1.28	10 (14%)	82,113,113	1.40	10 (12%)
23	CLA	C	514	-	69,73,73	1.27	8 (11%)	82,113,113	1.50	8 (9%)
25	BCR	B	619	-	41,41,41	1.23	4 (9%)	56,56,56	1.27	9 (16%)
33	LMG	D	411	-	26,26,55	0.83	1 (3%)	26,26,63	1.19	1 (3%)
24	PHO	d	401	-	58,69,69	2.07	10 (17%)	55,99,99	1.63	12 (21%)
28	DGD	H	102	-	63,63,67	1.35	12 (19%)	77,77,81	1.50	13 (16%)
28	DGD	c	517	-	63,63,67	1.18	6 (9%)	77,77,81	1.33	8 (10%)
23	CLA	c	506	-	69,73,73	1.87	11 (15%)	82,113,113	1.46	11 (13%)
27	SQD	A	410	-	50,52,54	1.09	6 (12%)	60,63,65	2.08	12 (20%)
23	CLA	c	510	-	69,73,73	1.24	9 (13%)	82,113,113	1.50	12 (14%)
33	LMG	c	519	-	37,37,55	1.13	4 (10%)	45,45,63	1.31	5 (11%)
23	CLA	B	612	-	69,73,73	1.62	7 (10%)	82,113,113	1.52	12 (14%)
33	LMG	C	501	-	48,48,55	1.17	6 (12%)	56,56,63	1.38	10 (17%)
23	CLA	C	510	-	69,73,73	1.18	9 (13%)	82,113,113	1.32	6 (7%)
25	BCR	C	520	-	41,41,41	1.06	3 (7%)	56,56,56	1.37	8 (14%)
34	HEM	E	103	6,5	50,50,50	1.38	7 (14%)	67,82,82	1.09	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	610	-	69,73,73	1.34	11 (15%)	82,113,113	1.25	9 (10%)
25	BCR	b	618	-	41,41,41	1.22	5 (12%)	56,56,56	1.32	6 (10%)
23	CLA	B	604	-	69,73,73	1.47	8 (11%)	82,113,113	1.41	10 (12%)
33	LMG	M	101	-	51,51,55	1.00	1 (1%)	59,59,63	1.48	10 (16%)
26	PL9	d	406	-	55,55,55	1.33	8 (14%)	68,69,69	1.74	14 (20%)
23	CLA	d	402	36	69,73,73	1.38	8 (11%)	82,113,113	1.84	13 (15%)
25	BCR	c	514	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	7 (12%)
24	PHO	D	401	-	58,69,69	2.07	9 (15%)	55,99,99	1.58	9 (16%)
25	BCR	C	515	-	41,41,41	1.30	5 (12%)	56,56,56	1.34	9 (16%)
25	BCR	B	617	-	41,41,41	1.31	4 (9%)	56,56,56	1.40	8 (14%)
25	BCR	T	101	-	41,41,41	1.23	4 (9%)	56,56,56	1.47	10 (17%)
23	CLA	b	612	-	69,73,73	1.55	9 (13%)	82,113,113	1.44	16 (19%)
25	BCR	B	618	-	41,41,41	1.39	4 (9%)	56,56,56	1.43	8 (14%)
27	SQD	A	411	-	38,38,54	1.11	4 (10%)	40,40,65	1.46	4 (10%)
33	LMG	b	622	-	55,55,55	1.08	4 (7%)	63,63,63	1.58	5 (7%)
27	SQD	f	101	-	39,41,54	1.12	4 (10%)	49,52,65	1.73	13 (26%)
33	LMG	d	410	-	21,21,55	1.01	1 (4%)	20,20,63	0.89	1 (5%)
23	CLA	A	407	-	58,62,73	1.53	10 (17%)	68,99,113	1.65	15 (22%)
29	LHG	D	409	-	46,46,48	1.09	3 (6%)	49,52,54	1.30	5 (10%)
23	CLA	B	616	-	64,68,73	1.72	9 (14%)	76,107,113	1.34	6 (7%)
33	LMG	c	522	-	48,48,55	1.19	7 (14%)	56,56,63	1.37	5 (8%)
23	CLA	C	505	36	63,67,73	1.95	13 (20%)	74,105,113	1.21	9 (12%)
29	LHG	d	408	-	48,48,48	0.70	0	51,54,54	1.22	4 (7%)
23	CLA	c	504	36	64,68,73	1.29	10 (15%)	76,107,113	1.26	6 (7%)
28	DGD	h	101	-	63,63,67	1.20	7 (11%)	77,77,81	1.58	16 (20%)
33	LMG	D	407	-	51,51,55	1.03	5 (9%)	59,59,63	1.21	3 (5%)
23	CLA	a	408	-	69,73,73	1.78	11 (15%)	82,113,113	1.24	8 (9%)
23	CLA	b	606	-	69,73,73	1.38	8 (11%)	82,113,113	1.70	17 (20%)
23	CLA	B	611	-	69,73,73	1.38	7 (10%)	82,113,113	1.42	11 (13%)
23	CLA	c	508	-	68,72,73	1.70	10 (14%)	80,111,113	1.24	10 (12%)
23	CLA	a	405	-	69,73,73	1.23	9 (13%)	82,113,113	1.40	12 (14%)
23	CLA	B	607	36	69,73,73	1.25	6 (8%)	82,113,113	1.25	7 (8%)
26	PL9	D	406	-	55,55,55	1.63	9 (16%)	68,69,69	1.59	14 (20%)
23	CLA	C	507	-	69,73,73	1.94	9 (13%)	82,113,113	1.33	11 (13%)
23	CLA	b	617	-	64,68,73	1.29	7 (10%)	76,107,113	1.55	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	613	-	69,73,73	1.41	9 (13%)	82,113,113	1.54	10 (12%)
23	CLA	B	602	-	69,73,73	1.25	9 (13%)	82,113,113	1.27	11 (13%)
29	LHG	d	407	-	48,48,48	0.83	1 (2%)	51,54,54	1.34	5 (9%)
23	CLA	c	512	-	69,73,73	1.25	8 (11%)	82,113,113	1.29	5 (6%)
23	CLA	a	406	36	69,73,73	1.08	5 (7%)	82,113,113	1.61	12 (14%)
23	CLA	b	609	-	69,73,73	1.44	9 (13%)	82,113,113	1.40	12 (14%)
27	SQD	F	101	-	34,36,54	0.92	1 (2%)	42,45,65	1.84	10 (23%)
25	BCR	d	405	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	8 (14%)
23	CLA	c	505	-	69,73,73	1.27	9 (13%)	82,113,113	1.20	6 (7%)
23	CLA	b	611	36	69,73,73	1.37	9 (13%)	82,113,113	1.27	12 (14%)
23	CLA	c	502	-	69,73,73	1.23	7 (10%)	82,113,113	1.44	11 (13%)
23	CLA	c	503	-	69,73,73	1.36	9 (13%)	82,113,113	1.47	11 (13%)
33	LMG	d	411	-	44,44,55	1.24	4 (9%)	52,52,63	1.49	6 (11%)
25	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.15	4 (7%)
31	BCT	A	415	21	3,3,3	1.25	0	2,3,3	2.90	1 (50%)
23	CLA	d	403	-	69,73,73	1.31	8 (11%)	82,113,113	1.18	6 (7%)
23	CLA	A	404	-	69,73,73	1.55	9 (13%)	82,113,113	1.35	8 (9%)
25	BCR	D	405	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	5 (8%)
29	LHG	E	101	-	48,48,48	0.93	3 (6%)	51,54,54	1.24	3 (5%)
23	CLA	b	607	-	69,73,73	1.33	7 (10%)	82,113,113	1.43	13 (15%)
28	DGD	C	517	-	63,63,67	1.24	10 (15%)	77,77,81	1.55	12 (15%)
25	BCR	a	409	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	6 (10%)
31	BCT	a	404	21	3,3,3	1.20	0	2,3,3	3.17	2 (100%)
25	BCR	x	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.41	9 (16%)
23	CLA	b	603	-	69,73,73	1.37	11 (15%)	82,113,113	1.46	12 (14%)
23	CLA	b	608	36	69,73,73	1.06	5 (7%)	82,113,113	1.28	9 (10%)
23	CLA	D	404	-	69,73,73	1.27	8 (11%)	82,113,113	1.33	12 (14%)
27	SQD	B	621	-	52,54,54	0.96	3 (5%)	62,65,65	1.81	15 (24%)
23	CLA	B	609	-	69,73,73	1.50	10 (14%)	82,113,113	1.44	16 (19%)
28	DGD	C	518	-	63,63,67	1.11	7 (11%)	77,77,81	1.42	10 (12%)
29	LHG	L	101	-	48,48,48	0.96	4 (8%)	51,54,54	1.09	2 (3%)
23	CLA	b	605	-	69,73,73	1.25	8 (11%)	82,113,113	1.39	12 (14%)
23	CLA	B	606	-	69,73,73	1.49	10 (14%)	82,113,113	1.64	13 (15%)
25	BCR	c	515	-	41,41,41	1.25	4 (9%)	56,56,56	1.42	10 (17%)
23	CLA	B	608	-	69,73,73	1.47	10 (14%)	82,113,113	1.20	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	c	521	-	41,41,41	1.02	3 (7%)	56,56,56	1.20	5 (8%)
29	LHG	A	413	-	48,48,48	0.89	2 (4%)	51,54,54	1.54	9 (17%)
23	CLA	C	512	3	69,73,73	1.62	9 (13%)	82,113,113	1.46	8 (9%)
23	CLA	B	614	-	69,73,73	1.26	8 (11%)	82,113,113	1.54	10 (12%)
23	CLA	A	405	36	69,73,73	1.35	9 (13%)	82,113,113	1.40	10 (12%)
23	CLA	c	501	-	69,73,73	1.42	7 (10%)	82,113,113	1.90	13 (15%)
33	LMG	D	410	-	31,31,55	1.18	3 (9%)	33,33,63	1.12	1 (3%)
23	CLA	b	616	-	69,73,73	2.09	10 (14%)	82,113,113	1.48	11 (13%)
24	PHO	A	406	-	58,69,69	1.95	10 (17%)	55,99,99	1.47	10 (18%)
29	LHG	e	101	-	41,41,48	0.89	3 (7%)	44,47,54	1.40	5 (11%)
27	SQD	a	412	-	35,35,54	1.08	2 (5%)	37,37,65	1.45	5 (13%)
34	HEM	e	102	6,5	50,50,50	1.46	6 (12%)	67,82,82	1.28	8 (11%)
23	CLA	C	506	-	69,73,73	1.14	6 (8%)	82,113,113	1.38	8 (9%)
23	CLA	b	615	-	69,73,73	1.36	11 (15%)	82,113,113	1.47	13 (15%)
23	CLA	b	613	-	69,73,73	1.28	6 (8%)	82,113,113	1.65	14 (17%)
33	LMG	C	519	-	48,48,55	1.03	6 (12%)	56,56,63	1.32	5 (8%)
29	LHG	D	408	-	48,48,48	1.07	3 (6%)	51,54,54	1.28	6 (11%)
23	CLA	C	503	-	69,73,73	1.21	7 (10%)	82,113,113	1.31	10 (12%)
33	LMG	m	101	-	51,51,55	0.98	4 (7%)	59,59,63	1.55	9 (15%)
28	DGD	C	516	-	63,63,67	1.38	7 (11%)	77,77,81	1.33	10 (12%)
24	PHO	a	407	-	58,69,69	1.93	11 (18%)	55,99,99	1.39	9 (16%)
28	DGD	c	516	-	63,63,67	1.20	6 (9%)	77,77,81	1.54	15 (19%)

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
28	DGD	A	412	-	-	28/55/95/95	0/2/2/2
23	CLA	c	511	3	1/1/20/20	9/39/115/115	-
23	CLA	c	507	36	1/1/20/20	10/39/115/115	-
25	BCR	K	101	-	-	12/29/63/63	0/2/2/2
23	CLA	C	502	-	1/1/20/20	4/39/115/115	-
25	BCR	b	619	-	-	12/29/63/63	0/2/2/2
23	CLA	D	403	-	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	404	-	1/1/20/20	7/39/115/115	-
23	CLA	B	601	36	1/1/20/20	13/39/115/115	-
29	LHG	d	409	-	-	11/43/43/53	-
23	CLA	B	610	36	1/1/20/20	9/39/115/115	-
26	PL9	a	410	-	-	20/53/73/73	0/1/1/1
29	LHG	l	101	-	-	16/53/53/53	-
25	BCR	A	408	-	-	8/29/63/63	0/2/2/2
28	DGD	a	413	-	-	21/45/45/95	-
23	CLA	C	513	-	1/1/20/20	12/39/115/115	-
23	CLA	b	604	-	1/1/20/20	9/39/115/115	-
25	BCR	t	101	-	-	7/29/63/63	0/2/2/2
27	SQD	b	601	-	-	22/44/64/69	0/1/1/1
27	SQD	a	411	-	-	23/49/69/69	0/1/1/1
35	HEC	V	201	16	-	6/14/54/54	-
35	HEC	v	201	16	-	6/14/54/54	-
23	CLA	c	513	-	1/1/20/20	9/39/115/115	-
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
25	BCR	H	101	-	-	9/29/63/63	0/2/2/2
23	CLA	B	603	-	1/1/20/20	11/39/115/115	-
23	CLA	C	508	36	1/1/20/20	7/39/115/115	-
25	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
26	PL9	A	409	-	-	19/53/73/73	0/1/1/1
23	CLA	C	509	-	1/1/20/20	4/39/115/115	-
23	CLA	C	511	-	1/1/20/20	10/39/115/115	-
28	DGD	c	518	-	-	22/51/91/95	0/2/2/2
23	CLA	B	615	-	1/1/20/20	9/39/115/115	-
23	CLA	b	602	36	1/1/20/20	17/39/115/115	-
23	CLA	C	504	-	-	6/39/115/115	-
23	CLA	B	605	-	1/1/20/20	12/39/115/115	-
23	CLA	c	509	-	1/1/20/20	15/39/115/115	-
33	LMG	c	524	-	-	16/44/64/70	0/1/1/1
23	CLA	D	402	36	1/1/20/20	3/39/115/115	-
23	CLA	b	614	-	1/1/20/20	9/39/115/115	-
23	CLA	C	514	-	1/1/20/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	619	-	-	5/29/63/63	0/2/2/2
33	LMG	D	411	-	-	15/22/22/70	-
24	PHO	d	401	-	-	3/37/103/103	0/5/6/6
28	DGD	H	102	-	-	16/51/91/95	0/2/2/2
28	DGD	c	517	-	-	19/51/91/95	0/2/2/2
23	CLA	c	506	-	1/1/20/20	17/39/115/115	-
27	SQD	A	410	-	-	19/47/67/69	0/1/1/1
23	CLA	c	510	-	1/1/20/20	13/39/115/115	-
33	LMG	c	519	-	-	12/31/51/70	0/1/1/1
23	CLA	B	612	-	1/1/20/20	17/39/115/115	-
33	LMG	C	501	-	-	21/43/63/70	0/1/1/1
23	CLA	C	510	-	1/1/20/20	7/39/115/115	-
25	BCR	C	520	-	-	10/29/63/63	0/2/2/2
34	HEM	E	103	6,5	-	2/14/54/54	-
23	CLA	b	610	-	1/1/20/20	10/39/115/115	-
25	BCR	b	618	-	-	4/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/20/20	9/39/115/115	-
33	LMG	M	101	-	-	19/46/66/70	0/1/1/1
26	PL9	d	406	-	-	18/53/73/73	0/1/1/1
23	CLA	d	402	36	1/1/20/20	4/39/115/115	-
25	BCR	c	514	-	-	14/29/63/63	0/2/2/2
24	PHO	D	401	-	-	0/37/103/103	0/5/6/6
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
25	BCR	B	617	-	-	11/29/63/63	0/2/2/2
25	BCR	T	101	-	-	2/29/63/63	0/2/2/2
23	CLA	b	612	-	1/1/20/20	11/39/115/115	-
25	BCR	B	618	-	-	3/29/63/63	0/2/2/2
27	SQD	A	411	-	-	14/39/39/69	-
33	LMG	b	622	-	-	19/50/70/70	0/1/1/1
27	SQD	f	101	-	-	16/36/56/69	0/1/1/1
33	LMG	d	410	-	-	15/17/17/70	-
23	CLA	A	407	-	1/1/17/20	5/26/102/115	-
29	LHG	D	409	-	-	23/51/51/53	-
23	CLA	B	616	-	1/1/19/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	c	522	-	-	21/43/63/70	0/1/1/1
23	CLA	C	505	36	1/1/18/20	9/32/108/115	-
29	LHG	d	408	-	-	18/53/53/53	-
23	CLA	c	504	36	1/1/19/20	9/33/109/115	-
28	DGD	h	101	-	-	18/51/91/95	0/2/2/2
33	LMG	D	407	-	-	18/46/66/70	0/1/1/1
23	CLA	a	408	-	1/1/20/20	6/39/115/115	-
23	CLA	b	606	-	1/1/20/20	7/39/115/115	-
23	CLA	B	611	-	1/1/20/20	6/39/115/115	-
23	CLA	c	508	-	-	12/38/114/115	-
23	CLA	a	405	-	1/1/20/20	4/39/115/115	-
23	CLA	B	607	36	1/1/20/20	7/39/115/115	-
26	PL9	D	406	-	-	11/53/73/73	0/1/1/1
23	CLA	C	507	-	-	16/39/115/115	-
23	CLA	b	617	-	1/1/19/20	7/33/109/115	-
23	CLA	B	613	-	1/1/20/20	5/39/115/115	-
23	CLA	B	602	-	1/1/20/20	7/39/115/115	-
29	LHG	d	407	-	-	21/53/53/53	-
23	CLA	c	512	-	1/1/20/20	22/39/115/115	-
23	CLA	a	406	36	1/1/20/20	13/39/115/115	-
23	CLA	b	609	-	1/1/20/20	6/39/115/115	-
27	SQD	F	101	-	-	13/28/48/69	0/1/1/1
25	BCR	d	405	-	-	12/29/63/63	0/2/2/2
23	CLA	c	505	-	1/1/20/20	7/39/115/115	-
23	CLA	b	611	36	1/1/20/20	3/39/115/115	-
23	CLA	c	502	-	-	7/39/115/115	-
23	CLA	c	503	-	1/1/20/20	11/39/115/115	-
33	LMG	d	411	-	-	8/39/59/70	0/1/1/1
25	BCR	k	101	-	-	13/29/63/63	0/2/2/2
23	CLA	d	403	-	-	10/39/115/115	-
23	CLA	A	404	-	1/1/20/20	4/39/115/115	-
25	BCR	D	405	-	-	3/29/63/63	0/2/2/2
29	LHG	E	101	-	-	26/53/53/53	-
23	CLA	b	607	-	1/1/20/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	C	517	-	-	18/51/91/95	0/2/2/2
25	BCR	a	409	-	-	2/29/63/63	0/2/2/2
25	BCR	x	102	-	-	10/29/63/63	0/2/2/2
23	CLA	b	603	-	1/1/20/20	7/39/115/115	-
23	CLA	b	608	36	1/1/20/20	13/39/115/115	-
23	CLA	D	404	-	-	14/39/115/115	-
27	SQD	B	621	-	-	23/49/69/69	0/1/1/1
23	CLA	B	609	-	-	6/39/115/115	-
28	DGD	C	518	-	-	15/51/91/95	0/2/2/2
29	LHG	L	101	-	-	23/53/53/53	-
23	CLA	b	605	-	1/1/20/20	10/39/115/115	-
23	CLA	B	606	-	1/1/20/20	11/39/115/115	-
25	BCR	c	515	-	-	5/29/63/63	0/2/2/2
23	CLA	B	608	-	-	0/39/115/115	-
25	BCR	c	521	-	-	7/29/63/63	0/2/2/2
29	LHG	A	413	-	-	15/53/53/53	-
23	CLA	C	512	3	1/1/20/20	7/39/115/115	-
23	CLA	B	614	-	1/1/20/20	11/39/115/115	-
23	CLA	A	405	36	1/1/20/20	2/39/115/115	-
23	CLA	c	501	-	1/1/20/20	6/39/115/115	-
33	LMG	D	410	-	-	17/33/33/70	-
23	CLA	b	616	-	1/1/20/20	8/39/115/115	-
24	PHO	A	406	-	-	8/37/103/103	0/5/6/6
29	LHG	e	101	-	-	30/46/46/53	-
27	SQD	a	412	-	-	19/37/37/69	-
34	HEM	e	102	6,5	-	3/14/54/54	-
23	CLA	C	506	-	1/1/20/20	12/39/115/115	-
23	CLA	b	615	-	1/1/20/20	13/39/115/115	-
23	CLA	b	613	-	1/1/20/20	12/39/115/115	-
33	LMG	C	519	-	-	17/43/63/70	0/1/1/1
29	LHG	D	408	-	-	26/53/53/53	-
23	CLA	C	503	-	1/1/20/20	11/39/115/115	-
33	LMG	m	101	-	-	20/46/66/70	0/1/1/1
28	DGD	C	516	-	-	22/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
28	DGD	c	516	-	-	23/51/91/95	0/2/2/2

All (965) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	MG-NB	11.78	2.29	2.05
23	b	616	CLA	MG-NA	11.51	2.33	2.06
23	C	507	CLA	MG-ND	-11.00	1.84	2.05
23	C	505	CLA	MG-ND	-10.38	1.85	2.05
23	c	508	CLA	MG-ND	9.89	2.25	2.05
24	D	401	PHO	C1B-C2B	9.76	1.50	1.39
23	c	506	CLA	MG-ND	-9.43	1.87	2.05
23	d	404	CLA	MG-ND	-9.35	1.87	2.05
23	B	612	CLA	MG-NB	9.11	2.23	2.05
24	d	401	PHO	C1B-C2B	8.84	1.49	1.39
23	C	512	CLA	MG-NA	8.81	2.27	2.06
23	C	511	CLA	MG-NB	8.65	2.22	2.05
24	A	406	PHO	C1B-C2B	8.53	1.48	1.39
24	a	407	PHO	C1B-C2B	8.29	1.48	1.39
23	C	504	CLA	MG-NA	8.14	2.25	2.06
23	B	616	CLA	MG-NB	-7.97	1.90	2.05
24	d	401	PHO	C3B-C4B	7.88	1.49	1.41
23	a	408	CLA	MG-NB	-7.73	1.90	2.05
23	C	502	CLA	MG-NA	7.70	2.24	2.06
23	B	604	CLA	MG-NA	7.45	2.24	2.06
24	a	407	PHO	C3B-C4B	7.43	1.49	1.41
23	C	513	CLA	MG-ND	-7.35	1.91	2.05
23	a	408	CLA	MG-NC	-7.30	1.88	2.06
23	b	602	CLA	MG-NA	7.14	2.23	2.06
23	c	511	CLA	MG-NA	7.07	2.23	2.06
23	b	616	CLA	MG-ND	-6.93	1.92	2.05
23	c	501	CLA	MG-NA	6.90	2.22	2.06
23	b	609	CLA	MG-ND	-6.86	1.92	2.05
23	c	506	CLA	MG-NB	6.79	2.19	2.05
23	B	603	CLA	MG-NA	6.61	2.22	2.06
23	b	612	CLA	MG-ND	6.57	2.18	2.05
23	B	606	CLA	MG-NA	6.30	2.21	2.06
23	B	611	CLA	MG-NA	6.29	2.21	2.06
24	D	401	PHO	C3B-C4B	6.29	1.47	1.41
23	A	407	CLA	MG-ND	-6.24	1.93	2.05
23	B	601	CLA	MG-NA	6.21	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	406	PL9	C6-C1	-6.16	1.38	1.48
35	v	201	HEC	CAB-C3B	6.15	1.55	1.35
24	A	406	PHO	C3B-C4B	6.01	1.47	1.41
35	v	201	HEC	CAC-C3C	5.99	1.54	1.35
23	b	606	CLA	MG-NB	5.97	2.17	2.05
35	V	201	HEC	CAC-C3C	5.92	1.54	1.35
23	B	615	CLA	MG-NC	5.58	2.19	2.06
23	b	613	CLA	MG-NB	5.57	2.16	2.05
23	A	404	CLA	MG-NB	5.55	2.16	2.05
23	B	601	CLA	MG-NB	-5.51	1.94	2.05
23	c	509	CLA	MG-ND	5.48	2.16	2.05
35	V	201	HEC	CAB-C3B	5.45	1.52	1.35
23	B	609	CLA	MG-NB	-5.44	1.95	2.05
28	a	413	DGD	O2G-C1B	5.42	1.49	1.34
23	b	616	CLA	MG-NC	-5.41	1.93	2.06
23	d	402	CLA	MG-NA	5.35	2.19	2.06
25	B	618	BCR	C30-C25	-5.22	1.47	1.53
23	C	505	CLA	MG-NB	5.19	2.16	2.05
23	A	405	CLA	MG-NC	5.10	2.18	2.06
23	B	609	CLA	MG-NC	-5.09	1.94	2.06
23	C	507	CLA	MG-NB	5.08	2.15	2.05
34	e	102	HEM	FE-NA	5.07	2.11	1.95
23	c	507	CLA	MG-ND	-4.99	1.95	2.05
23	B	613	CLA	MG-ND	-4.99	1.95	2.05
23	B	608	CLA	MG-ND	-4.97	1.95	2.05
23	B	608	CLA	MG-NB	4.97	2.15	2.05
33	d	411	LMG	O1-C7	-4.92	1.35	1.43
28	C	516	DGD	C4E-C3E	4.90	1.65	1.52
23	b	607	CLA	MG-NA	4.89	2.17	2.06
23	b	612	CLA	MG-NA	4.83	2.17	2.06
23	B	616	CLA	MG-ND	4.81	2.15	2.05
23	b	605	CLA	MG-ND	-4.73	1.96	2.05
23	C	507	CLA	MG-NA	4.72	2.17	2.06
23	C	509	CLA	MG-NA	4.70	2.17	2.06
23	c	503	CLA	MG-NC	4.67	2.17	2.06
23	B	607	CLA	MG-ND	-4.66	1.96	2.05
23	B	615	CLA	C4B-NB	4.65	1.44	1.37
23	b	611	CLA	MG-NB	-4.55	1.96	2.05
25	B	617	BCR	C1-C6	-4.55	1.48	1.53
23	c	509	CLA	MG-NC	4.53	2.17	2.06
24	d	401	PHO	C1D-C2D	4.52	1.44	1.39
25	K	101	BCR	C1-C6	-4.51	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	619	BCR	C30-C25	-4.50	1.48	1.53
25	H	101	BCR	C1-C6	-4.47	1.48	1.53
23	b	610	CLA	MG-ND	-4.45	1.97	2.05
23	B	613	CLA	MG-NA	4.40	2.16	2.06
23	A	405	CLA	MG-NA	-4.39	1.95	2.06
23	c	503	CLA	C4B-NB	4.37	1.43	1.37
28	A	412	DGD	C4D-C5D	4.33	1.62	1.53
23	A	404	CLA	MG-NC	-4.30	1.96	2.06
23	c	509	CLA	C1D-ND	4.25	1.43	1.37
25	H	101	BCR	C30-C25	-4.24	1.48	1.53
29	D	409	LHG	P-O6	4.23	1.76	1.59
23	B	608	CLA	C1B-NB	-4.23	1.32	1.37
23	c	511	CLA	MG-NB	-4.20	1.97	2.05
25	b	618	BCR	C1-C6	-4.18	1.48	1.53
23	C	508	CLA	MG-NA	4.18	2.16	2.06
25	K	101	BCR	C30-C25	-4.17	1.48	1.53
25	B	619	BCR	C1-C6	-4.17	1.48	1.53
23	D	403	CLA	MG-ND	4.16	2.14	2.05
25	x	102	BCR	C30-C25	-4.14	1.48	1.53
23	d	403	CLA	MG-NB	-4.13	1.97	2.05
33	D	410	LMG	C7-C8	4.12	1.61	1.51
23	C	514	CLA	MG-NC	4.11	2.16	2.06
35	V	201	HEC	CBB-CAB	-4.11	1.34	1.49
23	D	403	CLA	C1D-ND	4.08	1.43	1.37
23	B	615	CLA	MG-NB	-4.05	1.97	2.05
23	B	606	CLA	MG-NB	4.03	2.13	2.05
23	b	603	CLA	C1D-ND	4.02	1.43	1.37
35	v	201	HEC	CBB-CAB	-4.02	1.34	1.49
26	D	406	PL9	C52-C5	-4.02	1.42	1.50
26	A	409	PL9	C7-C3	-4.01	1.46	1.51
25	C	515	BCR	C1-C6	-3.99	1.48	1.53
23	B	605	CLA	MG-NC	-3.99	1.96	2.06
35	v	201	HEC	CBC-CAC	-3.99	1.34	1.49
23	A	404	CLA	C1B-C2B	3.98	1.52	1.43
28	a	413	DGD	C3G-C2G	3.98	1.60	1.51
23	a	405	CLA	C1D-ND	3.93	1.43	1.37
23	b	617	CLA	MG-NC	3.92	2.15	2.06
24	D	401	PHO	C4D-ND	-3.92	1.32	1.38
35	V	201	HEC	CBC-CAC	-3.92	1.35	1.49
25	b	619	BCR	C1-C6	-3.90	1.48	1.53
23	B	610	CLA	MG-NB	-3.87	1.98	2.05
23	b	614	CLA	MG-NA	3.86	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	C1D-ND	3.83	1.42	1.37
26	d	406	PL9	C7-C3	-3.82	1.46	1.51
23	C	512	CLA	C1D-ND	3.82	1.42	1.37
23	b	614	CLA	MG-ND	-3.79	1.98	2.05
23	C	512	CLA	C1B-C2B	3.78	1.52	1.43
25	A	408	BCR	C1-C6	-3.78	1.48	1.53
23	D	402	CLA	C1D-ND	3.78	1.42	1.37
25	Z	101	BCR	C30-C25	-3.77	1.49	1.53
27	b	601	SQD	O48-C23	3.77	1.44	1.33
23	c	506	CLA	C1D-ND	3.76	1.42	1.37
23	B	611	CLA	MG-NC	-3.74	1.97	2.06
25	d	405	BCR	C1-C6	-3.74	1.49	1.53
23	C	503	CLA	MG-NB	-3.74	1.98	2.05
23	B	606	CLA	MG-ND	-3.69	1.98	2.05
23	b	610	CLA	C1D-ND	3.68	1.42	1.37
28	c	517	DGD	C6E-C5E	3.67	1.64	1.51
28	H	102	DGD	O1G-C1G	-3.67	1.37	1.45
23	c	512	CLA	C1D-ND	3.66	1.42	1.37
33	c	524	LMG	C4-C5	3.66	1.60	1.53
23	D	404	CLA	C1D-ND	3.63	1.42	1.37
23	b	613	CLA	C1B-NB	-3.62	1.33	1.37
23	c	504	CLA	C4B-NB	3.61	1.42	1.37
23	B	601	CLA	C4B-NB	3.61	1.42	1.37
23	B	605	CLA	MG-ND	-3.59	1.98	2.05
23	c	513	CLA	MG-NA	3.56	2.14	2.06
28	A	412	DGD	C4E-C5E	3.55	1.60	1.53
29	D	408	LHG	O8-C6	-3.55	1.37	1.45
23	c	501	CLA	MG-ND	-3.55	1.98	2.05
27	a	412	SQD	O48-C23	3.54	1.43	1.33
24	D	401	PHO	C1D-C2D	3.53	1.43	1.39
23	b	611	CLA	MG-NA	3.53	2.14	2.06
24	D	401	PHO	CMC-C2C	-3.53	1.45	1.50
26	D	406	PL9	C11-C9	-3.53	1.44	1.51
23	c	505	CLA	CHC-C1C	3.53	1.45	1.38
23	c	511	CLA	MG-ND	3.52	2.12	2.05
23	a	408	CLA	CMD-C2D	-3.52	1.43	1.50
25	T	101	BCR	C30-C25	-3.51	1.49	1.53
23	B	616	CLA	MG-NC	3.50	2.14	2.06
23	d	403	CLA	MG-NA	3.50	2.14	2.06
23	A	407	CLA	MG-NA	-3.49	1.98	2.06
23	C	505	CLA	MG-NA	3.49	2.14	2.06
23	c	505	CLA	C4B-NB	3.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	MG-ND	-3.48	1.98	2.05
23	c	511	CLA	C4B-NB	3.48	1.42	1.37
28	c	518	DGD	C6D-C5D	3.48	1.62	1.51
23	C	508	CLA	C1B-NB	-3.47	1.33	1.37
23	A	404	CLA	MG-NA	3.47	2.14	2.06
24	A	406	PHO	C3B-C2B	-3.46	1.35	1.40
26	d	406	PL9	C3-C4	-3.45	1.44	1.49
23	B	614	CLA	MG-NA	3.43	2.14	2.06
23	b	607	CLA	C1D-ND	3.42	1.42	1.37
23	A	404	CLA	C1D-ND	3.42	1.42	1.37
25	C	520	BCR	C30-C25	-3.41	1.49	1.53
23	B	603	CLA	MG-NB	-3.41	1.99	2.05
23	b	615	CLA	MG-ND	3.40	2.12	2.05
28	c	516	DGD	O3G-C3G	-3.40	1.37	1.43
23	C	506	CLA	MG-NB	-3.40	1.99	2.05
23	B	605	CLA	MG-NA	3.39	2.14	2.06
23	b	606	CLA	MG-NC	-3.39	1.98	2.06
23	B	613	CLA	C1D-ND	3.39	1.42	1.37
28	h	101	DGD	O2D-C2D	-3.39	1.34	1.43
25	k	101	BCR	C30-C25	-3.38	1.49	1.53
23	B	614	CLA	C4B-NB	3.38	1.42	1.37
23	C	508	CLA	MG-NC	-3.38	1.98	2.06
25	b	618	BCR	C30-C25	-3.37	1.49	1.53
23	b	616	CLA	C1D-ND	3.37	1.42	1.37
23	C	511	CLA	C1B-C2B	3.36	1.51	1.43
24	d	401	PHO	CMC-C2C	-3.36	1.45	1.50
23	B	612	CLA	C1B-NB	-3.34	1.33	1.37
27	A	411	SQD	O48-C23	3.33	1.43	1.33
23	b	604	CLA	MG-NC	3.33	2.14	2.06
23	A	405	CLA	MG-NB	-3.32	1.99	2.05
23	B	614	CLA	MG-ND	-3.32	1.99	2.05
23	a	405	CLA	C1B-C2B	3.32	1.50	1.43
23	C	513	CLA	MG-NA	3.31	2.14	2.06
27	f	101	SQD	O47-C7	3.31	1.43	1.34
26	A	409	PL9	C37-C38	3.31	1.60	1.50
23	d	403	CLA	C1D-ND	3.31	1.42	1.37
23	B	615	CLA	CMB-C2B	-3.30	1.44	1.50
27	A	411	SQD	O47-C7	3.29	1.43	1.34
23	c	506	CLA	MG-NA	3.29	2.14	2.06
23	c	505	CLA	MG-NA	3.28	2.14	2.06
25	c	515	BCR	C1-C6	-3.28	1.49	1.53
23	c	510	CLA	C1D-ND	3.28	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C4B-NB	3.28	1.42	1.37
23	a	408	CLA	CHC-C4B	-3.26	1.32	1.39
24	A	406	PHO	C1D-C2D	3.26	1.43	1.39
33	d	411	LMG	O7-C8	-3.25	1.38	1.46
23	c	511	CLA	CHC-C1C	3.25	1.45	1.38
23	C	513	CLA	MG-NC	3.25	2.14	2.06
25	D	405	BCR	C1-C6	-3.25	1.49	1.53
23	b	605	CLA	C1D-ND	3.24	1.42	1.37
28	c	517	DGD	C3E-C2E	3.24	1.60	1.52
23	B	615	CLA	C1D-ND	3.23	1.42	1.37
25	b	620	BCR	C1-C6	-3.23	1.49	1.53
23	a	405	CLA	C4B-NB	3.23	1.42	1.37
25	a	409	BCR	C30-C25	-3.23	1.49	1.53
23	d	404	CLA	C4B-NB	3.22	1.42	1.37
28	c	518	DGD	O2G-C1B	3.22	1.43	1.34
23	a	408	CLA	C1B-C2B	3.22	1.50	1.43
23	c	509	CLA	CHC-C1C	3.22	1.44	1.38
33	C	519	LMG	O7-C8	-3.22	1.39	1.46
23	C	507	CLA	C1D-ND	3.22	1.42	1.37
27	B	621	SQD	O47-C7	3.21	1.43	1.34
23	b	615	CLA	CMB-C2B	-3.21	1.44	1.50
26	d	406	PL9	C6-C1	-3.21	1.43	1.48
23	c	512	CLA	C4B-NB	3.21	1.42	1.37
23	C	511	CLA	C1D-ND	3.20	1.42	1.37
23	B	616	CLA	C1B-C2B	3.20	1.50	1.43
23	b	603	CLA	C1B-C2B	3.20	1.50	1.43
27	a	412	SQD	O47-C7	3.20	1.43	1.34
23	b	615	CLA	C4B-NB	3.19	1.42	1.37
23	b	617	CLA	MG-NA	-3.19	1.98	2.06
23	D	404	CLA	CMD-C2D	-3.19	1.44	1.50
27	a	411	SQD	O48-C23	3.19	1.42	1.33
23	B	609	CLA	MG-NA	3.18	2.13	2.06
23	c	502	CLA	C1D-ND	3.18	1.42	1.37
23	C	507	CLA	C1B-NB	-3.18	1.33	1.37
23	B	605	CLA	C3B-C4B	3.18	1.52	1.42
24	A	406	PHO	CMD-C2D	-3.17	1.45	1.51
23	b	604	CLA	C1D-ND	3.17	1.42	1.37
27	B	621	SQD	O48-C23	3.17	1.42	1.33
23	b	603	CLA	C4B-NB	3.17	1.42	1.37
29	A	413	LHG	O7-C5	-3.17	1.39	1.46
23	B	602	CLA	C1D-ND	3.16	1.42	1.37
27	b	601	SQD	O47-C7	3.16	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	MG-NA	-3.16	1.98	2.06
23	b	602	CLA	C1D-ND	3.15	1.42	1.37
23	B	605	CLA	CHC-C1C	3.15	1.44	1.38
23	B	612	CLA	C1D-ND	3.15	1.42	1.37
33	C	501	LMG	C4-C5	3.15	1.59	1.53
23	a	405	CLA	C3B-C4B	3.14	1.51	1.42
23	b	609	CLA	CHC-C1C	3.14	1.44	1.38
33	m	101	LMG	O7-C8	-3.14	1.39	1.46
23	C	502	CLA	C4B-NB	3.14	1.42	1.37
23	B	602	CLA	MG-NA	3.14	2.13	2.06
23	c	504	CLA	CHC-C1C	3.13	1.44	1.38
23	b	607	CLA	C1B-C2B	3.13	1.50	1.43
23	C	511	CLA	MG-NA	3.13	2.13	2.06
23	b	602	CLA	C4B-NB	3.12	1.42	1.37
23	B	610	CLA	C4B-NB	3.12	1.42	1.37
23	d	402	CLA	C1B-C2B	3.12	1.50	1.43
25	a	409	BCR	C1-C6	-3.11	1.49	1.53
23	B	616	CLA	C1D-ND	3.11	1.42	1.37
23	B	603	CLA	C1D-ND	3.11	1.41	1.37
23	b	617	CLA	C1D-ND	3.11	1.41	1.37
27	A	410	SQD	O48-C23	3.11	1.42	1.33
27	f	101	SQD	O48-C23	3.11	1.42	1.33
23	b	615	CLA	MG-NB	-3.11	1.99	2.05
23	C	503	CLA	C1D-ND	3.10	1.41	1.37
26	a	410	PL9	C3-C4	-3.10	1.44	1.49
23	B	612	CLA	CMC-C2C	-3.10	1.44	1.50
23	D	404	CLA	MG-NA	-3.10	1.98	2.06
26	d	406	PL9	C30-C29	-3.09	1.43	1.50
23	c	513	CLA	C1B-C2B	3.09	1.50	1.43
23	B	608	CLA	C1D-ND	3.08	1.41	1.37
23	c	507	CLA	C1D-ND	3.08	1.41	1.37
25	T	101	BCR	C38-C26	-3.08	1.46	1.50
28	A	412	DGD	C6E-C5E	3.08	1.62	1.51
25	c	515	BCR	C30-C25	-3.08	1.49	1.53
23	A	404	CLA	C3B-C4B	3.06	1.51	1.42
24	D	401	PHO	CAC-C3C	-3.06	1.46	1.51
24	A	406	PHO	O2D-CGD	3.06	1.40	1.33
27	A	411	SQD	O47-C45	-3.05	1.41	1.47
23	c	508	CLA	C1D-ND	3.04	1.41	1.37
23	C	504	CLA	C1B-C2B	3.04	1.50	1.43
28	A	412	DGD	C3G-C2G	3.04	1.60	1.50
23	C	513	CLA	C1D-ND	3.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	MG-NA	3.03	2.13	2.06
33	c	522	LMG	C7-C8	3.03	1.60	1.50
26	a	410	PL9	C53-C6	-3.03	1.44	1.50
25	D	405	BCR	C30-C25	-3.03	1.49	1.53
23	b	612	CLA	MG-NB	-3.03	1.99	2.05
23	b	611	CLA	C1D-ND	3.02	1.41	1.37
23	b	602	CLA	MG-NB	-3.02	1.99	2.05
28	h	101	DGD	C1E-C2E	3.02	1.61	1.52
23	c	504	CLA	C1B-NB	-3.02	1.33	1.37
23	b	615	CLA	CMC-C2C	-3.01	1.44	1.50
25	c	521	BCR	C1-C6	-3.01	1.49	1.53
23	C	511	CLA	CHC-C1C	3.01	1.44	1.38
23	C	502	CLA	C1D-ND	3.01	1.41	1.37
23	b	614	CLA	C1D-ND	3.01	1.41	1.37
28	c	518	DGD	C4E-C5E	3.01	1.59	1.53
33	C	501	LMG	C4-C3	3.01	1.60	1.52
23	c	511	CLA	C1D-ND	2.99	1.41	1.37
24	d	401	PHO	C4D-ND	-2.99	1.34	1.38
23	b	610	CLA	MG-NA	2.99	2.13	2.06
28	A	412	DGD	C1E-C2E	2.98	1.61	1.52
23	d	404	CLA	MG-NA	2.98	2.13	2.06
33	D	410	LMG	C9-C8	2.98	1.60	1.50
23	c	503	CLA	C1D-ND	2.98	1.41	1.37
23	B	602	CLA	C4B-NB	2.98	1.41	1.37
23	c	502	CLA	MG-NA	2.98	2.13	2.06
23	c	512	CLA	C1B-C2B	2.98	1.50	1.43
23	b	610	CLA	C1B-C2B	2.97	1.50	1.43
23	B	601	CLA	CMB-C2B	-2.97	1.44	1.50
33	b	622	LMG	C4-C3	2.97	1.60	1.52
28	C	517	DGD	C4D-C3D	2.97	1.60	1.52
23	D	403	CLA	MG-NA	2.97	2.13	2.06
23	b	616	CLA	C4B-NB	2.97	1.41	1.37
23	b	606	CLA	C4B-NB	2.97	1.41	1.37
23	c	504	CLA	C1B-C2B	2.97	1.50	1.43
23	d	402	CLA	CHC-C1C	2.96	1.44	1.38
23	C	510	CLA	C1B-C2B	2.96	1.50	1.43
23	B	605	CLA	CMB-C2B	-2.96	1.44	1.50
23	C	512	CLA	C4B-NB	2.96	1.41	1.37
28	C	516	DGD	C3D-C2D	2.96	1.60	1.52
28	c	516	DGD	C4D-C3D	2.96	1.60	1.52
25	k	101	BCR	C1-C6	-2.95	1.50	1.53
23	d	402	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	C3B-C2B	-2.92	1.36	1.40
25	Z	101	BCR	C1-C6	-2.92	1.50	1.53
33	c	524	LMG	O6-C5	-2.92	1.37	1.44
23	c	509	CLA	C1B-C2B	2.91	1.50	1.43
23	C	509	CLA	CMB-C2B	-2.91	1.44	1.50
23	B	610	CLA	C1B-C2B	2.91	1.50	1.43
25	B	618	BCR	C1-C6	-2.90	1.50	1.53
23	B	614	CLA	MG-NC	2.90	2.13	2.06
27	A	410	SQD	O47-C7	2.90	1.42	1.34
23	B	610	CLA	CHC-C1C	2.90	1.44	1.38
28	c	518	DGD	C2A-C1A	-2.90	1.42	1.50
23	d	402	CLA	C4B-NB	2.90	1.41	1.37
26	D	406	PL9	C30-C29	-2.90	1.43	1.50
23	c	506	CLA	CAC-C3C	-2.89	1.43	1.51
23	B	601	CLA	C1D-ND	2.88	1.41	1.37
23	C	509	CLA	MG-NC	2.88	2.13	2.06
23	B	603	CLA	CMA-C3A	-2.88	1.47	1.53
23	c	511	CLA	C1B-C2B	2.88	1.49	1.43
28	A	412	DGD	O5D-C1E	2.87	1.45	1.40
23	C	505	CLA	C1D-ND	2.86	1.41	1.37
23	A	407	CLA	CHC-C4B	-2.86	1.33	1.39
23	B	610	CLA	CMB-C2B	-2.86	1.44	1.50
25	T	101	BCR	C1-C6	-2.86	1.50	1.53
26	a	410	PL9	C11-C9	-2.86	1.45	1.51
33	D	407	LMG	C6-C5	2.86	1.61	1.51
33	c	522	LMG	C1-C2	2.86	1.60	1.52
24	A	406	PHO	C3D-C4D	2.85	1.45	1.41
23	b	604	CLA	MG-ND	-2.85	2.00	2.05
23	C	504	CLA	C1D-ND	2.85	1.41	1.37
33	c	522	LMG	O1-C1	2.85	1.44	1.40
25	c	515	BCR	C33-C5	-2.85	1.46	1.50
23	c	513	CLA	C1D-ND	2.85	1.41	1.37
23	b	610	CLA	C4B-NB	2.85	1.41	1.37
23	B	616	CLA	CMC-C2C	-2.85	1.44	1.50
23	b	604	CLA	C4B-NB	2.84	1.41	1.37
27	F	101	SQD	O48-C23	2.84	1.41	1.33
23	B	609	CLA	CMD-C2D	-2.84	1.45	1.50
23	B	615	CLA	MG-NA	2.84	2.13	2.06
24	a	407	PHO	C1D-C2D	2.84	1.42	1.39
23	B	611	CLA	CMD-C2D	-2.83	1.45	1.50
23	B	602	CLA	C1B-C2B	2.83	1.49	1.43
29	e	101	LHG	O7-C5	-2.83	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C1B-NB	-2.83	1.34	1.37
25	d	405	BCR	C30-C25	-2.83	1.50	1.53
23	b	603	CLA	MG-NB	2.82	2.11	2.05
29	E	101	LHG	O7-C5	-2.82	1.40	1.46
28	h	101	DGD	O1G-C1G	-2.82	1.38	1.45
23	b	602	CLA	O2A-CGA	2.82	1.41	1.33
23	b	617	CLA	CMD-C2D	-2.81	1.45	1.50
24	A	406	PHO	C4D-ND	-2.81	1.34	1.38
23	C	509	CLA	C1D-ND	2.81	1.41	1.37
23	B	605	CLA	C4B-NB	2.81	1.41	1.37
23	b	603	CLA	CMD-C2D	-2.81	1.45	1.50
28	C	518	DGD	O2G-C2G	-2.80	1.40	1.46
35	V	201	HEC	C2A-C3A	-2.80	1.30	1.36
23	b	602	CLA	CHC-C1C	2.80	1.44	1.38
23	b	615	CLA	C3B-C4B	2.80	1.50	1.42
23	d	404	CLA	CMD-C2D	-2.79	1.45	1.50
25	c	514	BCR	C1-C6	-2.79	1.50	1.53
23	C	513	CLA	CMB-C2B	-2.79	1.45	1.50
23	B	605	CLA	C1D-ND	2.79	1.41	1.37
27	a	411	SQD	O47-C7	2.79	1.42	1.34
23	B	611	CLA	C1B-C2B	2.78	1.49	1.43
23	B	609	CLA	CMC-C2C	-2.78	1.45	1.50
23	c	511	CLA	C3B-C4B	2.77	1.50	1.42
23	D	404	CLA	MG-NC	2.77	2.12	2.06
23	c	510	CLA	MG-NB	2.77	2.11	2.05
23	c	505	CLA	C1B-C2B	2.77	1.49	1.43
35	v	201	HEC	C3B-C2B	-2.77	1.31	1.41
23	A	404	CLA	MG-ND	-2.76	2.00	2.05
23	C	503	CLA	C3B-C4B	2.76	1.50	1.42
23	B	612	CLA	C1B-C2B	2.76	1.49	1.43
23	B	612	CLA	MG-ND	-2.75	2.00	2.05
23	C	506	CLA	CHC-C1C	2.75	1.44	1.38
23	c	505	CLA	CMB-C2B	-2.75	1.45	1.50
23	B	613	CLA	C1B-C2B	2.75	1.49	1.43
23	c	511	CLA	MG-NC	2.75	2.12	2.06
23	b	605	CLA	MG-NB	2.74	2.11	2.05
23	C	513	CLA	CHC-C1C	2.74	1.44	1.38
23	c	512	CLA	MG-NC	2.74	2.12	2.06
28	c	517	DGD	O4E-C4E	-2.74	1.36	1.43
23	a	408	CLA	CMC-C2C	-2.74	1.45	1.50
28	H	102	DGD	O5D-C6D	-2.73	1.39	1.43
23	c	512	CLA	CHC-C1C	2.73	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	519	LMG	C4-C5	2.72	1.58	1.53
23	B	608	CLA	CMD-C2D	-2.72	1.45	1.50
23	b	605	CLA	C3B-C4B	2.72	1.50	1.42
25	C	515	BCR	C33-C5	-2.72	1.46	1.50
23	B	609	CLA	CHC-C4B	-2.72	1.33	1.39
23	B	616	CLA	CMD-C2D	-2.72	1.45	1.50
23	a	406	CLA	CMB-C2B	-2.72	1.45	1.50
23	c	507	CLA	CMB-C2B	-2.72	1.45	1.50
23	A	404	CLA	CHC-C1C	2.71	1.43	1.38
23	c	503	CLA	MG-NA	2.71	2.12	2.06
23	A	407	CLA	MG-NC	-2.71	1.99	2.06
26	a	410	PL9	C6-C1	-2.71	1.44	1.48
23	D	403	CLA	C1C-NC	-2.70	1.33	1.37
23	C	504	CLA	C4B-NB	2.70	1.41	1.37
23	b	611	CLA	C1B-C2B	2.70	1.49	1.43
28	C	518	DGD	C1G-C2G	2.70	1.59	1.50
23	C	509	CLA	MG-ND	-2.70	2.00	2.05
23	c	505	CLA	C3B-C4B	2.69	1.50	1.42
23	c	509	CLA	C3B-C4B	2.69	1.50	1.42
23	c	503	CLA	CMC-C2C	-2.69	1.45	1.50
28	C	516	DGD	O2G-C2G	-2.69	1.40	1.46
23	D	404	CLA	C1B-C2B	2.69	1.49	1.43
28	C	516	DGD	O1G-C1A	2.69	1.41	1.33
28	H	102	DGD	O3D-C3D	-2.69	1.36	1.43
35	V	201	HEC	CMD-C2D	2.68	1.56	1.50
23	B	609	CLA	C4B-NB	2.68	1.41	1.37
24	d	401	PHO	CMD-C2D	-2.68	1.46	1.51
23	c	501	CLA	CAC-C3C	-2.68	1.44	1.51
23	B	613	CLA	CHC-C4B	-2.67	1.33	1.39
23	C	502	CLA	CHC-C1C	2.67	1.43	1.38
25	B	617	BCR	C33-C5	-2.67	1.46	1.50
23	D	403	CLA	CMD-C2D	-2.66	1.45	1.50
23	A	407	CLA	CMC-C2C	-2.66	1.45	1.50
28	H	102	DGD	C1E-C2E	2.66	1.60	1.52
28	A	412	DGD	O2G-C1B	2.66	1.41	1.34
23	B	606	CLA	CMB-C2B	-2.65	1.45	1.50
23	c	501	CLA	C1D-ND	2.65	1.41	1.37
23	C	504	CLA	CMB-C2B	-2.65	1.45	1.50
23	b	609	CLA	C1D-ND	2.64	1.41	1.37
23	a	406	CLA	C1B-NB	-2.64	1.34	1.37
23	B	610	CLA	MG-ND	2.64	2.11	2.05
23	B	607	CLA	C1B-NB	-2.64	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	410	SQD	O2-C2	-2.64	1.36	1.43
23	C	504	CLA	CHC-C4B	-2.63	1.33	1.39
28	H	102	DGD	C4D-C5D	2.63	1.58	1.53
23	A	407	CLA	C1D-ND	2.63	1.41	1.37
23	c	504	CLA	MG-NC	2.63	2.12	2.06
23	c	507	CLA	MG-NA	-2.63	2.00	2.06
23	C	510	CLA	C3B-C4B	2.63	1.50	1.42
24	a	407	PHO	C4D-CHA	2.63	1.43	1.39
23	a	405	CLA	CMD-C2D	-2.63	1.45	1.50
23	c	506	CLA	C1B-C2B	2.62	1.49	1.43
24	a	407	PHO	CBD-CGD	-2.62	1.49	1.52
23	B	604	CLA	C1D-C2D	2.62	1.50	1.45
28	c	516	DGD	C3D-C2D	2.62	1.59	1.52
23	B	611	CLA	CMB-C2B	-2.62	1.45	1.50
23	c	503	CLA	C1B-C2B	2.61	1.49	1.43
23	B	605	CLA	C1B-C2B	2.61	1.49	1.43
23	C	510	CLA	C4B-NB	2.61	1.41	1.37
23	c	510	CLA	C3B-C4B	2.61	1.50	1.42
23	D	404	CLA	MG-NB	-2.61	2.00	2.05
23	a	405	CLA	MG-NA	2.61	2.12	2.06
23	C	511	CLA	C3B-C4B	2.61	1.50	1.42
23	b	602	CLA	C1B-C2B	2.61	1.49	1.43
28	H	102	DGD	O5D-C1E	2.60	1.44	1.40
23	C	505	CLA	C1B-NB	-2.60	1.34	1.37
23	B	606	CLA	C3B-C4B	2.60	1.50	1.42
23	c	507	CLA	C1B-C2B	2.60	1.49	1.43
23	c	509	CLA	C4B-NB	2.60	1.41	1.37
23	A	404	CLA	C4B-NB	2.59	1.41	1.37
33	c	522	LMG	C4-C3	2.59	1.59	1.52
35	V	201	HEC	C3B-C2B	-2.59	1.32	1.41
23	b	609	CLA	MG-NB	2.59	2.10	2.05
23	d	402	CLA	C3B-C4B	2.59	1.50	1.42
23	C	502	CLA	C1B-NB	-2.59	1.34	1.37
24	a	407	PHO	CMB-C2B	-2.59	1.46	1.51
23	C	505	CLA	C3B-C4B	2.59	1.50	1.42
33	d	411	LMG	O2-C2	-2.59	1.36	1.43
23	b	607	CLA	MG-NB	2.59	2.10	2.05
23	b	604	CLA	C1B-C2B	2.58	1.49	1.43
23	C	513	CLA	CMD-C2D	-2.58	1.45	1.50
24	A	406	PHO	CBD-CGD	-2.58	1.49	1.52
23	b	615	CLA	C1D-ND	2.58	1.41	1.37
25	C	515	BCR	C30-C25	-2.58	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	MG-NA	2.58	2.12	2.06
34	E	103	HEM	CAB-C3B	2.57	1.54	1.47
23	b	606	CLA	C3B-C4B	2.57	1.50	1.42
34	e	102	HEM	C2A-C3A	-2.57	1.32	1.38
23	b	603	CLA	MG-NA	2.57	2.12	2.06
23	c	501	CLA	C1B-C2B	2.57	1.49	1.43
23	b	604	CLA	CMC-C2C	-2.57	1.45	1.50
23	a	408	CLA	CMA-C3A	-2.57	1.47	1.53
23	C	514	CLA	C1B-C2B	2.57	1.49	1.43
23	D	402	CLA	C1B-C2B	2.57	1.49	1.43
24	A	406	PHO	CMC-C2C	-2.56	1.46	1.50
23	b	617	CLA	C1B-C2B	2.56	1.49	1.43
28	H	102	DGD	O2D-C2D	-2.56	1.36	1.43
23	b	617	CLA	CMB-C2B	-2.56	1.45	1.50
26	d	406	PL9	C53-C6	-2.56	1.45	1.50
29	L	101	LHG	O8-C23	2.56	1.40	1.33
29	l	101	LHG	O8-C23	2.56	1.40	1.33
23	b	611	CLA	C3B-C4B	2.55	1.50	1.42
25	B	617	BCR	C30-C25	-2.55	1.50	1.53
23	b	612	CLA	MG-NC	-2.55	2.00	2.06
23	B	604	CLA	CHC-C1C	2.55	1.43	1.38
23	c	507	CLA	CHC-C4B	-2.55	1.33	1.39
23	b	615	CLA	C1B-C2B	2.55	1.49	1.43
23	C	506	CLA	C4B-NB	2.54	1.41	1.37
23	c	508	CLA	CMC-C2C	-2.54	1.45	1.50
23	b	608	CLA	C1B-C2B	2.54	1.49	1.43
23	B	613	CLA	C1C-NC	-2.54	1.33	1.37
23	b	611	CLA	CMD-C2D	-2.53	1.45	1.50
23	d	403	CLA	CAA-C2A	-2.53	1.49	1.54
24	D	401	PHO	CMD-C2D	-2.53	1.46	1.51
23	C	508	CLA	C1D-ND	2.53	1.41	1.37
33	d	410	LMG	O7-C10	2.53	1.39	1.30
28	C	517	DGD	O3G-C3G	-2.53	1.39	1.43
23	b	604	CLA	CMD-C2D	-2.53	1.45	1.50
23	b	603	CLA	MG-ND	-2.53	2.00	2.05
23	A	407	CLA	C1B-C2B	2.53	1.49	1.43
23	B	602	CLA	C3B-C4B	2.53	1.50	1.42
23	b	608	CLA	C1C-NC	-2.52	1.33	1.37
23	B	604	CLA	MG-ND	2.52	2.10	2.05
23	B	607	CLA	C1D-ND	2.52	1.41	1.37
28	h	101	DGD	C4E-C3E	2.52	1.58	1.52
23	C	502	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	CMC-C2C	-2.51	1.45	1.50
23	b	603	CLA	CHC-C1C	2.51	1.43	1.38
23	c	502	CLA	C1B-C2B	2.51	1.49	1.43
33	b	622	LMG	O1-C7	-2.50	1.39	1.43
25	c	515	BCR	C38-C26	-2.50	1.47	1.50
29	E	101	LHG	O8-C23	2.50	1.40	1.33
23	b	608	CLA	CMD-C2D	-2.50	1.45	1.50
28	A	412	DGD	C4D-C3D	2.50	1.58	1.52
29	L	101	LHG	O7-C5	-2.49	1.40	1.46
28	C	518	DGD	C4E-C3E	2.49	1.58	1.52
23	C	512	CLA	C3B-C4B	2.49	1.50	1.42
23	B	601	CLA	C1B-C2B	2.49	1.49	1.43
23	c	502	CLA	MG-ND	2.49	2.10	2.05
23	c	504	CLA	C3B-C4B	2.49	1.50	1.42
23	c	503	CLA	CMB-C2B	-2.48	1.45	1.50
23	C	508	CLA	CMC-C2C	-2.48	1.45	1.50
26	A	409	PL9	C10-C9	-2.48	1.44	1.50
23	C	511	CLA	C4B-NB	2.47	1.41	1.37
23	B	603	CLA	C1B-C2B	2.47	1.48	1.43
23	c	508	CLA	C1B-C2B	2.47	1.48	1.43
23	C	506	CLA	C1B-NB	-2.47	1.34	1.37
23	b	603	CLA	CAC-C3C	-2.46	1.44	1.51
23	c	512	CLA	CMD-C2D	-2.46	1.45	1.50
29	D	408	LHG	C24-C23	2.46	1.57	1.50
33	M	101	LMG	C1-C2	2.46	1.59	1.52
33	m	101	LMG	O1-C7	-2.46	1.39	1.43
25	c	521	BCR	C38-C26	-2.45	1.47	1.50
24	a	407	PHO	CAC-C3C	-2.45	1.47	1.51
23	A	405	CLA	CMD-C2D	-2.45	1.45	1.50
23	B	613	CLA	CMC-C2C	-2.45	1.45	1.50
23	b	615	CLA	C1B-NB	-2.45	1.34	1.37
25	B	619	BCR	C30-C25	-2.44	1.50	1.53
23	c	510	CLA	C1B-NB	-2.44	1.34	1.37
23	c	506	CLA	MG-NC	2.44	2.12	2.06
29	D	408	LHG	O7-C5	-2.44	1.40	1.46
25	b	618	BCR	C33-C5	-2.44	1.47	1.50
33	C	501	LMG	O7-C8	-2.44	1.40	1.46
34	E	103	HEM	CMC-C2C	2.44	1.55	1.50
23	B	611	CLA	C3B-C4B	2.44	1.49	1.42
23	B	606	CLA	C1D-ND	2.43	1.41	1.37
23	C	502	CLA	C3D-C4D	2.43	1.49	1.44
23	b	605	CLA	MG-NC	2.43	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	MG-NC	2.43	2.12	2.06
28	C	517	DGD	C3E-C2E	2.42	1.58	1.52
33	m	101	LMG	O6-C5	-2.42	1.38	1.44
23	b	605	CLA	C1B-C2B	2.42	1.48	1.43
23	D	402	CLA	CHC-C1C	2.42	1.43	1.38
23	C	510	CLA	MG-ND	2.42	2.10	2.05
28	C	518	DGD	O3E-C3E	-2.42	1.37	1.43
34	e	102	HEM	CMC-C2C	2.42	1.55	1.50
23	C	509	CLA	C1B-C2B	2.42	1.48	1.43
23	B	613	CLA	CMD-C2D	-2.41	1.45	1.50
33	c	522	LMG	O6-C5	-2.41	1.38	1.44
23	C	512	CLA	C1D-C2D	2.41	1.50	1.45
23	B	614	CLA	MG-NB	-2.41	2.01	2.05
25	t	101	BCR	C30-C25	-2.40	1.50	1.53
23	c	505	CLA	MG-NB	-2.40	2.01	2.05
28	h	101	DGD	C4D-C5D	2.40	1.58	1.53
23	C	506	CLA	CMB-C2B	-2.40	1.45	1.50
35	v	201	HEC	CMD-C2D	2.39	1.55	1.50
25	T	101	BCR	C27-C26	-2.39	1.46	1.51
23	C	514	CLA	C4B-NB	2.39	1.41	1.37
34	E	103	HEM	C2A-C3A	-2.39	1.32	1.38
33	C	519	LMG	O3-C3	-2.39	1.37	1.43
23	d	404	CLA	CMB-C2B	-2.39	1.45	1.50
26	D	406	PL9	C27-C28	-2.39	1.43	1.50
23	b	612	CLA	CMB-C2B	-2.38	1.45	1.50
23	c	510	CLA	CHC-C1C	2.38	1.43	1.38
35	V	201	HEC	C3C-C2C	-2.38	1.33	1.41
23	A	407	CLA	CMD-C2D	-2.38	1.45	1.50
23	C	502	CLA	CMD-C2D	-2.38	1.45	1.50
23	C	511	CLA	C1B-NB	-2.38	1.34	1.37
29	L	101	LHG	P-O6	2.38	1.68	1.59
23	b	608	CLA	CMB-C2B	-2.38	1.45	1.50
24	D	401	PHO	CMB-C2B	-2.38	1.46	1.51
27	A	410	SQD	O3-C3	-2.38	1.37	1.43
23	c	501	CLA	CMD-C2D	-2.38	1.45	1.50
23	b	609	CLA	C3B-C4B	2.38	1.49	1.42
33	c	522	LMG	C3-C2	2.38	1.58	1.52
23	B	601	CLA	C1D-C2D	2.37	1.50	1.45
23	b	616	CLA	CMC-C2C	-2.37	1.45	1.50
23	B	601	CLA	CMD-C2D	-2.37	1.45	1.50
23	B	604	CLA	O2A-CGA	2.37	1.40	1.33
23	c	513	CLA	C4B-NB	2.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	519	LMG	O4-C4	-2.37	1.37	1.43
23	b	606	CLA	CMB-C2B	-2.37	1.45	1.50
23	B	611	CLA	C1D-ND	2.37	1.41	1.37
23	C	503	CLA	MG-NA	2.37	2.11	2.06
23	C	511	CLA	O2A-CGA	2.36	1.40	1.33
25	b	620	BCR	C30-C25	-2.36	1.50	1.53
23	b	616	CLA	C3B-C4B	2.36	1.49	1.42
28	A	412	DGD	C3E-C2E	2.36	1.58	1.52
33	d	411	LMG	C4-C5	2.36	1.58	1.53
23	C	505	CLA	CHC-C1C	2.36	1.43	1.38
23	c	504	CLA	CMB-C2B	-2.36	1.45	1.50
23	b	612	CLA	CHC-C1C	2.35	1.43	1.38
23	c	513	CLA	CMD-C2D	-2.35	1.46	1.50
23	a	405	CLA	CHC-C1C	2.35	1.43	1.38
24	d	401	PHO	CAC-C3C	-2.35	1.47	1.51
23	C	508	CLA	C4B-NB	2.35	1.40	1.37
28	H	102	DGD	C6D-C5D	2.34	1.58	1.51
33	b	622	LMG	C4-C5	2.34	1.58	1.53
23	a	408	CLA	CMB-C2B	-2.34	1.46	1.50
34	E	103	HEM	FE-NB	2.34	2.02	1.94
23	c	501	CLA	MG-NC	2.34	2.11	2.06
23	B	604	CLA	C3B-C4B	2.33	1.49	1.42
23	c	513	CLA	C3B-C4B	2.33	1.49	1.42
28	C	517	DGD	C1E-C2E	2.33	1.59	1.52
23	b	607	CLA	C4B-NB	2.33	1.40	1.37
29	e	101	LHG	P-O6	2.33	1.68	1.59
33	D	410	LMG	O8-C28	2.33	1.40	1.33
28	A	412	DGD	O6D-C1D	2.33	1.47	1.41
27	f	101	SQD	O2-C2	-2.33	1.37	1.43
23	b	611	CLA	CMB-C2B	-2.33	1.46	1.50
23	b	615	CLA	C1D-C2D	2.33	1.49	1.45
23	B	605	CLA	CMC-C2C	-2.32	1.46	1.50
29	d	409	LHG	P-O6	2.32	1.68	1.59
23	b	606	CLA	C1B-C2B	2.32	1.48	1.43
25	C	520	BCR	C1-C6	-2.32	1.50	1.53
29	D	409	LHG	O7-C7	2.32	1.40	1.34
23	c	512	CLA	C3D-C4D	2.32	1.49	1.44
28	C	516	DGD	C4D-C3D	2.32	1.58	1.52
27	A	410	SQD	O47-C45	-2.31	1.41	1.46
25	A	408	BCR	C33-C5	-2.31	1.47	1.50
23	B	614	CLA	CHC-C1C	2.31	1.43	1.38
23	d	403	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	519	LMG	O2-C2	-2.31	1.37	1.43
28	C	517	DGD	O4E-C4E	-2.31	1.37	1.43
23	C	510	CLA	CHC-C1C	2.31	1.43	1.38
23	B	610	CLA	C3B-C4B	2.31	1.49	1.42
23	b	614	CLA	C5-C3	-2.31	1.46	1.51
28	a	413	DGD	C1G-C2G	2.30	1.58	1.50
23	c	502	CLA	CHC-C1C	2.30	1.43	1.38
23	b	610	CLA	C3B-C4B	2.30	1.49	1.42
23	b	614	CLA	C1B-C2B	2.30	1.48	1.43
23	B	604	CLA	C1D-ND	2.30	1.40	1.37
25	D	405	BCR	C27-C26	-2.30	1.46	1.51
33	D	407	LMG	O8-C28	2.30	1.40	1.33
23	C	509	CLA	C4B-NB	2.30	1.40	1.37
33	D	411	LMG	O8-C28	2.29	1.38	1.30
28	c	518	DGD	O6E-C1E	-2.29	1.35	1.41
24	d	401	PHO	CAA-C2A	-2.29	1.49	1.54
33	D	407	LMG	O2-C2	-2.29	1.37	1.43
23	c	513	CLA	CMC-C2C	-2.29	1.46	1.50
23	c	508	CLA	C3B-C4B	2.28	1.49	1.42
26	D	406	PL9	C41-C39	-2.28	1.46	1.51
23	B	609	CLA	CAC-C3C	-2.28	1.45	1.51
33	C	501	LMG	C7-C8	2.28	1.57	1.50
23	c	506	CLA	C1B-NB	-2.28	1.34	1.37
26	A	409	PL9	C21-C19	2.28	1.56	1.51
23	b	602	CLA	C3B-C4B	2.27	1.49	1.42
23	B	604	CLA	MG-NC	-2.27	2.00	2.06
23	B	606	CLA	CMD-C2D	-2.27	1.46	1.50
23	B	603	CLA	C1A-CHA	-2.27	1.33	1.43
23	B	609	CLA	CMB-C2B	-2.27	1.46	1.50
25	C	515	BCR	C38-C26	-2.27	1.47	1.50
29	e	101	LHG	O8-C23	2.27	1.40	1.33
23	B	607	CLA	C1B-C2B	2.27	1.48	1.43
23	c	508	CLA	CMD-C2D	-2.27	1.46	1.50
23	b	607	CLA	CHC-C4B	-2.27	1.34	1.39
23	C	508	CLA	CMD-C2D	-2.26	1.46	1.50
26	D	406	PL9	C5-C4	-2.26	1.39	1.47
23	D	402	CLA	CMB-C2B	-2.26	1.46	1.50
23	D	404	CLA	C1B-NB	-2.26	1.34	1.37
23	C	508	CLA	C1B-C2B	2.26	1.48	1.43
28	c	517	DGD	C4E-C5E	2.26	1.57	1.53
25	x	102	BCR	C1-C6	-2.26	1.50	1.53
26	A	409	PL9	C3-C4	-2.26	1.46	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	516	DGD	O2D-C2D	-2.26	1.37	1.43
28	C	517	DGD	O6D-C5D	-2.25	1.38	1.44
33	C	501	LMG	O1-C1	2.25	1.43	1.40
33	C	519	LMG	C3-C2	2.25	1.58	1.52
29	d	409	LHG	C3-C2	2.25	1.58	1.51
23	D	402	CLA	C3B-C4B	2.25	1.49	1.42
28	A	412	DGD	O1G-C1A	2.25	1.39	1.33
23	C	511	CLA	CMD-C2D	-2.24	1.46	1.50
23	C	507	CLA	CAB-C3B	-2.24	1.41	1.47
23	B	606	CLA	C1B-C2B	2.24	1.48	1.43
23	c	504	CLA	C1D-ND	2.24	1.40	1.37
24	a	407	PHO	CMD-C2D	-2.24	1.47	1.51
25	A	408	BCR	C27-C26	-2.24	1.46	1.51
34	e	102	HEM	CAC-C3C	2.24	1.53	1.47
23	C	503	CLA	CMB-C2B	-2.24	1.46	1.50
23	C	504	CLA	CMC-C2C	-2.24	1.46	1.50
33	D	407	LMG	O6-C5	-2.24	1.38	1.44
23	a	406	CLA	MG-ND	-2.23	2.01	2.05
23	C	505	CLA	CMD-C2D	-2.23	1.46	1.50
23	c	508	CLA	CHC-C1C	2.23	1.43	1.38
23	b	613	CLA	O2D-CED	-2.23	1.40	1.45
28	H	102	DGD	C4E-C3E	2.23	1.58	1.52
29	D	409	LHG	O3-C3	-2.23	1.36	1.44
29	E	101	LHG	P-O6	2.23	1.68	1.59
23	b	614	CLA	CMB-C2B	-2.23	1.46	1.50
23	C	508	CLA	CMB-C2B	-2.23	1.46	1.50
25	C	515	BCR	C34-C9	-2.23	1.46	1.50
28	H	102	DGD	O2G-C2G	-2.23	1.41	1.46
28	C	517	DGD	O2G-C2G	-2.22	1.41	1.46
23	A	405	CLA	C1B-C2B	2.22	1.48	1.43
25	C	520	BCR	C38-C26	-2.22	1.47	1.50
23	d	402	CLA	C3D-C4D	2.22	1.49	1.44
23	C	514	CLA	C3B-C4B	2.22	1.49	1.42
23	a	408	CLA	C1C-NC	-2.22	1.34	1.37
23	d	403	CLA	C1B-C2B	2.22	1.48	1.43
28	c	518	DGD	O1G-C1G	-2.22	1.40	1.45
23	C	505	CLA	MG-NC	2.21	2.11	2.06
25	t	101	BCR	C1-C6	-2.21	1.50	1.53
23	D	402	CLA	C1B-NB	-2.21	1.35	1.37
23	b	610	CLA	CMB-C2B	-2.21	1.46	1.50
35	v	201	HEC	C3D-C2D	-2.21	1.33	1.38
25	B	618	BCR	C39-C30	-2.21	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C4B-NB	2.21	1.40	1.37
23	B	610	CLA	CMA-C3A	-2.21	1.48	1.53
23	B	613	CLA	C4B-NB	2.21	1.40	1.37
23	D	403	CLA	MG-NB	-2.21	2.01	2.05
23	C	507	CLA	C4B-NB	2.21	1.40	1.37
28	a	413	DGD	O1G-C1A	2.21	1.39	1.33
23	c	502	CLA	MG-NB	-2.20	2.01	2.05
28	H	102	DGD	C4E-C5E	2.20	1.57	1.53
25	B	619	BCR	C38-C26	-2.20	1.47	1.50
27	f	101	SQD	O3-C3	-2.20	1.37	1.43
23	D	403	CLA	C1B-C2B	2.20	1.48	1.43
28	c	518	DGD	O2D-C2D	-2.20	1.37	1.43
23	c	513	CLA	C1B-NB	-2.20	1.35	1.37
23	B	612	CLA	CMD-C2D	-2.20	1.46	1.50
23	b	613	CLA	CMC-C2C	-2.19	1.46	1.50
23	b	603	CLA	CHC-C4B	-2.19	1.34	1.39
23	b	614	CLA	CHC-C1C	2.19	1.42	1.38
28	C	516	DGD	C2B-C1B	-2.19	1.44	1.50
24	a	407	PHO	C3D-C4D	2.19	1.44	1.41
23	c	508	CLA	CMB-C2B	-2.19	1.46	1.50
33	b	622	LMG	C7-C8	2.19	1.57	1.50
23	c	505	CLA	CMD-C2D	-2.19	1.46	1.50
23	C	514	CLA	CMB-C2B	-2.19	1.46	1.50
23	C	510	CLA	MG-NA	2.19	2.11	2.06
23	c	502	CLA	CMC-C2C	-2.19	1.46	1.50
23	b	608	CLA	C1B-NB	-2.19	1.35	1.37
23	b	612	CLA	C1B-C2B	2.18	1.48	1.43
24	D	401	PHO	C3B-C2B	-2.18	1.37	1.40
35	v	201	HEC	C3C-C2C	-2.18	1.33	1.41
23	d	402	CLA	CMB-C2B	-2.18	1.46	1.50
29	l	101	LHG	P-O6	2.18	1.67	1.59
23	B	606	CLA	CMC-C2C	-2.18	1.46	1.50
23	a	405	CLA	CMC-C2C	-2.18	1.46	1.50
23	b	606	CLA	CMD-C2D	-2.18	1.46	1.50
23	B	603	CLA	C3B-C4B	2.18	1.49	1.42
23	C	505	CLA	C4B-NB	2.18	1.40	1.37
23	b	615	CLA	C1A-CHA	-2.18	1.34	1.43
28	c	516	DGD	O5D-C1E	2.18	1.43	1.40
28	A	412	DGD	O1G-C1G	-2.18	1.40	1.45
23	C	511	CLA	MG-NC	2.18	2.11	2.06
23	B	615	CLA	C5-C3	-2.18	1.46	1.51
33	c	519	LMG	O7-C8	-2.18	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CMB-C2B	-2.18	1.46	1.50
23	c	512	CLA	C3B-C4B	2.17	1.49	1.42
23	b	606	CLA	MG-NA	2.17	2.11	2.06
27	A	411	SQD	C46-C45	2.17	1.55	1.50
27	A	410	SQD	O4-C4	-2.17	1.37	1.43
28	C	518	DGD	C2A-C1A	-2.17	1.44	1.50
28	c	518	DGD	C1E-C2E	2.17	1.58	1.52
23	b	612	CLA	CMD-C2D	-2.17	1.46	1.50
23	B	602	CLA	CHC-C1C	2.17	1.42	1.38
23	B	608	CLA	MG-NA	-2.17	2.01	2.06
23	c	506	CLA	CHC-C1C	2.17	1.42	1.38
23	d	403	CLA	CMC-C2C	-2.17	1.46	1.50
29	A	413	LHG	O6-C4	-2.16	1.36	1.44
23	b	613	CLA	C3B-C4B	2.16	1.49	1.42
23	b	610	CLA	CMC-C2C	-2.16	1.46	1.50
23	d	404	CLA	C1B-C2B	2.16	1.48	1.43
26	d	406	PL9	C46-C44	-2.16	1.46	1.51
23	C	506	CLA	C4C-C3C	2.16	1.48	1.45
23	c	503	CLA	CHC-C1C	2.16	1.42	1.38
23	B	607	CLA	CAC-C3C	-2.16	1.45	1.51
34	e	102	HEM	CAB-C3B	2.16	1.53	1.47
23	a	406	CLA	MG-NB	2.16	2.10	2.05
23	b	616	CLA	C1B-C2B	2.16	1.48	1.43
34	E	103	HEM	CMB-C2B	2.16	1.55	1.50
23	b	616	CLA	CMD-C2D	-2.16	1.46	1.50
23	B	615	CLA	CMD-C2D	-2.16	1.46	1.50
27	a	411	SQD	O3-C3	-2.15	1.37	1.43
33	c	519	LMG	O8-C9	-2.15	1.40	1.45
23	C	511	CLA	CAA-C2A	-2.15	1.50	1.54
34	E	103	HEM	FE-NC	2.15	2.02	1.95
23	B	602	CLA	CMC-C2C	-2.15	1.46	1.50
23	C	507	CLA	CMA-C3A	-2.15	1.48	1.53
23	c	513	CLA	CMB-C2B	-2.15	1.46	1.50
23	B	608	CLA	O2D-CED	-2.15	1.40	1.45
23	a	408	CLA	C1D-ND	2.15	1.40	1.37
23	b	603	CLA	C3B-C4B	2.15	1.49	1.42
28	c	517	DGD	O2G-C2G	-2.14	1.41	1.46
24	a	407	PHO	CMC-C2C	-2.14	1.47	1.50
23	b	602	CLA	CMD-C2D	-2.14	1.46	1.50
23	A	405	CLA	CMB-C2B	-2.14	1.46	1.50
23	B	610	CLA	CMC-C2C	-2.14	1.46	1.50
28	C	517	DGD	O3D-C3D	-2.14	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C1B-C2B	2.14	1.48	1.43
23	b	617	CLA	CAB-C3B	-2.14	1.41	1.47
25	B	617	BCR	C38-C26	-2.14	1.47	1.50
23	C	505	CLA	CMB-C2B	-2.14	1.46	1.50
23	b	607	CLA	CMC-C2C	-2.14	1.46	1.50
23	C	507	CLA	C1A-CHA	-2.14	1.34	1.43
23	D	402	CLA	CMC-C2C	-2.14	1.46	1.50
25	b	620	BCR	C38-C26	-2.14	1.47	1.50
25	A	408	BCR	C30-C25	-2.14	1.51	1.53
23	A	405	CLA	C4B-NB	2.13	1.40	1.37
23	C	510	CLA	C1B-NB	-2.13	1.35	1.37
23	c	505	CLA	C1D-ND	2.13	1.40	1.37
23	B	615	CLA	C1B-C2B	2.13	1.48	1.43
25	k	101	BCR	C33-C5	-2.13	1.47	1.50
34	e	102	HEM	C3B-C2B	-2.13	1.32	1.37
23	c	507	CLA	CAB-C3B	-2.13	1.41	1.47
23	C	509	CLA	CMD-C2D	-2.13	1.46	1.50
23	b	609	CLA	C4B-NB	2.13	1.40	1.37
23	A	407	CLA	CMB-C2B	-2.13	1.46	1.50
23	B	608	CLA	CMB-C2B	-2.13	1.46	1.50
29	d	407	LHG	O7-C5	-2.12	1.41	1.46
23	b	604	CLA	CHC-C1C	2.12	1.42	1.38
23	C	512	CLA	CHC-C1C	2.12	1.42	1.38
23	B	608	CLA	C3D-C4D	2.12	1.49	1.44
23	c	510	CLA	C1B-C2B	2.12	1.48	1.43
33	c	524	LMG	O7-C8	-2.12	1.41	1.46
23	c	510	CLA	C5-C3	-2.11	1.46	1.51
23	C	513	CLA	C3B-C4B	2.11	1.48	1.42
23	C	503	CLA	CHC-C1C	2.11	1.42	1.38
23	b	604	CLA	CMB-C2B	-2.11	1.46	1.50
24	d	401	PHO	CMB-C2B	-2.10	1.47	1.51
28	C	517	DGD	C1G-C2G	2.10	1.57	1.50
25	a	409	BCR	C35-C13	-2.10	1.46	1.50
23	C	509	CLA	C1D-C2D	2.10	1.49	1.45
25	t	101	BCR	C33-C5	-2.10	1.47	1.50
23	d	404	CLA	C1D-ND	2.10	1.40	1.37
28	h	101	DGD	C3G-C2G	2.10	1.57	1.50
23	C	510	CLA	CMB-C2B	-2.10	1.46	1.50
23	b	609	CLA	CBD-CGD	-2.10	1.46	1.52
23	c	506	CLA	CMC-C2C	-2.09	1.46	1.50
23	D	404	CLA	CHC-C4B	-2.09	1.34	1.39
28	C	518	DGD	O1G-C1G	-2.09	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	518	DGD	O2E-C2E	-2.09	1.37	1.43
23	C	509	CLA	C3B-C4B	2.09	1.48	1.42
28	c	518	DGD	C3G-C2G	2.09	1.57	1.50
26	D	406	PL9	C45-C44	-2.09	1.45	1.50
23	A	405	CLA	C3B-C4B	2.09	1.48	1.42
23	B	603	CLA	MG-ND	2.09	2.09	2.05
23	b	611	CLA	C1C-NC	-2.09	1.34	1.37
23	c	510	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	614	CLA	C3B-C4B	2.09	1.48	1.42
23	c	504	CLA	C1C-C2C	2.09	1.48	1.44
23	c	506	CLA	CHC-C4B	-2.09	1.34	1.39
23	b	609	CLA	CAB-C3B	-2.09	1.41	1.47
23	b	602	CLA	CMC-C2C	-2.09	1.46	1.50
28	H	102	DGD	O2G-C1B	2.09	1.40	1.34
27	B	621	SQD	O2-C2	-2.08	1.37	1.43
23	b	611	CLA	CMA-C3A	-2.08	1.48	1.53
26	D	406	PL9	C21-C19	-2.08	1.47	1.51
25	H	101	BCR	C33-C5	-2.08	1.47	1.50
23	C	505	CLA	C4D-CHA	2.08	1.45	1.38
23	d	403	CLA	MG-NC	2.08	2.11	2.06
23	B	606	CLA	CHC-C4B	-2.08	1.34	1.39
23	b	610	CLA	CMD-C2D	-2.08	1.46	1.50
23	C	514	CLA	CMD-C2D	-2.08	1.46	1.50
23	B	603	CLA	C3C-C2C	2.07	1.41	1.36
23	b	605	CLA	CMB-C2B	-2.07	1.46	1.50
28	h	101	DGD	C6D-C5D	2.07	1.57	1.51
23	c	510	CLA	CMC-C2C	-2.07	1.46	1.50
23	c	509	CLA	C3C-C2C	2.07	1.41	1.36
25	A	408	BCR	C31-C1	-2.07	1.49	1.53
25	B	618	BCR	C33-C5	-2.07	1.47	1.50
23	a	408	CLA	C1B-NB	-2.07	1.35	1.37
33	D	407	LMG	C4-C3	2.07	1.57	1.52
27	a	411	SQD	O2-C2	-2.07	1.37	1.43
23	b	610	CLA	CMA-C3A	-2.07	1.48	1.53
25	B	619	BCR	C33-C5	-2.07	1.47	1.50
28	c	516	DGD	O3E-C3E	-2.06	1.37	1.43
23	C	504	CLA	C4D-CHA	2.06	1.45	1.38
23	a	405	CLA	CMB-C2B	-2.06	1.46	1.50
33	C	519	LMG	C4-C3	2.06	1.57	1.52
23	B	615	CLA	CAB-C3B	-2.06	1.41	1.47
23	B	605	CLA	C1B-NB	-2.06	1.35	1.37
23	c	508	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CMD-C2D	-2.06	1.46	1.50
33	C	519	LMG	C4-C5	2.06	1.57	1.53
33	m	101	LMG	O4-C4	-2.05	1.37	1.43
23	b	614	CLA	CMD-C2D	-2.05	1.46	1.50
23	A	407	CLA	CAC-C3C	-2.05	1.45	1.51
23	B	601	CLA	CAA-C2A	-2.05	1.50	1.54
34	E	103	HEM	CAC-C3C	2.05	1.52	1.47
28	c	517	DGD	O1G-C1A	2.05	1.39	1.33
23	d	404	CLA	C3B-C4B	2.05	1.48	1.42
23	b	602	CLA	C3D-C4D	2.05	1.48	1.44
23	B	605	CLA	CMD-C2D	-2.04	1.46	1.50
23	C	513	CLA	C1A-CHA	-2.04	1.34	1.43
23	b	610	CLA	C1A-CHA	-2.04	1.34	1.43
25	b	618	BCR	C38-C26	-2.04	1.47	1.50
23	C	512	CLA	C3D-C4D	2.04	1.48	1.44
33	c	522	LMG	O7-C8	-2.04	1.41	1.46
23	A	405	CLA	CAA-C2A	-2.04	1.50	1.54
23	B	603	CLA	CMC-C2C	-2.04	1.46	1.50
23	C	510	CLA	CMD-C2D	-2.04	1.46	1.50
23	B	602	CLA	CMB-C2B	-2.03	1.46	1.50
23	c	503	CLA	C1D-C2D	2.03	1.49	1.45
28	C	517	DGD	C4E-C5E	2.03	1.57	1.53
23	C	505	CLA	C3D-C4D	2.03	1.48	1.44
33	c	524	LMG	O8-C28	2.03	1.39	1.33
26	d	406	PL9	C23-C24	2.03	1.37	1.33
24	d	401	PHO	C4D-CHA	2.03	1.42	1.39
29	L	101	LHG	C4-C5	2.03	1.57	1.50
23	B	614	CLA	C3B-C4B	2.03	1.48	1.42
23	B	602	CLA	CMD-C2D	-2.03	1.46	1.50
25	c	521	BCR	C33-C5	-2.03	1.47	1.50
25	b	618	BCR	C5-C6	-2.02	1.31	1.34
33	c	524	LMG	C1-C2	2.02	1.58	1.52
23	c	511	CLA	C3C-C2C	2.02	1.41	1.36
23	c	509	CLA	O1D-CGD	2.02	1.26	1.21
23	B	609	CLA	C1B-NB	-2.02	1.35	1.37
33	C	501	LMG	C1-C2	2.02	1.58	1.52
26	d	406	PL9	C7-C8	-2.02	1.47	1.50
23	b	609	CLA	C1D-C2D	2.01	1.49	1.45
23	b	605	CLA	CHC-C1C	2.01	1.42	1.38
23	C	513	CLA	C1B-C2B	2.01	1.47	1.43
27	a	411	SQD	O4-C4	-2.01	1.38	1.43
23	C	512	CLA	C4D-CHA	2.01	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1B-NB	-2.01	1.35	1.37
23	B	614	CLA	CMD-C2D	-2.00	1.46	1.50
28	c	516	DGD	O1G-C1G	-2.00	1.40	1.45
23	C	503	CLA	C1B-C2B	2.00	1.47	1.43
23	a	406	CLA	CBD-CGD	-2.00	1.46	1.52

