



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:58 PM UTC

PDB ID : 6DHP / pdb_00006dhp
Title : RT XFEL structure of the three-flash state of Photosystem II (3F, S0-rich) at 2.04 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 : 2.04 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

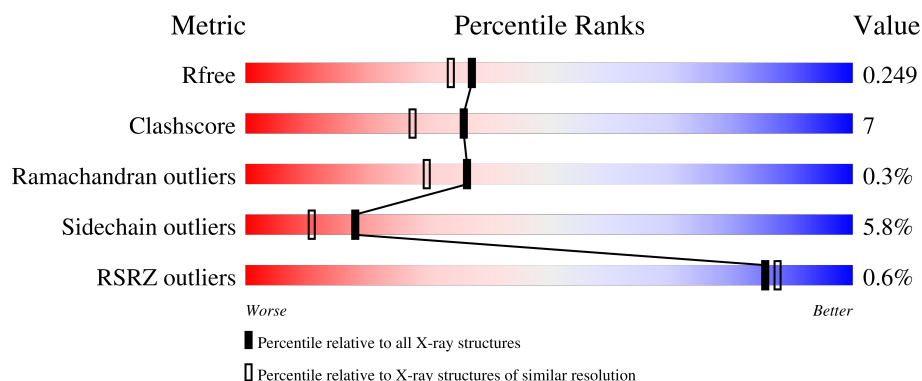
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

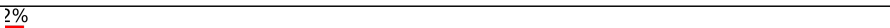
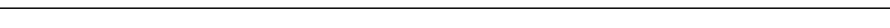
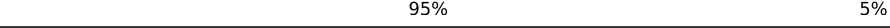
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Continued on next page...

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

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	a	334	 84% 14% .
2	B	505	 83% 16% .
2	b	505	 87% 12% .
3	C	451	 84% 13% ..
3	c	451	 84% 14% .
4	D	341	 88% 11% .
4	d	341	 85% 14% .
5	E	82	 63% 33% ..
5	e	82	 68% 30% .
6	F	34	 85% 12% .
6	f	34	 59% 35% 6% .
7	H	65	 75% 22% .
7	h	65	 68% 26% . .
8	I	36	 69% 28% .
8	i	36	 78% 19% .
9	J	36	 78% 22% .
9	j	36	 72% 22% 6% .
10	K	37	 65% 30% 5% .
10	k	37	 46% 46% 8% .
11	L	37	 95% 5% .
11	l	37	 70% 24% . .
12	M	33	 82% 15% .
12	m	33	 82% 15% .
13	O	244	 78% 20% .
13	o	244	 80% 18% .

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	603	X	-	-	-
23	CLA	A	607	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	603	X	-	-	-
23	CLA	a	606	X	-	-	-
23	CLA	a	612	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	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	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	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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	402	X	-	-	-
23	CLA	h	101	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105751 atoms, of which 52470 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	59	0
			6018	2010	2937	507	545	19			
1	a	334	Total	C	H	N	O	S	0	59	0
			6006	2007	2928	507	545	19			

- 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	7	0
			6868	2282	3392	579	601	14			
3	c	451	Total	C	H	N	O	S	0	8	0
			7017	2324	3464	596	619	14			

- 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	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	12			

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

- Molecule 14 is a protein called Photosystem II protein Y.

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

- Molecule 15 is a protein called Photosystem II reaction center protein T.

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

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

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

- Molecule 17 is a protein called Cytochrome c-550.

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

- 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			

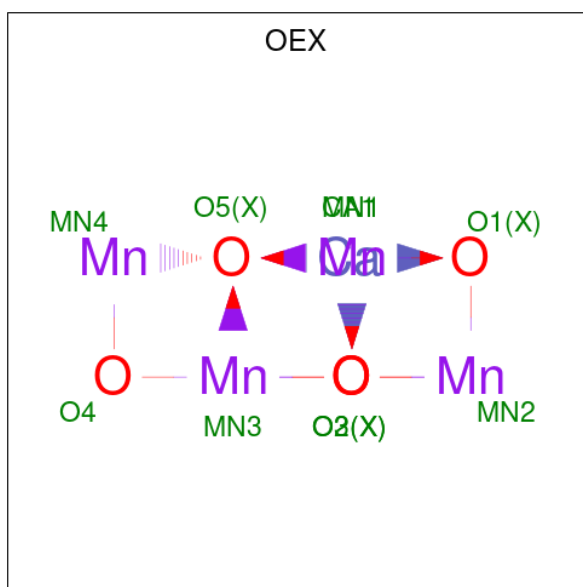
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

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

- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

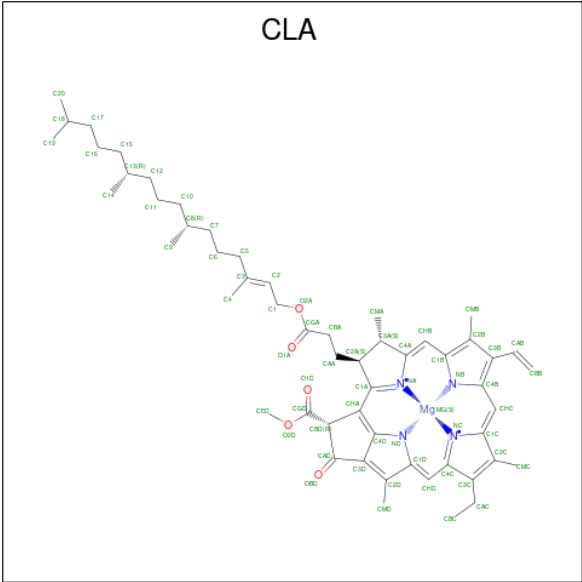


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- 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	A	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		

Continued on next page...

Continued from previous page...

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
			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		
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		

Continued on next page...

Continued from previous page...

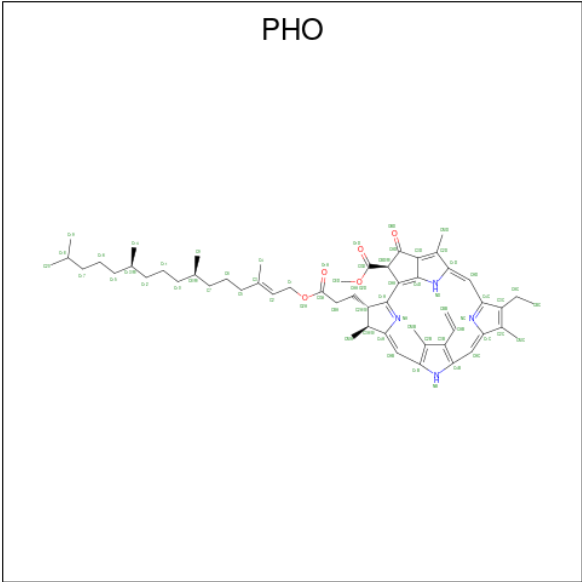
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total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

Continued on next page...

Continued from previous page...

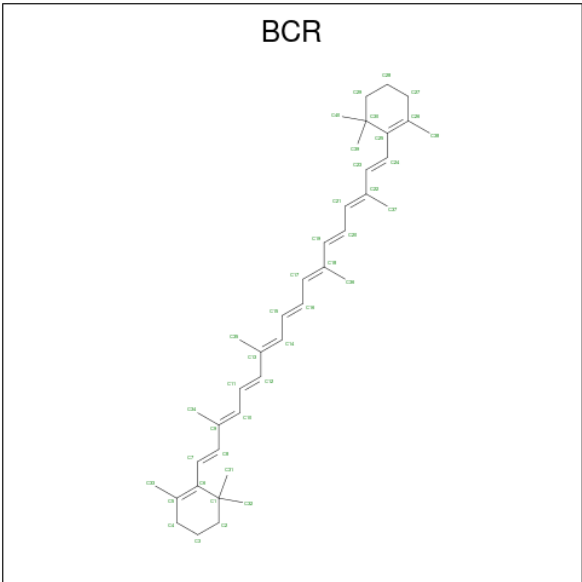
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 132	C 54	H 68	Mg 1	N 4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

- 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	A	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: $C_{40}H_{56}$).

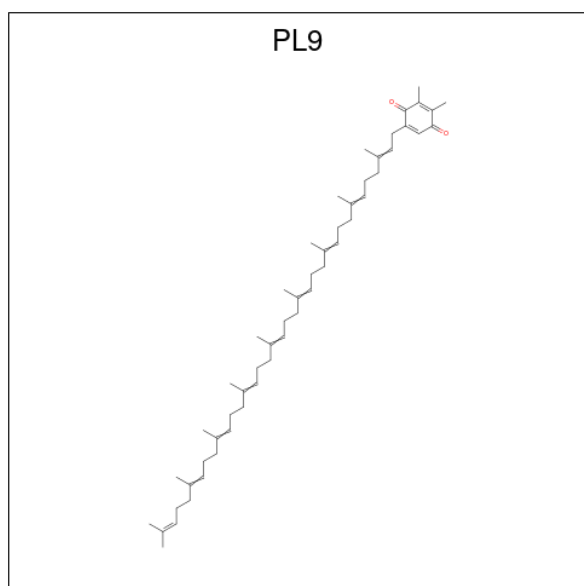


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total	C	H	0	0
			96	40	56		
25	H	1	Total	C	H	0	0
			96	40	56		
25	T	1	Total	C	H	0	0
			96	40	56		
25	Y	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		
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	k	1	Total	C	H	0	0
			96	40	56		
25	t	1	Total	C	H	0	0
			96	40	56		

- Molecule 26 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

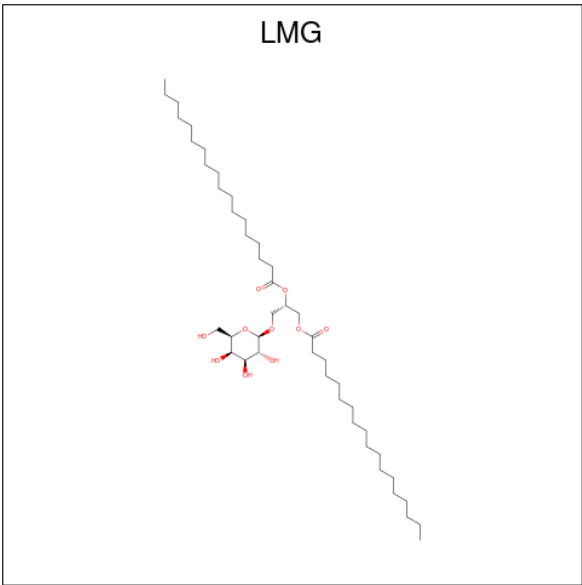
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	2	Total	Cl	0	0
			2	2		
26	a	2	Total	Cl	0	0
			2	2		

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



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

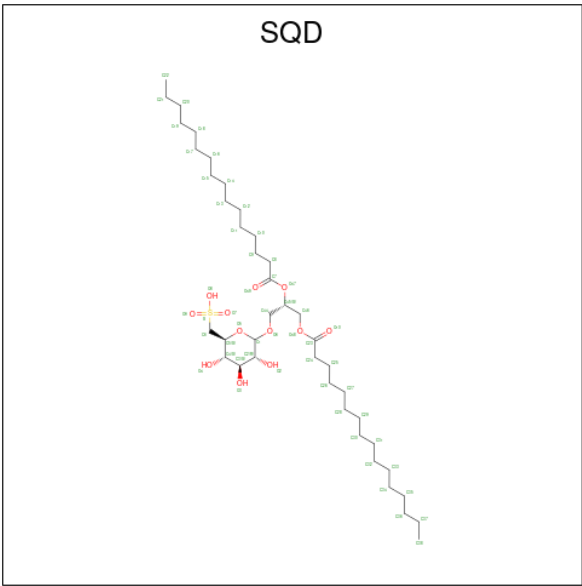
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

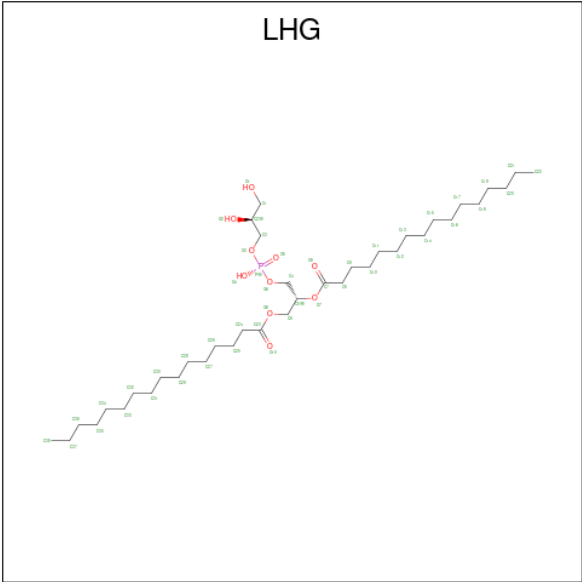
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



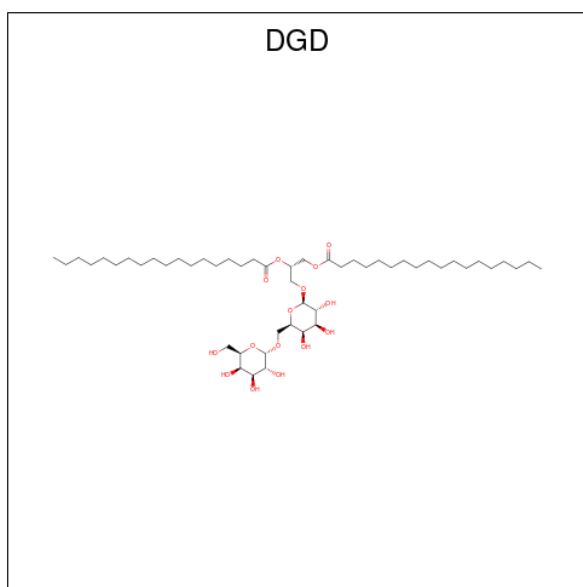
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



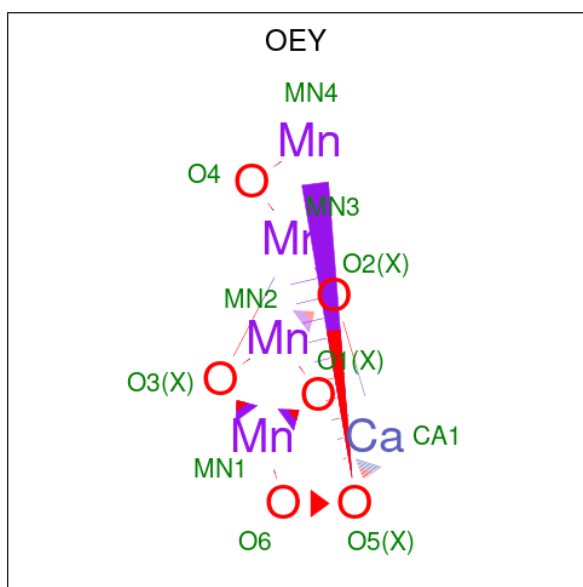
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	a	1	Total	C	H	O	P	0	0
			99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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



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

- Molecule 33 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

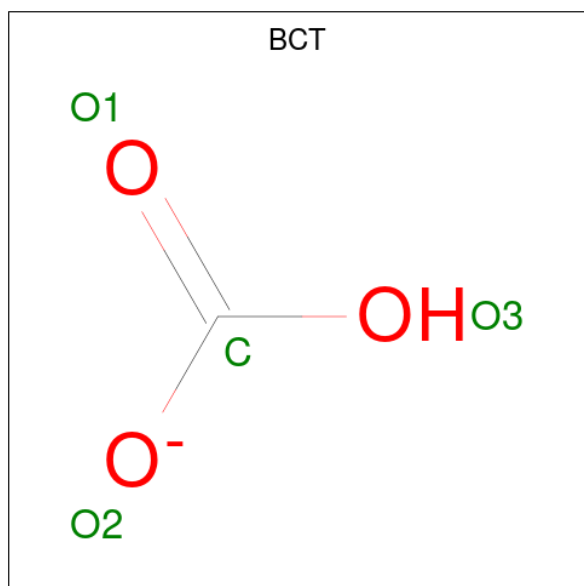
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	5	Total	C	H	O	0	0
			192	67	117	8		
33	C	3	Total	C	H	O	0	0
			103	36	63	4		
33	E	1	Total	C	H	O	0	0
			28	10	16	2		
33	H	1	Total	C	H		0	0
			53	18	35			
33	I	1	Total	C	H		0	0
			41	15	26			
33	J	1	Total	C	H	O	0	0
			28	10	16	2		
33	M	2	Total	C	H	O	0	0
			63	23	38	2		
33	T	2	Total	C	H		0	0
			91	31	60			
33	X	1	Total	C	H	O	0	0
			55	18	35	2		
33	a	1	Total	C	H	O	0	0
			28	10	16	2		

Continued on next page...

Continued from previous page...

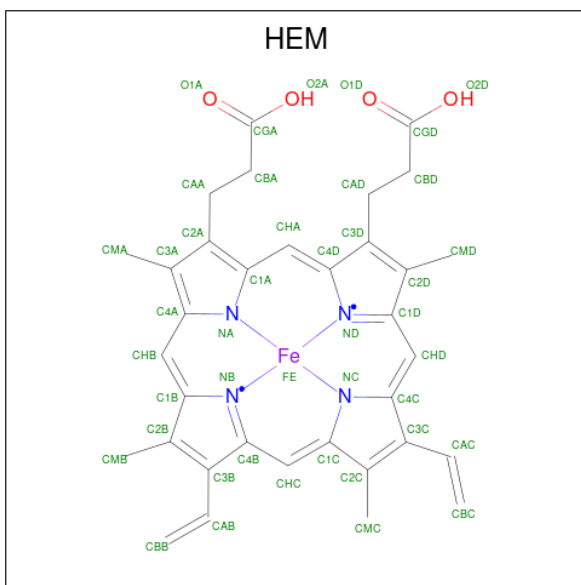
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	b	4	Total	C	H	O	0	0
			176	60	110	6		
33	c	2	Total	C	H	O	0	0
			83	28	51	4		
33	d	1	Total	C	H	O	0	0
			43	15	26	2		
33	j	1	Total	C	H	O	0	0
			28	10	16	2		
33	l	1	Total	C	H		0	0
			53	18	35			
33	m	1	Total	C	H	O	0	0
			28	10	16	2		
33	t	2	Total	C	H	O	0	0
			60	22	36	2		
33	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



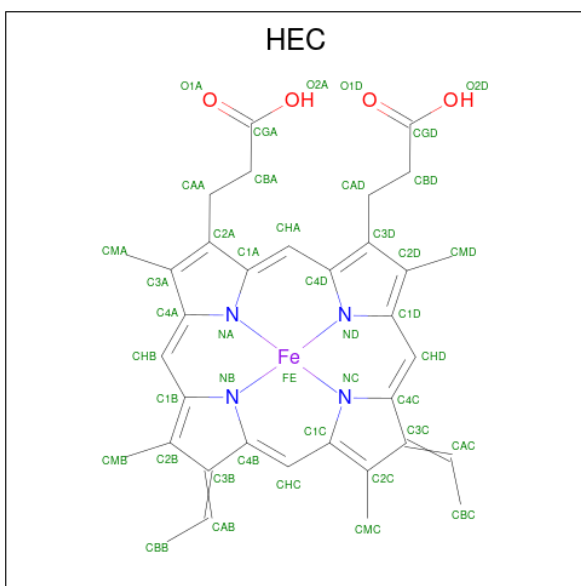
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	147	Total O 147 147	0	8
37	B	218	Total O 218 218	0	0
37	C	190	Total O 190 190	0	0
37	D	129	Total O 129 129	0	0
37	E	30	Total O 30 30	0	0
37	F	13	Total O 13 13	0	0
37	H	28	Total O 28 28	0	0
37	I	12	Total O 12 12	0	0
37	J	12	Total O 12 12	0	0
37	K	2	Total O 2 2	0	0
37	L	9	Total O 9 9	0	0
37	M	6	Total O 6 6	0	0
37	O	129	Total O 129 129	0	0
37	R	4	Total O 4 4	0	0
37	T	13	Total O 13 13	0	0
37	U	47	Total O 47 47	0	0
37	V	78	Total O 78 78	0	0
37	X	8	Total O 8 8	0	0
37	Y	5	Total O 5 5	0	0
37	Z	5	Total O 5 5	0	0
37	a	132	Total O 132 132	0	8

Continued on next page...

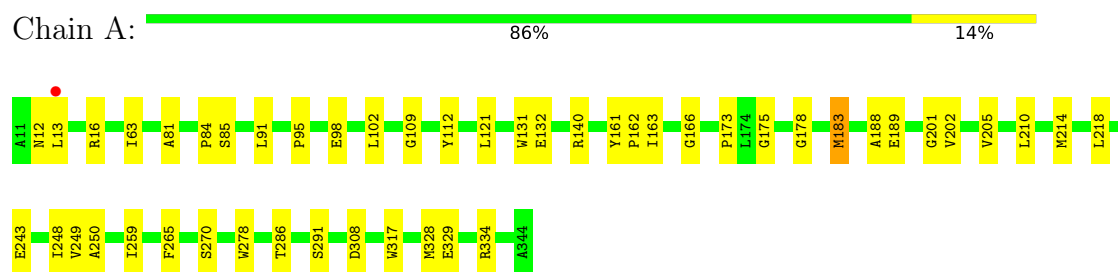
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	b	188	Total 188	O 188	0	0
37	c	155	Total 155	O 155	0	0
37	d	118	Total 118	O 118	0	0
37	e	19	Total 19	O 19	0	0
37	f	8	Total 8	O 8	0	0
37	h	19	Total 19	O 19	0	0
37	i	10	Total 10	O 10	0	0
37	j	10	Total 10	O 10	0	0
37	k	6	Total 6	O 6	0	0
37	l	13	Total 13	O 13	0	0
37	m	7	Total 7	O 7	0	0
37	o	109	Total 109	O 109	0	0
37	r	5	Total 5	O 5	0	0
37	t	14	Total 14	O 14	0	0
37	u	54	Total 54	O 54	0	0
37	v	59	Total 59	O 59	0	0
37	x	10	Total 10	O 10	0	0
37	y	4	Total 4	O 4	0	0
37	z	1	Total 1	O 1	0	0

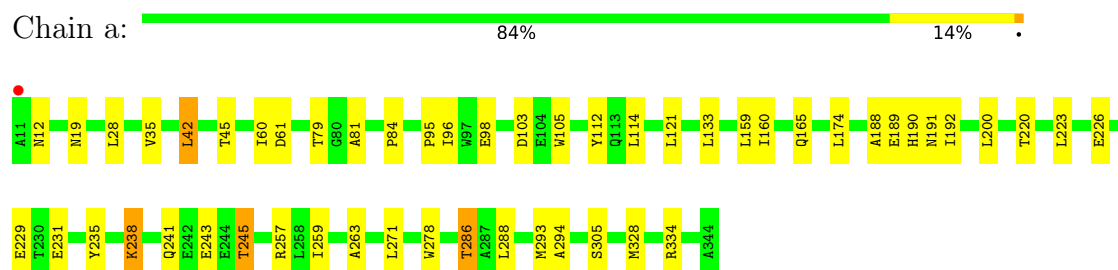
3 Residue-property plots

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

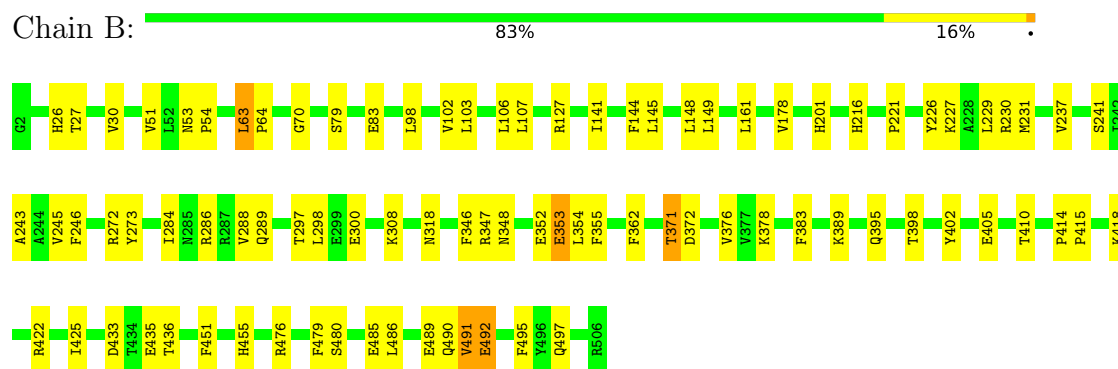
• Molecule 1: Photosystem II protein D1 1



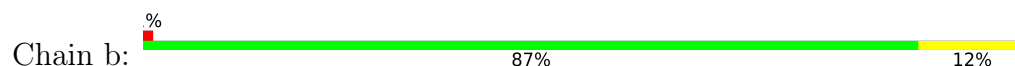
• Molecule 1: Photosystem II protein D1 1

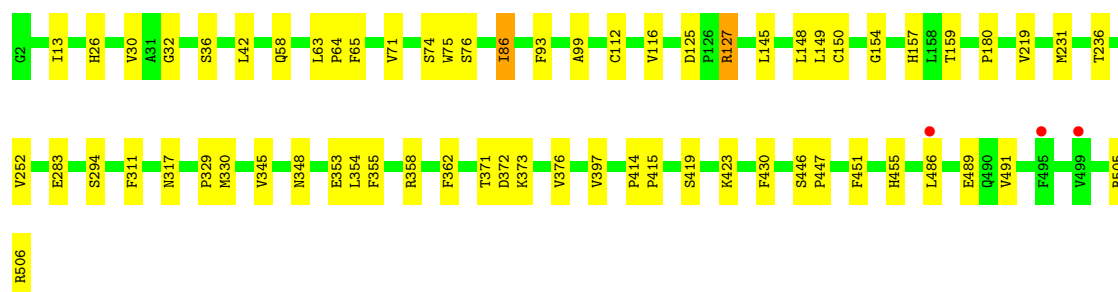


• Molecule 2: Photosystem II CP47 reaction center protein



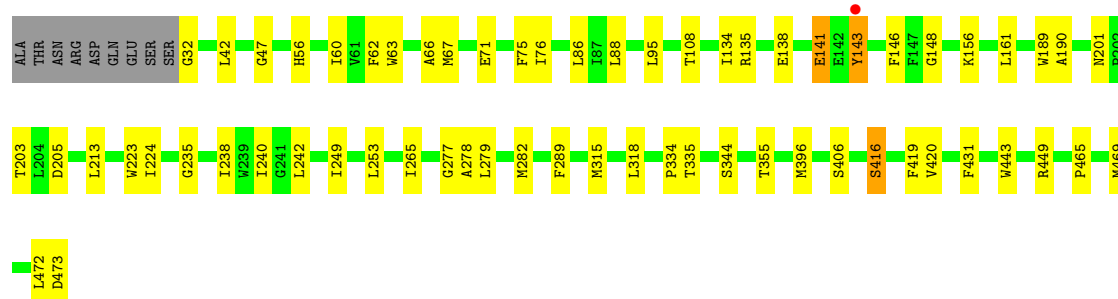
• Molecule 2: Photosystem II CP47 reaction center protein





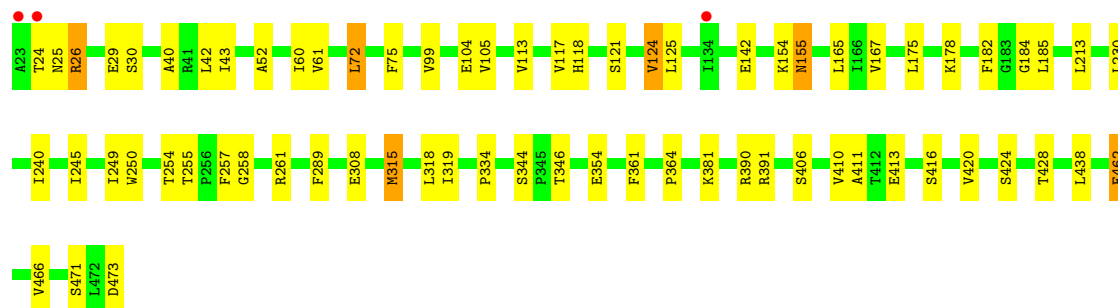
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 84% 13% ..



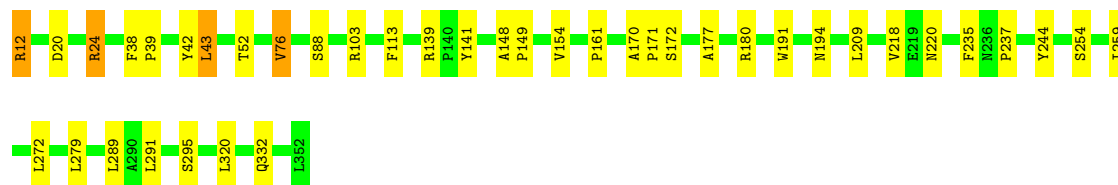
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 84% 14% .



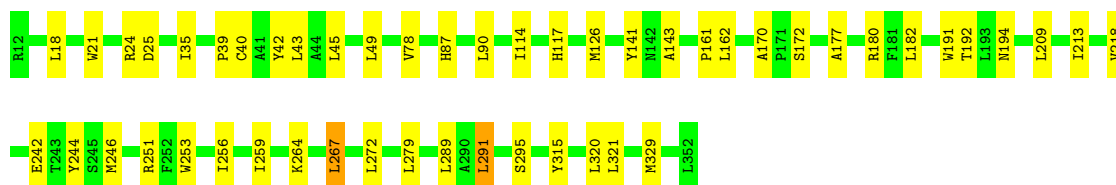
• Molecule 4: Photosystem II D2 protein

Chain D: 88% 11% .



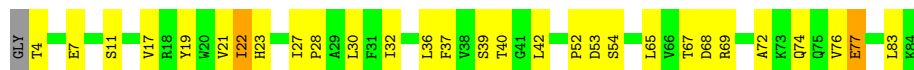
• Molecule 4: Photosystem II D2 protein

Chain d: 85% 14% .



• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 63% 33% ..



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 68% 30% .



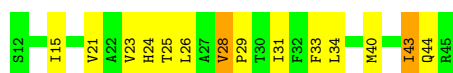
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 85% 12% .



• Molecule 6: Cytochrome b559 subunit beta

Chain f: 59% 35% 6%



• Molecule 7: Photosystem II reaction center protein H

Chain H: 75% 22% .



• Molecule 7: Photosystem II reaction center protein H

Chain h: 2% 68% 26% ..



• Molecule 8: Photosystem II reaction center protein I

Chain I:  69% 28% .



- Molecule 8: Photosystem II reaction center protein I

Chain i:  78% 19% .



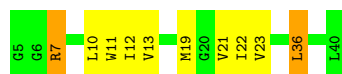
- Molecule 9: Photosystem II reaction center protein J

Chain J:  78% 22%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  72% 22% 6%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  3% 65% 30% 5%

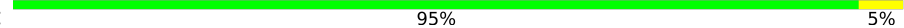


- Molecule 10: Photosystem II reaction center protein K

Chain k:  46% 46% 8%



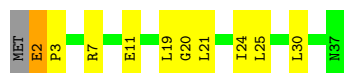
- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  70% 24% . .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  82% 15% .



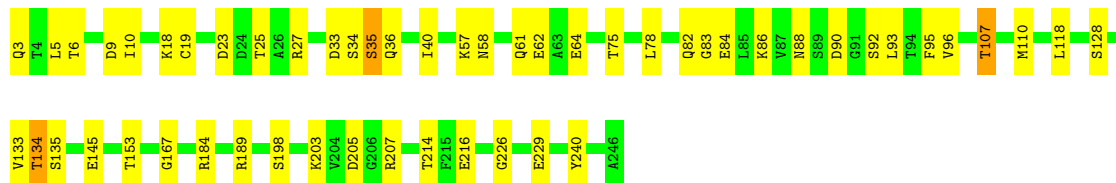
- Molecule 12: Photosystem II reaction center protein M

Chain m:  82% 15% .



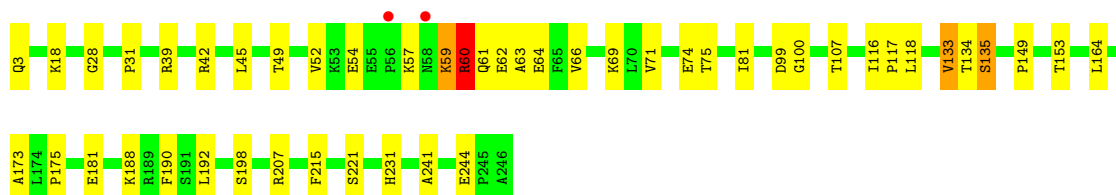
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  78% 20% .



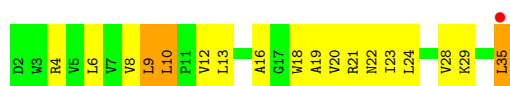
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  80% 18% .



- Molecule 14: Photosystem II protein Y

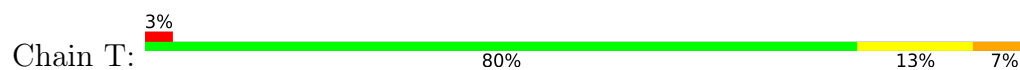
Chain R:  3% 47% 44% 9%



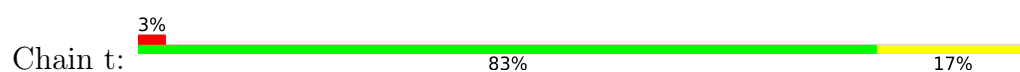
- Molecule 14: Photosystem II protein Y



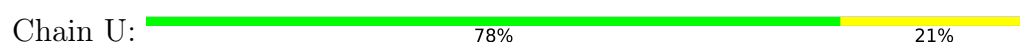
- Molecule 15: Photosystem II reaction center protein T



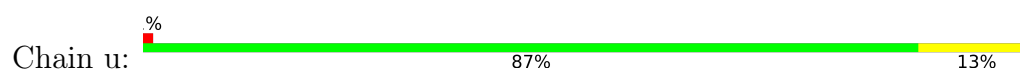
- Molecule 15: Photosystem II reaction center protein T



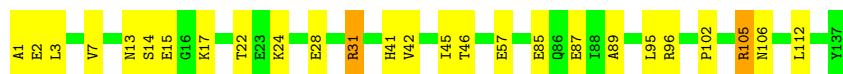
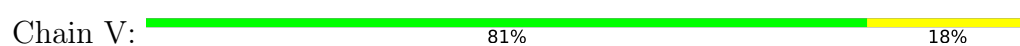
- Molecule 16: Photosystem II 12 kDa extrinsic protein



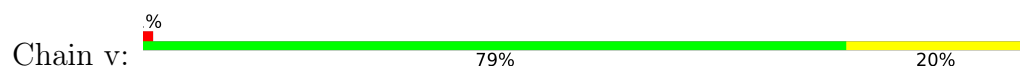
- Molecule 16: Photosystem II 12 kDa extrinsic protein



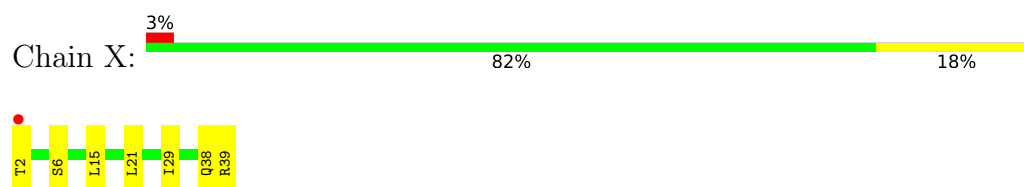
- Molecule 17: Cytochrome c-550



- Molecule 17: Cytochrome c-550



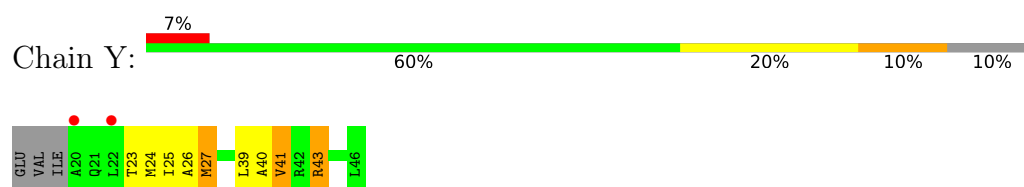
- Molecule 18: Photosystem II reaction center X protein



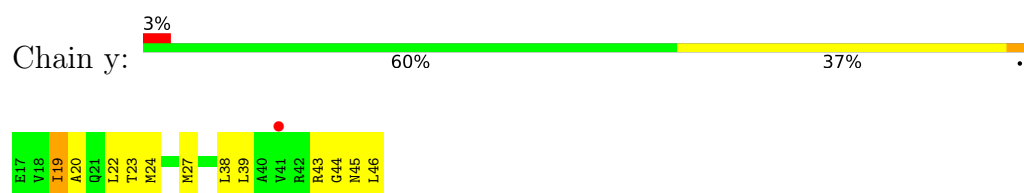
- Molecule 18: Photosystem II reaction center X protein



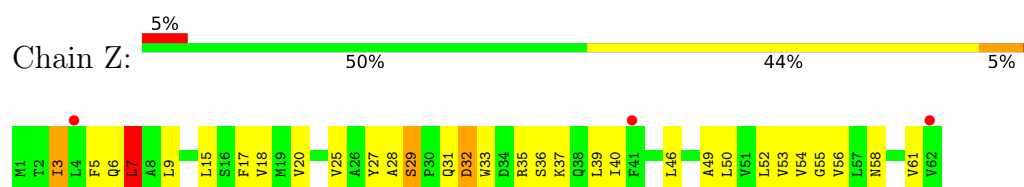
- Molecule 19: Photosystem II reaction center protein Ycf12



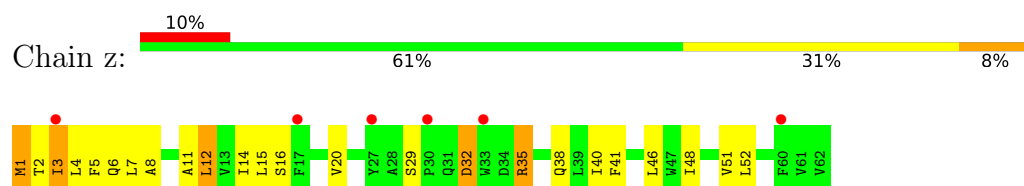
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.86Å 221.19Å 307.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 2.04 31.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.00-2.04) 88.5 (31.00-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.186 , 0.248 0.187 , 0.249	Depositor DCC
R_{free} test set	4461 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	105751	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, UNL, HEM, OEX, PHO, BCT, HEC, LMG, DGD, CLA, SQD, PL9, BCR, CL, OEY, FME, 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	0.60	0/3179	0.69	0/4331
1	a	0.56	0/3176	0.68	0/4327
2	B	0.65	0/4160	0.73	0/5668
2	b	0.62	0/4118	0.71	0/5611
3	C	0.61	0/3593	0.69	1/4891 (0.0%)
3	c	0.56	0/3673	0.69	0/4998
4	D	0.68	0/2820	0.75	0/3840
4	d	0.63	0/2829	0.70	0/3852
5	E	0.51	0/684	0.67	0/935
5	e	0.44	0/683	0.60	0/932
6	F	0.53	0/284	0.66	0/387
6	f	0.44	0/284	0.68	0/387
7	H	0.64	0/520	0.72	0/709
7	h	0.53	0/511	0.69	0/697
8	I	0.65	0/293	0.68	0/396
8	i	0.67	0/293	0.78	0/396
9	J	0.50	0/263	0.65	0/356
9	j	0.47	0/261	0.60	0/353
10	K	0.43	0/314	0.60	0/427
10	k	0.42	0/303	0.54	0/416
11	L	0.68	0/311	0.75	0/422
11	l	0.67	0/303	0.74	0/412
12	M	0.61	0/249	0.71	0/341
12	m	0.63	0/244	0.73	0/334
13	O	0.57	0/1914	0.70	0/2596
13	o	0.58	0/1905	0.70	0/2583
14	R	0.39	0/277	0.57	0/380
14	r	0.31	0/233	0.48	0/323
15	T	0.70	0/257	0.78	0/349
15	t	0.67	0/255	0.73	0/346
16	U	0.56	0/785	0.64	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.59	0/785	0.76	0/1064
17	V	0.59	0/1085	0.67	0/1473
17	v	0.53	0/1085	0.70	0/1473
18	X	0.50	0/284	0.63	0/384
18	x	0.39	0/284	0.47	0/384
19	Y	0.42	0/197	0.68	0/264
19	y	0.32	0/219	0.53	0/294
20	Z	0.44	0/490	0.59	0/669
20	z	0.37	0/488	0.57	0/666
All	All	0.59	0/43891	0.69	1/59730 (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
16	u	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	396	MET	CG-SD-CE	-6.00	87.69	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	u	52	ASN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3081	2937	2950	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3078	2928	2941	32	0
2	B	4004	3845	3864	54	0
2	b	3978	3811	3836	39	0
3	C	3476	3392	3405	43	0
3	c	3553	3464	3477	44	0
4	D	2726	2624	2632	35	0
4	d	2732	2630	2638	38	0
5	E	662	647	648	19	0
5	e	664	647	648	22	0
6	F	275	281	282	8	0
6	f	275	281	282	9	0
7	H	507	523	523	12	0
7	h	498	518	518	10	0
8	I	296	311	311	4	0
8	i	296	311	311	7	0
9	J	257	268	268	6	0
9	j	255	261	261	11	0
10	K	302	318	318	14	0
10	k	293	305	305	14	0
11	L	304	316	316	2	0
11	l	296	304	304	6	0
12	M	256	269	269	7	0
12	m	251	267	267	4	0
13	O	1880	1850	1852	33	0
13	o	1874	1844	1846	24	0
14	R	271	298	298	10	0
14	r	227	234	224	11	0
15	T	258	261	261	4	0
15	t	256	256	256	4	0
16	U	774	772	773	12	0
16	u	774	772	773	10	0
17	V	1064	1070	1073	16	0
17	v	1064	1070	1073	17	0
18	X	281	312	312	4	0
18	x	281	312	312	13	0
19	Y	196	208	217	6	0
19	y	218	241	241	6	0
20	Z	479	509	516	17	0
20	z	477	509	509	21	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	1	0	0	0	0
23	A	249	264	264	8	0
23	B	1035	1139	1139	24	0
23	C	839	922	922	14	0
23	D	130	144	144	2	0
23	a	260	288	288	12	0
23	b	970	1067	1067	27	0
23	c	839	919	919	15	0
23	d	130	144	144	2	0
23	h	65	72	72	3	0
24	A	128	148	148	3	0
24	a	64	74	74	2	0
24	d	64	74	74	4	0
25	A	40	56	56	1	0
25	B	120	168	168	7	0
25	C	120	168	168	4	0
25	D	40	56	56	4	0
25	H	40	56	56	4	0
25	T	40	56	56	5	0
25	Y	40	56	56	3	0
25	a	40	56	56	1	0
25	b	120	168	168	9	0
25	c	80	112	112	3	0
25	d	40	56	56	3	0
25	h	40	56	56	2	0
25	k	80	112	112	4	0
25	t	40	56	56	7	0
26	A	2	0	0	0	0
26	a	2	0	0	0	0
27	A	55	80	80	6	0
27	D	55	80	80	1	0
27	a	55	80	80	9	0
27	d	55	80	80	0	0
28	A	48	66	66	0	0
28	B	79	112	112	2	0
28	C	48	66	66	0	0
28	D	84	117	117	1	0
28	b	55	86	86	1	0
28	c	134	181	181	3	0
28	d	67	92	92	1	0
28	m	51	72	72	1	0
29	A	91	135	134	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B	54	78	78	0	0
29	F	36	45	45	0	0
29	a	90	134	134	6	0
29	b	49	65	64	2	0
29	f	41	49	49	3	0
30	A	49	74	74	1	0
30	B	49	74	74	4	0
30	D	96	141	141	3	0
30	L	49	74	74	0	0
30	a	42	57	57	3	0
30	d	137	199	199	7	0
30	l	49	74	74	0	0
31	A	66	96	96	2	0
31	C	186	246	245	3	0
31	H	62	82	81	1	0
31	a	44	75	75	4	0
31	c	186	246	242	1	0
31	h	62	82	81	2	0
32	A	11	0	0	2	0
32	a	11	0	0	2	0
33	B	75	117	0	0	0
33	C	40	63	0	0	0
33	E	12	16	0	0	0
33	H	18	35	0	0	0
33	I	15	26	0	0	0
33	J	12	16	0	0	0
33	M	25	38	0	0	0
33	T	31	60	0	0	0
33	X	20	35	0	1	0
33	a	12	16	0	0	0
33	b	66	110	0	0	0
33	c	32	51	0	0	0
33	d	17	26	0	0	0
33	j	12	16	0	0	0
33	l	18	35	0	0	0
33	m	12	16	0	0	0
33	t	24	36	0	0	0
33	x	20	35	0	1	0
34	D	4	1	1	0	0
34	a	4	1	1	0	0
35	F	43	30	30	3	0
35	f	43	30	30	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	43	30	30	1	0
36	v	43	30	30	1	0
37	A	147	0	0	6	0
37	B	218	0	0	6	0
37	C	190	0	0	4	1
37	D	129	0	0	3	0
37	E	30	0	0	1	0
37	F	13	0	0	2	0
37	H	28	0	0	2	1
37	I	12	0	0	1	0
37	J	12	0	0	2	0
37	K	2	0	0	0	0
37	L	9	0	0	0	0
37	M	6	0	0	0	0
37	O	129	0	0	10	0
37	R	4	0	0	0	0
37	T	13	0	0	1	0
37	U	47	0	0	2	0
37	V	78	0	0	5	0
37	X	8	0	0	0	0
37	Y	5	0	0	0	0
37	Z	5	0	0	0	0
37	a	132	0	0	3	0
37	b	188	0	0	6	0
37	c	155	0	0	6	0
37	d	118	0	0	2	0
37	e	19	0	0	0	0
37	f	8	0	0	0	0
37	h	19	0	0	2	0
37	i	10	0	0	0	0
37	j	10	0	0	1	0
37	k	6	0	0	1	0
37	l	13	0	0	1	0
37	m	7	0	0	1	0
37	o	109	0	0	2	0
37	r	5	0	0	1	0
37	t	14	0	0	0	0
37	u	54	0	0	3	0
37	v	59	0	0	2	0
37	x	10	0	0	3	0
37	y	4	0	0	0	0
37	z	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	53281	52470	51848	751	1

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

All (751) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:GLN:OE1	37:B:701:HOH:O	1.79	1.00
13:O:216:GLU:OE2	37:O:301:HOH:O	1.83	0.97
4:D:332:GLN:NE2	37:D:501:HOH:O	1.98	0.96
18:x:39:ARG:O	37:x:201:HOH:O	1.86	0.94
9:J:15:THR:HG22	9:J:19:MET:HE3	1.51	0.93
2:b:505:ARG:HG3	2:b:506:ARG:HG3	1.51	0.92
2:B:492:GLU:OE2	37:B:702:HOH:O	1.87	0.92
2:B:286:ARG:NH1	37:B:704:HOH:O	2.05	0.90
13:O:19:CYS:O	37:O:302:HOH:O	1.88	0.90
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.55	0.87
17:V:28:GLU:OE2	17:V:31:ARG:NH2	2.09	0.85
11:l:2:GLU:O	37:l:201:HOH:O	1.95	0.84
16:U:10:VAL:HG11	16:U:15:GLU:OE2	1.77	0.84
13:O:145:GLU:OE2	37:O:303:HOH:O	1.97	0.83
13:O:90:ASP:OD1	37:O:304:HOH:O	1.97	0.82
16:U:60:ASP:OD1	37:U:201:HOH:O	1.96	0.81
31:a:616:DGD:O3G	37:a:701:HOH:O	1.98	0.80
7:H:56:ASP:OD1	18:X:2:THR:N	2.15	0.80
17:V:2:GLU:OE2	37:V:301:HOH:O	1.97	0.79
13:o:28:GLY:O	37:o:301:HOH:O	2.00	0.79
12:m:5:GLN:O	37:m:201:HOH:O	2.00	0.79
2:B:410:THR:O	37:B:703:HOH:O	2.00	0.79
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.64	0.78
2:b:506:ARG:HG2	37:b:873:HOH:O	1.85	0.77
1:a:243:GLU:OE1	37:a:702:HOH:O	2.02	0.77
4:d:246:MET:HE3	4:d:264:LYS:CG	2.14	0.77
13:O:6:THR:HG22	13:O:9:ASP:OD2	1.85	0.76
3:C:213:LEU:HG	23:C:506:CLA:H193	1.67	0.76
3:c:391[A]:ARG:NH1	37:c:602:HOH:O	2.17	0.76
5:e:68:ASP:O	5:e:72:ALA:HB2	1.86	0.76
1:A:334[A]:ARG:NH2	37:A:701:HOH:O	2.19	0.75
8:i:33:LYS:O	8:i:35:LYS:NZ	2.20	0.75
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:779:HOH:O	13:O:107:THR:HG21	1.88	0.73
5:E:7:GLU:OE2	37:E:201:HOH:O	2.07	0.73
13:O:18:LYS:O	37:O:305:HOH:O	2.05	0.73
9:J:36:LEU:O	37:J:201:HOH:O	2.07	0.73
2:b:372:ASP:OD2	37:b:701:HOH:O	2.07	0.73
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.25	0.71
1:A:16:ARG:NH1	37:A:702:HOH:O	2.23	0.71
2:B:241:SER:O	2:B:245:VAL:HG23	1.90	0.71
9:J:15:THR:HG22	9:J:19:MET:CE	2.19	0.71
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.56	0.71
32:a:618[B]:OEY:O6	32:a:618[B]:OEY:O5	2.08	0.71
24:A:606:PHO:HBC3	4:D:279:LEU:HD22	1.72	0.71
3:C:277:GLY:C	23:C:505:CLA:HBC2	2.15	0.70
4:d:126:MET:HE3	4:d:143:ALA:O	1.92	0.70
4:d:242:GLU:OE2	37:d:501:HOH:O	2.10	0.70
23:c:501:CLA:H192	23:c:507:CLA:HBB1	1.73	0.69
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.73	0.69
3:C:146:PHE:O	3:C:156:LYS:NZ	2.23	0.69
2:B:352:GLU:OE2	37:B:705:HOH:O	2.09	0.69
23:b:603:CLA:H2	23:b:605:CLA:H91	1.74	0.69
3:C:205:ASP:OD1	37:C:601:HOH:O	2.10	0.69
3:C:473:ASP:OD2	15:T:24:ARG:HD3	1.92	0.68
4:d:246:MET:HE3	4:d:264:LYS:HG3	1.76	0.68
3:C:75:PHE:C	3:C:76:ILE:HD12	2.18	0.68
10:k:23:ASP:OD2	37:k:201:HOH:O	2.11	0.68
20:z:2:THR:HG23	20:z:3:ILE:H	1.58	0.68
4:d:267:LEU:C	4:d:267:LEU:HD23	2.20	0.67
32:A:618[B]:OEY:O5	32:A:618[B]:OEY:O6	2.11	0.67
25:t:101:BCR:H23C	25:t:101:BCR:H382	1.74	0.67
27:A:611:PL9:H361	6:F:25:THR:HG21	1.77	0.67
19:Y:39:LEU:HD21	20:Z:28:ALA:HB3	1.74	0.67
23:a:606:CLA:H42	8:i:9:TYR:CD2	2.29	0.67
4:D:272:LEU:C	4:D:272:LEU:HD23	2.19	0.67
16:u:50:VAL:O	16:u:53:ALA:HB2	1.95	0.67
5:e:14:ILE:HD11	9:j:10:LEU:HD11	1.76	0.67
20:z:1:MET:HB2	20:z:4:LEU:HD23	1.76	0.67
4:d:25:ASP:OD1	37:d:502:HOH:O	2.13	0.67
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.28	0.66
13:o:164:LEU:HD13	13:o:188:LYS:O	1.96	0.66
13:O:84:GLU:OE1	13:O:86:LYS:NZ	2.22	0.66
5:E:30:LEU:HD23	14:R:12:VAL:HG12	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:5:GLY:N	37:J:202:HOH:O	2.29	0.65
9:j:36:LEU:O	37:j:201:HOH:O	2.14	0.65
20:z:32:ASP:N	20:z:32:ASP:OD1	2.30	0.65
1:A:249:VAL:HG12	2:B:491:VAL:HG11	1.79	0.65
19:Y:23:THR:O	19:Y:27:MET:HE1	1.96	0.65
3:C:32:GLY:N	37:C:603:HOH:O	2.28	0.65
25:D:404:BCR:H331	25:D:404:BCR:C8	2.25	0.65
23:c:509:CLA:H43	23:c:509:CLA:O1A	1.97	0.65
25:D:404:BCR:H392	25:D:404:BCR:H23C	1.78	0.64
13:O:203:LYS:NZ	37:O:307:HOH:O	2.31	0.64
5:e:30:LEU:HD11	35:f:102:HEM:CBB	2.27	0.64
17:v:78:ASN:OD1	17:v:96:ARG:NH1	2.29	0.64
2:b:283:GLU:OE2	37:b:702:HOH:O	2.15	0.64
5:e:22:ILE:HG23	14:r:19:ALA:HB2	1.80	0.64
3:c:40:ALA:O	3:c:43:ILE:HD12	1.96	0.64
20:z:3:ILE:HG12	20:z:4:LEU:HD22	1.79	0.64
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.79	0.64
2:b:358:ARG:O	37:b:703:HOH:O	2.15	0.64
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.80	0.64
20:z:1:MET:SD	20:z:1:MET:N	2.57	0.64
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.80	0.64
16:U:45:LEU:HD21	16:U:71:GLN:HG2	1.80	0.63
16:U:70:ARG:NH2	17:V:85:GLU:OE1	2.32	0.63
17:v:103:LYS:NZ	37:v:305:HOH:O	2.28	0.63
14:R:18:TRP:O	14:R:22:ASN:ND2	2.32	0.63
13:o:18:LYS:NZ	13:o:74:GLU:OE1	2.32	0.63
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.81	0.63
10:k:10:LYS:HZ2	10:k:10:LYS:N	1.97	0.62
4:d:279:LEU:HD22	24:d:401:PHO:HBC3	1.79	0.62
5:e:63:ILE:HD12	5:e:63:ILE:N	2.14	0.62
2:B:106:LEU:HD11	29:a:615:SQD:H201	1.81	0.62
30:D:406:LHG:H321	15:T:21:ILE:HD11	1.80	0.62
23:b:602:CLA:H43	7:h:45:ILE:HG22	1.82	0.62
2:B:371:THR:HG23	2:B:372:ASP:O	1.99	0.62
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.80	0.62
25:T:101:BCR:H311	25:T:101:BCR:C8	2.29	0.62
3:c:175:LEU:HD22	23:c:501:CLA:C3D	2.30	0.61
10:K:22:VAL:HA	10:K:25:LEU:HD22	1.81	0.61
29:f:101:SQD:H351	18:x:27:VAL:HG21	1.83	0.61
13:O:92:SER:N	37:O:304:HOH:O	2.15	0.61
4:D:254:SER:OG	15:T:24:ARG:NH2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:NH2	37:A:706:HOH:O	2.33	0.61
20:Z:49:ALA:O	20:Z:53:VAL:HG23	2.02	0.60
3:c:473:ASP:OXT	15:t:28:ARG:NH1	2.35	0.60
23:B:605:CLA:HMC3	23:B:615:CLA:H43	1.83	0.60
3:c:315:MET:HE3	3:c:319:ILE:HD11	1.83	0.60
25:t:101:BCR:H321	25:t:101:BCR:HC8	1.83	0.60
23:B:606:CLA:H72	25:B:619:BCR:H311	1.82	0.60
14:r:2:ASP:N	37:r:101:HOH:O	2.34	0.60
3:C:406:SER:HA	3:C:420:VAL:HG23	1.84	0.60
35:f:102:HEM:HHC	35:f:102:HEM:HBB2	1.84	0.60
3:C:56:HIS:CE1	3:C:60:ILE:HD11	2.37	0.59
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.84	0.59
31:a:616:DGD:O1B	31:a:616:DGD:C1A	2.50	0.59
7:H:64:ALA:HB1	37:H:218:HOH:O	2.01	0.59
27:a:611:PL9:H161	27:a:611:PL9:H203	1.85	0.59
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.85	0.59
25:H:101:BCR:H331	25:H:101:BCR:C8	2.32	0.59
35:f:102:HEM:HMC1	35:f:102:HEM:HBC2	1.85	0.59
30:B:623:LHG:H222	12:M:18:PRO:HG3	1.83	0.59
27:a:611:PL9:H252	24:d:401:PHO:HBA2	1.83	0.59
2:b:30:VAL:HG12	23:b:605:CLA:HHD	1.85	0.59
13:O:184:ARG:NH2	13:O:229[A]:GLU:OE2	2.28	0.59
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.85	0.58
18:x:37:VAL:HG23	37:x:204:HOH:O	2.03	0.58
23:b:613:CLA:H203	30:d:405:LHG:C22	2.34	0.58
3:c:178:LYS:NZ	3:c:184:GLY:O	2.37	0.58
20:z:14:ILE:HG22	20:z:14:ILE:O	2.02	0.58
8:I:35:LYS:HD2	8:I:35:LYS:N	2.19	0.58
20:Z:5:PHE:O	20:Z:7:LEU:N	2.37	0.57
19:Y:40:ALA:O	19:Y:41:VAL:HB	2.03	0.57
17:V:41:HIS:HA	17:V:45:ILE:O	2.03	0.57
25:Y:101:BCR:H322	20:Z:17:PHE:CD1	2.39	0.57
2:b:317:ASN:HA	2:b:330:MET:HE1	1.87	0.57
19:y:23:THR:O	19:y:27:MET:HE2	2.05	0.57
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.19	0.57
23:B:606:CLA:H91	29:a:615:SQD:H211	1.87	0.57
5:e:17:VAL:HG23	9:j:7:ARG:HD2	1.85	0.57
2:B:141:ILE:O	2:B:145:LEU:HG	2.04	0.57
2:B:298:LEU:HD23	2:B:402:TYR:CE1	2.40	0.57
13:O:107:THR:HG22	37:O:330:HOH:O	2.03	0.57
1:a:45:THR:HG23	23:a:612:CLA:H201	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:381:LYS:NZ	13:o:99:ASP:OD2	2.29	0.57
16:U:58:VAL:O	16:U:61:VAL:HG22	2.03	0.56
7:h:12:ARG:NH2	7:h:15:ASN:O	2.37	0.56
25:T:101:BCR:H351	29:b:601:SQD:H202	1.87	0.56
25:c:515:BCR:C8	25:c:515:BCR:H331	2.35	0.56
4:d:209:LEU:HD23	4:d:209:LEU:C	2.30	0.56
1:a:103:ASP:OD2	13:o:69:LYS:NZ	2.34	0.56
10:k:40:GLN:HA	10:k:43:VAL:HG22	1.87	0.56
29:a:613:SQD:H381	9:j:22:ILE:HD11	1.87	0.56
4:d:141:TYR:OH	30:d:405:LHG:O4	2.10	0.56
8:i:16:VAL:O	8:i:20:VAL:HG23	2.05	0.56
14:r:29:LYS:O	14:r:31:VAL:N	2.39	0.56
25:d:404:BCR:H331	25:d:404:BCR:C8	2.36	0.56
15:T:2:GLU:OE1	37:T:201:HOH:O	2.17	0.56
13:O:3:GLN:N	37:O:309:HOH:O	2.39	0.55
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.87	0.55
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.42	0.55
25:T:101:BCR:H382	25:T:101:BCR:H23C	1.88	0.55
14:R:9:LEU:O	14:R:12:VAL:HG22	2.06	0.55
31:a:616:DGD:C3G	37:a:701:HOH:O	2.54	0.55
13:O:133:VAL:C	13:O:134:THR:HG23	2.31	0.55
3:c:245:ILE:HD13	28:c:521:LMG:H371	1.87	0.55
25:d:404:BCR:H381	28:d:406:LMG:H171	1.89	0.55
12:M:20:VAL:HG13	12:m:20:VAL:HG13	1.88	0.55
5:e:22:ILE:HD13	35:f:102:HEM:HMA3	1.89	0.55
20:z:2:THR:HG23	20:z:3:ILE:N	2.22	0.55
13:O:5:LEU:HD12	13:O:10:ILE:HD11	1.90	0.54
4:d:49:LEU:HD13	25:d:404:BCR:C15	2.37	0.54
13:o:52:VAL:O	13:o:66:VAL:HG22	2.07	0.54
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.90	0.54
1:a:220:THR:HA	1:a:223:LEU:HD13	1.90	0.54
1:a:165[B]:GLN:NE2	1:a:294:ALA:O	2.40	0.54
29:b:601:SQD:H101	23:b:614:CLA:H43	1.90	0.54
3:c:406:SER:HA	3:c:420:VAL:HG23	1.89	0.54
19:y:23:THR:HG23	19:y:24:MET:HE2	1.89	0.54
3:c:411:ALA:O	37:c:601:HOH:O	2.17	0.54
25:t:101:BCR:C8	25:t:101:BCR:H311	2.38	0.54
3:C:75:PHE:O	3:C:76:ILE:HD12	2.07	0.54
4:D:42:TYR:CE1	6:F:25:THR:HG23	2.43	0.54
4:D:170:ALA:HB1	4:D:171:PRO:HD2	1.89	0.54
3:c:26:ARG:O	10:k:46:ARG:HD2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:17:VAL:HG23	9:j:7:ARG:HB2	1.90	0.54
2:B:414:PRO:O	2:B:418:LYS:HG3	2.08	0.53
23:c:506:CLA:O1A	23:c:506:CLA:C2	2.55	0.53
17:v:41:HIS:HA	17:v:45:ILE:O	2.09	0.53
24:d:401:PHO:HMB3	24:d:401:PHO:HBB1	1.90	0.53
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.91	0.53
23:B:615:CLA:H93	23:B:616:CLA:H13	1.89	0.53
25:t:101:BCR:H23C	25:t:101:BCR:C38	2.38	0.53
25:t:101:BCR:HC8	25:t:101:BCR:H311	1.91	0.53
2:B:297:THR:HG23	2:B:300:GLU:CD	2.34	0.53
8:i:14:PHE:CZ	8:i:18:LEU:HD11	2.43	0.53
3:C:71:GLU:HB3	3:C:86:LEU:HD22	1.91	0.53
3:C:318:LEU:C	3:C:318:LEU:HD23	2.34	0.53
4:D:194:ASN:HA	4:D:295:SER:OG	2.09	0.53
10:K:43:VAL:HG21	10:K:46[A]:ARG:CZ	2.39	0.53
23:c:508:CLA:HMD2	30:d:409:LHG:H102	1.91	0.53
3:c:391[B]:ARG:NE	37:c:608:HOH:O	2.41	0.53
3:c:250:TRP:O	3:c:254:THR:HG23	2.07	0.53
11:l:20:GLY:O	11:l:24:ILE:HG12	2.08	0.53
1:a:257:ARG:NH1	2:b:491:VAL:O	2.36	0.52
5:e:30:LEU:HD11	35:f:102:HEM:HBB2	1.91	0.52
23:B:604:CLA:H172	23:B:604:CLA:H141	1.92	0.52
10:K:17:ILE:N	10:K:17:ILE:HD12	2.25	0.52
2:b:71:VAL:HG23	23:b:606:CLA:HMA2	1.91	0.52
4:D:218:VAL:HG22	4:D:244:TYR:CE2	2.45	0.52
7:H:50:ASN:OD1	7:H:52:THR:CG2	2.58	0.52
25:b:619:BCR:H331	25:b:619:BCR:C8	2.38	0.52
10:k:26:PRO:O	10:k:29:PRO:HD2	2.10	0.52
12:m:4:ASN:ND2	28:m:101:LMG:O10	2.43	0.52
1:A:218:LEU:HD12	27:A:611:PL9:C3	2.40	0.52
2:b:86:ILE:HD13	2:b:86:ILE:O	2.10	0.52
4:d:161:PRO:HB3	4:d:170:ALA:HB2	1.92	0.52
29:f:101:SQD:C31	18:x:27:VAL:HG11	2.40	0.52
25:k:101:BCR:H312	20:z:16:SER:HB3	1.90	0.52
13:O:58:ASN:HB3	37:b:706:HOH:O	2.10	0.52
18:X:38:GLN:O	18:X:39:ARG:HB2	2.09	0.51
23:a:603:CLA:HMB1	23:a:603:CLA:HBB1	1.92	0.51
25:b:617:BCR:H23C	25:b:617:BCR:H382	1.92	0.51
23:B:604:CLA:H43	23:B:605:CLA:H2	1.90	0.51
31:A:617:DGD:HD5	2:b:75:TRP:HB3	1.91	0.51
1:a:42:LEU:HD11	29:a:615:SQD:H302	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.74	0.51
5:E:68:ASP:O	5:E:72:ALA:HB2	2.10	0.51
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.93	0.51
7:H:12:ARG:HB3	7:H:13:PRO:HD3	1.93	0.51
2:B:237:VAL:HG22	23:B:610:CLA:HBC2	1.91	0.51
17:V:87:GLU:OE1	17:V:96:ARG:NH1	2.44	0.51
2:b:36:SER:OG	25:b:618:BCR:H362	2.10	0.51
1:A:91:LEU:HD11	1:A:163[A]:ILE:HA	1.93	0.51
1:A:334[B]:ARG:HD3	4:D:320:LEU:HD13	1.92	0.51
17:v:55:ARG:NH2	37:v:310:HOH:O	2.43	0.51
1:a:286:THR:HG23	23:a:603:CLA:HED3	1.93	0.50
25:b:618:BCR:H331	25:b:618:BCR:C8	2.40	0.50
5:e:17:VAL:H	9:j:7:ARG:HD2	1.76	0.50
13:o:3:GLN:HG3	37:o:402:HOH:O	2.11	0.50
4:d:18:LEU:HD22	18:x:29:ILE:HG12	1.94	0.50
5:e:14:ILE:O	5:e:20:TRP:NE1	2.44	0.50
16:U:18:GLY:O	37:U:202:HOH:O	2.19	0.50
5:e:25:ILE:HD12	5:e:25:ILE:N	2.26	0.50
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.45	0.50
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.92	0.50
23:C:502:CLA:H61	23:C:512:CLA:H42	1.93	0.50
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.94	0.50
23:b:613:CLA:H203	30:d:405:LHG:H222	1.92	0.50
3:c:334:PRO:HA	13:o:153:THR:OG1	2.11	0.50
5:E:53:ASP:O	17:V:1:ALA:N	2.44	0.50
23:a:606:CLA:H203	8:i:9:TYR:CD2	2.47	0.50
18:x:24:THR:HG22	18:x:28:LEU:HD12	1.93	0.50
13:O:83:GLY:HA3	13:O:96:VAL:O	2.12	0.50
1:a:271:LEU:HD13	1:a:271:LEU:C	2.37	0.50
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.94	0.50
23:c:513:CLA:HED2	23:c:513:CLA:OBD	2.12	0.50
3:C:156:LYS:NZ	37:C:608:HOH:O	2.42	0.50
20:Z:5:PHE:CE2	20:Z:54:VAL:HG13	2.46	0.50
1:A:162[A]:PRO:O	1:A:166[A]:GLY:N	2.43	0.49
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.47	0.49
2:B:102:VAL:HA	25:B:618:BCR:C40	2.42	0.49
17:V:102:PRO:HA	17:V:105:ARG:HD3	1.94	0.49
30:d:407:LHG:H292	15:t:17:PHE:CD1	2.47	0.49
2:B:347:ARG:HA	2:B:352:GLU:O	2.12	0.49
25:D:404:BCR:H331	25:D:404:BCR:HC8	1.95	0.49
23:b:614:CLA:H92	25:b:617:BCR:H362	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:VAL:O	5:E:21:VAL:HG23	2.12	0.49
5:E:22[A]:ILE:HD12	14:R:19:ALA:HB1	1.94	0.49
1:a:263:ALA:O	27:a:611:PL9:H152	2.13	0.49
4:D:20:ASP:O	4:D:24:ARG:HG2	2.12	0.49
1:A:201:GLY:HA3	1:A:286:THR:HB	1.94	0.49
6:f:26:LEU:O	6:f:29:PRO:HD2	2.12	0.49
1:A:189[B]:GLU:CD	32:A:618[B]:OEY:O6	2.51	0.49
2:B:221:PRO:HA	23:B:609:CLA:HED3	1.95	0.49
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49
3:C:67:MET:HB3	3:C:88:LEU:CD1	2.43	0.49
20:Z:52:LEU:O	20:Z:56:VAL:HG23	2.13	0.49
20:z:2:THR:HG23	20:z:3:ILE:HD13	1.95	0.49
16:u:92:VAL:HG12	16:u:97:ARG:HD2	1.95	0.49
23:B:613:CLA:H192	30:B:623:LHG:H223	1.95	0.48
6:f:21:VAL:O	6:f:25:THR:HG23	2.14	0.48
7:h:24:GLY:N	37:h:202:HOH:O	2.37	0.48
13:O:90:ASP:CG	37:O:304:HOH:O	2.51	0.48
17:v:100:ILE:C	17:v:102:PRO:HD3	2.38	0.48
18:x:3:ILE:N	18:x:3:ILE:HD12	2.28	0.48
23:B:609:CLA:NC	25:H:101:BCR:H332	2.28	0.48
3:C:143:TYR:CE1	23:C:513:CLA:HED3	2.48	0.48
10:K:28:ILE:N	10:K:29:PRO:CD	2.77	0.48
23:c:506:CLA:HBC2	23:c:506:CLA:HHD	1.93	0.48
4:D:209:LEU:HD23	4:D:209:LEU:C	2.37	0.48
12:M:17:VAL:HB	12:M:18:PRO:HD3	1.93	0.48
17:V:41:HIS:CE1	17:V:46:THR:OG1	2.66	0.48
13:o:59:LYS:C	13:o:60:ARG:HG3	2.37	0.48
23:d:403:CLA:H92	18:x:18:ALA:HB2	1.95	0.48
6:f:43:ILE:CD1	6:f:43:ILE:N	2.77	0.48
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.95	0.48
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.95	0.48
5:e:74:GLN:O	5:e:78:THR:HG23	2.13	0.48
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	1.95	0.48
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.96	0.48
16:u:9:LEU:HA	37:u:220:HOH:O	2.13	0.48
19:Y:41:VAL:HG12	19:Y:41:VAL:O	2.13	0.48
3:c:318:LEU:C	3:c:318:LEU:HD23	2.38	0.48
1:A:249:VAL:HG12	2:B:491:VAL:CG1	2.43	0.48
3:C:63:TRP:CZ2	3:C:67:MET:HG2	2.49	0.48
1:a:259:ILE:HG21	27:a:611:PL9:H202	1.96	0.48
2:b:414:PRO:N	2:b:415:PRO:HD2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:r:10:LEU:HB2	14:r:11:PRO:CD	2.44	0.48
27:A:611:PL9:H251	23:D:402:CLA:H141	1.96	0.47
30:B:623:LHG:O4	4:D:141:TYR:OH	2.29	0.47
2:b:157:HIS:C	2:b:157:HIS:CD2	2.92	0.47
3:c:121:SER:O	3:c:124:VAL:HG13	2.14	0.47
3:C:334:PRO:HA	13:O:153:THR:OG1	2.14	0.47
18:X:21:LEU:HD11	33:X:101:UNL:C18	2.45	0.47
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.97	0.47
24:A:605:PHO:NC	24:A:605:PHO:ND	2.62	0.47
2:B:63:LEU:N	2:B:64:PRO:HD2	2.28	0.47
10:K:13:GLU:OE1	10:K:13:GLU:N	2.45	0.47
3:c:75:PHE:O	10:k:10:LYS:NZ	2.45	0.47
3:c:364:PRO:HD2	37:c:644:HOH:O	2.14	0.47
20:z:32:ASP:CB	20:z:35:ARG:HB3	2.44	0.47
4:d:194:ASN:HA	4:d:295:SER:OG	2.14	0.47
13:o:62:GLU:OE2	13:o:63:ALA:O	2.32	0.47
16:U:45:LEU:HD21	16:U:71:GLN:CG	2.44	0.47
2:b:355:PHE:HE2	2:b:373:LYS:HG2	1.79	0.47
1:a:95:PRO:HG2	1:a:98:GLU:HG2	1.96	0.47
7:h:17:GLU:O	7:h:18:TYR:C	2.54	0.47
23:h:101:CLA:CHA	23:h:101:CLA:HBA2	2.45	0.47
13:O:35:SER:OG	13:O:36:GLN:N	2.48	0.47
14:R:4:ARG:O	14:R:8:VAL:HG23	2.14	0.47
6:f:24:HIS:O	6:f:28:VAL:HG13	2.15	0.47
25:h:102:BCR:H20C	25:h:102:BCR:H361	1.76	0.47
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.96	0.47
5:E:17:VAL:HG23	9:J:7:ARG:HG3	1.97	0.47
35:F:102:HEM:HBC2	35:F:102:HEM:HHD	1.96	0.47
10:K:15:TYR:O	10:K:17:ILE:N	2.48	0.47
4:d:291:LEU:CD1	31:h:103:DGD:CGB	2.93	0.47
1:A:183[B]:MET:HA	23:A:603:CLA:HMD1	1.97	0.47
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.96	0.47
23:A:613:CLA:HED1	27:D:407:PL9:H372	1.97	0.47
3:C:201:ASN:HB3	37:C:719:HOH:O	2.14	0.47
7:H:44:ILE:HG22	7:H:48:ILE:HD12	1.96	0.47
27:a:611:PL9:H151	30:a:614:LHG:H301	1.97	0.47
14:R:24:LEU:O	14:R:28:VAL:HG23	2.15	0.46
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.50	0.46
3:c:424:SER:O	3:c:428:THR:HG23	2.15	0.46
9:j:19:MET:HA	9:j:22:ILE:HD12	1.97	0.46
1:a:189[B]:GLU:OE1	32:a:618[B]:OEY:O6	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:154:LYS:NZ	37:c:612:HOH:O	2.47	0.46
13:o:71:VAL:HG22	13:o:107:THR:O	2.15	0.46
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.51	0.46
23:C:511:CLA:H143	20:Z:20:VAL:HG13	1.96	0.46
17:V:13:ASN:OD1	17:V:15:GLU:HB2	2.15	0.46
23:a:606:CLA:H203	23:a:606:CLA:H141	1.96	0.46
10:k:17:ILE:HD11	20:z:6:GLN:HG2	1.97	0.46
1:A:334[A]:ARG:HD3	4:D:320:LEU:HD13	1.98	0.46
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.03	0.46
8:I:31:ASN:HB2	8:I:32:PRO:HD2	1.98	0.46
2:b:58:GLN:C	2:b:329:PRO:HB3	2.41	0.46
23:b:607:CLA:H142	23:b:613:CLA:H202	1.98	0.46
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.95	0.46
6:f:29:PRO:O	6:f:33:PHE:HD2	1.98	0.46
17:v:26:TYR:OH	17:v:122:GLU:OE2	2.29	0.46
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.98	0.46
25:B:617:BCR:H322	28:B:620:LMG:H111	1.98	0.46
25:D:404:BCR:H352	6:F:29:PRO:HG2	1.97	0.46
11:L:36:PHE:HB3	12:M:3:VAL:HG22	1.97	0.46
20:Z:27:TYR:HE2	20:Z:33:TRP:CH2	2.33	0.46
30:a:614:LHG:HC2	5:e:11:SER:CB	2.45	0.46
17:v:76:MET:HE1	17:v:115:ILE:HD12	1.97	0.46
3:C:203:THR:O	3:C:235:GLY:HA3	2.16	0.46
10:K:15:TYR:C	10:K:17:ILE:N	2.72	0.46
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.51	0.46
23:B:608:CLA:H193	7:H:43:LEU:HD21	1.98	0.46
5:E:37:PHE:HD2	5:E:42:LEU:HD23	1.81	0.46
1:a:114:LEU:C	1:a:114:LEU:HD23	2.40	0.46
3:c:438:LEU:HD11	23:c:505:CLA:HBB1	1.97	0.46
19:y:39:LEU:O	19:y:44:GLY:N	2.48	0.46
3:C:141:GLU:HA	3:C:148:GLY:HA3	1.98	0.46
7:H:3:ARG:NH1	37:H:208:HOH:O	2.49	0.46
31:h:103:DGD:C1A	31:h:103:DGD:C1B	2.93	0.46
4:D:12:ARG:NE	4:D:12:ARG:HA	2.32	0.46
4:D:272:LEU:HD23	4:D:272:LEU:O	2.16	0.46
23:a:603:CLA:H143	24:a:605:PHO:H61	1.98	0.46
1:A:210:LEU:HD23	1:A:214:MET:HG2	1.97	0.45
2:B:229:LEU:O	2:B:230:ARG:C	2.58	0.45
3:C:472:LEU:HD12	37:D:608:HOH:O	2.16	0.45
25:C:514:BCR:H323	20:Z:55:GLY:HA2	1.98	0.45
13:O:58:ASN:OD1	13:O:61:GLN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:u:53:ALA:HB1	16:u:97:ARG:NH1	2.32	0.45
19:y:23:THR:CG2	19:y:24:MET:HE2	2.46	0.45
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.51	0.45
1:A:84:PRO:HA	1:A:112:TYR:CG	2.52	0.45
23:C:510:CLA:H2A	23:C:510:CLA:O2A	2.15	0.45
17:V:22:THR:HG21	37:V:322:HOH:O	2.16	0.45
2:b:63:LEU:N	2:b:64:PRO:HD2	2.31	0.45
10:k:39:TRP:O	10:k:42:ALA:HB3	2.16	0.45
29:a:613:SQD:O10	29:a:613:SQD:H262	2.17	0.45
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.16	0.45
23:c:504:CLA:H92	23:c:504:CLA:H62	1.84	0.45
2:B:237:VAL:CG2	23:B:610:CLA:HBC2	2.47	0.45
2:B:479[A]:PHE:O	4:D:139:ARG:NH2	2.48	0.45
4:D:272:LEU:C	4:D:272:LEU:CD2	2.89	0.45
10:K:17:ILE:H	10:K:17:ILE:CD1	2.30	0.45
3:c:155:ASN:OD1	3:c:255:THR:CG2	2.65	0.45
5:e:17:VAL:HG23	9:j:7:ARG:CD	2.46	0.45
3:C:249:ILE:O	3:C:253:LEU:HG	2.17	0.45
25:Y:101:BCR:H322	20:Z:17:PHE:CE1	2.51	0.45
23:b:609:CLA:H141	23:b:609:CLA:H172	1.98	0.45
17:v:108:THR:O	17:v:111:ASP:N	2.50	0.45
20:z:14:ILE:N	20:z:14:ILE:CD1	2.80	0.45
3:C:419:PHE:HA	31:C:517:DGD:O3E	2.16	0.45
4:D:43:LEU:HG	4:D:113:PHE:HZ	1.82	0.45
1:a:84:PRO:HA	1:a:112:TYR:CG	2.52	0.45
2:b:419:SER:O	2:b:423:LYS:HG2	2.17	0.45
4:d:39:PRO:O	4:d:43:LEU:HG	2.17	0.45
31:A:617:DGD:C2B	23:b:606:CLA:H201	2.47	0.45
2:B:353:GLU:HG2	2:B:355:PHE:CZ	2.51	0.45
23:B:606:CLA:H91	23:B:606:CLA:H112	1.80	0.45
30:B:623:LHG:C22	12:M:18:PRO:HG3	2.47	0.45
2:b:371:THR:HA	2:b:376:VAL:O	2.17	0.45
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.34	0.45
1:A:291:SER:HB3	3:C:431:PHE:CE2	2.52	0.45
3:C:189:TRP:O	3:C:190:ALA:C	2.58	0.45
16:U:57:SER:HA	16:U:84:VAL:HG21	1.98	0.45
2:b:32:GLY:HA3	25:b:618:BCR:H17C	1.99	0.45
23:b:606:CLA:HMB1	23:b:606:CLA:HBB1	1.97	0.45
23:b:613:CLA:H192	30:d:405:LHG:H222	1.99	0.45
23:b:616:CLA:HED2	23:b:616:CLA:C1A	2.46	0.45
10:k:25:LEU:N	10:k:26:PRO:CD	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:r:6:LEU:HD11	14:r:10:LEU:HD21	1.98	0.45
17:v:110:LYS:O	17:v:113:VAL:HG22	2.17	0.45
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.46	0.44
5:E:37:PHE:CD2	5:E:42:LEU:HD23	2.52	0.44
10:K:15:TYR:O	10:K:16:ALA:C	2.59	0.44
16:U:61:VAL:O	16:U:64:ILE:HG12	2.17	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.52	0.44
20:z:14:ILE:N	20:z:14:ILE:HD12	2.32	0.44
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.52	0.44
2:B:451:PHE:C	2:B:451:PHE:CD2	2.94	0.44
5:E:36:LEU:HA	5:E:39:SER:OG	2.16	0.44
8:I:30:ARG:HD3	37:I:204:HOH:O	2.17	0.44
35:f:102:HEM:HBC2	35:f:102:HEM:CMC	2.46	0.44
9:j:10:LEU:O	9:j:13:VAL:HG22	2.17	0.44
9:j:19:MET:O	9:j:23:VAL:HG23	2.17	0.44
6:F:45:ARG:NH1	9:J:40:LEU:OXT	2.45	0.44
7:H:38:PHE:HB2	25:H:101:BCR:C10	2.47	0.44
10:K:17:ILE:HD12	10:K:17:ILE:H	1.82	0.44
16:U:52:ASN:CB	16:U:64:ILE:HD12	2.47	0.44
3:c:257:PHE:O	3:c:261:ARG:HG3	2.17	0.44
18:x:36:LYS:NZ	37:x:203:HOH:O	2.49	0.44
25:C:514:BCR:C8	25:C:514:BCR:H331	2.46	0.44
5:E:74:GLN:N	5:E:74:GLN:CD	2.76	0.44
14:r:3:TRP:CD1	14:r:3:TRP:C	2.95	0.44
17:v:99:ASP:N	17:v:99:ASP:OD1	2.51	0.44
2:b:145:LEU:HD11	23:b:615:CLA:CMB	2.47	0.44
13:o:116:ILE:HD12	13:o:231:HIS:ND1	2.33	0.44
2:B:414:PRO:N	2:B:415:PRO:HD2	2.33	0.44
23:a:606:CLA:H162	8:i:9:TYR:HB3	1.99	0.44
16:u:53:ALA:HB1	16:u:97:ARG:HH12	1.83	0.44
1:A:95:PRO:HD2	1:A:98:GLU:HG3	2.00	0.44
1:A:250:ALA:HA	2:B:491:VAL:HG21	2.00	0.44
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.53	0.44
23:C:504:CLA:H92	31:C:517:DGD:HA92	1.99	0.44
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.81	0.44
8:I:7:THR:O	8:I:11:VAL:HG23	2.18	0.44
10:K:18:PHE:CE2	20:Z:9:LEU:HD21	2.53	0.44
2:b:311:PHE:HA	2:b:430:PHE:CZ	2.52	0.44
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.47	0.44
6:F:45:ARG:HG2	37:F:208:HOH:O	2.17	0.44
17:V:95:LEU:HD11	17:V:112:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:26:HIS:CE1	23:b:612:CLA:HMA2	2.52	0.44
25:c:515:BCR:H382	25:c:515:BCR:H23C	1.98	0.44
16:u:45:LEU:HD21	16:u:71:GLN:HB3	2.00	0.44
1:A:308:ASP:HB2	5:E:52:PRO:O	2.17	0.44
2:B:149[A]:LEU:HD21	23:B:606:CLA:HBB2	2.00	0.44
25:C:515:BCR:H15C	25:C:515:BCR:H351	1.87	0.44
25:H:101:BCR:H15C	25:H:101:BCR:H351	1.87	0.44
29:a:613:SQD:O10	29:a:613:SQD:C26	2.65	0.44
3:c:113:VAL:O	3:c:117:VAL:HG23	2.18	0.44
25:c:515:BCR:H11C	25:c:515:BCR:H341	1.84	0.44
10:k:20:PRO:O	10:k:24:VAL:HG13	2.17	0.44
12:M:20:VAL:HG13	12:m:20:VAL:CG1	2.47	0.43
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.99	0.43
25:k:101:BCR:H312	20:z:16:SER:CB	2.48	0.43
17:v:28:GLU:HA	17:v:28:GLU:OE1	2.17	0.43
23:B:607:CLA:HBC3	25:B:618:BCR:HC8	2.00	0.43
4:D:291:LEU:HD21	31:H:102:DGD:CGB	2.48	0.43
37:D:563:HOH:O	18:X:6:SER:HA	2.18	0.43
7:H:17:GLU:OE2	7:H:20:LYS:NZ	2.42	0.43
2:b:112:CYS:O	2:b:116:VAL:HG23	2.18	0.43
16:u:53:ALA:HB3	37:u:236:HOH:O	2.18	0.43
19:Y:41:VAL:O	19:Y:41:VAL:CG1	2.66	0.43
4:d:161:PRO:CG	4:d:170:ALA:HB2	2.47	0.43
7:h:3:ARG:NH2	37:h:204:HOH:O	2.51	0.43
11:l:25:LEU:HD23	11:l:25:LEU:HA	1.85	0.43
14:r:6:LEU:O	14:r:10:LEU:HG	2.19	0.43
17:v:40:CYS:SG	36:v:201:HEC:HMC1	2.59	0.43
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.99	0.43
2:B:103:LEU:O	2:B:107:LEU:HG	2.19	0.43
2:B:376:VAL:HG12	2:B:378:LYS:HD2	2.00	0.43
2:b:451:PHE:CE1	2:b:455:HIS:CE1	3.06	0.43
3:c:52:ALA:HB2	23:c:511:CLA:HMA2	2.00	0.43
23:B:602:CLA:H43	7:H:45:ILE:HG22	2.00	0.43
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.75	0.43
1:a:190[B]:HIS:O	1:a:191:ASN:C	2.61	0.43
27:a:611:PL9:H351	27:a:611:PL9:H371	1.79	0.43
23:B:604:CLA:H101	23:B:615:CLA:H42	1.99	0.43
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.99	0.43
25:C:515:BCR:H20C	25:C:515:BCR:H361	1.88	0.43
6:F:12:SER:N	37:F:203:HOH:O	2.52	0.43
13:O:88:ASN:ND2	13:O:92:SER:OG	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:606:CLA:H203	8:i:9:TYR:HD2	1.82	0.43
23:b:616:CLA:HED2	23:b:616:CLA:CHA	2.48	0.43
5:e:30:LEU:HA	5:e:30:LEU:HD23	1.78	0.43
20:z:8:ALA:O	20:z:11:ALA:HB3	2.19	0.43
1:A:161[B]:TYR:HB3	1:A:162[B]:PRO:HD3	2.00	0.43
13:O:27:ARG:HG3	13:O:27:ARG:HH11	1.84	0.43
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	2.00	0.43
20:Z:55:GLY:HA2	20:Z:58:ASN:HB3	2.01	0.43
20:z:48:ILE:O	20:z:52:LEU:HG	2.19	0.43
27:A:611:PL9:H152	30:A:615:LHG:H381	1.99	0.43
3:C:278:ALA:N	23:C:505:CLA:HBC2	2.34	0.43
13:O:110:MET:HE2	13:O:110:MET:HB3	1.95	0.43
27:a:611:PL9:H301	27:a:611:PL9:H321	1.78	0.43
5:e:22:ILE:HG23	14:r:19:ALA:CB	2.47	0.43
35:f:102:HEM:HMB3	14:r:19:ALA:HB3	1.99	0.43
20:z:12:LEU:HD11	20:z:51:VAL:HG22	1.99	0.43
19:Y:25:ILE:O	19:Y:26:ALA:C	2.60	0.43
20:Z:3:ILE:O	20:Z:7:LEU:HB2	2.19	0.43
31:a:616:DGD:O1B	31:a:616:DGD:O1G	2.36	0.43
2:b:345:VAL:HG13	2:b:353:GLU:OE2	2.19	0.43
5:e:63:ILE:N	5:e:63:ILE:CD1	2.79	0.43
7:h:28:THR:N	7:h:29:PRO:HD2	2.33	0.43
23:h:101:CLA:H93	25:h:102:BCR:H402	2.01	0.43
13:o:54:GLU:HG2	13:o:64:GLU:O	2.19	0.43
13:o:133:VAL:O	13:o:133:VAL:HG12	2.17	0.43
20:z:32:ASP:HB3	20:z:35:ARG:HB3	2.01	0.43
1:A:214:MET:O	1:A:218:LEU:HG	2.17	0.42
2:B:378:LYS:O	2:B:395:GLN:HG3	2.19	0.42
13:O:33:ASP:O	13:O:34:SER:C	2.62	0.42
1:a:79:THR:HG22	4:d:315:TYR:HB2	2.00	0.42
3:c:249:ILE:O	3:c:250:TRP:C	2.60	0.42
30:d:407:LHG:H242	11:l:19:LEU:HD23	2.00	0.42
25:k:101:BCR:H20C	25:k:101:BCR:H361	1.87	0.42
17:v:122:GLU:N	17:v:123:PRO:HD2	2.33	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.37	0.42
4:D:52:THR:CG2	4:D:76:VAL:HG13	2.49	0.42
23:D:403:CLA:H42	7:H:43:LEU:HD11	2.01	0.42
2:b:150:CYS:HB2	23:b:603:CLA:CMC	2.48	0.42
23:b:615:CLA:CBB	23:b:615:CLA:HHC	2.50	0.42
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.54	0.42
2:B:353:GLU:CG	2:B:355:PHE:CZ	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:65:PHE:HE1	23:b:604:CLA:HED2	1.84	0.42
23:c:501:CLA:C2D	23:c:503:CLA:H2	2.49	0.42
13:o:117:PRO:O	13:o:221:SER:HB2	2.19	0.42
20:z:40:ILE:HG13	20:z:41:PHE:N	2.34	0.42
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	2.00	0.42
1:a:235:TYR:OH	11:l:11:GLU:OE2	2.21	0.42
1:a:278:TRP:CD1	1:a:278:TRP:C	2.97	0.42
2:b:42:LEU:HD21	2:b:93:PHE:HB3	2.00	0.42
3:c:60:ILE:HG22	23:c:503:CLA:HHD	2.01	0.42
6:f:40:MET:HA	6:f:43:ILE:HD13	2.01	0.42
9:j:11:TRP:CZ2	9:j:12:ILE:HD11	2.54	0.42
11:l:2:GLU:N	11:l:3:PRO:HD3	2.34	0.42
19:y:19:ILE:HD12	19:y:19:ILE:C	2.45	0.42
24:A:606:PHO:HHD	24:A:606:PHO:HBC2	2.00	0.42
2:B:201:HIS:HB2	23:B:602:CLA:CHB	2.50	0.42
23:B:602:CLA:HBB1	23:B:602:CLA:HMB3	2.00	0.42
14:R:35:LEU:N	14:R:35:LEU:HD23	2.34	0.42
20:Z:36:SER:HA	20:Z:39:LEU:HD12	2.02	0.42
1:a:12:ASN:OD1	1:a:12:ASN:C	2.63	0.42
27:a:611:PL9:H151	30:a:614:LHG:C30	2.48	0.42
2:b:159:THR:O	2:b:180:PRO:HB3	2.19	0.42
2:b:373:LYS:HG3	37:b:705:HOH:O	2.19	0.42
23:b:610:CLA:H202	23:b:612:CLA:HMD3	2.00	0.42
13:o:45:LEU:HD23	13:o:215:PHE:CD2	2.54	0.42
3:C:135:ARG:O	3:C:135:ARG:HD3	2.20	0.42
1:a:334[B]:ARG:HD3	4:d:320:LEU:HD13	2.02	0.42
2:b:154:GLY:O	2:b:159:THR:HG23	2.19	0.42
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.55	0.42
4:d:180:ARG:HD3	4:d:180:ARG:C	2.44	0.42
13:o:81:ILE:HA	13:o:100:GLY:HA3	2.00	0.42
17:v:93:PRO:HA	17:v:101:PHE:CD2	2.55	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.42
17:V:57:GLU:H	17:V:57:GLU:CD	2.27	0.42
20:Z:29:SER:HB3	20:Z:31:GLN:HG3	2.01	0.42
7:h:25:TRP:O	7:h:26:GLY:C	2.61	0.42
25:B:618:BCR:H20C	25:B:618:BCR:H361	1.78	0.42
4:D:235:PHE:CE2	4:D:237:PRO:HA	2.55	0.42
10:K:27:VAL:HG12	10:K:27:VAL:O	2.19	0.42
25:b:617:BCR:H15C	25:b:617:BCR:H351	1.92	0.42
1:a:121:LEU:HD12	1:a:121:LEU:HA	1.92	0.42
1:a:133:LEU:HD23	4:d:256:ILE:HG12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:603:CLA:HBB1	23:a:603:CLA:CMB	2.49	0.42
3:c:462:GLU:HA	3:c:462:GLU:OE2	2.20	0.42
28:c:522:LMG:O9	28:c:522:LMG:C9	2.67	0.42
5:e:76:VAL:O	5:e:80:LEU:HG	2.20	0.42
7:h:36:GLY:O	7:h:40:VAL:HG12	2.19	0.42
2:B:107:LEU:HD23	2:B:107:LEU:HA	1.83	0.42
17:V:89:ALA:HB2	37:V:343:HOH:O	2.19	0.42
28:B:620:LMG:HC92	12:M:6:LEU:HD12	2.02	0.41
3:C:67:MET:HB3	3:C:88:LEU:HD12	2.01	0.41
4:d:21:TRP:HA	4:d:24:ARG:HG3	2.01	0.41
17:v:23:GLU:O	17:v:27:LEU:HG	2.20	0.41
1:A:81:ALA:HB2	1:A:175[A]:GLY:HA3	2.01	0.41
1:A:173[A]:PRO:HB2	1:A:178[A]:GLY:HA3	2.01	0.41
25:A:608:BCR:H11C	25:A:608:BCR:H341	1.78	0.41
3:C:47:GLY:N	3:C:138:GLU:O	2.53	0.41
3:C:465:PRO:O	3:C:469:MET:HG3	2.20	0.41
5:E:36:LEU:O	5:E:40:THR:HG23	2.20	0.41
24:a:605:PHO:H141	23:a:612:CLA:HBB1	2.01	0.41
2:b:99:ALA:HB1	23:b:606:CLA:H72	2.02	0.41
25:b:618:BCR:H20C	25:b:618:BCR:H361	1.90	0.41
7:h:4:ARG:NH2	7:h:9:ASP:OD2	2.46	0.41
19:y:20:ALA:O	19:y:23:THR:HG22	2.20	0.41
23:B:603:CLA:CMD	23:B:606:CLA:HMB2	2.50	0.41
30:D:406:LHG:HC62	11:L:15:THR:HG23	2.00	0.41
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.08	0.41
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.03	0.41
25:a:607:BCR:H20C	25:a:607:BCR:H361	1.91	0.41
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	2.03	0.41
3:c:61:VAL:HG13	3:c:118:HIS:HD2	1.86	0.41
5:e:26:THR:HA	14:r:15:ALA:HB1	2.02	0.41
13:O:93:LEU:O	13:O:128:SER:HA	2.20	0.41
13:O:205:ASP:OD1	13:O:207:ARG:HB2	2.20	0.41
14:R:16:ALA:O	14:R:20:VAL:HG23	2.20	0.41
3:c:258:GLY:HA2	3:c:261:ARG:CZ	2.50	0.41
31:c:518:DGD:HA52	31:c:518:DGD:HA81	1.85	0.41
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.02	0.41
4:d:272:LEU:C	4:d:272:LEU:HD23	2.46	0.41
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.54	0.41
15:t:8:PHE:HD1	25:t:101:BCR:H373	1.84	0.41
1:A:265:PHE:O	27:A:611:PL9:H532	2.21	0.41
27:A:611:PL9:H38	4:D:38:PHE:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:ARG:HG3	2:B:273:TYR:N	2.35	0.41
2:B:284:ILE:O	2:B:288:VAL:HG23	2.21	0.41
2:B:378:LYS:HE2	37:B:705:HOH:O	2.20	0.41
23:B:608:CLA:H43	23:B:609:CLA:H101	2.03	0.41
23:C:501:CLA:HBD	23:C:501:CLA:HAA1	2.02	0.41
5:E:22[A]:ILE:HD11	35:F:102:HEM:CHB	2.51	0.41
20:Z:32:ASP:CG	20:Z:35:ARG:HB3	2.45	0.41
23:b:616:CLA:HBC3	7:h:11:LEU:HD13	2.02	0.41
3:c:154:LYS:HE3	37:c:683:HOH:O	2.19	0.41
4:d:42:TYR:OH	6:f:25:THR:O	2.32	0.41
13:o:149:PRO:HA	13:o:192:LEU:HD12	2.02	0.41
1:A:202:VAL:HG11	23:A:604:CLA:C3D	2.50	0.41
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.02	0.41
3:C:344:SER:O	13:O:75:THR:HG22	2.21	0.41
17:V:28:GLU:HG2	37:V:328:HOH:O	2.21	0.41
4:d:40:CYS:HB3	4:d:117:HIS:O	2.21	0.41
23:h:101:CLA:H91	23:h:101:CLA:H111	1.84	0.41
3:C:62:PHE:C	3:C:62:PHE:CD2	2.98	0.41
3:C:134:ILE:HD13	23:C:511:CLA:H43	2.02	0.41
20:Z:25:VAL:O	20:Z:29:SER:HB2	2.20	0.41
13:o:31:PRO:HA	13:o:135:SER:OG	2.20	0.41
18:x:16:SER:HB3	33:x:101:UNL:C7	2.50	0.41
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.56	0.41
23:A:613:CLA:HBB1	23:A:613:CLA:HMB3	2.03	0.41
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.34	0.41
2:B:318:ASN:OD1	2:B:318:ASN:C	2.64	0.41
3:C:95:LEU:HD21	23:C:501:CLA:OBD	2.21	0.41
3:C:134:ILE:HD11	23:C:511:CLA:H92	2.03	0.41
4:D:38:PHE:N	4:D:39:PRO:CD	2.83	0.41
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.55	0.41
14:R:10:LEU:HD13	14:R:10:LEU:O	2.21	0.41
16:U:53:ALA:HB1	16:U:54:PRO:HA	2.03	0.41
17:V:41:HIS:O	17:V:42:VAL:C	2.61	0.41
1:a:160[A]:ILE:N	1:a:160[A]:ILE:HD13	2.35	0.41
1:a:238:LYS:HG2	1:a:241:GLN:HB3	2.03	0.41
3:c:466:VAL:HG13	4:d:251:ARG:HD2	2.02	0.41
23:c:504:CLA:H91	23:c:508:CLA:C17	2.51	0.41
4:d:267:LEU:C	4:d:267:LEU:CD2	2.92	0.41
29:f:101:SQD:H312	18:x:27:VAL:HG11	2.02	0.41
13:o:42:ARG:O	13:o:241:ALA:HA	2.20	0.41
16:u:66:GLY:O	16:u:67:LEU:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:u:85:THR:HB	37:u:233:HOH:O	2.20	0.41
20:z:32:ASP:HB2	20:z:35:ARG:HB3	2.02	0.41
1:A:85:SER:HA	1:A:109:GLY:HA3	2.03	0.41
23:A:604:CLA:H92	28:D:405:LMG:C25	2.51	0.41
23:A:604:CLA:HED1	31:C:518:DGD:HAH2	2.02	0.41
3:C:66:ALA:HB1	10:K:25:LEU:HB3	2.02	0.41
13:O:189:ARG:NH2	13:O:226:GLY:O	2.54	0.41
23:a:606:CLA:H111	23:a:606:CLA:H41	2.03	0.41
27:a:611:PL9:H303	4:d:45:LEU:CD2	2.50	0.41
2:b:125:ASP:OD2	2:b:127:ARG:HB2	2.21	0.41
23:b:615:CLA:H2	23:b:616:CLA:HBB2	2.02	0.41
3:c:26:ARG:HD3	10:k:46:ARG:NH1	2.35	0.41
3:c:167:VAL:HG22	23:c:512:CLA:H122	2.03	0.41
28:c:522:LMG:O9	28:c:522:LMG:HC91	2.21	0.41
4:d:45:LEU:HD12	4:d:45:LEU:HA	1.74	0.41
10:k:32:PHE:CE2	25:k:102:BCR:C21	3.04	0.41
13:o:173:ALA:C	13:o:175:PRO:HD3	2.46	0.41
1:A:329[A]:GLU:HG3	37:A:789:HOH:O	2.20	0.40
3:C:238:ILE:O	3:C:242:LEU:HG	2.21	0.40
3:c:344:SER:O	13:o:75:THR:HG22	2.21	0.40
4:d:218:VAL:HG22	4:d:244:TYR:CZ	2.57	0.40
13:o:39:ARG:HG2	13:o:244:GLU:O	2.21	0.40
18:x:3:ILE:HD12	18:x:3:ILE:H	1.87	0.40
2:B:26:HIS:O	2:B:30:VAL:HG23	2.20	0.40
3:C:443:TRP:CE2	23:C:508:CLA:HMD2	2.57	0.40
4:D:42:TYR:CE1	6:F:25:THR:CG2	3.04	0.40
13:O:240:TYR:CD2	13:O:240:TYR:C	2.99	0.40
2:b:148:LEU:HD23	2:b:148:LEU:HA	1.90	0.40
3:c:72:LEU:HD22	10:k:10:LYS:O	2.22	0.40
24:d:401:PHO:HBC2	24:d:401:PHO:HHH	2.02	0.40
15:t:14:ILE:HG22	25:t:101:BCR:H10C	2.03	0.40
2:B:53:ASN:N	2:B:54:PRO:CD	2.85	0.40
2:B:433:ASP:OD2	2:B:433:ASP:C	2.62	0.40
4:D:332:GLN:H	4:D:332:GLN:CD	2.29	0.40
10:K:17:ILE:N	10:K:17:ILE:CD1	2.84	0.40
1:a:60[A]:ILE:HG23	1:a:61[A]:ASP:N	2.37	0.40
23:b:605:CLA:HBB1	23:b:605:CLA:HHH	2.03	0.40
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.86	0.40
28:b:621:LMG:C10	28:b:621:LMG:O8	2.69	0.40
13:o:190:PHE:CD1	13:o:190:PHE:C	2.99	0.40
1:A:16:ARG:HG2	37:A:732:HOH:O	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:617:BCR:H371	25:B:617:BCR:H24C	1.83	0.40
25:B:619:BCR:H361	25:B:619:BCR:H20C	1.85	0.40
5:E:22[A]:ILE:HD11	35:F:102:HEM:C4A	2.56	0.40
6:F:15:ILE:HD13	14:R:23:ILE:HD11	2.04	0.40
7:H:11:LEU:O	7:H:12:ARG:C	2.64	0.40
17:V:28:GLU:OE2	17:V:31:ARG:CZ	2.68	0.40
1:a:81:ALA:HA	1:a:174[A]:LEU:O	2.21	0.40
2:b:231:MET:HE2	23:b:610:CLA:HMC2	2.02	0.40
3:c:390:ARG:HD3	17:v:100:ILE:HD12	2.03	0.40
1:A:183[A]:MET:HA	23:A:603:CLA:HMD1	2.03	0.40
1:A:278:TRP:CD1	1:A:278:TRP:C	2.99	0.40
23:A:603:CLA:HBB1	23:A:603:CLA:HMB1	2.04	0.40
2:B:243:ALA:HA	2:B:246:PHE:CE1	2.56	0.40
2:B:346:PHE:HA	2:B:398:THR:O	2.21	0.40
30:D:408:LHG:H341	30:D:408:LHG:H141	2.03	0.40
13:O:33:ASP:C	13:O:35:SER:N	2.75	0.40
36:V:201:HEC:HMD1	37:V:354:HOH:O	2.21	0.40
4:d:161:PRO:CB	4:d:170:ALA:HB2	2.52	0.40
5:e:19:TYR:CE2	5:e:23:HIS:CE1	3.09	0.40
6:f:31:ILE:HA	6:f:34:LEU:HD12	2.02	0.40
14:r:24:LEU:N	14:r:25:PRO:HD2	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:607:HOH:O	37:H:214:HOH:O[4_557]	2.14	0.06

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	390/334 (117%)	380 (97%)	9 (2%)	1 (0%)	36	30
1	a	390/334 (117%)	383 (98%)	7 (2%)	0	100	100
2	B	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
2	b	503/505 (100%)	491 (98%)	11 (2%)	1 (0%)	43	37
3	C	447/451 (99%)	435 (97%)	10 (2%)	2 (0%)	30	22
3	c	457/451 (101%)	439 (96%)	17 (4%)	1 (0%)	43	37
4	D	339/341 (99%)	329 (97%)	10 (3%)	0	100	100
4	d	340/341 (100%)	329 (97%)	11 (3%)	0	100	100
5	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
5	e	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	32 (94%)	1 (3%)	1 (3%)	3	0
9	j	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
10	K	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	3	0
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	m	30/33 (91%)	30 (100%)	0	0	100	100
13	O	243/244 (100%)	226 (93%)	16 (7%)	1 (0%)	30	22
13	o	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	16	9
14	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
14	r	29/34 (85%)	23 (79%)	5 (17%)	1 (3%)	3	0
15	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	v	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Y	25/30 (83%)	17 (68%)	6 (24%)	2 (8%)	1	0
19	y	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	2	0
20	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	0
20	z	60/62 (97%)	50 (83%)	9 (15%)	1 (2%)	7	2
All	All	5365/5326 (101%)	5165 (96%)	183 (3%)	17 (0%)	36	30

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	62	GLU
19	Y	41	VAL
19	Y	43	ARG
3	c	416	SER
13	o	60	ARG
14	r	30	GLN
20	Z	7	LEU
13	o	61	GLN
19	y	43	ARG
20	z	15	LEU
20	Z	6	GLN
2	b	127	ARG
3	C	143	TYR
9	J	6	GLY
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	319/270 (118%)	309 (97%)	10 (3%)	35	30
1	a	318/270 (118%)	304 (96%)	14 (4%)	25	19
2	B	407/403 (101%)	382 (94%)	25 (6%)	17	10
2	b	402/403 (100%)	390 (97%)	12 (3%)	36	32
3	C	351/352 (100%)	342 (97%)	9 (3%)	40	37
3	c	360/352 (102%)	338 (94%)	22 (6%)	17	10
4	D	277/276 (100%)	271 (98%)	6 (2%)	45	44
4	d	278/276 (101%)	270 (97%)	8 (3%)	37	33
5	E	72/72 (100%)	61 (85%)	11 (15%)	3	0
5	e	71/72 (99%)	63 (89%)	8 (11%)	5	1
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	26
6	f	28/28 (100%)	23 (82%)	5 (18%)	2	0
7	H	53/54 (98%)	50 (94%)	3 (6%)	18	11
7	h	53/54 (98%)	48 (91%)	5 (9%)	8	3
8	I	32/32 (100%)	27 (84%)	5 (16%)	2	0
8	i	32/32 (100%)	31 (97%)	1 (3%)	35	30
9	J	24/24 (100%)	23 (96%)	1 (4%)	26	20
9	j	23/24 (96%)	20 (87%)	3 (13%)	4	1
10	K	31/30 (103%)	29 (94%)	2 (6%)	15	9
10	k	30/30 (100%)	22 (73%)	8 (27%)	0	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	1
12	M	28/29 (97%)	26 (93%)	2 (7%)	13	7
12	m	28/29 (97%)	27 (96%)	1 (4%)	31	26
13	O	208/207 (100%)	195 (94%)	13 (6%)	16	9
13	o	207/207 (100%)	196 (95%)	11 (5%)	20	13
14	R	28/29 (97%)	21 (75%)	7 (25%)	0	0
14	r	19/29 (66%)	14 (74%)	5 (26%)	0	0
15	T	26/26 (100%)	22 (85%)	4 (15%)	2	0
15	t	25/26 (96%)	25 (100%)	0	100	100
16	U	84/84 (100%)	79 (94%)	5 (6%)	17	10
16	u	84/84 (100%)	84 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	117/117 (100%)	109 (93%)	8 (7%)	14	8
17	v	117/117 (100%)	112 (96%)	5 (4%)	26	20
18	X	31/31 (100%)	29 (94%)	2 (6%)	15	9
18	x	31/31 (100%)	29 (94%)	2 (6%)	15	9
19	Y	19/23 (83%)	16 (84%)	3 (16%)	2	0
19	y	22/23 (96%)	17 (77%)	5 (23%)	1	0
20	Z	52/52 (100%)	41 (79%)	11 (21%)	1	0
20	z	51/52 (98%)	41 (80%)	10 (20%)	1	0
All	All	4435/4348 (102%)	4178 (94%)	257 (6%)	18	11

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

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	102	LEU
1	A	121	LEU
1	A	183[A]	MET
1	A	183[B]	MET
1	A	205	VAL
1	A	243	GLU
1	A	248	ILE
1	A	270	SER
2	B	63	LEU
2	B	79	SER
2	B	83	GLU
2	B	98	LEU
2	B	127	ARG
2	B	161	LEU
2	B	227	LYS
2	B	289	GLN
2	B	353	GLU
2	B	362	PHE
2	B	371	THR
2	B	389	LYS
2	B	405	GLU
2	B	435	GLU
2	B	436	THR
2	B	476	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	480[A]	SER
2	B	480[B]	SER
2	B	485	GLU
2	B	486	LEU
2	B	489	GLU
2	B	490	GLN
2	B	491	VAL
2	B	492	GLU
2	B	495	PHE
3	C	108	THR
3	C	141	GLU
3	C	161	LEU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	355[A]	THR
3	C	355[B]	THR
3	C	416	SER
4	D	12	ARG
4	D	24	ARG
4	D	43	LEU
4	D	76	VAL
4	D	154	VAL
4	D	259	ILE
5	E	4	THR
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	32	ILE
5	E	54	SER
5	E	65	LEU
5	E	67	THR
5	E	76	VAL
5	E	77	GLU
5	E	83	LEU
6	F	25	THR
7	H	20	LYS
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	33	LYS
8	I	34	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	35	LYS
8	I	36	ASP
9	J	12	ILE
10	K	10	LYS
10	K	25	LEU
12	M	3	VAL
12	M	13	LEU
13	O	23	ASP
13	O	25	THR
13	O	35	SER
13	O	57	LYS
13	O	64	GLU
13	O	78	LEU
13	O	82	GLN
13	O	107	THR
13	O	118	LEU
13	O	134	THR
13	O	135	SER
13	O	198	SER
13	O	214	THR
14	R	6	LEU
14	R	9	LEU
14	R	10	LEU
14	R	13	LEU
14	R	21	ARG
14	R	29	LYS
14	R	35	LEU
15	T	2	GLU
15	T	24	ARG
15	T	25	GLU
15	T	29	ILE
16	U	37	GLN
16	U	39	ARG
16	U	59	GLU
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	14	SER
17	V	17	LYS
17	V	24	LYS
17	V	31	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	V	105	ARG
17	V	106	ASN
18	X	15	LEU
18	X	29	ILE
19	Y	24	MET
19	Y	27	MET
19	Y	43	ARG
20	Z	3	ILE
20	Z	7	LEU
20	Z	15	LEU
20	Z	18	VAL
20	Z	29	SER
20	Z	32	ASP
20	Z	37	LYS
20	Z	40	ILE
20	Z	46	LEU
20	Z	50	LEU
20	Z	61	VAL
1	a	19	ASN
1	a	28	LEU
1	a	35	VAL
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	226	GLU
1	a	229	GLU
1	a	231	GLU
1	a	238	LYS
1	a	245	THR
1	a	286	THR
1	a	288	LEU
1	a	305	SER
2	b	13	ILE
2	b	74	SER
2	b	76	SER
2	b	86	ILE
2	b	149	LEU
2	b	219	VAL
2	b	236	THR
2	b	252	VAL
2	b	294	SER
2	b	362	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	397	VAL
2	b	486	LEU
3	c	24	THR
3	c	25	ASN
3	c	26	ARG
3	c	29	GLU
3	c	30	SER
3	c	72	LEU
3	c	99	VAL
3	c	104	GLU
3	c	124	VAL
3	c	125	LEU
3	c	142	GLU
3	c	155	ASN
3	c	165	LEU
3	c	213	LEU
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	346	THR
3	c	354[A]	GLU
3	c	354[B]	GLU
3	c	462	GLU
3	c	471	SER
4	d	35	ILE
4	d	90	LEU
4	d	182	LEU
4	d	259	ILE
4	d	267	LEU
4	d	291	LEU
4	d	321	LEU
4	d	329	MET
5	e	8	ARG
5	e	39	SER
5	e	54	SER
5	e	61	ARG
5	e	63	ILE
5	e	75	GLN
5	e	82	GLN
5	e	83	LEU
6	f	15	ILE
6	f	23	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	f	28	VAL
6	f	43	ILE
6	f	44	GLN
7	h	3	ARG
7	h	7	LEU
7	h	40	VAL
7	h	43	LEU
7	h	56	ASP
8	i	33	LYS
9	j	7	ARG
9	j	21	VAL
9	j	36	LEU
10	k	10	LYS
10	k	19	ASP
10	k	22	VAL
10	k	24	VAL
10	k	27	VAL
10	k	30	VAL
10	k	35	LEU
10	k	46	ARG
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	49	THR
13	o	57	LYS
13	o	59	LYS
13	o	60	ARG
13	o	118	LEU
13	o	133	VAL
13	o	134	THR
13	o	135	SER
13	o	181	GLU
13	o	198	SER
13	o	207	ARG
14	r	3	TRP
14	r	6	LEU
14	r	9	LEU
14	r	14	LEU
14	r	23	ILE
17	v	6	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	v	15	GLU
17	v	23	GLU
17	v	24	LYS
17	v	90	GLU
18	x	8	LYS
18	x	15	LEU
19	y	19	ILE
19	y	22	LEU
19	y	38	LEU
19	y	45	ASN
19	y	46	LEU
20	z	1	MET
20	z	3	ILE
20	z	7	LEU
20	z	12	LEU
20	z	20	VAL
20	z	29	SER
20	z	32	ASP
20	z	35	ARG
20	z	38	GLN
20	z	46	LEU