All (1319) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C4A-NA-C1A	10.99	111.69	106.68
23	c	501	CLA	C4A-NA-C1A	10.50	111.47	106.68
23	C	502	CLA	C4A-NA-C1A	10.46	111.45	106.68
27	A	410	SQD	O6-C1-C2	10.43	124.11	108.27
23	d	402	CLA	C4A-NA-C1A	10.31	111.38	106.68
23	C	504	CLA	C4A-NA-C1A	9.14	110.85	106.68
23	D	403	CLA	C4A-NA-C1A	8.90	110.74	106.68
27	b	601	SQD	O6-C1-C2	8.62	121.37	108.27
23	B	606	CLA	C4A-NA-C1A	8.51	110.56	106.68
23	C	514	CLA	C4A-NA-C1A	8.35	110.49	106.68
27	a	411	SQD	O6-C1-C2	8.17	120.69	108.27
23	C	509	CLA	C4A-NA-C1A	8.04	110.35	106.68
23	C	512	CLA	C4A-NA-C1A	7.94	110.30	106.68
23	C	511	CLA	C4A-NA-C1A	7.69	110.19	106.68
23	B	612	CLA	C4A-NA-C1A	7.63	110.16	106.68
23	B	613	CLA	C4A-NA-C1A	7.40	110.06	106.68
23	c	511	CLA	C4A-NA-C1A	7.30	110.01	106.68
23	B	610	CLA	C4A-NA-C1A	7.29	110.00	106.68
33	b	622	LMG	O1-C1-C2	-6.96	97.70	108.27
23	b	613	CLA	C4A-NA-C1A	6.89	109.82	106.68
23	b	606	CLA	C4A-NA-C1A	6.77	109.77	106.68
23	c	502	CLA	C4A-NA-C1A	6.73	109.75	106.68
23	b	616	CLA	C4A-NA-C1A	6.47	109.63	106.68
23	c	507	CLA	C4A-NA-C1A	6.44	109.62	106.68
23	c	504	CLA	C4A-NA-C1A	6.30	109.55	106.68
23	C	510	CLA	C4A-NA-C1A	6.28	109.54	106.68
23	a	405	CLA	C4A-NA-C1A	6.06	109.45	106.68
23	A	407	CLA	O2D-CGD-O1D	-6.00	112.16	123.85
27	B	621	SQD	O6-C1-C2	5.96	117.33	108.27
23	A	404	CLA	C4A-NA-C1A	5.92	109.38	106.68
23	B	604	CLA	C4A-NA-C1A	5.92	109.38	106.68
23	B	603	CLA	O2D-CGD-O1D	-5.87	112.42	123.85
23	B	616	CLA	C4A-NA-C1A	5.82	109.33	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C4A-NA-C1A	5.81	109.33	106.68
23	c	503	CLA	C4A-NA-C1A	5.73	109.30	106.68
23	c	501	CLA	O2D-CGD-O1D	-5.73	112.69	123.85
23	B	614	CLA	O2D-CGD-O1D	-5.73	112.70	123.85
27	F	101	SQD	O6-C1-C2	5.72	116.96	108.27
27	f	101	SQD	O6-C1-C2	5.68	116.89	108.27
26	D	406	PL9	C7-C3-C4	5.63	121.55	116.91
35	v	201	HEC	CBC-CAC-C3C	-5.57	116.29	127.43
23	b	617	CLA	O2D-CGD-O1D	-5.57	113.01	123.85
23	B	611	CLA	C4A-NA-C1A	5.56	109.22	106.68
27	B	621	SQD	O47-C7-C8	5.54	123.48	111.48
23	c	506	CLA	C4A-NA-C1A	5.51	109.19	106.68
23	b	607	CLA	C4A-NA-C1A	5.50	109.19	106.68
23	b	609	CLA	C3B-C4B-NB	-5.40	105.70	110.53
28	H	102	DGD	O3G-C3G-C2G	-5.39	97.71	110.82
23	a	406	CLA	CHB-C4A-NA	5.33	132.09	124.40
26	a	410	PL9	C7-C3-C4	5.28	121.26	116.91
23	b	615	CLA	C4A-NA-C1A	5.15	109.03	106.68
23	c	512	CLA	C4A-NA-C1A	5.12	109.01	106.68
27	a	412	SQD	O47-C7-C8	5.09	122.49	111.48
23	C	502	CLA	C3B-C4B-NB	-5.06	106.01	110.53
27	b	601	SQD	O7-S-C6	5.01	114.24	106.76
27	A	410	SQD	O7-S-C6	5.00	114.22	106.76
26	A	409	PL9	C7-C3-C4	4.97	121.00	116.91
27	a	411	SQD	O9-S-C6	4.86	114.01	106.76
23	C	502	CLA	O2D-CGD-CBD	4.85	119.71	111.23
23	c	501	CLA	O2D-CGD-CBD	4.81	119.64	111.23
29	A	413	LHG	O4-P-O5	4.81	134.81	112.44
23	D	404	CLA	O2D-CGD-O1D	-4.80	114.51	123.85
23	b	614	CLA	C4A-NA-C1A	4.79	108.86	106.68
23	a	406	CLA	O2D-CGD-CBD	4.74	119.51	111.23
26	d	406	PL9	C40-C39-C41	4.72	123.42	115.23
27	F	101	SQD	O8-S-C6	4.70	115.05	105.97
35	V	201	HEC	CBB-CAB-C3B	-4.70	118.04	127.43
23	d	402	CLA	C3B-C4B-NB	-4.69	106.34	110.53
24	D	401	PHO	O1D-CGD-CBD	4.69	131.83	124.72
24	D	401	PHO	C2B-C1B-NB	-4.67	106.06	109.43
23	b	603	CLA	O2D-CGD-O1D	-4.65	114.79	123.85
23	b	617	CLA	C4A-NA-C1A	4.65	108.80	106.68
23	B	609	CLA	C4A-NA-C1A	4.62	108.79	106.68
35	v	201	HEC	CBB-CAB-C3B	-4.62	118.20	127.43
23	b	602	CLA	C3B-C4B-NB	-4.61	106.41	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C4A-NA-C1A	4.61	108.78	106.68
23	b	608	CLA	C4A-NA-C1A	4.59	108.77	106.68
23	b	604	CLA	C4A-NA-C1A	4.58	108.77	106.68
23	B	614	CLA	C3B-C4B-NB	-4.56	106.45	110.53
33	c	522	LMG	O6-C1-O1	-4.54	99.30	110.04
23	a	406	CLA	C4A-NA-C1A	4.54	108.75	106.68
23	B	601	CLA	C4A-NA-C1A	4.47	108.72	106.68
23	c	509	CLA	C3B-C4B-NB	-4.46	106.55	110.53
23	b	603	CLA	O2D-CGD-CBD	4.46	119.03	111.23
23	b	606	CLA	O2D-CGD-O1D	-4.46	115.17	123.85
23	A	405	CLA	O2D-CGD-CBD	4.45	119.00	111.23
29	e	101	LHG	O4-P-O5	4.44	133.09	112.44
23	C	509	CLA	O2D-CGD-O1D	-4.43	115.22	123.85
23	c	511	CLA	C3B-C4B-NB	-4.42	106.58	110.53
24	D	401	PHO	O2D-CGD-CBD	-4.42	106.09	110.95
29	d	407	LHG	O4-P-O5	4.42	133.00	112.44
23	A	405	CLA	O2D-CGD-O1D	-4.41	115.27	123.85
29	E	101	LHG	O4-P-O5	4.39	132.87	112.44
27	F	101	SQD	O9-S-C6	4.38	113.30	106.76
29	D	408	LHG	O4-P-O5	4.38	132.83	112.44
23	B	610	CLA	O2D-CGD-O1D	-4.37	115.34	123.85
28	C	518	DGD	O3G-C3G-C2G	-4.37	100.19	110.82
27	A	411	SQD	O47-C7-C8	4.37	120.93	111.48
29	d	409	LHG	O4-P-O5	4.36	132.74	112.44
23	A	404	CLA	CHB-C4A-NA	4.36	130.69	124.40
23	b	604	CLA	O2D-CGD-O1D	-4.33	115.42	123.85
28	A	412	DGD	C3G-C2G-C1G	-4.33	101.70	111.78
23	d	402	CLA	O2D-CGD-O1D	-4.32	115.45	123.85
23	b	604	CLA	O2D-CGD-CBD	4.31	118.77	111.23
23	c	506	CLA	CBC-CAC-C3C	-4.29	100.78	112.42
28	C	517	DGD	O3G-C3G-C2G	-4.28	100.41	110.82
23	c	510	CLA	O2D-CGD-O1D	-4.25	115.58	123.85
23	b	616	CLA	C3B-C4B-NB	-4.24	106.75	110.53
35	V	201	HEC	CBC-CAC-C3C	-4.23	118.97	127.43
29	d	408	LHG	O4-P-O5	4.22	132.09	112.44
29	D	409	LHG	O4-P-O5	4.21	132.04	112.44
23	c	513	CLA	C4A-NA-C1A	4.20	108.60	106.68
23	C	504	CLA	O2D-CGD-O1D	-4.20	115.68	123.85
27	b	601	SQD	O5-C5-C4	4.17	117.22	109.70
33	d	411	LMG	O1-C1-C2	-4.17	101.94	108.27
23	B	601	CLA	O2D-CGD-O1D	-4.16	115.76	123.85
33	d	411	LMG	O6-C5-C4	4.14	117.15	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410	PL9	C7-C3-C2	-4.13	118.52	123.39
23	B	615	CLA	CHC-C4B-NB	4.13	130.24	124.05
24	A	406	PHO	C3B-C4B-NB	-4.13	104.77	107.46
24	d	401	PHO	C2B-C1B-NB	-4.09	106.47	109.43
27	b	601	SQD	C1-C2-C3	-4.08	101.43	110.01
29	l	101	LHG	O4-P-O5	4.07	131.40	112.44
28	c	516	DGD	C3G-C2G-C1G	-4.07	102.29	111.78
23	c	503	CLA	C3B-C4B-NB	-4.07	106.90	110.53
23	a	406	CLA	CMA-C3A-C4A	-4.07	100.84	111.77
23	b	606	CLA	C1-C2-C3	-4.06	119.54	126.20
25	T	101	BCR	C27-C26-C25	4.06	128.19	122.70
23	B	612	CLA	CHB-C4A-NA	4.04	130.23	124.40
23	c	505	CLA	C3B-C4B-NB	-4.03	106.94	110.53
28	c	516	DGD	O3G-C3G-C2G	-4.00	101.09	110.82
28	c	518	DGD	C3G-C2G-C1G	-4.00	102.47	111.78
26	A	409	PL9	C7-C3-C2	-3.99	118.68	123.39
23	C	507	CLA	C3B-C4B-NB	-3.99	106.97	110.53
33	m	101	LMG	O7-C10-O9	-3.99	114.38	123.70
25	b	618	BCR	C2-C1-C6	3.98	116.22	110.44
23	a	406	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
23	c	510	CLA	C4A-NA-C1A	3.96	108.49	106.68
23	d	403	CLA	C4A-NA-C1A	3.96	108.49	106.68
23	b	613	CLA	CHB-C4A-NA	3.95	130.09	124.40
27	a	411	SQD	O9-S-O7	-3.94	101.00	113.82
23	b	603	CLA	CHB-C4A-NA	3.92	130.06	124.40
27	A	410	SQD	C1-C2-C3	-3.91	101.78	110.01
23	C	513	CLA	CHB-C4A-NA	3.91	130.05	124.40
28	H	102	DGD	C1D-O6D-C5D	-3.91	106.08	113.72
23	d	403	CLA	C3B-C4B-NB	-3.89	107.06	110.53
23	B	607	CLA	C4A-NA-C1A	3.88	108.45	106.68
23	b	617	CLA	O1D-CGD-CBD	3.85	132.11	124.52
23	b	606	CLA	CHD-C1D-ND	-3.84	119.40	124.80
31	A	415	BCT	O2-C-O1	3.84	129.49	119.68
23	c	512	CLA	C3B-C4B-NB	-3.83	107.11	110.53
24	d	401	PHO	O1D-CGD-CBD	3.83	130.53	124.72
23	B	603	CLA	C3B-C4B-NB	-3.82	107.12	110.53
28	C	517	DGD	C1D-C2D-C3D	-3.82	101.98	110.01
23	C	505	CLA	C4A-NA-C1A	3.82	108.42	106.68
25	b	618	BCR	C33-C5-C6	-3.81	120.33	124.48
23	B	615	CLA	C4A-NA-C1A	3.81	108.42	106.68
27	B	621	SQD	C1-O5-C5	-3.80	106.29	113.72
23	B	603	CLA	C4A-NA-C1A	3.80	108.41	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	C3B-C4B-NB	-3.80	107.14	110.53
23	C	510	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
23	C	502	CLA	O2D-CGD-O1D	-3.78	116.50	123.85
23	A	407	CLA	O2D-CGD-CBD	3.78	117.83	111.23
23	b	617	CLA	CHB-C4A-NA	3.77	129.84	124.40
23	b	603	CLA	CHC-C1C-NC	3.76	129.98	124.31
33	b	622	LMG	O2-C2-C1	-3.76	101.12	110.08
27	A	410	SQD	O47-C7-C8	3.75	119.58	111.48
23	c	510	CLA	CHB-C4A-NA	3.73	129.78	124.40
23	B	603	CLA	O2D-CGD-CBD	3.72	117.74	111.23
23	c	508	CLA	C4A-NA-C1A	3.72	108.38	106.68
27	A	410	SQD	O9-S-O7	-3.71	101.75	113.82
24	A	406	PHO	C2B-C1B-NB	-3.71	106.75	109.43
23	B	614	CLA	O1D-CGD-CBD	3.71	131.83	124.52
23	d	404	CLA	O2A-CGA-O1A	-3.70	114.37	123.63
23	C	508	CLA	O2D-CGD-CBD	3.70	117.69	111.23
23	B	616	CLA	C1-O2A-CGA	3.70	125.60	116.65
28	A	412	DGD	O5D-C1E-C2E	3.69	113.88	108.27
25	B	618	BCR	C35-C13-C14	-3.68	116.85	122.82
24	a	407	PHO	C2B-C1B-NB	-3.66	106.78	109.43
28	C	518	DGD	O6D-C1D-O3G	-3.66	101.39	110.04
23	B	604	CLA	C3B-C4B-NB	-3.65	107.27	110.53
34	e	102	HEM	CBD-CAD-C3D	-3.65	102.44	112.53
29	L	101	LHG	O4-P-O5	3.65	129.41	112.44
28	h	101	DGD	C4E-C3E-C2E	-3.65	104.43	110.83
23	B	611	CLA	C1-C2-C3	-3.65	120.22	126.20
23	C	507	CLA	C4A-NA-C1A	3.64	108.34	106.68
35	V	201	HEC	CHB-C4A-NA	3.63	128.41	124.45
23	c	510	CLA	C3B-C4B-NB	-3.63	107.29	110.53
23	c	509	CLA	CHB-C4A-NA	3.63	129.63	124.40
26	d	406	PL9	C22-C23-C24	-3.62	119.33	127.62
23	c	509	CLA	O2A-CGA-O1A	-3.60	114.61	123.63
29	A	413	LHG	O8-C23-C24	3.60	122.83	111.83
33	m	101	LMG	O1-C7-C8	-3.60	102.06	110.82
24	d	401	PHO	C4D-CHA-CBD	-3.60	106.73	108.45
25	B	618	BCR	C15-C16-C17	-3.60	116.16	123.52
26	D	406	PL9	C37-C38-C39	-3.59	119.40	127.62
23	b	604	CLA	C7-C6-C5	-3.59	103.69	113.26
23	C	503	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
33	c	524	LMG	C1-O6-C5	-3.58	106.72	113.72
23	b	602	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
23	B	602	CLA	O2D-CGD-CBD	3.58	117.49	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	CHD-C1D-ND	-3.58	119.77	124.80
29	d	407	LHG	O8-C23-C24	3.56	122.70	111.83
33	d	411	LMG	O2-C2-C1	-3.56	101.59	110.08
23	b	605	CLA	C4A-NA-C1A	3.56	108.30	106.68
26	d	406	PL9	C30-C29-C31	-3.56	109.05	115.23
23	B	616	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
23	B	606	CLA	C2A-C1A-CHA	3.54	130.00	123.87
31	a	404	BCT	O2-C-O1	3.53	128.71	119.68
23	a	406	CLA	CED-O2D-CGD	-3.53	107.91	115.92
23	b	609	CLA	CMA-C3A-C4A	-3.52	102.30	111.77
23	b	605	CLA	C3B-C4B-NB	-3.52	107.39	110.53
23	b	611	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
23	b	611	CLA	CAA-CBA-CGA	-3.51	103.24	113.21
25	x	102	BCR	C27-C26-C25	3.51	127.44	122.70
27	a	411	SQD	C1-C2-C3	-3.50	102.65	110.01
27	a	412	SQD	O48-C23-C24	3.49	122.49	111.83
25	b	619	BCR	C30-C25-C26	-3.48	117.88	122.64
23	B	602	CLA	CHB-C4A-NA	3.48	129.43	124.40
25	b	619	BCR	C8-C7-C6	-3.48	117.69	127.00
23	b	613	CLA	CMB-C2B-C1B	-3.47	120.13	125.42
28	c	516	DGD	C3E-C4E-C5E	-3.47	103.93	110.23
27	A	410	SQD	O47-C7-O49	-3.47	115.60	123.70
24	a	407	PHO	CMB-C2B-C3B	3.46	131.61	124.68
26	D	406	PL9	C7-C3-C2	-3.46	119.31	123.39
26	d	406	PL9	C7-C3-C4	3.46	119.76	116.91
23	C	511	CLA	C3B-C4B-NB	-3.45	107.45	110.53
25	Z	101	BCR	C15-C16-C17	-3.45	116.46	123.52
23	c	507	CLA	CHB-C4A-NA	3.45	129.38	124.40
23	c	503	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
27	b	601	SQD	O9-S-O7	-3.44	102.62	113.82
26	d	406	PL9	C45-C44-C46	-3.44	109.25	115.23
23	C	506	CLA	CAC-C3C-C4C	3.44	129.26	124.79
23	b	612	CLA	CHD-C1D-ND	-3.43	119.98	124.80
23	d	404	CLA	CHA-C1A-NA	-3.42	118.64	126.39
28	c	518	DGD	O6E-C5E-C4E	3.41	115.85	109.70
27	F	101	SQD	O5-C5-C4	3.41	115.84	109.70
23	A	405	CLA	CAC-C3C-C4C	3.41	129.22	124.79
23	b	602	CLA	C4A-NA-C1A	3.41	108.23	106.68
25	t	101	BCR	C29-C30-C25	3.41	115.39	110.44
28	h	101	DGD	O3G-C3G-C2G	-3.40	102.54	110.82
28	c	517	DGD	O6D-C1D-O3G	-3.39	102.03	110.04
27	f	101	SQD	O8-S-C6	3.39	112.52	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C3B-C4B-NB	-3.39	107.50	110.53
25	c	515	BCR	C27-C26-C25	3.39	127.28	122.70
23	B	604	CLA	O2A-CGA-O1A	-3.39	115.15	123.63
28	C	517	DGD	O5D-C1E-C2E	3.39	113.42	108.27
23	b	605	CLA	OBD-CAD-C3D	3.39	136.33	128.42
27	b	601	SQD	O8-S-C6	3.38	112.50	105.97
28	h	101	DGD	C1E-O6E-C5E	3.38	120.32	113.72
25	c	514	BCR	C27-C26-C25	3.38	127.27	122.70
27	a	411	SQD	O47-C7-O49	-3.37	115.82	123.70
23	c	512	CLA	C1-C2-C3	-3.37	120.67	126.20
23	b	608	CLA	O1D-CGD-CBD	3.37	131.17	124.52
23	B	607	CLA	CHD-C1D-ND	-3.37	120.06	124.80
25	c	521	BCR	C27-C26-C25	3.37	127.26	122.70
25	H	101	BCR	C29-C30-C25	3.36	115.32	110.44
25	Z	101	BCR	C2-C1-C6	3.35	115.31	110.44
33	m	101	LMG	O6-C1-O1	-3.35	102.12	110.04
27	F	101	SQD	O9-S-O7	-3.35	102.94	113.82
23	b	608	CLA	CHB-C4A-NA	3.34	129.22	124.40
23	C	506	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
23	D	403	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
25	c	515	BCR	C33-C5-C6	-3.32	120.86	124.48
25	B	618	BCR	C15-C14-C13	-3.32	122.62	127.28
23	B	613	CLA	C4-C3-C5	3.32	120.99	115.23
23	c	508	CLA	CHD-C1D-ND	-3.32	120.13	124.80
23	C	508	CLA	C4A-NA-C1A	3.32	108.19	106.68
25	C	520	BCR	C15-C16-C17	-3.31	116.75	123.52
23	B	611	CLA	O2D-CGD-CBD	3.31	117.02	111.23
23	C	509	CLA	O2D-CGD-CBD	3.31	117.01	111.23
23	b	613	CLA	CMB-C2B-C3B	3.31	134.33	126.55
23	B	605	CLA	CHD-C1D-ND	-3.29	120.17	124.80
26	A	409	PL9	C20-C19-C21	3.28	120.92	115.23
25	c	521	BCR	C11-C10-C9	-3.28	122.68	127.28
25	T	101	BCR	C7-C8-C9	-3.28	121.39	126.23
23	b	607	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
33	c	519	LMG	O6-C1-O1	-3.27	102.32	110.04
23	A	407	CLA	C4-C3-C5	3.26	120.89	115.23
26	d	406	PL9	C7-C8-C9	-3.26	121.21	126.83
25	C	520	BCR	C27-C26-C25	3.26	127.11	122.70
23	B	613	CLA	C1-C2-C3	-3.26	120.86	126.20
23	b	616	CLA	C1-O2A-CGA	3.26	124.53	116.65
27	B	621	SQD	O9-S-O7	-3.25	103.25	113.82
23	b	615	CLA	O2D-CGD-O1D	-3.25	117.52	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C27-C26-C25	3.25	127.09	122.70
33	c	524	LMG	O6-C1-O1	-3.25	102.37	110.04
29	d	408	LHG	O8-C23-C24	3.25	121.73	111.83
23	C	511	CLA	CHB-C4A-NA	3.24	129.08	124.40
23	C	506	CLA	O1D-CGD-CBD	3.24	130.92	124.52
25	H	101	BCR	C30-C25-C26	-3.24	118.21	122.64
23	B	613	CLA	CHB-C4A-NA	3.23	129.07	124.40
27	A	411	SQD	C45-O47-C7	3.23	122.45	117.78
23	B	609	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
23	B	614	CLA	CMB-C2B-C1B	-3.23	120.51	125.42
23	C	510	CLA	O1D-CGD-CBD	3.22	130.88	124.52
23	d	402	CLA	CHB-C4A-NA	3.22	129.04	124.40
23	c	513	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
23	C	508	CLA	CHD-C1D-ND	-3.22	120.28	124.80
33	C	519	LMG	O1-C7-C8	-3.22	103.00	110.82
23	A	405	CLA	C3B-C4B-NB	-3.21	107.66	110.53
29	A	413	LHG	O3-P-O5	-3.21	96.22	108.94
23	b	610	CLA	O1D-CGD-CBD	3.21	130.84	124.52
28	C	517	DGD	C1D-O6D-C5D	-3.20	107.47	113.72
23	B	606	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
23	b	606	CLA	O1D-CGD-CBD	3.19	130.81	124.52
28	A	412	DGD	C1D-C2D-C3D	-3.19	103.31	110.01
23	a	406	CLA	C3B-C4B-NB	-3.17	107.70	110.53
23	D	404	CLA	C2D-C1D-ND	-3.17	106.99	110.13
23	B	611	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
26	a	410	PL9	C22-C23-C24	-3.17	120.37	127.62
23	D	403	CLA	C3B-C4B-NB	-3.17	107.70	110.53
23	b	614	CLA	C7-C6-C5	-3.16	104.83	113.26
24	d	401	PHO	CBC-CAC-C3C	3.16	117.40	112.87
25	H	101	BCR	C27-C26-C25	3.16	126.97	122.70
23	c	502	CLA	C1-C2-C3	-3.16	121.02	126.20
29	E	101	LHG	O8-C23-C24	3.16	121.45	111.83
23	b	604	CLA	C3B-C4B-NB	-3.15	107.72	110.53
29	A	413	LHG	O8-C23-O10	-3.15	115.74	123.63
23	b	608	CLA	C3B-C4B-NB	-3.15	107.72	110.53
28	h	101	DGD	C4D-C3D-C2D	-3.15	105.31	110.83
24	A	406	PHO	C1A-C2A-C3A	-3.15	99.85	102.84
28	c	518	DGD	O3G-C3G-C2G	-3.14	103.17	110.82
23	b	612	CLA	CHD-C1D-C2D	3.14	132.02	125.49
24	d	401	PHO	C3B-C4B-NB	-3.14	105.42	107.46
25	C	515	BCR	C27-C26-C25	3.13	126.93	122.70
34	e	102	HEM	C3B-C2B-C1B	3.13	108.76	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	BCR	C37-C22-C21	-3.13	117.75	122.82
23	B	615	CLA	C3B-C4B-NB	-3.12	107.74	110.53
23	b	607	CLA	CHD-C4C-NC	3.12	129.07	124.23
27	B	621	SQD	O8-S-C6	3.12	111.99	105.97
23	C	513	CLA	C3B-C4B-NB	-3.11	107.75	110.53
25	b	620	BCR	C29-C30-C25	3.11	114.96	110.44
33	d	411	LMG	C6-C5-C4	-3.11	105.38	113.02
23	C	509	CLA	C3B-C4B-NB	-3.11	107.75	110.53
33	m	101	LMG	O3-C3-C2	-3.11	103.05	110.38
23	b	606	CLA	CHB-C4A-NA	3.11	128.88	124.40
23	b	613	CLA	CHD-C1D-ND	-3.10	120.43	124.80
23	c	506	CLA	C4-C3-C5	3.10	120.61	115.23
23	d	402	CLA	C2A-C1A-CHA	3.10	129.25	123.87
23	D	403	CLA	CHB-C4A-NA	3.10	128.88	124.40
23	B	610	CLA	C3B-C4B-NB	-3.10	107.76	110.53
23	B	610	CLA	CHB-C4A-NA	3.10	128.87	124.40
23	b	614	CLA	CED-O2D-CGD	3.10	122.94	115.92
25	B	617	BCR	C30-C25-C26	-3.10	118.41	122.64
23	B	605	CLA	C4-C3-C5	3.09	120.60	115.23
28	C	516	DGD	O2D-C2D-C1D	-3.09	102.71	110.08
23	b	616	CLA	CHB-C1B-NB	3.09	128.68	124.05
23	c	501	CLA	CMB-C2B-C1B	-3.09	120.72	125.42
23	B	605	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
23	b	609	CLA	CHB-C4A-NA	3.08	128.85	124.40
23	B	615	CLA	C7-C6-C5	-3.08	105.05	113.26
23	A	404	CLA	C3B-C4B-NB	-3.08	107.78	110.53
23	C	506	CLA	CHB-C4A-NA	3.08	128.84	124.40
23	C	514	CLA	CHB-C4A-NA	3.08	128.84	124.40
23	b	605	CLA	CHB-C4A-NA	3.08	128.84	124.40
24	d	401	PHO	CMB-C2B-C3B	3.07	130.82	124.68
23	C	504	CLA	C6-C5-C3	3.07	120.95	113.47
23	c	503	CLA	CHC-C4B-NB	3.07	128.65	124.05
27	a	412	SQD	O48-C23-O10	-3.07	115.95	123.63
23	c	502	CLA	C3A-C2A-C1A	3.07	105.93	101.34
25	B	617	BCR	C27-C26-C25	3.06	126.84	122.70
23	b	611	CLA	C4A-NA-C1A	3.06	108.08	106.68
23	a	408	CLA	CAA-CBA-CGA	-3.06	104.52	113.21
27	f	101	SQD	O9-S-C6	3.06	111.32	106.76
23	d	403	CLA	O2A-CGA-O1A	-3.06	115.98	123.63
33	C	501	LMG	O6-C1-C2	-3.06	104.09	110.37
27	A	411	SQD	O48-C23-O10	-3.05	115.99	123.63
28	h	101	DGD	C3G-C2G-C1G	-3.05	104.67	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	617	BCR	C2-C1-C6	3.05	114.87	110.44
23	a	408	CLA	CHB-C4A-NA	3.05	128.80	124.40
28	h	101	DGD	O3E-C3E-C4E	3.05	117.56	110.38
23	b	606	CLA	CHD-C4C-NC	3.05	128.96	124.23
25	H	101	BCR	C2-C1-C6	3.05	114.86	110.44
27	a	411	SQD	O47-C7-C8	3.05	118.07	111.48
23	A	407	CLA	C1D-ND-C4D	-3.04	104.18	106.31
33	D	407	LMG	O6-C1-O1	-3.04	102.86	110.04
23	B	612	CLA	C3B-C4B-NB	-3.04	107.82	110.53
23	c	501	CLA	C1C-C2C-C3C	-3.03	103.79	106.98
24	a	407	PHO	O1D-CGD-CBD	3.03	129.32	124.72
28	C	517	DGD	O6E-C1E-O5D	-3.03	102.88	110.04
25	K	101	BCR	C23-C22-C21	-3.02	114.25	119.01
23	D	404	CLA	O1D-CGD-CBD	3.02	130.48	124.52
23	B	612	CLA	O2A-CGA-O1A	-3.02	116.07	123.63
25	A	408	BCR	C29-C30-C25	3.01	114.82	110.44
28	C	517	DGD	O2D-C2D-C1D	-3.01	102.90	110.08
23	b	605	CLA	C1-C2-C3	-3.01	121.27	126.20
25	k	101	BCR	C27-C26-C25	3.01	126.77	122.70
33	M	101	LMG	O1-C1-C2	-3.01	103.71	108.27
23	d	402	CLA	CMC-C2C-C1C	3.01	129.73	125.03
23	b	613	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
23	a	405	CLA	C3A-C2A-C1A	3.00	105.83	101.34
28	H	102	DGD	O3E-C3E-C2E	-3.00	103.32	110.38
29	D	409	LHG	O8-C23-O10	-2.99	116.14	123.63
23	B	601	CLA	C3B-C4B-NB	-2.99	107.86	110.53
23	b	602	CLA	CHB-C1B-NB	2.99	128.53	124.05
23	b	612	CLA	CHD-C4C-NC	2.99	128.87	124.23
23	B	608	CLA	CHB-C4A-NA	2.99	128.71	124.40
23	C	510	CLA	CHB-C4A-NA	2.97	128.69	124.40
29	D	408	LHG	O8-C23-C24	2.97	120.89	111.83
27	b	601	SQD	O47-C45-C46	2.97	118.98	108.34
27	A	410	SQD	O2-C2-C1	2.97	117.14	110.08
23	C	503	CLA	C4A-NA-C1A	2.97	108.03	106.68
25	b	618	BCR	C27-C26-C25	2.96	126.71	122.70
23	b	612	CLA	O2D-CGD-CBD	2.96	116.41	111.23
25	D	405	BCR	C28-C27-C26	-2.96	108.77	114.06
23	b	610	CLA	C4A-NA-C1A	2.96	108.03	106.68
33	m	101	LMG	O1-C1-C2	-2.96	103.78	108.27
27	B	621	SQD	O5-C5-C4	2.96	115.03	109.70
33	C	501	LMG	C38-C37-C36	-2.96	99.42	114.37
33	D	407	LMG	O3-C3-C2	-2.96	103.41	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	514	BCR	C30-C25-C26	-2.95	118.60	122.64
23	C	504	CLA	C7-C6-C5	-2.94	105.42	113.26
23	A	407	CLA	C2C-C1C-NC	2.94	113.07	109.98
23	c	505	CLA	C4A-NA-C1A	2.94	108.02	106.68
27	F	101	SQD	O48-C23-C24	2.94	120.80	111.83
23	A	407	CLA	CHB-C4A-NA	2.93	128.63	124.40
23	A	407	CLA	CMB-C2B-C1B	-2.93	120.95	125.42
23	B	608	CLA	CHD-C1D-ND	-2.93	120.68	124.80
25	K	101	BCR	C33-C5-C6	-2.93	121.29	124.48
25	c	515	BCR	C2-C1-C6	2.93	114.69	110.44
23	D	404	CLA	C1-C2-C3	-2.92	121.41	126.20
33	b	622	LMG	C8-O7-C10	2.92	124.79	117.80
23	b	602	CLA	O2D-CGD-CBD	2.92	116.34	111.23
25	A	408	BCR	C38-C26-C27	-2.92	107.36	113.60
25	c	515	BCR	C30-C25-C26	-2.92	118.65	122.64
28	C	516	DGD	C4E-C3E-C2E	-2.92	105.70	110.83
23	d	402	CLA	O2D-CGD-CBD	2.92	116.33	111.23
23	c	501	CLA	O2A-CGA-O1A	-2.91	116.35	123.63
29	d	407	LHG	C11-C10-C9	-2.91	99.67	114.37
23	C	503	CLA	CHB-C1B-NB	2.91	128.41	124.05
23	b	609	CLA	O2A-CGA-O1A	-2.91	116.36	123.63
25	C	515	BCR	C2-C1-C6	2.91	114.66	110.44
28	c	518	DGD	O5E-C6E-C5E	-2.91	101.44	111.33
25	Z	101	BCR	C7-C8-C9	-2.90	121.94	126.23
27	b	601	SQD	O2-C2-C1	2.90	116.99	110.08
23	b	613	CLA	C1-C2-C3	-2.90	121.44	126.20
23	C	506	CLA	C4A-NA-C1A	2.90	108.00	106.68
23	B	609	CLA	C2C-C1C-NC	2.90	113.03	109.98
25	A	408	BCR	C27-C26-C25	2.90	126.62	122.70
23	b	617	CLA	CGD-CBD-CAD	-2.90	101.46	110.85
23	D	402	CLA	C16-C15-C13	-2.89	106.36	115.97
23	b	615	CLA	O1D-CGD-CBD	2.89	130.22	124.52
23	c	512	CLA	CHB-C4A-NA	2.89	128.57	124.40
23	b	613	CLA	C11-C12-C13	-2.89	106.36	115.97
23	b	614	CLA	C3B-C4B-NB	-2.89	107.95	110.53
29	e	101	LHG	O8-C23-C24	2.88	120.63	111.83
23	b	612	CLA	C3B-C4B-NB	-2.88	107.96	110.53
23	d	404	CLA	C1-C2-C3	-2.88	121.48	126.20
23	b	605	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
27	b	601	SQD	O47-C7-C8	2.87	117.70	111.48
23	c	510	CLA	O1D-CGD-CBD	2.87	130.18	124.52
23	B	605	CLA	C16-C15-C13	-2.87	106.43	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CHD-C1D-ND	-2.87	120.77	124.80
25	c	515	BCR	C29-C30-C25	2.87	114.60	110.44
23	C	506	CLA	C3B-C4B-NB	-2.86	107.97	110.53
23	c	505	CLA	C6-C7-C8	-2.86	106.45	115.97
23	b	615	CLA	CHD-C1D-C2D	2.85	131.42	125.49
23	b	614	CLA	CMB-C2B-C1B	-2.85	121.07	125.42
23	b	616	CLA	CMB-C2B-C1B	-2.85	121.07	125.42
28	H	102	DGD	C8B-C7B-C6B	-2.85	99.95	114.37
28	H	102	DGD	O3D-C3D-C4D	-2.85	103.66	110.38
23	b	612	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
25	b	619	BCR	C27-C26-C25	2.84	126.55	122.70
23	D	402	CLA	C4A-NA-C1A	2.84	107.98	106.68
27	b	601	SQD	C1-O5-C5	2.84	119.27	113.72
23	B	614	CLA	CHB-C1B-NB	2.84	128.31	124.05
23	B	602	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
25	C	520	BCR	C37-C22-C21	-2.84	118.22	122.82
25	a	409	BCR	C33-C5-C6	-2.83	121.39	124.48
23	C	513	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
25	a	409	BCR	C29-C30-C25	2.83	114.55	110.44
26	A	409	PL9	O1-C4-C3	-2.83	117.75	120.73
27	B	621	SQD	O47-C7-O49	-2.83	117.09	123.70
23	B	605	CLA	C3B-C4B-NB	-2.83	108.00	110.53
29	D	408	LHG	O8-C23-O10	-2.83	116.56	123.63
23	b	612	CLA	C4A-NA-C1A	2.83	107.97	106.68
23	B	606	CLA	CHA-C1A-NA	-2.82	120.00	126.39
27	a	411	SQD	C1-O5-C5	-2.82	108.22	113.72
23	C	504	CLA	O1D-CGD-CBD	2.81	130.07	124.52
23	b	613	CLA	C6-C5-C3	-2.81	106.62	113.47
26	d	406	PL9	C8-C7-C3	2.81	119.29	112.03
34	e	102	HEM	CBA-CAA-C2A	-2.81	104.77	112.53
23	D	402	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
23	C	507	CLA	CHB-C4A-NA	2.80	128.44	124.40
23	c	501	CLA	C2C-C1C-NC	2.80	112.92	109.98
26	D	406	PL9	C20-C19-C21	2.80	120.08	115.23
27	f	101	SQD	O5-C5-C4	2.79	114.73	109.70
23	c	507	CLA	CHC-C4B-NB	2.79	128.24	124.05
23	c	508	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
27	A	411	SQD	O48-C46-C45	2.79	116.29	108.35
26	d	406	PL9	C7-C3-C2	-2.78	120.11	123.39
28	c	516	DGD	CDB-CCB-CBB	-2.78	100.30	114.37
27	B	621	SQD	C45-O47-C7	2.78	124.46	117.80
33	M	101	LMG	O3-C3-C2	-2.78	103.82	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e	101	LHG	O8-C23-O10	-2.78	116.67	123.63
23	C	503	CLA	C3B-C4B-NB	-2.78	108.05	110.53
25	A	408	BCR	C40-C30-C25	2.78	114.60	110.24
26	a	410	PL9	C37-C38-C39	-2.78	121.26	127.62
23	B	615	CLA	C6-C5-C3	-2.78	106.70	113.47
23	b	615	CLA	C4D-CHA-C1A	2.78	124.56	121.24
24	a	407	PHO	C1-C2-C3	-2.77	121.65	126.20
25	k	101	BCR	C30-C25-C26	-2.77	118.85	122.64
23	b	606	CLA	C11-C12-C13	-2.77	106.76	115.97
27	f	101	SQD	O9-S-O7	-2.77	104.82	113.82
31	a	404	BCT	O3-C-O1	-2.77	112.60	119.68
23	b	602	CLA	CHB-C4A-NA	2.76	128.39	124.40
33	C	501	LMG	C1-O6-C5	-2.76	108.32	113.72
23	C	505	CLA	CHA-C1A-NA	-2.76	120.13	126.39
28	c	516	DGD	O3E-C3E-C2E	-2.76	103.86	110.38
23	d	403	CLA	CHC-C4B-NB	2.76	128.19	124.05
23	B	613	CLA	CED-O2D-CGD	2.76	122.18	115.92
25	Z	101	BCR	C35-C13-C14	-2.76	118.34	122.82
23	d	404	CLA	CBC-CAC-C3C	-2.76	104.94	112.42
23	c	507	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
23	B	602	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	C	515	BCR	C15-C16-C17	-2.76	117.88	123.52
28	C	518	DGD	CDB-CCB-CBB	-2.75	100.45	114.37
25	b	620	BCR	C37-C22-C21	-2.75	118.36	122.82
25	c	514	BCR	C15-C14-C13	-2.75	123.42	127.28
23	d	404	CLA	CHB-C4A-NA	2.75	128.37	124.40
23	b	607	CLA	O2D-CGD-CBD	2.75	116.04	111.23
27	A	410	SQD	O5-C1-C2	-2.75	104.72	110.37
27	a	411	SQD	O48-C23-C24	2.74	120.20	111.83
27	B	621	SQD	O7-S-C6	2.74	110.85	106.76
23	c	513	CLA	O1D-CGD-CBD	2.74	129.92	124.52
25	B	618	BCR	C2-C1-C6	2.74	114.41	110.44
23	a	406	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
23	b	614	CLA	CHB-C4A-NA	2.73	128.35	124.40
23	b	603	CLA	CHD-C1D-ND	-2.73	120.96	124.80
23	c	506	CLA	C1D-ND-C4D	2.73	108.23	106.31
23	c	506	CLA	CGD-CBD-CAD	-2.73	102.01	110.85
25	c	514	BCR	C39-C30-C25	2.73	114.52	110.24
29	e	101	LHG	C5-O7-C7	-2.73	111.27	117.80
23	b	606	CLA	CHD-C1D-C2D	2.72	131.15	125.49
23	C	502	CLA	C2B-C1B-NB	-2.72	107.50	110.33
26	d	406	PL9	C37-C38-C39	-2.72	121.40	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	x	102	BCR	C34-C9-C8	-2.72	113.93	118.09
23	C	511	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
23	C	508	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
23	C	512	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
23	A	407	CLA	O1D-CGD-CBD	2.71	129.87	124.52
23	A	407	CLA	CHD-C1D-ND	-2.71	120.99	124.80
25	x	102	BCR	C30-C25-C26	-2.71	118.94	122.64
23	D	404	CLA	CHB-C4A-NA	2.70	128.30	124.40
28	C	516	DGD	C3D-C4D-C5D	-2.70	105.34	110.23
23	c	508	CLA	CHD-C4C-NC	2.70	128.41	124.23
23	B	603	CLA	O1D-CGD-CBD	2.70	129.84	124.52
23	C	514	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
23	C	505	CLA	O2A-CGA-O1A	-2.70	116.89	123.63
23	B	613	CLA	CAC-C3C-C4C	2.69	128.29	124.79
25	Z	101	BCR	C15-C14-C13	-2.69	123.50	127.28
28	H	102	DGD	C1D-C2D-C3D	-2.69	104.36	110.01
23	D	403	CLA	C1-C2-C3	-2.69	121.79	126.20
23	b	612	CLA	C11-C10-C8	-2.68	107.05	115.97
25	H	101	BCR	C16-C15-C14	-2.68	118.03	123.52
23	B	605	CLA	CHD-C4C-NC	2.68	128.39	124.23
25	c	514	BCR	C15-C16-C17	-2.68	118.04	123.52
23	B	610	CLA	CHD-C1D-ND	-2.68	121.03	124.80
23	B	612	CLA	CED-O2D-CGD	-2.68	109.84	115.92
28	c	518	DGD	O3G-C1D-C2D	-2.67	104.21	108.27
26	a	410	PL9	C27-C28-C29	-2.67	121.50	127.62
25	x	102	BCR	C2-C1-C6	2.67	114.32	110.44
25	B	619	BCR	C33-C5-C6	-2.67	121.57	124.48
23	B	605	CLA	O1D-CGD-CBD	2.67	129.79	124.52
23	B	610	CLA	C1D-ND-C4D	-2.67	104.44	106.31
27	f	101	SQD	O48-C23-O10	-2.67	116.95	123.63
27	f	101	SQD	C1-O5-C5	-2.67	108.51	113.72
25	B	619	BCR	C27-C26-C25	2.67	126.31	122.70
23	b	615	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
28	a	413	DGD	O2G-C1B-C2B	2.66	117.24	111.48
35	V	201	HEC	CHD-C4C-NC	2.66	127.35	124.45
23	C	507	CLA	C2A-C3A-C4A	2.66	106.17	101.87
28	c	516	DGD	O2D-C2D-C1D	-2.66	103.74	110.08
27	f	101	SQD	O5-C1-C2	-2.66	104.91	110.37
23	d	402	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
23	b	612	CLA	CGD-CBD-CAD	-2.66	102.25	110.85
33	M	101	LMG	C40-C39-C38	-2.65	100.95	114.37
25	c	514	BCR	C2-C1-C6	2.65	114.29	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	405	BCR	C8-C7-C6	-2.65	119.91	127.00
33	c	522	LMG	C9-C8-C7	-2.65	105.60	111.78
23	b	612	CLA	CMD-C2D-C1D	2.65	129.39	124.73
25	B	619	BCR	C30-C25-C26	-2.65	119.02	122.64
23	B	609	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
23	b	602	CLA	CBA-CAA-C2A	2.65	121.67	113.79
33	C	501	LMG	O8-C28-O10	-2.65	117.00	123.63
23	a	405	CLA	C3B-C4B-NB	-2.65	108.17	110.53
23	B	604	CLA	CGD-CBD-CAD	-2.65	102.28	110.85
33	D	411	LMG	O8-C28-O10	-2.64	116.53	123.33
28	h	101	DGD	C3D-C4D-C5D	-2.64	105.44	110.23
26	D	406	PL9	C22-C23-C24	-2.64	121.58	127.62
23	B	604	CLA	CHD-C1D-ND	-2.64	121.09	124.80
23	C	503	CLA	CHA-C1A-NA	-2.64	120.42	126.39
23	B	606	CLA	CGD-CBD-CAD	-2.64	102.31	110.85
27	B	621	SQD	C1-C2-C3	-2.64	104.47	110.01
25	a	409	BCR	C2-C1-C6	2.64	114.27	110.44
23	C	509	CLA	CHB-C4A-NA	2.63	128.20	124.40
25	Z	101	BCR	C27-C26-C25	2.63	126.26	122.70
25	b	618	BCR	C29-C30-C25	2.63	114.26	110.44
23	b	605	CLA	C11-C10-C8	-2.63	107.22	115.97
23	c	501	CLA	CHC-C4B-NB	2.63	128.00	124.05
28	a	413	DGD	O1G-C1A-O1A	-2.63	117.05	123.63
25	d	405	BCR	C27-C26-C25	2.63	126.26	122.70
29	d	409	LHG	O8-C6-C5	-2.63	100.82	108.40
23	A	405	CLA	C4A-NA-C1A	2.62	107.88	106.68
23	c	505	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
23	b	611	CLA	CHB-C4A-NA	2.62	128.19	124.40
23	b	607	CLA	CHD-C1D-ND	-2.62	121.12	124.80
26	D	406	PL9	C36-C34-C33	-2.62	115.29	121.17
25	b	620	BCR	C27-C26-C25	2.62	126.24	122.70
24	D	401	PHO	C1-C2-C3	-2.62	121.91	126.20
25	t	101	BCR	C1-C6-C5	-2.62	119.06	122.64
25	A	408	BCR	C33-C5-C6	-2.61	121.63	124.48
25	T	101	BCR	C4-C5-C6	2.61	126.23	122.70
23	C	514	CLA	C3A-C2A-C1A	2.61	105.25	101.34
23	a	405	CLA	C4D-CHA-C1A	2.61	124.36	121.24
23	B	602	CLA	C2D-C1D-ND	-2.61	107.54	110.13
23	c	504	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
23	c	503	CLA	CAC-C3C-C4C	2.61	128.18	124.79
23	B	613	CLA	CHA-C1A-NA	-2.61	120.49	126.39
23	A	404	CLA	C7-C6-C5	-2.61	106.32	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	409	LHG	O8-C23-C24	2.61	119.78	111.83
28	a	413	DGD	C5B-C4B-C3B	-2.60	101.21	114.37
25	T	101	BCR	C15-C16-C17	-2.60	118.20	123.52
23	c	505	CLA	CED-O2D-CGD	-2.60	110.02	115.92
25	C	520	BCR	C35-C13-C12	2.60	122.06	118.09
26	a	410	PL9	C35-C34-C36	2.59	119.73	115.23
23	b	617	CLA	C3B-C4B-NB	-2.59	108.22	110.53
23	b	606	CLA	C16-C15-C13	-2.59	107.35	115.97
24	a	407	PHO	CBC-CAC-C3C	-2.59	109.17	112.87
23	b	605	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
25	b	619	BCR	C39-C30-C25	-2.59	106.19	110.24
29	D	408	LHG	C20-C19-C18	-2.58	101.31	114.37
24	A	406	PHO	OBD-CAD-CBD	-2.58	122.03	125.82
27	B	621	SQD	C3-C4-C5	2.58	114.92	110.23
23	C	506	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
28	c	517	DGD	C8B-C7B-C6B	-2.58	101.31	114.37
33	C	501	LMG	O3-C3-C2	-2.58	104.29	110.38
26	a	410	PL9	O2-C1-C6	2.58	124.58	120.48
23	B	605	CLA	C4A-NA-C1A	2.58	107.86	106.68
23	B	604	CLA	O2A-CGA-CBA	2.57	119.68	111.83
25	T	101	BCR	C38-C26-C27	-2.57	108.12	113.60
27	b	601	SQD	O48-C23-C24	2.57	119.67	111.83
28	c	518	DGD	O6D-C1D-O3G	-2.57	103.98	110.04
23	a	406	CLA	CAC-C3C-C4C	2.57	128.13	124.79
23	B	603	CLA	O2A-CGA-O1A	-2.56	117.21	123.63
23	b	603	CLA	CHD-C1D-C2D	2.56	130.82	125.49
23	b	606	CLA	CHC-C1C-NC	2.56	128.17	124.31
33	c	522	LMG	O7-C10-O9	-2.56	117.72	123.70
23	c	510	CLA	C7-C6-C5	-2.56	106.45	113.26
23	c	502	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
23	B	605	CLA	CHD-C4C-C3C	-2.55	121.05	124.77
23	B	610	CLA	O2D-CGD-CBD	2.55	115.69	111.23
24	A	406	PHO	CED-O2D-CGD	2.55	121.71	115.92
23	b	615	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
27	f	101	SQD	O47-C7-C8	2.55	120.29	110.93
23	B	610	CLA	O2A-CGA-O1A	-2.54	117.26	123.63
23	c	510	CLA	CMB-C2B-C3B	2.54	132.53	126.55
25	B	619	BCR	C29-C30-C25	2.54	114.13	110.44
33	b	622	LMG	C1-O6-C5	-2.54	108.76	113.72
35	V	201	HEC	C2A-C1A-NA	-2.54	107.87	110.32
28	C	517	DGD	C6D-O5D-C1E	2.54	119.24	113.80
23	C	510	CLA	C3B-C4B-NB	-2.54	108.26	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	CHB-C4A-NA	2.54	128.06	124.40
28	C	517	DGD	O6E-C5E-C4E	2.54	114.27	109.70
23	c	508	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
27	b	601	SQD	C3-C4-C5	2.53	114.83	110.23
23	A	405	CLA	CED-O2D-CGD	-2.53	110.17	115.92
23	B	607	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
23	B	609	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
23	C	511	CLA	C16-C15-C13	-2.53	107.55	115.97
24	d	401	PHO	CBA-CAA-C2A	-2.53	106.33	113.78
28	C	518	DGD	O3G-C1D-C2D	-2.53	104.43	108.27
23	C	507	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
25	T	101	BCR	C37-C22-C23	2.53	121.95	118.09
23	C	503	CLA	CHD-C1D-ND	-2.53	121.25	124.80
23	c	502	CLA	CHD-C1D-ND	-2.53	121.25	124.80
23	b	617	CLA	CHC-C4B-NB	2.52	127.84	124.05
23	b	610	CLA	CHA-C1A-NA	-2.52	120.68	126.39
26	d	406	PL9	C50-C49-C48	-2.52	115.08	122.66
23	C	508	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
23	c	505	CLA	C11-C10-C8	-2.52	107.58	115.97
25	C	515	BCR	C40-C30-C25	2.52	114.20	110.24
23	c	501	CLA	C3B-C4B-NB	-2.52	108.28	110.53
23	c	513	CLA	CHB-C4A-NA	2.52	128.04	124.40
28	H	102	DGD	C3E-C4E-C5E	-2.52	105.66	110.23
23	A	407	CLA	CMB-C2B-C3B	2.52	132.47	126.55
23	b	610	CLA	CHB-C4A-NA	2.52	128.03	124.40
23	b	603	CLA	C4A-NA-C1A	2.52	107.83	106.68
23	C	514	CLA	C3B-C4B-NB	-2.52	108.28	110.53
23	B	613	CLA	C2A-C1A-CHA	2.52	128.24	123.87
29	d	408	LHG	C20-C19-C18	-2.52	101.65	114.37
23	b	608	CLA	C1-C2-C3	-2.51	122.08	126.20
23	B	605	CLA	CHB-C1B-NB	2.51	127.82	124.05
23	A	404	CLA	CHD-C1D-ND	-2.51	121.26	124.80
28	c	516	DGD	O3D-C3D-C4D	-2.51	104.45	110.38
23	C	509	CLA	CED-O2D-CGD	-2.51	110.21	115.92
23	A	405	CLA	CHB-C4A-NA	2.51	128.03	124.40
29	d	409	LHG	C25-C24-C23	2.51	122.90	113.69
34	e	102	HEM	CHA-C4D-ND	2.51	127.47	124.37
28	A	412	DGD	CDB-CCB-CBB	-2.51	101.67	114.37
25	c	521	BCR	C33-C5-C6	-2.51	121.75	124.48
25	Z	101	BCR	C33-C5-C6	-2.51	121.75	124.48
23	b	605	CLA	C4D-C3D-CAD	-2.50	105.39	108.11
23	b	606	CLA	CMB-C2B-C1B	-2.50	121.61	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	M	101	LMG	C3-C4-C5	-2.50	105.70	110.23
23	C	509	CLA	CHB-C1B-NB	2.50	127.80	124.05
23	c	503	CLA	C2D-C1D-ND	-2.50	107.65	110.13
23	b	602	CLA	O2A-C1-C2	2.50	117.72	108.11
25	d	405	BCR	C38-C26-C25	-2.50	121.76	124.48
23	b	606	CLA	C3B-C4B-NB	-2.50	108.30	110.53
25	H	101	BCR	C33-C5-C6	-2.50	121.76	124.48
23	b	614	CLA	CHB-C1B-NB	2.49	127.79	124.05
25	c	515	BCR	C35-C13-C14	-2.49	118.78	122.82
25	B	618	BCR	C3-C4-C5	-2.49	109.61	114.06
28	C	518	DGD	O3E-C3E-C2E	-2.49	104.51	110.38
28	C	516	DGD	C1E-O6E-C5E	2.49	118.58	113.72
28	h	101	DGD	C6D-O5D-C1E	2.49	119.13	113.80
23	C	509	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
23	A	407	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
28	c	518	DGD	CAB-C9B-C8B	-2.49	101.80	114.37
23	d	402	CLA	CHC-C4B-NB	2.48	127.78	124.05
28	c	517	DGD	O2E-C2E-C1E	-2.48	104.16	110.08
23	B	609	CLA	CHA-C1A-NA	-2.48	120.77	126.39
33	c	524	LMG	O8-C28-O10	-2.48	117.42	123.63
23	B	611	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
25	k	101	BCR	C2-C1-C6	2.48	114.04	110.44
27	b	601	SQD	C45-O47-C7	2.48	123.73	117.80
23	b	610	CLA	O2D-CGD-CBD	-2.48	106.89	111.23
23	B	601	CLA	CAA-C2A-C3A	-2.48	106.31	113.00
27	a	412	SQD	O49-C7-C8	-2.48	114.10	123.78
23	b	608	CLA	C2D-C1D-ND	-2.47	107.68	110.13
23	B	605	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
23	b	610	CLA	CHD-C1D-ND	-2.47	121.33	124.80
25	x	102	BCR	C35-C13-C14	-2.47	118.82	122.82
28	H	102	DGD	C3G-C2G-C1G	-2.46	106.04	111.78
23	b	605	CLA	CGD-CBD-CAD	-2.46	102.87	110.85
23	a	405	CLA	CAC-C3C-C4C	2.46	128.00	124.79
27	F	101	SQD	C3-C4-C5	2.46	114.70	110.23
23	a	408	CLA	CHD-C4C-NC	2.46	128.05	124.23
23	B	613	CLA	C2C-C1C-NC	2.46	112.56	109.98
24	D	401	PHO	CMB-C2B-C3B	2.46	129.60	124.68
25	b	620	BCR	C2-C1-C6	2.46	114.01	110.44
23	C	504	CLA	CMC-C2C-C1C	-2.46	121.20	125.03
23	C	508	CLA	C3B-C4B-NB	-2.45	108.34	110.53
23	b	615	CLA	CHD-C4C-NC	2.45	128.03	124.23
23	C	507	CLA	CHC-C4B-NB	2.45	127.73	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	CLA	CMB-C2B-C3B	2.45	132.31	126.55
27	B	621	SQD	O10-C23-C24	-2.45	114.20	123.78
23	C	507	CLA	CHA-C1A-NA	-2.45	120.85	126.39
23	b	609	CLA	CHA-C1A-NA	-2.45	120.85	126.39
28	h	101	DGD	C3E-C4E-C5E	-2.45	105.80	110.23
26	a	410	PL9	O2-C1-C2	-2.45	116.27	121.83
25	D	405	BCR	C1-C6-C5	-2.44	119.30	122.64
23	b	609	CLA	CHB-C1B-NB	2.44	127.71	124.05
34	E	103	HEM	CBD-CAD-C3D	-2.44	105.79	112.53
25	K	101	BCR	C27-C26-C25	2.44	126.00	122.70
28	C	516	DGD	O3G-C3G-C2G	-2.44	104.89	110.82
27	f	101	SQD	C1-C2-C3	-2.44	104.88	110.01
25	t	101	BCR	C2-C1-C6	2.44	113.98	110.44
33	C	501	LMG	O5-C6-C5	-2.44	103.04	111.33
23	c	502	CLA	O1D-CGD-CBD	2.44	129.32	124.52
23	b	611	CLA	C3B-C4B-NB	-2.44	108.36	110.53
28	c	516	DGD	O2G-C1B-C2B	-2.44	106.21	111.48
23	B	604	CLA	O2A-C1-C2	2.43	117.48	108.11
23	b	614	CLA	CHA-C1A-NA	-2.43	120.88	126.39
26	d	406	PL9	C42-C43-C44	-2.43	122.05	127.62
23	b	617	CLA	C2A-C3A-C4A	2.43	105.80	101.87
28	c	516	DGD	C3D-C4D-C5D	-2.43	105.82	110.23
28	h	101	DGD	O6D-C1D-O3G	-2.43	104.31	110.04
23	B	606	CLA	CHB-C4A-NA	2.43	127.90	124.40
23	B	614	CLA	O2D-CGD-CBD	2.43	115.47	111.23
23	a	408	CLA	CHD-C1D-ND	-2.43	121.39	124.80
25	A	408	BCR	C31-C1-C6	-2.43	106.44	110.24
25	t	101	BCR	C35-C13-C14	-2.42	118.89	122.82
28	H	102	DGD	O6D-C1D-O3G	-2.42	104.32	110.04
26	a	410	PL9	C40-C39-C38	-2.42	117.41	123.63
24	d	401	PHO	C4B-NB-C1B	2.42	112.35	108.82
23	b	606	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
28	h	101	DGD	C1D-C2D-C3D	-2.42	104.92	110.01
25	b	620	BCR	C16-C15-C14	-2.42	118.58	123.52
23	c	504	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
25	t	101	BCR	C36-C18-C19	2.41	121.78	118.09
23	b	613	CLA	C3D-C4D-ND	2.41	113.91	109.99
34	E	103	HEM	CHC-C4B-NB	2.41	127.02	124.42
23	c	502	CLA	C1-O2A-CGA	2.41	122.49	116.65
23	B	601	CLA	O1D-CGD-CBD	2.41	129.27	124.52
23	A	405	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
25	a	409	BCR	C35-C13-C14	-2.41	118.91	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	C6-C5-C3	2.41	119.34	113.47
23	c	513	CLA	CAC-C3C-C4C	2.41	127.92	124.79
23	b	609	CLA	C6-C7-C8	-2.41	107.96	115.97
33	M	101	LMG	C38-C37-C36	-2.41	102.19	114.37
25	d	405	BCR	C30-C25-C26	-2.41	119.35	122.64
28	C	516	DGD	O6D-C1D-O3G	-2.41	104.36	110.04
23	B	605	CLA	C3D-C4D-ND	2.40	113.89	109.99
23	C	509	CLA	CHA-C1A-NA	-2.40	120.95	126.39
33	c	522	LMG	O3-C3-C2	-2.40	104.72	110.38
23	B	615	CLA	CHB-C1B-NB	2.40	127.65	124.05
28	C	517	DGD	CDB-CCB-CBB	-2.40	102.25	114.37
23	b	615	CLA	C6-C5-C3	-2.40	107.63	113.47
25	t	101	BCR	C15-C14-C13	-2.40	123.92	127.28
23	c	507	CLA	CHD-C1D-ND	-2.40	121.43	124.80
25	K	101	BCR	C8-C7-C6	-2.40	120.60	127.00
23	B	606	CLA	CHB-C1B-NB	2.39	127.64	124.05
28	c	517	DGD	CDB-CCB-CBB	-2.39	102.27	114.37
24	a	407	PHO	C3B-C4B-NB	-2.39	105.90	107.46
23	C	504	CLA	C6-C7-C8	-2.39	108.01	115.97
23	B	609	CLA	CHD-C1D-ND	-2.39	121.44	124.80
23	B	615	CLA	CHA-C1A-NA	-2.39	120.98	126.39
23	C	513	CLA	C16-C15-C13	-2.39	108.02	115.97
23	a	406	CLA	CHD-C1D-ND	-2.39	121.44	124.80
23	A	407	CLA	CHC-C1C-C2C	-2.39	120.16	126.95
26	A	409	PL9	C22-C23-C24	-2.39	122.16	127.62
23	B	607	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
25	B	618	BCR	C30-C25-C26	-2.39	119.37	122.64
23	B	602	CLA	CHA-C1A-NA	-2.39	120.99	126.39
23	B	614	CLA	CMB-C2B-C3B	2.39	132.16	126.55
33	m	101	LMG	C40-C39-C38	-2.39	102.31	114.37
23	b	603	CLA	CGD-CBD-CAD	-2.38	103.13	110.85
33	b	622	LMG	O7-C10-O9	-2.38	118.13	123.70
27	A	410	SQD	O48-C23-C24	2.38	119.10	111.83
23	C	505	CLA	C6-C5-C3	2.38	119.28	113.47
23	B	605	CLA	C1-O2A-CGA	-2.38	110.88	116.65
23	C	506	CLA	CMD-C2D-C1D	-2.38	120.53	124.73
23	D	403	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
27	b	601	SQD	O48-C23-O10	-2.38	117.67	123.63
23	B	609	CLA	CHB-C1B-NB	2.38	127.62	124.05
27	f	101	SQD	O48-C23-C24	2.38	119.08	111.83
23	b	606	CLA	O1A-CGA-CBA	2.38	133.08	123.78
23	C	505	CLA	CMB-C2B-C1B	-2.38	121.80	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	C3B-C4B-NB	-2.37	108.41	110.53
23	c	510	CLA	C16-C15-C13	-2.37	108.08	115.97
23	B	606	CLA	C7-C6-C5	-2.37	106.94	113.26
25	b	620	BCR	C11-C10-C9	-2.37	123.95	127.28
28	c	517	DGD	C3G-O3G-C1D	2.37	118.88	113.80
23	c	503	CLA	CMD-C2D-C1D	2.37	128.90	124.73
23	C	510	CLA	CHD-C1D-ND	-2.37	121.47	124.80
23	B	609	CLA	CHC-C1C-C2C	-2.37	120.22	126.95
25	d	405	BCR	C29-C30-C25	2.37	113.88	110.44
23	b	602	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
28	c	518	DGD	O1G-C1A-C2A	-2.37	104.61	111.83
23	b	611	CLA	C11-C10-C8	-2.37	108.10	115.97
23	c	502	CLA	CMB-C2B-C3B	2.37	132.11	126.55
23	B	615	CLA	C2B-C1B-NB	-2.36	107.87	110.33
25	b	619	BCR	C3-C4-C5	-2.36	109.84	114.06
23	B	606	CLA	C1-C2-C3	-2.36	122.33	126.20
33	c	519	LMG	O7-C10-O9	-2.36	118.44	122.99
23	C	513	CLA	C2D-C1D-ND	-2.36	107.79	110.13
23	C	507	CLA	O1D-CGD-CBD	2.36	129.16	124.52
25	Z	101	BCR	C24-C23-C22	-2.36	122.75	126.23
23	b	614	CLA	CGD-CBD-CAD	-2.35	103.22	110.85
23	D	403	CLA	O2D-CGD-CBD	2.35	115.34	111.23
23	B	606	CLA	C3B-C4B-NB	-2.35	108.43	110.53
23	a	408	CLA	CHD-C4C-C3C	-2.35	121.35	124.77
33	M	101	LMG	O6-C1-O1	-2.35	104.49	110.04
23	C	504	CLA	CMC-C2C-C3C	2.35	132.50	126.15
28	h	101	DGD	CDB-CCB-CBB	-2.35	102.50	114.37
23	C	512	CLA	CHB-C4A-NA	2.35	127.79	124.40
23	b	616	CLA	CAA-CBA-CGA	-2.35	106.54	113.21
26	D	406	PL9	C30-C29-C31	-2.35	111.15	115.23
23	C	512	CLA	CAC-C3C-C4C	2.35	127.84	124.79
35	V	201	HEC	C4A-C3A-C2A	2.35	110.46	106.97
23	b	616	CLA	CHA-C4D-ND	2.34	137.39	132.55
29	A	413	LHG	C18-C17-C16	-2.34	102.52	114.37
25	b	620	BCR	C30-C25-C26	-2.34	119.44	122.64
28	C	516	DGD	O1G-C1A-C2A	-2.34	104.70	111.83
26	A	409	PL9	C36-C34-C33	-2.34	115.91	121.17
28	c	517	DGD	O3G-C3G-C2G	-2.34	105.12	110.82
23	C	513	CLA	CAA-CBA-CGA	-2.34	106.57	113.21
23	a	405	CLA	C4-C3-C5	2.34	119.29	115.23
23	c	507	CLA	CHD-C4C-NC	2.34	127.86	124.23
28	c	516	DGD	CBB-CAB-C9B	-2.34	102.56	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	M	101	LMG	C8-O7-C10	2.34	123.39	117.80
24	A	406	PHO	CMB-C2B-C3B	2.34	129.35	124.68
25	a	409	BCR	C27-C26-C25	2.33	125.86	122.70
23	C	502	CLA	CAC-C3C-C4C	2.33	127.83	124.79
26	a	410	PL9	C12-C13-C14	-2.33	122.28	127.62
23	c	501	CLA	CHA-C4D-ND	2.33	137.36	132.55
26	d	406	PL9	C40-C39-C38	-2.32	117.66	123.63
23	B	615	CLA	C4-C3-C2	2.32	129.60	123.63
23	b	603	CLA	CHC-C1C-C2C	-2.32	120.34	126.95
25	B	619	BCR	C1-C6-C5	-2.32	119.46	122.64
23	c	504	CLA	C3B-C4B-NB	-2.32	108.46	110.53
23	b	604	CLA	CHD-C1D-C2D	2.32	130.32	125.49
23	c	508	CLA	CHD-C1D-C2D	2.32	130.32	125.49
33	c	524	LMG	O7-C10-O9	-2.32	118.28	123.70
23	D	404	CLA	CMB-C2B-C1B	2.32	128.95	125.42
23	a	405	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	B	619	BCR	C40-C30-C25	2.32	113.88	110.24
23	b	607	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	d	401	PHO	C1-C2-C3	-2.32	122.40	126.20
23	b	612	CLA	CHB-C4A-NA	2.32	127.74	124.40
23	B	615	CLA	C6-C7-C8	-2.31	108.28	115.97
23	b	613	CLA	C11-C10-C8	-2.31	108.28	115.97
23	b	608	CLA	C2C-C1C-NC	2.31	112.41	109.98
28	h	101	DGD	O3E-C3E-C2E	-2.31	104.93	110.38
23	A	405	CLA	CMB-C2B-C3B	2.31	131.99	126.55
33	D	410	LMG	O1-C7-C8	-2.31	105.83	111.77
23	B	616	CLA	O2D-CGD-CBD	2.31	115.27	111.23
23	b	604	CLA	C2D-C1D-ND	-2.31	107.84	110.13
28	h	101	DGD	CBB-CAB-C9B	-2.30	102.72	114.37
23	c	510	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
23	a	405	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
27	A	410	SQD	C1-O5-C5	-2.30	109.22	113.72
23	B	603	CLA	O1A-CGA-CBA	2.30	132.78	123.78
23	D	404	CLA	C6-C7-C8	-2.30	108.32	115.97
23	C	511	CLA	C3A-C2A-C1A	2.30	104.78	101.34
24	A	406	PHO	O2A-CGA-O1A	-2.30	117.88	123.63
24	A	406	PHO	C4B-NB-C1B	2.30	112.17	108.82
28	C	518	DGD	O3D-C3D-C4D	-2.30	104.96	110.38
23	d	402	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	B	617	BCR	C16-C15-C14	-2.29	118.83	123.52
28	c	516	DGD	O4D-C4D-C3D	2.29	115.78	110.38
23	B	614	CLA	CHC-C4B-NB	2.29	127.49	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CGD-CBD-CAD	-2.29	103.43	110.85
25	C	520	BCR	C38-C26-C25	-2.29	121.98	124.48
23	C	514	CLA	C2D-C1D-ND	-2.29	107.86	110.13
23	c	503	CLA	O1D-CGD-CBD	2.29	129.03	124.52
23	c	506	CLA	C4-C3-C2	-2.29	117.75	123.63
26	d	406	PL9	C32-C33-C34	-2.29	122.39	127.62
23	b	612	CLA	C1C-C2C-C3C	-2.29	104.57	106.98
23	C	511	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
25	a	409	BCR	C16-C15-C14	-2.29	118.84	123.52
23	b	607	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
23	a	405	CLA	CAA-C2A-C1A	-2.29	104.48	111.97
23	c	504	CLA	CMC-C2C-C1C	2.29	128.60	125.03
33	c	519	LMG	C9-C8-C7	-2.28	106.46	111.78
23	B	605	CLA	C3A-C2A-C1A	2.28	104.76	101.34
24	D	401	PHO	CBC-CAC-C3C	2.28	116.14	112.87
23	b	607	CLA	CHC-C1C-NC	2.28	127.75	124.31
23	a	408	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
25	B	617	BCR	C16-C17-C18	-2.28	124.08	127.28
23	c	507	CLA	C3A-C2A-C1A	2.28	104.75	101.34
33	d	410	LMG	O7-C10-O9	-2.28	117.47	123.33
26	D	406	PL9	C35-C34-C36	2.28	119.18	115.23
23	c	503	CLA	CHD-C1D-C2D	2.28	130.22	125.49
28	H	102	DGD	CDB-CCB-CBB	-2.28	102.86	114.37
23	b	613	CLA	CHD-C4C-C3C	-2.28	121.45	124.77
34	E	103	HEM	C1D-C2D-C3D	2.28	109.37	106.98
25	C	520	BCR	C2-C1-C6	2.27	113.74	110.44
23	C	513	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
33	C	501	LMG	O6-C1-O1	-2.27	104.67	110.04
25	d	405	BCR	C1-C6-C5	-2.27	119.53	122.64
24	d	401	PHO	C3D-C4D-ND	2.27	110.62	107.71
23	c	503	CLA	C1D-ND-C4D	2.27	107.91	106.31
28	h	101	DGD	C6D-C5D-C4D	2.27	116.83	112.07
23	b	616	CLA	CED-O2D-CGD	2.27	121.06	115.92
25	x	102	BCR	C35-C13-C12	2.27	121.55	118.09
23	b	605	CLA	O2D-CGD-CBD	2.27	115.19	111.23
25	A	408	BCR	C15-C16-C17	-2.27	118.88	123.52
25	C	515	BCR	C3-C4-C5	-2.27	110.02	114.06
33	d	411	LMG	C40-C39-C38	-2.27	102.92	114.37
33	C	501	LMG	O7-C10-O9	-2.27	118.41	123.70
26	a	410	PL9	O1-C4-C3	-2.26	118.34	120.73
25	D	405	BCR	C7-C8-C9	-2.26	122.89	126.23
23	C	504	CLA	CHB-C1B-NB	2.26	127.44	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	CHC-C4B-NB	2.26	127.44	124.05
33	d	411	LMG	O5-C6-C5	-2.26	103.63	111.33
23	b	613	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
23	c	507	CLA	O2D-CGD-CBD	2.26	115.18	111.23
25	Z	101	BCR	C34-C9-C8	-2.26	114.64	118.09
23	C	505	CLA	C2A-C1A-CHA	2.26	127.79	123.87
23	B	602	CLA	CHD-C1D-C2D	2.26	130.19	125.49
23	D	404	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
34	e	102	HEM	CHB-C1B-NB	2.26	127.16	124.37
23	B	610	CLA	O1D-CGD-CBD	2.25	128.96	124.52
23	b	606	CLA	CHC-C1C-C2C	-2.25	120.55	126.95
33	M	101	LMG	O8-C28-O10	-2.25	118.00	123.63
23	b	615	CLA	CMD-C2D-C1D	2.25	128.69	124.73
29	d	408	LHG	C18-C17-C16	-2.25	103.00	114.37
25	A	408	BCR	C8-C7-C6	-2.25	120.99	127.00
29	A	413	LHG	C20-C19-C18	-2.25	103.01	114.37
28	a	413	DGD	C1G-O1G-C1A	2.24	125.32	117.12
23	C	509	CLA	C7-C6-C5	-2.24	107.29	113.26
27	F	101	SQD	O48-C23-O10	-2.24	118.03	123.63
23	c	511	CLA	CHB-C1B-NB	2.24	127.41	124.05
23	B	601	CLA	CHC-C4B-NB	2.24	127.40	124.05
27	B	621	SQD	O5-C1-O6	2.24	115.33	110.04
25	t	101	BCR	C11-C10-C9	-2.24	124.14	127.28
25	c	521	BCR	C30-C25-C26	-2.23	119.58	122.64
23	b	611	CLA	CHA-C1A-NA	-2.23	121.33	126.39
23	B	609	CLA	CHD-C4C-NC	2.23	127.69	124.23
27	A	410	SQD	O48-C46-C45	2.23	114.83	108.40
23	B	606	CLA	CHD-C1D-ND	-2.23	121.67	124.80
23	b	610	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
23	C	505	CLA	C3B-C4B-NB	-2.23	108.54	110.53
23	B	604	CLA	CHB-C4A-NA	2.23	127.61	124.40
23	B	605	CLA	O1A-CGA-CBA	2.23	132.49	123.78
23	C	508	CLA	CHA-C1A-NA	-2.22	121.35	126.39
25	H	101	BCR	C35-C13-C14	-2.22	119.21	122.82
25	T	101	BCR	C1-C6-C5	-2.22	119.60	122.64
28	A	412	DGD	C4E-C3E-C2E	-2.22	106.93	110.83
23	d	404	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
25	t	101	BCR	C31-C1-C6	2.22	113.72	110.24
25	C	520	BCR	C15-C14-C13	-2.22	124.17	127.28
23	B	604	CLA	CMD-C2D-C1D	2.21	128.63	124.73
23	B	615	CLA	CHB-C4A-NA	2.21	127.59	124.40
23	B	609	CLA	C4B-CHC-C1C	-2.21	121.05	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	CHC-C1C-C2C	-2.21	120.67	126.95
29	E	101	LHG	O8-C23-O10	-2.21	118.10	123.63
23	B	612	CLA	C2A-C3A-C4A	2.21	105.44	101.87
23	C	508	CLA	CMB-C2B-C3B	2.21	131.75	126.55
27	a	411	SQD	O8-S-C6	2.21	110.24	105.97
23	B	612	CLA	CMC-C2C-C1C	-2.21	121.58	125.03
25	c	515	BCR	C4-C5-C6	2.21	125.69	122.70
23	C	509	CLA	C2A-C1A-CHA	2.21	127.70	123.87
23	b	607	CLA	CHA-C1A-NA	-2.21	121.39	126.39
28	H	102	DGD	C6D-C5D-C4D	2.21	116.70	112.07
23	a	405	CLA	O1D-CGD-CBD	2.21	128.87	124.52
23	c	512	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
23	A	407	CLA	C4A-NA-C1A	2.21	107.69	106.68
23	c	510	CLA	CHD-C1D-ND	-2.20	121.70	124.80
28	c	518	DGD	O6E-C1E-O5D	-2.20	104.84	110.04
24	a	407	PHO	O2A-CGA-O1A	-2.20	118.12	123.63
29	A	413	LHG	C5-O7-C7	-2.20	112.53	117.80
23	B	616	CLA	C1-C2-C3	2.20	129.81	126.20
34	e	102	HEM	CMA-C3A-C4A	2.20	128.77	125.42
33	D	407	LMG	O8-C28-O10	-2.20	118.12	123.63
23	B	608	CLA	CHD-C4C-NC	2.20	127.64	124.23
23	B	601	CLA	CHB-C4A-NA	2.20	127.57	124.40
25	d	405	BCR	C2-C1-C6	2.20	113.63	110.44
23	C	509	CLA	CHA-C4D-ND	2.20	137.08	132.55
23	b	612	CLA	C2D-C1D-ND	-2.19	107.96	110.13
23	C	507	CLA	C6-C7-C8	-2.19	108.68	115.97
23	B	609	CLA	O1D-CGD-CBD	2.19	128.84	124.52
25	c	515	BCR	C1-C6-C5	-2.19	119.64	122.64
28	C	517	DGD	O5E-C6E-C5E	-2.19	103.88	111.33
26	D	406	PL9	C42-C43-C44	-2.19	122.62	127.62
23	B	612	CLA	C11-C12-C13	-2.19	108.70	115.97
23	b	605	CLA	C7-C6-C5	-2.19	107.44	113.26
24	D	401	PHO	C3D-C4D-ND	2.18	110.50	107.71
27	A	410	SQD	C3-C4-C5	2.18	114.18	110.23
23	B	611	CLA	CHD-C4C-NC	2.18	127.61	124.23
28	c	517	DGD	O5D-C6D-C5D	-2.18	104.51	109.42
26	D	406	PL9	C31-C32-C33	-2.18	101.25	112.02
23	c	507	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
23	C	503	CLA	CHD-C4C-NC	2.18	127.61	124.23
23	b	611	CLA	O2A-C1-C2	2.18	116.48	108.11
23	b	612	CLA	CHA-C1A-NA	-2.18	121.46	126.39
23	b	602	CLA	CHD-C1D-ND	-2.18	121.74	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CHB-C4A-NA	2.17	127.54	124.40
23	C	502	CLA	CGD-CBD-CAD	-2.17	103.81	110.85
23	C	512	CLA	O2D-CGD-CBD	2.17	115.03	111.23
25	T	101	BCR	C37-C22-C21	-2.17	119.30	122.82
33	c	519	LMG	O8-C28-O10	-2.17	118.20	123.63
29	A	413	LHG	O4-P-O6	-2.17	97.73	107.57
28	a	413	DGD	C2G-O2G-C1B	2.17	122.99	117.80
25	d	405	BCR	C11-C10-C9	-2.17	124.23	127.28
27	f	101	SQD	O5-C1-O6	2.17	115.17	110.04
23	b	614	CLA	CMB-C2B-C3B	2.17	131.65	126.55
25	K	101	BCR	C24-C23-C22	-2.17	123.03	126.23
23	b	607	CLA	C4-C3-C5	2.17	118.99	115.23
23	C	504	CLA	O2A-C1-C2	-2.17	99.77	108.11
23	b	612	CLA	C3C-C4C-NC	-2.17	107.65	110.43
27	b	601	SQD	O8-S-O7	-2.17	105.98	111.40
23	c	501	CLA	C2A-C1A-CHA	2.16	127.62	123.87
24	A	406	PHO	C4D-CHA-CBD	-2.16	107.42	108.45
23	b	609	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
25	T	101	BCR	C33-C5-C6	-2.16	122.12	124.48
23	B	607	CLA	CMC-C2C-C1C	2.16	128.41	125.03
23	B	612	CLA	C1-C2-C3	-2.16	122.66	126.20
25	c	515	BCR	C15-C16-C17	-2.16	119.10	123.52
23	c	508	CLA	CHB-C4A-NA	2.16	127.51	124.40
23	c	509	CLA	C4D-CHA-C1A	2.16	123.82	121.24
23	C	502	CLA	C4-C3-C5	2.16	118.97	115.23
25	t	101	BCR	C27-C26-C25	2.15	125.62	122.70
27	B	621	SQD	O48-C23-C24	2.15	118.40	111.83
23	b	616	CLA	CHA-C1A-NA	-2.15	121.52	126.39
23	b	607	CLA	C2A-C1A-CHA	2.15	127.60	123.87
23	d	402	CLA	C1D-ND-C4D	2.15	107.82	106.31
23	C	514	CLA	C6-C7-C8	-2.15	108.81	115.97
25	D	405	BCR	C2-C1-C6	2.15	113.56	110.44
23	B	603	CLA	CHB-C1B-NB	2.15	127.27	124.05
25	C	515	BCR	C30-C25-C26	-2.15	119.70	122.64
28	c	516	DGD	C4B-C3B-C2B	-2.15	105.23	113.13
23	B	612	CLA	CHC-C1C-NC	2.15	127.55	124.31
23	B	609	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
24	d	401	PHO	CAA-C2A-C3A	-2.15	107.19	113.00
23	c	510	CLA	C9-C8-C10	2.15	118.93	111.27
23	b	607	CLA	CHD-C4C-C3C	-2.15	121.64	124.77
23	A	407	CLA	C3D-C4D-ND	2.15	113.48	109.99
23	b	603	CLA	CMD-C2D-C1D	2.15	128.51	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
23	a	405	CLA	CHD-C1D-ND	-2.14	121.78	124.80
25	t	101	BCR	C30-C25-C26	-2.14	119.70	122.64
23	b	610	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
25	C	520	BCR	C29-C30-C25	2.14	113.55	110.44
23	B	611	CLA	O1A-CGA-CBA	2.14	132.16	123.78
23	b	608	CLA	CHC-C4B-NB	2.14	127.26	124.05
23	b	609	CLA	C11-C10-C8	-2.14	108.85	115.97
23	d	404	CLA	CHB-C1B-NB	2.14	127.26	124.05
34	E	103	HEM	CHA-C1A-NA	2.13	127.73	123.86
23	B	609	CLA	OBD-CAD-C3D	2.13	133.40	128.42
25	t	101	BCR	C35-C13-C12	2.13	121.35	118.09
25	A	408	BCR	C2-C1-C6	2.13	113.53	110.44
33	C	501	LMG	C36-C35-C34	-2.13	103.60	114.37
25	t	101	BCR	C3-C4-C5	-2.13	110.26	114.06
33	M	101	LMG	O7-C10-O9	-2.13	118.72	123.70
25	x	102	BCR	C33-C5-C6	-2.13	122.16	124.48
27	F	101	SQD	C46-C45-C44	-2.13	106.79	113.67
23	D	404	CLA	C3D-C2D-C1D	2.13	108.74	105.83
25	T	101	BCR	C1-C6-C7	2.13	121.42	115.65
23	b	616	CLA	C2A-C1A-CHA	2.13	127.56	123.87
27	F	101	SQD	C1-C2-C3	-2.13	105.53	110.01
23	C	508	CLA	CHD-C4C-NC	2.13	127.53	124.23
25	b	619	BCR	C11-C10-C9	-2.12	124.30	127.28
29	L	101	LHG	C20-C19-C18	-2.12	103.64	114.37
23	C	502	CLA	OBD-CAD-C3D	2.12	133.38	128.42
29	d	407	LHG	C18-C17-C16	-2.12	103.64	114.37
33	m	101	LMG	O8-C28-O10	-2.12	118.32	123.63
27	a	412	SQD	O6-C44-C45	-2.12	106.32	111.77
23	b	611	CLA	O1D-CGD-CBD	2.12	128.70	124.52
29	l	101	LHG	C27-C26-C25	-2.12	103.66	114.37
23	c	506	CLA	CHA-C4D-ND	2.12	136.92	132.55
23	b	604	CLA	CHD-C1D-ND	-2.12	121.82	124.80
33	C	519	LMG	O3-C3-C2	-2.12	105.38	110.38
33	c	522	LMG	O8-C28-O10	-2.12	118.33	123.63
23	b	604	CLA	C4-C3-C5	2.12	118.91	115.23
23	b	611	CLA	C11-C12-C13	-2.12	108.93	115.97
23	D	404	CLA	O2D-CGD-CBD	2.12	114.93	111.23
23	B	605	CLA	CHD-C1D-C2D	2.12	129.89	125.49
27	f	101	SQD	C46-C45-C44	-2.12	106.85	111.78
23	b	607	CLA	CHD-C1D-C2D	2.12	129.89	125.49
33	C	501	LMG	C9-C8-C7	-2.11	106.85	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	617	BCR	C3-C4-C5	-2.11	110.28	114.06
23	C	513	CLA	C6-C5-C3	-2.11	108.32	113.47
23	C	503	CLA	CHB-C1B-C2B	-2.11	121.29	127.43
23	c	509	CLA	O2A-CGA-CBA	2.11	118.28	111.83
23	B	602	CLA	CHA-C4D-ND	2.11	136.91	132.55
33	C	519	LMG	O6-C1-O1	-2.11	105.05	110.04
26	a	410	PL9	C31-C29-C28	2.11	125.91	121.17
23	b	613	CLA	C1D-ND-C4D	-2.11	104.83	106.31
34	E	103	HEM	C4C-C3C-C2C	2.11	108.64	106.81
23	c	506	CLA	CHA-C1A-NA	-2.11	121.61	126.39
26	d	406	PL9	C36-C34-C33	-2.11	116.43	121.17
28	C	517	DGD	CBB-CAB-C9B	-2.11	103.71	114.37
23	A	405	CLA	C11-C12-C13	-2.11	108.96	115.97
23	B	601	CLA	O2D-CGD-CBD	2.11	114.91	111.23
27	B	621	SQD	O47-C45-C46	2.11	115.90	108.34
25	b	618	BCR	C38-C26-C25	-2.11	122.19	124.48
23	b	603	CLA	CHA-C4D-ND	2.10	136.89	132.55
23	D	404	CLA	CHD-C1D-C2D	2.10	129.86	125.49
23	A	404	CLA	C1D-ND-C4D	-2.10	104.84	106.31
25	t	101	BCR	C15-C16-C17	-2.10	119.22	123.52
35	v	201	HEC	CHA-C4D-ND	2.10	127.67	123.86
33	m	101	LMG	C9-C8-C7	-2.10	106.89	111.78
23	B	612	CLA	C16-C15-C13	-2.10	108.98	115.97
23	C	502	CLA	CMC-C2C-C1C	2.10	128.32	125.03
23	B	609	CLA	CHD-C4C-C3C	-2.10	121.71	124.77
23	b	609	CLA	C4D-CHA-C1A	2.10	123.75	121.24
23	a	408	CLA	C3D-C4D-ND	2.10	113.40	109.99
25	x	102	BCR	C16-C15-C14	-2.10	119.23	123.52
23	B	606	CLA	CMA-C3A-C4A	-2.10	106.14	111.77
26	A	409	PL9	O2-C1-C6	2.10	123.82	120.48
24	d	401	PHO	O2D-CGD-CBD	-2.10	108.64	110.95
28	C	516	DGD	C3E-C4E-C5E	-2.10	106.43	110.23
23	b	615	CLA	CHB-C1B-NB	2.10	127.19	124.05
28	C	516	DGD	O3D-C3D-C4D	-2.09	105.44	110.38
23	c	508	CLA	C3B-C4B-NB	-2.09	108.66	110.53
23	C	504	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
28	h	101	DGD	O6E-C5E-C4E	2.09	113.47	109.70
28	c	517	DGD	C3D-C4D-C5D	-2.09	106.44	110.23
23	b	612	CLA	C11-C12-C13	-2.09	109.01	115.97
23	B	610	CLA	CAA-CBA-CGA	-2.09	107.27	113.21
23	B	604	CLA	CHB-C1B-NB	2.09	127.18	124.05
23	B	611	CLA	C11-C10-C8	-2.09	109.02	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	617	CLA	O2D-CGD-CBD	2.09	114.88	111.23
23	C	512	CLA	C1-C2-C3	-2.09	122.78	126.20
23	B	601	CLA	CHA-C4D-ND	2.09	136.85	132.55
23	B	605	CLA	C1D-ND-C4D	-2.09	104.85	106.31
23	C	513	CLA	CHA-C1A-NA	-2.09	121.67	126.39
26	D	406	PL9	C11-C9-C8	-2.08	116.49	121.17
25	C	515	BCR	C29-C30-C25	2.08	113.47	110.44
24	D	401	PHO	C1A-C2A-C3A	-2.08	100.86	102.84
23	C	504	CLA	CHC-C4B-NB	2.08	127.17	124.05
23	c	509	CLA	C1D-ND-C4D	2.08	107.77	106.31
25	b	618	BCR	C32-C1-C6	-2.08	106.98	110.24
25	D	405	BCR	C16-C15-C14	-2.08	119.26	123.52
29	d	407	LHG	O8-C23-O10	-2.08	118.42	123.63
23	c	511	CLA	CHA-C1A-NA	-2.08	121.68	126.39
23	C	512	CLA	C4-C3-C5	2.08	118.84	115.23
35	v	201	HEC	CBD-CAD-C3D	-2.08	106.79	112.53
23	C	513	CLA	C11-C12-C13	-2.08	109.06	115.97
29	l	101	LHG	C11-C10-C9	-2.08	103.86	114.37
25	B	619	BCR	C2-C1-C6	2.08	113.46	110.44
28	c	518	DGD	C7A-C6A-C5A	-2.08	103.87	114.37
23	C	511	CLA	O2D-CGD-CBD	2.08	114.86	111.23
25	c	514	BCR	C1-C6-C5	-2.08	119.80	122.64
23	B	610	CLA	CHD-C4C-NC	2.08	127.45	124.23
23	b	602	CLA	C3C-C4C-NC	-2.08	107.77	110.43
26	a	410	PL9	C7-C8-C9	-2.08	123.26	126.83
23	C	504	CLA	CHA-C4D-ND	2.07	136.83	132.55
23	B	602	CLA	CMB-C2B-C3B	2.07	131.42	126.55
23	c	502	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
23	d	404	CLA	CMB-C2B-C3B	2.07	131.42	126.55
23	C	513	CLA	C4A-NA-C1A	2.07	107.62	106.68
33	c	519	LMG	C4-C3-C2	-2.07	107.19	110.83
33	C	519	LMG	O2-C2-C1	-2.07	105.14	110.08
23	B	606	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
23	d	402	CLA	C16-C17-C18	-2.07	106.69	115.94
23	C	509	CLA	CMD-C2D-C1D	2.07	128.37	124.73
23	C	511	CLA	CHD-C1D-ND	-2.07	121.89	124.80
23	c	510	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
25	A	408	BCR	C11-C10-C9	-2.07	124.38	127.28
28	c	518	DGD	O6E-C5E-C6E	-2.07	101.32	106.44
24	a	407	PHO	C1A-C2A-C3A	-2.07	100.87	102.84
23	c	508	CLA	O2D-CGD-CBD	2.07	114.84	111.23
26	a	410	PL9	C21-C19-C18	-2.07	116.53	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	516	DGD	C1D-C2D-C3D	-2.07	105.66	110.01
23	B	608	CLA	C6-C5-C3	-2.07	108.44	113.47
25	B	618	BCR	C40-C30-C25	2.06	113.48	110.24
24	D	401	PHO	OBD-CAD-CBD	-2.06	122.79	125.82
29	D	409	LHG	C6-C5-C4	2.06	116.60	111.78
23	c	504	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
25	K	101	BCR	C1-C6-C5	-2.06	119.82	122.64
23	C	502	CLA	CHB-C1B-NB	2.06	127.14	124.05
25	x	102	BCR	C7-C8-C9	-2.06	123.19	126.23
23	C	503	CLA	C4D-C3D-CAD	-2.06	105.87	108.11
29	D	408	LHG	C11-C10-C9	-2.06	103.95	114.37
23	D	404	CLA	C3D-C4D-ND	2.06	113.34	109.99
23	B	607	CLA	C2A-C1A-CHA	2.06	127.44	123.87
29	D	409	LHG	O8-C6-C5	-2.06	102.46	108.40
28	C	518	DGD	C3G-C2G-C1G	-2.06	106.98	111.78
23	b	611	CLA	CHA-C4D-ND	2.06	136.79	132.55
25	B	617	BCR	C15-C14-C13	-2.06	124.39	127.28
23	b	604	CLA	CHC-C4B-NB	2.06	127.14	124.05
28	C	518	DGD	C1D-C2D-C3D	-2.06	105.68	110.01
23	c	506	CLA	CMC-C2C-C1C	2.06	128.25	125.03
25	B	617	BCR	C33-C5-C6	-2.06	122.24	124.48
28	c	516	DGD	O3G-C1D-C2D	-2.06	105.15	108.27
23	d	403	CLA	C4D-CHA-C1A	2.05	123.69	121.24
23	b	609	CLA	O2D-CGD-CBD	2.05	114.82	111.23
23	b	610	CLA	CHD-C4C-NC	2.05	127.42	124.23
24	a	407	PHO	C4D-CHA-CBD	-2.05	107.47	108.45
26	A	409	PL9	C40-C39-C41	2.05	118.79	115.23
23	B	616	CLA	C2C-C1C-NC	2.05	112.14	109.98
23	b	608	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
23	c	503	CLA	CHD-C1D-ND	-2.05	121.92	124.80
23	b	606	CLA	CHD-C4C-C3C	-2.05	121.78	124.77
28	C	518	DGD	C5B-C4B-C3B	-2.05	104.01	114.37
23	a	406	CLA	CHD-C1D-C2D	2.05	129.75	125.49
23	D	402	CLA	CHC-C4B-NB	2.05	127.12	124.05
23	d	404	CLA	O2A-C1-C2	-2.05	100.23	108.11
26	a	410	PL9	C32-C33-C34	-2.05	122.94	127.62
28	c	516	DGD	O1G-C1A-C2A	-2.05	105.59	111.83
23	c	513	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
25	K	101	BCR	C15-C16-C17	-2.05	119.33	123.52
23	D	402	CLA	C7-C6-C5	-2.05	107.81	113.26
25	k	101	BCR	C1-C6-C5	-2.04	119.84	122.64
23	b	611	CLA	CAC-C3C-C4C	2.04	127.45	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C4-C3-C2	-2.04	118.38	123.63
23	C	505	CLA	CHA-C4D-ND	2.04	136.76	132.55
23	B	609	CLA	CHB-C4A-NA	2.04	127.34	124.40
23	A	404	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
23	c	502	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
28	H	102	DGD	O5D-C1E-C2E	2.04	111.37	108.27
34	e	102	HEM	CHC-C1C-NC	2.04	126.67	124.45
25	K	101	BCR	C32-C1-C6	-2.04	107.05	110.24
23	B	602	CLA	C1-C2-C3	-2.03	122.86	126.20
23	b	604	CLA	CHB-C4A-NA	2.03	127.34	124.40
23	c	501	CLA	CMC-C2C-C1C	2.03	128.21	125.03
23	c	509	CLA	C3A-C2A-C1A	2.03	104.39	101.34
26	D	406	PL9	C27-C28-C29	-2.03	122.97	127.62
34	e	102	HEM	CAB-C3B-C2B	-2.03	121.82	128.43
23	C	505	CLA	CMC-C2C-C1C	2.03	128.21	125.03
23	c	508	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
23	b	602	CLA	O2A-CGA-CBA	2.03	118.03	111.83
23	a	408	CLA	CHA-C1A-NA	-2.03	121.79	126.39
28	C	518	DGD	C8B-C7B-C6B	-2.03	104.10	114.37
35	V	201	HEC	CHC-C1C-NC	2.03	127.54	123.86
26	D	406	PL9	C7-C8-C9	-2.03	123.34	126.83
28	C	516	DGD	CCB-CBB-CAB	-2.03	104.13	114.37
23	b	604	CLA	C1-C2-C3	-2.03	122.88	126.20
23	C	503	CLA	O1D-CGD-CBD	2.03	128.51	124.52
23	B	605	CLA	OBD-CAD-C3D	2.03	133.15	128.42
25	K	101	BCR	C30-C25-C26	-2.03	119.87	122.64
23	b	615	CLA	CHB-C4A-NA	2.02	127.32	124.40
23	a	405	CLA	CHD-C1D-C2D	2.02	129.70	125.49
25	c	521	BCR	C24-C23-C22	-2.02	123.24	126.23
25	c	515	BCR	C8-C9-C10	2.02	122.19	119.01
23	B	610	CLA	C2D-C1D-ND	2.02	112.13	110.13
24	A	406	PHO	C1-C2-C3	-2.02	122.88	126.20
23	b	616	CLA	CHD-C4C-C3C	-2.02	121.83	124.77
23	C	508	CLA	C9-C8-C10	2.02	118.47	111.27
23	A	404	CLA	C4D-CHA-C1A	-2.02	118.83	121.24
33	M	101	LMG	O2-C2-C1	-2.02	105.26	110.08
28	C	517	DGD	O3D-C3D-C4D	-2.02	105.62	110.38
23	C	507	CLA	CMB-C2B-C3B	2.02	131.29	126.55
23	C	508	CLA	CHB-C4A-NA	2.02	127.31	124.40
23	C	507	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
23	d	402	CLA	C2B-C1B-NB	-2.02	108.23	110.33
33	C	519	LMG	C38-C37-C36	-2.01	104.18	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C14-C13-C15	-2.01	104.09	111.27
23	C	512	CLA	C3C-C4C-NC	-2.01	107.85	110.43
23	b	603	CLA	CMC-C2C-C3C	2.01	131.60	126.15
23	a	406	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
23	c	513	CLA	C16-C15-C13	-2.01	109.27	115.97
29	e	101	LHG	O10-C23-C24	-2.01	115.90	123.78
23	B	603	CLA	CHA-C4D-ND	2.01	136.70	132.55
29	A	413	LHG	C11-C10-C9	-2.01	104.19	114.37
23	B	607	CLA	CHA-C1A-NA	-2.01	121.83	126.39
23	B	612	CLA	CGD-CBD-CAD	2.01	117.36	110.85
25	C	515	BCR	C8-C7-C6	-2.01	121.62	127.00
23	C	514	CLA	CAC-C3C-C4C	2.01	127.41	124.79
23	c	506	CLA	C6-C5-C3	-2.01	108.57	113.47
23	d	404	CLA	C2C-C1C-NC	2.01	112.09	109.98
25	C	515	BCR	C34-C9-C10	-2.01	119.56	122.82
23	C	509	CLA	CMC-C2C-C3C	2.01	131.58	126.15
26	D	406	PL9	C37-C36-C34	-2.01	106.53	113.19
25	B	619	BCR	C40-C30-C29	-2.01	101.24	108.95
25	B	619	BCR	C34-C9-C10	-2.01	119.56	122.82
23	B	614	CLA	CHA-C1A-NA	-2.01	121.85	126.39
23	b	602	CLA	CHD-C4C-NC	2.01	127.34	124.23
29	D	408	LHG	C27-C26-C25	-2.00	104.23	114.37
33	m	101	LMG	O8-C9-C8	-2.00	102.62	108.40
23	d	403	CLA	CAA-CBA-CGA	-2.00	107.52	113.21
28	H	102	DGD	C5B-C4B-C3B	-2.00	104.24	114.37
28	c	518	DGD	CBB-CAB-C9B	-2.00	104.25	114.37

All (61) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	402	CLA	ND
23	a	405	CLA	ND
23	a	406	CLA	ND
23	a	408	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	c	501	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402	CLA	ND
23	d	404	CLA	ND

All (1687) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	C4B-C3B-CAB-CBB
23	B	606	CLA	C2B-C3B-CAB-CBB
23	B	606	CLA	C4B-C3B-CAB-CBB
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	615	CLA	C2B-C3B-CAB-CBB
23	B	615	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	C4-C3-C5-C6
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	513	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C12-C13-C15-C16
23	a	406	CLA	C4B-C3B-CAB-CBB
23	b	602	CLA	C1A-C2A-CAA-CBA
23	b	602	CLA	C4B-C3B-CAB-CBB
23	b	602	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	611	CLA	C2B-C3B-CAB-CBB
23	b	611	CLA	C4B-C3B-CAB-CBB
23	b	615	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	C2-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C11-C10-C8-C9
23	c	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	C6-C7-C8-C9
23	d	402	CLA	C2B-C3B-CAB-CBB
23	d	402	CLA	C4B-C3B-CAB-CBB
23	d	403	CLA	C2B-C3B-CAB-CBB
23	d	403	CLA	C4B-C3B-CAB-CBB
25	A	408	BCR	C7-C8-C9-C34
25	A	408	BCR	C20-C21-C22-C37
25	B	617	BCR	C16-C17-C18-C36
25	B	618	BCR	C35-C13-C14-C15
25	B	618	BCR	C16-C17-C18-C36
25	B	619	BCR	C11-C10-C9-C8
25	C	515	BCR	C11-C10-C9-C34
25	C	515	BCR	C11-C12-C13-C14
25	C	515	BCR	C11-C12-C13-C35
25	C	520	BCR	C16-C17-C18-C36
25	C	520	BCR	C18-C19-C20-C21
25	C	520	BCR	C20-C21-C22-C37
25	D	405	BCR	C37-C22-C23-C24
25	D	405	BCR	C23-C24-C25-C26
25	K	101	BCR	C17-C18-C19-C20
25	K	101	BCR	C21-C22-C23-C24
25	T	101	BCR	C20-C21-C22-C23
25	T	101	BCR	C20-C21-C22-C37
25	Z	101	BCR	C10-C11-C12-C13
25	Z	101	BCR	C11-C12-C13-C35
25	Z	101	BCR	C16-C17-C18-C19
25	Z	101	BCR	C16-C17-C18-C36
25	b	619	BCR	C11-C10-C9-C8
25	b	619	BCR	C11-C12-C13-C14
25	b	619	BCR	C20-C21-C22-C37
25	b	620	BCR	C11-C12-C13-C14
25	b	620	BCR	C11-C12-C13-C35
25	b	620	BCR	C37-C22-C23-C24
25	c	514	BCR	C7-C8-C9-C34
25	c	514	BCR	C35-C13-C14-C15
25	c	514	BCR	C18-C19-C20-C21
25	c	514	BCR	C20-C21-C22-C37
25	c	515	BCR	C35-C13-C14-C15
25	c	515	BCR	C20-C21-C22-C37
25	c	521	BCR	C17-C18-C19-C20
25	c	521	BCR	C36-C18-C19-C20
25	d	405	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	d	405	BCR	C7-C8-C9-C34
25	d	405	BCR	C20-C21-C22-C37
25	d	405	BCR	C37-C22-C23-C24
25	d	405	BCR	C22-C23-C24-C25
25	k	101	BCR	C11-C10-C9-C8
25	k	101	BCR	C11-C12-C13-C35
25	t	101	BCR	C12-C13-C14-C15
25	t	101	BCR	C35-C13-C14-C15
25	t	101	BCR	C14-C15-C16-C17
25	t	101	BCR	C20-C21-C22-C37
25	x	102	BCR	C23-C24-C25-C26
26	A	409	PL9	C9-C11-C12-C13
26	A	409	PL9	C12-C13-C14-C16
26	A	409	PL9	C22-C23-C24-C25
26	A	409	PL9	C22-C23-C24-C26
26	A	409	PL9	C32-C33-C34-C36
26	A	409	PL9	C37-C38-C39-C40
26	A	409	PL9	C37-C38-C39-C41
26	D	406	PL9	C32-C33-C34-C35
26	D	406	PL9	C32-C33-C34-C36
26	a	410	PL9	C22-C23-C24-C25
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C24-C26-C27-C28
26	a	410	PL9	C32-C33-C34-C36
26	a	410	PL9	C42-C43-C44-C46
26	d	406	PL9	C32-C33-C34-C35
26	d	406	PL9	C37-C38-C39-C40
26	d	406	PL9	C42-C43-C44-C45
26	d	406	PL9	C44-C46-C47-C48
27	A	410	SQD	C5-C6-S-O7
27	A	411	SQD	C46-C45-O47-C7
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O6-C44-C45-O47
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	a	411	SQD	O47-C45-C46-O48
27	a	412	SQD	O49-C7-O47-C45
27	a	412	SQD	O10-C23-O48-C46
27	f	101	SQD	O5-C1-O6-C44
28	A	412	DGD	C2B-C1B-O2G-C2G
28	A	412	DGD	O1B-C1B-O2G-C2G
28	A	412	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
28	a	413	DGD	O1A-C1A-O1G-C1G
28	a	413	DGD	O2G-C2G-C3G-O3G
29	A	413	LHG	O1-C1-C2-C3
29	A	413	LHG	C3-O3-P-O5
29	A	413	LHG	C3-O3-P-O6
29	D	408	LHG	O1-C1-C2-C3
29	D	408	LHG	O2-C2-C3-O3
29	D	408	LHG	C3-O3-P-O5
29	D	408	LHG	C3-O3-P-O6
29	D	408	LHG	C4-O6-P-O3
29	D	408	LHG	C4-O6-P-O4
29	D	409	LHG	C3-O3-P-O5
29	D	409	LHG	C3-O3-P-O6
29	E	101	LHG	C4-O6-P-O4
29	E	101	LHG	O10-C23-O8-C6
29	L	101	LHG	C4-O6-P-O3
29	L	101	LHG	C4-O6-P-O4
29	L	101	LHG	C4-O6-P-O5
29	d	407	LHG	O1-C1-C2-C3
29	d	407	LHG	C3-O3-P-O4
29	d	407	LHG	C3-O3-P-O5
29	d	407	LHG	C3-O3-P-O6
29	d	408	LHG	C4-O6-P-O3
29	d	408	LHG	C4-O6-P-O4
29	d	408	LHG	C4-O6-P-O5
29	e	101	LHG	O1-C1-C2-C3
29	e	101	LHG	C3-O3-P-O5
29	e	101	LHG	C3-O3-P-O6
29	e	101	LHG	C4-O6-P-O3
29	e	101	LHG	C4-O6-P-O4
29	e	101	LHG	C4-O6-P-O5
29	e	101	LHG	O10-C23-O8-C6
29	l	101	LHG	C4-O6-P-O5
33	C	501	LMG	O6-C1-O1-C7
33	C	501	LMG	O9-C10-O7-C8
33	C	519	LMG	C11-C10-O7-C8
33	D	410	LMG	O1-C7-C8-C9
33	D	410	LMG	O1-C7-C8-O7
33	D	410	LMG	C11-C10-O7-C8
33	b	622	LMG	O9-C10-O7-C8
33	b	622	LMG	C11-C10-O7-C8
33	c	524	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
33	c	524	LMG	O10-C28-O8-C9
33	c	524	LMG	C29-C28-O8-C9
35	V	201	HEC	C2B-C3B-CAB-CBB
35	V	201	HEC	C4B-C3B-CAB-CBB
35	V	201	HEC	C2C-C3C-CAC-CBC
35	V	201	HEC	C4C-C3C-CAC-CBC
35	v	201	HEC	C2B-C3B-CAB-CBB
35	v	201	HEC	C4B-C3B-CAB-CBB
35	v	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C4C-C3C-CAC-CBC
23	C	504	CLA	O1D-CGD-O2D-CED
23	b	602	CLA	O1D-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
26	D	406	PL9	C47-C48-C49-C50
23	c	510	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
27	a	412	SQD	C24-C23-O48-C46
29	E	101	LHG	C24-C23-O8-C6
29	e	101	LHG	C24-C23-O8-C6
27	F	101	SQD	O10-C23-O48-C46
33	c	522	LMG	O10-C28-O8-C9
23	B	601	CLA	O1D-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
24	d	401	PHO	CBD-CGD-O2D-CED
27	b	601	SQD	O10-C23-O48-C46
28	a	413	DGD	O1B-C1B-O2G-C2G
33	C	519	LMG	O9-C10-O7-C8
33	D	410	LMG	O9-C10-O7-C8
33	c	522	LMG	O9-C10-O7-C8
23	b	602	CLA	C3-C5-C6-C7
23	b	605	CLA	C3-C5-C6-C7
27	b	601	SQD	C24-C23-O48-C46
28	a	413	DGD	C2A-C1A-O1G-C1G
33	c	522	LMG	C29-C28-O8-C9
23	B	606	CLA	CBD-CGD-O2D-CED
23	C	502	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
27	a	412	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
33	C	501	LMG	C11-C10-O7-C8
23	c	503	CLA	O1D-CGD-O2D-CED
23	A	407	CLA	C4-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
26	a	410	PL9	C30-C29-C31-C32
26	d	406	PL9	C40-C39-C41-C42
23	A	407	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
26	A	409	PL9	C18-C19-C21-C22
26	a	410	PL9	C33-C34-C36-C37
26	d	406	PL9	C38-C39-C41-C42
23	b	607	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
23	b	607	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C3-C5-C6-C7
27	F	101	SQD	C24-C23-O48-C46
26	A	409	PL9	C12-C13-C14-C15
26	a	410	PL9	C42-C43-C44-C45
26	A	409	PL9	C17-C18-C19-C21
26	d	406	PL9	C32-C33-C34-C36
26	d	406	PL9	C42-C43-C44-C46
25	c	514	BCR	C9-C10-C11-C12
26	d	406	PL9	C47-C48-C49-C51
23	b	604	CLA	CBD-CGD-O2D-CED
29	D	409	LHG	O2-C2-C3-O3
27	F	101	SQD	C44-C45-C46-O48
28	c	518	DGD	O1A-C1A-O1G-C1G
23	c	508	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	CBD-CGD-O2D-CED
23	B	612	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
23	b	612	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
24	d	401	PHO	O1D-CGD-O2D-CED
33	C	501	LMG	O10-C28-O8-C9
28	h	101	DGD	O6E-C5E-C6E-O5E
26	A	409	PL9	C34-C36-C37-C38
26	A	409	PL9	C44-C46-C47-C48
26	a	410	PL9	C19-C21-C22-C23
26	a	410	PL9	C34-C36-C37-C38
26	d	406	PL9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	b	616	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	CBD-CGD-O2D-CED
33	c	524	LMG	O6-C5-C6-O5
33	C	501	LMG	O6-C5-C6-O5
23	b	617	CLA	O1D-CGD-O2D-CED
33	c	519	LMG	C11-C10-O7-C8
33	c	522	LMG	C4-C5-C6-O5
29	D	408	LHG	C1-C2-C3-O3
23	B	601	CLA	CBA-CGA-O2A-C1
27	A	411	SQD	C24-C23-O48-C46
27	f	101	SQD	C24-C23-O48-C46
33	c	519	LMG	C29-C28-O8-C9
33	c	524	LMG	C4-C5-C6-O5
23	b	613	CLA	O1D-CGD-O2D-CED
33	C	501	LMG	C28-C29-C30-C31
23	c	507	CLA	C4-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
23	B	605	CLA	C11-C10-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	B	614	CLA	C11-C12-C13-C14
23	B	614	CLA	C14-C13-C15-C16
23	C	503	CLA	C6-C7-C8-C9
23	C	508	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	b	602	CLA	C11-C10-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	b	607	CLA	C14-C13-C15-C16
23	c	502	CLA	C6-C7-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	c	509	CLA	C11-C12-C13-C14
23	d	404	CLA	C11-C12-C13-C14
24	A	406	PHO	C14-C13-C15-C16
33	C	519	LMG	C4-C5-C6-O5
23	c	511	CLA	O1D-CGD-O2D-CED
27	f	101	SQD	C2-C1-O6-C44
29	d	407	LHG	C7-C8-C9-C10
33	C	501	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
25	H	101	BCR	C11-C12-C13-C35
25	K	101	BCR	C7-C8-C9-C34
25	K	101	BCR	C11-C12-C13-C35
25	K	101	BCR	C37-C22-C23-C24
25	Z	101	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C34
25	b	619	BCR	C11-C12-C13-C35
25	c	514	BCR	C11-C12-C13-C35
25	c	521	BCR	C11-C12-C13-C35
25	d	405	BCR	C11-C12-C13-C35
25	k	101	BCR	C7-C8-C9-C34
25	x	102	BCR	C7-C8-C9-C34
25	x	102	BCR	C11-C12-C13-C35
25	x	102	BCR	C37-C22-C23-C24
25	d	405	BCR	C21-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C10
26	a	410	PL9	C47-C48-C49-C50
23	B	601	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	C10-C11-C12-C13
33	m	101	LMG	C10-C11-C12-C13
23	c	506	CLA	C2-C1-O2A-CGA
27	a	411	SQD	O10-C23-O48-C46
28	h	101	DGD	C4E-C5E-C6E-O5E
25	B	618	BCR	C14-C15-C16-C17
23	b	607	CLA	C15-C16-C17-C18
23	c	503	CLA	C5-C6-C7-C8
26	A	409	PL9	C47-C48-C49-C50
29	A	413	LHG	O1-C1-C2-O2
23	C	507	CLA	C3-C5-C6-C7
23	B	606	CLA	O1D-CGD-O2D-CED
26	d	406	PL9	C37-C38-C39-C41
23	B	612	CLA	C6-C7-C8-C10
29	e	101	LHG	C23-C24-C25-C26
25	B	619	BCR	C13-C14-C15-C16
23	b	606	CLA	C5-C6-C7-C8
23	c	512	CLA	C13-C15-C16-C17
33	c	519	LMG	O6-C5-C6-O5
29	D	409	LHG	C29-C30-C31-C32
28	c	517	DGD	C1B-C2B-C3B-C4B
33	D	411	LMG	C28-C29-C30-C31
23	c	507	CLA	CBD-CGD-O2D-CED
27	b	601	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C5-C6-C7-C8
23	b	615	CLA	C8-C10-C11-C12
33	C	519	LMG	O6-C5-C6-O5
23	b	602	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	O1D-CGD-O2D-CED
25	C	515	BCR	C10-C11-C12-C13
23	B	607	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	b	606	CLA	C15-C16-C17-C18
23	c	510	CLA	C15-C16-C17-C18
28	c	516	DGD	O6E-C5E-C6E-O5E
27	A	410	SQD	C7-C8-C9-C10
27	A	411	SQD	C7-C8-C9-C10
28	c	518	DGD	C1A-C2A-C3A-C4A
29	E	101	LHG	C7-C8-C9-C10
23	B	606	CLA	C15-C16-C17-C18
23	C	513	CLA	C10-C11-C12-C13
23	b	608	CLA	C10-C11-C12-C13
23	b	612	CLA	C10-C11-C12-C13
23	b	612	CLA	C13-C15-C16-C17
23	b	612	CLA	C15-C16-C17-C18
23	b	615	CLA	C5-C6-C7-C8
23	c	508	CLA	C13-C15-C16-C17
27	a	411	SQD	C12-C13-C14-C15
29	E	101	LHG	C32-C33-C34-C35
29	A	413	LHG	O2-C2-C3-O3
29	d	407	LHG	O2-C2-C3-O3
29	e	101	LHG	O2-C2-C3-O3
28	c	518	DGD	C2A-C1A-O1G-C1G
27	F	101	SQD	C23-C24-C25-C26
23	b	602	CLA	C15-C16-C17-C18
23	b	607	CLA	C10-C11-C12-C13
23	c	511	CLA	C13-C15-C16-C17
23	C	503	CLA	C3-C5-C6-C7
23	B	605	CLA	C5-C6-C7-C8
23	C	508	CLA	C10-C11-C12-C13
23	b	602	CLA	C8-C10-C11-C12
23	b	603	CLA	C13-C15-C16-C17
23	B	615	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C10-C11-C12-C13
23	B	609	CLA	C13-C15-C16-C17
23	b	610	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C8-C10-C11-C12
23	d	403	CLA	CBD-CGD-O2D-CED
33	M	101	LMG	O10-C28-O8-C9
23	c	505	CLA	C15-C16-C17-C18
28	A	412	DGD	O6D-C5D-C6D-O5D
29	A	413	LHG	C1-C2-C3-O3
29	d	407	LHG	C1-C2-C3-O3
29	e	101	LHG	C1-C2-C3-O3
23	B	606	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C2A-CAA-CBA-CGA
23	b	608	CLA	CBA-CGA-O2A-C1
33	C	501	LMG	C29-C28-O8-C9
33	C	519	LMG	C29-C28-O8-C9
27	b	601	SQD	C11-C10-C9-C8
23	B	615	CLA	C10-C11-C12-C13
23	a	406	CLA	C10-C11-C12-C13
23	c	503	CLA	C8-C10-C11-C12
33	c	522	LMG	C10-C11-C12-C13
23	A	404	CLA	C15-C16-C17-C18
23	B	611	CLA	C13-C15-C16-C17
23	a	408	CLA	C10-C11-C12-C13
23	B	607	CLA	C13-C15-C16-C17
23	C	506	CLA	C5-C6-C7-C8
23	C	510	CLA	C13-C15-C16-C17
23	c	509	CLA	C15-C16-C17-C18
23	c	512	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	C15-C16-C17-C18
23	c	508	CLA	C10-C11-C12-C13
28	a	413	DGD	C2B-C1B-O2G-C2G
27	B	621	SQD	C2-C1-O6-C44
28	A	412	DGD	C2E-C1E-O5D-C6D
28	C	517	DGD	C2E-C1E-O5D-C6D
28	c	517	DGD	C2E-C1E-O5D-C6D
27	B	621	SQD	C24-C23-O48-C46
23	B	616	CLA	C11-C12-C13-C14
23	c	506	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
23	B	613	CLA	C8-C10-C11-C12
25	A	408	BCR	C35-C13-C14-C15
25	B	617	BCR	C35-C13-C14-C15
25	B	617	BCR	C20-C21-C22-C37
25	C	515	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
25	C	520	BCR	C11-C10-C9-C34
25	H	101	BCR	C20-C21-C22-C37
25	K	101	BCR	C20-C21-C22-C37
25	Z	101	BCR	C20-C21-C22-C37
25	a	409	BCR	C20-C21-C22-C37
25	b	618	BCR	C20-C21-C22-C37
25	b	620	BCR	C20-C21-C22-C37
25	c	514	BCR	C16-C17-C18-C36
25	c	515	BCR	C16-C17-C18-C36
25	c	521	BCR	C16-C17-C18-C36
25	d	405	BCR	C16-C17-C18-C36
25	k	101	BCR	C11-C10-C9-C34
25	k	101	BCR	C16-C17-C18-C36
25	k	101	BCR	C20-C21-C22-C37
25	x	102	BCR	C16-C17-C18-C36
27	A	410	SQD	C23-C24-C25-C26
23	C	508	CLA	C13-C15-C16-C17
25	b	620	BCR	C36-C18-C19-C20
25	c	515	BCR	C37-C22-C23-C24
25	B	617	BCR	C17-C18-C19-C20
29	E	101	LHG	O1-C1-C2-C3
29	d	409	LHG	O1-C1-C2-C3
28	c	516	DGD	C1A-C2A-C3A-C4A
33	d	411	LMG	C28-C29-C30-C31
23	b	616	CLA	O1D-CGD-O2D-CED
25	c	514	BCR	C13-C14-C15-C16
23	C	503	CLA	C16-C17-C18-C19
23	b	604	CLA	O1D-CGD-O2D-CED
25	B	617	BCR	C12-C13-C14-C15
25	B	617	BCR	C20-C21-C22-C23
25	C	515	BCR	C11-C10-C9-C8
25	C	520	BCR	C16-C17-C18-C19
25	C	520	BCR	C20-C21-C22-C23
25	H	101	BCR	C11-C10-C9-C8
25	H	101	BCR	C20-C21-C22-C23
25	c	514	BCR	C12-C13-C14-C15
25	c	514	BCR	C20-C21-C22-C23
25	c	521	BCR	C16-C17-C18-C19
25	d	405	BCR	C11-C10-C9-C8
25	k	101	BCR	C20-C21-C22-C23
25	t	101	BCR	C16-C17-C18-C19
28	C	517	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	O6E-C1E-O5D-C6D
33	c	522	LMG	C11-C10-O7-C8
33	M	101	LMG	C10-C11-C12-C13
23	B	602	CLA	C13-C15-C16-C17
28	A	412	DGD	C4D-C5D-C6D-O5D
23	c	512	CLA	CBA-CGA-O2A-C1
27	a	411	SQD	C24-C23-O48-C46
28	c	516	DGD	O6D-C5D-C6D-O5D
23	A	405	CLA	C16-C17-C18-C20
23	D	404	CLA	C16-C17-C18-C19
23	c	506	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	B	614	CLA	C5-C6-C7-C8
27	A	410	SQD	C11-C12-C13-C14
33	d	411	LMG	C34-C35-C36-C37
25	b	619	BCR	C14-C15-C16-C17
27	a	411	SQD	C34-C35-C36-C37
28	A	412	DGD	C5B-C6B-C7B-C8B
28	C	517	DGD	CCB-CDB-CEB-CFB
29	L	101	LHG	C32-C33-C34-C35
29	e	101	LHG	C17-C18-C19-C20
33	M	101	LMG	C39-C40-C41-C42
33	c	522	LMG	C16-C17-C18-C19
33	d	410	LMG	C35-C36-C37-C38
23	b	603	CLA	O1D-CGD-O2D-CED
27	A	410	SQD	C33-C34-C35-C36
28	a	413	DGD	C5A-C6A-C7A-C8A
28	a	413	DGD	C8B-C9B-CAB-CBB
28	c	516	DGD	C3B-C4B-C5B-C6B
29	d	408	LHG	C11-C12-C13-C14
23	b	608	CLA	O1A-CGA-O2A-C1
26	d	406	PL9	C47-C48-C49-C50
27	A	411	SQD	C14-C15-C16-C17
27	a	411	SQD	C26-C27-C28-C29
27	a	412	SQD	C15-C16-C17-C18
28	A	412	DGD	CAA-CBA-CCA-CDA
28	A	412	DGD	C6B-C7B-C8B-C9B
28	C	517	DGD	C8B-C9B-CAB-CBB
28	C	518	DGD	CAA-CBA-CCA-CDA
28	H	102	DGD	C4B-C5B-C6B-C7B
29	D	409	LHG	C32-C33-C34-C35
29	e	101	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	e	101	LHG	C26-C27-C28-C29
33	c	524	LMG	C12-C13-C14-C15
28	C	516	DGD	O6E-C5E-C6E-O5E
33	c	522	LMG	O6-C5-C6-O5
29	D	408	LHG	O1-C1-C2-O2
29	d	407	LHG	O1-C1-C2-O2
29	e	101	LHG	O1-C1-C2-O2
28	A	412	DGD	C4A-C5A-C6A-C7A
33	D	407	LMG	C39-C40-C41-C42
23	b	612	CLA	O1D-CGD-O2D-CED
23	C	505	CLA	C4B-C3B-CAB-CBB
33	b	622	LMG	C11-C12-C13-C14
33	m	101	LMG	C11-C12-C13-C14
23	A	405	CLA	C16-C17-C18-C19
23	C	503	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C20
28	h	101	DGD	CBA-CCA-CDA-CEA
29	A	413	LHG	C14-C15-C16-C17
23	B	604	CLA	C13-C15-C16-C17
23	B	611	CLA	C15-C16-C17-C18
29	D	409	LHG	C27-C28-C29-C30
23	C	509	CLA	C12-C13-C15-C16
27	a	411	SQD	C11-C12-C13-C14
28	C	518	DGD	C5A-C6A-C7A-C8A
33	d	411	LMG	C39-C40-C41-C42
23	b	615	CLA	C13-C15-C16-C17
27	F	101	SQD	C33-C34-C35-C36
27	a	412	SQD	C12-C13-C14-C15
28	C	517	DGD	C9A-CAA-CBA-CCA
29	d	409	LHG	C30-C31-C32-C33
33	D	407	LMG	C20-C21-C22-C23
33	D	407	LMG	C35-C36-C37-C38
33	M	101	LMG	C38-C39-C40-C41
23	C	513	CLA	C3-C5-C6-C7
23	b	602	CLA	C3A-C2A-CAA-CBA
23	c	512	CLA	C3A-C2A-CAA-CBA
23	B	612	CLA	C13-C15-C16-C17
23	B	611	CLA	C16-C17-C18-C20
23	B	616	CLA	C11-C12-C13-C15
23	a	405	CLA	C16-C17-C18-C20
23	c	507	CLA	C16-C17-C18-C20
28	C	517	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
28	c	516	DGD	C4D-C5D-C6D-O5D
28	H	102	DGD	CCA-CDA-CEA-CFA
33	D	407	LMG	C34-C35-C36-C37
27	b	601	SQD	C18-C19-C20-C21
28	c	517	DGD	C8B-C9B-CAB-CBB
28	h	101	DGD	C2B-C3B-C4B-C5B
29	D	409	LHG	C34-C35-C36-C37
29	d	408	LHG	C14-C15-C16-C17
33	c	522	LMG	C34-C35-C36-C37
28	c	517	DGD	C1A-C2A-C3A-C4A
28	a	413	DGD	C4A-C5A-C6A-C7A
29	E	101	LHG	C15-C16-C17-C18
29	d	407	LHG	C17-C18-C19-C20
29	d	408	LHG	C29-C30-C31-C32
29	d	409	LHG	C27-C28-C29-C30
33	b	622	LMG	C15-C16-C17-C18
23	c	512	CLA	O1A-CGA-O2A-C1
27	F	101	SQD	C25-C26-C27-C28
27	f	101	SQD	C28-C29-C30-C31
27	f	101	SQD	C31-C32-C33-C34
29	E	101	LHG	C11-C10-C9-C8
33	C	501	LMG	C16-C17-C18-C19
27	A	411	SQD	C12-C13-C14-C15
28	a	413	DGD	C5B-C6B-C7B-C8B
28	c	516	DGD	C9A-CAA-CBA-CCA
28	c	518	DGD	C4B-C5B-C6B-C7B
26	D	406	PL9	C7-C8-C9-C10
29	d	408	LHG	C7-C8-C9-C10
23	B	605	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB
23	a	406	CLA	C2B-C3B-CAB-CBB
23	b	602	CLA	C2B-C3B-CAB-CBB
25	A	408	BCR	C1-C6-C7-C8
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	D	405	BCR	C23-C24-C25-C30
25	K	101	BCR	C1-C6-C7-C8
25	x	102	BCR	C23-C24-C25-C30
33	b	622	LMG	C31-C32-C33-C34
23	c	503	CLA	CBA-CGA-O2A-C1
23	b	607	CLA	C3-C5-C6-C7
28	C	516	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
29	d	409	LHG	C26-C27-C28-C29
33	d	410	LMG	C33-C34-C35-C36
23	C	512	CLA	O1D-CGD-O2D-CED
27	B	621	SQD	C13-C14-C15-C16
27	b	601	SQD	C10-C11-C12-C13
28	C	517	DGD	C5B-C6B-C7B-C8B
29	d	407	LHG	C30-C31-C32-C33
33	d	410	LMG	C37-C38-C39-C40
33	d	410	LMG	C38-C39-C40-C41
27	B	621	SQD	C9-C10-C11-C12
33	c	524	LMG	C38-C39-C40-C41
27	B	621	SQD	C11-C12-C13-C14
27	B	621	SQD	C17-C18-C19-C20
27	a	412	SQD	C10-C11-C12-C13
27	b	601	SQD	C16-C17-C18-C19
28	h	101	DGD	C5B-C6B-C7B-C8B
33	c	519	LMG	C31-C32-C33-C34
23	B	614	CLA	C4-C3-C5-C6
29	D	409	LHG	C25-C26-C27-C28
33	b	622	LMG	C18-C19-C20-C21
25	B	617	BCR	C18-C19-C20-C21
25	Z	101	BCR	C18-C19-C20-C21
25	x	102	BCR	C18-C19-C20-C21
23	b	602	CLA	C10-C11-C12-C13
28	A	412	DGD	CEA-CFA-CGA-CHA
29	d	408	LHG	C30-C31-C32-C33
33	b	622	LMG	C19-C20-C21-C22
33	m	101	LMG	C31-C32-C33-C34
23	c	505	CLA	O1D-CGD-O2D-CED
33	m	101	LMG	C29-C28-O8-C9
23	C	513	CLA	C11-C10-C8-C9
23	b	617	CLA	C11-C10-C8-C9
29	d	408	LHG	C32-C33-C34-C35
23	a	408	CLA	C13-C15-C16-C17
27	a	411	SQD	C30-C31-C32-C33
29	L	101	LHG	C27-C28-C29-C30
33	C	501	LMG	C14-C15-C16-C17
33	D	407	LMG	C11-C12-C13-C14
28	A	412	DGD	O6E-C1E-O5D-C6D
28	A	412	DGD	C2B-C3B-C4B-C5B
29	e	101	LHG	C12-C13-C14-C15
29	e	101	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
29	l	101	LHG	C13-C14-C15-C16
33	c	524	LMG	C34-C35-C36-C37
33	c	524	LMG	C2-C1-O1-C7
23	B	612	CLA	C10-C11-C12-C13
23	C	504	CLA	C8-C10-C11-C12
28	C	518	DGD	O1A-C1A-O1G-C1G
28	h	101	DGD	C3A-C4A-C5A-C6A
29	l	101	LHG	C29-C30-C31-C32
33	D	407	LMG	C14-C15-C16-C17
33	D	411	LMG	C33-C34-C35-C36
28	h	101	DGD	CCB-CDB-CEB-CFB
33	D	407	LMG	C19-C20-C21-C22
33	M	101	LMG	C36-C37-C38-C39
28	A	412	DGD	CEB-CFB-CGB-CHB
28	c	518	DGD	CBB-CCB-CDB-CEB
28	h	101	DGD	CAB-CBB-CCB-CDB
29	D	409	LHG	C9-C10-C11-C12
29	D	409	LHG	C11-C12-C13-C14
28	A	412	DGD	C2A-C1A-O1G-C1G
25	B	619	BCR	C15-C16-C17-C18
28	A	412	DGD	CCA-CDA-CEA-CFA
23	B	611	CLA	C8-C10-C11-C12
23	c	504	CLA	C5-C6-C7-C8
29	E	101	LHG	O9-C7-O7-C5
29	A	413	LHG	C12-C13-C14-C15
29	D	408	LHG	C30-C31-C32-C33
27	B	621	SQD	C29-C30-C31-C32
29	D	408	LHG	C10-C11-C12-C13
29	d	409	LHG	C29-C30-C31-C32
26	a	410	PL9	C47-C48-C49-C51
23	B	605	CLA	C10-C11-C12-C13
27	a	412	SQD	C18-C19-C20-C21
28	c	517	DGD	CAA-CBA-CCA-CDA
33	c	519	LMG	C36-C37-C38-C39
33	D	411	LMG	C11-C12-C13-C14
23	a	405	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C19
33	c	524	LMG	C13-C14-C15-C16
29	L	101	LHG	C23-C24-C25-C26
27	f	101	SQD	C29-C30-C31-C32
23	c	506	CLA	C5-C6-C7-C8
29	D	408	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	L	101	LHG	C30-C31-C32-C33
33	c	522	LMG	C32-C33-C34-C35
26	D	406	PL9	C47-C48-C49-C51
33	m	101	LMG	C17-C18-C19-C20
28	H	102	DGD	C8B-C9B-CAB-CBB
29	l	101	LHG	C16-C17-C18-C19
27	a	411	SQD	C8-C7-O47-C45
29	E	101	LHG	C8-C7-O7-C5
33	M	101	LMG	C11-C10-O7-C8
23	B	607	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C20
33	d	411	LMG	O6-C5-C6-O5
29	D	409	LHG	C24-C25-C26-C27
33	b	622	LMG	C16-C17-C18-C19
29	A	413	LHG	C7-C8-C9-C10
23	D	403	CLA	C15-C16-C17-C18
23	D	404	CLA	C5-C6-C7-C8
28	C	518	DGD	CCA-CDA-CEA-CFA
28	a	413	DGD	C3B-C4B-C5B-C6B
28	c	518	DGD	C8A-C9A-CAA-CBA
33	D	411	LMG	C32-C33-C34-C35
29	d	407	LHG	C28-C29-C30-C31
29	l	101	LHG	C27-C28-C29-C30
33	D	407	LMG	C13-C14-C15-C16
33	c	524	LMG	C16-C17-C18-C19
27	a	412	SQD	C11-C12-C13-C14
28	A	412	DGD	C4B-C5B-C6B-C7B
28	c	516	DGD	C4B-C5B-C6B-C7B
29	l	101	LHG	C9-C10-C11-C12
23	b	615	CLA	C15-C16-C17-C18
33	b	622	LMG	O6-C5-C6-O5
28	C	518	DGD	C3A-C4A-C5A-C6A
29	D	408	LHG	C11-C10-C9-C8
29	d	407	LHG	C32-C33-C34-C35
23	B	603	CLA	C16-C17-C18-C20
23	b	608	CLA	C16-C17-C18-C20
26	A	409	PL9	C47-C48-C49-C51
28	A	412	DGD	CBA-CCA-CDA-CEA
29	D	408	LHG	C11-C12-C13-C14
33	D	407	LMG	C30-C31-C32-C33
24	A	406	PHO	C2-C3-C5-C6
28	A	412	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	C6A-C7A-C8A-C9A
29	A	413	LHG	C27-C28-C29-C30
29	e	101	LHG	C10-C11-C12-C13
29	e	101	LHG	C14-C15-C16-C17
33	M	101	LMG	C12-C13-C14-C15
23	b	611	CLA	C2A-CAA-CBA-CGA
23	C	506	CLA	CBD-CGD-O2D-CED
33	c	522	LMG	C36-C37-C38-C39
33	d	410	LMG	C31-C32-C33-C34
33	M	101	LMG	C17-C18-C19-C20
33	c	519	LMG	C39-C40-C41-C42
33	b	622	LMG	C34-C35-C36-C37
23	a	408	CLA	C5-C6-C7-C8
23	c	507	CLA	O1D-CGD-O2D-CED
27	B	621	SQD	C10-C11-C12-C13
27	A	411	SQD	C10-C11-C12-C13
23	B	607	CLA	C1A-C2A-CAA-CBA
23	a	408	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	B	612	CLA	C5-C6-C7-C8
29	e	101	LHG	C27-C28-C29-C30
28	c	516	DGD	C8B-C9B-CAB-CBB
23	c	503	CLA	O1A-CGA-O2A-C1
28	A	412	DGD	C9B-CAB-CBB-CCB
29	D	409	LHG	C30-C31-C32-C33
23	C	513	CLA	C8-C10-C11-C12
29	E	101	LHG	O6-C4-C5-C6
29	l	101	LHG	O6-C4-C5-C6
27	a	411	SQD	C14-C15-C16-C17
28	c	516	DGD	C4A-C5A-C6A-C7A
29	D	408	LHG	C32-C33-C34-C35
23	B	614	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C10-C8-C7
23	C	507	CLA	C6-C7-C8-C10
23	a	406	CLA	C12-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C7
23	b	602	CLA	C11-C10-C8-C7
23	b	608	CLA	C6-C7-C8-C10
23	b	613	CLA	C12-C13-C15-C16
23	c	508	CLA	C12-C13-C15-C16
27	F	101	SQD	C26-C27-C28-C29
23	c	511	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	b	609	CLA	C5-C6-C7-C8
23	b	604	CLA	C8-C10-C11-C12
33	c	524	LMG	C28-C29-C30-C31
27	A	410	SQD	C31-C32-C33-C34
29	D	408	LHG	C29-C30-C31-C32
29	e	101	LHG	C16-C17-C18-C19
26	D	406	PL9	C30-C29-C31-C32
26	d	406	PL9	C28-C29-C31-C32
33	c	522	LMG	C38-C39-C40-C41
23	B	604	CLA	C11-C10-C8-C9
23	B	612	CLA	C6-C7-C8-C9
23	C	506	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C10-C8-C9
23	a	406	CLA	C14-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C9
23	b	604	CLA	C11-C12-C13-C14
23	b	605	CLA	C14-C13-C15-C16
23	b	609	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
23	c	508	CLA	C14-C13-C15-C16
23	c	511	CLA	C14-C13-C15-C16
33	c	522	LMG	C11-C12-C13-C14
28	C	517	DGD	O6E-C5E-C6E-O5E
28	a	413	DGD	CBA-CCA-CDA-CEA
29	L	101	LHG	C18-C19-C20-C21
28	h	101	DGD	C7A-C8A-C9A-CAA
29	d	409	LHG	C23-C24-C25-C26
26	D	406	PL9	C44-C46-C47-C48
27	B	621	SQD	O6-C44-C45-C46
27	a	411	SQD	C44-C45-C46-O48
27	a	412	SQD	C44-C45-C46-O48
27	b	601	SQD	C44-C45-C46-O48
28	C	516	DGD	O1G-C1G-C2G-C3G
28	C	517	DGD	C5A-C6A-C7A-C8A
29	D	408	LHG	C34-C35-C36-C37
33	D	410	LMG	C33-C34-C35-C36
28	c	518	DGD	CCA-CDA-CEA-CFA
23	B	601	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C5-C6-C7-C8
27	F	101	SQD	C31-C32-C33-C34
27	a	411	SQD	C10-C11-C12-C13
29	D	408	LHG	C25-C26-C27-C28
29	d	407	LHG	C25-C26-C27-C28
23	B	603	CLA	C16-C17-C18-C19
28	a	413	DGD	C7B-C8B-C9B-CAB
29	l	101	LHG	C32-C33-C34-C35
33	b	622	LMG	C23-C24-C25-C26
33	c	519	LMG	C35-C36-C37-C38
33	d	410	LMG	C32-C33-C34-C35
33	d	411	LMG	C14-C15-C16-C17
29	d	408	LHG	C34-C35-C36-C37
29	d	407	LHG	C33-C34-C35-C36
23	C	511	CLA	C4-C3-C5-C6
24	A	406	PHO	C4-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
23	d	404	CLA	C8-C10-C11-C12
23	b	608	CLA	C16-C17-C18-C19
28	C	517	DGD	C3A-C4A-C5A-C6A
33	D	411	LMG	C31-C32-C33-C34
33	M	101	LMG	C13-C14-C15-C16
28	H	102	DGD	O1A-C1A-O1G-C1G
23	b	612	CLA	C8-C10-C11-C12
23	c	506	CLA	C8-C10-C11-C12
33	D	407	LMG	O6-C5-C6-O5
27	B	621	SQD	C34-C35-C36-C37
33	C	501	LMG	C38-C39-C40-C41
24	a	407	PHO	O2A-C1-C2-C3
27	b	601	SQD	C46-C45-O47-C7
28	C	518	DGD	C7A-C8A-C9A-CAA
25	b	619	BCR	C10-C11-C12-C13
25	b	619	BCR	C18-C19-C20-C21
23	C	507	CLA	C13-C15-C16-C17
27	b	601	SQD	C13-C14-C15-C16
28	a	413	DGD	C2A-C3A-C4A-C5A
23	D	404	CLA	C16-C17-C18-C20
23	c	504	CLA	C11-C12-C13-C14
29	L	101	LHG	C33-C34-C35-C36
33	D	411	LMG	C16-C17-C18-C19
33	d	410	LMG	C34-C35-C36-C37
33	D	410	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	c	514	BCR	C16-C17-C18-C19
25	d	405	BCR	C20-C21-C22-C23
33	C	519	LMG	C11-C12-C13-C14
23	b	616	CLA	C5-C6-C7-C8
23	C	505	CLA	C11-C12-C13-C14
33	D	411	LMG	C34-C35-C36-C37
26	A	409	PL9	C25-C24-C26-C27
23	A	407	CLA	C6-C7-C8-C9
27	A	410	SQD	C24-C25-C26-C27
28	C	516	DGD	C2B-C3B-C4B-C5B
29	E	101	LHG	C24-C25-C26-C27
28	C	516	DGD	C4B-C5B-C6B-C7B
28	C	517	DGD	C2B-C3B-C4B-C5B
29	d	407	LHG	C16-C17-C18-C19
33	c	522	LMG	C40-C41-C42-C43
33	m	101	LMG	C37-C38-C39-C40
27	A	410	SQD	O6-C44-C45-O47
33	C	501	LMG	O1-C7-C8-O7
33	d	410	LMG	C28-C29-C30-C31
28	C	518	DGD	C6B-C7B-C8B-C9B
28	c	518	DGD	C6B-C7B-C8B-C9B
33	D	410	LMG	C28-C29-C30-C31
28	h	101	DGD	C6A-C7A-C8A-C9A
29	L	101	LHG	C12-C13-C14-C15
29	D	409	LHG	C17-C18-C19-C20
28	C	516	DGD	O6D-C5D-C6D-O5D
28	a	413	DGD	CFA-CGA-CHA-CIA
26	A	409	PL9	C24-C26-C27-C28
29	A	413	LHG	C18-C19-C20-C21
33	C	519	LMG	C40-C41-C42-C43
27	a	411	SQD	C18-C19-C20-C21
28	c	518	DGD	C5B-C6B-C7B-C8B
33	b	622	LMG	C38-C39-C40-C41
26	a	410	PL9	C32-C33-C34-C35
29	e	101	LHG	C28-C29-C30-C31
23	b	608	CLA	C8-C10-C11-C12
23	B	609	CLA	C4-C3-C5-C6
26	a	410	PL9	C40-C39-C41-C42
26	d	406	PL9	C45-C44-C46-C47
27	A	410	SQD	C15-C16-C17-C18
29	E	101	LHG	C13-C14-C15-C16
28	c	517	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
29	A	413	LHG	C25-C26-C27-C28
29	e	101	LHG	O9-C7-O7-C5
27	F	101	SQD	C45-C44-O6-C1
29	d	409	LHG	O1-C1-C2-O2
23	B	604	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C10-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C14
23	b	608	CLA	C6-C7-C8-C9
23	b	613	CLA	C14-C13-C15-C16
27	A	411	SQD	C27-C28-C29-C30
27	F	101	SQD	C30-C31-C32-C33
29	e	101	LHG	C11-C12-C13-C14
23	B	616	CLA	C5-C6-C7-C8
23	C	507	CLA	C8-C10-C11-C12
23	a	405	CLA	C15-C16-C17-C18
23	D	403	CLA	C4B-C3B-CAB-CBB
28	c	518	DGD	C2A-C3A-C4A-C5A
23	b	614	CLA	C8-C10-C11-C12
28	c	518	DGD	CDB-CEB-CFB-CGB
33	m	101	LMG	C32-C33-C34-C35
29	l	101	LHG	C24-C23-O8-C6
33	D	407	LMG	C38-C39-C40-C41
33	m	101	LMG	C19-C20-C21-C22
33	D	411	LMG	C37-C38-C39-C40
28	C	517	DGD	CCA-CDA-CEA-CFA
28	H	102	DGD	C3B-C4B-C5B-C6B
23	B	604	CLA	C11-C10-C8-C7
23	B	604	CLA	C12-C13-C15-C16
23	B	605	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C12-C13-C15
23	C	509	CLA	C11-C10-C8-C7
23	C	511	CLA	C12-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C7
23	D	404	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C12-C13-C15
23	b	605	CLA	C11-C12-C13-C15
23	b	605	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C10-C8-C7
23	b	609	CLA	C11-C12-C13-C15
23	b	610	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C12-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C15
23	c	505	CLA	C6-C7-C8-C10
23	c	509	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
24	a	407	PHO	C6-C7-C8-C10
33	D	410	LMG	C37-C38-C39-C40
28	C	518	DGD	CBA-CCA-CDA-CEA
27	a	412	SQD	C31-C32-C33-C34
33	m	101	LMG	C29-C30-C31-C32
27	f	101	SQD	C25-C26-C27-C28
23	B	604	CLA	C2C-C3C-CAC-CBC
28	c	517	DGD	CAB-CBB-CCB-CDB
29	d	407	LHG	C19-C20-C21-C22
33	C	501	LMG	C30-C31-C32-C33
33	D	411	LMG	C14-C15-C16-C17
33	C	519	LMG	C18-C19-C20-C21
23	C	514	CLA	C10-C11-C12-C13
23	c	513	CLA	C5-C6-C7-C8
29	d	407	LHG	C10-C11-C12-C13
27	a	412	SQD	C26-C27-C28-C29
29	l	101	LHG	C35-C36-C37-C38
33	M	101	LMG	C19-C20-C21-C22
23	B	603	CLA	CBA-CGA-O2A-C1
33	C	519	LMG	C31-C32-C33-C34
27	a	412	SQD	C17-C18-C19-C20
27	a	412	SQD	C29-C30-C31-C32
33	D	407	LMG	C40-C41-C42-C43
23	C	506	CLA	C16-C17-C18-C19
23	C	514	CLA	C13-C15-C16-C17
27	A	410	SQD	C32-C33-C34-C35
28	a	413	DGD	C1G-C2G-C3G-O3G
27	b	601	SQD	C25-C26-C27-C28
23	C	507	CLA	C4-C3-C5-C6
23	C	507	CLA	C2-C3-C5-C6
27	b	601	SQD	C30-C31-C32-C33
23	A	404	CLA	C4C-C3C-CAC-CBC
29	D	408	LHG	C16-C17-C18-C19
29	l	101	LHG	O6-C4-C5-O7
28	C	518	DGD	CDB-CEB-CFB-CGB
25	C	520	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	C	520	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C30
25	k	101	BCR	C1-C6-C7-C8
28	H	102	DGD	C1A-C2A-C3A-C4A
29	d	409	LHG	C32-C33-C34-C35
33	d	411	LMG	C35-C36-C37-C38
28	c	518	DGD	C3A-C4A-C5A-C6A
23	B	614	CLA	C8-C10-C11-C12
23	c	509	CLA	C2C-C3C-CAC-CBC
27	a	412	SQD	C11-C10-C9-C8
27	b	601	SQD	C26-C27-C28-C29
28	C	517	DGD	C8A-C9A-CAA-CBA
29	L	101	LHG	C25-C26-C27-C28
29	l	101	LHG	C24-C25-C26-C27
33	c	522	LMG	C12-C13-C14-C15
23	B	607	CLA	C16-C17-C18-C19
23	B	611	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	C	506	CLA	C16-C17-C18-C20
23	A	404	CLA	C2C-C3C-CAC-CBC
23	c	513	CLA	C13-C15-C16-C17
27	a	411	SQD	O6-C44-C45-O47
27	a	412	SQD	O47-C45-C46-O48
33	M	101	LMG	O7-C8-C9-O8
26	A	409	PL9	C4-C3-C7-C8
26	d	406	PL9	C4-C3-C7-C8
27	A	411	SQD	C28-C29-C30-C31
27	A	410	SQD	C26-C27-C28-C29
27	B	621	SQD	C23-C24-C25-C26
33	c	519	LMG	O10-C28-O8-C9
26	d	406	PL9	C15-C14-C16-C17
33	C	501	LMG	C33-C34-C35-C36
33	D	407	LMG	C16-C17-C18-C19
23	B	609	CLA	C2-C3-C5-C6
23	B	614	CLA	C2-C3-C5-C6
28	A	412	DGD	CFA-CGA-CHA-CIA
27	b	601	SQD	C15-C16-C17-C18
33	D	410	LMG	C12-C13-C14-C15
33	m	101	LMG	C14-C15-C16-C17
23	C	511	CLA	C10-C11-C12-C13
23	D	403	CLA	C10-C11-C12-C13
29	d	409	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C11-C10-C8-C9
23	b	609	CLA	C11-C10-C8-C9
23	c	509	CLA	C14-C13-C15-C16
33	c	524	LMG	C29-C30-C31-C32
27	A	411	SQD	C24-C25-C26-C27
29	D	408	LHG	C12-C13-C14-C15
25	k	101	BCR	C14-C15-C16-C17
29	E	101	LHG	C9-C10-C11-C12
23	c	507	CLA	C16-C17-C18-C19
28	C	516	DGD	C6B-C7B-C8B-C9B
29	d	409	LHG	C25-C26-C27-C28
33	d	411	LMG	C13-C14-C15-C16
23	b	616	CLA	C8-C10-C11-C12
24	A	406	PHO	C2C-C3C-CAC-CBC
29	D	408	LHG	C33-C34-C35-C36
27	a	412	SQD	O6-C44-C45-O47
28	A	412	DGD	C8B-C9B-CAB-CBB
23	B	613	CLA	C5-C6-C7-C8
27	A	411	SQD	C19-C20-C21-C22
29	E	101	LHG	O1-C1-C2-O2
29	d	408	LHG	O1-C1-C2-O2
25	K	101	BCR	C19-C20-C21-C22
26	D	406	PL9	C13-C14-C16-C17
26	D	406	PL9	C28-C29-C31-C32
23	B	601	CLA	C15-C16-C17-C18
23	c	504	CLA	C8-C10-C11-C12
28	c	517	DGD	C8A-C9A-CAA-CBA
29	d	408	LHG	C15-C16-C17-C18
27	F	101	SQD	C27-C28-C29-C30
28	a	413	DGD	CAB-CBB-CCB-CDB
29	E	101	LHG	C16-C17-C18-C19
25	H	101	BCR	C11-C10-C9-C34
25	H	101	BCR	C35-C13-C14-C15
25	H	101	BCR	C16-C17-C18-C36
25	K	101	BCR	C16-C17-C18-C36
25	a	409	BCR	C11-C10-C9-C34
25	b	618	BCR	C11-C10-C9-C34
25	t	101	BCR	C16-C17-C18-C36
27	f	101	SQD	O10-C23-O48-C46
29	D	408	LHG	C28-C29-C30-C31
23	c	501	CLA	C8-C10-C11-C12
23	c	508	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	c	516	DGD	C2A-C3A-C4A-C5A
29	E	101	LHG	C33-C34-C35-C36
29	D	409	LHG	O6-C4-C5-C6
25	C	520	BCR	C37-C22-C23-C24
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
23	C	510	CLA	C12-C13-C15-C16
23	C	511	CLA	C11-C10-C8-C7
23	C	514	CLA	C12-C13-C15-C16
23	D	404	CLA	C12-C13-C15-C16
23	b	605	CLA	C11-C10-C8-C7
23	d	404	CLA	C11-C12-C13-C15
27	a	411	SQD	C28-C29-C30-C31
33	D	410	LMG	C34-C35-C36-C37
25	K	101	BCR	C7-C8-C9-C10
25	x	102	BCR	C11-C12-C13-C14
25	x	102	BCR	C17-C18-C19-C20
23	B	612	CLA	CBA-CGA-O2A-C1
29	D	408	LHG	C18-C19-C20-C21
23	B	612	CLA	O1A-CGA-O2A-C1
28	c	517	DGD	O1A-C1A-O1G-C1G
33	C	519	LMG	O10-C28-O8-C9
27	A	410	SQD	C5-C6-S-O8
27	B	621	SQD	C45-C44-O6-C1
27	b	601	SQD	C5-C6-S-O8
28	C	517	DGD	C2G-C3G-O3G-C1D
28	C	517	DGD	C5D-C6D-O5D-C1E
29	D	409	LHG	C23-C24-C25-C26
28	c	516	DGD	O1B-C1B-O2G-C2G
26	A	409	PL9	C13-C14-C16-C17
29	E	101	LHG	C29-C30-C31-C32
29	d	408	LHG	O1-C1-C2-C3
33	D	410	LMG	C15-C16-C17-C18
23	d	403	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	O2A-C1-C2-C3
23	B	605	CLA	C15-C16-C17-C18
23	C	512	CLA	C8-C10-C11-C12
33	m	101	LMG	C40-C41-C42-C43
28	c	516	DGD	C2B-C3B-C4B-C5B
33	C	501	LMG	C17-C18-C19-C20
23	B	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	D	408	LHG	O10-C23-O8-C6
25	B	617	BCR	C16-C17-C18-C19
25	c	515	BCR	C12-C13-C14-C15
25	x	102	BCR	C11-C10-C9-C8
33	d	410	LMG	C39-C40-C41-C42
23	B	612	CLA	C15-C16-C17-C18
29	D	409	LHG	O6-C4-C5-O7
27	F	101	SQD	C32-C33-C34-C35
27	A	410	SQD	O6-C44-C45-C46
33	b	622	LMG	C7-C8-C9-O8
33	c	522	LMG	O1-C7-C8-C9
33	c	522	LMG	C7-C8-C9-O8
29	L	101	LHG	C35-C36-C37-C38
34	e	102	HEM	C4B-C3B-CAB-CBB
23	c	504	CLA	C11-C12-C13-C15
23	C	506	CLA	C4-C3-C5-C6
23	b	603	CLA	C8-C10-C11-C12
23	b	610	CLA	C3-C5-C6-C7
28	C	516	DGD	CBA-CCA-CDA-CEA
33	d	410	LMG	C36-C37-C38-C39
27	b	601	SQD	O6-C44-C45-O47
28	C	516	DGD	O2G-C2G-C3G-O3G
33	c	522	LMG	O7-C8-C9-O8
23	D	403	CLA	C14-C13-C15-C16
23	c	510	CLA	C11-C12-C13-C14
23	C	511	CLA	C16-C17-C18-C20
28	c	518	DGD	C2B-C3B-C4B-C5B
29	L	101	LHG	C10-C11-C12-C13
33	M	101	LMG	C33-C34-C35-C36
33	c	519	LMG	C38-C39-C40-C41
28	C	518	DGD	CBB-CCB-CDB-CEB
33	C	501	LMG	C39-C40-C41-C42
28	H	102	DGD	CBA-CCA-CDA-CEA
28	C	516	DGD	C4D-C5D-C6D-O5D
23	B	615	CLA	C16-C17-C18-C19
23	b	614	CLA	C13-C15-C16-C17
23	c	502	CLA	C3-C5-C6-C7
33	c	519	LMG	C28-C29-C30-C31
23	b	608	CLA	C5-C6-C7-C8
23	B	603	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C16-C17-C18-C19
29	d	408	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	M	101	LMG	C14-C15-C16-C17
29	L	101	LHG	C14-C15-C16-C17
27	a	411	SQD	C23-C24-C25-C26
23	B	610	CLA	C8-C10-C11-C12
23	c	513	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	CBA-CGA-O2A-C1
23	B	601	CLA	C4-C3-C5-C6
23	C	507	CLA	C10-C11-C12-C13
25	b	618	BCR	C6-C7-C8-C9
25	c	514	BCR	C22-C23-C24-C25
25	k	101	BCR	C17-C18-C19-C20
29	D	409	LHG	C31-C32-C33-C34
33	m	101	LMG	C30-C31-C32-C33
29	E	101	LHG	C10-C11-C12-C13
28	H	102	DGD	C5A-C6A-C7A-C8A
28	C	516	DGD	O1B-C1B-O2G-C2G
29	A	413	LHG	C24-C25-C26-C27
23	B	606	CLA	C11-C12-C13-C15
23	B	612	CLA	C11-C10-C8-C7
23	B	616	CLA	C6-C7-C8-C10
23	C	503	CLA	C6-C7-C8-C10
23	C	513	CLA	C12-C13-C15-C16
23	b	603	CLA	C6-C7-C8-C10
23	b	608	CLA	C11-C12-C13-C15
23	b	616	CLA	C11-C10-C8-C7
23	c	503	CLA	C11-C10-C8-C7
23	c	509	CLA	C11-C12-C13-C15
23	c	512	CLA	C11-C10-C8-C7
23	d	403	CLA	C6-C7-C8-C10
24	A	406	PHO	C12-C13-C15-C16
28	c	518	DGD	CCB-CDB-CEB-CFB
23	C	513	CLA	C16-C17-C18-C20
33	C	519	LMG	C30-C31-C32-C33
33	d	411	LMG	C38-C39-C40-C41
33	D	410	LMG	C11-C12-C13-C14
23	D	404	CLA	O1A-CGA-O2A-C1
23	C	507	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C4-C3-C5-C6
29	L	101	LHG	C19-C20-C21-C22
28	C	518	DGD	C3B-C4B-C5B-C6B
28	C	516	DGD	O1G-C1A-C2A-C3A
23	B	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	C36-C37-C38-C39
23	D	404	CLA	CBA-CGA-O2A-C1
27	f	101	SQD	C35-C36-C37-C38
23	c	513	CLA	C14-C13-C15-C16
25	b	619	BCR	C9-C10-C11-C12
25	d	405	BCR	C9-C10-C11-C12
23	B	610	CLA	C16-C17-C18-C19
23	b	614	CLA	O1D-CGD-O2D-CED
27	A	410	SQD	C25-C26-C27-C28
33	d	410	LMG	C11-C12-C13-C14
28	c	518	DGD	CAA-CBA-CCA-CDA
23	a	406	CLA	C15-C16-C17-C18
28	C	516	DGD	O1G-C1G-C2G-O2G
33	c	522	LMG	O1-C7-C8-O7
23	C	503	CLA	C10-C11-C12-C13
29	E	101	LHG	C18-C19-C20-C21
33	b	622	LMG	C35-C36-C37-C38
28	A	412	DGD	C1G-C2G-C3G-O3G
28	C	516	DGD	C1G-C2G-C3G-O3G
33	M	101	LMG	C7-C8-C9-O8
23	c	509	CLA	O1A-CGA-O2A-C1
23	C	506	CLA	C2-C3-C5-C6
27	f	101	SQD	C24-C25-C26-C27
28	H	102	DGD	C9B-CAB-CBB-CCB
23	B	601	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	C	514	CLA	CAD-CBD-CGD-O2D
23	b	606	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
33	b	622	LMG	C42-C43-C44-C45
28	C	517	DGD	O6D-C1D-O3G-C3G
23	c	507	CLA	C8-C10-C11-C12
23	b	610	CLA	C16-C17-C18-C19
27	B	621	SQD	C25-C26-C27-C28
28	c	516	DGD	C5B-C6B-C7B-C8B
23	C	512	CLA	O1A-CGA-O2A-C1
23	c	506	CLA	O1A-CGA-O2A-C1
27	A	411	SQD	C32-C33-C34-C35
28	c	518	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	514	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	617	CLA	CHA-CBD-CGD-O1D
23	b	617	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
25	K	101	BCR	C13-C14-C15-C16
25	c	514	BCR	C15-C16-C17-C18
25	c	521	BCR	C9-C10-C11-C12
29	D	408	LHG	C3-O3-P-O4
29	D	408	LHG	C4-O6-P-O5
29	E	101	LHG	C4-O6-P-O3
29	d	408	LHG	C3-O3-P-O5
29	l	101	LHG	C4-O6-P-O3
23	c	512	CLA	C4-C3-C5-C6
26	A	409	PL9	C20-C19-C21-C22
23	D	403	CLA	C2B-C3B-CAB-CBB
25	A	408	BCR	C5-C6-C7-C8
28	C	518	DGD	C2A-C3A-C4A-C5A
28	H	102	DGD	O2G-C1B-C2B-C3B
23	b	612	CLA	C2-C3-C5-C6
23	B	601	CLA	C8-C10-C11-C12
29	A	413	LHG	C19-C20-C21-C22
29	L	101	LHG	O9-C7-O7-C5
28	C	518	DGD	C4B-C5B-C6B-C7B
28	h	101	DGD	C5A-C6A-C7A-C8A
29	L	101	LHG	C31-C32-C33-C34
29	A	413	LHG	C29-C30-C31-C32
26	a	410	PL9	C4-C3-C7-C8
29	L	101	LHG	C29-C30-C31-C32
28	c	517	DGD	C7B-C8B-C9B-CAB
23	c	511	CLA	C15-C16-C17-C18
28	a	413	DGD	C1G-C2G-O2G-C1B
33	C	501	LMG	C9-C8-O7-C10
33	D	410	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
33	C	519	LMG	C14-C15-C16-C17
23	C	503	CLA	C15-C16-C17-C18
23	b	614	CLA	C5-C6-C7-C8
27	A	410	SQD	C30-C31-C32-C33
29	l	101	LHG	C19-C20-C21-C22
29	d	408	LHG	C13-C14-C15-C16
23	c	512	CLA	C16-C17-C18-C19
23	b	612	CLA	C5-C6-C7-C8
29	d	407	LHG	C27-C28-C29-C30
23	d	403	CLA	C3-C5-C6-C7
28	H	102	DGD	CCB-CDB-CEB-CFB
23	B	605	CLA	C14-C13-C15-C16
23	C	510	CLA	C14-C13-C15-C16
23	D	404	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C12-C13-C14
23	b	608	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
29	E	101	LHG	O6-C4-C5-O7
23	b	610	CLA	C16-C17-C18-C20
23	d	404	CLA	C16-C17-C18-C19
28	c	517	DGD	CDA-CEA-CFA-CGA
27	B	621	SQD	C11-C10-C9-C8
24	a	407	PHO	C4-C3-C5-C6
33	m	101	LMG	C15-C16-C17-C18
29	d	407	LHG	C31-C32-C33-C34
23	B	609	CLA	C16-C17-C18-C19
27	b	601	SQD	O47-C45-C46-O48
25	d	405	BCR	C19-C20-C21-C22
28	c	518	DGD	C5A-C6A-C7A-C8A
23	B	602	CLA	C16-C17-C18-C19
28	c	516	DGD	C8A-C9A-CAA-CBA
23	b	615	CLA	C2A-CAA-CBA-CGA
23	C	511	CLA	C16-C17-C18-C19
23	C	504	CLA	C10-C11-C12-C13
29	D	408	LHG	C23-C24-C25-C26
33	b	622	LMG	C30-C31-C32-C33
33	c	524	LMG	C19-C20-C21-C22
33	c	522	LMG	C37-C38-C39-C40
33	d	410	LMG	C29-C30-C31-C32
28	c	516	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	C5D-C6D-O5D-C1E
33	m	101	LMG	C8-C7-O1-C1
29	D	409	LHG	C16-C17-C18-C19
27	A	411	SQD	C30-C31-C32-C33
28	c	516	DGD	CAB-CBB-CCB-CDB
29	D	409	LHG	C1-C2-C3-O3
29	E	101	LHG	C30-C31-C32-C33
29	e	101	LHG	C7-C8-C9-C10
33	D	407	LMG	C28-C29-C30-C31
23	B	606	CLA	C11-C12-C13-C14
23	B	612	CLA	C11-C10-C8-C9
23	C	506	CLA	C14-C13-C15-C16
23	C	507	CLA	C11-C12-C13-C14
23	a	406	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	c	503	CLA	C11-C10-C8-C9
23	c	513	CLA	C6-C7-C8-C9
24	a	407	PHO	C6-C7-C8-C9
33	D	407	LMG	C15-C16-C17-C18
23	c	506	CLA	CBA-CGA-O2A-C1
33	c	524	LMG	C32-C33-C34-C35
28	C	516	DGD	CAA-CBA-CCA-CDA
23	A	407	CLA	CBA-CGA-O2A-C1
23	b	615	CLA	CBA-CGA-O2A-C1
24	A	406	PHO	CBA-CGA-O2A-C1
23	B	602	CLA	C8-C10-C11-C12
23	c	510	CLA	C4-C3-C5-C6
33	c	519	LMG	C4-C5-C6-O5
28	H	102	DGD	C6B-C7B-C8B-C9B
28	c	517	DGD	C3A-C4A-C5A-C6A
23	a	406	CLA	C13-C15-C16-C17
33	C	501	LMG	C11-C12-C13-C14
23	B	606	CLA	C6-C7-C8-C10
23	C	507	CLA	C11-C12-C13-C15
23	C	507	CLA	C12-C13-C15-C16
23	b	613	CLA	C6-C7-C8-C10
23	c	502	CLA	C11-C12-C13-C15
33	D	407	LMG	C21-C22-C23-C24
28	c	518	DGD	C9A-CAA-CBA-CCA
29	L	101	LHG	C24-C25-C26-C27
23	C	503	CLA	O1A-CGA-O2A-C1
28	c	517	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
33	b	622	LMG	O7-C8-C9-O8
26	a	410	PL9	C7-C8-C9-C10
29	l	101	LHG	C14-C15-C16-C17
23	B	601	CLA	C2-C3-C5-C6
23	c	512	CLA	C2-C3-C5-C6
27	a	411	SQD	C24-C25-C26-C27
28	H	102	DGD	CAA-CBA-CCA-CDA
25	B	619	BCR	C20-C21-C22-C37
25	C	515	BCR	C35-C13-C14-C15
28	A	412	DGD	CCB-CDB-CEB-CFB
23	a	406	CLA	C8-C10-C11-C12
29	E	101	LHG	C2-C3-O3-P
33	M	101	LMG	C40-C41-C42-C43
28	c	516	DGD	C7B-C8B-C9B-CAB
23	B	609	CLA	C5-C6-C7-C8
23	c	503	CLA	C15-C16-C17-C18
27	a	412	SQD	C27-C28-C29-C30
25	k	101	BCR	C11-C12-C13-C14
28	c	517	DGD	CCA-CDA-CEA-CFA
23	B	610	CLA	C16-C17-C18-C20
28	h	101	DGD	C7B-C8B-C9B-CAB
35	v	201	HEC	CAD-CBD-CGD-O1D
33	M	101	LMG	C32-C33-C34-C35
23	b	615	CLA	O1A-CGA-O2A-C1
23	C	507	CLA	C14-C13-C15-C16
23	C	512	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	b	613	CLA	C6-C7-C8-C9
23	b	615	CLA	C6-C7-C8-C9
23	c	502	CLA	C11-C12-C13-C14
23	c	512	CLA	C11-C12-C13-C14
29	l	101	LHG	C34-C35-C36-C37
28	C	516	DGD	CAB-CBB-CCB-CDB
27	f	101	SQD	C44-C45-O47-C7
27	f	101	SQD	C46-C45-O47-C7
23	C	506	CLA	C8-C10-C11-C12
34	E	103	HEM	CAD-CBD-CGD-O2D
28	H	102	DGD	C1B-C2B-C3B-C4B
23	B	602	CLA	C16-C17-C18-C20
27	F	101	SQD	O48-C23-C24-C25
23	A	407	CLA	O1A-CGA-O2A-C1
27	A	410	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
28	C	518	DGD	CDA-CEA-CFA-CGA
33	D	411	LMG	O8-C28-C29-C30
23	C	502	CLA	C2A-CAA-CBA-CGA
25	A	408	BCR	C20-C21-C22-C23
23	B	610	CLA	C2C-C3C-CAC-CBC
23	C	507	CLA	CBA-CGA-O2A-C1
35	v	201	HEC	CAD-CBD-CGD-O2D
28	a	413	DGD	C1A-C2A-C3A-C4A
33	c	522	LMG	C28-C29-C30-C31
29	e	101	LHG	C13-C14-C15-C16
23	B	601	CLA	C2B-C3B-CAB-CBB
23	D	404	CLA	C2B-C3B-CAB-CBB
25	K	101	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C26
33	d	410	LMG	O9-C10-C11-C12
33	M	101	LMG	O6-C5-C6-O5
23	b	602	CLA	C16-C17-C18-C20
28	A	412	DGD	C3B-C4B-C5B-C6B
34	e	102	HEM	CAD-CBD-CGD-O1D
23	B	613	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
27	A	410	SQD	C17-C18-C19-C20
24	A	406	PHO	O1A-CGA-O2A-C1
27	b	601	SQD	O49-C7-O47-C45
33	D	411	LMG	O10-C28-C29-C30
23	C	514	CLA	C11-C10-C8-C7
23	a	406	CLA	C6-C7-C8-C10
23	a	406	CLA	C11-C10-C8-C7
23	b	605	CLA	C6-C7-C8-C10
23	c	502	CLA	C6-C7-C8-C10
23	c	509	CLA	C12-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C10
23	c	512	CLA	C12-C13-C15-C16
28	a	413	DGD	O1G-C1G-C2G-O2G
29	e	101	LHG	O7-C5-C6-O8
33	D	410	LMG	C29-C30-C31-C32
26	a	410	PL9	C37-C38-C39-C40
28	a	413	DGD	O2G-C1B-C2B-C3B
23	c	512	CLA	C16-C17-C18-C20
23	c	508	CLA	C15-C16-C17-C18
26	a	410	PL9	C35-C34-C36-C37
23	c	510	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	B	621	SQD	C35-C36-C37-C38
33	b	622	LMG	C12-C13-C14-C15
23	b	616	CLA	C14-C13-C15-C16
23	c	505	CLA	C11-C10-C8-C9
33	D	410	LMG	C31-C32-C33-C34
23	b	609	CLA	C13-C15-C16-C17
28	A	412	DGD	CBB-CCB-CDB-CEB
34	E	103	HEM	CAD-CBD-CGD-O1D
25	b	619	BCR	C22-C23-C24-C25
29	d	409	LHG	C2-C3-O3-P
33	D	411	LMG	C29-C30-C31-C32
26	d	406	PL9	C33-C34-C36-C37
28	c	516	DGD	CCA-CDA-CEA-CFA
23	B	604	CLA	C15-C16-C17-C18
23	D	402	CLA	C13-C15-C16-C17
34	e	102	HEM	CAD-CBD-CGD-O2D
33	b	622	LMG	O8-C28-C29-C30
33	C	519	LMG	O1-C7-C8-C9
23	C	507	CLA	O1A-CGA-O2A-C1
23	c	501	CLA	C2A-CAA-CBA-CGA
23	D	403	CLA	C16-C17-C18-C19
29	D	409	LHG	C15-C16-C17-C18
33	m	101	LMG	C39-C40-C41-C42
28	C	517	DGD	C3B-C4B-C5B-C6B
33	M	101	LMG	C29-C30-C31-C32
23	b	604	CLA	C4B-C3B-CAB-CBB
23	c	506	CLA	C4B-C3B-CAB-CBB
28	C	517	DGD	O1A-C1A-O1G-C1G
29	d	407	LHG	C24-C25-C26-C27
33	d	410	LMG	O7-C10-C11-C12
29	d	408	LHG	C23-C24-C25-C26
28	h	101	DGD	O2G-C1B-C2B-C3B
28	A	412	DGD	CAB-CBB-CCB-CDB
23	C	502	CLA	C16-C17-C18-C20
33	c	519	LMG	C40-C41-C42-C43
27	A	411	SQD	C26-C27-C28-C29
29	E	101	LHG	C28-C29-C30-C31
27	a	411	SQD	C16-C17-C18-C19
23	c	509	CLA	C4C-C3C-CAC-CBC
28	c	518	DGD	C7A-C8A-C9A-CAA
28	C	516	DGD	O6E-C1E-O5D-C6D
28	c	516	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
33	C	519	LMG	O6-C1-O1-C7
23	d	404	CLA	C13-C15-C16-C17
33	d	410	LMG	C12-C13-C14-C15
26	d	406	PL9	C2-C3-C7-C8
23	c	512	CLA	C11-C12-C13-C15
23	b	610	CLA	O1D-CGD-O2D-CED
27	a	412	SQD	C19-C20-C21-C22
25	c	521	BCR	C13-C14-C15-C16
23	B	615	CLA	C11-C12-C13-C14
23	C	504	CLA	C6-C7-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	C	514	CLA	C14-C13-C15-C16
23	b	612	CLA	C11-C10-C8-C9
23	c	504	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
33	m	101	LMG	C33-C34-C35-C36
33	D	411	LMG	O7-C10-C11-C12
23	B	613	CLA	C2-C1-O2A-CGA
23	c	512	CLA	C2-C1-O2A-CGA
23	b	610	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CAA-CBA-CGA-O2A
28	c	516	DGD	CDB-CEB-CFB-CGB
23	B	602	CLA	C15-C16-C17-C18
23	D	404	CLA	O2A-C1-C2-C3
33	D	410	LMG	C14-C15-C16-C17
25	A	408	BCR	C18-C19-C20-C21
27	B	621	SQD	C33-C34-C35-C36
28	C	516	DGD	C5A-C6A-C7A-C8A
33	D	411	LMG	O9-C10-C11-C12
23	C	514	CLA	C4C-C3C-CAC-CBC
23	C	504	CLA	C15-C16-C17-C18
23	c	513	CLA	C3-C5-C6-C7
23	b	617	CLA	C10-C11-C12-C13
24	a	407	PHO	C2-C3-C5-C6
25	B	617	BCR	C11-C10-C9-C8
33	D	411	LMG	C30-C31-C32-C33
25	Z	101	BCR	C6-C7-C8-C9
23	b	606	CLA	C8-C10-C11-C12
23	C	503	CLA	CBA-CGA-O2A-C1
23	d	402	CLA	CBA-CGA-O2A-C1
27	b	601	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
28	c	516	DGD	O1G-C1G-C2G-C3G
29	e	101	LHG	C4-C5-C6-O8
33	C	501	LMG	O1-C7-C8-C9
23	b	610	CLA	C13-C15-C16-C17
23	b	604	CLA	C4-C3-C5-C6
35	V	201	HEC	CAD-CBD-CGD-O2D
23	b	604	CLA	C2-C3-C5-C6
29	L	101	LHG	C13-C14-C15-C16
23	B	604	CLA	C4C-C3C-CAC-CBC
23	B	610	CLA	C4C-C3C-CAC-CBC
23	C	510	CLA	C5-C6-C7-C8
35	V	201	HEC	CAD-CBD-CGD-O1D
28	H	102	DGD	C5B-C6B-C7B-C8B
23	b	614	CLA	CAA-CBA-CGA-O2A
28	C	516	DGD	CDA-CEA-CFA-CGA
29	e	101	LHG	C25-C26-C27-C28
23	B	603	CLA	C11-C10-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C10-C8-C9
33	c	524	LMG	O8-C28-C29-C30
23	B	605	CLA	C11-C10-C8-C7
23	B	612	CLA	C11-C12-C13-C15
23	B	615	CLA	C11-C12-C13-C15
23	C	512	CLA	C6-C7-C8-C10
23	D	402	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	b	616	CLA	C12-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C7
23	c	504	CLA	C11-C10-C8-C7
23	c	506	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	c	511	CLA	C12-C13-C15-C16
23	B	609	CLA	C2B-C3B-CAB-CBB
23	b	613	CLA	C2B-C3B-CAB-CBB
25	H	101	BCR	C23-C24-C25-C26
25	b	618	BCR	C1-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
23	B	603	CLA	C15-C16-C17-C18
33	C	519	LMG	C32-C33-C34-C35
23	A	404	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	C2-C1-O2A-CGA
23	B	606	CLA	C16-C17-C18-C19
29	d	407	LHG	C11-C10-C9-C8
23	B	612	CLA	CAA-CBA-CGA-O2A
28	c	516	DGD	CBB-CCB-CDB-CEB
23	B	616	CLA	O1D-CGD-O2D-CED
33	D	407	LMG	C31-C32-C33-C34
27	A	410	SQD	O47-C7-C8-C9
23	B	614	CLA	C2A-CAA-CBA-CGA
27	B	621	SQD	O47-C7-C8-C9
23	C	509	CLA	C16-C17-C18-C19
23	b	613	CLA	CAA-CBA-CGA-O2A
27	a	411	SQD	C25-C26-C27-C28
23	B	603	CLA	C4-C3-C5-C6
33	m	101	LMG	O8-C28-C29-C30
23	B	602	CLA	C2A-CAA-CBA-CGA
29	d	408	LHG	C31-C32-C33-C34
33	C	501	LMG	C34-C35-C36-C37
23	b	613	CLA	C8-C10-C11-C12
29	D	409	LHG	C28-C29-C30-C31
28	H	102	DGD	CDB-CEB-CFB-CGB
23	C	513	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C10-C8-C9
23	B	613	CLA	CAA-CBA-CGA-O2A
29	L	101	LHG	O7-C7-C8-C9
23	c	508	CLA	O1A-CGA-O2A-C1
27	f	101	SQD	C44-C45-C46-O48
28	h	101	DGD	C1G-C2G-C3G-O3G
23	B	601	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C4B-C3B-CAB-CBB
23	D	404	CLA	C4B-C3B-CAB-CBB
23	c	504	CLA	C4B-C3B-CAB-CBB
23	c	512	CLA	C4B-C3B-CAB-CBB
23	C	514	CLA	CBA-CGA-O2A-C1
23	d	404	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	C3-C5-C6-C7
28	c	518	DGD	C9B-CAB-CBB-CCB
27	a	411	SQD	O47-C7-C8-C9
26	D	406	PL9	C21-C22-C23-C24
25	B	619	BCR	C11-C12-C13-C14
25	Z	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	Z	101	BCR	C11-C12-C13-C14
25	t	101	BCR	C17-C18-C19-C20
25	C	520	BCR	C19-C20-C21-C22
23	b	602	CLA	C16-C17-C18-C19
28	h	101	DGD	C3B-C4B-C5B-C6B
23	c	506	CLA	C10-C11-C12-C13
23	c	501	CLA	CAA-CBA-CGA-O2A
27	a	411	SQD	O48-C23-C24-C25
23	B	607	CLA	C15-C16-C17-C18
23	C	510	CLA	C8-C10-C11-C12
23	b	602	CLA	C13-C15-C16-C17
28	C	516	DGD	C3B-C4B-C5B-C6B
33	m	101	LMG	C21-C22-C23-C24
23	c	509	CLA	C8-C10-C11-C12
27	A	410	SQD	C5-C6-S-O9
27	b	601	SQD	C5-C6-S-O7
27	a	411	SQD	C29-C30-C31-C32
23	C	514	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	D	403	CLA	C6-C7-C8-C10
23	D	403	CLA	C11-C10-C8-C7
23	b	612	CLA	C6-C7-C8-C10
23	d	403	CLA	C11-C12-C13-C15
23	C	514	CLA	C2C-C3C-CAC-CBC
23	b	602	CLA	O2A-C1-C2-C3
23	B	603	CLA	C5-C6-C7-C8
23	b	614	CLA	C15-C16-C17-C18
27	b	601	SQD	C14-C15-C16-C17
23	B	610	CLA	C2A-CAA-CBA-CGA
27	A	411	SQD	C16-C17-C18-C19
23	B	603	CLA	C10-C11-C12-C13
27	B	621	SQD	C7-C8-C9-C10
28	a	413	DGD	C7A-C8A-C9A-CAA
23	b	605	CLA	C13-C15-C16-C17
29	E	101	LHG	C14-C15-C16-C17
23	c	510	CLA	CAA-CBA-CGA-O2A
26	a	410	PL9	C38-C39-C41-C42
28	c	517	DGD	C9A-CAA-CBA-CCA
25	A	408	BCR	C16-C17-C18-C19
28	h	101	DGD	C6B-C7B-C8B-C9B
23	C	514	CLA	O1A-CGA-O2A-C1
29	D	409	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
28	A	412	DGD	C7A-C8A-C9A-CAA
23	C	508	CLA	C5-C6-C7-C8
28	h	101	DGD	O6E-C1E-O5D-C6D
27	f	101	SQD	C27-C28-C29-C30
27	f	101	SQD	C26-C27-C28-C29
23	d	402	CLA	C2C-C3C-CAC-CBC
23	B	605	CLA	C11-C12-C13-C14
23	B	616	CLA	C6-C7-C8-C9
23	D	402	CLA	C11-C12-C13-C14
23	a	406	CLA	C11-C10-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	d	403	CLA	C6-C7-C8-C9
28	c	518	DGD	O1B-C1B-C2B-C3B
29	e	101	LHG	O10-C23-C24-C25
23	B	610	CLA	CBD-CGD-O2D-CED
27	f	101	SQD	C30-C31-C32-C33
29	D	409	LHG	O10-C23-C24-C25
23	c	505	CLA	C10-C11-C12-C13
28	C	518	DGD	C8A-C9A-CAA-CBA
29	L	101	LHG	C11-C12-C13-C14
23	b	614	CLA	CBD-CGD-O2D-CED
25	H	101	BCR	C17-C18-C19-C20
25	c	514	BCR	C7-C8-C9-C10
23	B	612	CLA	CAA-CBA-CGA-O1A
23	c	501	CLA	CAA-CBA-CGA-O1A
27	a	411	SQD	C45-C44-O6-C1
28	h	101	DGD	O2G-C2G-C3G-O3G
33	C	519	LMG	O1-C7-C8-O7
23	a	406	CLA	C3-C5-C6-C7
23	b	613	CLA	CAA-CBA-CGA-O1A
23	b	614	CLA	CAA-CBA-CGA-O1A
27	B	621	SQD	O49-C7-C8-C9
33	D	407	LMG	O7-C10-C11-C12
33	C	519	LMG	C39-C40-C41-C42
28	C	516	DGD	C6A-C7A-C8A-C9A
28	c	516	DGD	C1G-C2G-C3G-O3G
28	C	516	DGD	O1B-C1B-C2B-C3B
29	L	101	LHG	C15-C16-C17-C18
23	c	509	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	b	601	SQD	O47-C7-C8-C9
33	m	101	LMG	O7-C10-C11-C12
23	B	606	CLA	C13-C15-C16-C17
28	c	517	DGD	O6D-C5D-C6D-O5D
33	C	501	LMG	C37-C38-C39-C40
23	d	404	CLA	O1A-CGA-O2A-C1
26	a	410	PL9	C21-C22-C23-C24
33	D	410	LMG	C16-C17-C18-C19
24	d	401	PHO	C2C-C3C-CAC-CBC
28	c	518	DGD	O1G-C1A-C2A-C3A
23	B	603	CLA	C13-C15-C16-C17
23	B	607	CLA	C5-C6-C7-C8
23	C	506	CLA	CAA-CBA-CGA-O2A
23	C	513	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	C2C-C3C-CAC-CBC
26	D	406	PL9	C37-C38-C39-C41
23	c	510	CLA	CAA-CBA-CGA-O1A
33	M	101	LMG	O10-C28-C29-C30

There are no ring outliers.

98 monomers are involved in 177 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	412	DGD	5	0
23	c	511	CLA	1	0
23	c	507	CLA	1	0
25	K	101	BCR	4	0
23	C	502	CLA	2	0
25	b	619	BCR	3	0
23	D	403	CLA	2	0
30	a	415	OEX	1	0
23	d	404	CLA	1	0
23	B	601	CLA	3	0
29	d	409	LHG	1	0
26	a	410	PL9	3	0
28	a	413	DGD	2	0
23	b	604	CLA	4	0
25	t	101	BCR	7	0
27	b	601	SQD	1	0
27	a	411	SQD	1	0
25	H	101	BCR	4	0
23	C	508	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	101	BCR	1	0
26	A	409	PL9	1	0
23	C	509	CLA	1	0
23	C	511	CLA	1	0
23	B	615	CLA	1	0
23	b	602	CLA	2	0
33	c	524	LMG	3	0
23	D	402	CLA	1	0
23	b	614	CLA	2	0
23	C	514	CLA	1	0
25	B	619	BCR	2	0
33	D	411	LMG	1	0
24	d	401	PHO	3	0
28	H	102	DGD	1	0
23	c	506	CLA	2	0
23	c	510	CLA	2	0
23	C	510	CLA	4	0
34	E	103	HEM	4	0
23	b	610	CLA	2	0
25	b	618	BCR	4	0
23	B	604	CLA	1	0
33	M	101	LMG	1	0
23	d	402	CLA	1	0
25	c	514	BCR	3	0
24	D	401	PHO	3	0
25	C	515	BCR	5	0
25	B	617	BCR	1	0
25	T	101	BCR	2	0
23	b	612	CLA	1	0
25	B	618	BCR	3	0
27	A	411	SQD	2	0
27	f	101	SQD	2	0
23	B	616	CLA	1	0
29	d	408	LHG	1	0
33	D	407	LMG	3	0
23	a	408	CLA	1	0
23	b	606	CLA	2	0
23	c	508	CLA	1	0
23	a	405	CLA	1	0
26	D	406	PL9	1	0
23	C	507	CLA	2	0
23	b	617	CLA	2	0

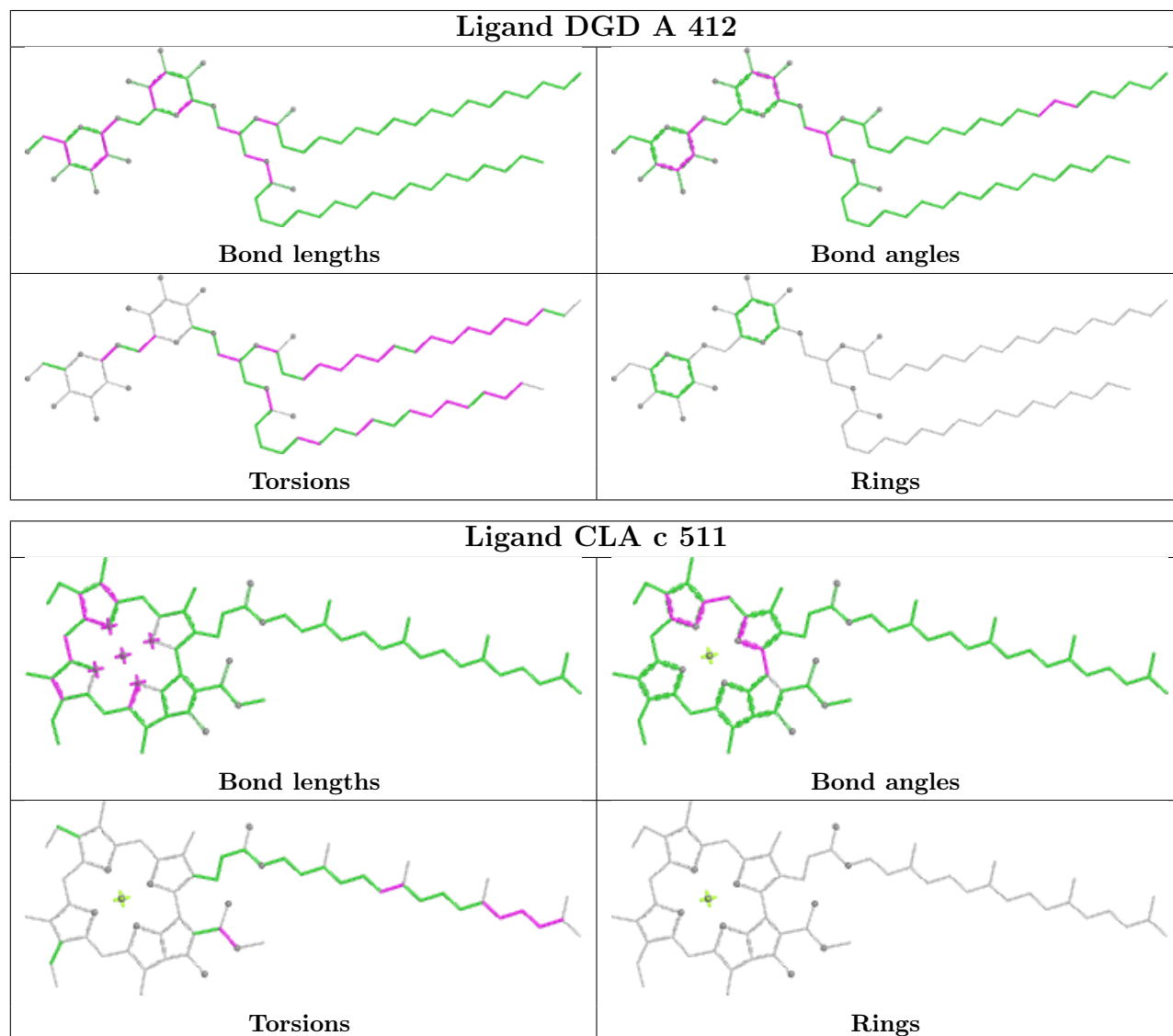
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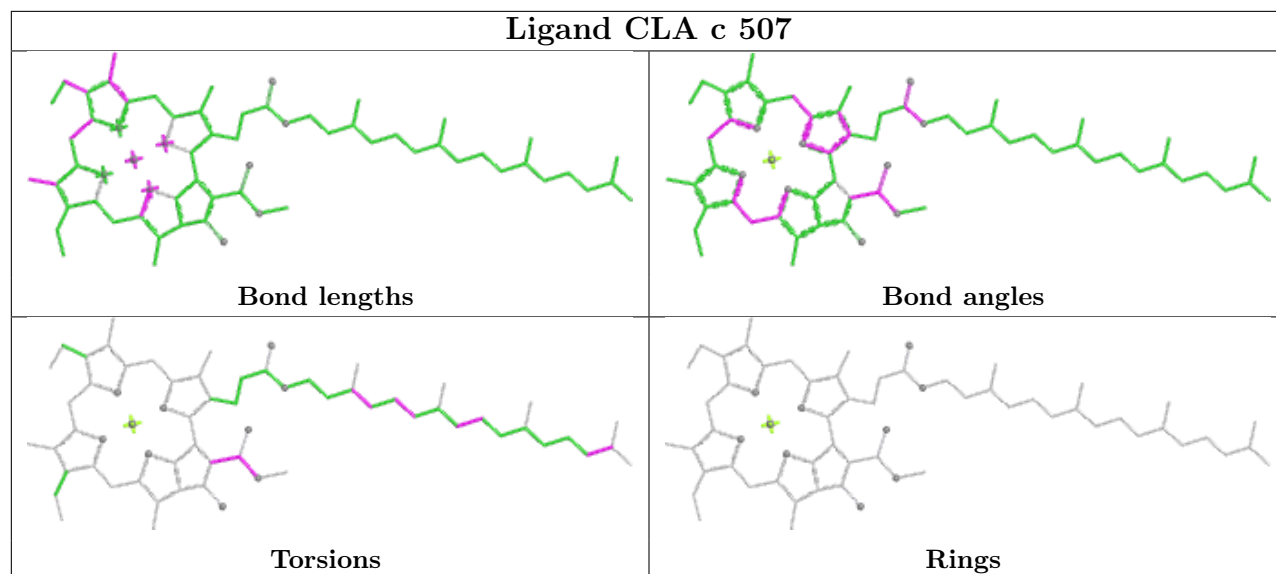
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	613	CLA	3	0
23	B	602	CLA	1	0
29	d	407	LHG	2	0
27	F	101	SQD	2	0
25	d	405	BCR	3	0
23	c	505	CLA	3	0
33	d	411	LMG	1	0
25	k	101	BCR	1	0
23	d	403	CLA	2	0
23	A	404	CLA	1	0
25	D	405	BCR	6	0
23	b	607	CLA	2	0
25	a	409	BCR	1	0
23	b	608	CLA	1	0
27	B	621	SQD	1	0
23	B	609	CLA	1	0
28	C	518	DGD	1	0
29	L	101	LHG	3	0
23	b	605	CLA	1	0
23	B	606	CLA	1	0
25	c	515	BCR	3	0
25	c	521	BCR	1	0
29	A	413	LHG	4	0
23	C	512	CLA	2	0
23	B	614	CLA	1	0
23	A	405	CLA	1	0
23	c	501	CLA	2	0
23	b	616	CLA	3	0
24	A	406	PHO	1	0
29	e	101	LHG	1	0
27	a	412	SQD	3	0
34	e	102	HEM	5	0
23	C	506	CLA	2	0
23	b	615	CLA	3	0
29	D	408	LHG	2	0
33	m	101	LMG	1	0
24	a	407	PHO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

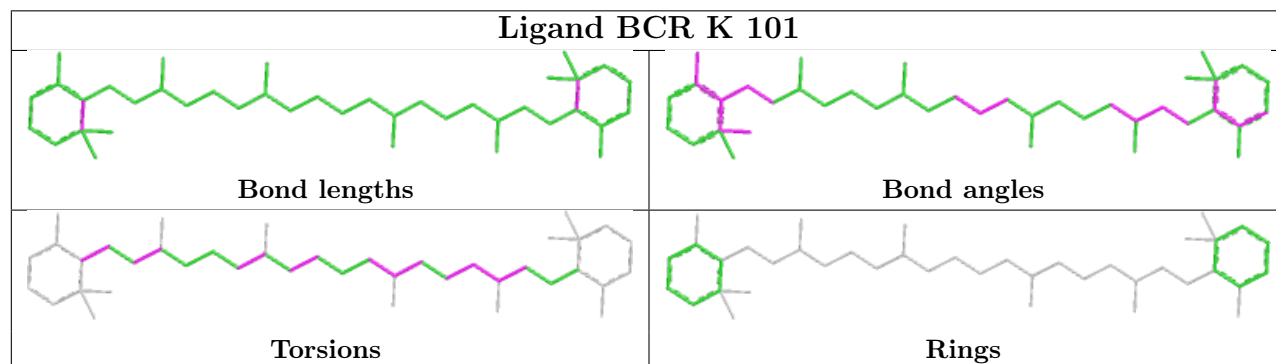
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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



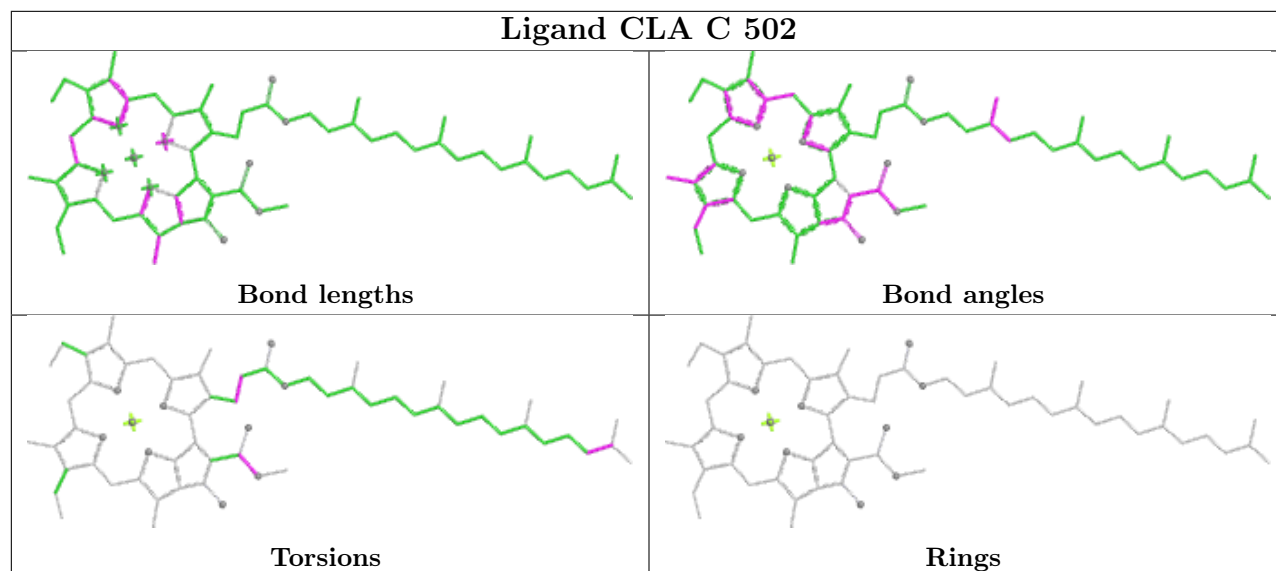
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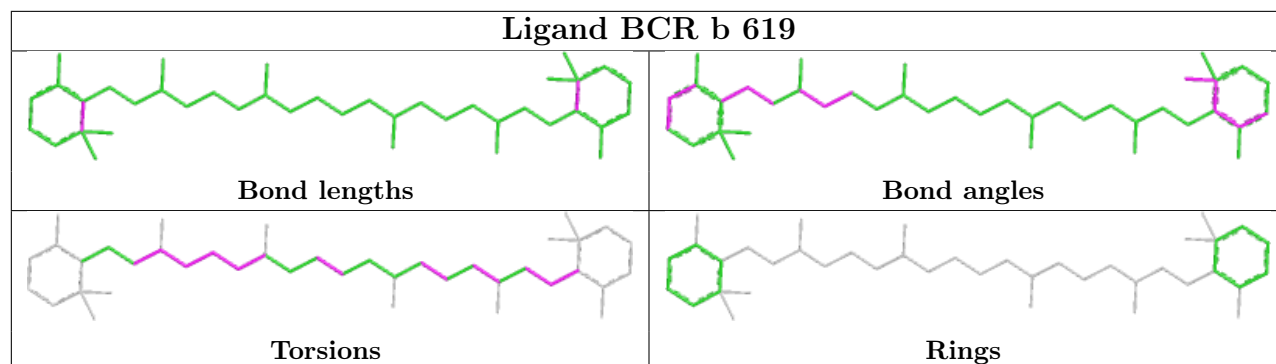
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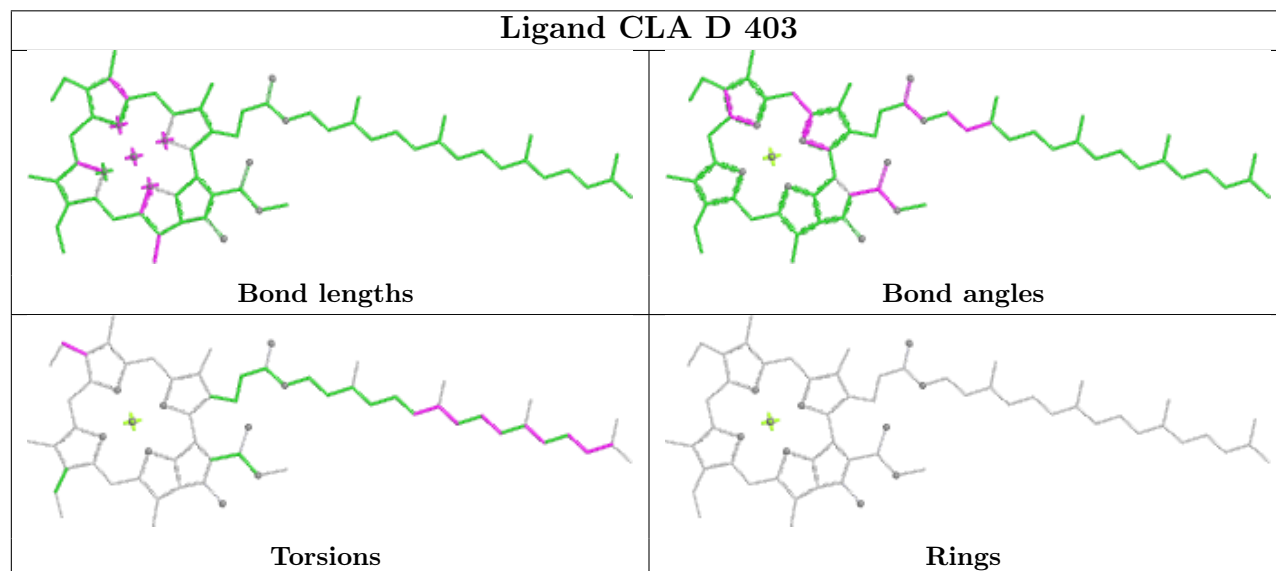
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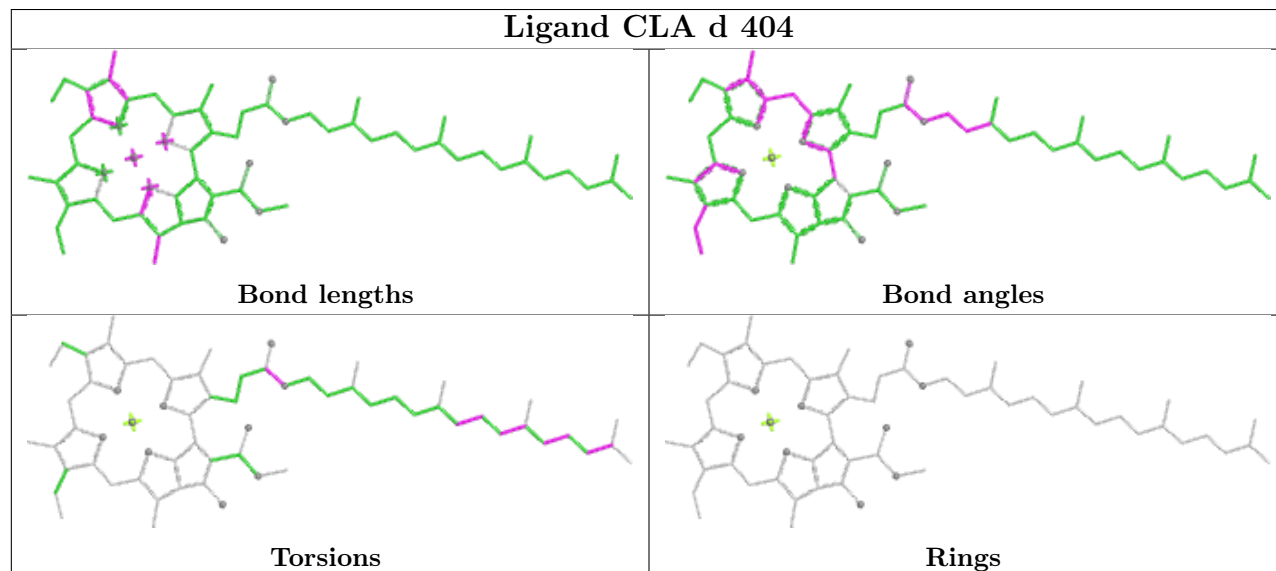
Ligand BCR b 619



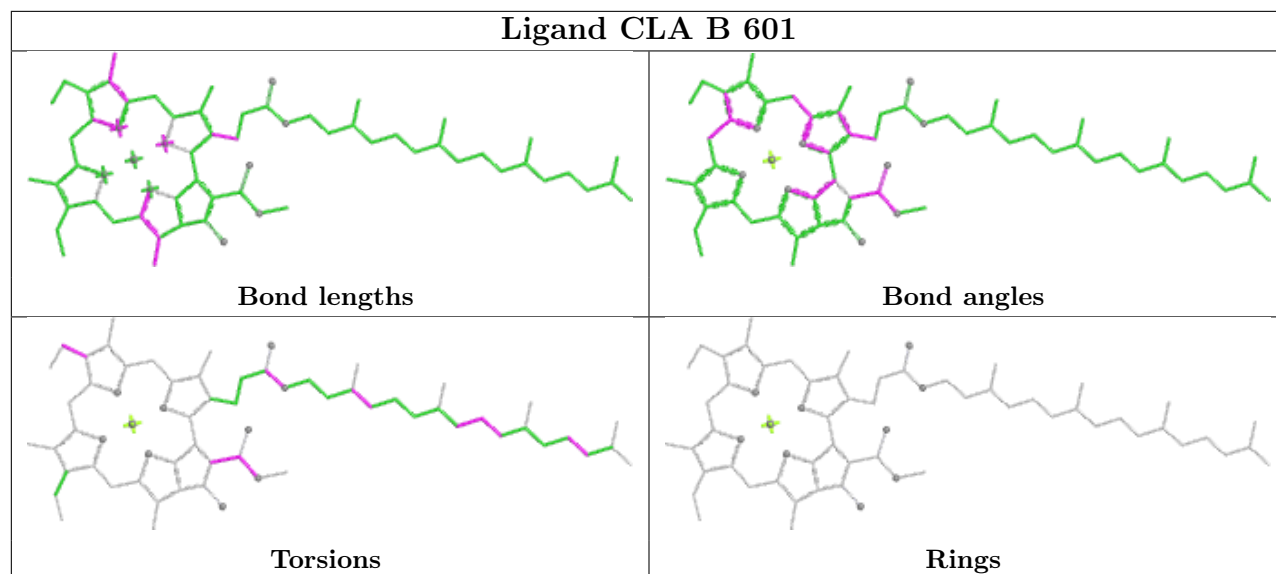
Ligand CLA D 403



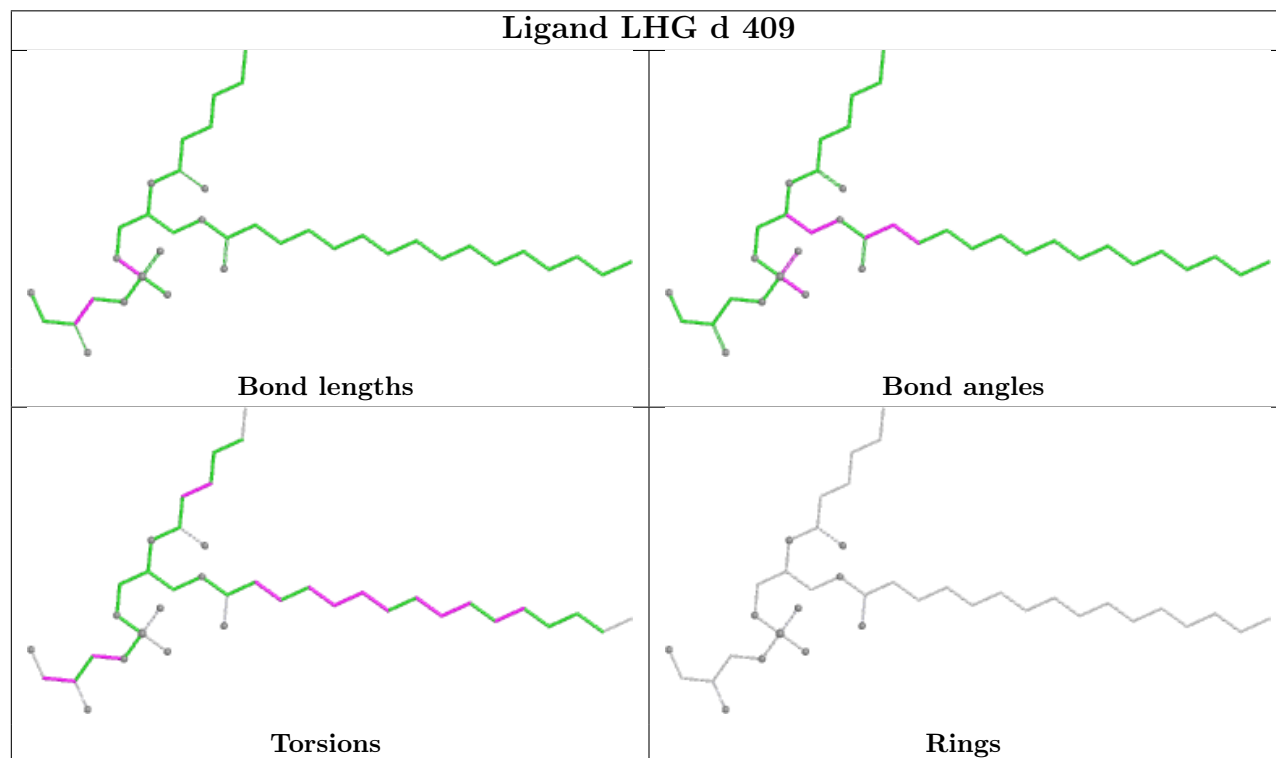
Ligand CLA d 404

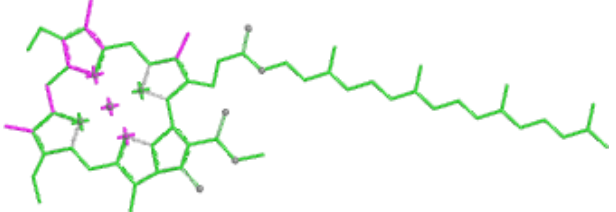
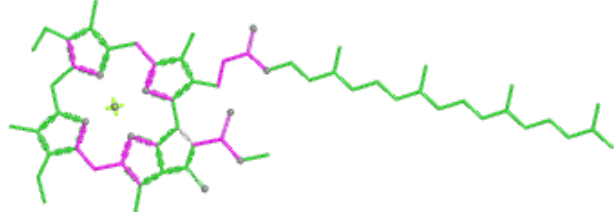
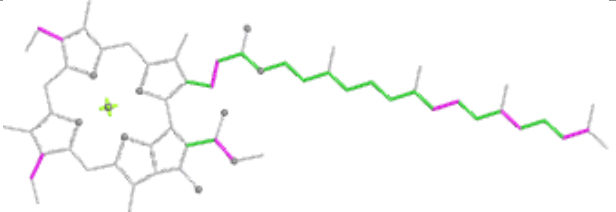
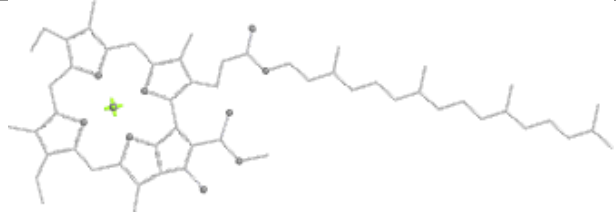


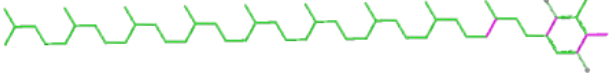
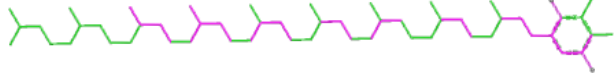
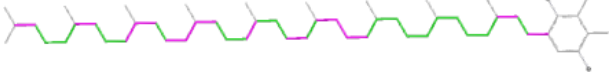
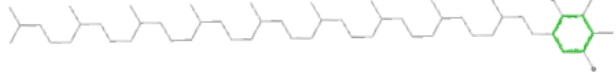
Ligand CLA B 601

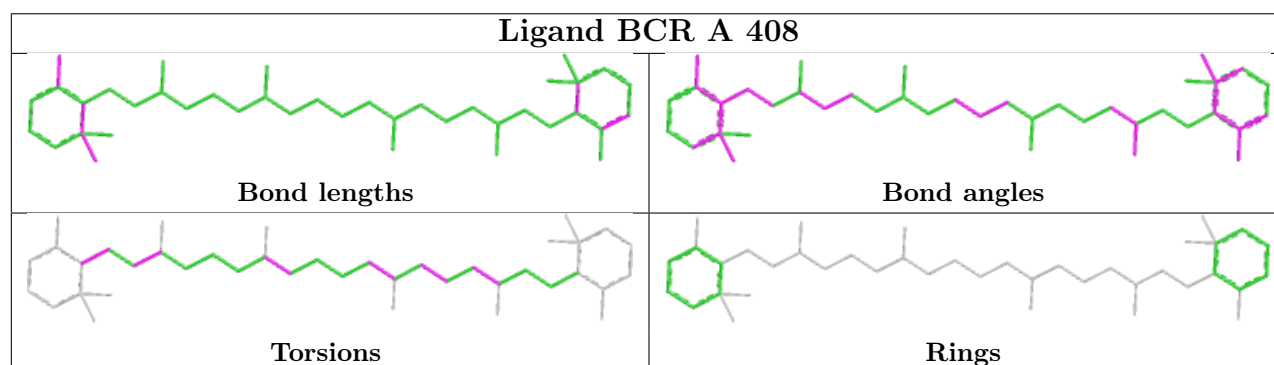
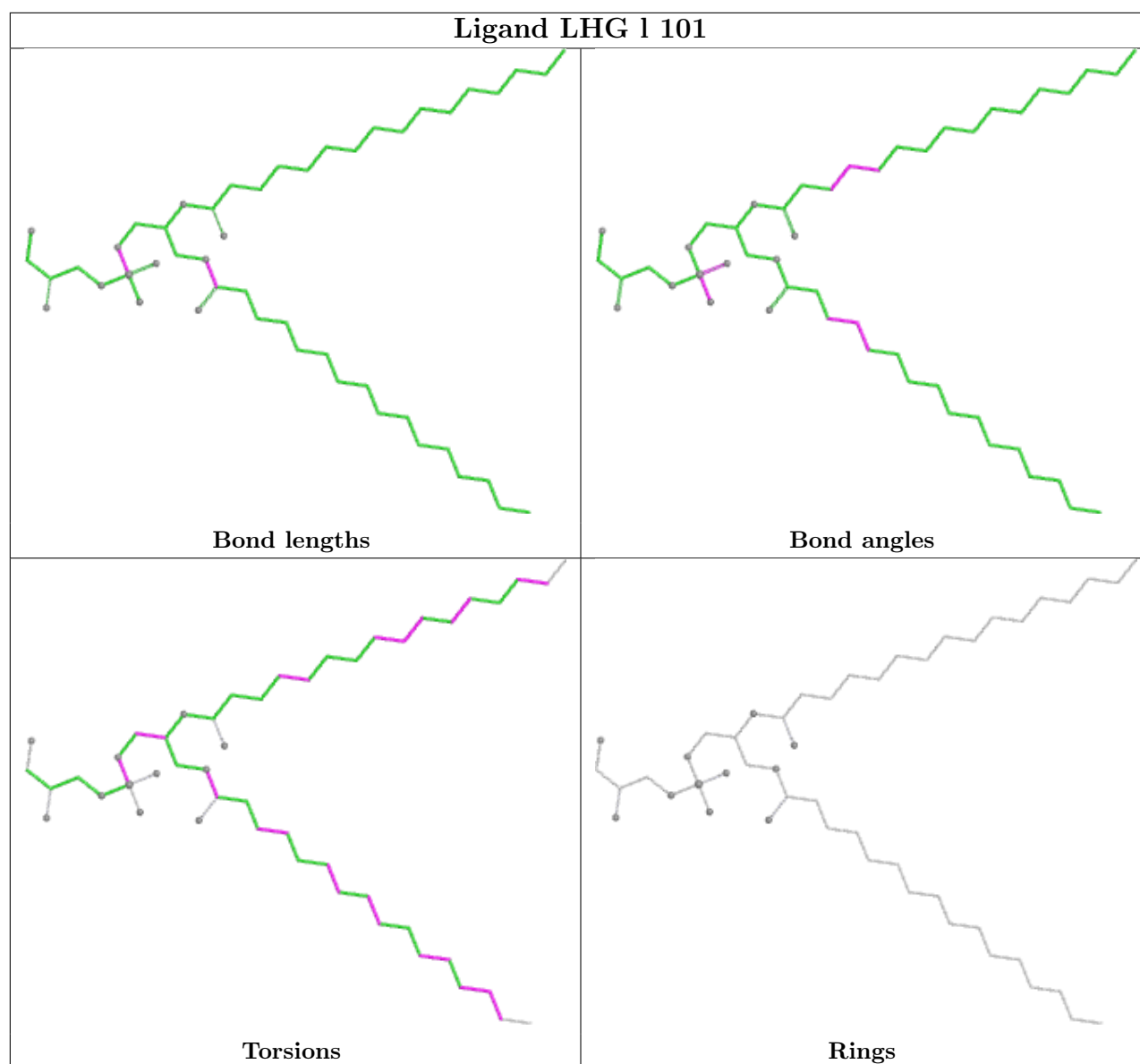


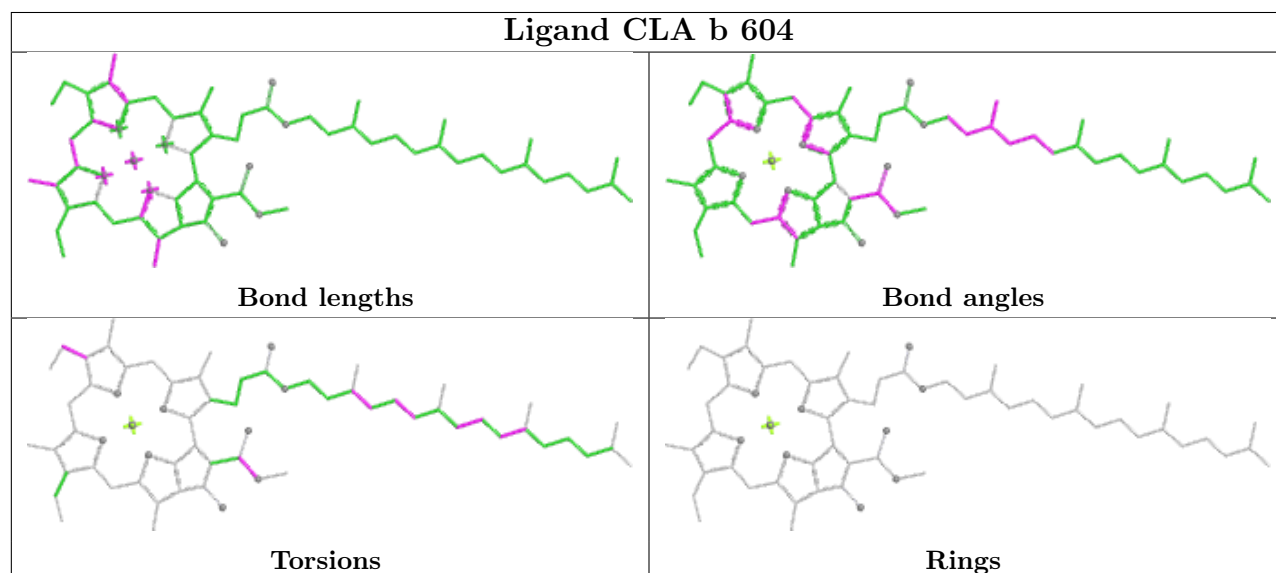
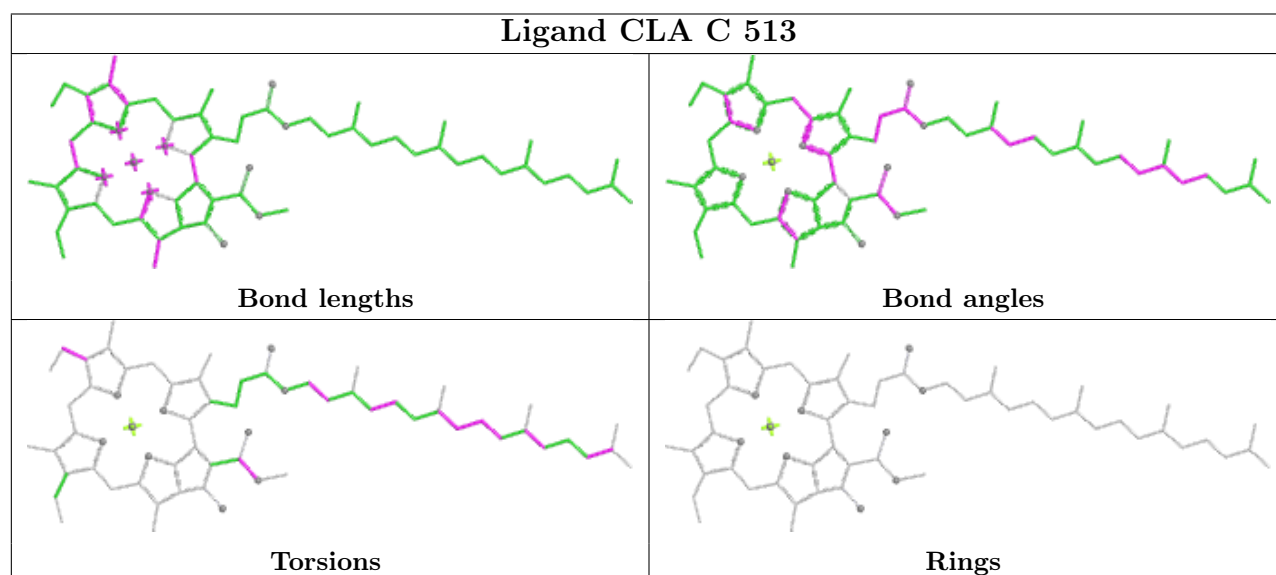
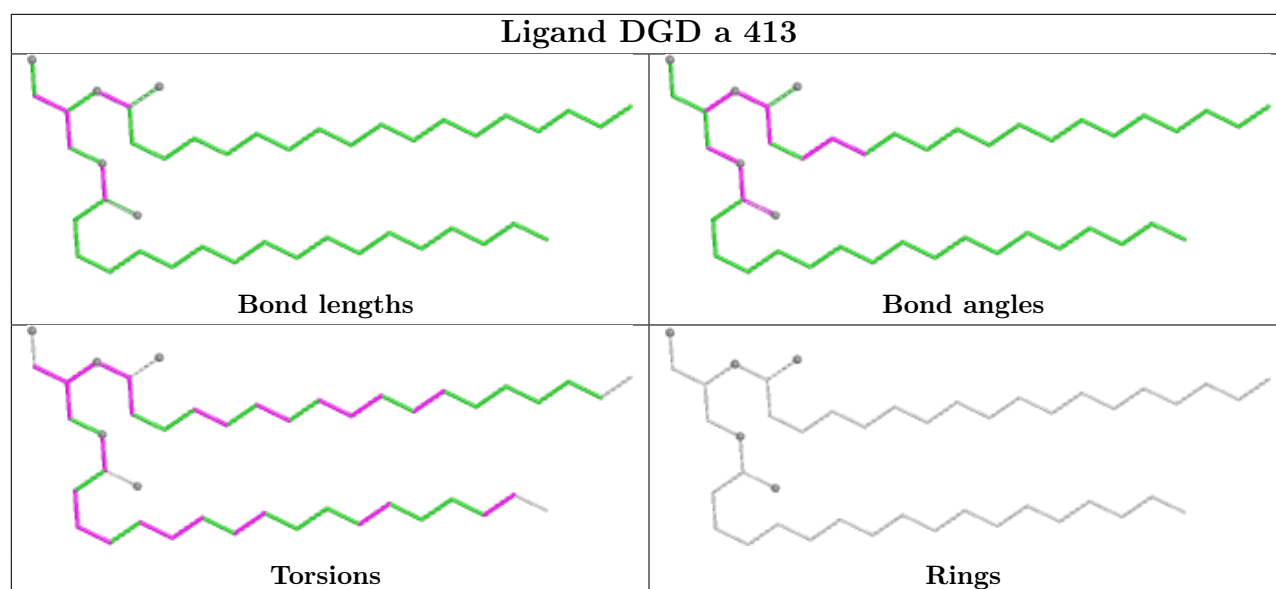
Ligand LHG d 409