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

Mol	Chain	Res	Type
1	A	75	ASN
1	A	261	GLN
2	B	223	GLN
2	B	338	GLN
2	B	394	GLN
2	B	490	GLN
3	C	327	ASN
3	C	382	ASN
4	D	61	HIS
4	D	336	HIS
13	O	82	GLN
13	O	88	ASN
13	O	130	GLN
16	U	73	GLN
18	X	38	GLN
19	Y	21	GLN
19	Y	45	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	Z	6	GLN
1	a	199	GLN
2	b	338	GLN
2	b	409	GLN
3	c	25	ASN
3	c	28	GLN
3	c	201	ASN
3	c	322	GLN
3	c	382	ASN
3	c	418	ASN
4	d	250	ASN
11	l	6	ASN
13	o	58	ASN
13	o	219	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.90	0	8,9,11	1.51	2 (25%)
15	FME	t	1	15	8,9,10	1.16	1 (12%)	8,9,11	1.07	0
15	FME	T	1	15	8,9,10	1.21	1 (12%)	8,9,11	1.87	3 (37%)
12	FME	m	1	12	8,9,10	0.90	0	8,9,11	0.96	1 (12%)
8	FME	i	1	8	8,9,10	1.07	0	8,9,11	1.52	2 (25%)
12	FME	M	1	12	8,9,10	1.00	0	8,9,11	0.73	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
8	FME	I	1	8	-	2/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.75	1.42	1.46
15	T	1	FME	CA-N	-2.10	1.43	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.83	114.96	109.50
15	T	1	FME	CA-N-CN	-2.81	118.50	122.82
15	T	1	FME	C-CA-N	2.71	114.72	109.50
8	I	1	FME	C-CA-N	2.59	114.50	109.50
15	T	1	FME	O1-CN-N	-2.25	119.50	125.32
8	i	1	FME	CA-N-CN	-2.15	119.51	122.82
8	I	1	FME	CB-CA-N	2.07	114.28	110.52
12	m	1	FME	CB-CA-N	2.04	114.23	110.52

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 188 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	f	101	-	39,41,54	1.16	4 (10%)	49,52,65	1.56	9 (18%)
23	CLA	C	504	37	63,67,73	1.38	9 (14%)	74,105,113	1.32	10 (13%)
25	BCR	D	404	-	41,41,41	1.19	2 (4%)	56,56,56	1.19	6 (10%)
31	DGD	C	516	-	63,63,67	1.30	10 (15%)	77,77,81	1.32	8 (10%)
23	CLA	c	513	-	69,73,73	1.41	10 (14%)	82,113,113	1.03	5 (6%)
23	CLA	c	511	3	69,73,73	1.48	9 (13%)	82,113,113	1.31	9 (10%)
23	CLA	B	602	-	69,73,73	1.20	8 (11%)	82,113,113	1.24	10 (12%)
23	CLA	b	608	-	69,73,73	1.23	6 (8%)	82,113,113	1.35	12 (14%)
31	DGD	h	103	-	63,63,67	1.02	2 (3%)	77,77,81	1.42	9 (11%)
28	LMG	D	409	-	31,31,55	1.47	5 (16%)	33,33,63	1.12	4 (12%)
23	CLA	b	612	-	69,73,73	1.18	8 (11%)	82,113,113	1.46	14 (17%)
30	LHG	D	408	-	46,46,48	1.08	3 (6%)	49,52,54	1.38	5 (10%)
36	HEC	v	201	17	46,50,50	1.87	5 (10%)	58,82,82	1.53	6 (10%)
30	LHG	d	407	-	48,48,48	0.96	2 (4%)	51,54,54	1.17	3 (5%)
23	CLA	b	615	-	69,73,73	1.73	10 (14%)	82,113,113	1.49	13 (15%)
28	LMG	D	405	-	51,51,55	1.11	3 (5%)	59,59,63	1.18	5 (8%)
29	SQD	A	614	-	50,52,54	1.09	4 (8%)	60,63,65	2.36	14 (23%)
23	CLA	b	602	-	69,73,73	1.19	8 (11%)	82,113,113	1.52	10 (12%)
25	BCR	A	608	-	41,41,41	1.20	2 (4%)	56,56,56	1.48	11 (19%)
25	BCR	C	514	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	9 (16%)
25	BCR	C	520	-	41,41,41	1.11	4 (9%)	56,56,56	1.22	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DGD	H	102	-	63,63,67	1.54	10 (15%)	77,77,81	1.55	13 (16%)
23	CLA	B	616	-	64,68,73	1.53	9 (14%)	76,107,113	1.43	10 (13%)
23	CLA	d	403	-	69,73,73	1.15	6 (8%)	82,113,113	1.25	10 (12%)
21	OEX	a	601[A]	37,1,3	0,15,15	-	-	-		
23	CLA	B	610	37	69,73,73	1.28	9 (13%)	82,113,113	1.54	11 (13%)
23	CLA	C	507	37	69,73,73	1.12	6 (8%)	82,113,113	1.50	11 (13%)
23	CLA	C	512	-	69,73,73	1.64	11 (15%)	82,113,113	1.36	9 (10%)
35	HEM	F	102	5,6	50,50,50	1.40	8 (16%)	67,82,82	1.17	6 (8%)
23	CLA	A	613	37	69,73,73	1.42	10 (14%)	82,113,113	1.36	8 (9%)
25	BCR	B	617	-	41,41,41	1.20	3 (7%)	56,56,56	1.29	5 (8%)
31	DGD	c	517	-	63,63,67	1.31	11 (17%)	77,77,81	1.45	12 (15%)
31	DGD	C	518	-	63,63,67	0.92	3 (4%)	77,77,81	1.38	9 (11%)
23	CLA	A	607	-	58,62,73	1.62	9 (15%)	68,99,113	1.64	11 (16%)
25	BCR	d	404	-	41,41,41	1.32	3 (7%)	56,56,56	1.27	6 (10%)
23	CLA	C	505	-	69,73,73	1.12	5 (7%)	82,113,113	1.28	10 (12%)
23	CLA	d	402	-	69,73,73	1.41	9 (13%)	82,113,113	1.31	6 (7%)
30	LHG	A	615	-	48,48,48	0.97	3 (6%)	51,54,54	1.17	3 (5%)
25	BCR	c	515	-	41,41,41	1.38	4 (9%)	56,56,56	1.54	14 (25%)
25	BCR	a	607	-	41,41,41	1.22	4 (9%)	56,56,56	1.41	8 (14%)
23	CLA	b	616	-	64,68,73	1.19	8 (12%)	76,107,113	1.47	10 (13%)
30	LHG	a	614	-	41,41,48	0.81	0	44,47,54	1.31	4 (9%)
29	SQD	a	613	-	52,54,54	0.94	3 (5%)	62,65,65	1.89	12 (19%)
27	PL9	A	611	-	55,55,55	0.98	2 (3%)	68,69,69	1.60	13 (19%)
28	LMG	B	622	-	26,26,55	0.91	2 (7%)	26,26,63	1.11	2 (7%)
23	CLA	B	615	-	69,73,73	1.39	12 (17%)	82,113,113	1.37	12 (14%)
23	CLA	c	512	-	69,73,73	1.30	9 (13%)	82,113,113	1.39	9 (10%)
25	BCR	k	102	-	41,41,41	1.01	2 (4%)	56,56,56	1.30	7 (12%)
28	LMG	m	101	-	51,51,55	0.85	2 (3%)	59,59,63	1.57	12 (20%)
23	CLA	a	612	37	69,73,73	1.48	10 (14%)	82,113,113	1.47	9 (10%)
23	CLA	B	609	-	69,73,73	1.42	9 (13%)	82,113,113	1.40	6 (7%)
28	LMG	b	621	-	55,55,55	0.90	2 (3%)	63,63,63	1.39	8 (12%)
23	CLA	a	604	37	69,73,73	1.40	10 (14%)	82,113,113	1.39	12 (14%)
23	CLA	C	511	3	69,73,73	1.64	7 (10%)	82,113,113	1.42	6 (7%)
28	LMG	B	620	-	51,51,55	1.11	4 (7%)	59,59,63	1.49	11 (18%)
29	SQD	b	601	-	47,49,54	0.97	4 (8%)	57,60,65	2.07	14 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	604	-	69,73,73	1.20	9 (13%)	82,113,113	1.52	11 (13%)
31	DGD	a	616	-	43,43,67	1.34	4 (9%)	45,45,81	1.43	5 (11%)
23	CLA	D	402	-	69,73,73	1.31	8 (11%)	82,113,113	1.23	8 (9%)
23	CLA	B	601	37	69,73,73	1.71	9 (13%)	82,113,113	1.71	8 (9%)
28	LMG	C	519	-	48,48,55	1.20	5 (10%)	56,56,63	1.29	4 (7%)
23	CLA	C	506	-	69,73,73	1.66	8 (11%)	82,113,113	1.16	8 (9%)
23	CLA	B	607	37	69,73,73	1.68	11 (15%)	82,113,113	1.17	6 (7%)
30	LHG	L	101	-	48,48,48	0.91	1 (2%)	51,54,54	1.13	3 (5%)
25	BCR	B	619	-	41,41,41	1.29	3 (7%)	56,56,56	1.49	9 (16%)
24	PHO	A	606	-	58,69,69	1.96	11 (18%)	55,99,99	1.28	5 (9%)
27	PL9	D	407	-	55,55,55	1.76	12 (21%)	68,69,69	1.52	12 (17%)
31	DGD	c	518	-	63,63,67	1.11	7 (11%)	77,77,81	1.44	13 (16%)
25	BCR	c	514	-	41,41,41	1.18	3 (7%)	56,56,56	1.37	10 (17%)
27	PL9	d	408	-	55,55,55	1.57	9 (16%)	68,69,69	1.75	15 (22%)
32	OEY	a	618[B]	37,1,3	0,16,16	-	-	-	-	-
31	DGD	A	617	-	67,67,67	1.46	10 (14%)	81,81,81	1.44	12 (14%)
23	CLA	C	508	-	69,73,73	1.15	7 (10%)	82,113,113	1.33	9 (10%)
23	CLA	B	614	-	69,73,73	1.43	7 (10%)	82,113,113	1.44	11 (13%)
29	SQD	a	615	-	35,35,54	1.14	2 (5%)	37,37,65	1.46	7 (18%)
23	CLA	b	607	37	69,73,73	1.15	6 (8%)	82,113,113	1.34	10 (12%)
25	BCR	T	101	-	41,41,41	1.22	5 (12%)	56,56,56	1.41	8 (14%)
23	CLA	h	101	37	69,73,73	1.42	10 (14%)	82,113,113	1.47	13 (15%)
23	CLA	C	502	-	69,73,73	1.33	6 (8%)	82,113,113	1.26	6 (7%)
30	LHG	D	406	-	48,48,48	0.88	1 (2%)	51,54,54	1.30	8 (15%)
23	CLA	B	604	-	69,73,73	1.41	7 (10%)	82,113,113	1.69	8 (9%)
23	CLA	b	610	37	69,73,73	1.26	11 (15%)	82,113,113	1.25	7 (8%)
36	HEC	V	201	17	46,50,50	1.94	10 (21%)	58,82,82	1.35	3 (5%)
23	CLA	b	611	-	69,73,73	1.23	9 (13%)	82,113,113	1.55	19 (23%)
25	BCR	b	617	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	7 (12%)
30	LHG	d	405	-	48,48,48	0.69	0	51,54,54	1.29	4 (7%)
32	OEY	A	618[B]	37,1,3	0,16,16	-	-	-	-	-
23	CLA	b	614	-	69,73,73	1.18	9 (13%)	82,113,113	1.42	12 (14%)
25	BCR	b	619	-	41,41,41	1.20	3 (7%)	56,56,56	1.28	6 (10%)
23	CLA	B	606	-	69,73,73	1.55	10 (14%)	82,113,113	1.55	13 (15%)
29	SQD	A	616	-	38,38,54	1.04	3 (7%)	40,40,65	1.54	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DGD	c	516	-	63,63,67	1.17	7 (11%)	77,77,81	1.35	11 (14%)
30	LHG	B	623	-	48,48,48	0.89	1 (2%)	51,54,54	1.46	9 (17%)
28	LMG	A	612	-	48,48,55	1.02	3 (6%)	56,56,63	1.43	11 (19%)
23	CLA	c	505	-	69,73,73	1.17	9 (13%)	82,113,113	1.43	13 (15%)
25	BCR	B	618	-	41,41,41	1.26	3 (7%)	56,56,56	1.24	6 (10%)
23	CLA	c	510	-	69,73,73	1.23	10 (14%)	82,113,113	1.39	10 (12%)
23	CLA	A	604	37	69,73,73	1.19	5 (7%)	82,113,113	1.32	10 (12%)
24	PHO	d	401	-	58,69,69	2.14	10 (17%)	55,99,99	1.74	13 (23%)
23	CLA	B	603	-	69,73,73	1.33	9 (13%)	82,113,113	1.44	11 (13%)
23	CLA	b	609	-	69,73,73	1.32	8 (11%)	82,113,113	1.32	10 (12%)
23	CLA	C	503	-	69,73,73	1.47	10 (14%)	82,113,113	1.55	13 (15%)
24	PHO	A	605	-	58,69,69	2.00	10 (17%)	55,99,99	1.96	8 (14%)
23	CLA	B	605	-	69,73,73	1.34	7 (10%)	82,113,113	1.58	16 (19%)
23	CLA	B	611	-	69,73,73	1.36	10 (14%)	82,113,113	1.40	11 (13%)
23	CLA	c	503	-	69,73,73	1.33	10 (14%)	82,113,113	1.42	12 (14%)
30	LHG	l	101	-	48,48,48	0.77	2 (4%)	51,54,54	1.33	8 (15%)
23	CLA	b	613	-	69,73,73	1.39	8 (11%)	82,113,113	1.53	14 (17%)
27	PL9	a	611	-	55,55,55	1.13	5 (9%)	68,69,69	1.58	13 (19%)
28	LMG	d	406	-	44,44,55	1.27	4 (9%)	52,52,63	1.34	6 (11%)
23	CLA	b	603	-	69,73,73	1.32	8 (11%)	82,113,113	1.42	12 (14%)
25	BCR	h	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.48	11 (19%)
23	CLA	C	501	-	69,73,73	1.46	11 (15%)	82,113,113	1.54	12 (14%)
28	LMG	d	410	-	21,21,55	0.75	0	20,20,63	1.03	0
23	CLA	c	509	-	69,73,73	1.14	5 (7%)	82,113,113	1.45	12 (14%)
23	CLA	C	509	-	69,73,73	1.45	8 (11%)	82,113,113	1.18	6 (7%)
29	SQD	B	624	-	52,54,54	0.92	3 (5%)	62,65,65	1.72	13 (20%)
23	CLA	b	605	-	69,73,73	1.24	8 (11%)	82,113,113	1.67	16 (19%)
34	BCT	a	610	22	3,3,3	1.31	0	2,3,3	2.62	1 (50%)
23	CLA	c	508	-	68,72,73	1.32	10 (14%)	80,111,113	1.18	10 (12%)
25	BCR	k	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.10	4 (7%)
35	HEM	f	102	5,6	50,50,50	1.40	6 (12%)	67,82,82	1.14	4 (5%)
23	CLA	c	504	37	64,68,73	1.33	6 (9%)	76,107,113	1.30	8 (10%)
23	CLA	A	603	-	69,73,73	1.37	14 (20%)	82,113,113	1.21	9 (10%)
25	BCR	H	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.50	9 (16%)
25	BCR	Y	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCT	D	401	22	3,3,3	1.04	0	2,3,3	3.28	2 (100%)
28	LMG	c	522	-	49,49,55	1.04	2 (4%)	57,57,63	1.32	4 (7%)
25	BCR	t	101	-	41,41,41	1.17	4 (9%)	56,56,56	1.60	13 (23%)
23	CLA	a	606	-	69,73,73	1.44	13 (18%)	82,113,113	1.50	7 (8%)
23	CLA	C	513	-	69,73,73	1.29	9 (13%)	82,113,113	1.32	7 (8%)
29	SQD	F	101	-	34,36,54	1.07	3 (8%)	42,45,65	1.86	10 (23%)
31	DGD	C	517	-	63,63,67	1.24	6 (9%)	77,77,81	1.58	12 (15%)
23	CLA	c	502	-	69,73,73	1.08	6 (8%)	82,113,113	1.64	12 (14%)
23	CLA	B	608	-	69,73,73	1.03	3 (4%)	82,113,113	1.43	8 (9%)
23	CLA	b	606	-	69,73,73	1.47	8 (11%)	82,113,113	1.44	7 (8%)
23	CLA	a	603	-	69,73,73	1.44	8 (11%)	82,113,113	1.60	11 (13%)
28	LMG	c	521	-	48,48,55	1.18	5 (10%)	56,56,63	1.34	6 (10%)
23	CLA	c	501	-	69,73,73	1.36	10 (14%)	82,113,113	1.69	17 (20%)
23	CLA	B	613	-	69,73,73	1.27	8 (11%)	82,113,113	1.34	9 (10%)
25	BCR	b	618	-	41,41,41	1.39	4 (9%)	56,56,56	1.31	10 (17%)
23	CLA	c	507	37	69,73,73	1.29	10 (14%)	82,113,113	1.60	12 (14%)
21	OEX	A	601[A]	37,1,3	0,15,15	-	-	-	-	-
25	BCR	C	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.20	6 (10%)
24	PHO	a	605	-	58,69,69	2.04	12 (20%)	55,99,99	1.56	6 (10%)
23	CLA	D	403	-	69,73,73	1.65	9 (13%)	82,113,113	1.15	11 (13%)
23	CLA	C	510	-	69,73,73	1.26	13 (18%)	82,113,113	1.41	9 (10%)
30	LHG	d	409	-	38,38,48	0.98	1 (2%)	41,44,54	1.27	4 (9%)
28	LMG	c	519	-	37,37,55	1.21	3 (8%)	45,45,63	1.22	4 (8%)
23	CLA	B	612	-	69,73,73	1.15	5 (7%)	82,113,113	1.38	8 (9%)
23	CLA	c	506	-	69,73,73	1.83	9 (13%)	82,113,113	1.38	11 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	f	101	-	-	18/36/56/69	0/1/1/1
23	CLA	C	504	37	1/1/18/20	8/32/108/115	-
25	BCR	D	404	-	-	7/29/63/63	0/2/2/2
31	DGD	C	516	-	-	18/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	513	-	1/1/20/20	4/39/115/115	-
23	CLA	c	511	3	1/1/20/20	10/39/115/115	-
23	CLA	B	602	-	1/1/20/20	4/39/115/115	-
23	CLA	b	608	-	-	8/39/115/115	-
31	DGD	h	103	-	-	18/51/91/95	0/2/2/2
28	LMG	D	409	-	-	17/33/33/70	-
23	CLA	b	612	-	1/1/20/20	6/39/115/115	-
30	LHG	D	408	-	-	20/51/51/53	-
36	HEC	v	201	17	-	6/14/54/54	-
30	LHG	d	407	-	-	19/53/53/53	-
23	CLA	b	615	-	1/1/20/20	8/39/115/115	-
28	LMG	D	405	-	-	17/46/66/70	0/1/1/1
29	SQD	A	614	-	-	23/47/67/69	0/1/1/1
23	CLA	b	602	-	1/1/20/20	6/39/115/115	-
25	BCR	A	608	-	-	6/29/63/63	0/2/2/2
25	BCR	C	514	-	-	7/29/63/63	0/2/2/2
25	BCR	C	520	-	-	7/29/63/63	0/2/2/2
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
23	CLA	B	616	-	1/1/19/20	9/33/109/115	-
23	CLA	d	403	-	-	6/39/115/115	-
23	CLA	B	610	37	1/1/20/20	5/39/115/115	-
23	CLA	C	507	37	1/1/20/20	10/39/115/115	-
23	CLA	C	512	-	1/1/20/20	14/39/115/115	-
35	HEM	F	102	5,6	-	2/14/54/54	-
23	CLA	A	613	37	-	2/39/115/115	-
25	BCR	B	617	-	-	5/29/63/63	0/2/2/2
31	DGD	c	517	-	-	20/51/91/95	0/2/2/2
31	DGD	C	518	-	-	17/51/91/95	0/2/2/2
23	CLA	A	607	-	1/1/17/20	3/26/102/115	-
25	BCR	d	404	-	-	8/29/63/63	0/2/2/2
23	CLA	C	505	-	1/1/20/20	11/39/115/115	-
23	CLA	d	402	-	1/1/20/20	11/39/115/115	-
30	LHG	A	615	-	-	27/53/53/53	-
25	BCR	c	515	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	a	607	-	-	3/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/19/20	6/33/109/115	-
30	LHG	a	614	-	-	28/46/46/53	-
29	SQD	a	613	-	-	25/49/69/69	0/1/1/1
27	PL9	A	611	-	-	28/53/73/73	0/1/1/1
28	LMG	B	622	-	-	11/22/22/70	-
23	CLA	B	615	-	1/1/20/20	11/39/115/115	-
23	CLA	c	512	-	1/1/20/20	15/39/115/115	-
25	BCR	k	102	-	-	3/29/63/63	0/2/2/2
28	LMG	m	101	-	-	20/46/66/70	0/1/1/1
23	CLA	a	612	37	1/1/20/20	1/39/115/115	-
23	CLA	B	609	-	-	5/39/115/115	-
28	LMG	b	621	-	-	16/50/70/70	0/1/1/1
23	CLA	a	604	37	-	10/39/115/115	-
23	CLA	C	511	3	1/1/20/20	7/39/115/115	-
28	LMG	B	620	-	-	22/46/66/70	0/1/1/1
29	SQD	b	601	-	-	18/44/64/69	0/1/1/1
23	CLA	b	604	-	1/1/20/20	10/39/115/115	-
31	DGD	a	616	-	-	26/45/45/95	-
23	CLA	D	402	-	-	6/39/115/115	-
23	CLA	B	601	37	1/1/20/20	16/39/115/115	-
28	LMG	C	519	-	-	15/43/63/70	0/1/1/1
23	CLA	C	506	-	-	11/39/115/115	-
23	CLA	B	607	37	1/1/20/20	11/39/115/115	-
30	LHG	L	101	-	-	18/53/53/53	-
25	BCR	B	619	-	-	8/29/63/63	0/2/2/2
24	PHO	A	606	-	-	4/37/103/103	0/5/6/6
27	PL9	D	407	-	-	11/53/73/73	0/1/1/1
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
25	BCR	c	514	-	-	16/29/63/63	0/2/2/2
27	PL9	d	408	-	-	20/53/73/73	0/1/1/1
31	DGD	A	617	-	-	24/55/95/95	0/2/2/2
23	CLA	C	508	-	-	9/39/115/115	-
23	CLA	B	614	-	1/1/20/20	14/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	a	615	-	-	18/37/37/69	-
23	CLA	b	607	37	1/1/20/20	12/39/115/115	-
25	BCR	T	101	-	-	10/29/63/63	0/2/2/2
23	CLA	h	101	37	1/1/20/20	19/39/115/115	-
23	CLA	C	502	-	1/1/20/20	7/39/115/115	-
30	LHG	D	406	-	-	20/53/53/53	-
23	CLA	B	604	-	1/1/20/20	7/39/115/115	-
23	CLA	b	610	37	1/1/20/20	8/39/115/115	-
36	HEC	V	201	17	-	6/14/54/54	-
23	CLA	b	611	-	1/1/20/20	6/39/115/115	-
25	BCR	b	617	-	-	0/29/63/63	0/2/2/2
30	LHG	d	405	-	-	24/53/53/53	-
23	CLA	b	614	-	1/1/20/20	16/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	B	606	-	1/1/20/20	7/39/115/115	-
29	SQD	A	616	-	-	17/39/39/69	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
30	LHG	B	623	-	-	15/53/53/53	-
28	LMG	A	612	-	-	21/43/63/70	0/1/1/1
23	CLA	c	505	-	1/1/20/20	8/39/115/115	-
25	BCR	B	618	-	-	5/29/63/63	0/2/2/2
23	CLA	c	510	-	1/1/20/20	12/39/115/115	-
23	CLA	A	604	37	-	6/39/115/115	-
24	PHO	d	401	-	-	7/37/103/103	0/5/6/6
23	CLA	B	603	-	1/1/20/20	14/39/115/115	-
23	CLA	b	609	-	1/1/20/20	13/39/115/115	-
23	CLA	C	503	-	1/1/20/20	3/39/115/115	-
24	PHO	A	605	-	-	5/37/103/103	0/5/6/6
23	CLA	B	605	-	-	10/39/115/115	-
23	CLA	B	611	-	-	8/39/115/115	-
23	CLA	c	503	-	1/1/20/20	7/39/115/115	-
30	LHG	l	101	-	-	19/53/53/53	-
23	CLA	b	613	-	1/1/20/20	8/39/115/115	-
27	PL9	a	611	-	-	25/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	d	406	-	-	13/39/59/70	0/1/1/1
23	CLA	b	603	-	1/1/20/20	8/39/115/115	-
25	BCR	h	102	-	-	11/29/63/63	0/2/2/2
23	CLA	C	501	-	1/1/20/20	4/39/115/115	-
28	LMG	d	410	-	-	10/17/17/70	-
23	CLA	c	509	-	1/1/20/20	12/39/115/115	-
23	CLA	C	509	-	1/1/20/20	14/39/115/115	-
29	SQD	B	624	-	-	23/49/69/69	0/1/1/1
23	CLA	b	605	-	1/1/20/20	5/39/115/115	-
23	CLA	c	508	-	1/1/19/20	9/38/114/115	-
25	BCR	k	101	-	-	9/29/63/63	0/2/2/2
35	HEM	f	102	5,6	-	3/14/54/54	-
23	CLA	c	504	37	1/1/19/20	8/33/109/115	-
23	CLA	A	603	-	1/1/20/20	2/39/115/115	-
25	BCR	H	101	-	-	6/29/63/63	0/2/2/2
25	BCR	Y	101	-	-	12/29/63/63	0/2/2/2
28	LMG	c	522	-	-	25/44/64/70	0/1/1/1
25	BCR	t	101	-	-	9/29/63/63	0/2/2/2
23	CLA	a	606	-	1/1/20/20	10/39/115/115	-
23	CLA	C	513	-	1/1/20/20	7/39/115/115	-
29	SQD	F	101	-	-	16/28/48/69	0/1/1/1
31	DGD	C	517	-	-	21/51/91/95	0/2/2/2
23	CLA	c	502	-	-	3/39/115/115	-
23	CLA	b	606	-	1/1/20/20	11/39/115/115	-
23	CLA	B	608	-	-	1/39/115/115	-
23	CLA	a	603	-	1/1/20/20	1/39/115/115	-
28	LMG	c	521	-	-	20/43/63/70	0/1/1/1
23	CLA	c	501	-	1/1/20/20	5/39/115/115	-
23	CLA	B	613	-	1/1/20/20	7/39/115/115	-
25	BCR	b	618	-	-	6/29/63/63	0/2/2/2
23	CLA	c	507	37	1/1/20/20	10/39/115/115	-
25	BCR	C	515	-	-	6/29/63/63	0/2/2/2
24	PHO	a	605	-	-	8/37/103/103	0/5/6/6
23	CLA	D	403	-	1/1/20/20	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	510	-	1/1/20/20	5/39/115/115	-
30	LHG	d	409	-	-	13/43/43/53	-
28	LMG	c	519	-	-	10/31/51/70	0/1/1/1
23	CLA	B	612	-	1/1/20/20	11/39/115/115	-
23	CLA	c	506	-	1/1/20/20	18/39/115/115	-

All (918) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	MG-ND	-10.99	1.84	2.05
23	b	615	CLA	MG-NA	9.73	2.29	2.06
24	d	401	PHO	C1B-C2B	9.70	1.50	1.39
23	C	511	CLA	MG-NA	9.42	2.28	2.06
24	a	605	PHO	C1B-C2B	9.27	1.49	1.39
24	d	401	PHO	C3B-C4B	8.71	1.50	1.41
24	A	605	PHO	C1B-C2B	8.43	1.48	1.39
24	A	606	PHO	C1B-C2B	7.84	1.48	1.39
23	C	509	CLA	MG-NB	-7.69	1.90	2.05
23	C	512	CLA	MG-NB	7.53	2.20	2.05
23	B	601	CLA	MG-ND	-7.49	1.90	2.05
23	B	614	CLA	MG-ND	-7.42	1.91	2.05
23	B	607	CLA	MG-NB	-7.36	1.91	2.05
24	a	605	PHO	C3B-C4B	7.33	1.48	1.41
24	A	605	PHO	C3B-C4B	7.23	1.48	1.41
23	D	403	CLA	MG-ND	-7.12	1.91	2.05
24	A	606	PHO	C3B-C4B	7.07	1.48	1.41
23	C	506	CLA	MG-NB	7.04	2.19	2.05
23	A	607	CLA	MG-ND	-6.81	1.92	2.05
23	C	512	CLA	MG-ND	-6.72	1.92	2.05
23	b	606	CLA	MG-NA	6.63	2.22	2.06
31	A	617	DGD	C4D-C5D	6.62	1.67	1.53
23	a	612	CLA	MG-NA	6.61	2.22	2.06
23	B	601	CLA	MG-NA	6.61	2.22	2.06
23	a	603	CLA	MG-NA	6.60	2.22	2.06
23	B	606	CLA	MG-NA	6.50	2.21	2.06
23	B	604	CLA	MG-NA	6.45	2.21	2.06
36	v	201	HEC	CAC-C3C	6.27	1.55	1.35
36	v	201	HEC	CAB-C3B	6.27	1.55	1.35
36	V	201	HEC	CAC-C3C	6.10	1.54	1.35
23	a	606	CLA	MG-ND	-6.01	1.93	2.05
31	H	102	DGD	O5D-C1E	5.93	1.50	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	408	PL9	C6-C1	-5.90	1.38	1.48
23	C	506	CLA	MG-ND	-5.85	1.94	2.05
36	V	201	HEC	CAB-C3B	5.76	1.53	1.35
23	c	511	CLA	MG-NC	5.76	2.20	2.06
27	D	407	PL9	C6-C1	-5.60	1.39	1.48
28	d	406	LMG	O7-C8	-5.57	1.33	1.46
23	B	603	CLA	MG-NB	5.54	2.16	2.05
23	C	502	CLA	MG-ND	5.48	2.16	2.05
23	C	501	CLA	MG-NA	5.48	2.19	2.06
23	B	605	CLA	MG-NB	5.48	2.16	2.05
23	c	513	CLA	MG-NB	-5.37	1.95	2.05
23	b	609	CLA	MG-NA	5.35	2.19	2.06
23	a	604	CLA	MG-NC	5.33	2.18	2.06
23	d	402	CLA	MG-NB	-5.31	1.95	2.05
23	c	504	CLA	MG-ND	-5.30	1.95	2.05
23	h	101	CLA	MG-NA	5.27	2.18	2.06
23	C	503	CLA	MG-NB	5.25	2.16	2.05
23	b	613	CLA	MG-NA	5.23	2.18	2.06
23	c	513	CLA	MG-NA	5.11	2.18	2.06
23	A	613	CLA	MG-NA	5.11	2.18	2.06
23	B	616	CLA	MG-NA	5.05	2.18	2.06
27	d	408	PL9	C3-C4	-4.89	1.41	1.49
25	C	515	BCR	C1-C6	-4.87	1.47	1.53
23	B	609	CLA	MG-NA	4.87	2.17	2.06
25	d	404	BCR	C1-C6	-4.83	1.47	1.53
23	D	402	CLA	MG-NB	-4.77	1.96	2.05
23	b	615	CLA	MG-NC	-4.77	1.94	2.06
25	H	101	BCR	C30-C25	-4.73	1.47	1.53
23	C	504	CLA	MG-NC	-4.72	1.95	2.06
23	B	616	CLA	MG-NB	-4.70	1.96	2.05
23	B	611	CLA	MG-NA	4.61	2.17	2.06
23	C	513	CLA	MG-NA	4.60	2.17	2.06
23	B	607	CLA	MG-NC	4.59	2.17	2.06
25	B	619	BCR	C1-C6	-4.56	1.47	1.53
24	A	605	PHO	C4D-ND	-4.55	1.31	1.38
25	b	618	BCR	C30-C25	-4.53	1.48	1.53
23	D	403	CLA	MG-NB	-4.52	1.96	2.05
23	b	603	CLA	MG-NB	-4.46	1.96	2.05
27	D	407	PL9	C11-C9	-4.46	1.42	1.51
25	c	515	BCR	C30-C25	-4.45	1.48	1.53
23	A	613	CLA	C1D-ND	4.44	1.43	1.37
25	B	617	BCR	C1-C6	-4.43	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	MG-NB	4.43	2.14	2.05
23	B	613	CLA	MG-ND	-4.41	1.97	2.05
23	D	403	CLA	C1D-ND	4.41	1.43	1.37
23	c	511	CLA	MG-NA	4.37	2.16	2.06
23	B	606	CLA	MG-NC	-4.37	1.95	2.06
23	c	508	CLA	MG-NB	4.36	2.14	2.05
25	D	404	BCR	C30-C25	-4.35	1.48	1.53
25	C	514	BCR	C1-C6	-4.34	1.48	1.53
23	c	501	CLA	MG-NB	-4.29	1.97	2.05
23	b	606	CLA	C1D-ND	4.28	1.43	1.37
23	c	507	CLA	MG-NA	4.24	2.16	2.06
25	h	102	BCR	C30-C25	-4.23	1.48	1.53
30	D	408	LHG	P-O6	4.22	1.75	1.59
31	C	516	DGD	O5D-C6D	-4.22	1.36	1.43
23	C	501	CLA	MG-ND	-4.21	1.97	2.05
23	B	609	CLA	MG-NB	-4.20	1.97	2.05
23	B	607	CLA	MG-NA	4.18	2.16	2.06
23	C	506	CLA	MG-NC	-4.16	1.96	2.06
23	A	607	CLA	C1D-ND	4.16	1.43	1.37
25	b	619	BCR	C1-C6	-4.13	1.48	1.53
23	c	506	CLA	C1D-ND	4.13	1.43	1.37
35	f	102	HEM	FE-NA	4.12	2.08	1.95
23	B	616	CLA	C1D-ND	4.11	1.43	1.37
23	B	607	CLA	C1D-ND	4.10	1.43	1.37
24	d	401	PHO	C1D-C2D	4.09	1.44	1.39
28	C	519	LMG	O7-C8	-4.07	1.37	1.46
27	D	407	PL9	C52-C5	-4.07	1.42	1.50
31	a	616	DGD	O2G-C1B	4.07	1.45	1.34
25	B	618	BCR	C30-C25	-4.06	1.48	1.53
31	C	517	DGD	C4D-C3D	4.05	1.62	1.52
31	c	516	DGD	O2E-C2E	-4.01	1.33	1.43
23	C	507	CLA	MG-NA	4.00	2.15	2.06
23	C	509	CLA	C1D-ND	4.00	1.43	1.37
23	C	504	CLA	MG-NA	3.99	2.15	2.06
30	L	101	LHG	O7-C5	-3.99	1.37	1.46
28	D	409	LMG	C7-C8	3.98	1.60	1.51
24	a	605	PHO	C1D-C2D	3.97	1.43	1.39
23	b	613	CLA	MG-NC	-3.97	1.96	2.06
23	c	503	CLA	MG-NC	3.96	2.15	2.06
23	C	508	CLA	MG-ND	3.96	2.13	2.05
23	D	402	CLA	C1D-ND	3.96	1.43	1.37
25	A	608	BCR	C1-C6	-3.95	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	C1D-ND	3.94	1.43	1.37
23	A	607	CLA	MG-NC	-3.93	1.96	2.06
28	c	521	LMG	O1-C1	3.93	1.46	1.40
23	B	609	CLA	C1D-ND	3.91	1.43	1.37
23	c	512	CLA	MG-NC	3.90	2.15	2.06
23	D	403	CLA	MG-NC	3.89	2.15	2.06
31	H	102	DGD	C4D-C5D	3.89	1.61	1.53
25	Y	101	BCR	C30-C25	-3.88	1.48	1.53
23	B	610	CLA	MG-ND	-3.88	1.98	2.05
23	c	501	CLA	C1D-ND	3.87	1.42	1.37
25	b	617	BCR	C30-C25	-3.84	1.48	1.53
23	A	604	CLA	C1D-ND	3.81	1.42	1.37
24	A	606	PHO	C1D-C2D	3.79	1.43	1.39
23	c	501	CLA	MG-NA	3.79	2.15	2.06
28	D	405	LMG	C4-C3	3.77	1.62	1.52
25	c	515	BCR	C1-C6	-3.77	1.49	1.53
25	T	101	BCR	C30-C25	-3.76	1.49	1.53
29	a	615	SQD	O47-C7	3.76	1.44	1.34
23	B	616	CLA	MG-ND	3.75	2.13	2.05
23	C	502	CLA	MG-NB	-3.75	1.98	2.05
25	b	618	BCR	C1-C6	-3.74	1.49	1.53
25	Y	101	BCR	C1-C6	-3.73	1.49	1.53
29	a	615	SQD	O48-C23	3.72	1.44	1.33
23	a	604	CLA	C1D-ND	3.72	1.42	1.37
23	b	609	CLA	C4B-NB	3.72	1.42	1.37
31	c	517	DGD	O3G-C1D	-3.72	1.34	1.40
23	b	603	CLA	C1D-ND	3.72	1.42	1.37
25	C	520	BCR	C30-C25	-3.72	1.49	1.53
25	c	514	BCR	C1-C6	-3.71	1.49	1.53
23	a	603	CLA	C1D-ND	3.67	1.42	1.37
23	d	402	CLA	MG-NC	3.66	2.15	2.06
23	B	606	CLA	MG-ND	3.66	2.13	2.05
23	b	605	CLA	C1D-ND	3.64	1.42	1.37
36	V	201	HEC	CBC-CAC	-3.64	1.36	1.49
29	a	613	SQD	O48-C23	3.63	1.43	1.33
23	b	610	CLA	C1D-ND	3.60	1.42	1.37
36	V	201	HEC	CBB-CAB	-3.60	1.36	1.49
31	C	517	DGD	O3D-C3D	-3.59	1.34	1.43
23	C	501	CLA	C1D-ND	3.59	1.42	1.37
23	c	510	CLA	MG-NC	-3.59	1.97	2.06
25	d	404	BCR	C30-C25	-3.58	1.49	1.53
25	A	608	BCR	C33-C5	-3.57	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	MG-NA	3.56	2.14	2.06
23	B	610	CLA	C4B-NB	3.56	1.42	1.37
23	a	603	CLA	C1B-C2B	3.55	1.51	1.43
23	b	610	CLA	MG-NB	-3.54	1.98	2.05
31	C	516	DGD	C4E-C3E	3.51	1.61	1.52
23	A	603	CLA	C1B-C2B	3.51	1.51	1.43
23	B	601	CLA	C4B-NB	3.49	1.42	1.37
27	D	407	PL9	C5-C4	-3.49	1.35	1.47
31	c	517	DGD	O5D-C1E	3.48	1.46	1.40
23	C	503	CLA	MG-NC	3.48	2.14	2.06
23	B	610	CLA	C1D-ND	3.48	1.42	1.37
31	C	518	DGD	O2G-C2G	-3.48	1.38	1.46
23	B	604	CLA	MG-NB	3.47	2.12	2.05
24	A	605	PHO	CMC-C2C	-3.47	1.45	1.50
23	C	511	CLA	C1D-ND	3.47	1.42	1.37
23	c	511	CLA	C4B-NB	3.47	1.42	1.37
23	B	614	CLA	C4B-NB	3.47	1.42	1.37
36	v	201	HEC	CBB-CAB	-3.46	1.36	1.49
24	A	606	PHO	C4D-ND	-3.46	1.33	1.38
23	c	507	CLA	C1B-C2B	3.46	1.51	1.43
23	D	403	CLA	CMD-C2D	-3.45	1.43	1.50
23	b	608	CLA	CHC-C1C	3.45	1.45	1.38
36	v	201	HEC	CBC-CAC	-3.44	1.36	1.49
30	D	406	LHG	O8-C6	-3.43	1.37	1.45
23	A	603	CLA	MG-ND	-3.43	1.99	2.05
23	h	101	CLA	C1D-ND	3.43	1.42	1.37
31	H	102	DGD	O2D-C2D	-3.42	1.34	1.43
23	a	603	CLA	MG-NB	3.42	2.12	2.05
25	C	514	BCR	C30-C25	-3.41	1.49	1.53
23	c	511	CLA	CHC-C1C	3.40	1.45	1.38
23	b	602	CLA	C1D-ND	3.40	1.42	1.37
25	B	618	BCR	C1-C6	-3.40	1.49	1.53
23	A	604	CLA	MG-NB	-3.39	1.99	2.05
29	F	101	SQD	O48-C23	3.39	1.43	1.33
25	a	607	BCR	C30-C25	-3.38	1.49	1.53
29	b	601	SQD	O48-C23	3.36	1.43	1.33
23	B	615	CLA	MG-NA	3.36	2.14	2.06
25	b	617	BCR	C1-C6	-3.36	1.49	1.53
29	f	101	SQD	O47-C7	3.35	1.43	1.34
27	a	611	PL9	C53-C6	-3.35	1.43	1.50
23	c	512	CLA	MG-NB	3.35	2.12	2.05
23	C	507	CLA	C1B-NB	-3.34	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	620	LMG	O1-C7	-3.34	1.38	1.43
28	c	522	LMG	C4-C5	3.33	1.60	1.53
23	B	605	CLA	C1B-C2B	3.33	1.50	1.43
23	A	613	CLA	CHC-C1C	3.32	1.45	1.38
23	b	616	CLA	CMB-C2B	-3.32	1.44	1.50
23	C	508	CLA	MG-NB	-3.32	1.99	2.05
31	A	617	DGD	C4D-C3D	3.32	1.60	1.52
31	a	616	DGD	O1G-C1A	3.30	1.43	1.33
23	b	607	CLA	MG-NA	3.30	2.14	2.06
23	B	611	CLA	MG-ND	3.30	2.12	2.05
23	c	504	CLA	C1B-NB	-3.29	1.33	1.37
23	C	501	CLA	C4B-NB	3.29	1.42	1.37
23	b	611	CLA	CHC-C1C	3.29	1.45	1.38
23	a	612	CLA	CMD-C2D	-3.29	1.44	1.50
25	h	102	BCR	C1-C6	-3.28	1.49	1.53
25	T	101	BCR	C1-C6	-3.27	1.49	1.53
29	A	616	SQD	O48-C23	3.26	1.42	1.33
23	B	615	CLA	C4B-NB	3.25	1.42	1.37
24	a	605	PHO	CMC-C2C	-3.25	1.45	1.50
28	D	409	LMG	C9-C8	3.25	1.61	1.50
31	H	102	DGD	O1G-C1G	-3.24	1.37	1.45
23	C	506	CLA	C1D-ND	3.24	1.42	1.37
23	B	614	CLA	MG-NA	3.24	2.14	2.06
25	c	515	BCR	C33-C5	-3.23	1.45	1.50
23	b	611	CLA	C1B-C2B	3.23	1.50	1.43
29	f	101	SQD	O48-C23	3.22	1.42	1.33
30	D	408	LHG	O3-C3	-3.22	1.32	1.44
23	B	607	CLA	C1C-NC	-3.22	1.32	1.37
25	t	101	BCR	C1-C6	-3.21	1.49	1.53
23	B	613	CLA	C4B-NB	3.21	1.42	1.37
23	C	511	CLA	C1B-C2B	3.21	1.50	1.43
23	d	403	CLA	CMD-C2D	-3.21	1.44	1.50
23	B	606	CLA	MG-NB	3.21	2.12	2.05
23	A	604	CLA	MG-NA	3.20	2.13	2.06
23	C	513	CLA	MG-NB	-3.20	1.99	2.05
24	A	605	PHO	C3D-C4D	3.20	1.45	1.41
31	A	617	DGD	C1E-C2E	3.19	1.61	1.52
27	d	408	PL9	C53-C6	-3.19	1.44	1.50
23	d	402	CLA	C1D-ND	3.19	1.42	1.37
31	A	617	DGD	O6D-C1D	3.18	1.50	1.41
23	b	603	CLA	CMC-C2C	-3.17	1.44	1.50
28	B	620	LMG	C9-C8	3.17	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	614	SQD	O48-C23	3.17	1.42	1.33
23	d	402	CLA	MG-ND	3.16	2.12	2.05
27	D	407	PL9	C36-C37	-3.15	1.43	1.53
23	C	505	CLA	C1D-ND	3.15	1.42	1.37
31	c	518	DGD	C6D-C5D	3.15	1.61	1.51
23	h	101	CLA	C1B-C2B	3.14	1.50	1.43
23	b	614	CLA	MG-NA	3.14	2.13	2.06
23	B	604	CLA	C1D-ND	3.12	1.42	1.37
23	a	612	CLA	C1B-C2B	3.12	1.50	1.43
23	b	611	CLA	C4B-NB	3.12	1.42	1.37
23	B	615	CLA	CMB-C2B	-3.12	1.44	1.50
35	F	102	HEM	FE-NB	3.12	2.04	1.94
23	C	510	CLA	MG-NB	3.11	2.12	2.05
23	b	613	CLA	MG-ND	-3.11	1.99	2.05
25	k	101	BCR	C1-C6	-3.11	1.49	1.53
23	c	503	CLA	C4B-NB	3.10	1.41	1.37
23	D	402	CLA	CMD-C2D	-3.10	1.44	1.50
23	C	511	CLA	C4B-NB	3.10	1.41	1.37
27	D	407	PL9	C46-C44	-3.09	1.44	1.51
31	C	517	DGD	O2G-C2G	-3.09	1.39	1.46
24	A	605	PHO	C3D-CAD	-3.08	1.41	1.47
27	A	611	PL9	C7-C3	-3.08	1.47	1.51
23	B	611	CLA	C1B-C2B	3.08	1.50	1.43
23	C	503	CLA	MG-NA	3.08	2.13	2.06
28	c	519	LMG	C4-C3	3.07	1.60	1.52
23	c	512	CLA	C1B-C2B	3.07	1.50	1.43
25	a	607	BCR	C1-C6	-3.07	1.49	1.53
29	A	616	SQD	O47-C7	3.06	1.42	1.34
23	c	507	CLA	MG-NC	-3.06	1.99	2.06
23	C	510	CLA	C1D-ND	3.05	1.41	1.37
23	b	609	CLA	C1D-ND	3.05	1.41	1.37
23	b	611	CLA	CMD-C2D	-3.05	1.44	1.50
23	b	606	CLA	MG-ND	3.05	2.11	2.05
23	c	506	CLA	MG-NC	3.05	2.13	2.06
23	C	503	CLA	C1D-ND	3.05	1.41	1.37
23	B	602	CLA	C1D-ND	3.05	1.41	1.37
30	A	615	LHG	O8-C23	3.04	1.42	1.33
23	B	605	CLA	C3B-C4B	3.04	1.51	1.42
23	c	503	CLA	MG-NB	3.04	2.11	2.05
23	b	605	CLA	C1B-C2B	3.03	1.50	1.43
23	c	506	CLA	MG-NA	3.03	2.13	2.06
23	B	602	CLA	C1B-C2B	3.02	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C1D-ND	3.01	1.41	1.37
23	B	609	CLA	C4B-NB	3.01	1.41	1.37
24	d	401	PHO	C4D-ND	-3.01	1.34	1.38
29	b	601	SQD	O47-C7	3.01	1.42	1.34
25	B	617	BCR	C33-C5	-3.01	1.46	1.50
23	b	607	CLA	MG-NB	-3.01	1.99	2.05
23	a	606	CLA	C1B-C2B	3.00	1.50	1.43
23	c	504	CLA	C4B-NB	2.99	1.41	1.37
29	B	624	SQD	O47-C7	2.99	1.42	1.34
23	a	606	CLA	MG-NB	-2.99	1.99	2.05
23	b	604	CLA	MG-NB	2.99	2.11	2.05
23	b	614	CLA	C4B-NB	2.98	1.41	1.37
24	A	606	PHO	CAC-C3C	-2.98	1.46	1.51
23	B	601	CLA	C1D-ND	2.98	1.41	1.37
24	A	606	PHO	CMB-C2B	-2.98	1.45	1.51
23	b	603	CLA	CMD-C2D	-2.97	1.44	1.50
31	c	516	DGD	C4E-C3E	2.97	1.60	1.52
35	f	102	HEM	CAB-C3B	2.97	1.55	1.47
31	C	517	DGD	O5D-C6D	-2.96	1.38	1.43
23	B	613	CLA	C1B-C2B	2.96	1.50	1.43
23	b	604	CLA	MG-NC	2.96	2.13	2.06
25	c	514	BCR	C30-C25	-2.96	1.50	1.53
23	b	604	CLA	C1D-ND	2.96	1.41	1.37
23	B	606	CLA	CMD-C2D	-2.95	1.44	1.50
23	A	603	CLA	MG-NC	-2.94	1.99	2.06
29	B	624	SQD	O48-C23	2.94	1.41	1.33
31	C	516	DGD	C2A-C1A	-2.94	1.42	1.50
23	c	510	CLA	CMB-C2B	-2.93	1.44	1.50
23	b	608	CLA	C1B-NB	-2.93	1.34	1.37
36	V	201	HEC	C3D-C2D	-2.93	1.31	1.38
30	d	409	LHG	P-O6	2.92	1.70	1.59
23	b	604	CLA	C4B-NB	2.92	1.41	1.37
23	C	510	CLA	C4B-NB	2.91	1.41	1.37
23	C	513	CLA	C1D-ND	2.91	1.41	1.37
28	c	519	LMG	O1-C1	2.91	1.45	1.40
29	A	614	SQD	O47-C7	2.90	1.42	1.34
28	C	519	LMG	C4-C5	2.90	1.59	1.53
23	A	613	CLA	C1B-C2B	2.90	1.49	1.43
23	C	503	CLA	CHC-C1C	2.90	1.44	1.38
23	c	513	CLA	C1B-C2B	2.89	1.49	1.43
23	B	605	CLA	CHC-C1C	2.89	1.44	1.38
23	B	606	CLA	CHC-C1C	2.88	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C1B-NB	-2.88	1.34	1.37
25	C	515	BCR	C30-C25	-2.88	1.50	1.53
23	C	512	CLA	C1B-C2B	2.87	1.49	1.43
23	B	603	CLA	MG-NA	-2.86	1.99	2.06
23	c	501	CLA	C4B-NB	2.86	1.41	1.37
23	c	509	CLA	C1B-C2B	2.86	1.49	1.43
31	H	102	DGD	C1E-C2E	2.85	1.60	1.52
23	c	507	CLA	CHC-C4B	-2.85	1.33	1.39
23	a	606	CLA	C1D-ND	2.84	1.41	1.37
31	c	517	DGD	O3E-C3E	-2.84	1.35	1.43
23	h	101	CLA	O2A-CGA	2.83	1.41	1.33
23	b	609	CLA	MG-NB	-2.83	2.00	2.05
23	b	605	CLA	MG-NA	2.82	2.13	2.06
23	b	612	CLA	MG-NC	-2.82	1.99	2.06
23	b	612	CLA	C3B-C4B	2.82	1.50	1.42
31	c	518	DGD	C1D-C2D	2.82	1.60	1.52
31	H	102	DGD	C3E-C2E	2.81	1.59	1.52
23	B	610	CLA	CMB-C2B	-2.81	1.45	1.50
23	c	512	CLA	C1D-ND	2.81	1.41	1.37
23	a	604	CLA	C1B-NB	-2.81	1.34	1.37
23	a	606	CLA	C4B-NB	2.80	1.41	1.37
23	A	613	CLA	MG-NB	2.80	2.11	2.05
23	B	608	CLA	CMD-C2D	-2.80	1.45	1.50
28	B	622	LMG	O8-C28	2.79	1.40	1.30
25	b	619	BCR	C30-C25	-2.79	1.50	1.53
24	a	605	PHO	C4D-ND	-2.79	1.34	1.38
28	D	409	LMG	O8-C28	2.79	1.41	1.33
35	F	102	HEM	FE-NC	2.78	2.04	1.95
28	A	612	LMG	C4-C5	2.78	1.59	1.53
23	b	605	CLA	CMB-C2B	-2.78	1.45	1.50
23	c	508	CLA	CMD-C2D	-2.78	1.45	1.50
35	f	102	HEM	CAC-C3C	2.78	1.54	1.47
29	a	613	SQD	O47-C7	2.77	1.42	1.34
23	C	503	CLA	C1B-C2B	2.77	1.49	1.43
28	c	519	LMG	C1-C2	2.77	1.60	1.52
23	B	608	CLA	C1B-C2B	2.77	1.49	1.43
23	a	606	CLA	CMA-C3A	-2.77	1.47	1.53
23	b	603	CLA	C4B-NB	2.77	1.41	1.37
23	B	611	CLA	MG-NC	-2.76	1.99	2.06
31	c	517	DGD	O5D-C6D	2.76	1.48	1.43
23	B	613	CLA	C1B-NB	-2.76	1.34	1.37
23	B	614	CLA	CMC-C2C	-2.76	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	517	DGD	C1E-C2E	2.76	1.60	1.52
23	b	612	CLA	C1B-C2B	2.76	1.49	1.43
23	d	403	CLA	C1B-C2B	2.76	1.49	1.43
23	B	606	CLA	C1B-C2B	2.76	1.49	1.43
23	c	511	CLA	MG-ND	2.76	2.11	2.05
31	H	102	DGD	O2G-C2G	-2.76	1.40	1.46
23	b	612	CLA	CMC-C2C	-2.75	1.45	1.50
23	C	512	CLA	C3B-C4B	2.75	1.50	1.42
23	c	503	CLA	C1B-C2B	2.75	1.49	1.43
23	b	610	CLA	CMB-C2B	-2.75	1.45	1.50
23	b	614	CLA	C1D-ND	2.75	1.41	1.37
25	b	617	BCR	C33-C5	-2.75	1.46	1.50
23	C	511	CLA	C3B-C4B	2.74	1.50	1.42
23	B	603	CLA	C3B-C4B	2.73	1.50	1.42
23	C	510	CLA	C1B-C2B	2.73	1.49	1.43
23	b	602	CLA	C1B-C2B	2.73	1.49	1.43
24	d	401	PHO	C4D-CHA	2.73	1.43	1.39
23	C	502	CLA	C1B-C2B	2.72	1.49	1.43
23	c	508	CLA	C1B-NB	-2.72	1.34	1.37
23	c	502	CLA	CMD-C2D	-2.72	1.45	1.50
23	a	612	CLA	MG-ND	2.72	2.11	2.05
23	a	604	CLA	CHC-C1C	2.72	1.43	1.38
23	h	101	CLA	C4B-NB	2.72	1.41	1.37
23	c	503	CLA	C1D-ND	2.72	1.41	1.37
30	A	615	LHG	P-O6	2.71	1.70	1.59
23	b	602	CLA	CMD-C2D	-2.71	1.45	1.50
31	C	518	DGD	C6D-C5D	2.71	1.59	1.51
23	b	613	CLA	MG-NB	-2.70	2.00	2.05
31	h	103	DGD	C4D-C3D	2.70	1.59	1.52
31	H	102	DGD	C4E-C5E	2.70	1.58	1.53
25	D	404	BCR	C1-C6	-2.69	1.50	1.53
28	m	101	LMG	C4-C3	2.69	1.59	1.52
23	c	508	CLA	C1B-C2B	2.69	1.49	1.43
23	C	513	CLA	C4B-NB	2.69	1.41	1.37
23	B	615	CLA	C1B-C2B	2.69	1.49	1.43
23	c	508	CLA	C1D-ND	2.68	1.41	1.37
23	B	615	CLA	CMD-C2D	-2.68	1.45	1.50
23	b	606	CLA	C3B-C4B	2.68	1.50	1.42
23	c	508	CLA	MG-ND	2.68	2.11	2.05
23	c	505	CLA	MG-NA	-2.67	1.99	2.06
23	A	603	CLA	C1D-ND	2.67	1.41	1.37
23	b	614	CLA	CHC-C1C	2.67	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C4B-NB	2.67	1.41	1.37
23	b	613	CLA	C1D-ND	2.67	1.41	1.37
23	A	613	CLA	C3B-C4B	2.67	1.50	1.42
23	B	613	CLA	C1D-ND	2.66	1.41	1.37
27	D	407	PL9	C41-C39	-2.66	1.45	1.51
23	B	602	CLA	MG-NA	2.66	2.12	2.06
23	A	607	CLA	C4B-NB	2.66	1.41	1.37
23	c	505	CLA	CHC-C1C	2.66	1.43	1.38
23	c	512	CLA	C1B-NB	-2.66	1.34	1.37
23	D	403	CLA	CMB-C2B	-2.66	1.45	1.50
23	C	509	CLA	C4B-NB	2.66	1.41	1.37
23	c	509	CLA	C3B-C4B	2.65	1.50	1.42
28	c	521	LMG	C1-C2	2.65	1.60	1.52
27	d	408	PL9	C15-C14	-2.65	1.44	1.50
23	D	402	CLA	MG-NC	2.64	2.12	2.06
23	b	614	CLA	CMC-C2C	-2.64	1.45	1.50
23	C	506	CLA	C1B-C2B	2.64	1.49	1.43
23	c	510	CLA	C4B-NB	2.64	1.41	1.37
23	c	505	CLA	MG-NB	2.64	2.11	2.05
23	D	403	CLA	C4B-NB	2.63	1.41	1.37
28	c	522	LMG	O8-C9	-2.63	1.39	1.45
23	b	615	CLA	C1B-C2B	2.63	1.49	1.43
24	A	606	PHO	C3B-C2B	-2.63	1.36	1.40
23	C	509	CLA	C1B-C2B	2.63	1.49	1.43
31	C	516	DGD	C4D-C3D	2.63	1.59	1.52
23	b	615	CLA	CMD-C2D	-2.62	1.45	1.50
23	B	601	CLA	CMC-C2C	-2.62	1.45	1.50
23	c	508	CLA	C3B-C4B	2.62	1.50	1.42
23	C	509	CLA	CMD-C2D	-2.62	1.45	1.50
23	b	603	CLA	CMB-C2B	-2.62	1.45	1.50
23	c	504	CLA	C1B-C2B	2.62	1.49	1.43
23	b	616	CLA	C1D-ND	2.62	1.41	1.37
28	B	620	LMG	O7-C8	-2.62	1.40	1.46
29	A	614	SQD	O2-C2	-2.62	1.36	1.43
31	c	517	DGD	O2E-C2E	-2.61	1.36	1.43
23	C	511	CLA	CMC-C2C	-2.61	1.45	1.50
23	b	602	CLA	C3B-C4B	2.61	1.50	1.42
23	C	503	CLA	C1D-C2D	2.61	1.50	1.45
23	d	402	CLA	C1B-C2B	2.61	1.49	1.43
23	c	511	CLA	C3B-C4B	2.61	1.50	1.42
25	k	101	BCR	C30-C25	-2.60	1.50	1.53
23	a	604	CLA	C4B-NB	2.60	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	616	SQD	O47-C45	-2.60	1.42	1.47
23	B	611	CLA	C4B-NB	2.60	1.41	1.37
23	C	501	CLA	C1B-NB	-2.60	1.34	1.37
23	A	607	CLA	C3D-C4D	2.60	1.50	1.44
31	c	516	DGD	C6D-C5D	2.59	1.59	1.51
23	C	513	CLA	C1B-C2B	2.59	1.49	1.43
23	b	607	CLA	CMD-C2D	-2.59	1.45	1.50
23	a	603	CLA	C3B-C4B	2.59	1.50	1.42
25	B	619	BCR	C30-C25	-2.58	1.50	1.53
23	B	602	CLA	C3B-C4B	2.58	1.50	1.42
36	V	201	HEC	C2A-C3A	-2.57	1.31	1.36
35	F	102	HEM	CAB-C3B	2.57	1.54	1.47
23	B	605	CLA	MG-ND	-2.57	2.00	2.05
23	B	616	CLA	C4B-NB	2.56	1.41	1.37
28	c	521	LMG	C7-C8	2.56	1.58	1.50
31	c	516	DGD	C4D-C3D	2.56	1.59	1.52
23	A	613	CLA	CAC-C3C	-2.55	1.44	1.51
23	C	507	CLA	C1D-ND	2.55	1.41	1.37
23	a	604	CLA	MG-NB	2.55	2.10	2.05
23	c	505	CLA	C4B-NB	2.55	1.41	1.37
23	B	609	CLA	C1B-C2B	2.55	1.49	1.43
23	B	611	CLA	CMB-C2B	-2.55	1.45	1.50
29	F	101	SQD	O2-C2	-2.55	1.36	1.43
23	b	613	CLA	CAA-C2A	-2.54	1.49	1.54
23	B	610	CLA	C1B-NB	-2.54	1.34	1.37
24	A	606	PHO	CMC-C2C	-2.54	1.46	1.50
23	A	604	CLA	MG-ND	-2.54	2.00	2.05
23	B	612	CLA	C1B-NB	-2.53	1.34	1.37
28	C	519	LMG	C7-C8	2.52	1.58	1.50
27	D	407	PL9	C20-C19	-2.52	1.44	1.50
25	t	101	BCR	C30-C25	-2.52	1.50	1.53
24	a	605	PHO	CMB-C2B	-2.52	1.46	1.51
23	C	501	CLA	CHC-C1C	2.52	1.43	1.38
23	c	512	CLA	C4B-NB	2.51	1.41	1.37
23	C	513	CLA	C1B-NB	-2.51	1.34	1.37
23	b	605	CLA	C1B-NB	-2.51	1.34	1.37
23	c	508	CLA	CHC-C1C	2.51	1.43	1.38
23	c	507	CLA	C4B-NB	2.51	1.41	1.37
23	b	615	CLA	CMC-C2C	-2.51	1.45	1.50
23	B	609	CLA	CMD-C2D	-2.50	1.45	1.50
31	A	617	DGD	O2G-C1B	2.50	1.41	1.34
23	c	503	CLA	CMB-C2B	-2.50	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C4B-NB	2.50	1.41	1.37
24	A	606	PHO	CMD-C2D	-2.50	1.46	1.51
25	T	101	BCR	C27-C26	-2.50	1.46	1.51
23	b	606	CLA	C1B-C2B	2.49	1.49	1.43
35	F	102	HEM	CMA-C3A	2.49	1.55	1.50
23	A	603	CLA	CMD-C2D	-2.49	1.45	1.50
23	C	510	CLA	CHC-C1C	2.49	1.43	1.38
23	c	505	CLA	MG-NC	2.49	2.12	2.06
23	b	616	CLA	CAA-C2A	-2.49	1.49	1.54
24	d	401	PHO	CAC-C3C	-2.49	1.47	1.51
24	d	401	PHO	CMD-C2D	-2.49	1.46	1.51
23	b	605	CLA	CHC-C4B	-2.48	1.33	1.39
35	f	102	HEM	CMC-C2C	2.48	1.55	1.50
23	a	612	CLA	CMB-C2B	-2.48	1.45	1.50
23	d	403	CLA	CMC-C2C	-2.48	1.45	1.50
31	c	517	DGD	O3D-C3D	-2.48	1.36	1.43
23	C	504	CLA	CMB-C2B	-2.48	1.45	1.50
23	d	402	CLA	CMB-C2B	-2.47	1.45	1.50
23	A	607	CLA	CHC-C4B	-2.47	1.33	1.39
23	b	614	CLA	C3B-C4B	2.47	1.49	1.42
23	D	403	CLA	C3B-C4B	2.47	1.49	1.42
23	b	608	CLA	C3B-C4B	2.47	1.49	1.42
23	c	513	CLA	MG-NC	-2.47	2.00	2.06
23	c	513	CLA	C4B-NB	2.47	1.41	1.37
23	C	510	CLA	CMD-C2D	-2.47	1.45	1.50
23	c	501	CLA	CMB-C2B	-2.47	1.45	1.50
23	b	611	CLA	C3B-C4B	2.46	1.49	1.42
31	c	518	DGD	O4D-C4D	-2.46	1.36	1.43
25	t	101	BCR	C27-C26	-2.46	1.46	1.51
27	a	611	PL9	C6-C1	-2.46	1.44	1.48
31	c	517	DGD	C1D-C2D	2.46	1.59	1.52
24	a	605	PHO	C3D-C4D	2.46	1.44	1.41
27	D	407	PL9	C27-C28	-2.45	1.43	1.50
23	C	501	CLA	C1B-C2B	2.45	1.48	1.43
23	c	506	CLA	C1B-C2B	2.45	1.48	1.43
28	D	409	LMG	C30-C29	2.45	1.61	1.52
23	B	605	CLA	O2D-CED	-2.45	1.39	1.45
23	b	604	CLA	C1B-C2B	2.45	1.48	1.43
23	B	615	CLA	C5-C3	-2.45	1.46	1.51
28	d	406	LMG	O6-C5	-2.45	1.38	1.44
27	D	407	PL9	C45-C44	-2.45	1.44	1.50
23	h	101	CLA	C1D-C2D	2.44	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C3B-C4B	2.44	1.49	1.42
24	a	605	PHO	O2D-CGD	2.44	1.39	1.33
23	b	610	CLA	MG-ND	-2.44	2.00	2.05
24	A	605	PHO	CHA-CBD	-2.44	1.48	1.51
23	C	510	CLA	C1B-NB	-2.44	1.34	1.37
23	B	607	CLA	CMC-C2C	-2.44	1.45	1.50
23	C	506	CLA	C1B-NB	-2.43	1.34	1.37
23	d	403	CLA	C4B-NB	2.43	1.41	1.37
29	B	624	SQD	O2-C2	-2.43	1.36	1.43
31	A	617	DGD	C3G-C2G	2.43	1.58	1.50
23	C	508	CLA	C1D-ND	2.43	1.41	1.37
23	b	610	CLA	C1B-C2B	2.42	1.48	1.43
23	c	512	CLA	CMD-C2D	-2.42	1.45	1.50
23	b	607	CLA	C1B-C2B	2.42	1.48	1.43
23	B	601	CLA	C1B-C2B	2.42	1.48	1.43
27	d	408	PL9	C23-C24	2.42	1.38	1.33
28	C	519	LMG	C1-C2	2.42	1.59	1.52
24	A	605	PHO	C4D-CHA	2.41	1.43	1.39
23	B	603	CLA	C1B-C2B	2.41	1.48	1.43
23	B	606	CLA	CMC-C2C	-2.41	1.45	1.50
23	B	602	CLA	C4B-NB	2.41	1.41	1.37
23	A	603	CLA	CMC-C2C	-2.40	1.45	1.50
23	B	614	CLA	C3B-C4B	2.40	1.49	1.42
23	D	402	CLA	CHC-C4B	-2.40	1.34	1.39
23	C	505	CLA	C1B-C2B	2.40	1.48	1.43
23	b	611	CLA	MG-NA	2.40	2.12	2.06
28	D	409	LMG	O8-C9	2.40	1.50	1.45
23	b	602	CLA	MG-NB	2.40	2.10	2.05
23	b	612	CLA	CMB-C2B	-2.40	1.45	1.50
30	d	407	LHG	P-O3	2.40	1.68	1.59
29	f	101	SQD	O2-C2	-2.40	1.37	1.43
23	C	501	CLA	CMD-C2D	-2.39	1.45	1.50
23	b	604	CLA	CHC-C1C	2.39	1.43	1.38
23	B	606	CLA	C4B-NB	2.39	1.41	1.37
23	C	504	CLA	CMD-C2D	-2.39	1.45	1.50
29	f	101	SQD	O3-C3	-2.39	1.37	1.43
23	C	504	CLA	C4B-NB	2.39	1.41	1.37
23	c	513	CLA	CMB-C2B	-2.39	1.45	1.50
23	b	604	CLA	CMC-C2C	-2.39	1.45	1.50
23	d	403	CLA	C3B-C4B	2.39	1.49	1.42
31	C	517	DGD	C6D-C5D	2.38	1.58	1.51
25	C	515	BCR	C33-C5	-2.38	1.47	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	516	DGD	O6D-C1D	2.38	1.48	1.41
23	C	510	CLA	MG-NC	2.38	2.11	2.06
23	c	513	CLA	C3B-C4B	2.37	1.49	1.42
23	C	504	CLA	C3B-C4B	2.37	1.49	1.42
23	c	503	CLA	CHC-C1C	2.37	1.43	1.38
27	d	408	PL9	C46-C44	-2.37	1.46	1.51
23	c	511	CLA	C1D-ND	2.37	1.41	1.37
23	b	613	CLA	CMD-C2D	-2.36	1.45	1.50
23	c	503	CLA	C1B-NB	-2.36	1.34	1.37
23	C	504	CLA	CMA-C3A	-2.36	1.48	1.53
31	a	616	DGD	CFA-CEA	2.36	1.63	1.51
23	A	603	CLA	C1B-NB	-2.36	1.34	1.37
23	C	512	CLA	C1A-CHA	-2.36	1.33	1.43
23	b	602	CLA	C4B-NB	2.35	1.41	1.37
25	C	515	BCR	C36-C18	-2.35	1.46	1.50
23	a	606	CLA	C1C-NC	-2.35	1.34	1.37
23	c	503	CLA	CMC-C2C	-2.35	1.46	1.50
23	B	610	CLA	C1B-C2B	2.35	1.48	1.43
23	b	613	CLA	CMC-C2C	-2.35	1.46	1.50
23	c	508	CLA	CMC-C2C	-2.34	1.46	1.50
23	d	402	CLA	C3B-C4B	2.34	1.49	1.42
23	A	613	CLA	C3C-C2C	2.34	1.41	1.36
23	a	603	CLA	CHC-C1C	2.34	1.43	1.38
24	A	605	PHO	O2D-CGD	2.34	1.39	1.33
23	b	605	CLA	C3B-C4B	2.34	1.49	1.42
24	a	605	PHO	CAC-C3C	-2.34	1.47	1.51
23	b	609	CLA	C1B-C2B	2.33	1.48	1.43
23	c	513	CLA	CHC-C1C	2.33	1.43	1.38
23	B	616	CLA	C1B-NB	-2.33	1.34	1.37
23	C	509	CLA	CMC-C2C	-2.33	1.46	1.50
23	B	607	CLA	CAC-C3C	-2.33	1.45	1.51
31	H	102	DGD	O3E-C3E	-2.33	1.37	1.43
23	B	611	CLA	C1D-ND	2.32	1.40	1.37
25	k	101	BCR	C33-C5	-2.32	1.47	1.50
23	A	613	CLA	C4B-NB	2.32	1.40	1.37
23	B	603	CLA	MG-NC	2.32	2.11	2.06
23	C	501	CLA	CMB-C2B	-2.32	1.46	1.50
23	C	512	CLA	C1D-ND	2.32	1.40	1.37
23	C	505	CLA	CHC-C1C	2.32	1.43	1.38
23	B	604	CLA	C4B-NB	2.32	1.40	1.37
31	c	517	DGD	O1G-C1A	2.31	1.40	1.33
35	F	102	HEM	CAC-C3C	2.31	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	613	SQD	O2-C2	-2.31	1.37	1.43
23	A	603	CLA	C3B-C4B	2.31	1.49	1.42
36	V	201	HEC	C3B-C2B	-2.31	1.33	1.41
31	h	103	DGD	C1E-C2E	2.31	1.59	1.52
23	b	604	CLA	C3B-C4B	2.30	1.49	1.42
23	b	602	CLA	CHC-C1C	2.30	1.43	1.38
23	B	602	CLA	CMB-C2B	-2.30	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.30	1.46	1.50
23	b	616	CLA	CAB-C3B	-2.30	1.41	1.47
23	C	505	CLA	MG-ND	-2.30	2.01	2.05
30	l	101	LHG	P-O6	2.30	1.68	1.59
31	c	517	DGD	O2G-C2G	-2.30	1.41	1.46
23	c	511	CLA	CMB-C2B	-2.30	1.46	1.50
31	C	516	DGD	C2B-C1B	-2.30	1.44	1.50
24	A	605	PHO	CMD-C2D	-2.30	1.47	1.51
23	c	509	CLA	C4B-NB	2.30	1.40	1.37
23	C	512	CLA	CMD-C2D	-2.29	1.46	1.50
23	c	504	CLA	CMB-C2B	-2.29	1.46	1.50
24	A	606	PHO	CAA-C2A	-2.29	1.49	1.54
23	c	510	CLA	CHC-C1C	2.29	1.43	1.38
23	c	513	CLA	C1D-ND	2.29	1.40	1.37
23	c	503	CLA	C1D-C2D	2.29	1.49	1.45
23	c	501	CLA	CMD-C2D	-2.28	1.46	1.50
23	b	610	CLA	CMD-C2D	-2.28	1.46	1.50
25	c	514	BCR	C33-C5	-2.28	1.47	1.50
23	b	616	CLA	O2D-CED	-2.28	1.40	1.45
23	C	513	CLA	CMB-C2B	-2.28	1.46	1.50
23	C	503	CLA	C1B-NB	-2.28	1.34	1.37
35	f	102	HEM	C3B-C2B	-2.28	1.32	1.37
35	F	102	HEM	CMC-C2C	2.27	1.55	1.50
23	B	604	CLA	C3B-C4B	2.27	1.49	1.42
27	a	611	PL9	C3-C4	-2.27	1.46	1.49
23	A	603	CLA	C1D-C2D	2.27	1.49	1.45
23	a	606	CLA	MG-NC	-2.27	2.00	2.06
23	B	604	CLA	C1B-C2B	2.27	1.48	1.43
27	A	611	PL9	C6-C1	-2.26	1.44	1.48
25	C	520	BCR	C33-C5	-2.26	1.47	1.50
28	c	521	LMG	C4-C3	2.26	1.58	1.52
23	h	101	CLA	CHC-C1C	2.26	1.43	1.38
23	C	509	CLA	O2D-CGD	2.26	1.38	1.33
23	b	606	CLA	CAC-C3C	-2.25	1.45	1.51
23	h	101	CLA	CMC-C2C	-2.25	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	CMB-C2B	-2.25	1.46	1.50
23	B	615	CLA	C3D-C4D	2.25	1.49	1.44
23	B	609	CLA	CMC-C2C	-2.25	1.46	1.50
23	B	607	CLA	CMB-C2B	-2.25	1.46	1.50
23	c	506	CLA	C4B-NB	2.25	1.40	1.37
28	A	612	LMG	O1-C7	-2.25	1.39	1.43
23	B	614	CLA	CMD-C2D	-2.25	1.46	1.50
30	A	615	LHG	P-O3	2.25	1.68	1.59
29	b	601	SQD	O2-C2	-2.24	1.37	1.43
23	a	604	CLA	C1B-C2B	2.24	1.48	1.43
23	c	510	CLA	C1B-C2B	2.24	1.48	1.43
23	a	606	CLA	MG-NA	2.24	2.11	2.06
23	B	606	CLA	C3B-C4B	2.24	1.49	1.42
23	c	512	CLA	C3B-C4B	2.24	1.49	1.42
23	c	504	CLA	CMD-C2D	-2.24	1.46	1.50
23	C	510	CLA	O2A-CGA	2.24	1.39	1.33
25	b	618	BCR	C4-C5	-2.24	1.46	1.51
23	c	511	CLA	C1B-C2B	2.24	1.48	1.43
23	b	610	CLA	CHC-C4B	-2.24	1.34	1.39
23	D	402	CLA	C1A-CHA	-2.23	1.33	1.43
28	b	621	LMG	O8-C28	2.23	1.39	1.33
23	A	603	CLA	C4B-NB	2.23	1.40	1.37
23	B	615	CLA	C1B-NB	-2.23	1.34	1.37
23	A	607	CLA	C1B-C2B	2.23	1.48	1.43
23	c	506	CLA	CAC-C3C	-2.23	1.45	1.51
28	m	101	LMG	O1-C7	-2.23	1.39	1.43
28	B	620	LMG	C1-C2	2.23	1.59	1.52
25	T	101	BCR	C33-C5	-2.23	1.47	1.50
23	B	615	CLA	O2D-CED	-2.23	1.40	1.45
23	C	511	CLA	CHC-C1C	2.23	1.42	1.38
28	D	405	LMG	C34-C33	2.23	1.62	1.51
23	b	610	CLA	C3D-C4D	2.22	1.49	1.44
27	a	611	PL9	C46-C44	-2.22	1.46	1.51
31	c	516	DGD	O3E-C3E	-2.22	1.37	1.43
23	B	605	CLA	CMC-C2C	-2.22	1.46	1.50
23	b	615	CLA	C3B-C4B	2.22	1.49	1.42
31	H	102	DGD	O6E-C1E	2.22	1.47	1.41
23	A	603	CLA	C1A-CHA	-2.22	1.34	1.43
23	c	513	CLA	CMD-C2D	-2.22	1.46	1.50
35	f	102	HEM	C2A-C3A	-2.21	1.33	1.38
23	B	604	CLA	CMA-C3A	-2.21	1.48	1.53
23	a	604	CLA	C3B-C4B	2.21	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C1B-NB	-2.21	1.35	1.37
23	b	612	CLA	C4C-C3C	2.21	1.48	1.45
27	D	407	PL9	C10-C9	-2.21	1.45	1.50
31	C	516	DGD	C6D-C5D	2.21	1.58	1.51
23	a	604	CLA	CMD-C2D	-2.21	1.46	1.50
23	C	512	CLA	C3D-C4D	2.21	1.49	1.44
23	B	607	CLA	MG-ND	-2.21	2.01	2.05
23	B	602	CLA	MG-ND	-2.21	2.01	2.05
23	C	504	CLA	O2D-CGD	2.21	1.38	1.33
23	b	610	CLA	C1B-NB	-2.21	1.35	1.37
23	b	616	CLA	C3B-C4B	2.20	1.49	1.42
23	b	609	CLA	C1B-NB	-2.20	1.35	1.37
28	B	622	LMG	O7-C10	2.20	1.38	1.30
23	d	402	CLA	O2D-CED	-2.20	1.40	1.45
23	b	611	CLA	C1D-C2D	2.20	1.49	1.45
23	c	507	CLA	MG-ND	-2.20	2.01	2.05
23	b	608	CLA	CMD-C2D	-2.20	1.46	1.50
27	d	408	PL9	C16-C14	-2.20	1.46	1.51
23	B	603	CLA	C1B-NB	-2.19	1.35	1.37
30	d	407	LHG	C6-C5	2.19	1.57	1.50
23	c	502	CLA	MG-NB	-2.19	2.01	2.05
31	c	517	DGD	C3E-C2E	2.19	1.58	1.52
23	b	604	CLA	CMB-C2B	-2.19	1.46	1.50
23	C	509	CLA	C3B-C4B	2.19	1.49	1.42
23	c	509	CLA	O2D-CED	-2.19	1.40	1.45
31	c	518	DGD	O5D-C1E	2.18	1.43	1.40
23	b	614	CLA	C1A-CHA	-2.18	1.34	1.43
25	T	101	BCR	C38-C26	-2.18	1.47	1.50
23	b	608	CLA	C1C-C2C	2.18	1.48	1.44
36	V	201	HEC	CMD-C2D	2.18	1.55	1.50
23	C	508	CLA	C1B-C2B	2.18	1.48	1.43
36	V	201	HEC	C3C-C2C	-2.18	1.33	1.41
23	b	612	CLA	C1D-ND	2.18	1.40	1.37
23	b	614	CLA	O2D-CED	-2.17	1.40	1.45
23	B	613	CLA	CMC-C2C	-2.17	1.46	1.50
23	B	607	CLA	C1B-C2B	2.17	1.48	1.43
23	c	510	CLA	C1B-NB	-2.17	1.35	1.37
23	C	503	CLA	C3D-C4D	2.17	1.49	1.44
23	b	615	CLA	CMB-C2B	-2.17	1.46	1.50
25	b	619	BCR	C33-C5	-2.17	1.47	1.50
23	c	510	CLA	C1D-ND	2.17	1.40	1.37
23	b	610	CLA	CMC-C2C	-2.17	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	CMA-C3A	-2.17	1.48	1.53
28	C	519	LMG	O1-C1	2.17	1.43	1.40
23	b	611	CLA	CMC-C2C	-2.17	1.46	1.50
25	C	520	BCR	C1-C6	-2.16	1.51	1.53
23	a	603	CLA	C1B-NB	-2.16	1.35	1.37
23	c	502	CLA	C3B-C4B	2.16	1.49	1.42
23	b	616	CLA	CAC-C3C	-2.16	1.45	1.51
23	A	607	CLA	MG-NB	-2.16	2.01	2.05
23	a	612	CLA	MG-NB	2.16	2.10	2.05
23	c	508	CLA	CMB-C2B	-2.16	1.46	1.50
23	C	502	CLA	C4B-NB	2.16	1.40	1.37
23	c	506	CLA	CMD-C2D	-2.15	1.46	1.50
28	b	621	LMG	O1-C7	-2.15	1.40	1.43
31	A	617	DGD	C4E-C5E	2.15	1.57	1.53
23	c	506	CLA	C3B-C4B	2.15	1.49	1.42
25	d	404	BCR	C33-C5	-2.15	1.47	1.50
23	A	603	CLA	CHC-C1C	2.15	1.42	1.38
23	b	602	CLA	CMB-C2B	-2.15	1.46	1.50
27	D	407	PL9	C3-C4	-2.15	1.46	1.49
31	c	518	DGD	C2A-C1A	-2.15	1.44	1.50
31	C	516	DGD	O6E-C1E	2.15	1.47	1.41
28	D	405	LMG	C4-C5	2.15	1.57	1.53
31	a	616	DGD	C2B-C1B	2.15	1.56	1.50
23	a	606	CLA	CMD-C2D	-2.15	1.46	1.50
23	B	603	CLA	C1A-CHA	-2.15	1.34	1.43
28	d	406	LMG	O1-C7	-2.14	1.40	1.43
23	C	503	CLA	C3B-C4B	2.14	1.49	1.42
23	B	608	CLA	C1D-ND	2.14	1.40	1.37
23	c	501	CLA	C1B-NB	-2.14	1.35	1.37
23	b	615	CLA	C1D-ND	2.14	1.40	1.37
30	D	408	LHG	C6-C5	2.14	1.57	1.50
23	B	611	CLA	C3B-C4B	2.14	1.49	1.42
23	d	403	CLA	CAB-C3B	-2.14	1.41	1.47
25	b	618	BCR	C29-C30	-2.14	1.49	1.54
23	a	612	CLA	O2D-CED	-2.14	1.40	1.45
23	A	603	CLA	CAC-C3C	-2.13	1.45	1.51
23	b	606	CLA	C4B-NB	2.13	1.40	1.37
24	d	401	PHO	CMA-C3A	-2.13	1.49	1.53
23	c	505	CLA	C3B-C4B	2.13	1.48	1.42
23	C	501	CLA	C3D-C4D	2.13	1.49	1.44
23	b	607	CLA	C3B-C4B	2.13	1.48	1.42
23	c	502	CLA	C1B-NB	-2.13	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	101	SQD	O3-C3	-2.13	1.37	1.43
23	a	603	CLA	CMC-C2C	-2.12	1.46	1.50
27	d	408	PL9	C47-C48	-2.12	1.44	1.50
31	C	518	DGD	O6E-C1E	2.12	1.47	1.41
23	C	512	CLA	C4B-NB	2.12	1.40	1.37
25	C	520	BCR	C38-C26	-2.12	1.47	1.50
23	C	505	CLA	MG-NB	-2.12	2.01	2.05
23	B	601	CLA	CAC-C3C	-2.12	1.45	1.51
29	A	614	SQD	O47-C45	-2.12	1.41	1.46
23	B	611	CLA	CHC-C1C	2.12	1.42	1.38
23	C	507	CLA	CHC-C1C	2.12	1.42	1.38
23	b	609	CLA	CAC-C3C	-2.11	1.45	1.51
23	B	601	CLA	C1B-NB	-2.11	1.35	1.37
23	b	609	CLA	C3D-C4D	2.11	1.48	1.44
30	B	623	LHG	P-O4	-2.11	1.45	1.55
23	c	501	CLA	C1B-C2B	2.11	1.48	1.43
23	c	502	CLA	C1B-C2B	2.11	1.48	1.43
31	c	517	DGD	C6D-C5D	2.11	1.57	1.51
36	v	201	HEC	C3B-C2B	-2.11	1.34	1.41
23	c	510	CLA	CMD-C2D	-2.11	1.46	1.50
23	B	614	CLA	CHC-C1C	2.11	1.42	1.38
23	B	601	CLA	CMB-C2B	-2.11	1.46	1.50
23	B	615	CLA	C1D-C2D	2.11	1.49	1.45
23	C	508	CLA	CMC-C2C	-2.11	1.46	1.50
25	k	102	BCR	C30-C25	-2.10	1.51	1.53
28	c	521	LMG	O6-C5	-2.10	1.39	1.44
23	B	616	CLA	CHC-C4B	-2.10	1.34	1.39
23	B	610	CLA	CHC-C1C	2.10	1.42	1.38
23	B	610	CLA	CAC-C3C	-2.10	1.45	1.51
28	d	406	LMG	O3-C3	-2.10	1.37	1.43
23	b	606	CLA	MG-NC	2.10	2.11	2.06
30	l	101	LHG	O8-C23	2.10	1.39	1.33
31	c	518	DGD	C2B-C1B	-2.10	1.44	1.50
23	a	606	CLA	CHC-C4B	-2.10	1.34	1.39
23	D	402	CLA	C1B-C2B	2.10	1.48	1.43
23	C	508	CLA	C3B-C4B	2.10	1.48	1.42
23	c	502	CLA	CMC-C2C	-2.10	1.46	1.50
29	b	601	SQD	O3-C3	-2.09	1.37	1.43
23	h	101	CLA	C3B-C4B	2.09	1.48	1.42
23	b	603	CLA	C3B-C4B	2.09	1.48	1.42
23	B	613	CLA	MG-NA	2.09	2.11	2.06
27	a	611	PL9	C52-C5	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	PHO	CMC-C2C	-2.09	1.47	1.50
24	d	401	PHO	CMB-C2B	-2.09	1.47	1.51
23	C	502	CLA	O2D-CGD	2.09	1.38	1.33
23	b	607	CLA	C1D-C2D	2.09	1.49	1.45
23	c	510	CLA	MG-NB	2.08	2.09	2.05
31	A	617	DGD	C6D-C5D	2.08	1.57	1.51
25	B	617	BCR	C30-C25	-2.08	1.51	1.53
36	V	201	HEC	C4D-ND	-2.08	1.35	1.39
23	a	612	CLA	C4B-NB	2.08	1.40	1.37
23	B	609	CLA	C3B-C4B	2.08	1.48	1.42
23	b	615	CLA	CAC-C3C	-2.08	1.45	1.51
23	c	507	CLA	C1D-ND	2.08	1.40	1.37
23	C	510	CLA	CMC-C2C	-2.08	1.46	1.50
23	D	402	CLA	C1C-NC	-2.07	1.34	1.37
23	B	612	CLA	C1A-CHA	-2.07	1.34	1.43
31	C	516	DGD	C3D-C2D	2.07	1.57	1.52
23	A	613	CLA	C3D-C4D	2.07	1.48	1.44
23	B	616	CLA	CMD-C2D	-2.07	1.46	1.50
23	B	616	CLA	C1B-C2B	2.07	1.48	1.43
23	c	512	CLA	C1D-C2D	2.07	1.49	1.45
23	a	612	CLA	CHC-C1C	2.07	1.42	1.38
23	B	610	CLA	C3D-C4D	2.07	1.48	1.44
23	C	507	CLA	C1B-C2B	2.06	1.48	1.43
35	F	102	HEM	C2A-C3A	-2.06	1.33	1.38
31	A	617	DGD	C6E-C5E	2.06	1.58	1.51
23	b	616	CLA	CMD-C2D	-2.06	1.46	1.50
23	B	613	CLA	CMB-C2B	-2.06	1.46	1.50
23	c	507	CLA	MG-NB	-2.06	2.01	2.05
31	C	516	DGD	C1D-C2D	2.06	1.58	1.52
23	C	510	CLA	C3D-C4D	2.06	1.48	1.44
23	B	615	CLA	C1D-ND	2.06	1.40	1.37
31	c	518	DGD	C4D-C5D	2.06	1.57	1.53
31	c	516	DGD	O3G-C3G	-2.06	1.40	1.43
25	k	102	BCR	C1-C6	-2.06	1.51	1.53
23	b	605	CLA	MG-ND	-2.05	2.01	2.05
23	b	611	CLA	MG-NB	2.05	2.09	2.05
23	C	512	CLA	CAA-C2A	-2.05	1.50	1.54
23	C	501	CLA	CMC-C2C	-2.05	1.46	1.50
23	C	510	CLA	C3B-C4B	2.05	1.48	1.42
23	B	615	CLA	CAC-C3C	-2.05	1.45	1.51
23	c	505	CLA	CMC-C2C	-2.04	1.46	1.50
28	A	612	LMG	C1-C2	2.04	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	408	PL9	O2-C1	-2.04	1.19	1.24
23	B	612	CLA	C3B-C4B	2.04	1.48	1.42
23	C	512	CLA	CHC-C1C	2.04	1.42	1.38
23	B	602	CLA	O2D-CED	-2.04	1.40	1.45
23	C	506	CLA	C3B-C4B	2.04	1.48	1.42
23	b	610	CLA	C1C-NC	-2.04	1.34	1.37
23	a	604	CLA	CMB-C2B	-2.04	1.46	1.50
23	c	507	CLA	CMC-C2C	-2.04	1.46	1.50
35	F	102	HEM	CMB-C2B	2.04	1.55	1.50
23	b	608	CLA	O2A-CGA	2.04	1.39	1.33
25	B	619	BCR	C33-C5	-2.04	1.47	1.50
23	B	607	CLA	CAA-C2A	2.04	1.57	1.54
23	c	501	CLA	CAC-C3C	-2.04	1.45	1.51
23	B	609	CLA	O2D-CGD	2.04	1.38	1.33
23	C	510	CLA	C3C-C2C	2.03	1.41	1.36
31	C	516	DGD	O5D-C1E	2.03	1.43	1.40
23	A	603	CLA	C5-C3	-2.03	1.47	1.51
23	a	606	CLA	C1B-NB	-2.03	1.35	1.37
25	H	101	BCR	C33-C5	-2.03	1.47	1.50
23	A	607	CLA	CMD-C2D	-2.03	1.46	1.50
31	A	617	DGD	O4D-C4D	-2.03	1.37	1.43
23	B	611	CLA	C1B-NB	-2.03	1.35	1.37
23	C	513	CLA	C3B-C4B	2.02	1.48	1.42
23	c	510	CLA	CMC-C2C	-2.02	1.46	1.50
23	d	402	CLA	MG-NA	2.02	2.11	2.06
23	c	505	CLA	C1B-C2B	2.02	1.47	1.43
24	a	605	PHO	CMD-C2D	-2.02	1.47	1.51
23	h	101	CLA	C3D-C4D	2.02	1.48	1.44
23	c	501	CLA	MG-ND	-2.02	2.01	2.05
23	a	606	CLA	O1D-CGD	2.02	1.26	1.21
25	t	101	BCR	C33-C5	-2.02	1.47	1.50
24	a	605	PHO	C3B-C2B	-2.02	1.37	1.40
23	a	612	CLA	C1B-NB	-2.02	1.35	1.37
25	a	607	BCR	C27-C26	-2.02	1.47	1.51
24	A	606	PHO	CBD-CGD	-2.01	1.50	1.52
23	b	614	CLA	C1B-C2B	2.01	1.47	1.43
23	D	403	CLA	C1A-CHA	-2.01	1.34	1.43
24	a	605	PHO	C3A-C2A	-2.01	1.53	1.54
25	c	515	BCR	C36-C18	-2.01	1.46	1.50
23	A	604	CLA	CAC-C3C	-2.01	1.46	1.51
25	a	607	BCR	C32-C1	-2.01	1.50	1.53
23	C	507	CLA	CAB-C3B	-2.01	1.42	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	CMB-C2B	-2.01	1.46	1.50
25	B	618	BCR	C4-C5	-2.00	1.47	1.51
23	C	513	CLA	CMD-C2D	-2.00	1.46	1.50
23	c	507	CLA	CAB-C3B	-2.00	1.42	1.47

All (1314) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C4A-NA-C1A	10.98	111.69	106.68
29	A	614	SQD	O6-C1-C2	10.25	123.84	108.27
23	B	601	CLA	C4A-NA-C1A	10.00	111.24	106.68
29	b	601	SQD	O6-C1-C2	9.81	123.17	108.27
24	A	605	PHO	C4D-CHA-CBD	-9.67	103.82	108.45
23	c	502	CLA	C4A-NA-C1A	9.59	111.05	106.68
23	a	606	CLA	C4A-NA-C1A	8.82	110.70	106.68
29	a	613	SQD	O6-C1-C2	8.67	121.44	108.27
23	C	511	CLA	C4A-NA-C1A	8.41	110.52	106.68
23	C	510	CLA	C4A-NA-C1A	8.29	110.46	106.68
23	a	603	CLA	C4A-NA-C1A	8.26	110.45	106.68
23	c	507	CLA	C4A-NA-C1A	8.10	110.38	106.68
29	A	614	SQD	O7-S-C6	7.97	118.66	106.76
23	C	507	CLA	C4A-NA-C1A	7.54	110.12	106.68
23	C	501	CLA	C4A-NA-C1A	7.43	110.07	106.68
23	a	612	CLA	C4A-NA-C1A	7.42	110.06	106.68
23	b	604	CLA	C4A-NA-C1A	7.35	110.03	106.68
23	B	606	CLA	C4A-NA-C1A	6.96	109.85	106.68
23	C	513	CLA	C4A-NA-C1A	6.95	109.85	106.68
29	A	616	SQD	C45-O47-C7	6.86	127.67	117.78
23	b	606	CLA	C4A-NA-C1A	6.77	109.77	106.68
23	B	609	CLA	C4A-NA-C1A	6.75	109.76	106.68
23	B	612	CLA	C4A-NA-C1A	6.53	109.66	106.68
23	c	501	CLA	C4A-NA-C1A	6.46	109.63	106.68
23	C	503	CLA	C4A-NA-C1A	6.46	109.62	106.68
23	d	402	CLA	C4A-NA-C1A	6.36	109.58	106.68
23	B	614	CLA	O2D-CGD-O1D	-6.16	111.85	123.85
23	c	509	CLA	C4A-NA-C1A	6.10	109.46	106.68
36	V	201	HEC	CBB-CAB-C3B	-6.06	115.32	127.43
23	b	602	CLA	C4A-NA-C1A	6.03	109.43	106.68
24	a	605	PHO	C4D-CHA-CBD	-6.02	105.57	108.45
36	v	201	HEC	CBC-CAC-C3C	-5.97	115.51	127.43
23	A	613	CLA	C4A-NA-C1A	5.91	109.37	106.68
23	B	610	CLA	C4A-NA-C1A	5.90	109.37	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C4A-NA-C1A	5.82	109.33	106.68
27	a	611	PL9	C7-C3-C4	5.79	121.68	116.91
23	b	607	CLA	C4A-NA-C1A	5.78	109.32	106.68
24	d	401	PHO	C4D-CHA-CBD	-5.77	105.69	108.45
23	c	501	CLA	O2D-CGD-O1D	-5.68	112.80	123.85
24	A	605	PHO	O2D-CGD-CBD	5.63	117.13	110.95
23	c	511	CLA	C4A-NA-C1A	5.61	109.24	106.68
29	F	101	SQD	O6-C1-C2	5.60	116.77	108.27
23	b	605	CLA	C4A-NA-C1A	5.55	109.21	106.68
27	A	611	PL9	C7-C3-C4	5.49	121.43	116.91
29	F	101	SQD	O8-S-C6	5.32	116.24	105.97
23	b	613	CLA	C4A-NA-C1A	5.30	109.10	106.68
23	c	505	CLA	C3B-C4B-NB	-5.28	105.82	110.53
31	C	517	DGD	O3G-C3G-C2G	-5.27	98.00	110.82
23	B	616	CLA	C4A-NA-C1A	5.26	109.08	106.68
31	H	102	DGD	O3G-C3G-C2G	-5.18	98.23	110.82
23	B	608	CLA	C4A-NA-C1A	5.18	109.04	106.68
23	b	602	CLA	O2D-CGD-O1D	-5.07	113.99	123.85
23	B	613	CLA	C4A-NA-C1A	5.06	108.99	106.68
23	b	615	CLA	C3B-C4B-NB	-5.06	106.02	110.53
27	D	407	PL9	C7-C3-C4	5.03	121.05	116.91
23	A	607	CLA	O2D-CGD-O1D	-4.98	114.15	123.85
23	b	614	CLA	C4A-NA-C1A	4.95	108.94	106.68
23	c	506	CLA	C4A-NA-C1A	4.95	108.94	106.68
23	B	608	CLA	O2D-CGD-O1D	-4.94	114.23	123.85
23	b	608	CLA	C3B-C4B-NB	-4.93	106.12	110.53
29	f	101	SQD	O6-C1-C2	4.91	115.73	108.27
23	C	503	CLA	C7-C6-C5	-4.86	100.30	113.26
23	a	604	CLA	C4A-NA-C1A	4.81	108.87	106.68
31	a	616	DGD	C2G-O2G-C1B	4.77	129.21	117.80
23	h	101	CLA	C4A-NA-C1A	4.75	108.85	106.68
36	V	201	HEC	CBC-CAC-C3C	-4.74	117.95	127.43
27	d	408	PL9	C7-C3-C4	4.73	120.80	116.91
23	b	612	CLA	C4A-NA-C1A	4.72	108.83	106.68
29	B	624	SQD	O6-C1-C2	4.72	115.45	108.27
29	a	615	SQD	O47-C7-C8	4.71	121.67	111.48
23	b	616	CLA	O2D-CGD-O1D	-4.71	114.68	123.85
30	D	408	LHG	O4-P-O5	4.68	134.20	112.44
23	c	512	CLA	C4A-NA-C1A	4.67	108.81	106.68
24	d	401	PHO	O1D-CGD-CBD	4.67	131.81	124.72
23	C	505	CLA	CAC-C3C-C4C	4.66	130.85	124.79
23	b	603	CLA	O2D-CGD-O1D	-4.62	114.86	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	m	101	LMG	O7-C10-O9	-4.62	112.91	123.70
23	B	611	CLA	O2D-CGD-O1D	-4.59	114.91	123.85
27	a	611	PL9	C7-C3-C2	-4.59	117.98	123.39
30	a	614	LHG	O4-P-O5	4.44	133.11	112.44
23	C	512	CLA	O2D-CGD-O1D	-4.44	115.20	123.85
29	a	613	SQD	O8-S-C6	4.42	114.51	105.97
23	c	503	CLA	C4A-NA-C1A	4.42	108.69	106.68
36	v	201	HEC	CBB-CAB-C3B	-4.41	118.62	127.43
23	c	511	CLA	C3B-C4B-NB	-4.41	106.59	110.53
23	B	610	CLA	O2D-CGD-O1D	-4.40	115.28	123.85
29	A	614	SQD	O9-S-O7	-4.38	99.58	113.82
29	A	614	SQD	O47-C7-C8	4.37	120.93	111.48
25	H	101	BCR	C38-C26-C25	-4.34	119.75	124.48
23	C	501	CLA	O2D-CGD-CBD	4.32	118.79	111.23
30	d	405	LHG	O4-P-O5	4.31	132.50	112.44
23	c	510	CLA	CHB-C4A-NA	4.29	130.60	124.40
30	B	623	LHG	O4-P-O5	4.29	132.40	112.44
29	B	624	SQD	O7-S-C6	4.29	113.16	106.76
23	c	509	CLA	O2A-CGA-O1A	-4.28	112.92	123.63
31	A	617	DGD	C3G-C2G-C1G	-4.25	101.86	111.78
23	C	508	CLA	O2D-CGD-O1D	-4.24	115.59	123.85
30	d	407	LHG	O4-P-O5	4.24	132.17	112.44
23	C	510	CLA	C3B-C4B-NB	-4.24	106.75	110.53
24	d	401	PHO	C2B-C1B-NB	-4.23	106.37	109.43
23	B	604	CLA	C3B-C4B-NB	-4.23	106.75	110.53
23	b	602	CLA	O2D-CGD-CBD	4.20	118.57	111.23
28	c	521	LMG	O6-C1-O1	-4.19	100.14	110.04
23	b	604	CLA	C3B-C4B-NB	-4.19	106.79	110.53
29	b	601	SQD	C1-C2-C3	-4.18	101.21	110.01
23	C	501	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
23	C	507	CLA	C3B-C4B-NB	-4.18	106.80	110.53
30	A	615	LHG	O4-P-O5	4.16	131.79	112.44
31	H	102	DGD	C1D-O6D-C5D	-4.16	105.60	113.72
29	A	614	SQD	C1-C2-C3	-4.15	101.28	110.01
23	A	607	CLA	C4A-NA-C1A	4.15	108.57	106.68
23	B	605	CLA	C3B-C4B-NB	-4.13	106.84	110.53
23	B	603	CLA	C4A-NA-C1A	4.13	108.56	106.68
23	c	501	CLA	O2D-CGD-CBD	4.10	118.41	111.23
23	C	512	CLA	CHB-C4A-NA	4.10	130.32	124.40
31	C	516	DGD	O1G-C1A-C2A	-4.10	99.35	111.83
23	B	607	CLA	C4A-NA-C1A	4.09	108.55	106.68
23	b	602	CLA	CHB-C4A-NA	4.09	130.30	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	409	LHG	O4-P-O5	4.08	131.41	112.44
23	b	611	CLA	O2D-CGD-O1D	-4.08	115.91	123.85
30	D	406	LHG	O4-P-O5	4.06	131.33	112.44
23	a	604	CLA	CMA-C3A-C4A	-4.05	100.88	111.77
31	c	516	DGD	O3G-C3G-C2G	-4.03	101.01	110.82
29	f	101	SQD	O9-S-C6	4.01	112.74	106.76
23	c	507	CLA	O2D-CGD-O1D	-4.01	116.05	123.85
23	a	612	CLA	C3B-C4B-NB	-4.00	106.96	110.53
23	c	512	CLA	C1-C2-C3	-3.99	119.66	126.20
24	A	606	PHO	C1-C2-C3	-3.99	119.66	126.20
31	C	518	DGD	O3G-C3G-C2G	-3.97	101.17	110.82
23	B	614	CLA	C3B-C4B-NB	-3.95	107.00	110.53
25	B	617	BCR	C2-C1-C6	3.94	116.16	110.44
30	l	101	LHG	O4-P-O5	3.93	130.71	112.44
23	c	510	CLA	O2D-CGD-O1D	-3.92	116.21	123.85
29	A	614	SQD	C3-C4-C5	3.90	117.31	110.23
23	b	605	CLA	O2D-CGD-O1D	-3.90	116.26	123.85
23	B	601	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
23	B	610	CLA	CED-O2D-CGD	-3.88	107.11	115.92
29	F	101	SQD	C46-C45-C44	-3.87	101.17	113.67
23	b	605	CLA	C1-C2-C3	-3.86	119.87	126.20
34	D	401	BCT	O2-C-O1	3.86	129.55	119.68
23	c	501	CLA	C2C-C1C-NC	3.85	114.03	109.98
23	B	606	CLA	C4D-CHA-C1A	3.85	125.84	121.24
31	C	517	DGD	C1D-C2D-C3D	-3.85	101.92	110.01
23	a	604	CLA	C3B-C4B-NB	-3.84	107.10	110.53
23	B	605	CLA	CMB-C2B-C1B	3.84	131.26	125.42
23	B	614	CLA	O1D-CGD-CBD	3.83	132.07	124.52
29	a	613	SQD	C1-O5-C5	-3.83	106.25	113.72
23	A	613	CLA	C3B-C4B-NB	-3.83	107.11	110.53
23	b	616	CLA	C3B-C4B-NB	-3.82	107.12	110.53
29	b	601	SQD	O2-C2-C1	3.81	119.16	110.08
23	h	101	CLA	O2D-CGD-O1D	-3.80	116.44	123.85
24	A	605	PHO	CMA-C3A-C4A	-3.79	106.45	114.61
25	T	101	BCR	C27-C26-C25	3.78	127.81	122.70
23	C	502	CLA	C3B-C4B-NB	-3.77	107.17	110.53
23	B	602	CLA	CHB-C4A-NA	3.74	129.81	124.40
23	c	512	CLA	CHB-C4A-NA	3.72	129.78	124.40
23	c	508	CLA	C3B-C4B-NB	-3.71	107.22	110.53
23	h	101	CLA	C3B-C4B-NB	-3.70	107.23	110.53
25	A	608	BCR	C11-C10-C9	-3.69	122.10	127.28
29	B	624	SQD	C1-O5-C5	-3.69	106.51	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CHB-C4A-NA	3.68	129.71	124.40
29	B	624	SQD	O9-S-O7	-3.67	101.88	113.82
29	b	601	SQD	O5-C5-C4	3.67	116.31	109.70
25	C	520	BCR	C27-C26-C25	3.67	127.66	122.70
23	C	509	CLA	C4A-NA-C1A	3.66	108.35	106.68
30	d	409	LHG	O8-C23-O10	-3.64	114.51	123.63
27	d	408	PL9	C7-C3-C2	-3.64	119.10	123.39
31	h	103	DGD	O3G-C3G-C2G	-3.62	102.01	110.82
24	a	605	PHO	C1-C2-C3	-3.61	120.28	126.20
23	c	510	CLA	C4A-NA-C1A	3.61	108.33	106.68
29	B	624	SQD	O47-C7-C8	3.61	119.30	111.48
23	B	611	CLA	O2D-CGD-CBD	3.61	117.53	111.23
23	B	605	CLA	C3B-C2B-C1B	-3.60	102.92	107.17
30	B	623	LHG	O8-C23-O10	-3.60	114.62	123.63
23	B	606	CLA	CHD-C1D-ND	-3.60	119.73	124.80
23	b	613	CLA	C3B-C4B-NB	-3.60	107.32	110.53
23	B	609	CLA	O2D-CGD-O1D	-3.59	116.85	123.85
25	k	102	BCR	C27-C26-C25	3.59	127.55	122.70
23	c	504	CLA	C4A-NA-C1A	3.59	108.31	106.68
31	h	103	DGD	C1E-O6E-C5E	3.58	120.72	113.72
23	a	604	CLA	CHB-C4A-NA	3.58	129.56	124.40
31	A	617	DGD	C1D-C2D-C3D	-3.58	102.48	110.01
27	A	611	PL9	C7-C3-C2	-3.57	119.18	123.39
23	b	610	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
23	h	101	CLA	O2D-CGD-CBD	3.56	117.46	111.23
30	L	101	LHG	O4-P-O5	3.55	128.98	112.44
23	B	615	CLA	C4A-NA-C1A	3.55	108.30	106.68
23	B	615	CLA	CMB-C2B-C1B	-3.55	120.02	125.42
23	c	503	CLA	C3B-C4B-NB	-3.54	107.37	110.53
23	b	614	CLA	C1-C2-C3	-3.54	120.39	126.20
31	c	517	DGD	C1D-C2D-C3D	-3.54	102.57	110.01
23	b	613	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
23	b	606	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
23	b	605	CLA	CBC-CAC-C3C	-3.53	102.85	112.42
23	b	612	CLA	CMB-C2B-C1B	-3.52	120.06	125.42
25	t	101	BCR	C15-C16-C17	-3.52	116.32	123.52
31	C	517	DGD	O3G-C1D-C2D	-3.52	102.93	108.27
23	c	502	CLA	O2D-CGD-O1D	-3.52	117.01	123.85
35	f	102	HEM	CBD-CAD-C3D	-3.51	102.81	112.53
23	b	612	CLA	C11-C12-C13	-3.51	104.29	115.97
24	a	605	PHO	O2A-CGA-O1A	-3.50	114.87	123.63
23	C	512	CLA	O2D-CGD-CBD	3.50	117.35	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
23	a	606	CLA	CHB-C4A-NA	3.50	129.45	124.40
25	B	619	BCR	C37-C22-C21	-3.49	117.16	122.82
23	B	610	CLA	O2A-CGA-O1A	-3.49	114.89	123.63
23	c	509	CLA	CHB-C4A-NA	3.47	129.41	124.40
23	C	506	CLA	CHB-C4A-NA	3.47	129.41	124.40
28	c	522	LMG	C1-O6-C5	-3.46	106.97	113.72
23	b	614	CLA	CHD-C1D-ND	-3.46	119.94	124.80
23	C	503	CLA	C3B-C4B-NB	-3.45	107.45	110.53
31	C	516	DGD	O3G-C3G-C2G	-3.45	102.42	110.82
23	d	402	CLA	C4-C3-C5	3.45	121.22	115.23
28	b	621	LMG	C1-O6-C5	-3.45	106.99	113.72
23	c	503	CLA	C1D-ND-C4D	3.42	108.71	106.31
25	t	101	BCR	C27-C26-C25	3.41	127.31	122.70
23	B	601	CLA	CAA-C2A-C3A	-3.40	103.81	113.00
30	D	408	LHG	O8-C23-O10	-3.40	115.13	123.63
23	b	605	CLA	C16-C15-C13	-3.39	104.69	115.97
27	D	407	PL9	C37-C38-C39	-3.39	119.86	127.62
23	b	603	CLA	C4A-NA-C1A	3.39	108.23	106.68
23	b	603	CLA	C3B-C4B-NB	-3.39	107.50	110.53
23	B	604	CLA	CHB-C4A-NA	3.39	129.29	124.40
23	D	402	CLA	C3B-C4B-NB	-3.39	107.51	110.53
23	C	501	CLA	C3B-C4B-NB	-3.38	107.51	110.53
29	B	624	SQD	C3-C4-C5	3.38	116.36	110.23
23	C	508	CLA	C3B-C4B-NB	-3.38	107.51	110.53
23	C	506	CLA	C4A-NA-C1A	3.38	108.22	106.68
23	A	607	CLA	C1D-ND-C4D	-3.37	103.94	106.31
23	A	604	CLA	O2A-CGA-O1A	-3.37	115.20	123.63
31	a	616	DGD	O1G-C1A-O1A	-3.37	115.20	123.63
23	b	613	CLA	CMB-C2B-C1B	-3.37	120.29	125.42
27	a	611	PL9	C35-C34-C36	3.36	121.07	115.23
23	b	612	CLA	O1D-CGD-CBD	3.36	131.15	124.52
23	b	611	CLA	CHD-C4C-NC	3.36	129.44	124.23
23	b	611	CLA	CHD-C1D-C2D	3.36	132.47	125.49
23	B	610	CLA	CHB-C4A-NA	3.35	129.24	124.40
29	A	614	SQD	O4-C4-C3	-3.35	102.48	110.38
25	b	617	BCR	C11-C10-C9	-3.35	122.58	127.28
23	A	607	CLA	O2D-CGD-CBD	3.33	117.06	111.23
31	h	103	DGD	O3E-C3E-C2E	-3.33	102.52	110.38
25	b	619	BCR	C29-C30-C25	3.33	115.28	110.44
23	C	502	CLA	C4A-NA-C1A	3.33	108.20	106.68
23	b	609	CLA	CMB-C2B-C1B	-3.32	120.36	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	O2D-CGD-CBD	3.32	117.04	111.23
25	C	514	BCR	C27-C26-C25	3.32	127.19	122.70
23	A	603	CLA	CHB-C4A-NA	3.31	129.18	124.40
23	B	606	CLA	CHD-C4C-NC	3.31	129.36	124.23
25	d	404	BCR	C27-C26-C25	3.31	127.18	122.70
28	B	620	LMG	O1-C1-C2	-3.31	103.25	108.27
23	B	612	CLA	CHB-C4A-NA	3.31	129.17	124.40
23	b	609	CLA	C3B-C4B-NB	-3.30	107.58	110.53
31	c	518	DGD	O6D-C1D-O3G	-3.30	102.25	110.04
23	a	603	CLA	CAC-C3C-C4C	3.30	129.08	124.79
23	D	402	CLA	CED-O2D-CGD	3.30	123.40	115.92
27	D	407	PL9	C22-C23-C24	-3.30	120.07	127.62
23	B	612	CLA	C11-C12-C13	-3.29	105.03	115.97
27	A	611	PL9	C40-C39-C38	-3.29	115.18	123.63
25	b	617	BCR	C33-C5-C6	-3.29	120.90	124.48
23	c	505	CLA	O2D-CGD-CBD	3.28	116.97	111.23
34	a	610	BCT	O2-C-O1	3.28	128.06	119.68
27	d	408	PL9	C40-C39-C41	3.28	120.92	115.23
23	B	603	CLA	CHD-C1D-ND	-3.27	120.20	124.80
23	h	101	CLA	CHB-C4A-NA	3.27	129.12	124.40
23	B	607	CLA	C1-C2-C3	-3.26	120.86	126.20
23	B	605	CLA	O2A-CGA-O1A	-3.26	115.47	123.63
23	c	508	CLA	CHB-C4A-NA	3.26	129.10	124.40
23	h	101	CLA	CHD-C1D-ND	-3.25	120.23	124.80
25	T	101	BCR	C38-C26-C27	-3.25	106.67	113.60
23	b	616	CLA	O2D-CGD-CBD	3.23	116.88	111.23
23	d	402	CLA	C3B-C4B-NB	-3.23	107.65	110.53
23	C	502	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
23	B	616	CLA	O2A-CGA-O1A	-3.23	115.55	123.63
23	b	602	CLA	CMB-C2B-C1B	-3.22	120.51	125.42
23	b	613	CLA	C7-C6-C5	-3.22	104.68	113.26
23	h	101	CLA	CBA-CAA-C2A	3.22	123.37	113.79
23	b	613	CLA	CHB-C4A-NA	3.22	129.04	124.40
23	b	605	CLA	C4D-CHA-C1A	3.21	125.07	121.24
27	d	408	PL9	C45-C44-C46	-3.20	109.67	115.23
28	b	621	LMG	O1-C1-C2	-3.20	103.42	108.27
24	A	605	PHO	CMB-C2B-C3B	3.19	131.06	124.68
25	c	515	BCR	C27-C26-C25	3.19	127.01	122.70
28	c	522	LMG	O8-C28-O10	-3.18	115.68	123.63
25	B	619	BCR	C33-C5-C6	-3.18	121.02	124.48
23	b	611	CLA	O2D-CGD-CBD	3.18	116.78	111.23
23	c	505	CLA	O2D-CGD-O1D	-3.18	117.67	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	O2D-CGD-CBD	3.17	116.77	111.23
23	c	505	CLA	O2A-CGA-O1A	-3.17	115.71	123.63
28	m	101	LMG	O8-C28-O10	-3.16	115.72	123.63
29	B	624	SQD	O8-S-C6	3.16	112.08	105.97
27	d	408	PL9	C22-C23-C24	-3.16	120.39	127.62
23	b	611	CLA	CHD-C1D-ND	-3.15	120.37	124.80
29	a	613	SQD	O9-S-C6	3.15	111.46	106.76
25	B	619	BCR	C29-C30-C25	3.15	115.01	110.44
23	b	611	CLA	CHB-C4A-NA	3.14	128.94	124.40
25	Y	101	BCR	C15-C16-C17	-3.14	117.09	123.52
25	t	101	BCR	C38-C26-C27	-3.14	106.90	113.60
29	A	616	SQD	O47-C45-C46	3.13	113.42	106.21
31	H	102	DGD	O5D-C1E-C2E	3.13	113.03	108.27
23	B	606	CLA	CHD-C4C-C3C	-3.13	120.21	124.77
25	H	101	BCR	C27-C26-C25	3.12	126.92	122.70
29	F	101	SQD	O9-S-C6	3.12	111.42	106.76
29	A	614	SQD	O2-C2-C1	3.12	117.51	110.08
35	F	102	HEM	CBD-CAD-C3D	-3.12	103.91	112.53
27	d	408	PL9	C35-C34-C36	3.12	120.64	115.23
25	B	619	BCR	C38-C26-C25	-3.12	121.08	124.48
23	c	508	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
23	b	605	CLA	O1D-CGD-CBD	3.11	130.65	124.52
28	B	620	LMG	O6-C1-O1	-3.11	102.70	110.04
25	h	102	BCR	C27-C26-C25	3.11	126.91	122.70
23	a	603	CLA	C3B-C4B-NB	-3.11	107.75	110.53
27	A	611	PL9	C20-C19-C21	3.11	120.62	115.23
29	F	101	SQD	O9-S-O7	-3.10	103.73	113.82
30	A	615	LHG	O8-C23-C24	3.10	121.28	111.83
23	b	605	CLA	CHB-C1B-NB	3.09	128.69	124.05
23	C	511	CLA	CHB-C4A-NA	3.09	128.86	124.40
23	B	610	CLA	C3B-C4B-NB	-3.09	107.77	110.53
29	b	601	SQD	O48-C23-C24	3.09	121.25	111.83
29	B	624	SQD	O5-C5-C4	3.08	115.25	109.70
29	A	614	SQD	O47-C7-O49	-3.08	116.50	123.70
25	C	514	BCR	C33-C5-C6	-3.08	121.12	124.48
27	d	408	PL9	C8-C7-C3	3.08	119.99	112.03
27	d	408	PL9	C7-C8-C9	-3.08	121.53	126.83
23	B	612	CLA	C7-C6-C5	-3.08	105.06	113.26
25	c	514	BCR	C27-C26-C25	3.08	126.86	122.70
23	B	602	CLA	O2D-CGD-CBD	3.07	116.60	111.23
29	a	613	SQD	O47-C7-C8	3.07	118.12	111.48
23	b	604	CLA	CHB-C4A-NA	3.07	128.83	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	BCR	C38-C26-C25	-3.06	121.14	124.48
29	A	614	SQD	C1-O5-C5	-3.06	107.74	113.72
23	b	614	CLA	C3B-C4B-NB	-3.06	107.80	110.53
23	c	507	CLA	CHC-C4B-NB	3.06	128.64	124.05
23	B	605	CLA	C16-C15-C13	-3.06	105.81	115.97
27	D	407	PL9	C7-C3-C2	-3.05	119.79	123.39
23	B	605	CLA	CHB-C4A-NA	3.05	128.81	124.40
23	d	403	CLA	CHD-C1D-ND	-3.05	120.51	124.80
25	B	617	BCR	C29-C30-C25	3.05	114.86	110.44
25	a	607	BCR	C27-C26-C25	3.05	126.82	122.70
23	c	504	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
25	c	515	BCR	C2-C1-C6	3.04	114.86	110.44
23	b	616	CLA	CMB-C2B-C1B	-3.04	120.78	125.42
23	A	604	CLA	C3B-C4B-NB	-3.04	107.82	110.53
29	a	613	SQD	O9-S-O7	-3.04	103.94	113.82
31	A	617	DGD	C6D-O5D-C1E	3.03	120.30	113.80
29	a	615	SQD	O49-C7-C8	-3.03	111.93	123.78
31	c	517	DGD	O3D-C3D-C4D	-3.03	103.24	110.38
28	d	406	LMG	C3-C4-C5	-3.03	104.74	110.23
23	c	505	CLA	CHB-C4A-NA	3.03	128.77	124.40
23	b	611	CLA	C1-C2-C3	-3.02	121.24	126.20
25	t	101	BCR	C34-C9-C10	-3.02	117.92	122.82
23	a	603	CLA	C4D-CHA-C1A	3.02	124.85	121.24
29	b	601	SQD	C3-C4-C5	3.02	115.71	110.23
23	b	611	CLA	C2D-C1D-ND	-3.02	107.14	110.13
25	H	101	BCR	C2-C1-C6	3.02	114.82	110.44
25	b	617	BCR	C27-C26-C25	3.02	126.78	122.70
23	b	604	CLA	C11-C10-C8	-3.01	105.95	115.97
23	c	505	CLA	C4A-NA-C1A	3.01	108.05	106.68
25	c	515	BCR	C36-C18-C17	-3.01	117.94	122.82
23	B	606	CLA	O2A-CGA-O1A	-3.01	116.10	123.63
24	d	401	PHO	CMB-C2B-C3B	3.01	130.69	124.68
23	A	607	CLA	CHD-C1D-ND	-3.00	120.58	124.80
24	A	606	PHO	C2B-C1B-NB	-2.99	107.27	109.43
23	c	502	CLA	C3B-C4B-NB	-2.99	107.86	110.53
25	H	101	BCR	C16-C15-C14	-2.99	117.40	123.52
23	b	607	CLA	O1D-CGD-CBD	2.99	130.41	124.52
23	B	601	CLA	C2A-C1A-CHA	2.98	129.04	123.87
23	c	504	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
23	A	607	CLA	C4-C3-C5	2.97	120.39	115.23
25	b	619	BCR	C38-C26-C25	-2.97	121.24	124.48
23	A	613	CLA	O2D-CGD-CBD	2.97	116.42	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	518	DGD	O3D-C3D-C4D	-2.97	103.37	110.38
23	C	508	CLA	O2D-CGD-CBD	2.97	116.42	111.23
30	l	101	LHG	O8-C23-O10	-2.97	116.20	123.63
23	b	608	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
23	C	512	CLA	CAA-CBA-CGA	-2.97	104.79	113.21
25	h	102	BCR	C34-C9-C8	-2.96	113.56	118.09
23	c	509	CLA	C3B-C4B-NB	-2.96	107.89	110.53
23	B	603	CLA	C3B-C4B-NB	-2.95	107.89	110.53
27	a	611	PL9	C22-C23-C24	-2.95	120.87	127.62
23	A	604	CLA	C4A-NA-C1A	2.95	108.02	106.68
23	B	613	CLA	C1-C2-C3	-2.95	121.37	126.20
28	c	519	LMG	O6-C1-O1	-2.95	103.08	110.04
29	b	601	SQD	O47-C7-C8	2.95	117.86	111.48
23	a	612	CLA	CHB-C4A-NA	2.94	128.65	124.40
31	C	517	DGD	O5D-C1E-C2E	2.94	112.74	108.27
27	d	408	PL9	C20-C19-C21	2.94	120.34	115.23
30	B	623	LHG	O3-P-O5	-2.94	97.28	108.94
30	a	614	LHG	O8-C23-C24	2.93	120.77	111.83
25	C	514	BCR	C34-C9-C10	-2.93	118.07	122.82
23	b	612	CLA	CHB-C4A-NA	2.93	128.62	124.40
23	D	402	CLA	O2A-CGA-O1A	-2.93	116.31	123.63
23	b	614	CLA	CMD-C2D-C1D	2.92	129.88	124.73
23	C	511	CLA	CAC-C3C-C4C	2.92	128.59	124.79
23	B	613	CLA	CHB-C4A-NA	2.92	128.62	124.40
35	f	102	HEM	CHB-C1B-NB	2.92	127.98	124.37
23	d	403	CLA	C3B-C4B-NB	-2.92	107.93	110.53
25	B	618	BCR	C27-C26-C25	2.91	126.64	122.70
23	B	615	CLA	C3B-C4B-NB	-2.91	107.93	110.53
25	c	515	BCR	C35-C13-C14	-2.90	118.11	122.82
31	h	103	DGD	O6E-C5E-C4E	2.90	114.93	109.70
28	A	612	LMG	C38-C37-C36	-2.90	99.69	114.37
23	c	512	CLA	C3B-C4B-NB	-2.90	107.94	110.53
31	C	518	DGD	O3E-C3E-C2E	-2.90	103.54	110.38
23	c	510	CLA	C3B-C4B-NB	-2.90	107.94	110.53
31	c	517	DGD	C3E-C4E-C5E	-2.90	104.98	110.23
23	B	602	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
25	T	101	BCR	C2-C1-C6	2.89	114.64	110.44
23	B	615	CLA	CHB-C1B-NB	2.89	128.39	124.05
28	d	406	LMG	O6-C1-O1	-2.89	103.22	110.04
25	k	101	BCR	C27-C26-C25	2.89	126.61	122.70
25	b	617	BCR	C2-C1-C6	2.89	114.63	110.44
31	A	617	DGD	C4E-C3E-C2E	-2.89	105.76	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	102	HEM	C4C-C3C-C2C	2.88	109.31	106.81
23	B	601	CLA	C1-C2-C3	-2.88	121.47	126.20
35	f	102	HEM	C3B-C2B-C1B	2.88	108.58	106.41
28	C	519	LMG	O7-C10-O9	-2.88	116.97	123.70
27	D	407	PL9	C42-C43-C44	-2.88	121.03	127.62
23	d	403	CLA	CHA-C1A-NA	-2.88	119.87	126.39
23	B	614	CLA	C1-C2-C3	-2.88	121.48	126.20
23	C	513	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
23	B	615	CLA	CHB-C4A-NA	2.87	128.55	124.40
23	C	504	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	C	512	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	B	603	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
23	B	611	CLA	CHD-C1D-ND	-2.87	120.77	124.80
29	B	624	SQD	O48-C23-C24	2.86	120.57	111.83
25	D	404	BCR	C2-C1-C6	2.86	114.59	110.44
23	b	605	CLA	C11-C12-C13	-2.86	106.47	115.97
25	a	607	BCR	C30-C25-C26	-2.85	118.74	122.64
23	B	606	CLA	C6-C5-C3	-2.85	106.53	113.47
27	A	611	PL9	O2-C1-C2	-2.85	115.35	121.83
28	D	405	LMG	O8-C28-O10	-2.85	116.51	123.63
31	c	518	DGD	O1G-C1A-O1A	-2.84	116.51	123.63
25	h	102	BCR	C2-C1-C6	2.84	114.57	110.44
23	A	604	CLA	CED-O2D-CGD	-2.84	109.48	115.92
25	b	617	BCR	C29-C30-C25	2.84	114.56	110.44
23	C	509	CLA	C1-C2-C3	-2.84	121.55	126.20
23	B	605	CLA	CED-O2D-CGD	2.84	122.35	115.92
23	b	603	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
23	a	603	CLA	O1D-CGD-CBD	2.83	130.10	124.52
23	C	509	CLA	C3B-C4B-NB	-2.82	108.01	110.53
23	b	612	CLA	CMB-C2B-C3B	2.82	133.18	126.55
25	d	404	BCR	C1-C6-C5	-2.82	118.78	122.64
23	b	608	CLA	CHA-C1A-NA	-2.82	120.01	126.39
31	C	518	DGD	O3G-C1D-C2D	-2.82	103.99	108.27
23	C	501	CLA	C1D-ND-C4D	-2.82	104.34	106.31
30	l	101	LHG	O8-C23-C24	2.82	120.42	111.83
23	B	603	CLA	CHD-C4C-NC	2.81	128.59	124.23
25	c	515	BCR	C30-C25-C26	-2.81	118.79	122.64
23	B	602	CLA	O2A-CGA-O1A	-2.81	116.59	123.63
23	b	602	CLA	CHC-C1C-NC	2.81	128.55	124.31
25	A	608	BCR	C27-C26-C25	2.81	126.50	122.70
23	c	502	CLA	C1-C2-C3	-2.81	121.59	126.20
23	A	607	CLA	C2C-C1C-NC	2.81	112.93	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	101	SQD	C1-C2-C3	-2.80	104.11	110.01
25	Y	101	BCR	C27-C26-C25	2.80	126.49	122.70
30	D	406	LHG	C20-C19-C18	-2.80	100.20	114.37
27	D	407	PL9	C36-C34-C33	-2.80	114.88	121.17
23	h	101	CLA	O2A-CGA-O1A	-2.80	116.62	123.63
23	C	504	CLA	CHD-C1D-ND	-2.80	120.86	124.80
23	c	503	CLA	O1D-CGD-CBD	2.79	130.03	124.52
23	A	603	CLA	O1D-CGD-CBD	2.79	130.03	124.52
23	b	614	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
25	b	618	BCR	C15-C14-C13	-2.79	123.36	127.28
28	A	612	LMG	O6-C1-O1	-2.79	103.45	110.04
30	L	101	LHG	O8-C23-O10	-2.79	116.66	123.63
23	B	608	CLA	O2D-CGD-CBD	2.78	116.10	111.23
30	d	407	LHG	C20-C19-C18	-2.78	100.30	114.37
23	b	606	CLA	C4D-CHA-C1A	2.78	124.56	121.24
23	d	403	CLA	CHB-C4A-NA	2.78	128.41	124.40
31	C	516	DGD	O6D-C1D-O3G	-2.77	103.49	110.04
23	C	506	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
31	C	517	DGD	O6D-C1D-O3G	-2.77	103.49	110.04
28	d	406	LMG	O2-C2-C1	-2.77	103.47	110.08
23	b	605	CLA	CHD-C1D-ND	-2.77	120.90	124.80
23	b	613	CLA	O1D-CGD-CBD	2.77	129.99	124.52
23	B	602	CLA	C4A-NA-C1A	2.77	107.94	106.68
25	C	514	BCR	C11-C10-C9	-2.77	123.39	127.28
23	B	611	CLA	C3B-C4B-NB	-2.77	108.06	110.53
30	l	101	LHG	C29-C28-C27	-2.77	100.37	114.37
23	B	614	CLA	O2D-CGD-CBD	2.77	116.07	111.23
23	c	504	CLA	O2D-CGD-CBD	2.77	116.07	111.23
23	C	506	CLA	O1D-CGD-CBD	2.77	129.97	124.52
25	Y	101	BCR	C39-C30-C25	-2.77	105.91	110.24
31	h	103	DGD	C3D-C4D-C5D	-2.77	105.22	110.23
25	k	101	BCR	C33-C5-C6	-2.76	121.47	124.48
23	c	501	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
25	h	102	BCR	C30-C25-C26	-2.76	118.86	122.64
23	B	608	CLA	C2C-C1C-NC	2.76	112.88	109.98
29	A	616	SQD	O47-C7-C8	2.76	117.45	111.48
23	b	616	CLA	CMB-C2B-C3B	2.76	133.03	126.55
28	B	622	LMG	O7-C10-O9	-2.76	116.25	123.33
28	C	519	LMG	O8-C28-O10	-2.75	116.74	123.63
31	C	516	DGD	C3D-C4D-C5D	-2.75	105.24	110.23
27	A	611	PL9	O2-C1-C6	2.75	124.85	120.48
31	a	616	DGD	C1G-C2G-C3G	-2.74	105.47	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C3A-C2A-C1A	2.74	105.45	101.34
25	t	101	BCR	C35-C13-C12	2.74	122.28	118.09
28	D	405	LMG	O2-C2-C1	-2.74	103.54	110.08
29	a	613	SQD	C3-C4-C5	2.74	115.20	110.23
25	C	514	BCR	C15-C14-C13	-2.74	123.44	127.28
24	A	605	PHO	O2D-CGD-O1D	-2.74	118.52	123.85
23	C	503	CLA	C4D-CHA-C1A	2.74	124.51	121.24
28	m	101	LMG	O3-C3-C2	-2.73	103.93	110.38
29	a	613	SQD	O48-C23-C24	2.73	120.16	111.83
23	A	603	CLA	C6-C5-C3	2.73	120.11	113.47
29	f	101	SQD	O8-S-C6	2.72	111.23	105.97
25	T	101	BCR	C1-C6-C5	-2.72	118.92	122.64
23	b	610	CLA	CAA-CBA-CGA	-2.72	105.49	113.21
25	c	515	BCR	C34-C9-C10	-2.72	118.41	122.82
25	H	101	BCR	C35-C13-C14	-2.72	118.42	122.82
23	b	609	CLA	O1D-CGD-CBD	2.71	129.87	124.52
23	C	508	CLA	C4A-NA-C1A	2.71	107.92	106.68
23	c	501	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
29	a	613	SQD	O47-C7-O49	-2.71	117.36	123.70
23	b	603	CLA	CHB-C1B-NB	2.71	128.12	124.05
31	c	517	DGD	C3G-O3G-C1D	2.71	119.61	113.80
25	a	607	BCR	C29-C30-C25	2.71	114.37	110.44
29	F	101	SQD	C1-O5-C5	-2.70	108.44	113.72
28	c	519	LMG	O8-C28-O10	-2.70	116.88	123.63
25	a	607	BCR	C38-C26-C27	-2.70	107.84	113.60
25	C	515	BCR	C33-C5-C6	-2.70	121.54	124.48
24	a	605	PHO	C2B-C1B-NB	-2.70	107.48	109.43
28	c	519	LMG	O7-C10-O9	-2.69	117.79	122.99
25	c	515	BCR	C33-C5-C6	-2.69	121.54	124.48
23	b	615	CLA	CHB-C1B-NB	2.69	128.09	124.05
23	b	611	CLA	C1D-ND-C4D	2.69	108.20	106.31
31	c	518	DGD	O3G-C3G-C2G	-2.69	104.27	110.82
23	c	509	CLA	C4D-C3D-CAD	-2.69	105.18	108.11
25	C	515	BCR	C15-C16-C17	-2.69	118.01	123.52
23	C	501	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
23	b	613	CLA	CMB-C2B-C3B	2.69	132.87	126.55
23	c	506	CLA	C6-C5-C3	-2.69	106.93	113.47
29	a	615	SQD	O48-C23-C24	2.69	120.02	111.83
23	B	603	CLA	C9-C8-C7	-2.68	101.70	111.27
23	c	502	CLA	C3A-C2A-C1A	2.68	105.36	101.34
25	C	515	BCR	C36-C18-C17	-2.68	118.47	122.82
31	c	517	DGD	O2E-C2E-C1E	-2.68	103.69	110.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
23	b	605	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
25	T	101	BCR	C15-C14-C13	-2.68	123.52	127.28
23	C	504	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
28	A	612	LMG	O8-C28-O10	-2.68	116.93	123.63
28	m	101	LMG	C1-C2-C3	-2.68	104.38	110.01
29	f	101	SQD	O9-S-O7	-2.67	105.13	113.82
28	c	521	LMG	O3-C3-C2	-2.67	104.08	110.38
23	A	604	CLA	O2D-CGD-CBD	2.67	115.90	111.23
23	c	505	CLA	CHD-C1D-ND	-2.67	121.05	124.80
25	C	514	BCR	C38-C26-C25	-2.67	121.58	124.48
23	b	604	CLA	CMC-C2C-C1C	-2.66	120.87	125.03
31	H	102	DGD	O2G-C1B-O1B	-2.66	117.48	123.70
30	B	623	LHG	C11-C10-C9	-2.66	100.92	114.37
31	C	517	DGD	O5D-C6D-C5D	-2.66	103.42	109.42
30	d	405	LHG	O8-C6-C5	-2.66	100.73	108.40
27	d	408	PL9	C37-C38-C39	-2.66	121.54	127.62
23	b	606	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
30	a	614	LHG	O8-C23-O10	-2.66	116.98	123.63
23	D	403	CLA	C3B-C4B-NB	-2.66	108.16	110.53
23	b	609	CLA	CMB-C2B-C3B	2.66	132.80	126.55
25	a	607	BCR	C35-C13-C14	-2.65	118.52	122.82
23	b	609	CLA	CHD-C4C-NC	2.65	128.35	124.23
31	h	103	DGD	C1D-C2D-C3D	-2.65	104.43	110.01
31	H	102	DGD	O2D-C2D-C1D	-2.65	103.76	110.08
30	D	408	LHG	O8-C23-C24	2.65	119.91	111.83
31	H	102	DGD	C3E-C4E-C5E	-2.65	105.43	110.23
23	A	613	CLA	CAA-C2A-C1A	-2.65	103.30	111.97
23	B	603	CLA	CHD-C1D-C2D	2.64	130.99	125.49
23	b	608	CLA	O2A-CGA-O1A	-2.64	117.01	123.63
24	a	605	PHO	CMB-C2B-C3B	2.64	129.97	124.68
25	b	618	BCR	C15-C16-C17	-2.64	118.11	123.52
30	d	405	LHG	C11-C10-C9	-2.64	101.02	114.37
23	a	604	CLA	CED-O2D-CGD	-2.64	109.93	115.92
31	c	517	DGD	O3G-C3G-C2G	-2.64	104.40	110.82
31	c	517	DGD	CDB-CCB-CBB	-2.64	101.03	114.37
23	b	616	CLA	CHB-C4A-NA	2.64	128.21	124.40
24	d	401	PHO	O2D-CGD-CBD	-2.64	108.05	110.95
35	F	102	HEM	O2D-CGD-CBD	2.64	122.33	114.00
31	c	518	DGD	O3E-C3E-C2E	-2.64	104.16	110.38
31	C	518	DGD	CDB-CCB-CBB	-2.63	101.05	114.37
23	b	608	CLA	CHD-C4C-C3C	-2.63	120.94	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	517	DGD	C8B-C7B-C6B	-2.63	101.08	114.37
29	b	601	SQD	O10-C23-C24	-2.63	113.51	123.78
23	b	609	CLA	CHC-C4B-NB	2.63	127.99	124.05
25	A	608	BCR	C2-C1-C6	2.62	114.25	110.44
25	a	607	BCR	C33-C5-C6	-2.62	121.62	124.48
23	B	605	CLA	O1D-CGD-CBD	2.62	129.69	124.52
23	B	614	CLA	CHB-C1B-NB	2.62	127.98	124.05
23	b	608	CLA	C6-C7-C8	-2.62	107.26	115.97
23	C	504	CLA	C6-C5-C3	2.62	119.84	113.47
23	C	503	CLA	C5-C3-C2	-2.62	115.30	121.17
25	b	619	BCR	C27-C26-C25	2.61	126.23	122.70
23	a	604	CLA	O2D-CGD-CBD	2.61	115.80	111.23
25	H	101	BCR	C35-C13-C12	2.61	122.08	118.09
23	B	613	CLA	CAC-C3C-C4C	2.61	128.19	124.79
23	b	605	CLA	CHA-C1A-NA	-2.61	120.48	126.39
23	C	509	CLA	CHB-C4A-NA	2.61	128.17	124.40
23	b	614	CLA	CMB-C2B-C3B	2.61	132.69	126.55
23	B	608	CLA	O1D-CGD-CBD	2.61	129.66	124.52
23	c	502	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
24	d	401	PHO	CMA-C3A-C4A	-2.61	108.99	114.61
31	c	518	DGD	O1G-C1A-C2A	-2.61	103.89	111.83
23	C	512	CLA	C4A-NA-C1A	2.60	107.87	106.68
23	C	502	CLA	CHD-C1D-ND	-2.60	121.14	124.80
28	A	612	LMG	O7-C10-O9	-2.60	117.62	123.70
23	B	603	CLA	C7-C6-C5	-2.60	106.33	113.26
23	D	402	CLA	C1D-CHD-C4C	-2.60	120.49	126.02
28	B	622	LMG	O8-C28-O10	-2.60	116.65	123.33
23	b	612	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
23	b	610	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	D	404	BCR	C27-C26-C25	2.60	126.21	122.70
25	B	618	BCR	C2-C1-C6	2.59	114.20	110.44
27	A	611	PL9	C22-C23-C24	-2.59	121.69	127.62
23	B	602	CLA	C1-C2-C3	-2.59	121.95	126.20
23	B	606	CLA	CHD-C1D-C2D	2.59	130.87	125.49
25	b	619	BCR	C2-C1-C6	2.59	114.20	110.44
23	c	506	CLA	CGD-CBD-CAD	-2.59	102.47	110.85
27	D	407	PL9	C27-C28-C29	-2.59	121.70	127.62
23	b	606	CLA	C6-C5-C3	2.59	119.77	113.47
23	c	510	CLA	O2D-CGD-CBD	2.58	115.75	111.23
25	B	619	BCR	C2-C1-C6	2.58	114.19	110.44
28	c	521	LMG	O8-C28-O10	-2.58	117.17	123.63
23	c	503	CLA	CAC-C3C-C4C	2.58	128.15	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	518	DGD	C3D-C4D-C5D	-2.58	105.56	110.23
25	h	102	BCR	C38-C26-C25	-2.58	121.67	124.48
23	c	513	CLA	C4A-NA-C1A	2.58	107.86	106.68
29	b	601	SQD	O9-S-C6	2.58	110.60	106.76
23	c	509	CLA	CMD-C2D-C3D	2.57	133.59	127.69
28	A	612	LMG	C36-C35-C34	-2.57	101.36	114.37
30	B	623	LHG	O8-C23-C24	2.57	119.67	111.83
31	C	518	DGD	O6D-C1D-O3G	-2.57	103.97	110.04
31	c	516	DGD	O3E-C3E-C2E	-2.57	104.32	110.38
23	b	612	CLA	CHD-C1D-ND	-2.57	121.19	124.80
34	D	401	BCT	O3-C-O1	-2.56	113.12	119.68
23	C	505	CLA	C3B-C4B-NB	-2.56	108.24	110.53
31	C	516	DGD	O5D-C6D-C5D	-2.56	103.65	109.42
23	b	602	CLA	C3B-C4B-NB	-2.56	108.24	110.53
25	c	515	BCR	C8-C9-C10	2.56	123.03	119.01
25	A	608	BCR	C4-C5-C6	2.56	126.16	122.70
31	A	617	DGD	CDB-CCB-CBB	-2.55	101.46	114.37
23	c	506	CLA	CAC-C3C-C4C	2.55	128.11	124.79
23	C	507	CLA	CHD-C1D-ND	-2.55	121.21	124.80
23	a	603	CLA	C2A-C1A-CHA	2.55	128.29	123.87
23	C	504	CLA	CHB-C1B-NB	2.55	127.87	124.05
23	B	616	CLA	CAC-C3C-C4C	2.55	128.11	124.79
25	B	617	BCR	C11-C10-C9	-2.54	123.71	127.28
23	B	606	CLA	CGD-CBD-CAD	-2.54	102.62	110.85
23	C	503	CLA	CHD-C1D-ND	-2.54	121.23	124.80
25	c	514	BCR	C11-C10-C9	-2.54	123.72	127.28
25	c	514	BCR	C15-C14-C13	-2.53	123.72	127.28
23	C	507	CLA	C2A-C1A-CHA	2.53	128.26	123.87
23	c	509	CLA	O2A-CGA-CBA	2.53	119.56	111.83
23	c	513	CLA	C3B-C4B-NB	-2.53	108.27	110.53
31	c	518	DGD	C7B-C6B-C5B	-2.53	101.57	114.37
23	B	603	CLA	C6-C5-C3	2.53	119.63	113.47
23	B	602	CLA	CHA-C1A-NA	-2.53	120.66	126.39
23	b	611	CLA	C4-C3-C2	-2.53	117.14	123.63
23	B	605	CLA	CHD-C1D-ND	-2.52	121.25	124.80
23	c	501	CLA	CED-O2D-CGD	-2.52	110.19	115.92
29	a	613	SQD	C1-C2-C3	-2.52	104.71	110.01
28	D	405	LMG	O1-C7-C8	-2.52	104.69	110.82
23	C	503	CLA	O1D-CGD-CBD	2.52	129.49	124.52
24	a	605	PHO	CMD-C2D-C3D	2.52	129.71	124.68
25	B	618	BCR	C35-C13-C14	-2.52	118.74	122.82
30	d	407	LHG	O8-C23-C24	2.52	119.51	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	606	CLA	O2D-CGD-CBD	2.51	115.62	111.23
23	B	616	CLA	C1-O2A-CGA	2.51	122.74	116.65
23	c	508	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
23	B	610	CLA	CHD-C1D-ND	-2.51	121.27	124.80
23	A	603	CLA	O2D-CGD-CBD	-2.51	106.84	111.23
28	b	621	LMG	C8-O7-C10	2.51	123.80	117.80
23	b	616	CLA	CHD-C1D-ND	-2.51	121.27	124.80
23	c	512	CLA	C2D-C1D-ND	-2.51	107.64	110.13
23	B	609	CLA	C7-C6-C5	-2.51	106.58	113.26
23	C	501	CLA	CAC-C3C-C4C	2.50	128.05	124.79
23	B	611	CLA	CHD-C1D-C2D	2.50	130.70	125.49
23	b	603	CLA	CHD-C1D-ND	-2.50	121.28	124.80
23	b	611	CLA	C3C-C4C-NC	-2.50	107.22	110.43
25	A	608	BCR	C34-C9-C10	-2.50	118.76	122.82
23	B	615	CLA	C4-C3-C2	2.50	130.05	123.63
23	c	502	CLA	C4D-CHA-C1A	2.50	124.23	121.24
23	A	607	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
25	A	608	BCR	C33-C5-C6	-2.50	121.76	124.48
25	c	514	BCR	C30-C25-C26	-2.50	119.23	122.64
28	d	406	LMG	C1-C2-C3	-2.50	104.76	110.01
23	C	508	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
25	C	520	BCR	C11-C10-C9	-2.49	123.78	127.28
23	c	505	CLA	C6-C7-C8	-2.49	107.68	115.97
24	A	605	PHO	C2D-C1D-ND	2.49	111.23	109.43
30	d	405	LHG	O8-C23-O10	-2.49	117.40	123.63
23	C	507	CLA	CHD-C4C-NC	2.49	128.09	124.23
23	c	511	CLA	CHB-C1B-NB	2.49	127.78	124.05
29	a	615	SQD	O48-C23-O10	-2.49	117.40	123.63
23	B	605	CLA	C4A-NA-C1A	2.49	107.81	106.68
30	D	408	LHG	C25-C24-C23	2.49	122.82	113.69
23	c	507	CLA	C2C-C1C-NC	2.49	112.60	109.98
25	c	514	BCR	C24-C23-C22	-2.48	122.56	126.23
23	a	612	CLA	C1-O2A-CGA	2.48	122.66	116.65
29	F	101	SQD	O7-S-C6	-2.48	103.05	106.76
27	D	407	PL9	C20-C19-C21	2.48	119.54	115.23
23	B	616	CLA	CHA-C1A-NA	-2.48	120.77	126.39
23	D	403	CLA	O2D-CGD-CBD	2.48	115.57	111.23
23	D	402	CLA	CHB-C4A-NA	2.48	127.98	124.40
31	c	516	DGD	C3D-C4D-C5D	-2.48	105.74	110.23
29	b	601	SQD	O7-S-C6	2.48	110.46	106.76
28	A	612	LMG	C40-C39-C38	-2.48	101.84	114.37
23	c	510	CLA	CHD-C1D-ND	-2.48	121.31	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	102	BCR	C16-C17-C18	-2.48	123.80	127.28
23	c	507	CLA	O1D-CGD-CBD	2.48	129.40	124.52
27	a	611	PL9	C27-C28-C29	-2.48	121.95	127.62
23	c	511	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
23	b	604	CLA	C1-C2-C3	-2.47	122.14	126.20
28	d	406	LMG	O1-C7-C8	-2.47	104.80	110.82
23	B	605	CLA	C1-O2A-CGA	-2.47	110.66	116.65
23	c	506	CLA	CHA-C1A-NA	-2.47	120.79	126.39
29	f	101	SQD	O5-C5-C4	2.47	114.16	109.70
23	C	511	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
23	c	510	CLA	C2A-C3A-C4A	2.47	105.86	101.87
29	F	101	SQD	O48-C23-O10	-2.47	117.45	123.63
36	v	201	HEC	CHA-C1A-C2A	2.47	128.76	124.86
23	B	613	CLA	CHA-C1A-NA	-2.47	120.80	126.39
23	c	503	CLA	CHD-C1D-C2D	2.47	130.61	125.49
25	D	404	BCR	C16-C15-C14	-2.46	118.48	123.52
23	C	506	CLA	C3B-C4B-NB	-2.46	108.33	110.53
25	c	515	BCR	C15-C14-C13	-2.46	123.82	127.28
31	H	102	DGD	C1E-O6E-C5E	2.46	118.53	113.72
23	B	601	CLA	O1D-CGD-CBD	2.46	129.38	124.52
23	b	612	CLA	O2D-CGD-CBD	-2.46	106.93	111.23
23	b	609	CLA	CHD-C1D-ND	-2.46	121.34	124.80
23	B	613	CLA	C4-C3-C5	2.46	119.50	115.23
23	b	604	CLA	CHC-C1C-NC	2.46	128.01	124.31
29	a	613	SQD	O5-C5-C4	2.46	114.13	109.70
23	c	507	CLA	CHD-C4C-C3C	-2.46	121.19	124.77
31	a	616	DGD	C1G-O1G-C1A	2.46	126.09	117.12
23	B	611	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
23	C	510	CLA	O2D-CGD-CBD	2.45	115.52	111.23
23	D	403	CLA	CHB-C1B-NB	2.45	127.73	124.05
31	A	617	DGD	O5D-C6D-C5D	-2.45	103.89	109.42
23	C	507	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
23	C	504	CLA	CHD-C4C-NC	2.45	128.03	124.23
23	C	504	CLA	CHB-C4A-NA	2.45	127.93	124.40
23	A	613	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
31	A	617	DGD	C3E-C4E-C5E	-2.45	105.79	110.23
23	D	403	CLA	CAA-CBA-CGA	-2.45	106.26	113.21
23	A	604	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
25	b	619	BCR	C11-C10-C9	-2.44	123.85	127.28
29	b	601	SQD	O9-S-O7	-2.44	105.88	113.82
28	m	101	LMG	O6-C1-O1	-2.44	104.27	110.04
28	d	406	LMG	O1-C1-C2	-2.44	104.56	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	102	BCR	C11-C10-C9	-2.44	123.85	127.28
25	A	608	BCR	C19-C18-C17	-2.44	115.17	119.01
27	a	611	PL9	O2-C1-C6	2.44	124.36	120.48
25	D	404	BCR	C24-C23-C22	-2.44	122.62	126.23
23	C	510	CLA	CHB-C4A-NA	2.44	127.92	124.40
28	B	620	LMG	O3-C3-C2	-2.44	104.62	110.38
23	a	606	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
23	c	508	CLA	O2D-CGD-CBD	2.43	115.49	111.23
23	A	603	CLA	CAC-C3C-C4C	2.43	127.96	124.79
28	A	612	LMG	C9-C8-C7	-2.43	106.13	111.78
23	b	613	CLA	C2C-C1C-NC	2.43	112.53	109.98
23	B	608	CLA	CED-O2D-CGD	-2.43	110.41	115.92
31	C	517	DGD	O6E-C1E-O5D	-2.43	104.31	110.04
23	C	508	CLA	CHB-C4A-NA	2.42	127.90	124.40
23	b	607	CLA	C3B-C4B-NB	-2.42	108.37	110.53
23	c	513	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
31	H	102	DGD	C1D-C2D-C3D	-2.42	104.92	110.01
23	A	607	CLA	CHC-C1C-C2C	-2.42	120.08	126.95
23	B	614	CLA	CHB-C1B-C2B	-2.42	120.41	127.43
28	m	101	LMG	O1-C7-C8	-2.42	104.94	110.82
23	c	501	CLA	CHB-C1B-NB	2.42	127.67	124.05
23	B	601	CLA	CHA-C4D-ND	2.41	137.53	132.55
23	c	503	CLA	C4-C3-C5	2.41	119.42	115.23
23	B	614	CLA	CHC-C4B-NB	2.41	127.67	124.05
23	b	610	CLA	CHA-C1A-NA	-2.41	120.93	126.39
25	t	101	BCR	C4-C5-C6	2.41	125.96	122.70
25	c	515	BCR	C1-C6-C5	-2.41	119.34	122.64
23	D	403	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
23	C	507	CLA	CHB-C4A-NA	2.41	127.87	124.40
23	B	612	CLA	CED-O2D-CGD	-2.41	110.46	115.92
23	B	613	CLA	C2A-C1A-CHA	2.40	128.04	123.87
23	C	505	CLA	CAC-C3C-C2C	-2.40	123.14	127.56
28	A	612	LMG	C4-C3-C2	-2.40	106.61	110.83
29	B	624	SQD	O47-C7-O49	-2.40	118.09	123.70
29	B	624	SQD	O48-C23-O10	-2.40	117.62	123.63
23	A	613	CLA	CHB-C4A-NA	2.40	127.86	124.40
30	D	406	LHG	O8-C23-C24	2.40	119.15	111.83
23	c	501	CLA	C3B-C4B-NB	-2.40	108.39	110.53
25	t	101	BCR	C7-C8-C9	-2.40	122.69	126.23
35	f	102	HEM	CAB-C3B-C2B	-2.40	120.64	128.43
23	A	613	CLA	C3C-C4C-NC	-2.39	107.36	110.43
24	A	606	PHO	O1D-CGD-CBD	2.39	128.35	124.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	516	DGD	O6E-C5E-C4E	2.39	114.01	109.70
23	B	610	CLA	O2D-CGD-CBD	2.39	115.42	111.23
23	c	503	CLA	C2D-C1D-ND	-2.39	107.76	110.13
25	c	515	BCR	C11-C10-C9	-2.39	123.92	127.28
23	B	616	CLA	CHB-C1B-NB	2.39	127.64	124.05
23	B	612	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
23	a	603	CLA	C14-C13-C15	-2.39	102.77	111.27
27	A	611	PL9	C27-C28-C29	-2.39	122.16	127.62
23	c	508	CLA	C1D-ND-C4D	2.39	107.99	106.31
23	c	509	CLA	CMB-C2B-C3B	2.39	132.16	126.55
23	b	608	CLA	O2D-CGD-CBD	2.38	115.39	111.23
23	B	605	CLA	C3A-C2A-C1A	2.38	104.90	101.34
25	b	618	BCR	C27-C26-C25	2.38	125.92	122.70
23	b	611	CLA	CMA-C3A-C4A	-2.38	105.39	111.77
25	H	101	BCR	C30-C25-C26	-2.38	119.39	122.64
30	D	406	LHG	O8-C23-O10	-2.37	117.69	123.63
25	c	514	BCR	C15-C16-C17	-2.37	118.66	123.52
31	C	518	DGD	O1G-C1A-C2A	-2.37	104.61	111.83
23	C	512	CLA	CMB-C2B-C3B	2.37	132.12	126.55
24	d	401	PHO	O2A-CGA-O1A	-2.37	117.70	123.63
23	a	604	CLA	C4D-C3D-CAD	-2.37	105.53	108.11
36	v	201	HEC	O2D-CGD-CBD	2.37	121.48	114.00
23	c	501	CLA	CHA-C1A-NA	-2.37	121.03	126.39
23	B	613	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
31	C	516	DGD	CCB-CBB-CAB	-2.36	102.42	114.37
25	Y	101	BCR	C40-C30-C25	2.36	113.95	110.24
25	A	608	BCR	C37-C22-C21	-2.36	118.99	122.82
23	B	606	CLA	C3B-C4B-NB	-2.36	108.42	110.53
23	c	506	CLA	C2A-C1A-CHA	2.36	127.96	123.87
23	b	611	CLA	C4A-NA-C1A	2.36	107.75	106.68
30	D	406	LHG	C27-C26-C25	-2.36	102.45	114.37
25	c	514	BCR	C33-C5-C6	-2.36	121.91	124.48
29	A	614	SQD	O8-S-O7	-2.36	105.50	111.40
28	b	621	LMG	O2-C2-C1	-2.36	104.46	110.08
23	B	610	CLA	O1D-CGD-CBD	2.36	129.17	124.52
27	d	408	PL9	C50-C49-C48	-2.36	115.58	122.66
23	b	602	CLA	CMB-C2B-C3B	2.36	132.09	126.55
23	b	615	CLA	O2D-CGD-CBD	2.36	115.35	111.23
31	c	517	DGD	O6D-C1D-O3G	-2.35	104.48	110.04
23	B	606	CLA	CHC-C1C-NC	2.35	127.86	124.31
23	C	504	CLA	C1-O2A-CGA	2.35	122.34	116.65
25	T	101	BCR	C7-C8-C9	-2.35	122.76	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	519	LMG	O6-C1-O1	-2.35	104.49	110.04
28	b	621	LMG	O6-C5-C6	2.35	112.26	106.44
27	A	611	PL9	C41-C39-C38	-2.35	115.89	121.17
28	c	522	LMG	O6-C1-O1	-2.35	104.49	110.04
27	a	611	PL9	C12-C13-C14	-2.35	122.25	127.62
31	h	103	DGD	O2D-C2D-C1D	-2.35	104.48	110.08
25	d	404	BCR	C16-C15-C14	-2.35	118.71	123.52
23	C	508	CLA	CHD-C1D-ND	-2.35	121.50	124.80
23	b	605	CLA	CHC-C1C-C2C	-2.35	120.28	126.95
23	A	604	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	C	514	BCR	C15-C16-C17	-2.34	118.72	123.52
27	d	408	PL9	C36-C34-C33	-2.34	115.91	121.17
23	C	503	CLA	C4-C3-C5	2.34	119.30	115.23
23	c	511	CLA	CHA-C1A-NA	-2.34	121.09	126.39
25	B	619	BCR	C12-C13-C14	-2.34	115.33	119.01
28	m	101	LMG	O1-C1-C2	-2.34	104.72	108.27
28	B	620	LMG	O8-C28-O10	-2.34	117.77	123.63
23	b	615	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
23	b	610	CLA	O2D-CGD-CBD	2.34	115.32	111.23
23	C	512	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
25	Y	101	BCR	C23-C24-C25	-2.34	120.75	127.00
23	B	616	CLA	CED-O2D-CGD	2.34	121.22	115.92
24	A	606	PHO	C3B-C4B-NB	-2.34	105.94	107.46
31	h	103	DGD	O5E-C6E-C5E	-2.34	103.38	111.33
31	A	617	DGD	C1E-O6E-C5E	2.34	118.28	113.72
23	a	603	CLA	C1D-ND-C4D	2.33	107.95	106.31
31	H	102	DGD	C8B-C7B-C6B	-2.33	102.57	114.37
23	B	605	CLA	C4B-C3B-C2B	2.33	110.20	107.30
23	c	502	CLA	CMB-C2B-C3B	2.33	132.04	126.55
23	B	614	CLA	CMB-C2B-C3B	2.33	132.03	126.55
23	B	605	CLA	OBD-CAD-C3D	2.33	133.87	128.42
23	c	507	CLA	CHD-C4C-NC	2.33	127.85	124.23
25	b	618	BCR	C30-C25-C26	-2.33	119.45	122.64
31	c	517	DGD	O3G-C1D-C2D	-2.33	104.73	108.27
23	b	615	CLA	CHD-C4C-C3C	-2.33	121.38	124.77
23	B	607	CLA	CHB-C1B-NB	2.33	127.54	124.05
31	c	518	DGD	O2D-C2D-C3D	-2.33	104.89	110.38
23	B	605	CLA	CAC-C3C-C4C	2.33	127.81	124.79
23	b	615	CLA	C6-C5-C3	-2.32	107.81	113.47
23	B	614	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
25	c	515	BCR	C29-C30-C25	2.32	113.81	110.44
23	C	503	CLA	CHA-C1A-NA	-2.32	121.13	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	101	BCR	C11-C10-C9	-2.32	124.02	127.28
25	k	102	BCR	C2-C1-C6	2.32	113.81	110.44
23	c	501	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
25	H	101	BCR	C24-C23-C22	-2.32	122.81	126.23
23	D	403	CLA	CHB-C1B-C2B	-2.32	120.70	127.43
28	B	620	LMG	C40-C39-C38	-2.31	102.67	114.37
23	a	603	CLA	CMC-C2C-C1C	2.31	128.65	125.03
23	c	501	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
28	m	101	LMG	O8-C9-C8	-2.31	101.73	108.40
28	B	620	LMG	O1-C7-C8	-2.31	105.20	110.82
31	c	518	DGD	C3G-C2G-C1G	-2.31	106.41	111.78
31	c	517	DGD	O2G-C1B-O1B	-2.31	118.31	123.70
23	C	512	CLA	C1-C2-C3	-2.30	122.42	126.20
23	d	403	CLA	C1-C2-C3	-2.30	122.42	126.20
23	A	603	CLA	CHA-C1A-NA	-2.30	121.18	126.39
23	c	504	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
24	d	401	PHO	C1-C2-C3	-2.30	122.43	126.20
23	c	512	CLA	O1D-CGD-CBD	2.30	129.06	124.52
25	A	608	BCR	C16-C15-C14	-2.30	118.81	123.52
23	c	504	CLA	CMB-C2B-C3B	2.30	131.96	126.55
28	B	620	LMG	C38-C37-C36	-2.30	102.74	114.37
23	B	616	CLA	CAA-CBA-CGA	-2.30	106.68	113.21
25	t	101	BCR	C1-C6-C5	-2.30	119.50	122.64
27	D	407	PL9	C12-C13-C14	-2.30	122.37	127.62
23	B	604	CLA	C2B-C1B-NB	-2.29	107.95	110.33
23	c	506	CLA	O2A-C1-C2	-2.29	99.29	108.11
23	d	403	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
23	c	503	CLA	C11-C12-C13	-2.29	108.35	115.97
25	C	514	BCR	C7-C8-C9	-2.29	122.85	126.23
25	k	101	BCR	C38-C26-C25	-2.29	121.98	124.48
23	B	607	CLA	CHC-C4B-NB	2.29	127.48	124.05
23	A	607	CLA	CMB-C2B-C3B	2.29	131.93	126.55
23	C	505	CLA	OBD-CAD-C3D	2.29	133.76	128.42
23	B	602	CLA	CHA-C4D-ND	2.29	137.26	132.55
23	d	403	CLA	O1D-CGD-CBD	2.28	129.02	124.52
24	A	606	PHO	CMB-C2B-C3B	2.28	129.25	124.68
25	c	515	BCR	C15-C16-C17	-2.28	118.85	123.52
27	D	407	PL9	C50-C49-C48	-2.28	115.80	122.66
31	A	617	DGD	O6D-C1D-O3G	-2.28	104.65	110.04
23	D	402	CLA	C1-C2-C3	-2.28	122.46	126.20
23	B	601	CLA	CHA-C1A-NA	-2.28	121.23	126.39
25	a	607	BCR	C19-C18-C17	-2.28	115.42	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
25	B	619	BCR	C15-C16-C17	-2.28	118.86	123.52
23	a	612	CLA	C2B-C1B-NB	-2.28	107.96	110.33
25	b	618	BCR	C37-C22-C21	-2.28	119.13	122.82
35	F	102	HEM	CHC-C4B-NB	2.28	126.87	124.42
30	a	614	LHG	C11-C10-C9	-2.28	102.86	114.37
23	c	503	CLA	CHD-C1D-ND	-2.27	121.60	124.80
29	A	614	SQD	O8-S-C6	2.27	110.36	105.97
23	b	616	CLA	C4A-NA-C1A	2.27	107.72	106.68
23	C	513	CLA	C3B-C4B-NB	-2.27	108.50	110.53
25	C	515	BCR	C27-C26-C25	2.27	125.77	122.70
28	D	409	LMG	O7-C10-O9	-2.27	118.41	123.70
23	B	608	CLA	CHC-C1C-C2C	-2.26	120.51	126.95
23	B	615	CLA	CHC-C4B-NB	2.26	127.44	124.05
25	A	608	BCR	C1-C6-C5	-2.26	119.55	122.64
25	c	515	BCR	C4-C5-C6	2.26	125.76	122.70
23	b	609	CLA	CHB-C1B-NB	2.26	127.44	124.05
23	b	608	CLA	CHB-C1B-NB	2.26	127.44	124.05
25	t	101	BCR	C36-C18-C19	2.26	121.54	118.09
23	b	614	CLA	CHD-C1D-C2D	2.26	130.18	125.49
23	b	606	CLA	O2D-CGD-CBD	2.26	115.17	111.23
23	c	507	CLA	CHB-C4A-NA	2.26	127.66	124.40
28	A	612	LMG	O3-C3-C2	-2.25	105.06	110.38
23	B	602	CLA	C2A-C1A-CHA	2.25	127.78	123.87
23	C	501	CLA	OBD-CAD-C3D	2.25	133.68	128.42
23	C	501	CLA	CHB-C1B-NB	2.25	127.43	124.05
25	B	618	BCR	C15-C14-C13	-2.25	124.12	127.28
24	d	401	PHO	C4B-NB-C1B	2.25	112.10	108.82
23	a	604	CLA	CHA-C1A-NA	-2.25	121.30	126.39
25	c	514	BCR	C34-C9-C10	-2.25	119.17	122.82
23	C	506	CLA	CHD-C1D-ND	-2.25	121.64	124.80
23	B	612	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
27	a	611	PL9	C30-C29-C28	-2.25	117.85	123.63
27	a	611	PL9	C37-C38-C39	-2.25	122.48	127.62
23	A	603	CLA	C7-C6-C5	-2.25	107.27	113.26
23	c	503	CLA	CHB-C4A-NA	2.25	127.64	124.40
28	D	409	LMG	O1-C7-C8	-2.25	106.00	111.77
23	C	504	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
31	c	517	DGD	CBB-CAB-C9B	-2.25	103.02	114.37
23	c	506	CLA	O1A-CGA-CBA	2.25	132.56	123.78
25	k	102	BCR	C11-C10-C9	-2.24	124.13	127.28
23	c	505	CLA	C4D-C3D-CAD	-2.24	105.67	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	O2A-C1-C2	-2.24	99.49	108.11
31	a	616	DGD	O3G-C3G-C2G	-2.24	106.02	111.77
30	D	408	LHG	C11-C10-C9	-2.24	103.06	114.37
28	b	621	LMG	C6-C5-C4	-2.24	107.53	113.02
23	A	604	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
23	C	503	CLA	CHB-C1B-NB	2.24	127.40	124.05
23	B	608	CLA	C11-C12-C13	-2.23	108.54	115.97
23	d	403	CLA	CHD-C1D-C2D	2.23	130.13	125.49
23	C	508	CLA	CMB-C2B-C3B	2.23	131.80	126.55
28	c	521	LMG	C9-C8-C7	-2.23	106.58	111.78
23	b	605	CLA	CHD-C1D-C2D	2.23	130.13	125.49
23	c	508	CLA	CHD-C1D-C2D	2.23	130.13	125.49
23	c	511	CLA	C4D-CHA-C1A	2.23	123.90	121.24
31	H	102	DGD	CDB-CCB-CBB	-2.23	103.11	114.37
31	C	517	DGD	CDB-CCB-CBB	-2.23	103.11	114.37
23	C	508	CLA	CHD-C1D-C2D	2.22	130.11	125.49
27	a	611	PL9	C40-C39-C38	-2.22	117.92	123.63
23	a	612	CLA	C3A-C2A-C1A	2.22	104.67	101.34
25	B	619	BCR	C16-C15-C14	-2.22	118.97	123.52
31	H	102	DGD	O6E-C5E-C4E	2.22	113.70	109.70
23	b	615	CLA	CHA-C4D-ND	2.22	137.13	132.55
25	k	102	BCR	C16-C15-C14	-2.22	118.97	123.52
30	l	101	LHG	C20-C19-C18	-2.22	103.15	114.37
23	b	609	CLA	CHA-C1A-NA	-2.22	121.37	126.39
25	A	608	BCR	C40-C30-C39	-2.22	102.28	108.63
23	c	505	CLA	CAC-C3C-C4C	2.22	127.67	124.79
29	b	601	SQD	O8-S-C6	2.21	110.25	105.97
29	B	624	SQD	O9-S-C6	2.21	110.06	106.76
25	B	617	BCR	C33-C5-C6	-2.21	122.07	124.48
23	B	602	CLA	C6-C5-C3	-2.21	108.08	113.47
28	C	519	LMG	O1-C7-C8	-2.21	105.43	110.82
25	Y	101	BCR	C8-C7-C6	-2.21	121.09	127.00
25	b	618	BCR	C11-C10-C9	-2.21	124.18	127.28
30	D	406	LHG	O2-C2-C3	-2.21	102.06	109.70
23	B	606	CLA	OBD-CAD-C3D	2.21	133.58	128.42
23	D	403	CLA	CHB-C4A-NA	2.21	127.59	124.40
23	b	605	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
28	B	620	LMG	C1-O6-C5	-2.21	109.41	113.72
23	B	611	CLA	C1-C2-C3	-2.21	122.58	126.20
31	c	518	DGD	C9B-C8B-C7B	-2.21	103.22	114.37
30	d	409	LHG	C27-C26-C25	-2.21	103.22	114.37
23	C	513	CLA	CMB-C2B-C1B	-2.20	122.06	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CHC-C4B-NB	2.20	127.36	124.05
23	B	610	CLA	CHA-C1A-NA	-2.20	121.40	126.39
25	B	617	BCR	C3-C4-C5	-2.20	110.13	114.06
31	h	103	DGD	CDB-CCB-CBB	-2.20	103.24	114.37
23	B	615	CLA	C6-C7-C8	-2.20	108.65	115.97
23	c	505	CLA	C4D-CHA-C1A	2.20	123.87	121.24
31	c	516	DGD	CBB-CAB-C9B	-2.20	103.24	114.37
27	A	611	PL9	C11-C9-C8	-2.20	116.23	121.17
30	B	623	LHG	C20-C19-C18	-2.20	103.26	114.37
23	B	605	CLA	CHA-C1A-NA	-2.20	121.42	126.39
23	c	507	CLA	C1-C2-C3	-2.20	122.60	126.20
28	A	612	LMG	C3-C4-C5	-2.20	106.25	110.23
31	H	102	DGD	O3E-C3E-C2E	-2.19	105.21	110.38
35	F	102	HEM	CBA-CAA-C2A	-2.19	106.48	112.53
23	b	610	CLA	C4A-NA-C1A	2.19	107.68	106.68
23	a	603	CLA	CAA-C2A-C1A	-2.19	104.80	111.97
23	C	506	CLA	CMC-C2C-C1C	2.19	128.45	125.03
36	V	201	HEC	CHC-C4B-C3B	2.19	128.90	125.21
23	C	503	CLA	C4D-C3D-CAD	-2.19	105.73	108.11
23	B	609	CLA	CHA-C1A-NA	-2.19	121.44	126.39
23	C	507	CLA	O2D-CGD-CBD	2.19	115.05	111.23
23	c	501	CLA	C4D-CHA-C1A	2.19	123.85	121.24
31	c	516	DGD	O2D-C2D-C1D	-2.19	104.87	110.08
23	c	509	CLA	OBD-CAD-C3D	2.18	133.52	128.42
23	C	513	CLA	O2D-CGD-CBD	2.18	115.05	111.23
30	l	101	LHG	O10-C23-C24	-2.18	115.24	123.78
23	b	611	CLA	C5-C3-C2	2.18	126.07	121.17
23	c	507	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
30	l	101	LHG	C27-C26-C25	-2.18	103.33	114.37
23	B	615	CLA	CMB-C2B-C3B	2.18	131.68	126.55
25	k	102	BCR	C40-C30-C25	2.18	113.67	110.24
23	b	612	CLA	CHD-C4C-C3C	-2.18	121.59	124.77
23	C	502	CLA	CAC-C3C-C4C	2.18	127.63	124.79
23	b	613	CLA	CHB-C1B-NB	2.18	127.32	124.05
23	D	403	CLA	CHA-C1A-NA	-2.18	121.46	126.39
27	A	611	PL9	C7-C8-C9	-2.18	123.08	126.83
23	b	604	CLA	CMC-C2C-C3C	2.18	132.03	126.15
23	b	607	CLA	C2C-C1C-NC	2.17	112.26	109.98
23	C	505	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
23	B	611	CLA	C9-C8-C10	-2.17	103.54	111.27
23	B	615	CLA	CHD-C1D-ND	-2.17	121.75	124.80
23	a	604	CLA	C2D-C1D-ND	-2.17	107.98	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CBC-CAC-C3C	2.17	118.30	112.42
25	b	618	BCR	C7-C8-C9	-2.17	123.03	126.23
36	v	201	HEC	CBD-CAD-C3D	-2.16	106.55	112.53
27	d	408	PL9	C40-C39-C38	-2.16	118.07	123.63
28	c	519	LMG	O3-C3-C2	-2.16	105.28	110.38
25	d	404	BCR	C4-C5-C6	2.16	125.63	122.70
23	b	612	CLA	CAC-C3C-C4C	2.16	127.61	124.79
23	B	604	CLA	C11-C10-C8	-2.16	108.77	115.97
23	b	614	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
25	t	101	BCR	C15-C14-C13	-2.16	124.24	127.28
29	a	615	SQD	C45-O47-C7	2.16	122.97	117.80
23	B	611	CLA	CHD-C4C-NC	2.16	127.58	124.23
23	b	616	CLA	CHD-C4C-NC	2.16	127.58	124.23
27	D	407	PL9	O2-C1-C2	-2.16	116.91	121.83
25	C	515	BCR	C4-C5-C6	2.16	125.62	122.70
23	C	510	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
23	b	607	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
25	k	101	BCR	C16-C15-C14	-2.16	119.10	123.52
25	k	102	BCR	C24-C23-C22	-2.16	123.04	126.23
28	m	101	LMG	C9-C8-C7	-2.16	106.76	111.78
25	T	101	BCR	C33-C5-C6	-2.16	122.13	124.48
25	B	618	BCR	C8-C7-C6	-2.15	121.24	127.00
25	b	617	BCR	C15-C16-C17	-2.15	119.11	123.52
23	b	604	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
23	D	403	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
23	b	605	CLA	C2C-C1C-NC	2.15	112.24	109.98
30	D	406	LHG	C18-C17-C16	-2.15	103.50	114.37
23	b	606	CLA	C1-O2A-CGA	2.15	121.85	116.65
23	D	403	CLA	C3D-C4D-ND	2.15	113.48	109.99
28	m	101	LMG	C40-C39-C38	-2.15	103.52	114.37
23	d	402	CLA	CHD-C1D-ND	-2.15	121.78	124.80
25	b	618	BCR	C34-C9-C10	-2.14	119.34	122.82
23	C	501	CLA	CHD-C1D-ND	-2.14	121.78	124.80
23	a	612	CLA	C2D-C1D-ND	-2.14	108.00	110.13
23	B	607	CLA	CHA-C1A-NA	-2.14	121.54	126.39
23	a	604	CLA	C2A-C1A-CHA	2.14	127.58	123.87
23	b	604	CLA	C11-C12-C13	-2.14	108.85	115.97
23	b	608	CLA	CHB-C4A-NA	2.14	127.49	124.40
23	b	603	CLA	CHD-C1D-C2D	2.14	129.94	125.49
23	c	507	CLA	C2A-C1A-CHA	2.14	127.58	123.87
25	b	618	BCR	C10-C11-C12	-2.14	117.00	123.20
23	b	615	CLA	O2A-CGA-O1A	-2.14	118.28	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	409	LMG	C8-O7-C10	2.14	122.91	117.80
23	c	501	CLA	O1D-CGD-CBD	2.14	128.73	124.52
23	C	505	CLA	CHA-C1A-NA	-2.14	121.55	126.39
29	f	101	SQD	C45-O47-C7	2.14	122.91	117.80
23	b	611	CLA	C11-C10-C8	-2.14	108.87	115.97
31	A	617	DGD	CAB-C9B-C8B	-2.14	103.57	114.37
23	b	611	CLA	C11-C12-C13	-2.14	108.87	115.97
23	d	403	CLA	CGD-CBD-CAD	-2.13	103.94	110.85
31	C	518	DGD	C4A-C3A-C2A	-2.13	105.28	113.13
23	a	603	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
23	A	613	CLA	CMB-C2B-C3B	2.13	131.57	126.55
23	h	101	CLA	C2A-C3A-C4A	2.13	105.31	101.87
23	c	504	CLA	CHB-C4A-NA	2.13	127.48	124.40
23	c	505	CLA	CED-O2D-CGD	-2.13	111.08	115.92
27	A	611	PL9	O1-C4-C3	-2.13	118.48	120.73
28	c	521	LMG	O7-C10-O9	-2.13	118.72	123.70
30	l	101	LHG	C11-C10-C9	-2.13	103.60	114.37
25	h	102	BCR	C35-C13-C12	2.13	121.34	118.09
25	H	101	BCR	C29-C30-C25	2.13	113.53	110.44
28	B	620	LMG	C37-C36-C35	-2.13	103.60	114.37
23	b	607	CLA	C3A-C2A-C1A	2.13	104.53	101.34
23	h	101	CLA	O2A-CGA-CBA	2.13	118.33	111.83
23	c	509	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
31	C	517	DGD	C4E-C3E-C2E	-2.13	107.09	110.83
23	A	603	CLA	CMB-C2B-C3B	2.13	131.56	126.55
23	C	501	CLA	C3D-C4D-ND	2.13	113.45	109.99
23	a	604	CLA	O1A-CGA-CBA	2.13	132.10	123.78
23	C	511	CLA	C1-C2-C3	-2.13	122.71	126.20
23	b	613	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
23	B	610	CLA	O1A-CGA-CBA	2.13	132.10	123.78
31	C	517	DGD	C7B-C6B-C5B	-2.13	103.62	114.37
25	c	514	BCR	C7-C8-C9	-2.13	123.09	126.23
31	C	517	DGD	CAB-C9B-C8B	-2.12	103.64	114.37
27	a	611	PL9	C36-C34-C33	-2.12	116.40	121.17
23	c	501	CLA	CHC-C4B-NB	2.12	127.23	124.05
23	c	508	CLA	CHD-C1D-ND	-2.12	121.82	124.80
23	b	611	CLA	C3B-C4B-NB	-2.12	108.64	110.53
29	f	101	SQD	O47-C7-C8	2.12	118.71	110.93
24	d	401	PHO	CED-O2D-CGD	2.12	120.72	115.92
25	h	102	BCR	C7-C8-C9	-2.12	123.10	126.23
23	C	509	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
24	d	401	PHO	C6-C7-C8	-2.12	108.93	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	CBA-CAA-C2A	2.12	120.09	113.79
23	c	510	CLA	CED-O2D-CGD	2.12	120.72	115.92
23	c	509	CLA	CMD-C2D-C1D	-2.12	121.00	124.73
23	c	502	CLA	O2D-CGD-CBD	2.11	114.93	111.23
25	Y	101	BCR	C33-C5-C6	-2.11	122.18	124.48
29	a	615	SQD	C10-C9-C8	-2.11	105.36	113.13
25	a	607	BCR	C37-C22-C21	-2.11	119.39	122.82
23	b	611	CLA	CHA-C1A-NA	-2.11	121.61	126.39
28	m	101	LMG	C6-C5-C4	-2.11	107.84	113.02
23	A	607	CLA	O1D-CGD-CBD	2.11	128.68	124.52
28	D	405	LMG	O6-C1-O1	-2.11	105.06	110.04
23	c	502	CLA	CHB-C4A-NA	2.11	127.44	124.40
23	b	614	CLA	CAC-C3C-C4C	2.11	127.53	124.79
25	d	404	BCR	C30-C25-C26	-2.11	119.75	122.64
23	C	510	CLA	CHC-C4B-NB	2.11	127.21	124.05
25	t	101	BCR	C40-C30-C25	2.11	113.55	110.24
27	d	408	PL9	C12-C13-C14	-2.11	122.80	127.62
23	c	506	CLA	CHC-C4B-NB	2.11	127.21	124.05
31	c	516	DGD	CDB-CCB-CBB	-2.10	103.73	114.37
23	c	506	CLA	CHB-C1B-C2B	-2.10	121.32	127.43
23	b	607	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
23	c	504	CLA	C1C-C2C-C3C	-2.10	104.77	106.98
25	C	514	BCR	C35-C13-C14	-2.10	119.41	122.82
24	d	401	PHO	C3B-C4B-NB	-2.10	106.09	107.46
23	h	101	CLA	CHD-C1D-C2D	2.10	129.86	125.49
36	v	201	HEC	CHA-C4D-ND	2.10	127.67	123.86
23	B	613	CLA	O1D-CGD-CBD	2.10	128.66	124.52
23	b	613	CLA	C16-C15-C13	-2.10	108.99	115.97
23	C	513	CLA	C3A-C2A-C1A	2.10	104.48	101.34
23	b	603	CLA	CMB-C2B-C3B	2.10	131.49	126.55
23	A	603	CLA	C1D-ND-C4D	-2.10	104.84	106.31
28	A	612	LMG	C1-O6-C5	-2.10	109.62	113.72
31	A	617	DGD	C7B-C6B-C5B	-2.10	103.77	114.37
23	b	607	CLA	C3D-C4D-ND	2.09	113.39	109.99
29	b	601	SQD	O48-C23-O10	-2.09	118.39	123.63
23	b	612	CLA	C1-C2-C3	-2.09	122.77	126.20
23	C	507	CLA	CHC-C4B-NB	2.09	127.19	124.05
23	D	403	CLA	C1D-ND-C4D	-2.09	104.84	106.31
23	c	508	CLA	C2D-C1D-ND	-2.09	108.05	110.13
23	h	101	CLA	O2A-C1-C2	2.09	116.16	108.11
23	b	608	CLA	CAC-C3C-C4C	2.09	127.51	124.79
25	t	101	BCR	C11-C10-C9	-2.09	124.35	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	CHD-C4C-NC	2.09	127.47	124.23
24	d	401	PHO	CMC-C2C-C1C	-2.08	120.98	124.73
30	d	409	LHG	O7-C7-O9	-2.08	118.83	123.70
27	D	407	PL9	C7-C8-C9	-2.08	123.24	126.83
23	b	612	CLA	C2C-C1C-NC	2.08	112.17	109.98
23	a	606	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
23	a	612	CLA	CHD-C1D-C2D	2.08	129.82	125.49
23	A	604	CLA	CMB-C2B-C3B	2.08	131.45	126.55
23	b	613	CLA	C2A-C3A-C4A	2.08	105.23	101.87
23	b	615	CLA	C2A-C1A-CHA	2.08	127.48	123.87
25	h	102	BCR	C35-C13-C14	-2.08	119.45	122.82
23	C	502	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
27	d	408	PL9	C11-C9-C8	-2.07	116.51	121.17
28	D	409	LMG	C38-C37-C36	-2.07	103.88	114.37
23	B	612	CLA	C16-C15-C13	-2.07	109.07	115.97
23	b	602	CLA	C6-C5-C3	-2.07	108.42	113.47
23	C	503	CLA	CHD-C1D-C2D	2.07	129.80	125.49
23	C	511	CLA	C3B-C4B-NB	-2.07	108.68	110.53
25	C	515	BCR	C29-C30-C25	2.07	113.45	110.44
29	f	101	SQD	C1-C2-C3	-2.07	105.65	110.01
27	a	611	PL9	C21-C19-C18	-2.07	116.52	121.17
23	b	614	CLA	CHB-C4A-NA	2.07	127.39	124.40
31	c	518	DGD	C3E-C4E-C5E	-2.07	106.48	110.23
23	d	402	CLA	CBA-CAA-C2A	-2.07	107.64	113.79
27	A	611	PL9	C36-C34-C33	-2.07	116.52	121.17
23	c	506	CLA	CHD-C4C-C3C	2.07	127.79	124.77
23	C	510	CLA	C3A-C2A-C1A	2.07	104.44	101.34
23	c	501	CLA	CHD-C1D-ND	-2.07	121.89	124.80
28	c	521	LMG	C42-C41-C40	-2.07	103.92	114.37
31	C	517	DGD	O3D-C3D-C4D	-2.07	105.50	110.38
28	c	522	LMG	O5-C6-C5	-2.07	104.30	111.33
30	B	623	LHG	C9-C8-C7	-2.07	106.13	113.69
31	c	516	DGD	C3G-C2G-C1G	-2.07	106.97	111.78
24	A	605	PHO	C5-C3-C2	2.06	125.80	121.17
23	C	509	CLA	CMB-C2B-C3B	2.06	131.40	126.55
31	C	518	DGD	C1D-C2D-C3D	-2.06	105.67	110.01
23	d	402	CLA	C6-C5-C3	2.06	118.49	113.47
23	C	505	CLA	CMB-C2B-C3B	2.06	131.40	126.55
23	c	511	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
23	b	603	CLA	CMD-C2D-C1D	2.06	128.36	124.73
28	D	405	LMG	O3-C3-C2	-2.06	105.52	110.38
23	C	505	CLA	C11-C10-C8	-2.06	109.12	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C4-C3-C5	-2.06	111.66	115.23
23	b	615	CLA	CHA-C1A-NA	-2.06	121.73	126.39
28	B	620	LMG	C8-O7-C10	2.06	122.72	117.80
23	b	615	CLA	C2B-C1B-NB	-2.06	108.19	110.33
23	b	609	CLA	C1C-C2C-C3C	-2.06	104.82	106.98
23	b	607	CLA	CMA-C3A-C4A	2.06	117.30	111.77
27	a	611	PL9	O2-C1-C2	-2.06	117.15	121.83
23	c	510	CLA	C4-C3-C5	2.06	118.80	115.23
25	B	619	BCR	C40-C30-C29	-2.06	101.06	108.95
23	B	604	CLA	CHA-C4D-ND	2.06	136.79	132.55
23	B	604	CLA	C2A-C3A-C4A	2.05	105.19	101.87
31	c	516	DGD	O6D-C1D-O3G	-2.05	105.19	110.04
23	C	505	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
23	C	510	CLA	CHD-C1D-ND	-2.05	121.91	124.80
25	t	101	BCR	C40-C30-C29	-2.05	101.07	108.95
23	a	606	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
29	B	624	SQD	O47-C45-C46	2.05	115.71	108.34
23	b	615	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
23	c	505	CLA	CHC-C1C-NC	2.05	127.40	124.31
25	C	520	BCR	C2-C1-C6	2.05	113.42	110.44
29	A	614	SQD	O2-C2-C3	-2.05	105.54	110.38
29	a	615	SQD	C9-C8-C7	-2.05	106.18	113.69
31	A	617	DGD	C6D-C5D-C4D	2.05	116.37	112.07
29	a	613	SQD	O10-C23-C24	-2.05	115.77	123.78
23	C	505	CLA	O1D-CGD-CBD	2.05	128.56	124.52
25	D	404	BCR	C38-C26-C25	-2.05	122.25	124.48
23	c	508	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
25	k	102	BCR	C29-C30-C25	2.05	113.41	110.44
23	B	616	CLA	C4D-CHA-C1A	2.05	123.68	121.24
31	c	516	DGD	C5B-C4B-C3B	-2.04	104.03	114.37
25	B	618	BCR	C15-C16-C17	-2.04	119.34	123.52
28	B	620	LMG	C22-C21-C20	-2.04	104.04	114.37
23	A	604	CLA	CHC-C4B-NB	2.04	127.11	124.05
23	a	604	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
23	B	616	CLA	CHC-C4B-NB	2.04	127.11	124.05
23	B	606	CLA	CHB-C4A-NA	2.04	127.35	124.40
29	f	101	SQD	O47-C45-C46	2.04	115.67	108.34
23	c	512	CLA	C1D-ND-C4D	2.04	107.74	106.31
31	c	518	DGD	CDB-CCB-CBB	-2.04	104.05	114.37
23	c	513	CLA	CHB-C4A-NA	2.04	127.34	124.40
23	b	603	CLA	C7-C6-C5	-2.04	107.83	113.26
23	B	611	CLA	O2A-CGA-O1A	-2.04	118.53	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C2A-C1A-CHA	2.04	127.40	123.87
23	b	611	CLA	CMD-C2D-C1D	2.04	128.31	124.73
23	B	607	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
35	F	102	HEM	C2D-C1D-ND	-2.03	107.55	109.90
23	B	603	CLA	C4D-CHA-C1A	2.03	123.67	121.24
23	d	403	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
30	D	406	LHG	C11-C10-C9	-2.03	104.09	114.37
25	b	619	BCR	C16-C15-C14	-2.03	119.36	123.52
23	c	502	CLA	CHC-C4B-NB	2.03	127.10	124.05
23	c	507	CLA	C3A-C2A-C1A	2.03	104.38	101.34
29	F	101	SQD	O48-C23-C24	2.03	118.03	111.83
23	a	612	CLA	C1D-ND-C4D	2.03	107.74	106.31
23	c	513	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	b	608	CLA	CHD-C1D-ND	-2.03	121.95	124.80
30	B	623	LHG	C18-C17-C16	-2.03	104.12	114.37
23	c	511	CLA	C2A-C1A-CHA	2.03	127.39	123.87
23	B	614	CLA	CAC-C3C-C4C	2.03	127.43	124.79
23	c	512	CLA	CHA-C1A-NA	-2.03	121.80	126.39
28	m	101	LMG	C19-C18-C17	-2.03	104.12	114.37
24	A	605	PHO	C3B-C4B-NB	-2.03	106.14	107.46
28	b	621	LMG	O5-C6-C5	-2.03	104.44	111.33
23	C	510	CLA	CHD-C4C-NC	2.02	127.37	124.23
23	C	504	CLA	CHD-C1D-C2D	2.02	129.70	125.49
30	A	615	LHG	C27-C26-C25	-2.02	104.14	114.37
23	D	402	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
25	D	404	BCR	C36-C18-C19	-2.02	115.00	118.09
28	b	621	LMG	C42-C41-C40	-2.02	104.14	114.37
31	H	102	DGD	O4E-C4E-C5E	2.02	114.31	109.32
23	b	608	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
31	C	516	DGD	C9B-C8B-C7B	-2.02	104.14	114.37
29	A	614	SQD	O48-C23-O10	-2.02	118.57	123.63
25	h	102	BCR	C15-C14-C13	-2.02	124.45	127.28
31	c	518	DGD	C5B-C4B-C3B	-2.02	104.16	114.37
23	B	615	CLA	C7-C6-C5	-2.02	107.88	113.26
23	D	402	CLA	CHB-C1B-NB	2.02	127.08	124.05
23	c	502	CLA	CHD-C1D-ND	-2.02	121.97	124.80
23	a	606	CLA	CAA-CBA-CGA	-2.02	107.48	113.21
23	c	503	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
23	b	616	CLA	C6-C5-C3	2.01	118.38	113.47
23	B	615	CLA	C4-C3-C5	-2.01	111.73	115.23
25	c	514	BCR	C2-C1-C6	2.01	113.36	110.44
30	B	623	LHG	O10-C23-C24	-2.01	115.91	123.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C16-C15-C13	-2.01	109.28	115.97
23	b	612	CLA	CMD-C2D-C3D	2.01	132.30	127.69
25	T	101	BCR	C4-C5-C6	2.01	125.42	122.70
23	h	101	CLA	C7-C6-C5	2.01	118.62	113.26
23	b	604	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
23	b	613	CLA	CHA-C1A-NA	-2.01	121.84	126.39
25	b	617	BCR	C16-C15-C14	-2.01	119.41	123.52
31	C	516	DGD	O3D-C3D-C4D	-2.01	105.64	110.38
23	c	511	CLA	O1A-CGA-CBA	2.01	131.64	123.78
23	C	507	CLA	CAA-CBA-CGA	-2.01	107.50	113.21
23	c	501	CLA	C11-C10-C8	-2.01	109.30	115.97
23	c	509	CLA	O1D-CGD-CBD	2.01	128.47	124.52
23	b	603	CLA	CHB-C1B-C2B	-2.01	121.61	127.43
29	b	601	SQD	O47-C45-C46	2.00	115.54	108.34
25	b	618	BCR	C2-C1-C6	2.00	113.35	110.44
23	C	506	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
25	C	520	BCR	C30-C25-C26	-2.00	119.90	122.64
30	L	101	LHG	C12-C11-C10	-2.00	104.24	114.37
31	c	516	DGD	O5D-C6D-C5D	-2.00	104.91	109.42
23	B	611	CLA	CMB-C2B-C1B	-2.00	122.37	125.42

All (57) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	603	CLA	ND
23	A	607	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	610	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	C	505	CLA	ND
23	C	507	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	403	CLA	ND
23	a	603	CLA	ND
23	a	606	CLA	ND
23	a	612	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	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	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
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	d	402	CLA	ND
23	h	101	CLA	ND