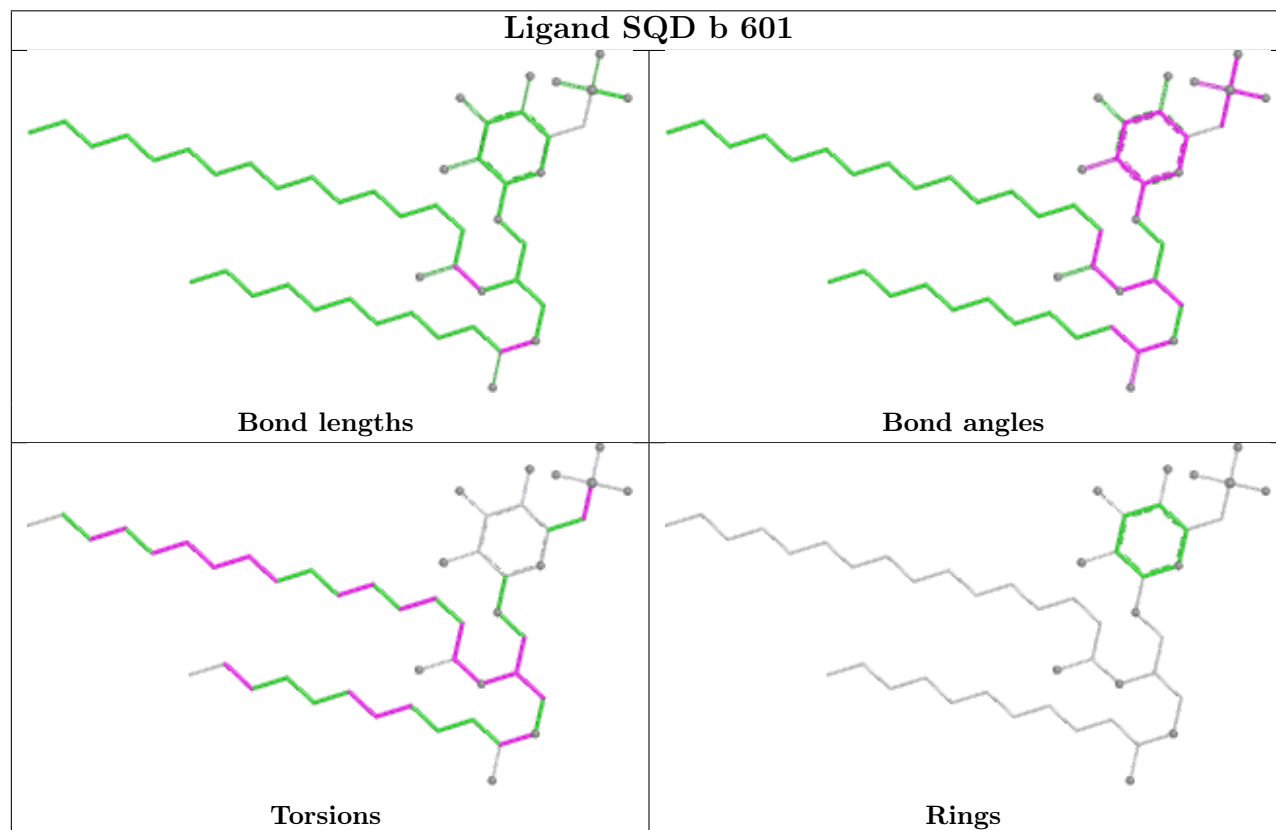
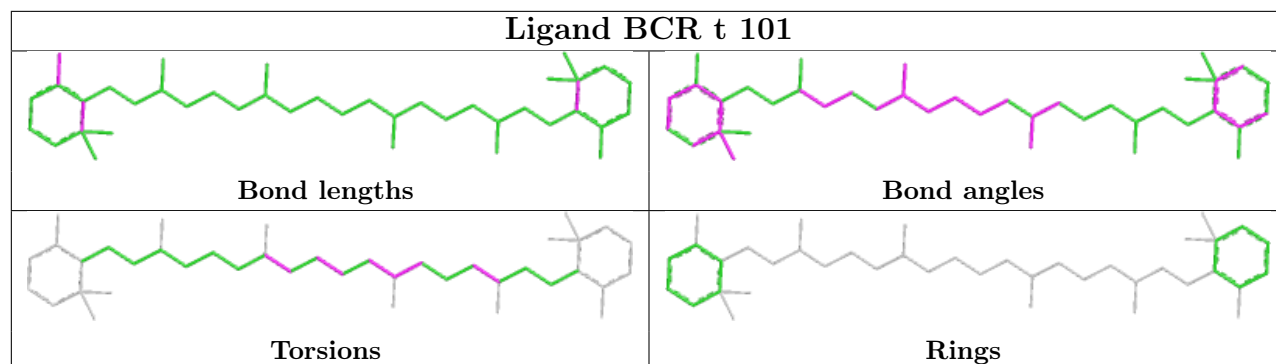


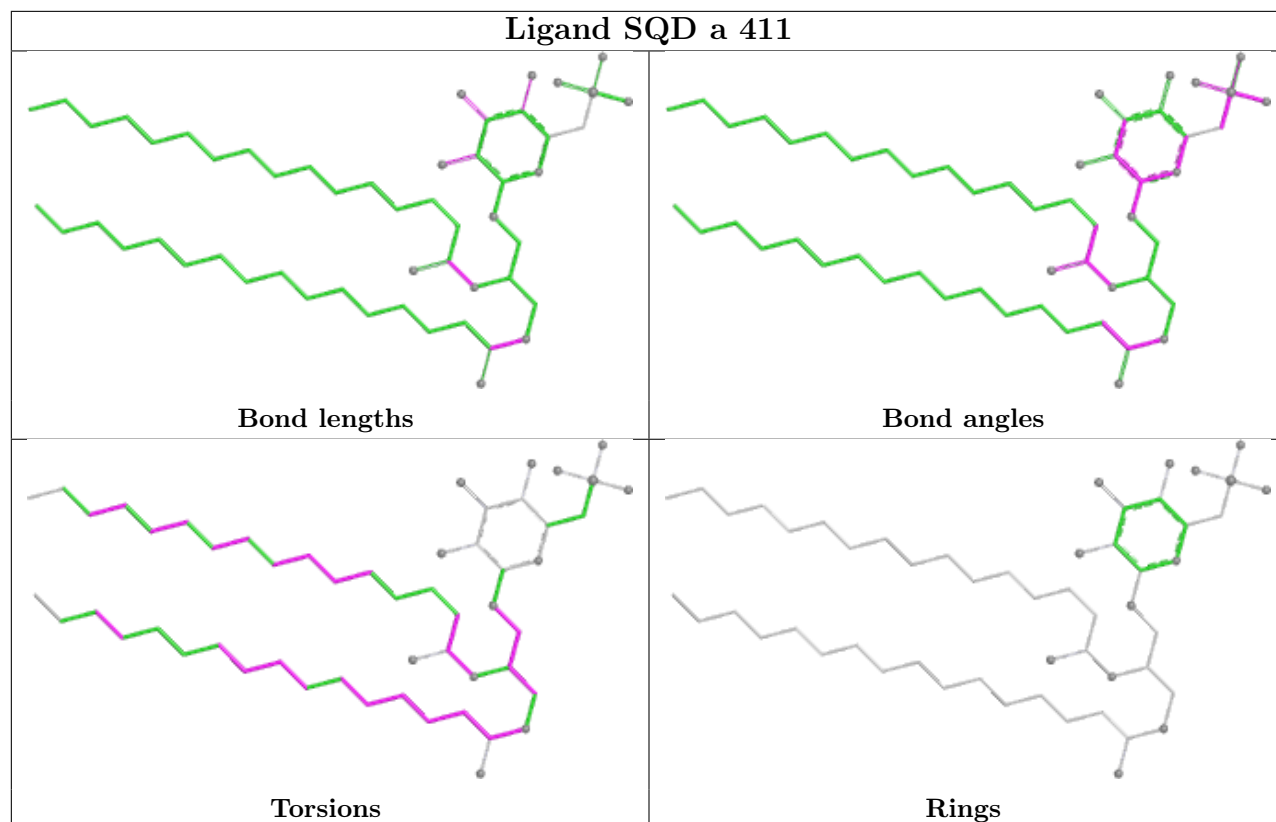
Ligand CLA B 610			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand PL9 a 410			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

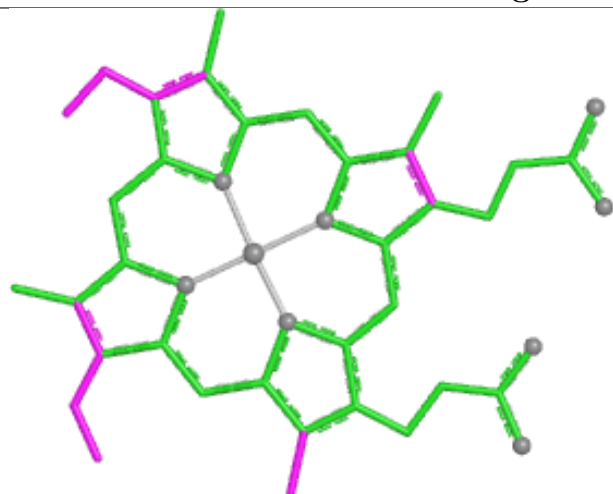




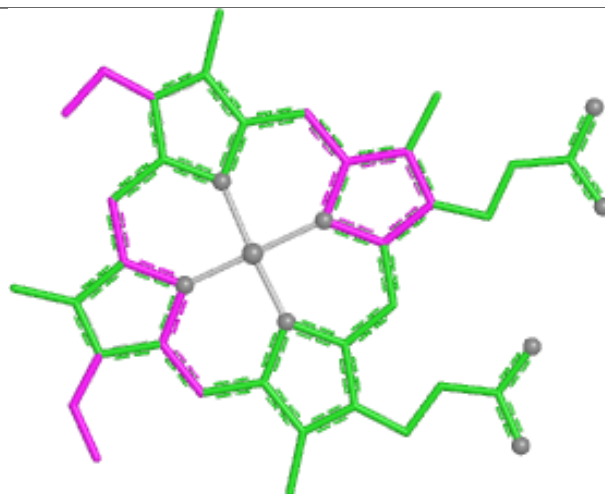




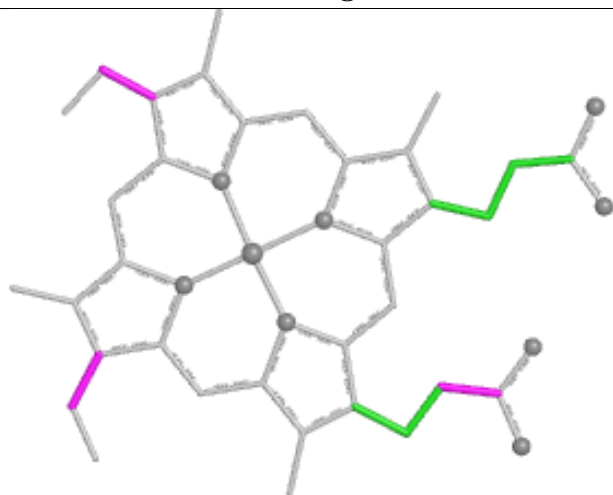
Ligand HEC V 201



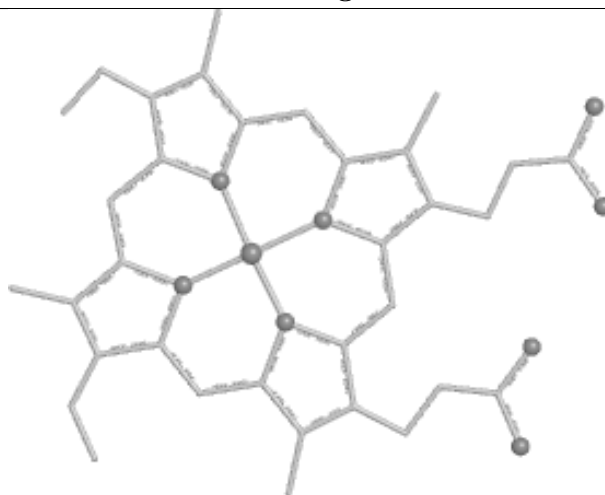
Bond lengths



Bond angles

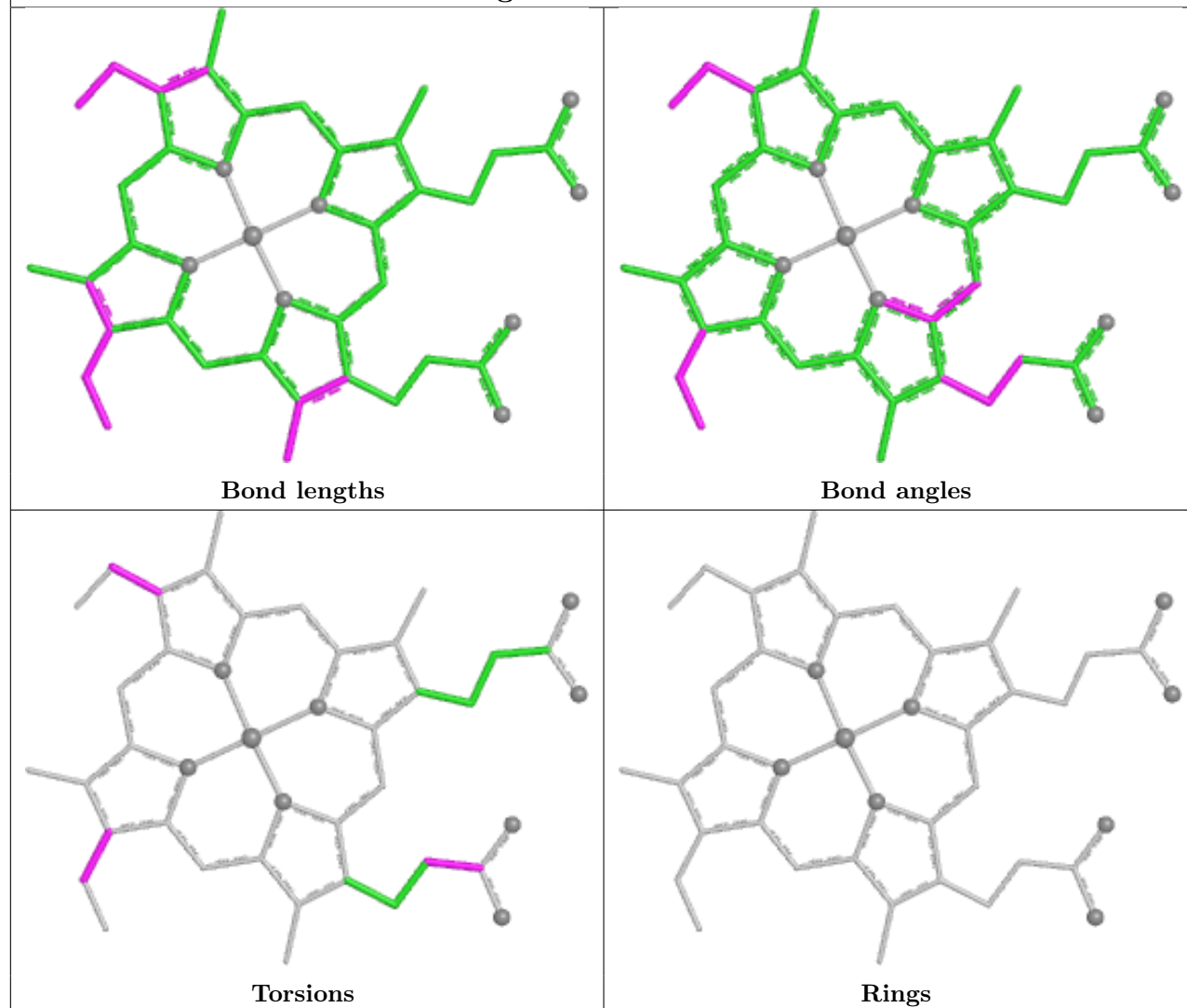


Torsions

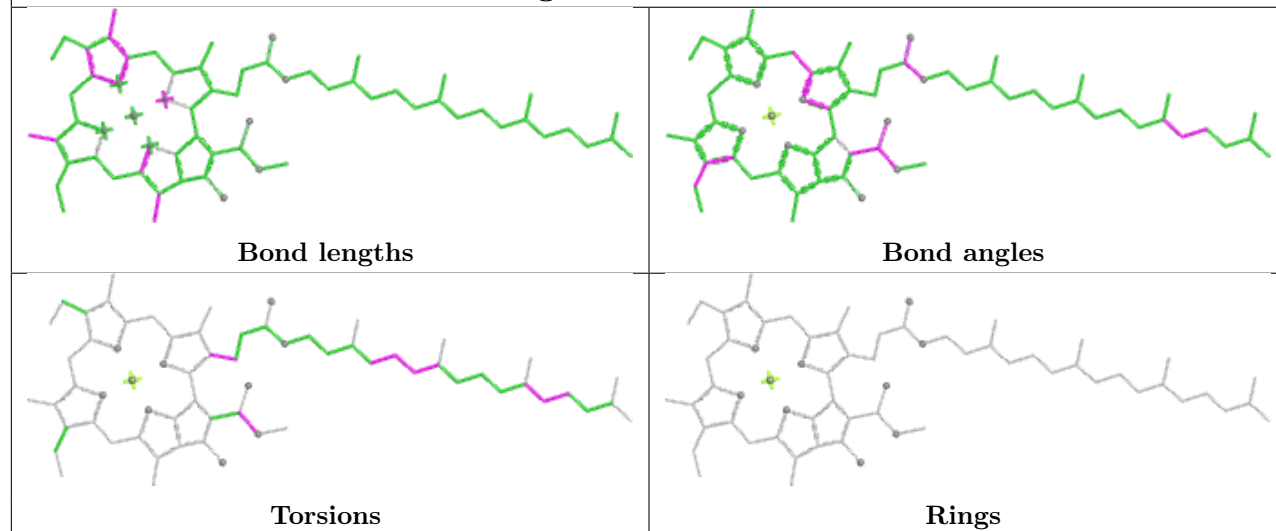


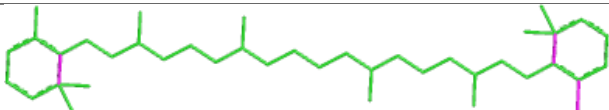
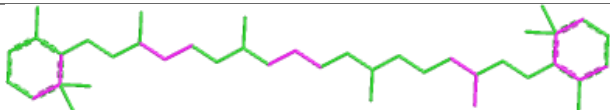
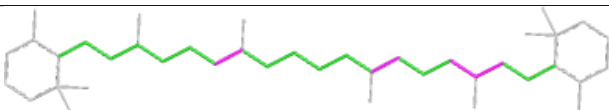
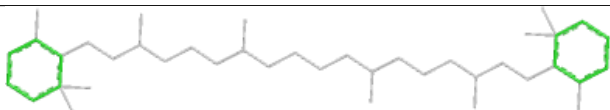
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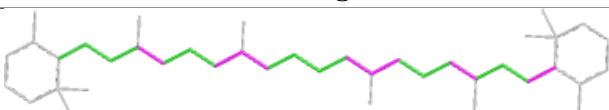
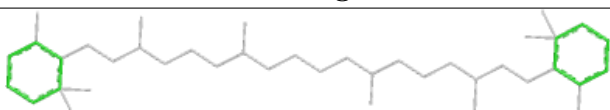
Ligand HEC v 201

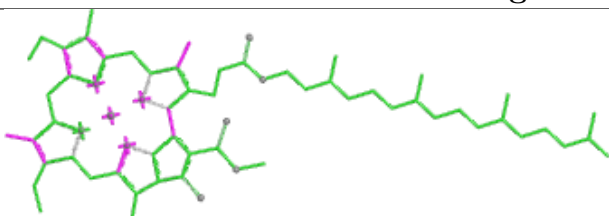
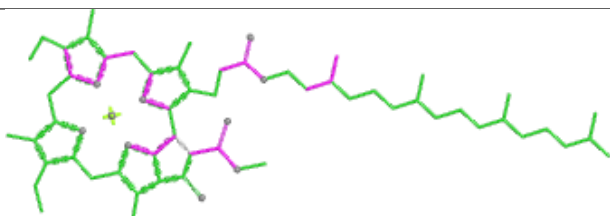
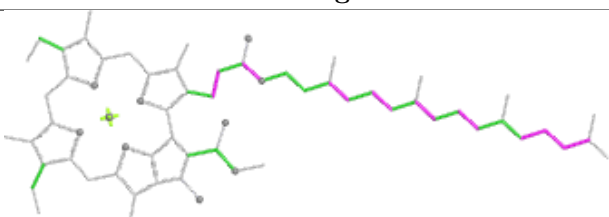
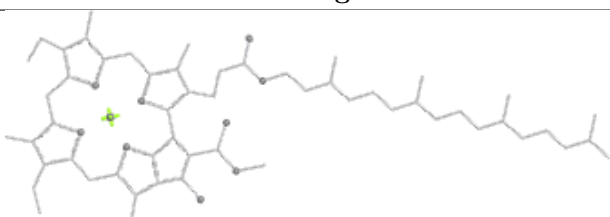


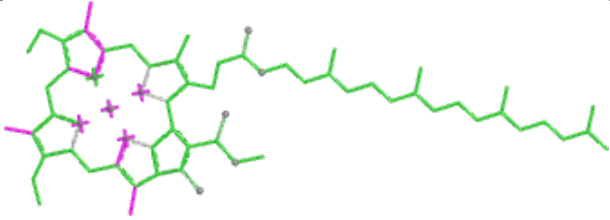
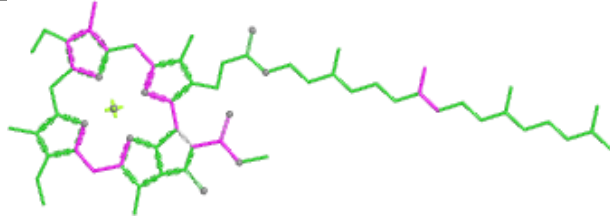
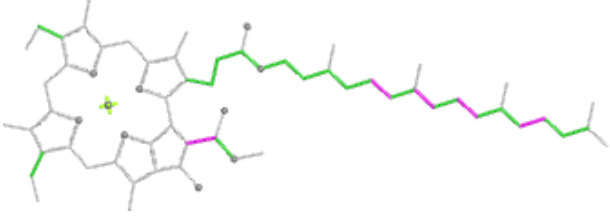
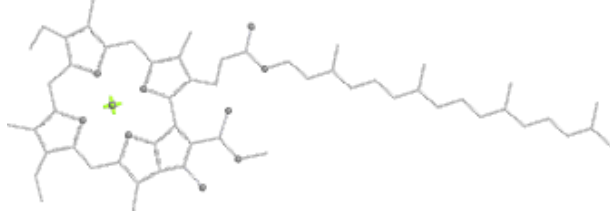
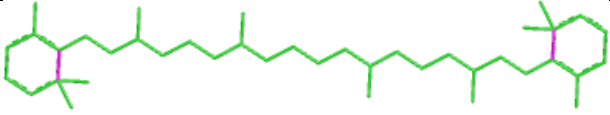
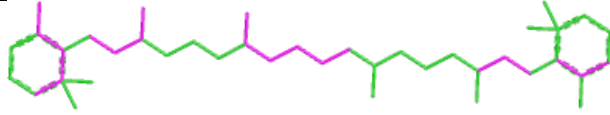
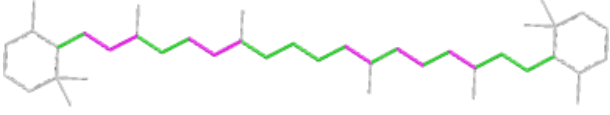
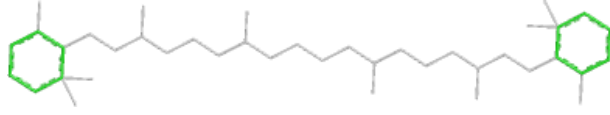
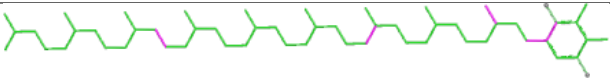
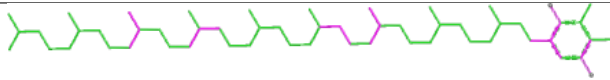
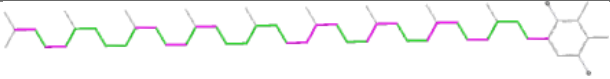
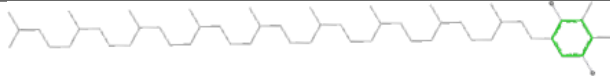
Ligand CLA c 513

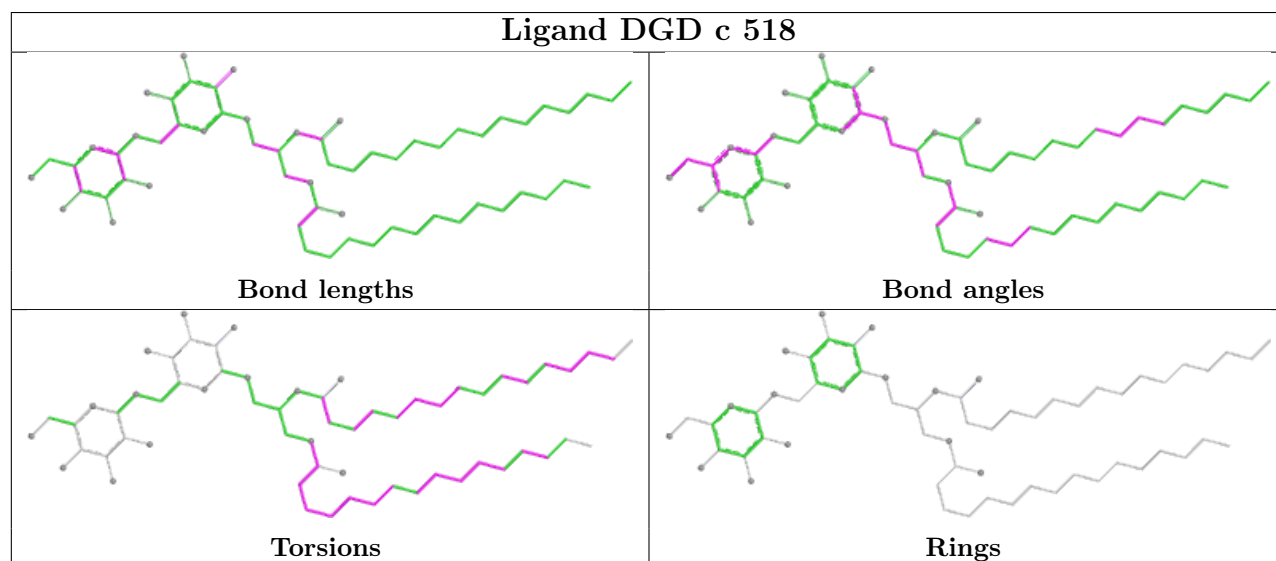
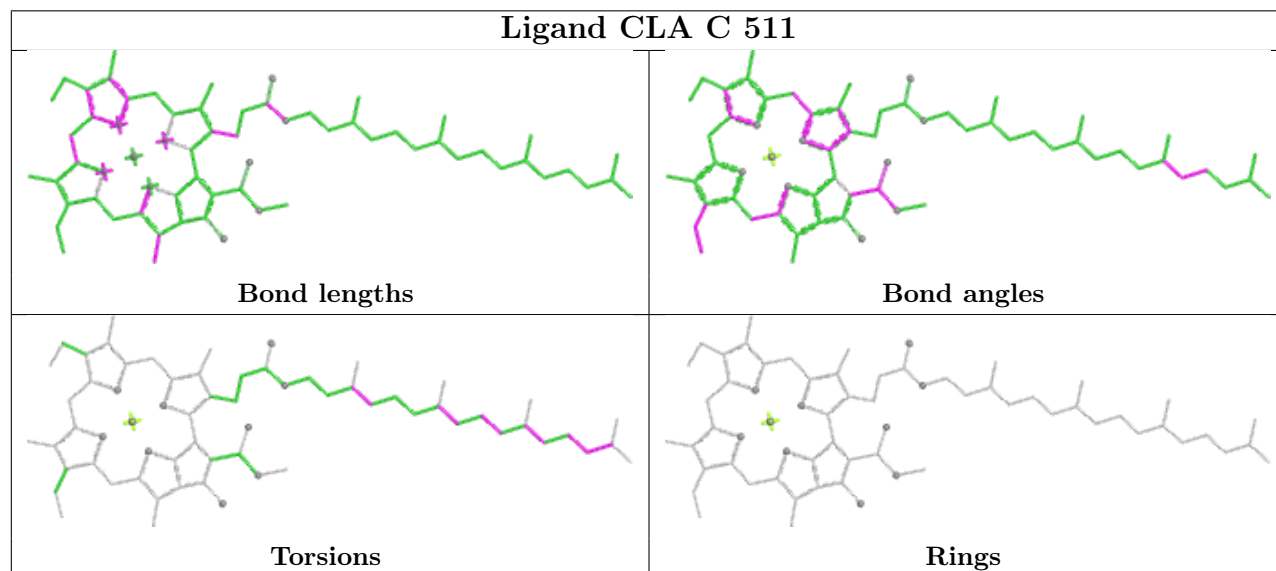
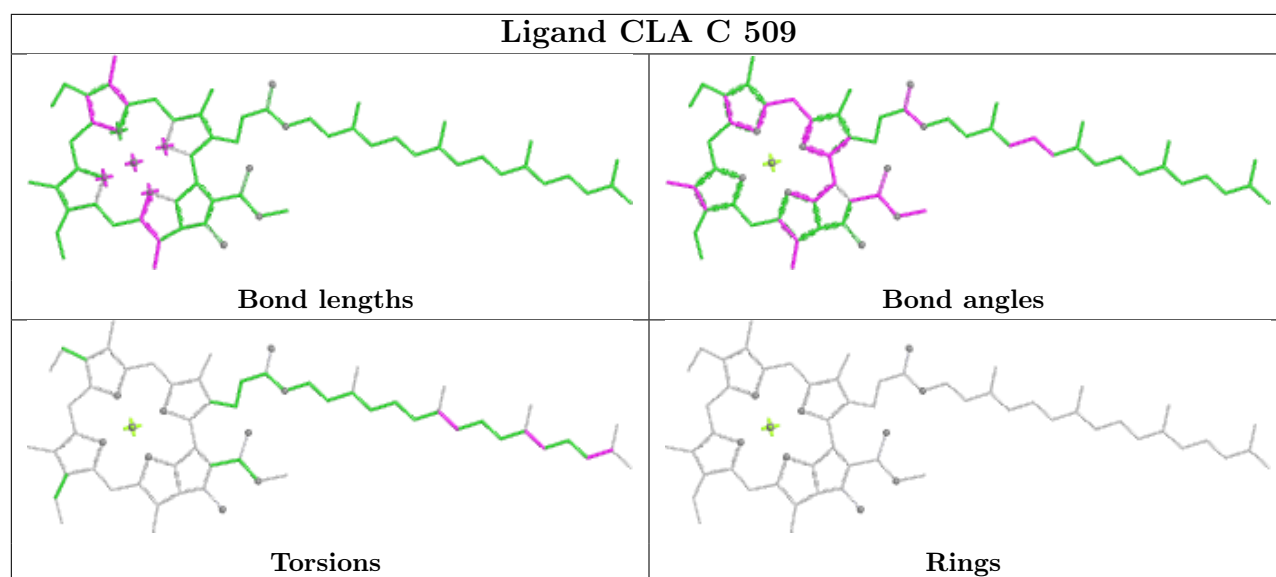


Ligand BCR b 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

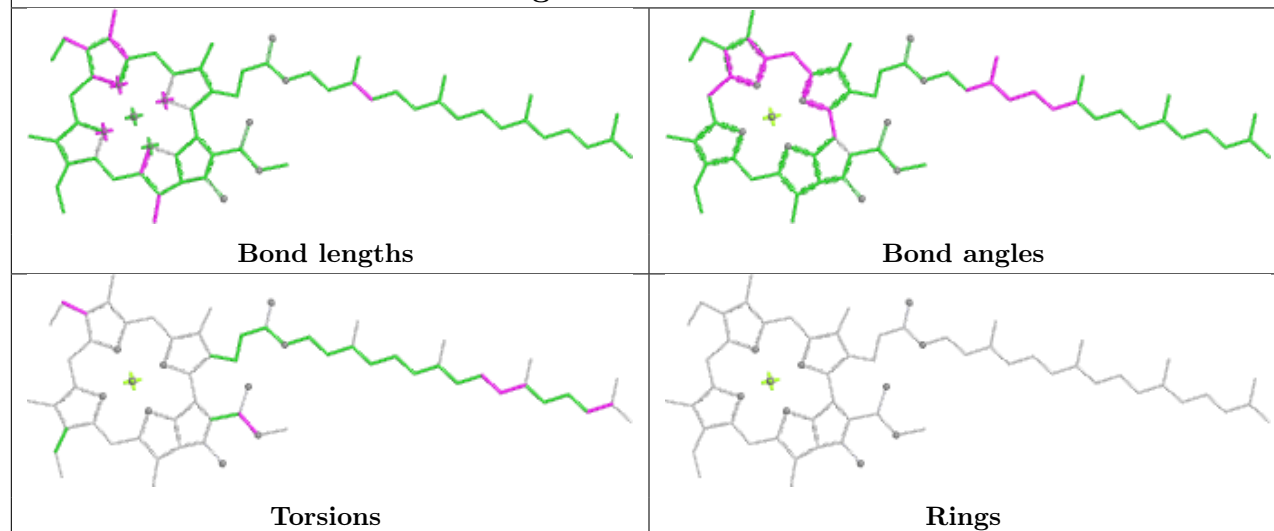
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

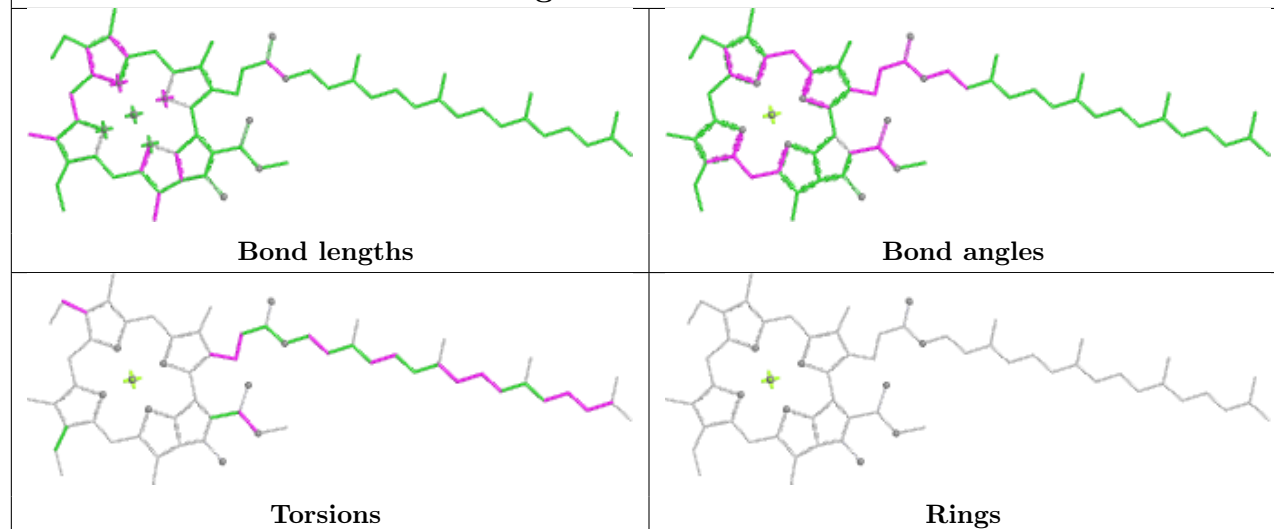
Ligand CLA C 508	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings



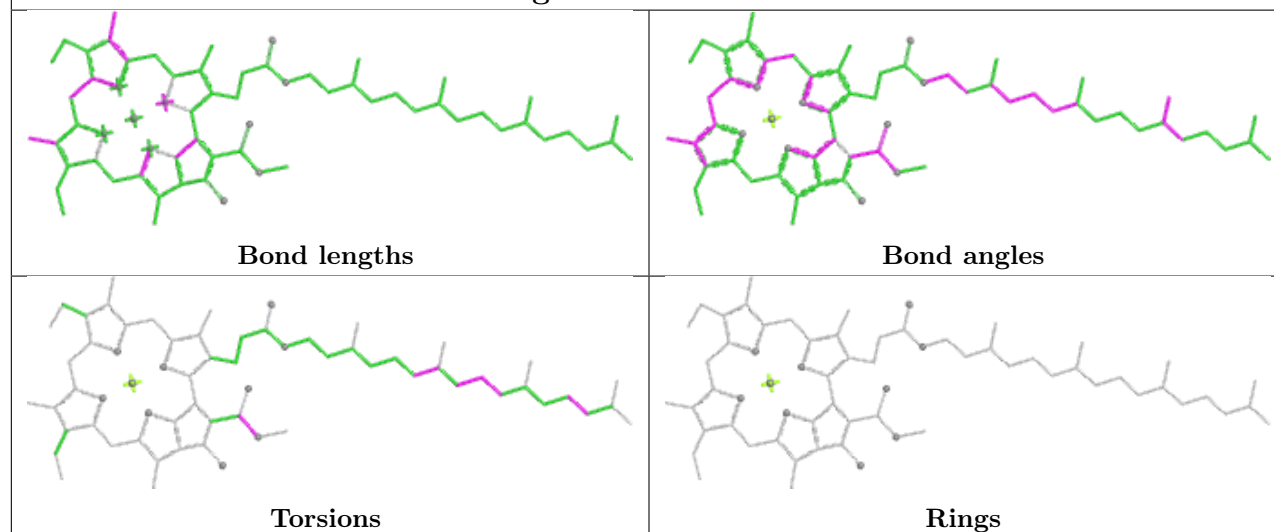
Ligand CLA B 615

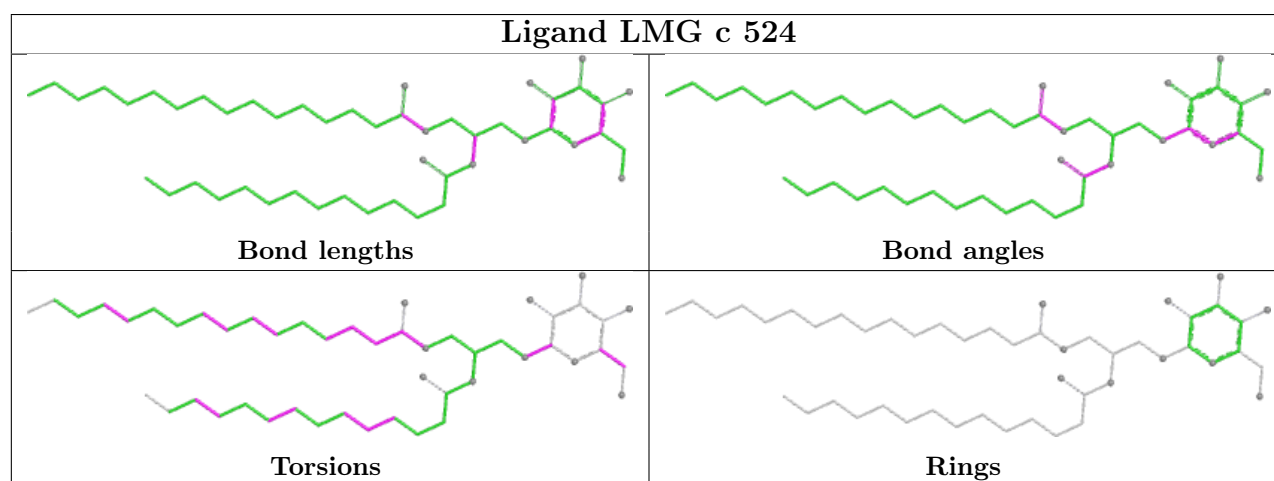
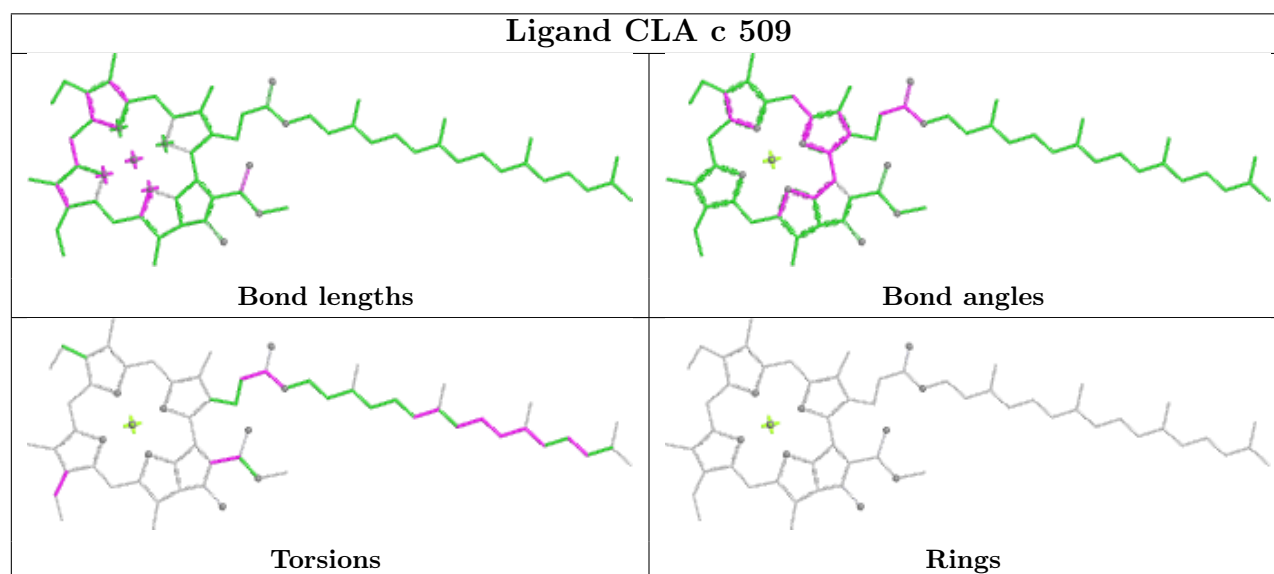
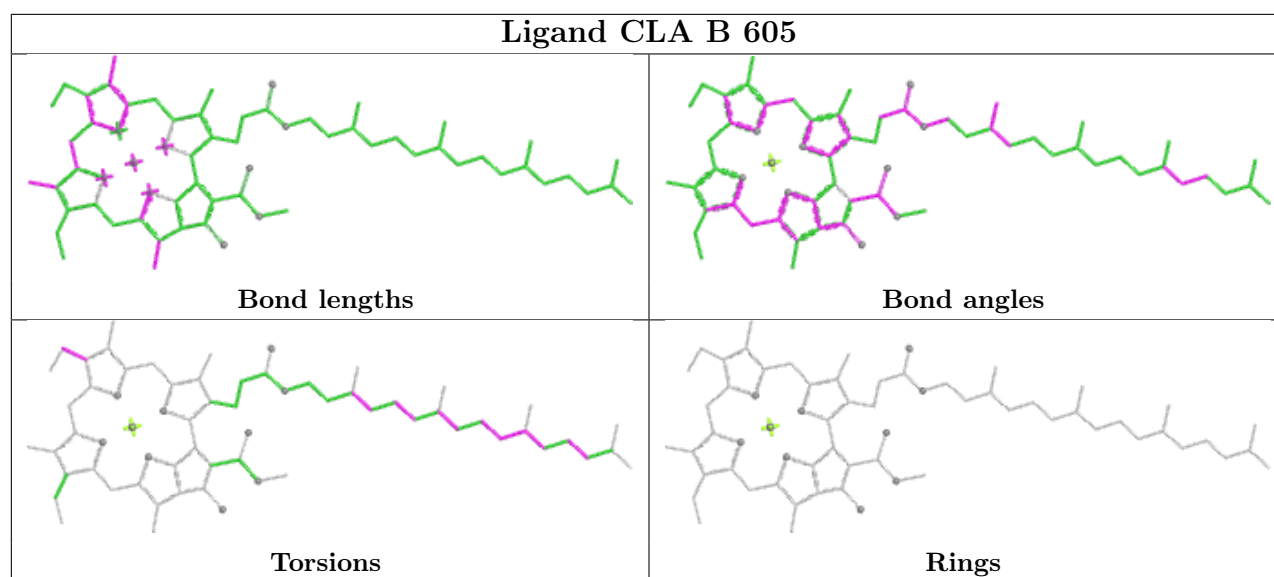


Ligand CLA b 602

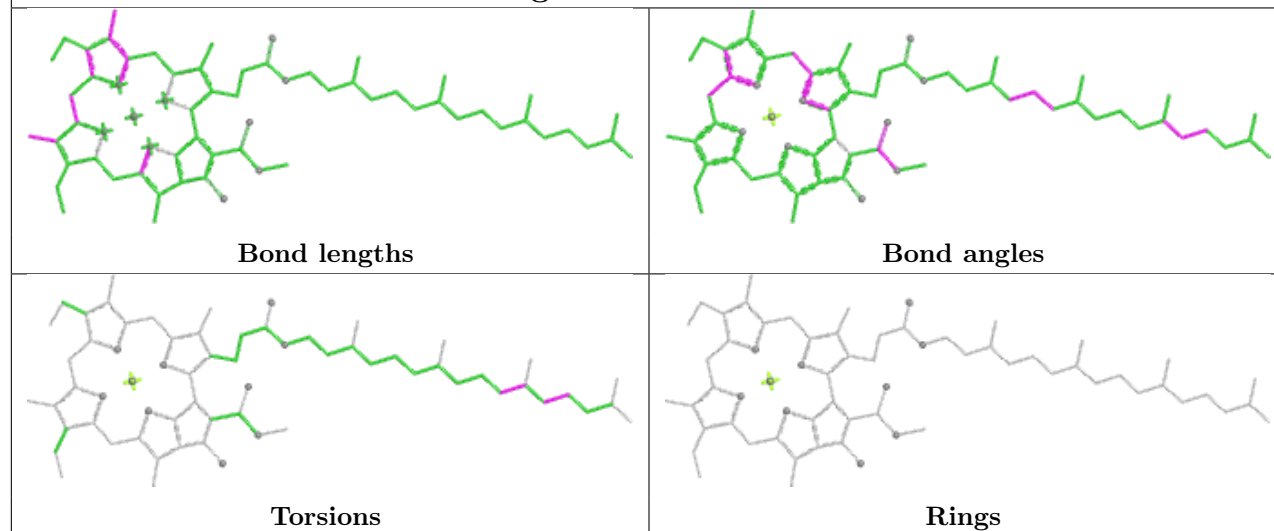


Ligand CLA C 504

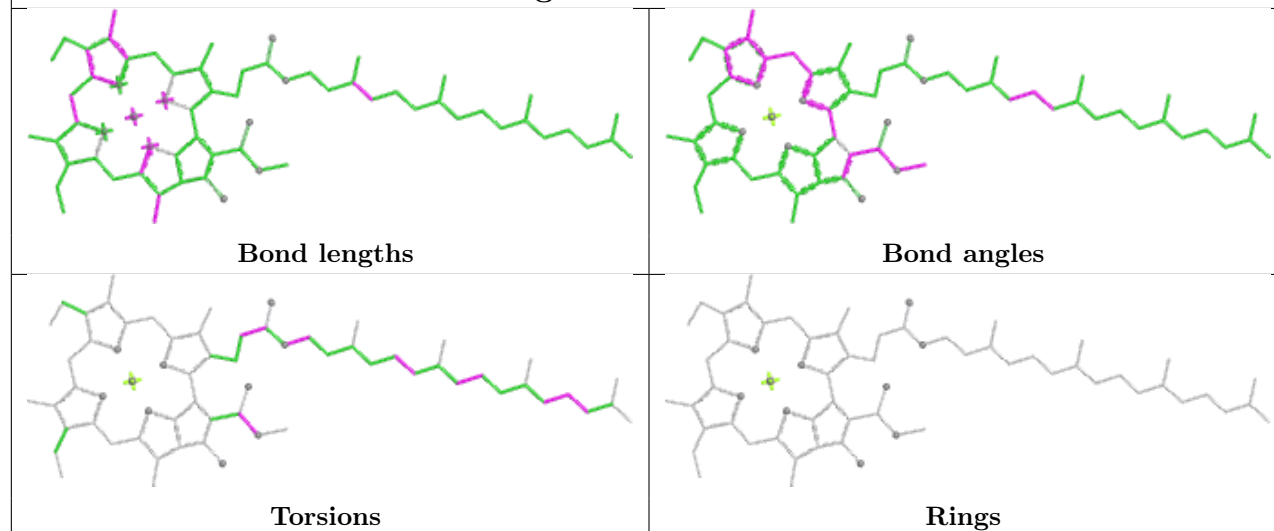




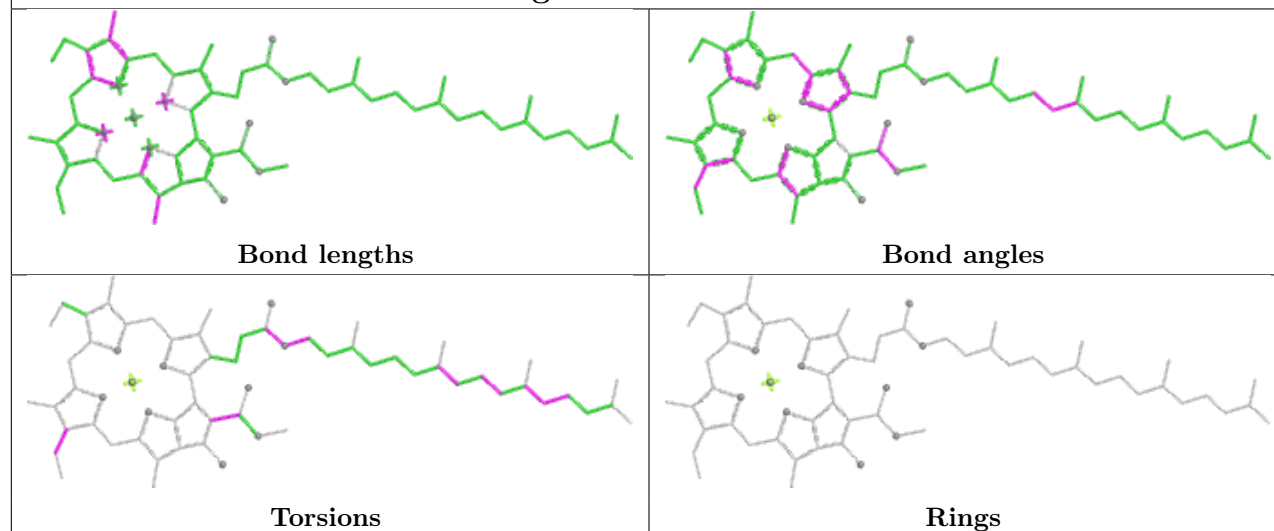
Ligand CLA D 402

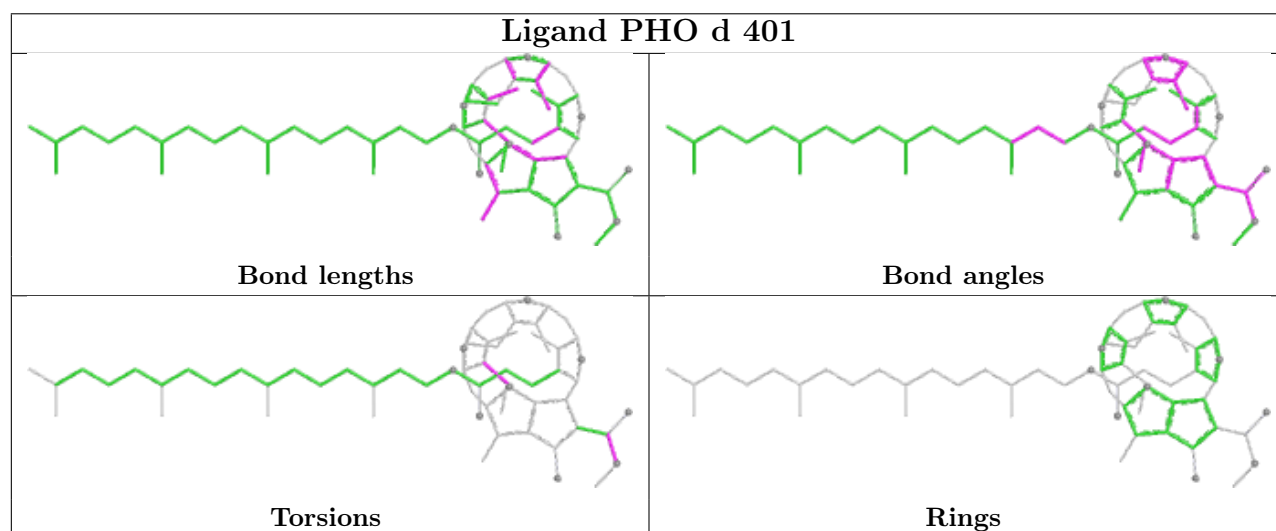
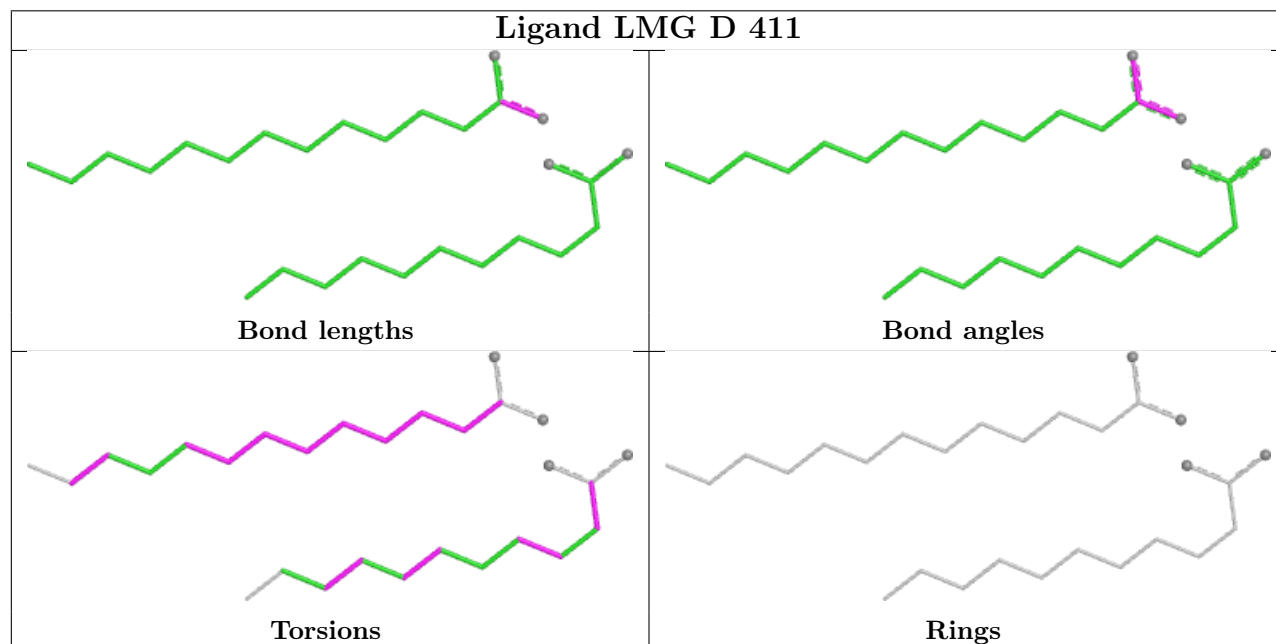
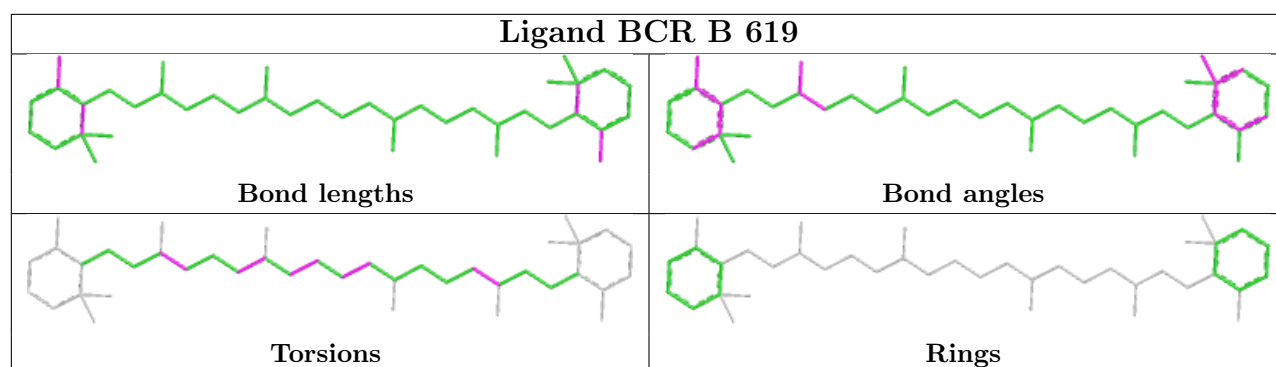


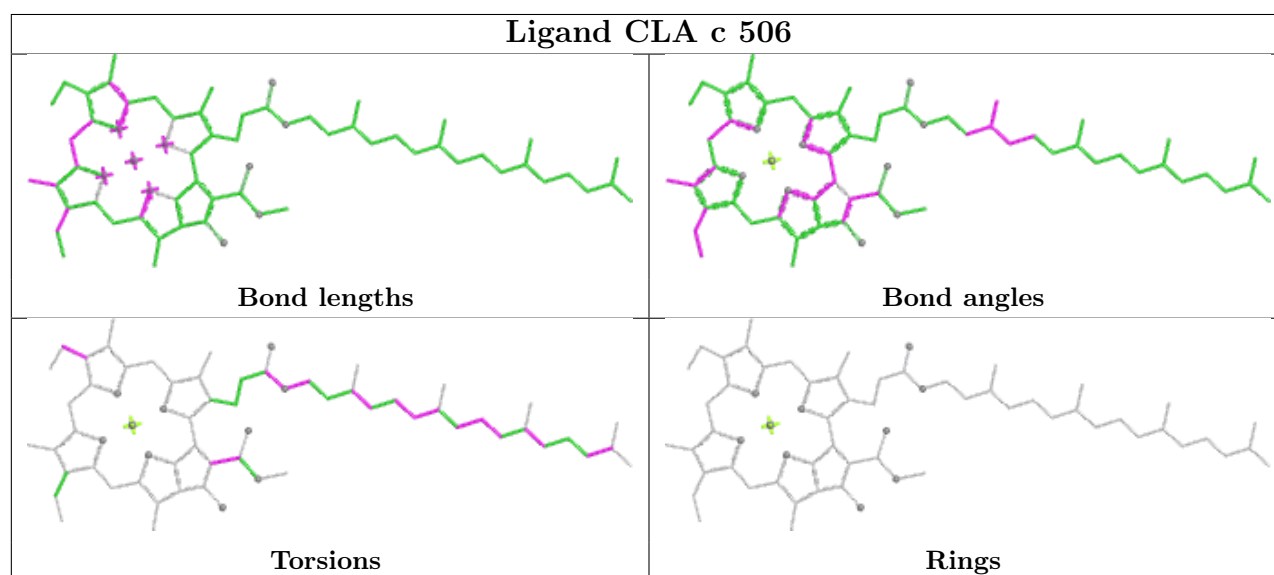
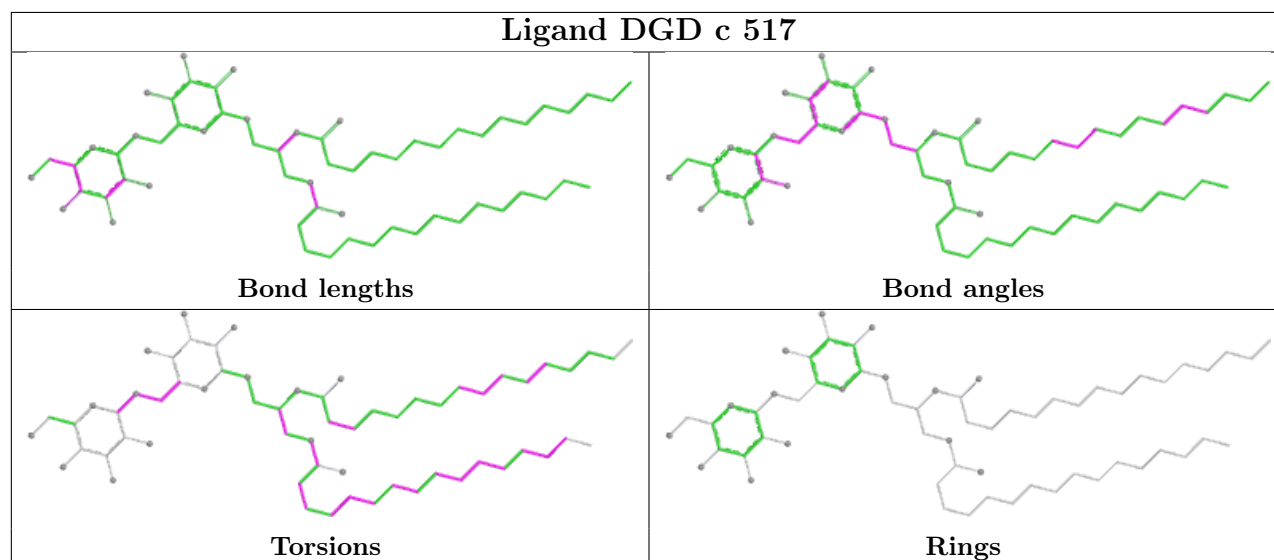
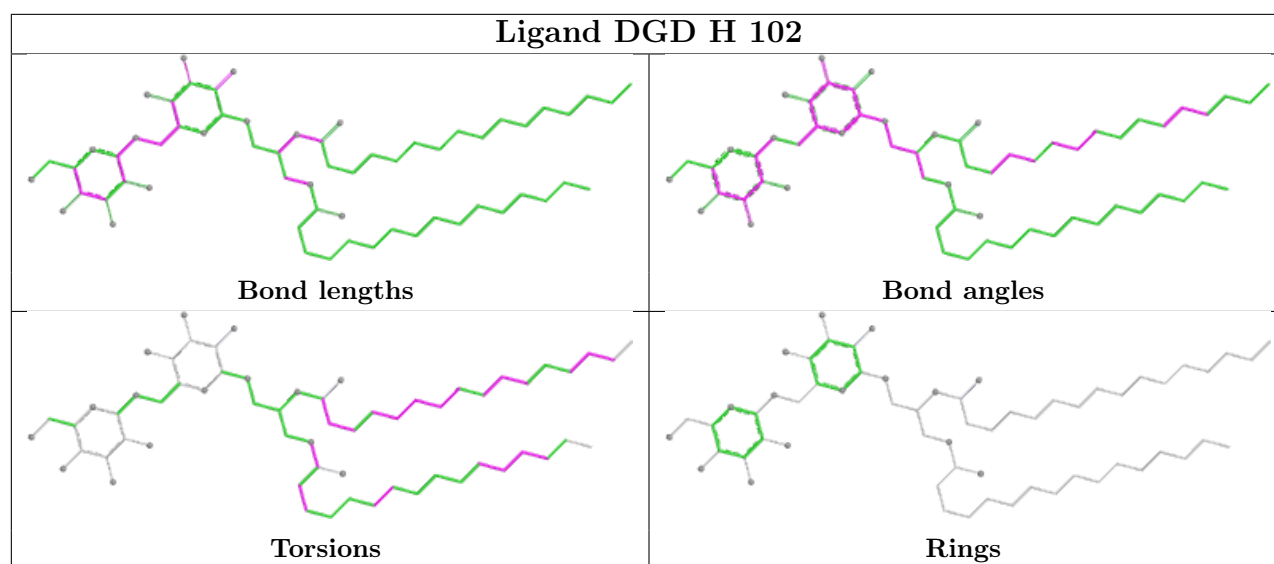
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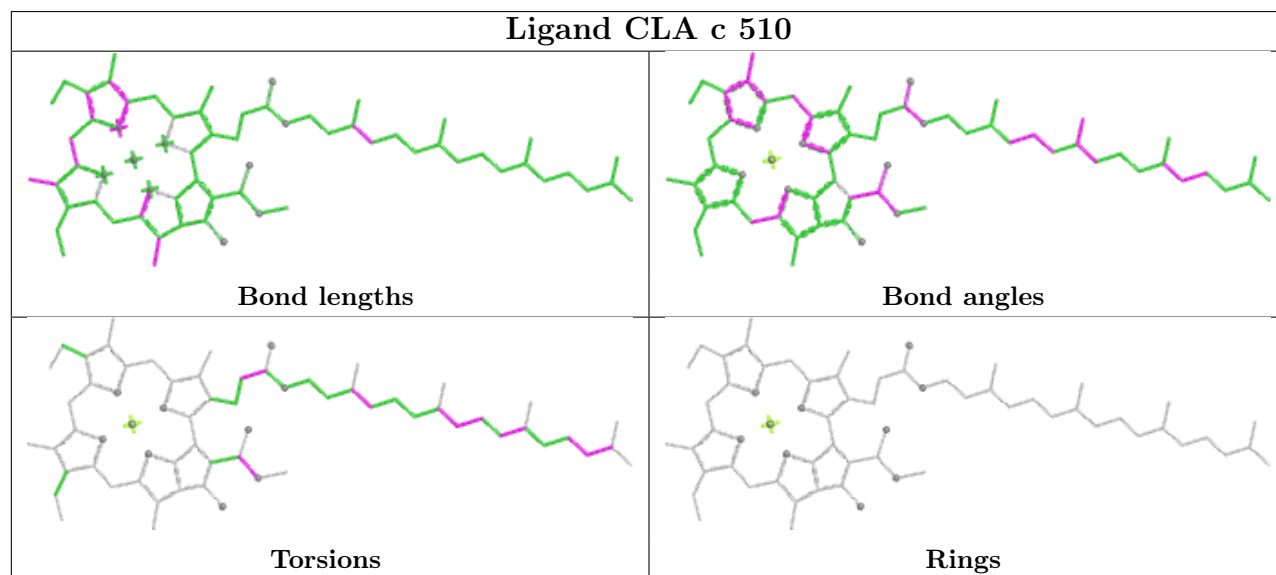
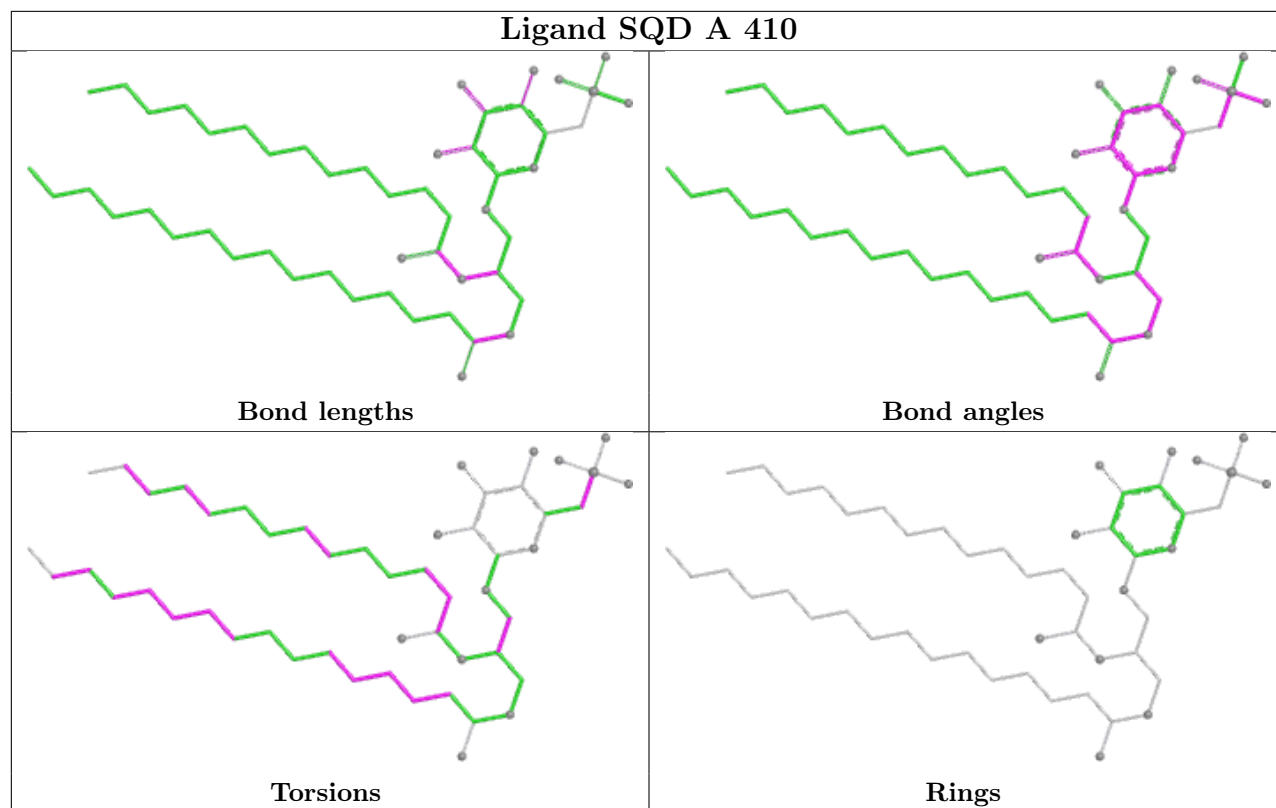


Ligand CLA C 514

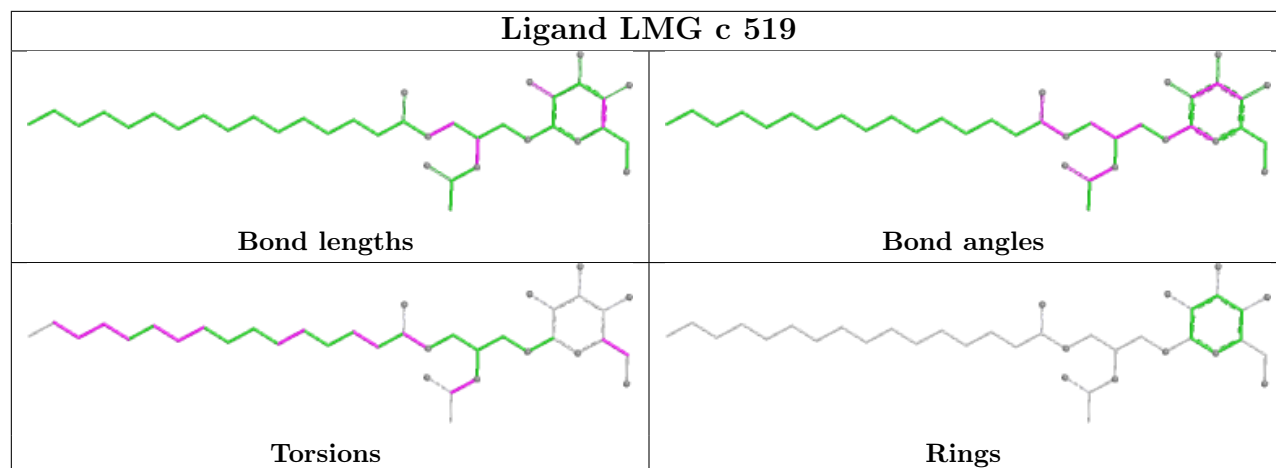




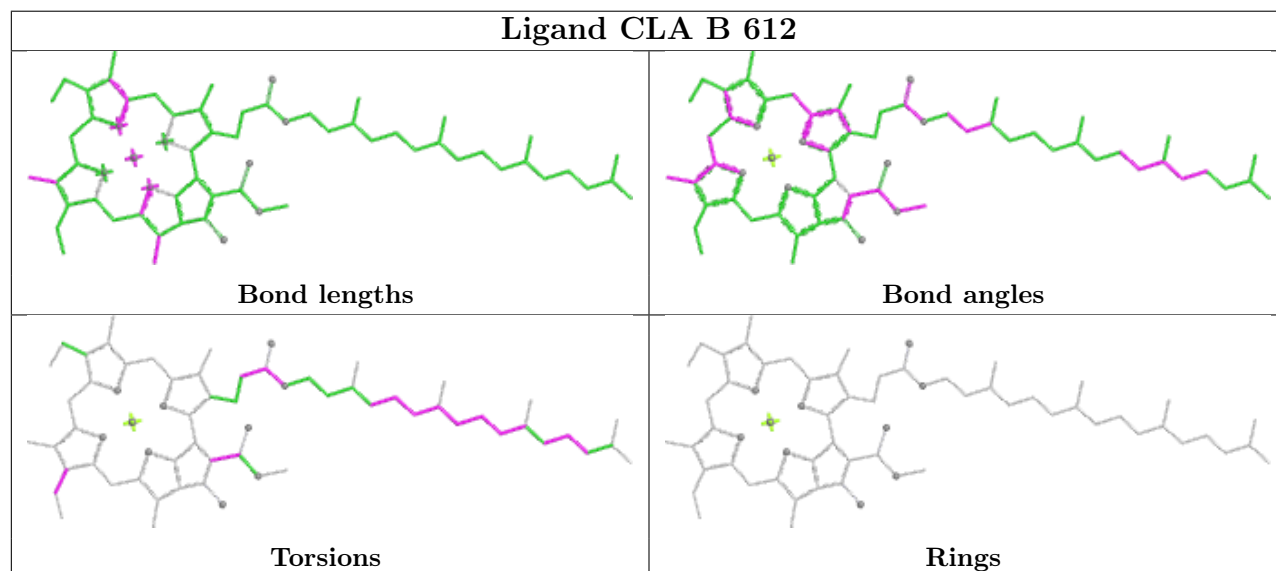




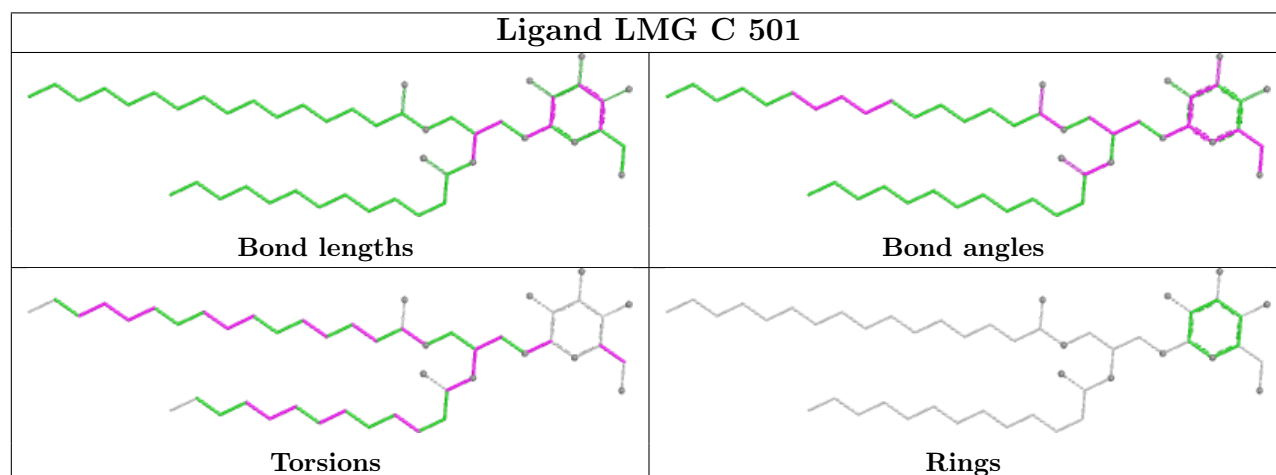
Ligand LMG c 519

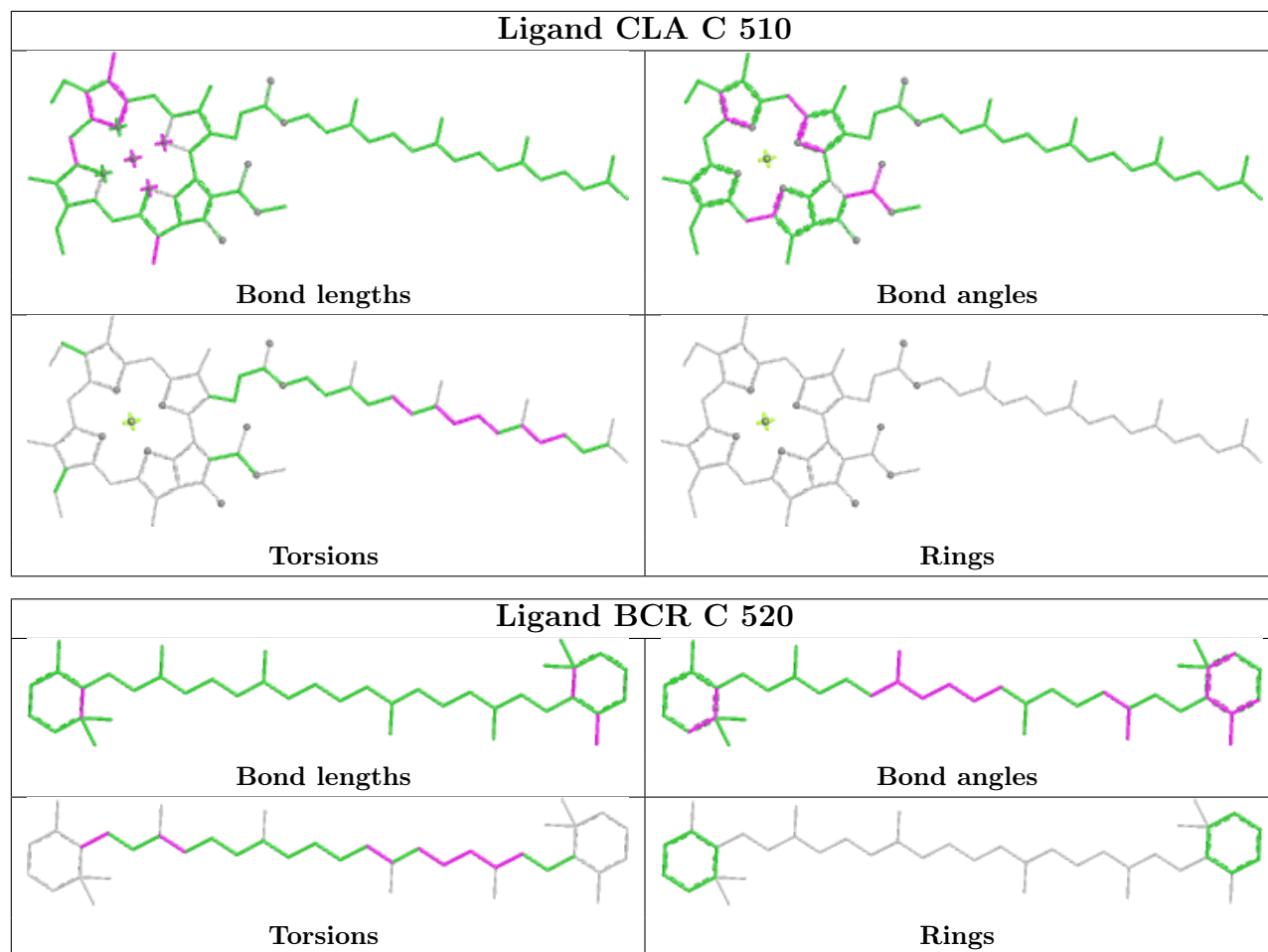


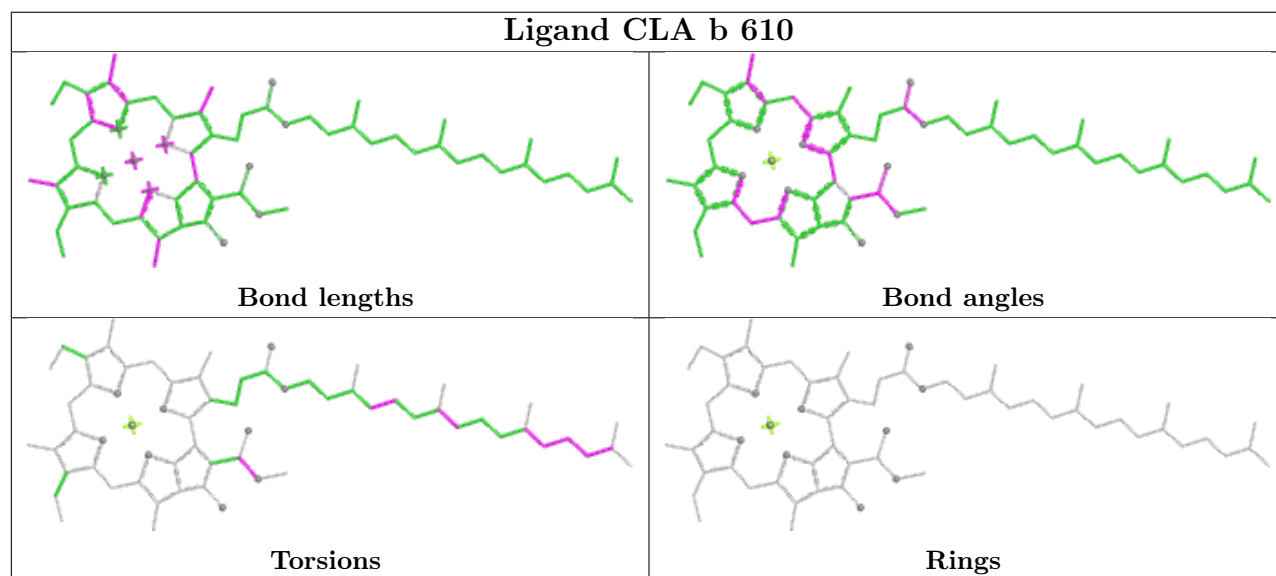
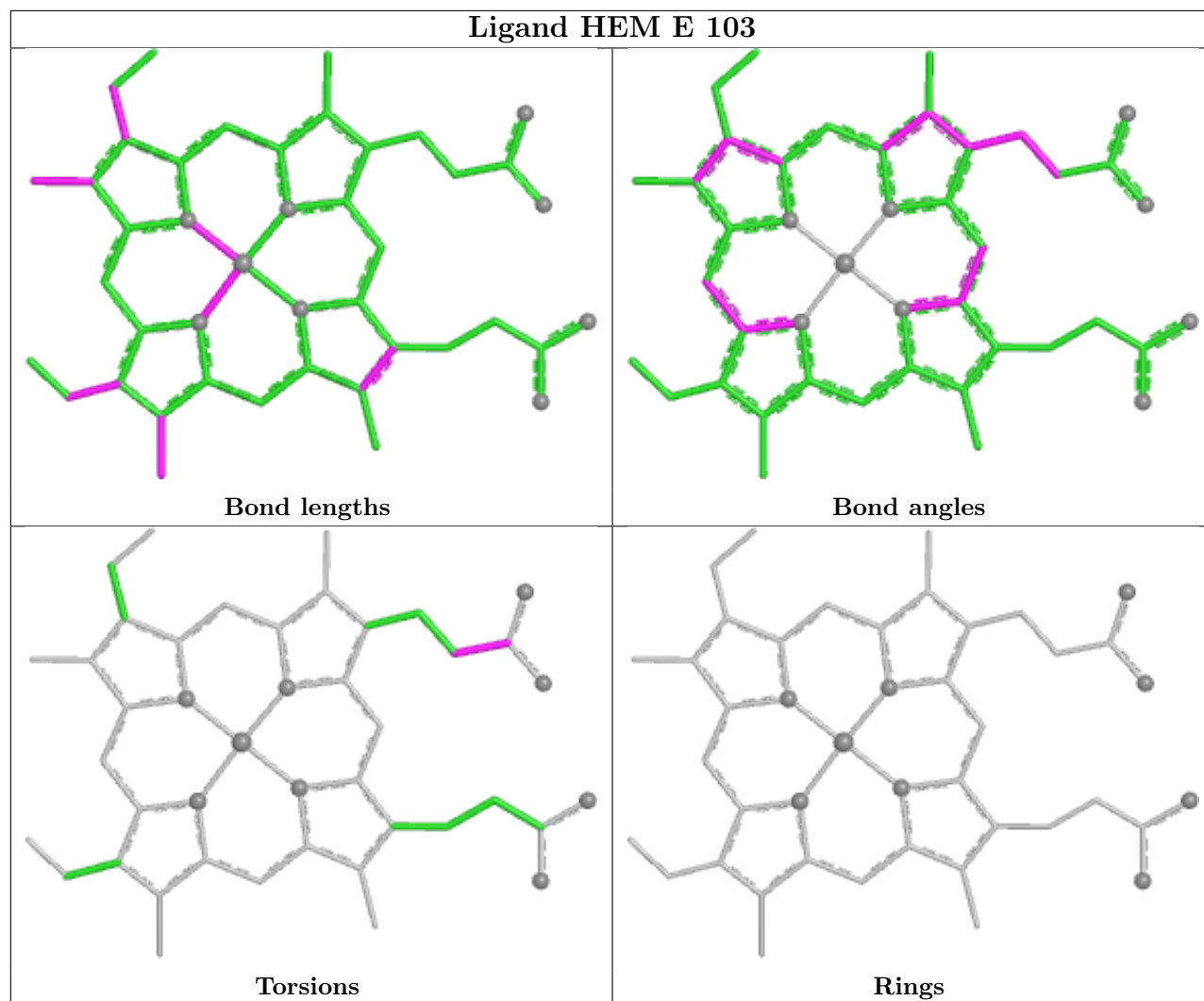
Ligand CLA B 612



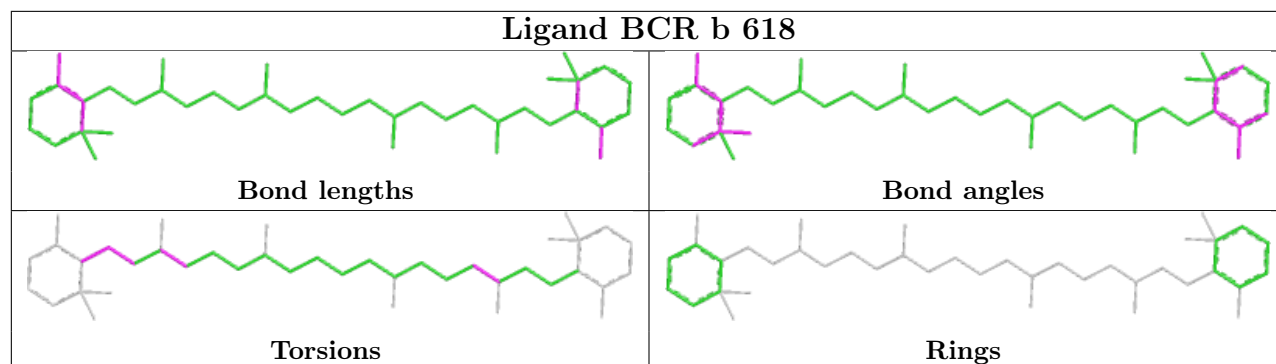
Ligand LMG C 501



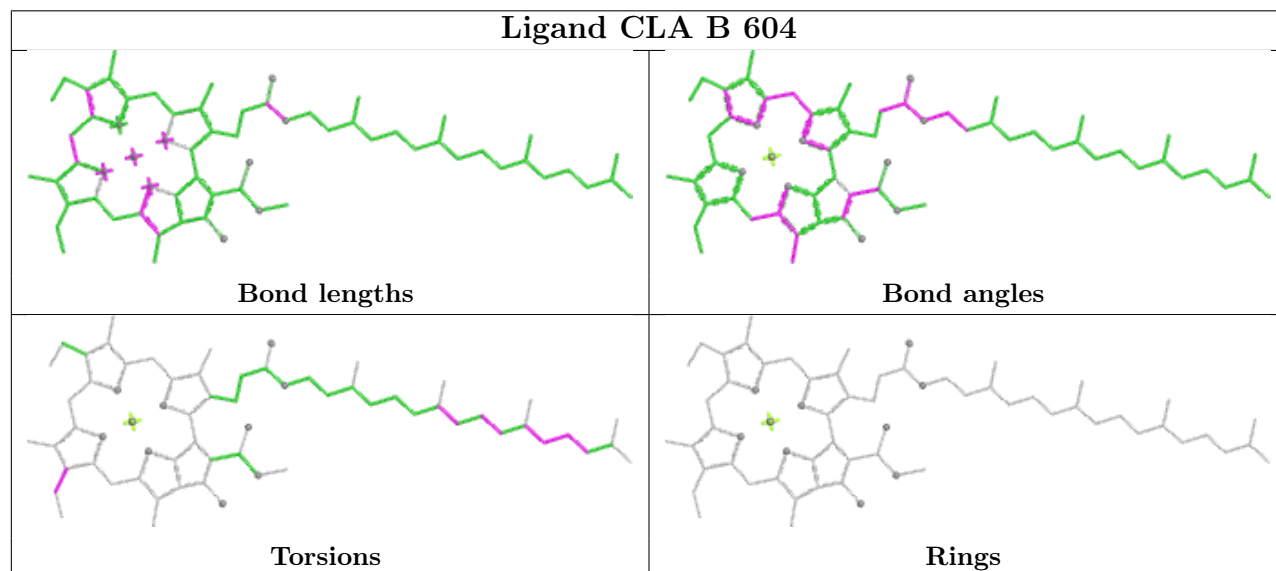




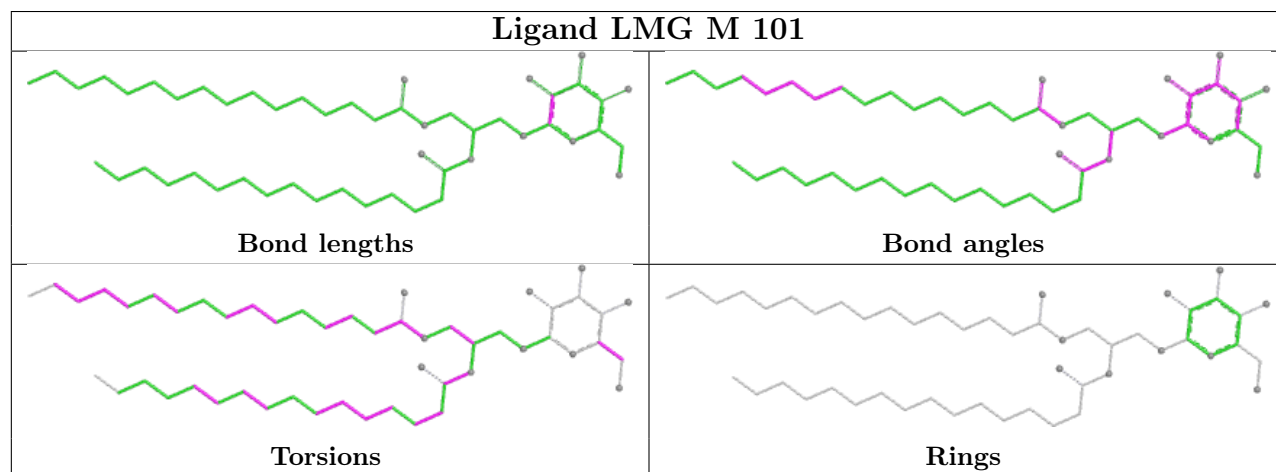
Ligand BCR b 618



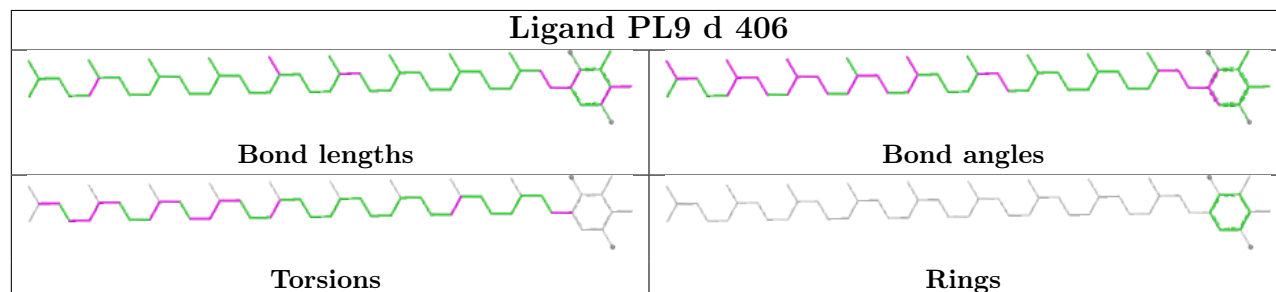
Ligand CLA B 604



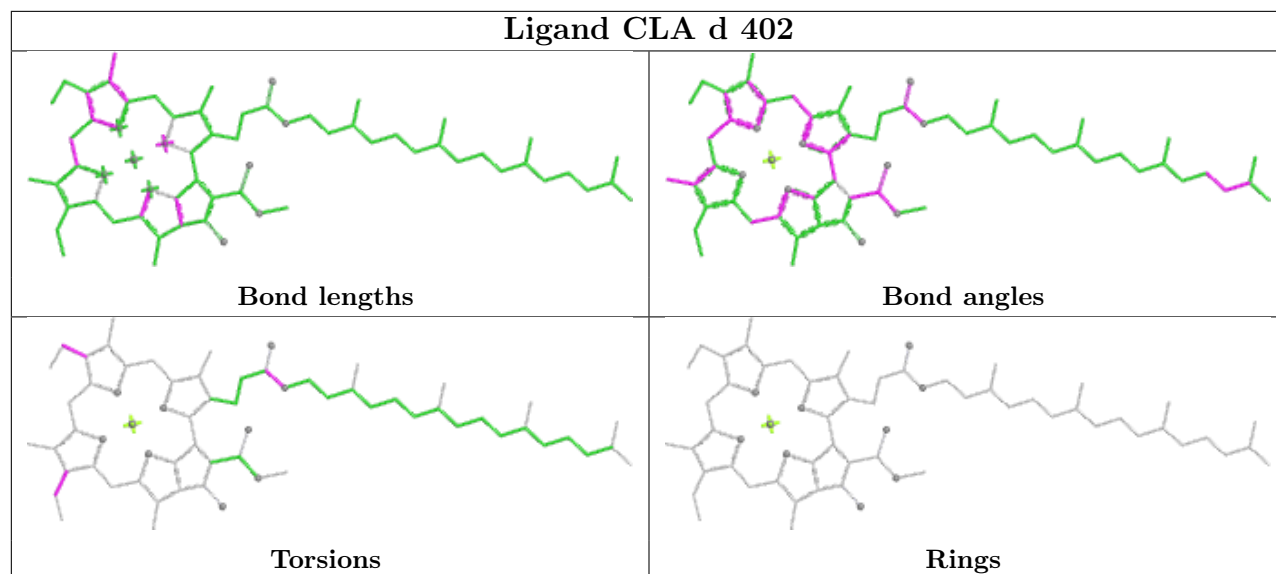
Ligand LMG M 101



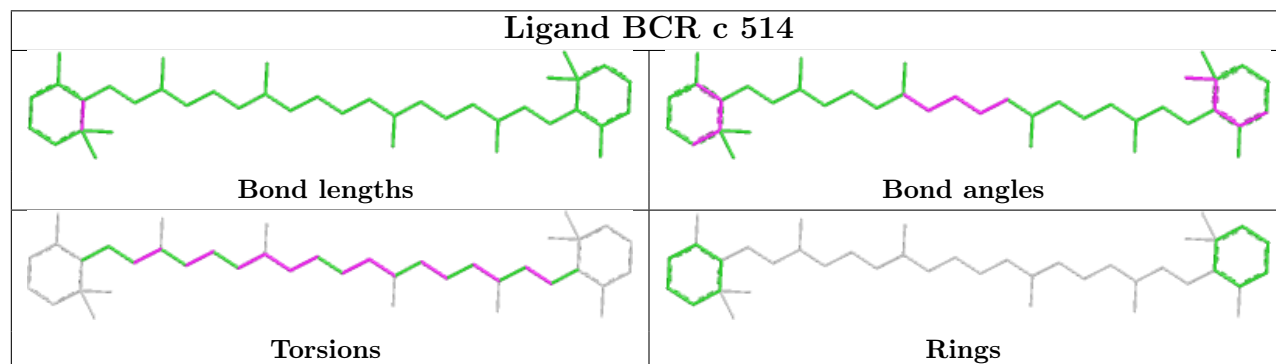
Ligand PL9 d 406



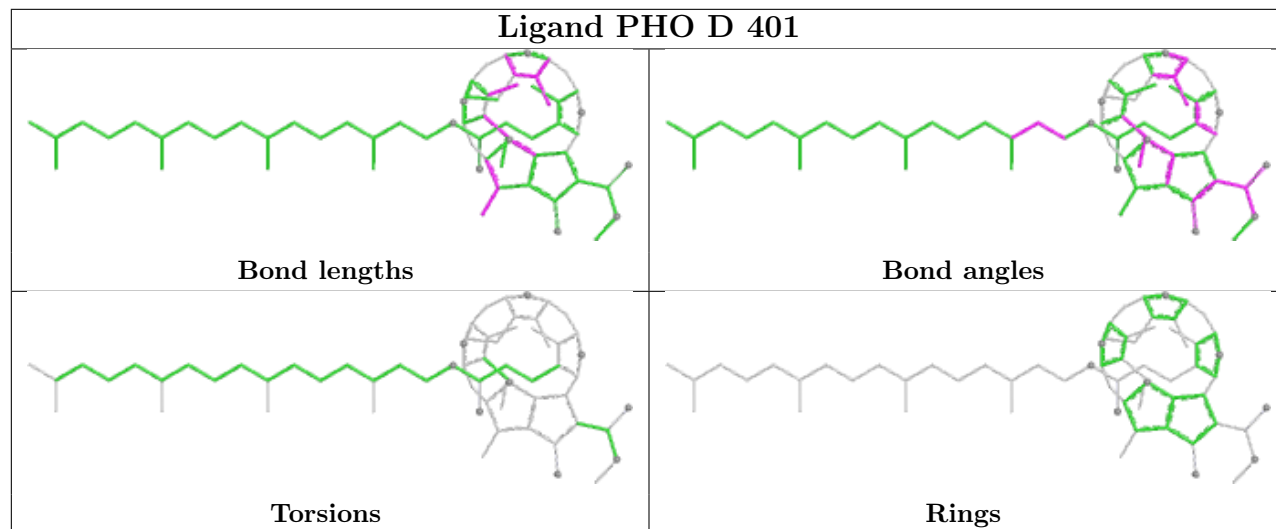
Ligand CLA d 402

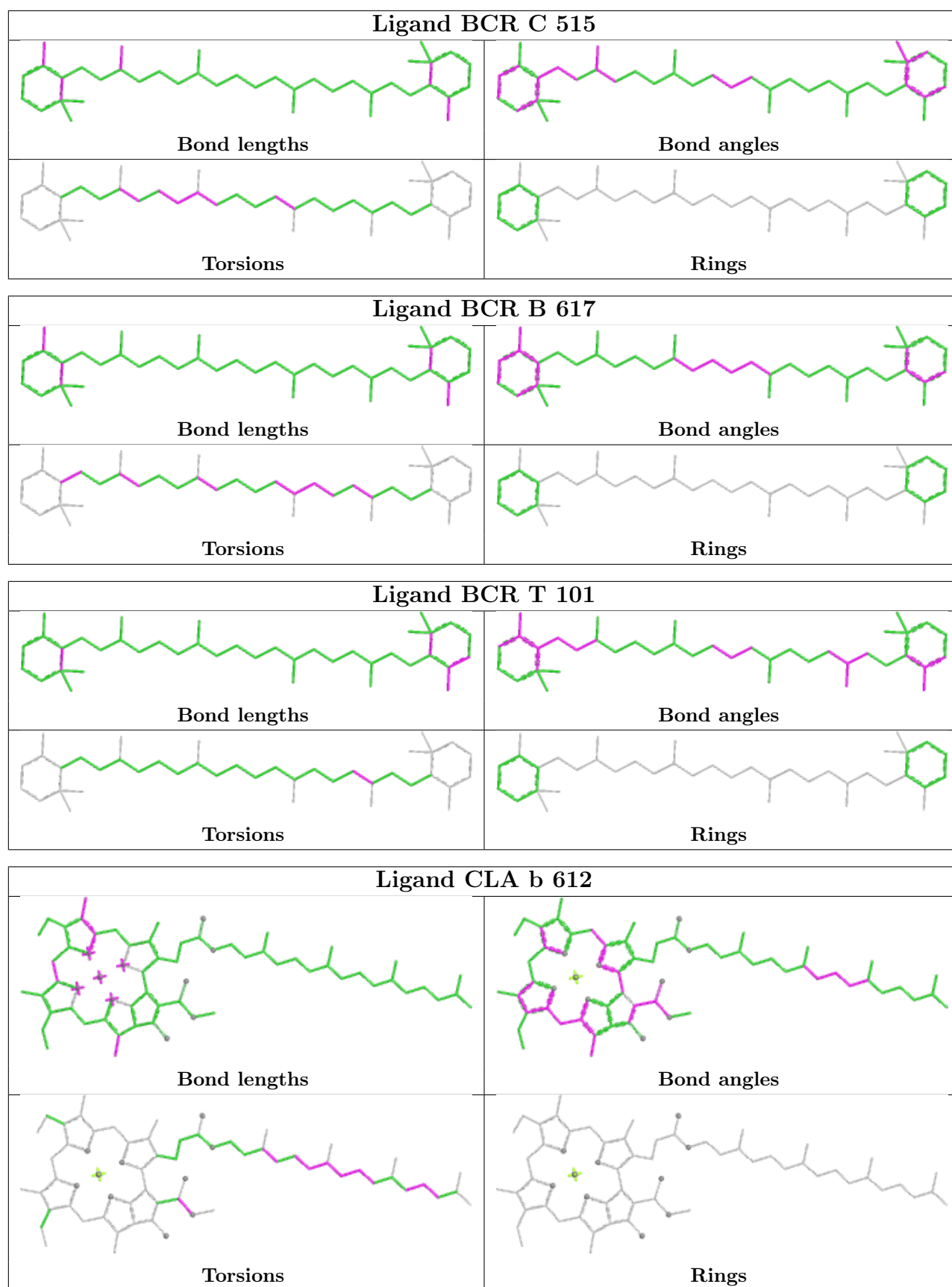


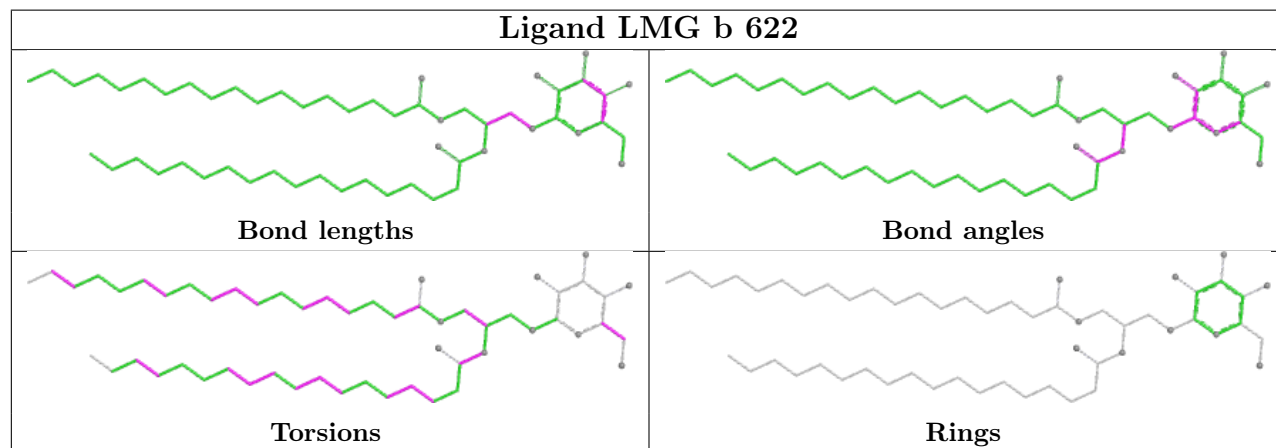
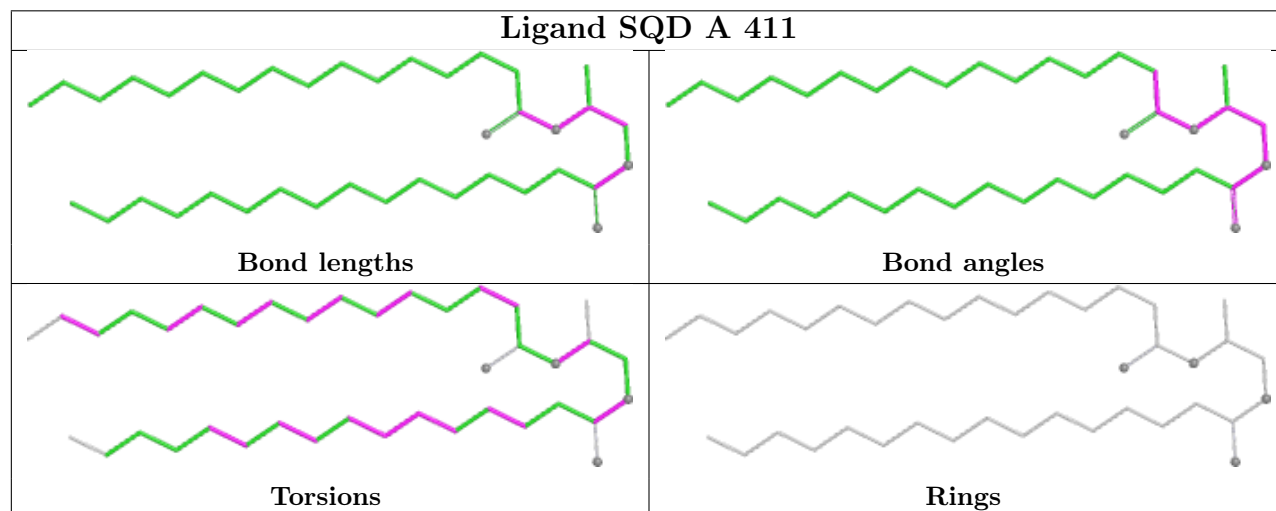
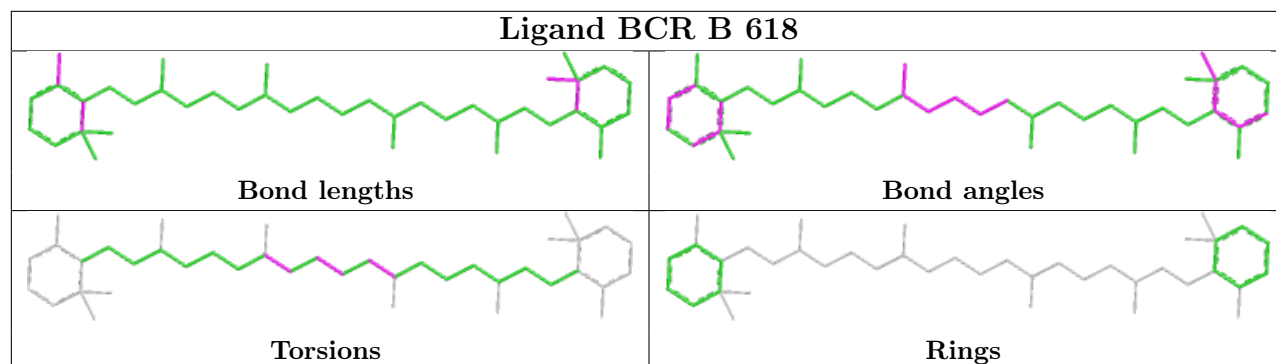
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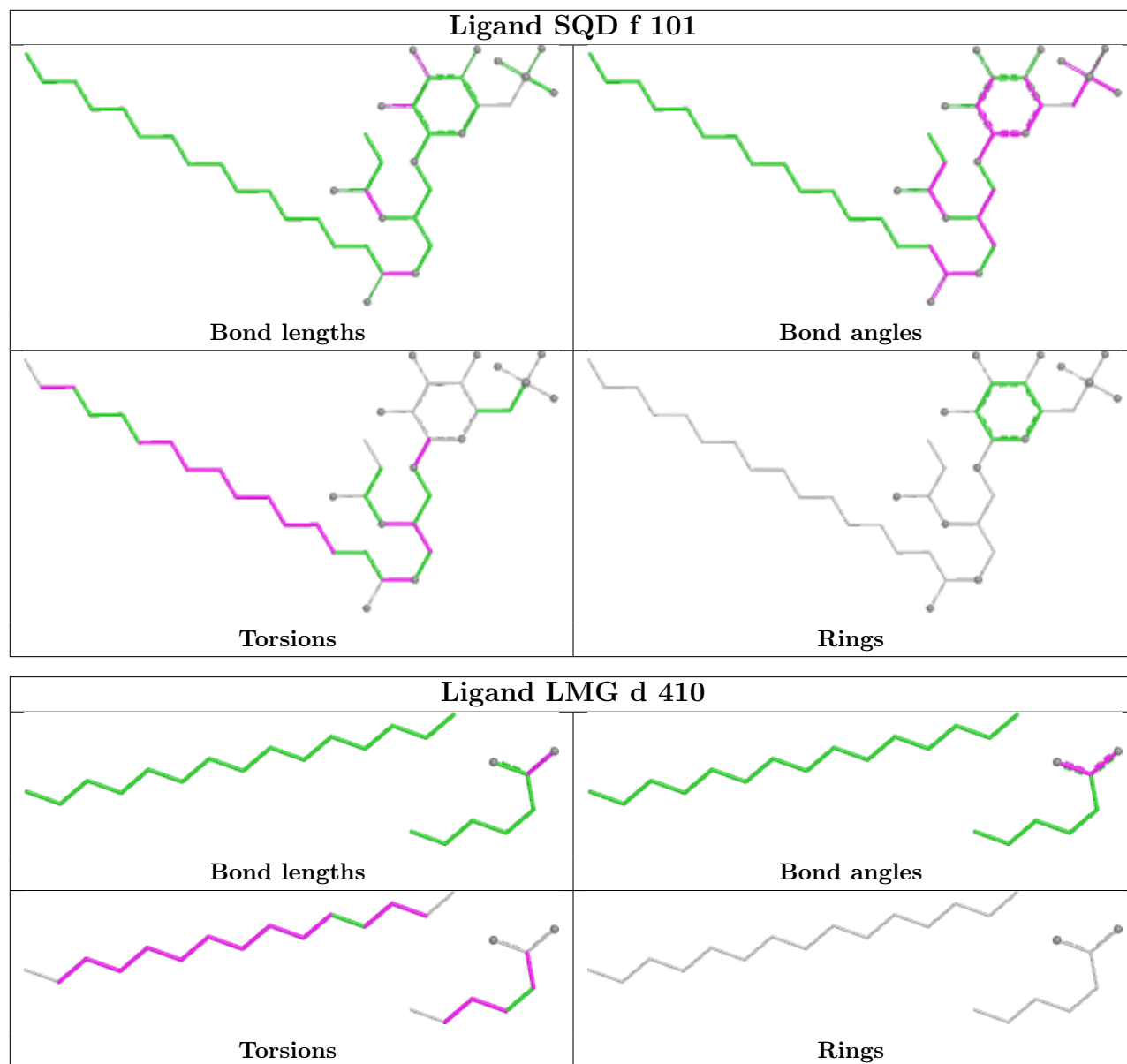