All (1653) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C11-C12-C13-C14
23	B	615	CLA	C2B-C3B-CAB-CBB
23	B	615	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C2-C3-C5-C6
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	C2B-C3B-CAB-CBB
23	C	512	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C6-C7-C8-C9
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CBD-CGD-O2D-CED
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	CBD-CGD-O2D-CED
23	d	403	CLA	C11-C12-C13-C14
23	h	101	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	CAD-CBD-CGD-O1D
23	h	101	CLA	CAD-CBD-CGD-O2D
25	A	608	BCR	C7-C8-C9-C34
25	B	619	BCR	C35-C13-C14-C15
25	C	514	BCR	C7-C8-C9-C34
25	C	514	BCR	C11-C12-C13-C35
25	C	514	BCR	C16-C17-C18-C19
25	C	514	BCR	C16-C17-C18-C36
25	C	515	BCR	C21-C22-C23-C24
25	C	520	BCR	C7-C8-C9-C10
25	C	520	BCR	C7-C8-C9-C34
25	C	520	BCR	C20-C21-C22-C37
25	D	404	BCR	C16-C17-C18-C36
25	D	404	BCR	C22-C23-C24-C25
25	D	404	BCR	C23-C24-C25-C26
25	H	101	BCR	C11-C12-C13-C14
25	T	101	BCR	C11-C12-C13-C14
25	Y	101	BCR	C5-C6-C7-C8
25	Y	101	BCR	C11-C10-C9-C34
25	Y	101	BCR	C20-C21-C22-C37
25	b	619	BCR	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	619	BCR	C11-C12-C13-C35
25	c	514	BCR	C7-C8-C9-C10
25	c	514	BCR	C11-C10-C9-C34
25	c	514	BCR	C11-C12-C13-C14
25	c	514	BCR	C13-C14-C15-C16
25	c	514	BCR	C15-C16-C17-C18
25	c	514	BCR	C18-C19-C20-C21
25	c	515	BCR	C21-C22-C23-C24
25	c	515	BCR	C37-C22-C23-C24
25	h	102	BCR	C20-C21-C22-C37
25	k	101	BCR	C7-C8-C9-C10
25	k	101	BCR	C7-C8-C9-C34
25	t	101	BCR	C11-C10-C9-C34
25	t	101	BCR	C10-C11-C12-C13
25	t	101	BCR	C17-C18-C19-C20
25	t	101	BCR	C20-C21-C22-C37
25	t	101	BCR	C37-C22-C23-C24
27	A	611	PL9	C11-C12-C13-C14
27	A	611	PL9	C12-C13-C14-C15
27	A	611	PL9	C12-C13-C14-C16
27	A	611	PL9	C17-C18-C19-C20
27	A	611	PL9	C17-C18-C19-C21
27	A	611	PL9	C22-C23-C24-C25
27	A	611	PL9	C22-C23-C24-C26
27	A	611	PL9	C32-C33-C34-C36
27	A	611	PL9	C37-C38-C39-C40
27	A	611	PL9	C37-C38-C39-C41
27	D	407	PL9	C32-C33-C34-C36
27	D	407	PL9	C47-C48-C49-C51
27	a	611	PL9	C16-C17-C18-C19
27	a	611	PL9	C17-C18-C19-C21
27	a	611	PL9	C22-C23-C24-C25
27	a	611	PL9	C22-C23-C24-C26
27	a	611	PL9	C32-C33-C34-C35
27	a	611	PL9	C34-C36-C37-C38
27	a	611	PL9	C42-C43-C44-C46
27	d	408	PL9	C12-C13-C14-C15
27	d	408	PL9	C32-C33-C34-C35
27	d	408	PL9	C32-C33-C34-C36
27	d	408	PL9	C37-C38-C39-C41
27	d	408	PL9	C42-C43-C44-C46
27	d	408	PL9	C47-C48-C49-C51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	A	612	LMG	O9-C10-O7-C8
28	A	612	LMG	C11-C10-O7-C8
28	C	519	LMG	C11-C10-O7-C8
28	D	409	LMG	O1-C7-C8-C9
28	D	409	LMG	O1-C7-C8-O7
28	D	409	LMG	C11-C10-O7-C8
28	b	621	LMG	O9-C10-O7-C8
28	c	522	LMG	O6-C1-O1-C7
28	c	522	LMG	O10-C28-O8-C9
28	c	522	LMG	C29-C28-O8-C9
29	A	616	SQD	C44-C45-C46-O48
29	A	616	SQD	C46-C45-O47-C7
29	B	624	SQD	C2-C1-O6-C44
29	B	624	SQD	O5-C1-O6-C44
29	B	624	SQD	O6-C44-C45-O47
29	B	624	SQD	O49-C7-O47-C45
29	B	624	SQD	C8-C7-O47-C45
29	a	613	SQD	O47-C45-C46-O48
29	a	613	SQD	C5-C6-S-O7
29	a	613	SQD	C5-C6-S-O8
29	b	601	SQD	C8-C7-O47-C45
29	b	601	SQD	C24-C23-O48-C46
29	f	101	SQD	O5-C1-O6-C44
30	A	615	LHG	O10-C23-O8-C6
30	B	623	LHG	O1-C1-C2-C3
30	B	623	LHG	C3-O3-P-O4
30	D	406	LHG	O1-C1-C2-C3
30	D	406	LHG	C3-O3-P-O5
30	D	406	LHG	C3-O3-P-O6
30	D	406	LHG	C4-O6-P-O4
30	D	408	LHG	C3-O3-P-O5
30	D	408	LHG	C3-O3-P-O6
30	L	101	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O3
30	L	101	LHG	C4-O6-P-O4
30	a	614	LHG	C3-O3-P-O5
30	a	614	LHG	C4-O6-P-O3
30	a	614	LHG	C4-O6-P-O5
30	a	614	LHG	O10-C23-O8-C6
30	d	405	LHG	O1-C1-C2-C3
30	d	405	LHG	C3-O3-P-O6
30	d	407	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	d	407	LHG	C3-O3-P-O4
30	d	407	LHG	C4-O6-P-O3
30	d	407	LHG	C4-O6-P-O4
30	l	101	LHG	C4-O6-P-O3
30	l	101	LHG	C4-O6-P-O4
30	l	101	LHG	C4-O6-P-O5
31	A	617	DGD	O1B-C1B-O2G-C2G
31	A	617	DGD	O2G-C2G-C3G-O3G
31	a	616	DGD	C2A-C1A-O1G-C1G
31	a	616	DGD	O1A-C1A-O1G-C1G
31	a	616	DGD	O1G-C1G-C2G-O2G
36	V	201	HEC	C2B-C3B-CAB-CBB
36	V	201	HEC	C2C-C3C-CAC-CBC
36	V	201	HEC	C4C-C3C-CAC-CBC
36	v	201	HEC	C2B-C3B-CAB-CBB
36	v	201	HEC	C2C-C3C-CAC-CBC
36	v	201	HEC	C4C-C3C-CAC-CBC
23	c	513	CLA	O1D-CGD-O2D-CED
23	h	101	CLA	O1D-CGD-O2D-CED
28	c	519	LMG	C11-C10-O7-C8
23	b	616	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
23	h	101	CLA	CBD-CGD-O2D-CED
29	b	601	SQD	O10-C23-O48-C46
27	d	408	PL9	C47-C48-C49-C50
30	A	615	LHG	C24-C23-O8-C6
30	a	614	LHG	C24-C23-O8-C6
29	a	615	SQD	O10-C23-O48-C46
23	B	604	CLA	C13-C15-C16-C17
23	B	601	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	O1D-CGD-O2D-CED
28	D	409	LMG	O9-C10-O7-C8
29	a	615	SQD	O49-C7-O47-C45
31	a	616	DGD	O1B-C1B-O2G-C2G
23	C	506	CLA	C3-C5-C6-C7
23	b	602	CLA	C3-C5-C6-C7
23	h	101	CLA	C3-C5-C6-C7
23	C	508	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	614	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
23	d	403	CLA	CBD-CGD-O2D-CED
28	b	621	LMG	C11-C10-O7-C8
29	a	615	SQD	C8-C7-O47-C45
31	A	617	DGD	C2B-C1B-O2G-C2G
23	B	605	CLA	C4-C3-C5-C6
23	C	504	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
27	A	611	PL9	C15-C14-C16-C17
27	a	611	PL9	C35-C34-C36-C37
27	d	408	PL9	C40-C39-C41-C42
23	b	603	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
27	A	611	PL9	C23-C24-C26-C27
23	b	614	CLA	C3-C5-C6-C7
23	B	616	CLA	CBA-CGA-O2A-C1
29	f	101	SQD	C24-C23-O48-C46
27	a	611	PL9	C17-C18-C19-C20
27	d	408	PL9	C37-C38-C39-C40
27	a	611	PL9	C27-C28-C29-C31
27	a	611	PL9	C32-C33-C34-C36
28	A	612	LMG	O10-C28-O8-C9
28	c	521	LMG	O10-C28-O8-C9
29	F	101	SQD	O10-C23-O48-C46
29	a	613	SQD	O10-C23-O48-C46
28	B	620	LMG	O6-C5-C6-O5
27	D	407	PL9	C47-C48-C49-C50
23	B	607	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CBD-CGD-O2D-CED
30	D	408	LHG	O2-C2-C3-O3
23	d	403	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CBA-CGA-O2A-C1
31	c	518	DGD	O1A-C1A-O1G-C1G
28	c	521	LMG	C4-C5-C6-O5
28	B	620	LMG	C4-C5-C6-O5
28	c	522	LMG	C4-C5-C6-O5
31	h	103	DGD	O6E-C5E-C6E-O5E
29	a	613	SQD	C24-C23-O48-C46
29	a	615	SQD	C24-C23-O48-C46
23	A	607	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	A	611	PL9	C20-C19-C21-C22
27	A	611	PL9	C40-C39-C41-C42
23	A	607	CLA	C2-C3-C5-C6
27	A	611	PL9	C18-C19-C21-C22
27	a	611	PL9	C28-C29-C31-C32
27	d	408	PL9	C38-C39-C41-C42
23	B	616	CLA	O1A-CGA-O2A-C1
28	B	620	LMG	O10-C28-O8-C9
27	A	611	PL9	C24-C26-C27-C28
27	A	611	PL9	C44-C46-C47-C48
27	a	611	PL9	C14-C16-C17-C18
27	a	611	PL9	C19-C21-C22-C23
27	a	611	PL9	C24-C26-C27-C28
27	d	408	PL9	C9-C11-C12-C13
23	c	511	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	C13-C15-C16-C17
27	A	611	PL9	C47-C48-C49-C50
23	B	601	CLA	O1A-CGA-O2A-C1
28	C	519	LMG	C29-C28-O8-C9
28	c	522	LMG	O6-C5-C6-O5
28	c	521	LMG	O6-C5-C6-O5
23	b	614	CLA	O1D-CGD-O2D-CED
28	A	612	LMG	C29-C28-O8-C9
28	c	521	LMG	C29-C28-O8-C9
29	F	101	SQD	C24-C23-O48-C46
23	B	605	CLA	C2-C3-C5-C6
27	A	611	PL9	C13-C14-C16-C17
27	a	611	PL9	C33-C34-C36-C37
23	B	605	CLA	C11-C10-C8-C9
23	B	614	CLA	C14-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C12-C13-C14
23	b	613	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C10-C8-C9
23	c	511	CLA	C14-C13-C15-C16
24	A	605	PHO	C14-C13-C15-C16
23	C	508	CLA	O1D-CGD-O2D-CED
23	C	512	CLA	O1D-CGD-O2D-CED
30	D	406	LHG	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	h	103	DGD	C4E-C5E-C6E-O5E
23	c	512	CLA	O1D-CGD-O2D-CED
25	B	618	BCR	C7-C8-C9-C34
25	B	619	BCR	C11-C12-C13-C35
25	C	515	BCR	C7-C8-C9-C34
25	C	515	BCR	C37-C22-C23-C24
25	H	101	BCR	C11-C12-C13-C35
25	Y	101	BCR	C37-C22-C23-C24
25	c	514	BCR	C11-C12-C13-C35
25	h	102	BCR	C7-C8-C9-C34
25	k	101	BCR	C37-C22-C23-C24
25	t	101	BCR	C36-C18-C19-C20
23	b	613	CLA	O1D-CGD-O2D-CED
29	A	614	SQD	O6-C44-C45-O47
29	a	613	SQD	O6-C44-C45-O47
28	m	101	LMG	C29-C28-O8-C9
23	c	511	CLA	C15-C16-C17-C18
27	d	408	PL9	C27-C28-C29-C30
23	B	611	CLA	C13-C15-C16-C17
23	C	513	CLA	C13-C15-C16-C17
23	b	604	CLA	C3-C5-C6-C7
29	A	614	SQD	C7-C8-C9-C10
29	B	624	SQD	C23-C24-C25-C26
23	c	504	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	CBA-CGA-O2A-C1
28	B	620	LMG	C29-C28-O8-C9
28	c	519	LMG	O6-C5-C6-O5
30	A	615	LHG	O9-C7-O7-C5
27	A	611	PL9	C9-C11-C12-C13
27	A	611	PL9	C34-C36-C37-C38
27	d	408	PL9	C44-C46-C47-C48
28	A	612	LMG	C4-C5-C6-O5
30	a	614	LHG	C7-C8-C9-C10
30	d	405	LHG	C23-C24-C25-C26
31	a	616	DGD	C1A-C2A-C3A-C4A
23	C	512	CLA	C10-C11-C12-C13
23	b	606	CLA	C15-C16-C17-C18
23	c	506	CLA	C10-C11-C12-C13
23	B	606	CLA	C2A-CAA-CBA-CGA
23	h	101	CLA	C2A-CAA-CBA-CGA
29	B	624	SQD	C29-C30-C31-C32
25	B	619	BCR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	520	BCR	C18-C19-C20-C21
23	B	605	CLA	C10-C11-C12-C13
23	B	607	CLA	C5-C6-C7-C8
23	B	607	CLA	C8-C10-C11-C12
23	B	612	CLA	C10-C11-C12-C13
23	C	505	CLA	C5-C6-C7-C8
23	C	505	CLA	C8-C10-C11-C12
23	C	511	CLA	C8-C10-C11-C12
23	c	510	CLA	C15-C16-C17-C18
28	D	409	LMG	C10-C11-C12-C13
28	c	522	LMG	C28-C29-C30-C31
28	d	406	LMG	C28-C29-C30-C31
30	D	408	LHG	C7-C8-C9-C10
23	b	607	CLA	C10-C11-C12-C13
23	b	608	CLA	C13-C15-C16-C17
23	b	614	CLA	C8-C10-C11-C12
23	b	614	CLA	C15-C16-C17-C18
29	a	613	SQD	C12-C13-C14-C15
30	d	405	LHG	O2-C2-C3-O3
31	C	517	DGD	O6E-C5E-C6E-O5E
23	C	501	CLA	CBD-CGD-O2D-CED
29	f	101	SQD	O10-C23-O48-C46
31	C	518	DGD	O1A-C1A-O1G-C1G
29	F	101	SQD	C23-C24-C25-C26
23	B	604	CLA	C10-C11-C12-C13
23	a	606	CLA	C10-C11-C12-C13
23	a	606	CLA	C13-C15-C16-C17
23	c	513	CLA	C5-C6-C7-C8
23	B	614	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	C5-C6-C7-C8
23	c	505	CLA	C15-C16-C17-C18
27	A	611	PL9	C43-C44-C46-C47
28	B	622	LMG	C28-C29-C30-C31
30	A	615	LHG	C7-C8-C9-C10
31	C	517	DGD	C1B-C2B-C3B-C4B
31	c	518	DGD	C1A-C2A-C3A-C4A
23	B	605	CLA	C15-C16-C17-C18
23	b	614	CLA	C5-C6-C7-C8
23	c	507	CLA	C5-C6-C7-C8
23	c	512	CLA	C5-C6-C7-C8
25	c	514	BCR	C9-C10-C11-C12
29	f	101	SQD	O49-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	B	624	SQD	C24-C23-O48-C46
23	b	611	CLA	C8-C10-C11-C12
23	c	504	CLA	C5-C6-C7-C8
23	c	506	CLA	C5-C6-C7-C8
23	c	506	CLA	C13-C15-C16-C17
23	h	101	CLA	C8-C10-C11-C12
23	b	609	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	C3-C5-C6-C7
23	B	612	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
23	a	603	CLA	C15-C16-C17-C18
23	a	604	CLA	C8-C10-C11-C12
23	b	616	CLA	C10-C11-C12-C13
23	c	503	CLA	C8-C10-C11-C12
23	c	512	CLA	C13-C15-C16-C17
28	c	519	LMG	O9-C10-O7-C8
27	a	611	PL9	C30-C29-C31-C32
23	A	603	CLA	C15-C16-C17-C18
23	b	612	CLA	C3-C5-C6-C7
23	D	402	CLA	C11-C10-C8-C9
23	B	607	CLA	O1D-CGD-O2D-CED
27	A	611	PL9	C42-C43-C44-C45
27	D	407	PL9	C7-C8-C9-C10
28	c	521	LMG	O9-C10-O7-C8
31	C	517	DGD	C2E-C1E-O5D-C6D
31	c	517	DGD	C2E-C1E-O5D-C6D
23	B	607	CLA	C13-C15-C16-C17
23	b	607	CLA	C5-C6-C7-C8
25	A	608	BCR	C20-C21-C22-C37
25	B	617	BCR	C16-C17-C18-C36
25	B	618	BCR	C20-C21-C22-C37
25	B	619	BCR	C11-C10-C9-C34
25	C	514	BCR	C20-C21-C22-C37
25	C	520	BCR	C11-C10-C9-C34
25	D	404	BCR	C20-C21-C22-C37
25	T	101	BCR	C11-C10-C9-C34
25	T	101	BCR	C20-C21-C22-C37
25	Y	101	BCR	C35-C13-C14-C15
25	a	607	BCR	C35-C13-C14-C15
25	a	607	BCR	C16-C17-C18-C36
25	b	618	BCR	C16-C17-C18-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	619	BCR	C16-C17-C18-C36
25	c	514	BCR	C16-C17-C18-C36
25	d	404	BCR	C35-C13-C14-C15
25	h	102	BCR	C16-C17-C18-C36
25	k	101	BCR	C35-C13-C14-C15
25	k	101	BCR	C20-C21-C22-C37
25	k	102	BCR	C35-C13-C14-C15
25	k	102	BCR	C20-C21-C22-C37
25	t	101	BCR	C16-C17-C18-C36
28	A	612	LMG	O6-C5-C6-O5
23	C	504	CLA	C8-C10-C11-C12
23	C	507	CLA	C10-C11-C12-C13
25	c	514	BCR	C7-C8-C9-C34
25	c	514	BCR	C36-C18-C19-C20
25	d	404	BCR	C37-C22-C23-C24
23	c	506	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	C2A-CAA-CBA-CGA
23	B	611	CLA	C8-C10-C11-C12
23	a	606	CLA	C5-C6-C7-C8
30	d	409	LHG	O1-C1-C2-C3
28	D	409	LMG	C9-C8-O7-C10
29	b	601	SQD	C46-C45-O47-C7
23	A	604	CLA	C16-C17-C18-C19
23	B	610	CLA	C16-C17-C18-C20
23	C	502	CLA	C16-C17-C18-C19
25	B	619	BCR	C11-C10-C9-C8
25	C	520	BCR	C20-C21-C22-C23
25	H	101	BCR	C11-C10-C9-C8
25	Y	101	BCR	C11-C10-C9-C8
25	Y	101	BCR	C12-C13-C14-C15
25	h	102	BCR	C11-C10-C9-C8
25	h	102	BCR	C20-C21-C22-C23
25	k	101	BCR	C11-C10-C9-C8
28	A	612	LMG	O6-C1-O1-C7
31	C	517	DGD	O6E-C1E-O5D-C6D
31	c	517	DGD	O6E-C1E-O5D-C6D
31	a	616	DGD	C2B-C1B-O2G-C2G
23	c	503	CLA	C5-C6-C7-C8
30	a	614	LHG	C23-C24-C25-C26
23	B	616	CLA	C2-C1-O2A-CGA
23	c	507	CLA	C2-C1-O2A-CGA
23	C	502	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	609	CLA	C16-C17-C18-C20
29	b	601	SQD	C11-C10-C9-C8
23	b	611	CLA	C13-C15-C16-C17
23	c	511	CLA	O1D-CGD-O2D-CED
28	A	612	LMG	C16-C17-C18-C19
28	C	519	LMG	C11-C12-C13-C14
28	b	621	LMG	C16-C17-C18-C19
30	B	623	LHG	C14-C15-C16-C17
30	d	405	LHG	C30-C31-C32-C33
30	d	407	LHG	C34-C35-C36-C37
25	T	101	BCR	C14-C15-C16-C17
28	B	620	LMG	C13-C14-C15-C16
28	B	622	LMG	C16-C17-C18-C19
28	c	521	LMG	C41-C42-C43-C44
28	c	522	LMG	C38-C39-C40-C41
29	a	613	SQD	C24-C25-C26-C27
29	a	615	SQD	C12-C13-C14-C15
30	A	615	LHG	C27-C28-C29-C30
30	B	623	LHG	C29-C30-C31-C32
31	A	617	DGD	C5B-C6B-C7B-C8B
31	c	516	DGD	C9A-CAA-CBA-CCA
31	C	517	DGD	C5A-C6A-C7A-C8A
28	c	519	LMG	C29-C28-O8-C9
31	c	516	DGD	O6D-C5D-C6D-O5D
28	D	405	LMG	C30-C31-C32-C33
28	c	521	LMG	C11-C12-C13-C14
29	B	624	SQD	C11-C12-C13-C14
29	a	613	SQD	C34-C35-C36-C37
30	a	614	LHG	C17-C18-C19-C20
30	d	407	LHG	C33-C34-C35-C36
30	d	409	LHG	C30-C31-C32-C33
30	l	101	LHG	C16-C17-C18-C19
31	c	518	DGD	C9A-CAA-CBA-CCA
29	F	101	SQD	C45-C44-O6-C1
30	B	623	LHG	O1-C1-C2-O2
28	B	620	LMG	C16-C17-C18-C19
28	B	622	LMG	C14-C15-C16-C17
30	d	405	LHG	C10-C11-C12-C13
23	B	606	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB
23	h	101	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	614	SQD	C23-C24-C25-C26
28	c	519	LMG	C36-C37-C38-C39
28	c	522	LMG	C35-C36-C37-C38
31	C	517	DGD	CCB-CDB-CEB-CFB
31	H	102	DGD	C3B-C4B-C5B-C6B
23	A	604	CLA	C16-C17-C18-C20
23	b	609	CLA	C16-C17-C18-C19
23	b	606	CLA	C2A-CAA-CBA-CGA
28	c	521	LMG	C32-C33-C34-C35
29	A	616	SQD	C14-C15-C16-C17
30	d	407	LHG	C31-C32-C33-C34
31	A	617	DGD	C9B-CAB-CBB-CCB
23	B	613	CLA	C8-C10-C11-C12
30	a	614	LHG	C8-C7-O7-C5
23	C	506	CLA	C12-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C15
29	f	101	SQD	C28-C29-C30-C31
29	f	101	SQD	C32-C33-C34-C35
31	A	617	DGD	C4A-C5A-C6A-C7A
31	A	617	DGD	C2B-C3B-C4B-C5B
23	C	509	CLA	C10-C11-C12-C13
28	B	620	LMG	C36-C37-C38-C39
28	c	522	LMG	C12-C13-C14-C15
30	A	615	LHG	C28-C29-C30-C31
30	l	101	LHG	C28-C29-C30-C31
23	c	512	CLA	C3A-C2A-CAA-CBA
23	h	101	CLA	C3A-C2A-CAA-CBA
28	c	522	LMG	C34-C35-C36-C37
29	A	614	SQD	C30-C31-C32-C33
28	A	612	LMG	C30-C31-C32-C33
30	a	614	LHG	C13-C14-C15-C16
31	c	517	DGD	C6A-C7A-C8A-C9A
31	c	518	DGD	CCA-CDA-CEA-CFA
23	C	513	CLA	C10-C11-C12-C13
28	D	405	LMG	C18-C19-C20-C21
29	F	101	SQD	C34-C35-C36-C37
23	D	403	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
28	c	522	LMG	C11-C12-C13-C14
28	d	406	LMG	C13-C14-C15-C16
30	a	614	LHG	C16-C17-C18-C19
30	l	101	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C8-C10-C11-C12
31	c	516	DGD	C4D-C5D-C6D-O5D
29	f	101	SQD	C31-C32-C33-C34
30	L	101	LHG	C31-C32-C33-C34
23	c	506	CLA	C2C-C3C-CAC-CBC
28	B	622	LMG	C29-C30-C31-C32
28	b	621	LMG	C31-C32-C33-C34
30	B	623	LHG	C25-C26-C27-C28
30	D	408	LHG	C27-C28-C29-C30
30	d	405	LHG	C7-C8-C9-C10
28	C	519	LMG	C32-C33-C34-C35
28	D	405	LMG	C17-C18-C19-C20
28	b	621	LMG	C34-C35-C36-C37
28	d	410	LMG	C31-C32-C33-C34
29	A	614	SQD	C31-C32-C33-C34
29	F	101	SQD	C27-C28-C29-C30
30	D	408	LHG	C11-C12-C13-C14
30	d	405	LHG	C32-C33-C34-C35
31	C	517	DGD	C7A-C8A-C9A-CAA
31	h	103	DGD	C2B-C3B-C4B-C5B
30	L	101	LHG	O10-C23-O8-C6
29	A	616	SQD	C28-C29-C30-C31
30	l	101	LHG	C24-C25-C26-C27
31	C	518	DGD	C2A-C3A-C4A-C5A
31	h	103	DGD	C9A-CAA-CBA-CCA
23	c	504	CLA	O1D-CGD-O2D-CED
28	B	620	LMG	C39-C40-C41-C42
31	c	516	DGD	C4B-C5B-C6B-C7B
31	c	516	DGD	C5B-C6B-C7B-C8B
30	d	409	LHG	C26-C27-C28-C29
30	l	101	LHG	C14-C15-C16-C17
31	A	617	DGD	C8B-C9B-CAB-CBB
31	C	517	DGD	CAA-CBA-CCA-CDA
23	D	403	CLA	C2B-C3B-CAB-CBB
23	a	604	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C1-C6-C7-C8
25	D	404	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	h	102	BCR	C23-C24-C25-C26
25	h	102	BCR	C23-C24-C25-C30
28	d	410	LMG	C38-C39-C40-C41
29	F	101	SQD	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	614	LHG	C14-C15-C16-C17
23	B	603	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
31	c	518	DGD	C8A-C9A-CAA-CBA
31	h	103	DGD	C5B-C6B-C7B-C8B
28	m	101	LMG	C10-C11-C12-C13
28	D	405	LMG	C14-C15-C16-C17
28	b	621	LMG	C11-C12-C13-C14
28	c	522	LMG	C29-C30-C31-C32
28	d	410	LMG	C11-C12-C13-C14
31	A	617	DGD	CDB-CEB-CFB-CGB
29	b	601	SQD	O49-C7-O47-C45
29	A	614	SQD	C32-C33-C34-C35
29	B	624	SQD	C9-C10-C11-C12
29	f	101	SQD	C24-C25-C26-C27
25	C	514	BCR	C18-C19-C20-C21
25	d	404	BCR	C10-C11-C12-C13
23	b	614	CLA	C2-C3-C5-C6
27	A	611	PL9	C47-C48-C49-C51
29	F	101	SQD	C33-C34-C35-C36
29	a	613	SQD	C26-C27-C28-C29
23	B	611	CLA	C11-C12-C13-C14
23	h	101	CLA	C11-C10-C8-C9
31	C	517	DGD	C6B-C7B-C8B-C9B
31	a	616	DGD	C2A-C3A-C4A-C5A
31	c	516	DGD	CCB-CDB-CEB-CFB
31	h	103	DGD	CAB-CBB-CCB-CDB
29	A	616	SQD	C26-C27-C28-C29
30	a	614	LHG	C26-C27-C28-C29
31	A	617	DGD	CBA-CCA-CDA-CEA
25	h	102	BCR	C14-C15-C16-C17
28	D	405	LMG	C20-C21-C22-C23
29	a	615	SQD	C10-C11-C12-C13
30	d	407	LHG	C11-C12-C13-C14
28	c	522	LMG	C2-C1-O1-C7
29	f	101	SQD	C2-C1-O6-C44
23	c	509	CLA	C10-C11-C12-C13
28	D	405	LMG	C39-C40-C41-C42
29	A	616	SQD	C12-C13-C14-C15
30	D	406	LHG	C11-C10-C9-C8
28	b	621	LMG	C18-C19-C20-C21
28	c	521	LMG	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	522	LMG	C19-C20-C21-C22
23	b	615	CLA	C8-C10-C11-C12
31	c	518	DGD	C2A-C1A-O1G-C1G
23	c	507	CLA	C16-C17-C18-C20
28	c	521	LMG	C11-C10-O7-C8
29	f	101	SQD	C8-C7-O47-C45
30	A	615	LHG	C8-C7-O7-C5
31	C	516	DGD	C1B-C2B-C3B-C4B
31	C	518	DGD	C6A-C7A-C8A-C9A
31	a	616	DGD	C4A-C5A-C6A-C7A
23	B	602	CLA	C13-C15-C16-C17
28	C	519	LMG	O9-C10-O7-C8
29	A	616	SQD	O49-C7-O47-C45
30	D	408	LHG	C32-C33-C34-C35
30	d	409	LHG	C27-C28-C29-C30
31	C	516	DGD	C9A-CAA-CBA-CCA
23	D	403	CLA	C15-C16-C17-C18
28	c	521	LMG	C10-C11-C12-C13
31	h	103	DGD	C7B-C8B-C9B-CAB
31	C	517	DGD	C5D-C6D-O5D-C1E
23	B	603	CLA	C16-C17-C18-C19
23	B	603	CLA	C16-C17-C18-C20
23	c	506	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C19
23	c	511	CLA	C16-C17-C18-C20
23	c	512	CLA	C4-C3-C5-C6
28	c	521	LMG	C34-C35-C36-C37
31	H	102	DGD	CBB-CCB-CDB-CEB
28	C	519	LMG	O10-C28-O8-C9
23	B	610	CLA	C8-C10-C11-C12
23	b	603	CLA	C5-C6-C7-C8
23	h	101	CLA	C15-C16-C17-C18
28	m	101	LMG	C28-C29-C30-C31
31	c	517	DGD	CAB-CBB-CCB-CDB
31	C	518	DGD	CAA-CBA-CCA-CDA
23	D	403	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C8-C10-C11-C12
23	d	403	CLA	C15-C16-C17-C18
23	h	101	CLA	C10-C11-C12-C13
23	c	510	CLA	C16-C17-C18-C19
29	f	101	SQD	C33-C34-C35-C36
30	A	615	LHG	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	409	LMG	C14-C15-C16-C17
28	c	521	LMG	C38-C39-C40-C41
31	C	516	DGD	CBA-CCA-CDA-CEA
23	C	506	CLA	C15-C16-C17-C18
29	A	614	SQD	C14-C15-C16-C17
31	c	516	DGD	C8B-C9B-CAB-CBB
23	B	601	CLA	C3-C5-C6-C7
23	c	505	CLA	CBD-CGD-O2D-CED
29	b	601	SQD	O47-C45-C46-O48
30	d	405	LHG	C17-C18-C19-C20
23	c	512	CLA	CBA-CGA-O2A-C1
28	d	406	LMG	C34-C35-C36-C37
29	A	614	SQD	C28-C29-C30-C31
30	d	405	LHG	C24-C25-C26-C27
31	a	616	DGD	CBA-CCA-CDA-CEA
31	a	616	DGD	CEA-CFA-CGA-CHA
31	c	516	DGD	C4A-C5A-C6A-C7A
23	C	503	CLA	C5-C6-C7-C8
31	C	518	DGD	C9A-CAA-CBA-CCA
28	D	405	LMG	C37-C38-C39-C40
28	b	621	LMG	C37-C38-C39-C40
29	A	614	SQD	C11-C10-C9-C8
30	A	615	LHG	C11-C10-C9-C8
31	a	616	DGD	C5B-C6B-C7B-C8B
23	b	616	CLA	C2-C1-O2A-CGA
23	C	509	CLA	C16-C17-C18-C20
29	a	615	SQD	C18-C19-C20-C21
23	B	614	CLA	C4-C3-C5-C6
23	B	614	CLA	C2-C3-C5-C6
30	d	405	LHG	C1-C2-C3-O3
23	B	606	CLA	C15-C16-C17-C18
31	C	517	DGD	C6A-C7A-C8A-C9A
28	c	521	LMG	C40-C41-C42-C43
28	d	410	LMG	C36-C37-C38-C39
27	a	611	PL9	C47-C48-C49-C50
28	A	612	LMG	C14-C15-C16-C17
28	c	519	LMG	C35-C36-C37-C38
30	L	101	LHG	C18-C19-C20-C21
23	B	603	CLA	C10-C11-C12-C13
30	d	405	LHG	O1-C1-C2-O2
30	d	407	LHG	O1-C1-C2-O2
28	m	101	LMG	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	L	101	LHG	C12-C13-C14-C15
23	a	606	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
28	b	621	LMG	O6-C5-C6-O5
31	a	616	DGD	CDA-CEA-CFA-CGA
31	c	517	DGD	C7B-C8B-C9B-CAB
31	c	518	DGD	C3A-C4A-C5A-C6A
28	d	410	LMG	C32-C33-C34-C35
31	a	616	DGD	C5A-C6A-C7A-C8A
28	D	405	LMG	O6-C5-C6-O5
28	d	406	LMG	O6-C5-C6-O5
31	c	516	DGD	O1B-C1B-O2G-C2G
28	D	409	LMG	C16-C17-C18-C19
29	A	614	SQD	C10-C11-C12-C13
29	a	613	SQD	C18-C19-C20-C21
23	B	604	CLA	C11-C10-C8-C7
23	B	605	CLA	C11-C10-C8-C7
23	B	614	CLA	C11-C12-C13-C15
23	B	615	CLA	C6-C7-C8-C10
23	C	506	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C10-C8-C7
23	C	509	CLA	C11-C10-C8-C7
23	a	604	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	605	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7
23	b	607	CLA	C6-C7-C8-C10
23	b	612	CLA	C6-C7-C8-C10
23	c	505	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C10-C8-C7
23	c	506	CLA	C6-C7-C8-C10
23	c	508	CLA	C12-C13-C15-C16
28	D	409	LMG	C34-C35-C36-C37
23	B	615	CLA	C16-C17-C18-C20
23	b	606	CLA	C10-C11-C12-C13
23	c	512	CLA	O1A-CGA-O2A-C1
30	d	405	LHG	O10-C23-O8-C6
28	c	519	LMG	C39-C40-C41-C42
31	C	516	DGD	C5B-C6B-C7B-C8B
23	c	512	CLA	C2-C3-C5-C6
27	D	407	PL9	C28-C29-C31-C32
27	a	611	PL9	C38-C39-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	b	621	LMG	C39-C40-C41-C42
28	d	406	LMG	C35-C36-C37-C38
30	L	101	LHG	C27-C28-C29-C30
31	c	518	DGD	C5B-C6B-C7B-C8B
23	B	613	CLA	C13-C15-C16-C17
23	B	615	CLA	C11-C12-C13-C14
23	C	510	CLA	C11-C10-C8-C9
23	a	604	CLA	C11-C10-C8-C9
23	b	603	CLA	C11-C12-C13-C14
23	b	604	CLA	C11-C12-C13-C14
23	b	605	CLA	C11-C12-C13-C14
23	b	606	CLA	C6-C7-C8-C9
23	b	607	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C10-C8-C9
24	A	606	PHO	C6-C7-C8-C9
28	m	101	LMG	C19-C20-C21-C22
29	f	101	SQD	C30-C31-C32-C33
30	d	409	LHG	C24-C23-O8-C6
29	a	613	SQD	C30-C31-C32-C33
30	a	614	LHG	O9-C7-O7-C5
30	l	101	LHG	C32-C33-C34-C35
28	D	409	LMG	C7-C8-C9-O8
29	B	624	SQD	O6-C44-C45-C46
29	a	613	SQD	C44-C45-C46-O48
31	A	617	DGD	C1G-C2G-C3G-O3G
29	B	624	SQD	C34-C35-C36-C37
30	a	614	LHG	C11-C10-C9-C8
30	B	623	LHG	C12-C13-C14-C15
30	D	406	LHG	C25-C26-C27-C28
23	C	504	CLA	C11-C12-C13-C14
23	b	610	CLA	C15-C16-C17-C18
30	L	101	LHG	C11-C12-C13-C14
30	d	405	LHG	C25-C26-C27-C28
31	c	516	DGD	O6E-C5E-C6E-O5E
23	C	509	CLA	C16-C17-C18-C19
30	A	615	LHG	C15-C16-C17-C18
25	T	101	BCR	C35-C13-C14-C15
29	a	615	SQD	C11-C12-C13-C14
30	A	615	LHG	C33-C34-C35-C36
30	D	406	LHG	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	616	SQD	C7-C8-C9-C10
29	A	614	SQD	C24-C25-C26-C27
23	C	506	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
23	B	607	CLA	C16-C17-C18-C20
28	D	405	LMG	C11-C12-C13-C14
28	D	405	LMG	C33-C34-C35-C36
31	C	516	DGD	O6E-C5E-C6E-O5E
25	h	102	BCR	C21-C22-C23-C24
23	B	610	CLA	C15-C16-C17-C18
23	b	613	CLA	C13-C15-C16-C17
23	b	614	CLA	C13-C15-C16-C17
31	c	517	DGD	CAA-CBA-CCA-CDA
29	B	624	SQD	C13-C14-C15-C16
29	a	615	SQD	C11-C10-C9-C8
31	h	103	DGD	CBA-CCA-CDA-CEA
31	A	617	DGD	C1A-C2A-C3A-C4A
28	c	521	LMG	C36-C37-C38-C39
28	d	410	LMG	C37-C38-C39-C40
31	C	518	DGD	CBA-CCA-CDA-CEA
30	a	614	LHG	C19-C20-C21-C22
23	C	512	CLA	O2A-C1-C2-C3
30	d	405	LHG	C27-C28-C29-C30
23	c	511	CLA	C13-C15-C16-C17
28	c	519	LMG	C33-C34-C35-C36
25	h	102	BCR	C9-C10-C11-C12
28	D	409	LMG	C28-C29-C30-C31
31	C	517	DGD	C8B-C9B-CAB-CBB
31	c	516	DGD	C3B-C4B-C5B-C6B
25	Y	101	BCR	C20-C21-C22-C23
30	D	406	LHG	C1-C2-C3-O3
30	a	614	LHG	O6-C4-C5-O7
31	A	617	DGD	O6D-C5D-C6D-O5D
23	B	611	CLA	C15-C16-C17-C18
28	c	522	LMG	C16-C17-C18-C19
30	d	409	LHG	C29-C30-C31-C32
28	m	101	LMG	C13-C14-C15-C16
29	a	613	SQD	C16-C17-C18-C19
30	B	623	LHG	C24-C25-C26-C27
31	A	617	DGD	C6B-C7B-C8B-C9B
23	B	601	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	A	612	LMG	C12-C13-C14-C15
28	B	622	LMG	C11-C12-C13-C14
28	d	406	LMG	C14-C15-C16-C17
29	a	613	SQD	C11-C10-C9-C8
30	D	408	LHG	C25-C26-C27-C28
30	d	407	LHG	C14-C15-C16-C17
28	B	620	LMG	C15-C16-C17-C18
28	D	405	LMG	C35-C36-C37-C38
29	a	615	SQD	O47-C45-C46-O48
31	c	516	DGD	CAB-CBB-CCB-CDB
29	a	615	SQD	C13-C14-C15-C16
31	H	102	DGD	CBA-CCA-CDA-CEA
28	C	519	LMG	C29-C30-C31-C32
31	H	102	DGD	C9B-CAB-CBB-CCB
30	L	101	LHG	C19-C20-C21-C22
28	D	409	LMG	C15-C16-C17-C18
30	D	406	LHG	C15-C16-C17-C18
23	c	506	CLA	C16-C17-C18-C19
31	h	103	DGD	CDA-CEA-CFA-CGA
28	c	521	LMG	C13-C14-C15-C16
23	b	607	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	C16-C17-C18-C19
31	H	102	DGD	CDB-CEB-CFB-CGB
28	m	101	LMG	C29-C30-C31-C32
30	A	615	LHG	C24-C25-C26-C27
23	B	602	CLA	C8-C10-C11-C12
31	h	103	DGD	CBB-CCB-CDB-CEB
23	B	603	CLA	C8-C10-C11-C12
23	C	507	CLA	C13-C15-C16-C17
23	B	606	CLA	C16-C17-C18-C19
23	B	615	CLA	C4-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
29	B	624	SQD	C35-C36-C37-C38
28	c	522	LMG	C13-C14-C15-C16
30	A	615	LHG	C31-C32-C33-C34
23	c	503	CLA	CBA-CGA-O2A-C1
28	B	622	LMG	C30-C31-C32-C33
30	d	405	LHG	C15-C16-C17-C18
23	B	601	CLA	C6-C7-C8-C9
23	B	604	CLA	C11-C10-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	B	613	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C6-C7-C8-C9
23	C	506	CLA	C6-C7-C8-C9
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	a	604	CLA	C14-C13-C15-C16
23	b	604	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
23	b	606	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C10-C8-C9
30	D	406	LHG	C12-C13-C14-C15
31	A	617	DGD	C3B-C4B-C5B-C6B
23	C	506	CLA	C13-C15-C16-C17
23	b	605	CLA	C15-C16-C17-C18
23	c	513	CLA	C8-C10-C11-C12
23	C	502	CLA	C4B-C3B-CAB-CBB
23	a	604	CLA	C4B-C3B-CAB-CBB
23	b	610	CLA	C4B-C3B-CAB-CBB
23	d	402	CLA	C4B-C3B-CAB-CBB
30	A	615	LHG	C29-C30-C31-C32
30	D	406	LHG	C11-C12-C13-C14
31	h	103	DGD	CCA-CDA-CEA-CFA
23	B	610	CLA	C16-C17-C18-C19
30	D	408	LHG	C17-C18-C19-C20
31	C	516	DGD	CCA-CDA-CEA-CFA
23	C	503	CLA	C8-C10-C11-C12
28	D	405	LMG	C34-C35-C36-C37
28	D	409	LMG	C33-C34-C35-C36
30	L	101	LHG	C15-C16-C17-C18
31	A	617	DGD	CEB-CFB-CGB-CHB
31	c	517	DGD	C8B-C9B-CAB-CBB
30	A	615	LHG	O6-C4-C5-C6
31	c	518	DGD	CBB-CCB-CDB-CEB
31	A	617	DGD	CFA-CGA-CHA-CIA
23	B	607	CLA	C11-C10-C8-C7
23	B	613	CLA	C6-C7-C8-C10
23	B	615	CLA	C11-C12-C13-C15
23	C	505	CLA	C11-C12-C13-C15
23	C	505	CLA	C12-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C7
23	D	403	CLA	C12-C13-C15-C16
23	a	604	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	603	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C10-C8-C7
23	b	604	CLA	C12-C13-C15-C16
23	b	609	CLA	C12-C13-C15-C16
23	d	403	CLA	C11-C12-C13-C15
23	b	607	CLA	C8-C10-C11-C12
28	c	522	LMG	C40-C41-C42-C43
23	b	602	CLA	C16-C17-C18-C20
30	A	615	LHG	C19-C20-C21-C22
29	A	614	SQD	C11-C12-C13-C14
27	D	407	PL9	C30-C29-C31-C32
27	d	408	PL9	C15-C14-C16-C17
31	C	516	DGD	O6D-C5D-C6D-O5D
31	H	102	DGD	O2G-C1B-C2B-C3B
31	H	102	DGD	C4B-C5B-C6B-C7B
23	c	507	CLA	C8-C10-C11-C12
23	b	606	CLA	CBA-CGA-O2A-C1
25	k	101	BCR	C19-C20-C21-C22
31	h	103	DGD	C3A-C4A-C5A-C6A
31	h	103	DGD	C6A-C7A-C8A-C9A
23	C	507	CLA	C15-C16-C17-C18
30	l	101	LHG	C7-C8-C9-C10
28	d	410	LMG	C28-C29-C30-C31
31	H	102	DGD	CCA-CDA-CEA-CFA
31	a	616	DGD	CDB-CEB-CFB-CGB
23	B	615	CLA	C13-C15-C16-C17
28	B	620	LMG	C7-C8-C9-O8
28	C	519	LMG	O1-C7-C8-C9
28	c	521	LMG	C7-C8-C9-O8
29	A	614	SQD	O6-C44-C45-C46
29	a	613	SQD	O6-C44-C45-C46
31	c	516	DGD	O1G-C1G-C2G-C3G
23	c	506	CLA	C3-C5-C6-C7
28	c	521	LMG	C16-C17-C18-C19
30	d	407	LHG	C26-C27-C28-C29
31	a	616	DGD	CEB-CFB-CGB-CHB
23	B	601	CLA	C16-C17-C18-C19
24	a	605	PHO	C16-C17-C18-C20
30	a	614	LHG	C28-C29-C30-C31
30	D	408	LHG	C30-C31-C32-C33
30	d	409	LHG	C25-C26-C27-C28
31	C	517	DGD	CCA-CDA-CEA-CFA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C4-C3-C5-C6
27	a	611	PL9	C15-C14-C16-C17
23	b	609	CLA	O1D-CGD-O2D-CED
30	l	101	LHG	C19-C20-C21-C22
29	A	616	SQD	O47-C45-C46-O48
23	B	607	CLA	C16-C17-C18-C19
23	B	616	CLA	C11-C12-C13-C14
30	A	615	LHG	O6-C4-C5-O7
23	h	101	CLA	C2B-C3B-CAB-CBB
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
23	c	509	CLA	C15-C16-C17-C18
28	B	620	LMG	C12-C13-C14-C15
29	a	615	SQD	C15-C16-C17-C18
31	c	518	DGD	C8B-C9B-CAB-CBB
23	c	507	CLA	C16-C17-C18-C19
23	c	509	CLA	CAA-CBA-CGA-O2A
28	A	612	LMG	O1-C7-C8-O7
28	B	620	LMG	O7-C8-C9-O8
29	A	614	SQD	O47-C45-C46-O48
23	B	604	CLA	C2C-C3C-CAC-CBC
28	d	406	LMG	C40-C41-C42-C43
31	c	517	DGD	CDA-CEA-CFA-CGA
23	B	601	CLA	C4-C3-C5-C6
25	c	514	BCR	C10-C11-C12-C13
23	b	611	CLA	C10-C11-C12-C13
23	B	615	CLA	C2-C3-C5-C6
27	d	408	PL9	C13-C14-C16-C17
28	D	405	LMG	C13-C14-C15-C16
28	d	406	LMG	C33-C34-C35-C36
29	a	615	SQD	C9-C10-C11-C12
30	l	101	LHG	C30-C31-C32-C33
23	B	615	CLA	C16-C17-C18-C19
28	A	612	LMG	C32-C33-C34-C35
31	c	518	DGD	C6B-C7B-C8B-C9B
30	D	408	LHG	C23-C24-C25-C26
23	C	501	CLA	O1D-CGD-O2D-CED
30	D	408	LHG	C11-C10-C9-C8
23	B	611	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C14
23	b	612	CLA	C14-C13-C15-C16
23	b	615	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C14-C13-C15-C16
30	B	623	LHG	C31-C32-C33-C34
23	C	510	CLA	C15-C16-C17-C18
31	a	616	DGD	CFA-CGA-CHA-CIA
25	d	404	BCR	C22-C23-C24-C25
29	a	613	SQD	C10-C11-C12-C13
31	A	617	DGD	CAA-CBA-CCA-CDA
31	A	617	DGD	CCA-CDA-CEA-CFA
25	t	101	BCR	C14-C15-C16-C17
28	m	101	LMG	C37-C38-C39-C40
31	h	103	DGD	C7A-C8A-C9A-CAA
23	D	403	CLA	C16-C17-C18-C20
30	l	101	LHG	C24-C23-O8-C6
29	f	101	SQD	C25-C26-C27-C28
27	A	611	PL9	C19-C21-C22-C23
30	d	405	LHG	C28-C29-C30-C31
30	d	409	LHG	O1-C1-C2-O2
31	C	517	DGD	C4B-C5B-C6B-C7B
23	C	505	CLA	C2-C3-C5-C6
23	B	606	CLA	C16-C17-C18-C20
28	c	519	LMG	C4-C5-C6-O5
30	l	101	LHG	C23-C24-C25-C26
28	C	519	LMG	O6-C5-C6-O5
24	d	401	PHO	O1D-CGD-O2D-CED
23	b	604	CLA	C10-C11-C12-C13
30	D	408	LHG	C1-C2-C3-O3
30	a	614	LHG	C1-C2-C3-O3
30	D	408	LHG	C31-C32-C33-C34
25	B	619	BCR	C20-C21-C22-C37
25	H	101	BCR	C11-C10-C9-C34
25	b	618	BCR	C11-C10-C9-C34
25	d	404	BCR	C16-C17-C18-C36
25	d	404	BCR	C20-C21-C22-C37
23	c	503	CLA	O1A-CGA-O2A-C1
30	d	407	LHG	C23-C24-C25-C26
23	b	613	CLA	C8-C10-C11-C12
31	c	516	DGD	CBB-CCB-CDB-CEB
25	c	515	BCR	C36-C18-C19-C20
31	a	616	DGD	CAA-CBA-CCA-CDA
23	B	616	CLA	C6-C7-C8-C10
23	C	504	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C12-C13-C15-C16
23	C	509	CLA	C12-C13-C15-C16
23	C	513	CLA	C12-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C10-C8-C7
23	b	616	CLA	C11-C10-C8-C7
23	c	503	CLA	C11-C10-C8-C7
23	c	509	CLA	C12-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C12-C13-C15-C16
24	a	605	PHO	C6-C7-C8-C10
30	D	406	LHG	C10-C11-C12-C13
31	C	517	DGD	CDA-CEA-CFA-CGA
23	B	603	CLA	O1D-CGD-O2D-CED
29	F	101	SQD	O48-C23-C24-C25
23	C	509	CLA	C3-C5-C6-C7
23	C	506	CLA	C8-C10-C11-C12
23	c	512	CLA	C8-C10-C11-C12
25	C	520	BCR	C11-C12-C13-C14
31	C	518	DGD	C5A-C6A-C7A-C8A
23	b	607	CLA	O1A-CGA-O2A-C1
31	c	517	DGD	O1A-C1A-O1G-C1G
31	c	517	DGD	C2G-C3G-O3G-C1D
31	c	517	DGD	C5D-C6D-O5D-C1E
31	c	516	DGD	C6B-C7B-C8B-C9B
28	D	409	LMG	C11-C12-C13-C14
28	m	101	LMG	C35-C36-C37-C38
30	a	614	LHG	C18-C19-C20-C21
30	d	407	LHG	C10-C11-C12-C13
23	c	510	CLA	C4-C3-C5-C6
23	b	606	CLA	O1A-CGA-O2A-C1
31	c	516	DGD	O1A-C1A-O1G-C1G
29	B	624	SQD	C45-C46-O48-C23
28	m	101	LMG	C39-C40-C41-C42
30	D	406	LHG	C29-C30-C31-C32
30	d	405	LHG	C33-C34-C35-C36
23	D	403	CLA	O2A-C1-C2-C3
24	a	605	PHO	O2A-C1-C2-C3
31	a	616	DGD	C1G-C2G-O2G-C1B
28	d	406	LMG	C29-C30-C31-C32
23	B	607	CLA	C15-C16-C17-C18
24	A	606	PHO	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	615	LHG	O2-C2-C3-O3
31	c	518	DGD	CDB-CEB-CFB-CGB
25	T	101	BCR	C16-C17-C18-C19
25	b	618	BCR	C16-C17-C18-C19
31	A	617	DGD	CCB-CDB-CEB-CFB
28	C	519	LMG	C34-C35-C36-C37
29	B	624	SQD	C11-C10-C9-C8
28	C	519	LMG	O6-C1-O1-C7
29	a	615	SQD	C44-C45-C46-O48
31	a	616	DGD	O1G-C1G-C2G-C3G
35	f	102	HEM	C4B-C3B-CAB-CBB
23	b	602	CLA	C16-C17-C18-C19
30	d	407	LHG	C18-C19-C20-C21
23	B	601	CLA	C2-C3-C5-C6
27	A	611	PL9	C38-C39-C41-C42
28	m	101	LMG	C15-C16-C17-C18
31	C	517	DGD	C3A-C4A-C5A-C6A
28	C	519	LMG	O1-C7-C8-O7
28	D	409	LMG	O7-C8-C9-O8
29	b	601	SQD	O6-C44-C45-O47
31	C	516	DGD	O1G-C1G-C2G-O2G
23	b	604	CLA	C11-C10-C8-C9
30	D	406	LHG	C34-C35-C36-C37
28	b	621	LMG	C41-C42-C43-C44
28	d	410	LMG	C29-C30-C31-C32
29	A	614	SQD	C33-C34-C35-C36
29	A	616	SQD	C10-C11-C12-C13
29	F	101	SQD	C31-C32-C33-C34
29	B	624	SQD	C33-C34-C35-C36
29	F	101	SQD	C29-C30-C31-C32
30	L	101	LHG	C24-C25-C26-C27
29	A	614	SQD	C26-C27-C28-C29
29	b	601	SQD	C25-C26-C27-C28
30	D	408	LHG	C9-C10-C11-C12
31	a	616	DGD	C4B-C5B-C6B-C7B
31	C	516	DGD	C4D-C5D-C6D-O5D
23	B	607	CLA	C10-C11-C12-C13
30	d	409	LHG	C2-C3-O3-P
23	A	607	CLA	C6-C7-C8-C9
31	C	518	DGD	CBB-CCB-CDB-CEB
31	C	517	DGD	C3B-C4B-C5B-C6B
27	d	408	PL9	C43-C44-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C5-C6-C7-C8
23	d	403	CLA	C5-C6-C7-C8
31	C	518	DGD	C7B-C8B-C9B-CAB
30	B	623	LHG	O10-C23-O8-C6
30	l	101	LHG	C11-C12-C13-C14
30	a	614	LHG	C12-C13-C14-C15
30	d	405	LHG	C16-C17-C18-C19
23	A	613	CLA	C16-C17-C18-C19
23	B	616	CLA	C11-C12-C13-C15
27	a	611	PL9	C44-C46-C47-C48
31	A	617	DGD	C4D-C5D-C6D-O5D
23	B	601	CLA	C4B-C3B-CAB-CBB
23	B	605	CLA	C4B-C3B-CAB-CBB
28	B	620	LMG	C32-C33-C34-C35
23	C	510	CLA	C4-C3-C5-C6
25	c	514	BCR	C22-C23-C24-C25
25	h	102	BCR	C22-C23-C24-C25
25	k	102	BCR	C6-C7-C8-C9
31	c	517	DGD	C3B-C4B-C5B-C6B
25	C	515	BCR	C7-C8-C9-C10
25	T	101	BCR	C7-C8-C9-C10
25	Y	101	BCR	C7-C8-C9-C10
30	l	101	LHG	C35-C36-C37-C38
28	c	521	LMG	C31-C32-C33-C34
23	a	606	CLA	O1A-CGA-O2A-C1
30	l	101	LHG	O6-C4-C5-C6
31	c	517	DGD	C2B-C3B-C4B-C5B
29	A	614	SQD	C5-C6-S-O7
29	a	613	SQD	C5-C6-S-O9
29	f	101	SQD	C5-C6-S-O7
23	B	612	CLA	C11-C10-C8-C7
23	C	505	CLA	C6-C7-C8-C10
23	C	512	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C12-C13-C15
23	b	607	CLA	C11-C12-C13-C15
23	b	608	CLA	C11-C10-C8-C7
23	b	614	CLA	C11-C12-C13-C15
23	c	501	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
23	d	402	CLA	C6-C7-C8-C10
23	h	101	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	605	PHO	C12-C13-C15-C16
28	A	612	LMG	C33-C34-C35-C36
31	C	516	DGD	C3A-C4A-C5A-C6A
23	B	614	CLA	C16-C17-C18-C20
23	C	501	CLA	C16-C17-C18-C20
24	a	605	PHO	C16-C17-C18-C19
23	B	604	CLA	O1D-CGD-O2D-CED
23	a	606	CLA	CBA-CGA-O2A-C1
31	A	617	DGD	C6A-C7A-C8A-C9A
23	c	508	CLA	O1D-CGD-O2D-CED
30	L	101	LHG	C11-C10-C9-C8
31	c	518	DGD	CCB-CDB-CEB-CFB
36	V	201	HEC	C4B-C3B-CAB-CBB
36	v	201	HEC	C4B-C3B-CAB-CBB
23	C	512	CLA	C16-C17-C18-C19
30	A	615	LHG	C13-C14-C15-C16
23	B	607	CLA	C11-C10-C8-C9
23	B	612	CLA	C11-C10-C8-C9
23	B	616	CLA	C6-C7-C8-C9
23	C	504	CLA	C11-C10-C8-C9
23	C	509	CLA	C14-C13-C15-C16
23	D	403	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C9
23	c	509	CLA	C14-C13-C15-C16
24	a	605	PHO	C6-C7-C8-C9
29	a	615	SQD	C19-C20-C21-C22
23	c	506	CLA	C8-C10-C11-C12
29	A	614	SQD	C12-C13-C14-C15
31	a	616	DGD	C7B-C8B-C9B-CAB
28	c	521	LMG	O7-C8-C9-O8
29	f	101	SQD	O47-C45-C46-O48
30	A	615	LHG	O7-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-O2G
30	L	101	LHG	C26-C27-C28-C29
31	H	102	DGD	C7A-C8A-C9A-CAA
28	A	612	LMG	C28-C29-C30-C31
28	b	621	LMG	C7-C8-C9-O8
29	f	101	SQD	C44-C45-C46-O48
31	C	516	DGD	O1G-C1G-C2G-C3G
31	C	516	DGD	O1A-C1A-O1G-C1G
29	B	624	SQD	C14-C15-C16-C17
23	B	612	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
30	B	623	LHG	C19-C20-C21-C22
31	C	516	DGD	C4B-C5B-C6B-C7B
28	c	522	LMG	C31-C32-C33-C34
23	B	612	CLA	C16-C17-C18-C19
31	C	518	DGD	CCA-CDA-CEA-CFA
30	A	615	LHG	C30-C31-C32-C33
28	m	101	LMG	C31-C32-C33-C34
29	A	616	SQD	C32-C33-C34-C35
28	d	410	LMG	C34-C35-C36-C37
23	B	612	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
25	d	404	BCR	C9-C10-C11-C12
30	D	406	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O5
30	a	614	LHG	C4-O6-P-O4
30	d	405	LHG	C3-O3-P-O5
30	d	407	LHG	C4-O6-P-O5
30	D	408	LHG	C35-C36-C37-C38
24	d	401	PHO	C2C-C3C-CAC-CBC
23	B	606	CLA	C2B-C3B-CAB-CBB
25	k	101	BCR	C1-C6-C7-C8
23	c	510	CLA	C2-C3-C5-C6
30	A	615	LHG	C9-C10-C11-C12
23	C	508	CLA	C13-C15-C16-C17
31	H	102	DGD	CCB-CDB-CEB-CFB
29	a	613	SQD	C13-C14-C15-C16
30	d	407	LHG	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	611	PL9	C4-C3-C7-C8
28	d	406	LMG	C30-C31-C32-C33
30	d	409	LHG	C33-C34-C35-C36
28	A	612	LMG	C9-C8-O7-C10
29	B	624	SQD	C44-C45-O47-C7
23	b	609	CLA	C4-C3-C5-C6
23	C	512	CLA	C16-C17-C18-C20
28	D	405	LMG	C36-C37-C38-C39
30	a	614	LHG	O6-C4-C5-C6
23	B	608	CLA	C6-C7-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	513	CLA	C14-C13-C15-C16
23	b	602	CLA	C11-C10-C8-C9
23	b	609	CLA	C14-C13-C15-C16
23	b	612	CLA	C6-C7-C8-C9
23	c	501	CLA	C11-C12-C13-C14
31	c	516	DGD	C8A-C9A-CAA-CBA
23	b	612	CLA	C12-C13-C15-C16
23	b	613	CLA	C6-C7-C8-C10
25	A	608	BCR	C20-C21-C22-C23
25	T	101	BCR	C20-C21-C22-C23
30	A	615	LHG	C10-C11-C12-C13
30	l	101	LHG	O6-C4-C5-O7
31	c	516	DGD	C2A-C3A-C4A-C5A
31	h	103	DGD	O2G-C1B-C2B-C3B
23	D	403	CLA	C13-C15-C16-C17
29	F	101	SQD	C24-C25-C26-C27
30	D	408	LHG	C16-C17-C18-C19
31	a	616	DGD	C8B-C9B-CAB-CBB
31	C	518	DGD	C2A-C1A-O1G-C1G
23	D	402	CLA	C15-C16-C17-C18
28	A	612	LMG	C19-C20-C21-C22
23	c	506	CLA	C4-C3-C5-C6
30	L	101	LHG	C30-C31-C32-C33
28	D	405	LMG	C31-C32-C33-C34
29	b	601	SQD	O6-C44-C45-C46
29	F	101	SQD	O6-C44-C45-C46
31	C	516	DGD	O1G-C1A-C2A-C3A
31	a	616	DGD	O2G-C1B-C2B-C3B
25	A	608	BCR	C36-C18-C19-C20
25	B	617	BCR	C7-C8-C9-C34
25	T	101	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	T	101	BCR	C36-C18-C19-C20
23	b	615	CLA	C16-C17-C18-C20
23	a	604	CLA	C15-C16-C17-C18
29	A	616	SQD	C11-C12-C13-C14
31	c	516	DGD	C5D-C6D-O5D-C1E
28	b	621	LMG	C23-C24-C25-C26
25	B	619	BCR	C15-C16-C17-C18
25	D	404	BCR	C9-C10-C11-C12
25	d	404	BCR	C13-C14-C15-C16
30	D	406	LHG	C14-C15-C16-C17
27	a	611	PL9	C25-C24-C26-C27
23	C	510	CLA	C2-C3-C5-C6
31	a	616	DGD	CFB-CGB-CHB-CIB
31	C	517	DGD	C8A-C9A-CAA-CBA
28	B	620	LMG	C28-C29-C30-C31
23	b	607	CLA	C11-C12-C13-C14
23	c	503	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	d	402	CLA	C6-C7-C8-C9
23	c	503	CLA	C4B-C3B-CAB-CBB
29	a	613	SQD	C27-C28-C29-C30
24	A	605	PHO	C15-C16-C17-C18
28	m	101	LMG	C22-C23-C24-C25
23	B	612	CLA	CBA-CGA-O2A-C1
23	C	502	CLA	C10-C11-C12-C13
29	F	101	SQD	C45-C46-O48-C23
28	m	101	LMG	C11-C12-C13-C14
28	d	410	LMG	C39-C40-C41-C42
27	d	408	PL9	C34-C36-C37-C38
29	A	614	SQD	C17-C18-C19-C20
29	A	614	SQD	C15-C16-C17-C18
23	a	606	CLA	C11-C10-C8-C7
23	b	602	CLA	C6-C7-C8-C10
23	b	605	CLA	C12-C13-C15-C16
23	h	101	CLA	C13-C15-C16-C17
29	a	615	SQD	C17-C18-C19-C20
30	a	614	LHG	C25-C26-C27-C28
23	d	402	CLA	C2C-C3C-CAC-CBC
29	B	624	SQD	C10-C11-C12-C13
23	B	603	CLA	C4-C3-C5-C6
23	B	609	CLA	C3A-C2A-CAA-CBA
25	c	515	BCR	C35-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	516	DGD	O6E-C1E-O5D-C6D
29	a	615	SQD	C26-C27-C28-C29
31	h	103	DGD	C8B-C9B-CAB-CBB
23	B	603	CLA	C5-C6-C7-C8
29	A	616	SQD	C30-C31-C32-C33
29	A	616	SQD	C16-C17-C18-C19
23	d	402	CLA	C3-C5-C6-C7
23	c	502	CLA	C15-C16-C17-C18
25	b	618	BCR	C37-C22-C23-C24
31	a	616	DGD	C9B-CAB-CBB-CCB
28	d	406	LMG	C32-C33-C34-C35
23	B	609	CLA	C13-C15-C16-C17
23	C	506	CLA	C10-C11-C12-C13
23	c	510	CLA	C10-C11-C12-C13
29	b	601	SQD	C15-C16-C17-C18
31	c	517	DGD	O1B-C1B-O2G-C2G
30	B	623	LHG	C18-C19-C20-C21
30	A	615	LHG	C1-C2-C3-O3
23	c	508	CLA	O1A-CGA-O2A-C1
27	D	407	PL9	C44-C46-C47-C48
30	A	615	LHG	C4-C5-C6-O8
29	a	615	SQD	C27-C28-C29-C30
28	B	622	LMG	O9-C10-C11-C12
23	C	508	CLA	C11-C12-C13-C14
23	C	511	CLA	C6-C7-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	b	602	CLA	C6-C7-C8-C9
23	b	610	CLA	C14-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C9
23	b	614	CLA	C11-C12-C13-C14
23	c	509	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	b	615	CLA	C16-C17-C18-C19
28	B	620	LMG	C35-C36-C37-C38
35	f	102	HEM	CAD-CBD-CGD-O1D
36	V	201	HEC	CAD-CBD-CGD-O2D
28	c	522	LMG	C9-C8-O7-C10
29	B	624	SQD	C46-C45-O47-C7
29	f	101	SQD	C46-C45-O47-C7
23	c	508	CLA	C13-C15-C16-C17
30	d	405	LHG	C18-C19-C20-C21
30	a	614	LHG	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	v	201	HEC	CAD-CBD-CGD-O1D
28	D	409	LMG	C31-C32-C33-C34
31	C	518	DGD	C4A-C5A-C6A-C7A
31	c	516	DGD	O1G-C1A-C2A-C3A
28	c	522	LMG	C33-C34-C35-C36
30	D	406	LHG	O1-C1-C2-O2
36	v	201	HEC	CAD-CBD-CGD-O2D
31	c	518	DGD	CBA-CCA-CDA-CEA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	B	602	CLA	C1A-C2A-CAA-CBA
25	C	514	BCR	C11-C10-C9-C8
30	L	101	LHG	C23-C24-C25-C26
23	A	604	CLA	C2B-C3B-CAB-CBB
23	B	601	CLA	C2B-C3B-CAB-CBB
23	B	605	CLA	C2B-C3B-CAB-CBB
23	C	502	CLA	C2B-C3B-CAB-CBB
23	D	402	CLA	C2B-C3B-CAB-CBB
23	b	603	CLA	C2B-C3B-CAB-CBB
23	b	610	CLA	C2B-C3B-CAB-CBB
23	b	611	CLA	C2B-C3B-CAB-CBB
23	d	402	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C5-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C30
25	C	515	BCR	C1-C6-C7-C8
25	C	515	BCR	C5-C6-C7-C8
25	b	618	BCR	C23-C24-C25-C30
25	c	514	BCR	C1-C6-C7-C8
25	c	514	BCR	C5-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
24	d	401	PHO	CBD-CGD-O2D-CED
23	c	508	CLA	CBA-CGA-O2A-C1
23	C	508	CLA	C16-C17-C18-C19
31	A	617	DGD	C4E-C5E-C6E-O5E
23	D	403	CLA	C2-C3-C5-C6
29	a	613	SQD	C15-C16-C17-C18
23	c	501	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	CBD-CGD-O2D-CED
29	a	613	SQD	C7-C8-C9-C10
23	b	603	CLA	C8-C10-C11-C12
23	B	603	CLA	C6-C7-C8-C10
23	B	605	CLA	C12-C13-C15-C16
23	c	504	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C2A-CAA-CBA-CGA
31	C	516	DGD	C6A-C7A-C8A-C9A
23	B	609	CLA	C10-C11-C12-C13
31	h	103	DGD	C3B-C4B-C5B-C6B
28	A	612	LMG	C39-C40-C41-C42
29	a	613	SQD	C29-C30-C31-C32
29	b	601	SQD	C13-C14-C15-C16
30	d	409	LHG	C24-C25-C26-C27
24	d	401	PHO	C3-C5-C6-C7
28	B	620	LMG	C40-C41-C42-C43
29	F	101	SQD	C26-C27-C28-C29
27	d	408	PL9	C35-C34-C36-C37
25	D	404	BCR	C18-C19-C20-C21
23	C	505	CLA	C10-C11-C12-C13
23	D	402	CLA	C10-C11-C12-C13
23	d	402	CLA	C2-C1-O2A-CGA
28	b	621	LMG	C29-C28-O8-C9
29	A	616	SQD	C33-C34-C35-C36
23	a	606	CLA	C11-C10-C8-C9
28	m	101	LMG	C32-C33-C34-C35
30	D	408	LHG	C24-C25-C26-C27
31	H	102	DGD	C8B-C9B-CAB-CBB
25	t	101	BCR	C13-C14-C15-C16
36	V	201	HEC	CAD-CBD-CGD-O1D
28	D	405	LMG	C40-C41-C42-C43
28	A	612	LMG	C17-C18-C19-C20
28	B	622	LMG	O7-C10-C11-C12
28	B	622	LMG	O8-C28-C29-C30
23	c	506	CLA	C4C-C3C-CAC-CBC
30	d	405	LHG	C31-C32-C33-C34
23	B	603	CLA	C13-C15-C16-C17
23	B	605	CLA	C5-C6-C7-C8
31	C	517	DGD	O1B-C1B-O2G-C2G
23	b	610	CLA	O1D-CGD-O2D-CED
28	m	101	LMG	O10-C28-O8-C9
23	c	501	CLA	C2A-CAA-CBA-CGA
35	f	102	HEM	CAD-CBD-CGD-O2D
30	a	614	LHG	O1-C1-C2-O2
30	d	405	LHG	O6-C4-C5-O7
23	d	402	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	623	LHG	C32-C33-C34-C35
23	A	604	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	c	504	CLA	C11-C12-C13-C14
23	h	101	CLA	C16-C17-C18-C20
23	C	507	CLA	C5-C6-C7-C8
31	C	518	DGD	C3A-C4A-C5A-C6A
24	A	606	PHO	CHA-CBD-CGD-O1D
24	a	605	PHO	CHA-CBD-CGD-O1D
30	d	409	LHG	C9-C10-C11-C12
28	b	621	LMG	O7-C8-C9-O8
28	B	620	LMG	C10-C11-C12-C13
31	C	517	DGD	O6D-C1D-O3G-C3G
30	d	407	LHG	C16-C17-C18-C19
23	c	506	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
28	m	101	LMG	C30-C31-C32-C33
29	b	601	SQD	C19-C20-C21-C22
31	c	517	DGD	C5B-C6B-C7B-C8B
25	Y	101	BCR	C13-C14-C15-C16
25	b	618	BCR	C9-C10-C11-C12
31	c	516	DGD	C3A-C4A-C5A-C6A
28	d	406	LMG	C10-C11-C12-C13
31	h	103	DGD	O1B-C1B-C2B-C3B
23	C	512	CLA	C14-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C9
23	a	604	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C10-C8-C9
23	h	101	CLA	C11-C12-C13-C14
28	B	620	LMG	C8-C7-O1-C1
29	A	614	SQD	C5-C6-S-O8
28	C	519	LMG	C14-C15-C16-C17
31	C	518	DGD	C3B-C4B-C5B-C6B
23	B	613	CLA	C2-C1-O2A-CGA
23	c	512	CLA	C2-C1-O2A-CGA
31	c	516	DGD	C1A-C2A-C3A-C4A
23	B	602	CLA	C3A-C2A-CAA-CBA
23	B	603	CLA	C2-C3-C5-C6
23	b	608	CLA	C2C-C3C-CAC-CBC
28	C	519	LMG	C37-C38-C39-C40
28	b	621	LMG	C42-C43-C44-C45
23	A	613	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	d	402	CLA	C16-C17-C18-C19
23	c	505	CLA	C4-C3-C5-C6
31	H	102	DGD	CDA-CEA-CFA-CGA
28	c	522	LMG	C37-C38-C39-C40
23	B	614	CLA	C16-C17-C18-C19
31	c	517	DGD	C9A-CAA-CBA-CCA
31	c	517	DGD	CCB-CDB-CEB-CFB
30	d	407	LHG	C19-C20-C21-C22
28	c	522	LMG	O1-C7-C8-C9
29	A	614	SQD	C44-C45-C46-O48
29	b	601	SQD	C44-C45-C46-O48
23	B	612	CLA	O1A-CGA-O2A-C1
27	D	407	PL9	C37-C38-C39-C40
30	A	615	LHG	C14-C15-C16-C17
23	C	511	CLA	CBA-CGA-O2A-C1
31	C	517	DGD	C9A-CAA-CBA-CCA
25	b	619	BCR	C9-C10-C11-C12
31	c	518	DGD	C2A-C3A-C4A-C5A
31	C	518	DGD	C8A-C9A-CAA-CBA
31	H	102	DGD	C5B-C6B-C7B-C8B
28	B	620	LMG	C14-C15-C16-C17
30	d	407	LHG	C32-C33-C34-C35
31	c	517	DGD	CCA-CDA-CEA-CFA
31	C	518	DGD	C4B-C5B-C6B-C7B
31	H	102	DGD	C7B-C8B-C9B-CAB
23	c	509	CLA	CAA-CBA-CGA-O1A
31	A	617	DGD	C2A-C3A-C4A-C5A
25	B	619	BCR	C14-C15-C16-C17
23	C	508	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	b	607	CLA	C16-C17-C18-C19
23	b	607	CLA	C16-C17-C18-C20
25	B	618	BCR	C7-C8-C9-C10
23	b	609	CLA	C3-C5-C6-C7
28	A	612	LMG	C38-C39-C40-C41
23	b	610	CLA	C13-C15-C16-C17
23	d	402	CLA	C10-C11-C12-C13
29	b	601	SQD	C26-C27-C28-C29
28	B	620	LMG	C18-C19-C20-C21
23	c	505	CLA	C2-C3-C5-C6
23	B	603	CLA	C12-C13-C15-C16
23	C	511	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C11-C10-C8-C7
23	D	403	CLA	C11-C10-C8-C7
23	a	604	CLA	C6-C7-C8-C10
23	b	614	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
28	m	101	LMG	C38-C39-C40-C41
23	A	603	CLA	C2B-C3B-CAB-CBB
25	A	608	BCR	C1-C6-C7-C8
25	A	608	BCR	C5-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C26
25	Y	101	BCR	C23-C24-C25-C30
25	a	607	BCR	C1-C6-C7-C8
23	C	512	CLA	C2-C1-O2A-CGA
23	b	608	CLA	CBD-CGD-O2D-CED
30	D	408	LHG	C24-C23-O8-C6
29	B	624	SQD	C16-C17-C18-C19
23	B	612	CLA	CAA-CBA-CGA-O2A
28	c	522	LMG	O8-C28-C29-C30
29	a	613	SQD	O47-C7-C8-C9
23	B	609	CLA	C2-C3-C5-C6
23	b	609	CLA	C2-C3-C5-C6
27	D	407	PL9	C13-C14-C16-C17
27	a	611	PL9	C13-C14-C16-C17
23	b	607	CLA	C13-C15-C16-C17
27	A	611	PL9	C4-C3-C7-C8
28	B	622	LMG	C31-C32-C33-C34
35	F	102	HEM	CAD-CBD-CGD-O1D
23	B	611	CLA	O1A-CGA-O2A-C1
31	c	518	DGD	C7B-C8B-C9B-CAB
28	B	622	LMG	C13-C14-C15-C16
23	B	611	CLA	C2-C3-C5-C6
27	A	611	PL9	C12-C11-C9-C8
27	d	408	PL9	C33-C34-C36-C37
29	b	601	SQD	C16-C17-C18-C19
30	d	405	LHG	O9-C7-O7-C5
30	B	623	LHG	C27-C28-C29-C30
29	F	101	SQD	C35-C36-C37-C38
23	B	603	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C10-C8-C9
23	C	512	CLA	C8-C10-C11-C12
28	B	620	LMG	O1-C7-C8-C9
31	c	516	DGD	C1G-C2G-C3G-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	605	PHO	O1D-CGD-O2D-CED
23	c	507	CLA	C4B-C3B-CAB-CBB
23	B	609	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	c	504	CLA	C8-C10-C11-C12
30	B	623	LHG	C16-C17-C18-C19
23	c	510	CLA	CAA-CBA-CGA-O2A
29	A	614	SQD	O47-C7-C8-C9
30	L	101	LHG	O7-C7-C8-C9
31	C	516	DGD	O2G-C1B-C2B-C3B
31	C	518	DGD	C8B-C9B-CAB-CBB
23	C	507	CLA	C2-C3-C5-C6
25	B	617	BCR	C11-C12-C13-C14
23	C	509	CLA	C5-C6-C7-C8
23	c	511	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	C15-C16-C17-C18
23	b	613	CLA	CAA-CBA-CGA-O2A
28	m	101	LMG	O8-C28-C29-C30
29	a	613	SQD	C19-C20-C21-C22
24	d	401	PHO	C8-C10-C11-C12
23	C	512	CLA	C4-C3-C5-C6
27	a	611	PL9	C40-C39-C41-C42
27	d	408	PL9	C30-C29-C31-C32
23	D	402	CLA	C2-C1-O2A-CGA
23	B	601	CLA	C12-C13-C15-C16
23	a	606	CLA	C12-C13-C15-C16
23	b	606	CLA	C12-C13-C15-C16
23	b	608	CLA	C6-C7-C8-C10
23	b	609	CLA	C11-C12-C13-C15
24	A	605	PHO	C6-C7-C8-C10
29	A	616	SQD	C24-C23-O48-C46
28	d	406	LMG	C12-C13-C14-C15
29	f	101	SQD	C44-C45-O47-C7
23	C	511	CLA	O1A-CGA-O2A-C1
31	a	616	DGD	C7A-C8A-C9A-CAA
23	h	101	CLA	C16-C17-C18-C19
30	D	406	LHG	C33-C34-C35-C36
30	D	408	LHG	C2-C3-O3-P
28	c	522	LMG	C32-C33-C34-C35
27	D	407	PL9	C22-C23-C24-C25
23	B	601	CLA	C3A-C2A-CAA-CBA
31	c	517	DGD	C1A-C2A-C3A-C4A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	514	BCR	C12-C13-C14-C15
23	D	402	CLA	C3-C5-C6-C7
28	B	620	LMG	C38-C39-C40-C41
30	D	406	LHG	C16-C17-C18-C19
29	b	601	SQD	C10-C11-C12-C13
35	F	102	HEM	CAD-CBD-CGD-O2D
31	c	517	DGD	C8A-C9A-CAA-CBA
27	D	407	PL9	C21-C22-C23-C24
23	b	613	CLA	C16-C17-C18-C19
23	B	611	CLA	C6-C7-C8-C9
23	C	505	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	b	609	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
30	a	614	LHG	O2-C2-C3-O3
23	B	613	CLA	CAA-CBA-CGA-O2A
23	b	611	CLA	C2-C3-C5-C6
23	A	604	CLA	C15-C16-C17-C18
23	c	510	CLA	CAA-CBA-CGA-O1A
31	c	516	DGD	O1B-C1B-C2B-C3B
23	a	612	CLA	C2C-C3C-CAC-CBC
23	b	612	CLA	C8-C10-C11-C12
24	d	401	PHO	C5-C6-C7-C8
29	b	601	SQD	C45-C44-O6-C1
28	c	522	LMG	O7-C8-C9-O8
23	B	612	CLA	CAA-CBA-CGA-O1A
30	a	614	LHG	O10-C23-C24-C25
28	D	405	LMG	C19-C20-C21-C22
28	c	519	LMG	C34-C35-C36-C37
28	D	409	LMG	C35-C36-C37-C38
28	m	101	LMG	O9-C10-C11-C12
30	d	409	LHG	O10-C23-C24-C25
23	C	509	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
31	C	516	DGD	O1B-C1B-C2B-C3B
31	C	516	DGD	CDB-CEB-CFB-CGB
23	C	501	CLA	CAD-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
24	A	606	PHO	CAD-CBD-CGD-O2D
24	a	605	PHO	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	d	401	PHO	CAD-CBD-CGD-O2D
29	A	616	SQD	C34-C35-C36-C37
23	a	606	CLA	CAA-CBA-CGA-O2A
30	A	615	LHG	C12-C13-C14-C15
28	C	519	LMG	C17-C18-C19-C20
31	H	102	DGD	C5A-C6A-C7A-C8A
31	c	518	DGD	O1B-C1B-C2B-C3B
23	B	614	CLA	C5-C6-C7-C8
29	B	624	SQD	O47-C7-C8-C9
24	A	605	PHO	O1A-CGA-O2A-C1
23	B	613	CLA	CAA-CBA-CGA-O1A
23	A	604	CLA	C13-C15-C16-C17
30	l	101	LHG	C33-C34-C35-C36
28	A	612	LMG	C37-C38-C39-C40

There are no ring outliers.

116 monomers are involved in 229 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	f	101	SQD	3	0
23	C	504	CLA	1	0
25	D	404	BCR	4	0
23	c	513	CLA	1	0
23	c	511	CLA	2	0
23	B	602	CLA	3	0
31	h	103	DGD	2	0
23	b	612	CLA	2	0
30	D	408	LHG	1	0
36	v	201	HEC	1	0
30	d	407	LHG	2	0
23	b	615	CLA	4	0
28	D	405	LMG	1	0
23	b	602	CLA	1	0
25	A	608	BCR	1	0
25	C	514	BCR	2	0
31	H	102	DGD	1	0
23	B	616	CLA	2	0
23	d	403	CLA	1	0
23	B	610	CLA	2	0
23	C	512	CLA	1	0
35	F	102	HEM	3	0
23	A	613	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	617	BCR	2	0
31	C	518	DGD	1	0
25	d	404	BCR	3	0
23	C	505	CLA	2	0
23	d	402	CLA	1	0
30	A	615	LHG	1	0
25	c	515	BCR	3	0
25	a	607	BCR	1	0
23	b	616	CLA	4	0
30	a	614	LHG	3	0
29	a	613	SQD	3	0
27	A	611	PL9	6	0
23	B	615	CLA	3	0
23	c	512	CLA	1	0
25	k	102	BCR	1	0
28	m	101	LMG	1	0
23	a	612	CLA	2	0
23	B	609	CLA	4	0
28	b	621	LMG	1	0
23	C	511	CLA	4	0
28	B	620	LMG	2	0
29	b	601	SQD	2	0
23	b	604	CLA	1	0
31	a	616	DGD	4	0
23	D	402	CLA	1	0
23	C	506	CLA	1	0
23	B	607	CLA	1	0
25	B	619	BCR	2	0
24	A	606	PHO	2	0
27	D	407	PL9	1	0
31	c	518	DGD	1	0
32	a	618[B]	OEY	2	0
31	A	617	DGD	2	0
23	C	508	CLA	1	0
29	a	615	SQD	3	0
23	b	607	CLA	1	0
25	T	101	BCR	5	0
23	h	101	CLA	3	0
23	C	502	CLA	1	0
30	D	406	LHG	2	0
23	B	604	CLA	3	0
23	b	610	CLA	2	0

Continued on next page...

Continued from previous page...

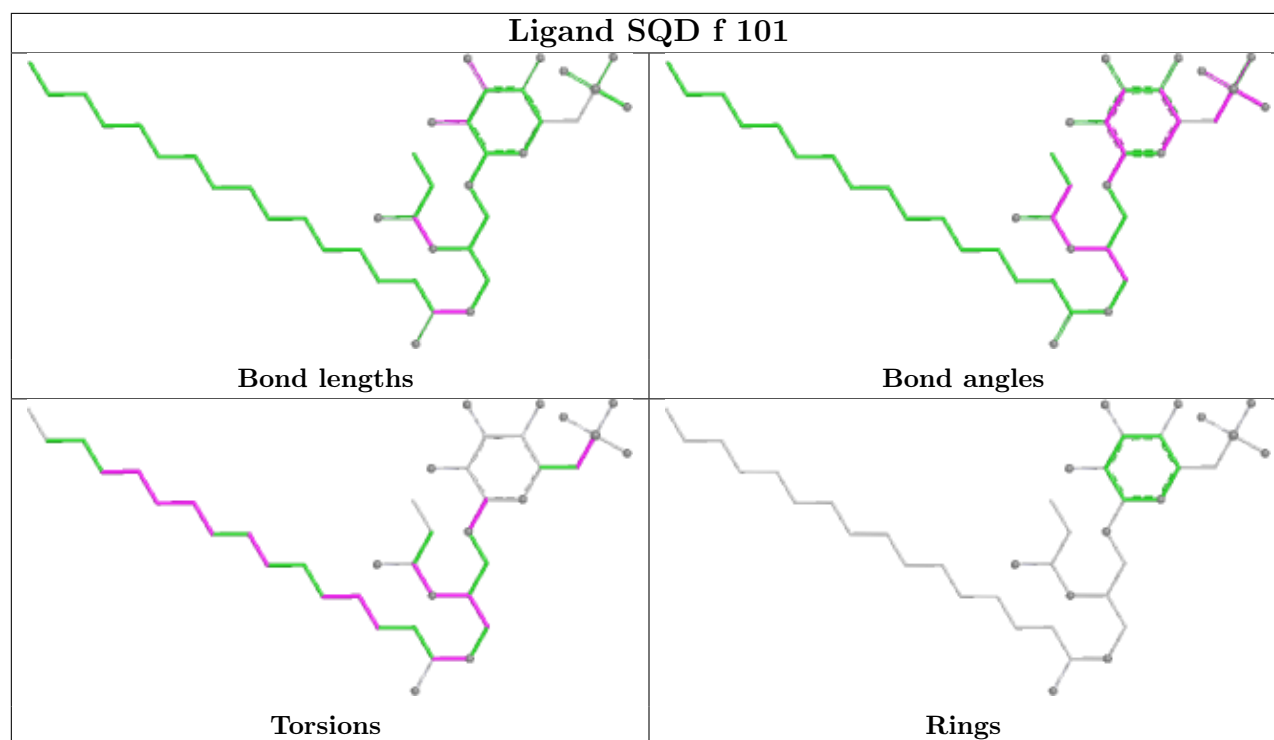
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	V	201	HEC	1	0
25	b	617	BCR	3	0
30	d	405	LHG	4	0
32	A	618[B]	OEY	2	0
23	b	614	CLA	2	0
25	b	619	BCR	1	0
23	B	606	CLA	5	0
30	B	623	LHG	4	0
23	c	505	CLA	1	0
25	B	618	BCR	3	0
23	A	604	CLA	3	0
24	d	401	PHO	4	0
23	B	603	CLA	1	0
23	b	609	CLA	1	0
24	A	605	PHO	1	0
23	B	605	CLA	2	0
23	c	503	CLA	2	0
23	b	613	CLA	4	0
27	a	611	PL9	9	0
28	d	406	LMG	1	0
23	b	603	CLA	2	0
25	h	102	BCR	2	0
23	C	501	CLA	2	0
23	c	509	CLA	1	0
23	b	605	CLA	3	0
23	c	508	CLA	2	0
25	k	101	BCR	3	0
35	f	102	HEM	7	0
23	c	504	CLA	2	0
23	A	603	CLA	3	0
25	H	101	BCR	4	0
25	Y	101	BCR	3	0
28	c	522	LMG	2	0
25	t	101	BCR	7	0
23	a	606	CLA	6	0
23	C	513	CLA	1	0
31	C	517	DGD	2	0
23	B	608	CLA	2	0
23	b	606	CLA	4	0
23	a	603	CLA	4	0
28	c	521	LMG	1	0
23	c	501	CLA	3	0

Continued on next page...

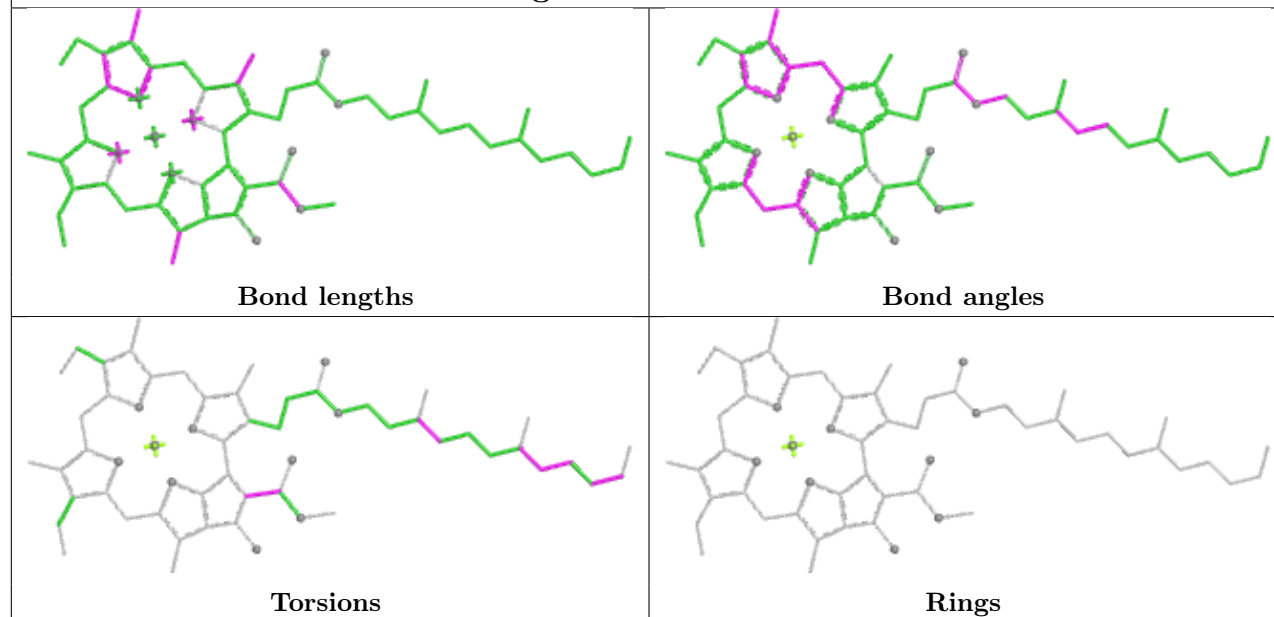
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	613	CLA	2	0
25	b	618	BCR	5	0
23	c	507	CLA	1	0
25	C	515	BCR	2	0
24	a	605	PHO	2	0
23	D	403	CLA	1	0
23	C	510	CLA	1	0
30	d	409	LHG	1	0
23	c	506	CLA	2	0

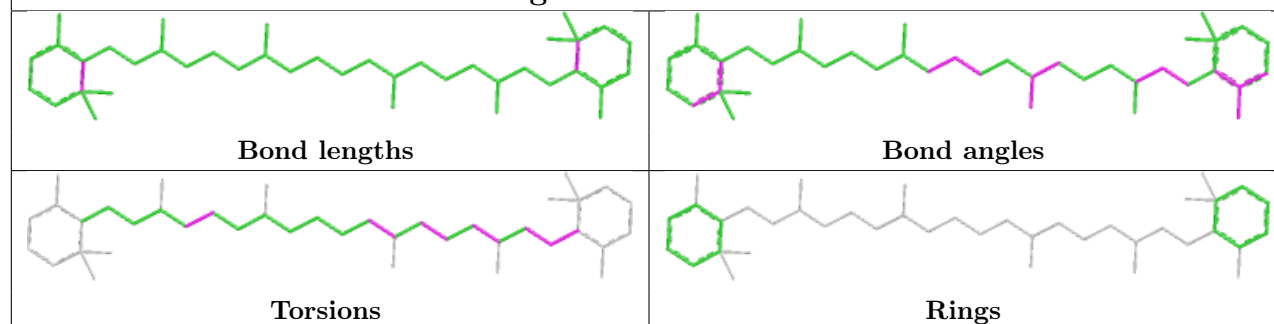
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



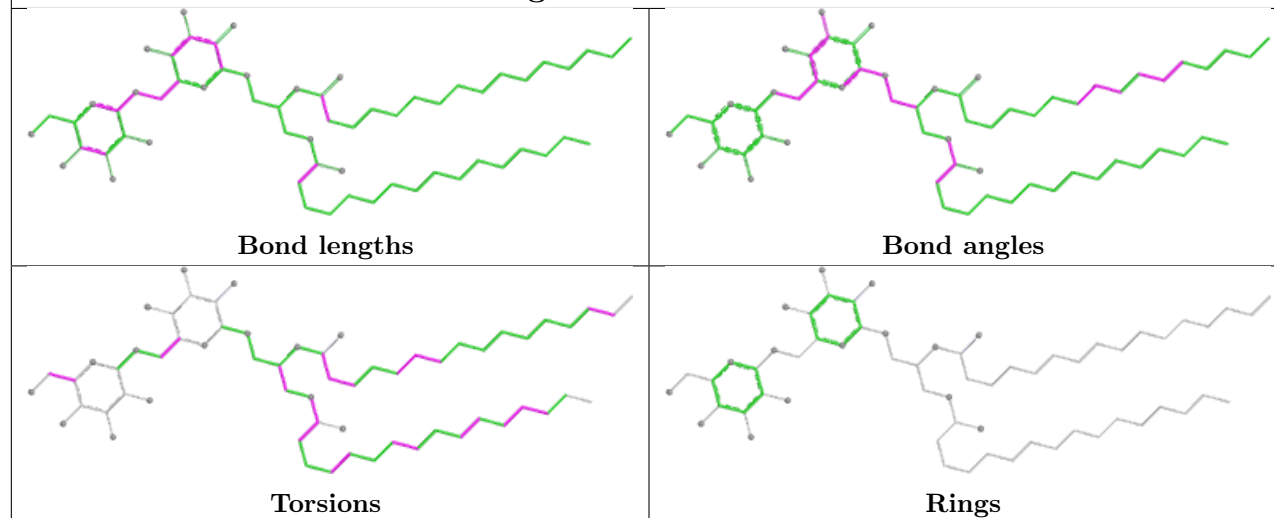
Ligand CLA C 504



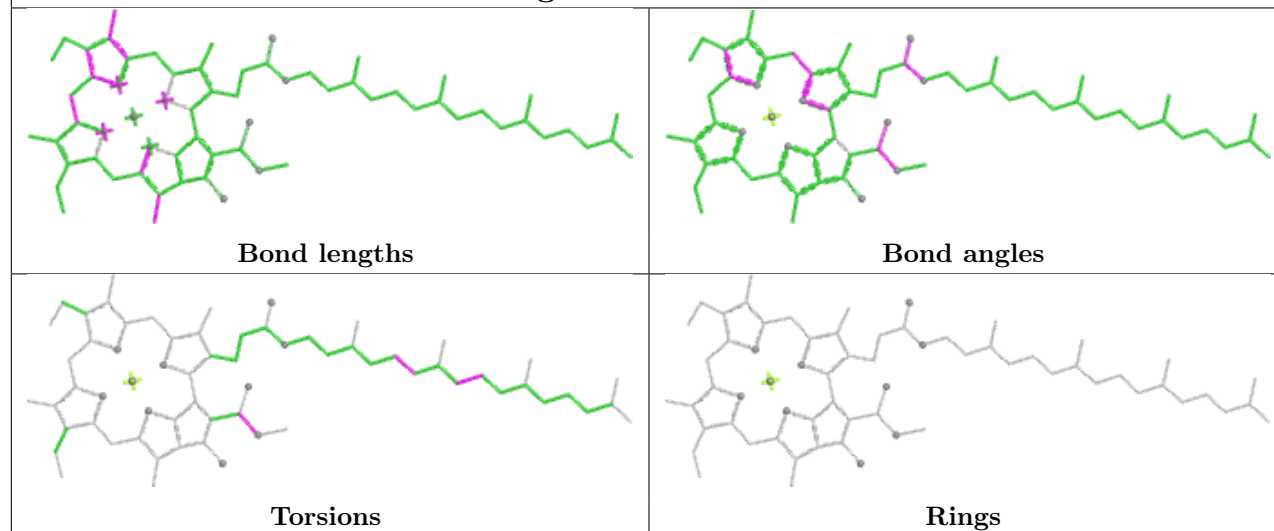
Ligand BCR D 404



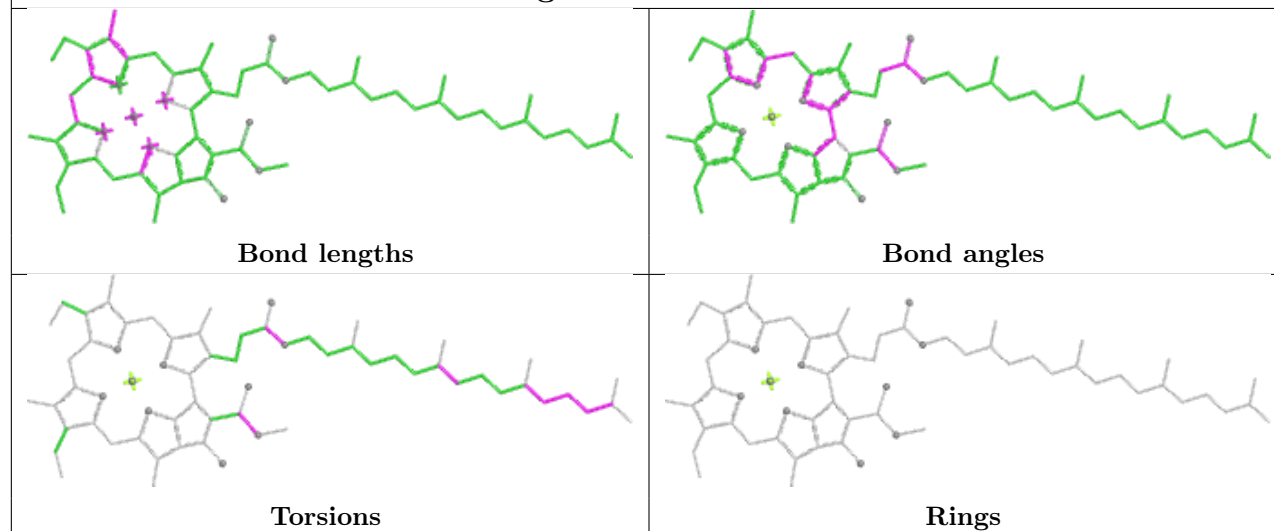
Ligand DGD C 516



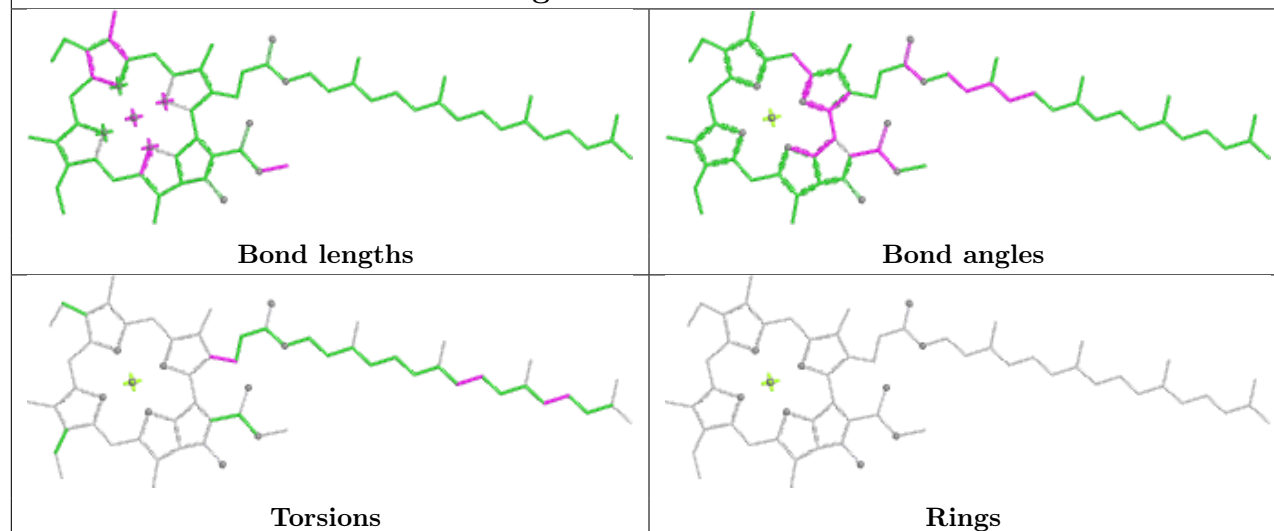
Ligand CLA c 513

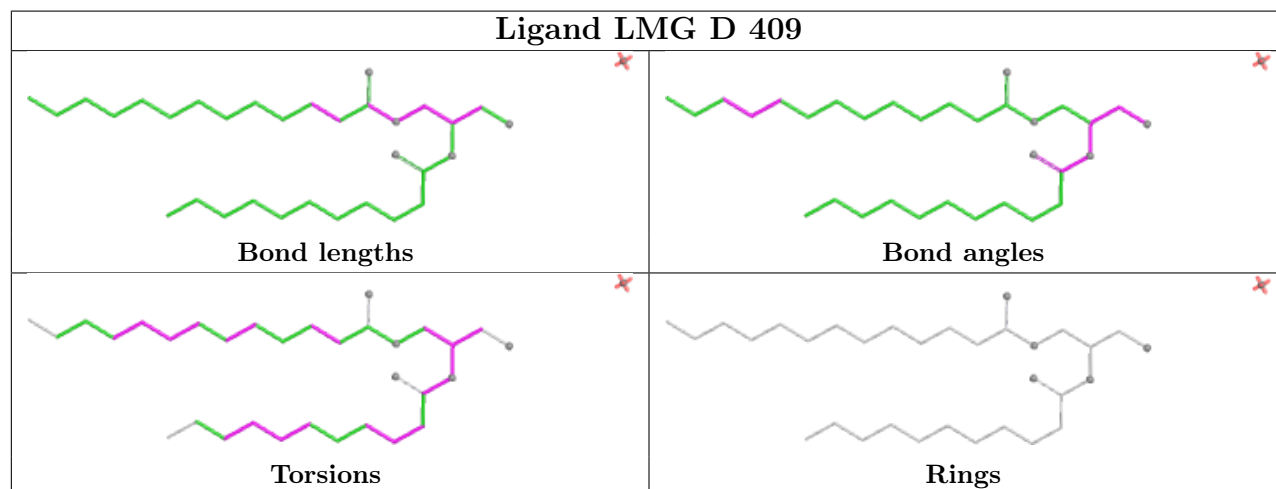
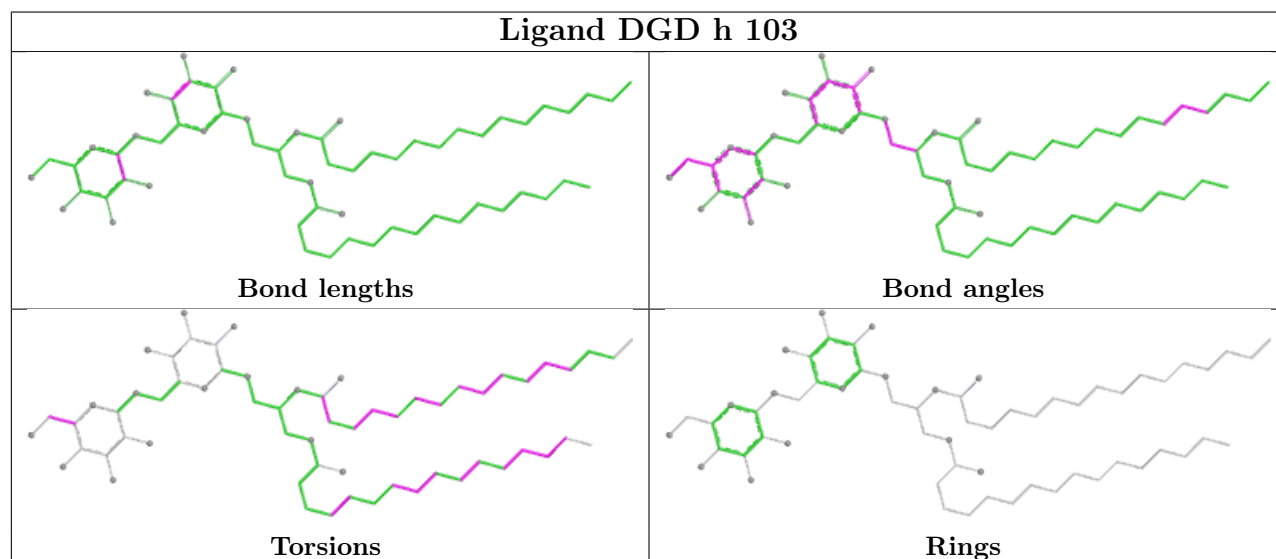
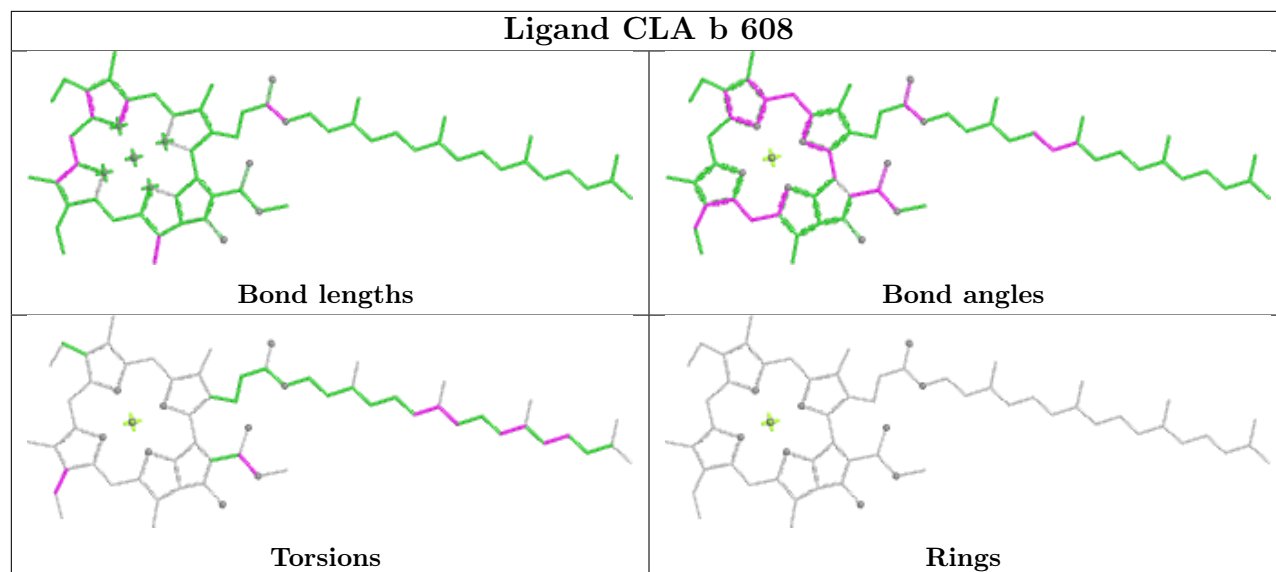


Ligand CLA c 511

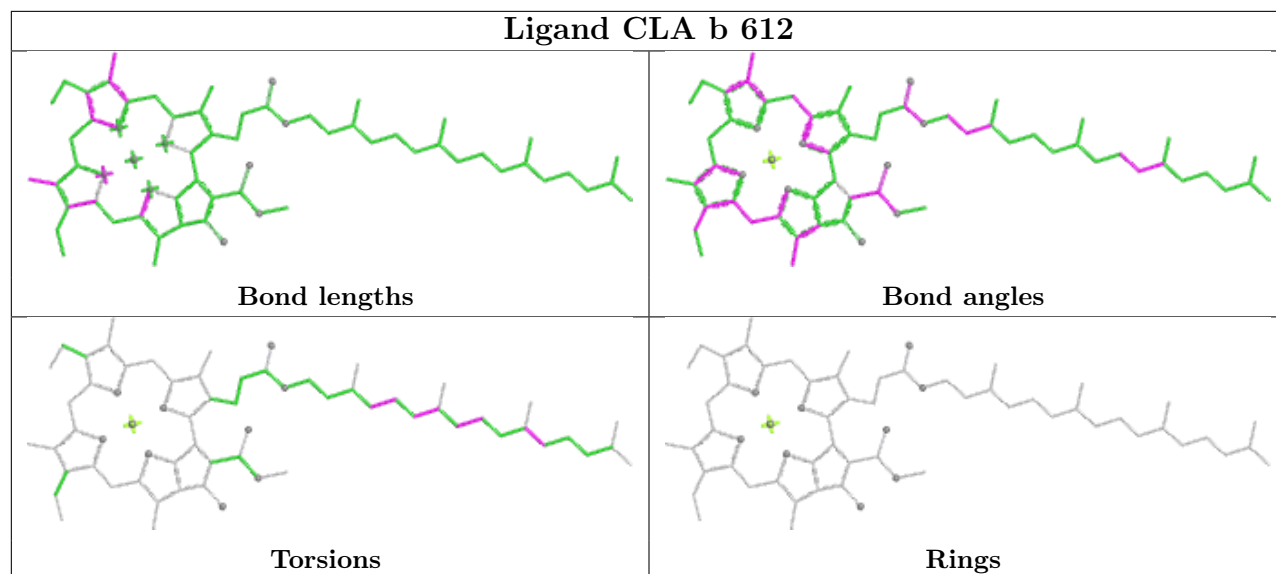


Ligand CLA B 602

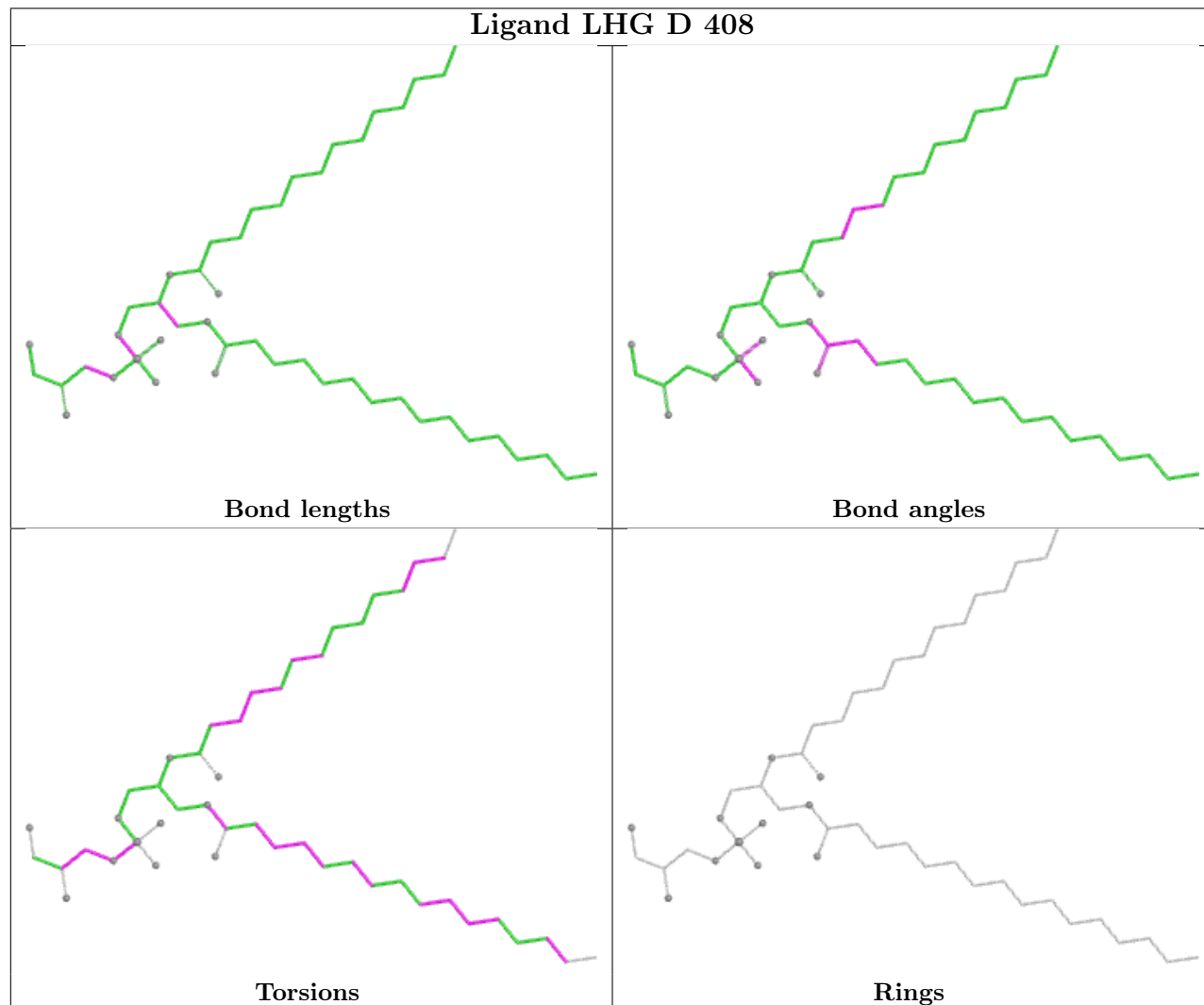




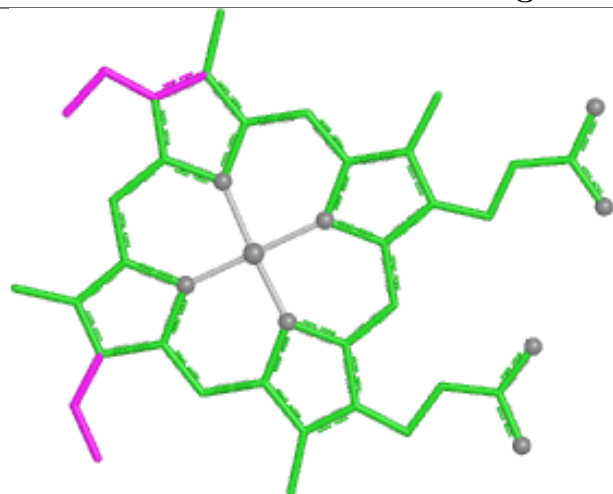
Ligand CLA b 612



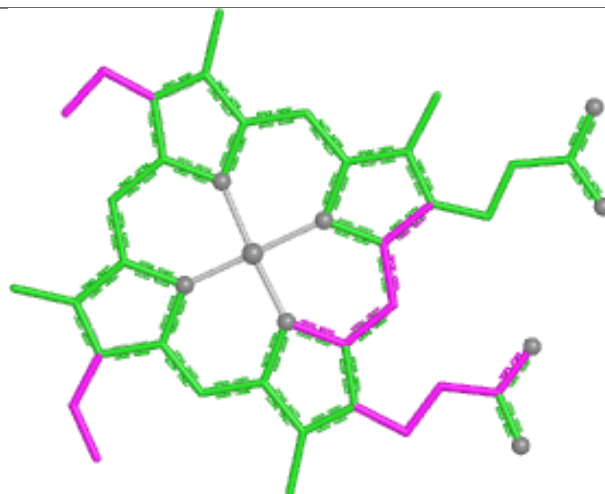
Ligand LHG D 408



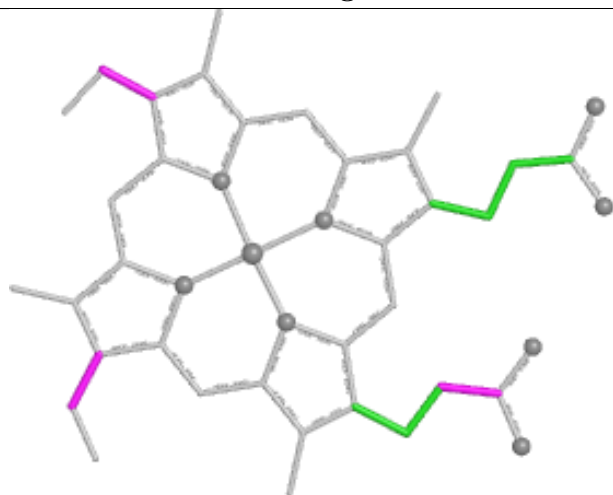
Ligand HEC v 201



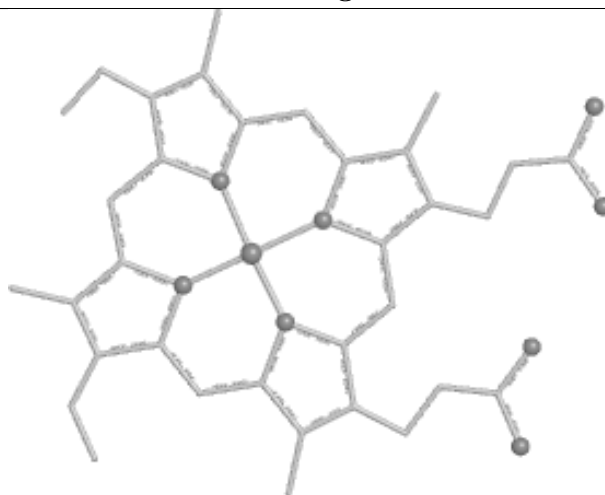
Bond lengths



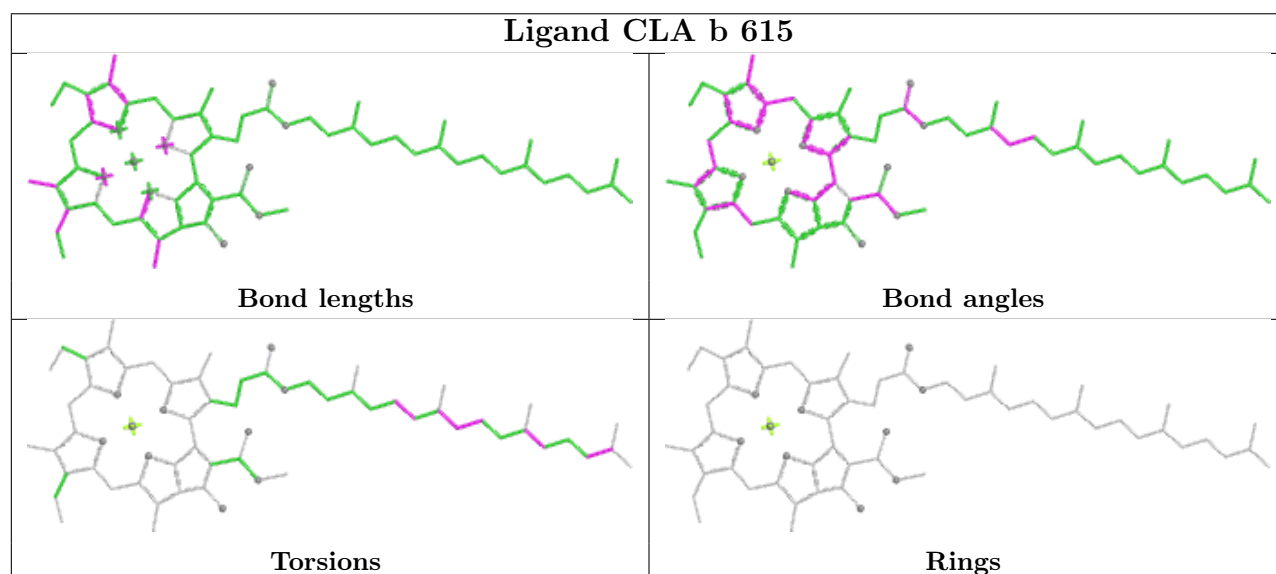
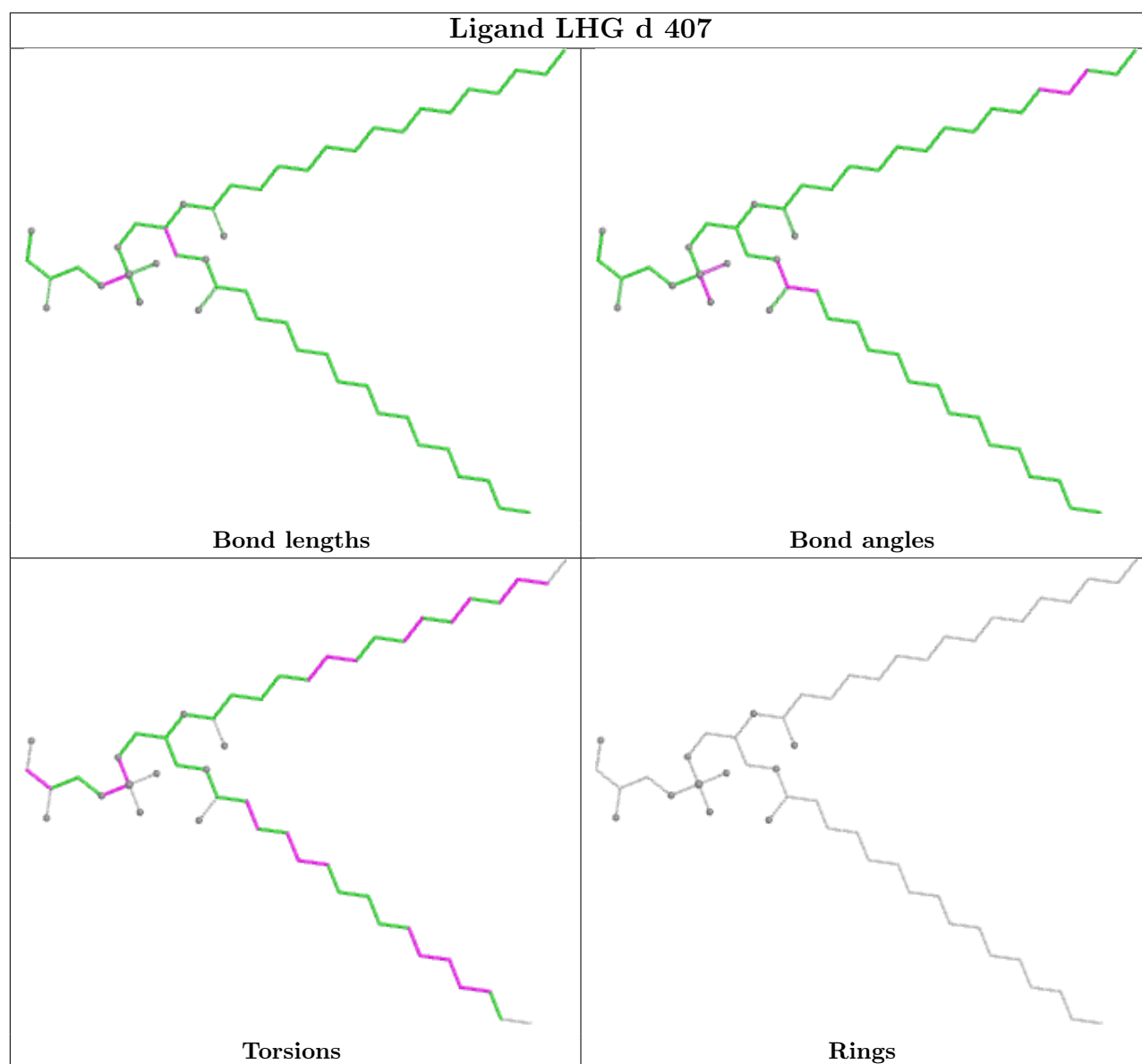
Bond angles

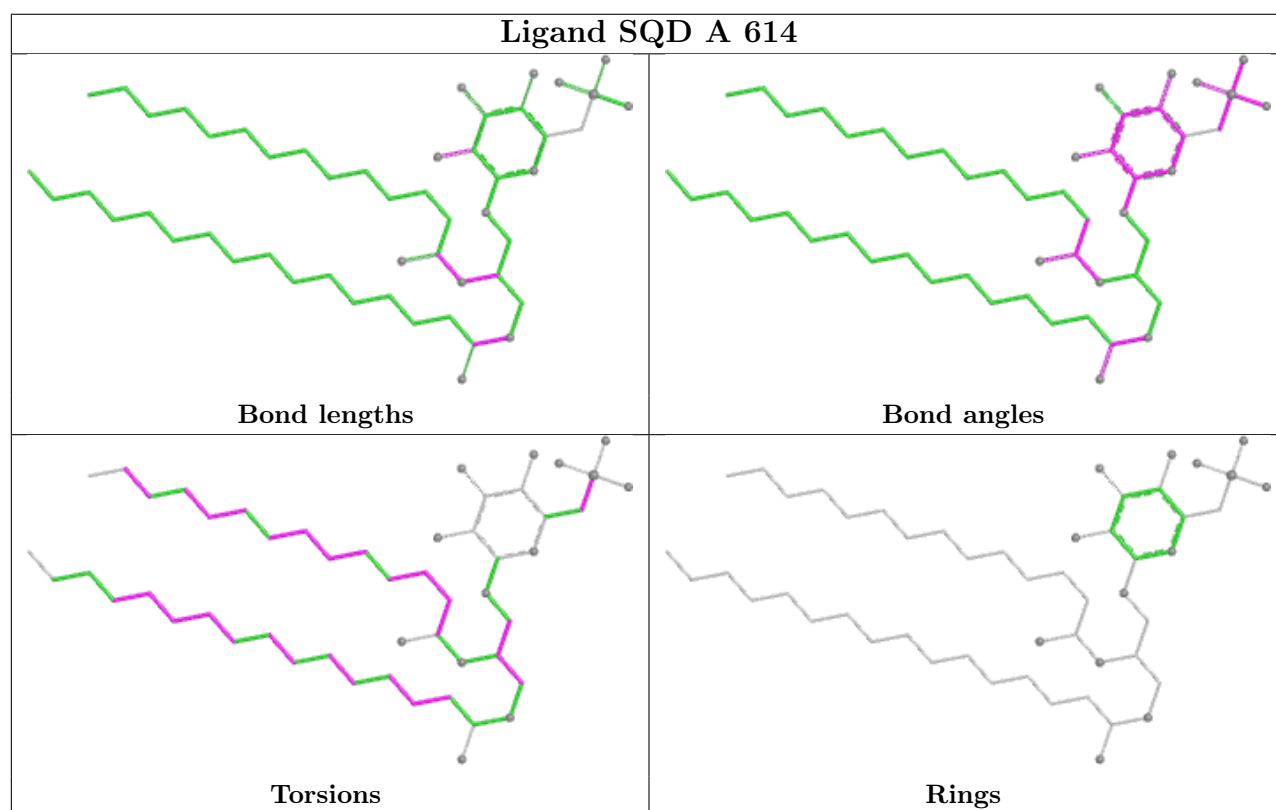
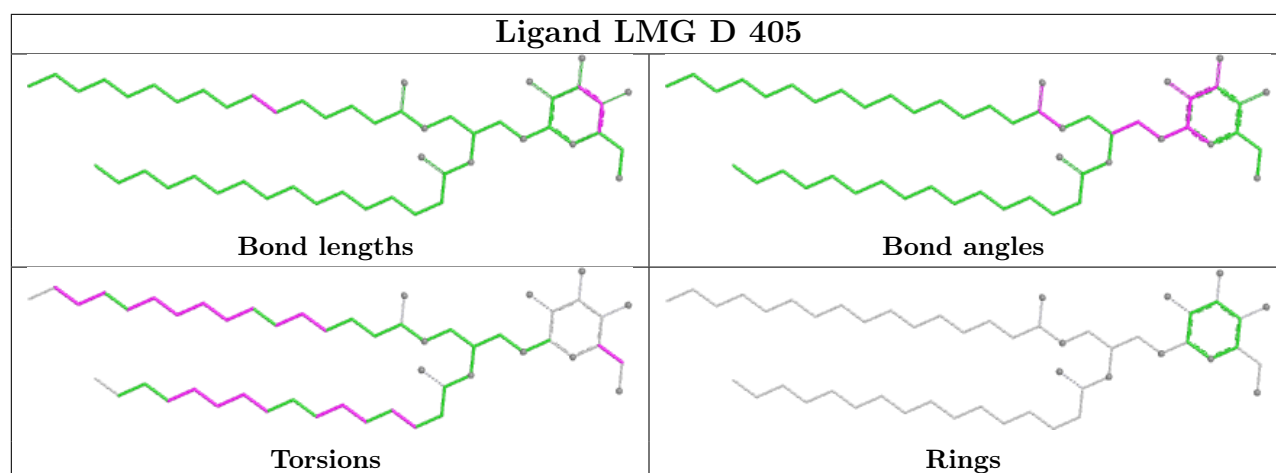


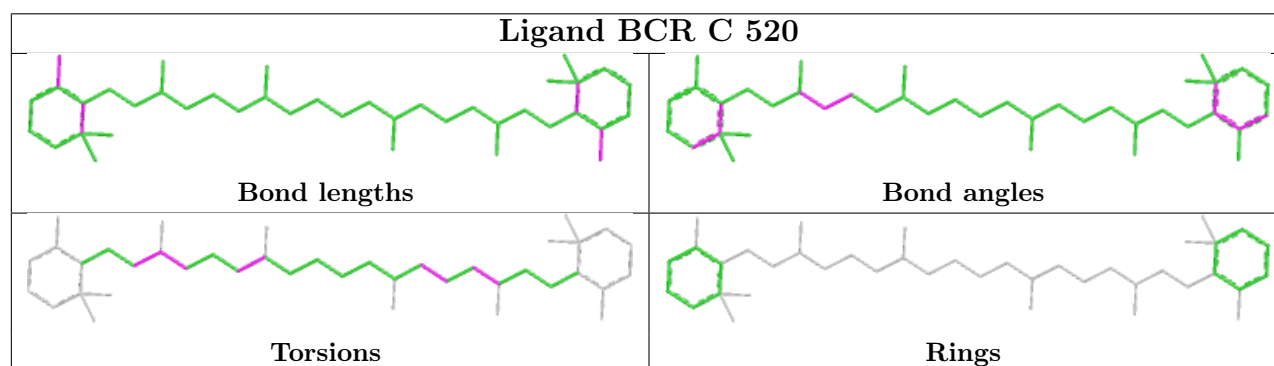
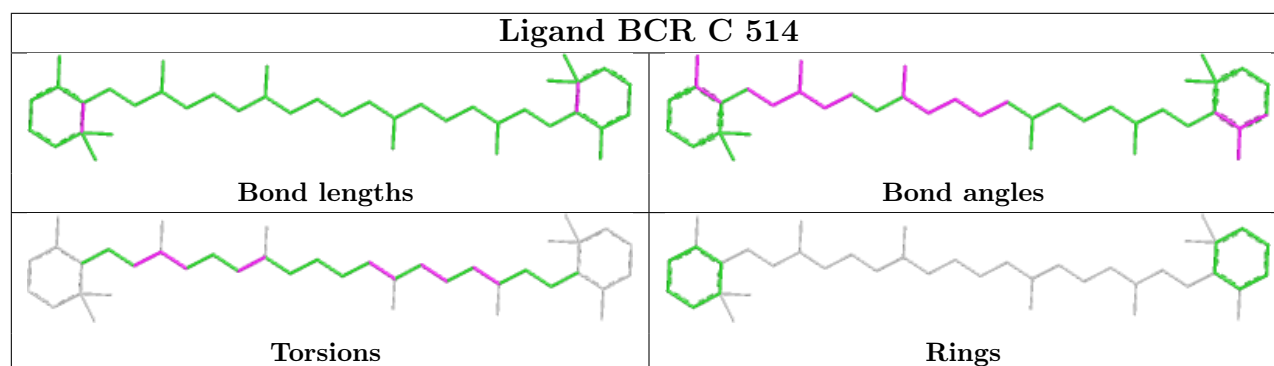
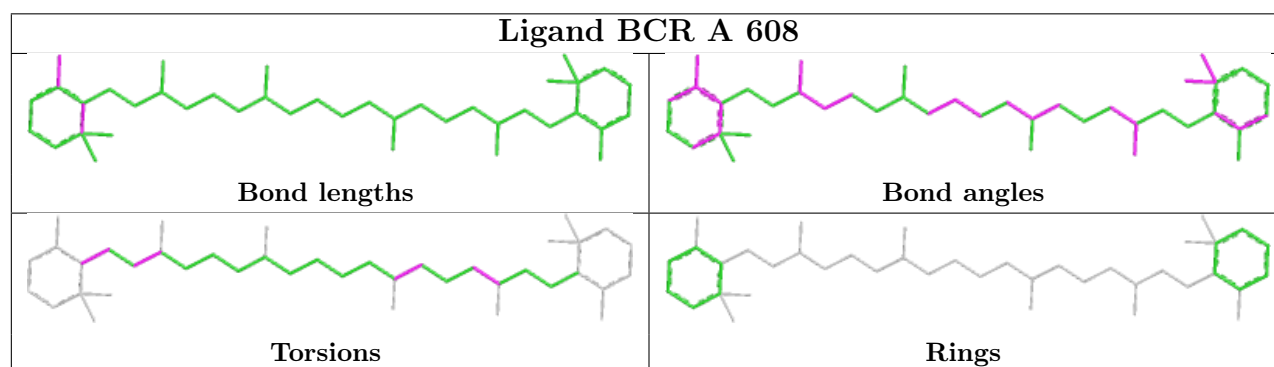
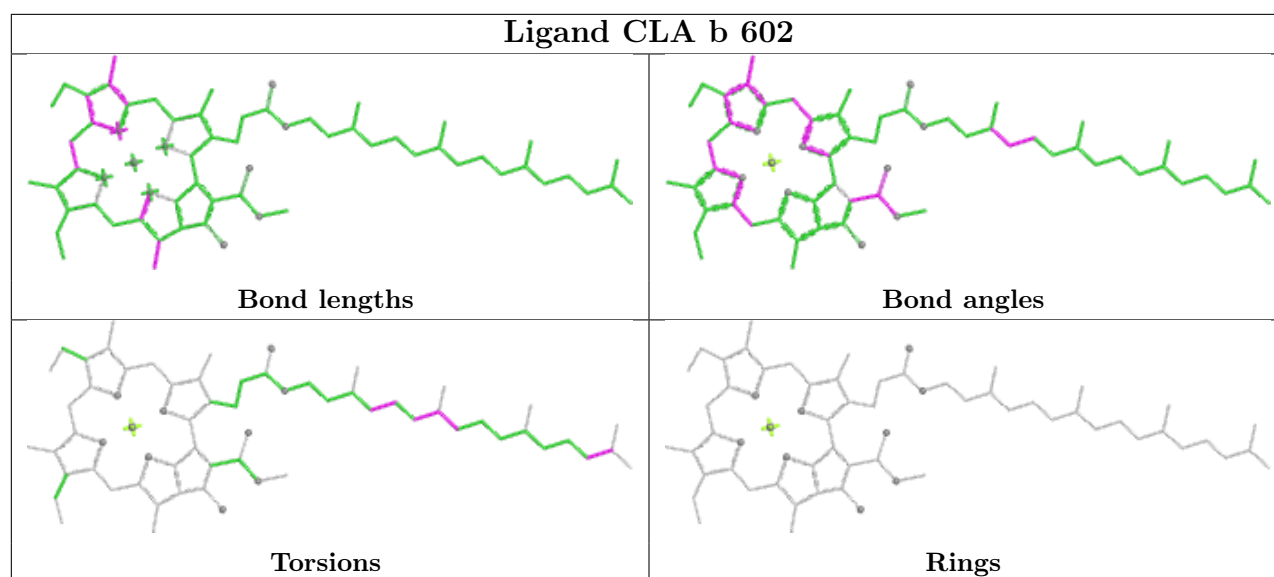
Torsions

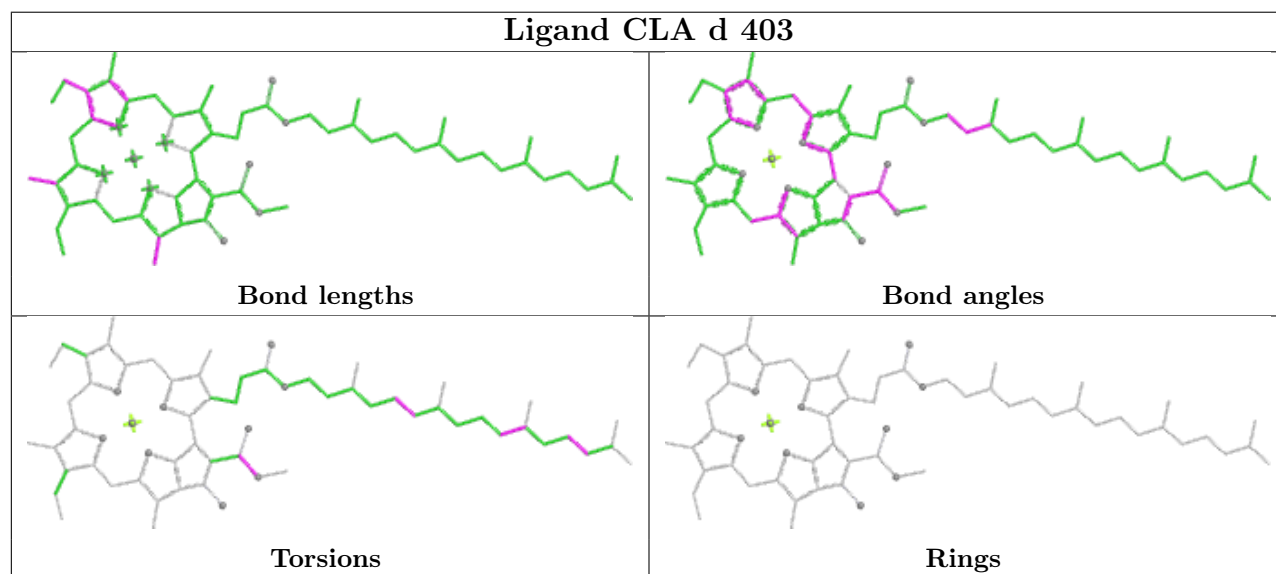
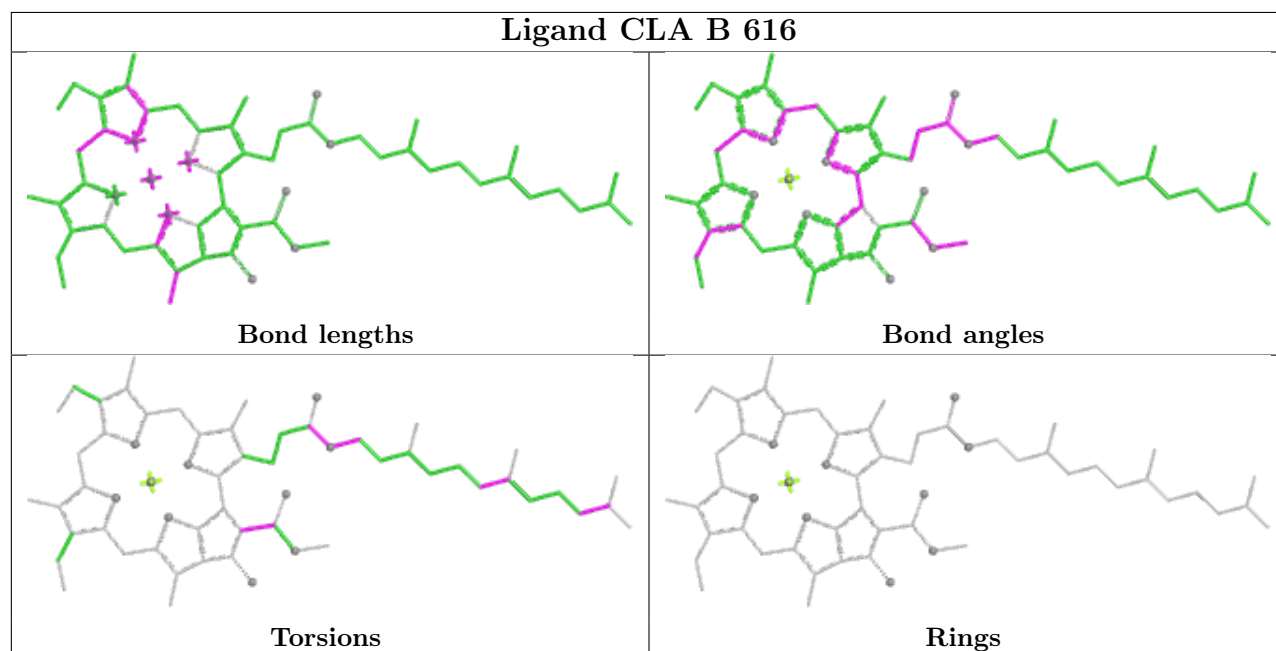
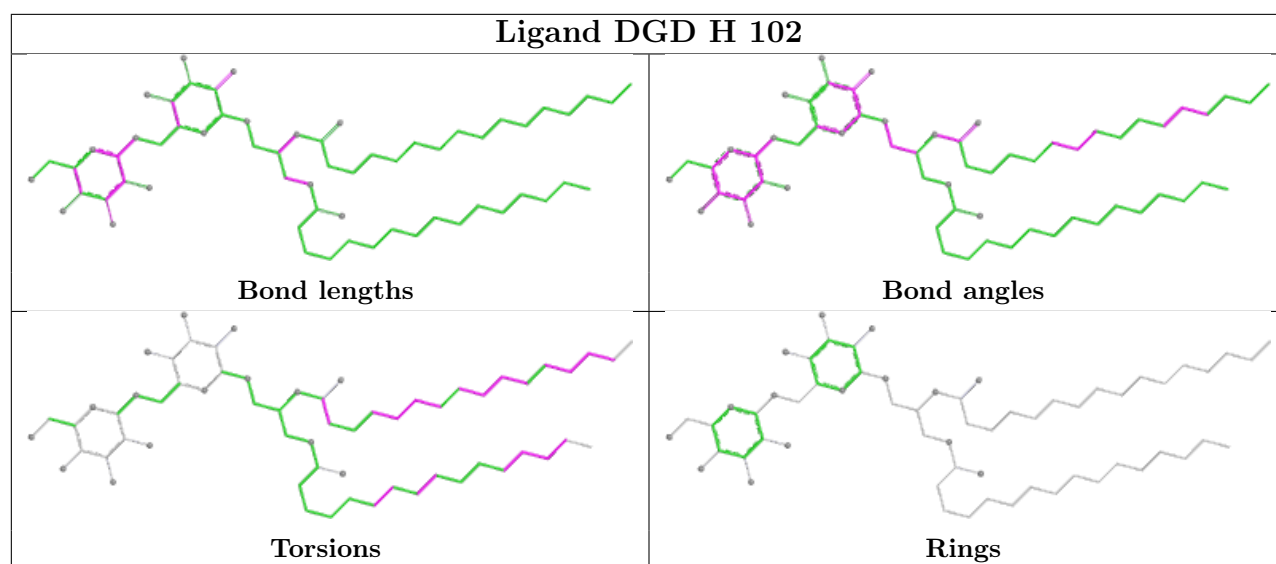


Rings

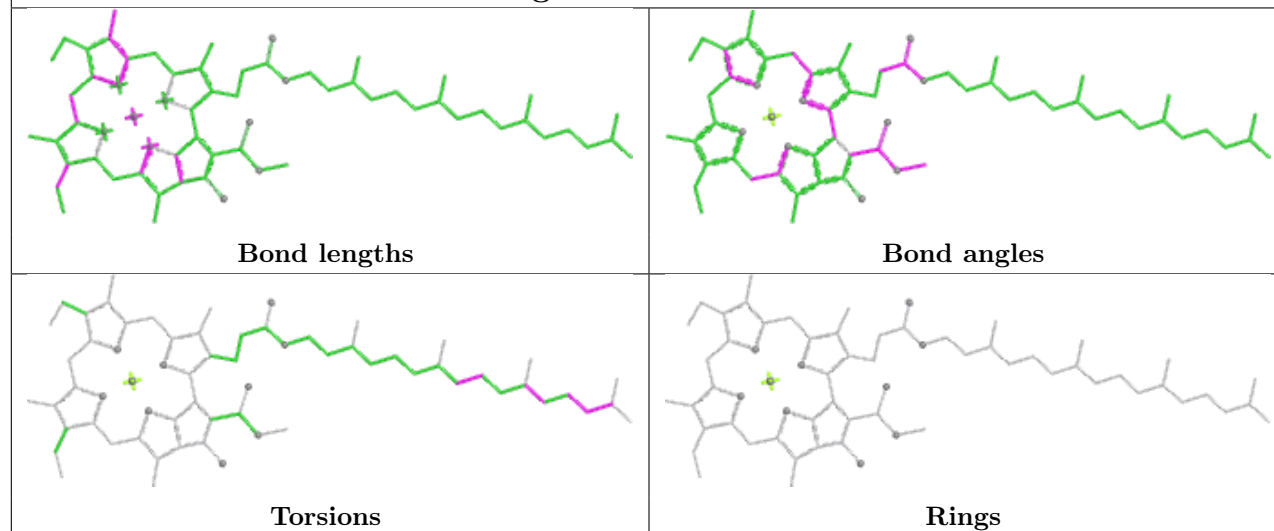




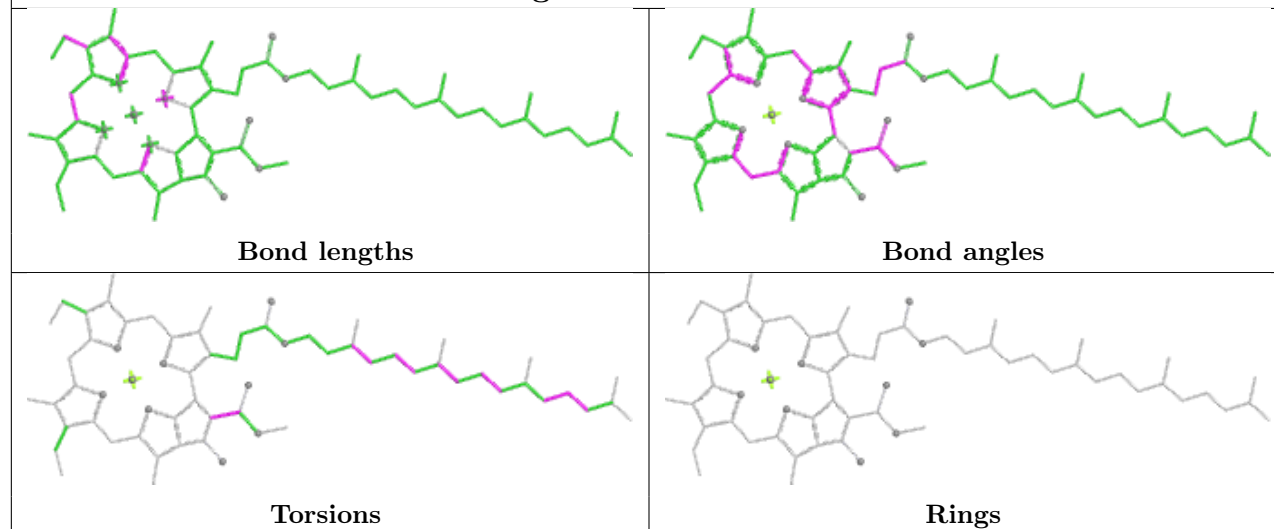




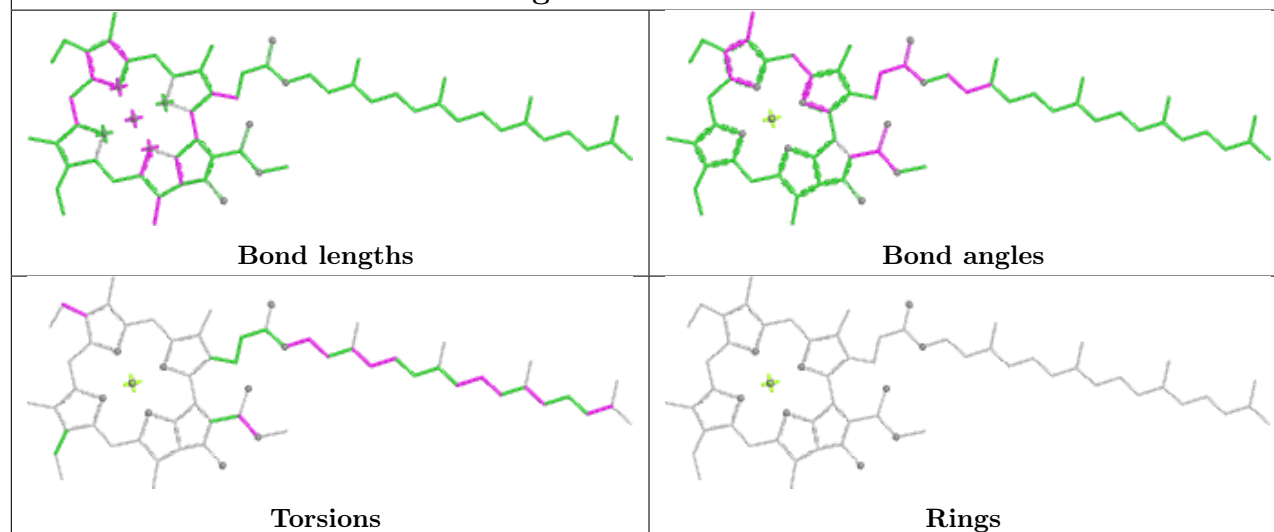
Ligand CLA B 610

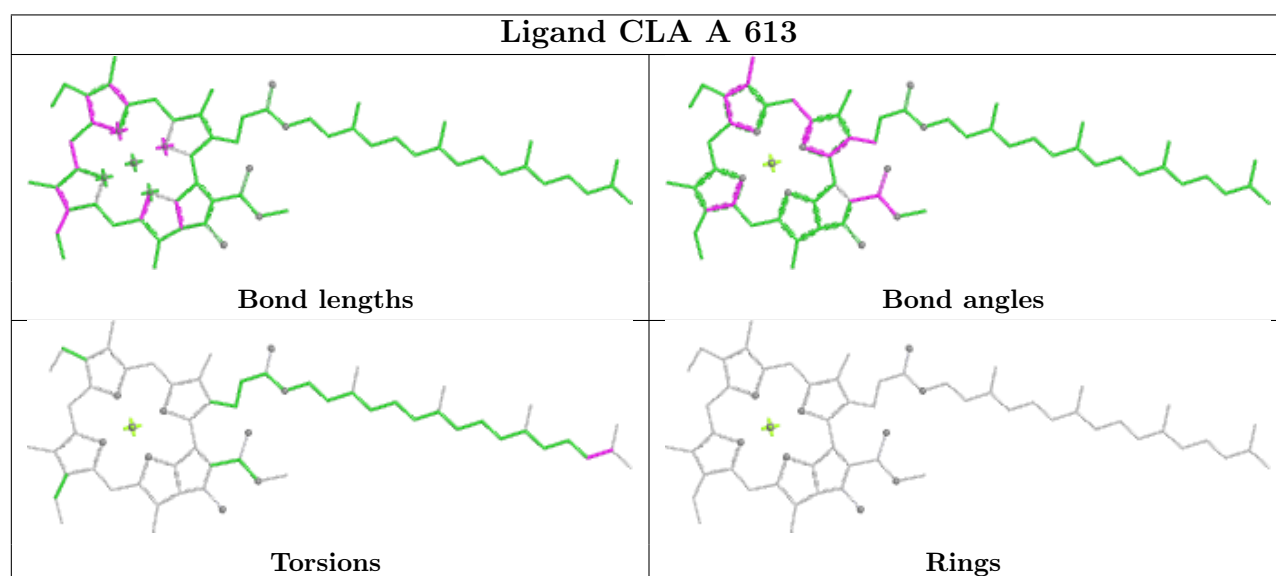
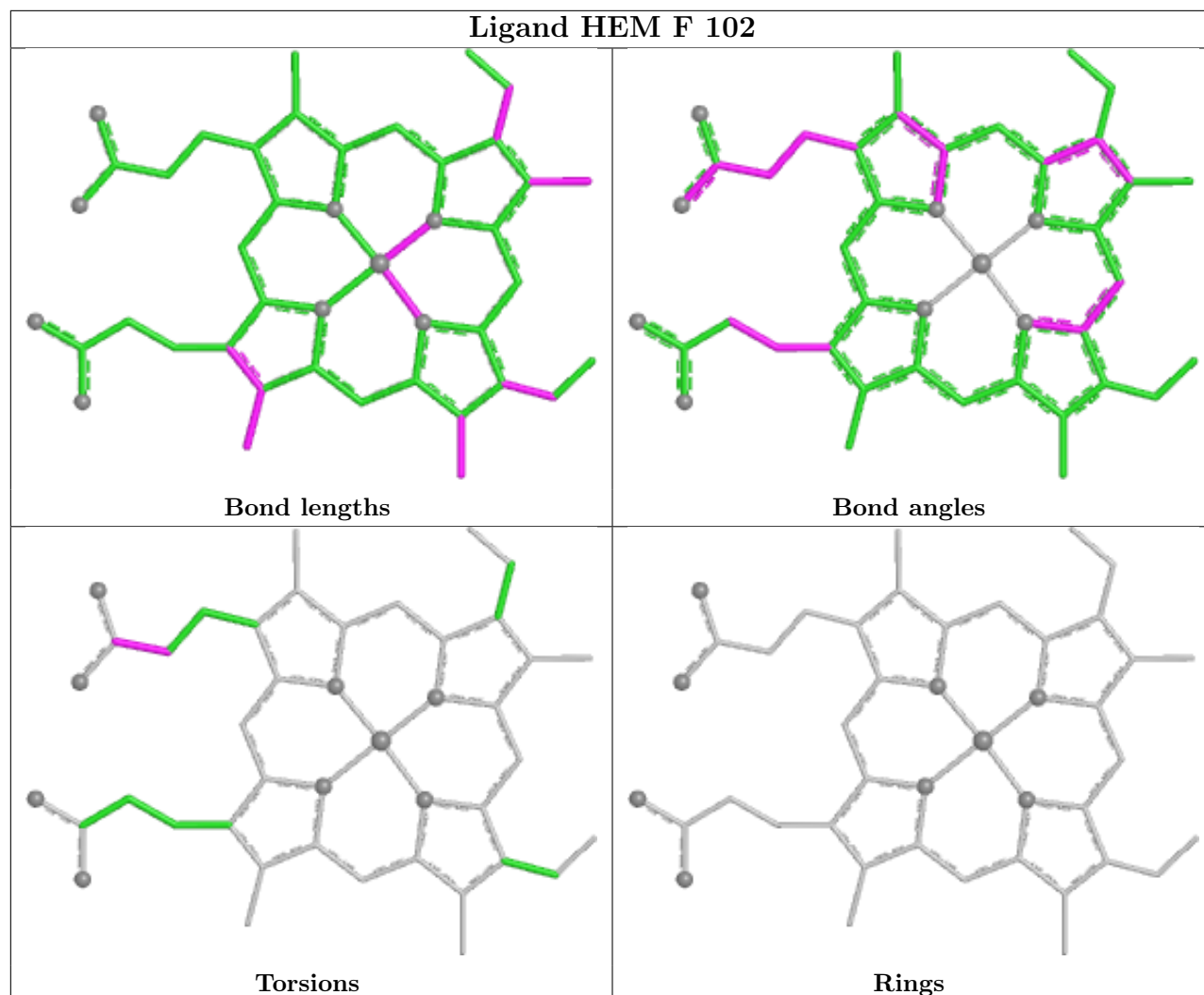


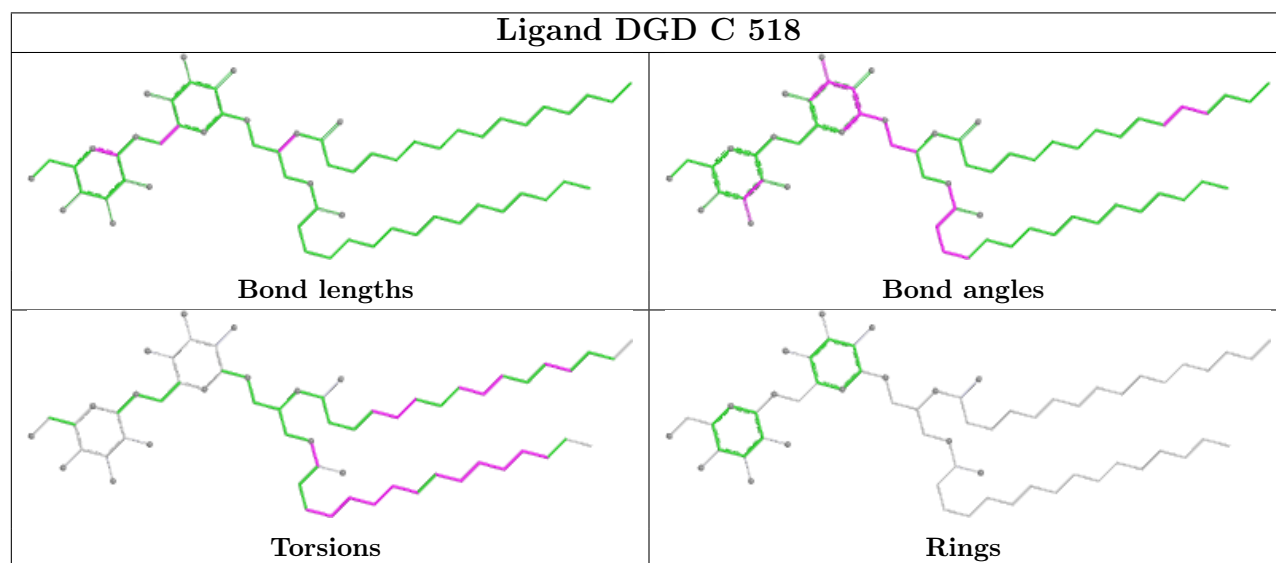
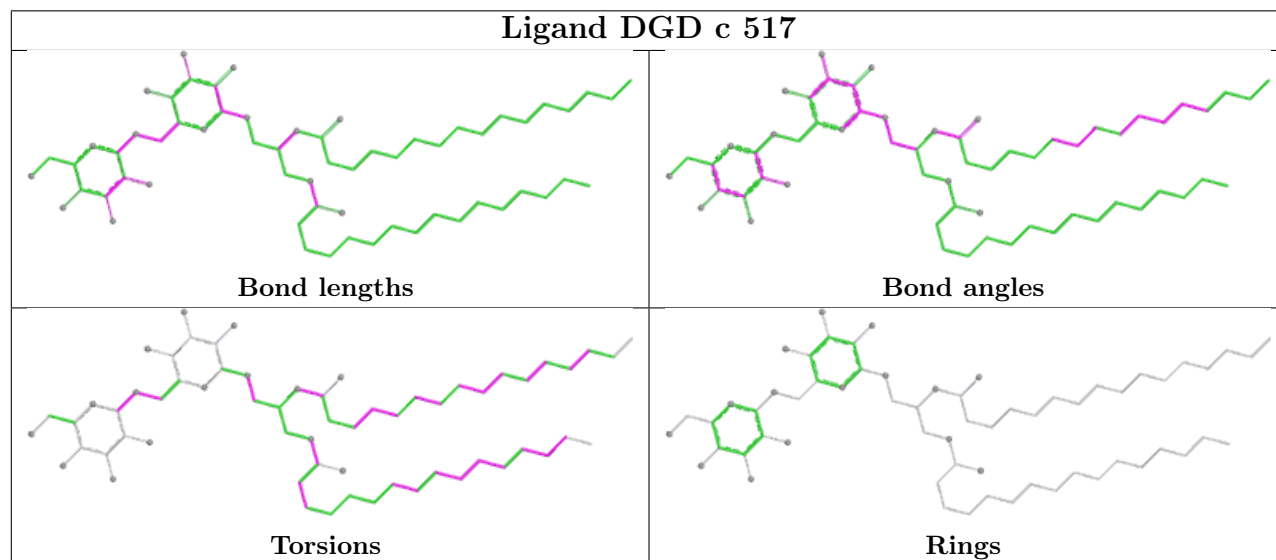
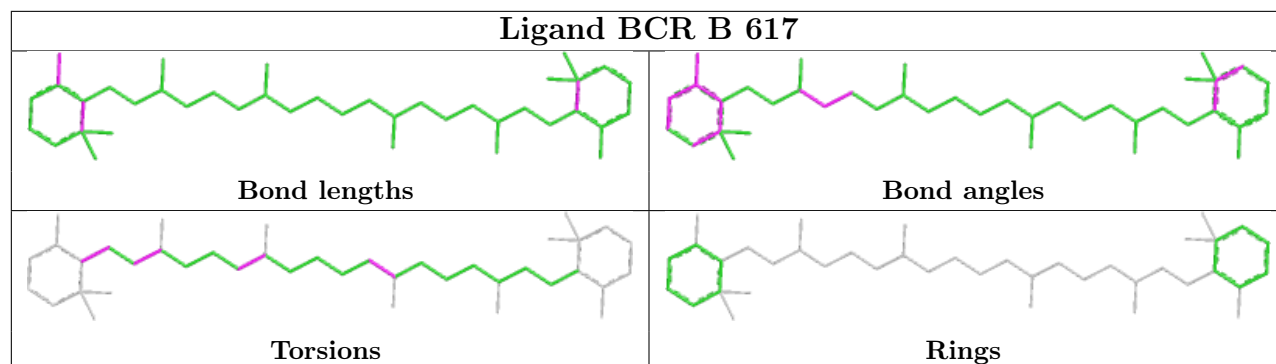
Ligand CLA C 507

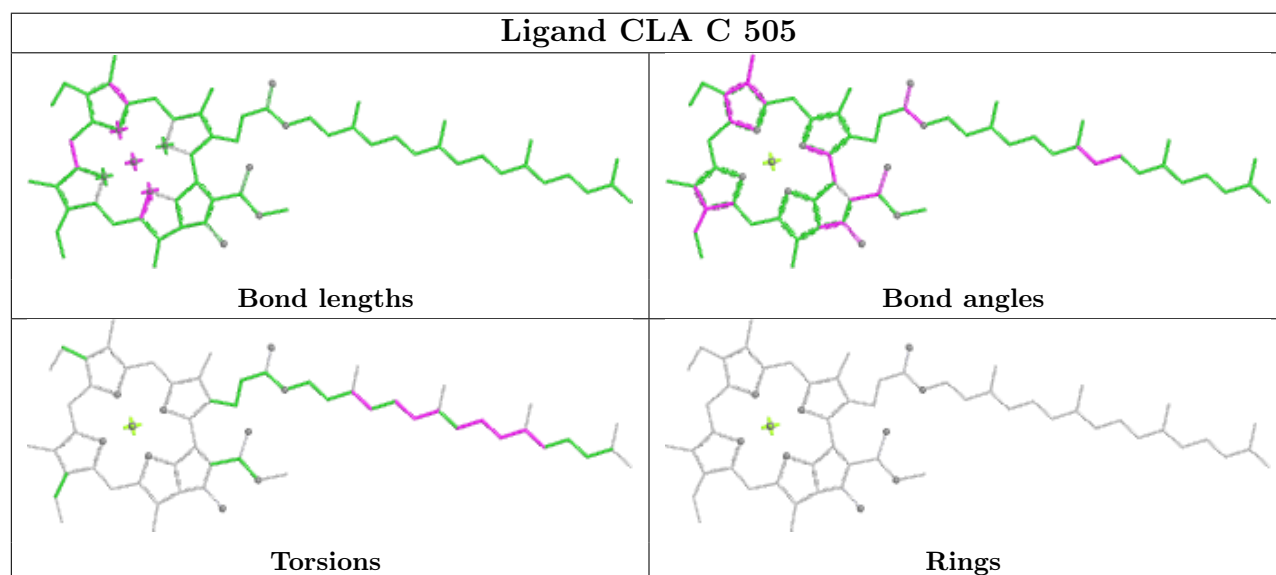
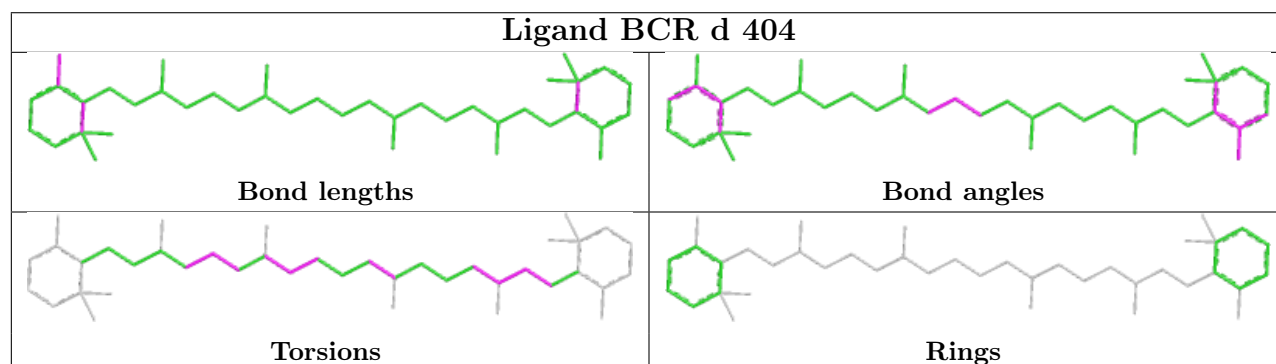
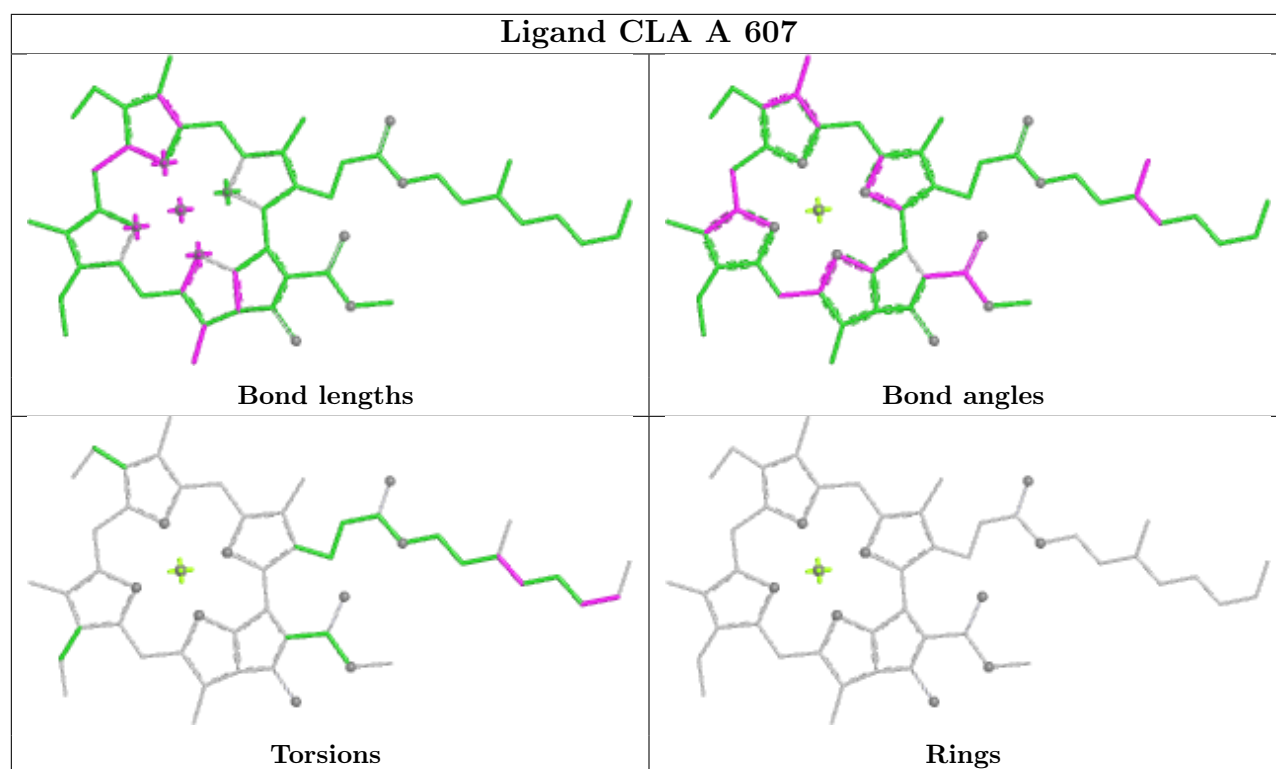


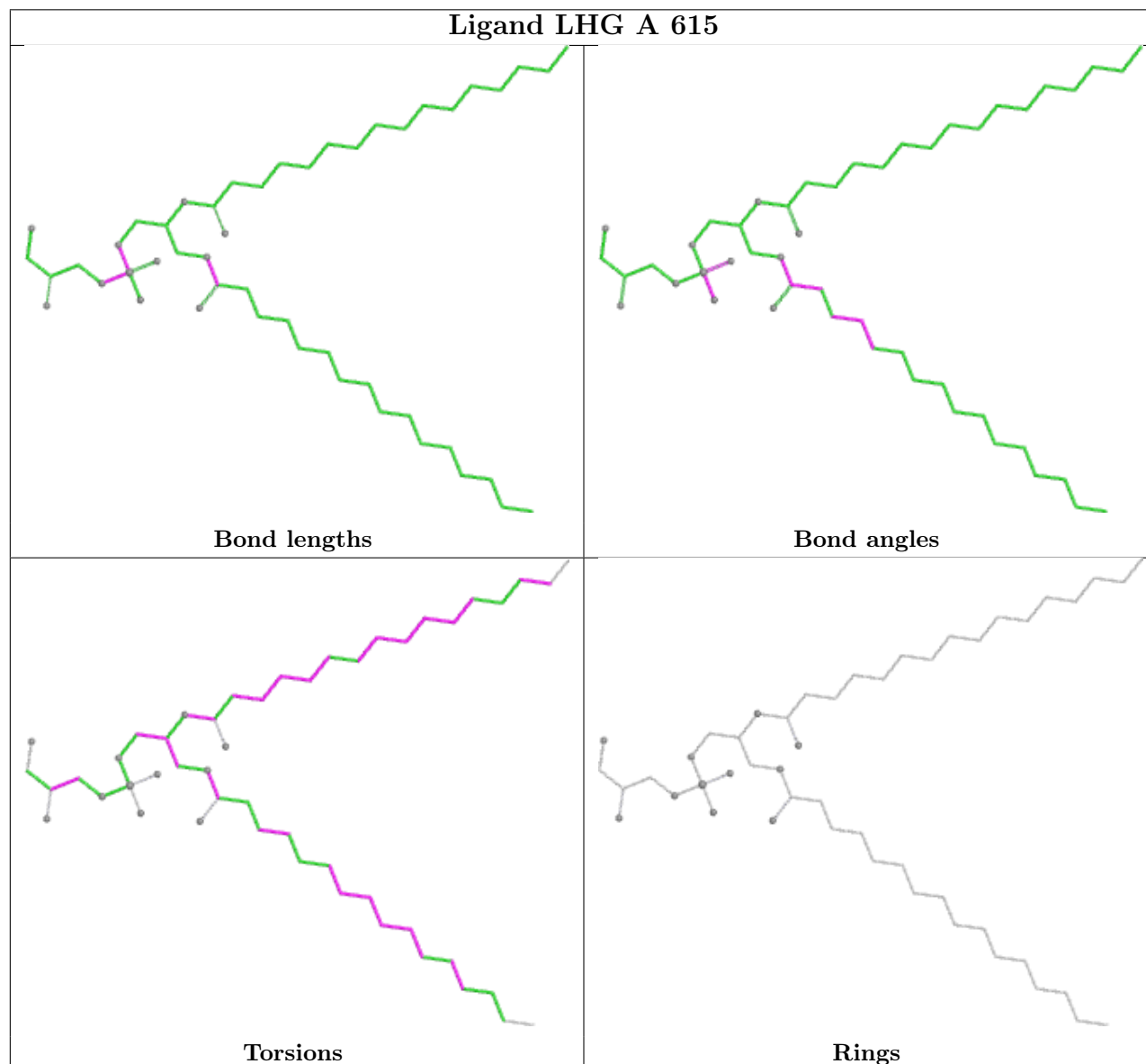
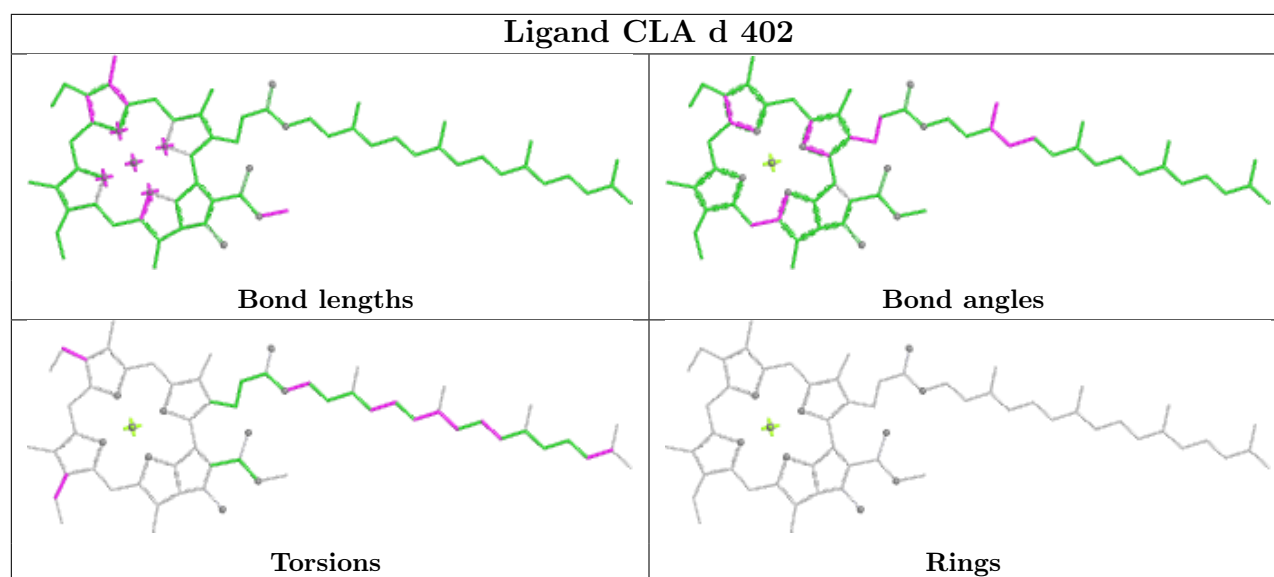
Ligand CLA C 512

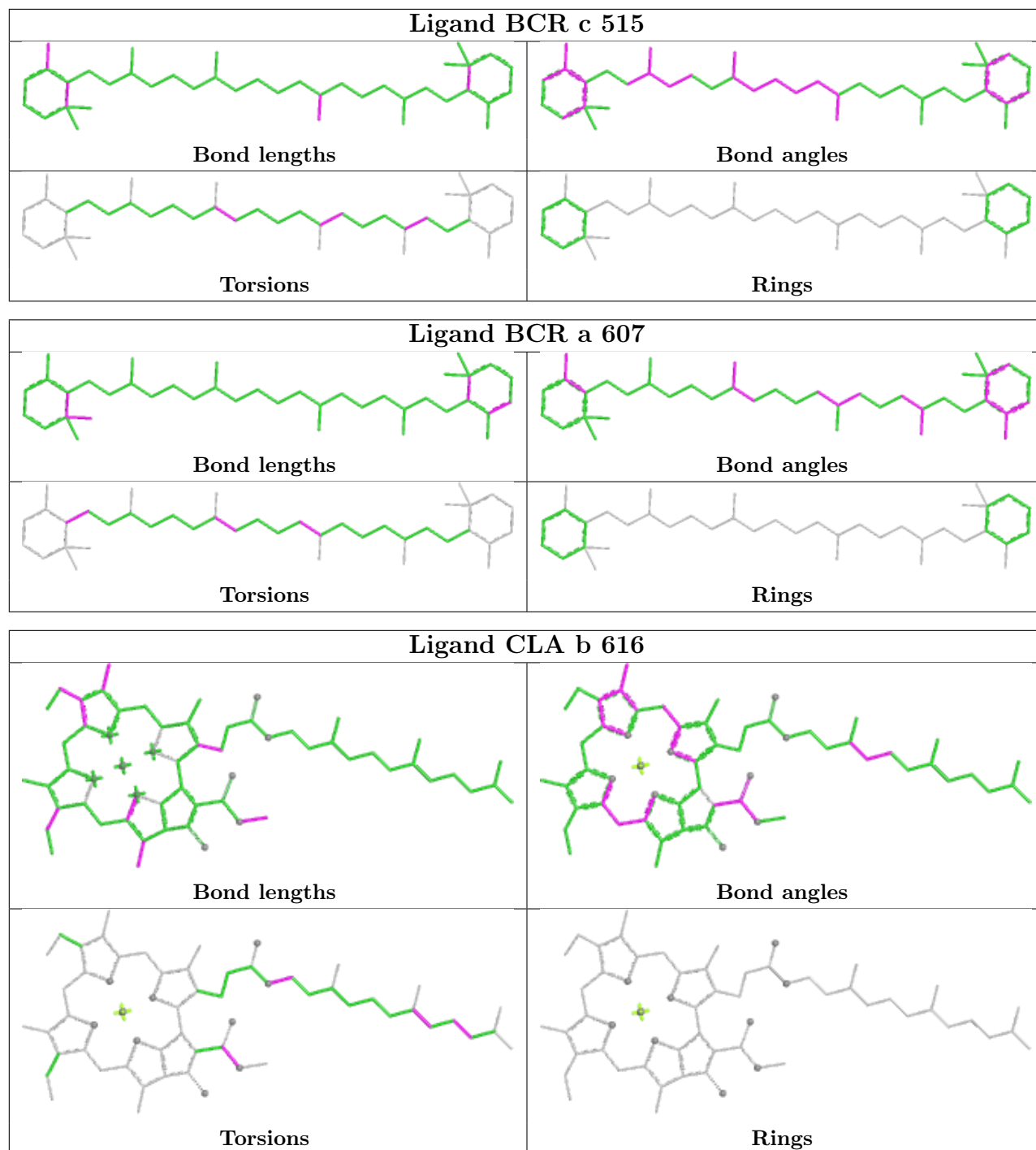


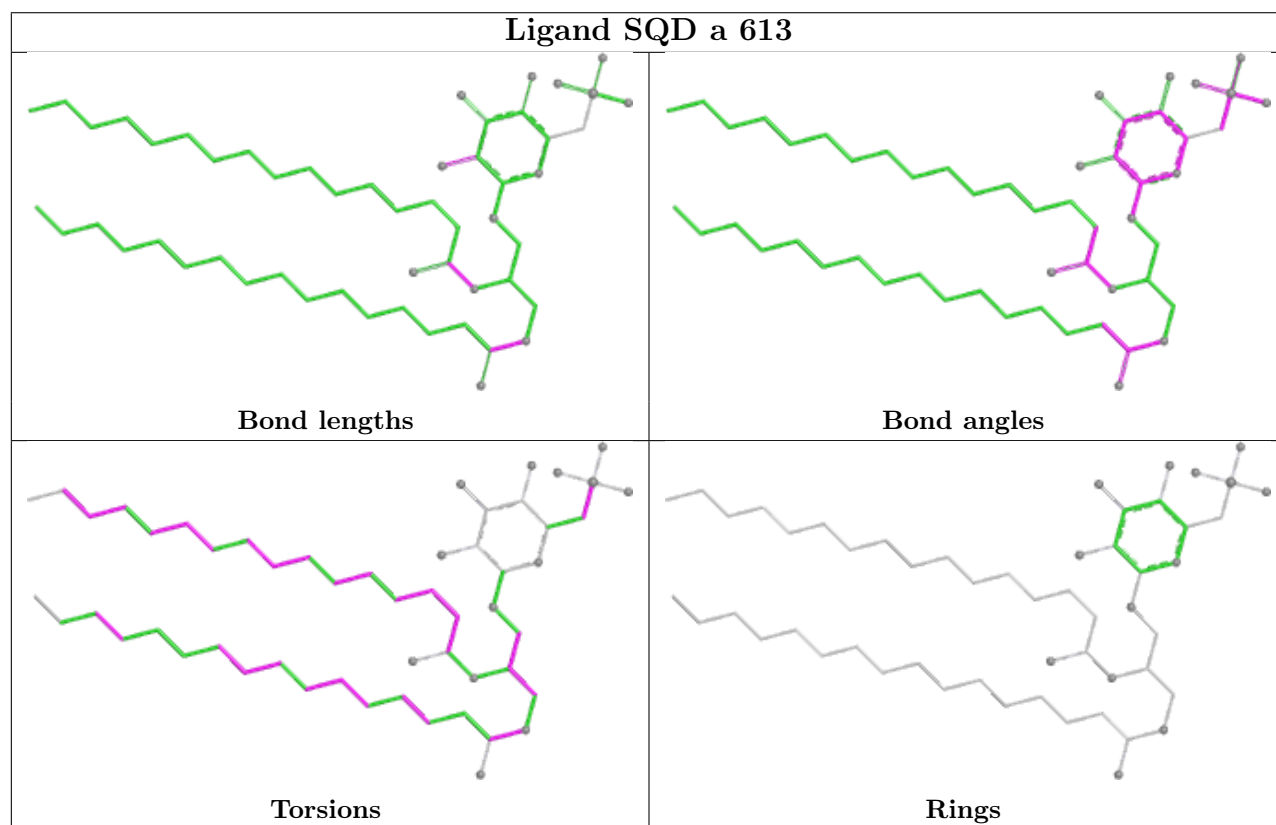
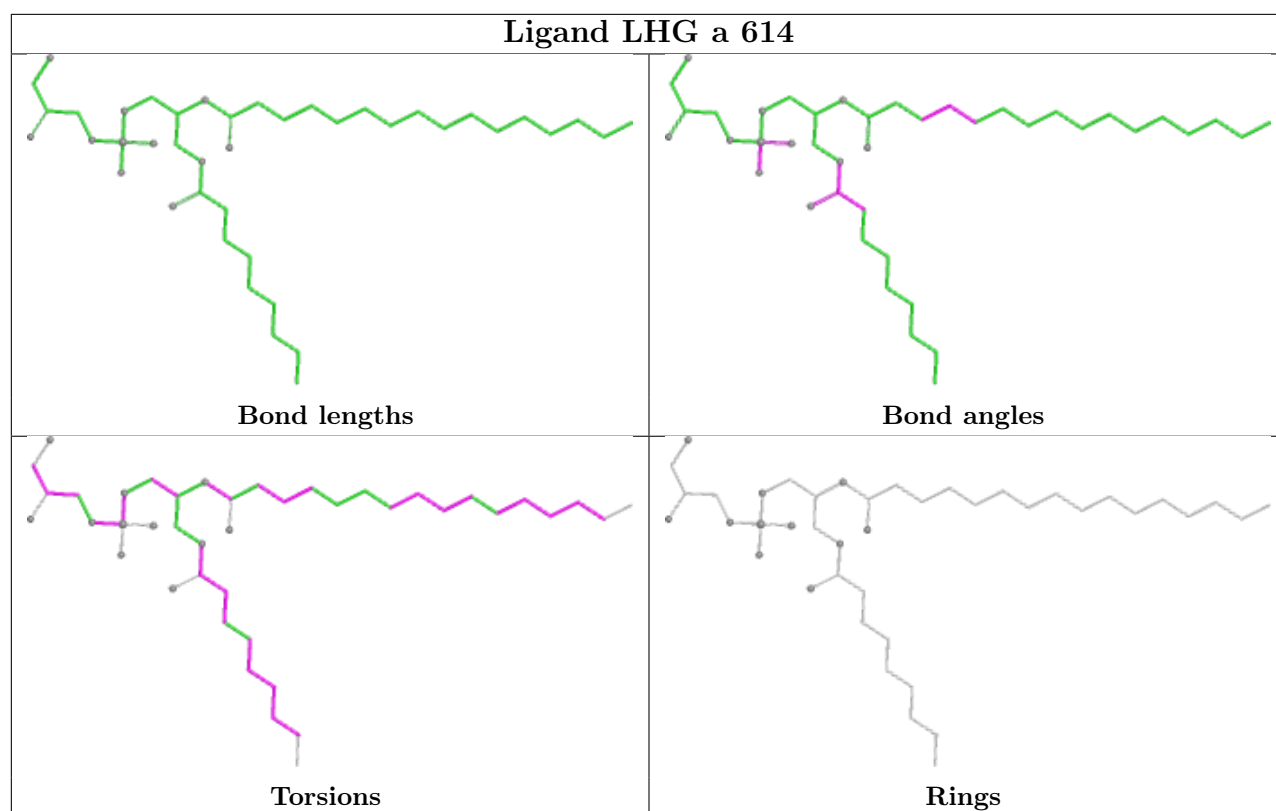


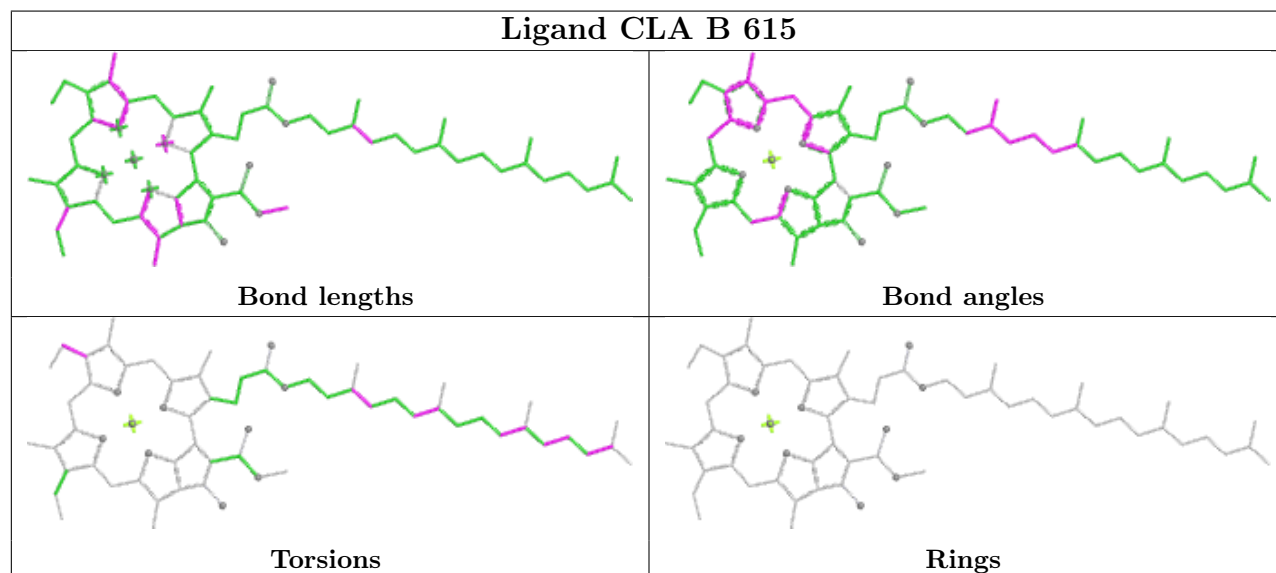
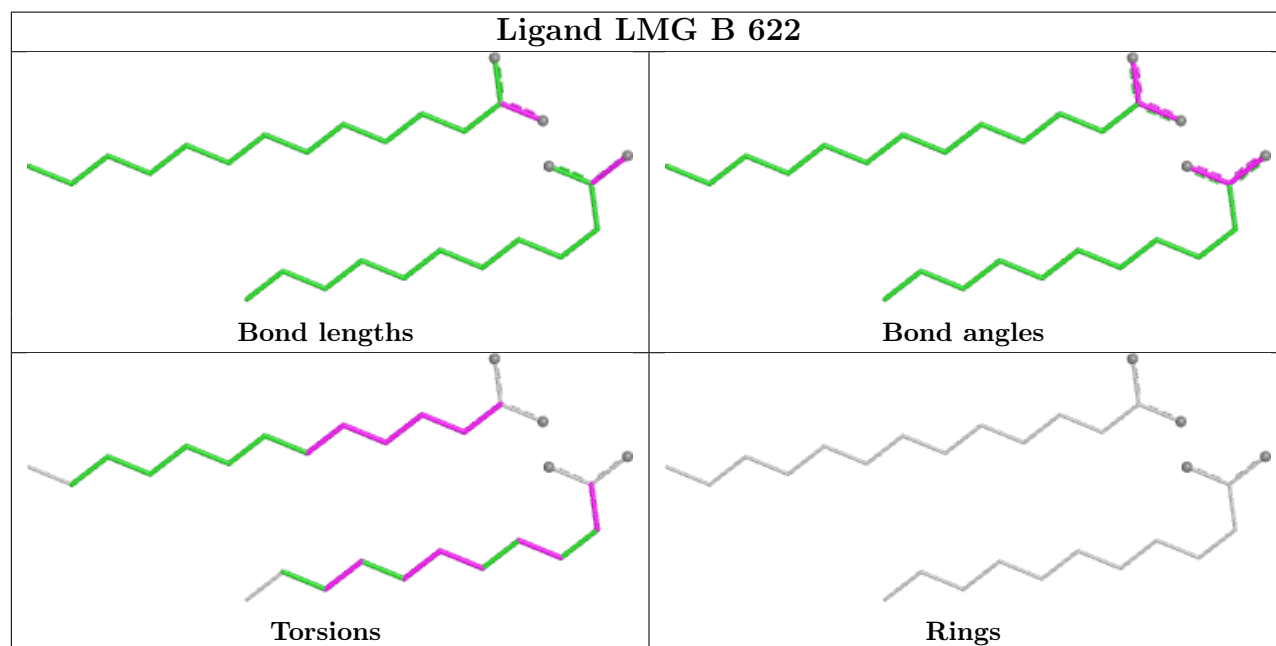
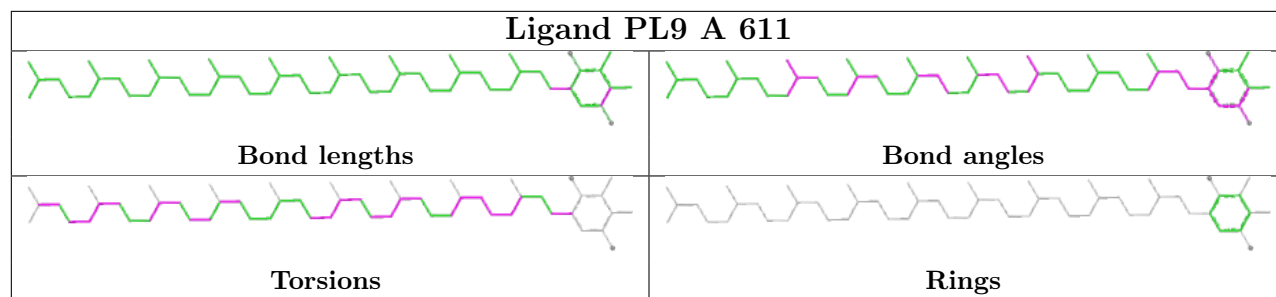


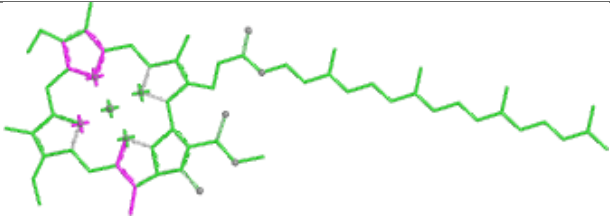
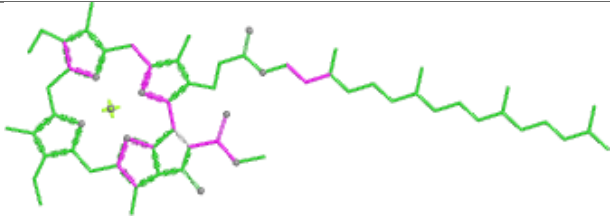
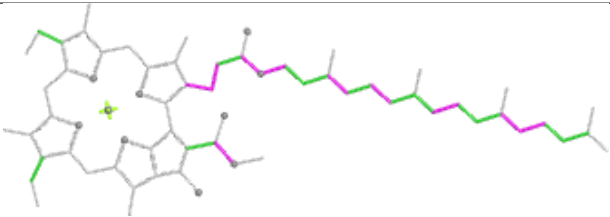
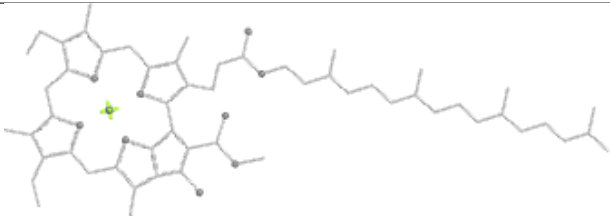
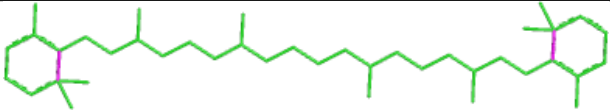
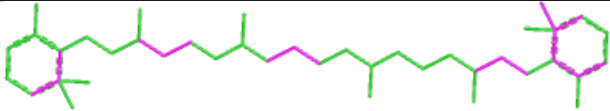
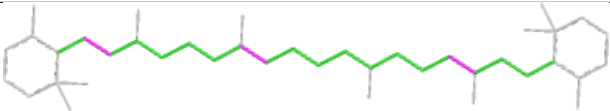
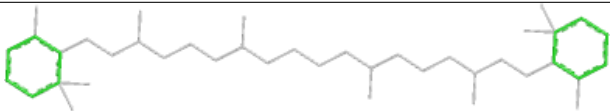
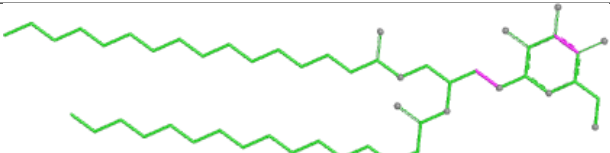
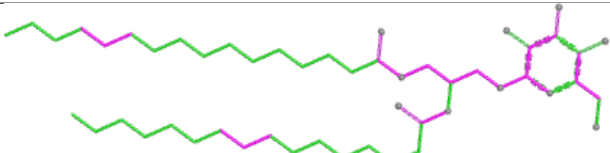
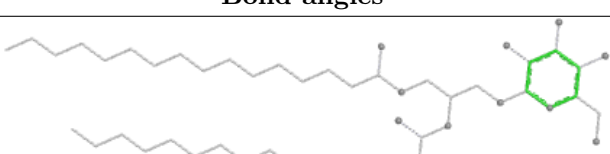




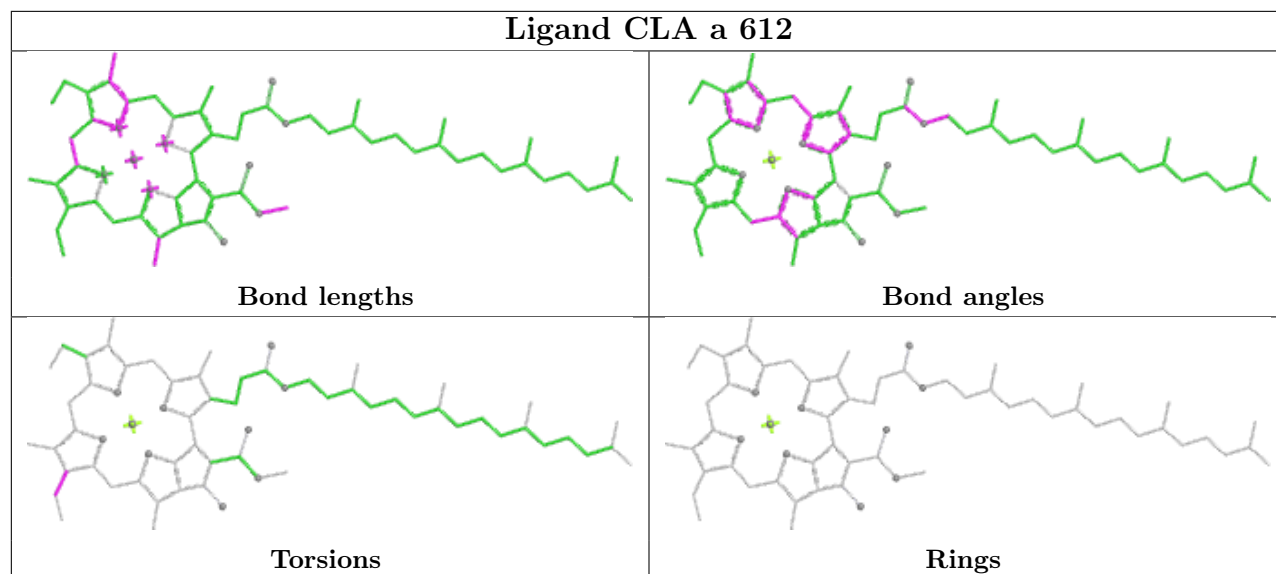




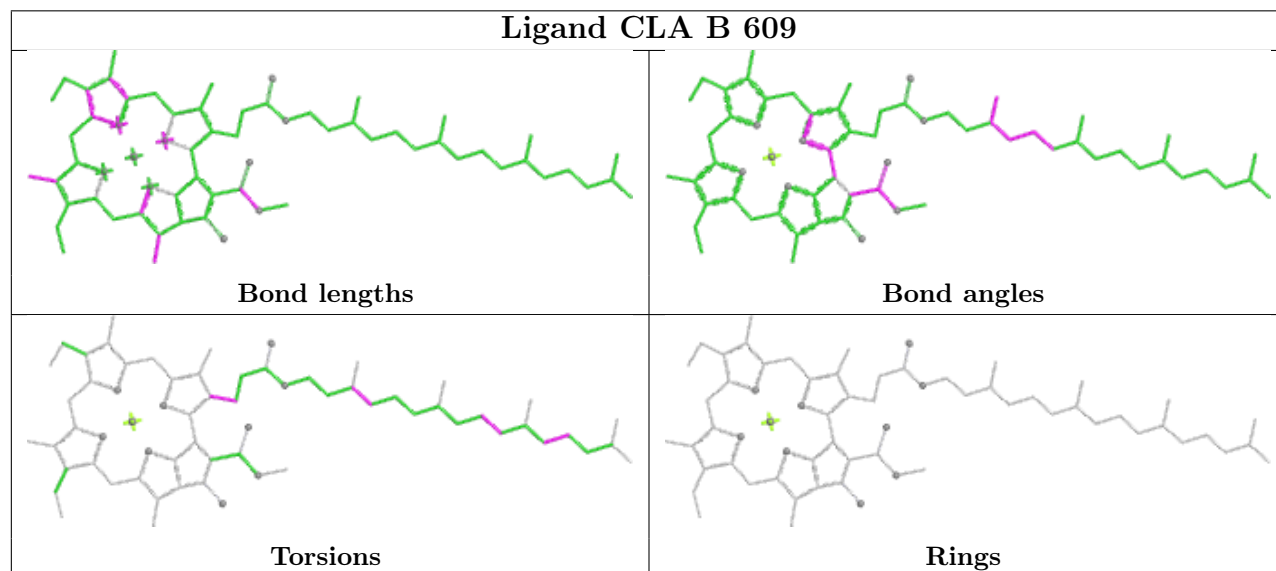


Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

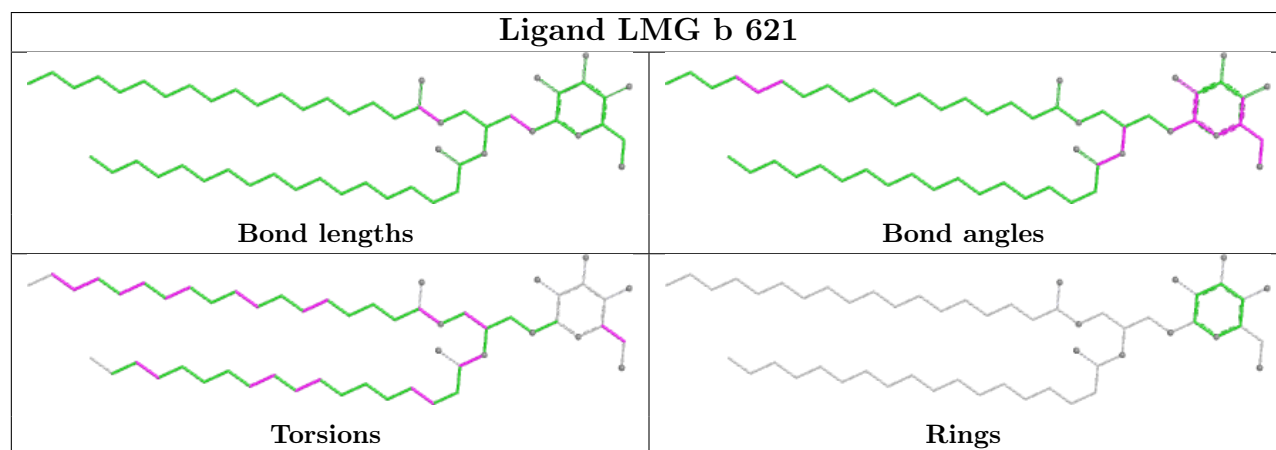
Ligand CLA a 612

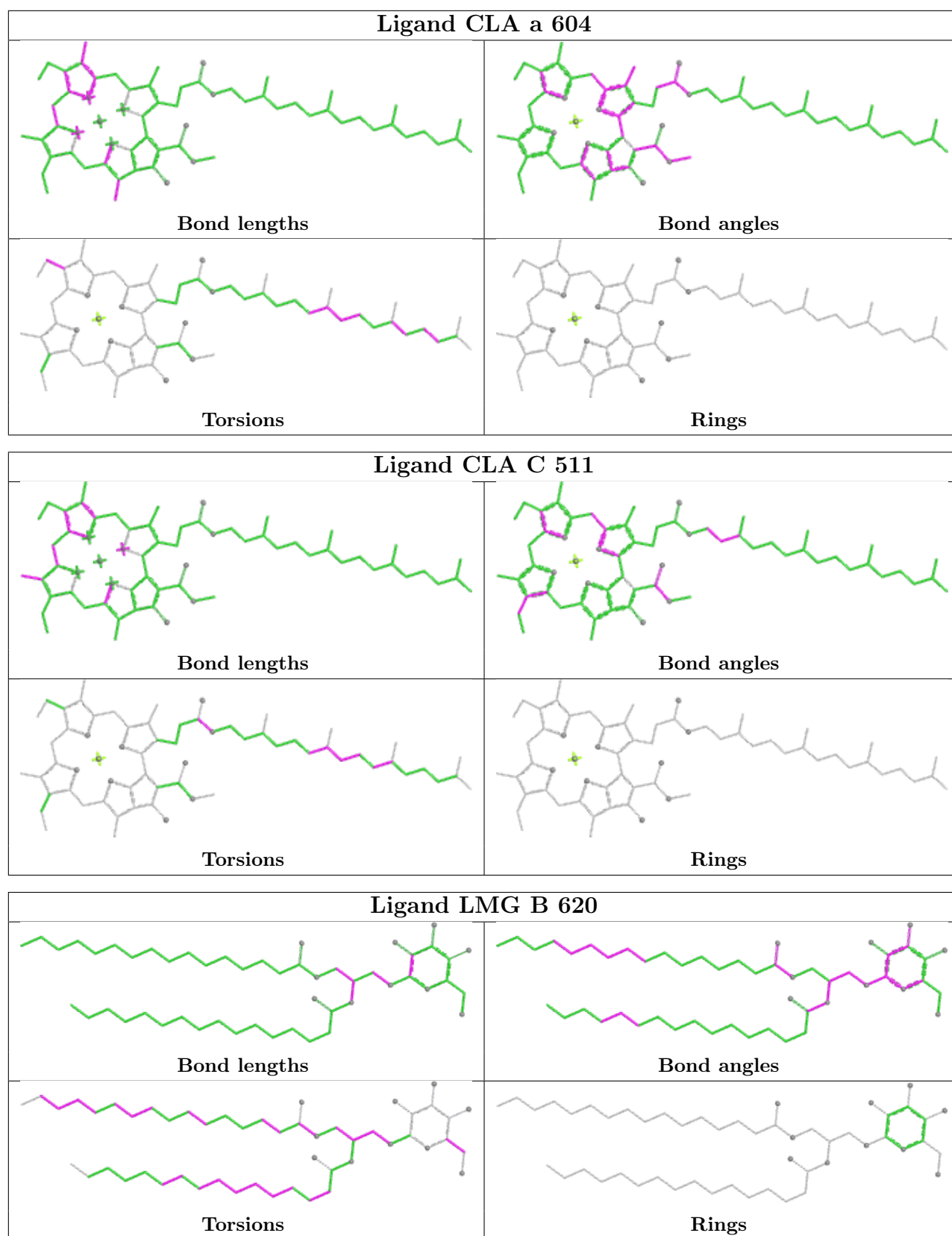


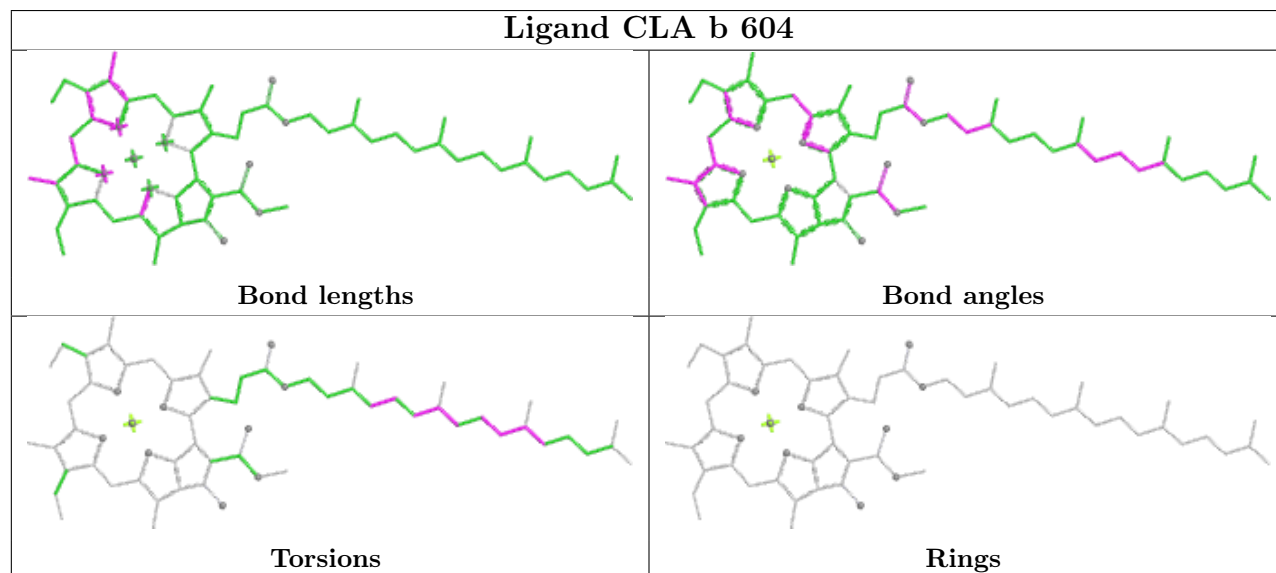
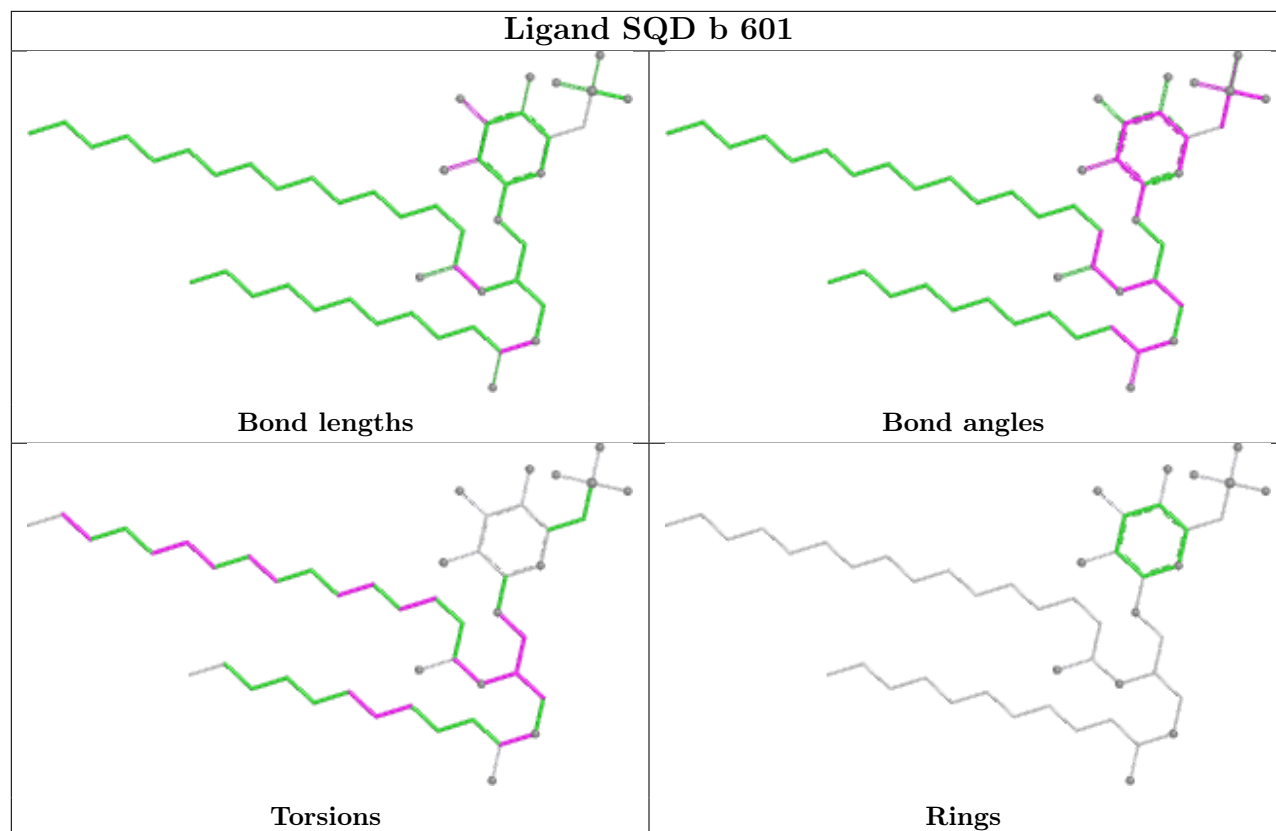
Ligand CLA B 609

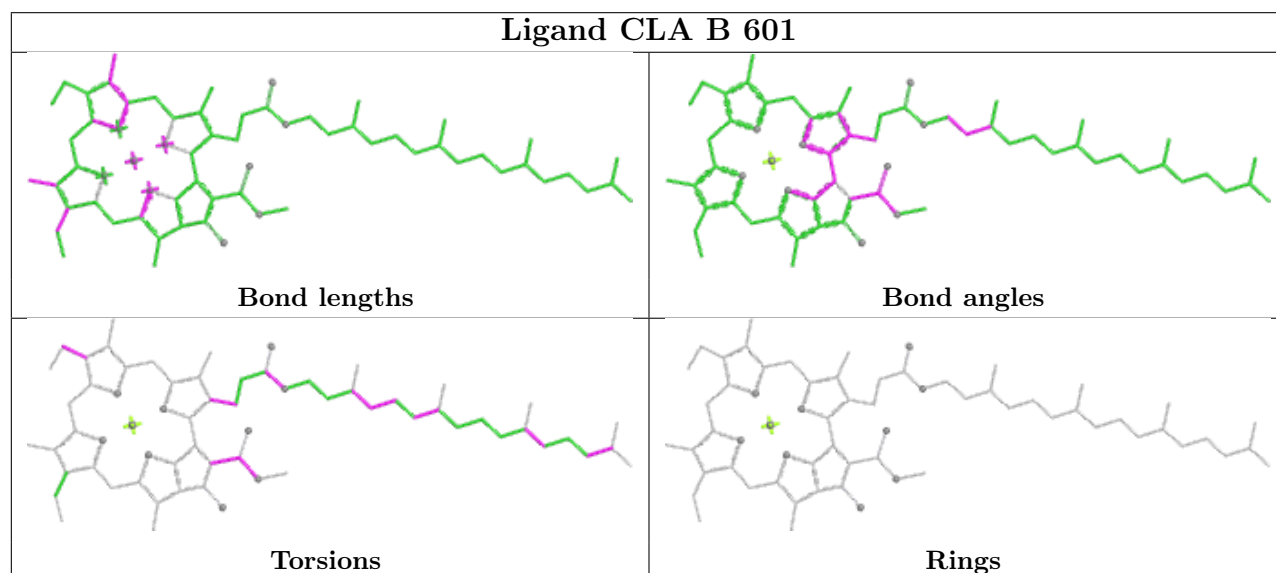
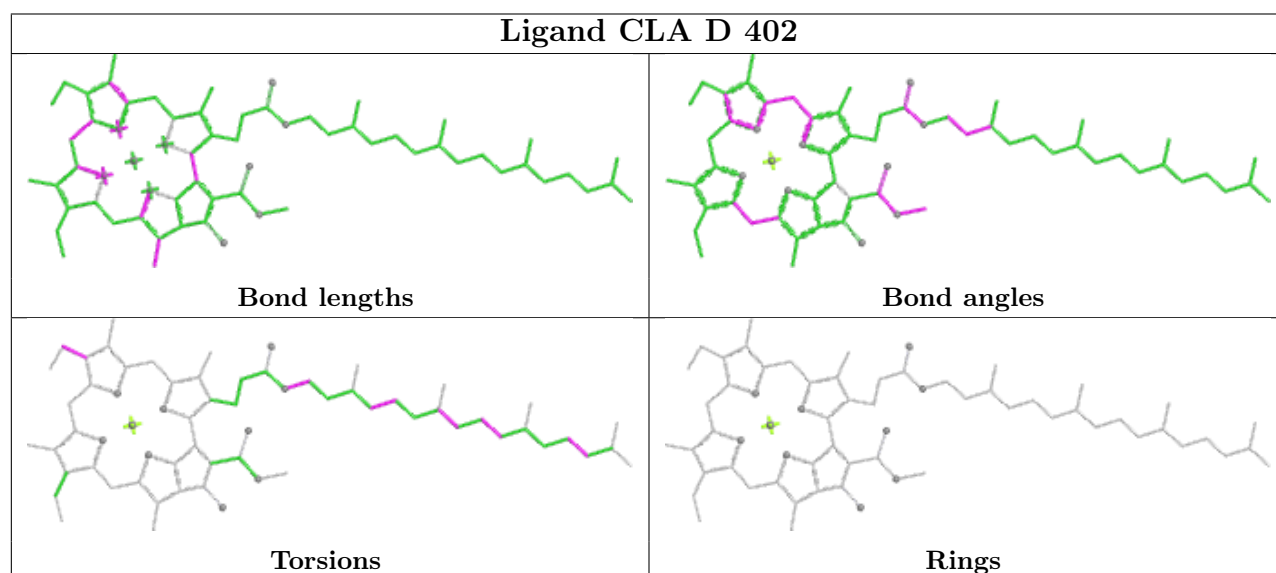
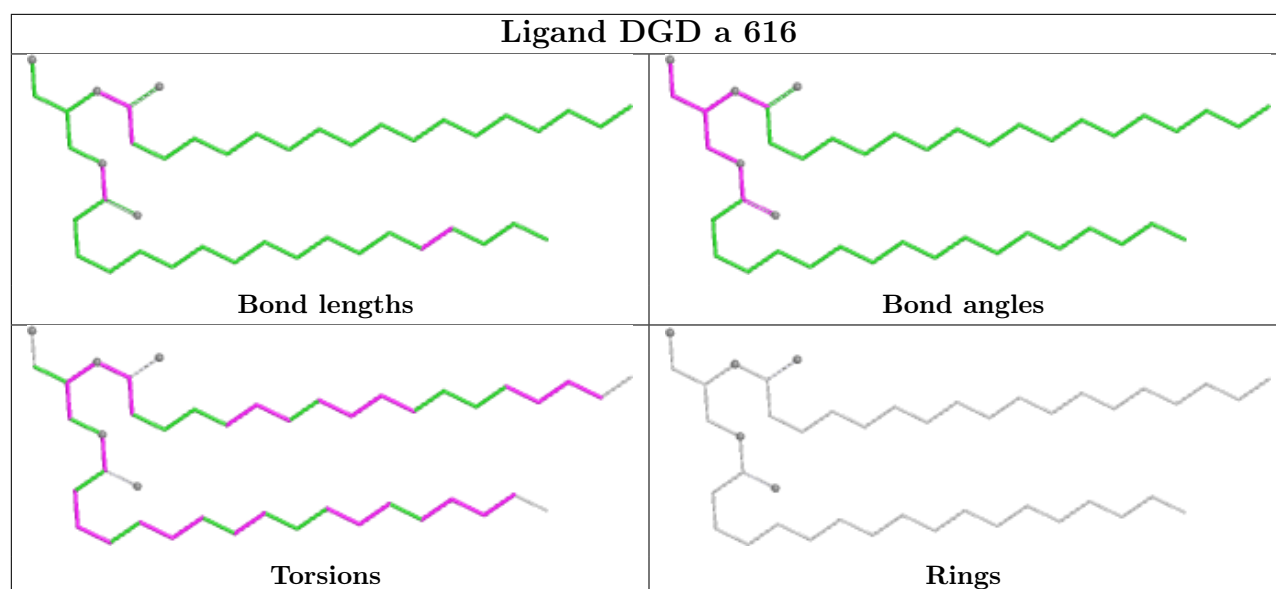


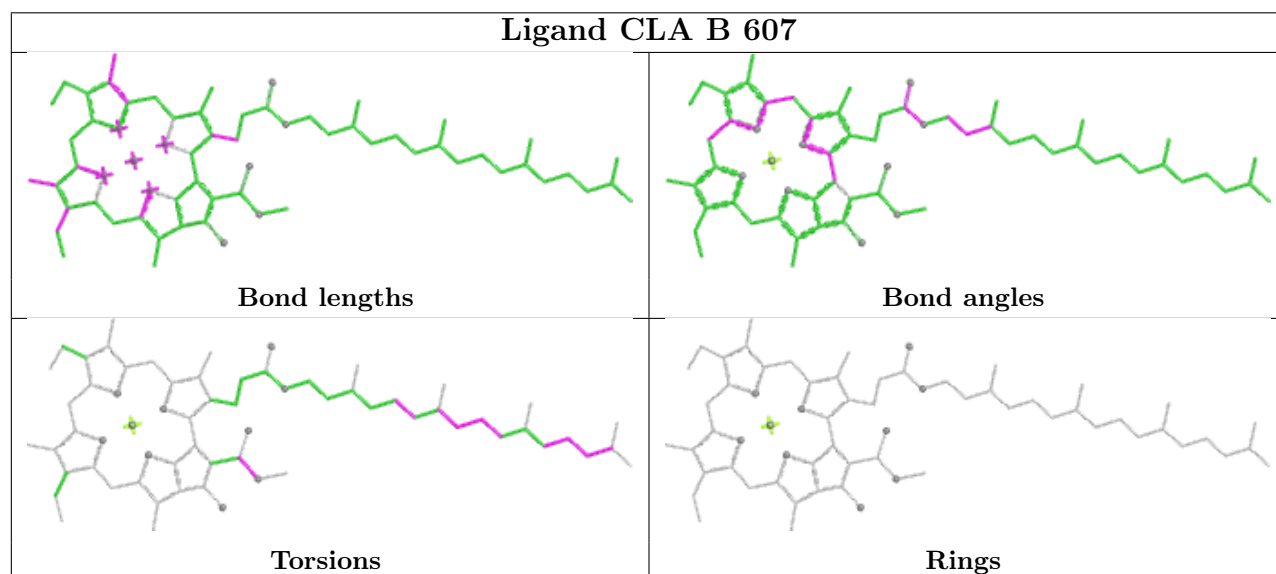
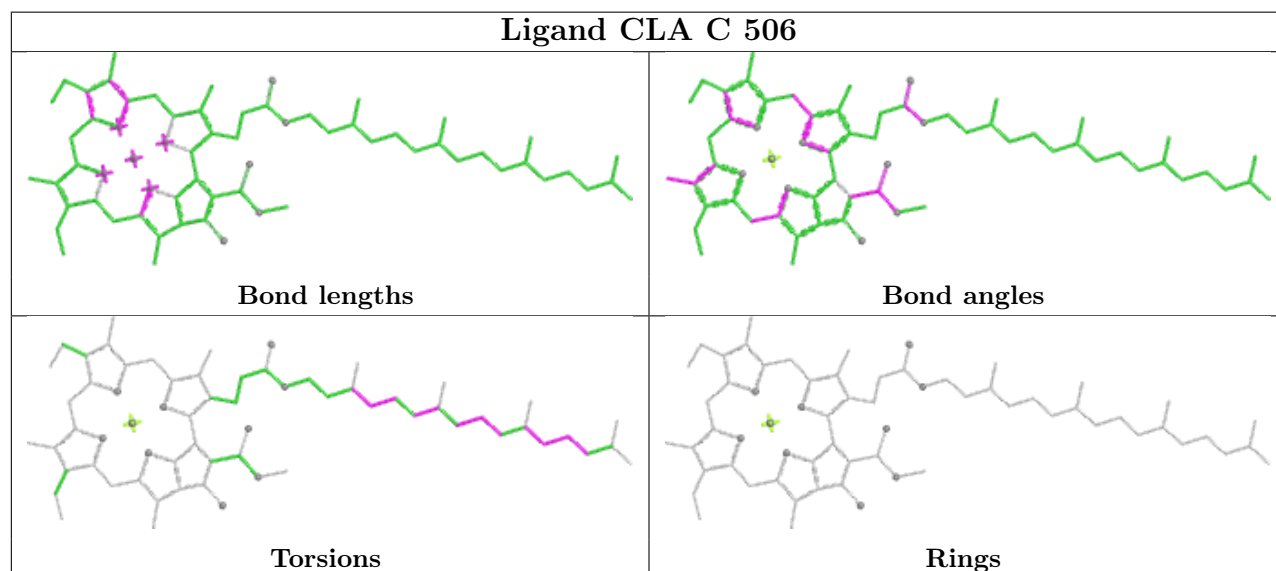
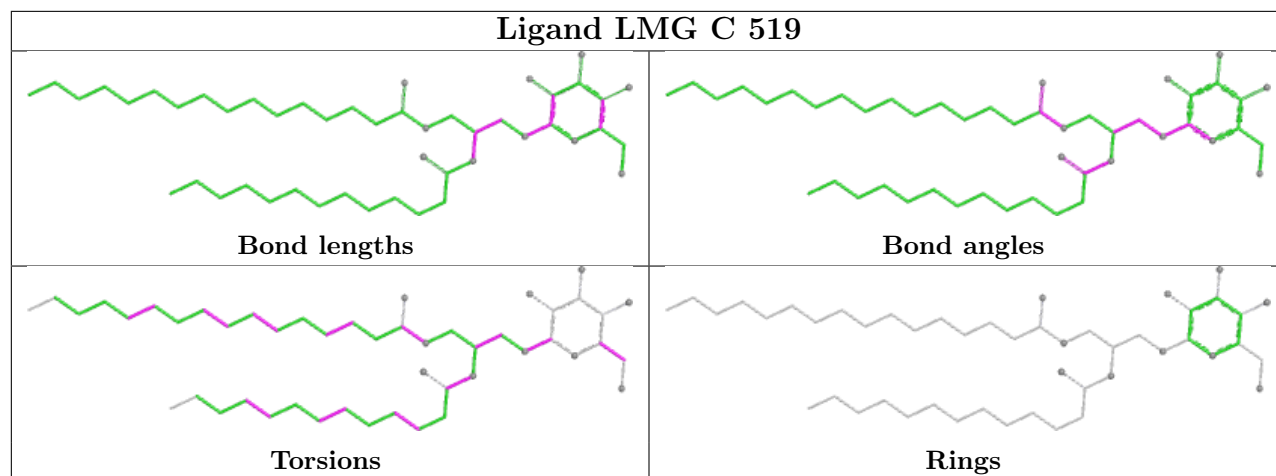
Ligand LMG b 621

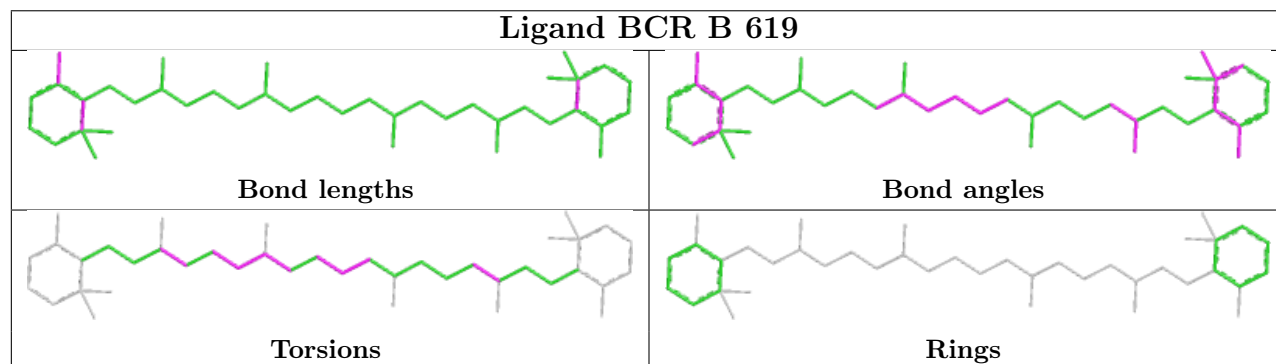
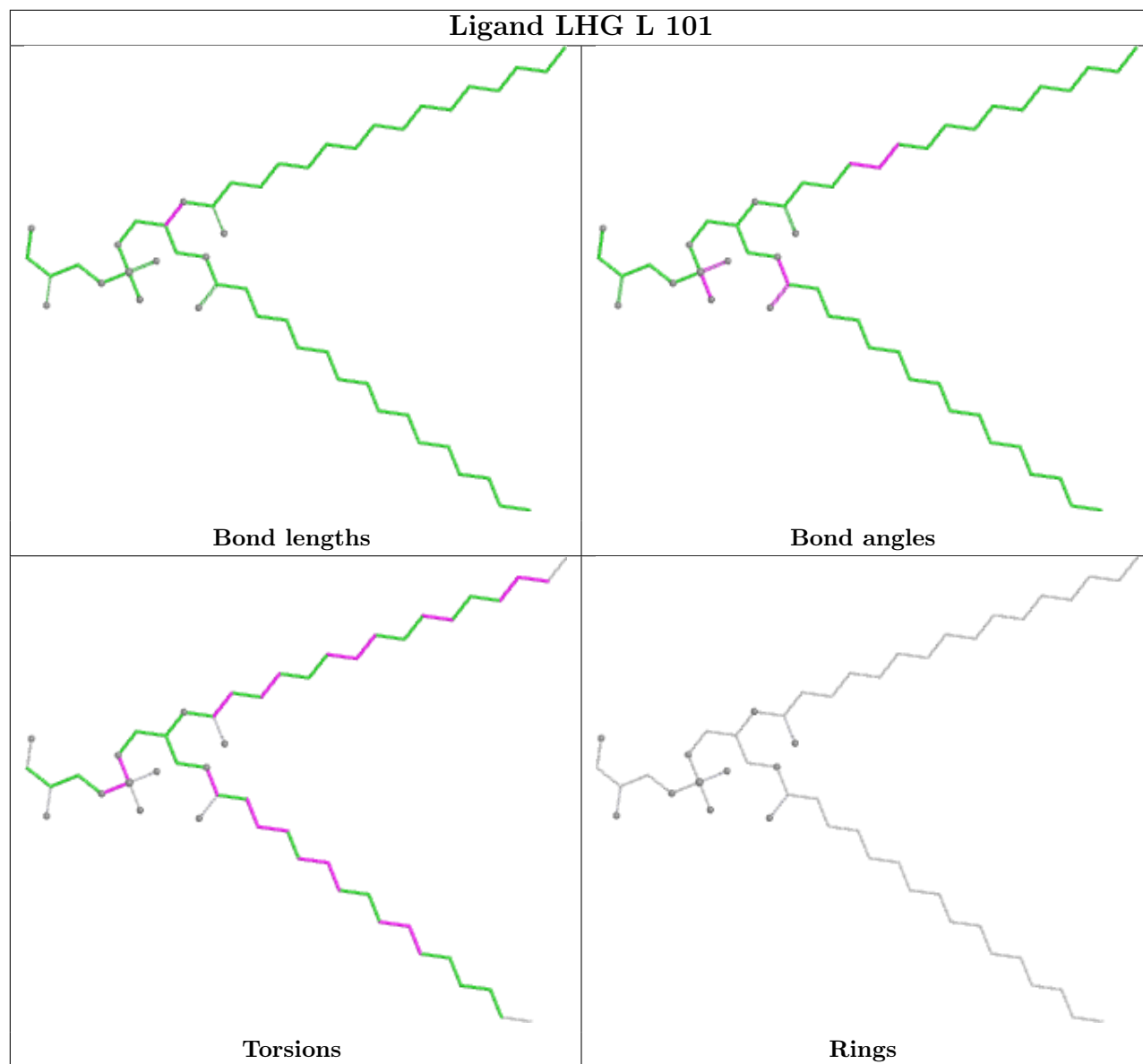


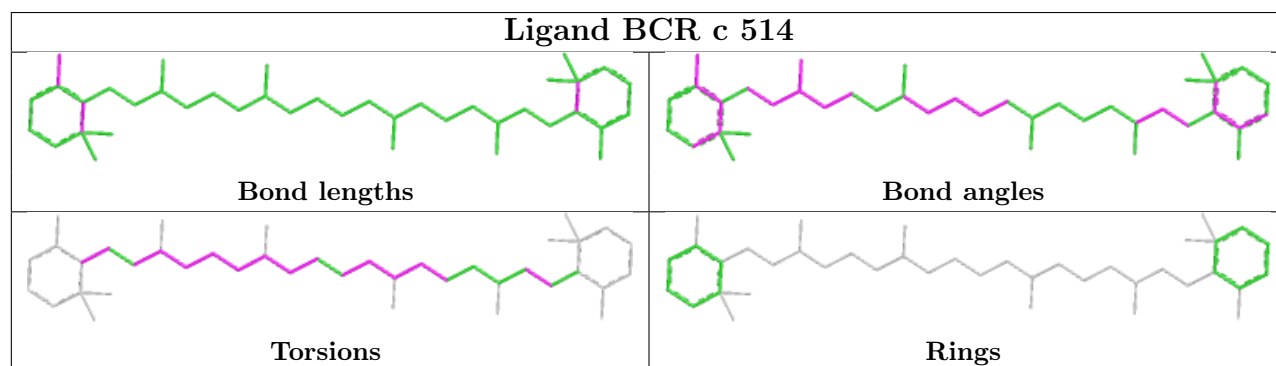
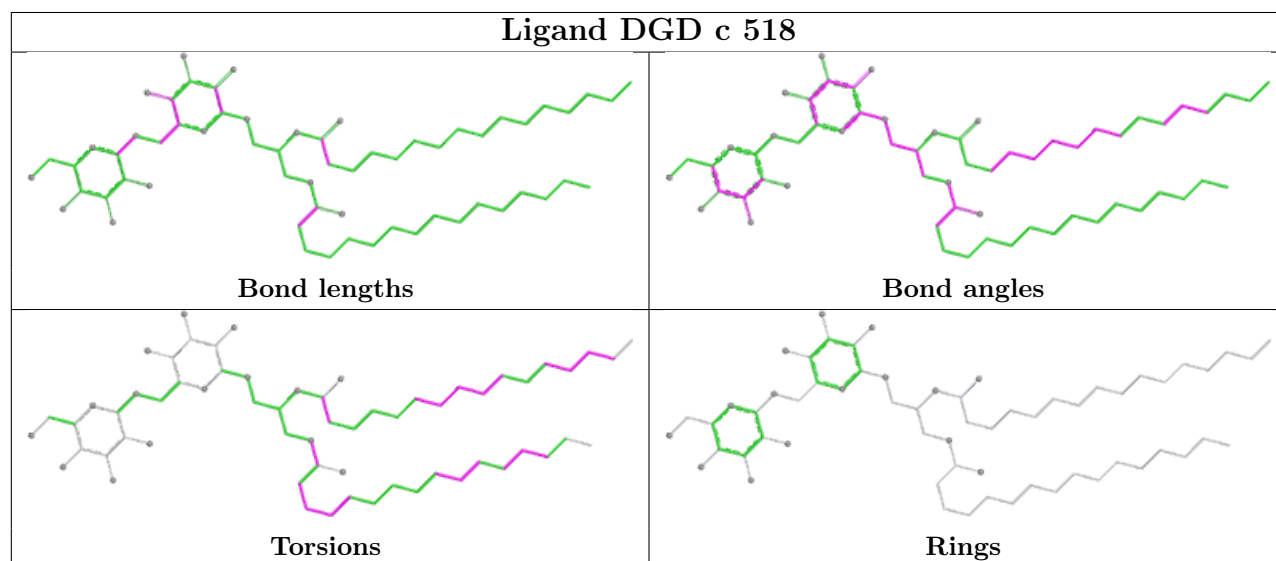
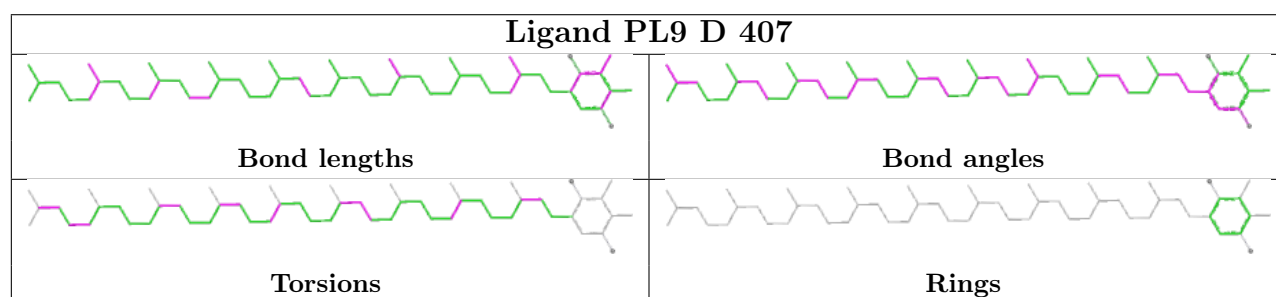
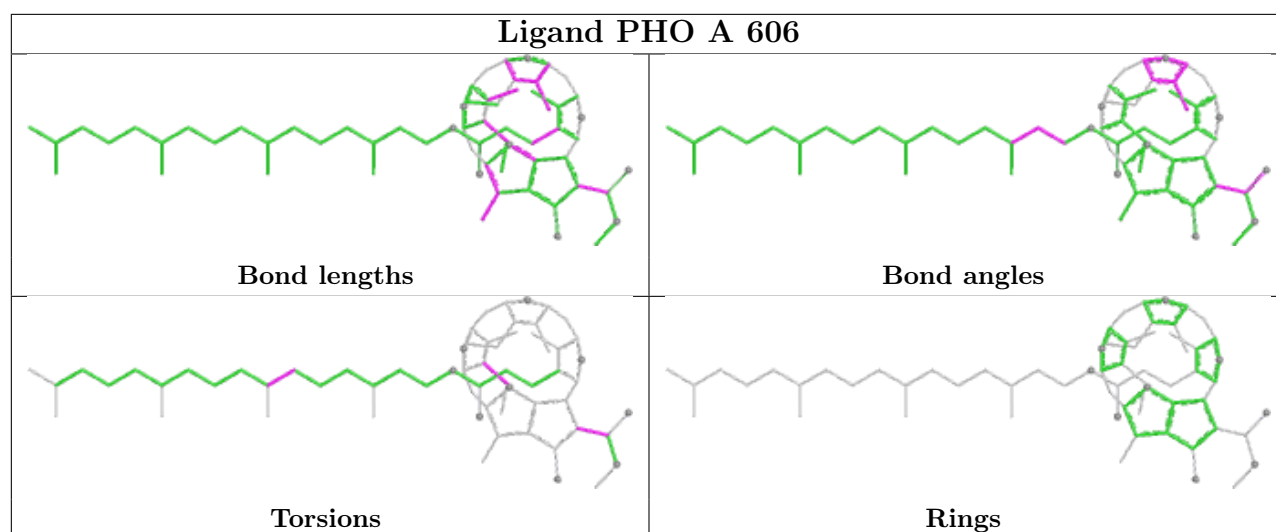


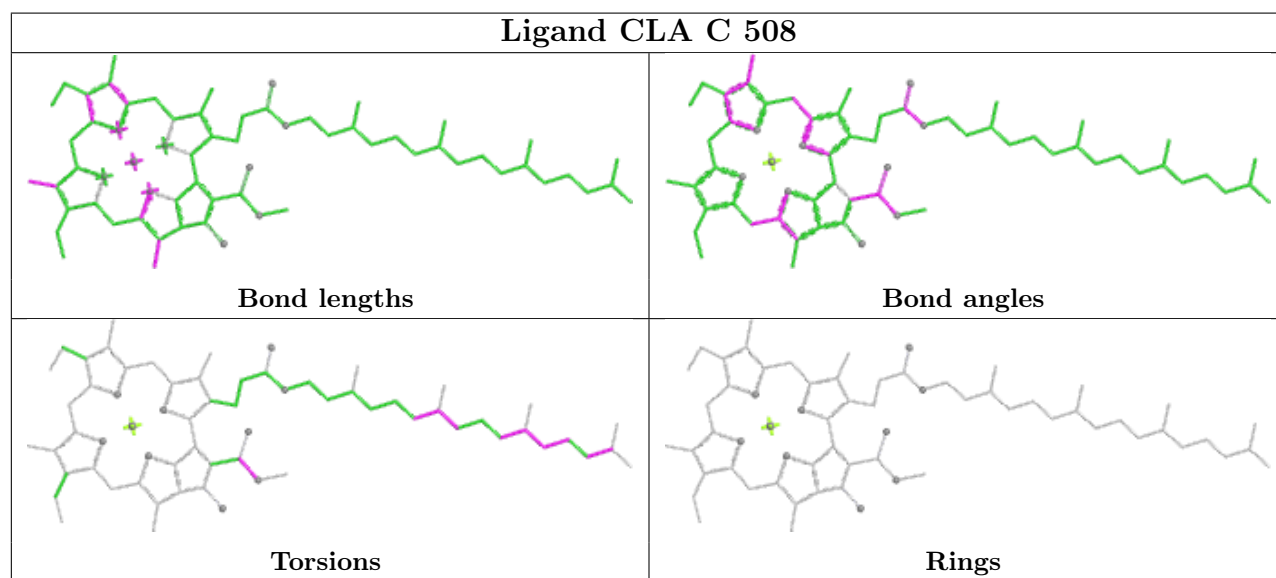
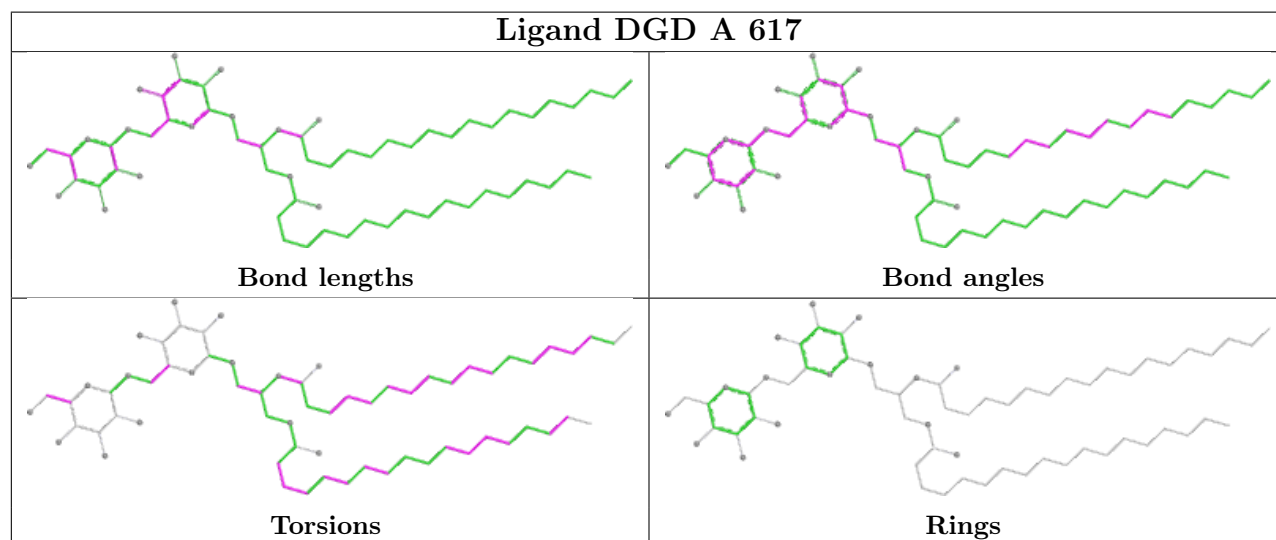
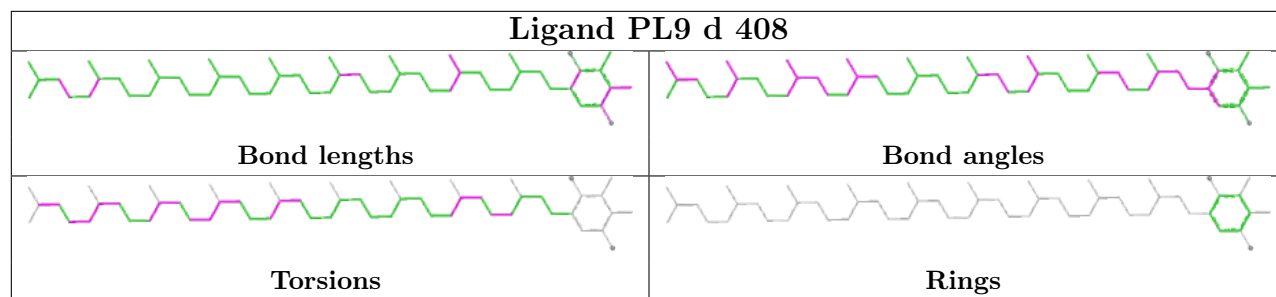


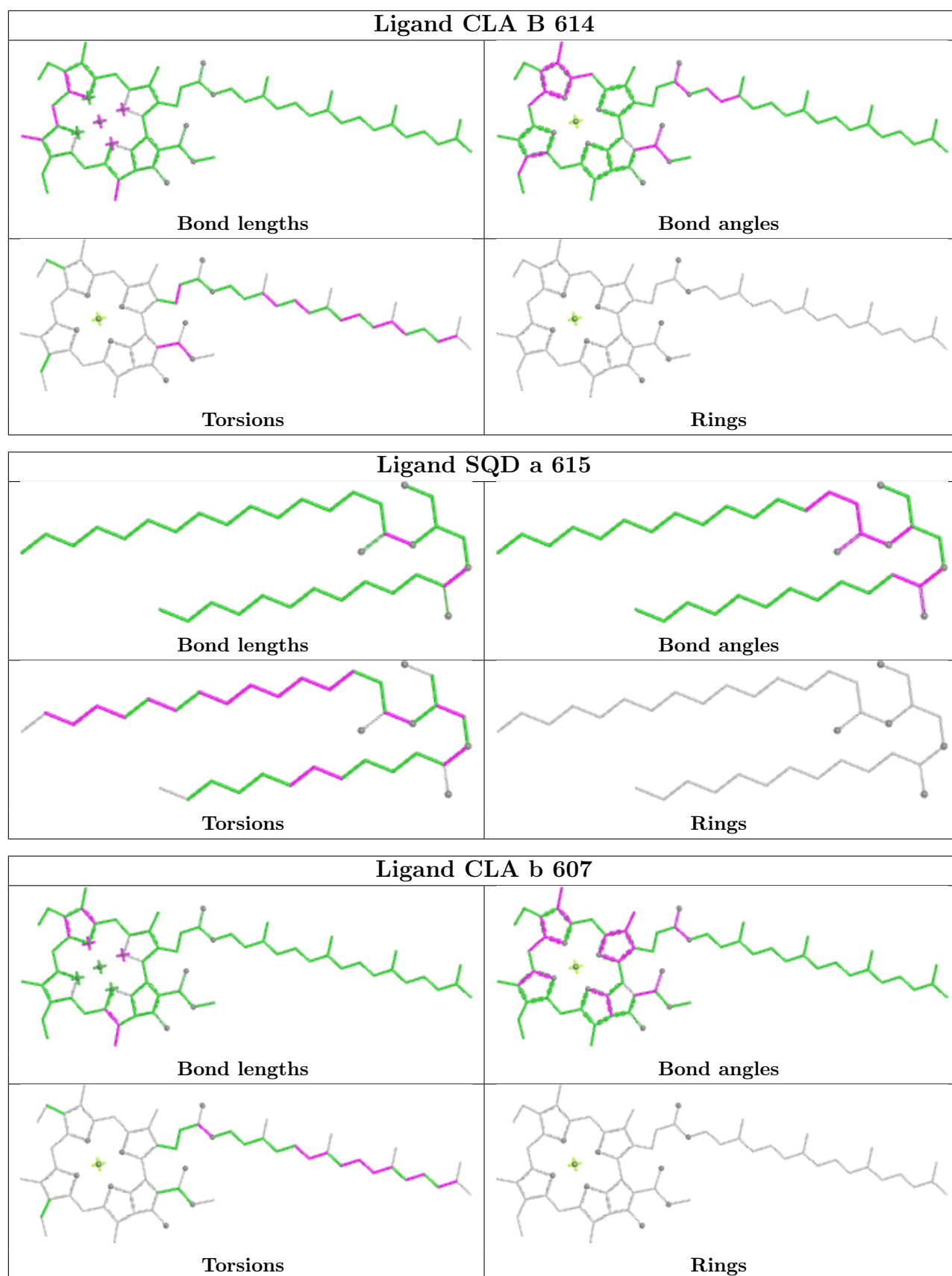


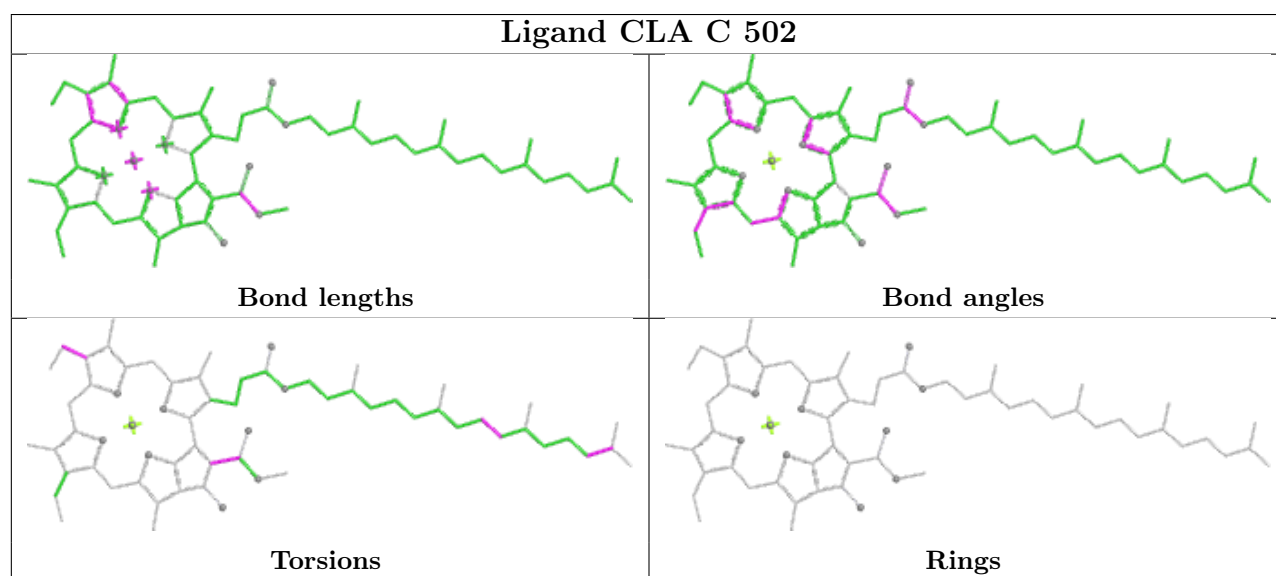
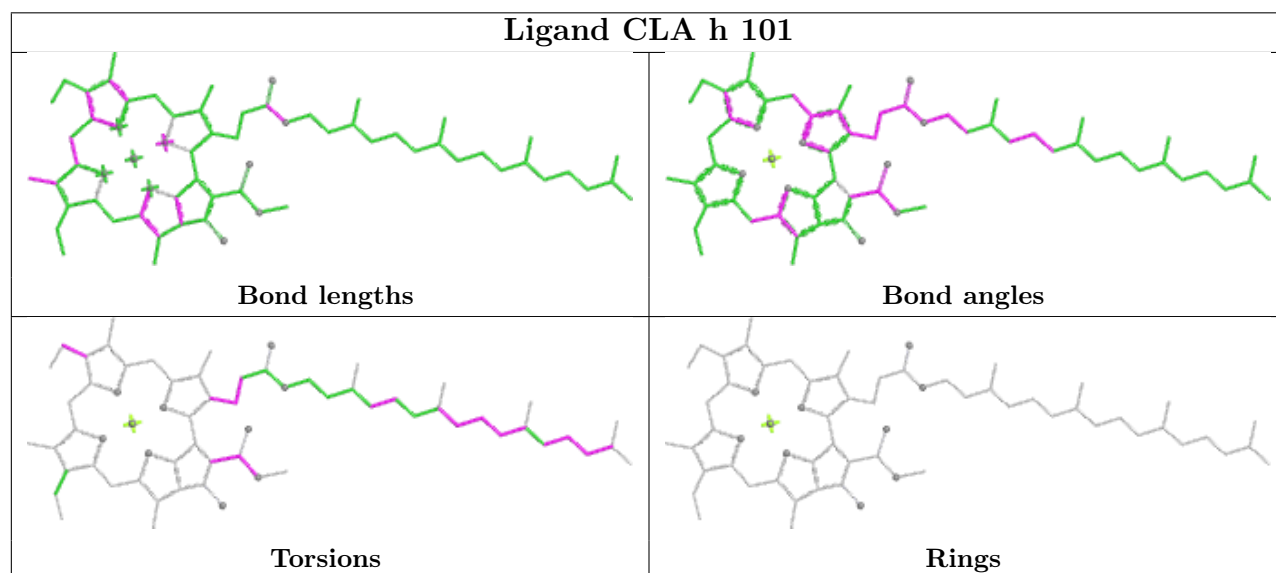
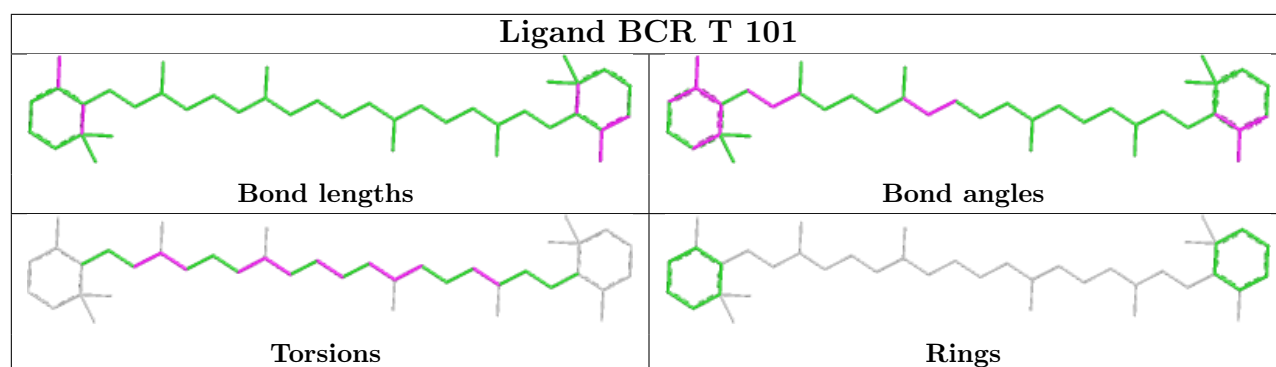


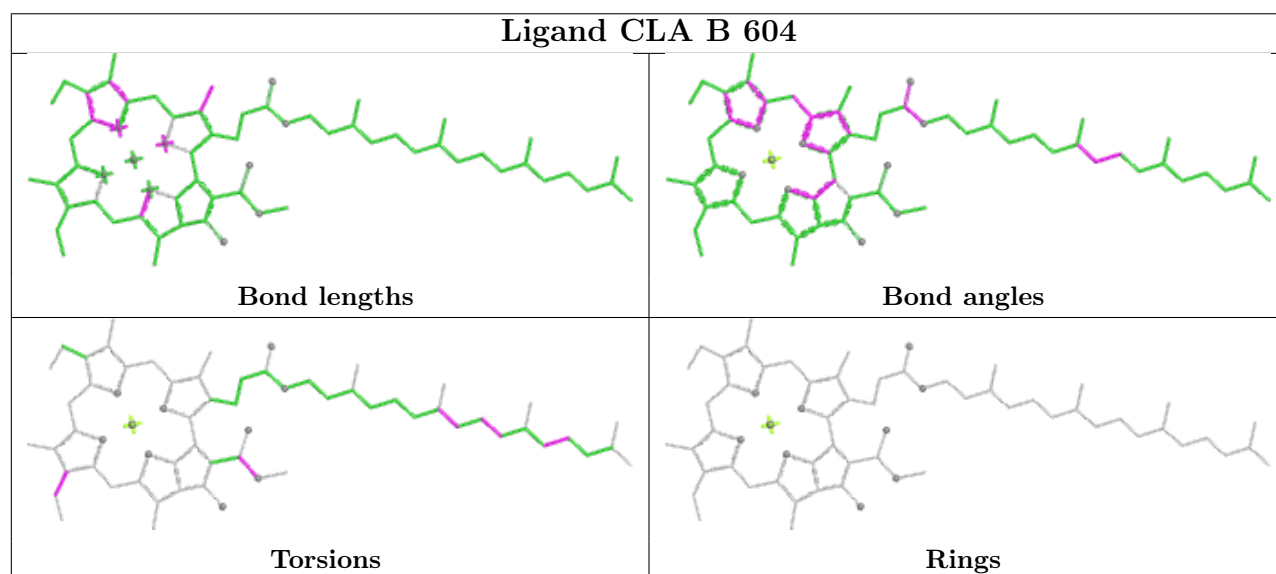
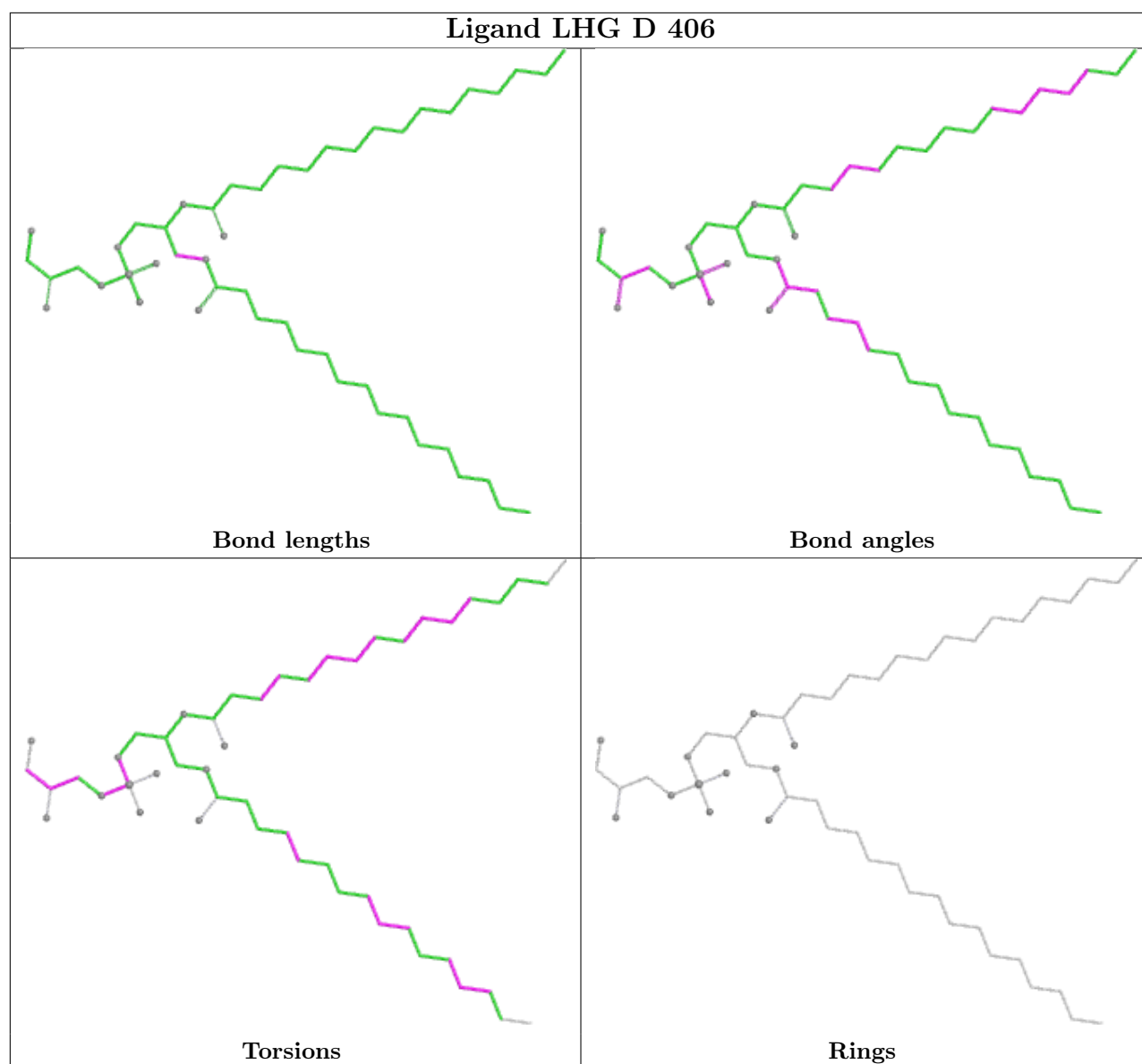