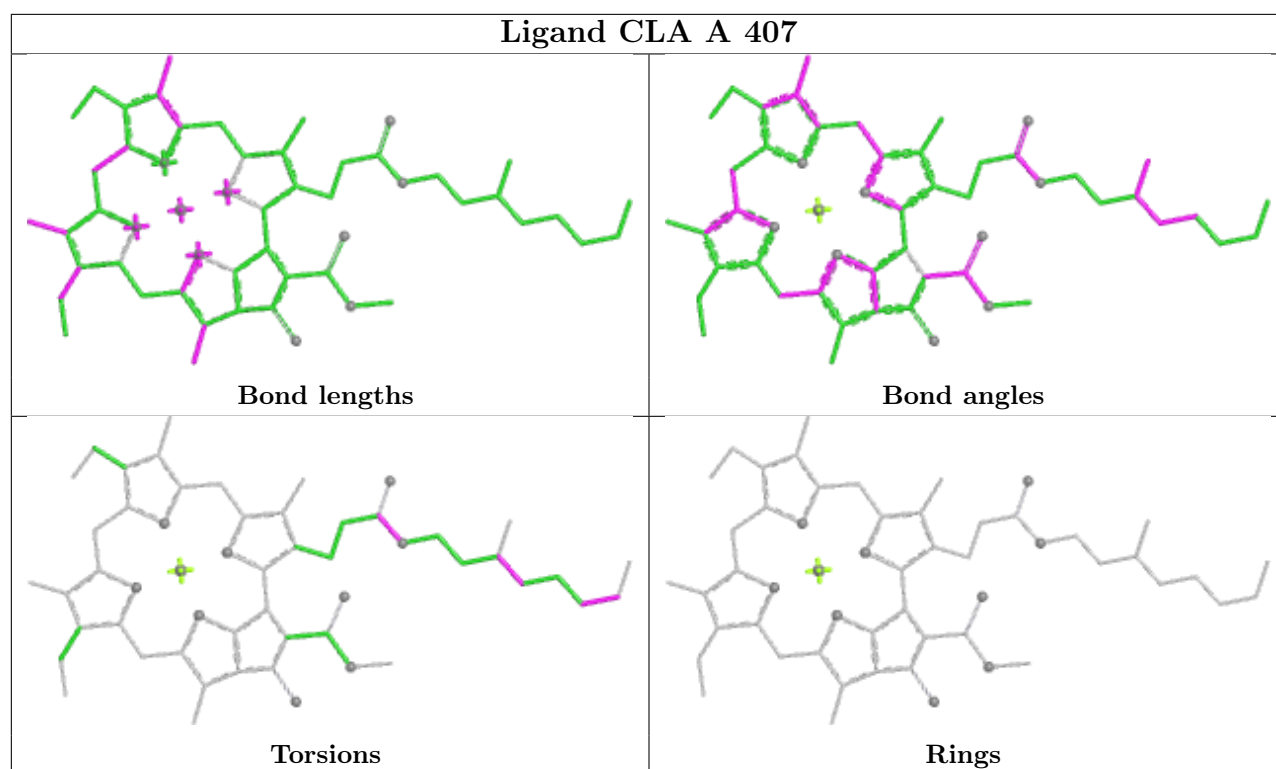
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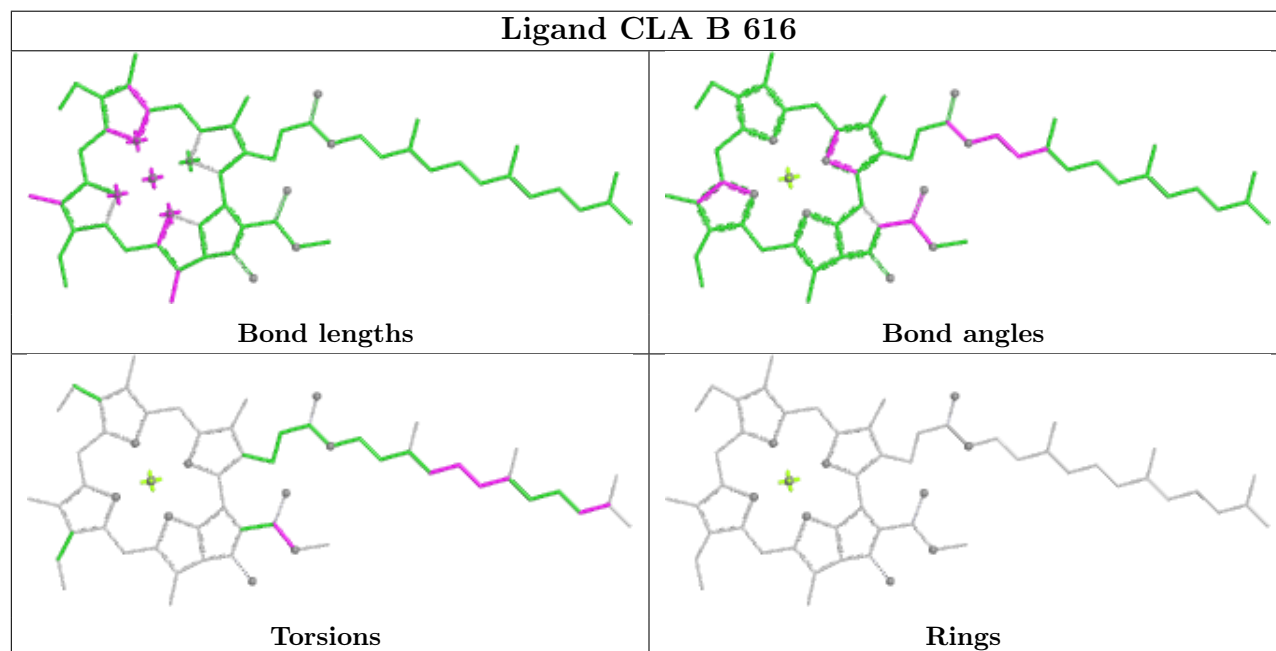
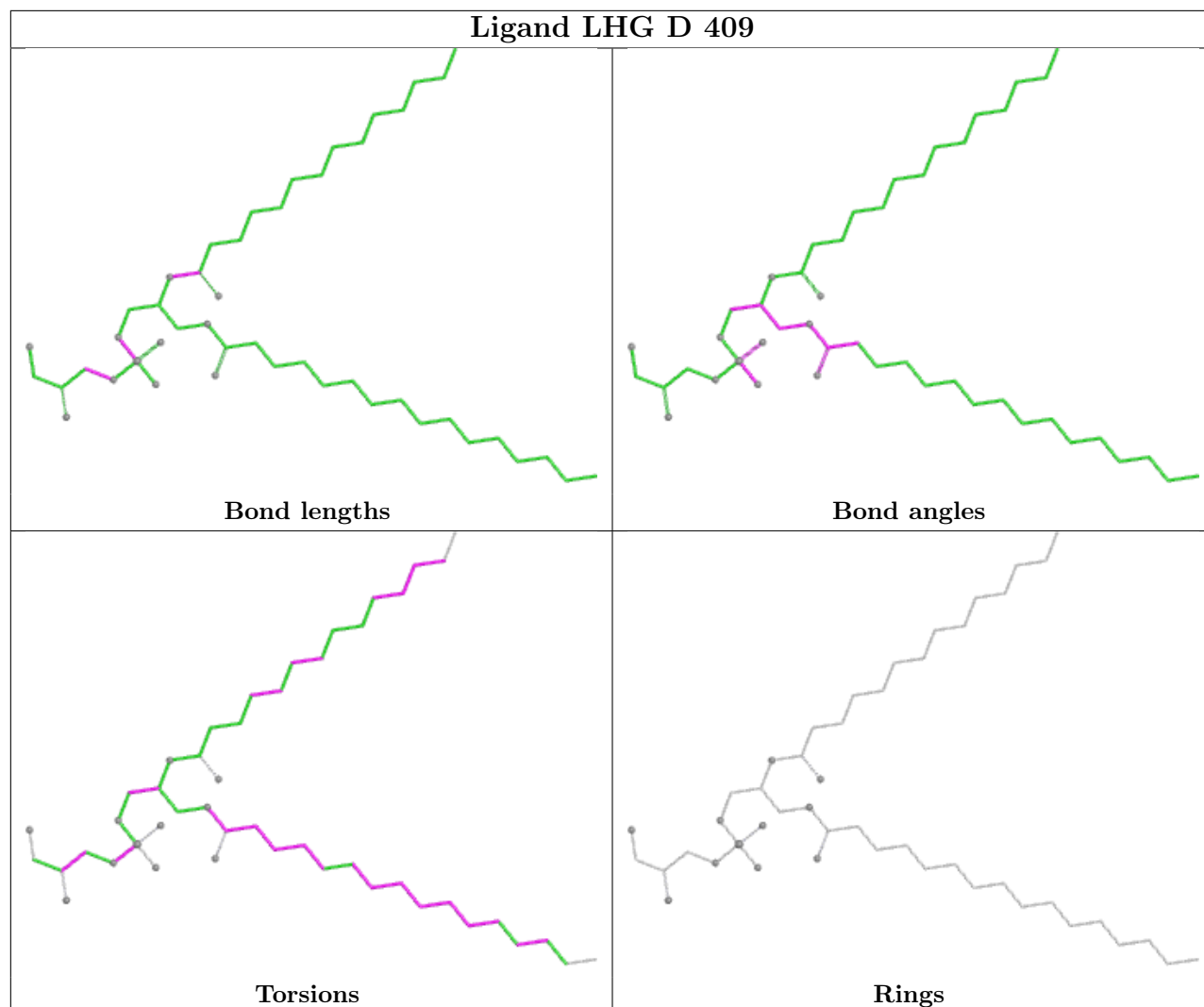


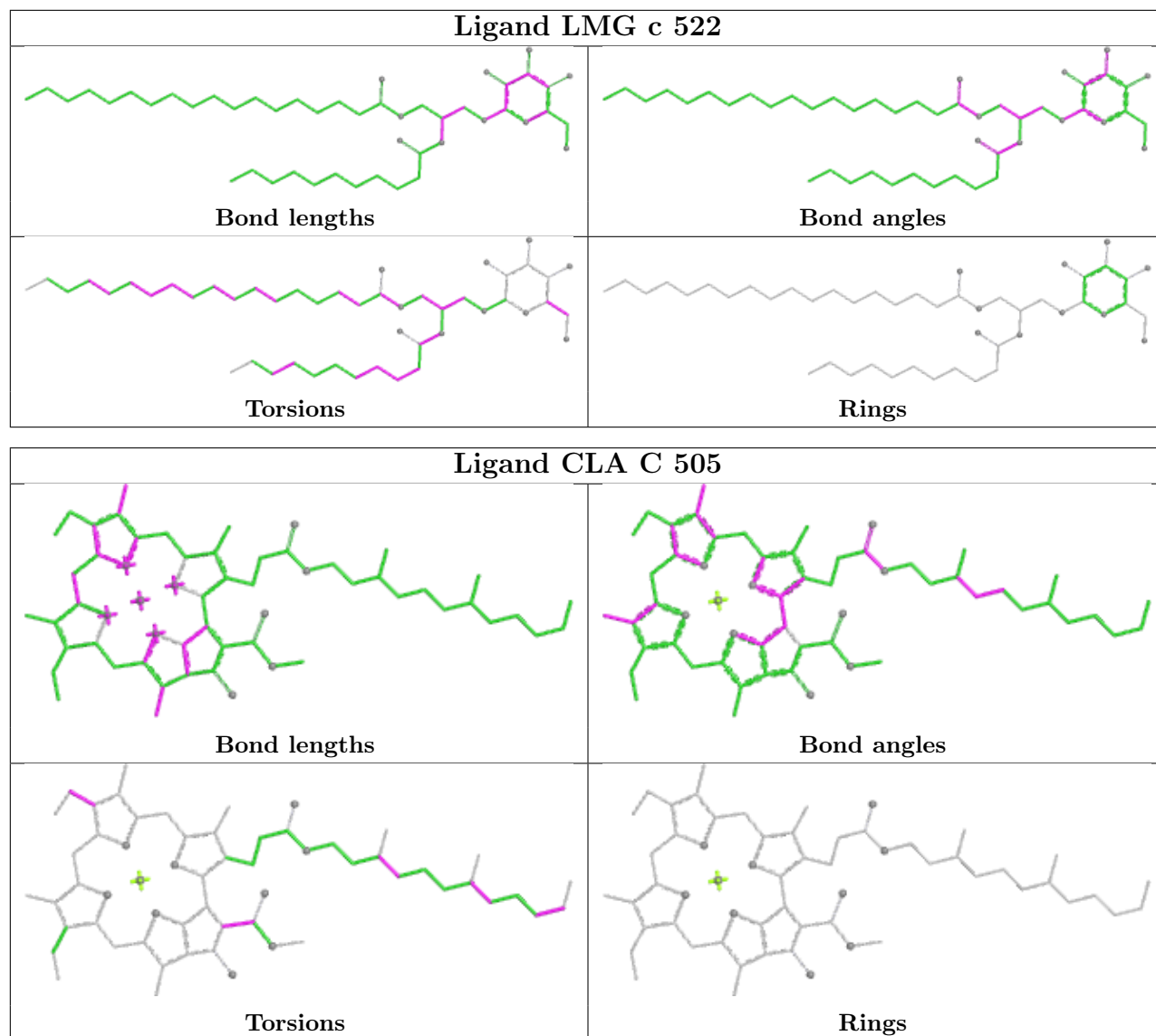


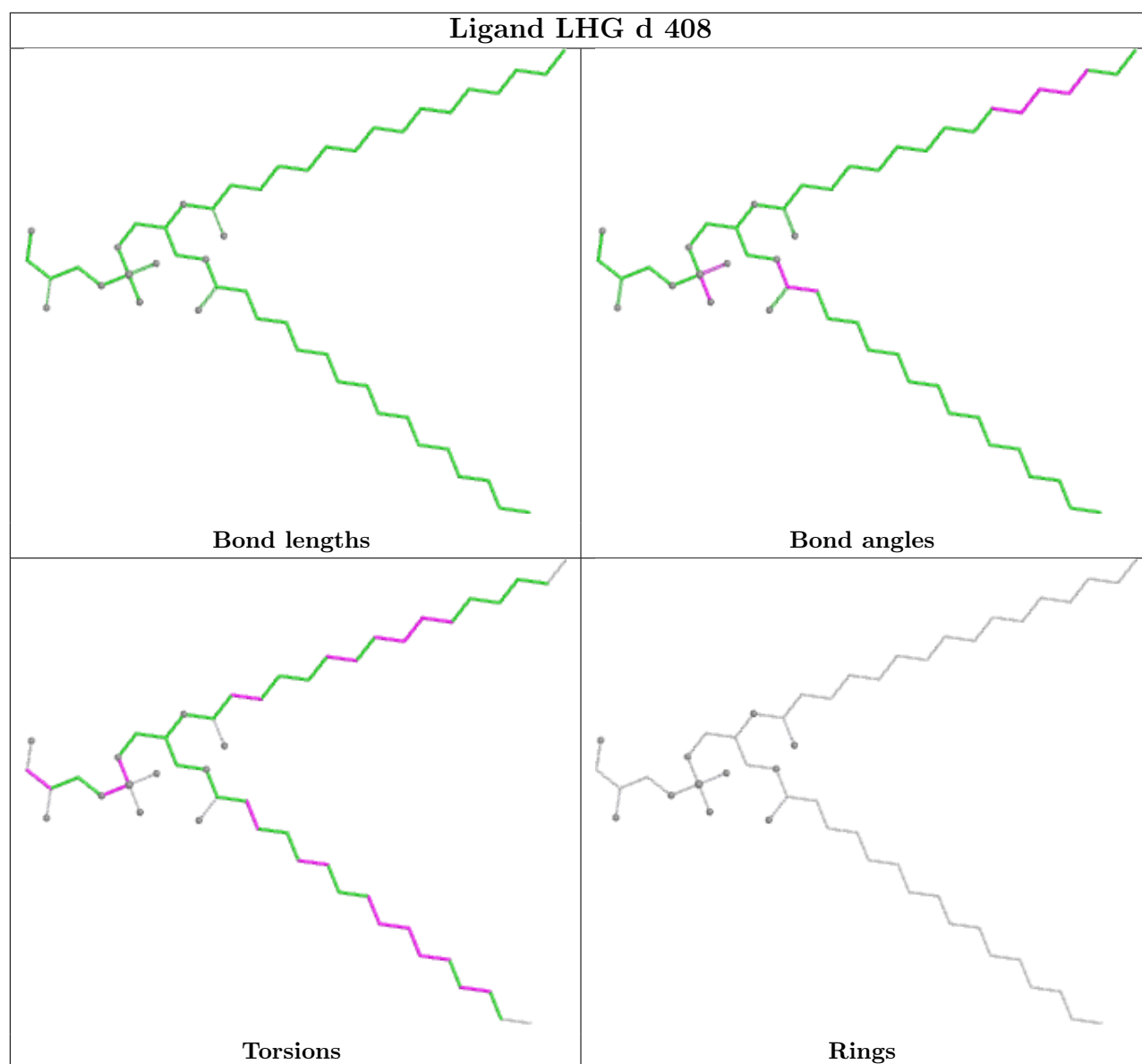




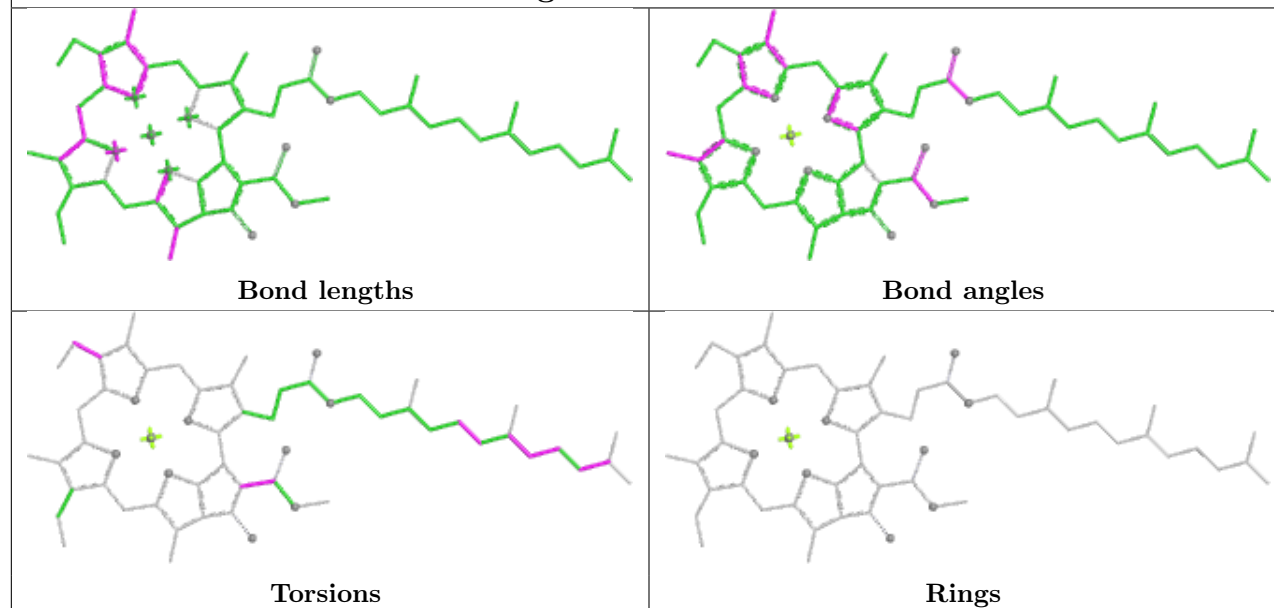




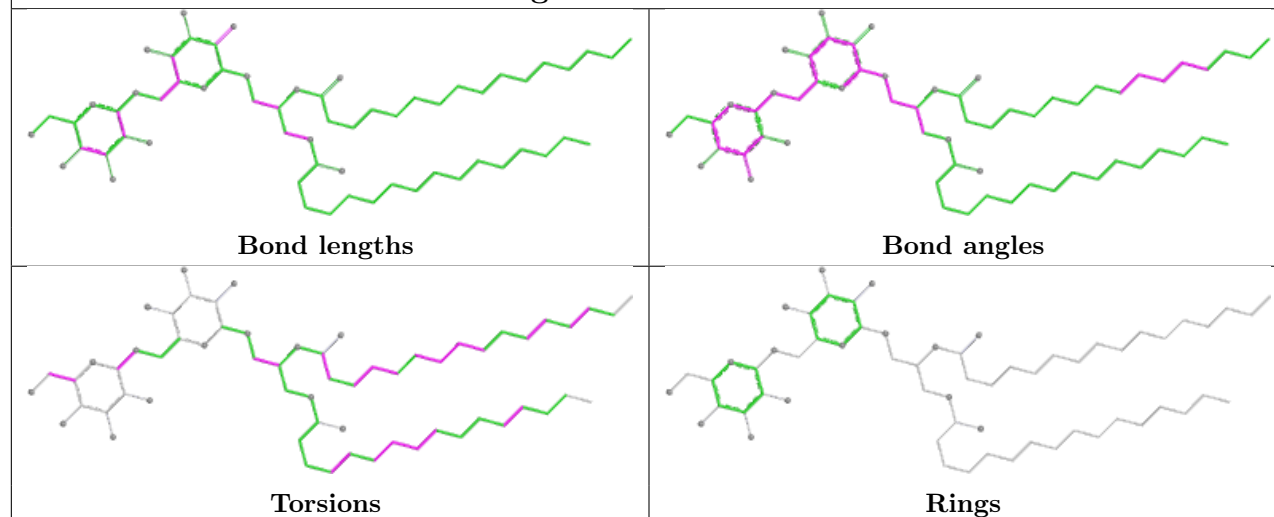




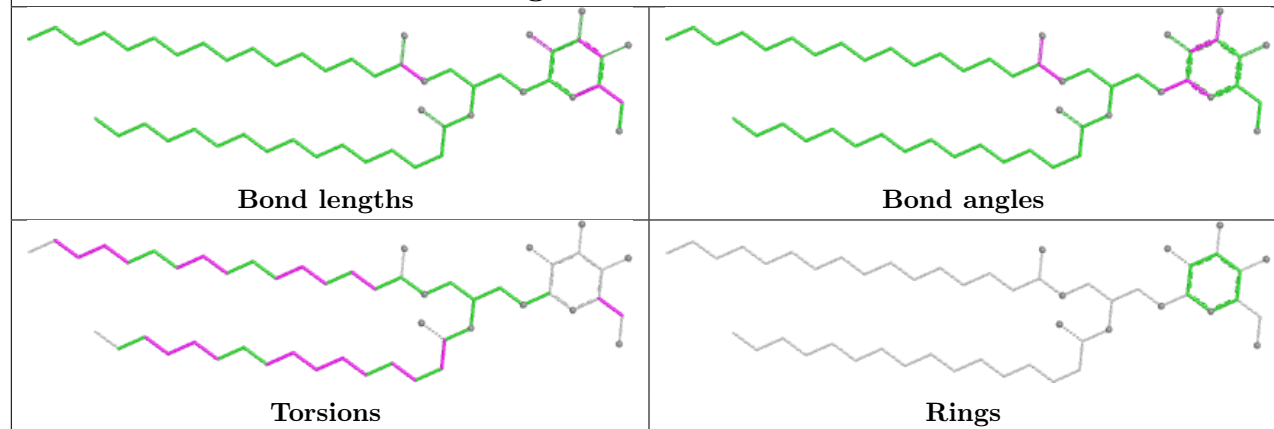
Ligand CLA c 504



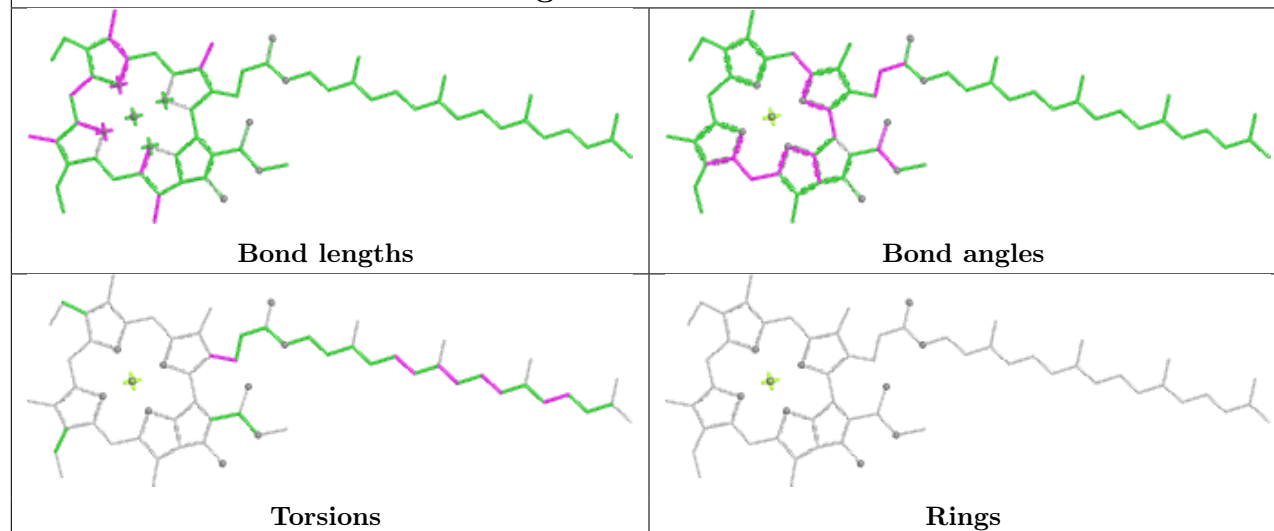
Ligand DGD h 101



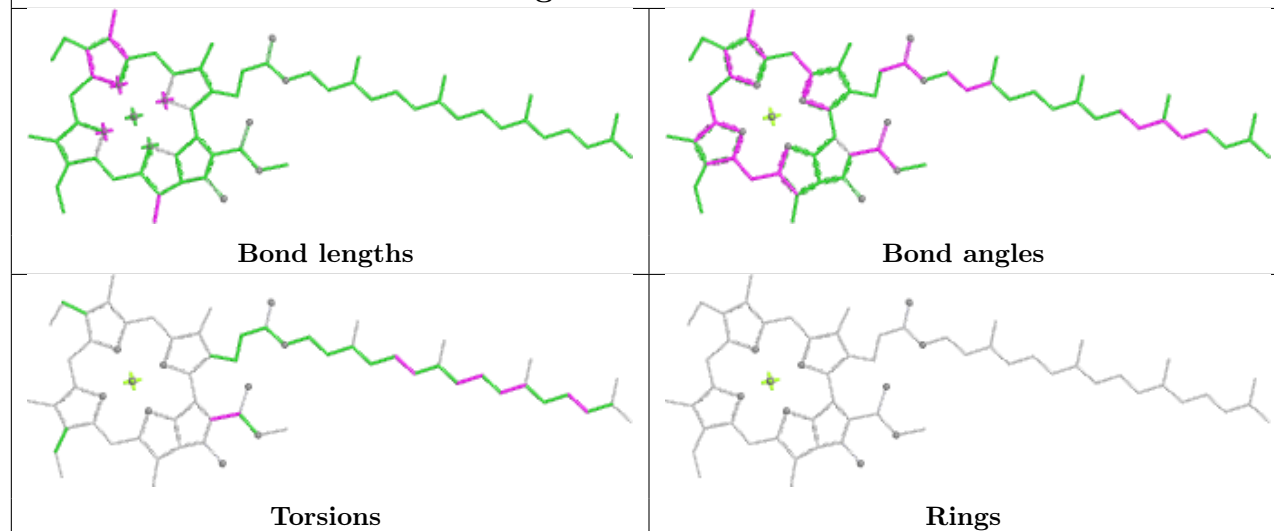
Ligand LMG D 407



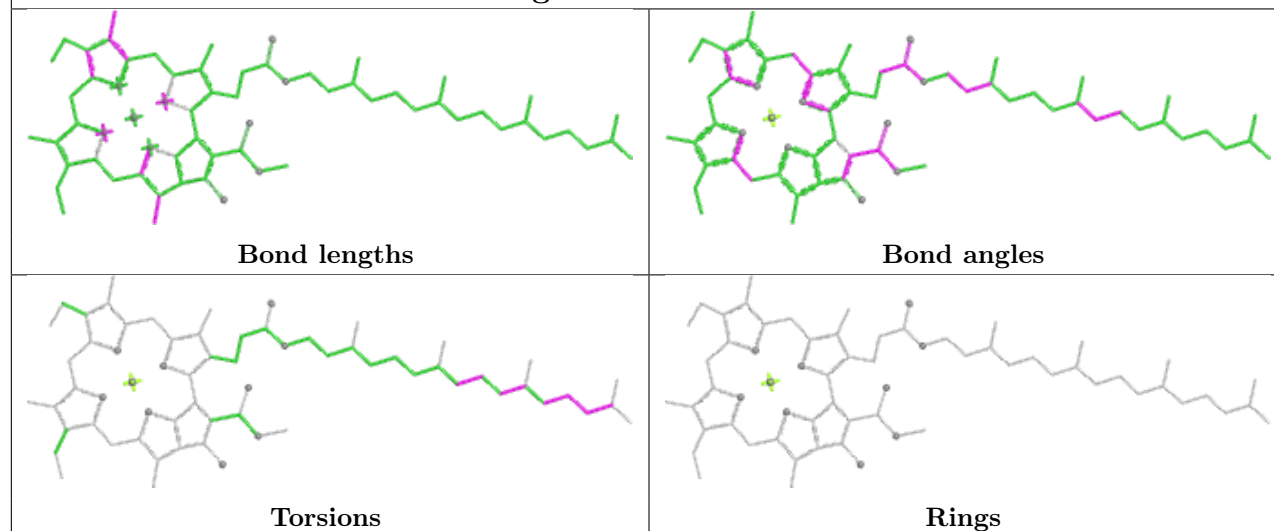
Ligand CLA a 408



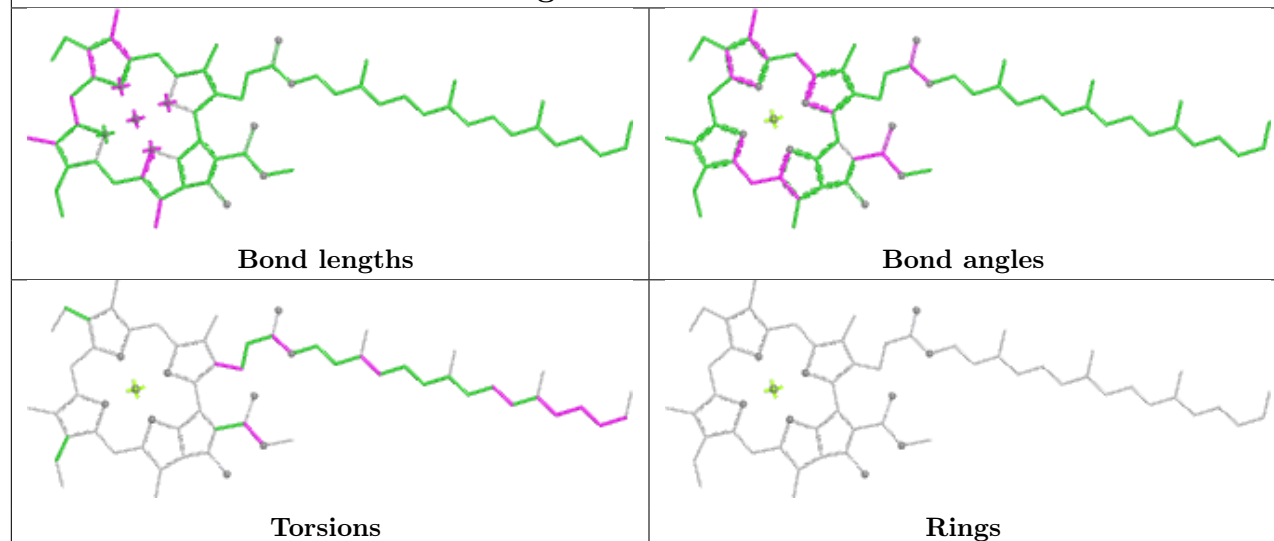
Ligand CLA b 606



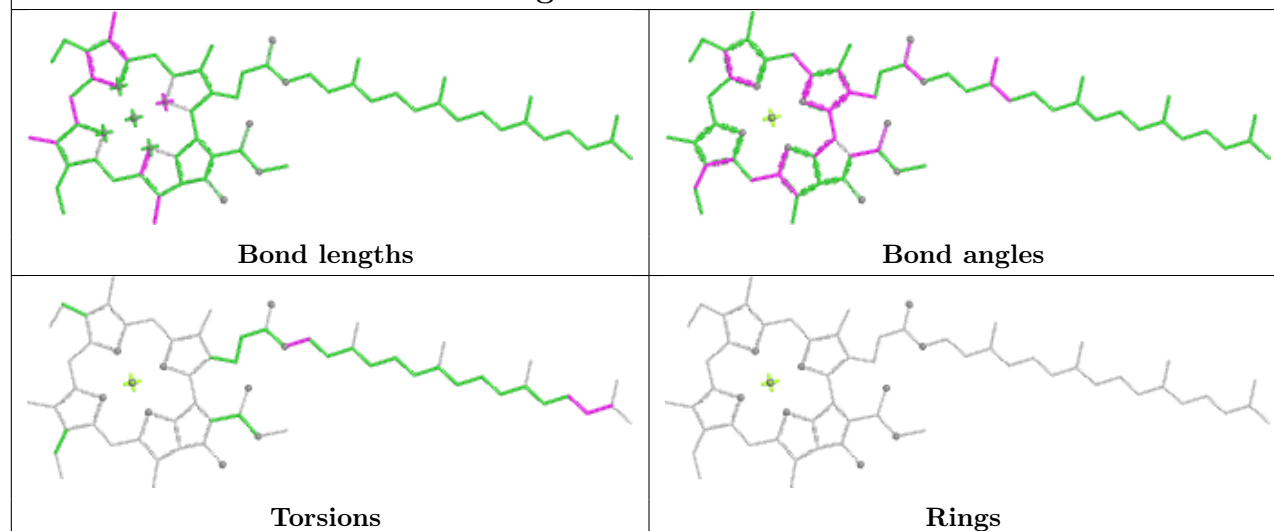
Ligand CLA B 611



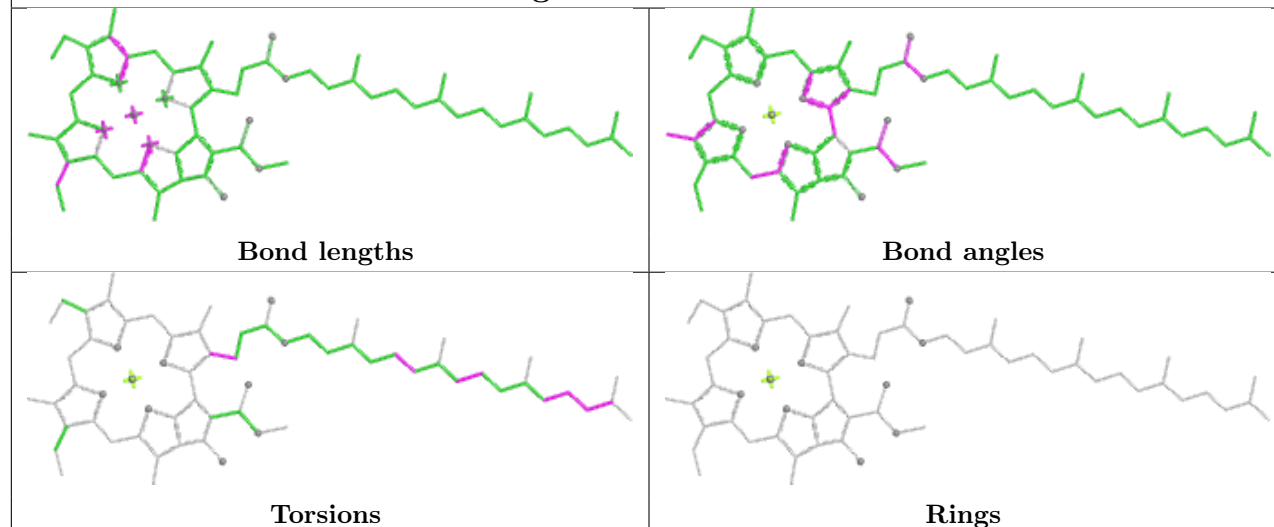
Ligand CLA c 508

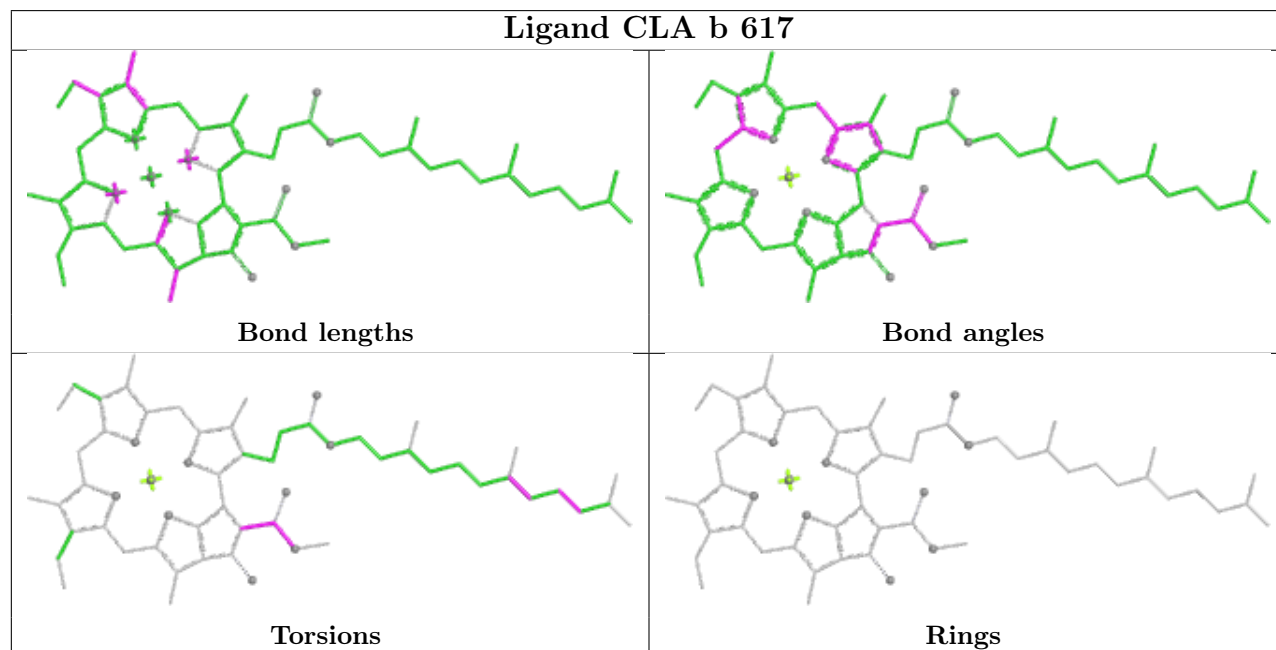
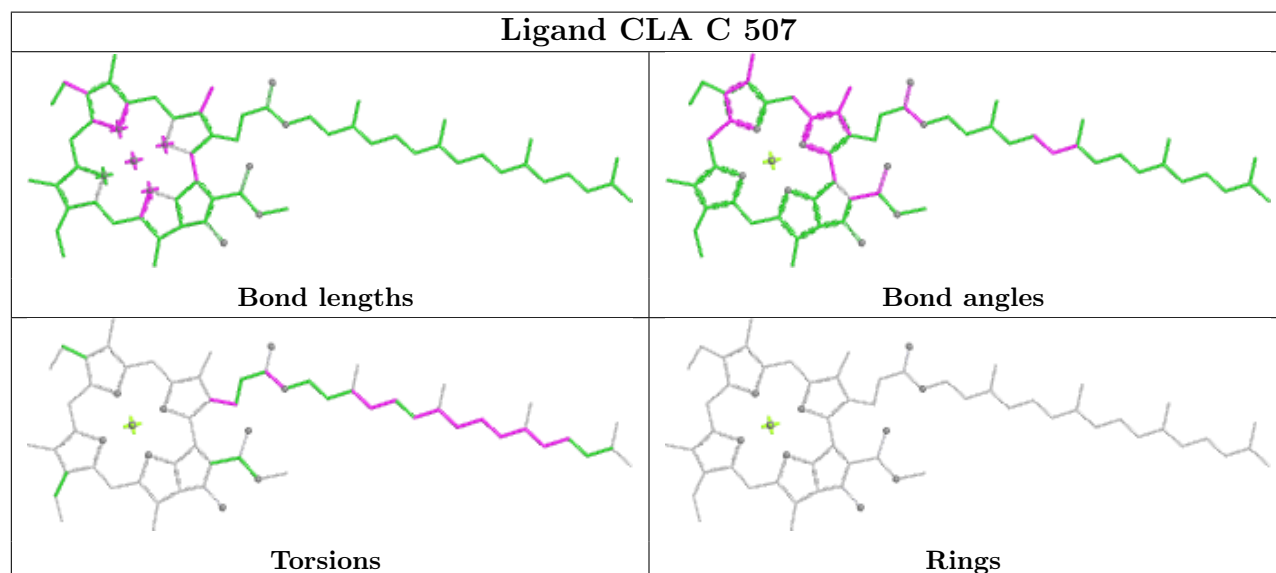
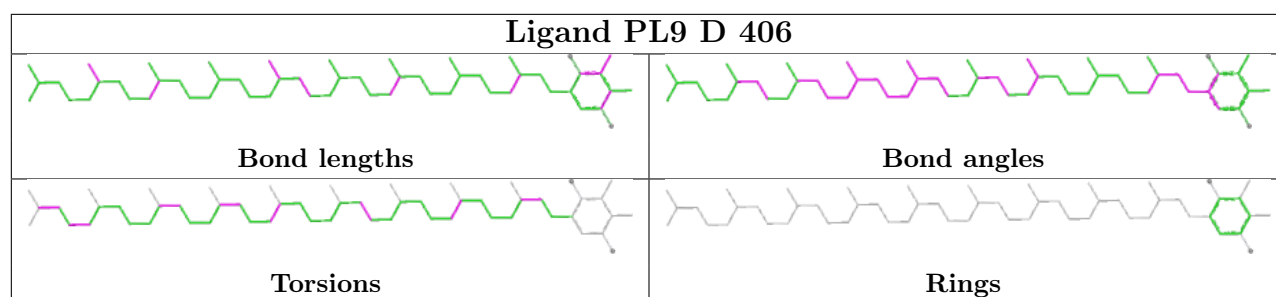


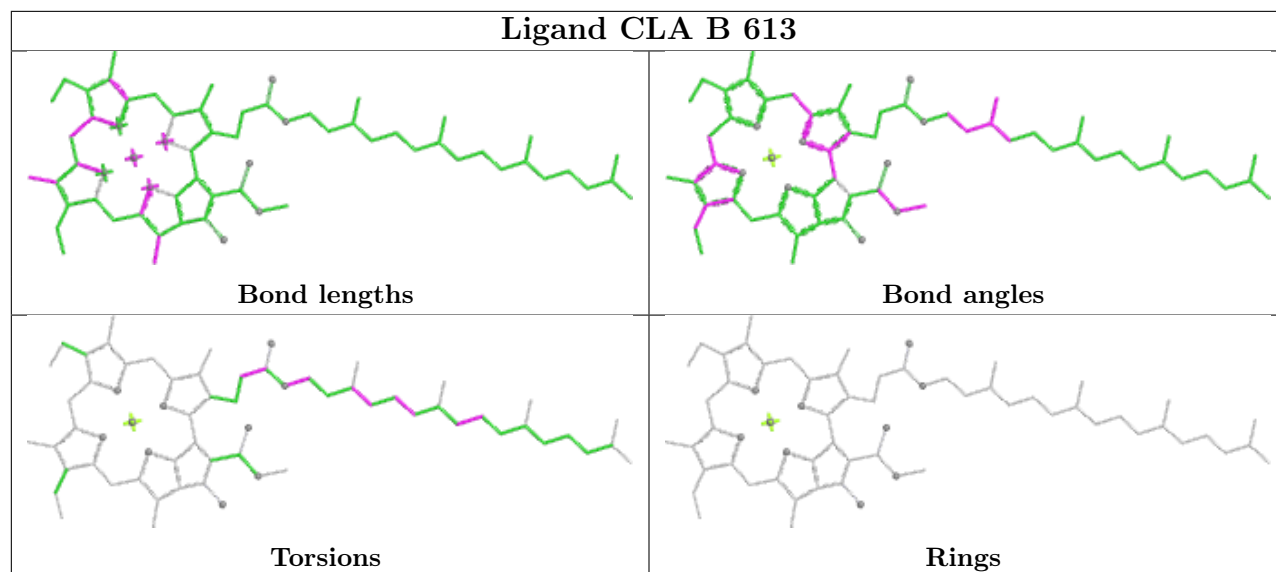
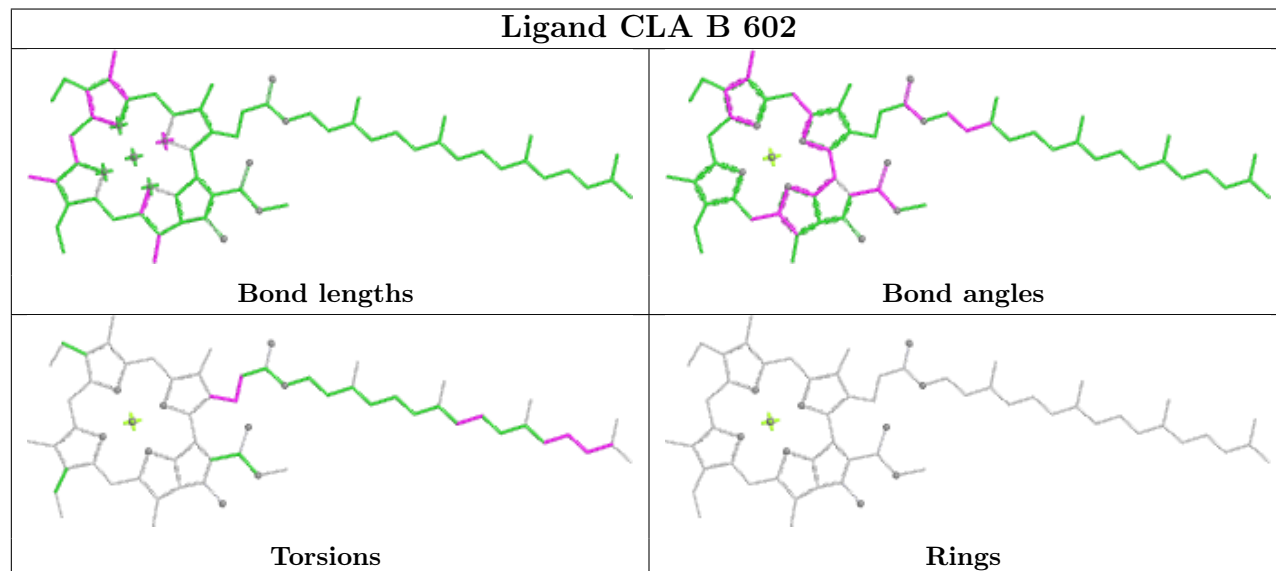
Ligand CLA a 405

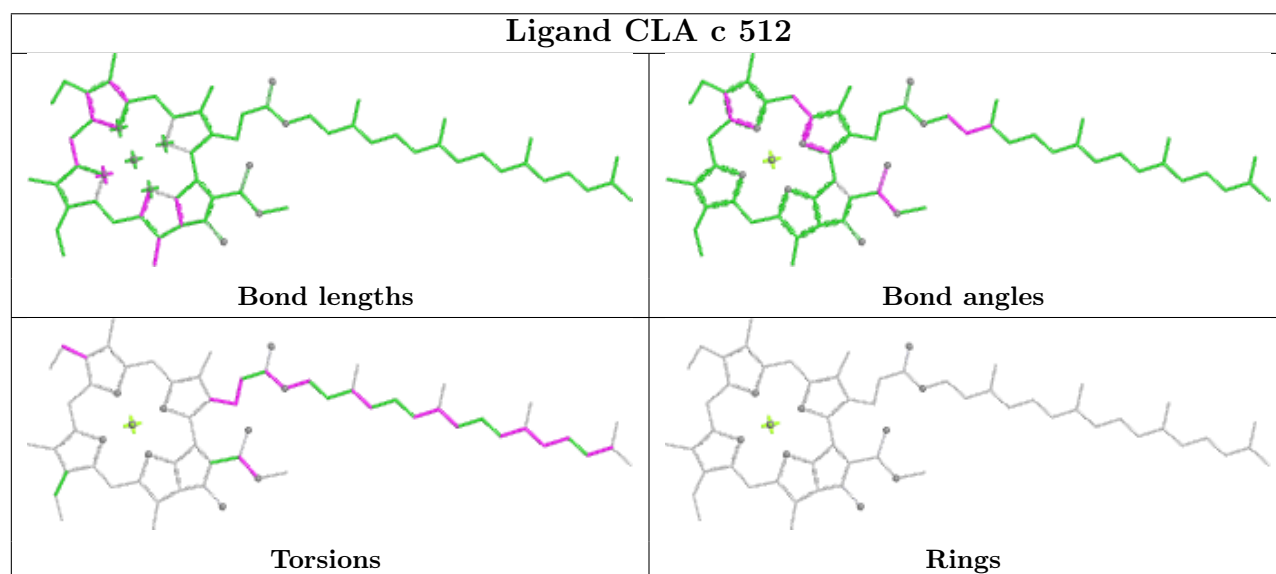
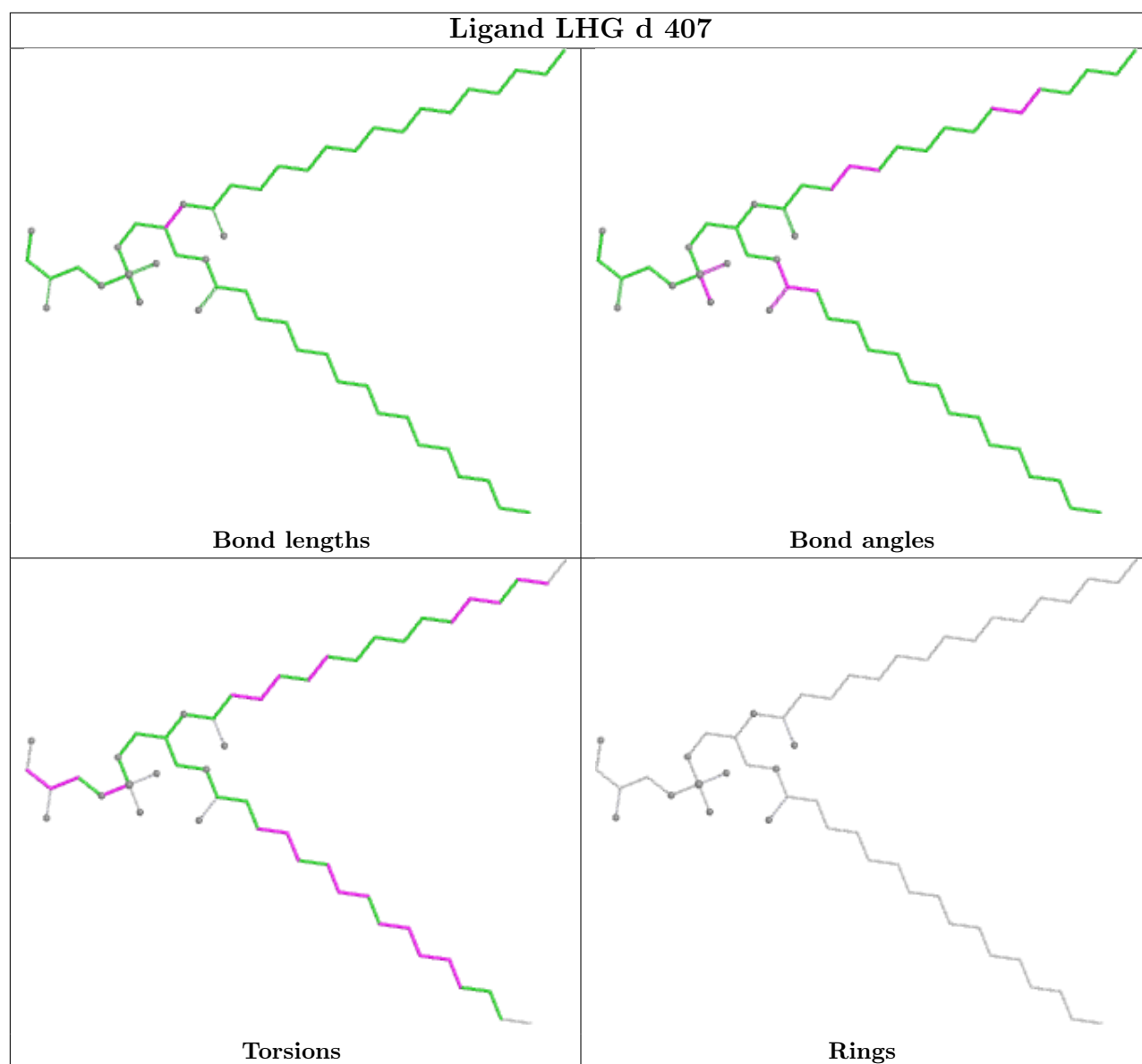


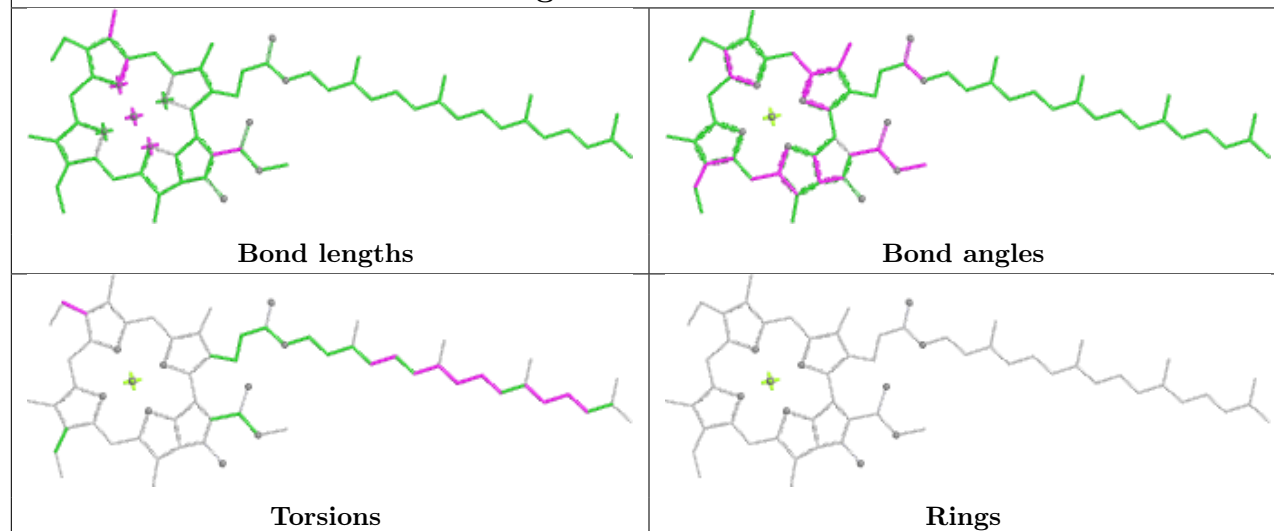
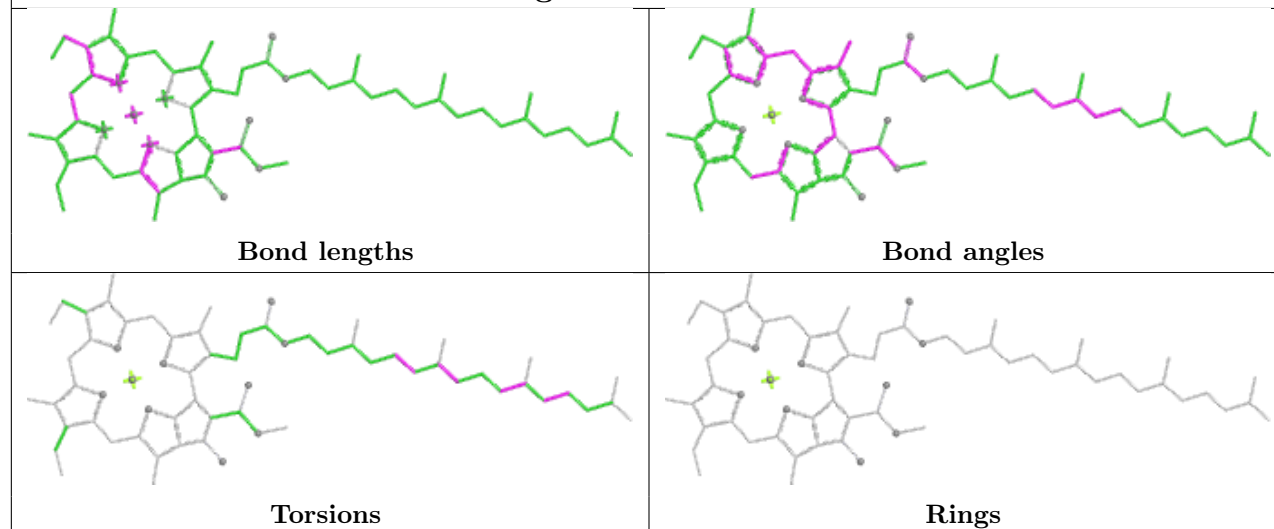
Ligand CLA B 607

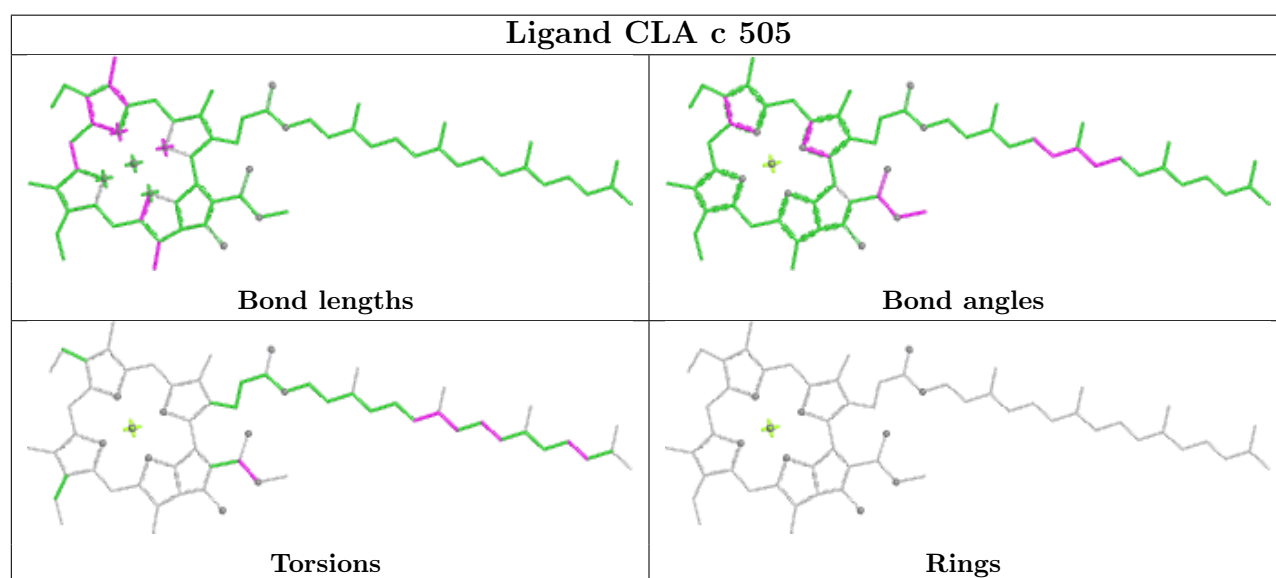
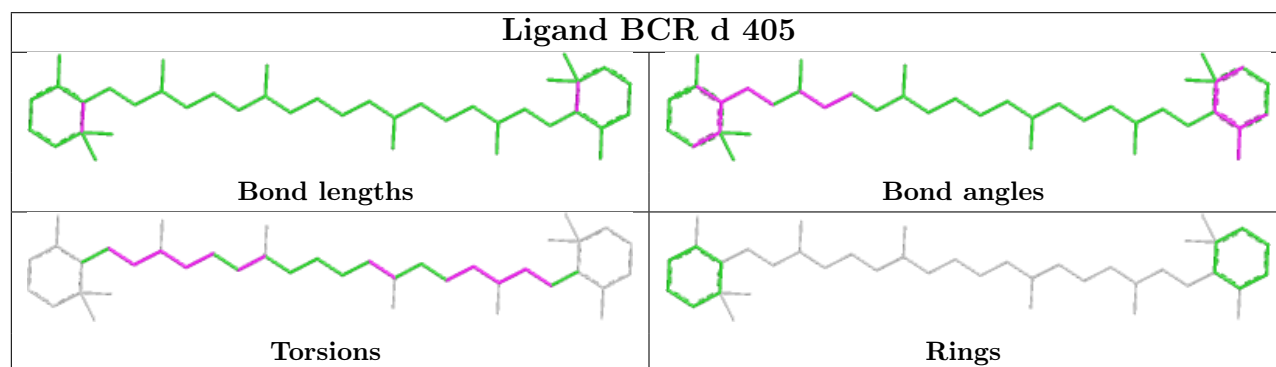
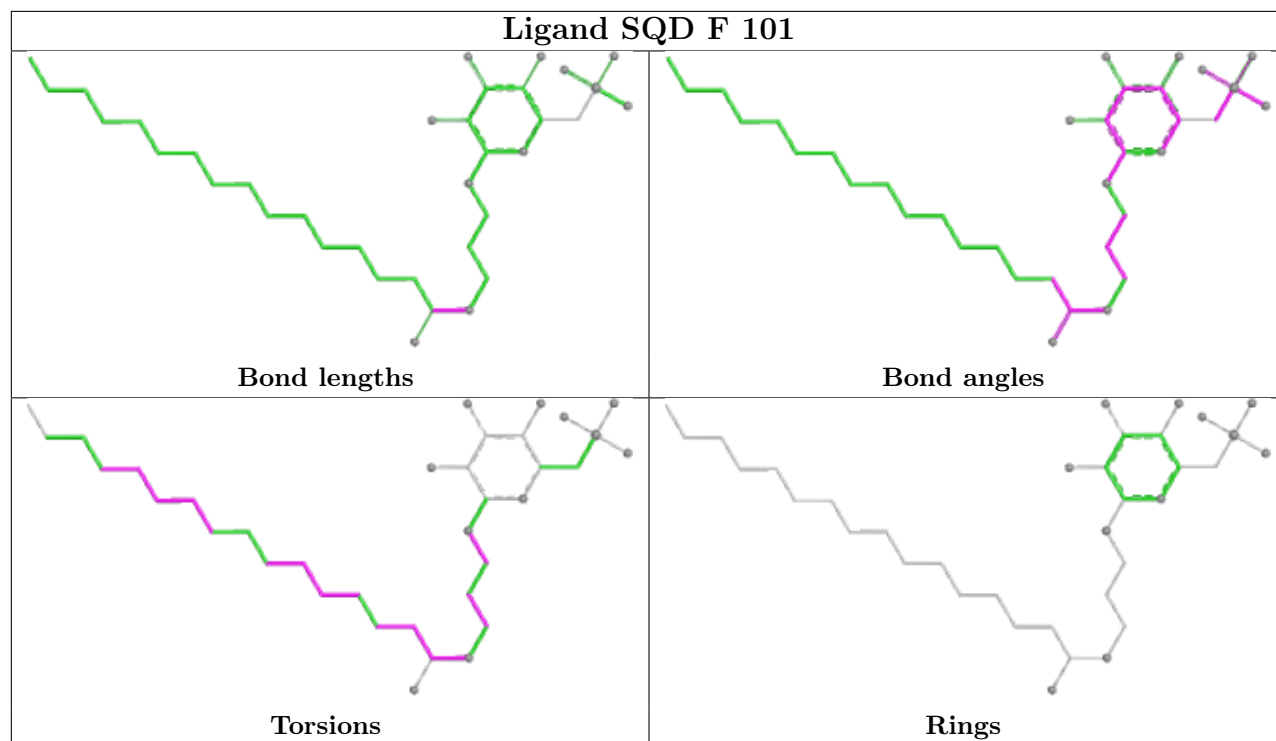




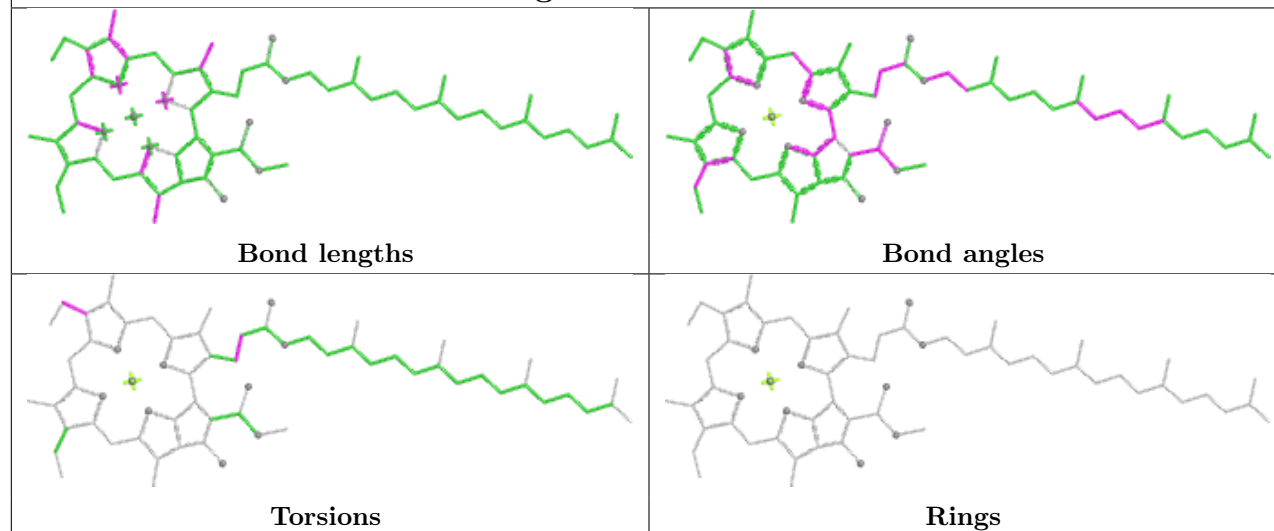
Ligand CLA B 613**Ligand CLA B 602**



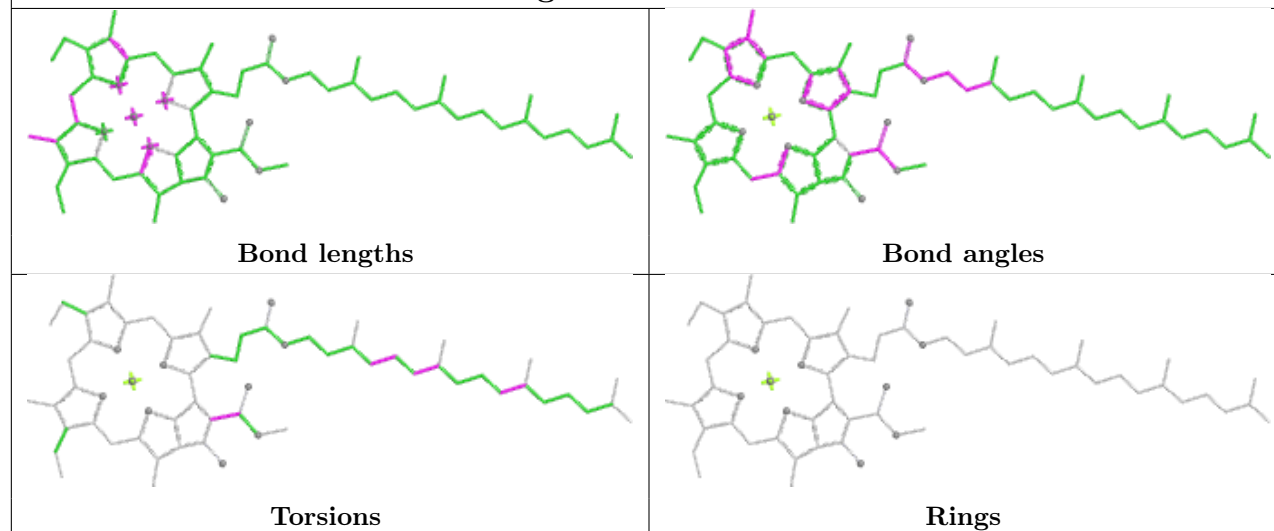
Ligand CLA a 406**Ligand CLA b 609**



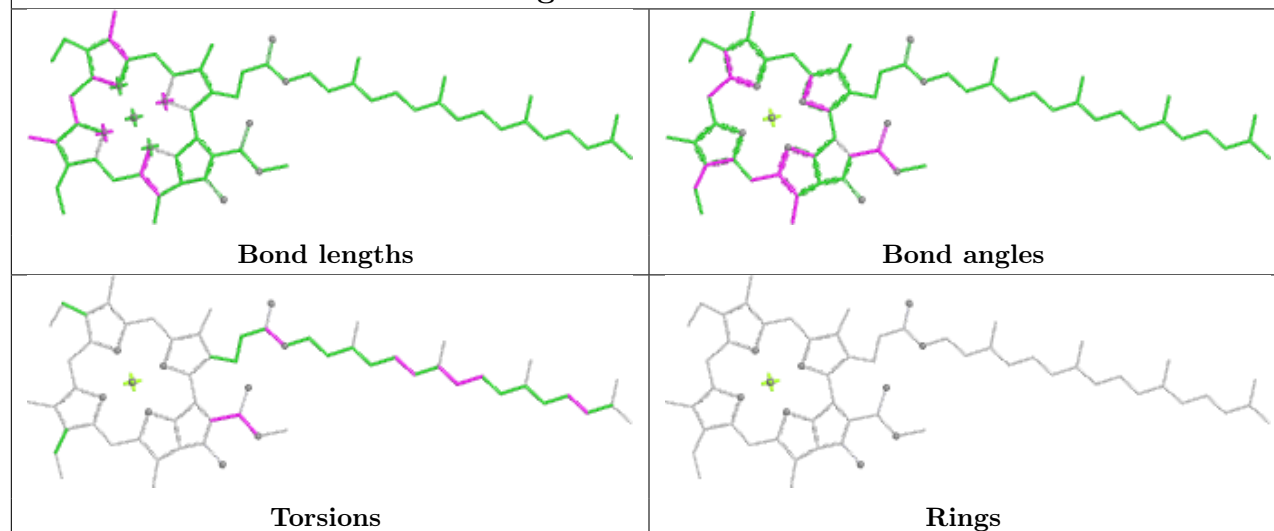
Ligand CLA b 611

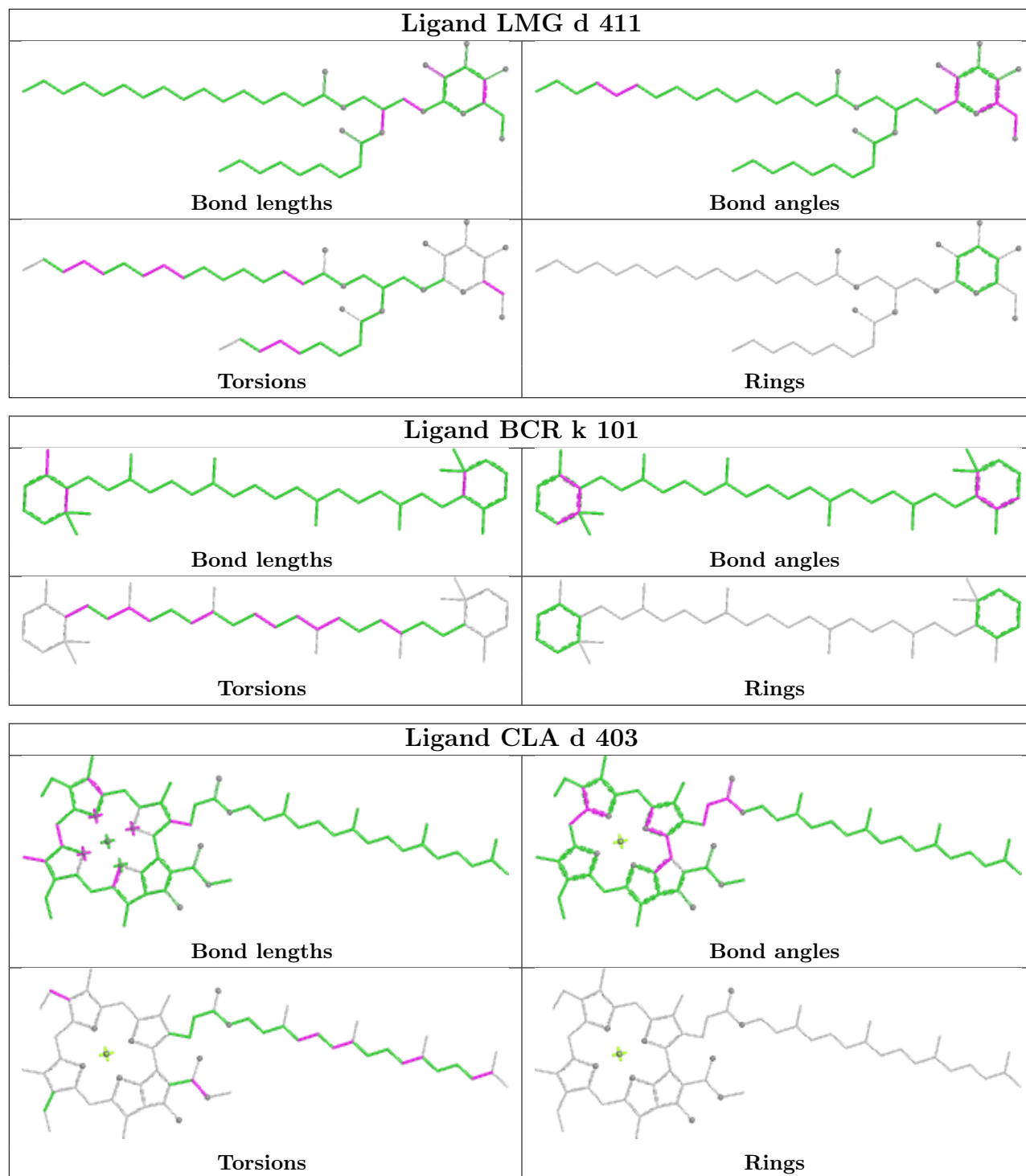


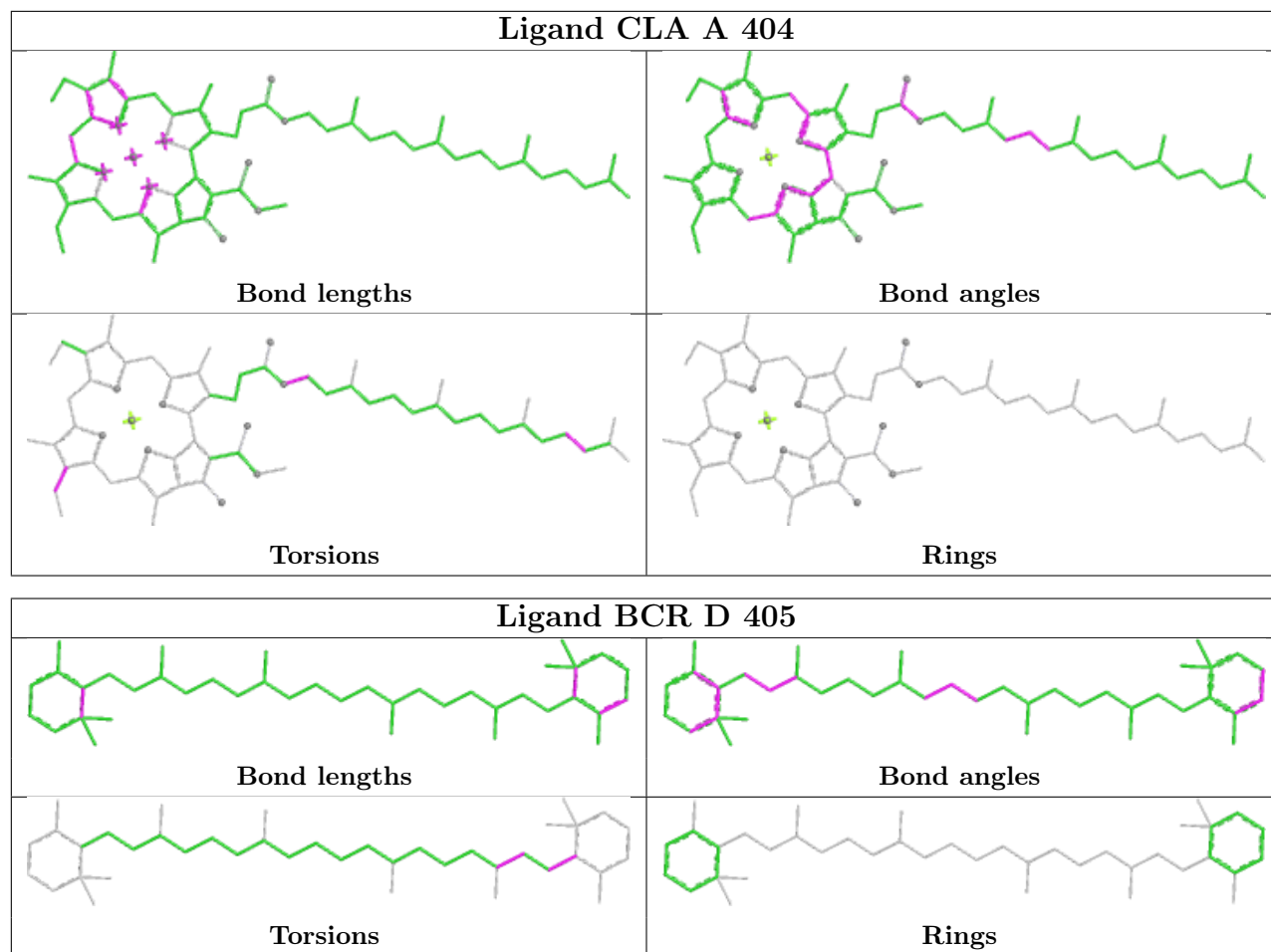
Ligand CLA c 502

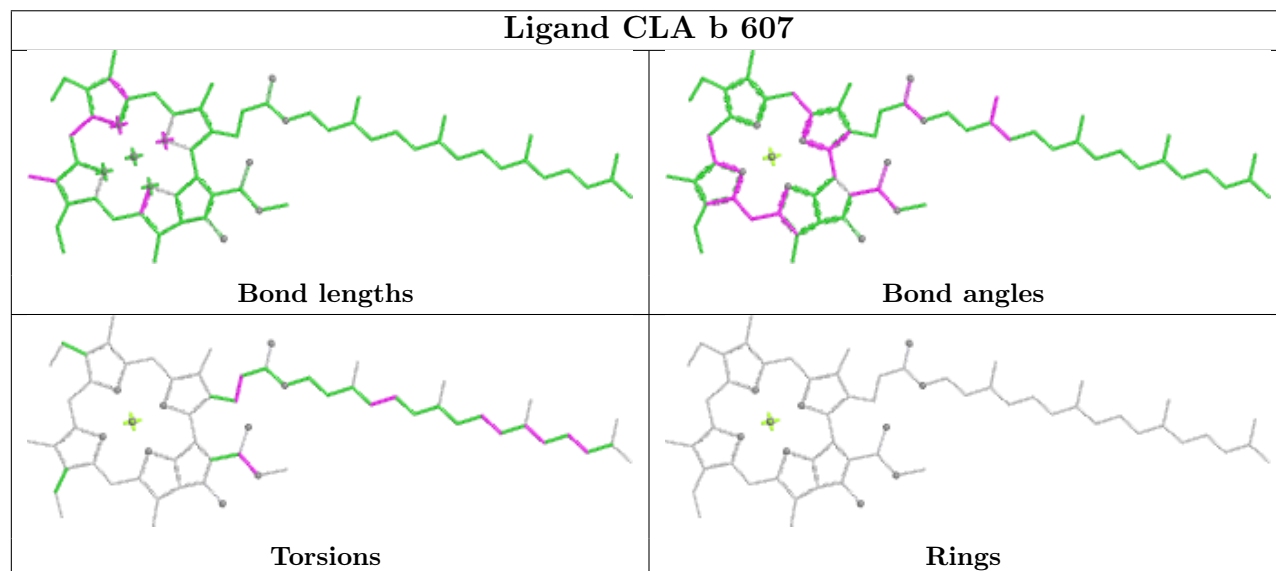
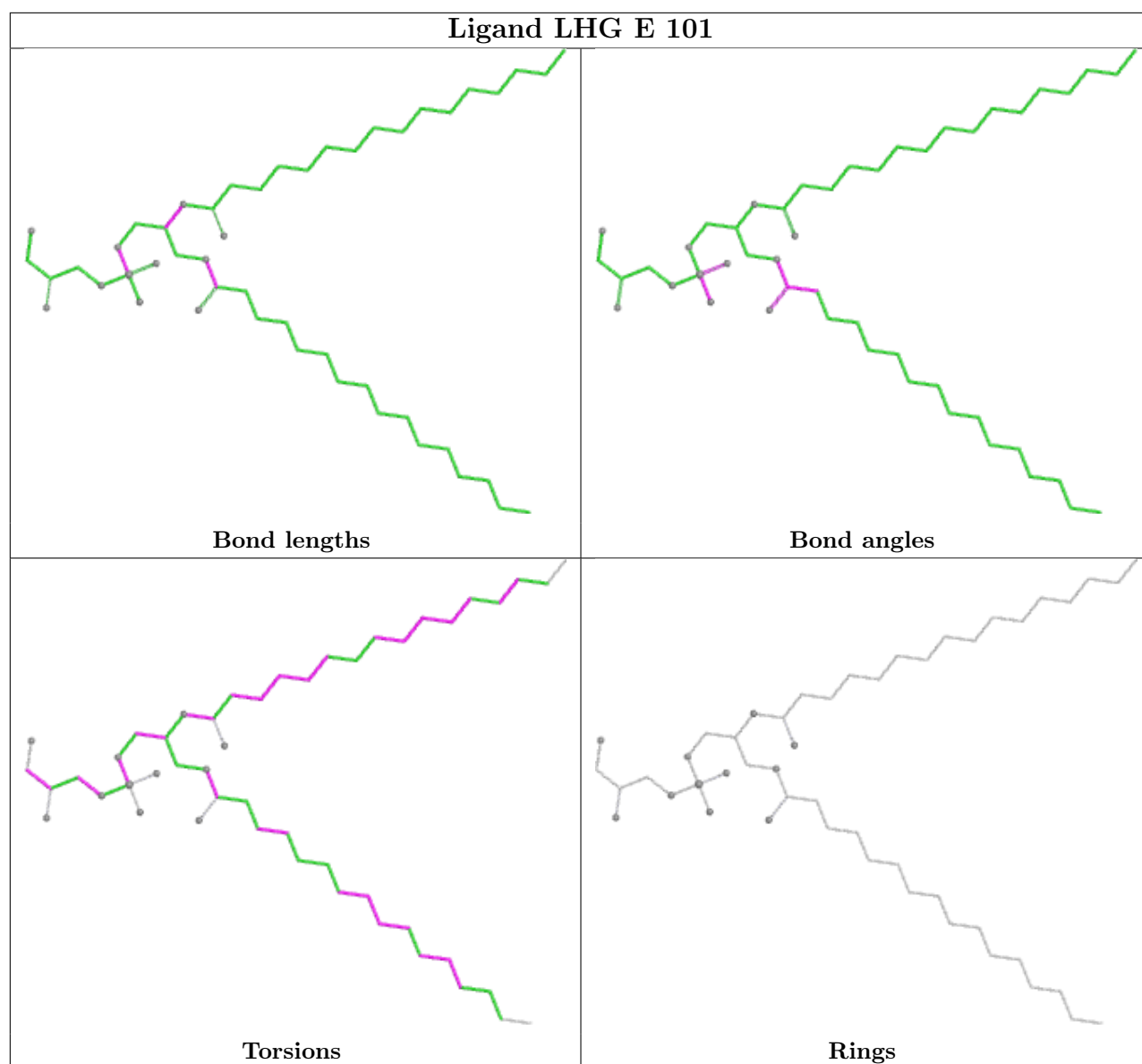


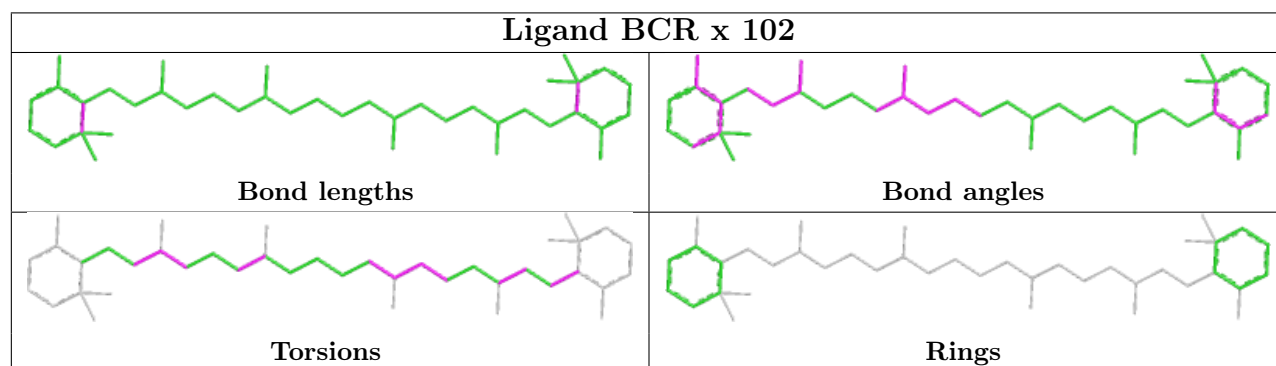
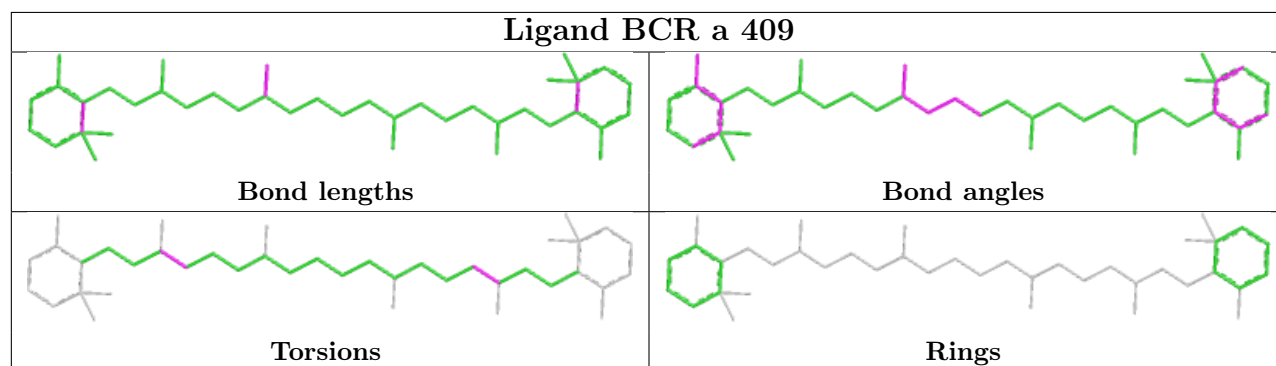
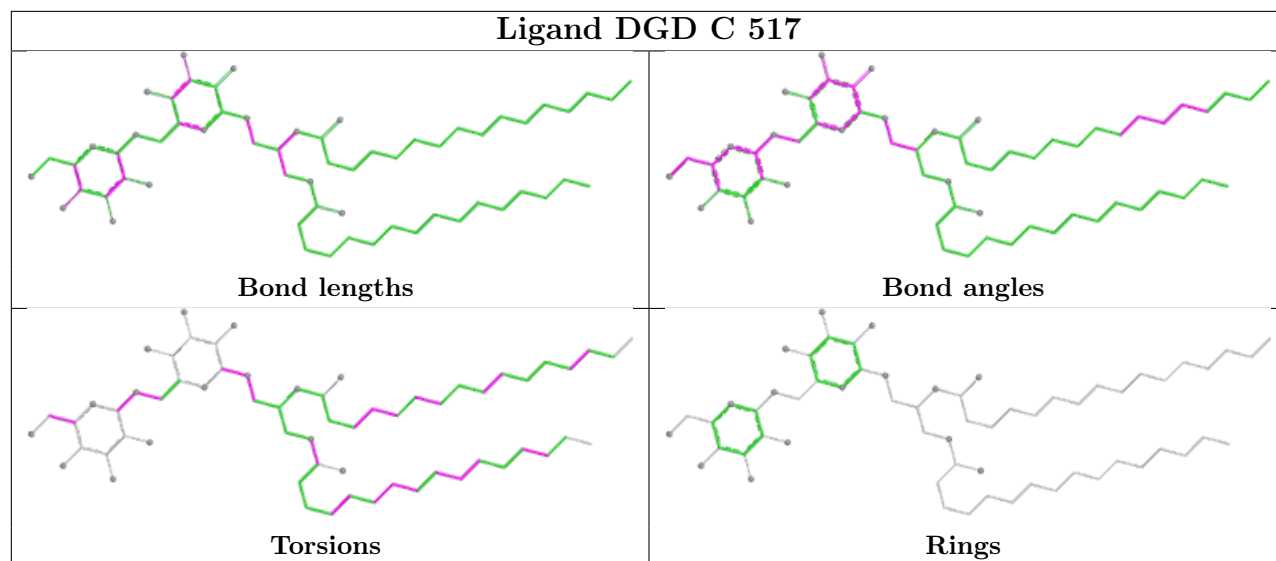
Ligand CLA c 503



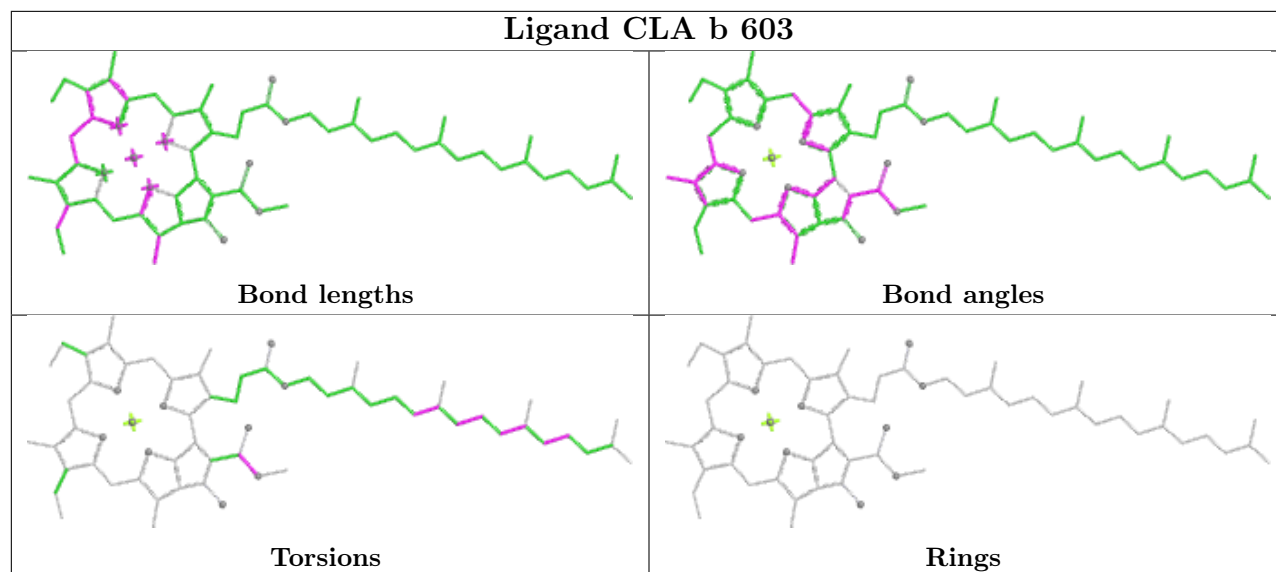




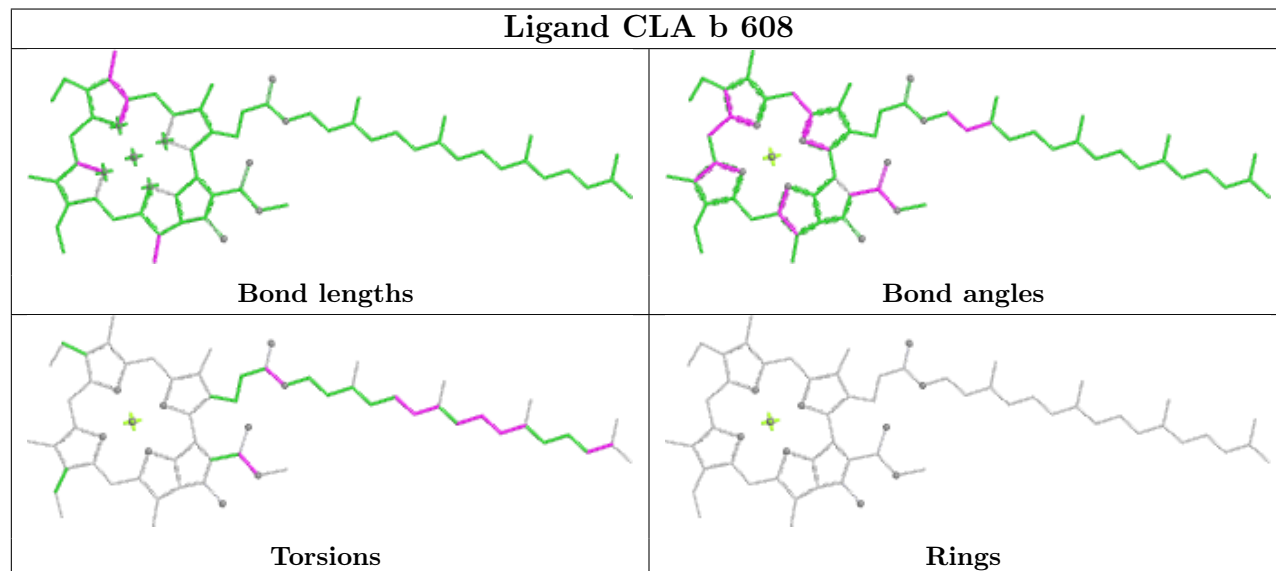




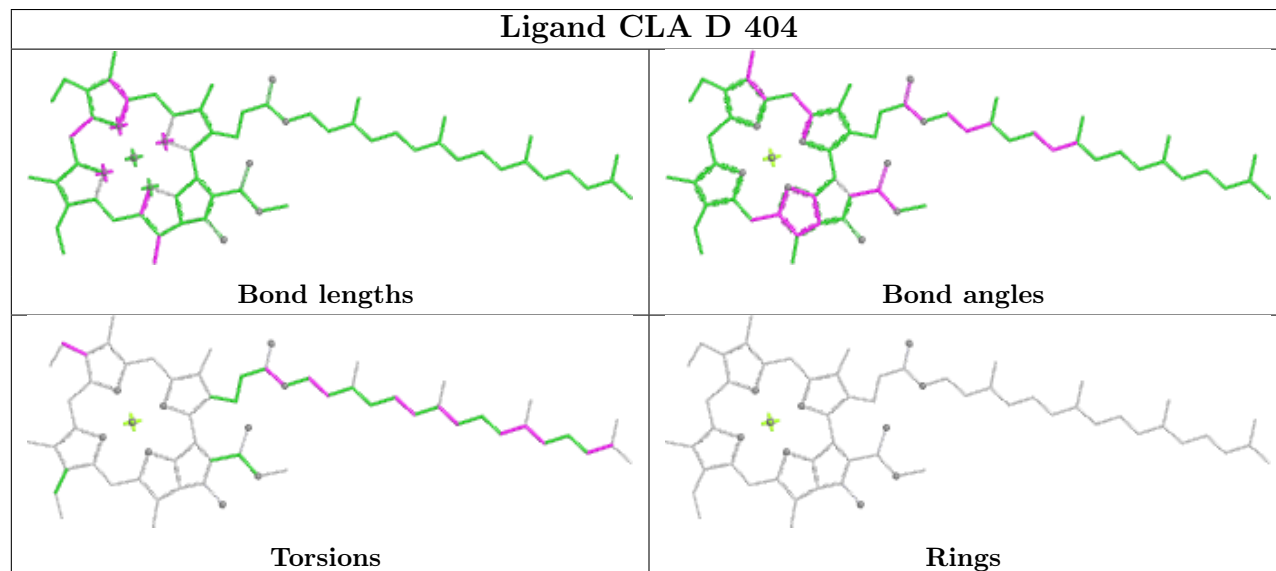
Ligand CLA b 603

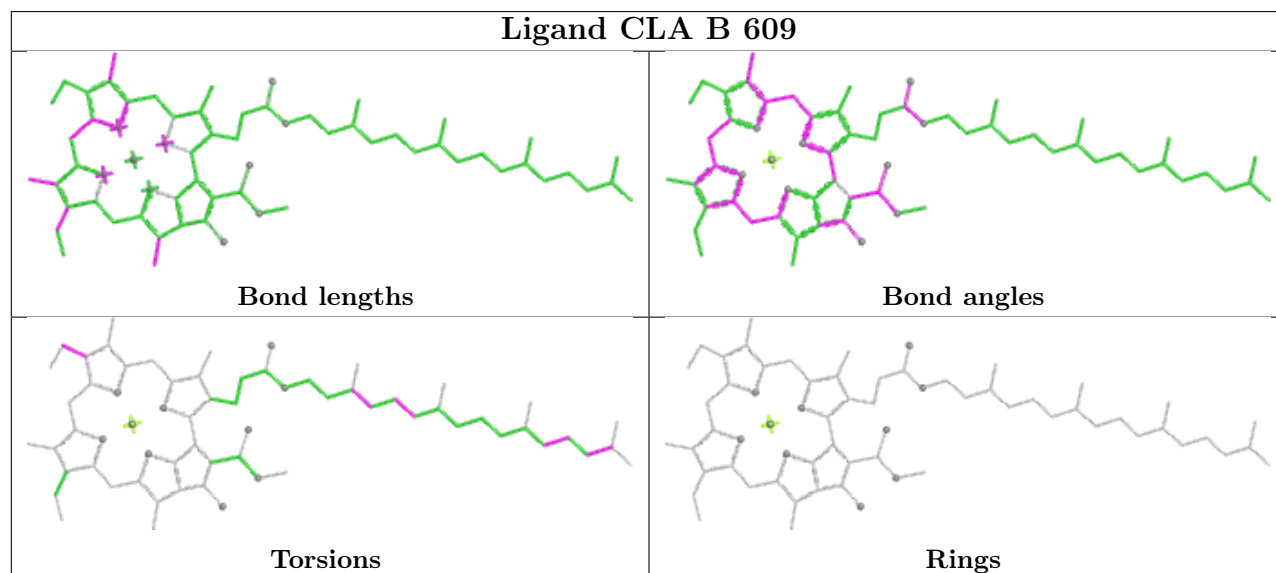
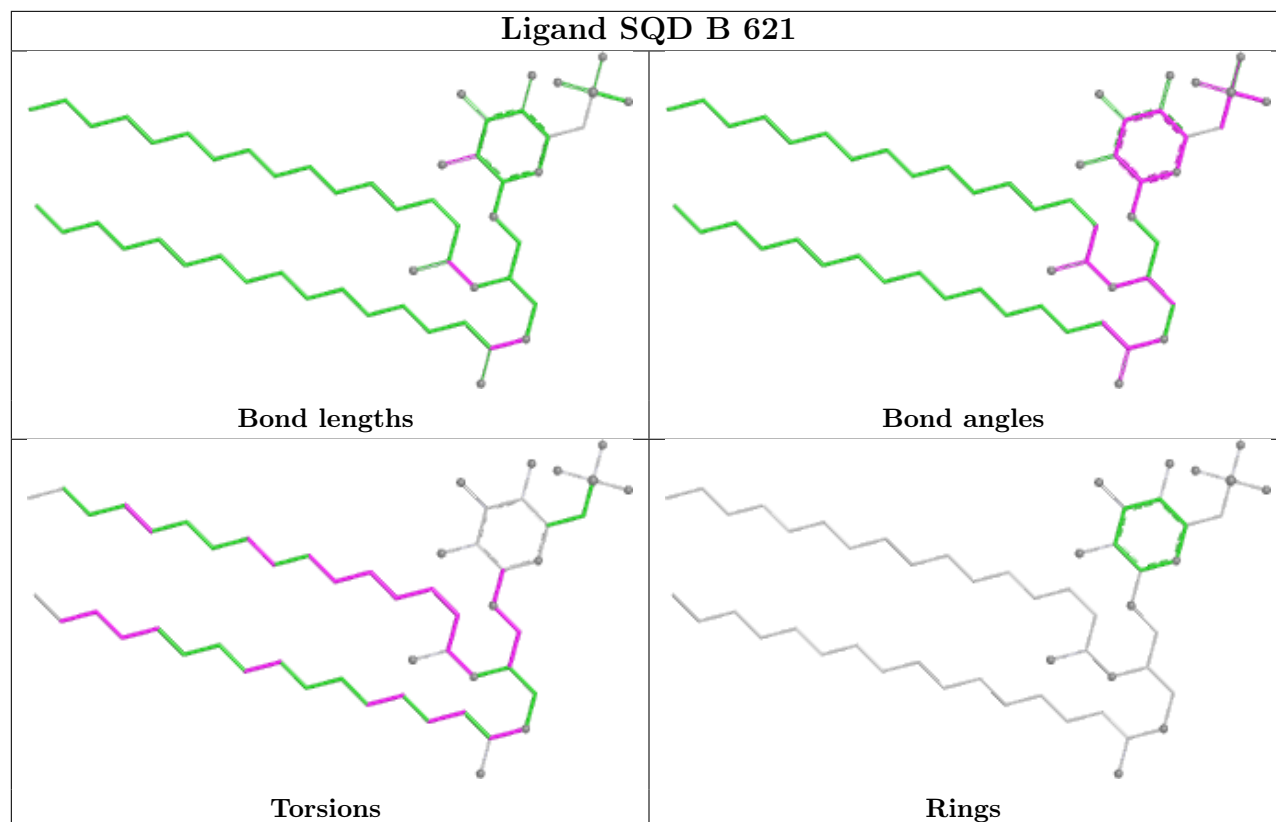


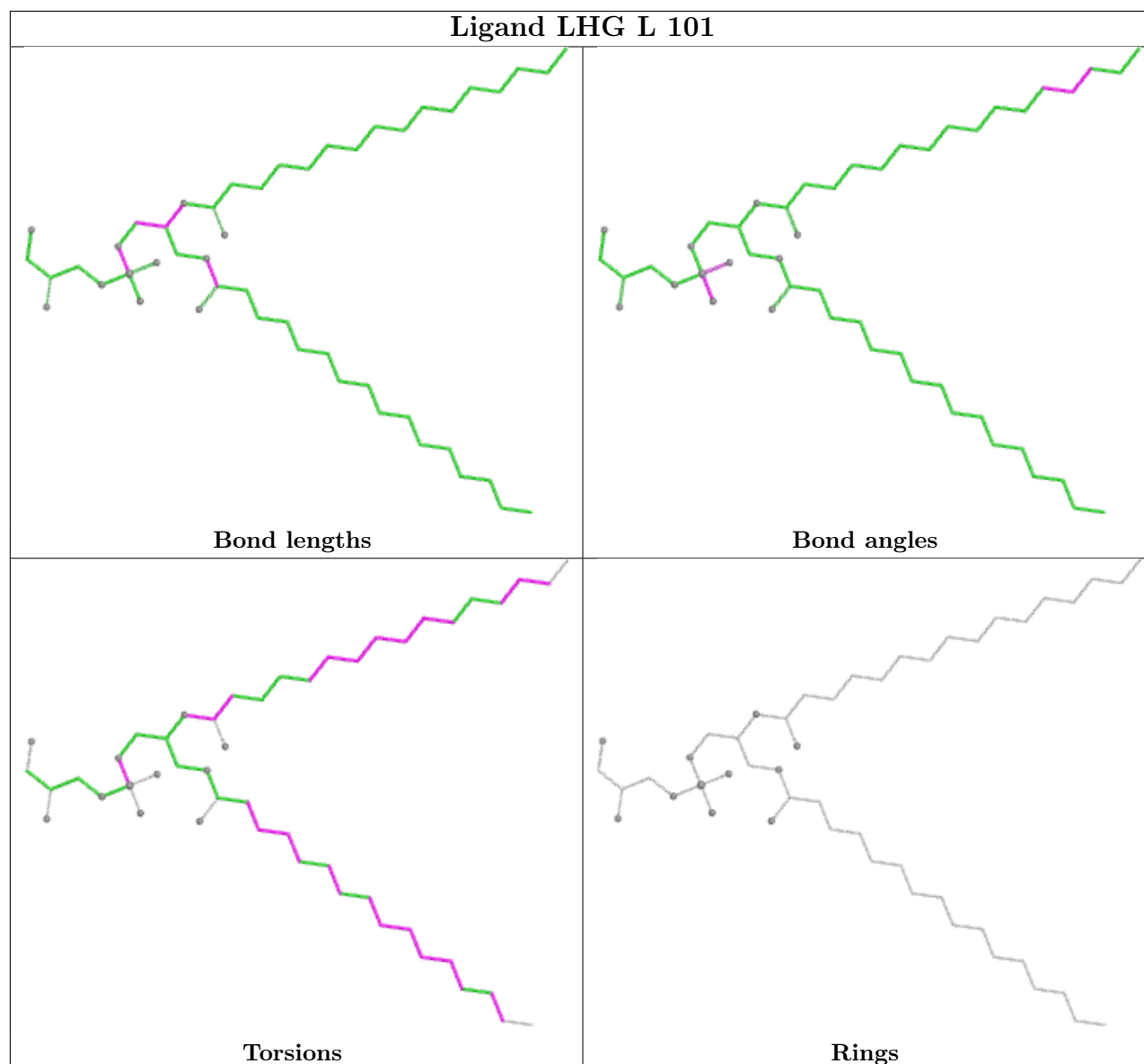
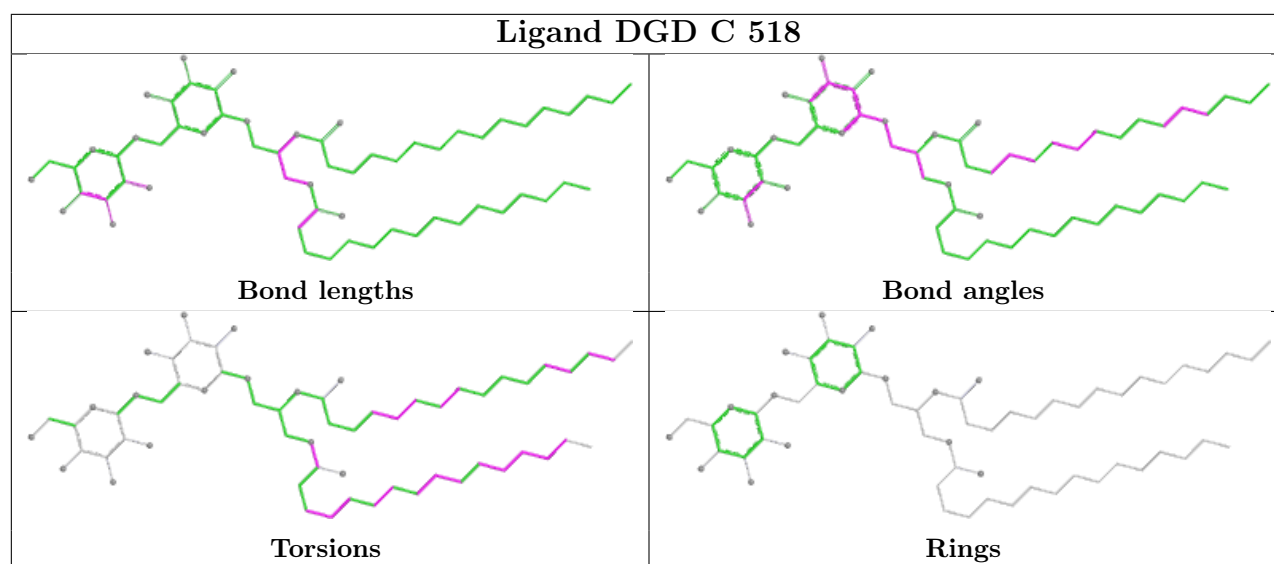
Ligand CLA b 608

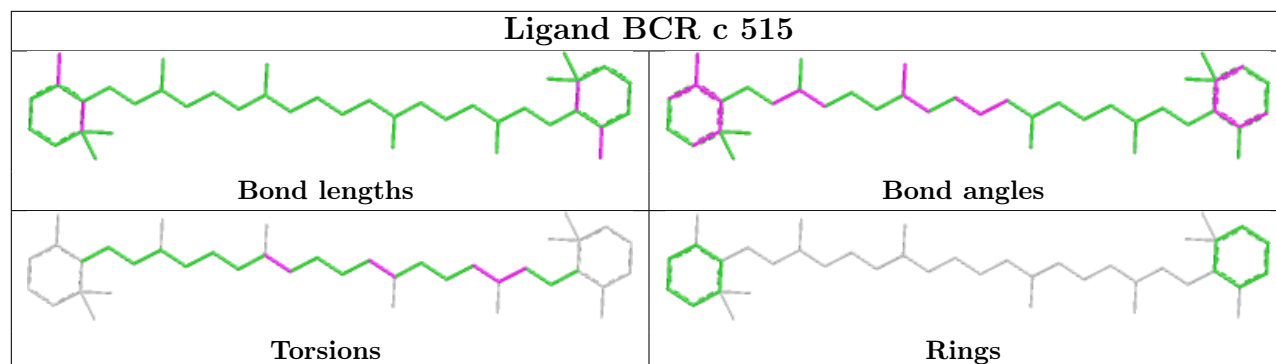
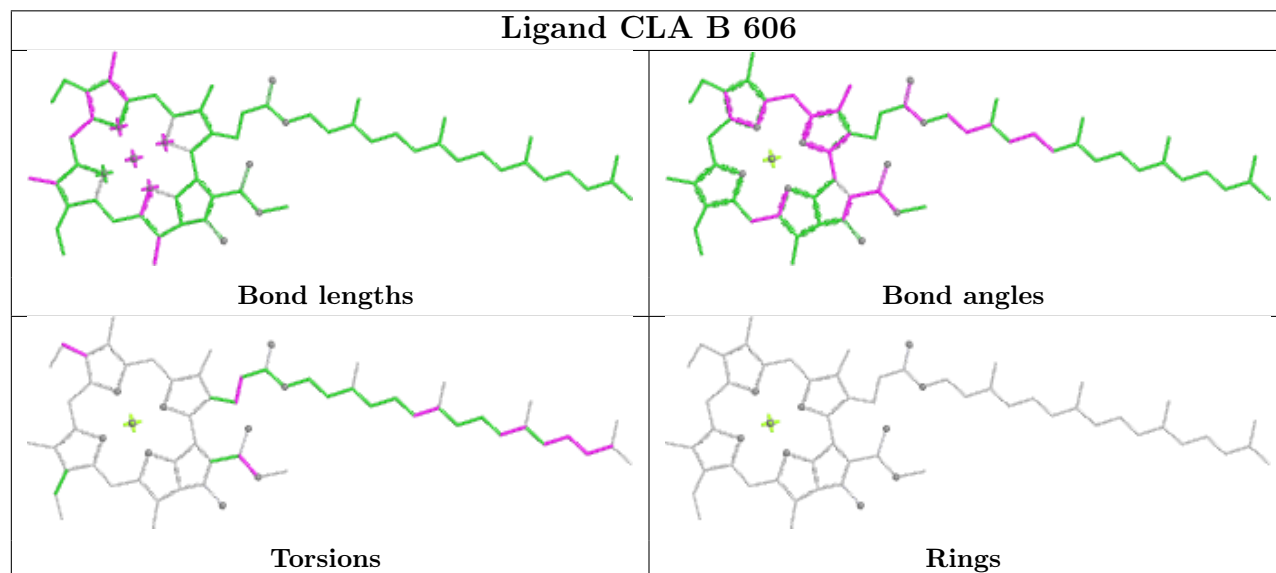
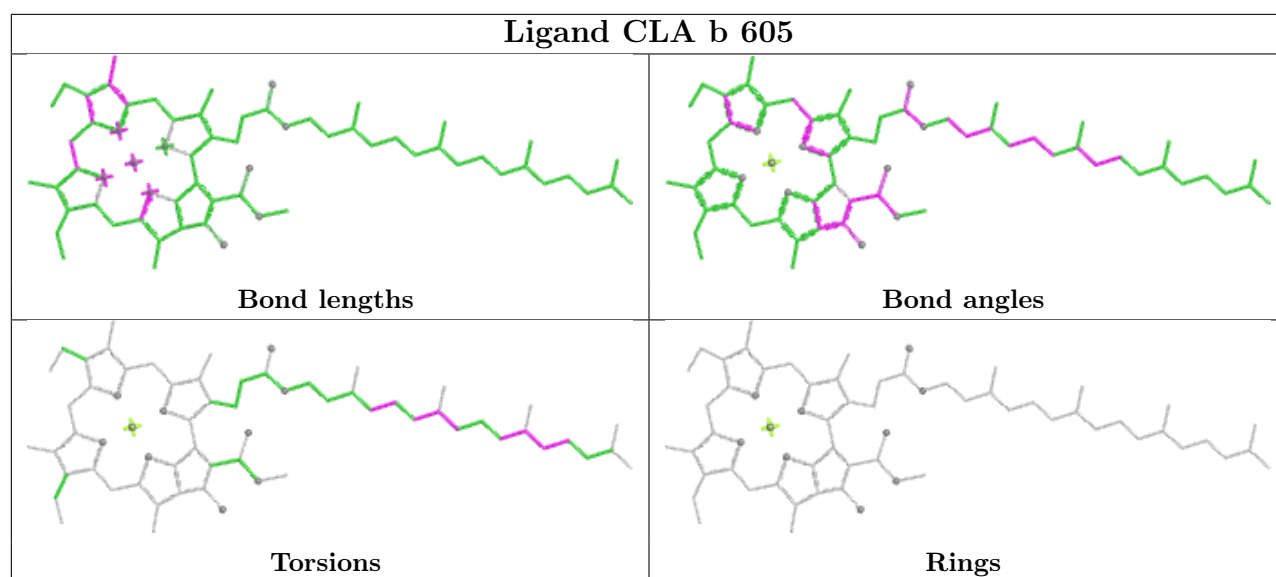


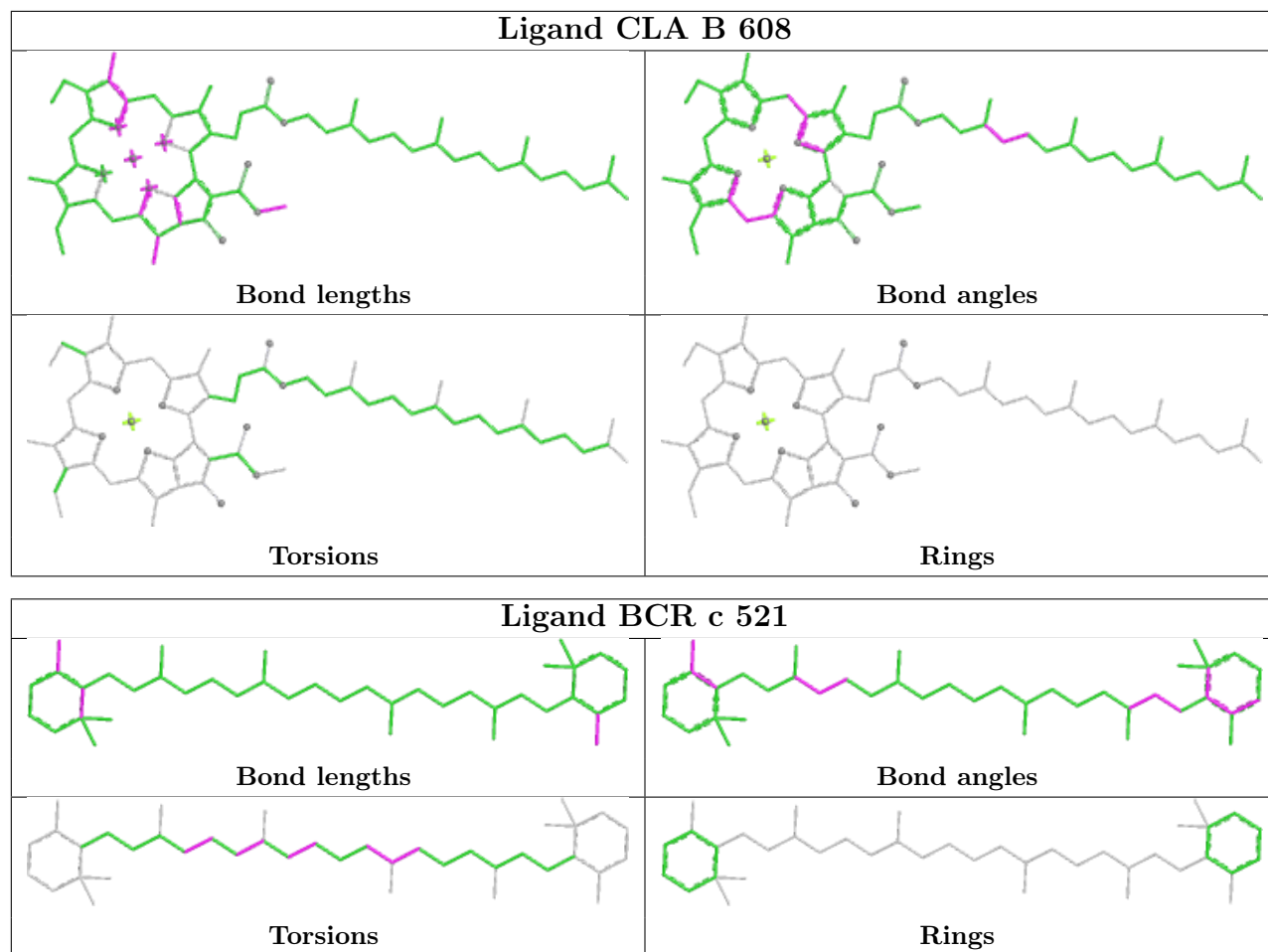
Ligand CLA D 404

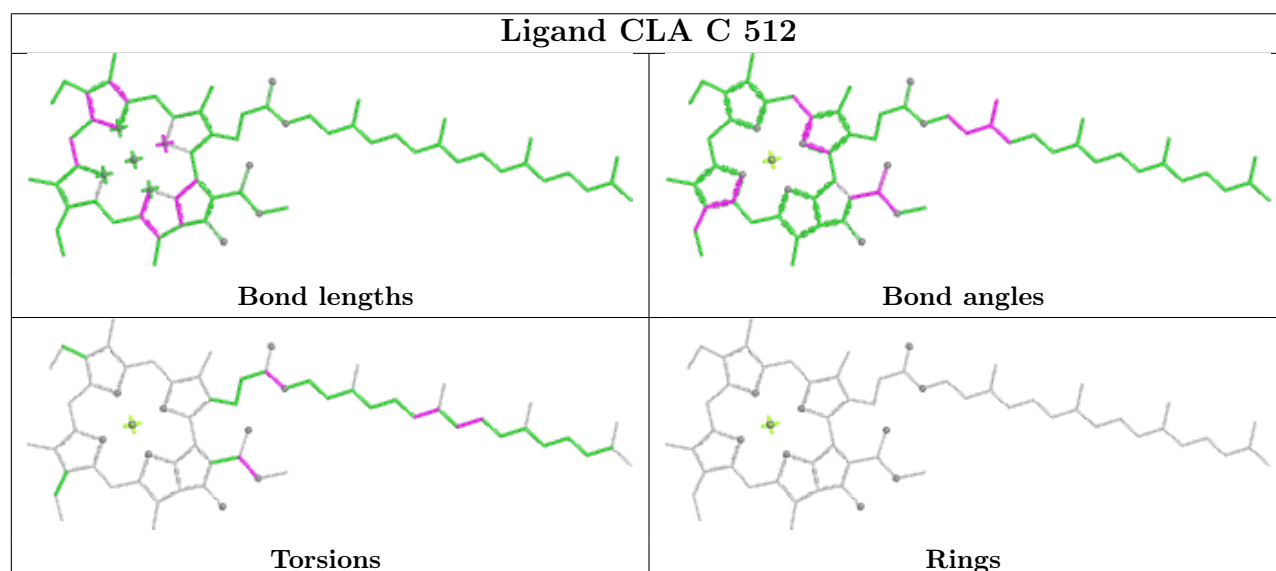
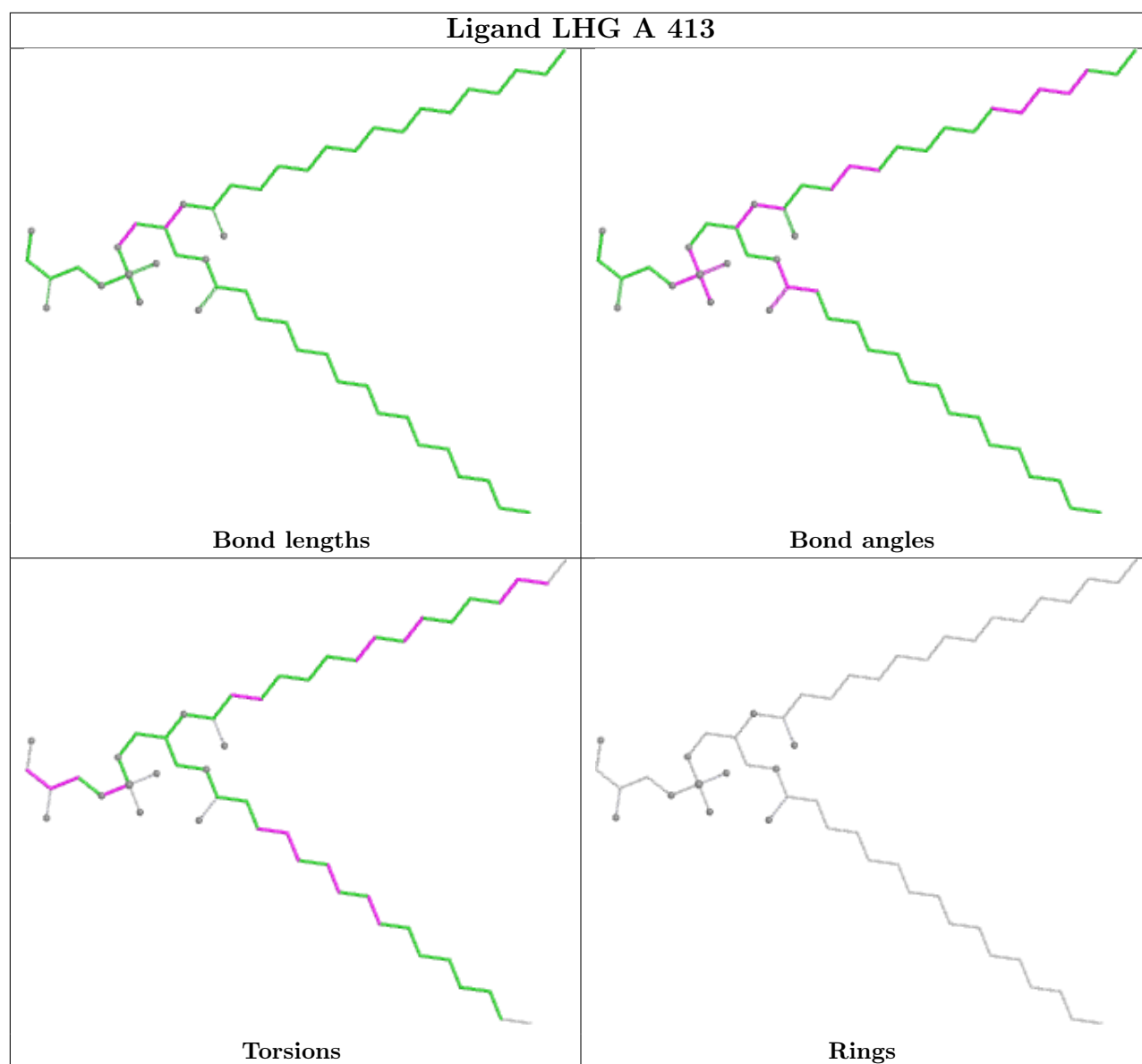




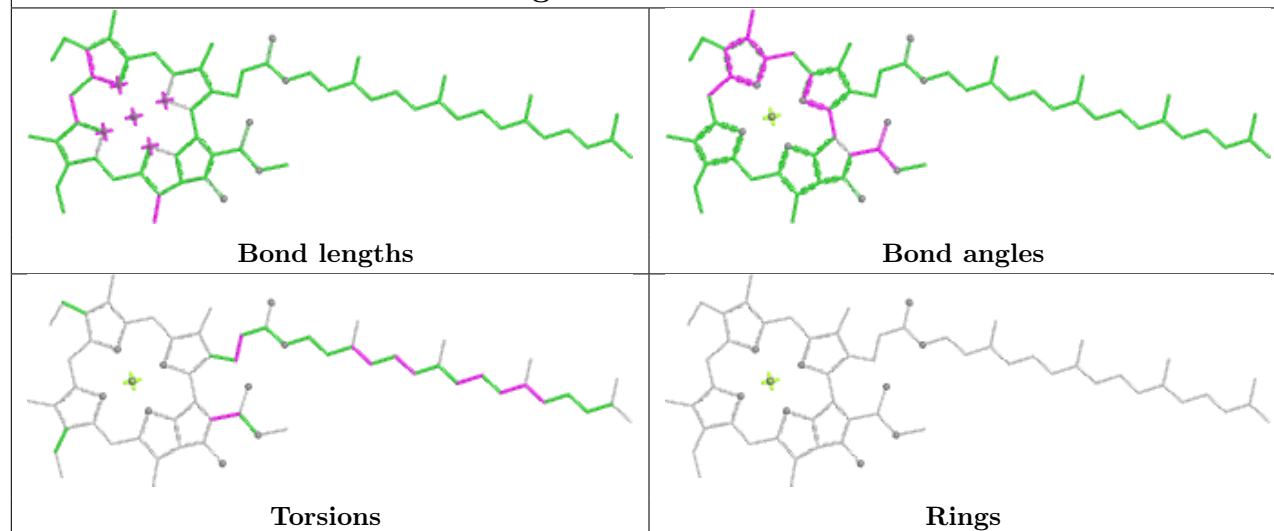




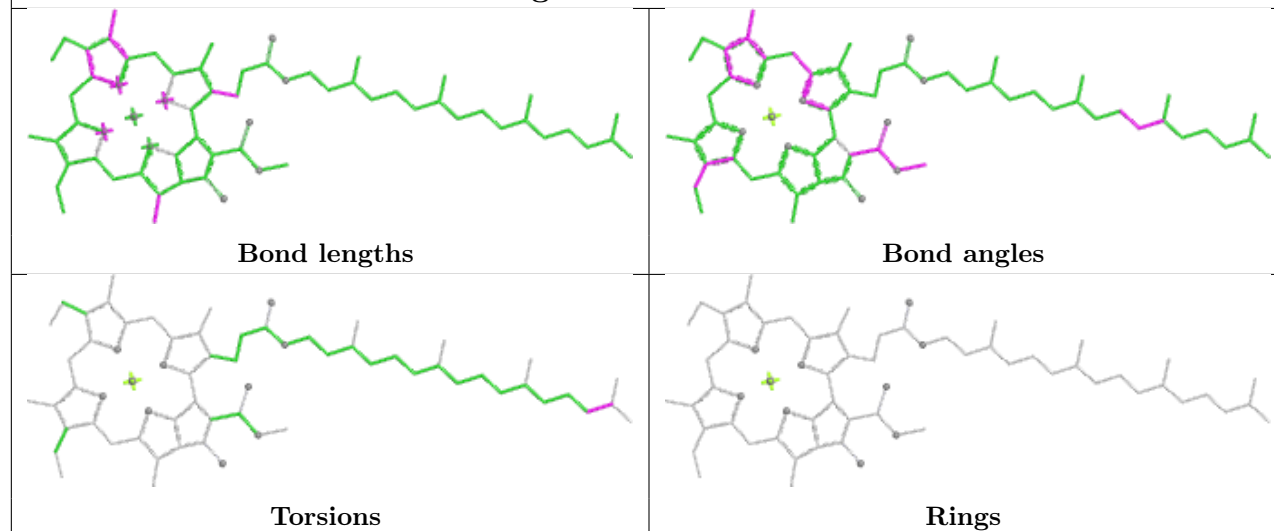




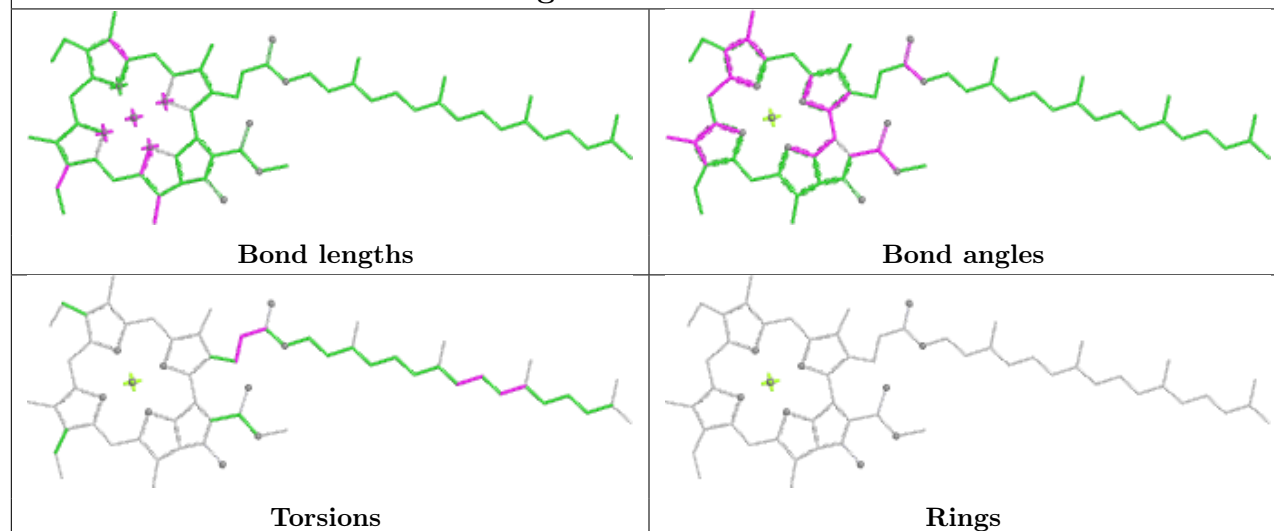
Ligand CLA B 614

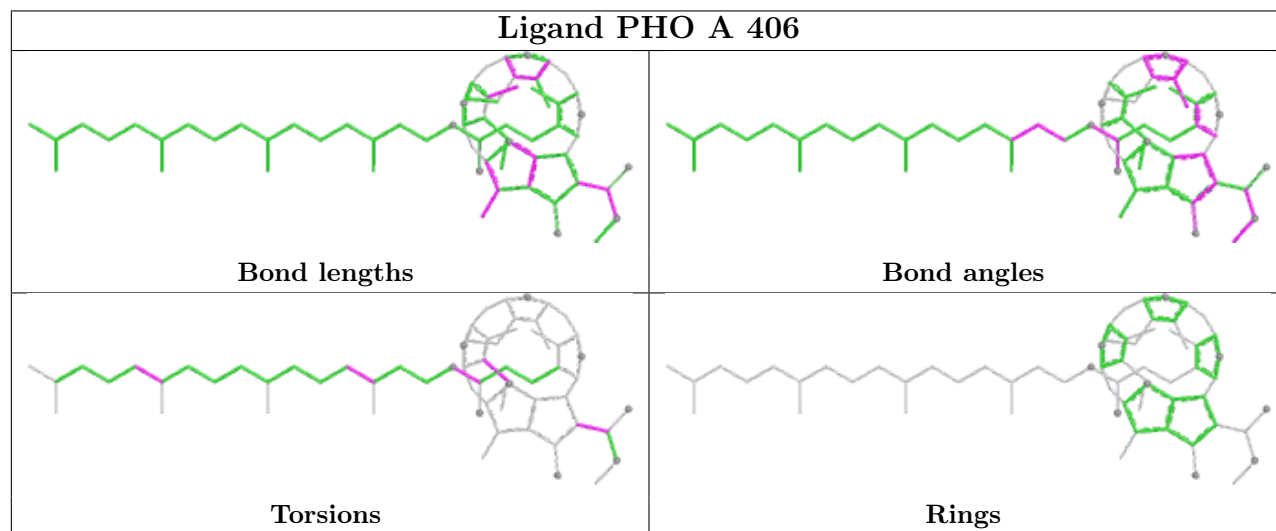
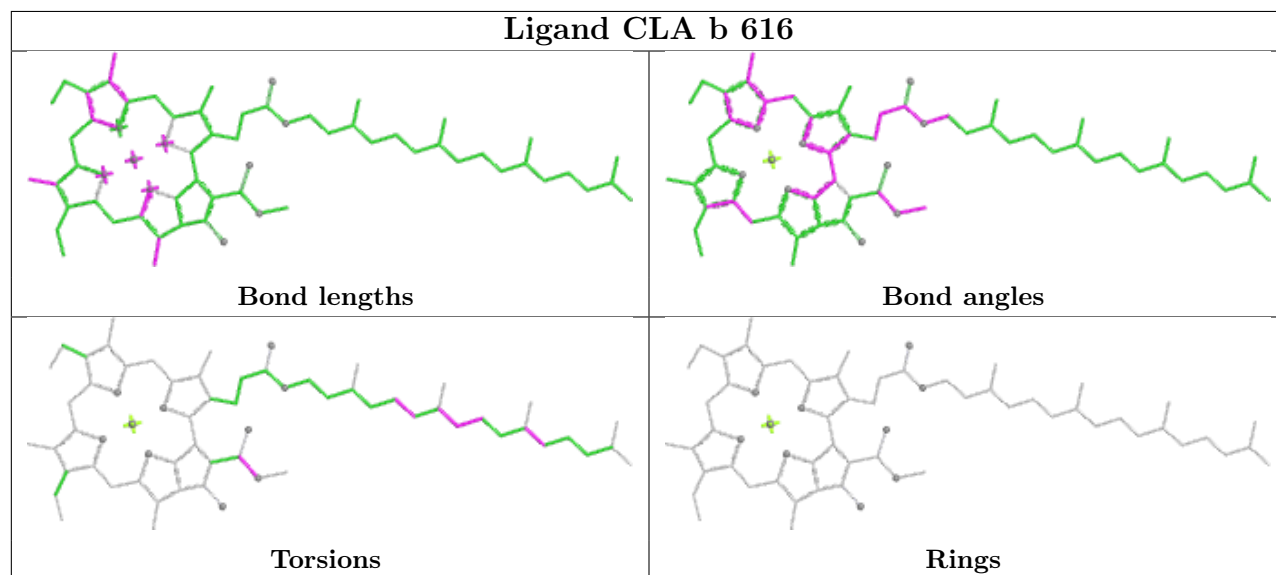
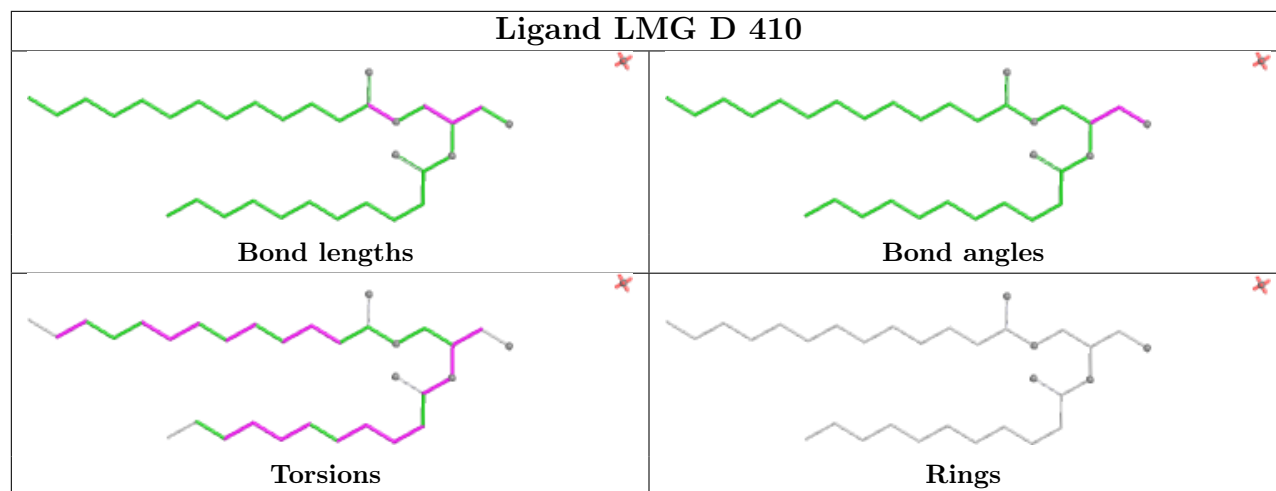


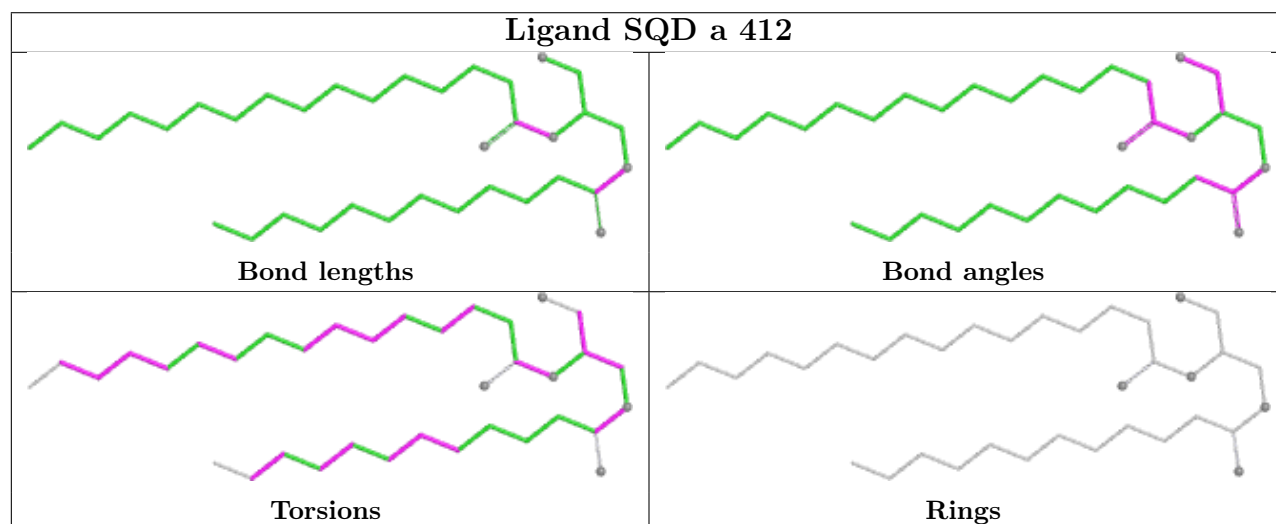
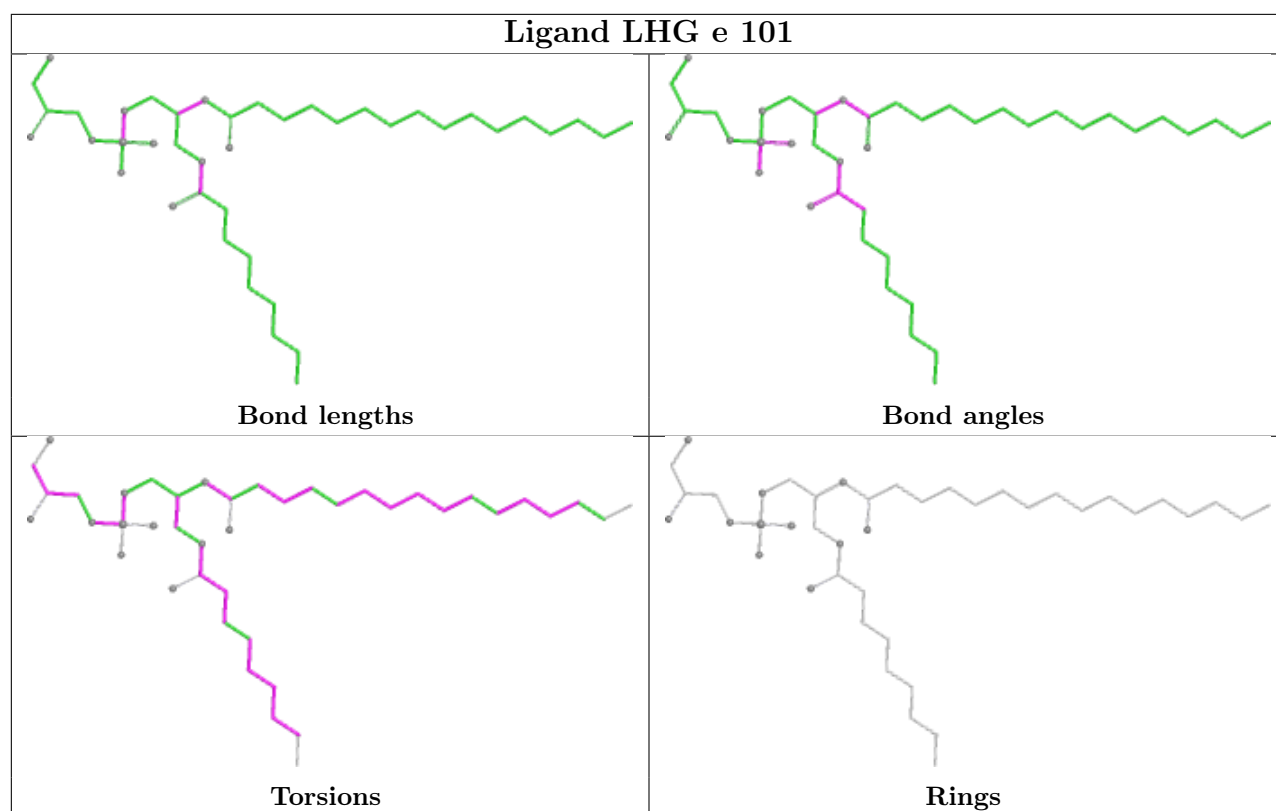
Ligand CLA A 405



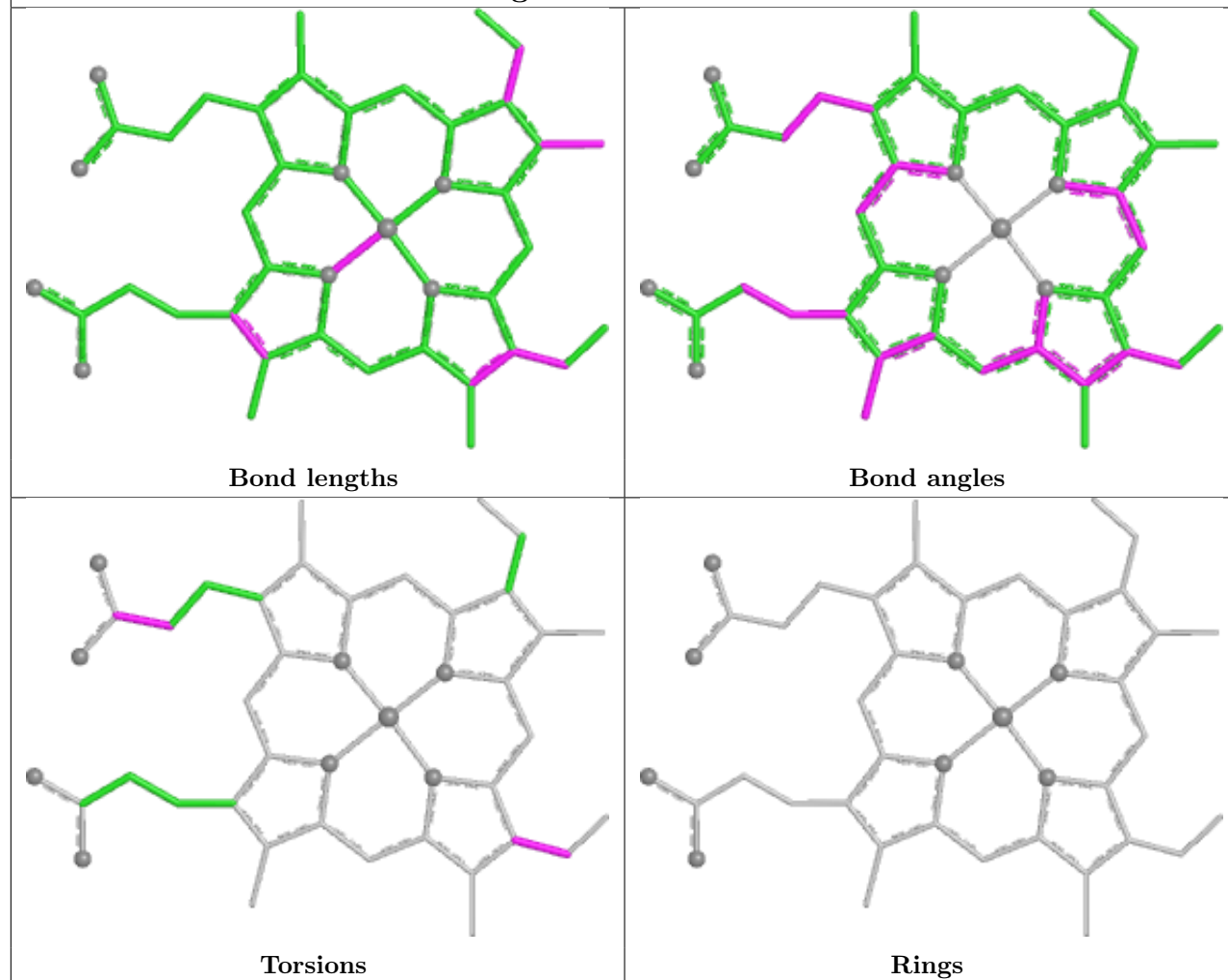
Ligand CLA c 501



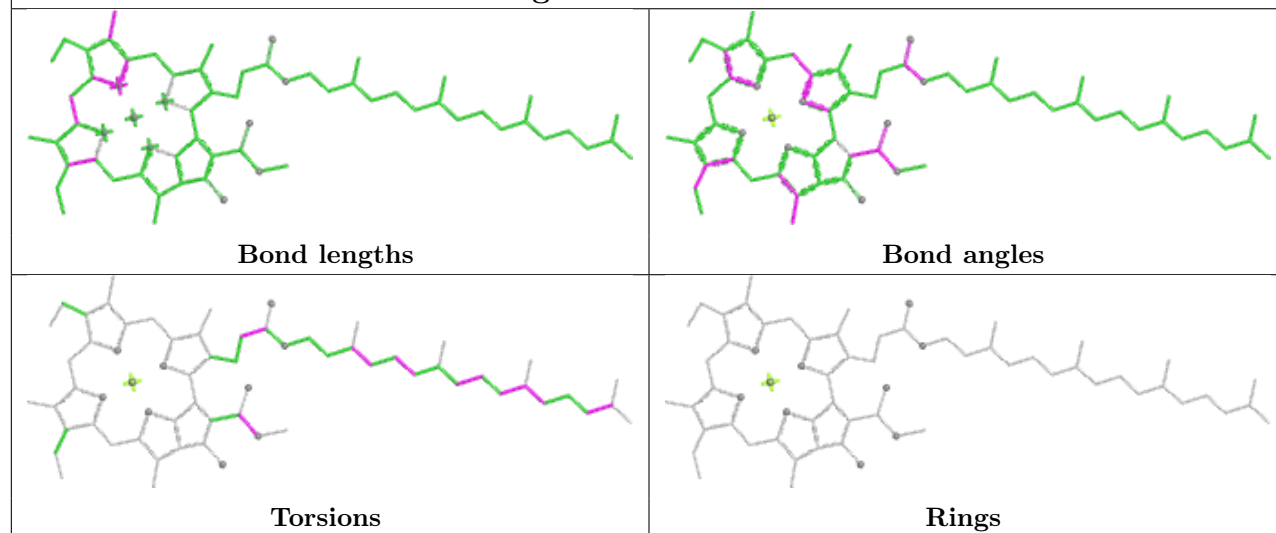




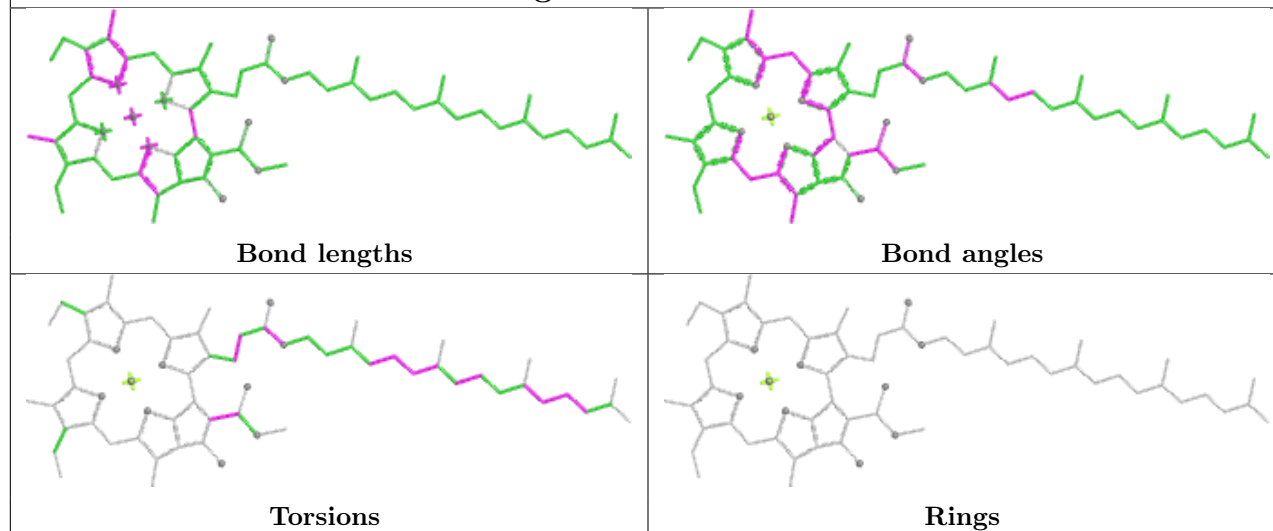
Ligand HEM e 102



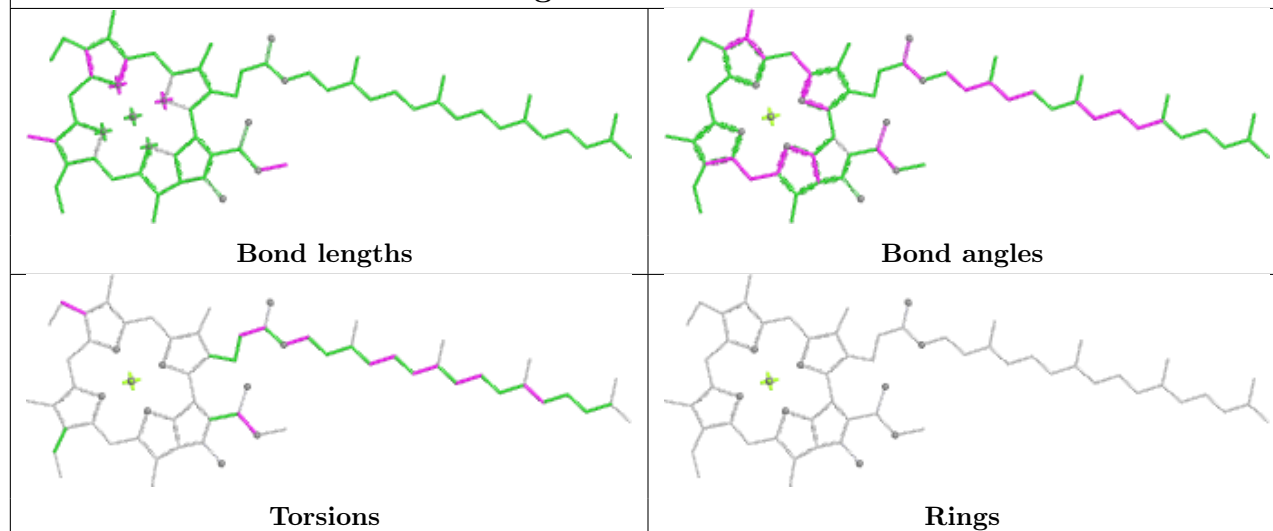
Ligand CLA C 506



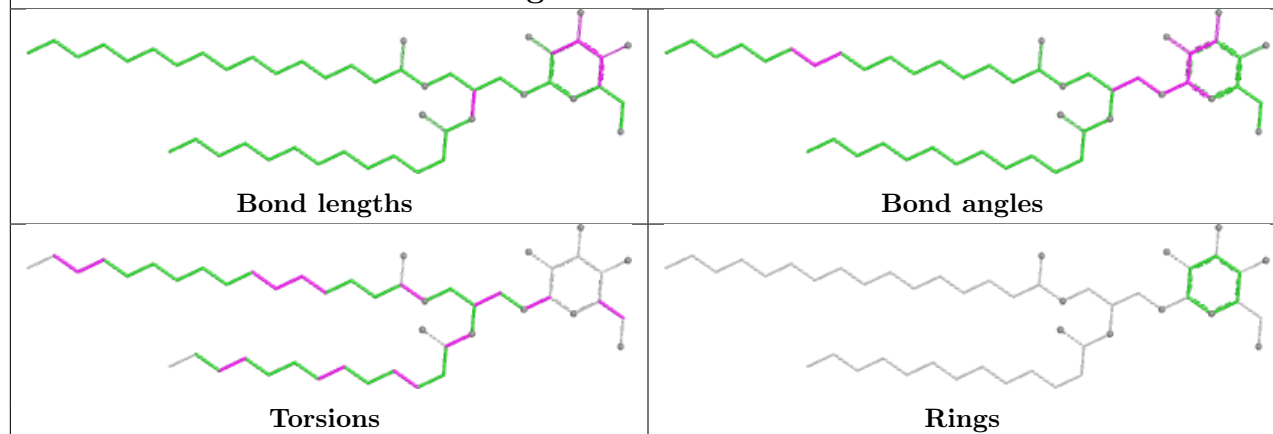
Ligand CLA b 615

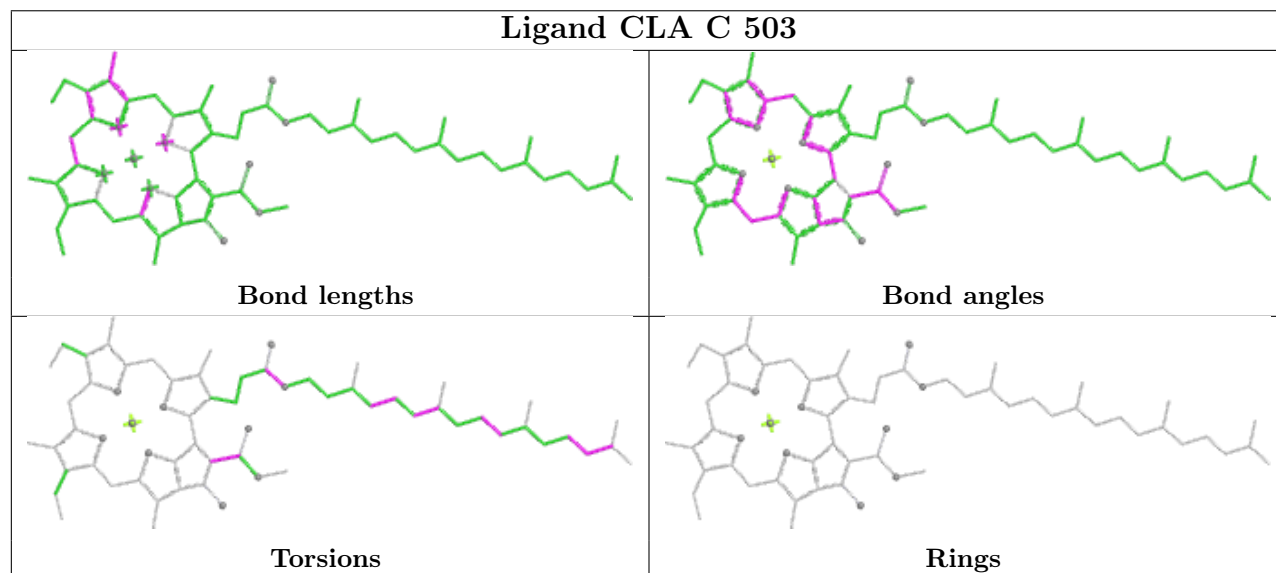
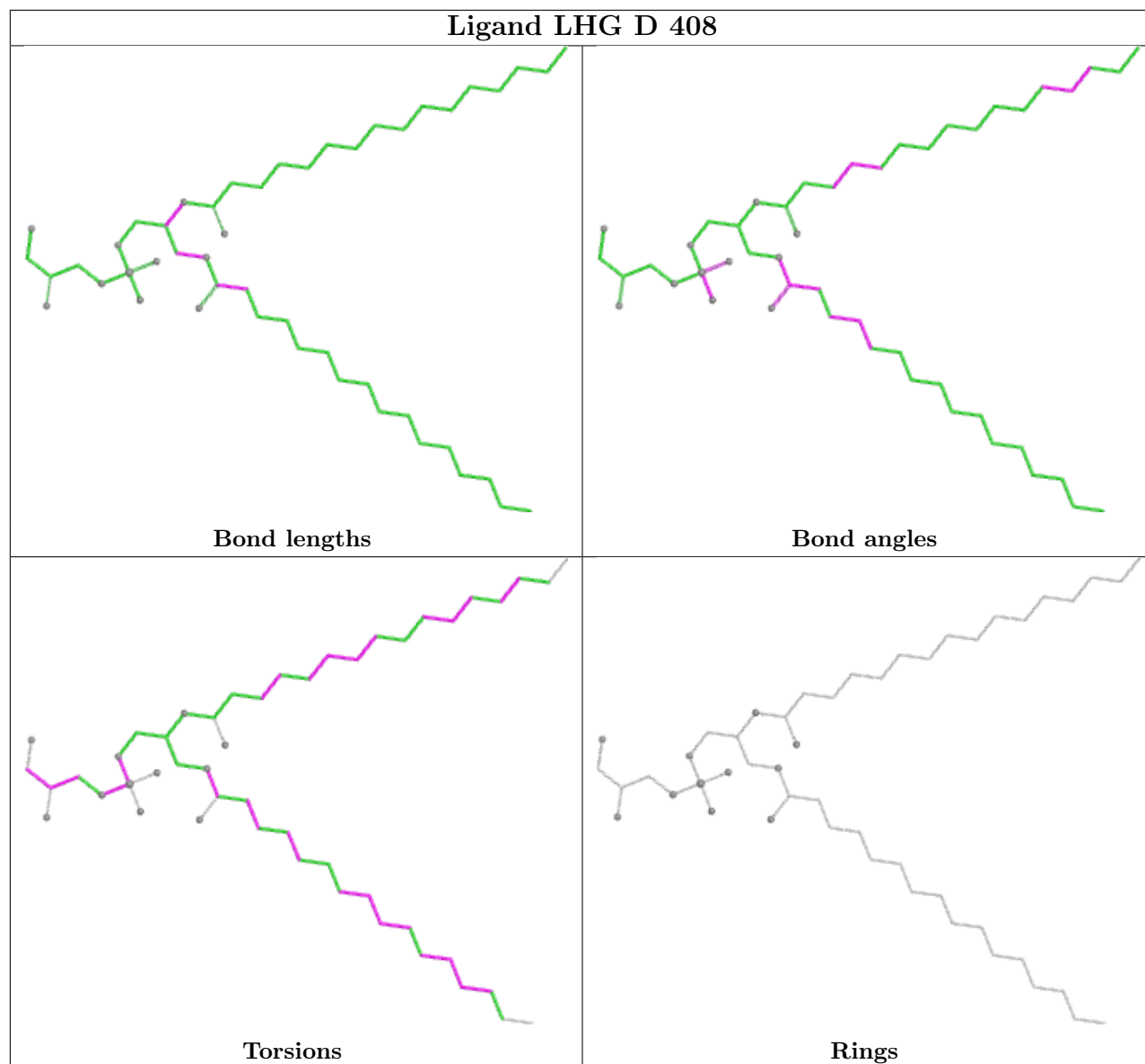


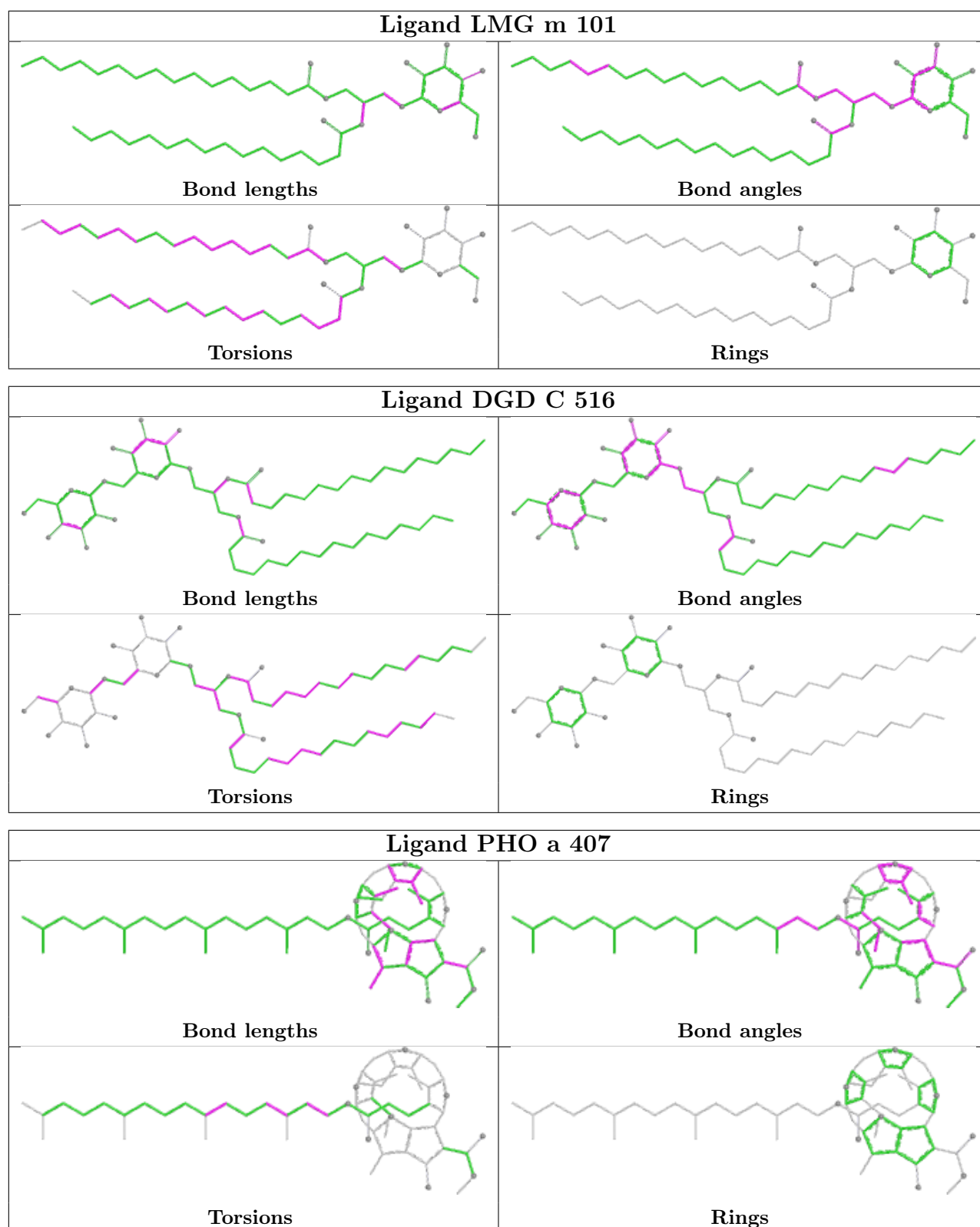
Ligand CLA b 613

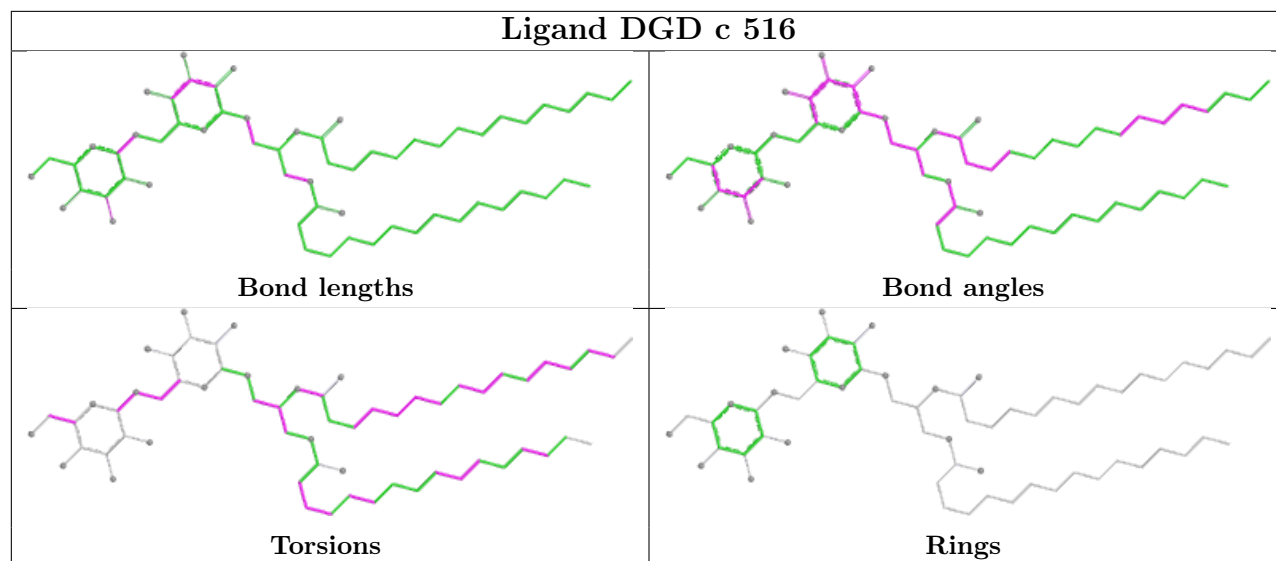


Ligand LMG C 519









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.74	0 100 100	30, 38, 59, 96	0
1	a	334/334 (100%)	-0.63	0 100 100	29, 40, 69, 91	0
2	B	505/505 (100%)	-0.61	0 100 100	21, 43, 75, 121	4 (0%)
2	b	505/505 (100%)	-0.50	0 100 100	31, 46, 84, 117	0
3	C	442/451 (98%)	-0.57	0 100 100	31, 46, 65, 90	0
3	c	451/451 (100%)	-0.50	1 (0%) 91 89	26, 51, 75, 120	1 (0%)
4	D	341/341 (100%)	-0.73	0 100 100	29, 40, 59, 103	0
4	d	341/341 (100%)	-0.59	0 100 100	31, 44, 70, 100	1 (0%)
5	E	81/82 (98%)	-0.17	1 (1%) 76 73	35, 62, 77, 97	1 (1%)
5	e	82/82 (100%)	0.01	1 (1%) 76 73	47, 71, 94, 105	0
6	F	34/34 (100%)	-0.38	0 100 100	47, 53, 76, 91	0
6	f	34/34 (100%)	-0.12	0 100 100	54, 60, 90, 106	0
7	H	65/65 (100%)	-0.47	1 (1%) 72 68	41, 49, 73, 90	0
7	h	63/65 (96%)	-0.31	0 100 100	47, 60, 80, 90	0
8	I	35/36 (97%)	-0.57	0 100 100	37, 48, 82, 86	0
8	i	35/36 (97%)	-0.38	0 100 100	35, 51, 93, 100	0
9	J	36/36 (100%)	-0.28	0 100 100	48, 60, 85, 117	0
9	j	36/36 (100%)	-0.16	0 100 100	47, 64, 99, 109	0
10	K	37/37 (100%)	-0.20	1 (2%) 56 51	39, 65, 82, 85	1 (2%)
10	k	37/37 (100%)	0.02	0 100 100	64, 74, 87, 92	0
11	L	37/37 (100%)	-0.74	0 100 100	32, 40, 80, 87	0
11	l	36/37 (97%)	-0.75	0 100 100	33, 41, 81, 94	0
12	M	32/33 (96%)	-0.59	0 100 100	34, 42, 75, 85	0
12	m	31/33 (93%)	-0.64	0 100 100	37, 43, 59, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.41	0 100 100	29, 52, 93, 165	1 (0%)
13	o	244/244 (100%)	-0.46	0 100 100	30, 50, 99, 144	0
14	T	29/30 (96%)	-0.71	0 100 100	32, 42, 75, 82	0
14	t	29/30 (96%)	-0.60	1 (3%) 48 43	34, 41, 98, 102	0
15	U	97/97 (100%)	-0.45	0 100 100	39, 53, 84, 112	0
15	u	97/97 (100%)	-0.43	0 100 100	38, 51, 68, 106	0
16	V	137/137 (100%)	-0.59	0 100 100	35, 51, 67, 97	0
16	v	137/137 (100%)	-0.34	0 100 100	41, 58, 82, 105	0
17	Y	27/30 (90%)	0.72	2 (7%) 20 18	62, 85, 123, 131	0
17	y	30/30 (100%)	0.37	0 100 100	67, 86, 106, 126	0
18	X	38/38 (100%)	-0.22	0 100 100	45, 59, 90, 91	0
18	x	38/38 (100%)	-0.08	0 100 100	55, 70, 96, 103	0
19	Z	62/62 (100%)	0.26	0 100 100	60, 77, 124, 139	0
19	z	62/62 (100%)	0.46	2 (3%) 50 46	66, 86, 134, 144	0
20	R	34/34 (100%)	0.24	1 (2%) 53 49	71, 83, 108, 117	0
20	r	31/34 (91%)	0.90	1 (3%) 50 46	83, 105, 114, 121	0
All	All	5300/5326 (99%)	-0.48	12 (0%) 91 89	21, 48, 88, 165	9 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	23	ALA	3.6
19	z	33	TRP	3.2
7	H	66	GLY	3.1
14	t	30	THR	3.0
20	r	32	GLN	2.9
20	R	35	LEU	2.8
17	Y	20	ALA	2.6
5	E	79	PHE	2.6
10	K	46[A]	ARG	2.4
19	z	27	TYR	2.4
5	e	79	PHE	2.4
17	Y	22	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.95	0.09	41,55,69,80	0
8	FME	I	1	10/11	0.96	0.07	48,61,72,83	0
14	FME	T	1	10/11	0.96	0.08	33,58,80,90	0
8	FME	i	1	10/11	0.96	0.07	39,54,68,78	0
12	FME	m	1	10/11	0.96	0.08	37,54,75,81	0
14	FME	t	1	10/11	0.96	0.06	36,55,82,88	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	UNL	H	103	53/-	0.75	0.17	44,89,115,116	0
32	UNL	c	523	28/-	0.78	0.13	55,80,93,95	0
32	UNL	b	626	26/-	0.80	0.16	52,65,76,78	0
32	UNL	a	414	28/-	0.80	0.13	44,66,82,84	0
29	LHG	e	101	42/49	0.81	0.14	68,92,115,158	0
29	LHG	E	101	49/49	0.82	0.14	54,88,118,126	0
32	UNL	B	626	47/-	0.82	0.15	54,73,88,96	0
28	DGD	A	412	66/66	0.83	0.13	41,75,100,124	0
32	UNL	b	623	40/-	0.83	0.15	52,68,91,100	0
33	LMG	c	522	48/55	0.83	0.15	42,89,123,138	0
33	LMG	d	410	23/55	0.83	0.17	43,73,104,105	0
33	LMG	D	410	33/55	0.84	0.13	34,61,107,111	0
32	UNL	x	101	55/-	0.85	0.13	43,71,92,94	0
32	UNL	b	624	44/-	0.85	0.15	48,68,88,89	0
33	LMG	b	622	55/55	0.85	0.14	48,80,99,104	0
32	UNL	B	624	46/-	0.85	0.13	55,68,83,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	UNL	T	102	47/-	0.85	0.14	34,52,79,81	0
32	UNL	t	102	26/-	0.86	0.15	56,75,87,88	0
32	UNL	C	523	47/-	0.86	0.12	47,60,78,78	0
32	UNL	B	620	43/-	0.86	0.12	41,59,81,83	0
26	PL9	A	409	55/55	0.86	0.14	35,70,101,113	0
28	DGD	a	413	44/66	0.86	0.12	36,62,86,88	0
32	UNL	j	101	28/-	0.86	0.12	53,67,81,85	0
32	UNL	b	621	55/-	0.87	0.13	42,68,96,118	0
32	UNL	c	520	55/-	0.87	0.12	48,72,94,101	0
32	UNL	B	625	28/-	0.87	0.14	47,67,91,99	0
23	CLA	b	602	65/65	0.87	0.11	55,76,104,110	0
32	UNL	b	625	55/-	0.87	0.12	50,73,87,98	0
32	UNL	m	102	28/-	0.88	0.13	38,58,78,78	0
27	SQD	A	411	39/54	0.88	0.12	43,73,96,111	0
32	UNL	C	521	28/-	0.88	0.11	35,50,62,67	0
33	LMG	C	519	48/55	0.88	0.12	53,85,105,121	0
27	SQD	a	412	36/54	0.88	0.12	40,72,101,113	0
33	LMG	D	411	28/55	0.88	0.12	34,58,76,80	0
26	PL9	a	410	55/55	0.88	0.12	42,77,101,112	0
32	UNL	d	412	43/-	0.88	0.12	50,62,78,83	0
32	UNL	M	103	26/-	0.88	0.13	36,54,72,72	0
27	SQD	B	621	54/54	0.89	0.10	43,67,104,121	0
33	LMG	C	501	48/55	0.89	0.10	40,67,86,111	0
33	LMG	c	519	37/55	0.89	0.11	45,74,99,105	0
23	CLA	c	512	65/65	0.89	0.11	45,68,99,114	0
32	UNL	E	102	28/-	0.89	0.13	66,88,97,103	0
23	CLA	B	601	65/65	0.90	0.10	36,65,116,139	0
32	UNL	C	522	28/-	0.90	0.11	41,61,81,83	0
27	SQD	f	101	41/54	0.90	0.13	58,91,129,142	0
32	UNL	B	622	34/-	0.90	0.10	38,55,71,72	0
23	CLA	C	514	65/65	0.90	0.11	48,77,110,115	0
25	BCR	d	405	40/40	0.90	0.10	39,59,110,121	0
33	LMG	c	524	49/55	0.90	0.10	31,60,96,125	0
25	BCR	x	102	40/40	0.90	0.10	40,62,84,87	0
33	LMG	m	101	51/55	0.90	0.10	37,60,85,98	0
32	UNL	I	101	41/-	0.91	0.12	42,62,95,99	0
32	UNL	J	101	28/-	0.91	0.12	48,62,74,75	0
27	SQD	b	601	49/54	0.91	0.10	47,68,101,117	0
25	BCR	K	101	40/40	0.91	0.09	38,60,75,91	0
27	SQD	a	411	54/54	0.91	0.10	45,75,97,102	0
28	DGD	C	517	62/66	0.91	0.09	40,62,111,122	0
32	UNL	D	412	55/-	0.91	0.11	35,65,88,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	k	101	40/40	0.91	0.10	45,71,86,89	0
28	DGD	c	517	62/66	0.91	0.10	37,62,94,112	0
29	LHG	d	407	49/49	0.92	0.10	38,59,98,112	0
25	BCR	b	620	40/40	0.92	0.08	34,58,75,80	0
25	BCR	c	514	40/40	0.92	0.09	44,65,80,80	0
33	LMG	M	101	51/55	0.92	0.09	33,54,75,89	0
25	BCR	B	619	40/40	0.92	0.08	33,49,66,84	0
32	UNL	l	102	53/-	0.92	0.12	36,55,96,102	0
32	UNL	B	623	28/-	0.92	0.09	36,52,70,76	0
25	BCR	D	405	40/40	0.92	0.09	34,50,95,115	0
23	CLA	c	513	65/65	0.92	0.10	47,74,109,113	0
33	LMG	d	411	44/55	0.92	0.09	41,63,94,112	0
25	BCR	Z	101	40/40	0.92	0.09	41,63,81,84	0
28	DGD	h	101	62/66	0.93	0.09	35,55,69,73	0
25	BCR	B	618	40/40	0.93	0.07	29,45,68,69	0
25	BCR	H	101	40/40	0.93	0.09	35,51,65,69	0
23	CLA	c	503	65/65	0.93	0.08	33,54,68,71	0
25	BCR	T	101	40/40	0.93	0.07	30,50,64,70	0
27	SQD	A	410	52/54	0.93	0.09	37,68,94,102	0
32	UNL	M	102	37/-	0.93	0.09	37,51,63,73	0
25	BCR	B	617	40/40	0.94	0.08	32,48,61,67	0
23	CLA	c	504	60/65	0.94	0.08	36,54,83,87	0
25	BCR	c	515	40/40	0.94	0.09	32,52,66,80	0
25	BCR	c	521	40/40	0.94	0.09	39,61,68,74	0
28	DGD	H	102	62/66	0.94	0.08	32,52,68,76	0
23	CLA	c	506	65/65	0.94	0.09	35,60,114,126	0
25	BCR	C	515	40/40	0.94	0.09	24,46,60,75	0
28	DGD	c	518	62/66	0.94	0.08	30,63,82,92	0
25	BCR	C	520	40/40	0.94	0.10	42,60,75,79	0
33	LMG	D	407	51/55	0.94	0.09	34,64,86,98	0
29	LHG	D	409	47/49	0.94	0.09	36,56,90,108	0
23	CLA	c	508	64/65	0.94	0.08	32,54,97,122	0
23	CLA	c	509	65/65	0.94	0.10	37,56,73,83	0
29	LHG	d	409	39/49	0.94	0.09	35,56,75,81	0
23	CLA	c	511	65/65	0.94	0.10	45,66,85,88	0
23	CLA	b	617	60/65	0.94	0.08	33,50,94,105	0
23	CLA	B	616	60/65	0.94	0.08	24,45,91,96	0
27	SQD	F	101	36/54	0.94	0.10	48,76,102,107	0
25	BCR	b	618	40/40	0.94	0.07	31,50,67,67	0
25	BCR	b	619	40/40	0.94	0.07	33,46,58,62	0
23	CLA	C	509	65/65	0.95	0.07	28,51,114,130	0
23	CLA	C	510	65/65	0.95	0.08	35,51,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	510	65/65	0.95	0.08	39,57,78,89	0
29	LHG	A	413	49/49	0.95	0.08	31,53,82,87	0
23	CLA	C	512	65/65	0.95	0.08	37,58,76,83	0
23	CLA	C	513	65/65	0.95	0.09	35,62,112,146	0
23	CLA	B	615	65/65	0.95	0.07	27,46,70,81	0
25	BCR	t	101	40/40	0.95	0.07	31,45,57,65	0
23	CLA	d	402	65/65	0.95	0.07	26,39,50,54	0
29	LHG	l	101	49/49	0.95	0.07	38,51,63,81	0
23	CLA	d	404	65/65	0.95	0.09	31,56,111,137	0
25	BCR	A	408	40/40	0.95	0.06	25,37,50,51	0
26	PL9	d	406	55/55	0.95	0.07	27,41,49,54	0
23	CLA	a	408	65/65	0.95	0.08	22,41,107,114	0
23	CLA	B	606	65/65	0.95	0.08	26,43,85,94	0
23	CLA	b	607	65/65	0.95	0.07	30,48,78,87	0
23	CLA	b	611	65/65	0.95	0.07	26,41,59,70	0
23	CLA	b	615	65/65	0.95	0.08	24,46,85,89	0
23	CLA	C	503	65/65	0.95	0.07	37,51,67,80	0
23	CLA	c	501	65/65	0.95	0.07	30,46,58,67	0
23	CLA	c	502	65/65	0.95	0.07	36,52,71,82	0
23	CLA	C	504	65/65	0.95	0.07	30,50,63,68	0
28	DGD	C	516	62/66	0.95	0.08	27,44,87,103	0
23	CLA	C	506	65/65	0.95	0.08	27,46,69,79	0
28	DGD	C	518	62/66	0.95	0.08	32,58,86,104	0
23	CLA	c	505	65/65	0.95	0.08	31,48,70,79	0
23	CLA	C	507	65/65	0.95	0.08	27,49,103,114	0
26	PL9	D	406	55/55	0.96	0.07	22,38,49,55	0
23	CLA	D	404	65/65	0.96	0.08	26,47,133,138	0
23	CLA	a	405	65/65	0.96	0.06	25,37,55,65	0
23	CLA	a	406	65/65	0.96	0.08	31,48,99,114	0
23	CLA	B	603	65/65	0.96	0.07	26,42,69,76	0
23	CLA	C	502	65/65	0.96	0.06	25,43,59,68	0
23	CLA	d	403	65/65	0.96	0.07	24,41,75,83	0
23	CLA	b	603	65/65	0.96	0.08	28,50,75,82	0
24	PHO	D	401	64/64	0.96	0.06	26,37,47,51	0
24	PHO	a	407	64/64	0.96	0.07	24,36,48,50	0
24	PHO	d	401	64/64	0.96	0.07	32,45,59,68	0
23	CLA	b	604	65/65	0.96	0.07	28,44,70,74	0
23	CLA	b	605	65/65	0.96	0.07	25,42,84,98	0
23	CLA	b	606	65/65	0.96	0.07	27,43,57,61	0
23	CLA	B	604	65/65	0.96	0.08	25,41,92,98	0
23	CLA	b	608	65/65	0.96	0.07	23,42,73,81	0
23	CLA	b	609	65/65	0.96	0.07	27,48,72,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	DGD	c	516	62/66	0.96	0.07	25,46,78,94	0
23	CLA	b	610	65/65	0.96	0.07	27,48,67,93	0
23	CLA	B	605	65/65	0.96	0.07	23,39,55,60	0
23	CLA	b	613	65/65	0.96	0.07	24,40,56,65	0
23	CLA	b	614	65/65	0.96	0.07	23,41,92,97	0
23	CLA	C	505	59/65	0.96	0.07	30,52,92,107	0
25	BCR	a	409	40/40	0.96	0.06	25,42,57,63	0
29	LHG	L	101	49/49	0.96	0.07	31,46,63,69	0
23	CLA	b	616	65/65	0.96	0.07	33,48,69,80	0
23	CLA	A	405	65/65	0.96	0.08	23,41,104,122	0
23	CLA	B	607	65/65	0.96	0.07	18,41,77,85	0
23	CLA	C	508	65/65	0.96	0.07	29,44,66,71	0
31	BCT	a	404	4/4	0.96	0.09	27,36,48,58	0
23	CLA	B	609	65/65	0.96	0.07	23,42,59,66	0
23	CLA	B	610	65/65	0.96	0.07	25,39,55,62	0
23	CLA	C	511	65/65	0.96	0.07	35,55,81,86	0
23	CLA	B	613	65/65	0.96	0.07	24,36,71,82	0
23	CLA	c	507	65/65	0.96	0.07	35,51,66,69	0
23	CLA	B	614	65/65	0.96	0.08	25,46,93,105	0
23	CLA	B	602	65/65	0.96	0.07	28,44,72,77	0
24	PHO	A	406	64/64	0.97	0.06	20,35,49,55	0
23	CLA	D	402	65/65	0.97	0.06	22,35,54,60	0
31	BCT	A	415	4/4	0.97	0.09	32,35,39,42	0
23	CLA	D	403	65/65	0.97	0.06	22,37,58,68	0
23	CLA	b	612	65/65	0.97	0.06	26,38,58,62	0
29	LHG	D	408	49/49	0.97	0.06	30,46,62,65	0
23	CLA	A	404	65/65	0.97	0.06	19,33,54,68	0
23	CLA	B	611	65/65	0.97	0.06	20,34,47,48	0
23	CLA	B	612	65/65	0.97	0.06	23,38,55,59	0
23	CLA	B	608	65/65	0.97	0.05	24,40,58,65	0
29	LHG	d	408	49/49	0.97	0.07	27,48,66,67	0
23	CLA	A	407	54/65	0.97	0.07	25,38,83,85	0
34	HEM	E	103	43/43	0.97	0.08	39,53,69,76	0
34	HEM	e	102	43/43	0.97	0.09	46,63,79,83	0
22	CL	a	402	1/1	0.98	0.04	34,34,34,34	0
35	HEC	V	201	43/43	0.98	0.05	28,38,50,51	0
30	OEX	a	415	10/10	0.99	0.03	29,33,38,39	0
22	CL	A	402	1/1	0.99	0.03	36,36,36,36	0
22	CL	A	403	1/1	0.99	0.03	36,36,36,36	0
21	FE2	a	401	1/1	0.99	0.03	39,39,39,39	0
22	CL	a	403	1/1	0.99	0.10	32,32,32,32	0
35	HEC	v	201	43/43	0.99	0.06	37,45,57,61	0

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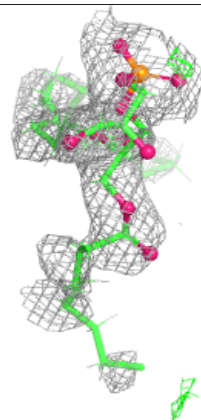
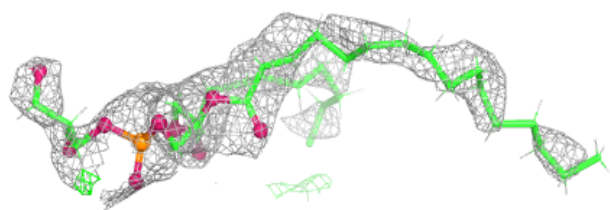
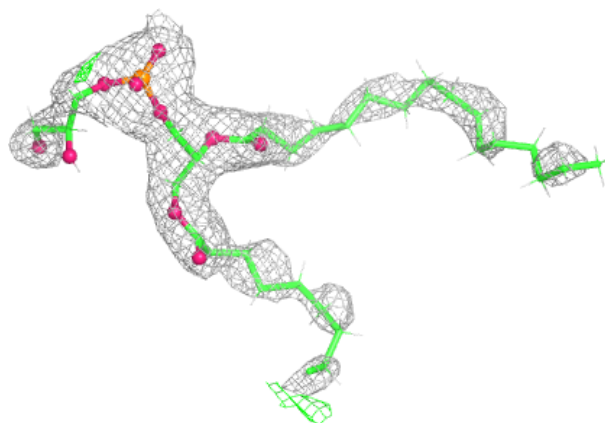
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	OEX	A	414	10/10	1.00	0.03	31,36,39,42	0
21	FE2	A	401	1/1	1.00	0.01	32,32,32,32	0

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

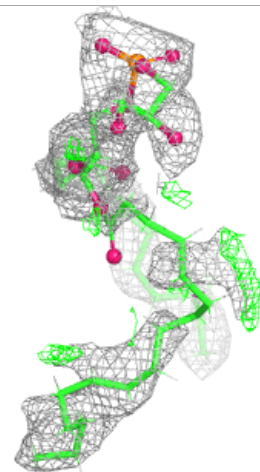
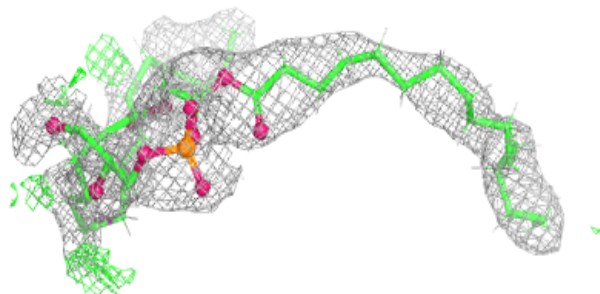
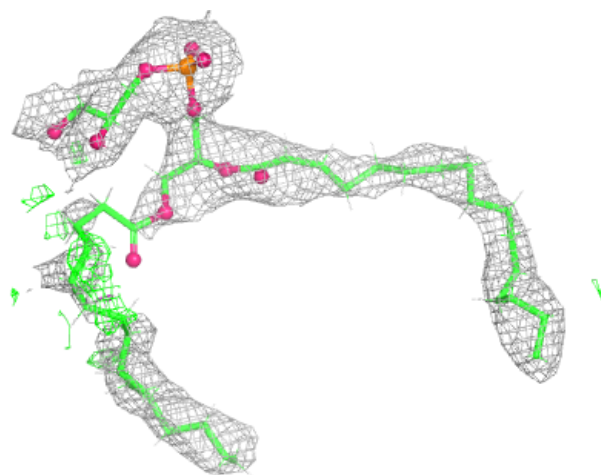
Electron density around LHG e 101:

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



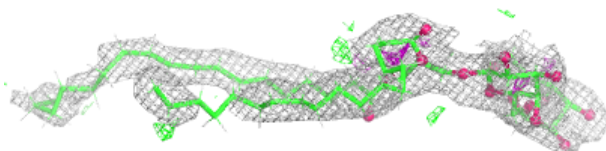
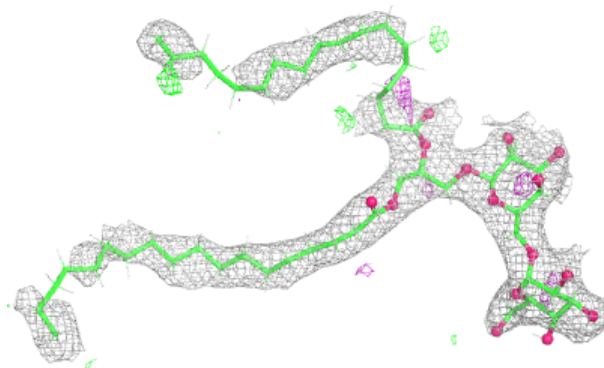
Electron density around LHG E 101:

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

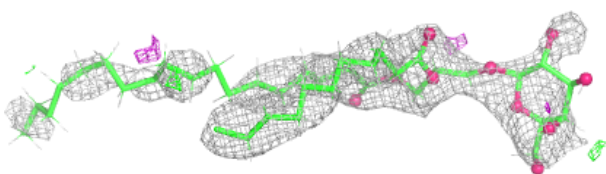
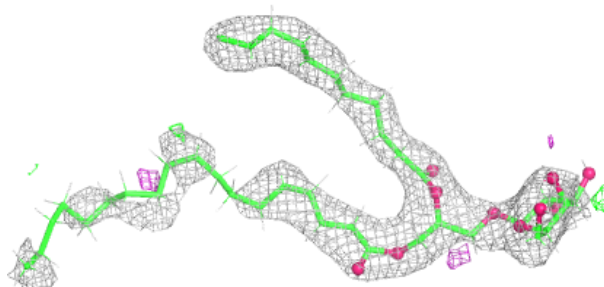


Electron density around DGD A 412:

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

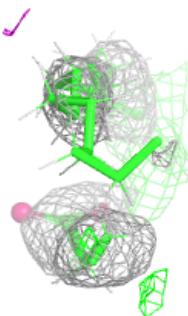
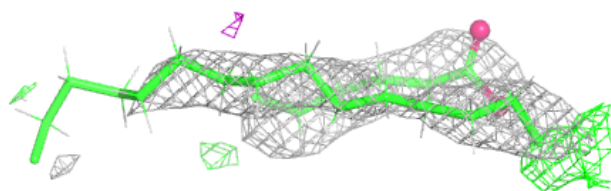
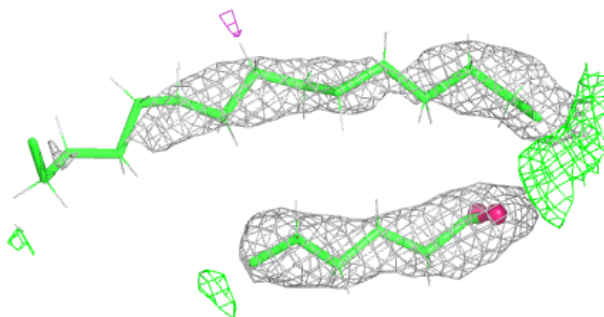
**Electron density around LMG c 522:**

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

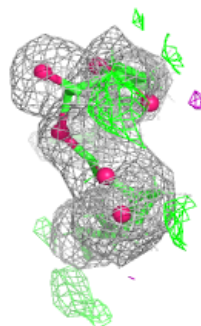
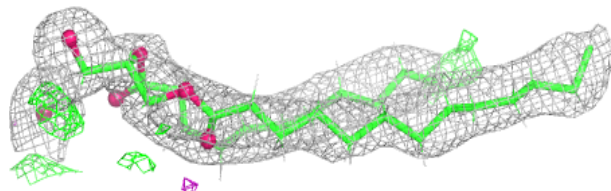
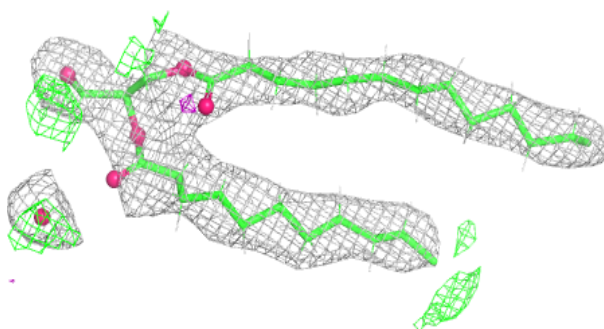


Electron density around LMG d 410:

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

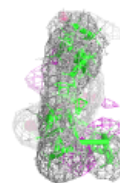
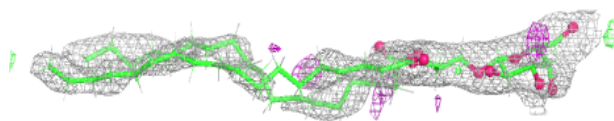
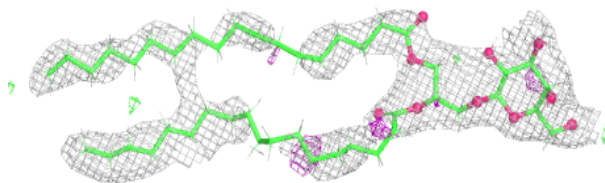
**Electron density around LMG D 410:**

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

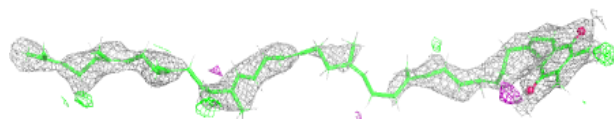
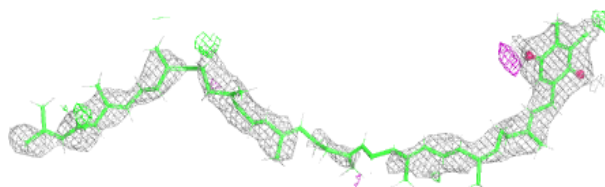