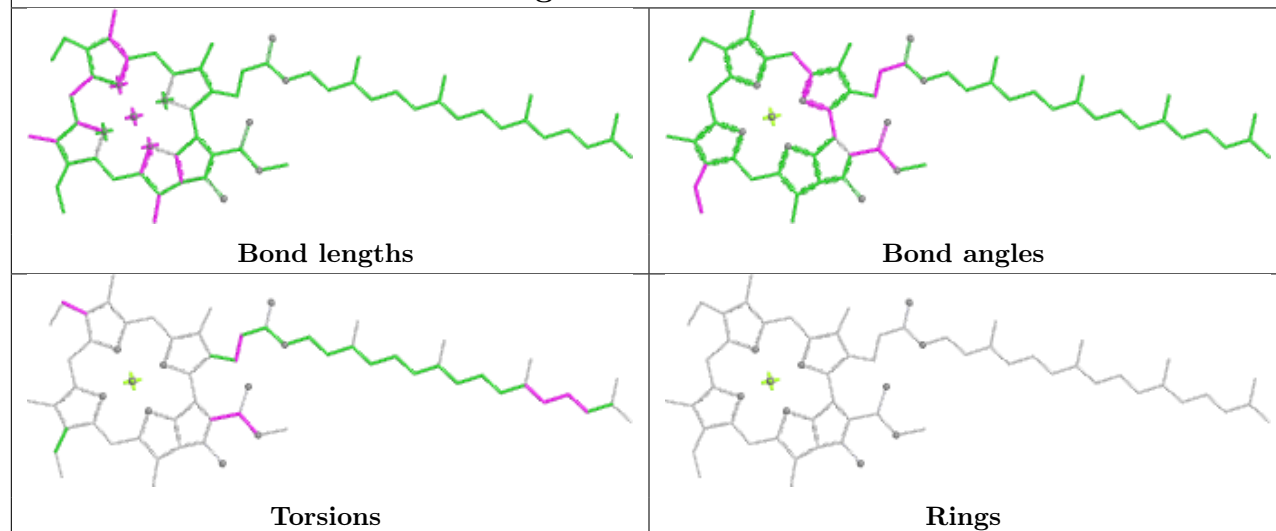




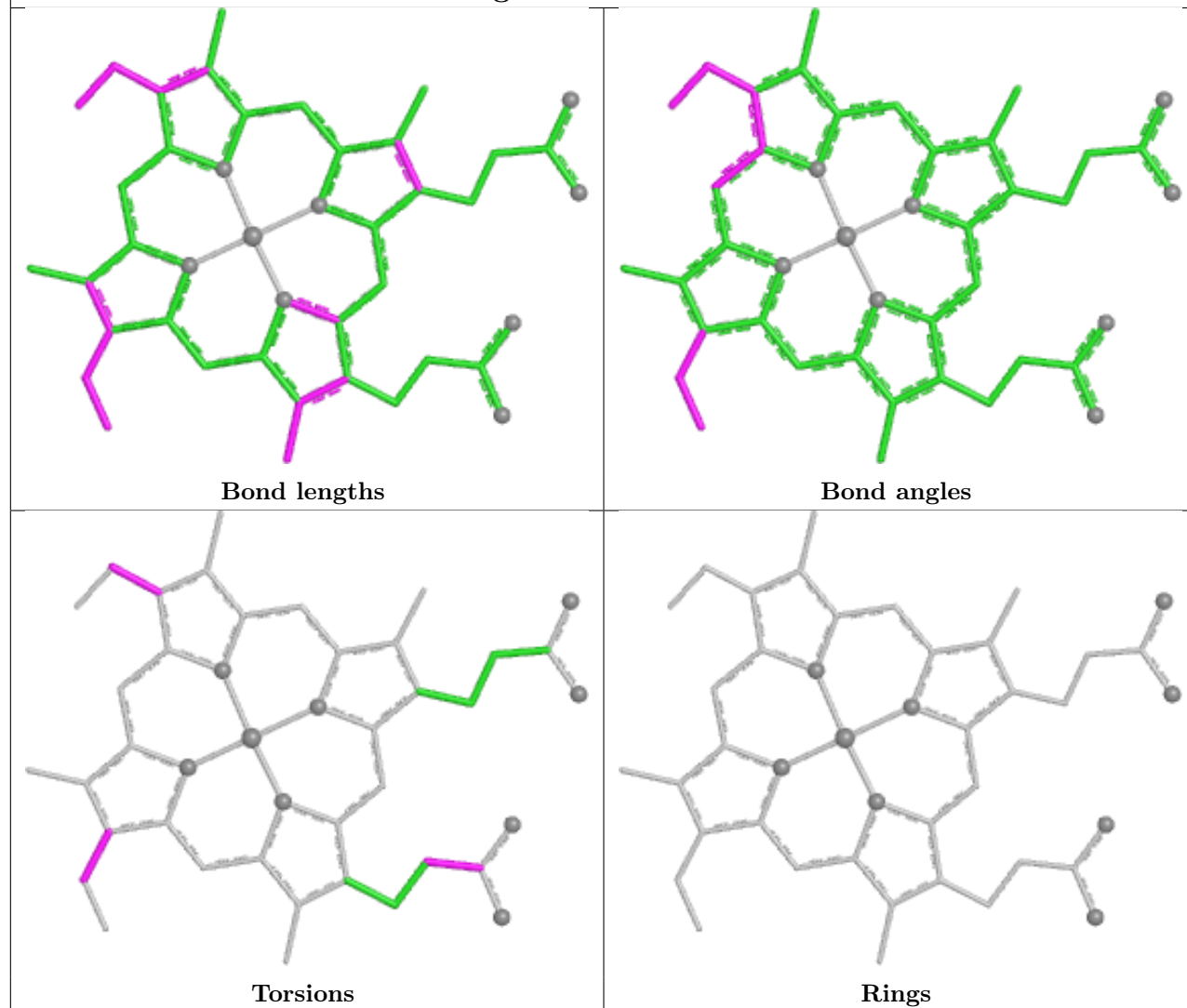


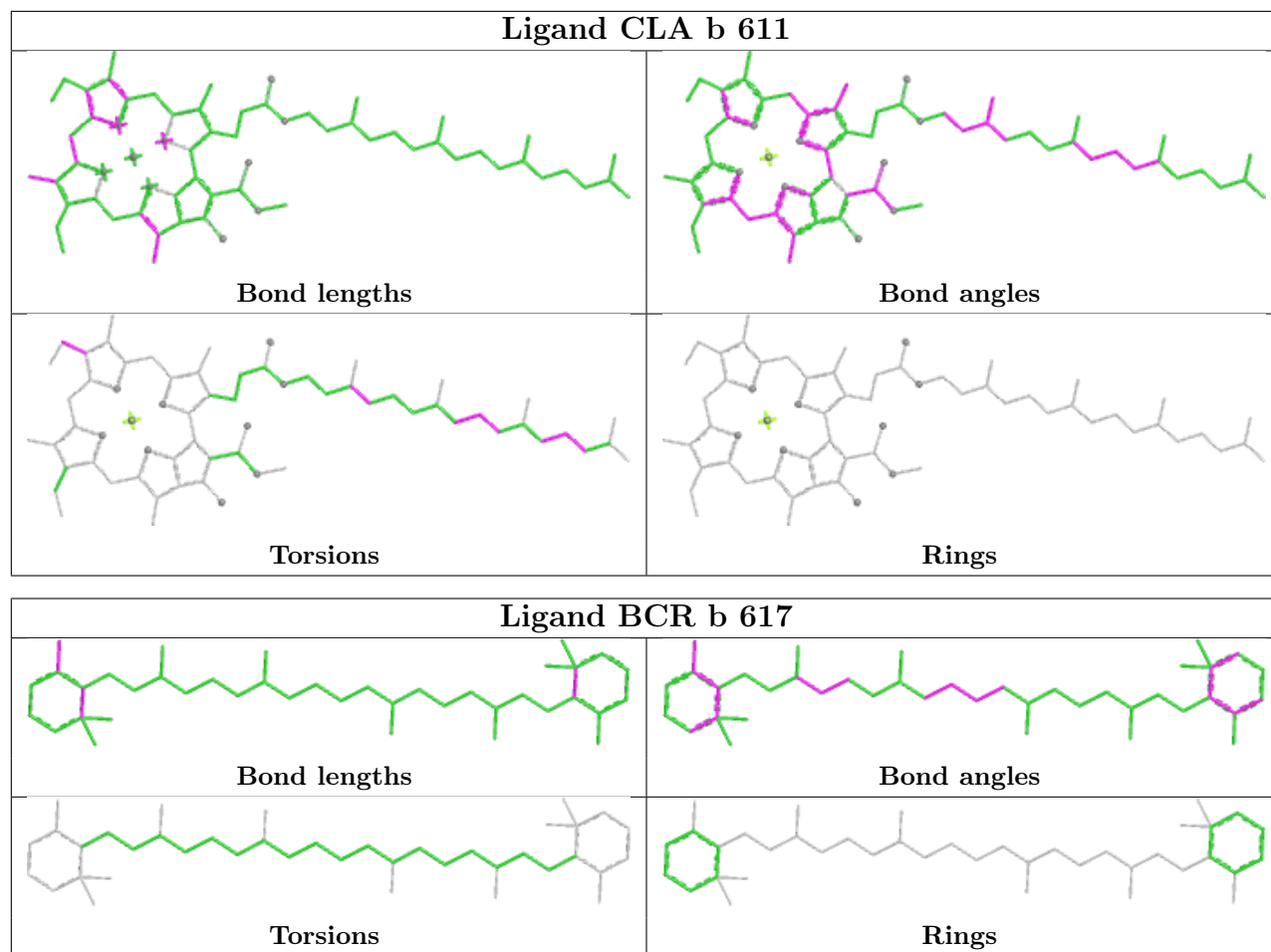


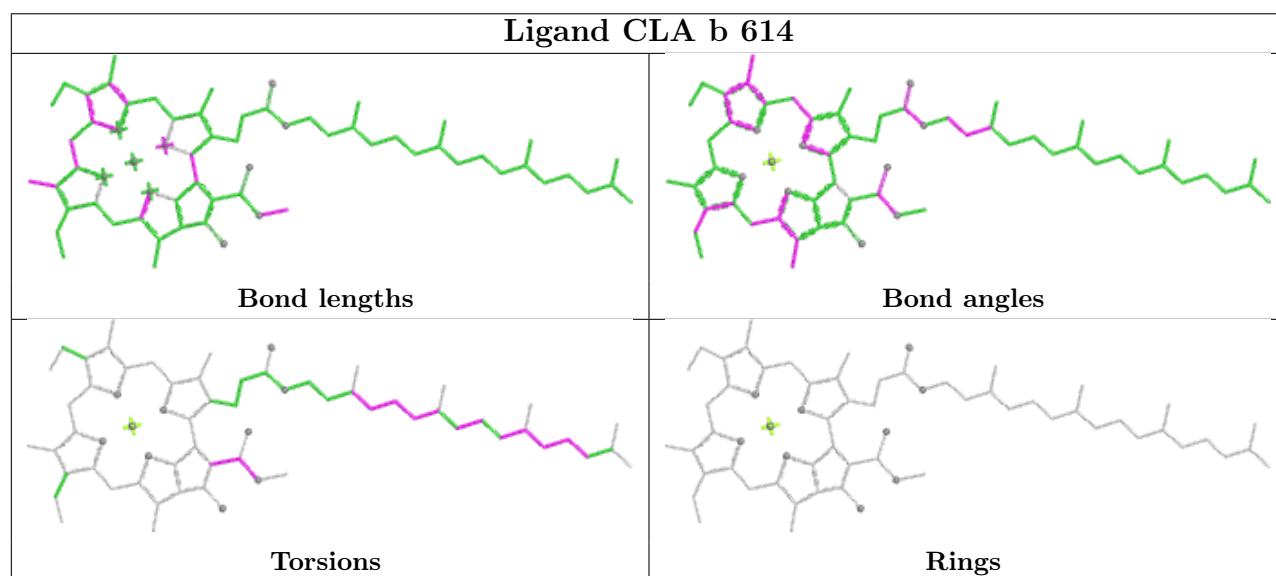
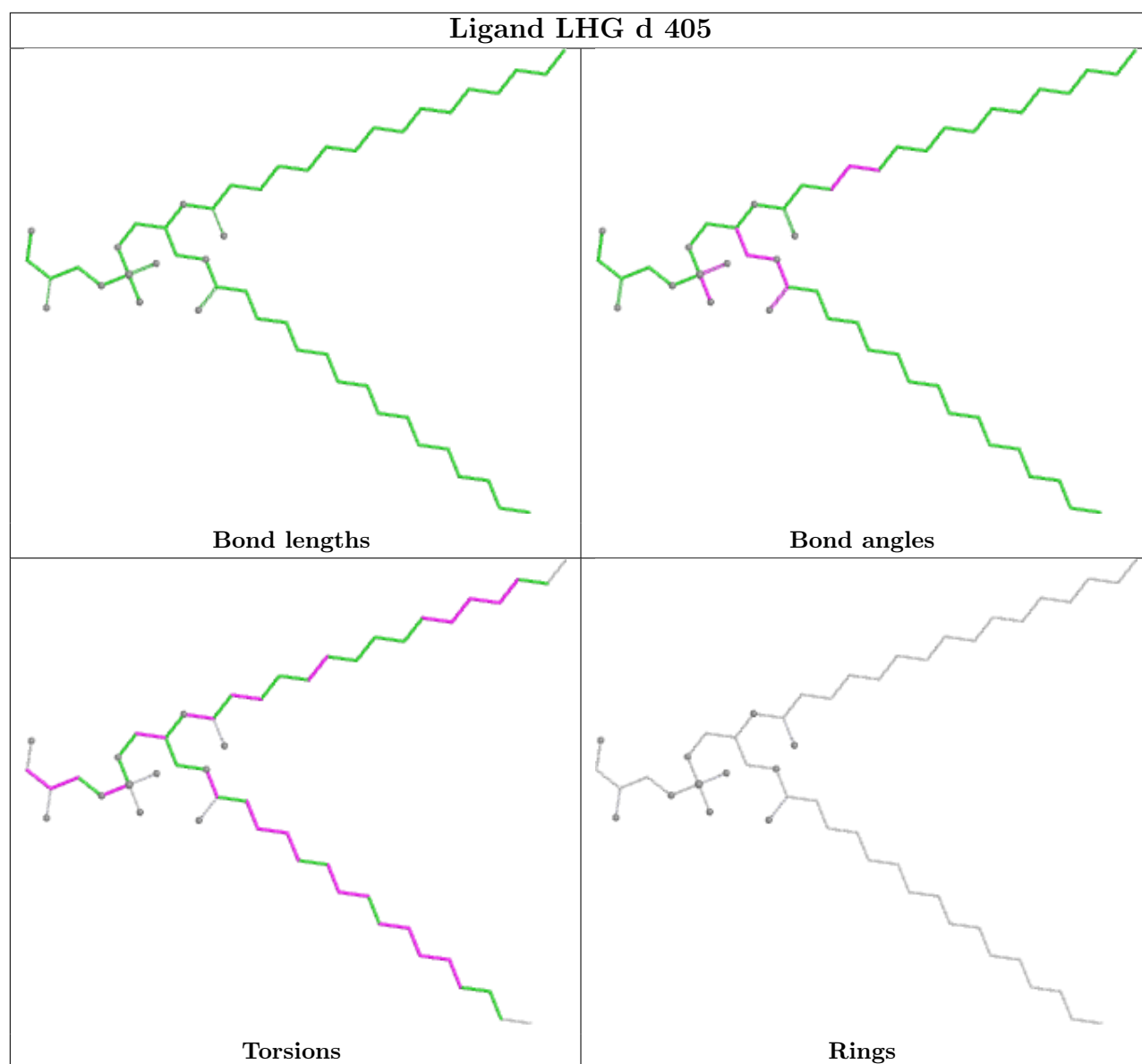
Ligand CLA b 610



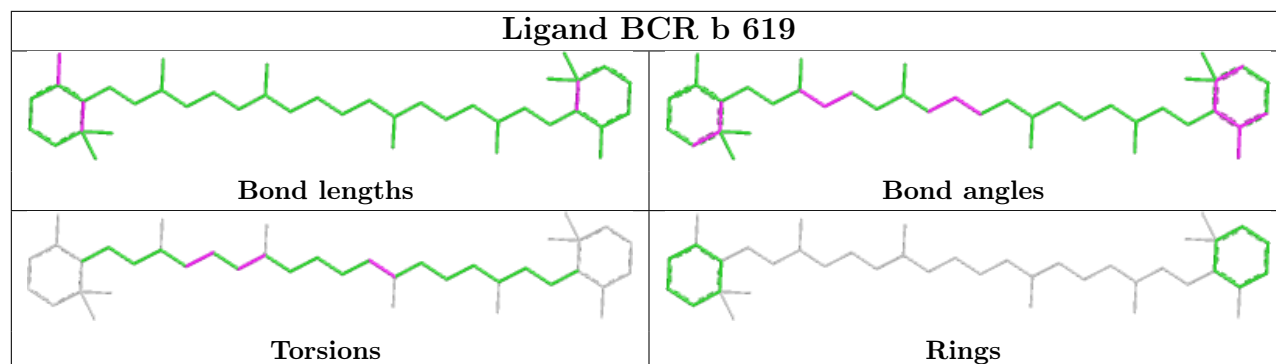
Ligand HEC V 201



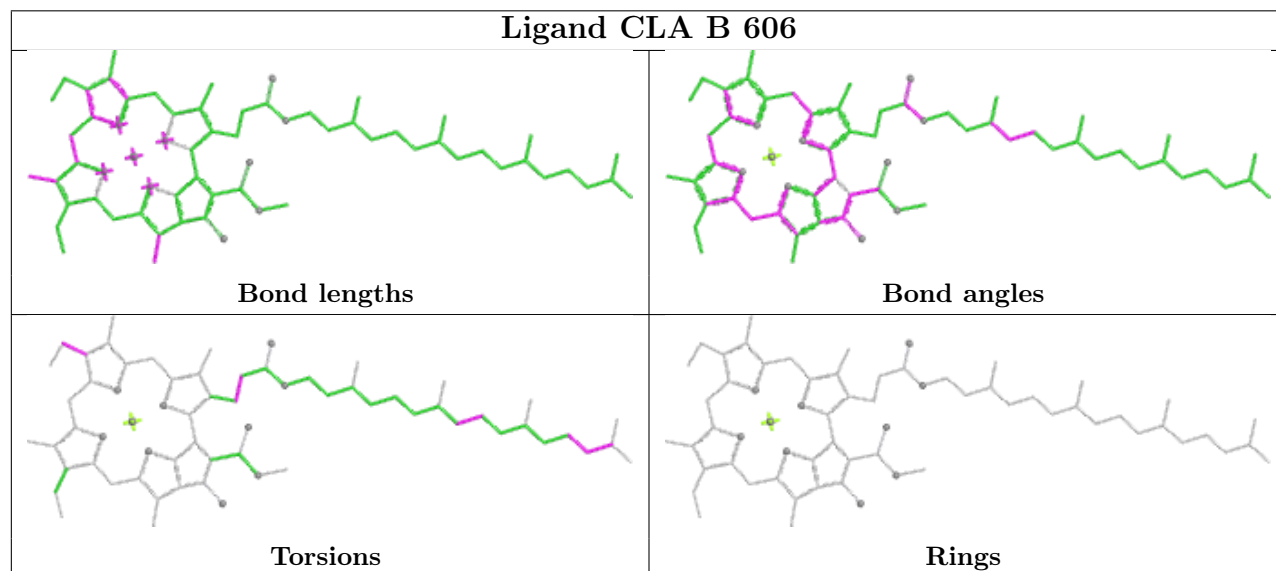




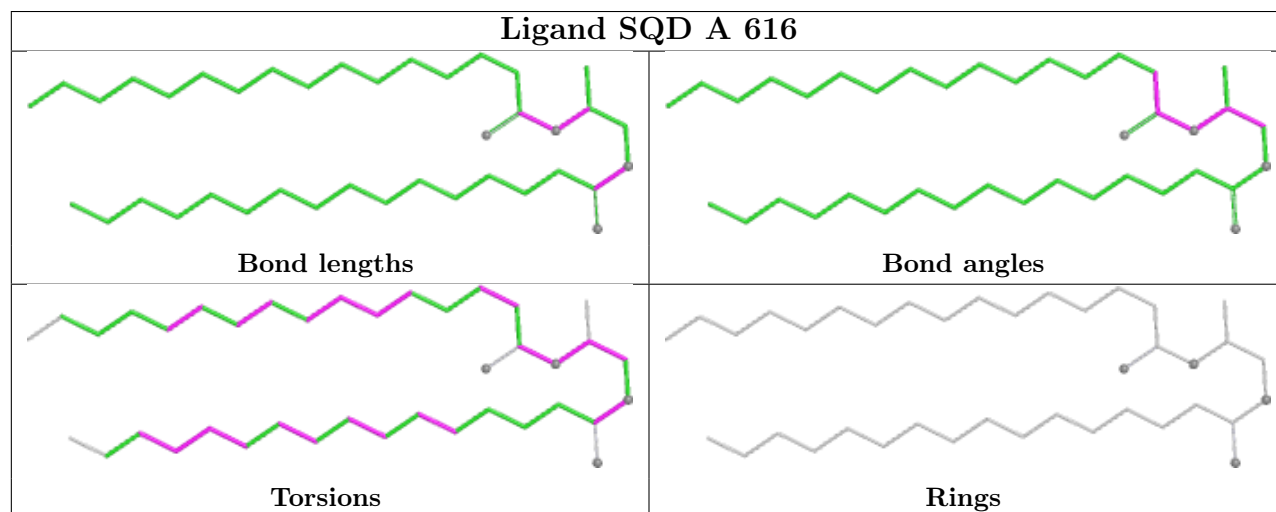
Ligand BCR b 619

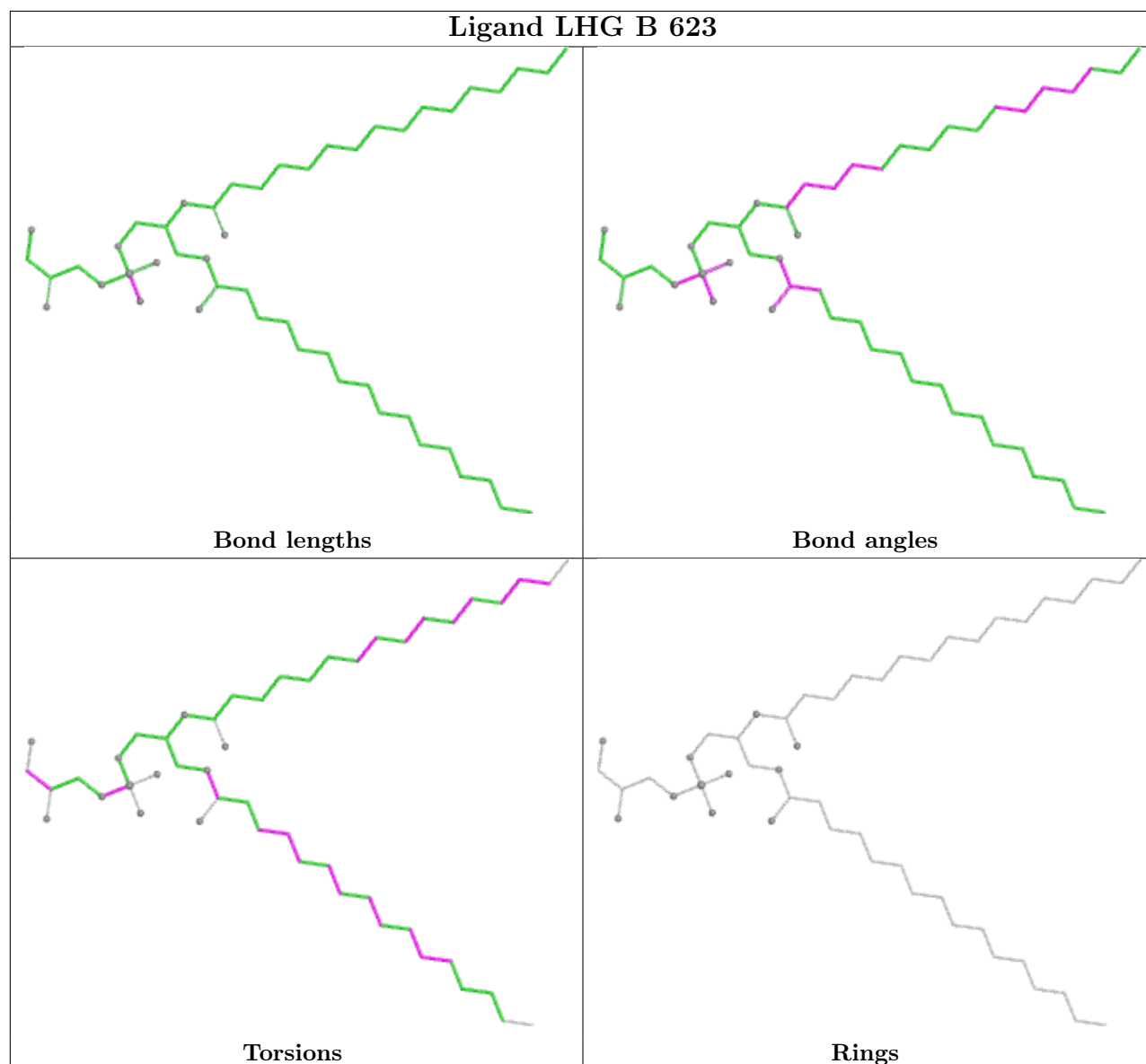
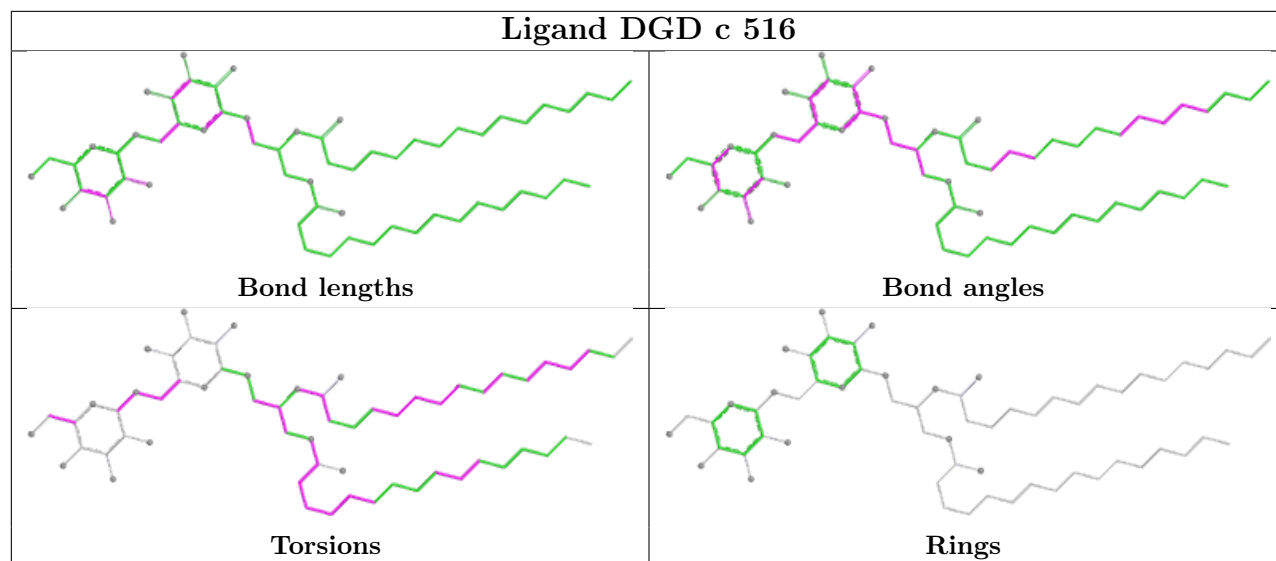


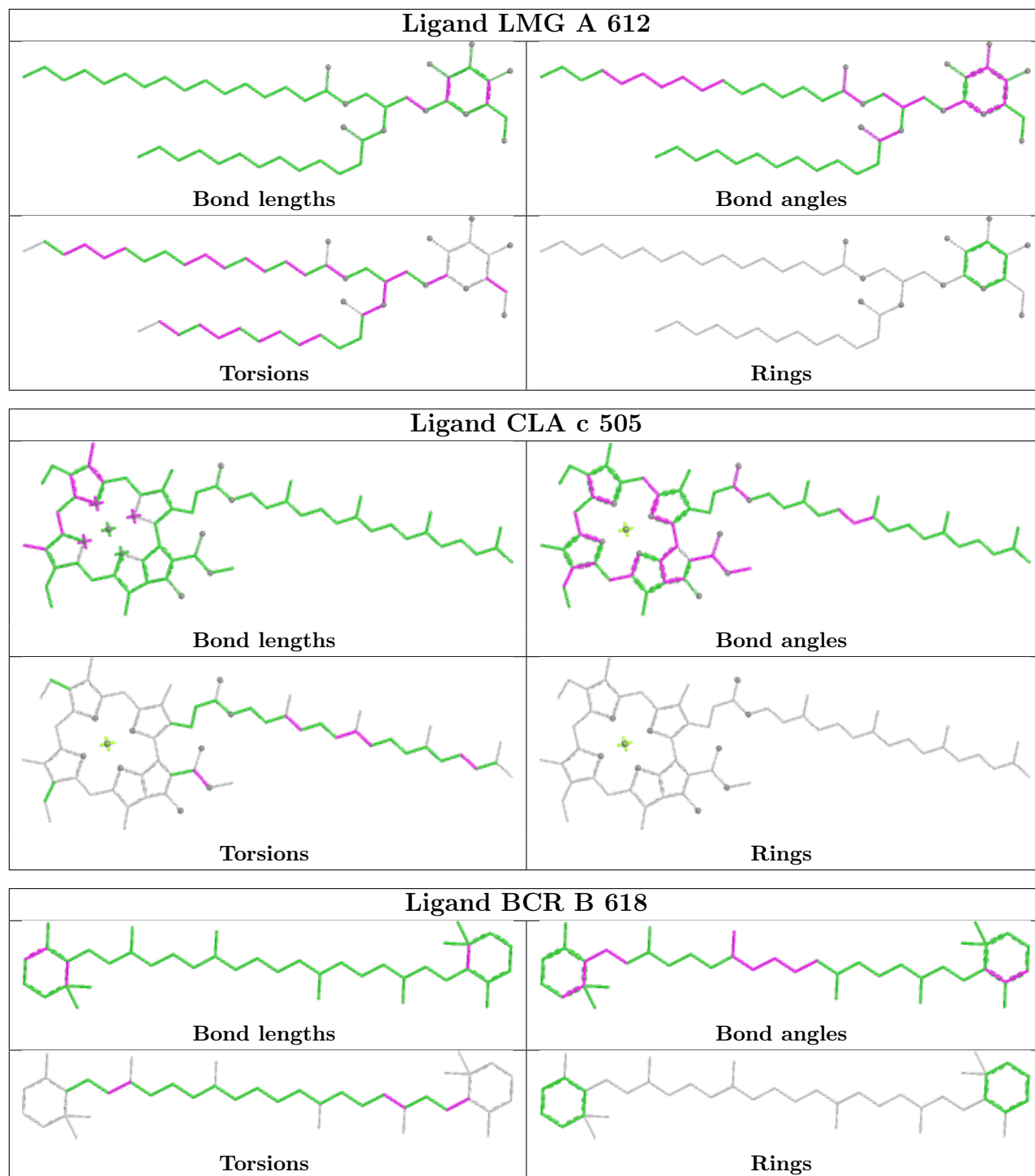
Ligand CLA B 606

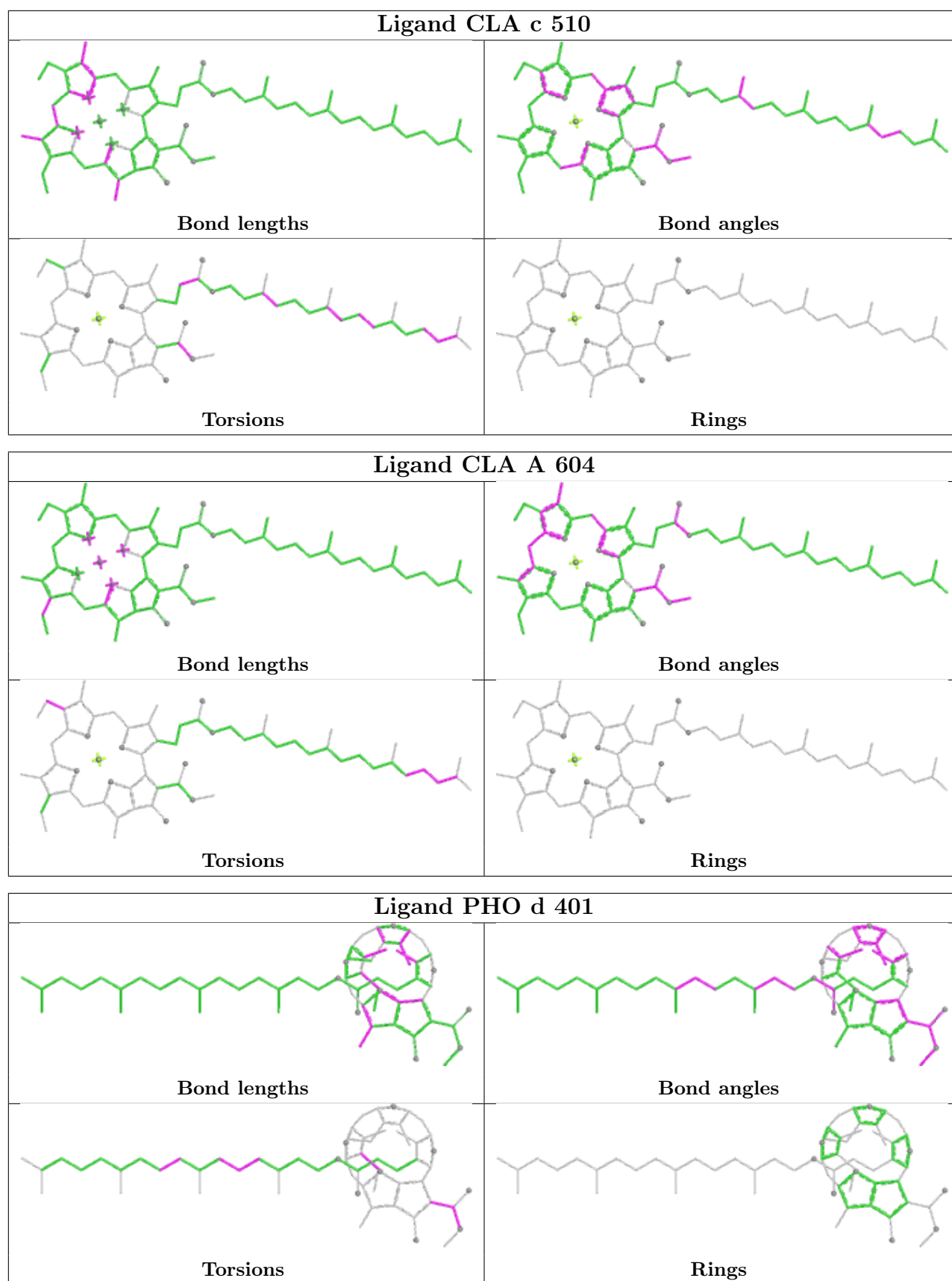


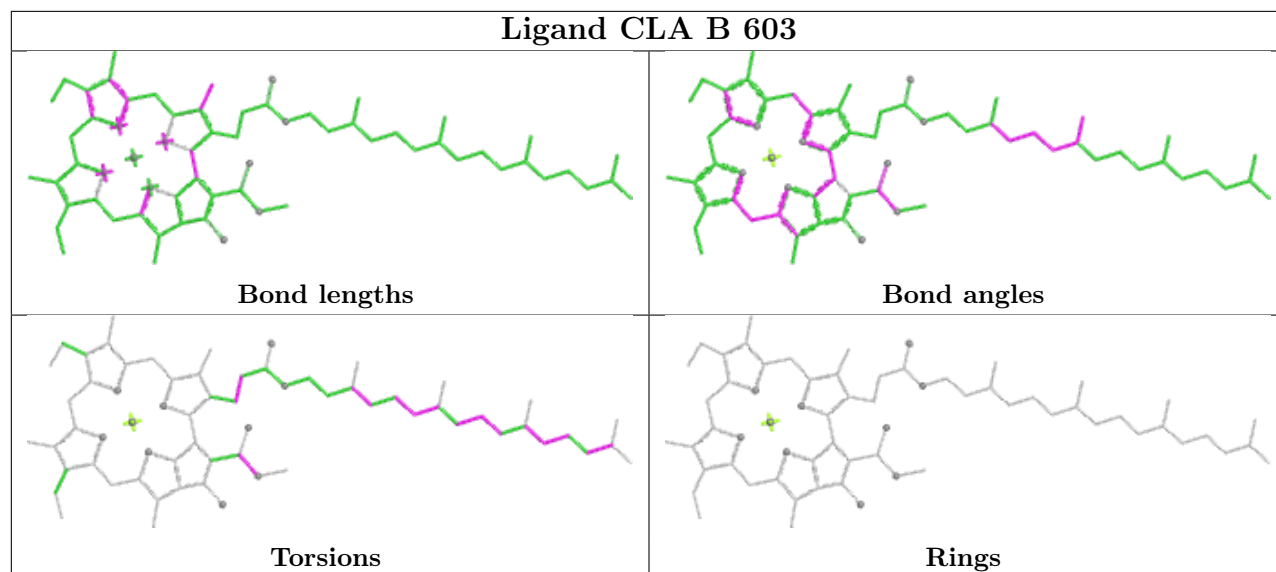
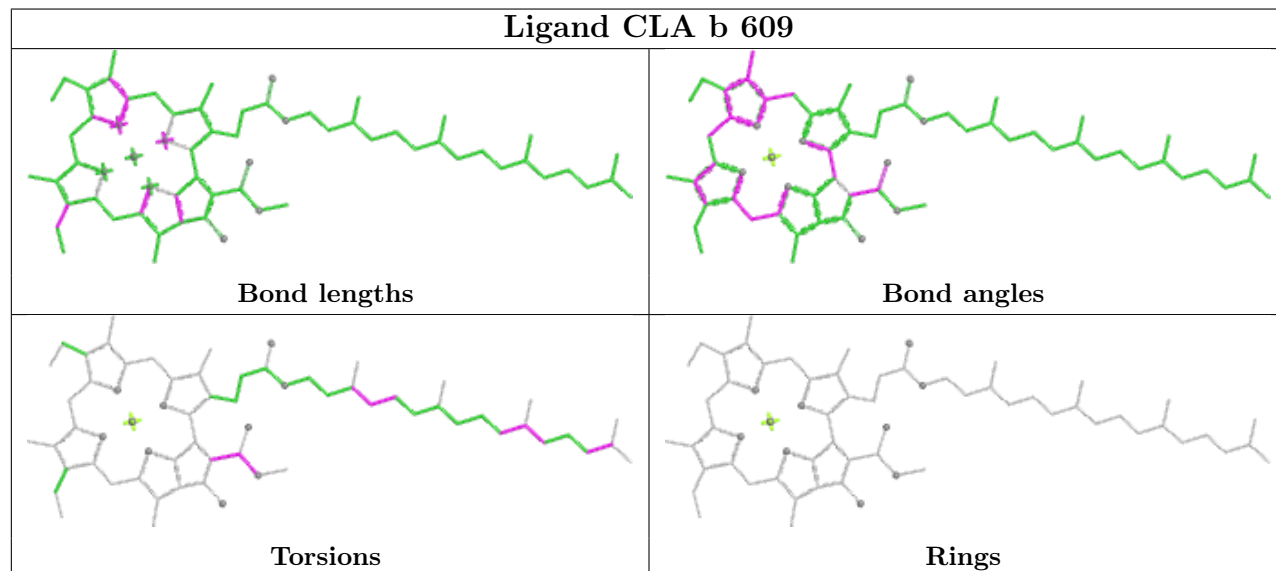
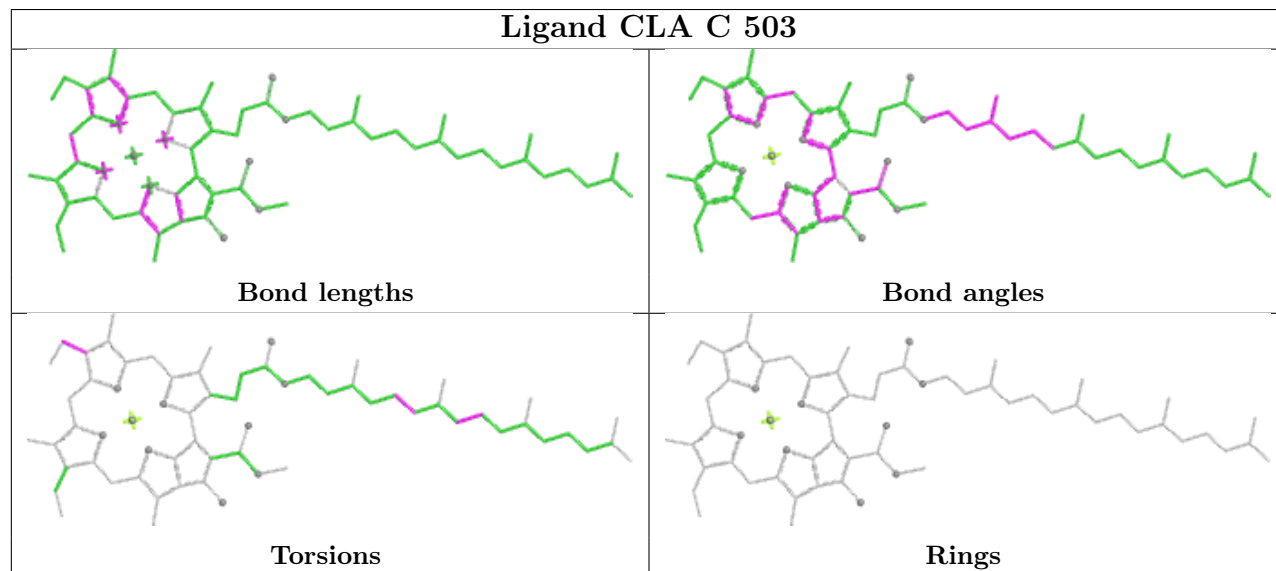
Ligand SQD A 616

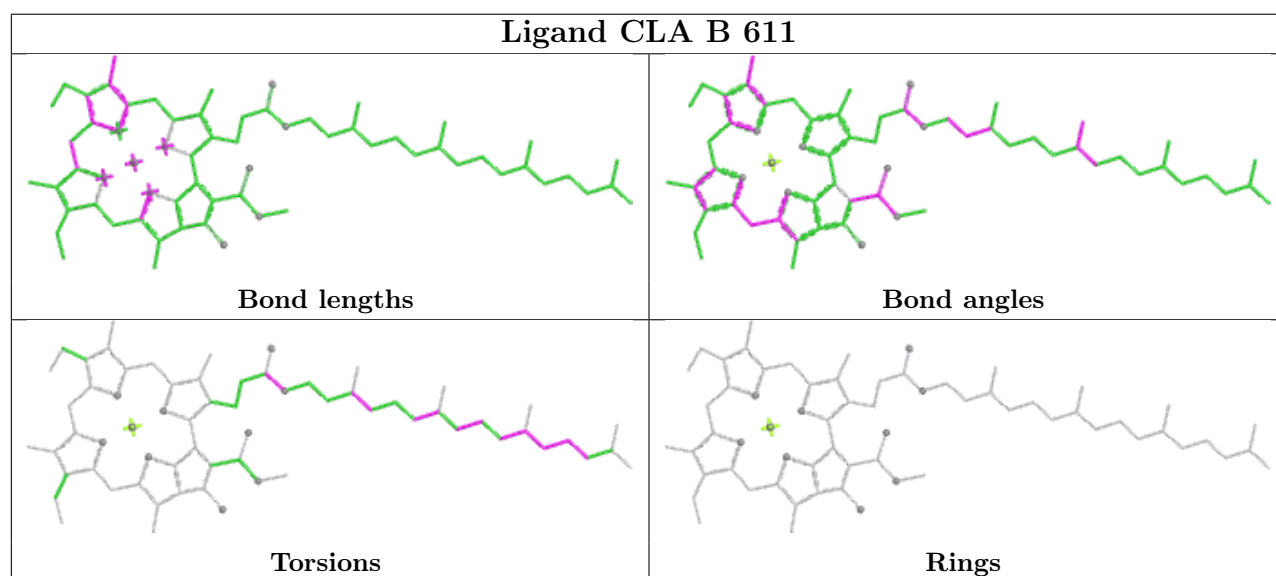
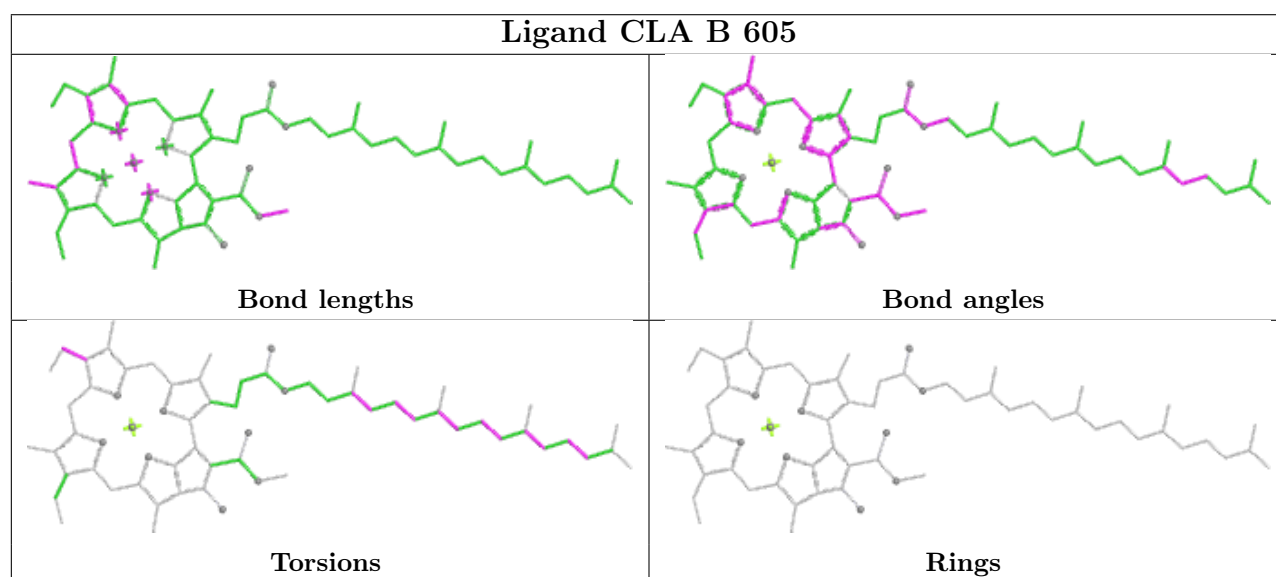
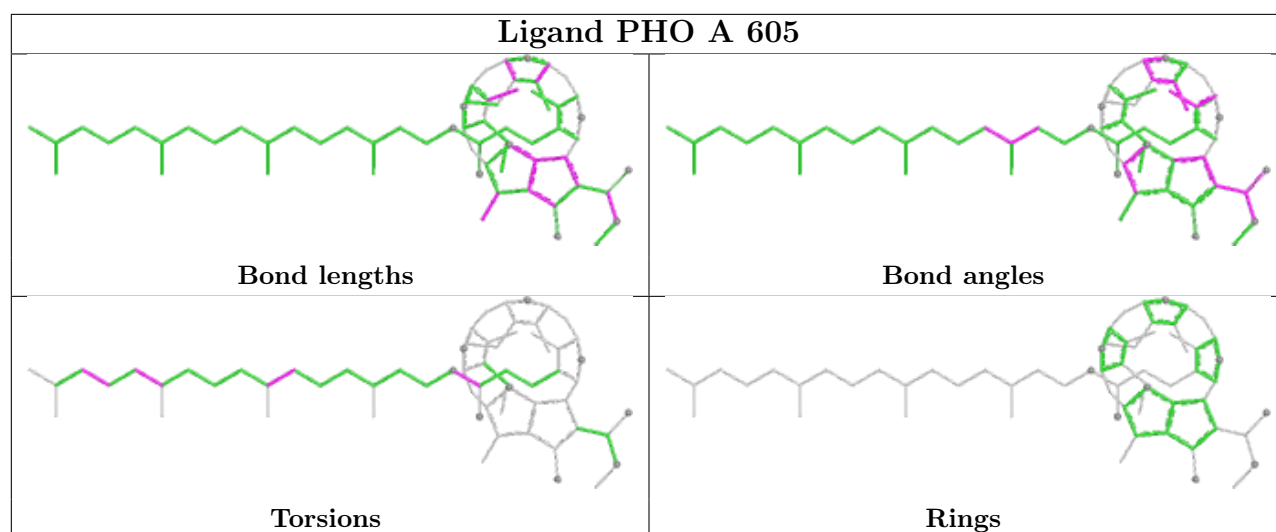


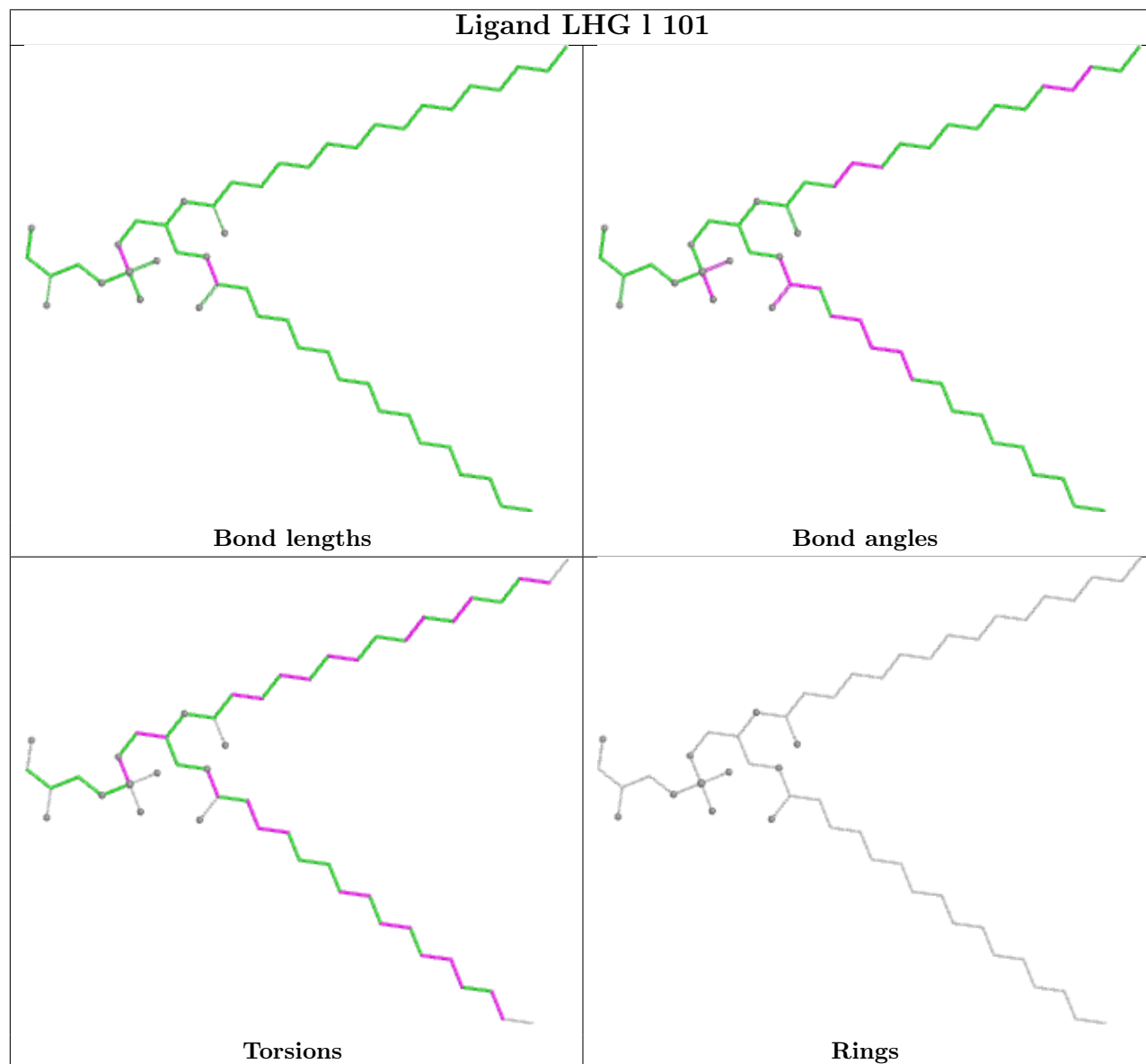
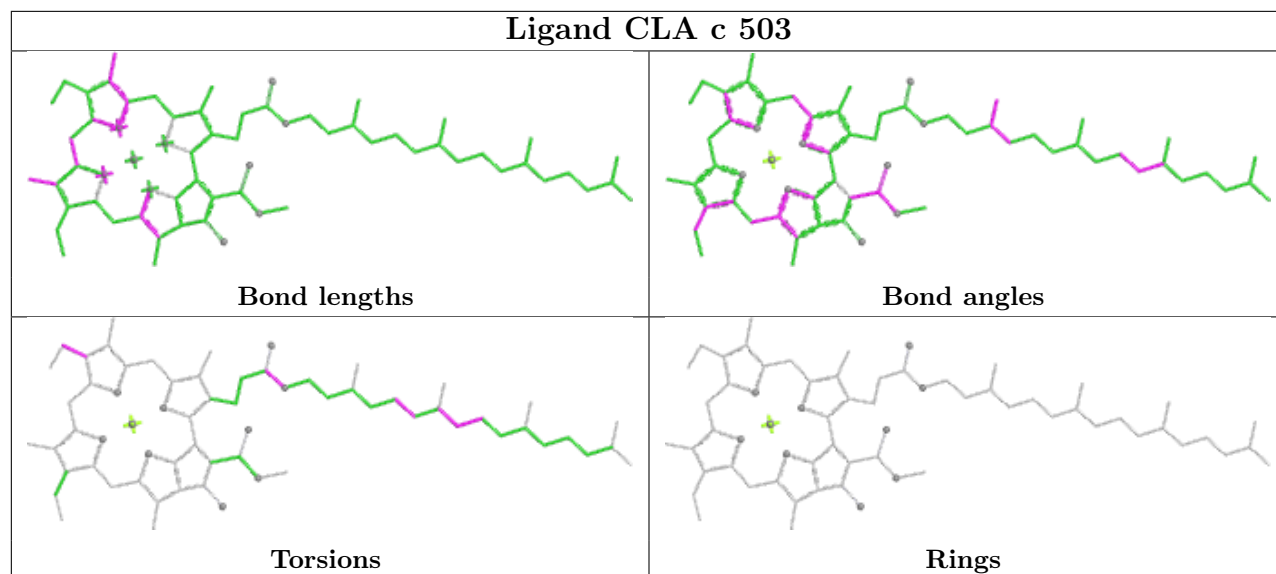


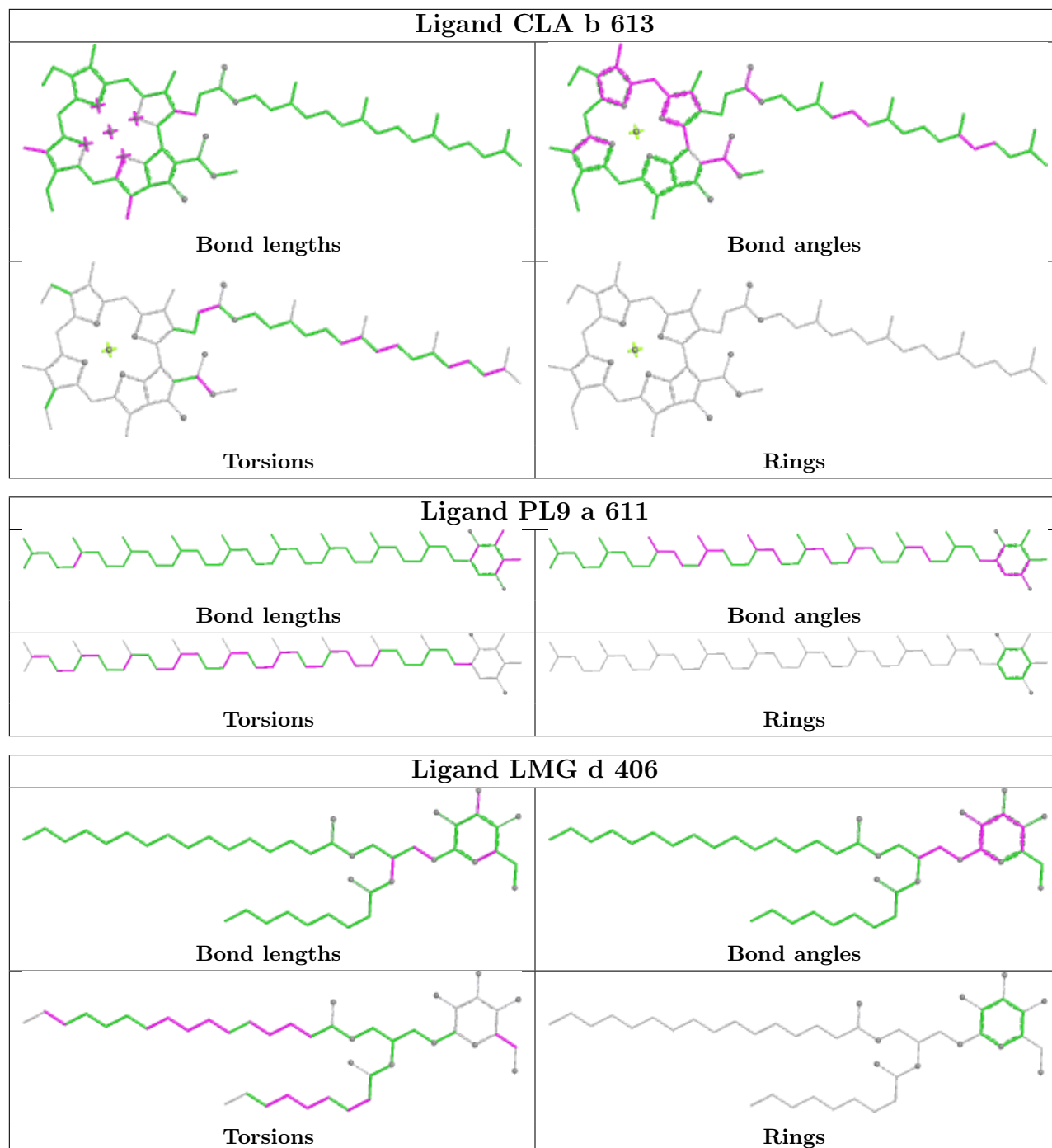


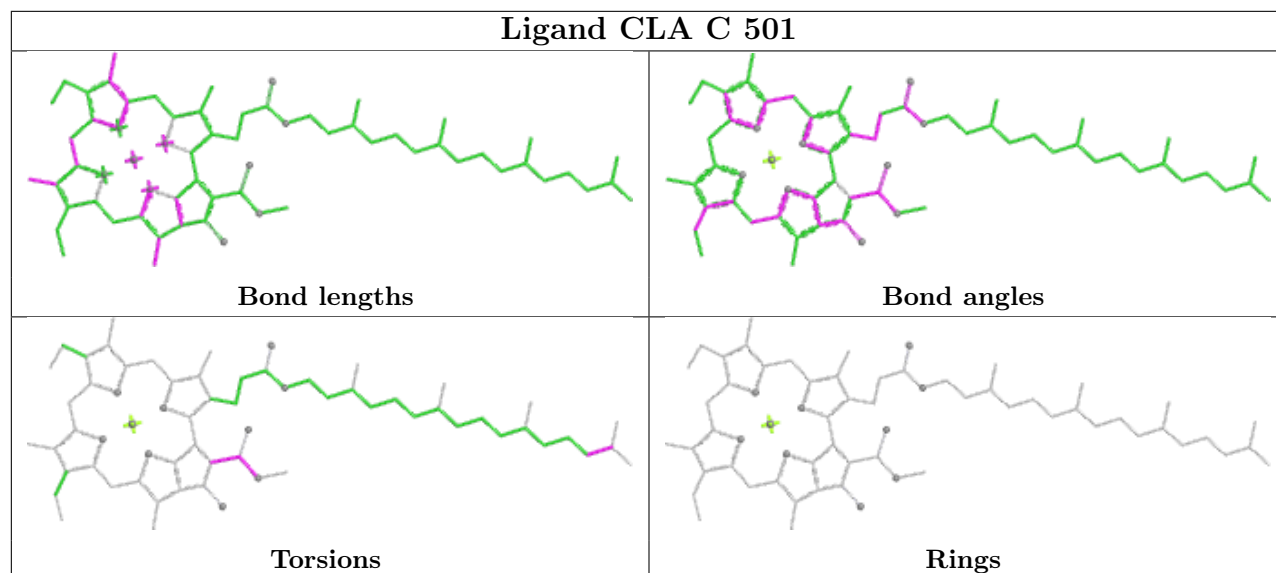
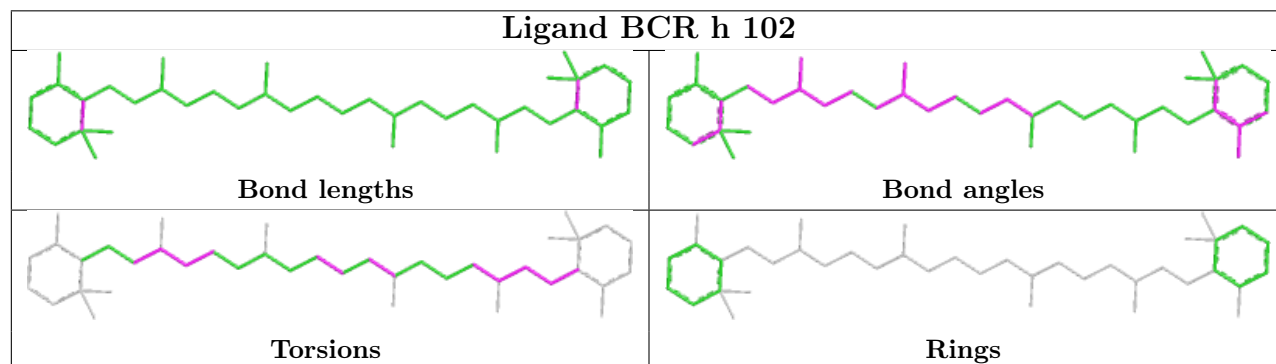
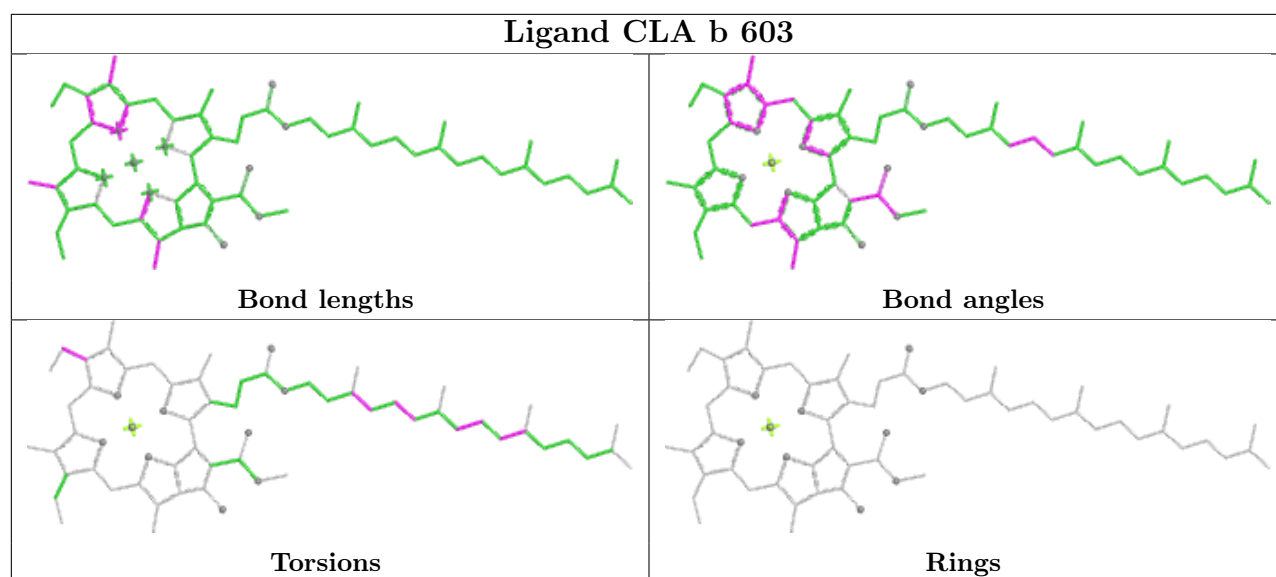


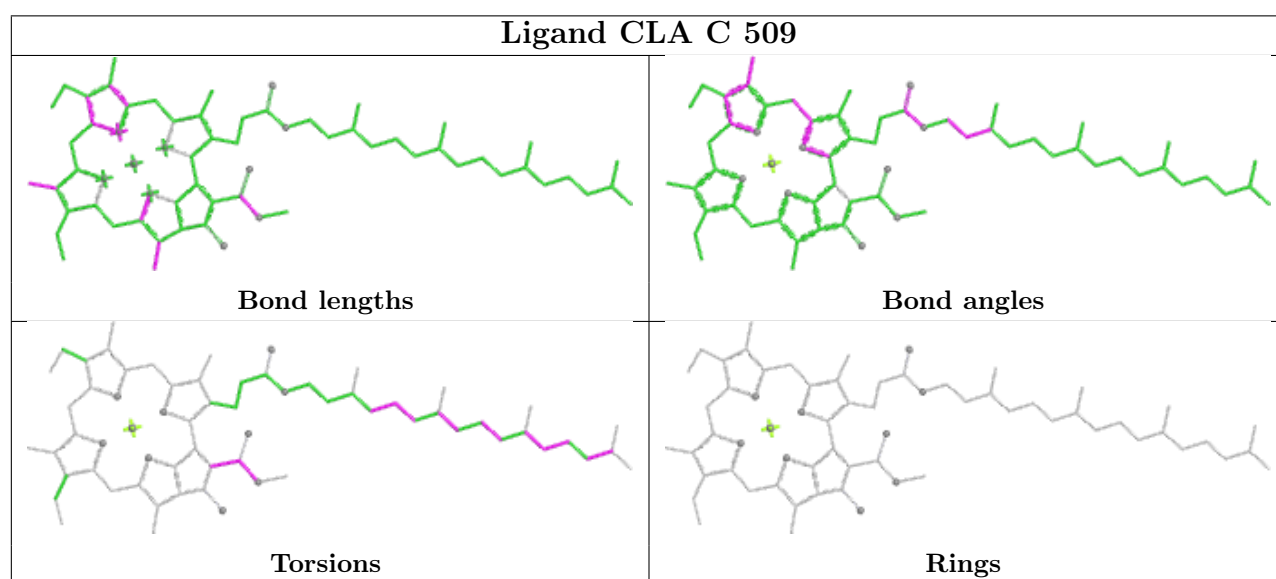
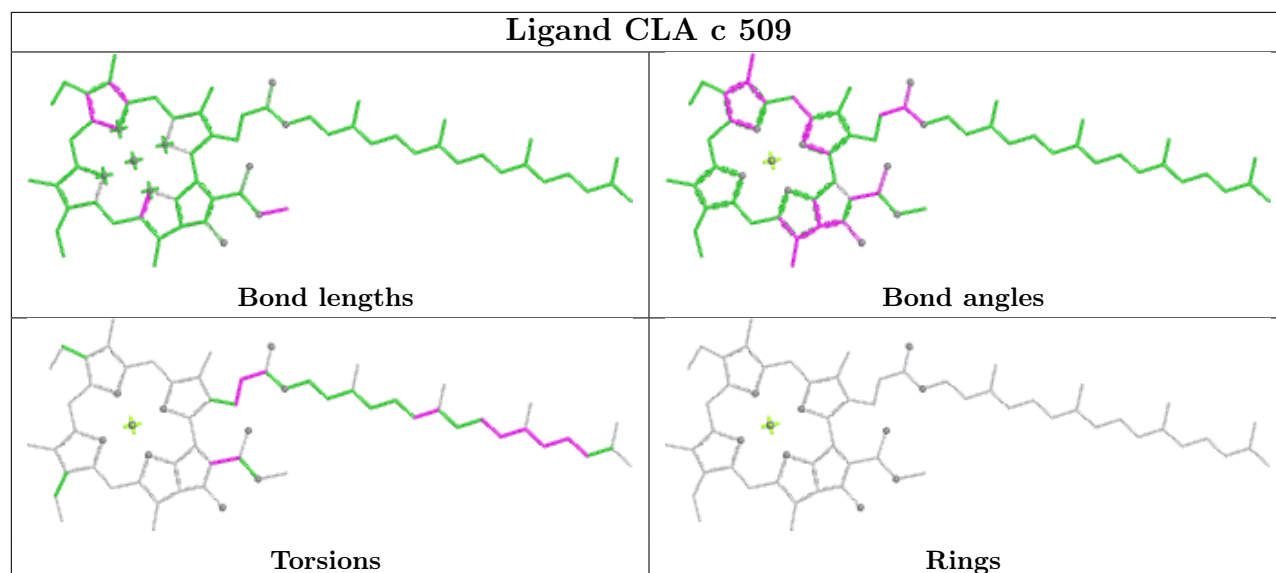
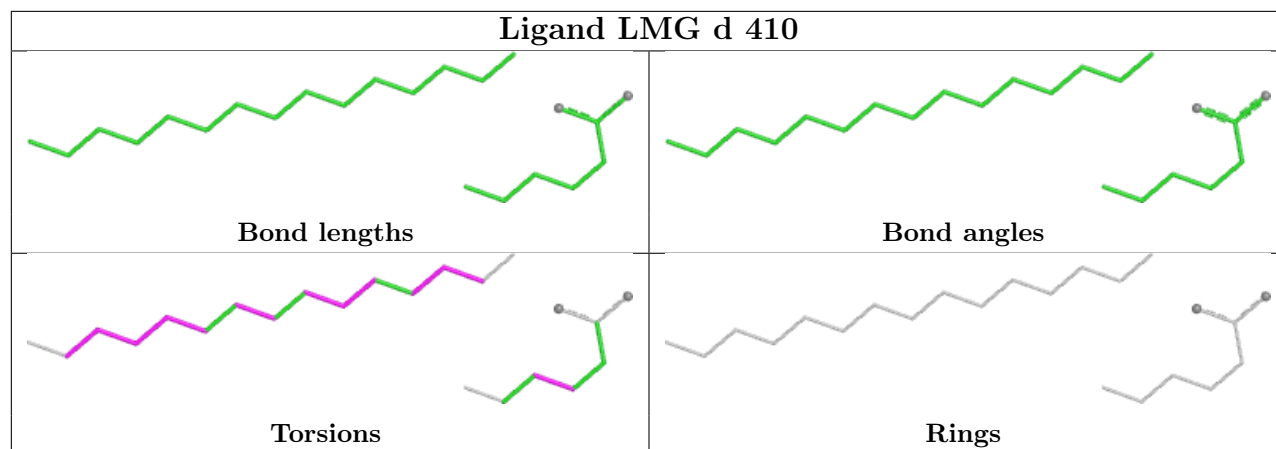
Ligand CLA B 603**Ligand CLA b 609****Ligand CLA C 503**

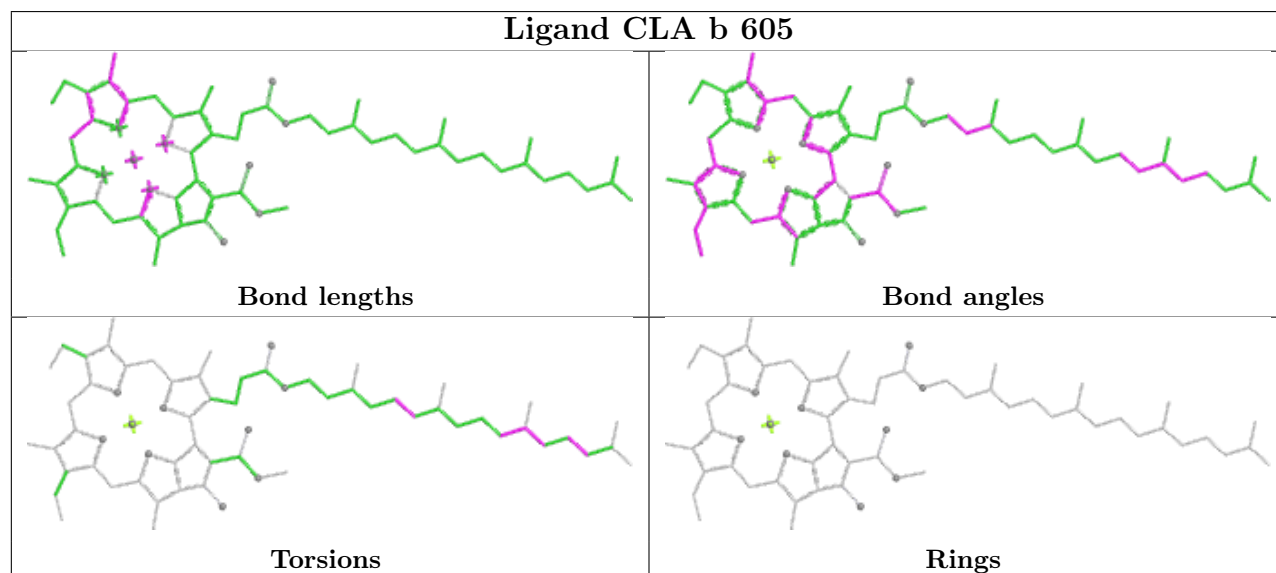
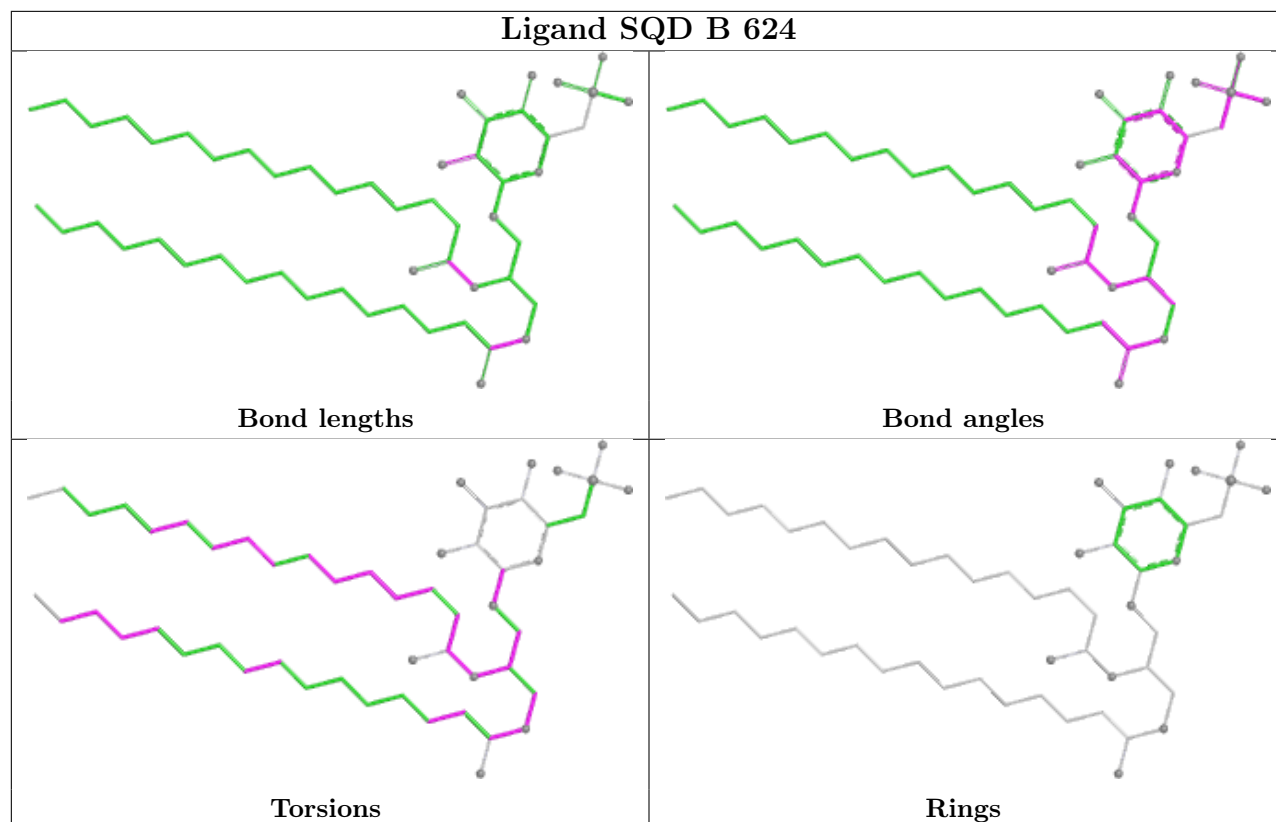


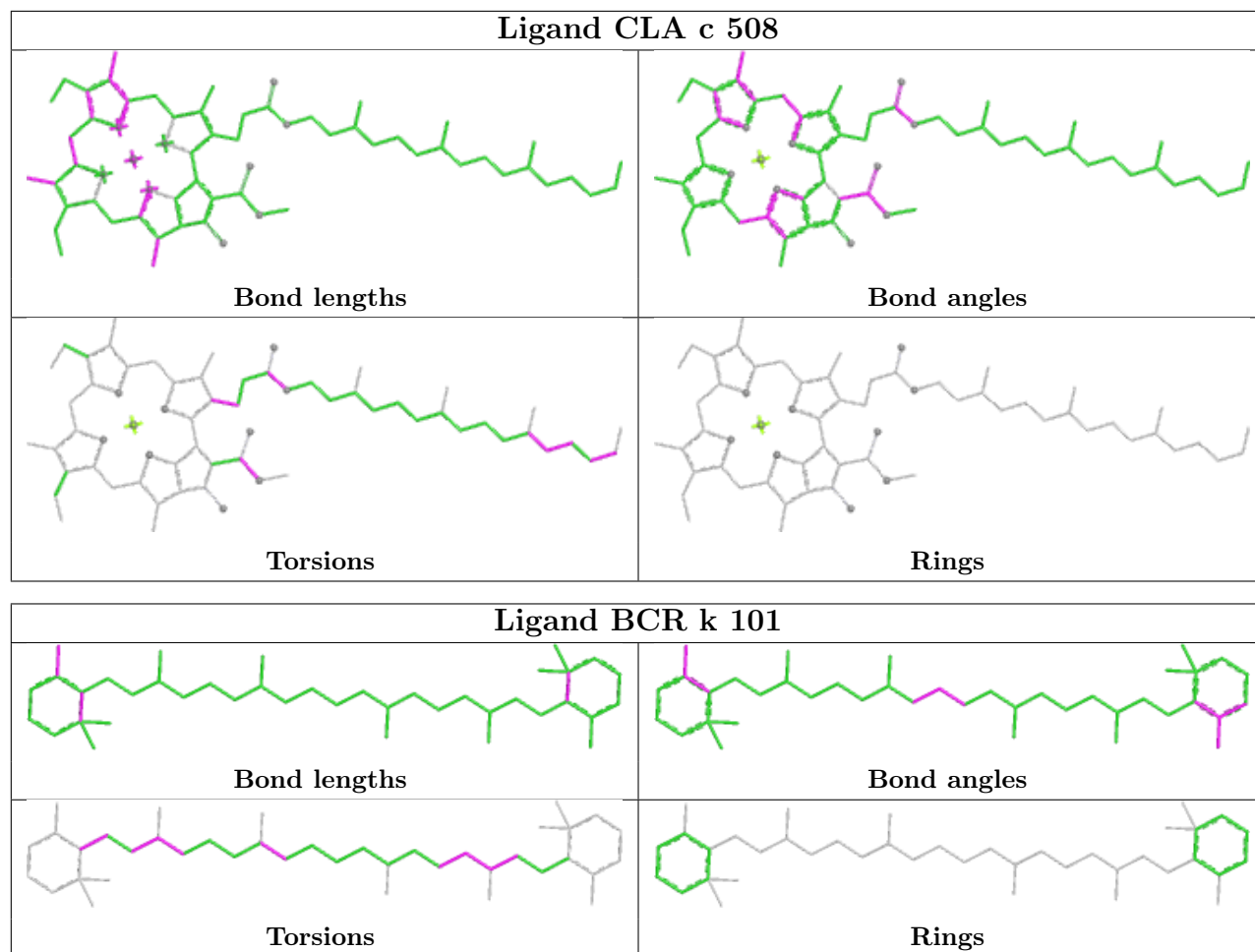




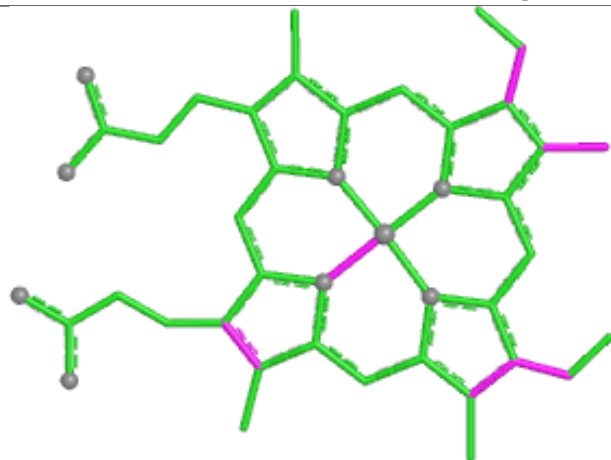




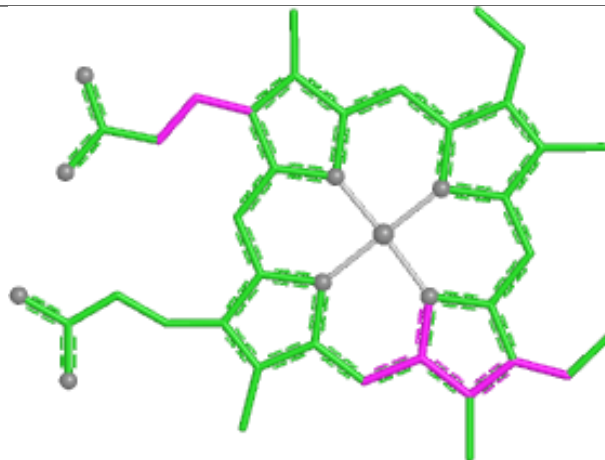




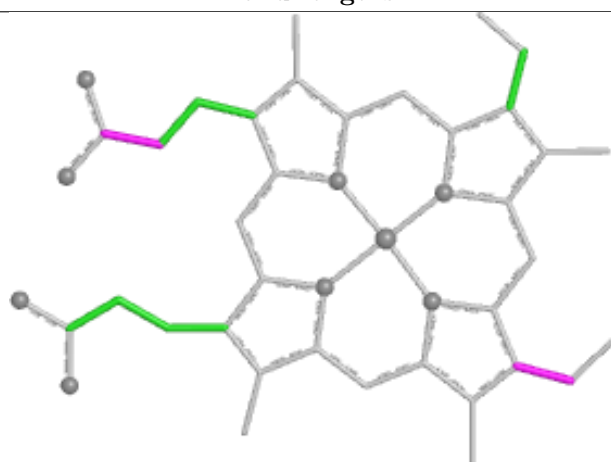
Ligand HEM f 102



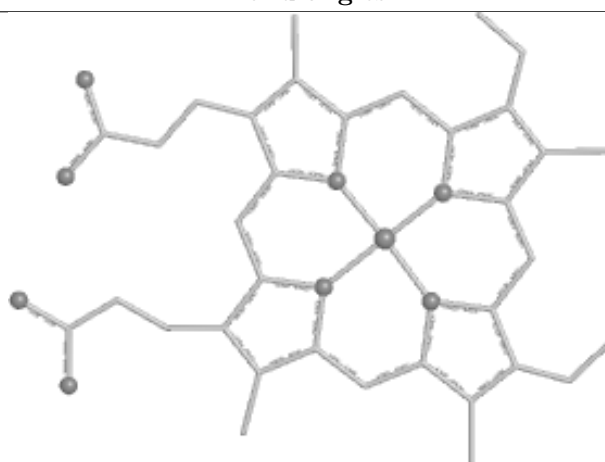
Bond lengths



Bond angles

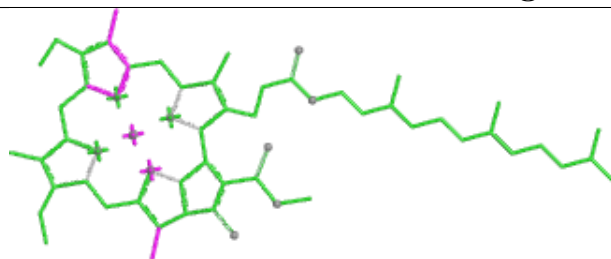


Torsions

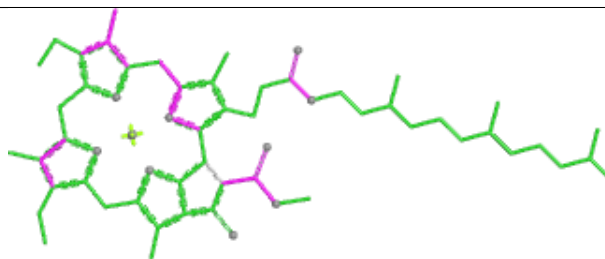


Rings

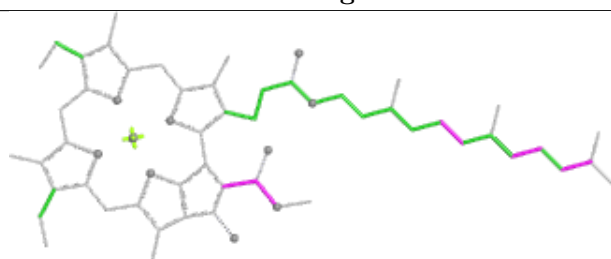
Ligand CLA c 504



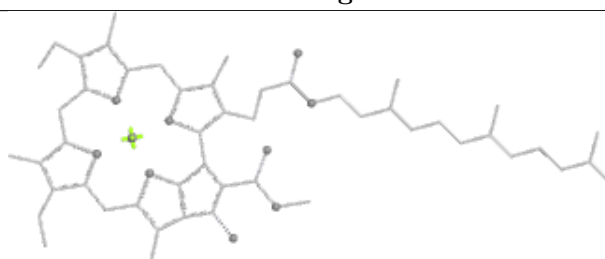
Bond lengths



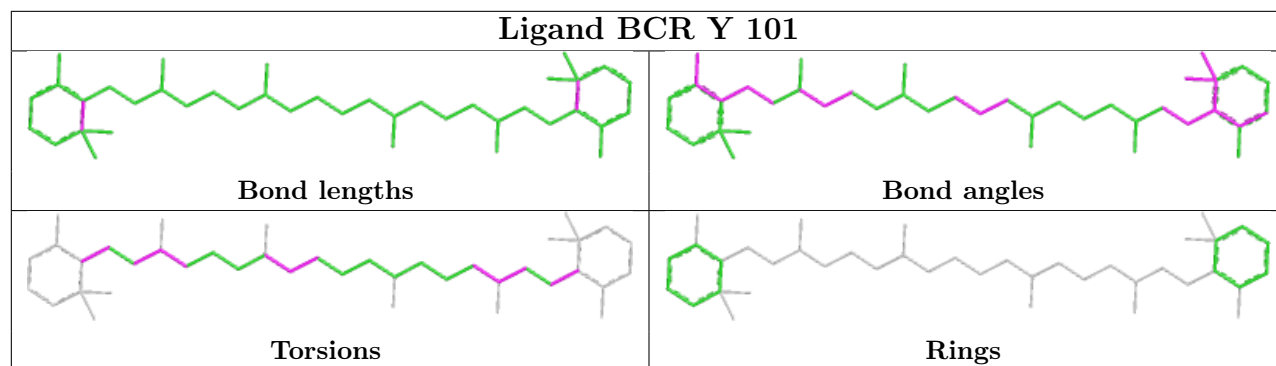
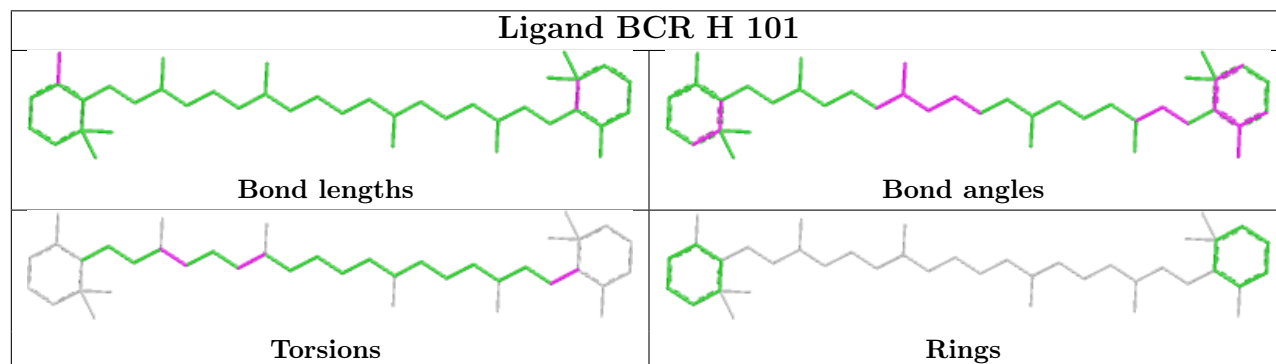
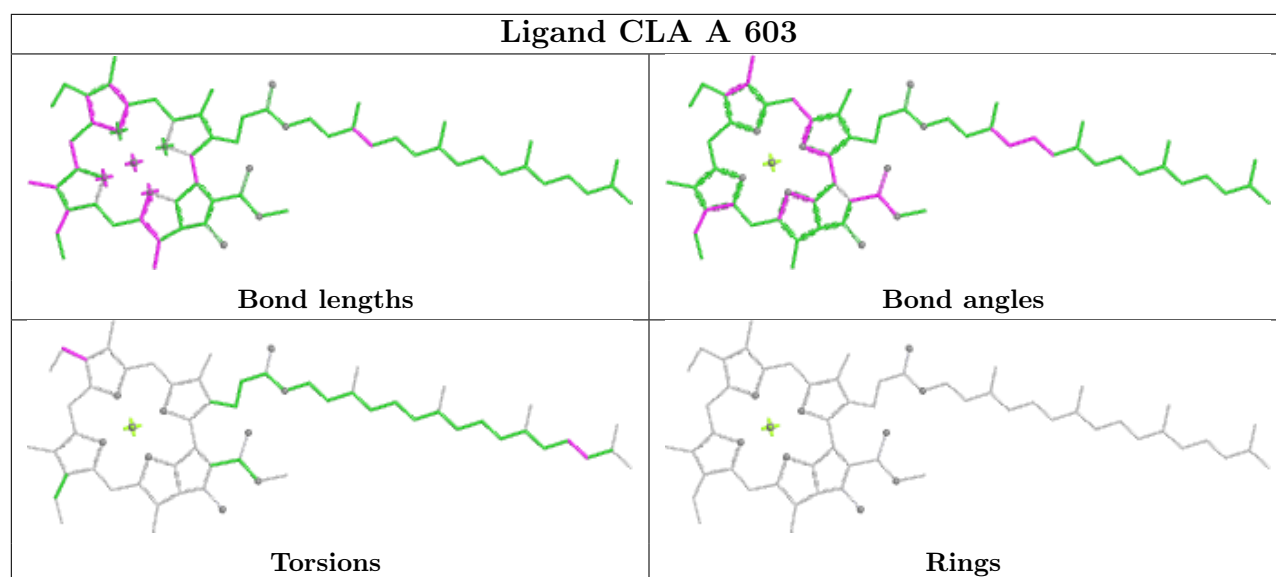
Bond angles

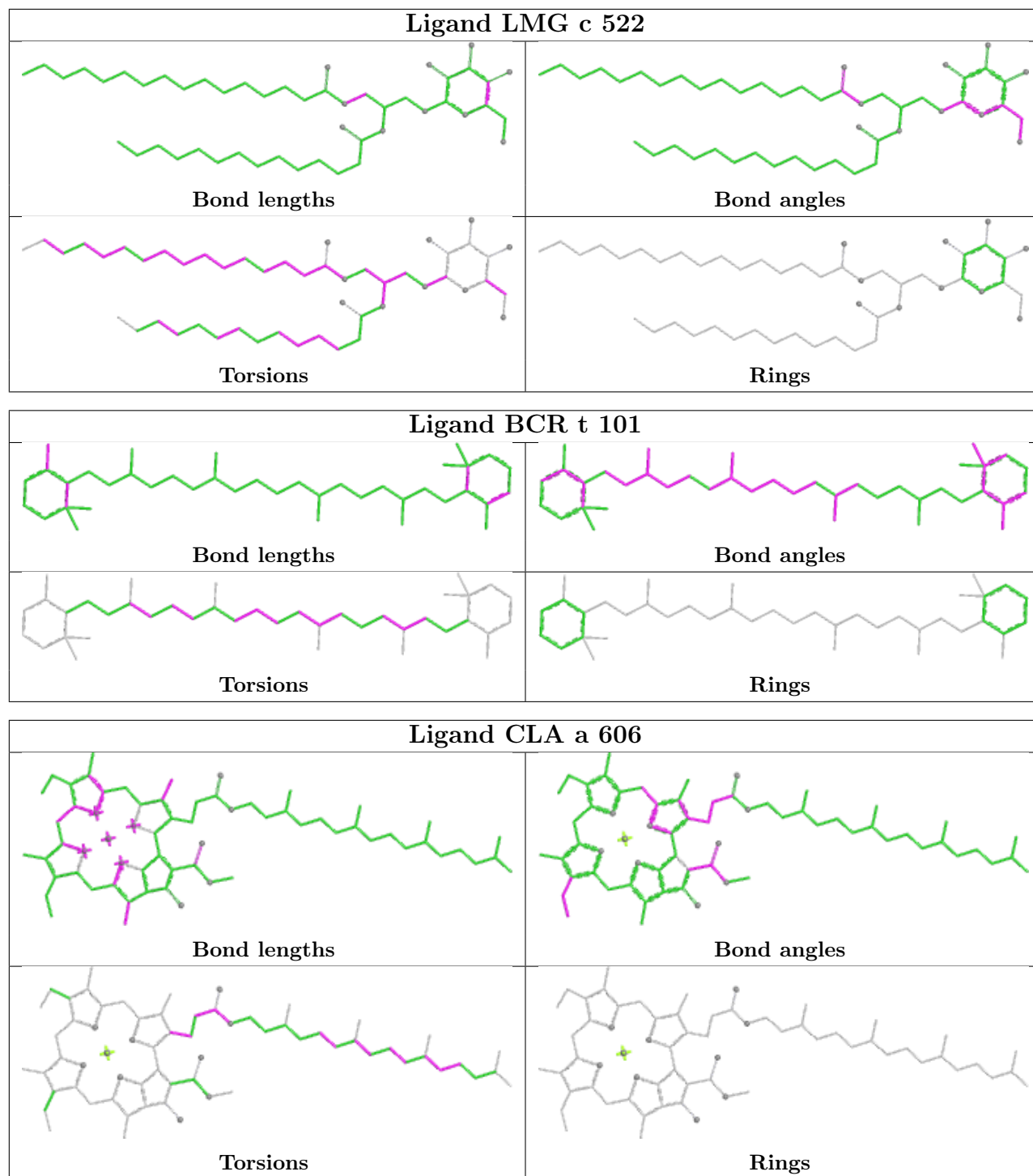


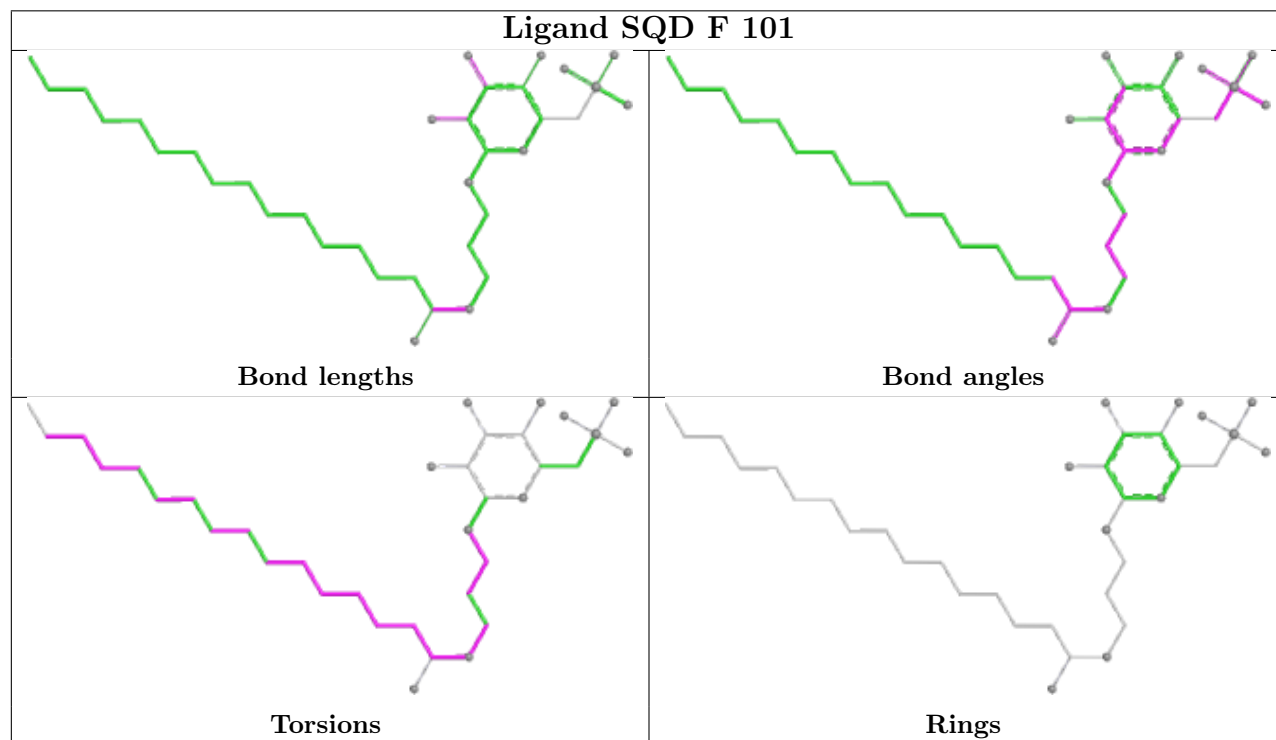
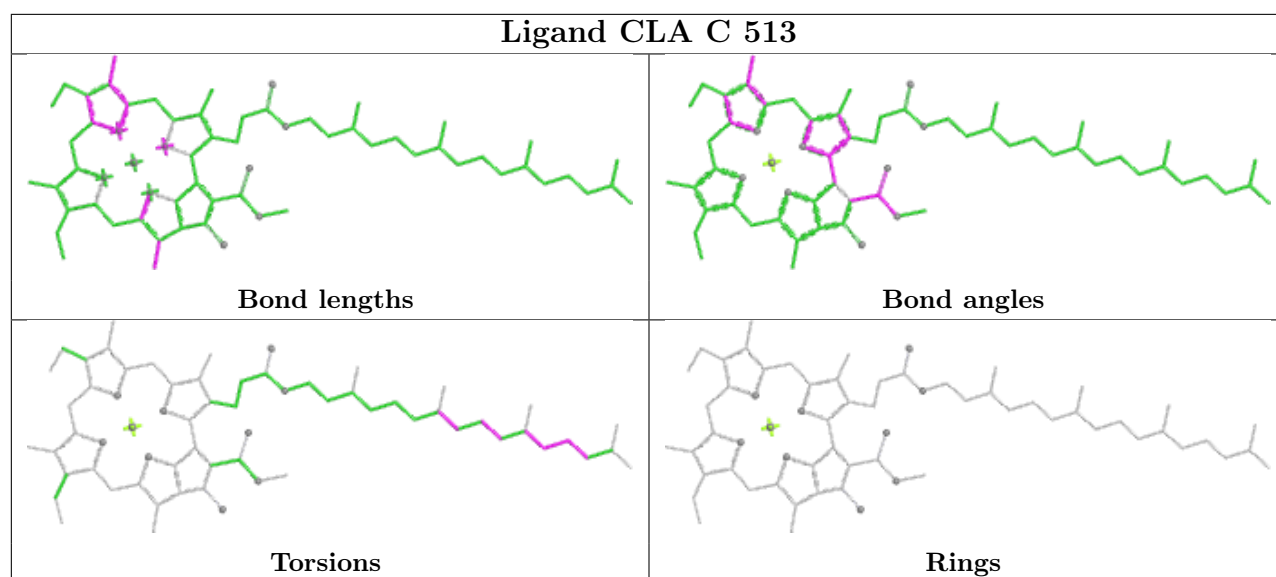
Torsions

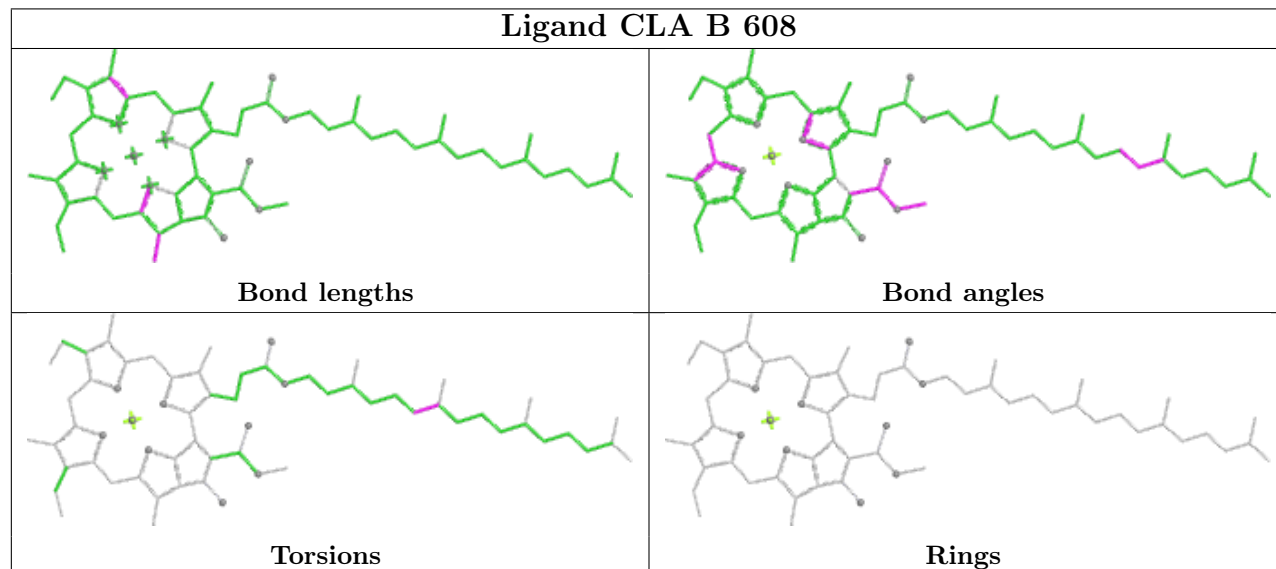
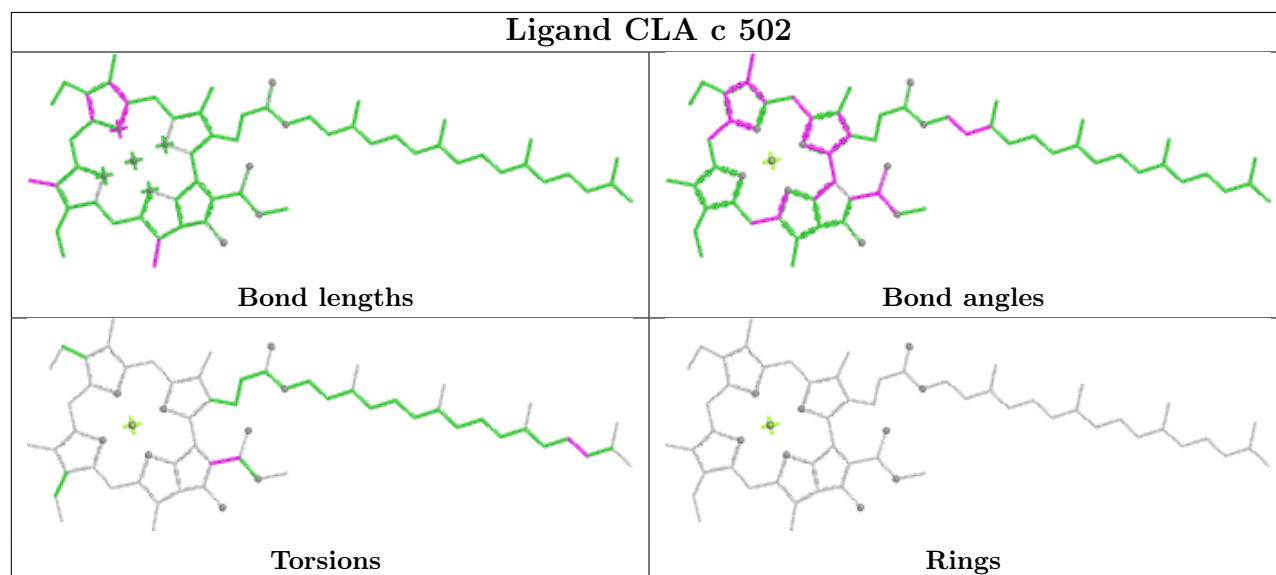
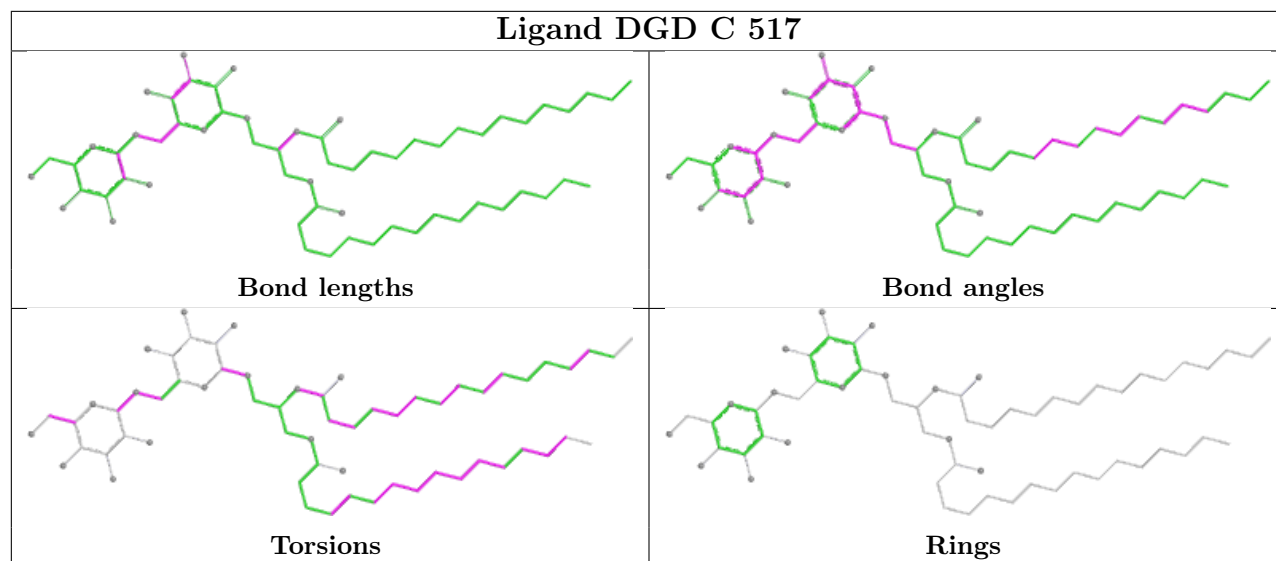


Rings

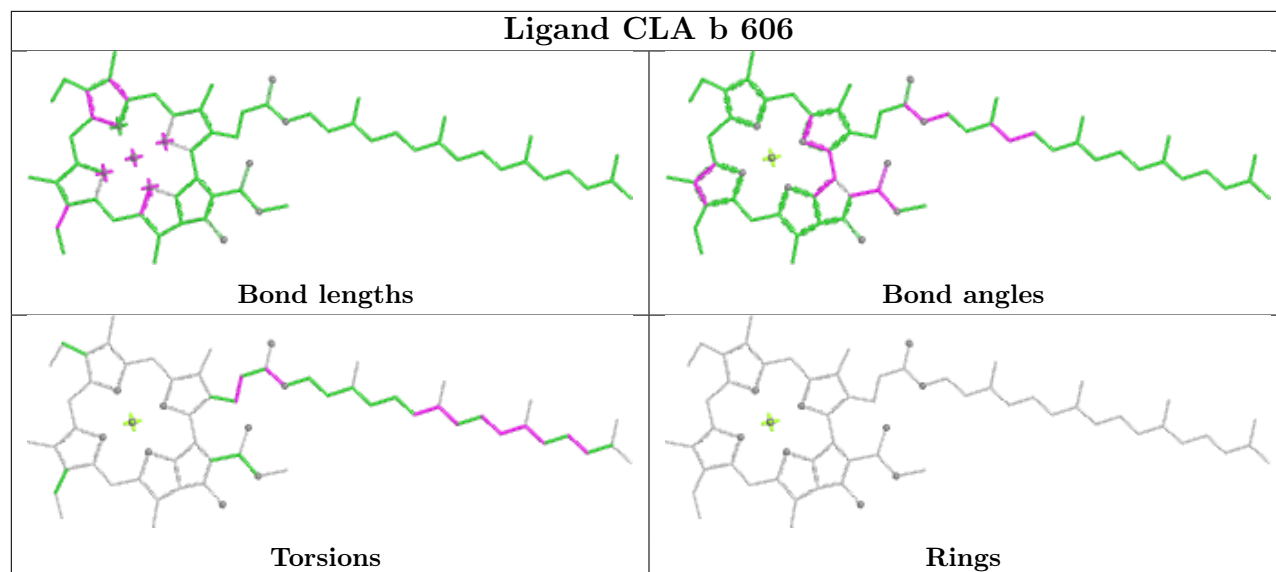




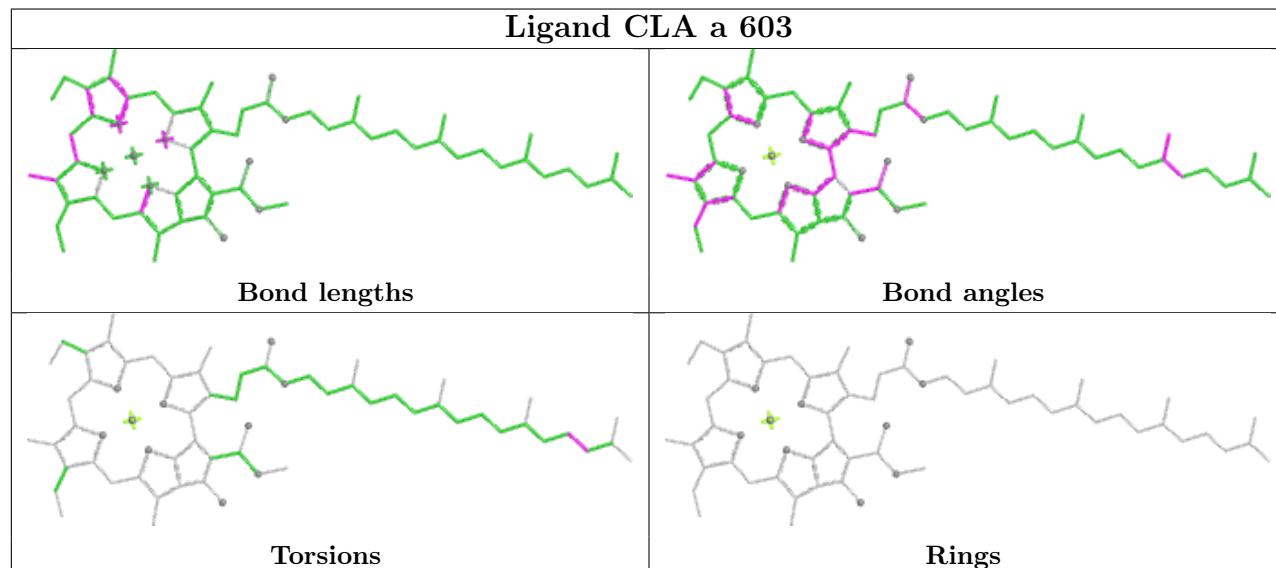




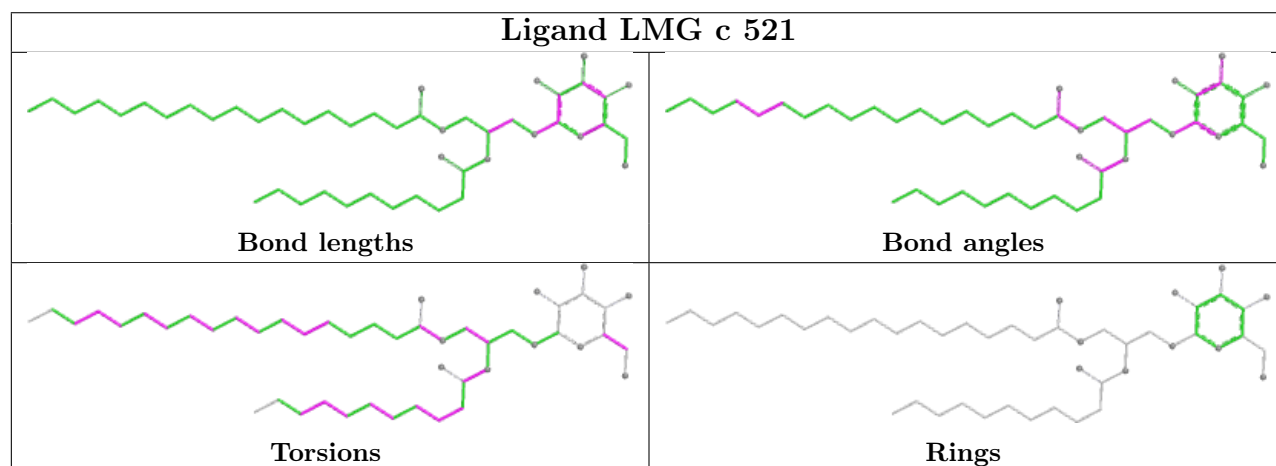
Ligand CLA b 606

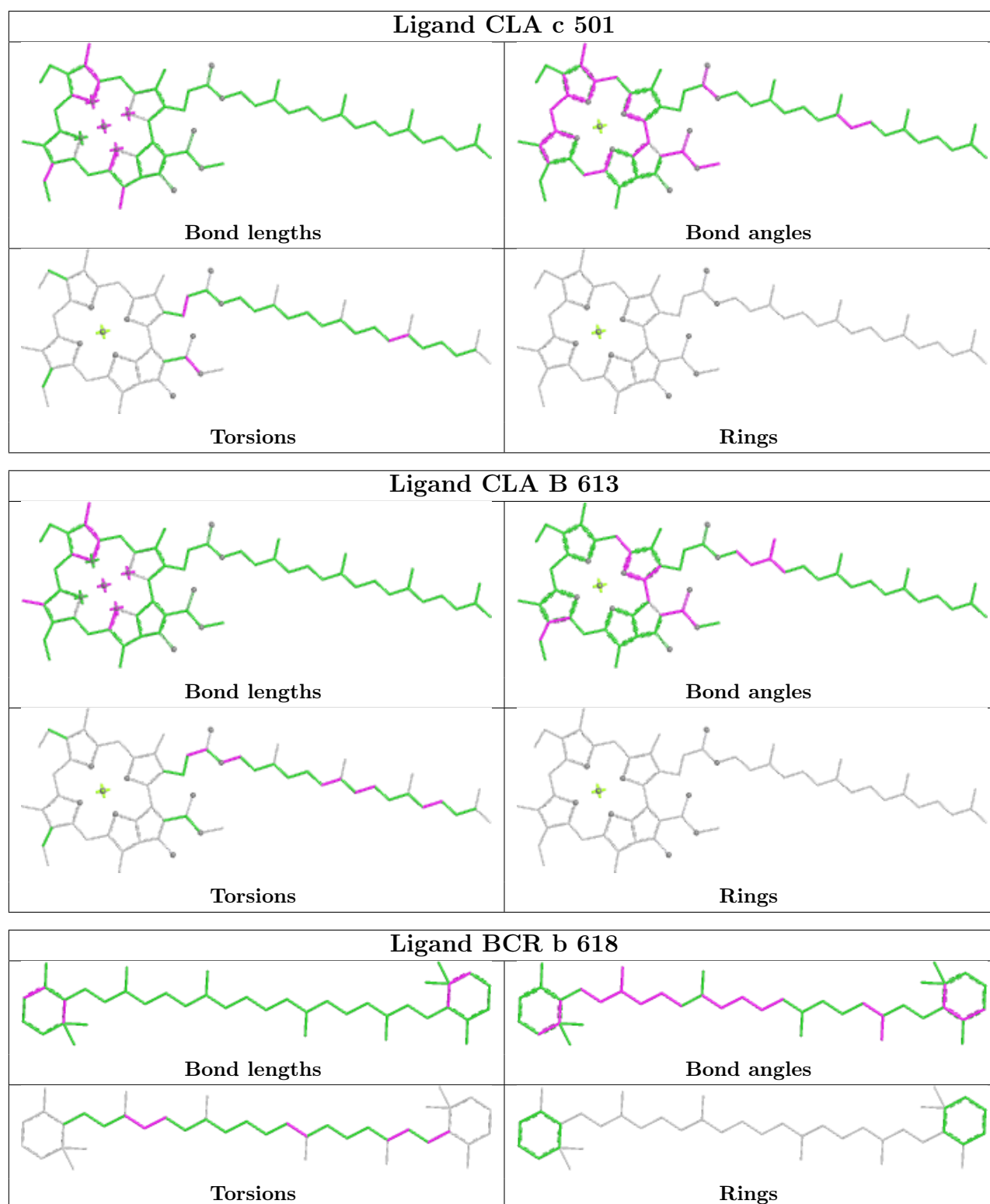


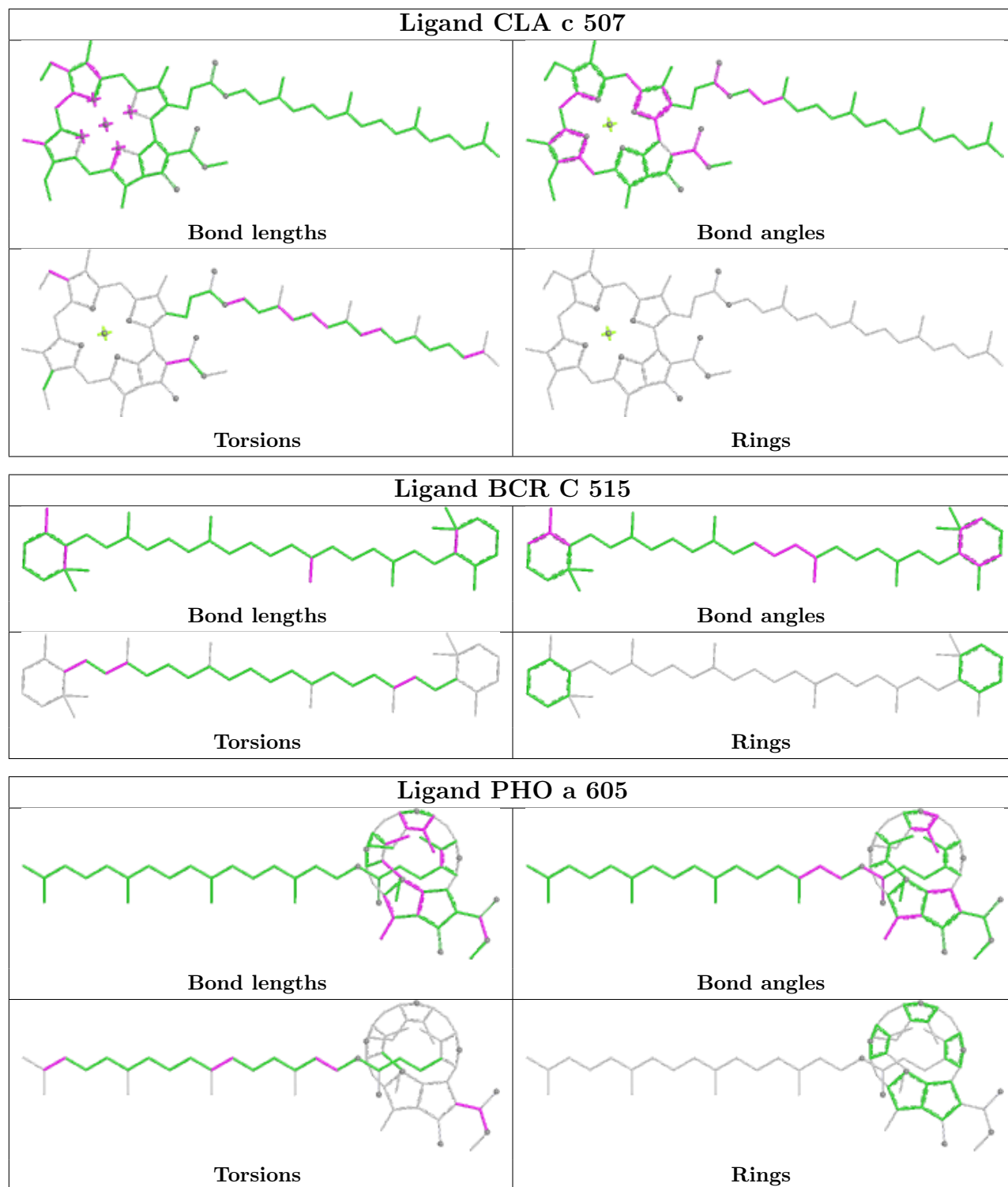
Ligand CLA a 603



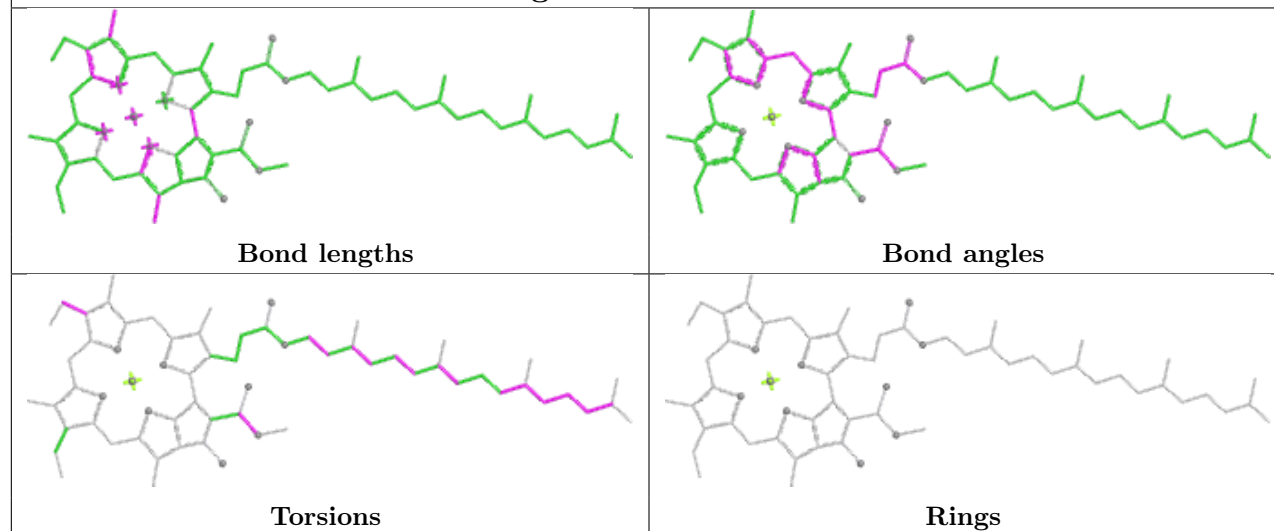
Ligand LMG c 521



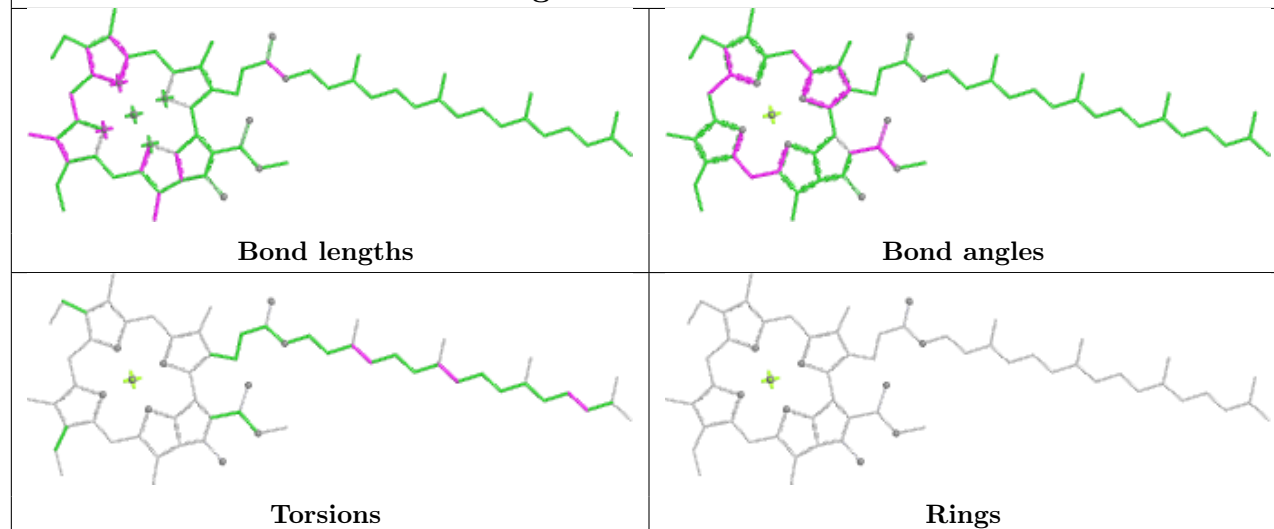


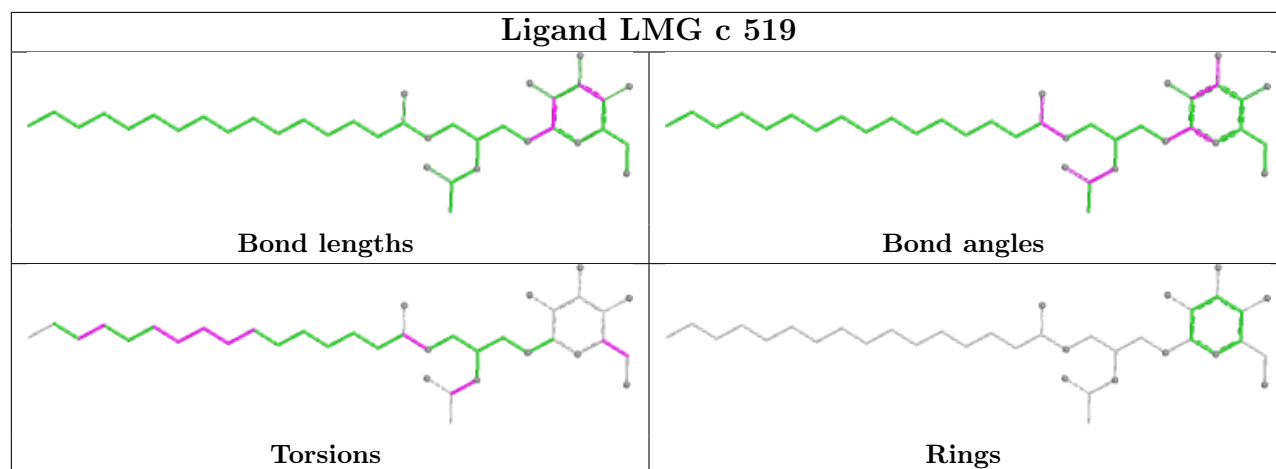
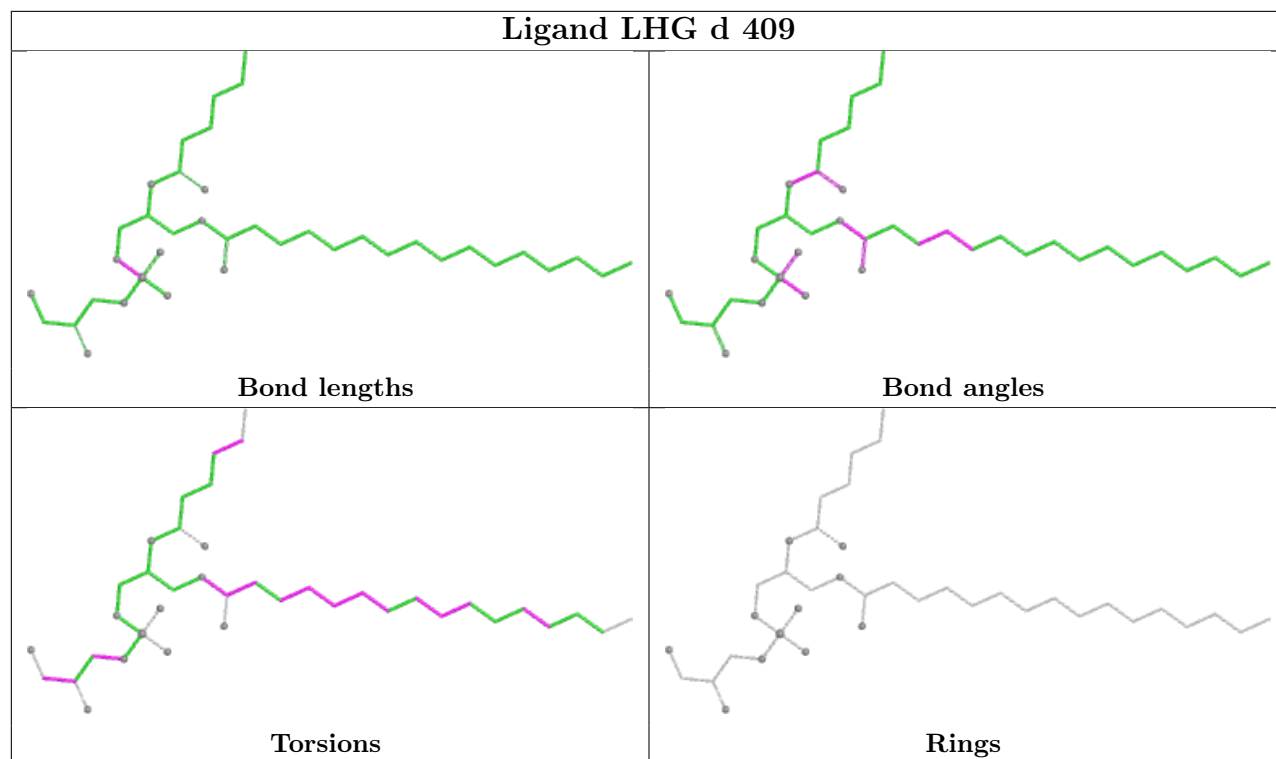