Electron density around LMG b 622:

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

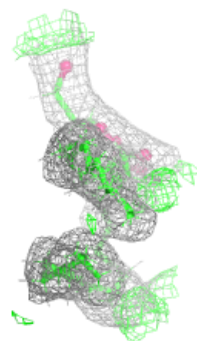
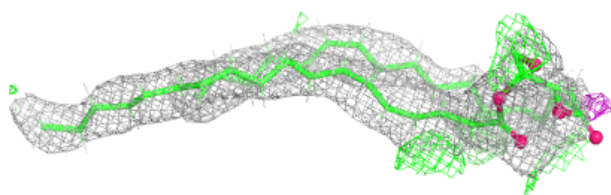
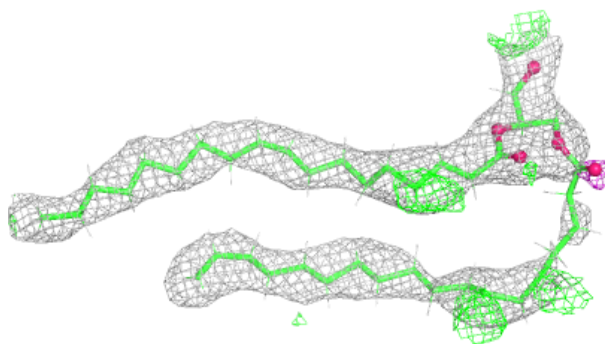
**Electron density around PL9 A 409:**

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

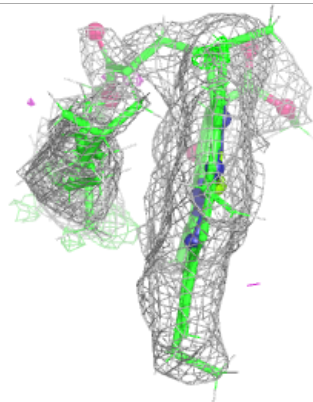
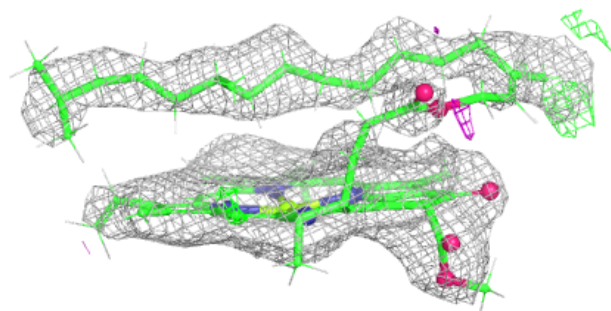
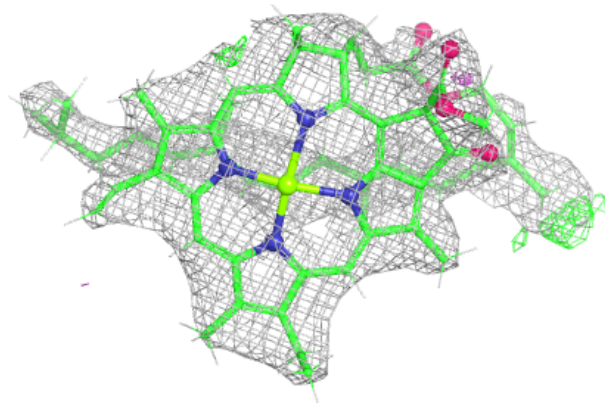


Electron density around DGD a 413:

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

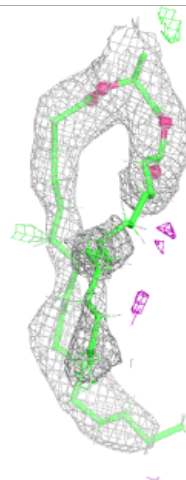
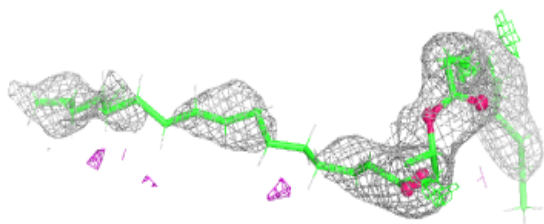
**Electron density around CLA b 602:**

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



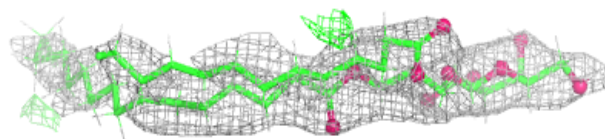
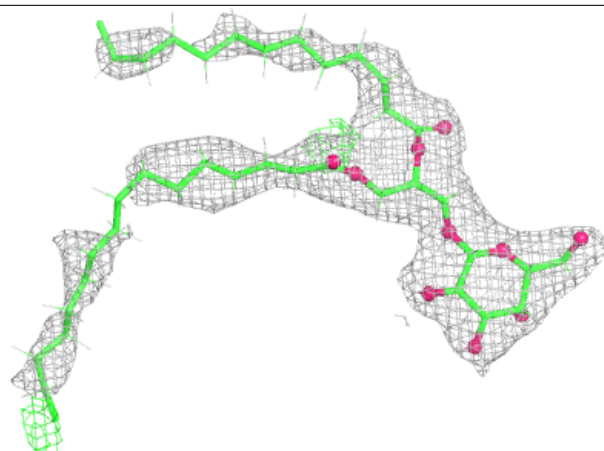
Electron density around SQD A 411:

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



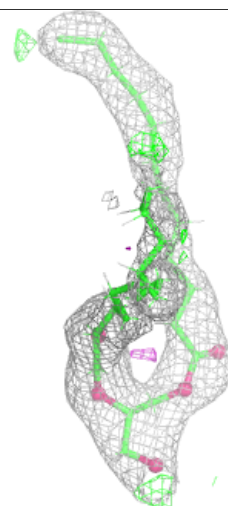
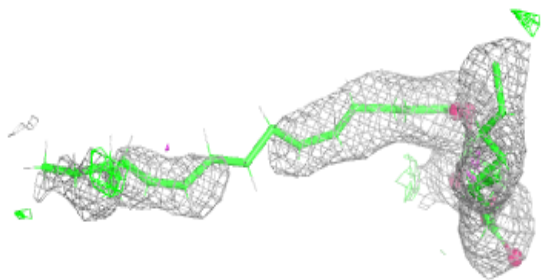
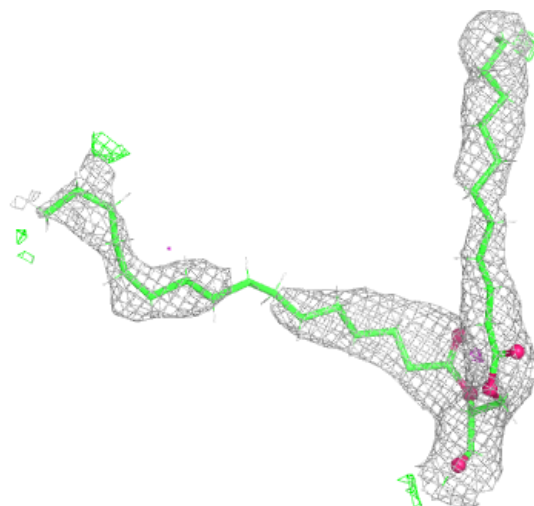
Electron density around LMG C 519:

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



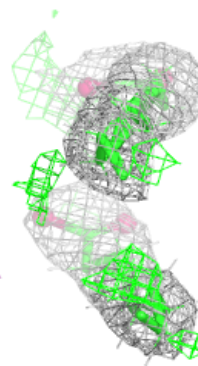
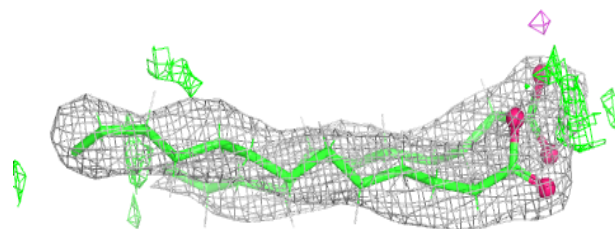
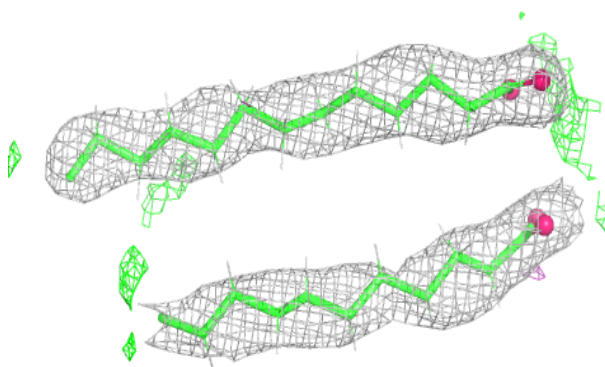
Electron density around SQD a 412:

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and green (positive)

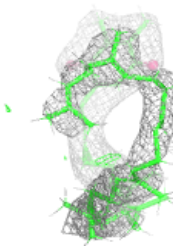
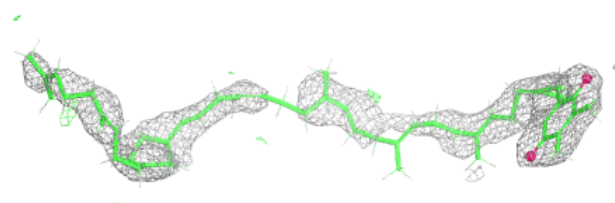
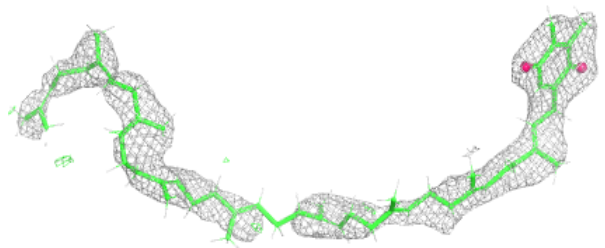


Electron density around LMG D 411:

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

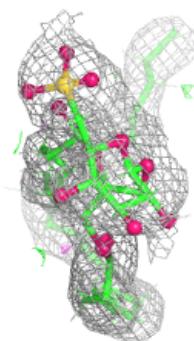
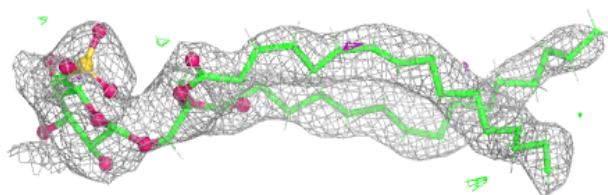
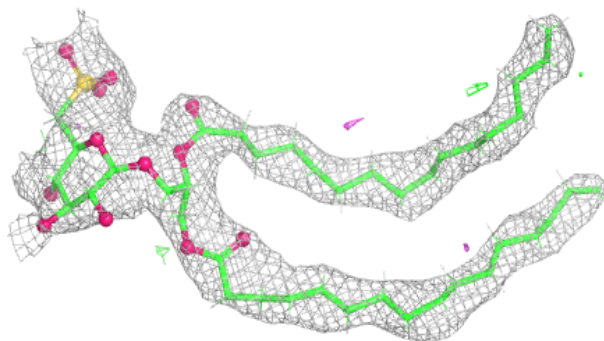
**Electron density around PL9 a 410:**

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

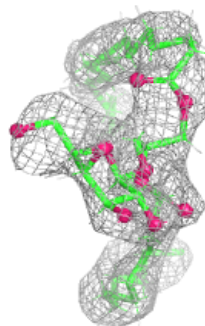
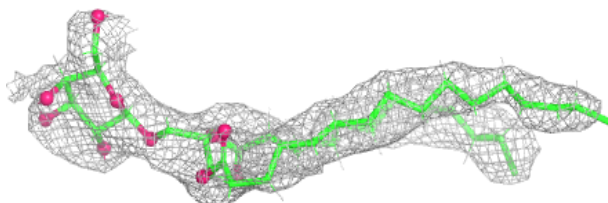
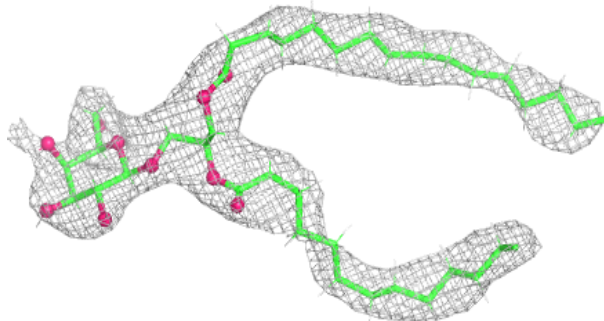


Electron density around SQD B 621:

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

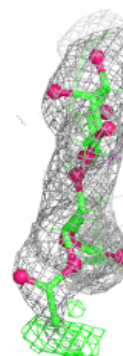
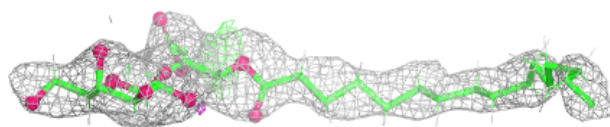
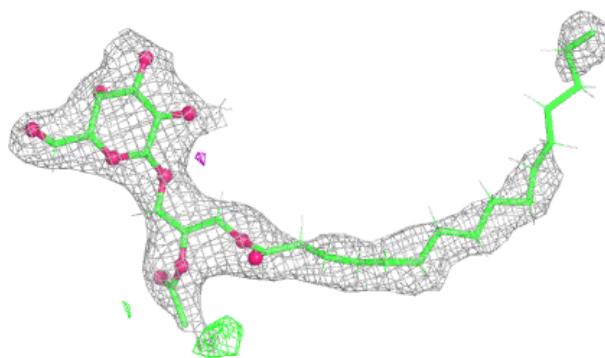
**Electron density around LMG C 501:**

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



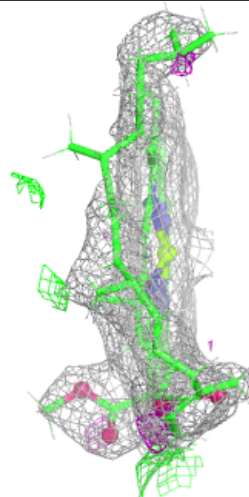
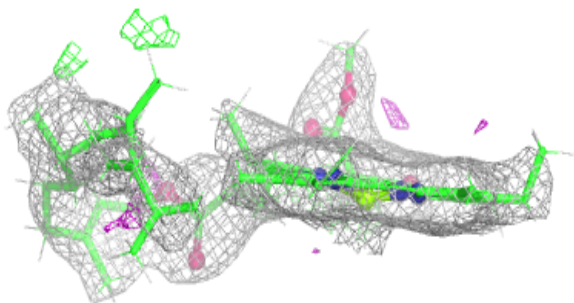
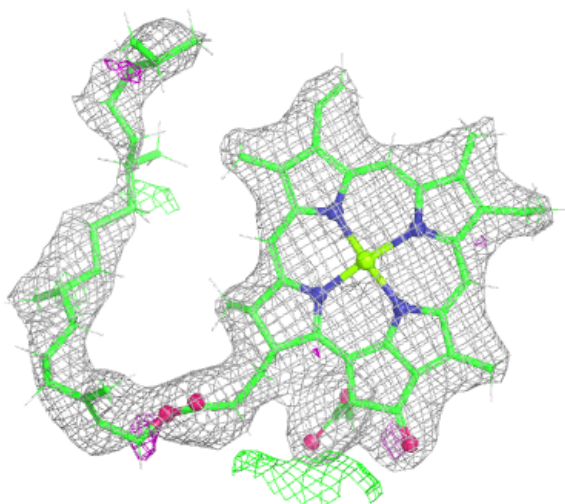
Electron density around LMG c 519:

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



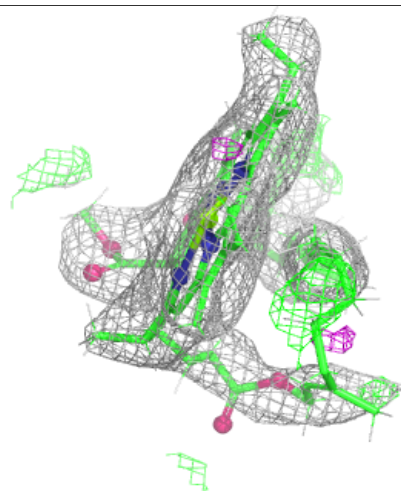
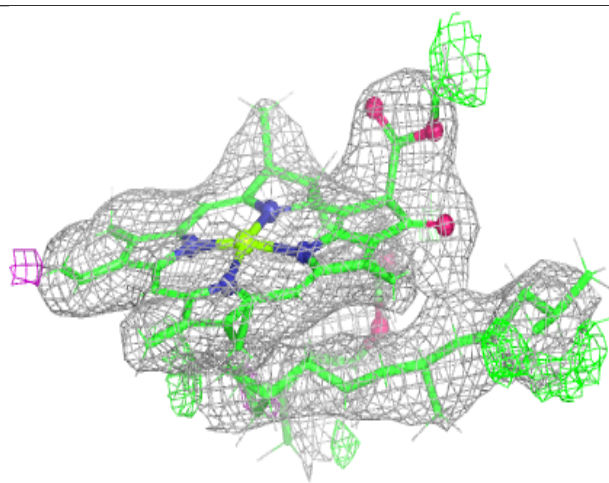
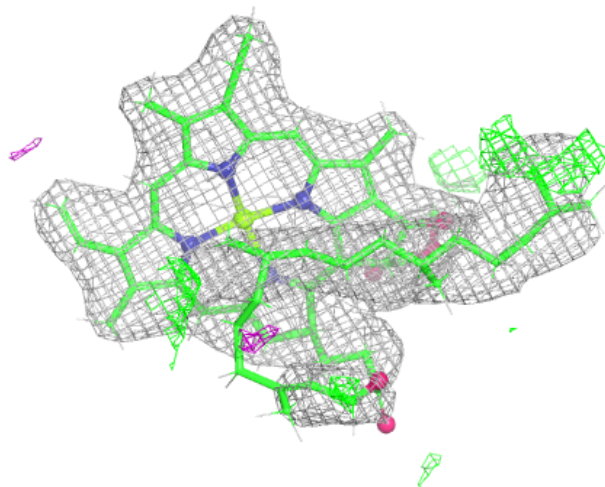
Electron density around CLA c 512:

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



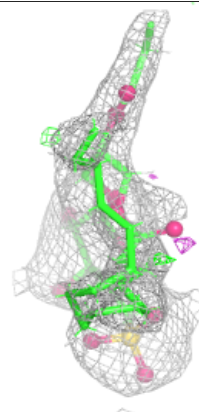
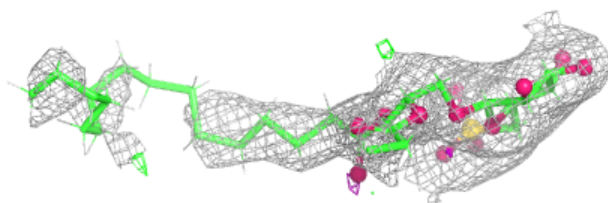
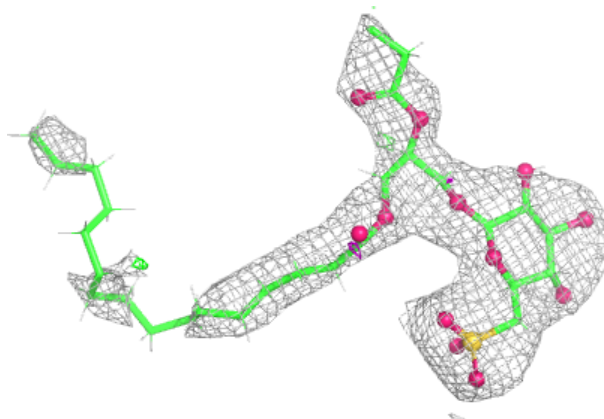
Electron density around CLA B 601:

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

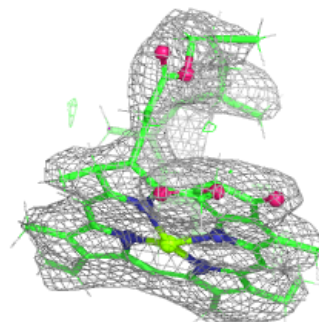
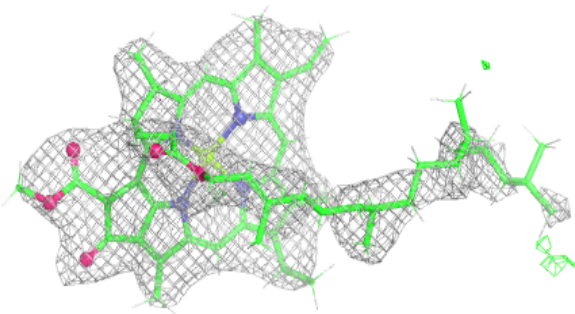
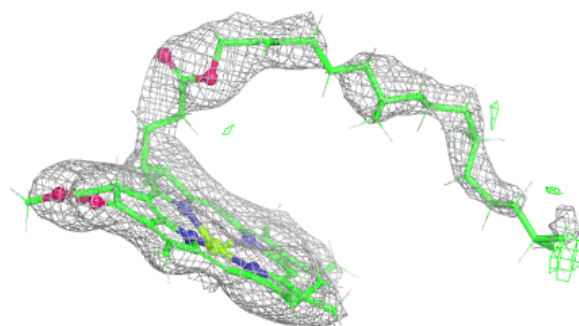


Electron density around SQD f 101:

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

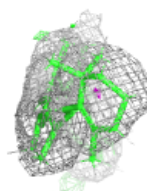
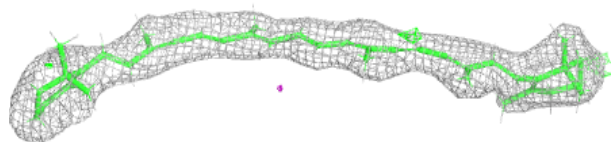
**Electron density around CLA C 514:**

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

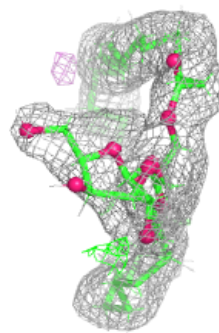
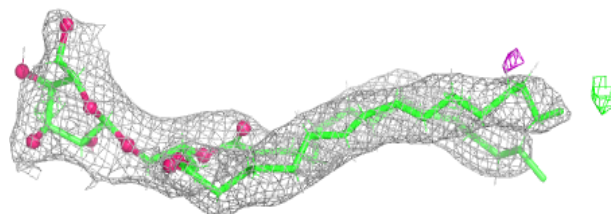
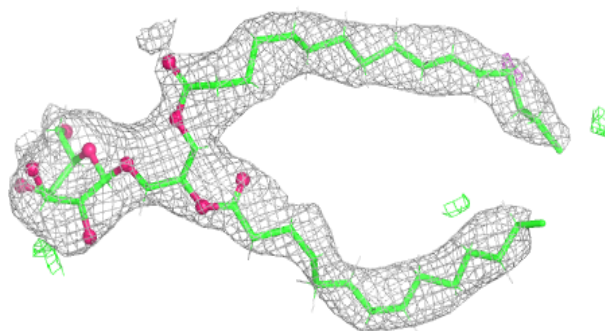


Electron density around BCR d 405:

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

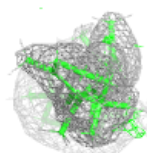
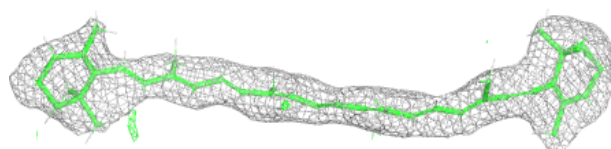
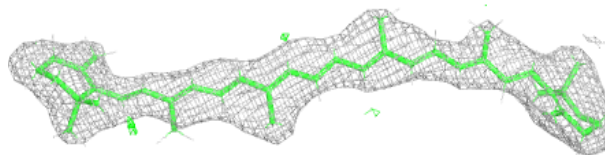
**Electron density around LMG c 524:**

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

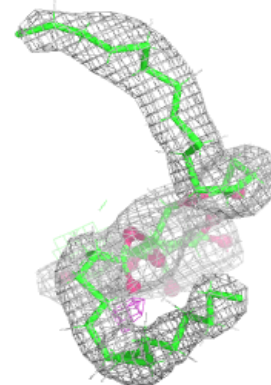
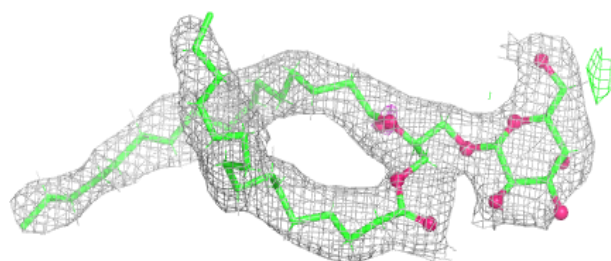
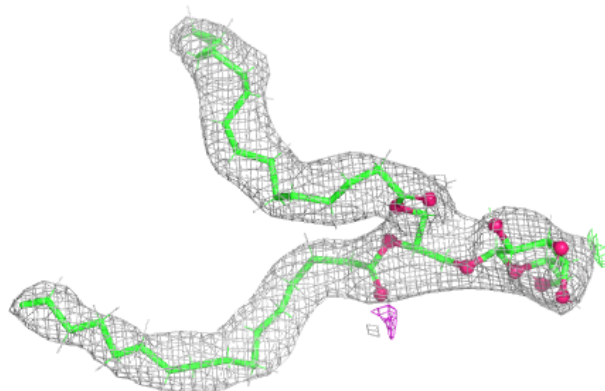


Electron density around BCR x 102:

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

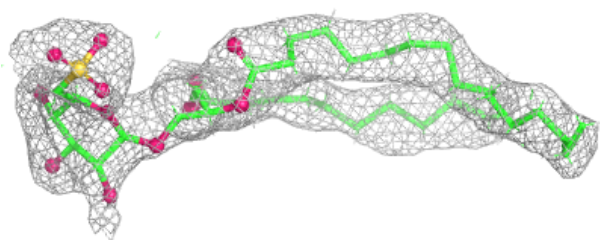
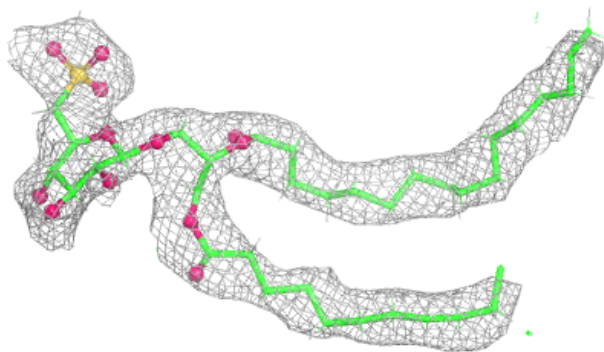
**Electron density around LMG m 101:**

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

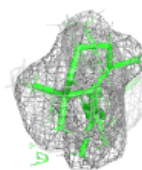
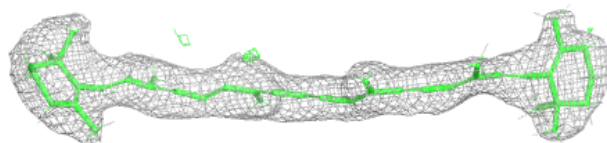
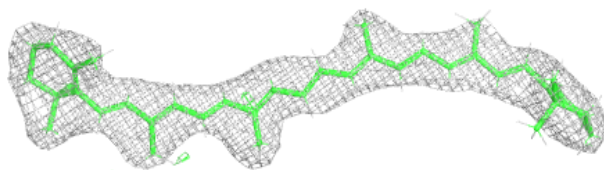


Electron density around SQD b 601:

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

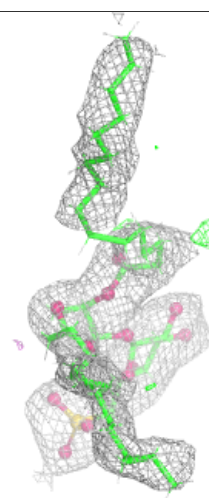
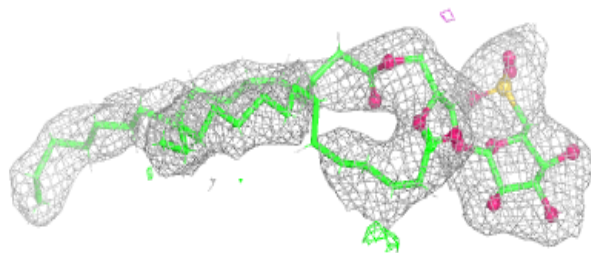
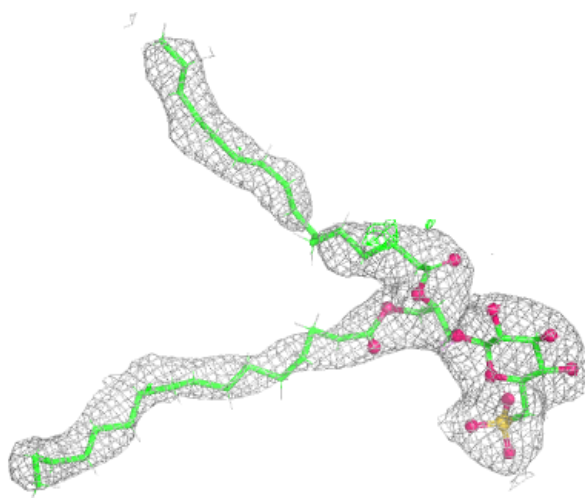
**Electron density around BCR K 101:**

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



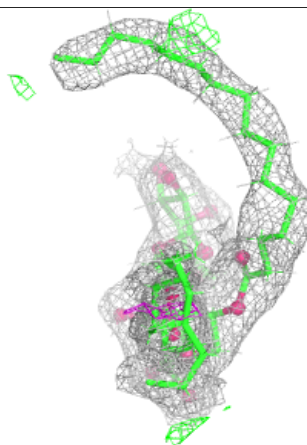
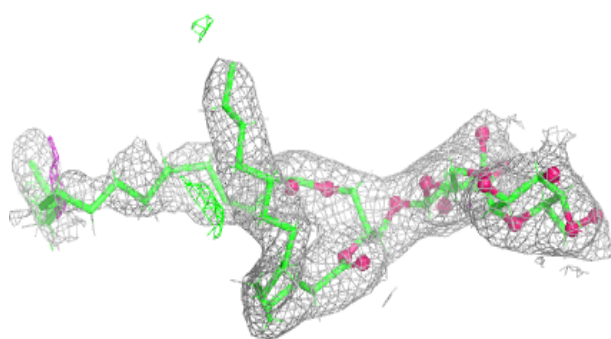
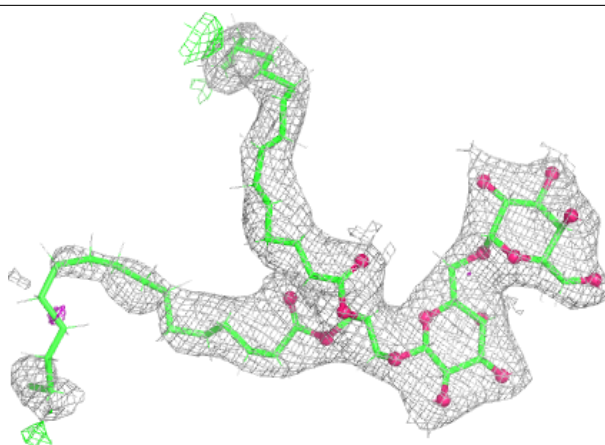
Electron density around SQD a 411:

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

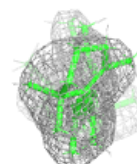
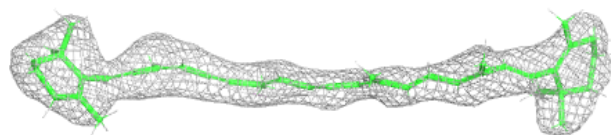


Electron density around DGD C 517:

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

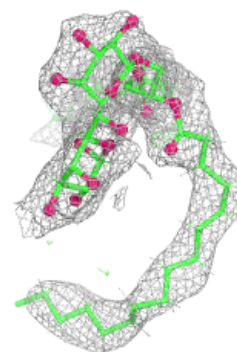
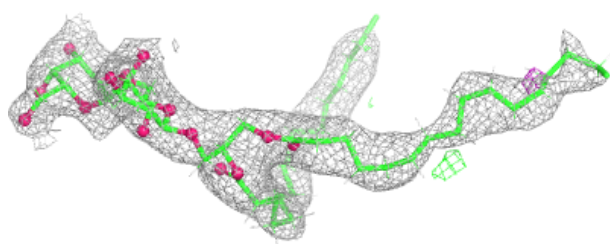
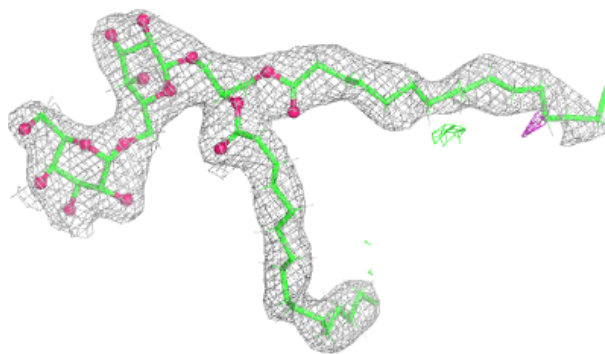
**Electron density around BCR k 101:**

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

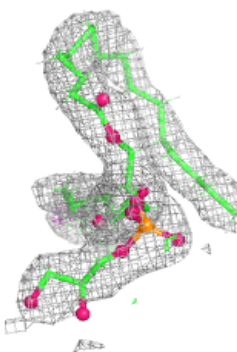
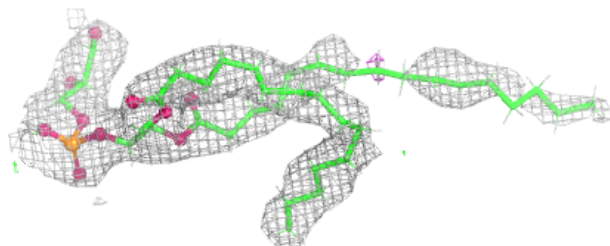
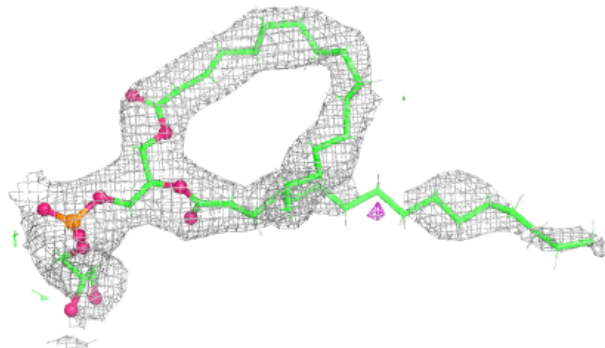


Electron density around DGD c 517:

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

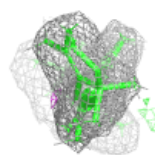
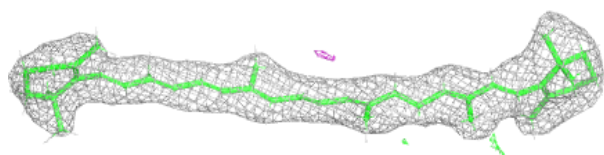
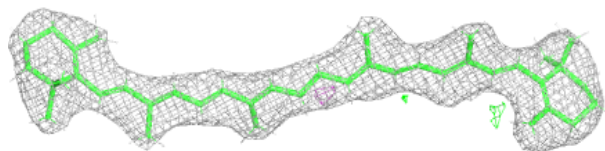
**Electron density around LHG d 407:**

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

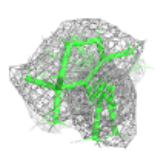
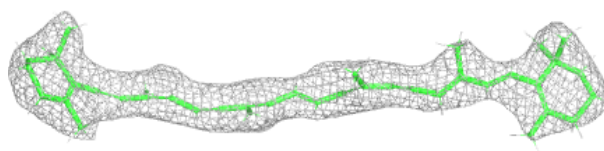
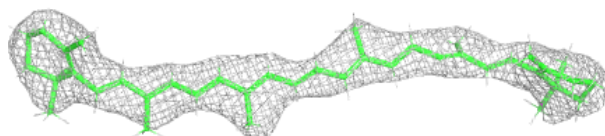


Electron density around BCR b 620:

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

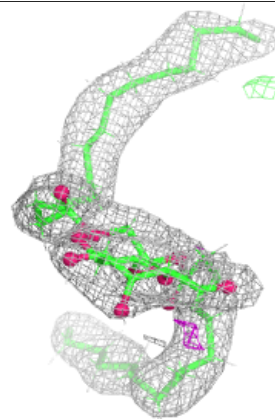
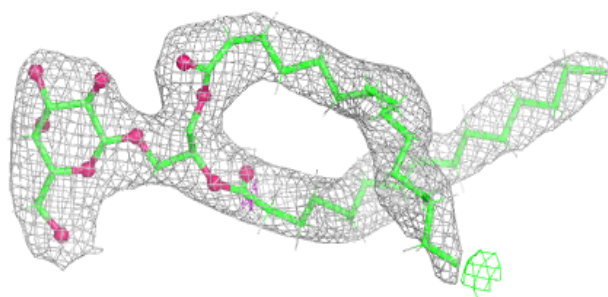
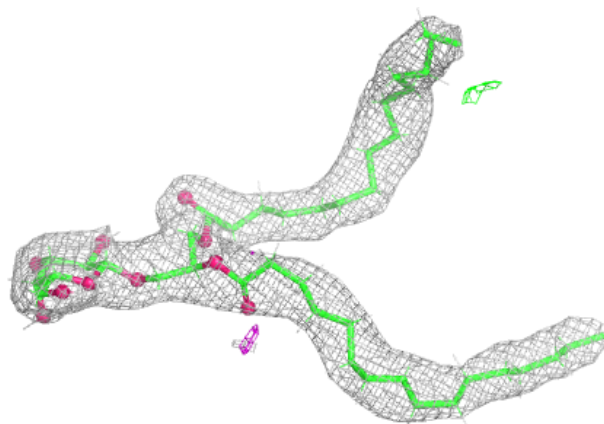
**Electron density around BCR c 514:**

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

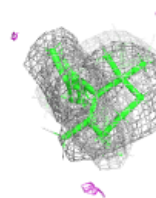
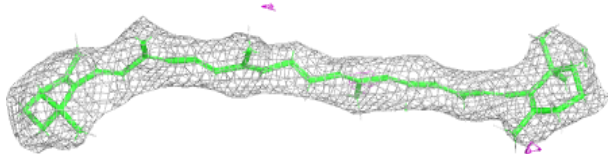
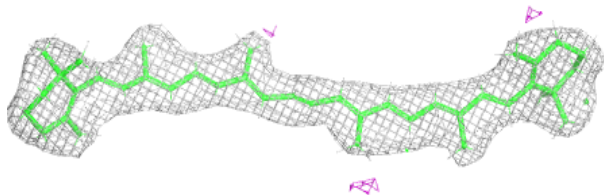


Electron density around LMG M 101:

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

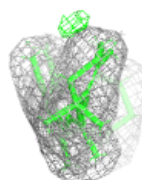
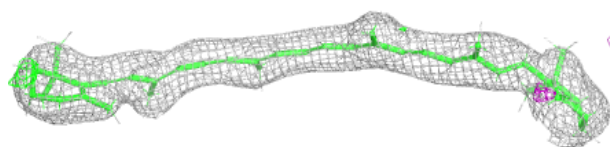
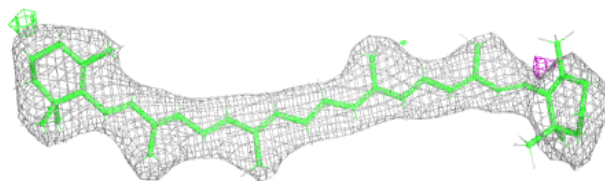
**Electron density around BCR B 619:**

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

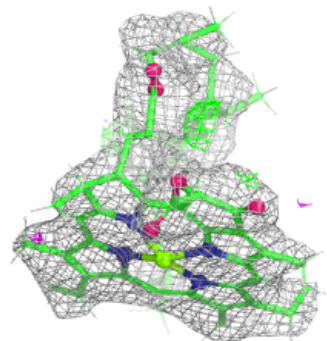
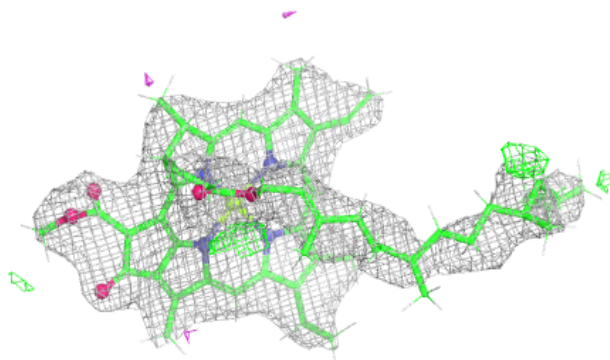
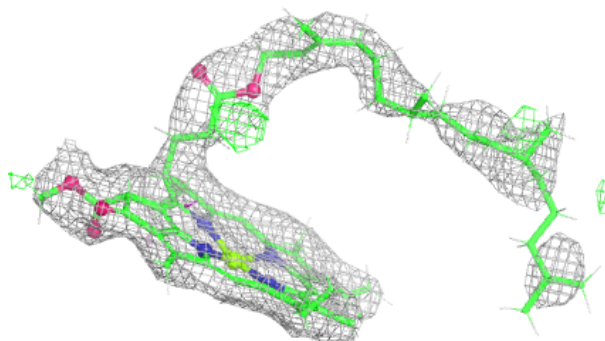


Electron density around BCR D 405:

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

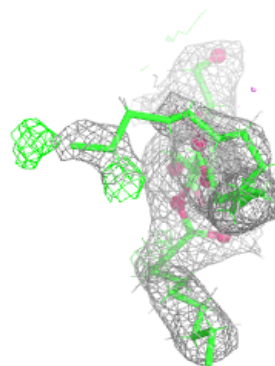
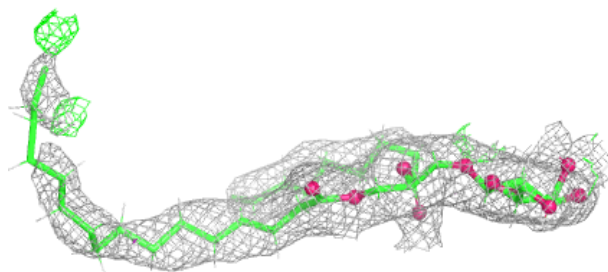
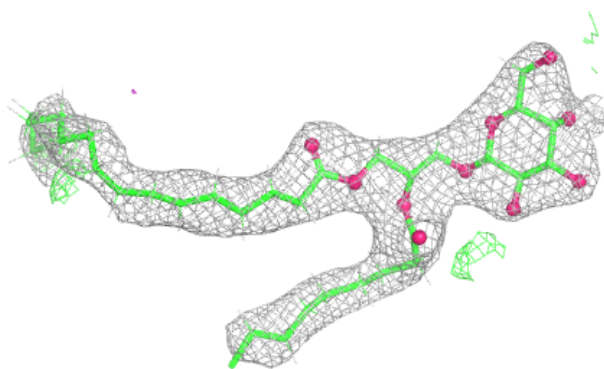
**Electron density around CLA c 513:**

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

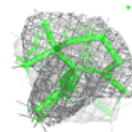


Electron density around LMG d 411:

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

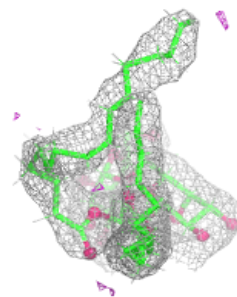
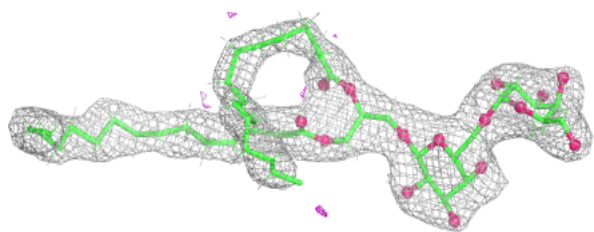
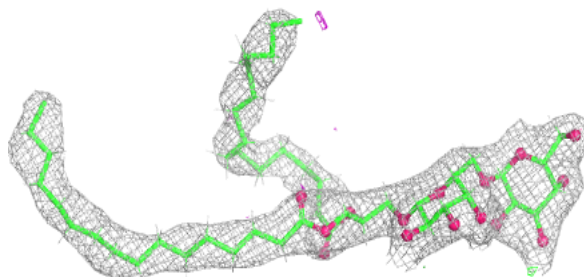
**Electron density around BCR Z 101:**

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

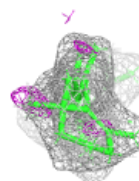
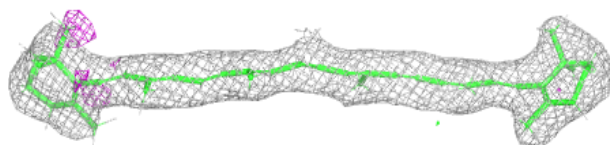
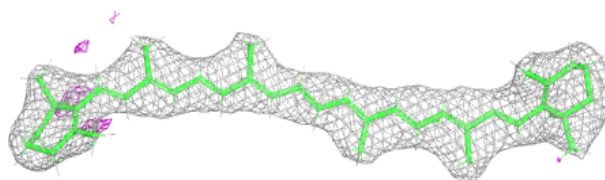


Electron density around DGD h 101:

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

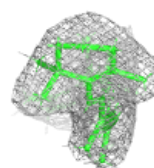
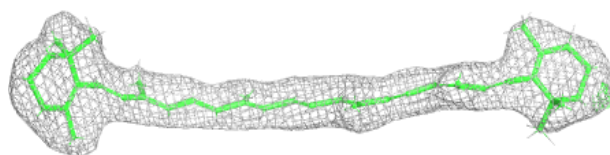
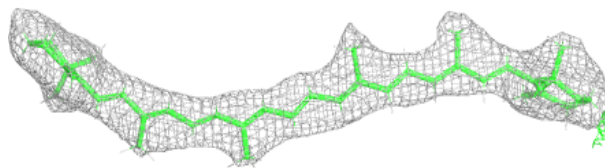
**Electron density around BCR B 618:**

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



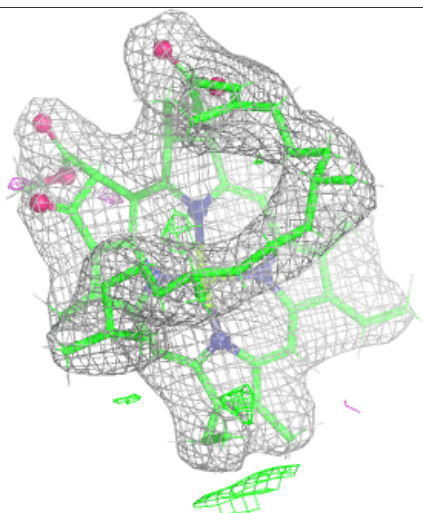
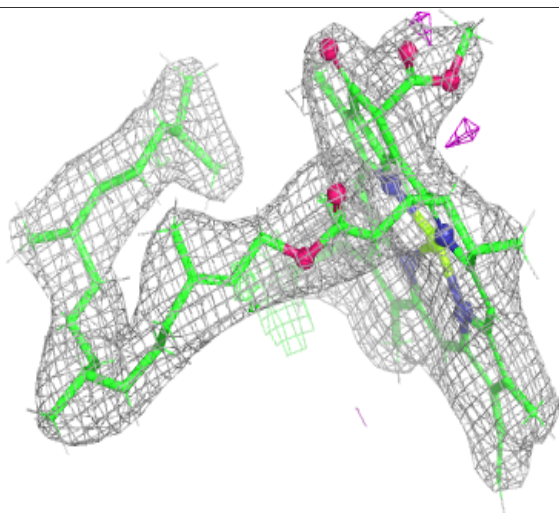
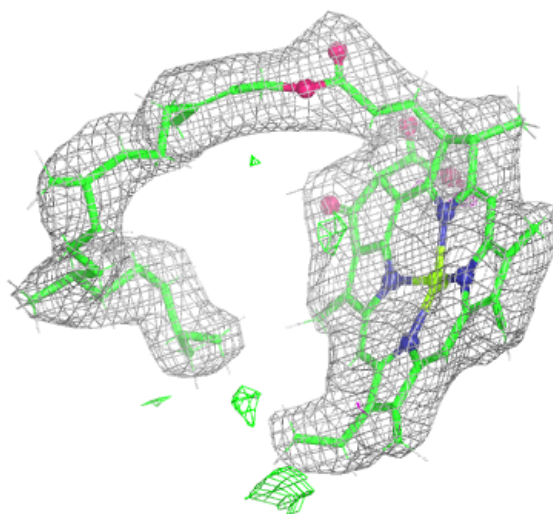
Electron density around BCR H 101:

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



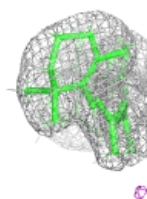
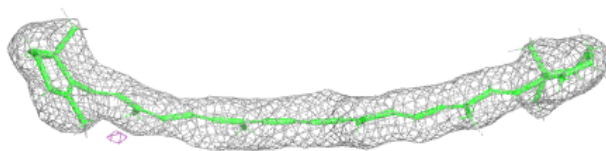
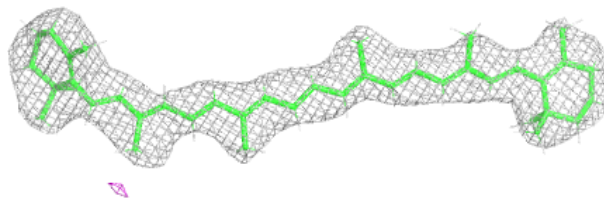
Electron density around CLA c 503:

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



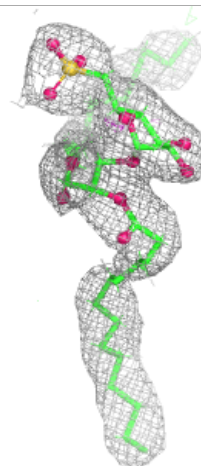
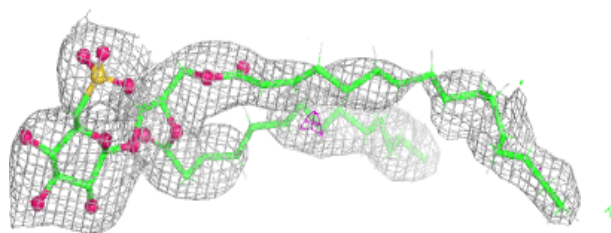
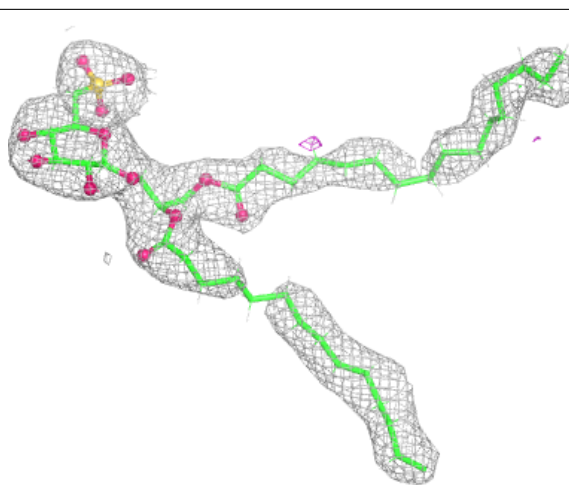
Electron density around BCR T 101:

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



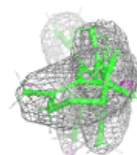
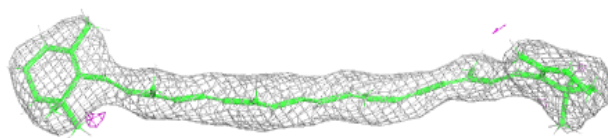
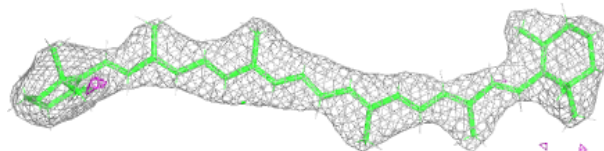
Electron density around SQD A 410:

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

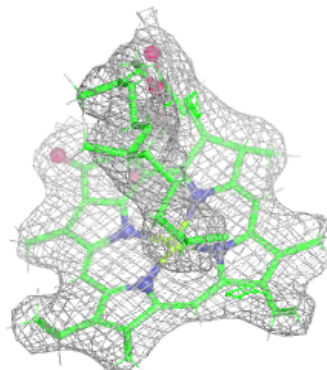
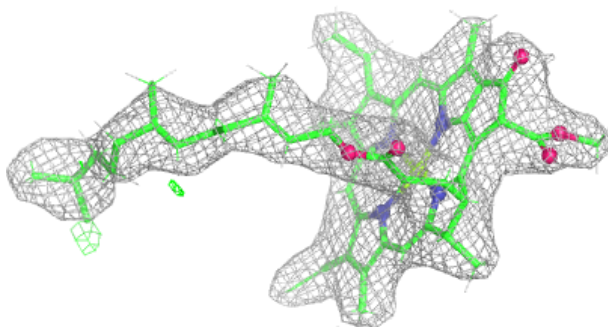
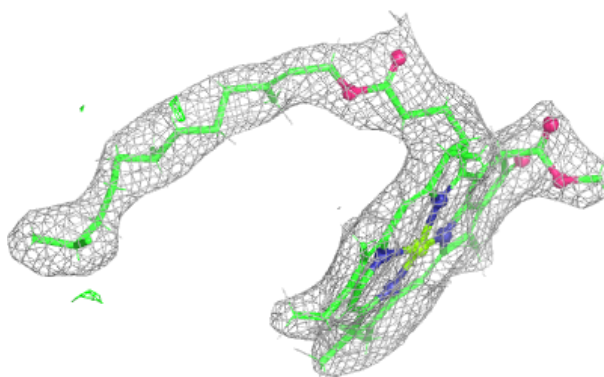


Electron density around BCR B 617:

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

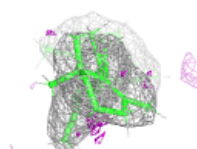
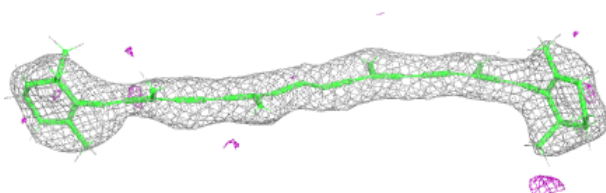
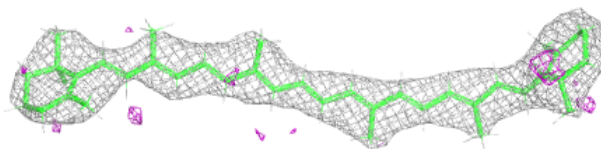
**Electron density around CLA c 504:**

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

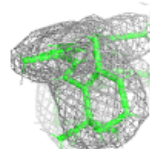
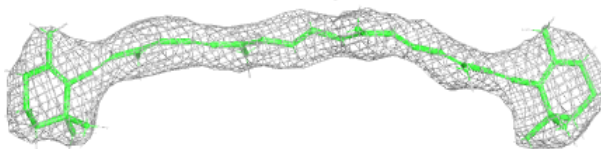


Electron density around BCR c 515:

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

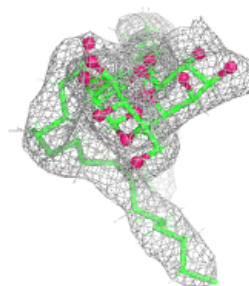
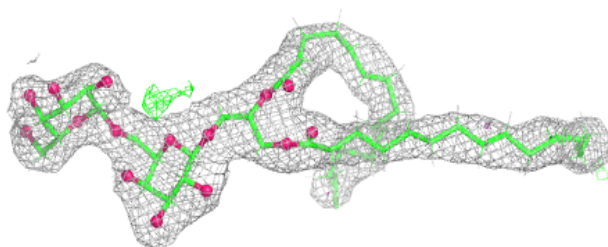
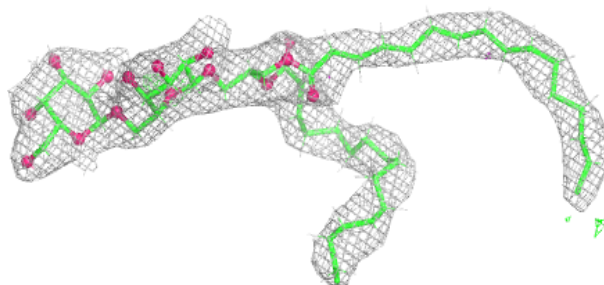
**Electron density around BCR c 521:**

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

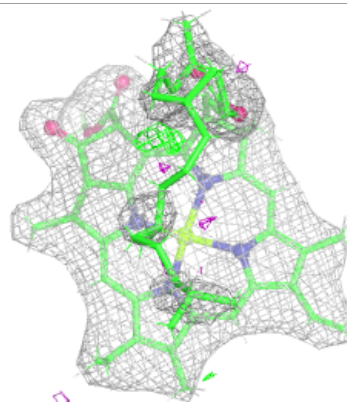
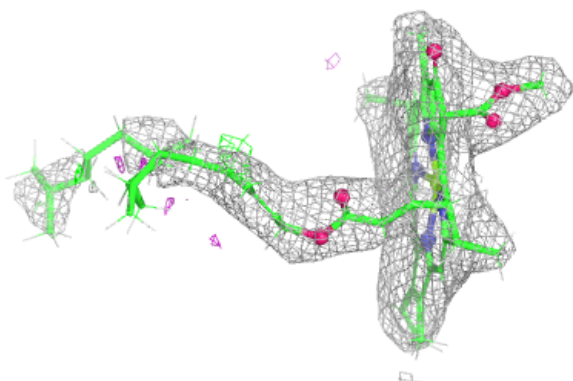
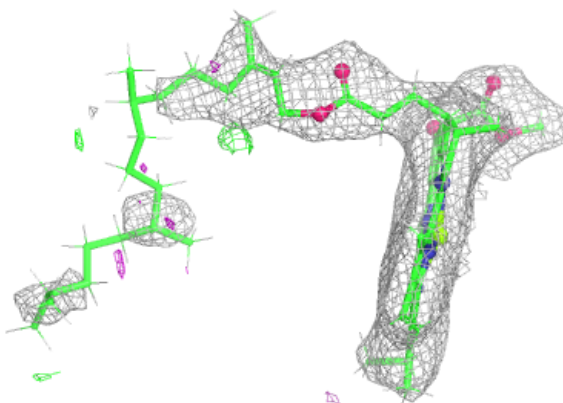


Electron density around DGD H 102:

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

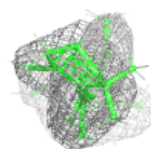
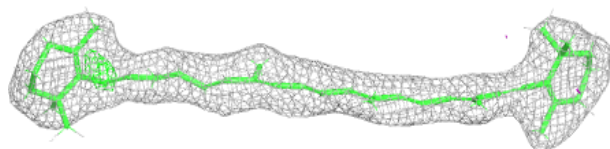
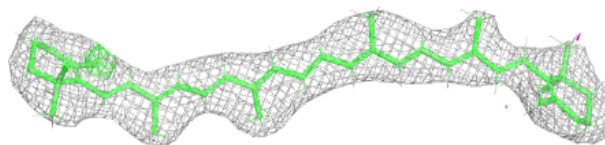
**Electron density around CLA c 506:**

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

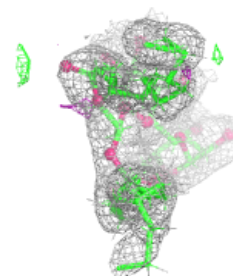
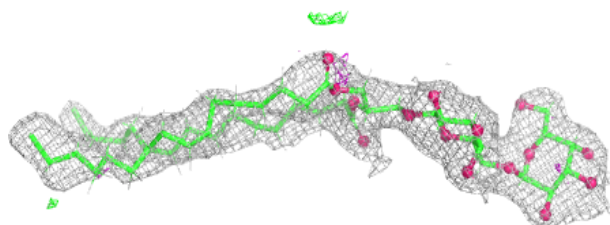
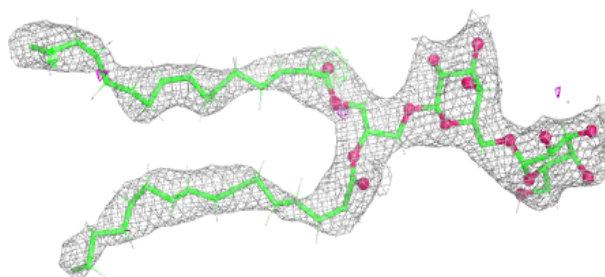


Electron density around BCR C 515:

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

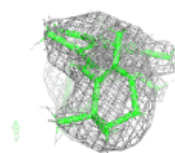
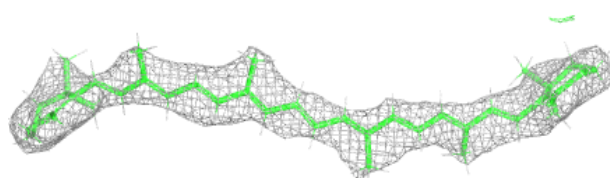
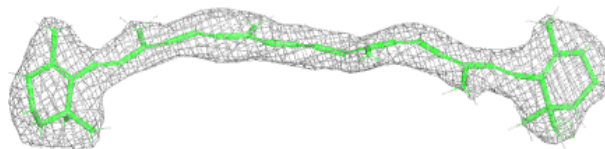
**Electron density around DGD c 518:**

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

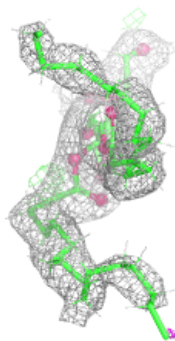
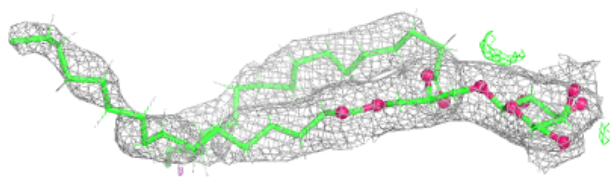
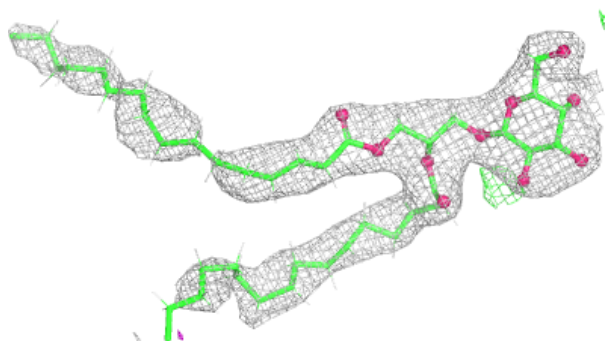


Electron density around BCR C 520:

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

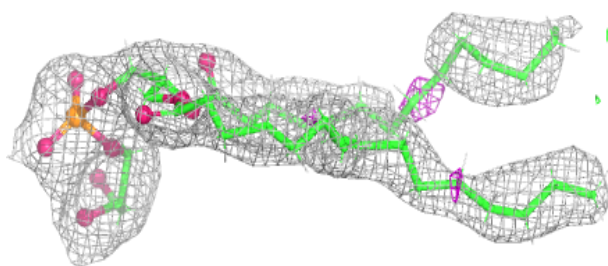
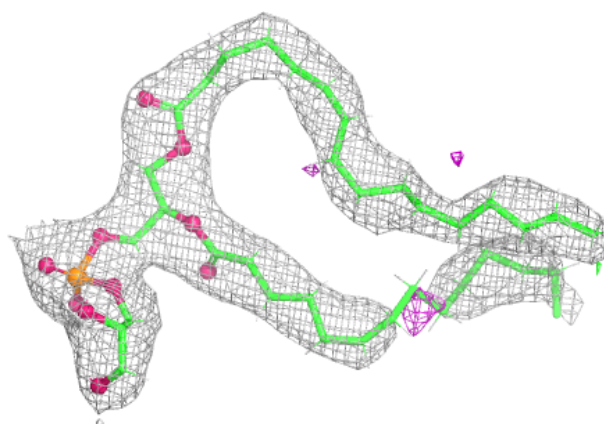
**Electron density around LMG D 407:**

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

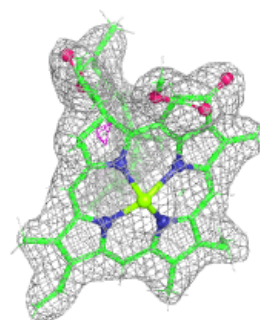
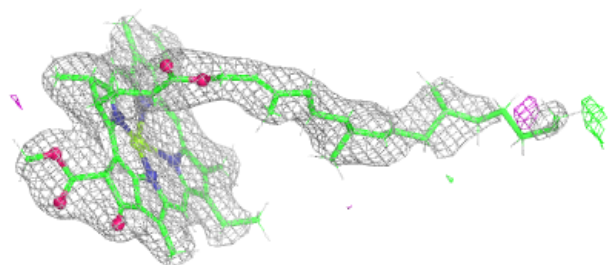
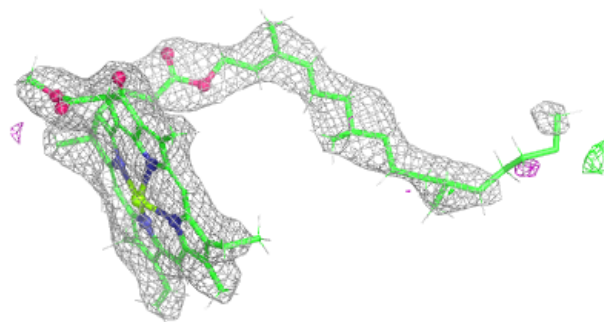


Electron density around LHG D 409:

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

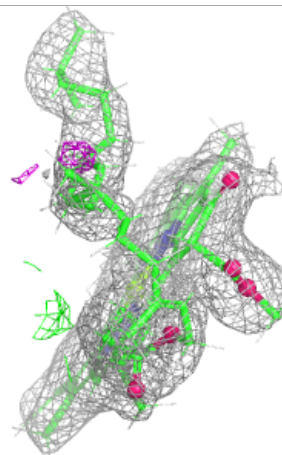
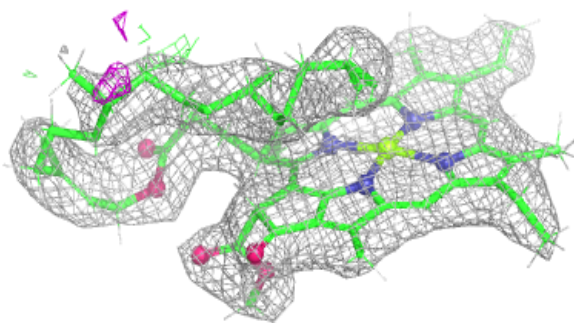
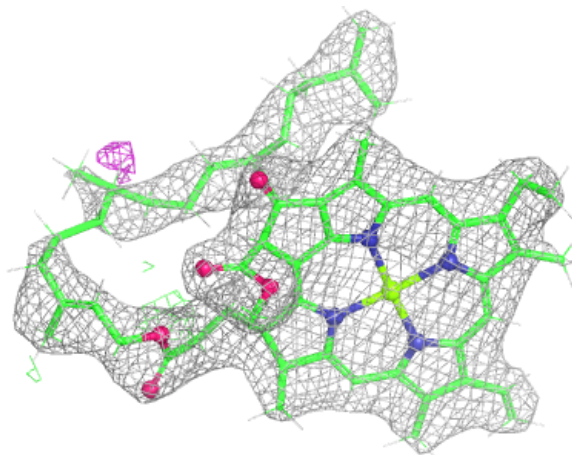
**Electron density around CLA c 508:**

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



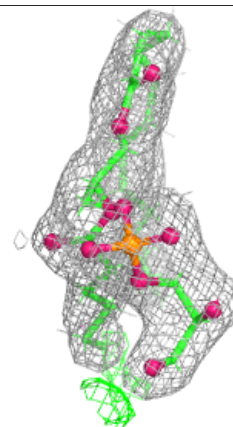
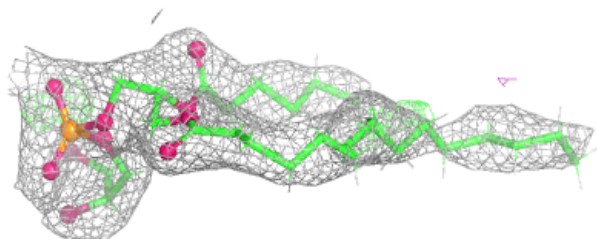
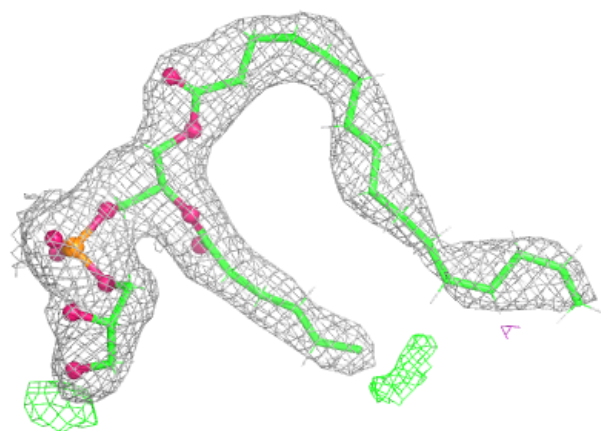
Electron density around CLA c 509:

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

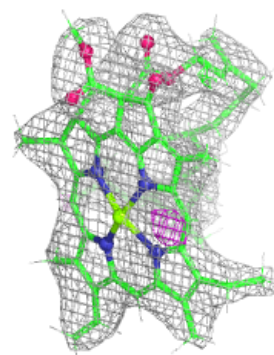
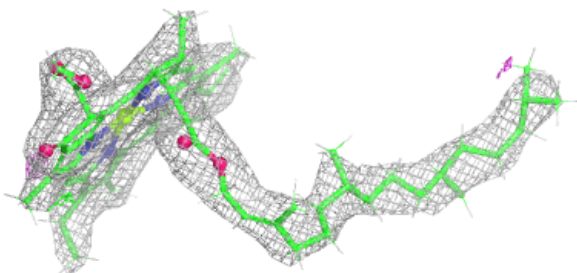
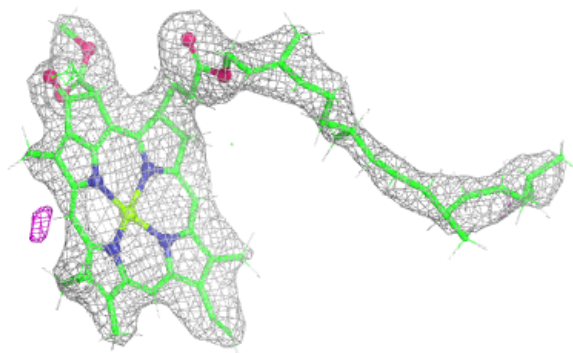


Electron density around LHG d 409:

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

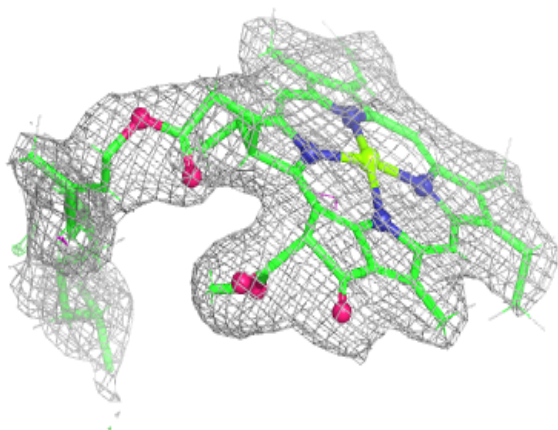
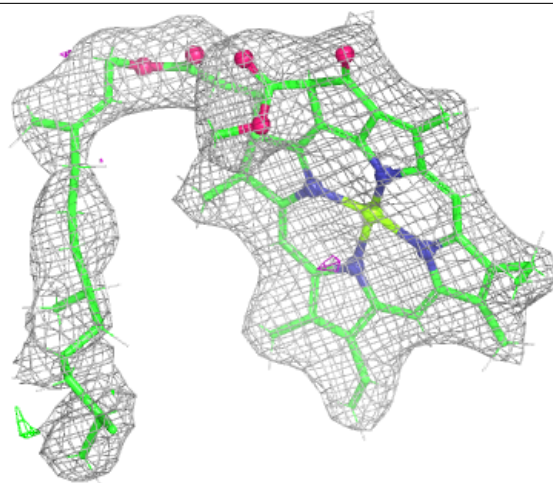
**Electron density around CLA c 511:**

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



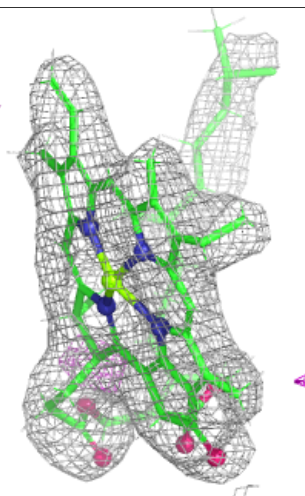
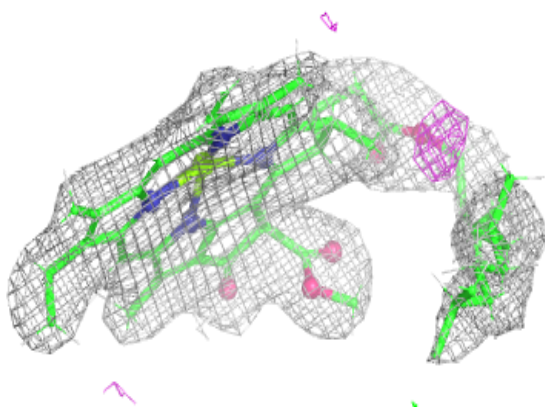
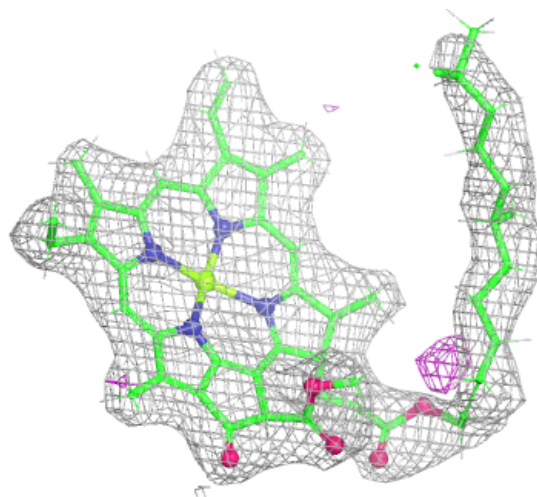
Electron density around CLA b 617:

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



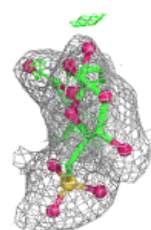
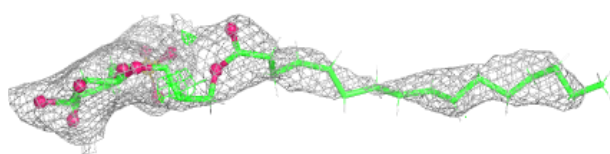
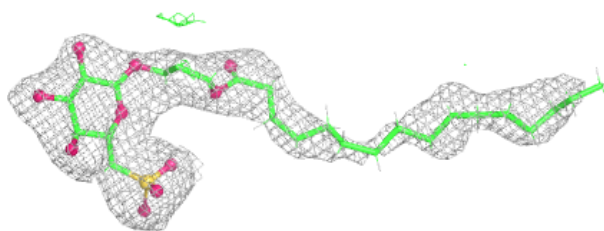
Electron density around CLA B 616:

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

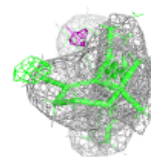
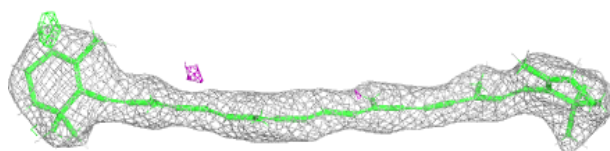


Electron density around SQD F 101:

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

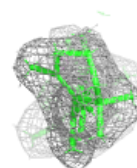
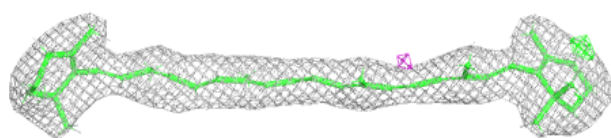
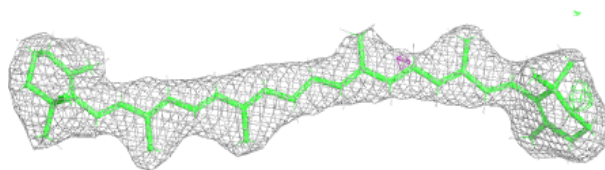
**Electron density around BCR b 618:**

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

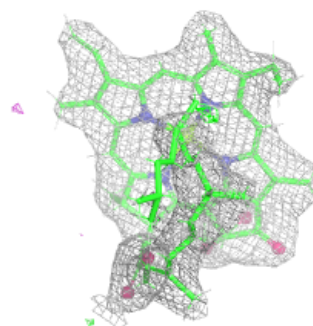
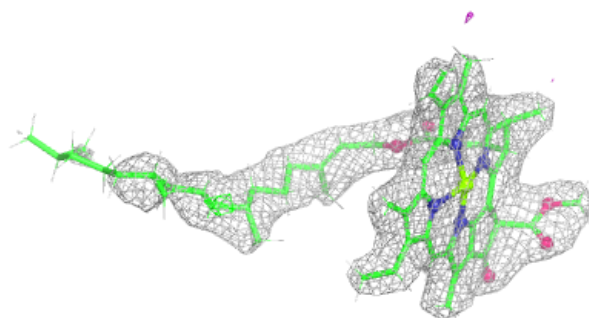
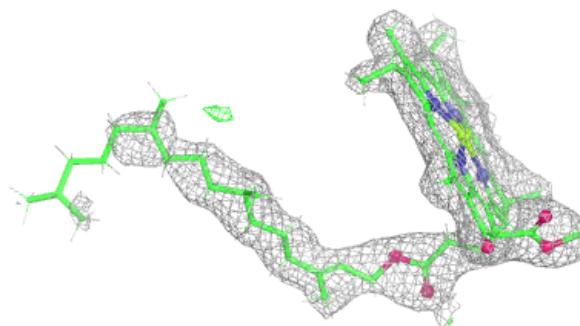


Electron density around BCR b 619:

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

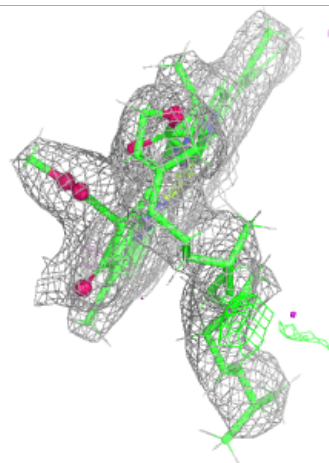
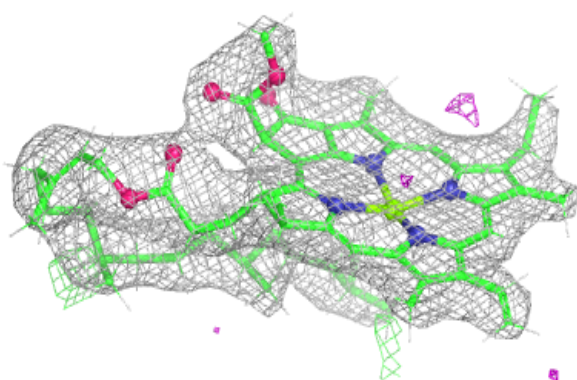
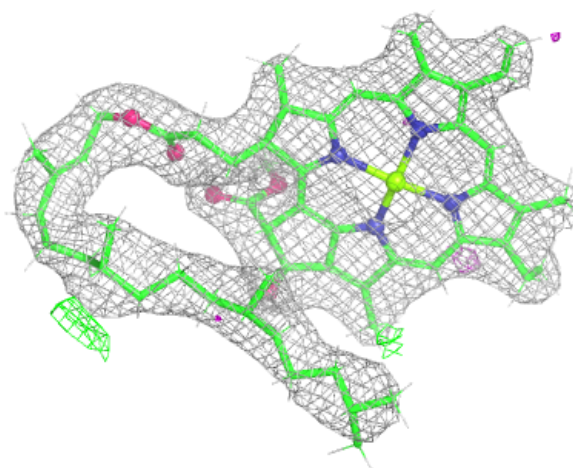
**Electron density around CLA C 509:**

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



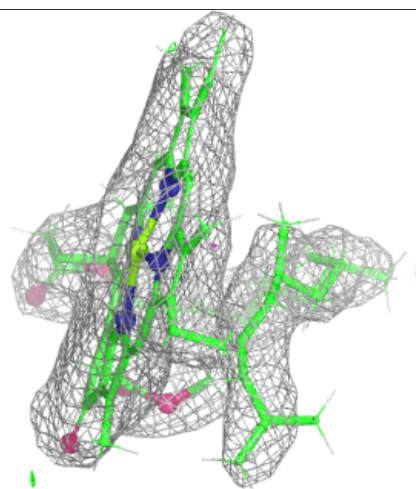
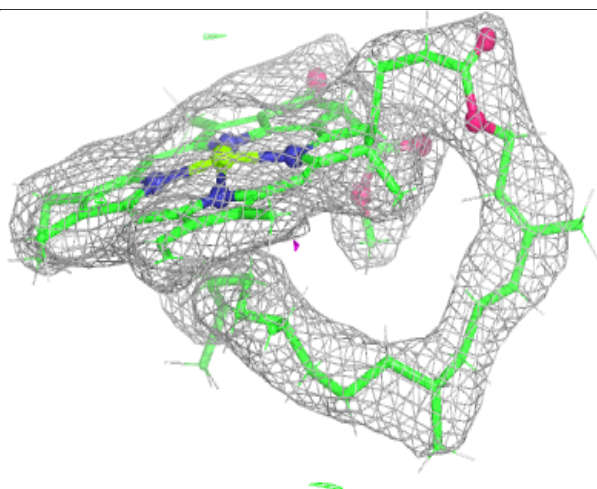
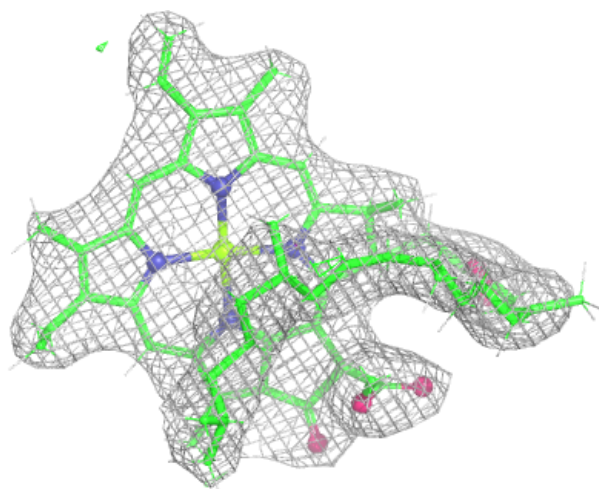
Electron density around CLA C 510:

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



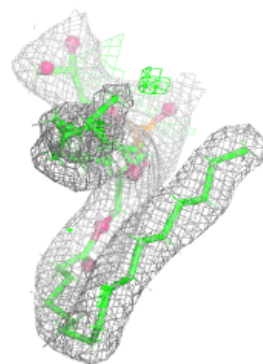
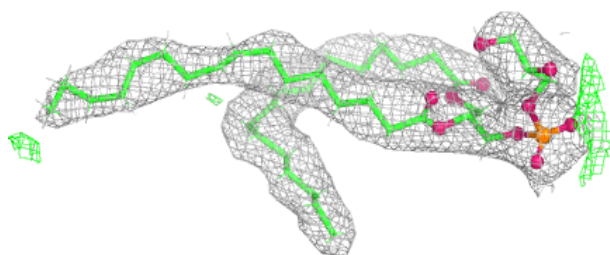
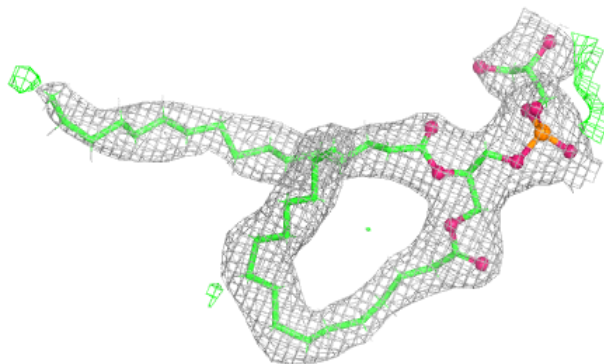
Electron density around CLA c 510:

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

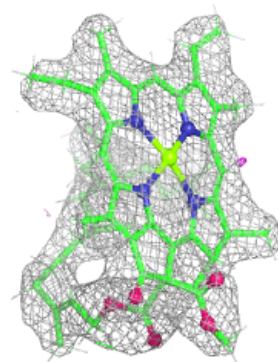
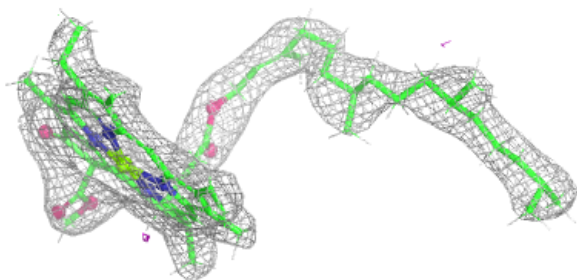
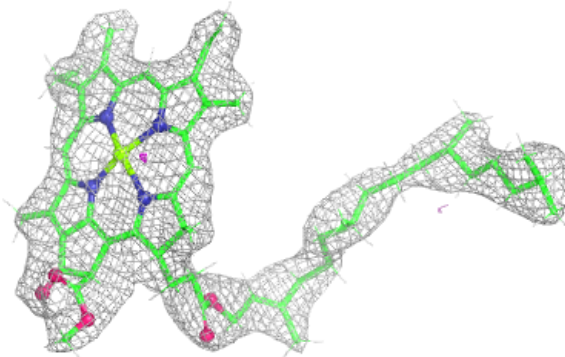


Electron density around LHG A 413:

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

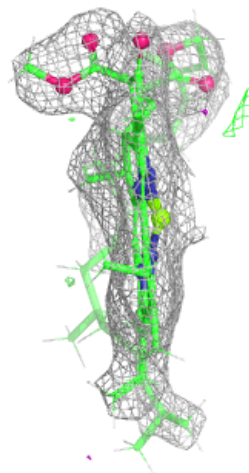
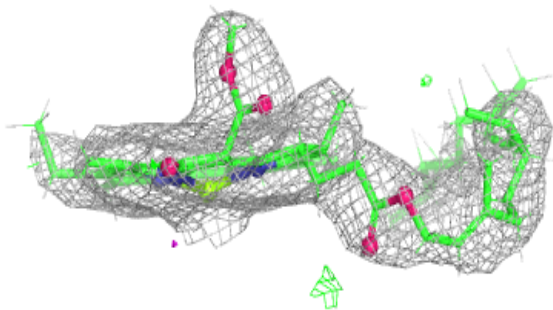
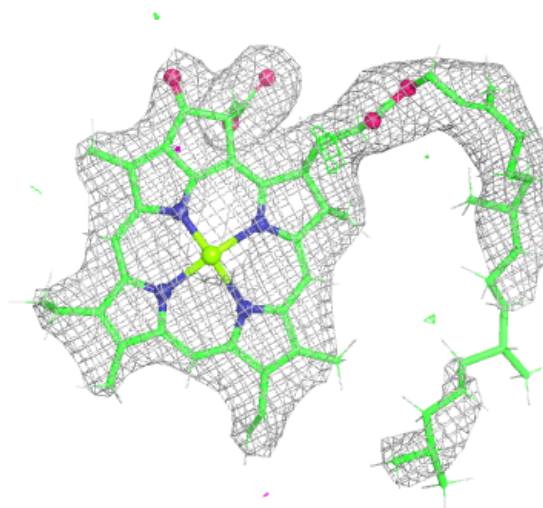
**Electron density around CLA C 512:**

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



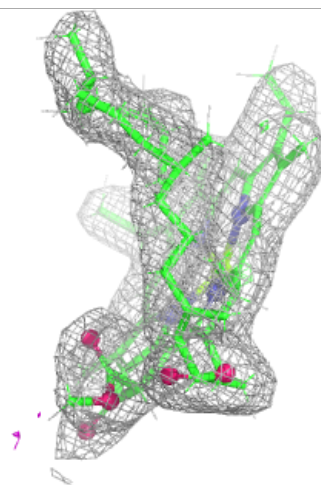
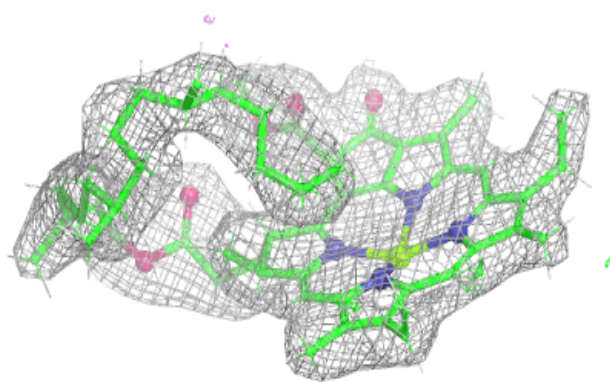
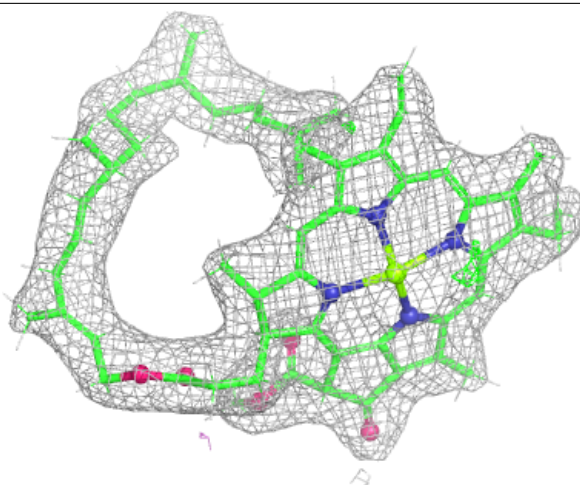
Electron density around CLA C 513:

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



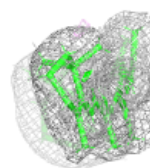
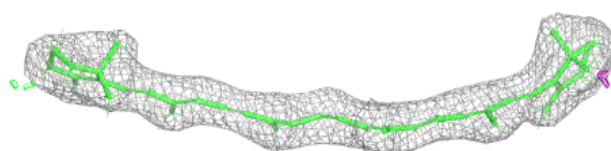
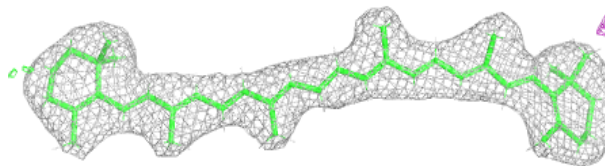
Electron density around CLA B 615:

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

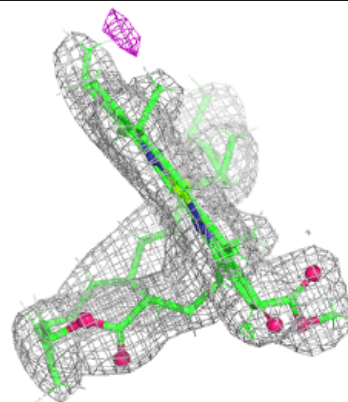
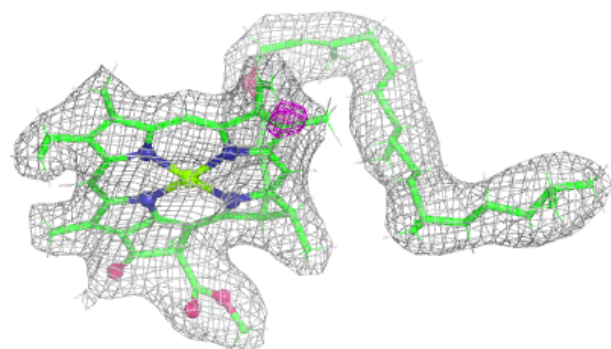
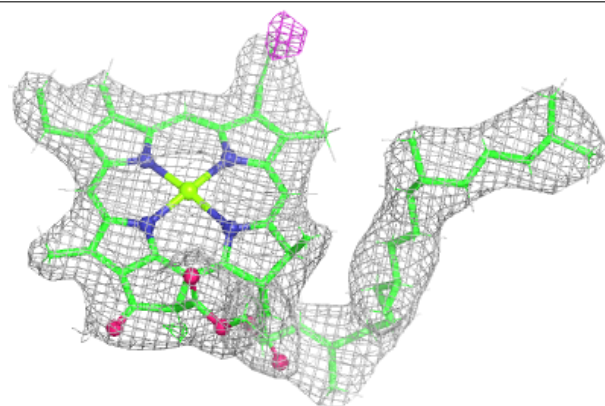


Electron density around BCR t 101:

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

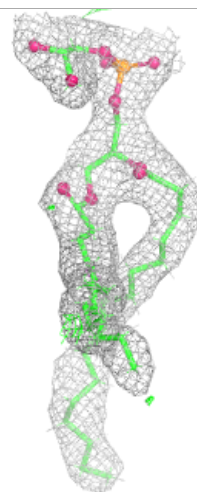
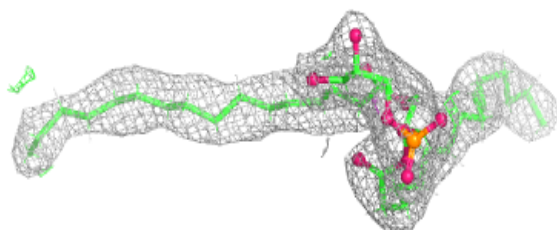
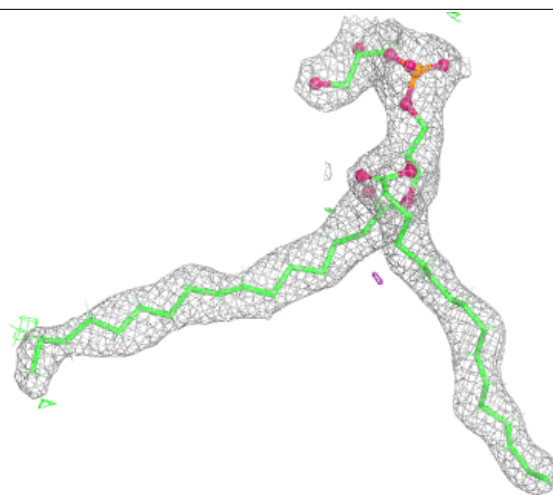
**Electron density around CLA d 402:**

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



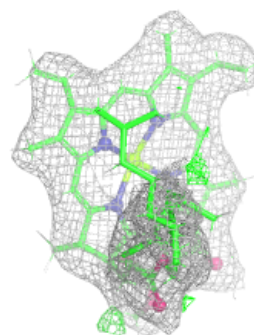
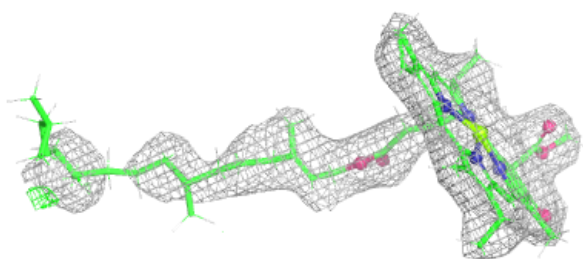
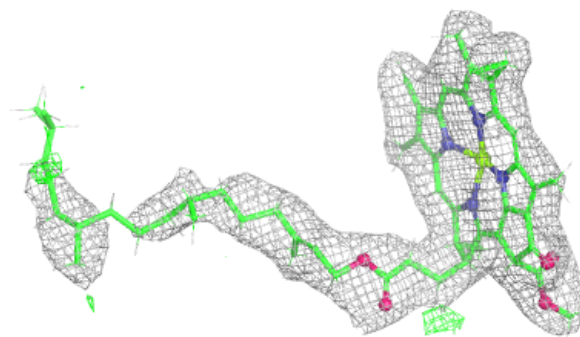
Electron density around LHG 1 101:

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

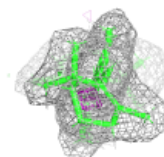
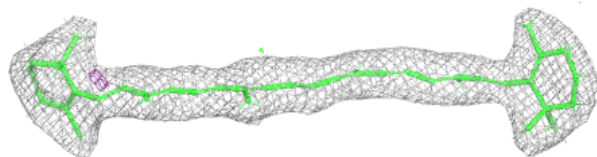
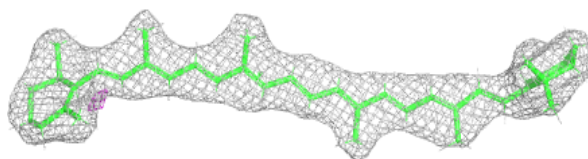


Electron density around CLA d 404:

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

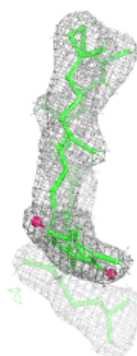
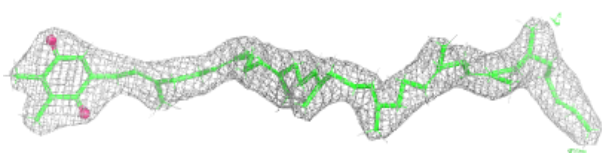
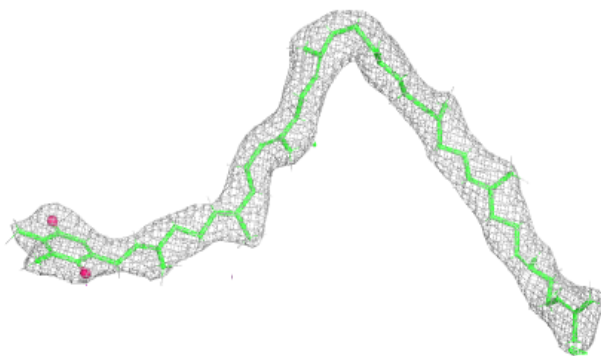
**Electron density around BCR A 408:**

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

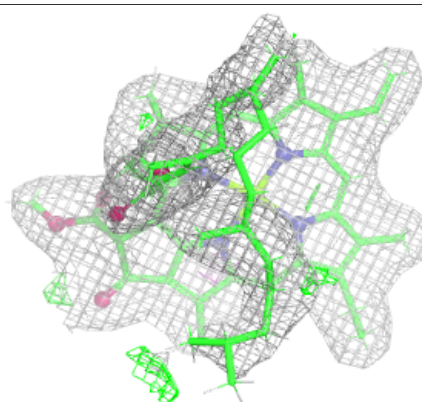
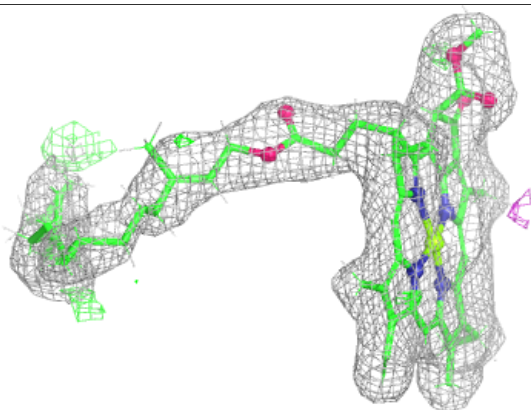
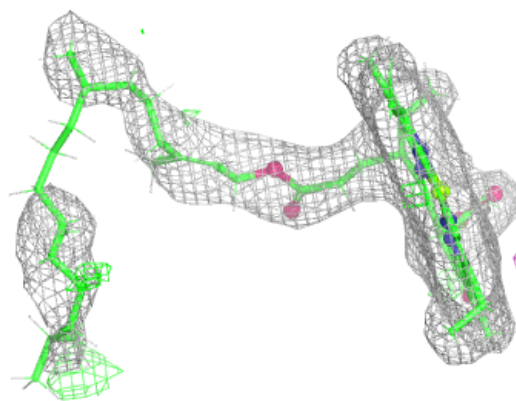


Electron density around PL9 d 406:

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

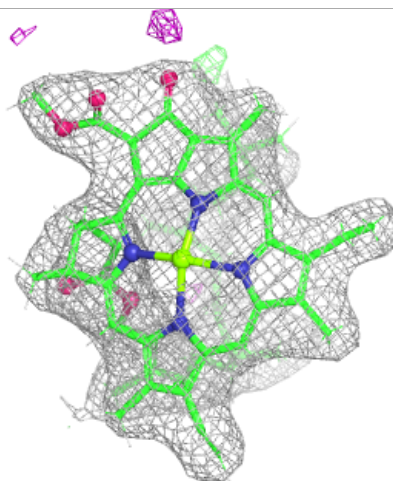
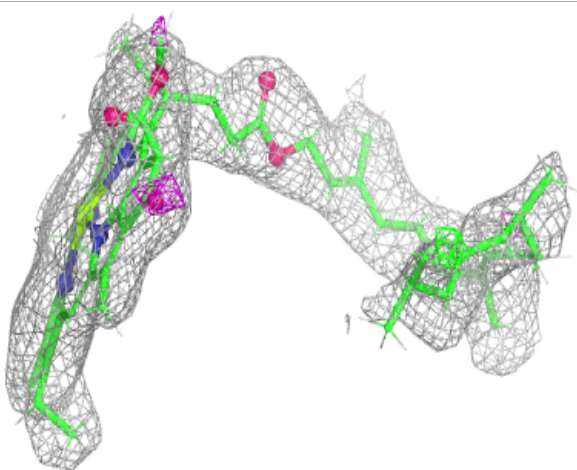
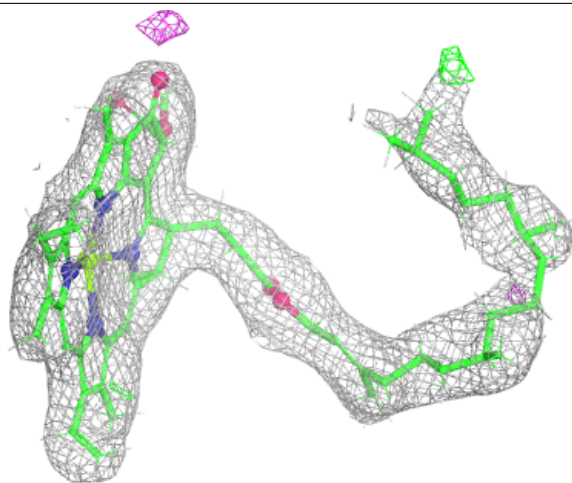
**Electron density around CLA a 408:**

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



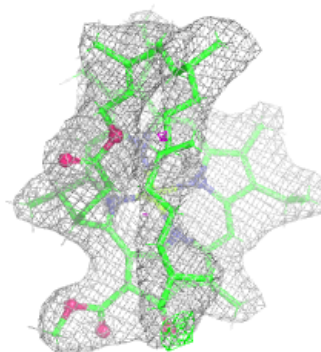
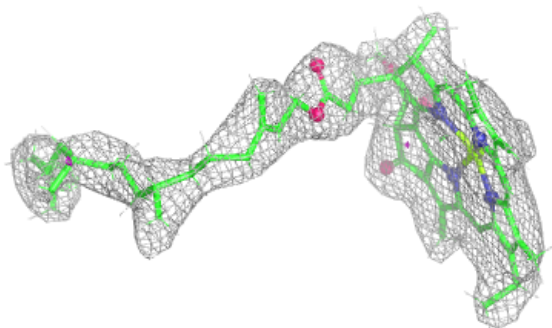
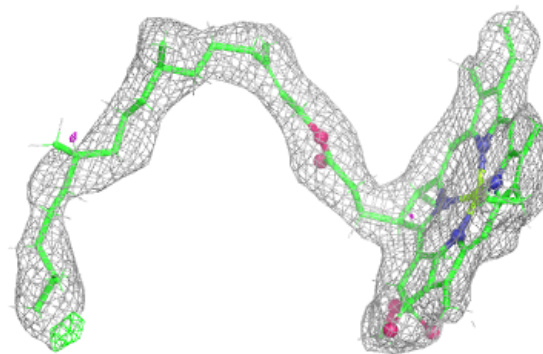
Electron density around CLA B 606:

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

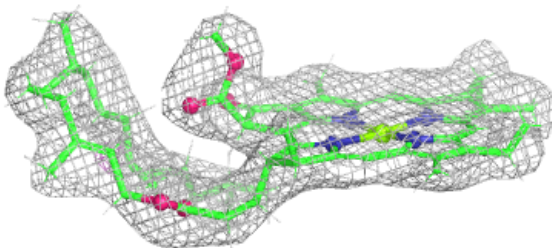
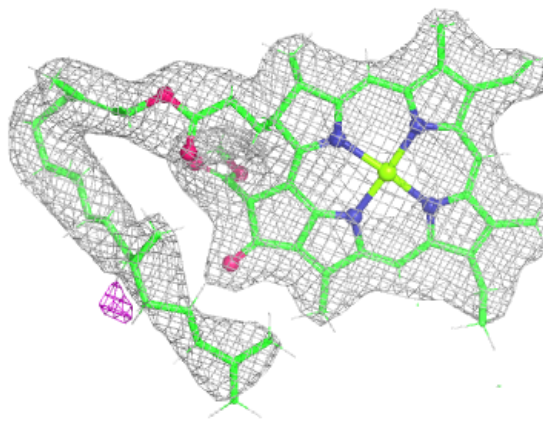


Electron density around CLA b 607:

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

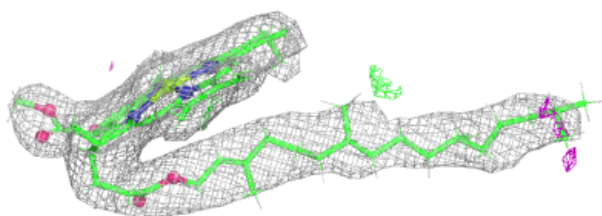
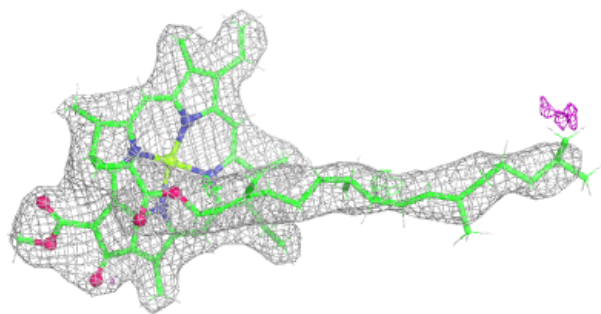
**Electron density around CLA b 611:**

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

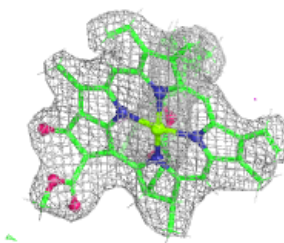
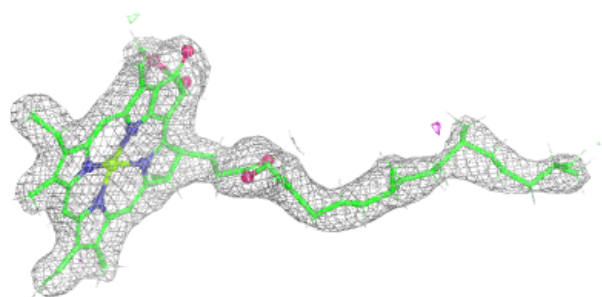
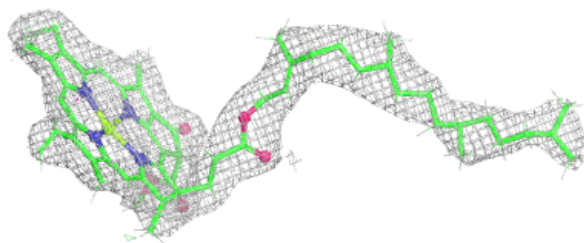


Electron density around CLA b 615:

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

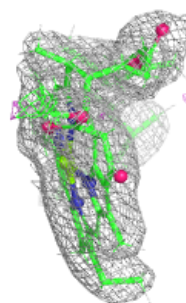
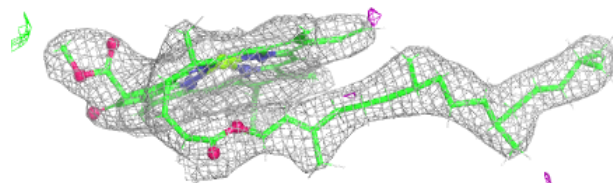
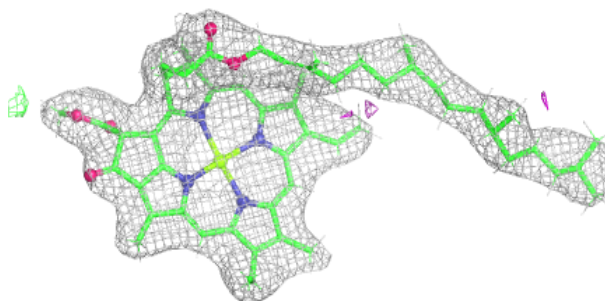
**Electron density around CLA C 503:**

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

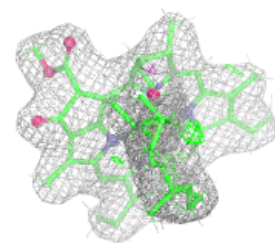
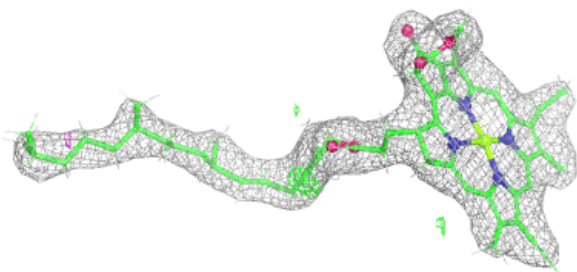
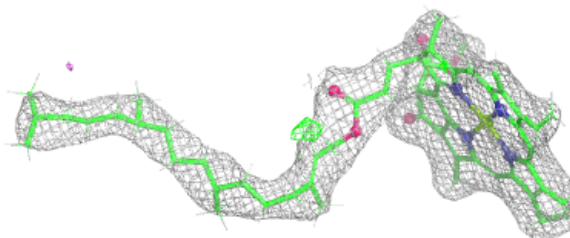


Electron density around CLA c 501:

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

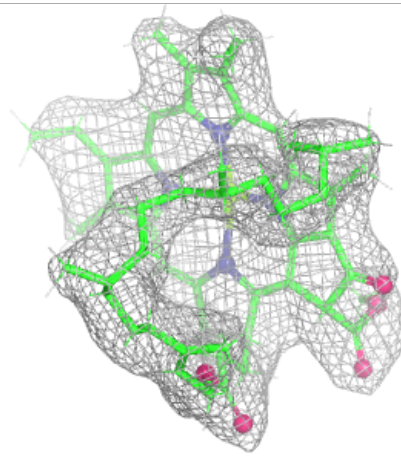
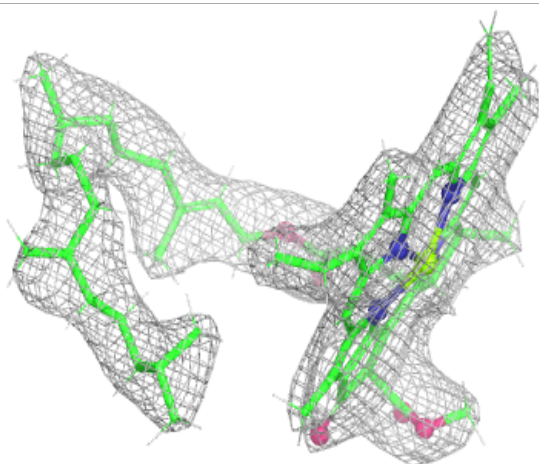
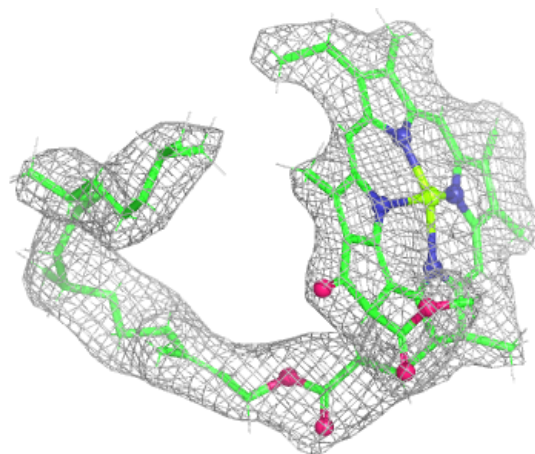
**Electron density around CLA c 502:**

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



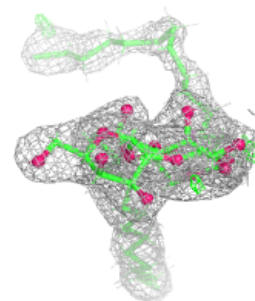
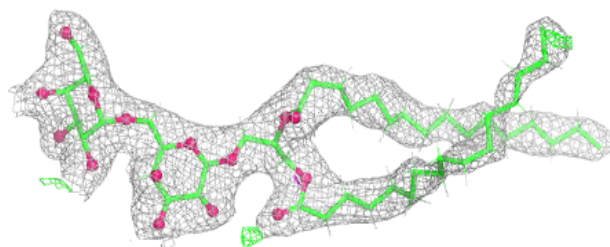
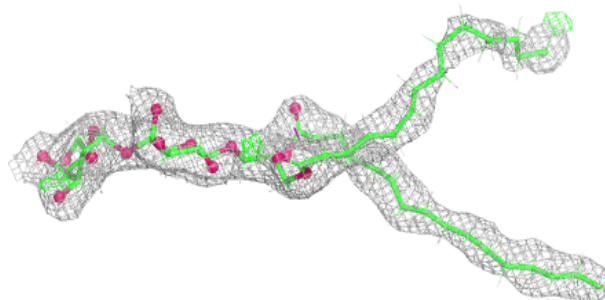
Electron density around CLA C 504:

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

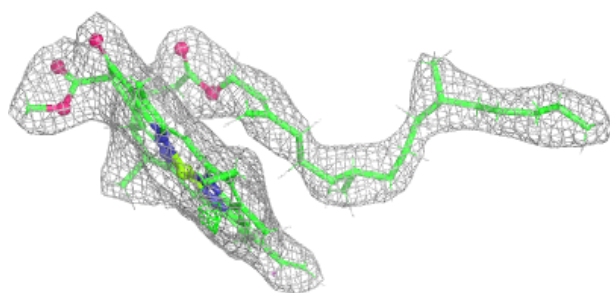
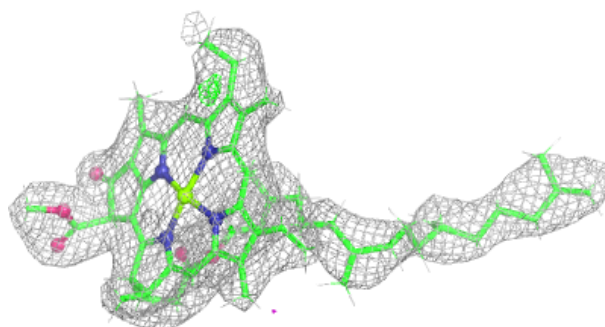


Electron density around DGD C 516:

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

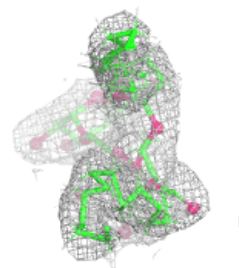
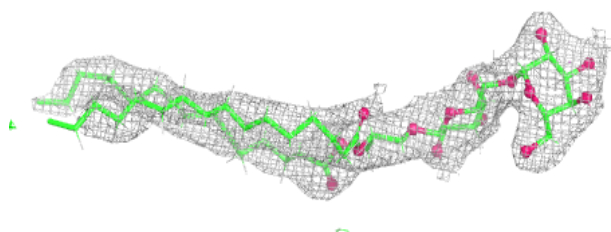
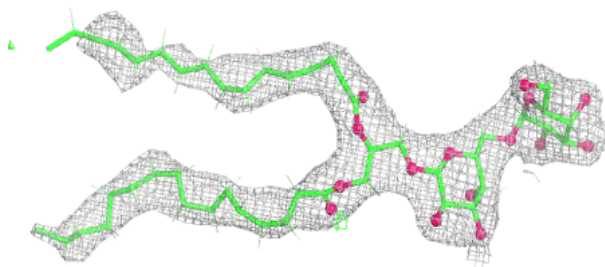
**Electron density around CLA C 506:**

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

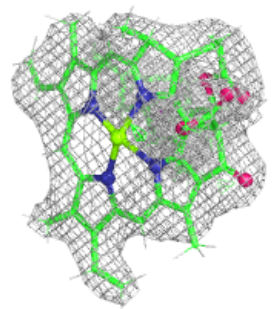
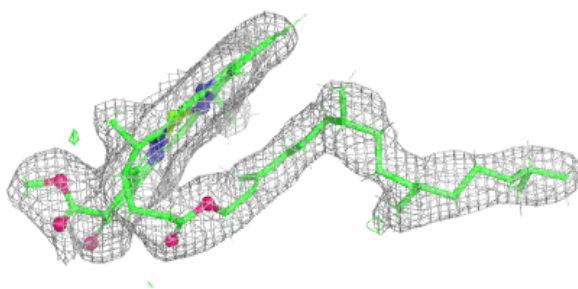
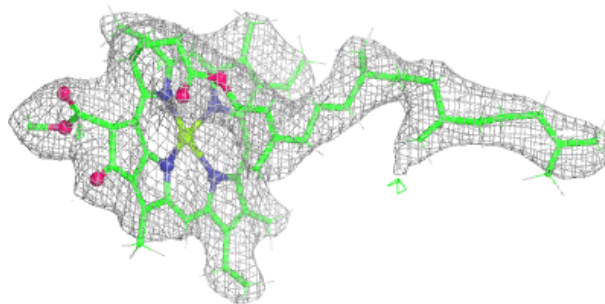


Electron density around DGD C 518:

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

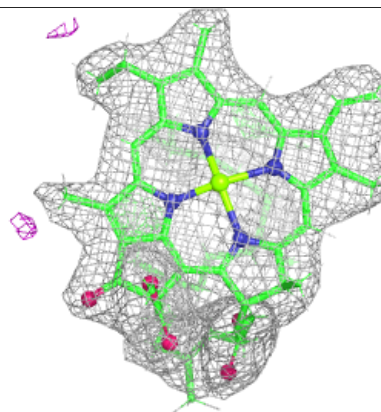
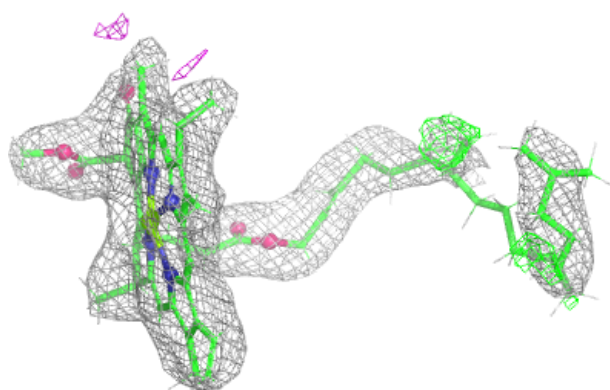
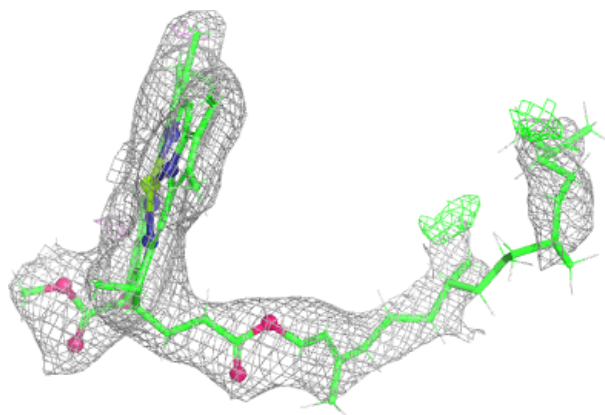
**Electron density around CLA c 505:**

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

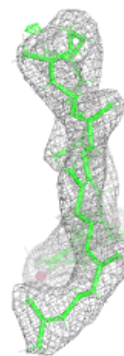
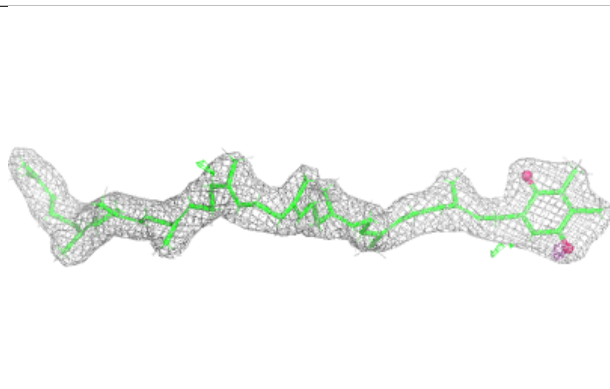
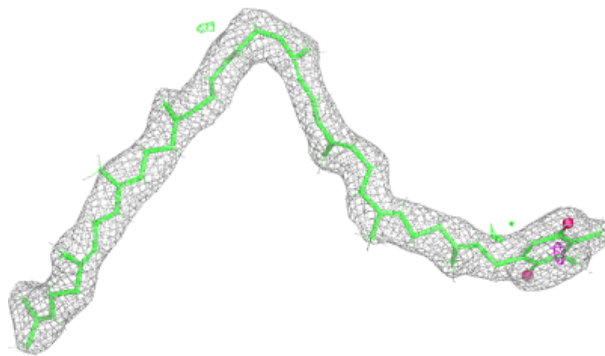


Electron density around CLA C 507:

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

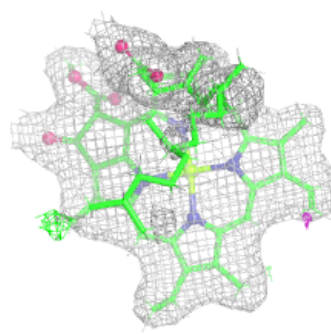
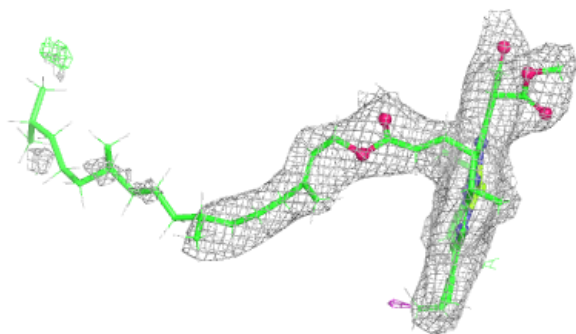
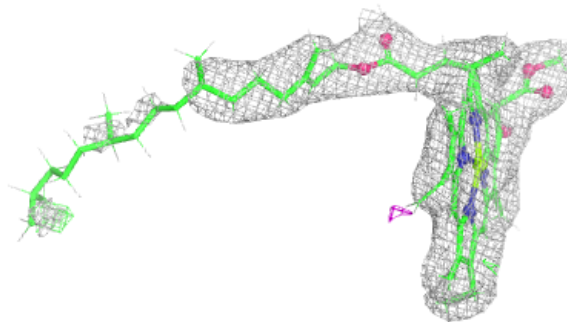
**Electron density around PL9 D 406:**

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

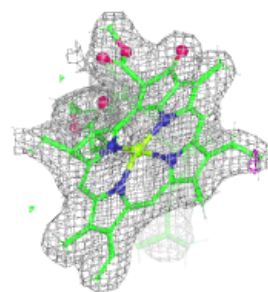
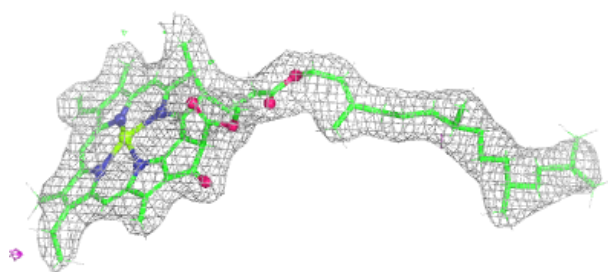
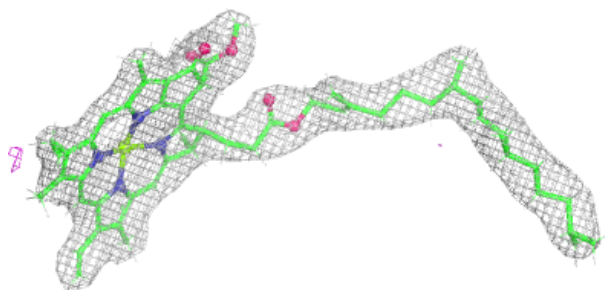


Electron density around CLA D 404:

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

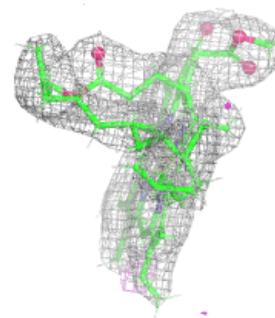
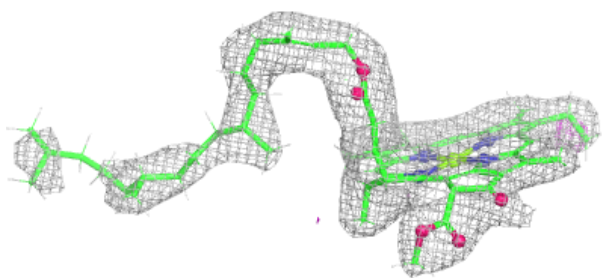
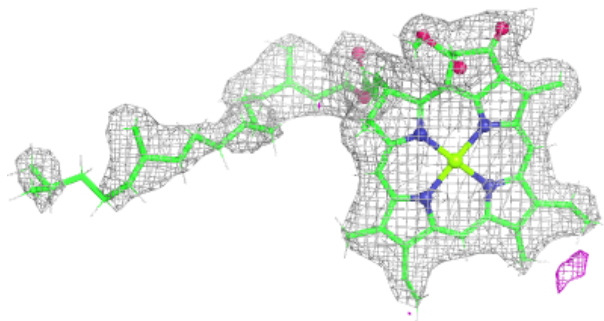
**Electron density around CLA a 405:**

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

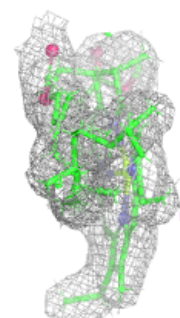
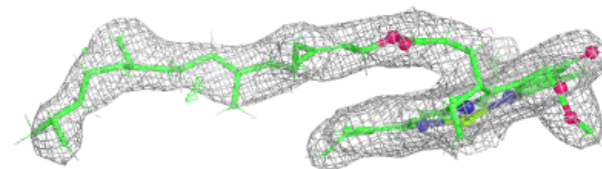
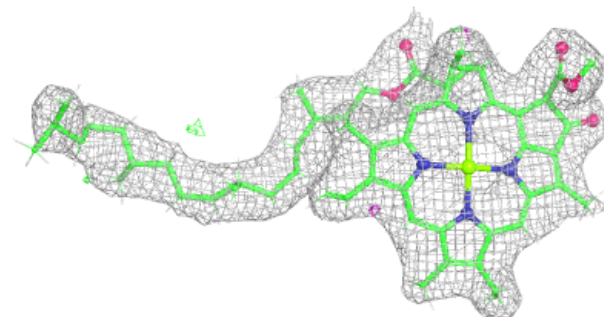


Electron density around CLA a 406:

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

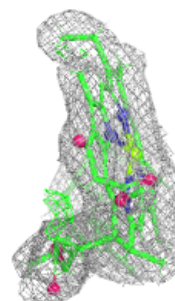
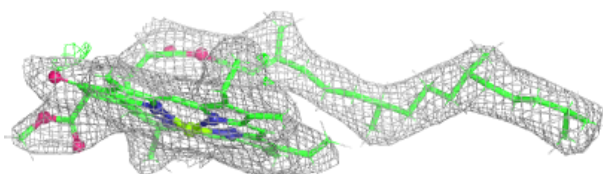
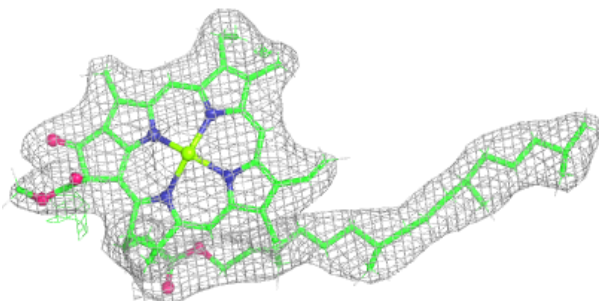
**Electron density around CLA B 603:**

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

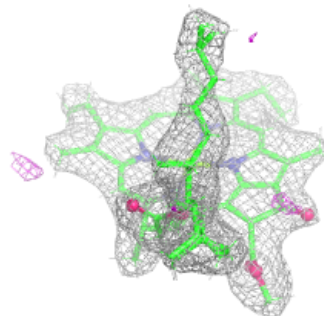
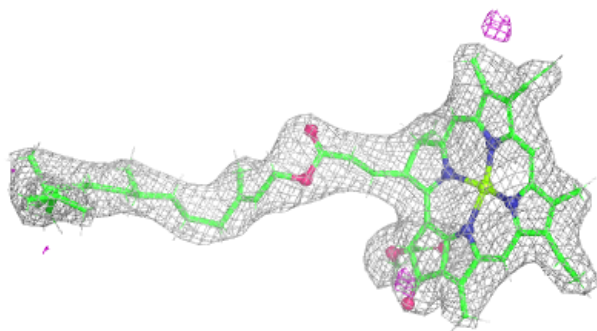
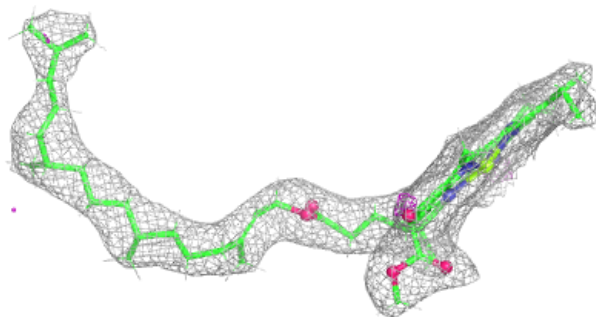


Electron density around CLA C 502:

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

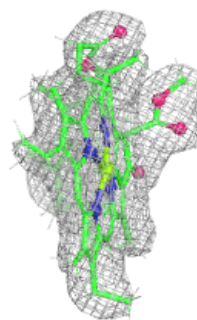
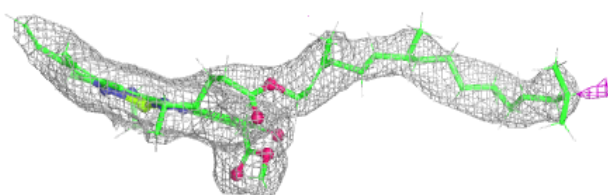
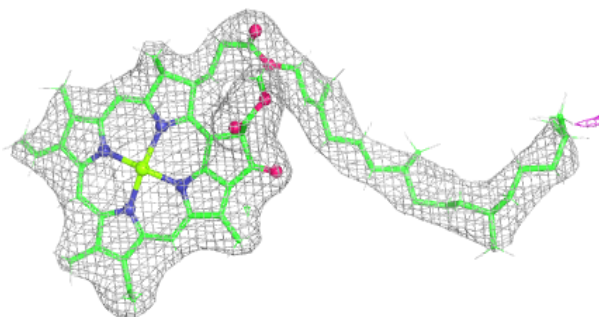
**Electron density around CLA d 403:**

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

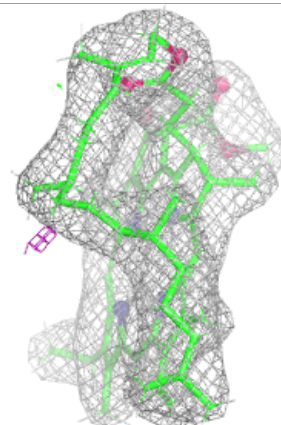
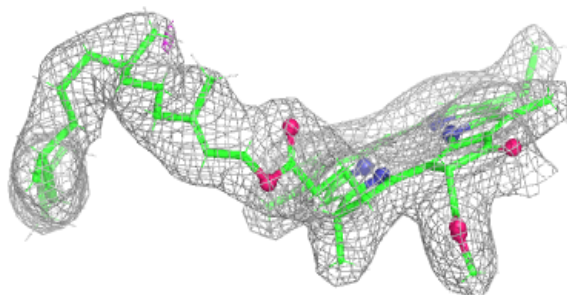
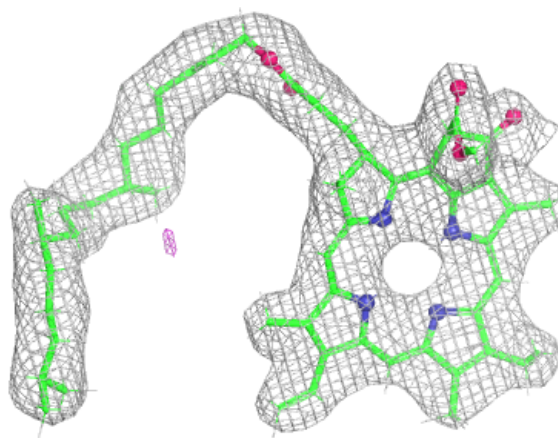


Electron density around CLA b 603:

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

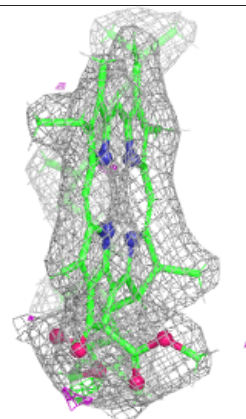
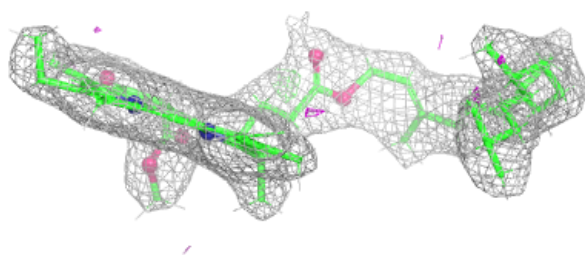
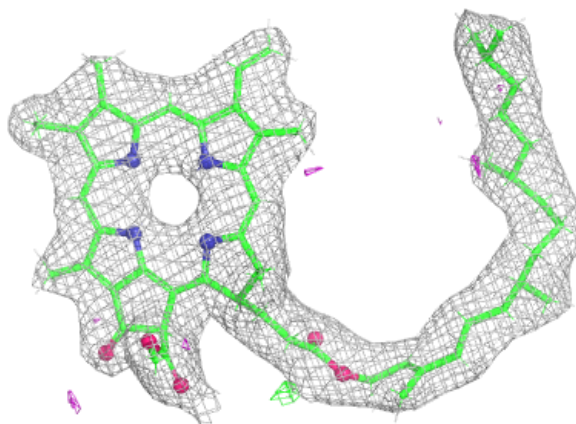
**Electron density around PHO D 401:**

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



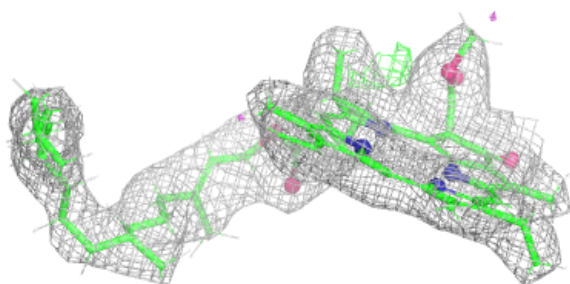
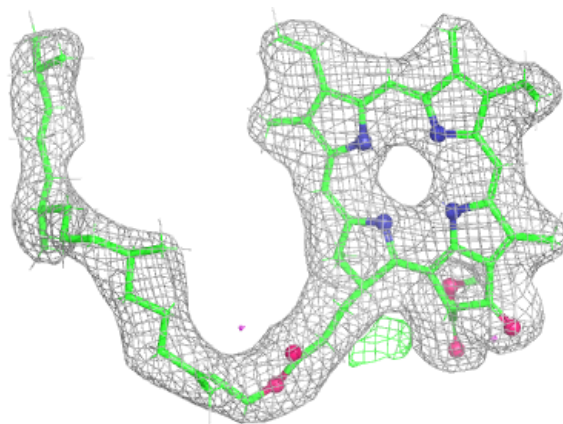
Electron density around PHO a 407:

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

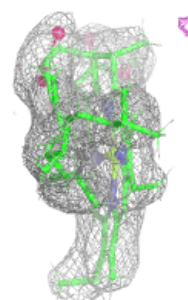
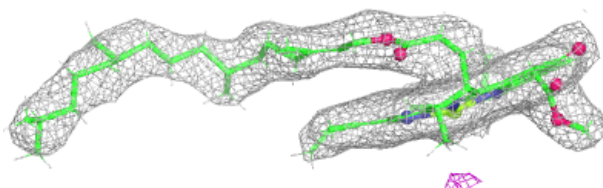
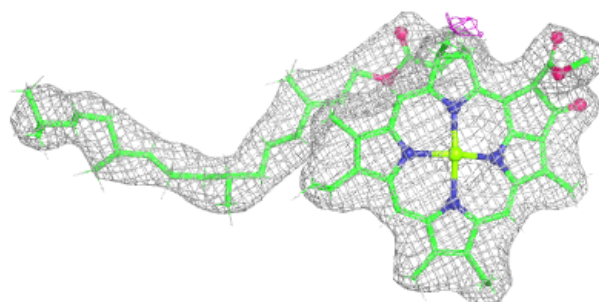


Electron density around PHO d 401:

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

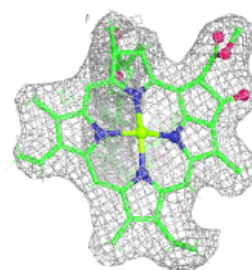
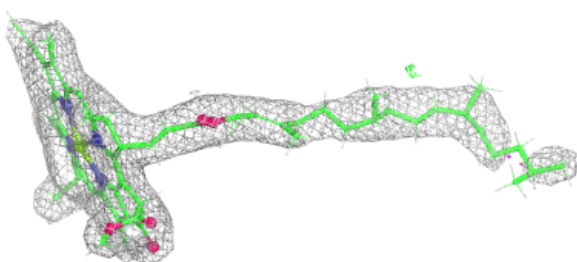
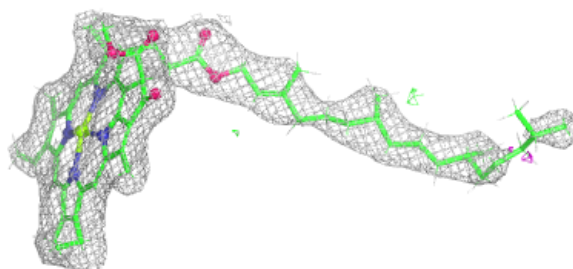
**Electron density around CLA b 604:**

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

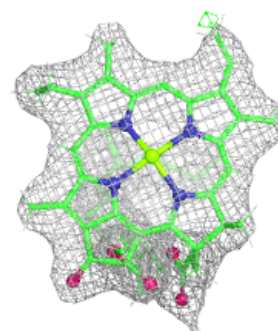
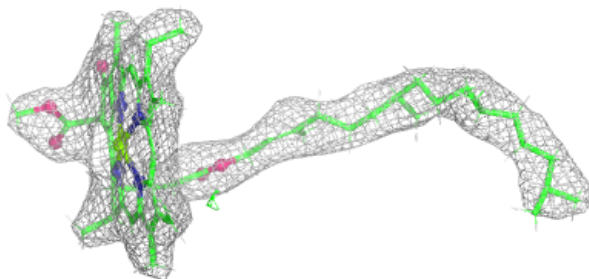
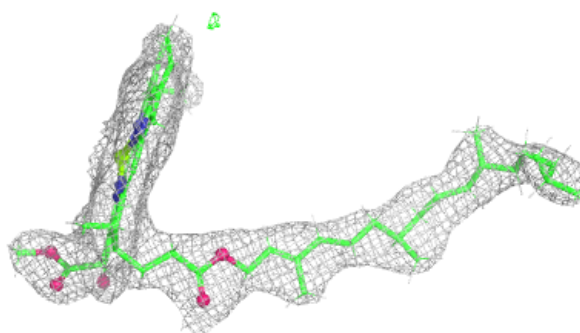


Electron density around CLA b 605:

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

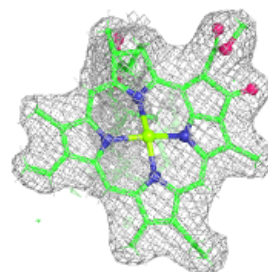
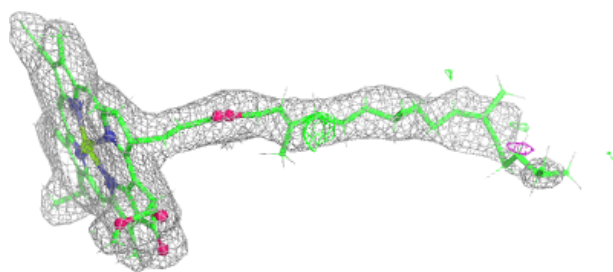
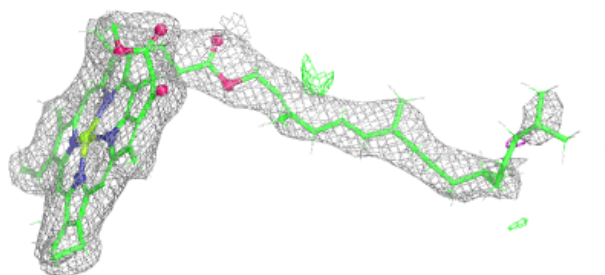
**Electron density around CLA b 606:**

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

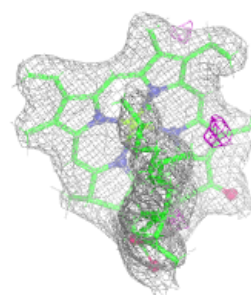
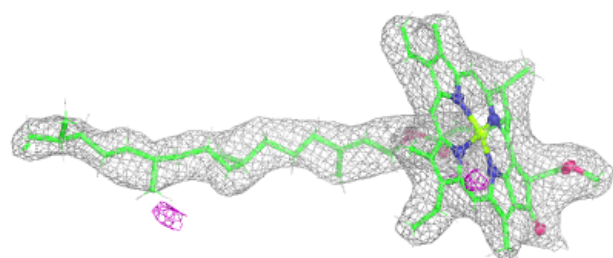
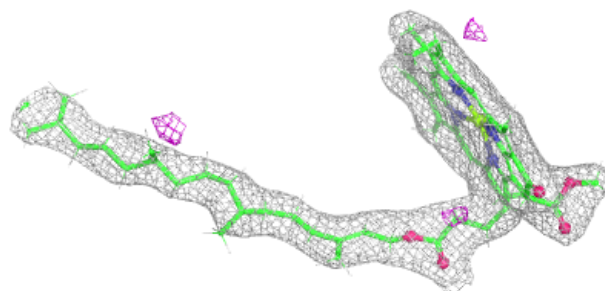


Electron density around CLA B 604:

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

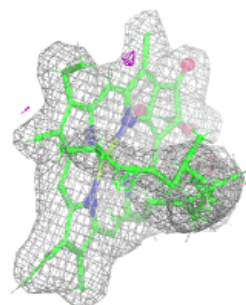
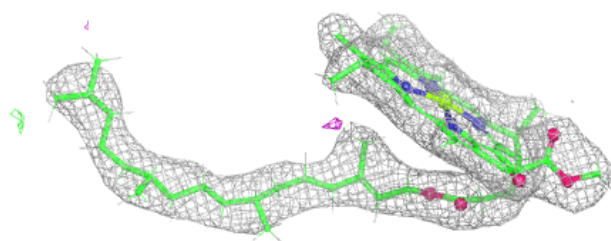
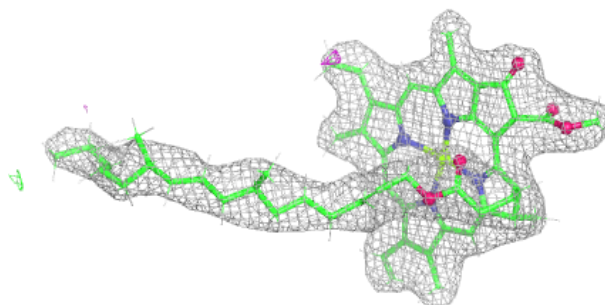
**Electron density around CLA b 608:**

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

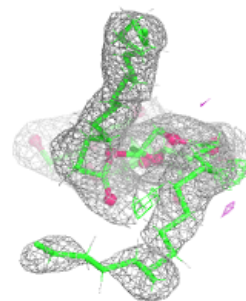
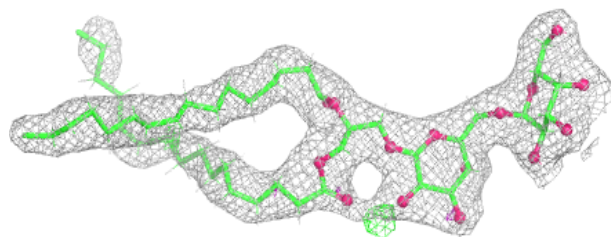
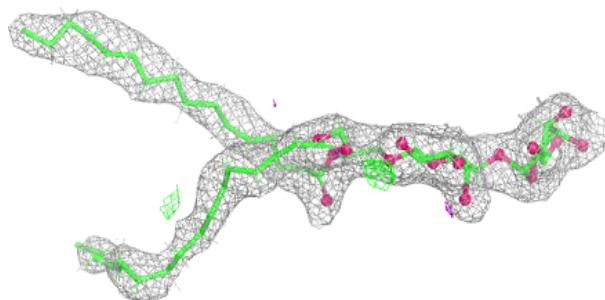


Electron density around CLA b 609:

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

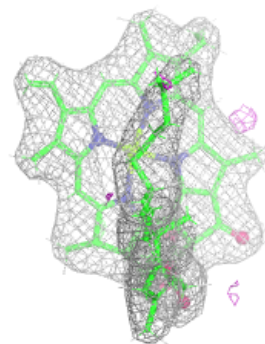
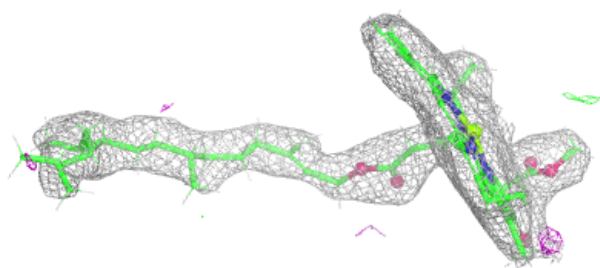
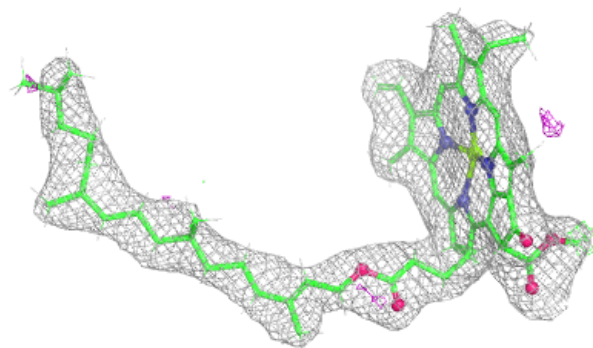
**Electron density around DGD c 516:**

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

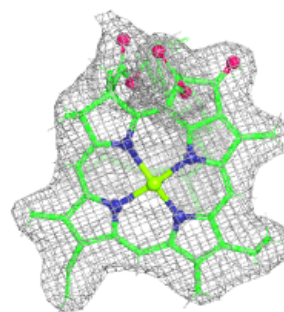
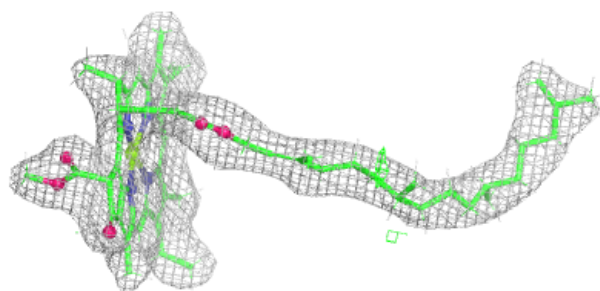
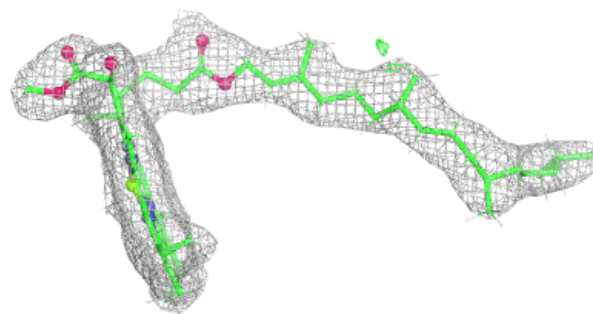


Electron density around CLA b 610:

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

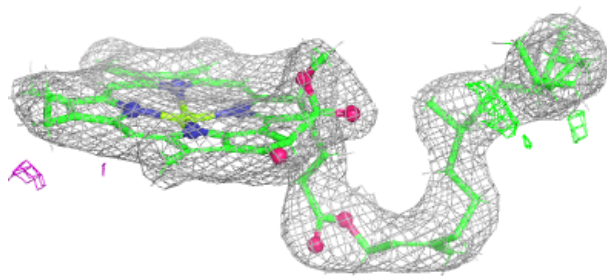
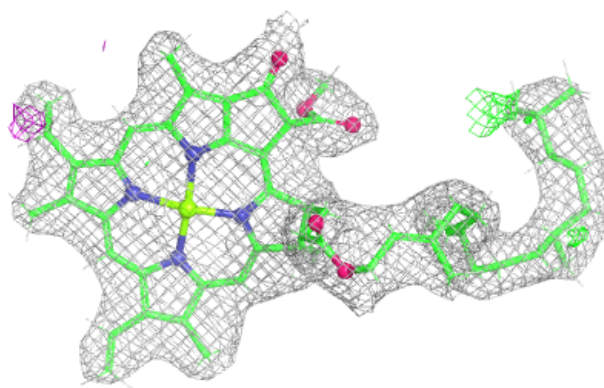
**Electron density around CLA B 605:**

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



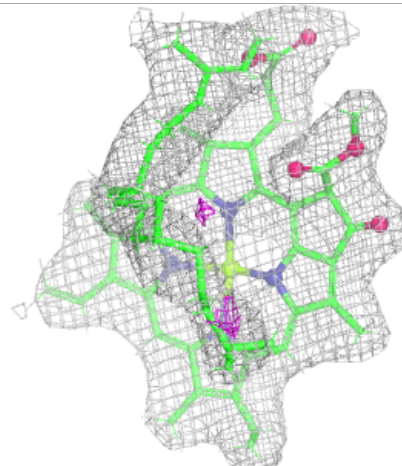
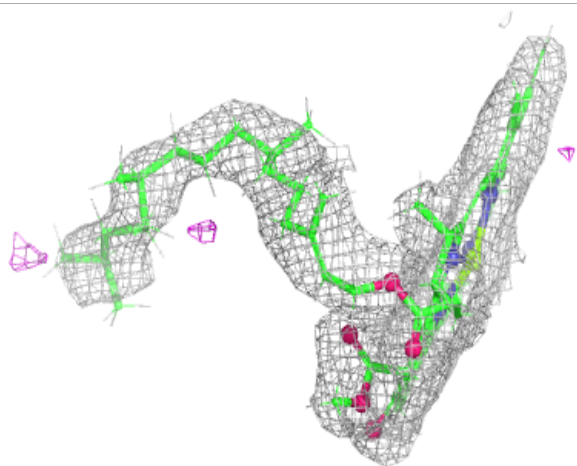
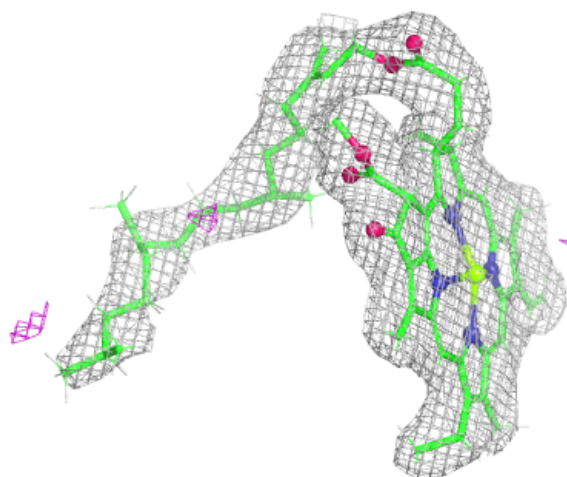
Electron density around CLA b 613:

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



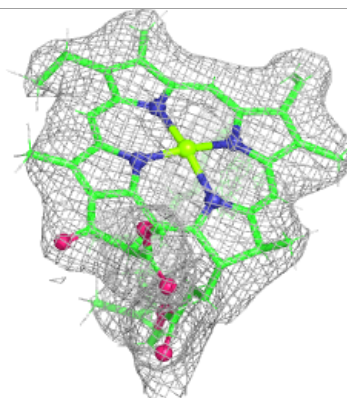
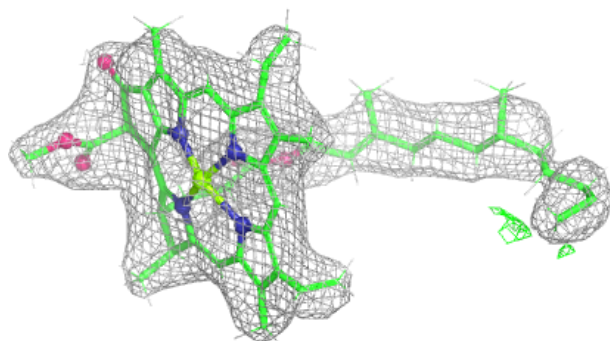
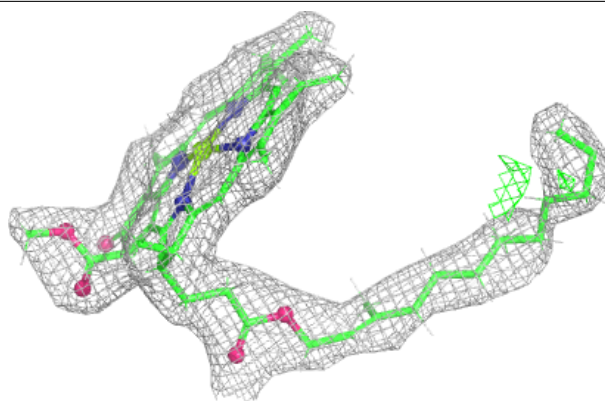
Electron density around CLA b 614:

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

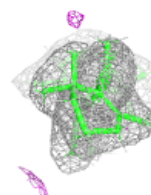
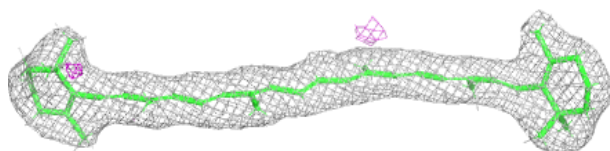
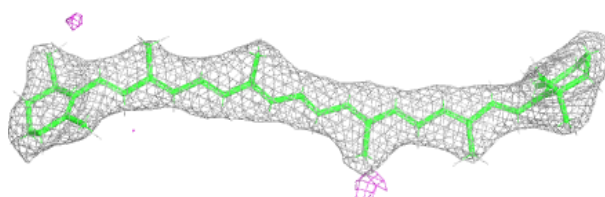


Electron density around CLA C 505:

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

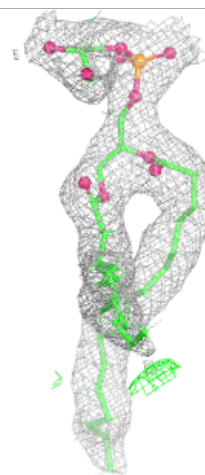
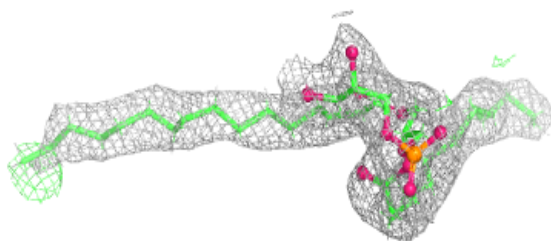
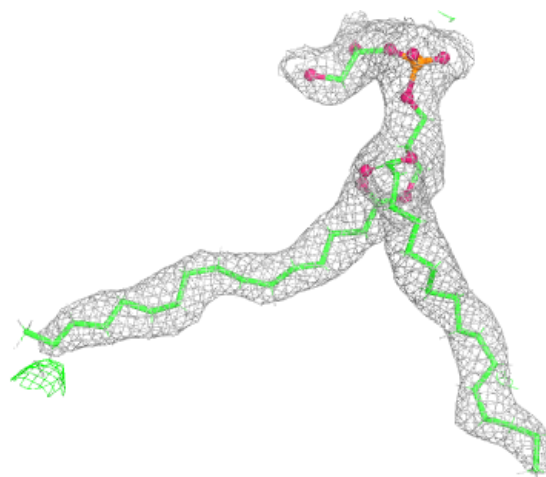
**Electron density around BCR a 409:**

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



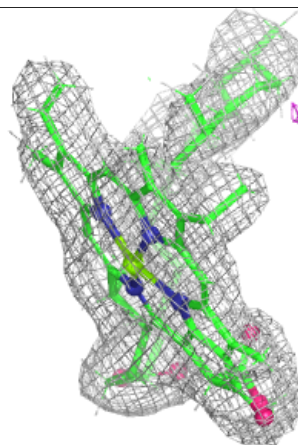
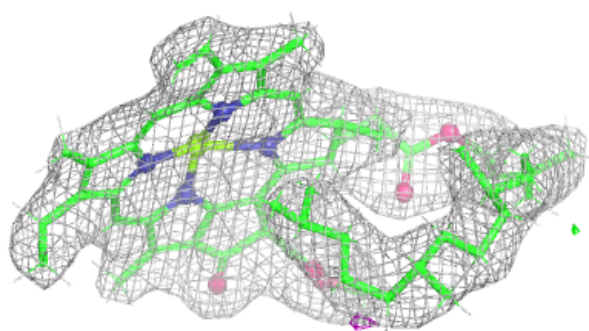
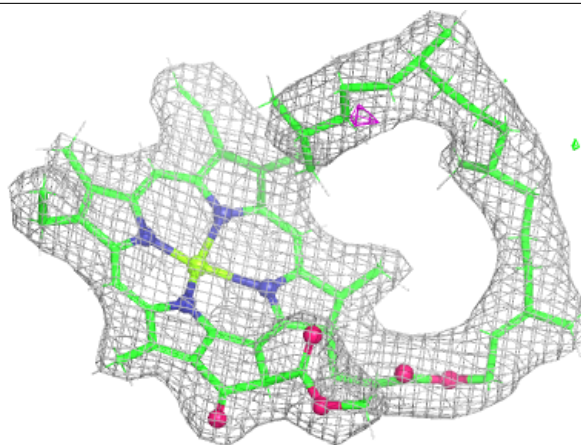
Electron density around LHG L 101:

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

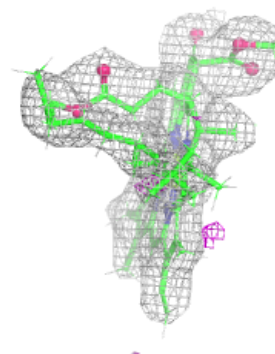
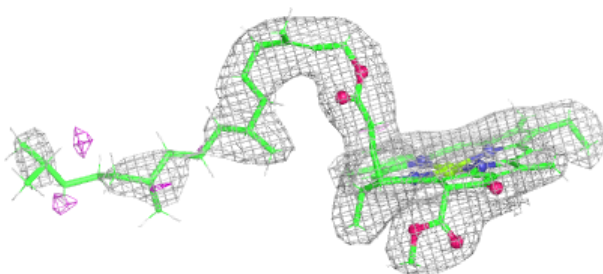
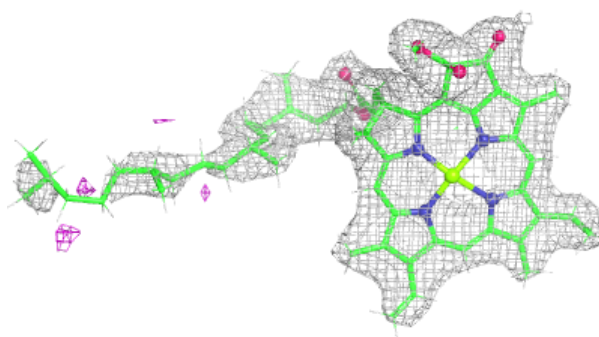


Electron density around CLA b 616:

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

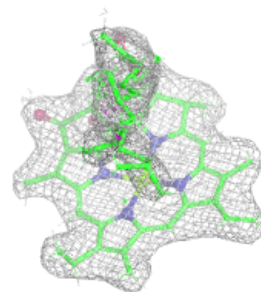
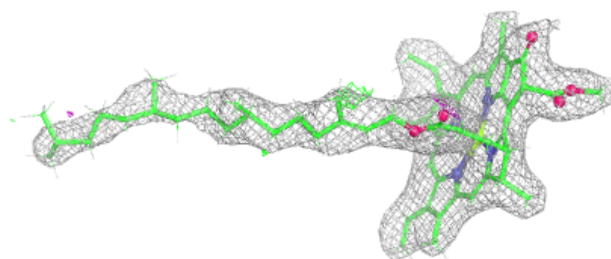
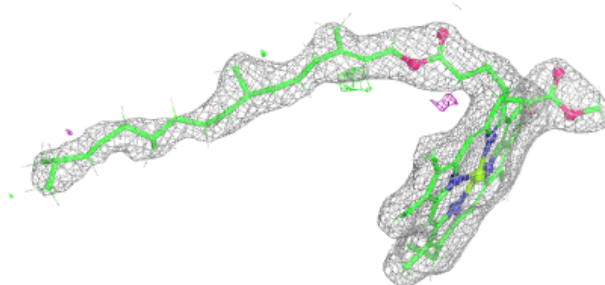
**Electron density around CLA A 405:**

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



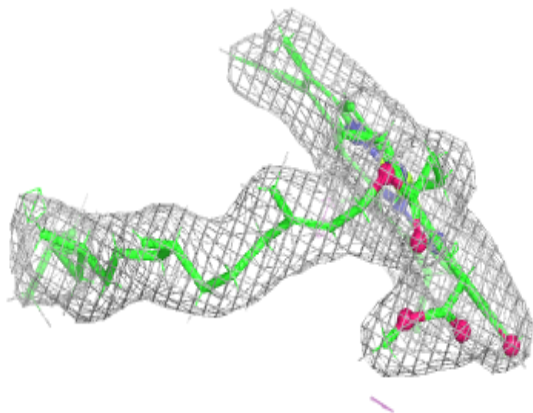
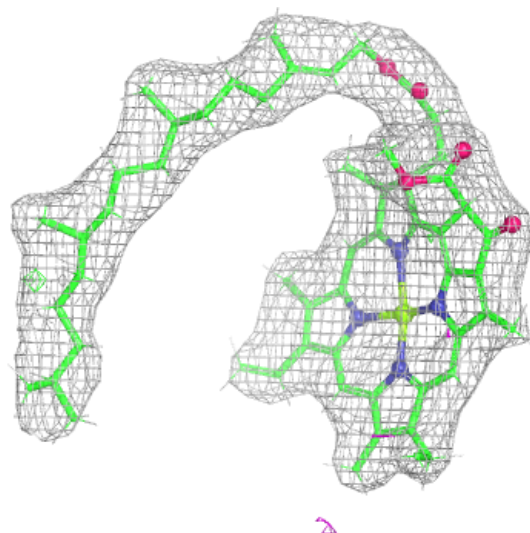
Electron density around CLA B 607:

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



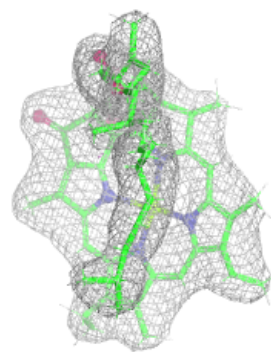
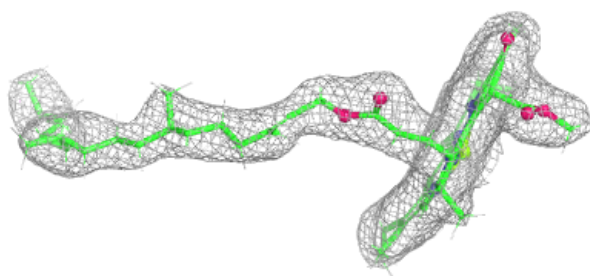
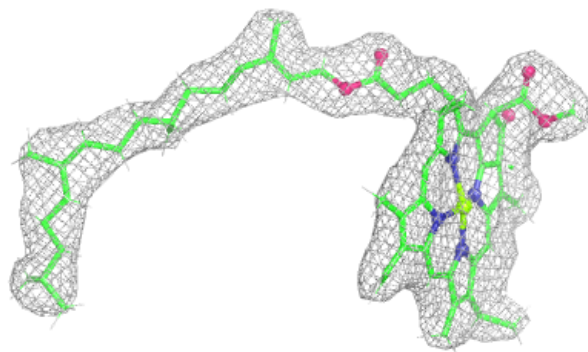
Electron density around CLA C 508:

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



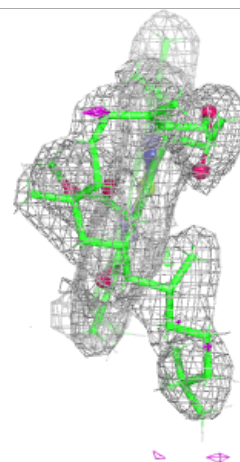
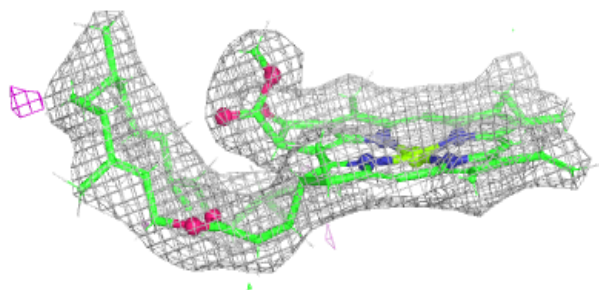
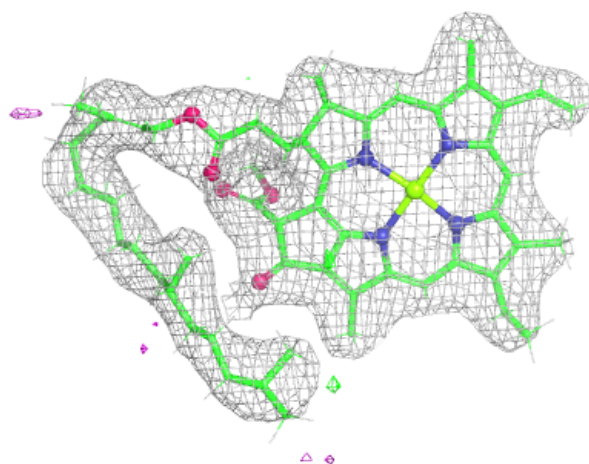
Electron density around CLA B 609:

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



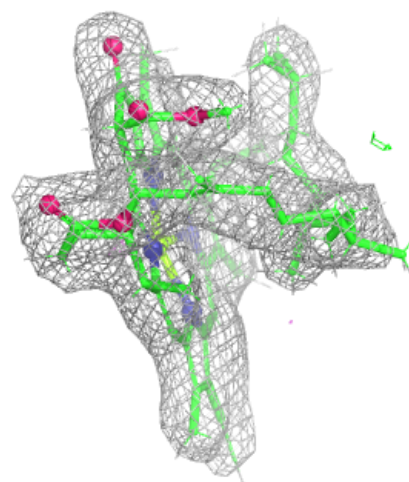
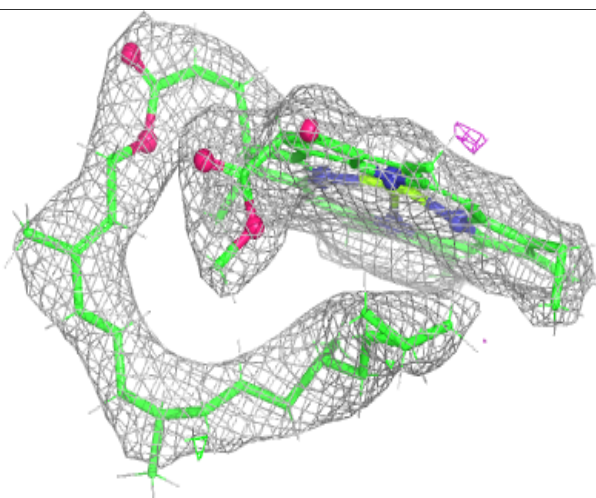
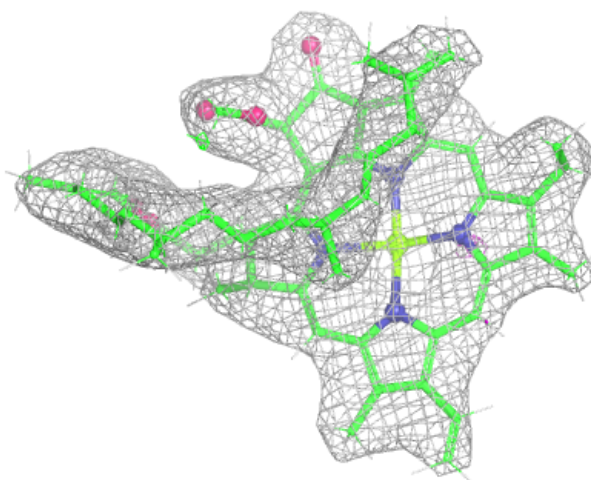
Electron density around CLA B 610:

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



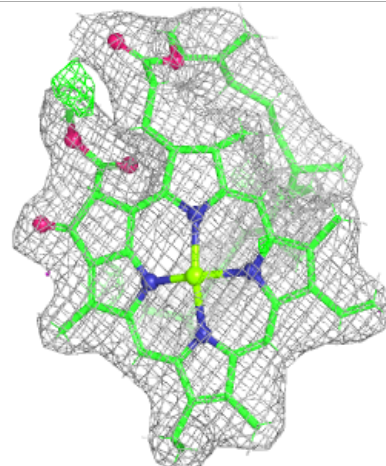
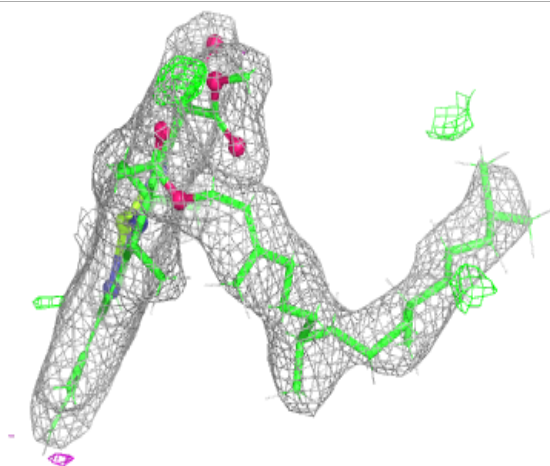
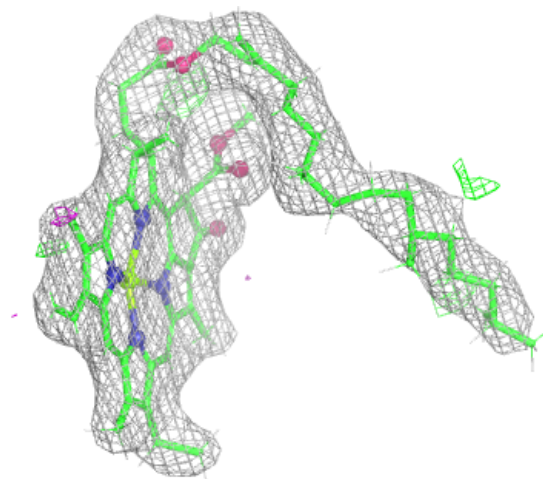
Electron density around CLA C 511:

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



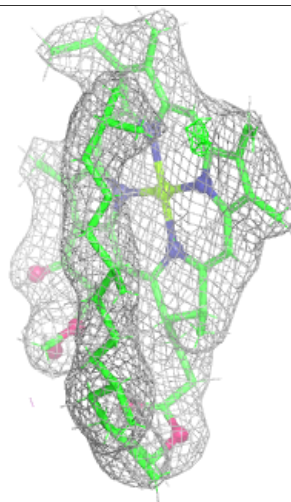
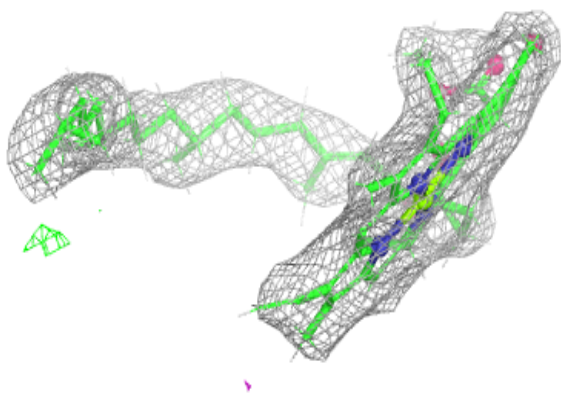
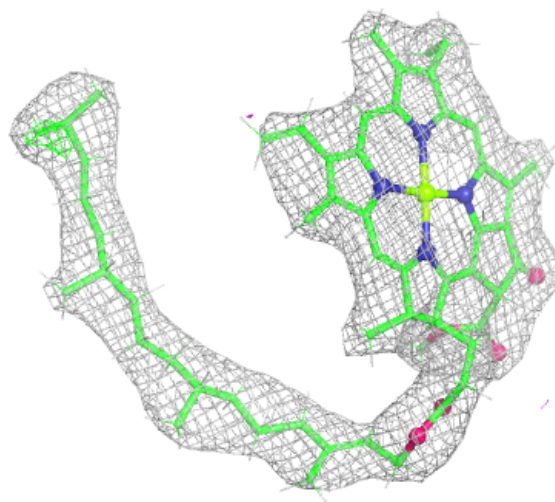
Electron density around CLA B 613:

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



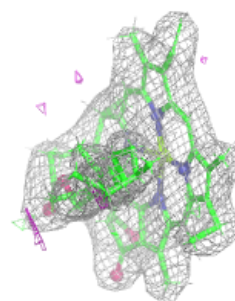
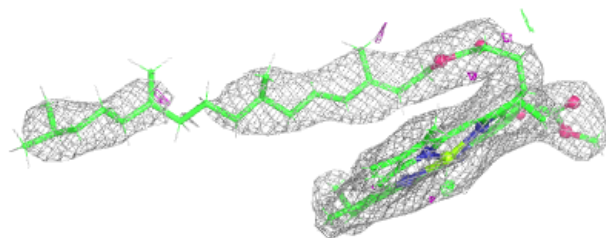
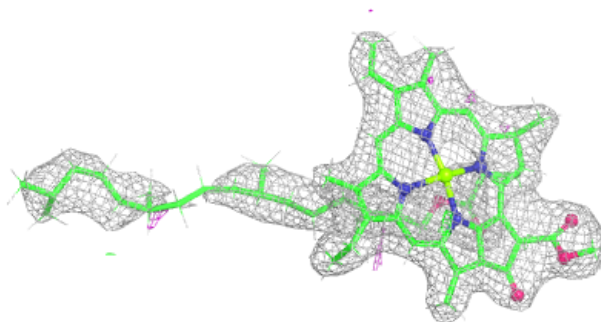
Electron density around CLA c 507:

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

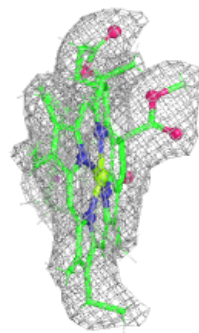
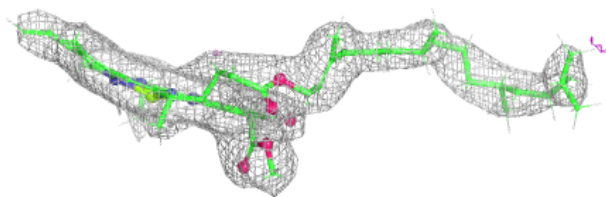
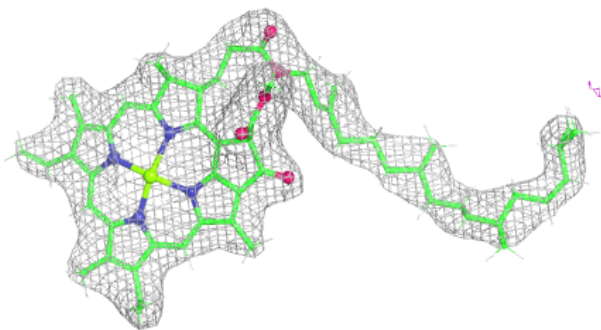


Electron density around CLA B 614:

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

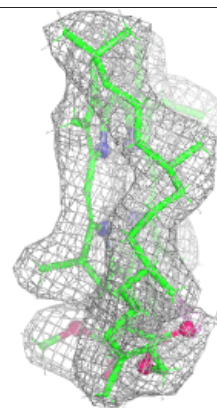
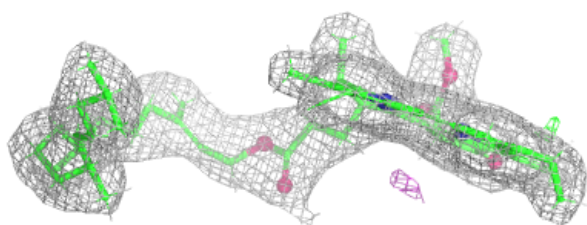
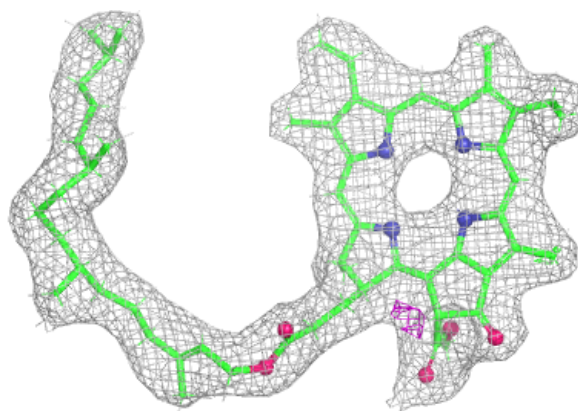
**Electron density around CLA B 602:**

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

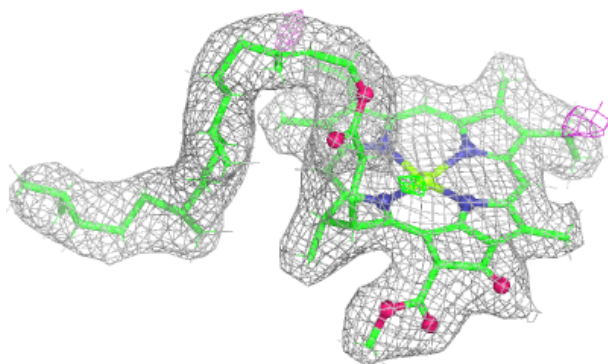
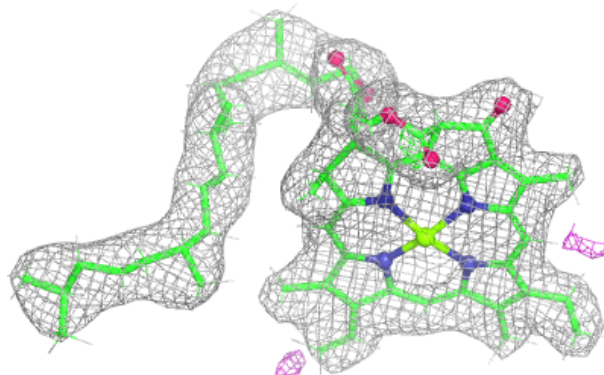


Electron density around PHO A 406:

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

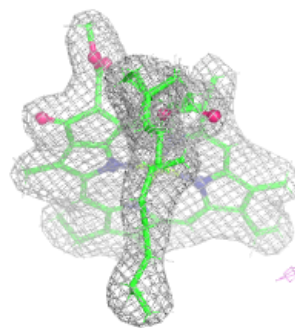
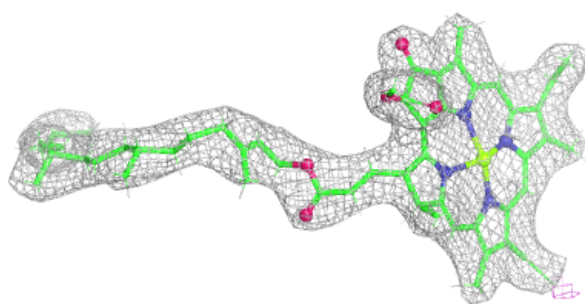
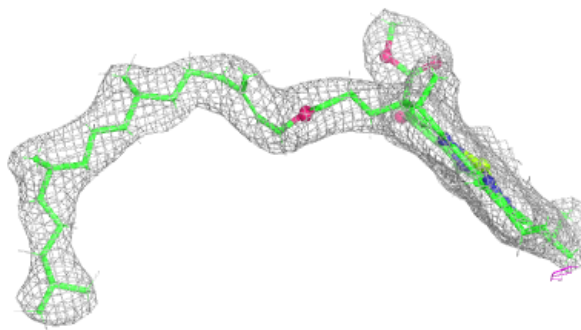
**Electron density around CLA D 402:**

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



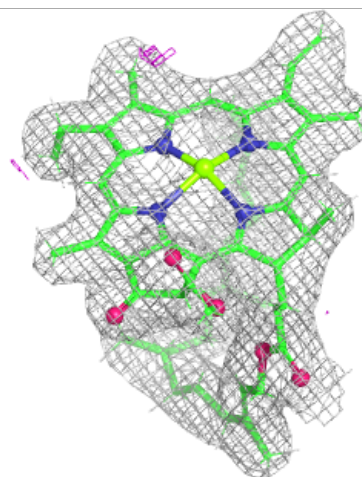
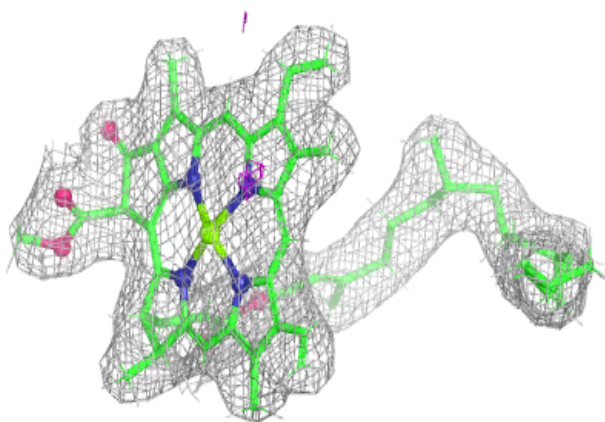
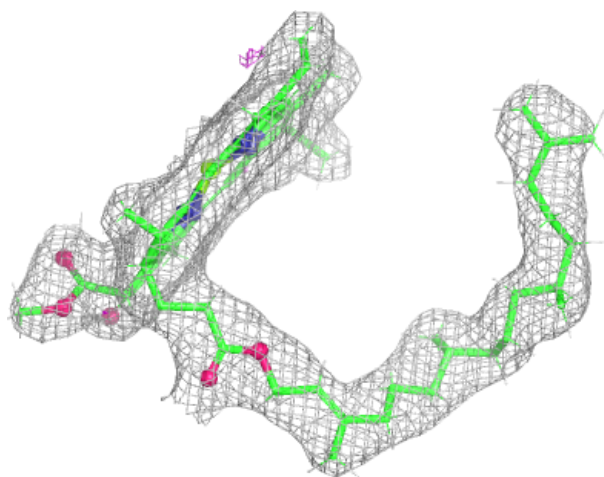
Electron density around CLA D 403:

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



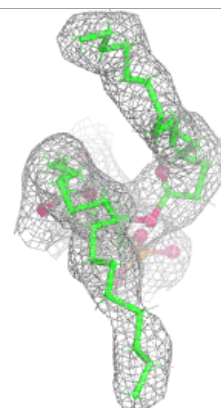
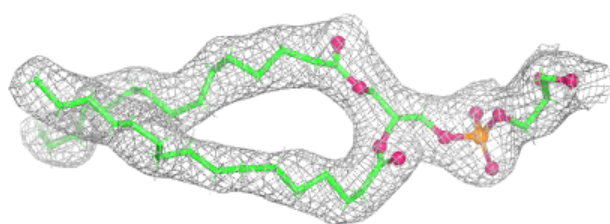
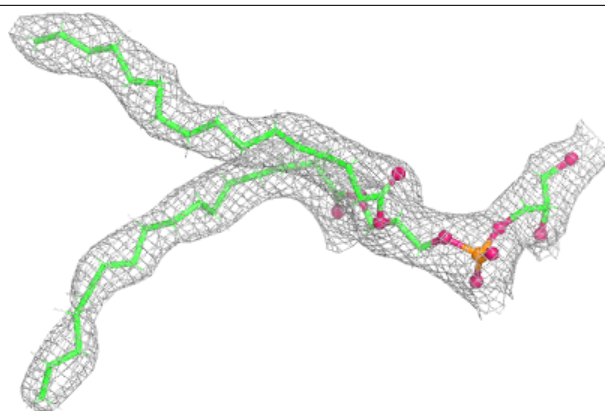
Electron density around CLA b 612:

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

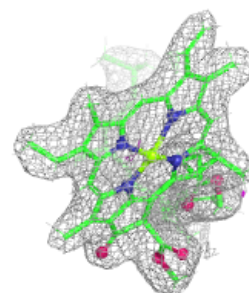
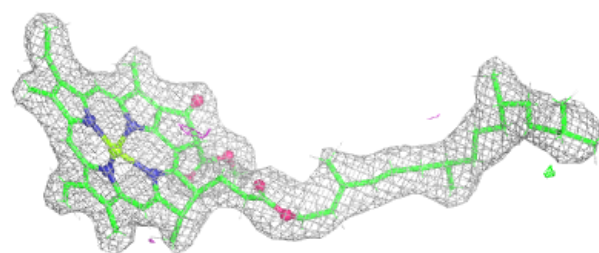
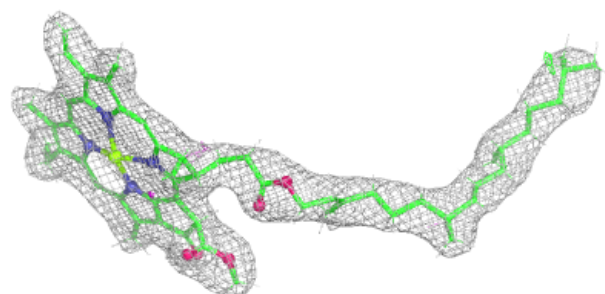


Electron density around LHG D 408:

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

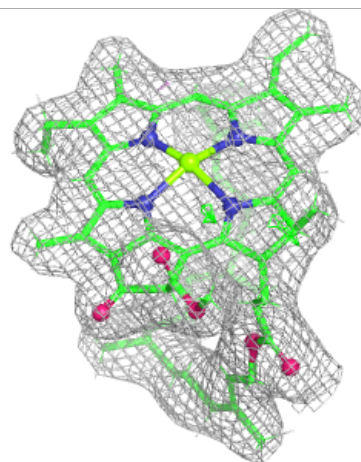
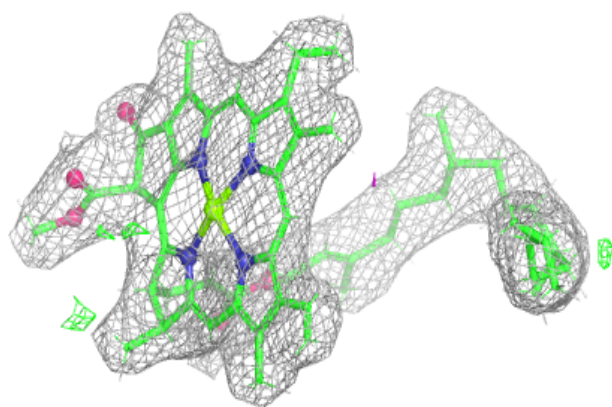
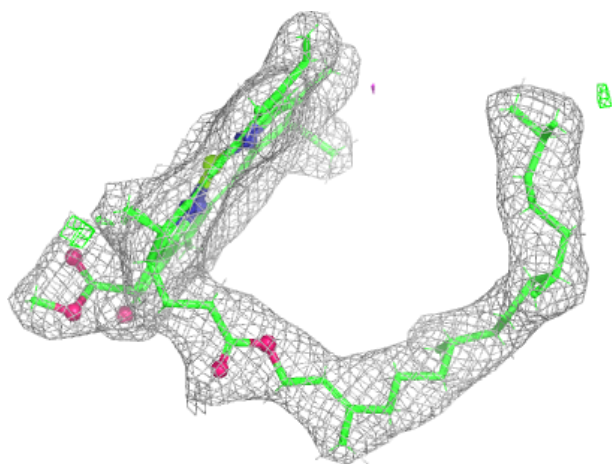
**Electron density around CLA A 404:**

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



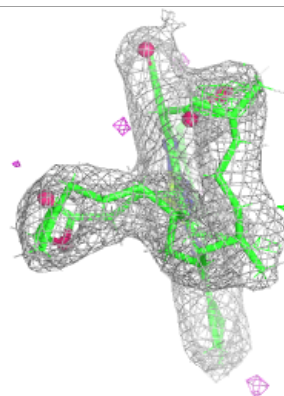
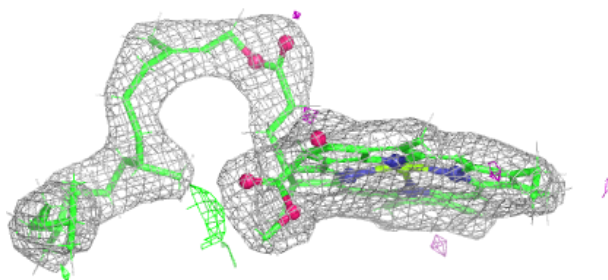
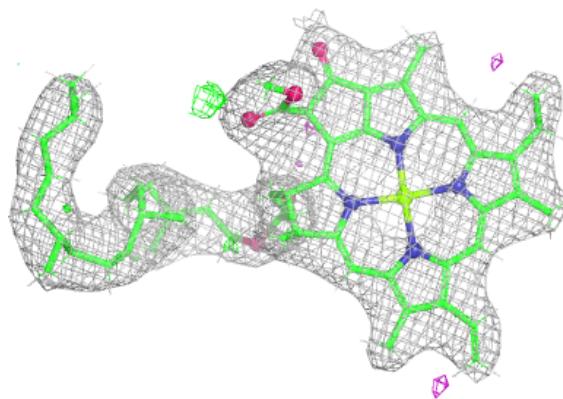
Electron density around CLA B 611:

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

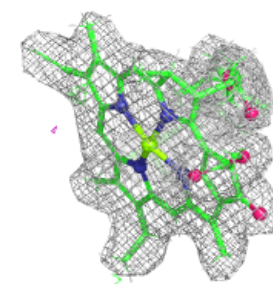
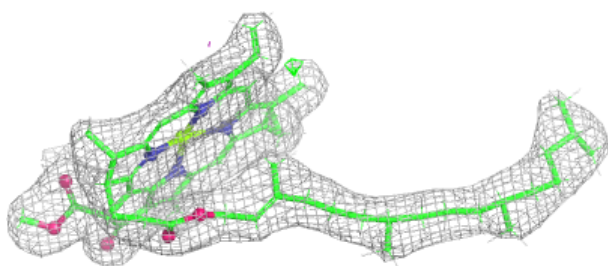
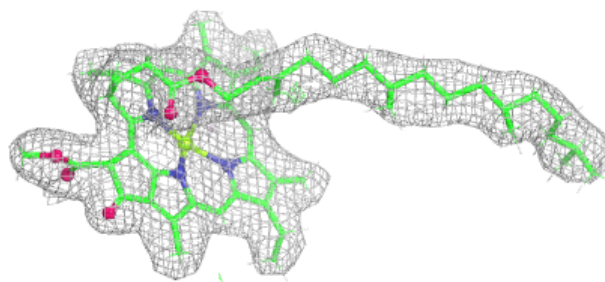


Electron density around CLA B 612:

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

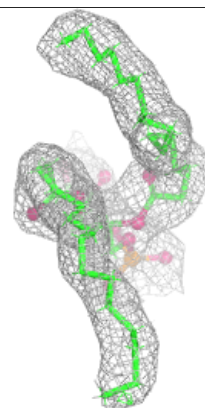
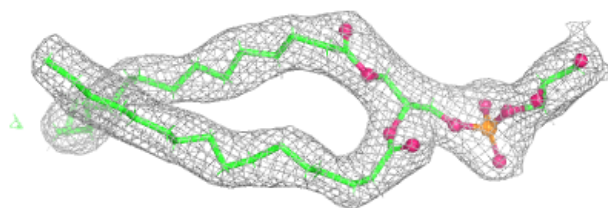
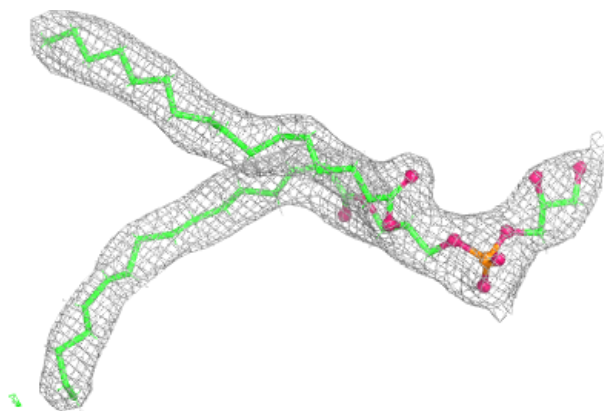
**Electron density around CLA B 608:**

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

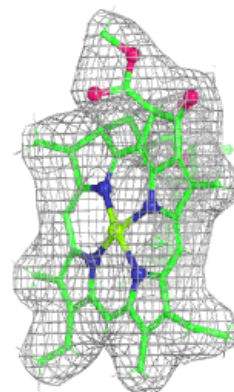
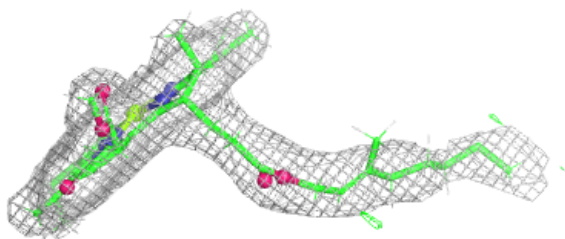
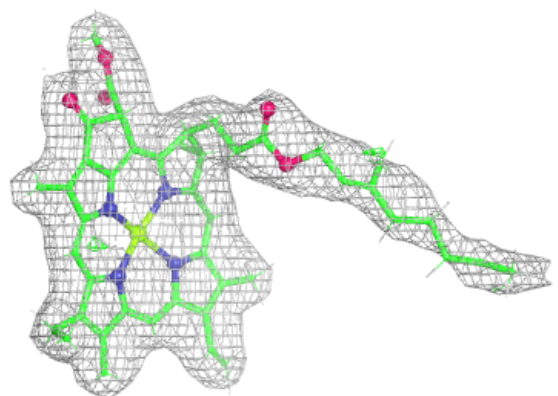


Electron density around LHG d 408:

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

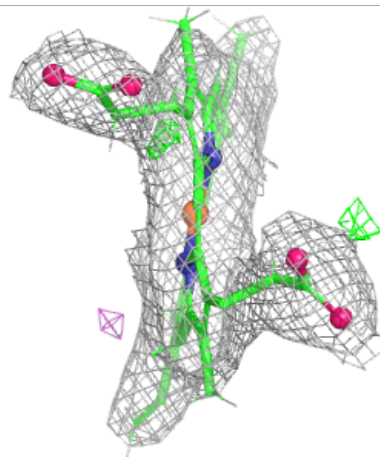
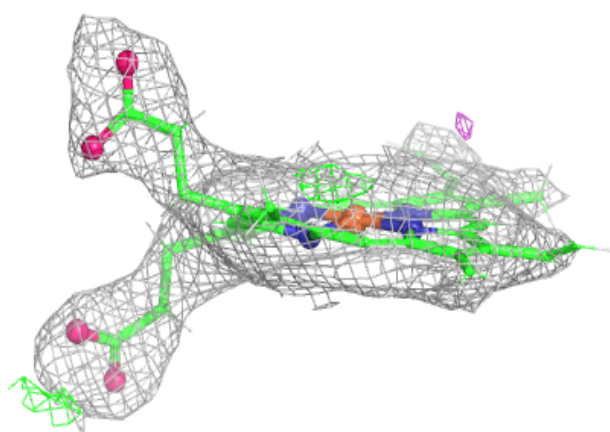
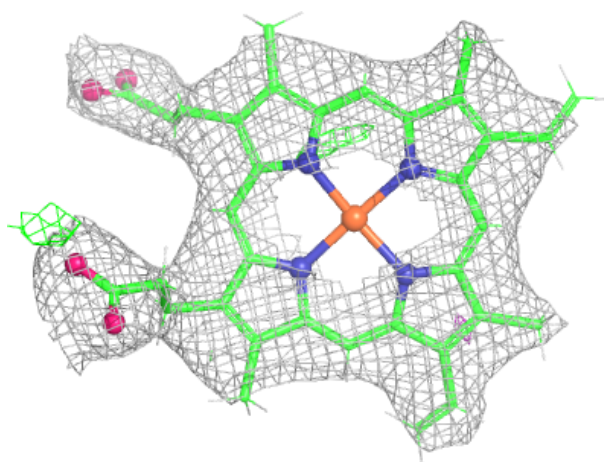
**Electron density around CLA A 407:**

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



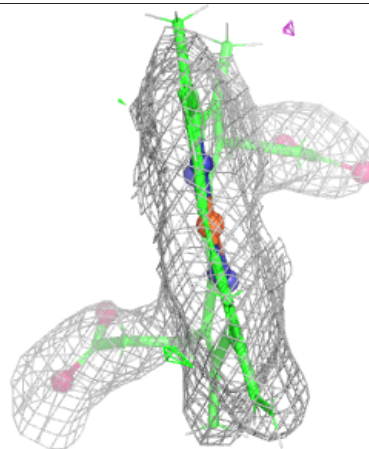
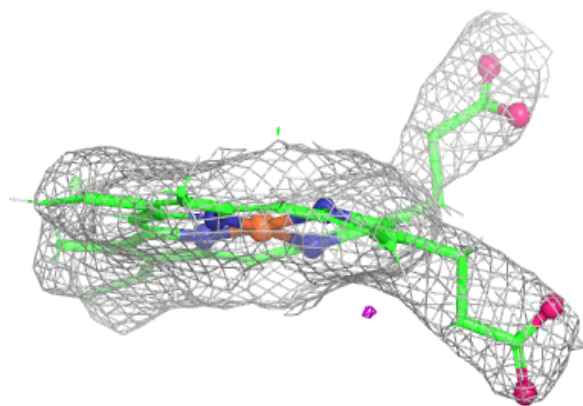
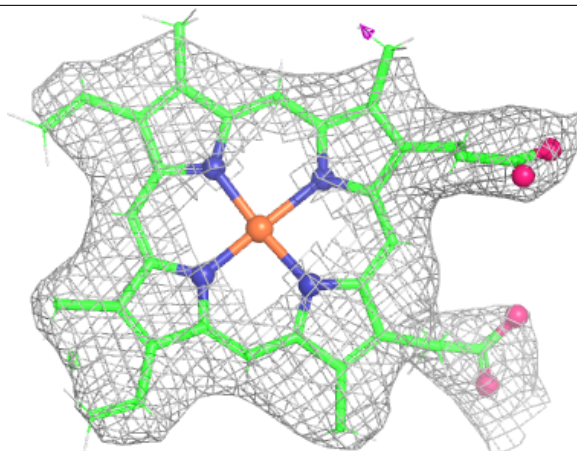
Electron density around HEM E 103:

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



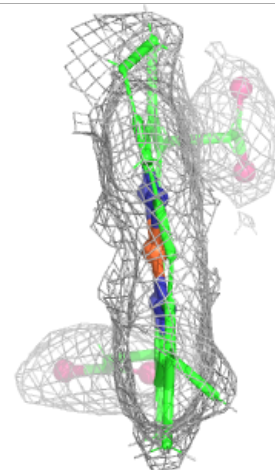
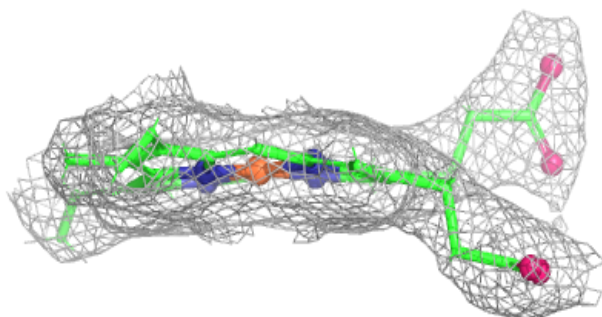
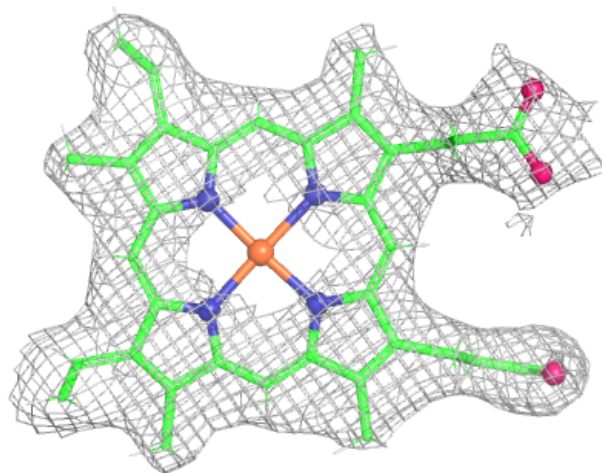
Electron density around HEM e 102:

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



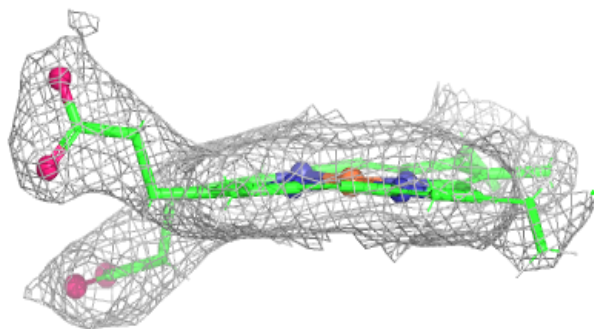
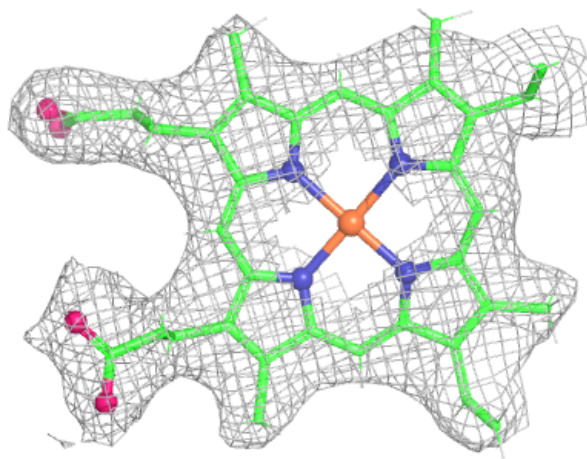
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.