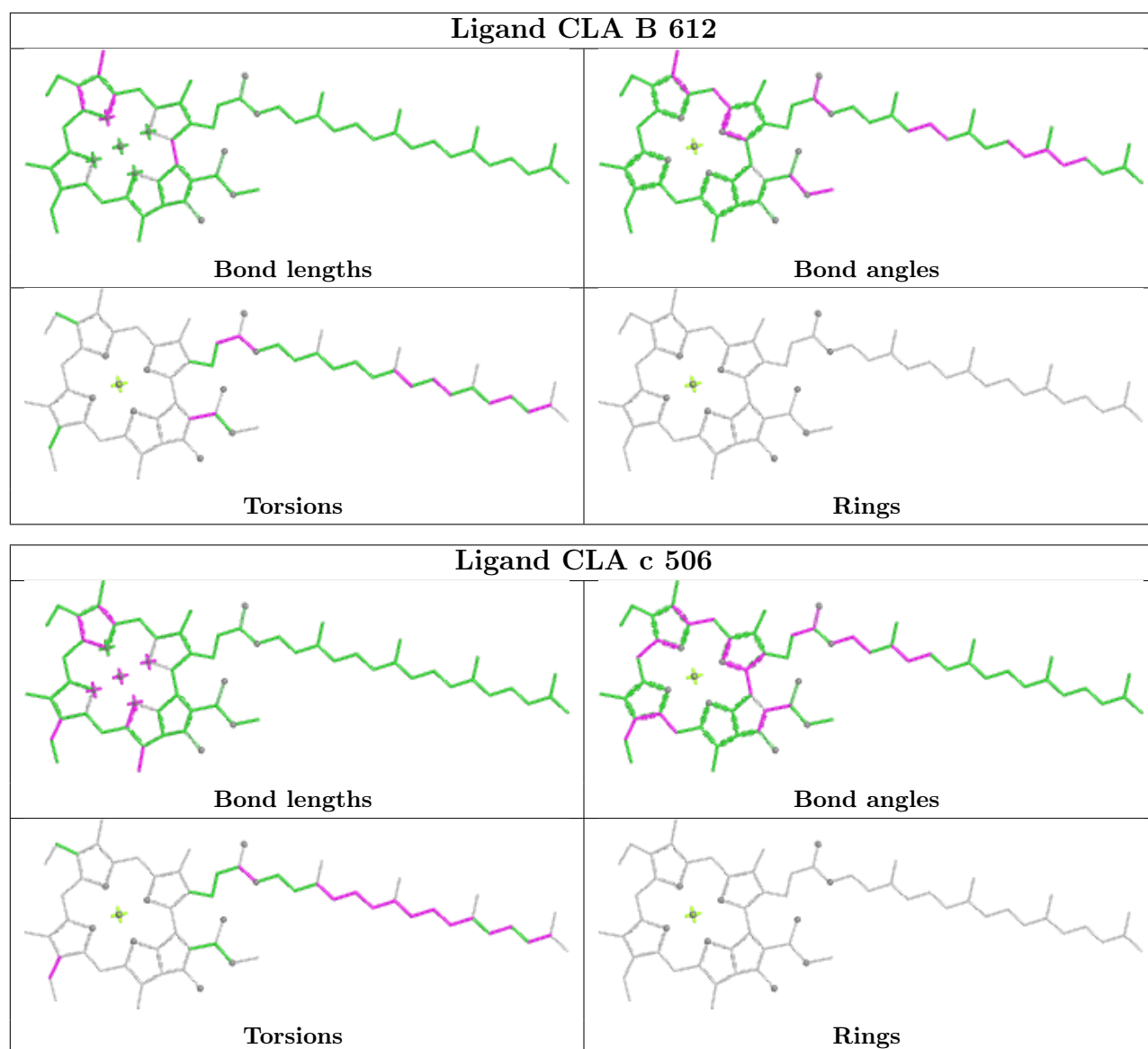
Ligand CLA D 403



Ligand CLA C 510







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%)	-0.69	1 (0%) 90 92	12, 28, 50, 81	59 (17%)
1	a	334/334 (100%)	-0.59	1 (0%) 90 92	12, 31, 62, 85	59 (17%)
2	B	505/505 (100%)	-0.55	0 100 100	15, 34, 65, 106	4 (0%)
2	b	505/505 (100%)	-0.42	3 (0%) 85 87	24, 38, 77, 118	0
3	C	442/451 (98%)	-0.49	1 (0%) 91 93	13, 37, 57, 81	7 (1%)
3	c	451/451 (100%)	-0.39	3 (0%) 84 85	14, 42, 66, 107	8 (1%)
4	D	341/341 (100%)	-0.69	0 100 100	15, 31, 50, 95	1 (0%)
4	d	341/341 (100%)	-0.53	0 100 100	16, 35, 62, 86	2 (0%)
5	E	81/82 (98%)	0.03	0 100 100	29, 54, 75, 95	1 (1%)
5	e	82/82 (100%)	0.21	0 100 100	40, 62, 90, 98	0
6	F	34/34 (100%)	-0.22	0 100 100	35, 45, 64, 83	0
6	f	34/34 (100%)	0.16	0 100 100	45, 54, 87, 94	0
7	H	65/65 (100%)	-0.33	0 100 100	33, 41, 64, 80	0
7	h	63/65 (96%)	-0.03	1 (1%) 70 72	40, 53, 63, 76	0
8	I	35/36 (97%)	-0.39	0 100 100	30, 39, 71, 82	0
8	i	35/36 (97%)	-0.26	0 100 100	33, 43, 75, 80	0
9	J	36/36 (100%)	-0.18	0 100 100	35, 51, 82, 102	0
9	j	36/36 (100%)	0.08	0 100 100	39, 54, 91, 99	0
10	K	37/37 (100%)	0.03	1 (2%) 56 58	32, 54, 73, 76	1 (2%)
10	k	37/37 (100%)	0.21	0 100 100	48, 61, 77, 86	0
11	L	37/37 (100%)	-0.75	0 100 100	24, 30, 71, 74	0
11	l	36/37 (97%)	-0.66	0 100 100	24, 32, 74, 86	0
12	M	32/33 (96%)	-0.53	0 100 100	27, 35, 66, 77	0
12	m	31/33 (93%)	-0.52	0 100 100	28, 37, 52, 72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.33	0 100 100	22, 44, 88, 150	1 (0%)
13	o	244/244 (100%)	-0.34	2 (0%) 82 84	24, 42, 83, 145	0
14	R	34/34 (100%)	0.66	1 (2%) 53 55	62, 76, 92, 100	0
14	r	31/34 (91%)	1.14	3 (9%) 13 13	70, 95, 107, 116	0
15	T	29/30 (96%)	-0.67	1 (3%) 48 48	26, 33, 63, 78	0
15	t	29/30 (96%)	-0.50	1 (3%) 48 48	25, 32, 83, 97	0
16	U	97/97 (100%)	-0.30	0 100 100	32, 44, 72, 102	0
16	u	97/97 (100%)	-0.34	1 (1%) 79 81	30, 42, 59, 94	0
17	V	137/137 (100%)	-0.45	0 100 100	27, 42, 59, 85	0
17	v	137/137 (100%)	-0.20	1 (0%) 84 85	34, 49, 76, 87	0
18	X	38/38 (100%)	-0.02	1 (2%) 57 59	39, 54, 81, 95	0
18	x	38/38 (100%)	0.12	0 100 100	49, 65, 91, 106	0
19	Y	27/30 (90%)	0.93	2 (7%) 20 21	56, 81, 125, 130	0
19	y	30/30 (100%)	0.59	1 (3%) 49 49	63, 80, 108, 113	0
20	Z	62/62 (100%)	0.58	3 (4%) 35 36	53, 70, 123, 142	0
20	z	62/62 (100%)	0.78	6 (9%) 13 13	57, 76, 123, 135	0
All	All	5300/5326 (99%)	-0.38	34 (0%) 85 87	12, 39, 79, 150	143 (2%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	z	33	TRP	3.3
14	R	35	LEU	3.2
16	u	53	ALA	2.7
1	A	13	LEU	2.7
18	X	2	THR	2.7
3	c	23	ALA	2.6
19	Y	22	LEU	2.6
15	t	30	THR	2.6
14	r	26	TYR	2.5
1	a	11	ALA	2.5
2	b	495	PHE	2.5
14	r	14	LEU	2.4
19	Y	20	ALA	2.4
10	K	46[A]	ARG	2.3
19	y	41	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	z	3	ILE	2.2
20	Z	62	VAL	2.2
13	o	58	ASN	2.2
20	Z	41	PHE	2.2
20	z	27	TYR	2.2
7	h	64	ALA	2.1
2	b	486	LEU	2.1
20	z	60	PHE	2.1
14	r	28	VAL	2.1
17	v	21	LEU	2.1
13	o	56	PRO	2.1
2	b	499	VAL	2.1
20	Z	4	LEU	2.0
3	c	24	THR	2.0
20	z	30	PRO	2.0
3	c	134	ILE	2.0
20	z	17	PHE	2.0
15	T	30	THR	2.0
3	C	143	TYR	2.0

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

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	0.08	36,45,71,81	0
15	FME	T	1	10/11	0.95	0.10	27,45,71,71	0
8	FME	i	1	10/11	0.95	0.07	35,43,56,58	0
8	FME	I	1	10/11	0.96	0.06	34,47,61,64	0
15	FME	t	1	10/11	0.96	0.07	19,33,65,69	0
12	FME	m	1	10/11	0.97	0.08	26,49,72,73	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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
33	UNL	b	624	26/-	0.77	0.16	39,54,65,72	0
33	UNL	H	103	53/-	0.79	0.14	45,74,95,103	0
30	LHG	A	615	49/49	0.82	0.13	48,80,108,117	0
33	UNL	c	523	28/-	0.82	0.11	45,67,86,88	0
28	LMG	c	521	48/55	0.83	0.14	39,81,114,121	0
33	UNL	b	623	55/-	0.83	0.12	42,64,85,85	0
28	LMG	D	409	33/55	0.84	0.12	34,53,93,95	0
33	UNL	J	101	28/-	0.84	0.12	48,62,68,70	0
33	UNL	a	617	28/-	0.84	0.11	42,65,78,78	0
28	LMG	b	621	55/55	0.84	0.14	40,76,103,112	0
31	DGD	A	617	66/66	0.84	0.12	42,64,85,111	0
33	UNL	E	101	28/-	0.84	0.12	45,71,88,95	0
30	LHG	a	614	42/49	0.85	0.12	58,86,109,122	0
33	UNL	T	103	44/-	0.85	0.14	38,57,79,84	0
33	UNL	B	627	47/-	0.85	0.14	44,63,79,79	0
33	UNL	d	411	43/-	0.85	0.13	39,55,66,70	0
33	UNL	t	103	26/-	0.85	0.12	35,59,76,83	0
33	UNL	x	101	55/-	0.85	0.11	39,58,75,75	0
28	LMG	d	410	23/55	0.86	0.15	31,71,94,98	0
33	UNL	B	628	28/-	0.86	0.17	52,70,102,107	0
27	PL9	A	611	55/55	0.86	0.14	35,58,81,84	135
27	PL9	a	611	55/55	0.86	0.14	38,69,88,94	0
28	LMG	B	622	28/55	0.86	0.12	31,48,58,63	0
33	UNL	j	101	28/-	0.86	0.12	46,61,70,74	0
33	UNL	T	102	47/-	0.86	0.13	35,51,66,74	0
31	DGD	a	616	44/66	0.86	0.12	33,56,77,89	0
33	UNL	B	621	43/-	0.87	0.11	31,50,71,76	0
29	SQD	A	616	39/54	0.87	0.12	41,65,88,92	0
33	UNL	I	101	41/-	0.87	0.13	36,53,72,79	0
33	UNL	b	620	55/-	0.87	0.11	37,60,83,90	0
33	UNL	b	622	40/-	0.87	0.11	43,59,81,83	0
29	SQD	a	615	36/54	0.87	0.12	30,66,85,87	0
33	UNL	B	626	46/-	0.88	0.11	39,59,72,77	0
28	LMG	c	519	37/55	0.88	0.12	38,69,88,92	0
28	LMG	C	519	48/55	0.88	0.11	46,73,95,106	0
33	UNL	C	522	28/-	0.88	0.10	43,54,64,66	0
29	SQD	f	101	41/54	0.89	0.12	45,84,111,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	h	101	65/65	0.89	0.10	41,62,91,97	0
33	UNL	c	520	55/-	0.89	0.11	34,54,93,94	0
28	LMG	A	612	48/55	0.89	0.10	31,56,74,91	0
29	SQD	B	624	54/54	0.89	0.10	37,59,97,109	0
33	UNL	C	523	47/-	0.89	0.10	37,53,71,75	0
33	UNL	t	102	34/-	0.89	0.10	35,50,56,63	0
28	LMG	c	522	49/55	0.89	0.10	32,56,91,110	0
29	SQD	b	601	49/54	0.89	0.10	39,58,99,111	0
33	UNL	X	101	55/-	0.90	0.10	33,52,73,79	0
25	BCR	h	102	40/40	0.90	0.10	35,54,74,82	0
33	UNL	m	102	28/-	0.90	0.12	42,63,77,78	0
29	SQD	a	613	54/54	0.91	0.09	39,67,93,101	0
23	CLA	C	513	65/65	0.91	0.10	43,62,88,97	0
28	LMG	m	101	51/55	0.91	0.09	33,51,81,98	0
33	UNL	M	101	37/-	0.91	0.10	31,43,63,70	0
33	UNL	M	102	26/-	0.91	0.11	30,50,60,62	0
25	BCR	k	101	40/40	0.91	0.10	44,63,75,80	0
23	CLA	B	601	65/65	0.91	0.10	25,60,104,130	0
28	LMG	B	620	51/55	0.92	0.08	25,49,73,87	0
23	CLA	c	513	65/65	0.92	0.09	44,69,104,112	0
23	CLA	c	512	65/65	0.92	0.10	38,55,94,108	0
33	UNL	B	625	28/-	0.92	0.09	26,48,64,71	0
33	UNL	l	102	53/-	0.92	0.12	25,48,87,99	0
25	BCR	Y	101	40/40	0.92	0.09	33,53,73,76	0
25	BCR	c	514	40/40	0.92	0.09	39,60,71,72	0
25	BCR	d	404	40/40	0.92	0.08	32,51,90,97	0
33	UNL	C	521	28/-	0.92	0.09	28,40,53,66	0
25	BCR	C	514	40/40	0.93	0.09	35,54,66,68	0
25	BCR	D	404	40/40	0.93	0.09	28,43,98,109	0
25	BCR	H	101	40/40	0.93	0.07	29,45,59,68	0
29	SQD	A	614	52/54	0.93	0.09	31,58,84,89	0
30	LHG	d	409	39/49	0.93	0.09	27,47,66,70	0
25	BCR	k	102	40/40	0.93	0.10	36,51,72,74	0
31	DGD	C	517	62/66	0.93	0.09	32,51,107,118	0
31	DGD	H	102	62/66	0.93	0.09	30,48,61,73	0
23	CLA	c	511	65/65	0.93	0.10	36,54,72,75	0
31	DGD	c	517	62/66	0.93	0.08	29,50,83,96	0
31	DGD	h	103	62/66	0.93	0.08	31,48,61,74	0
29	SQD	F	101	36/54	0.93	0.10	45,67,87,92	0
25	BCR	b	618	40/40	0.93	0.07	25,37,53,60	0
23	CLA	C	512	65/65	0.93	0.09	31,53,103,112	0
31	DGD	c	518	62/66	0.94	0.08	27,50,77,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	B	619	40/40	0.94	0.07	20,39,59,66	0
25	BCR	b	619	40/40	0.94	0.07	25,47,58,64	0
28	LMG	D	405	51/55	0.94	0.09	26,54,98,102	0
30	LHG	d	405	49/49	0.94	0.09	35,50,72,88	0
25	BCR	t	101	40/40	0.94	0.07	24,36,57,63	0
25	BCR	B	618	40/40	0.94	0.06	21,37,56,56	0
25	BCR	c	515	40/40	0.94	0.08	28,41,52,71	0
25	BCR	C	520	40/40	0.94	0.09	36,51,66,69	0
25	BCR	b	617	40/40	0.94	0.07	24,42,54,58	0
28	LMG	d	406	44/55	0.94	0.08	31,54,94,113	0
30	LHG	D	408	47/49	0.95	0.08	23,46,81,103	0
23	CLA	c	509	65/65	0.95	0.08	28,46,64,68	0
23	CLA	C	511	65/65	0.95	0.08	28,50,68,68	0
23	CLA	C	503	65/65	0.95	0.07	24,39,51,63	0
30	LHG	l	101	49/49	0.95	0.07	29,43,59,64	0
23	CLA	C	510	65/65	0.95	0.07	28,45,67,73	0
23	CLA	a	604	65/65	0.95	0.08	26,40,89,107	0
24	PHO	d	401	64/64	0.95	0.06	25,38,46,65	0
25	BCR	B	617	40/40	0.95	0.07	25,39,53,56	0
31	DGD	c	516	62/66	0.95	0.08	19,41,75,84	0
23	CLA	b	609	65/65	0.95	0.08	27,45,69,79	0
23	CLA	b	616	60/65	0.95	0.08	25,42,90,95	0
23	CLA	c	503	65/65	0.95	0.07	32,44,57,62	0
25	BCR	C	515	40/40	0.95	0.07	21,35,50,54	0
27	PL9	D	407	55/55	0.95	0.06	20,31,40,48	0
23	CLA	c	504	60/65	0.95	0.08	31,45,79,90	0
27	PL9	d	408	55/55	0.95	0.06	21,33,43,47	0
23	CLA	c	505	65/65	0.95	0.08	22,41,66,73	0
23	CLA	c	506	65/65	0.95	0.09	31,52,107,111	0
25	BCR	T	101	40/40	0.95	0.06	25,42,61,68	0
23	CLA	c	508	64/65	0.95	0.08	28,44,83,104	0
30	LHG	B	623	49/49	0.95	0.08	25,42,70,73	0
23	CLA	B	616	60/65	0.96	0.08	21,39,94,99	0
23	CLA	C	502	65/65	0.96	0.06	26,40,54,61	0
23	CLA	c	510	65/65	0.96	0.07	33,49,67,74	0
23	CLA	B	606	65/65	0.96	0.07	17,32,74,80	0
23	CLA	a	606	65/65	0.96	0.08	17,34,86,104	0
23	CLA	a	612	65/65	0.96	0.06	18,28,38,44	0
23	CLA	d	403	65/65	0.96	0.07	31,48,100,105	0
23	CLA	b	602	65/65	0.96	0.07	23,41,65,75	0
24	PHO	a	605	64/64	0.96	0.05	18,29,38,43	0
30	LHG	D	406	49/49	0.96	0.07	22,38,54,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	606	65/65	0.96	0.07	20,38,69,74	0
25	BCR	A	608	40/40	0.96	0.06	20,32,40,46	0
23	CLA	b	608	65/65	0.96	0.06	24,39,61,64	0
23	CLA	C	505	65/65	0.96	0.07	20,39,71,83	0
23	CLA	b	610	65/65	0.96	0.07	22,36,53,55	0
23	CLA	b	612	65/65	0.96	0.07	16,33,47,56	0
31	DGD	C	516	62/66	0.96	0.08	21,41,76,90	0
23	CLA	b	615	65/65	0.96	0.06	25,40,55,65	0
31	DGD	C	518	62/66	0.96	0.07	25,44,75,84	0
23	CLA	C	506	65/65	0.96	0.08	25,40,101,113	0
23	CLA	c	501	65/65	0.96	0.06	27,38,49,55	0
23	CLA	c	502	65/65	0.96	0.07	28,41,65,67	0
23	CLA	C	508	65/65	0.96	0.07	23,40,100,118	0
23	CLA	C	509	65/65	0.96	0.07	22,41,63,64	0
25	BCR	a	607	40/40	0.96	0.06	15,31,41,49	0
23	CLA	B	609	65/65	0.96	0.06	23,35,58,66	0
23	CLA	B	615	65/65	0.96	0.07	22,37,67,83	0
23	CLA	c	507	65/65	0.96	0.07	23,42,57,66	0
34	BCT	a	610	4/4	0.96	0.07	26,32,41,50	0
23	CLA	B	605	65/65	0.97	0.06	17,29,47,49	0
23	CLA	b	613	65/65	0.97	0.06	18,32,65,75	0
23	CLA	b	614	65/65	0.97	0.07	22,36,77,87	0
23	CLA	A	604	65/65	0.97	0.08	14,33,101,121	0
23	CLA	C	507	65/65	0.97	0.06	20,38,60,68	0
23	CLA	B	607	65/65	0.97	0.06	15,31,59,67	0
23	CLA	B	608	65/65	0.97	0.05	20,33,52,64	0
23	CLA	A	613	65/65	0.97	0.05	14,26,48,58	0
23	CLA	B	610	65/65	0.97	0.06	18,30,43,47	0
23	CLA	B	611	65/65	0.97	0.05	18,30,47,53	0
23	CLA	B	612	65/65	0.97	0.06	19,30,44,44	0
23	CLA	D	402	65/65	0.97	0.06	16,30,56,64	0
23	CLA	D	403	65/65	0.97	0.07	19,39,104,113	0
23	CLA	a	603	65/65	0.97	0.05	16,29,43,51	0
23	CLA	B	613	65/65	0.97	0.06	17,30,68,73	0
23	CLA	B	614	65/65	0.97	0.07	20,34,82,95	0
30	LHG	L	101	49/49	0.97	0.07	24,39,54,65	0
23	CLA	A	603	65/65	0.97	0.05	13,25,44,57	0
23	CLA	B	602	65/65	0.97	0.06	22,34,59,63	0
30	LHG	d	407	49/49	0.97	0.06	25,42,60,64	0
23	CLA	d	402	65/65	0.97	0.06	20,34,64,70	0
23	CLA	b	603	65/65	0.97	0.06	21,36,69,76	0
23	CLA	b	604	65/65	0.97	0.07	20,34,80,90	0

Continued on next page...

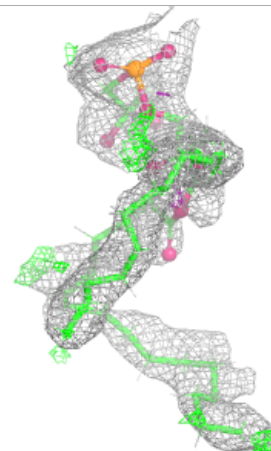
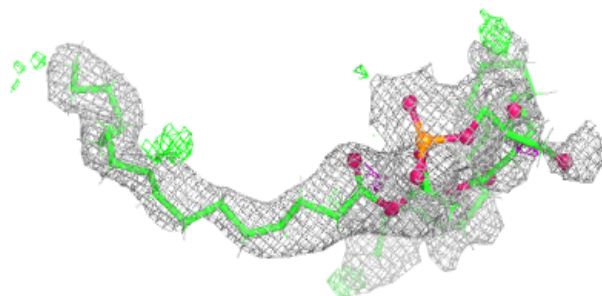
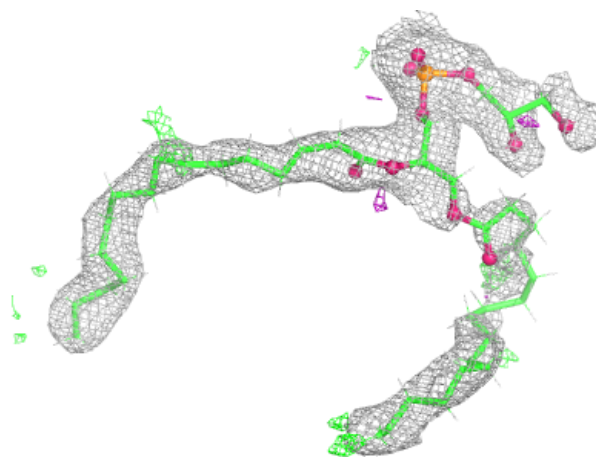
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	PHO	A	605	64/64	0.97	0.05	12,27,36,40	0
24	PHO	A	606	64/64	0.97	0.05	19,30,44,50	0
23	CLA	b	605	65/65	0.97	0.06	19,33,47,56	0
23	CLA	C	501	65/65	0.97	0.06	23,35,49,60	0
23	CLA	b	607	65/65	0.97	0.07	19,36,61,68	0
23	CLA	B	603	65/65	0.97	0.06	14,31,62,69	0
23	CLA	B	604	65/65	0.97	0.07	18,31,82,93	0
23	CLA	C	504	59/65	0.97	0.07	24,42,80,85	0
34	BCT	D	401	4/4	0.97	0.05	26,27,32,37	0
23	CLA	b	611	65/65	0.97	0.06	20,34,51,55	0
35	HEM	F	102	43/43	0.97	0.08	34,48,68,69	0
35	HEM	f	102	43/43	0.97	0.09	41,55,76,78	0
23	CLA	A	607	54/65	0.98	0.06	15,28,62,69	0
36	HEC	v	201	43/43	0.98	0.06	27,36,49,53	0
21	OEX	a	601[A]	10/10	0.99	0.03	19,22,28,28	10
26	CL	A	609	1/1	0.99	0.03	27,27,27,27	0
26	CL	A	610	1/1	0.99	0.03	24,24,24,24	0
26	CL	a	608	1/1	0.99	0.03	25,25,25,25	0
32	OEY	A	618[B]	11/11	0.99	0.03	23,27,30,31	11
32	OEY	a	618[B]	11/11	0.99	0.03	22,28,30,31	11
36	HEC	V	201	43/43	0.99	0.05	21,31,42,46	0
21	OEX	A	601[A]	10/10	0.99	0.03	21,25,28,32	10
22	FE2	a	602	1/1	1.00	0.02	30,30,30,30	0
22	FE2	A	602	1/1	1.00	0.01	25,25,25,25	0
26	CL	a	609	1/1	1.00	0.10	25,25,25,25	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.

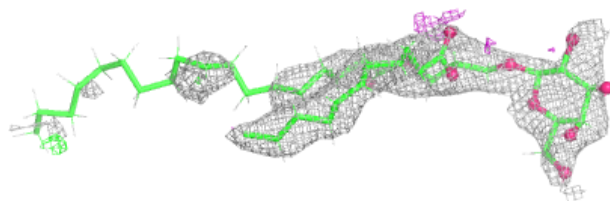
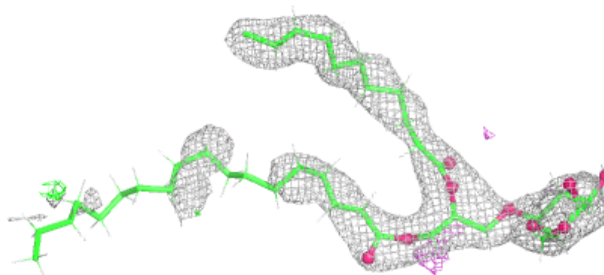
Electron density around LHG A 615:

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

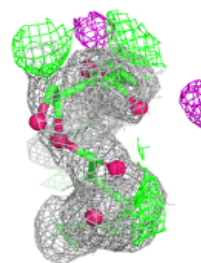
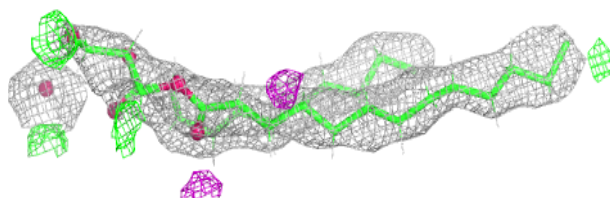
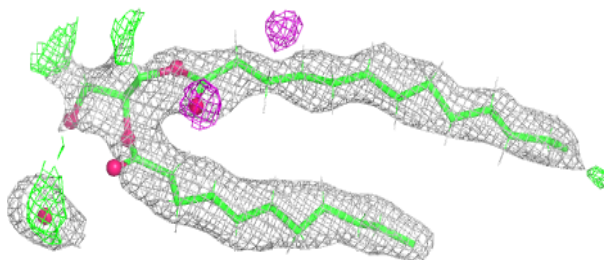


Electron density around LMG c 521:

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

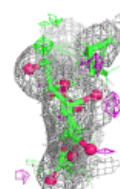
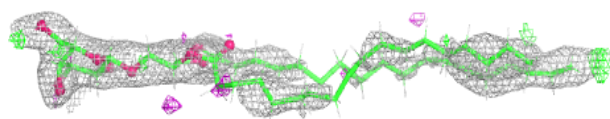
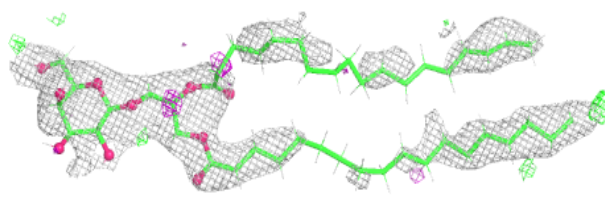
**Electron density around LMG D 409:**

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

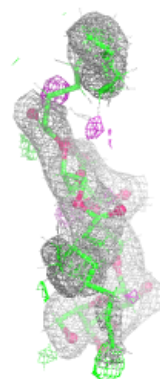
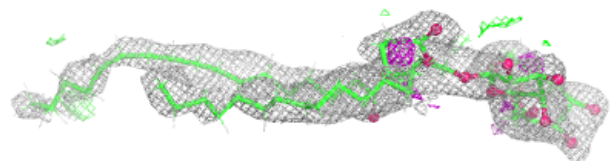
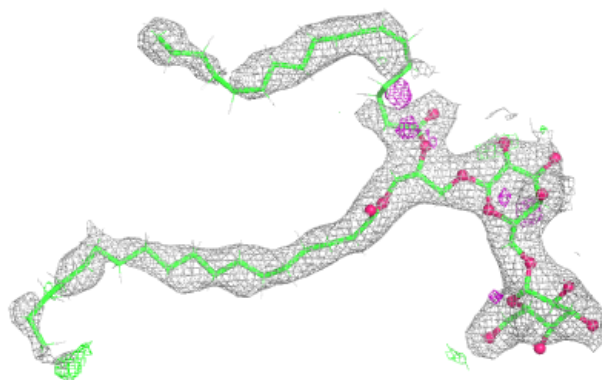


Electron density around LMG b 621:

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

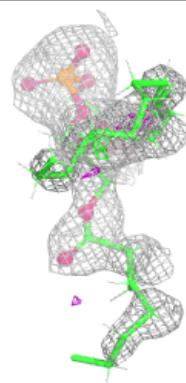
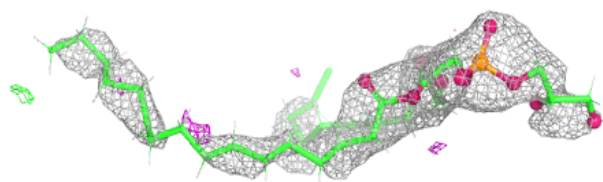
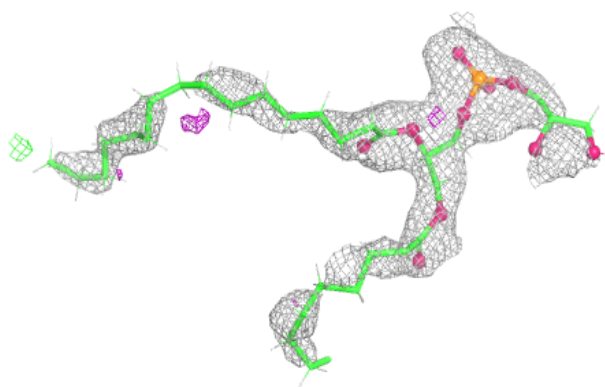
**Electron density around DGD A 617:**

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

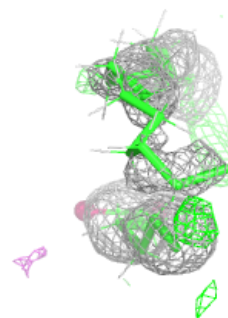
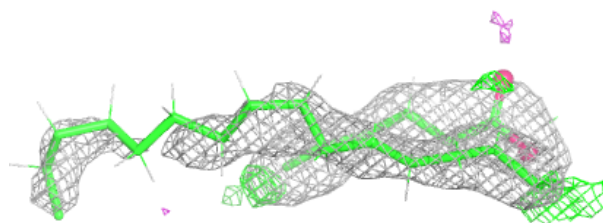
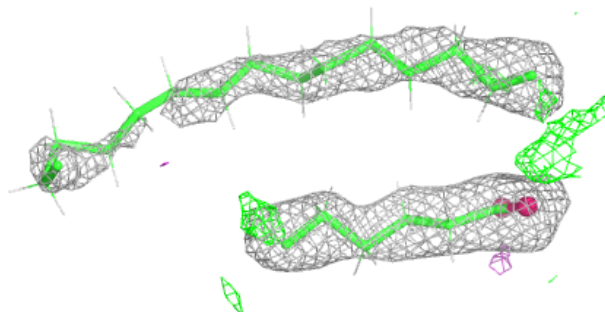


Electron density around LHG a 614:

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

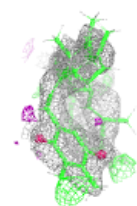
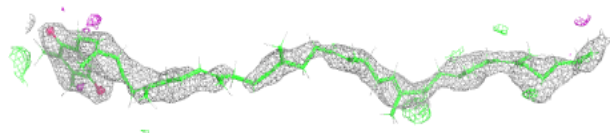
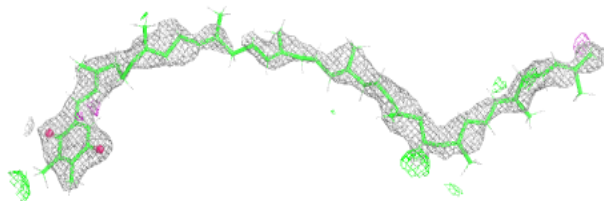
**Electron density around LMG d 410:**

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

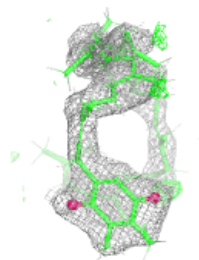
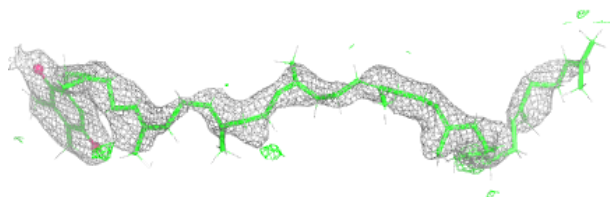
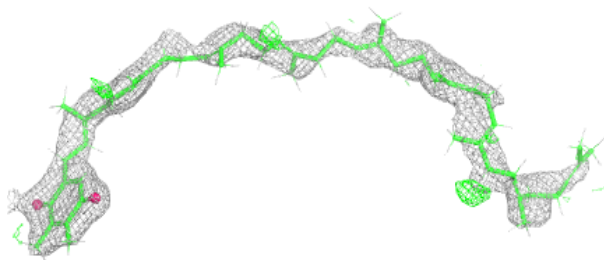


Electron density around PL9 A 611:

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

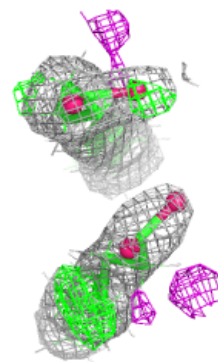
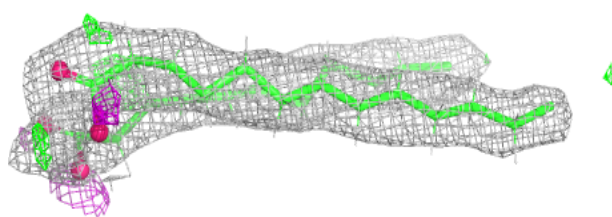
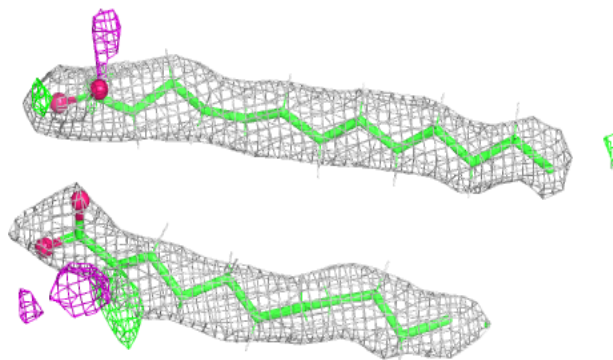
**Electron density around PL9 a 611:**

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

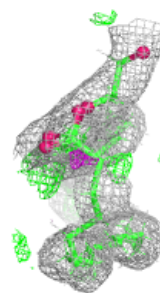
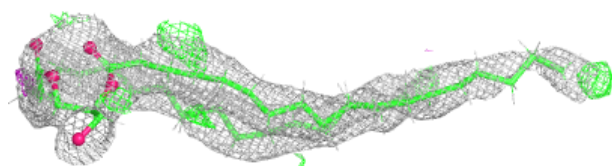
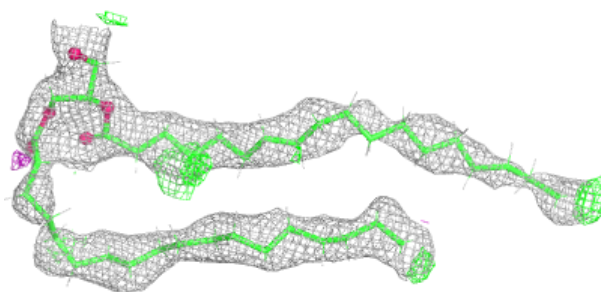


Electron density around LMG B 622:

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

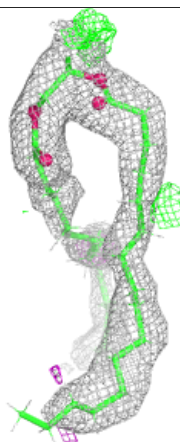
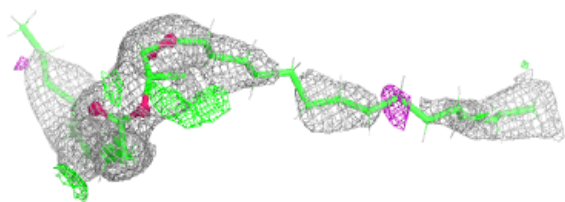
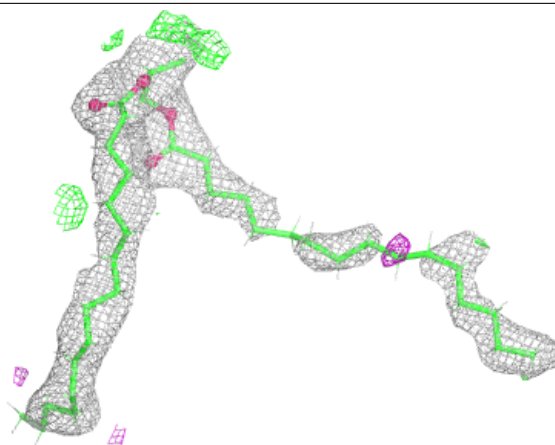
**Electron density around DGD a 616:**

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



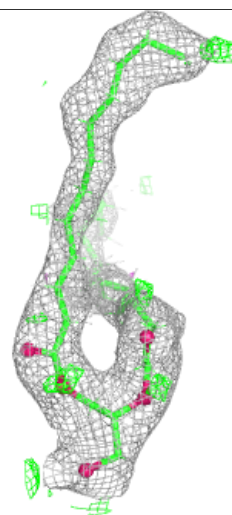
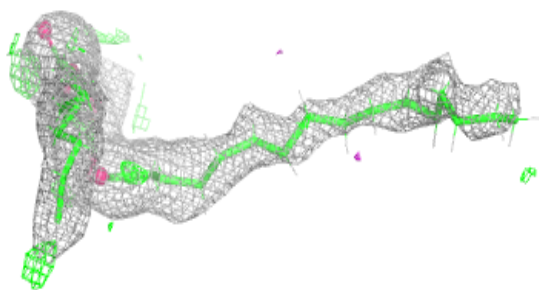
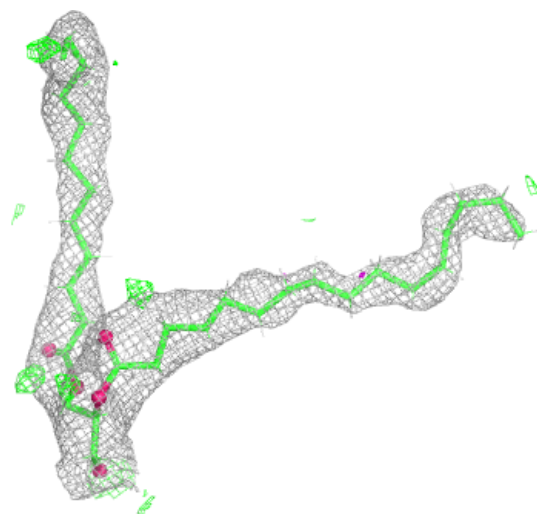
Electron density around SQD A 616:

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



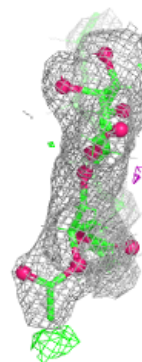
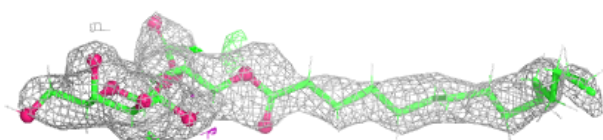
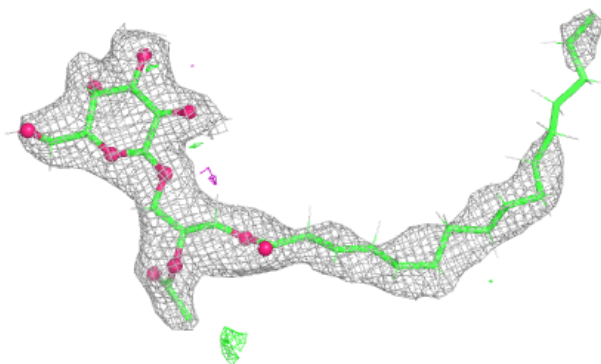
Electron density around SQD a 615:

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



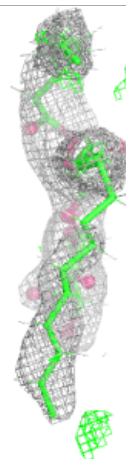
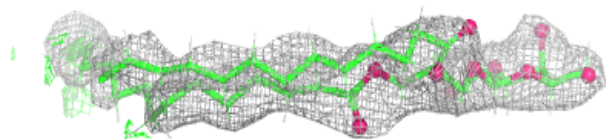
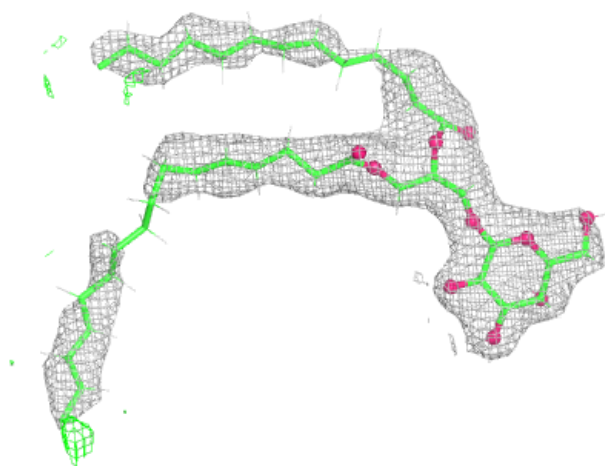
Electron density around LMG c 519:

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



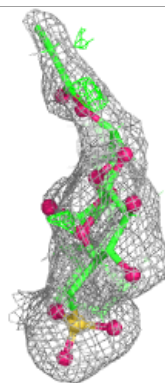
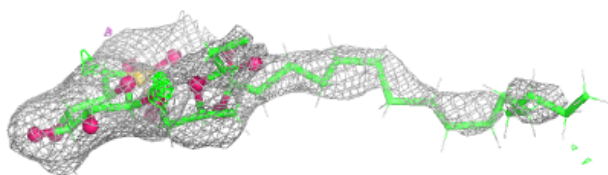
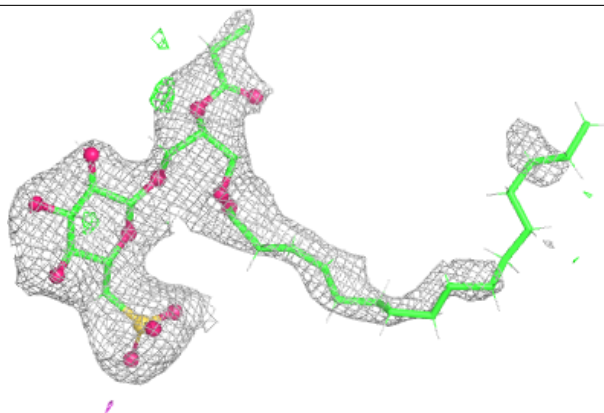
Electron density around LMG C 519:

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

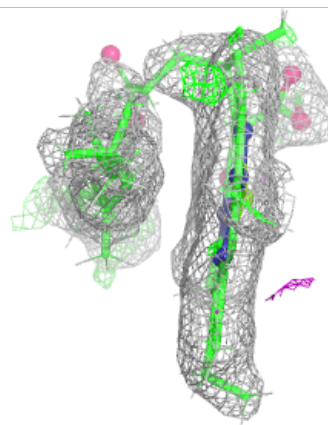
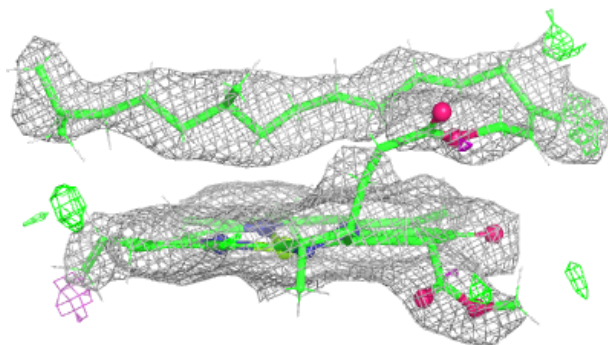
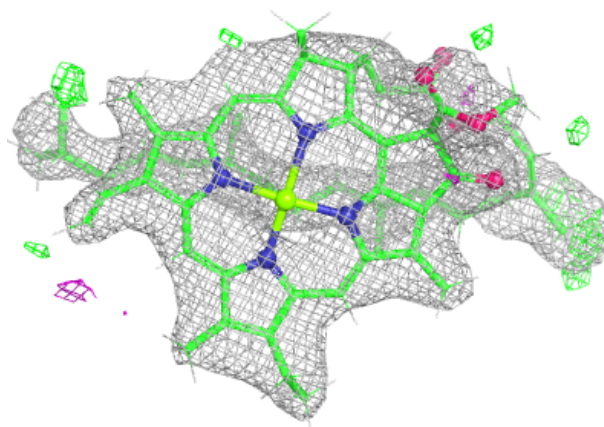


Electron density around SQD f 101:

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

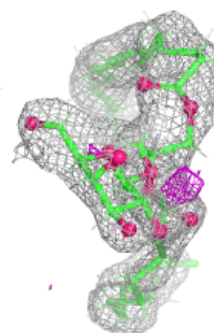
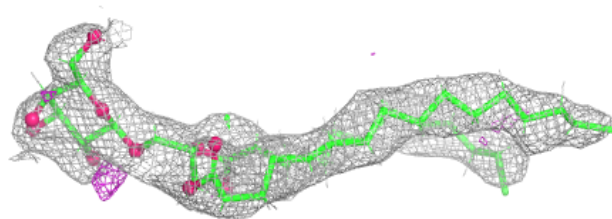
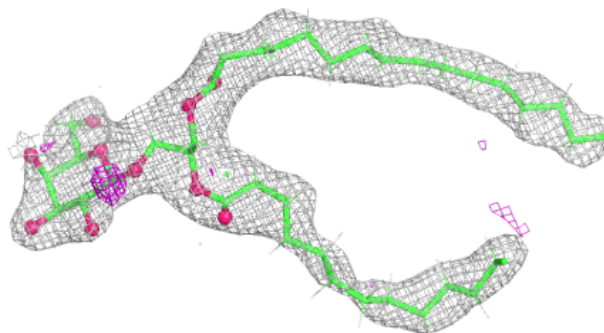
**Electron density around CLA h 101:**

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

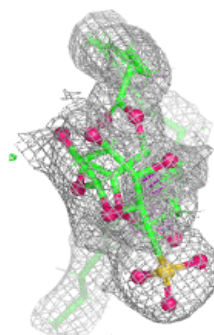
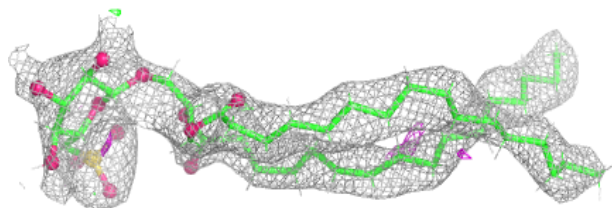
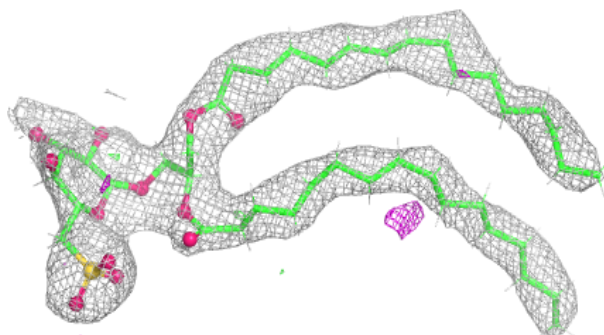


Electron density around LMG A 612:

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

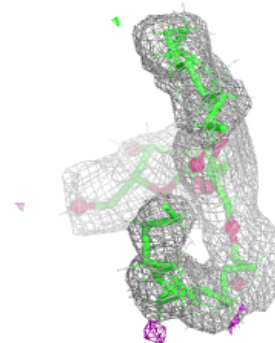
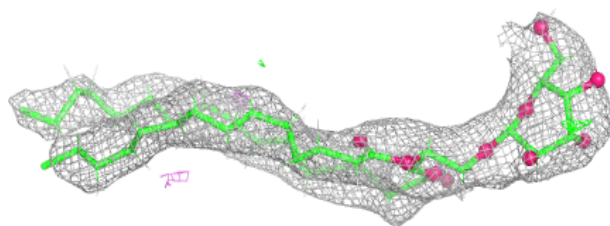
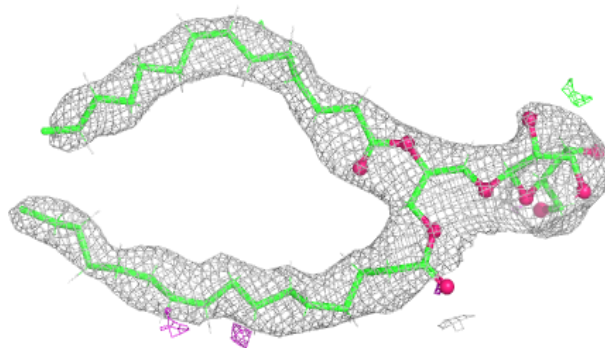
**Electron density around SQD B 624:**

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

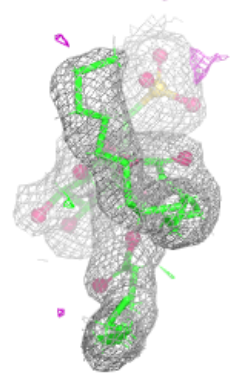
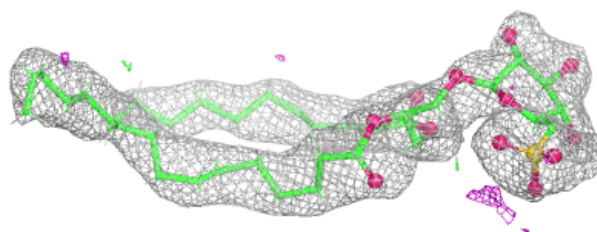
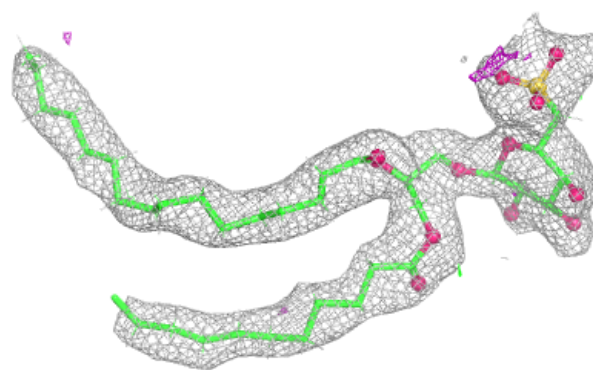


Electron density around LMG c 522:

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

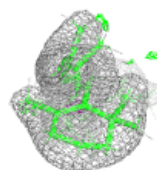
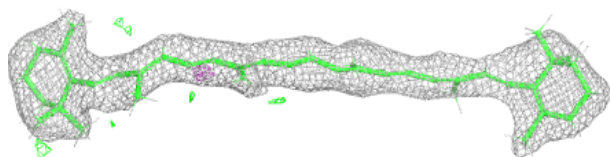
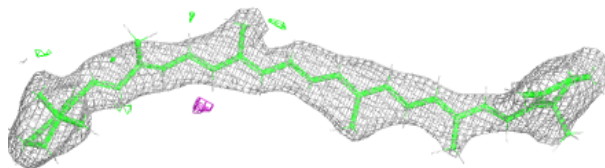
**Electron density around SQD b 601:**

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



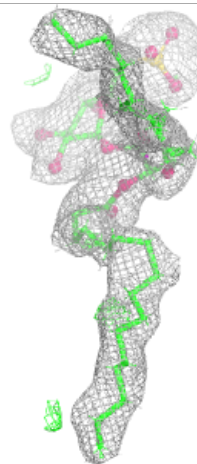
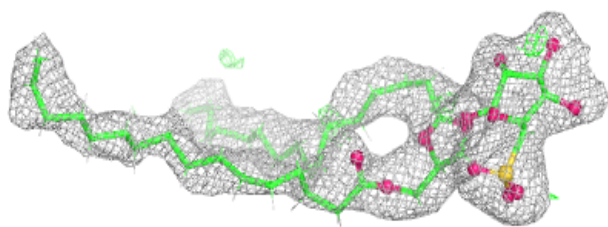
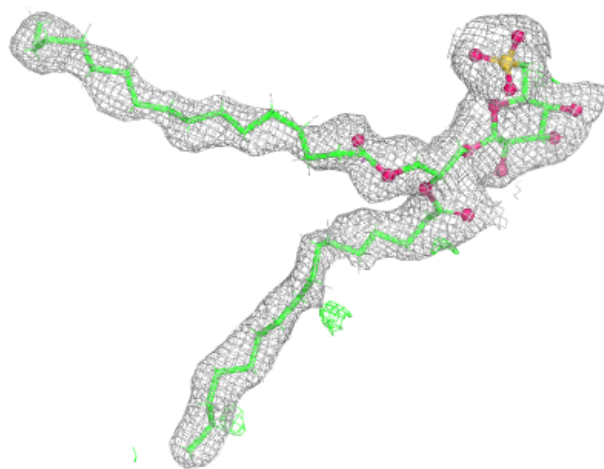
Electron density around BCR h 102:

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



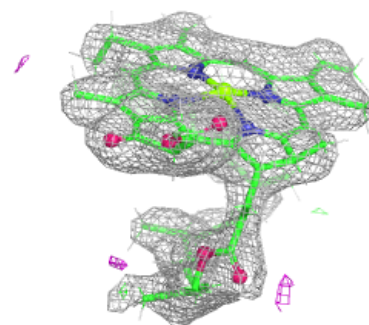
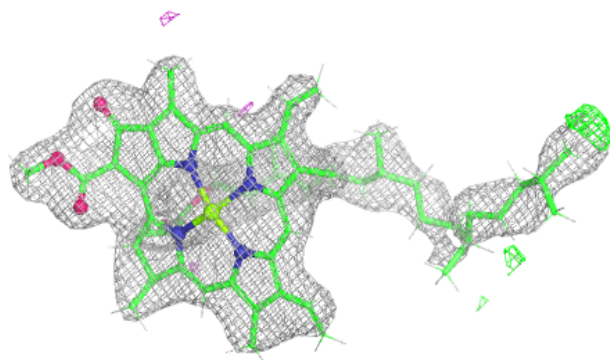
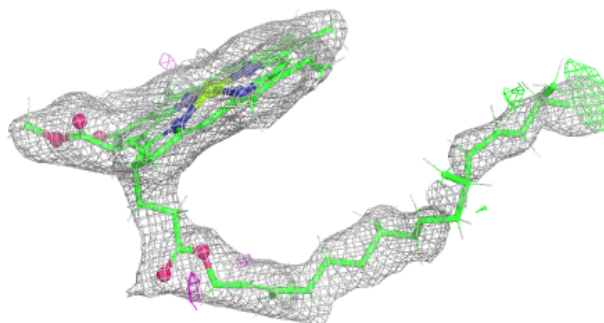
Electron density around SQD a 613:

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

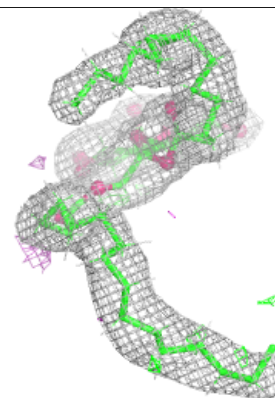
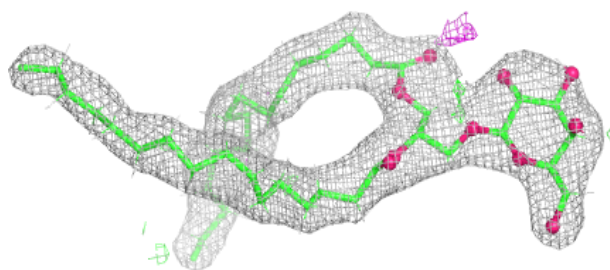
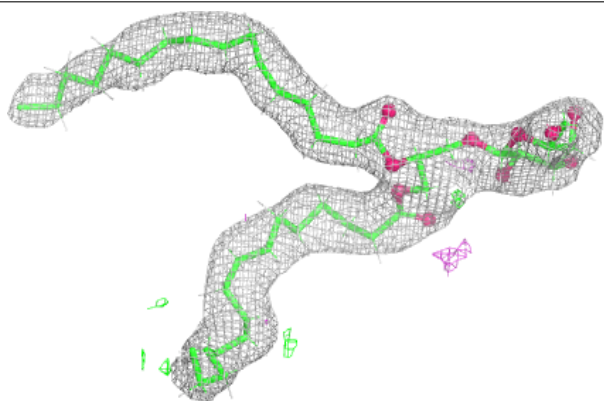


Electron density around CLA C 513:

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

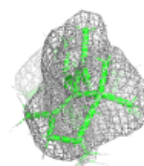
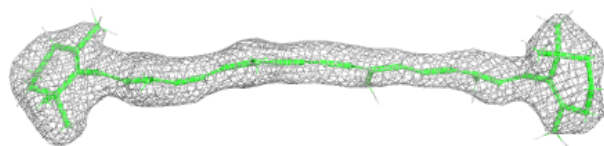
**Electron density around LMG m 101:**

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

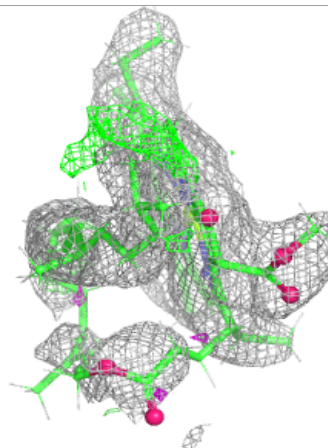
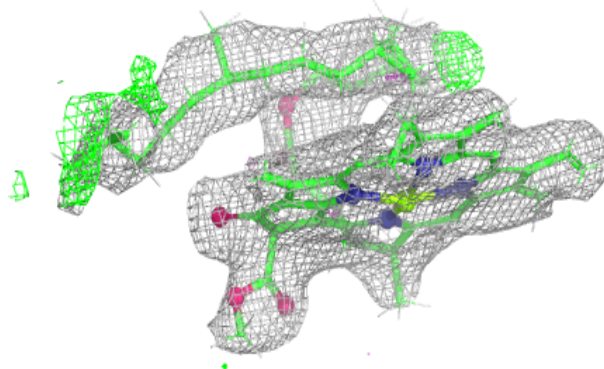
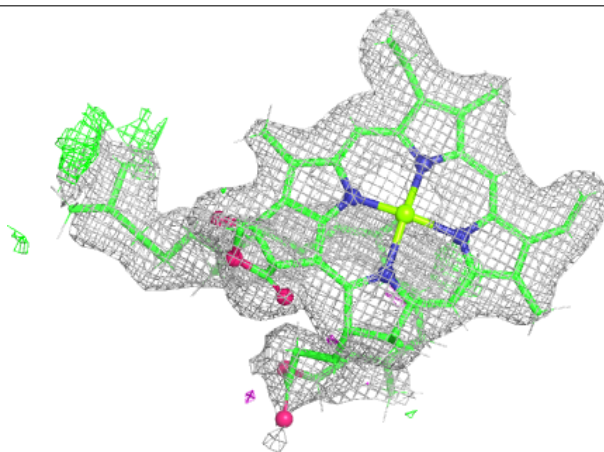


Electron density around BCR k 101:

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

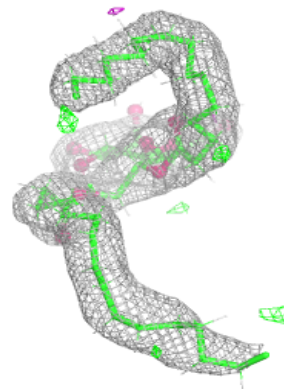
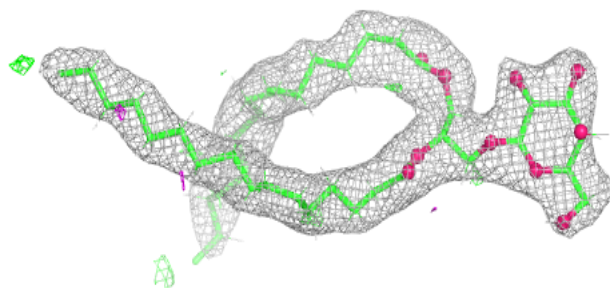
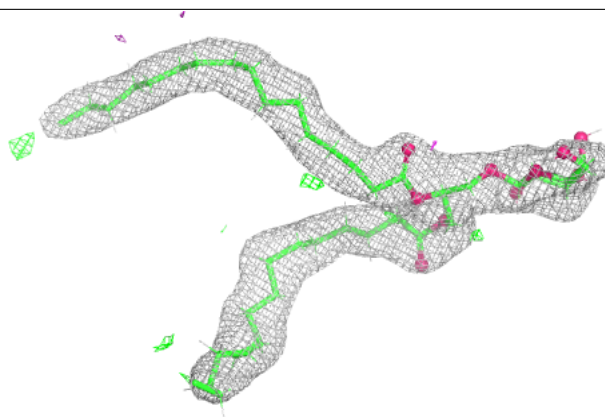
**Electron density around CLA B 601:**

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

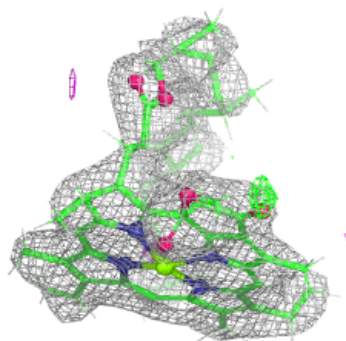
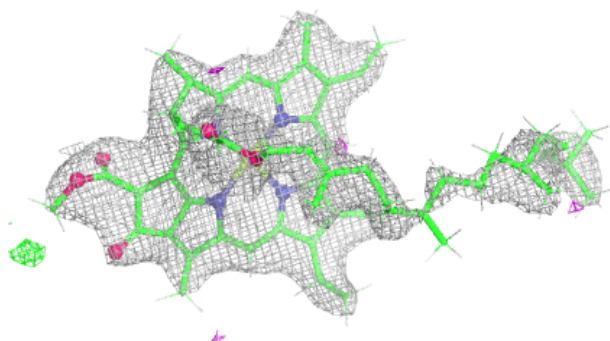
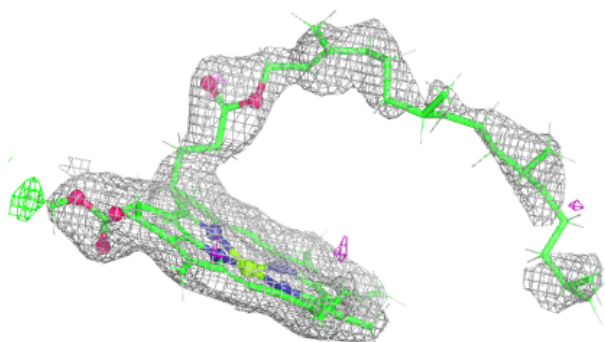


Electron density around LMG B 620:

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

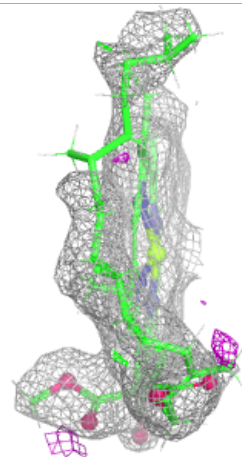
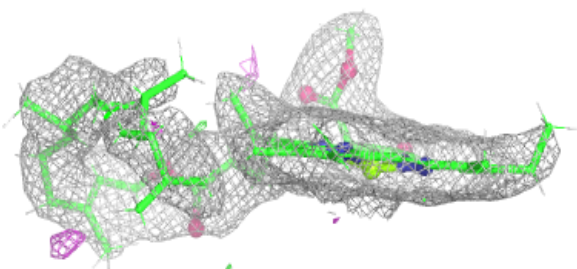
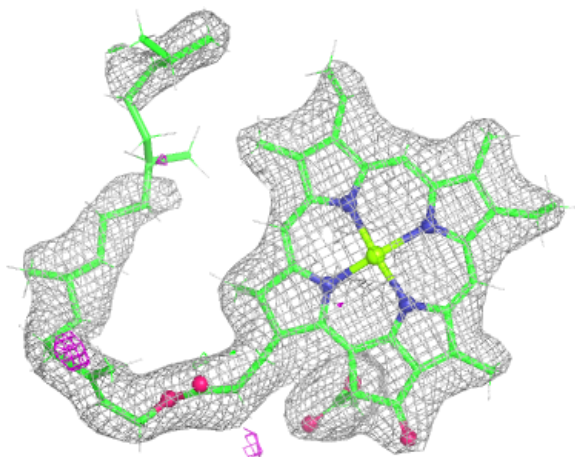
**Electron density around CLA c 513:**

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



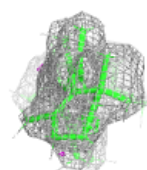
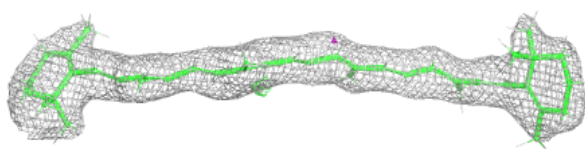
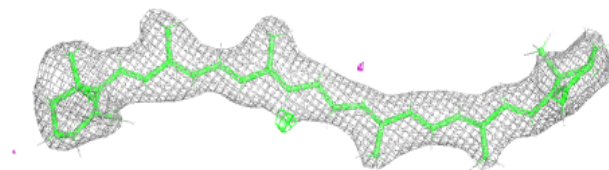
Electron density around CLA c 512:

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

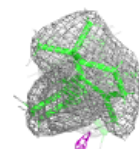
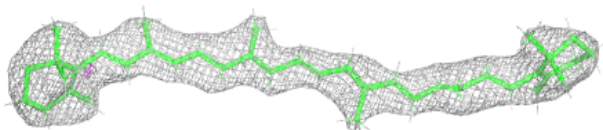
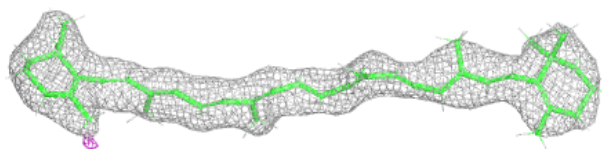


Electron density around BCR Y 101:

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

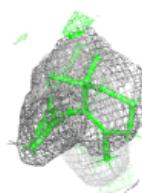
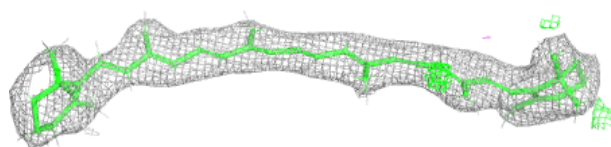
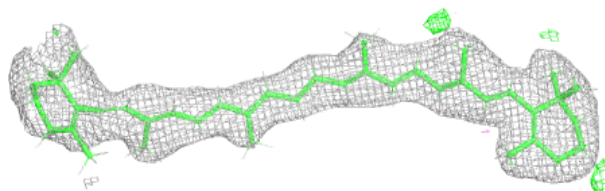
**Electron density around BCR c 514:**

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

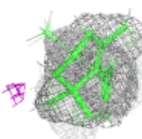
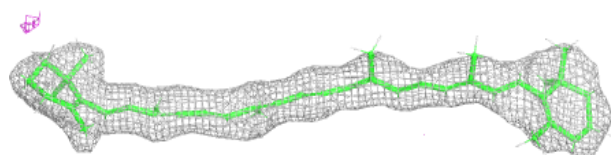
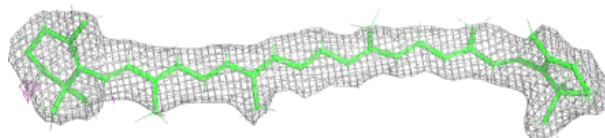


Electron density around BCR d 404:

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

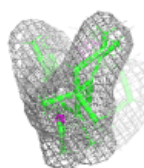
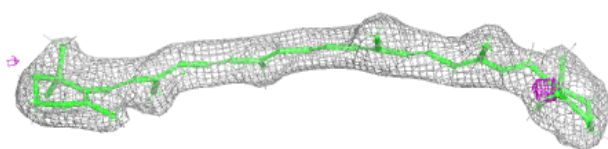
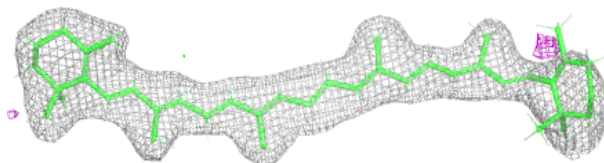
**Electron density around BCR C 514:**

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

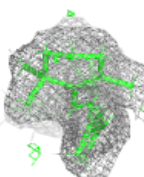
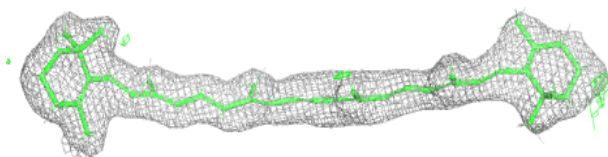
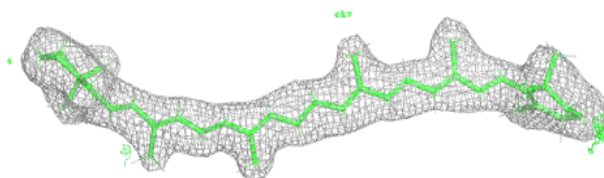


Electron density around BCR D 404:

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

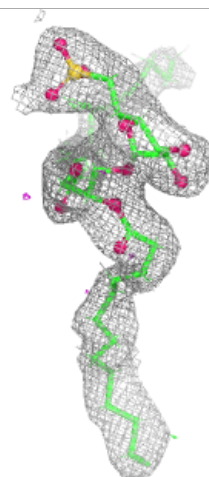
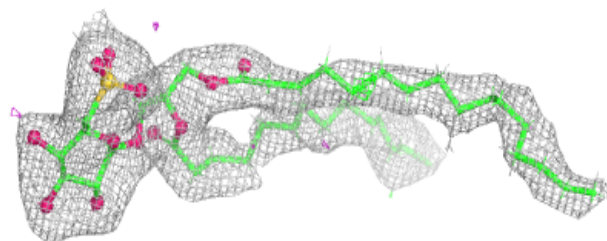
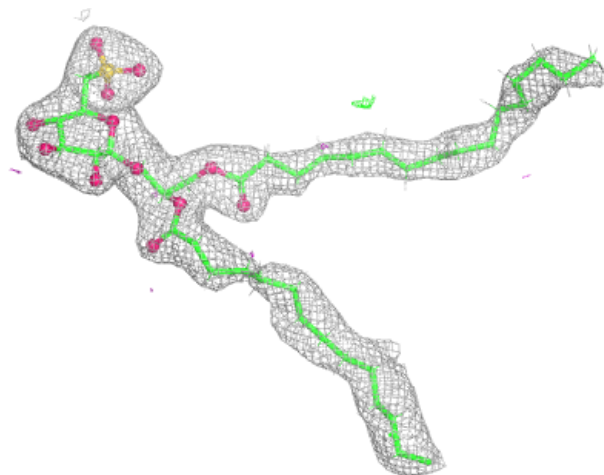
**Electron density around BCR H 101:**

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



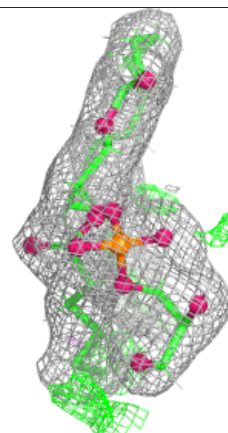
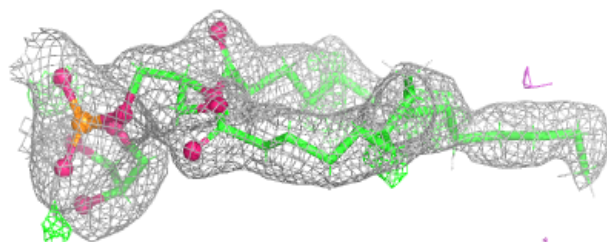
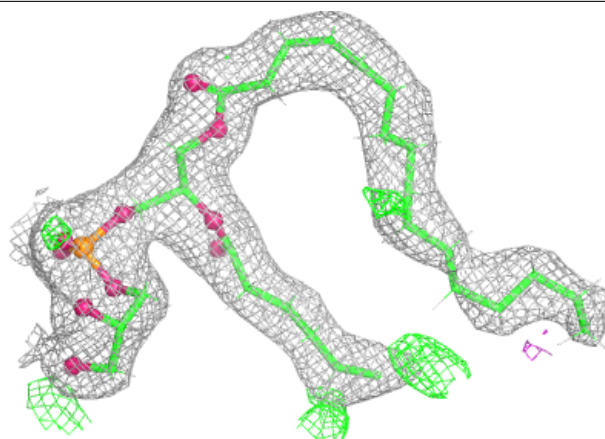
Electron density around SQD A 614:

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

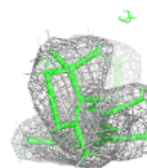
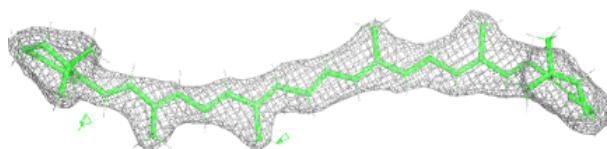
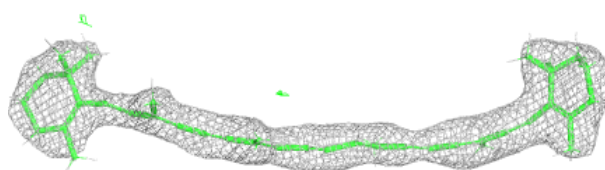


Electron density around LHG d 409:

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

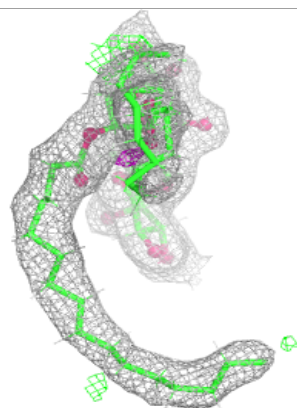
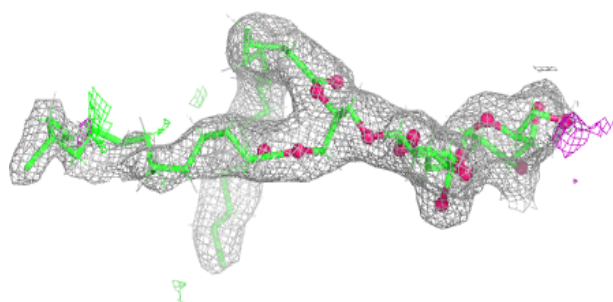
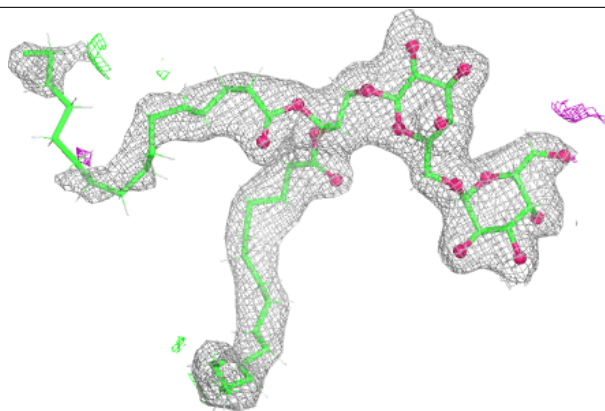
**Electron density around BCR k 102:**

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

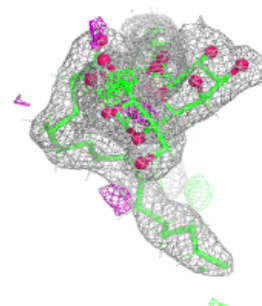
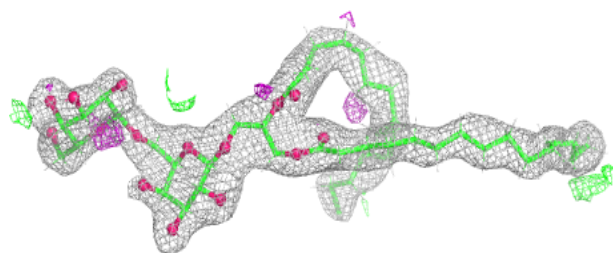
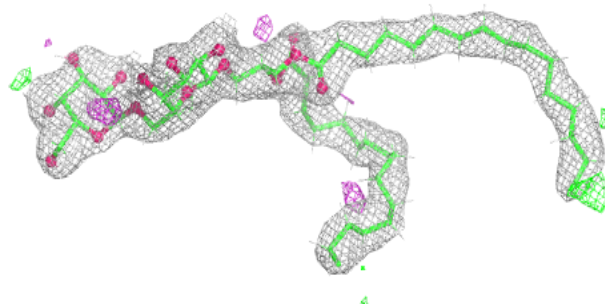


Electron density around DGD C 517:

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

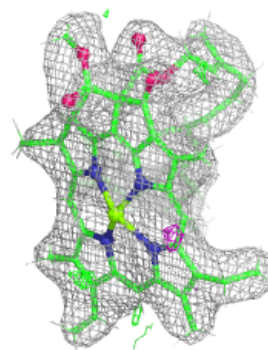
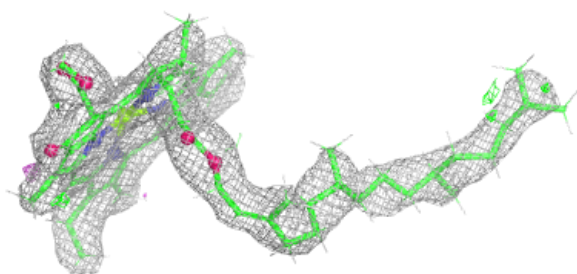
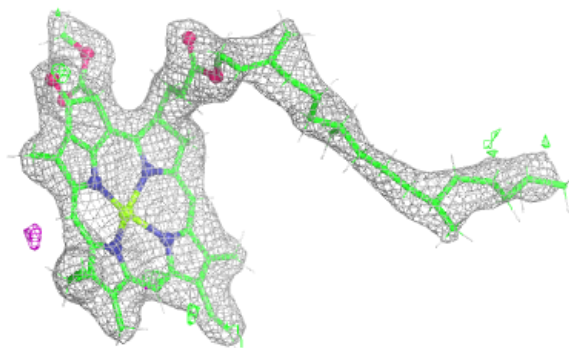
**Electron density around DGD H 102:**

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

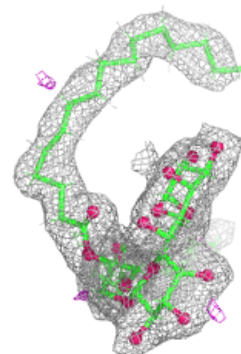
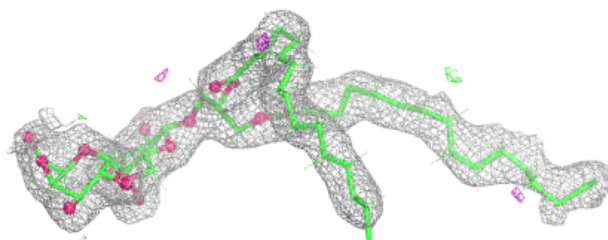
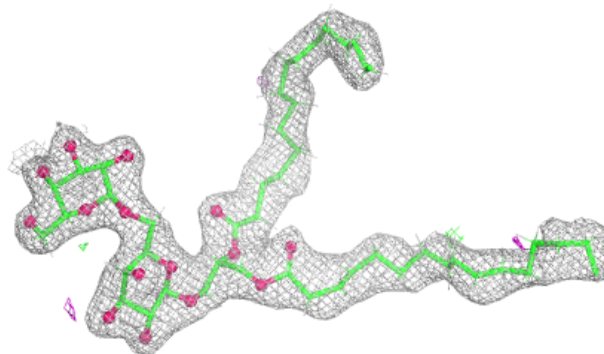


Electron density around CLA c 511:

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

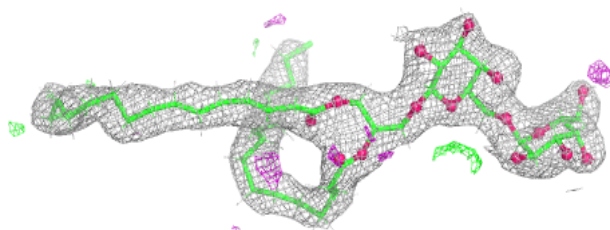
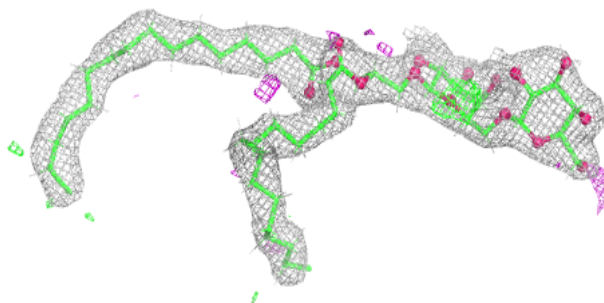
**Electron density around DGD c 517:**

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

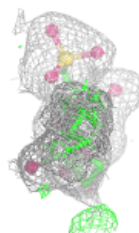
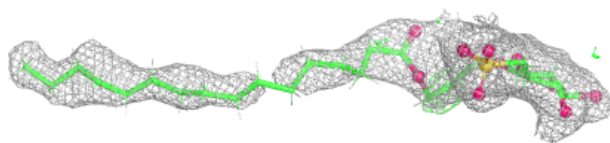
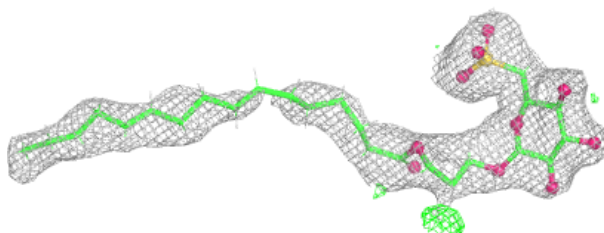


Electron density around DGD h 103:

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

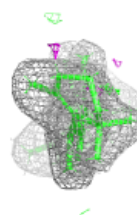
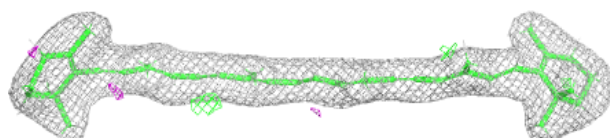
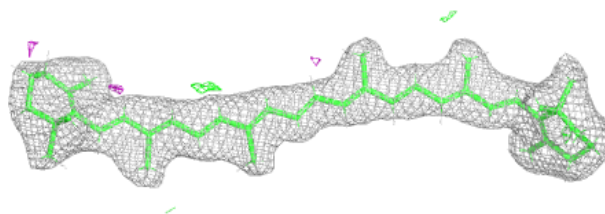
**Electron density around SQD F 101:**

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



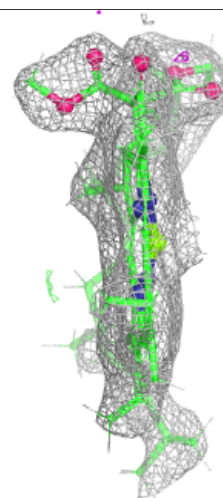
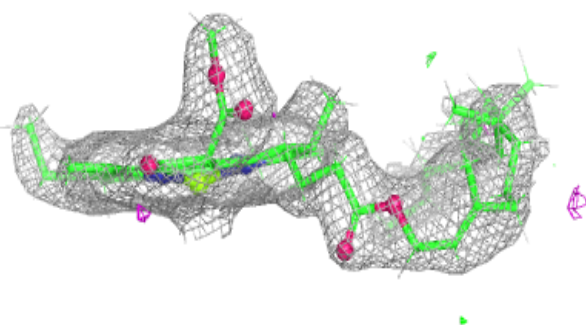
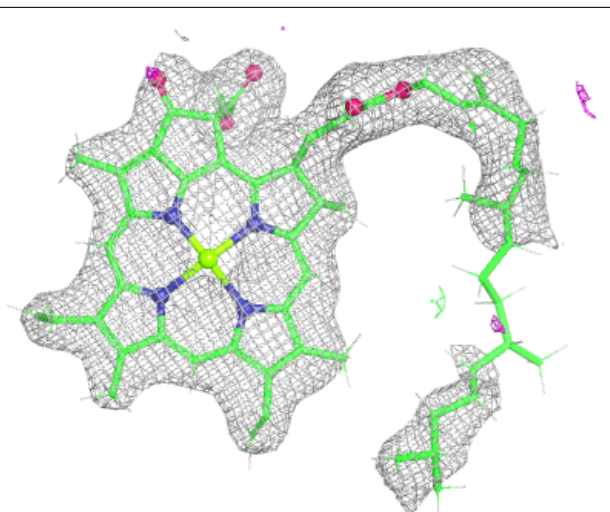
Electron density around BCR b 618:

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



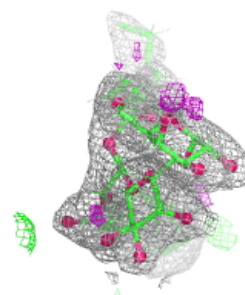
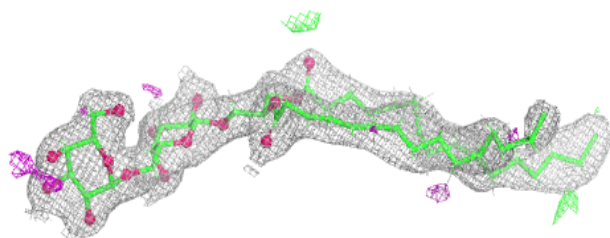
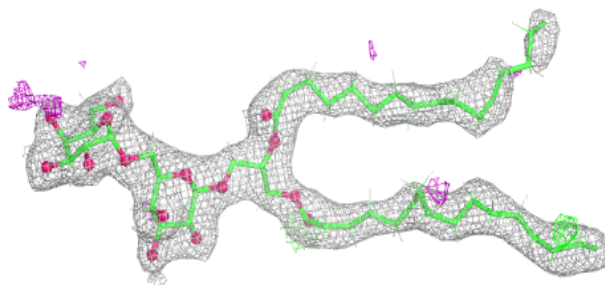
Electron density around CLA C 512:

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

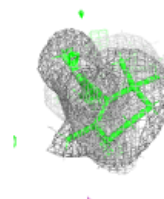
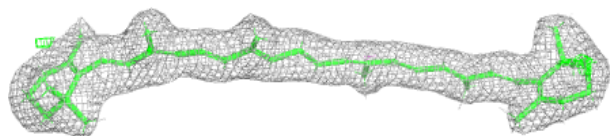
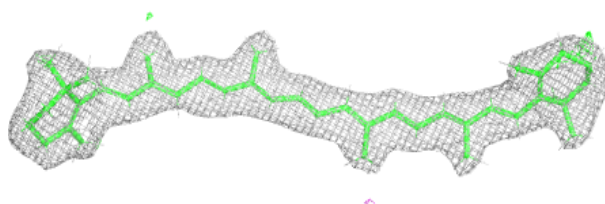


Electron density around DGD c 518:

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

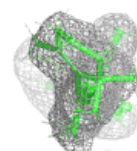
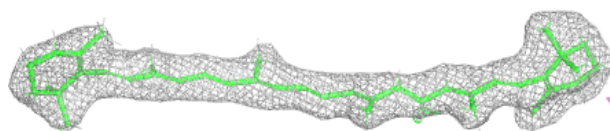
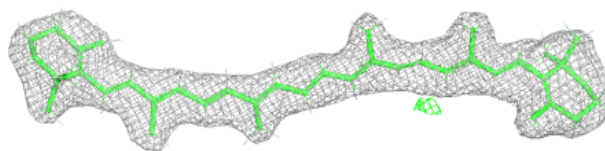
**Electron density around BCR B 619:**

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

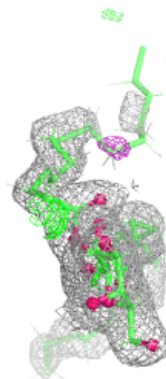
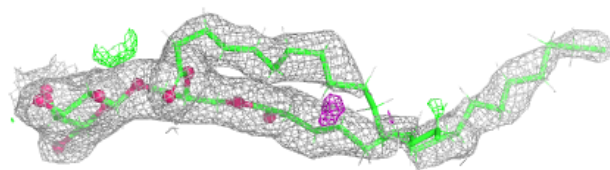
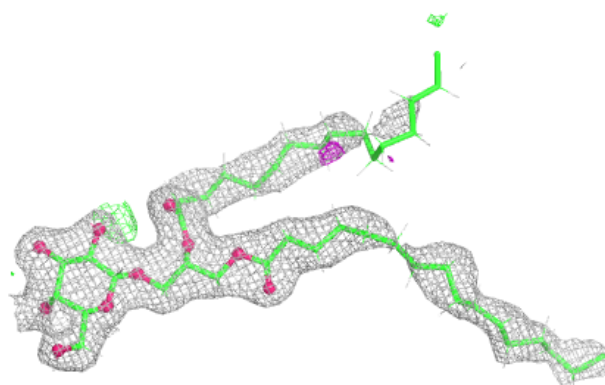


Electron density around BCR b 619:

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

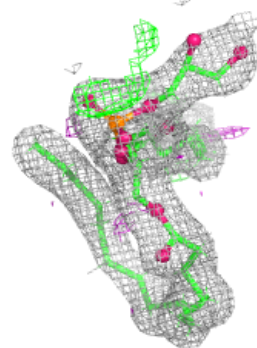
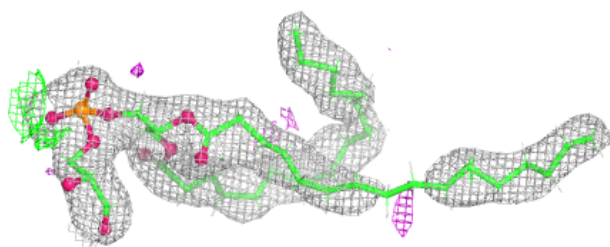
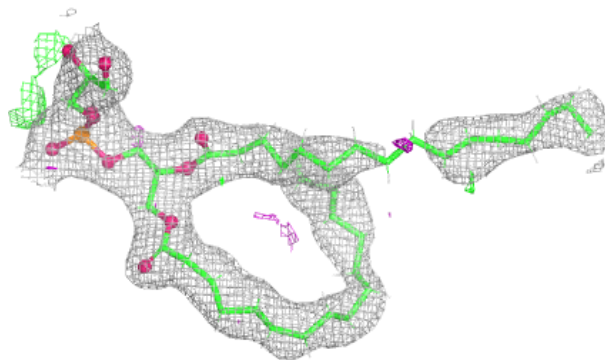
**Electron density around LMG D 405:**

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

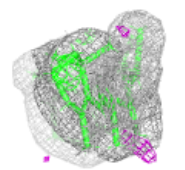
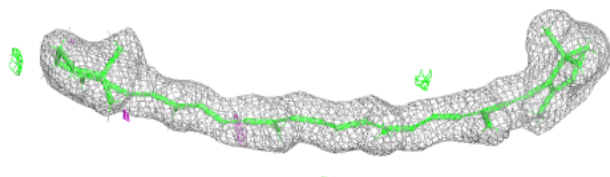
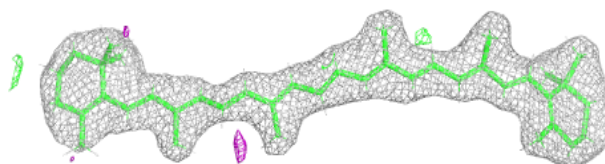


Electron density around LHG d 405:

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

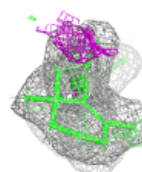
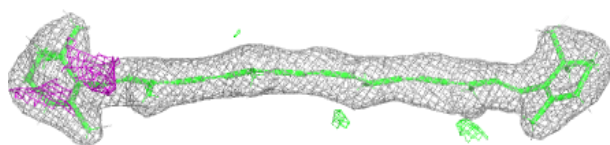
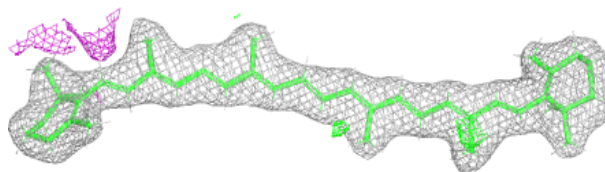
**Electron density around BCR t 101:**

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

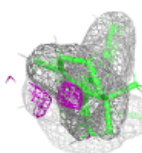
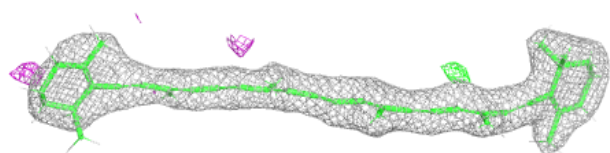
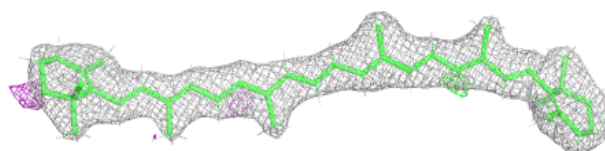


Electron density around BCR B 618:

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

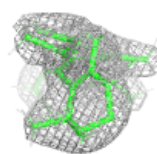
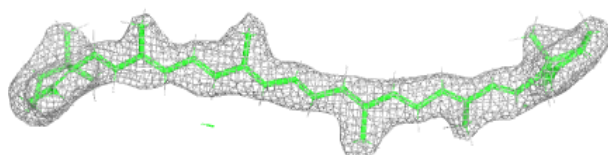
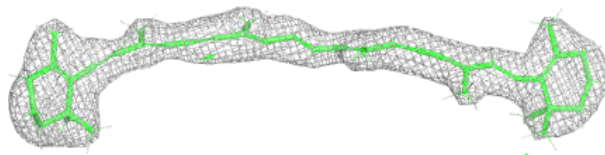
**Electron density around BCR c 515:**

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

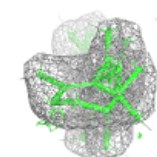
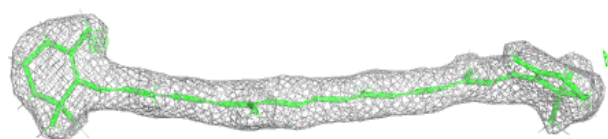
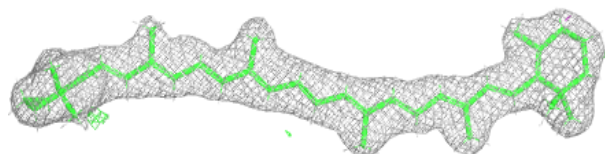


Electron density around BCR C 520:

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

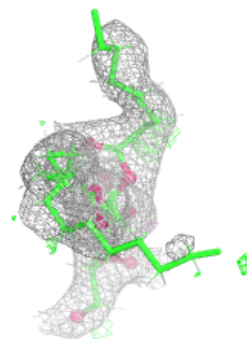
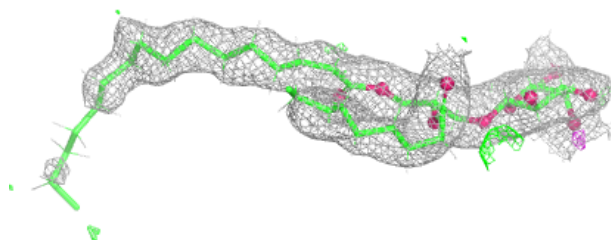
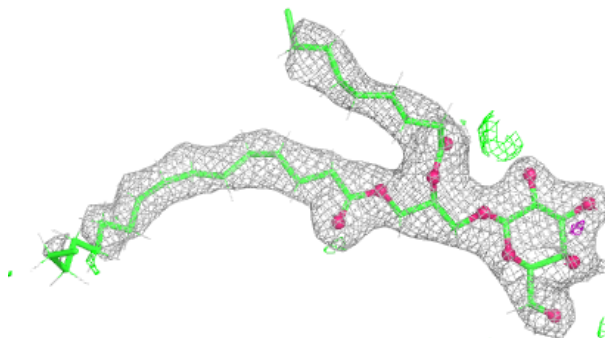
**Electron density around BCR b 617:**

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

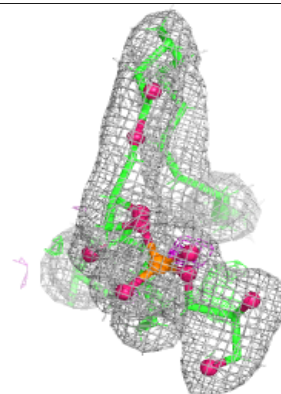
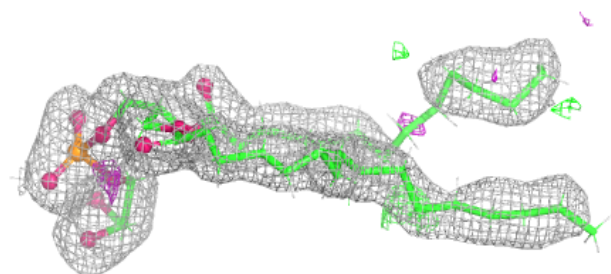
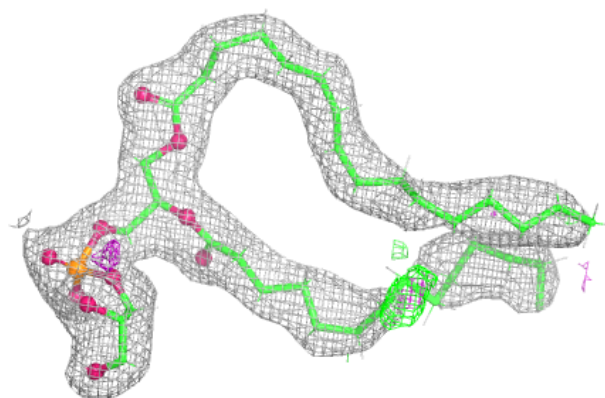


Electron density around LMG d 406:

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

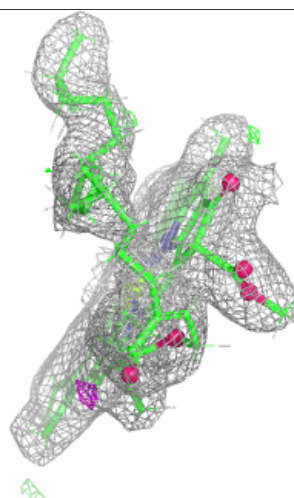
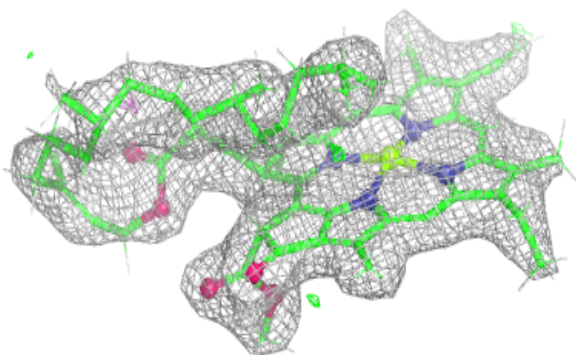
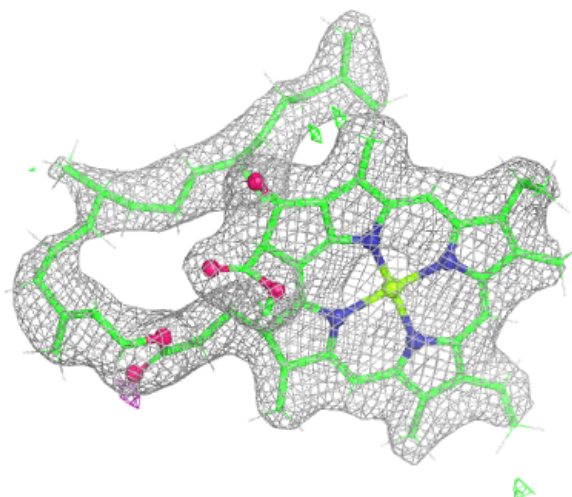
**Electron density around LHG D 408:**

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



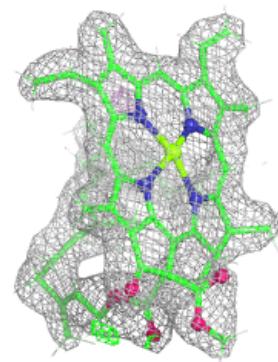
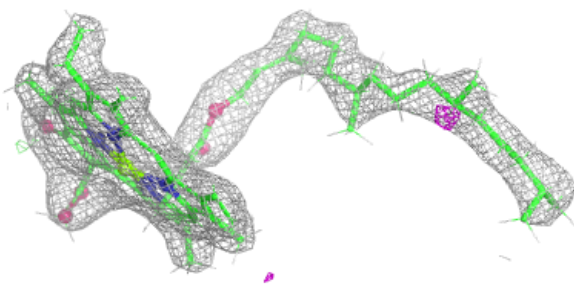
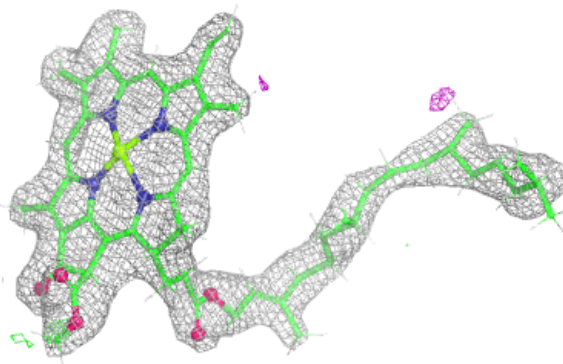
Electron density around CLA c 509:

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



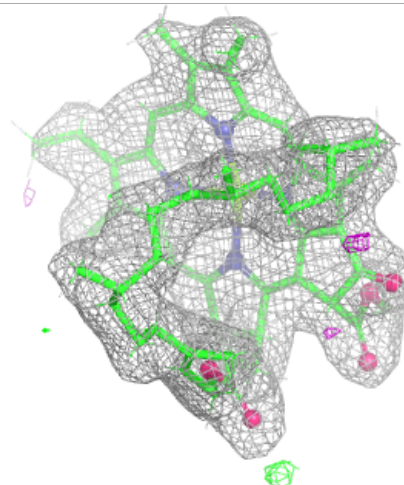
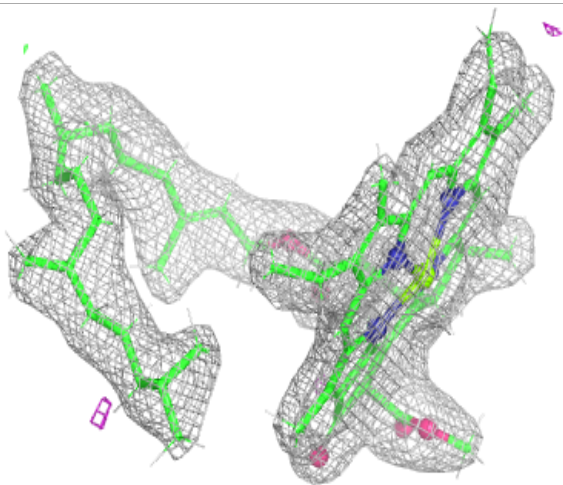
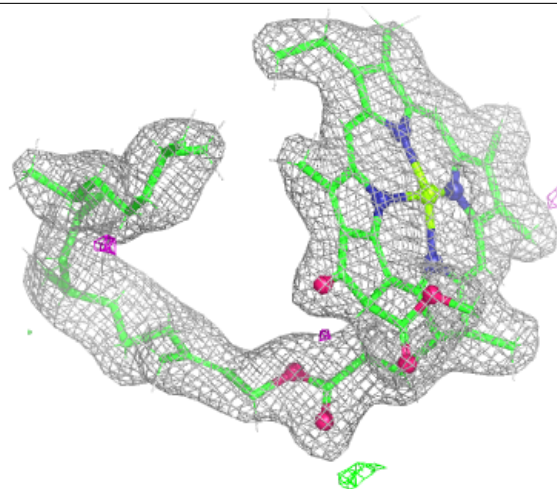
Electron density around CLA C 511:

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



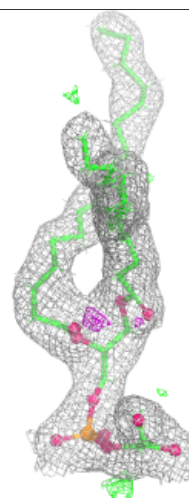
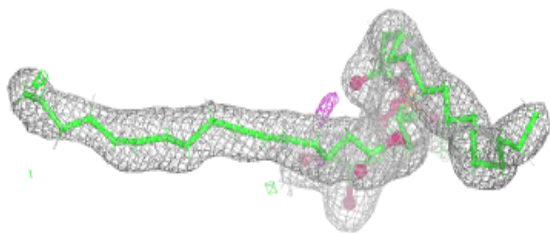
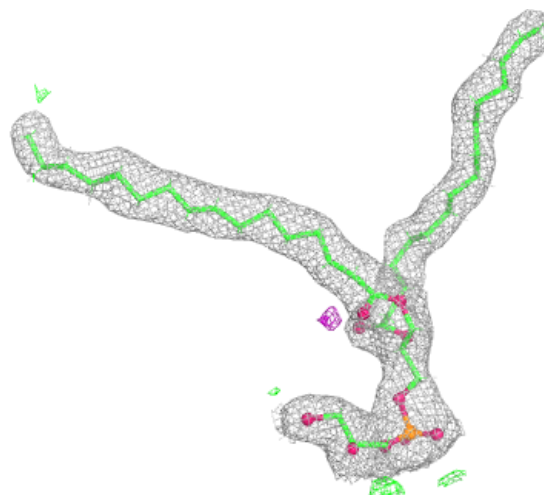
Electron density around CLA C 503:

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



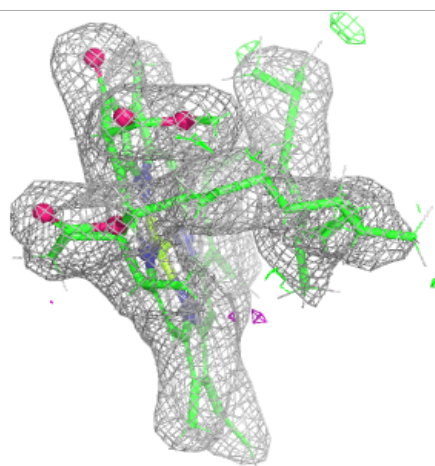
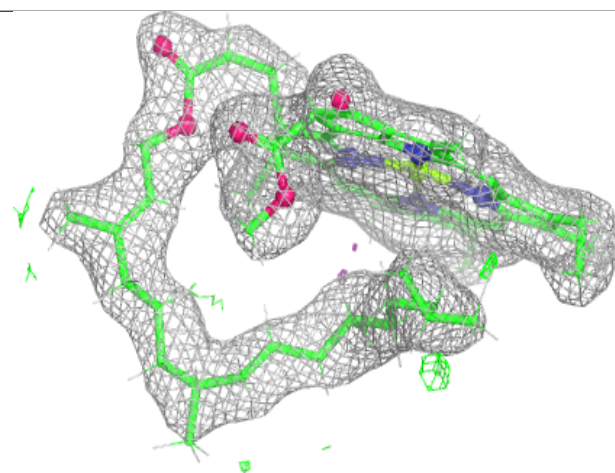
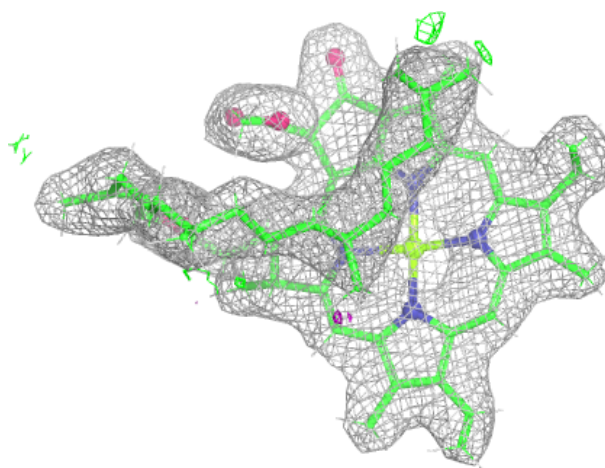
Electron density around LHG 1 101:

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



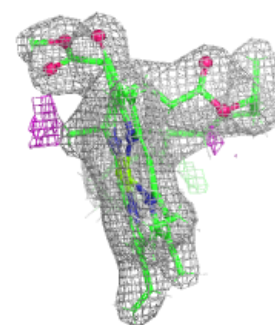
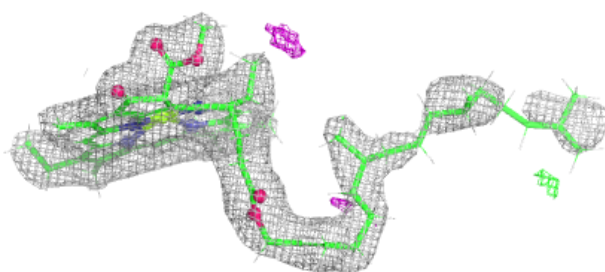
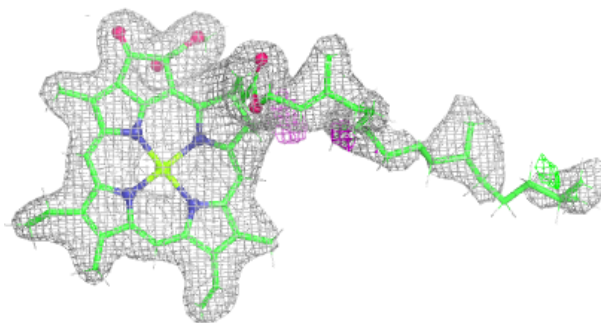
Electron density around CLA C 510:

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

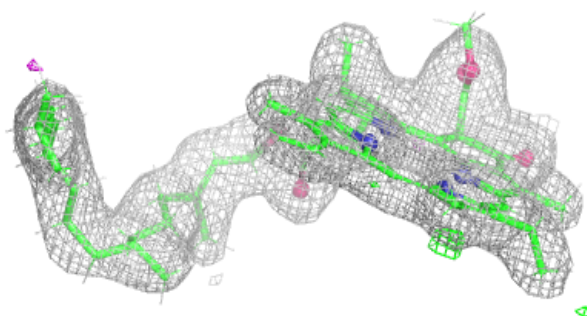
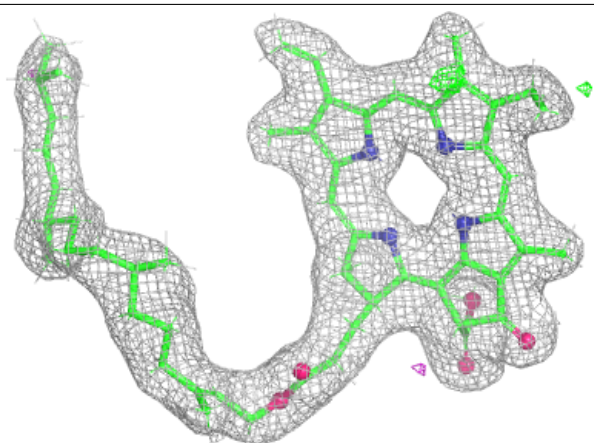


Electron density around CLA a 604:

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

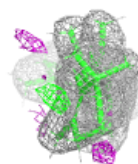
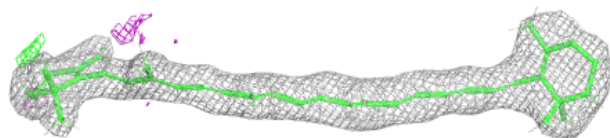
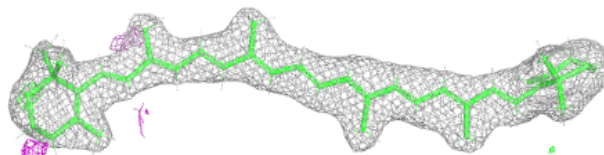
**Electron density around PHO d 401:**

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

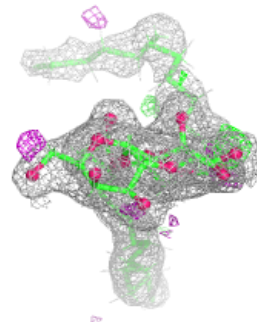
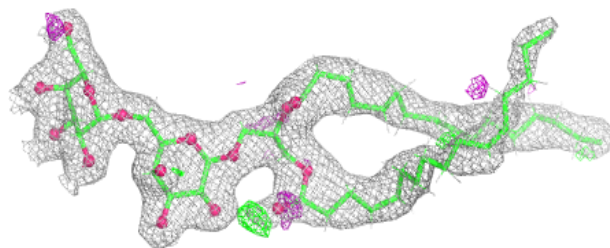
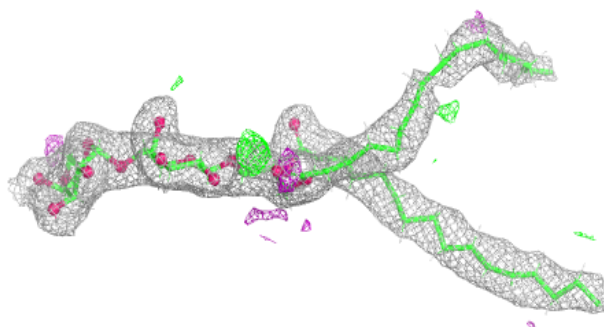


Electron density around BCR B 617:

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

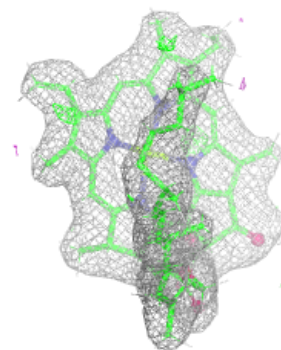
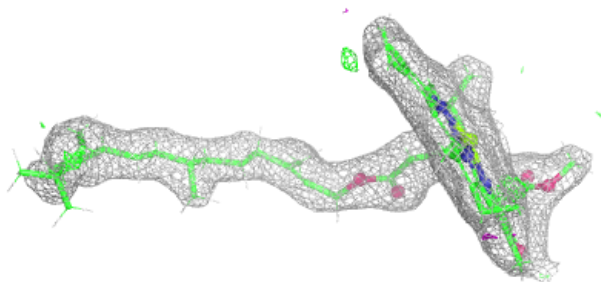
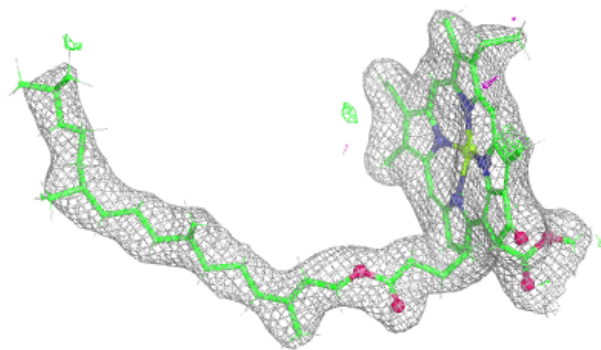
**Electron density around DGD c 516:**

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



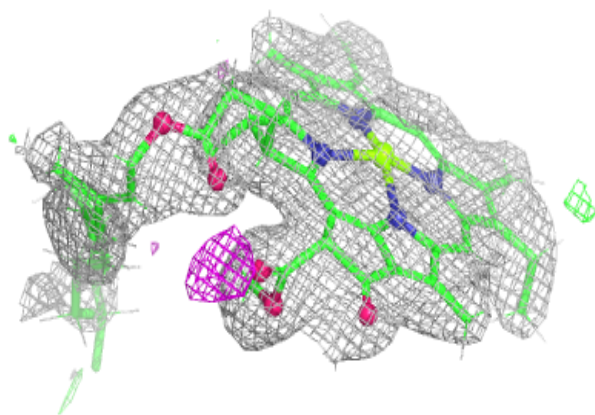
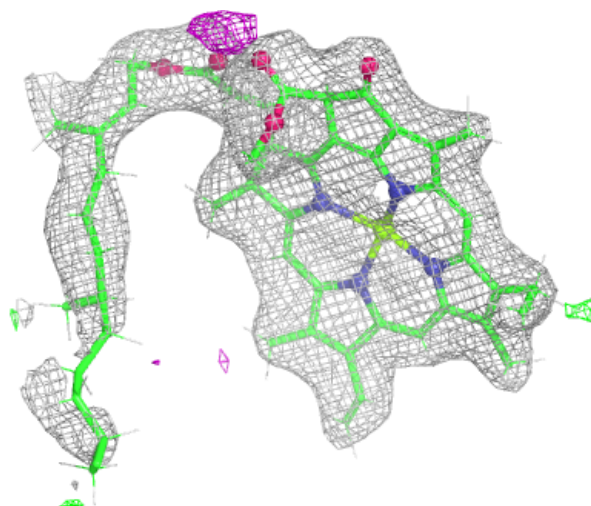
Electron density around CLA b 609:

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



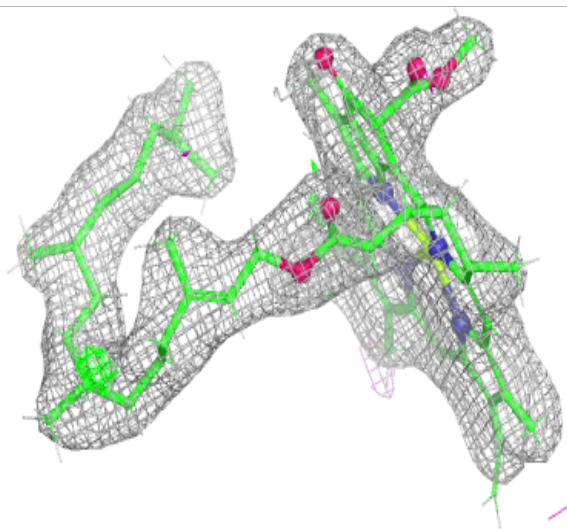
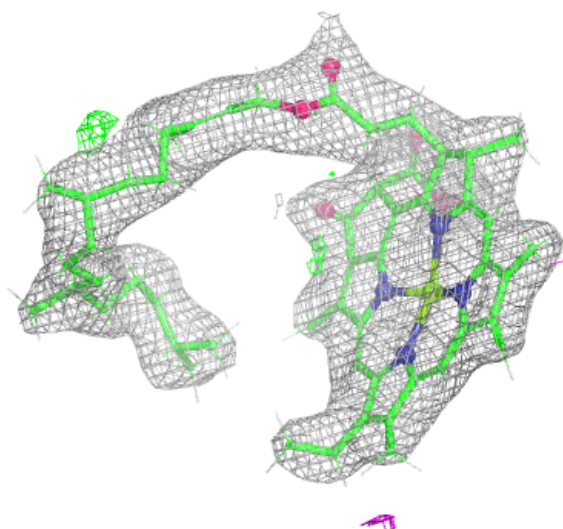
Electron density around CLA b 616:

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



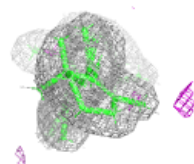
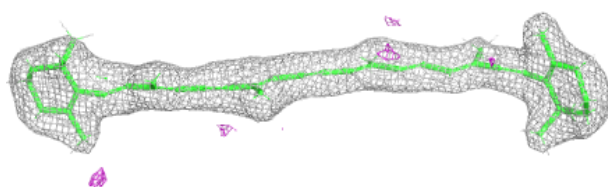
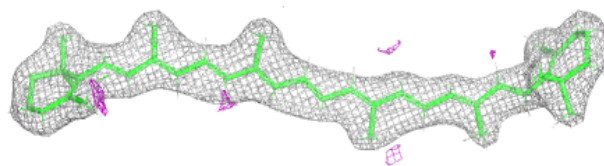
Electron density around CLA c 503:

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

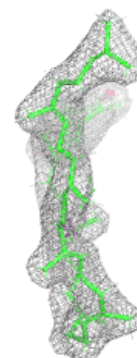
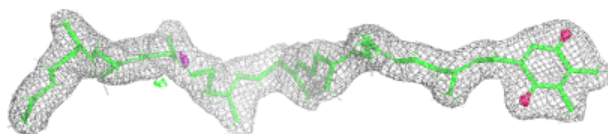
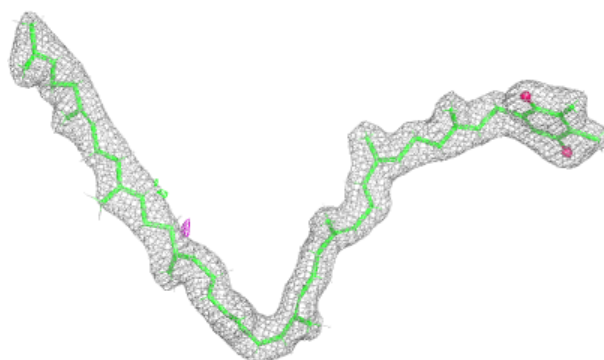


Electron density around BCR C 515:

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

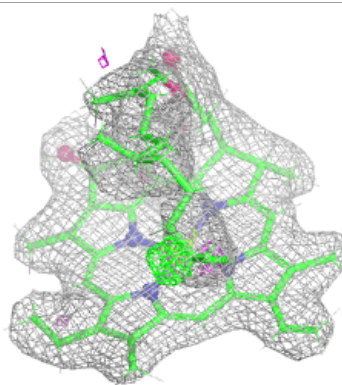
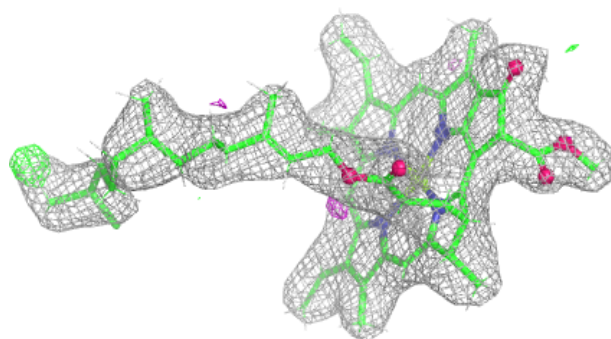
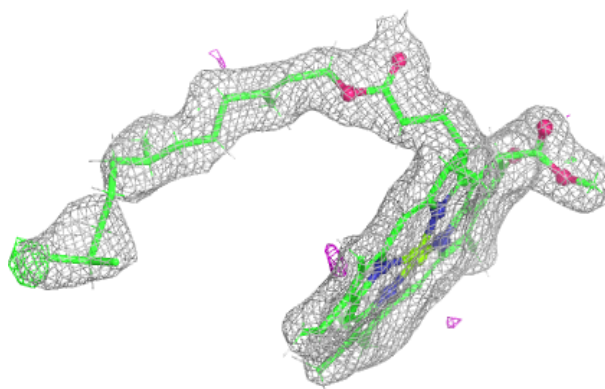
**Electron density around PL9 D 407:**

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

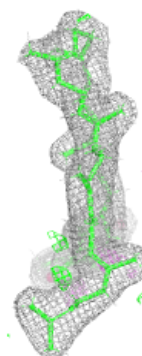
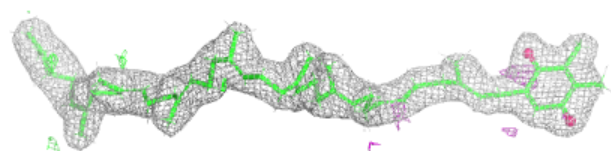
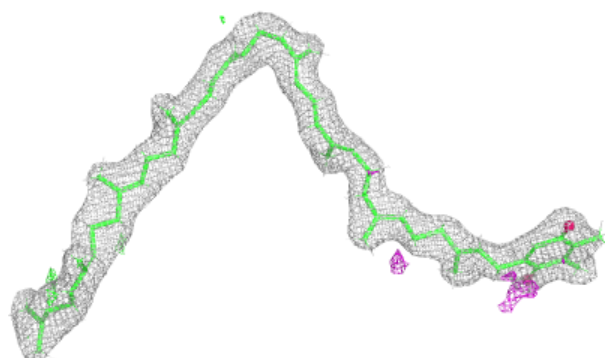


Electron density around CLA c 504:

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

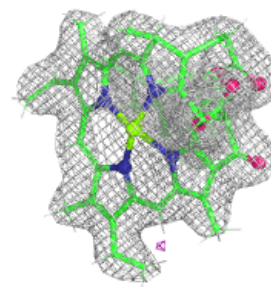
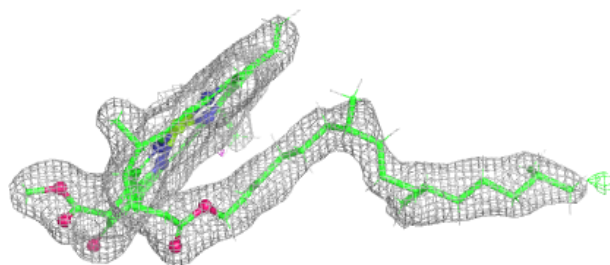
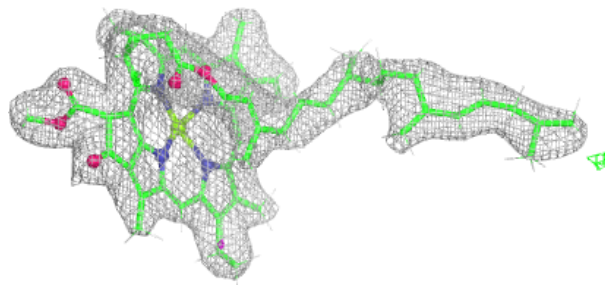
**Electron density around PL9 d 408:**

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

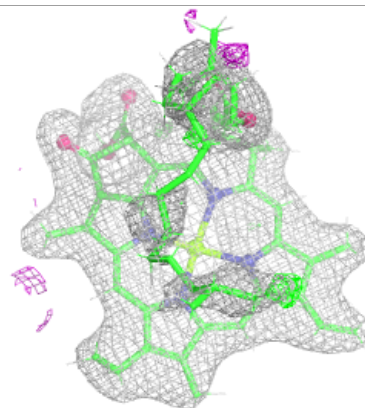
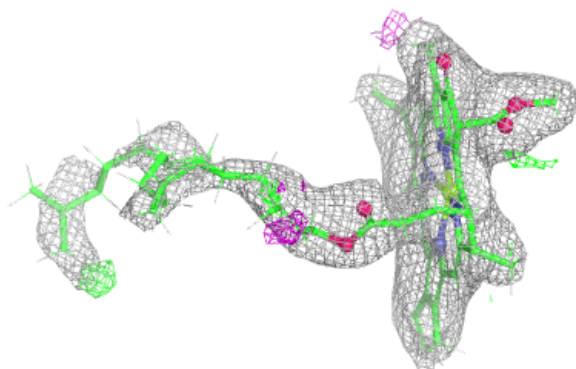
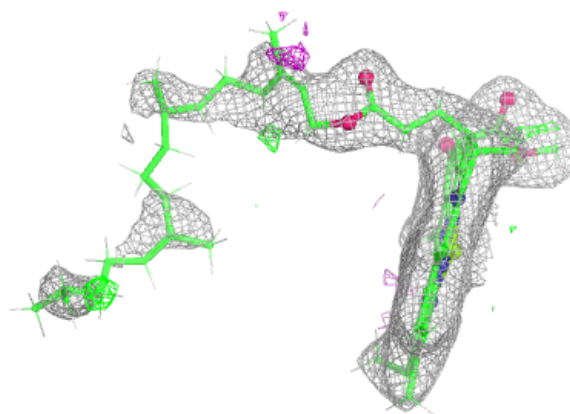


Electron density around CLA c 505:

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

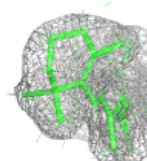
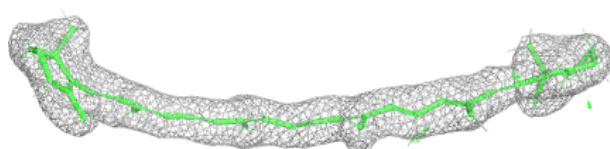
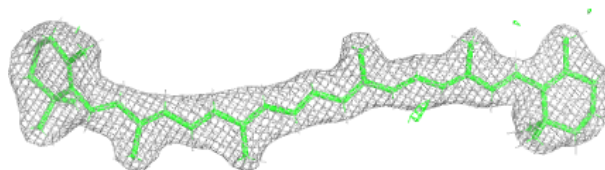
**Electron density around CLA c 506:**

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

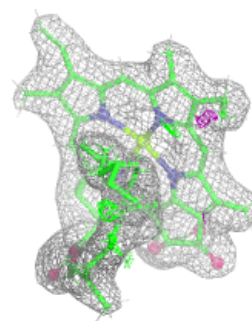
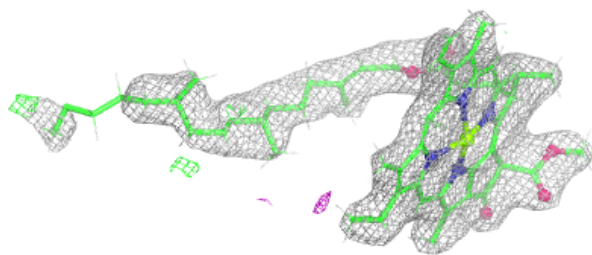
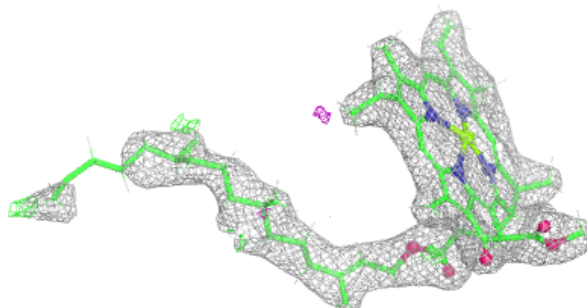


Electron density around BCR T 101:

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

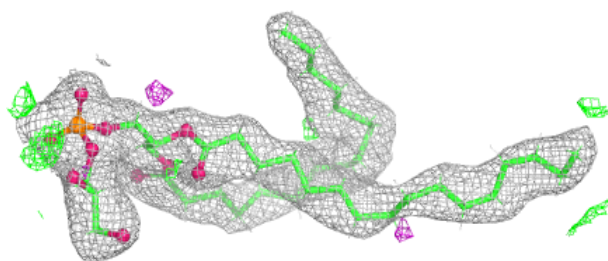
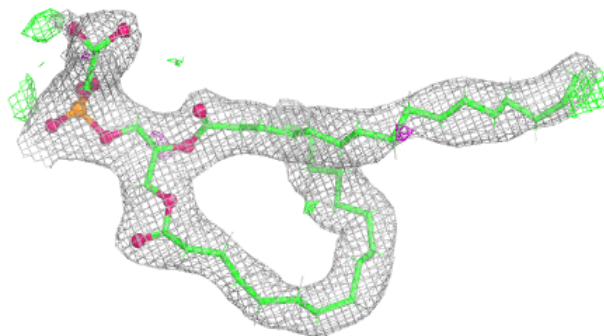
**Electron density around CLA c 508:**

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



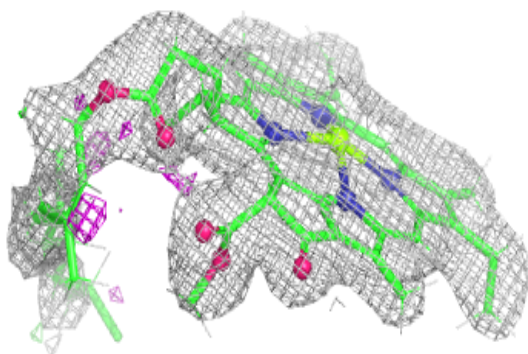
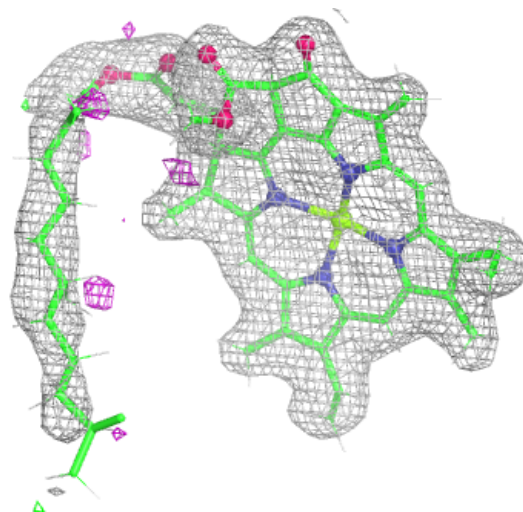
Electron density around LHG B 623:

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



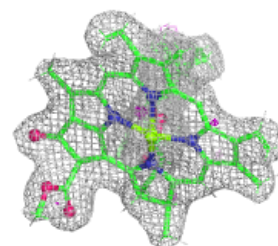
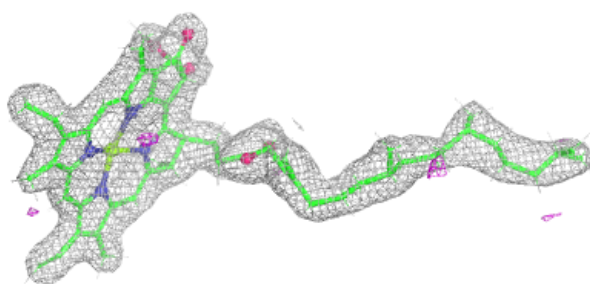
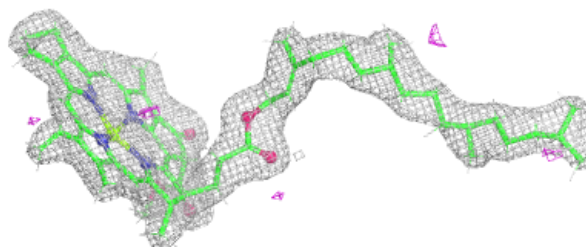
Electron density around CLA B 616:

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



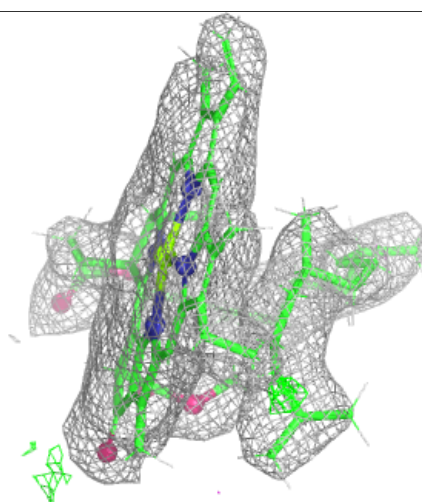
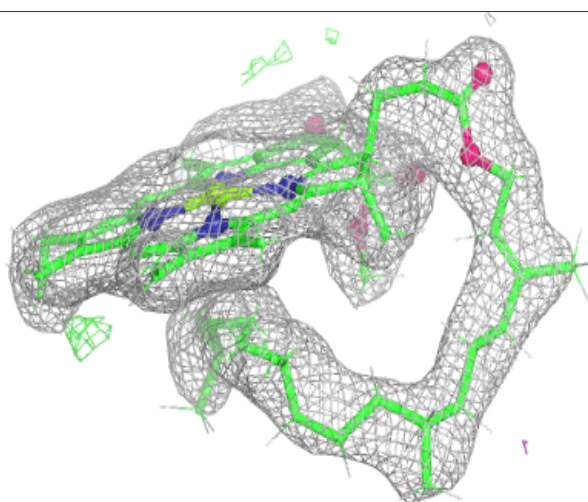
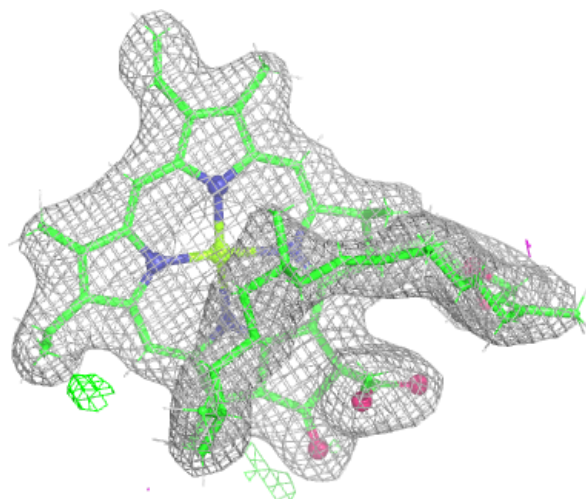
Electron density around CLA C 502:

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



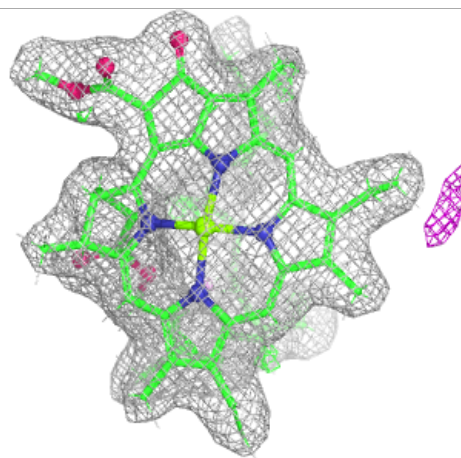
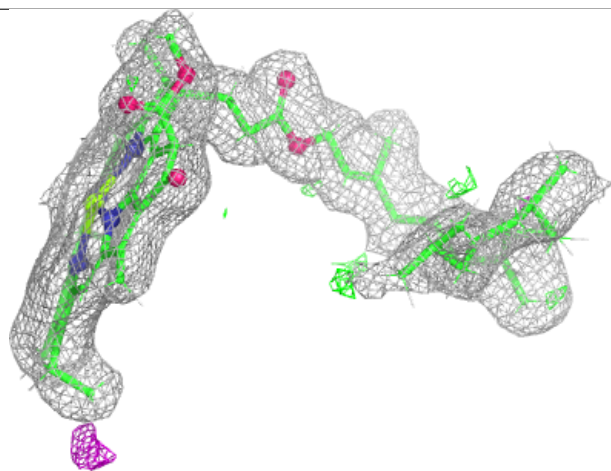
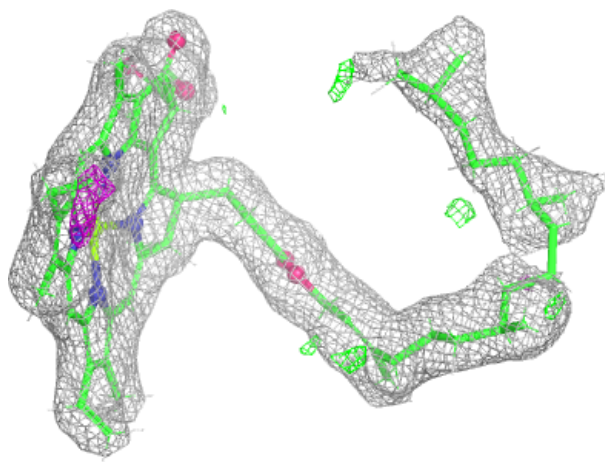
Electron density around CLA c 510:

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



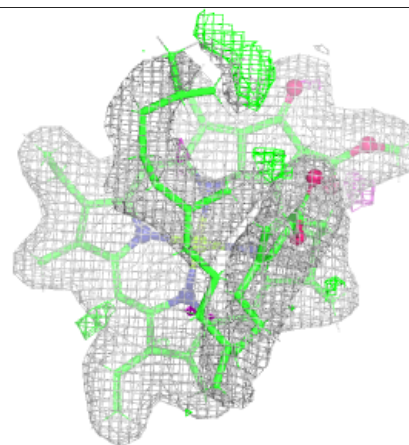
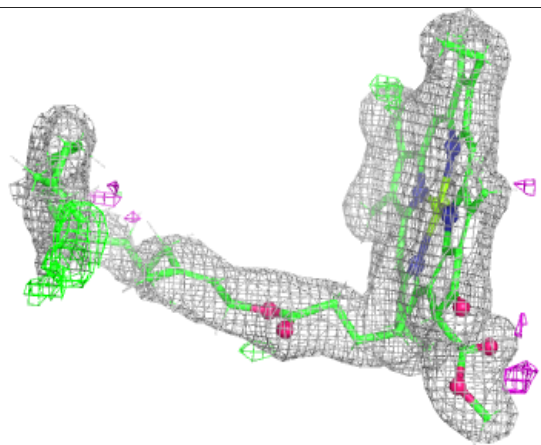
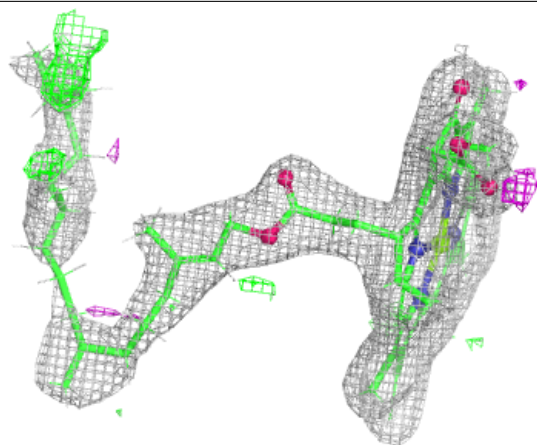
Electron density around CLA B 606:

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

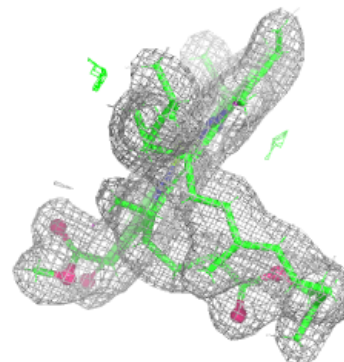
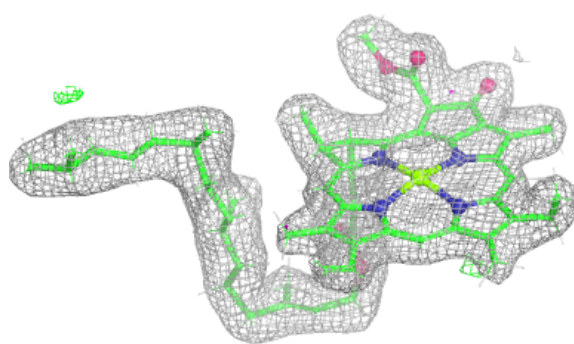
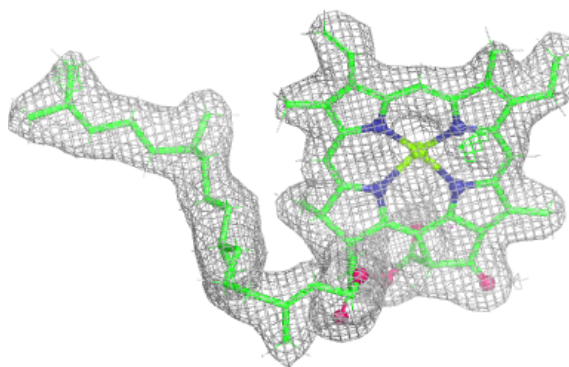


Electron density around CLA a 606:

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

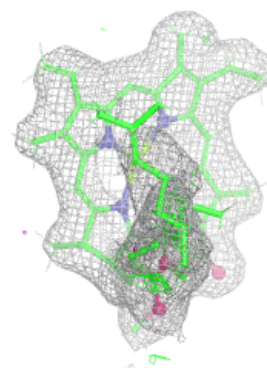
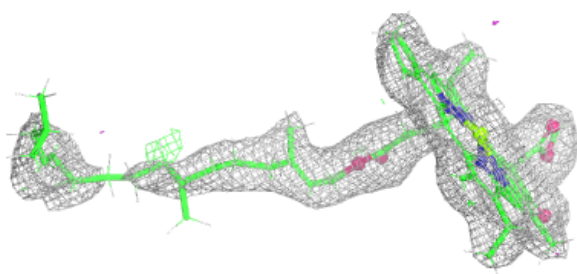
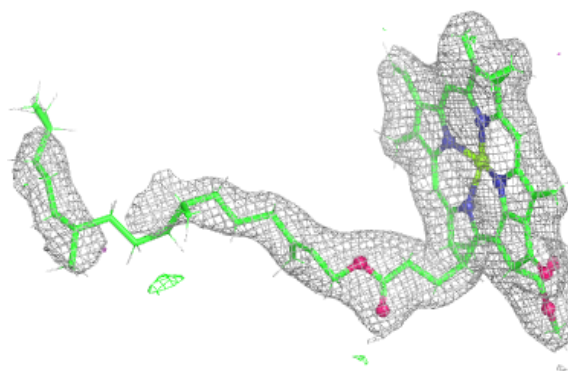
**Electron density around CLA a 612:**

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

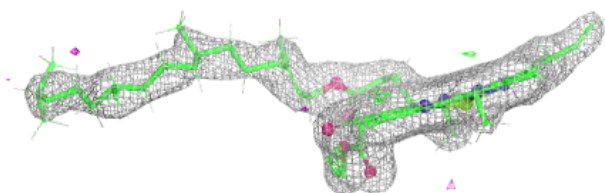
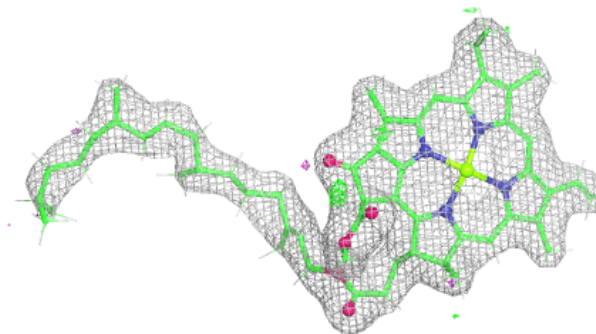


Electron density around CLA d 403:

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

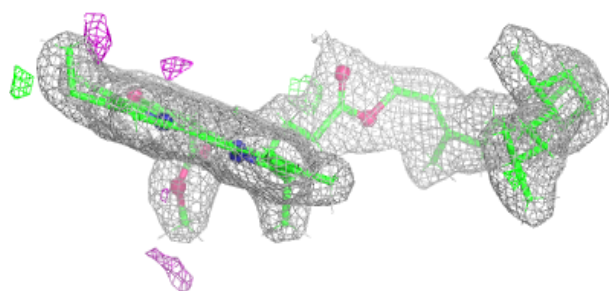
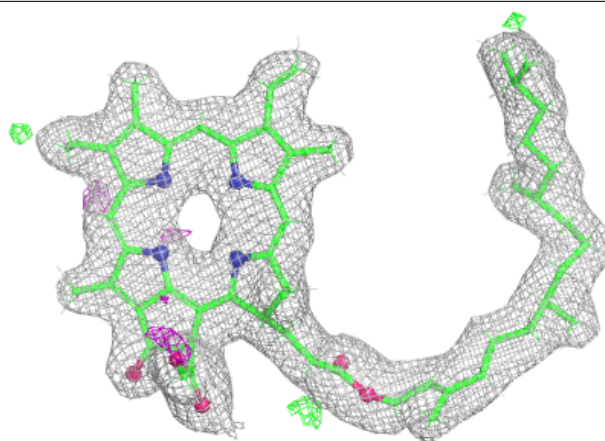
**Electron density around CLA b 602:**

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



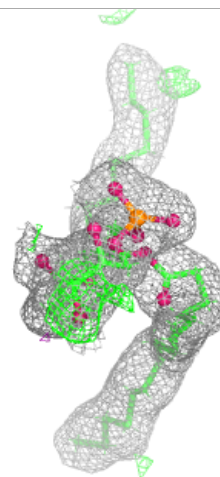
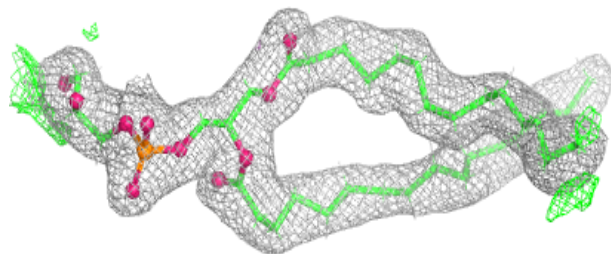
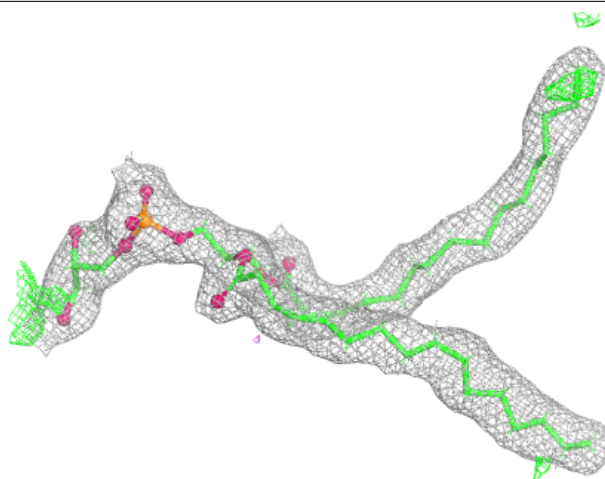
Electron density around PHO a 605:

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



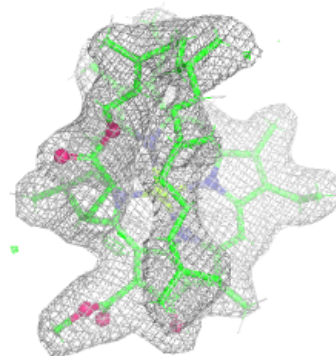
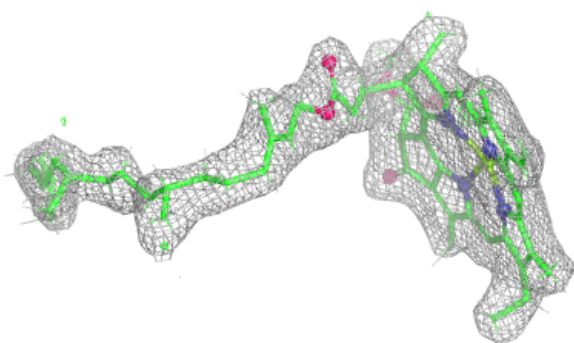
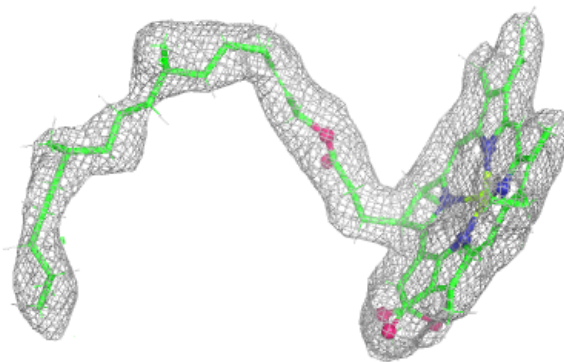
Electron density around LHG D 406:

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

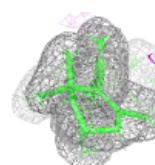
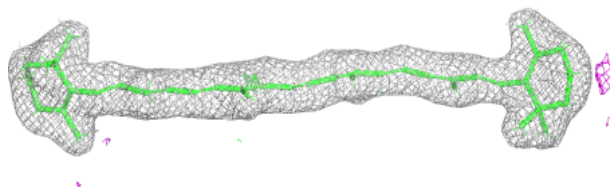
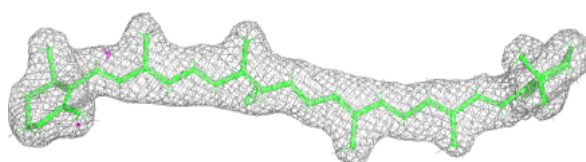


Electron density around CLA b 606:

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

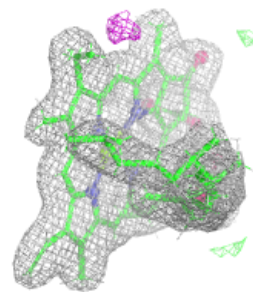
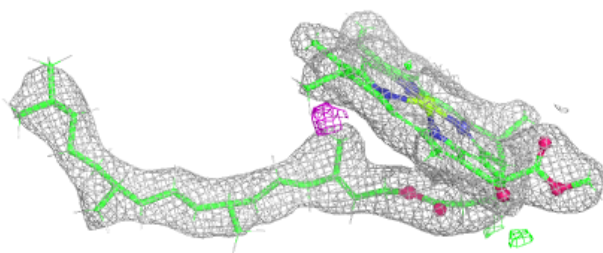
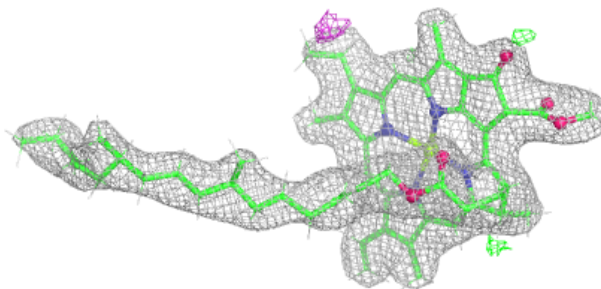
**Electron density around BCR A 608:**

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

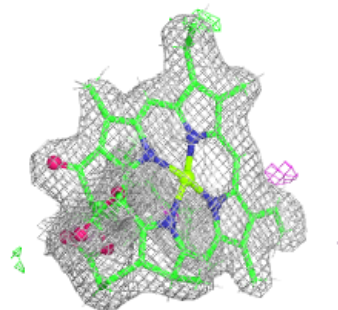
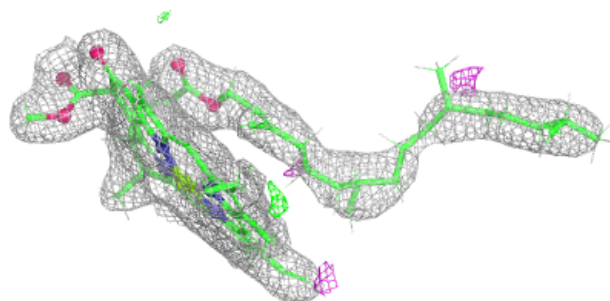
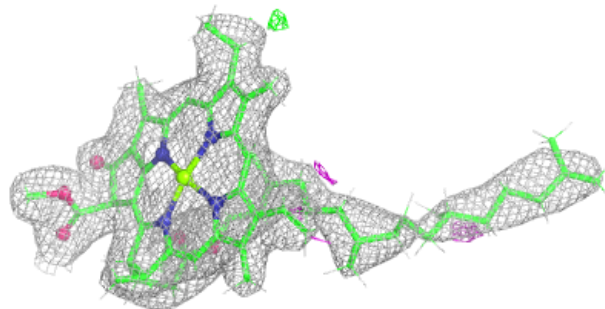


Electron density around CLA b 608:

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

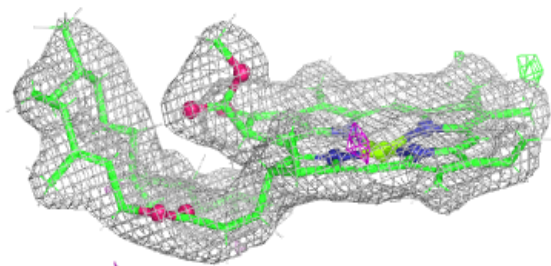
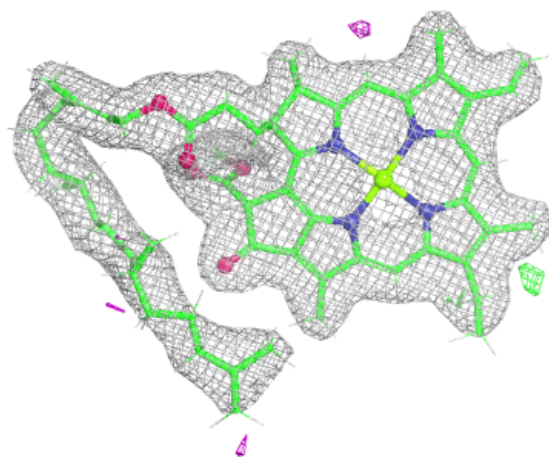
**Electron density around CLA C 505:**

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



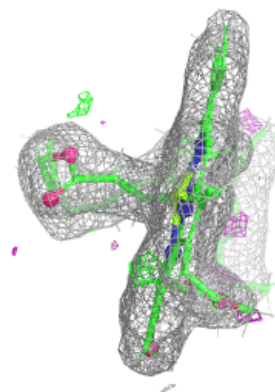
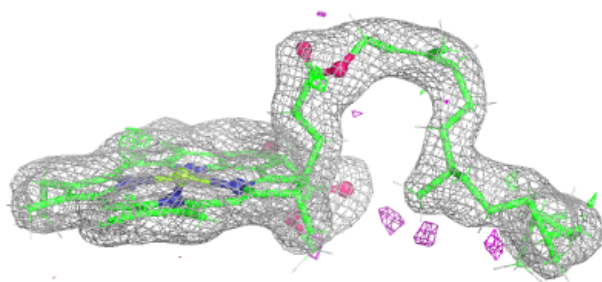
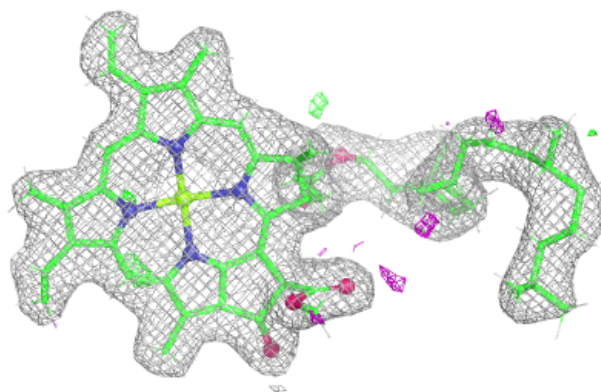
Electron density around CLA b 610:

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

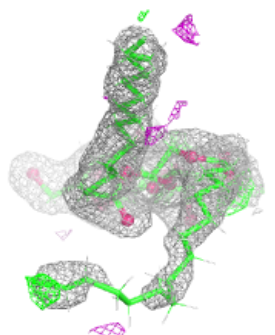
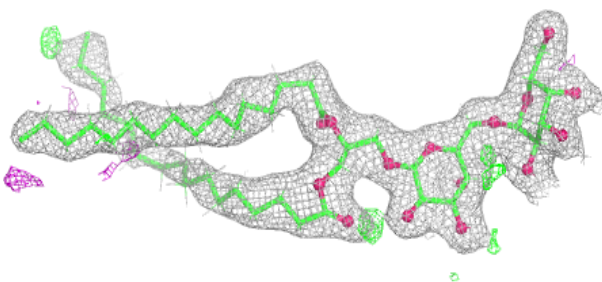
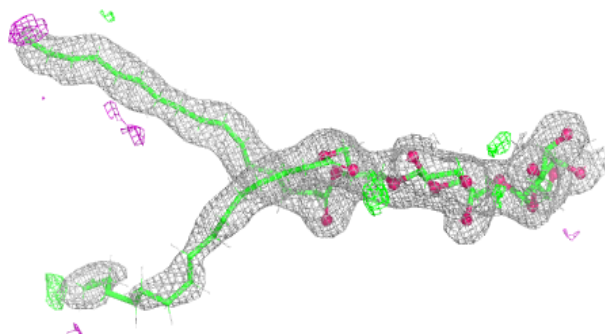


Electron density around CLA b 612:

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

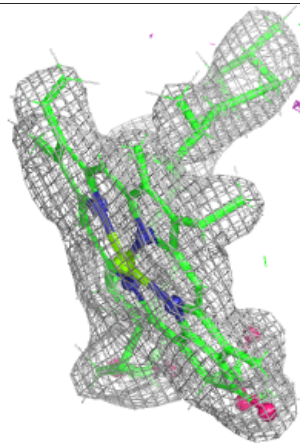
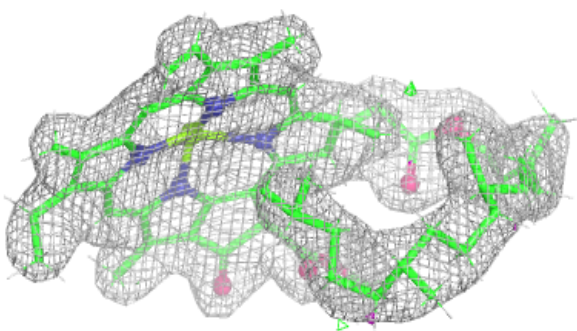
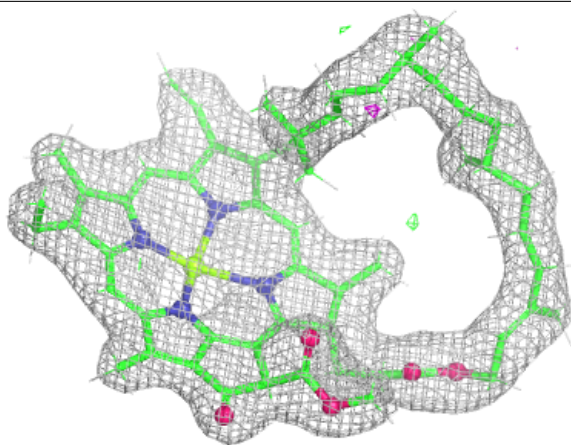
**Electron density around DGD C 516:**

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

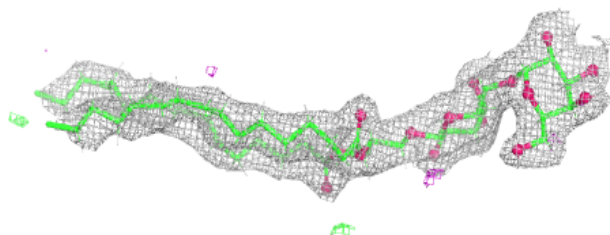
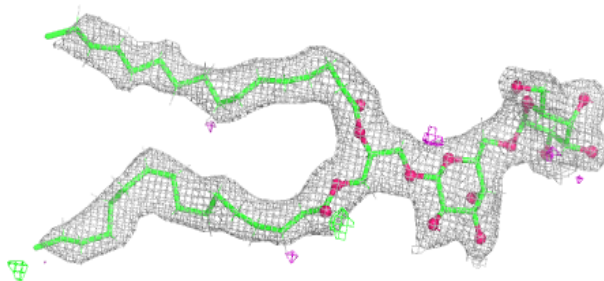


Electron density around CLA b 615:

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

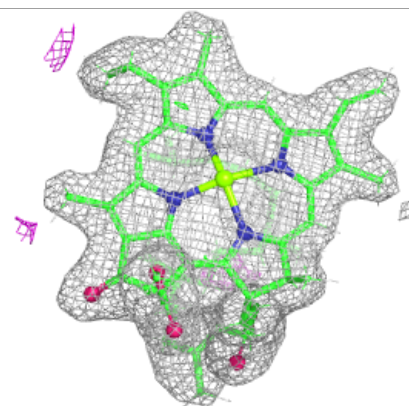
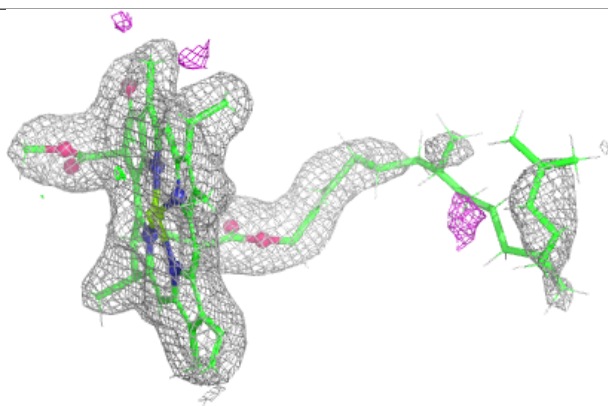
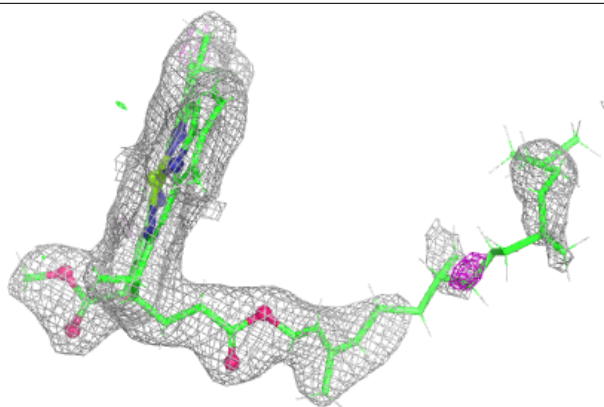
**Electron density around DGD C 518:**

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

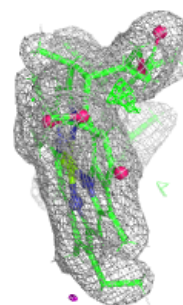
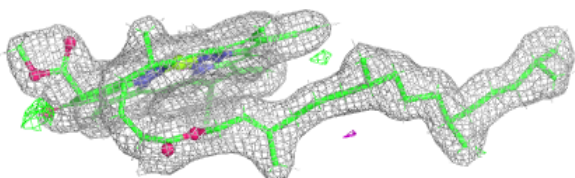
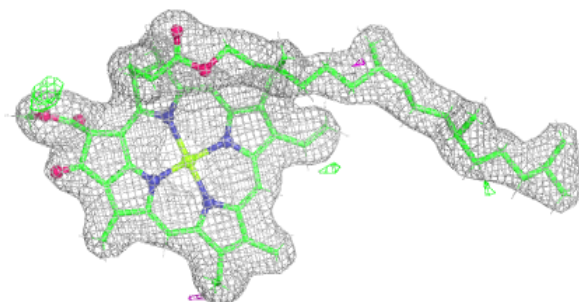


Electron density around CLA C 506:

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

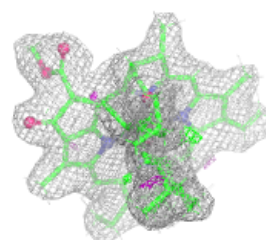
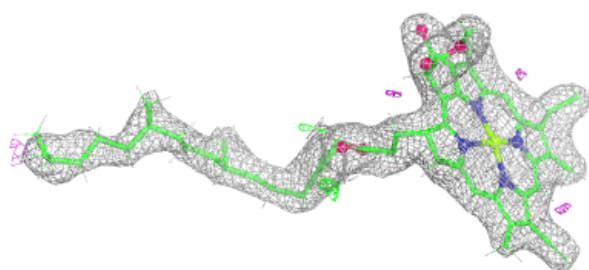
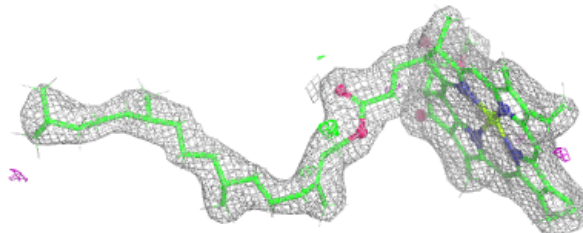
**Electron density around CLA c 501:**

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

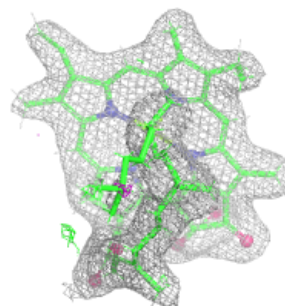
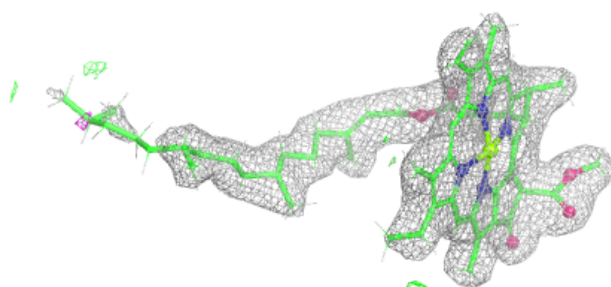
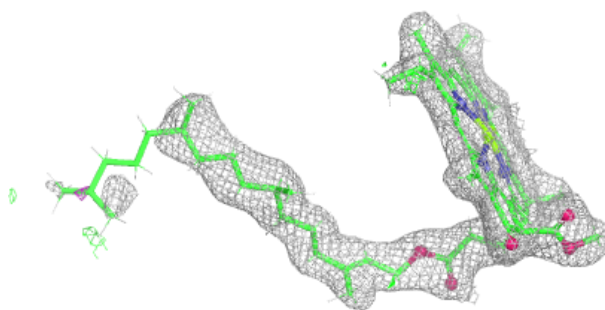


Electron density around CLA c 502:

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

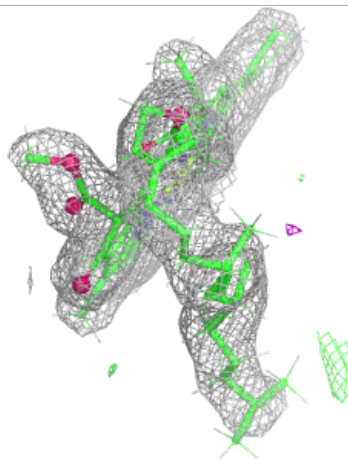
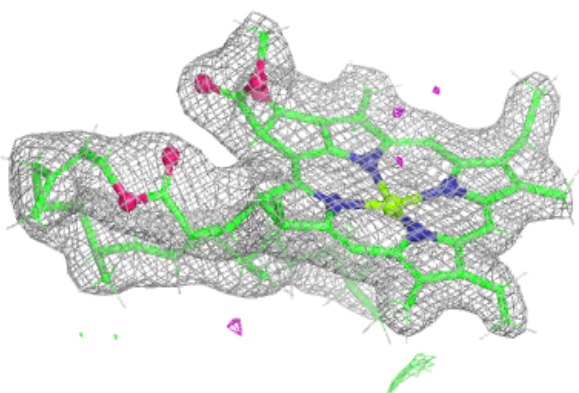
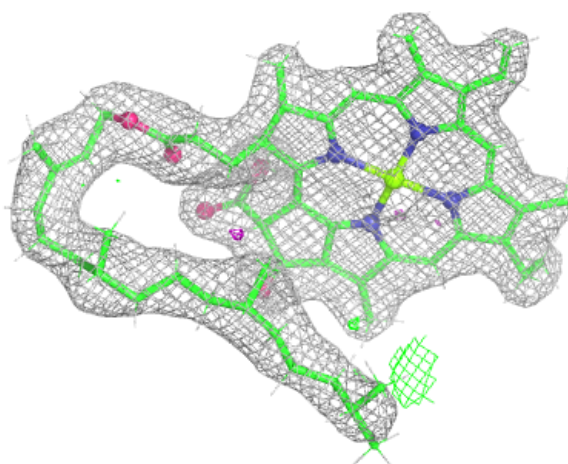
**Electron density around CLA C 508:**

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



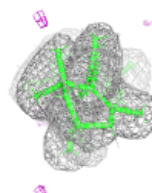
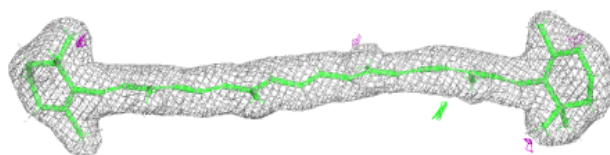
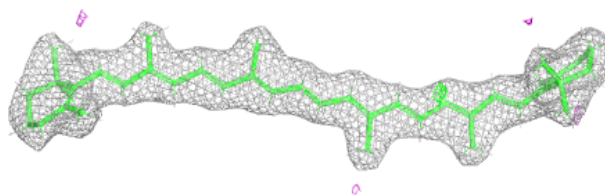
Electron density around CLA C 509:

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

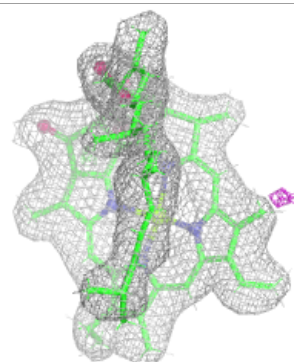
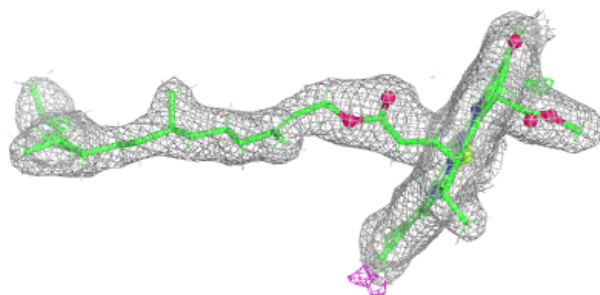
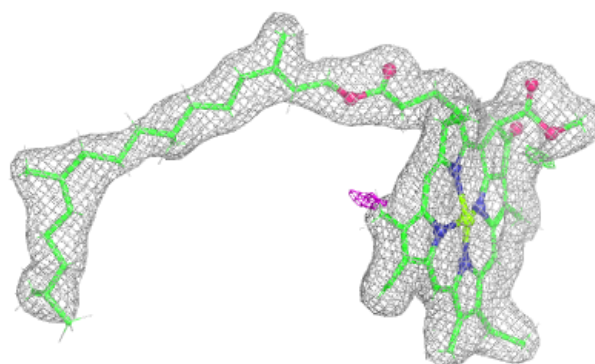


Electron density around BCR a 607:

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

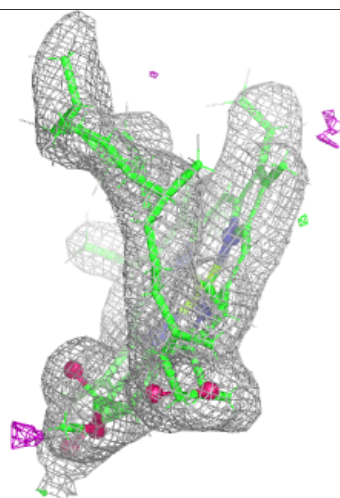
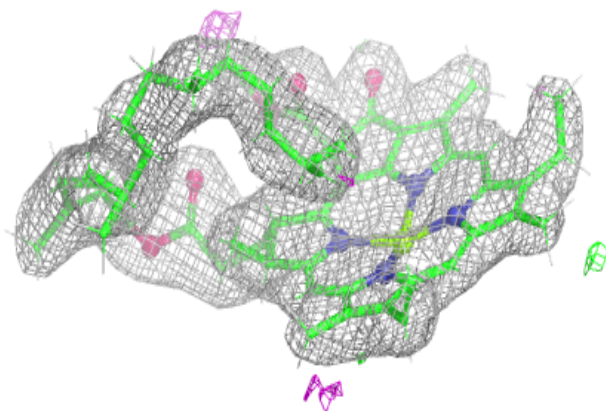
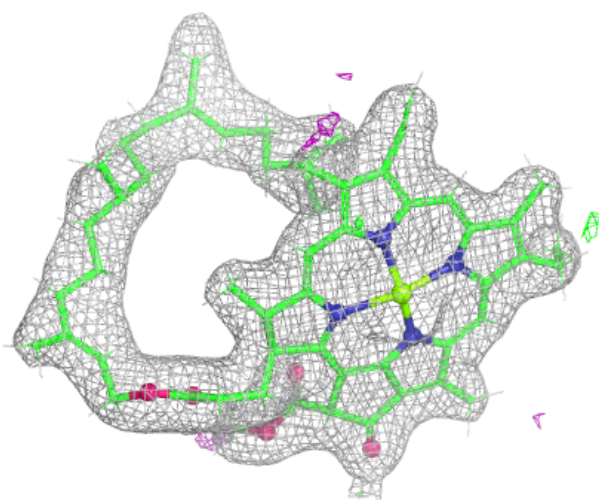
**Electron density around CLA B 609:**

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



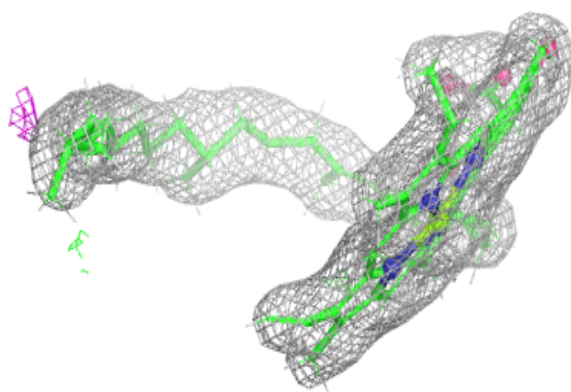
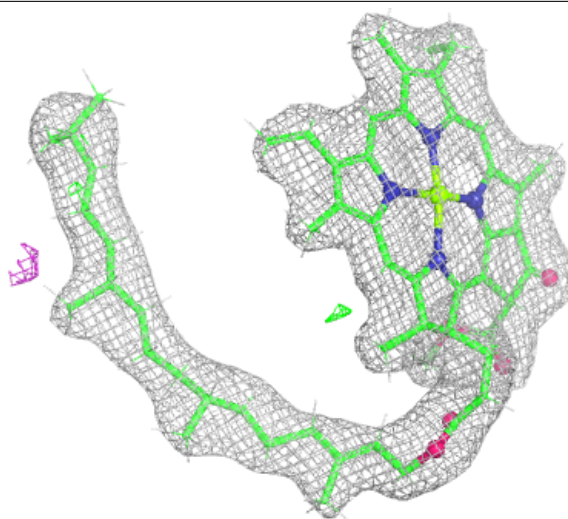
Electron density around CLA B 615:

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



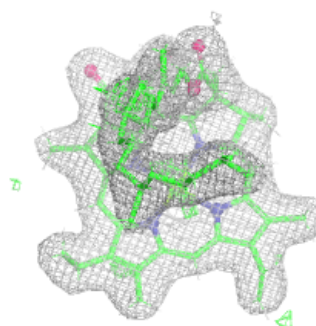
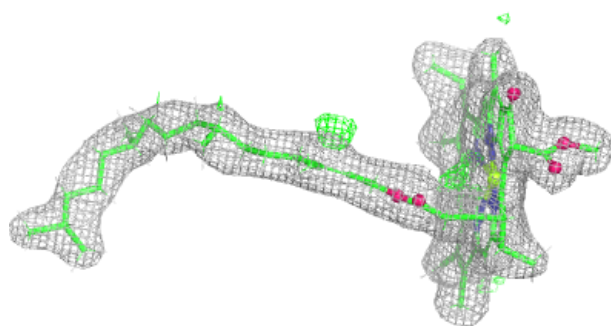
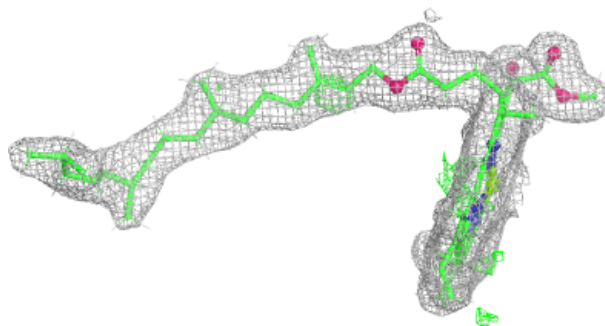
Electron density around CLA c 507:

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



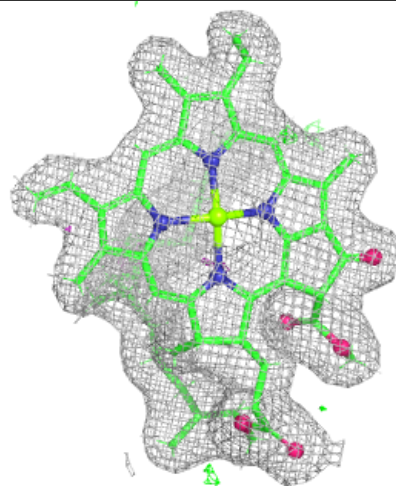
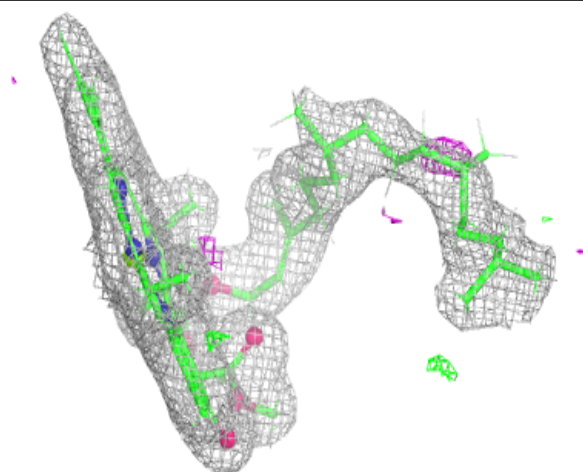
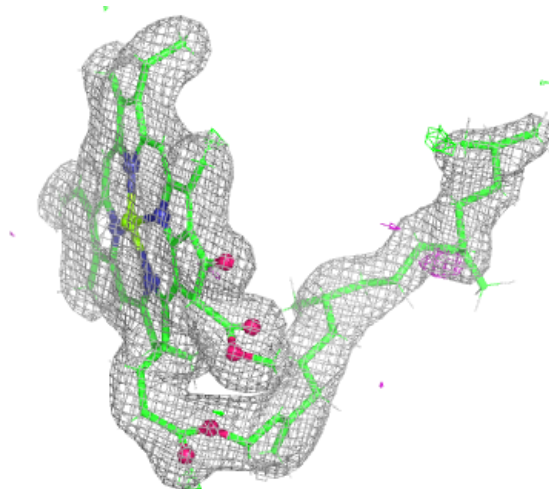
Electron density around CLA B 605:

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



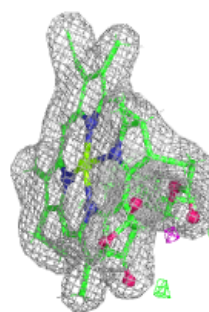
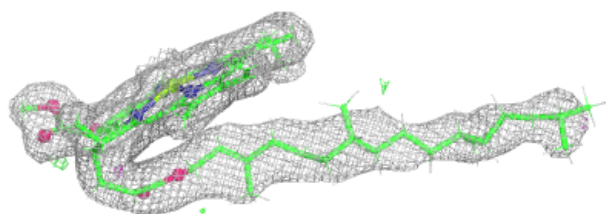
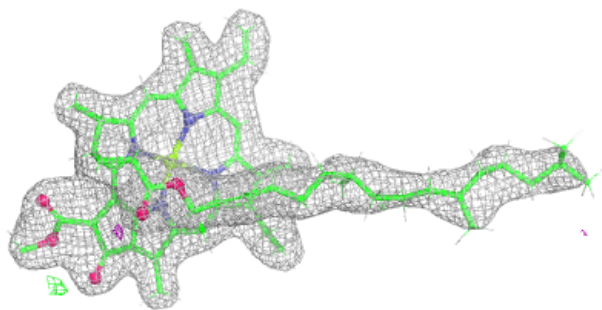
Electron density around CLA b 613:

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

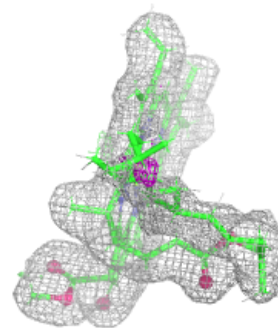
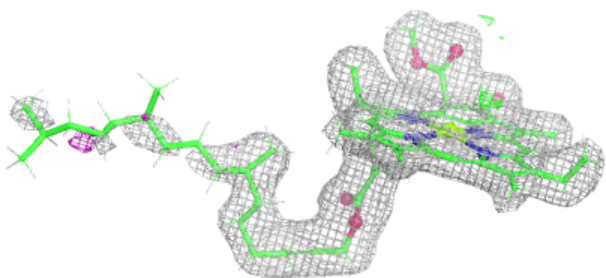
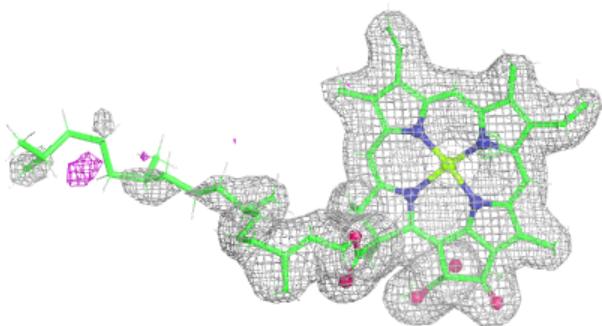


Electron density around CLA b 614:

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

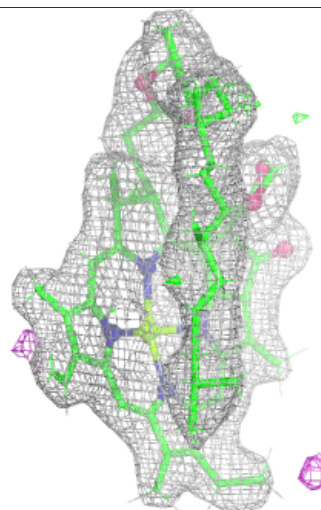
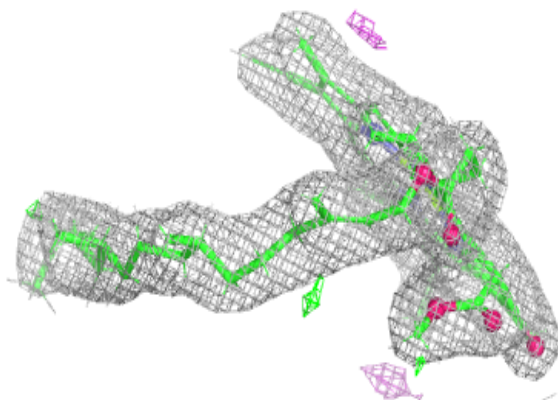
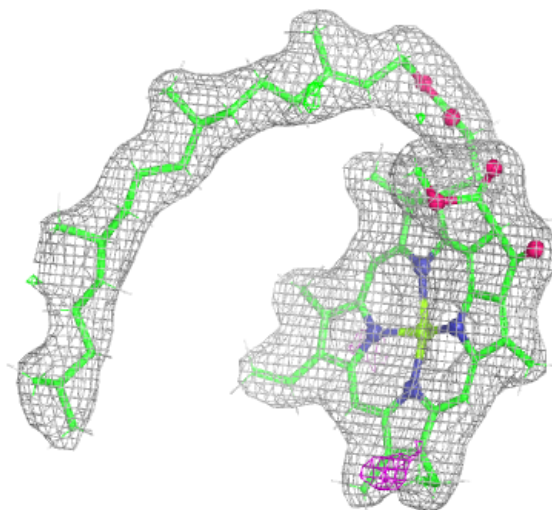
**Electron density around CLA A 604:**

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



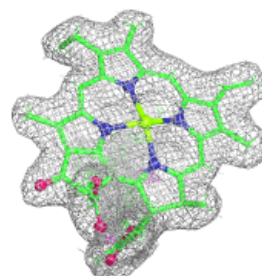
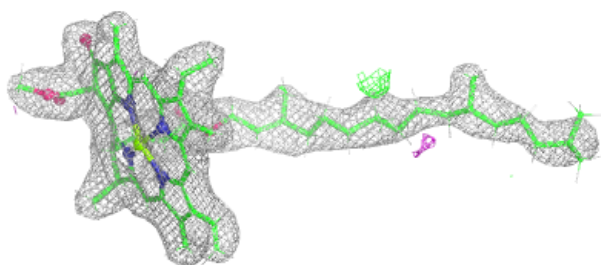
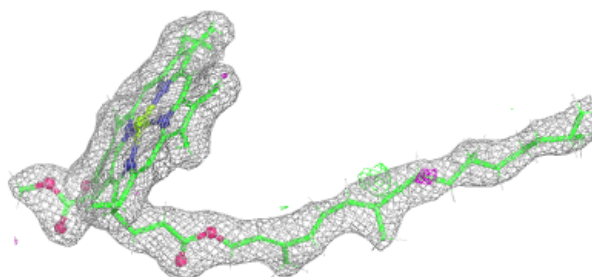
Electron density around CLA C 507:

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

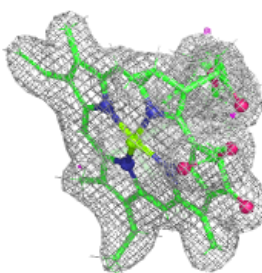
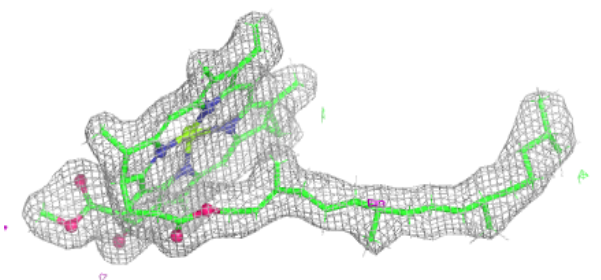
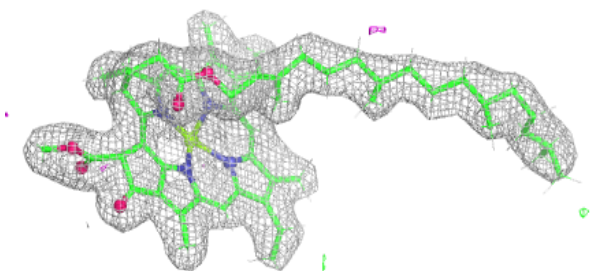


Electron density around CLA B 607:

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

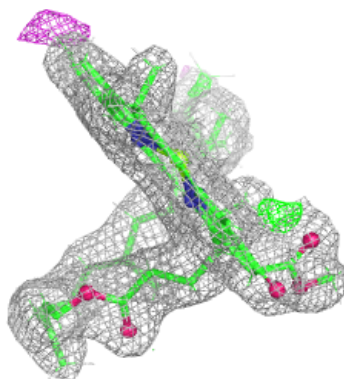
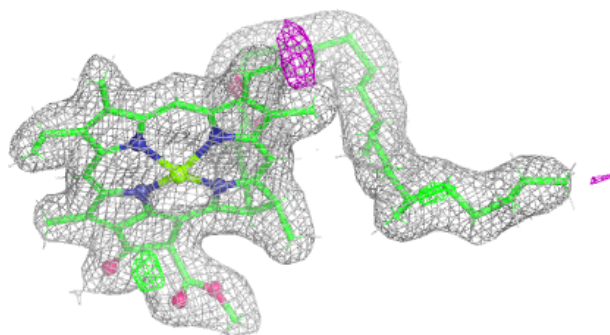
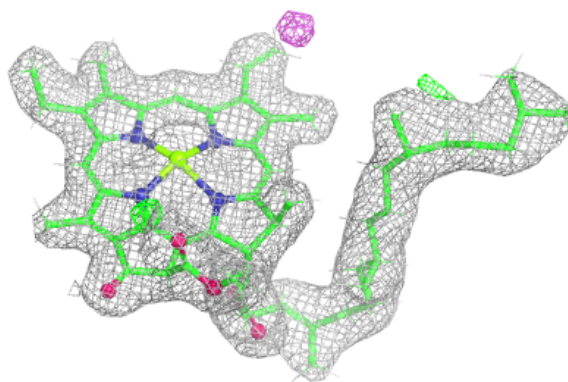
**Electron density around CLA B 608:**

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

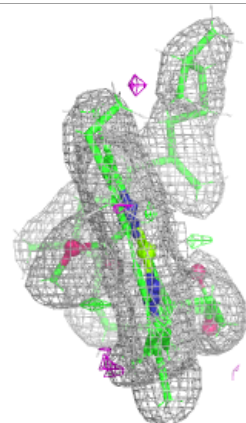
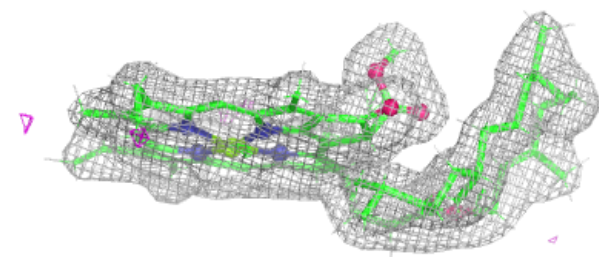
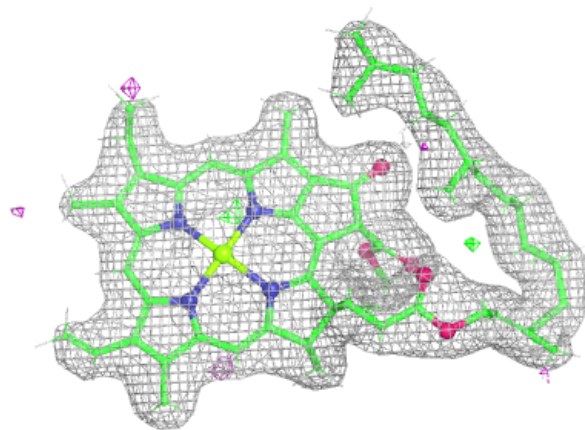


Electron density around CLA A 613:

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

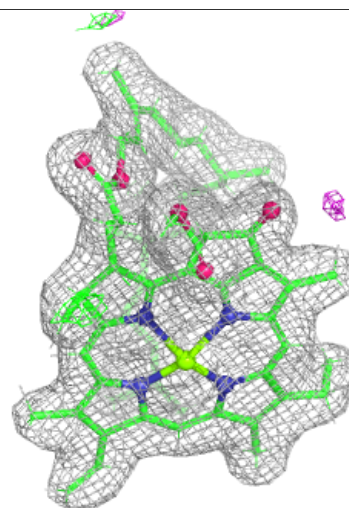
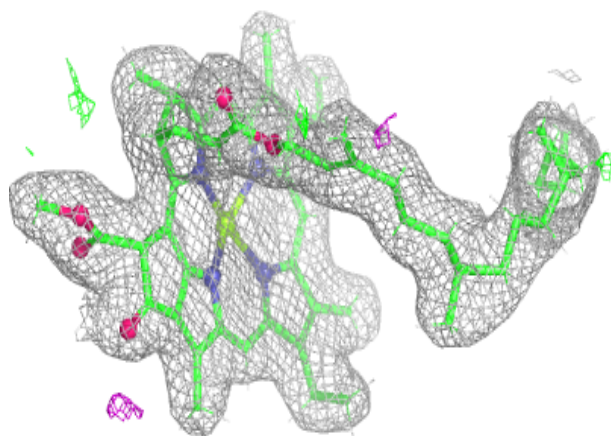
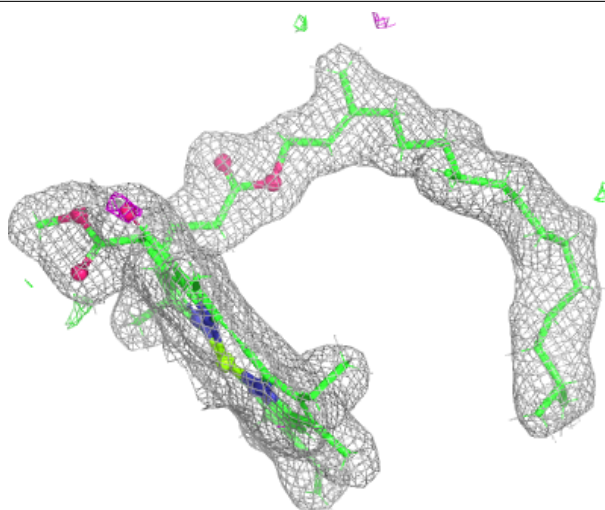
**Electron density around CLA B 610:**

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



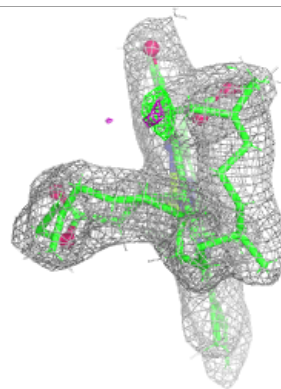
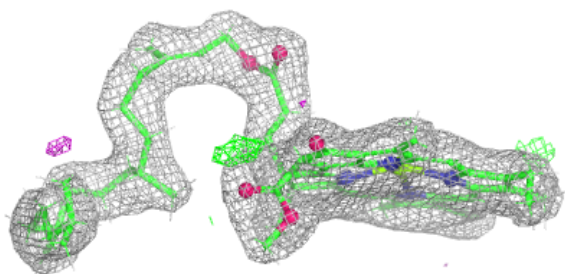
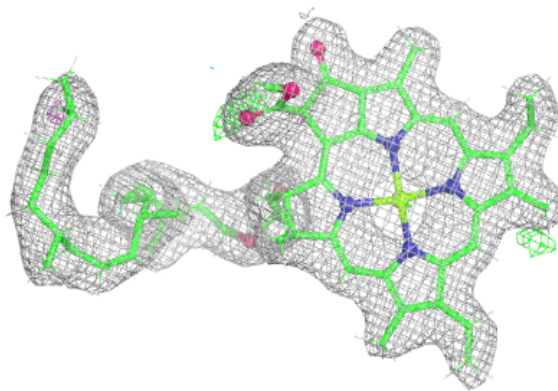
Electron density around CLA B 611:

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

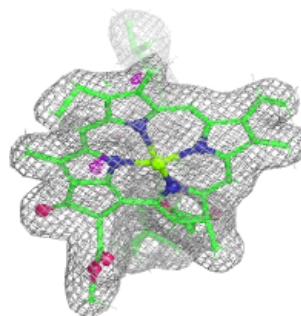
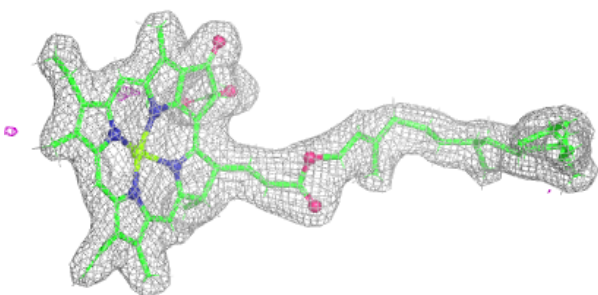
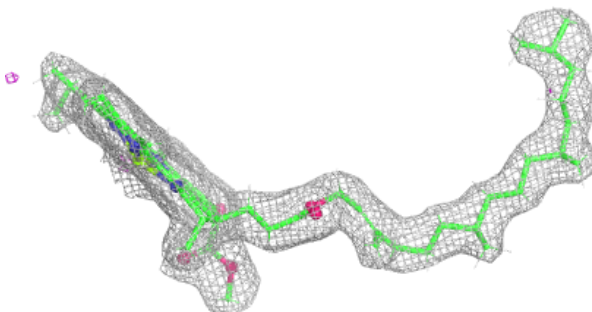


Electron density around CLA B 612:

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

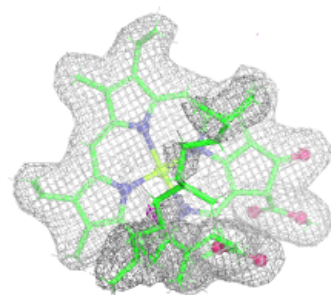
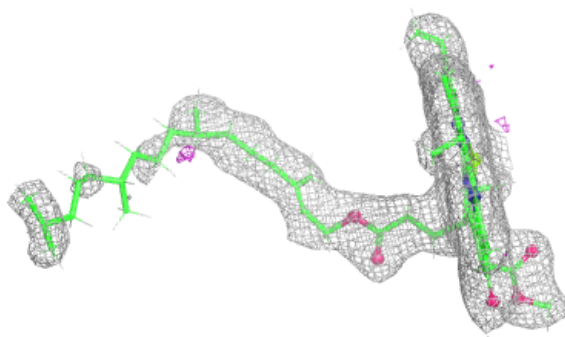
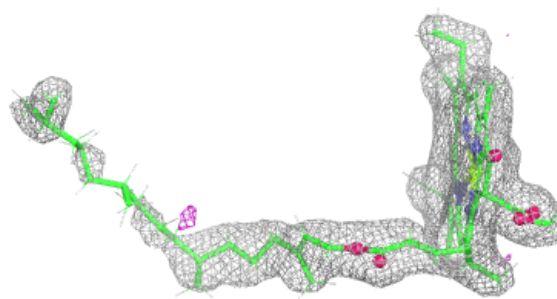
**Electron density around CLA D 402:**

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

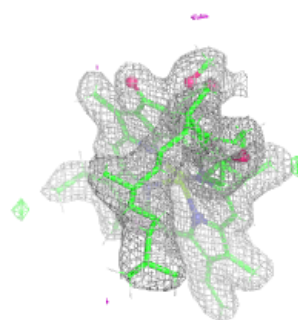
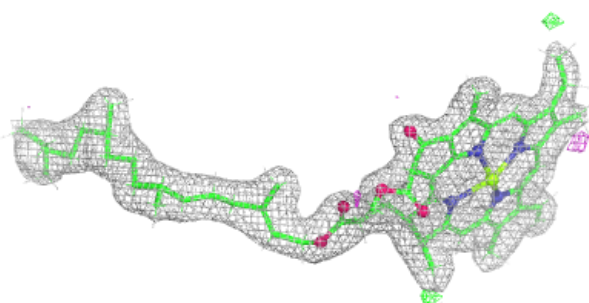
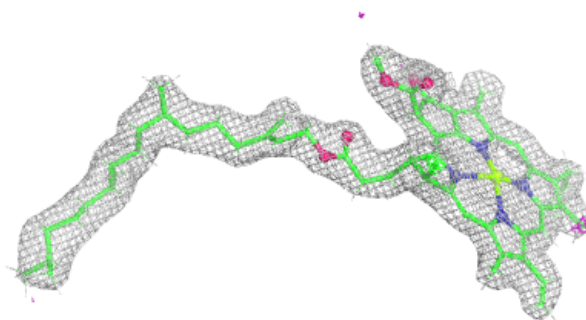


Electron density around CLA D 403:

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

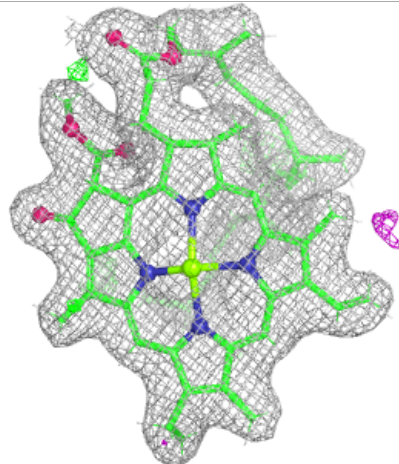
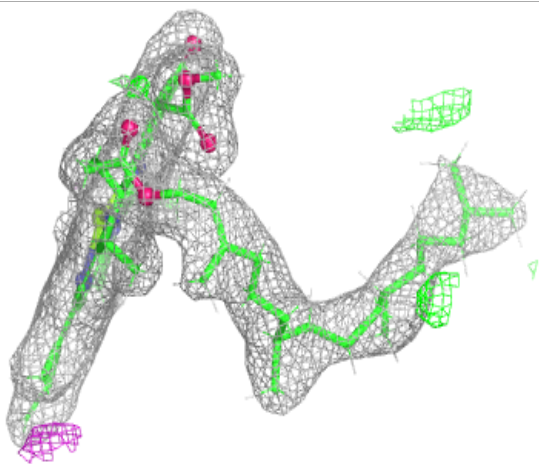
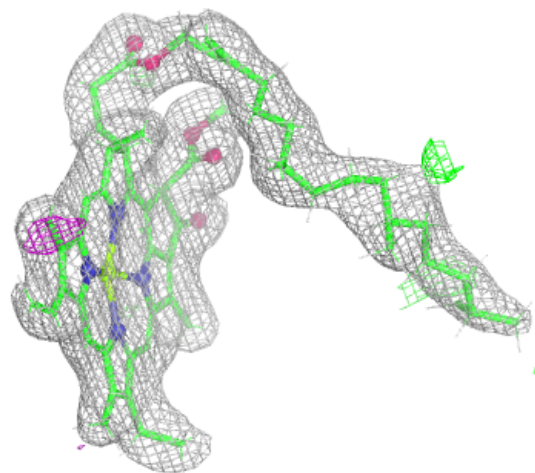
**Electron density around CLA a 603:**

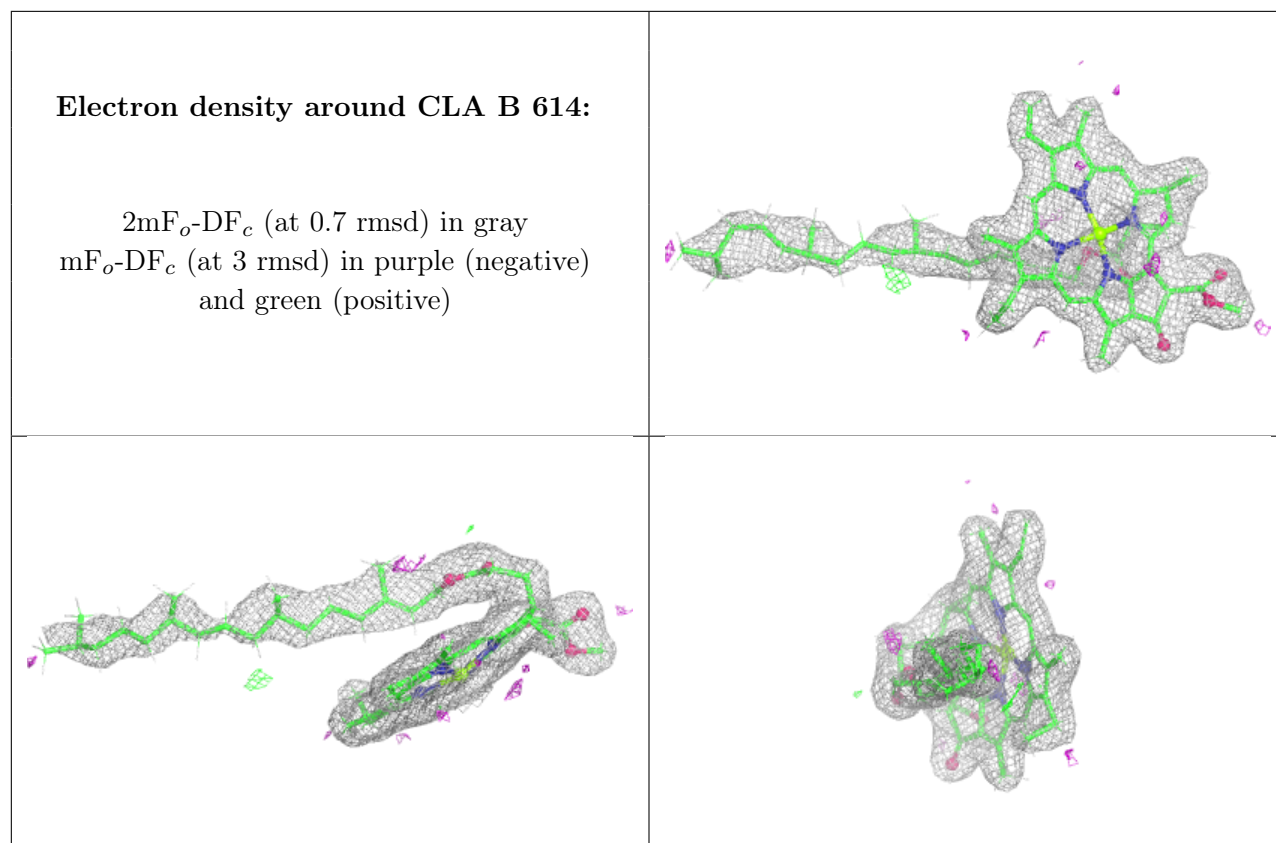
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 613:

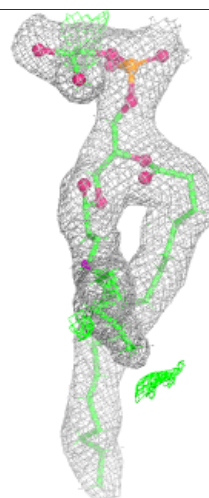
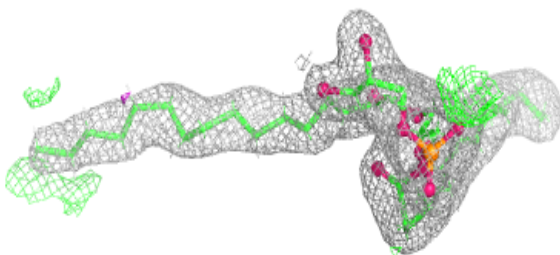
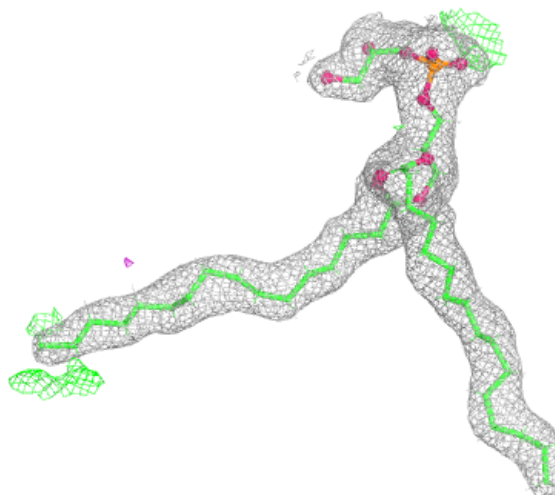
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





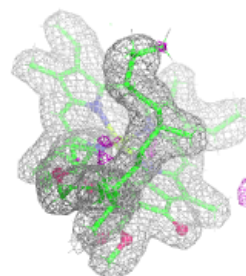
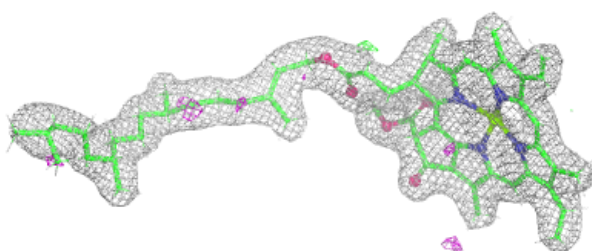
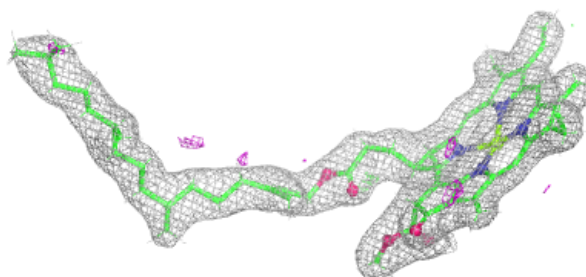
Electron density around LHG L 101:

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

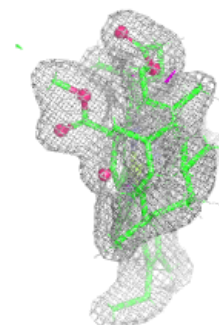
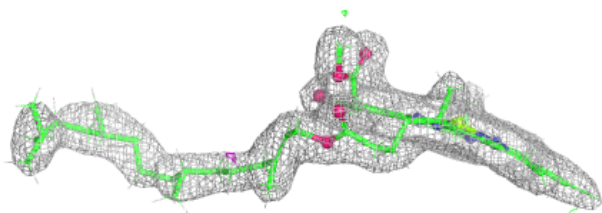
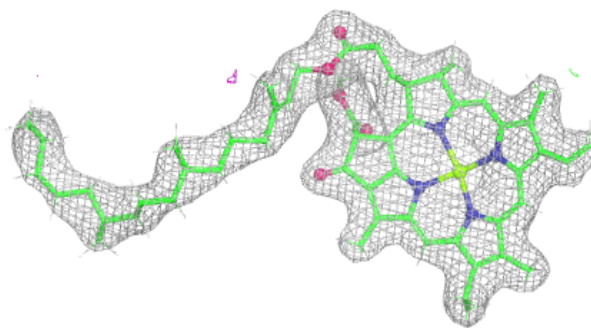


Electron density around CLA A 603:

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

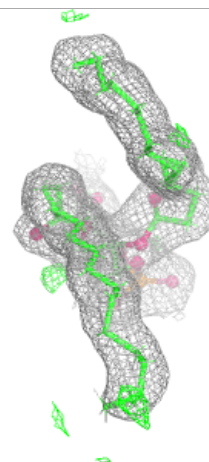
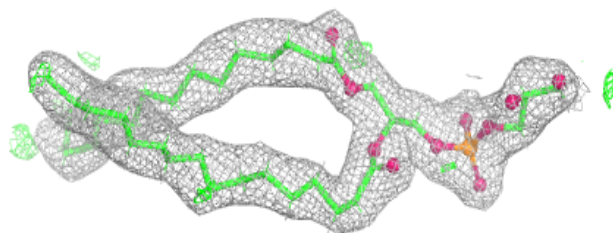
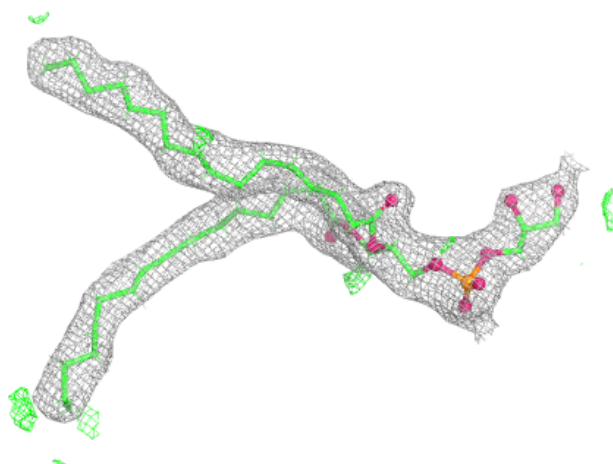
**Electron density around CLA B 602:**

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



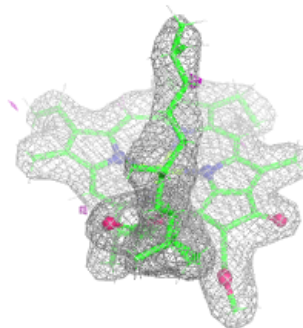
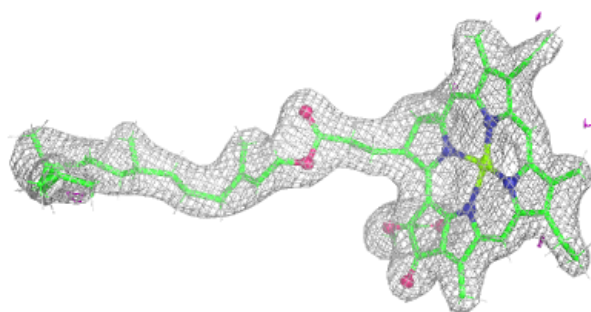
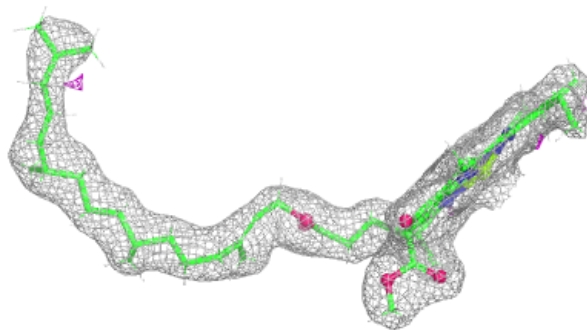
Electron density around LHG d 407:

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

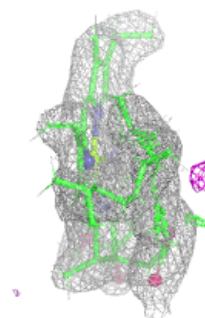
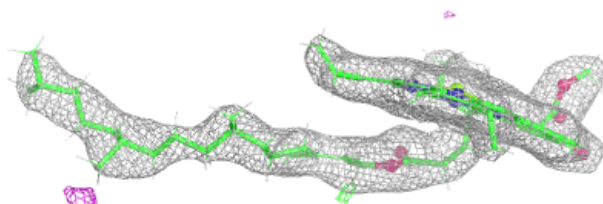
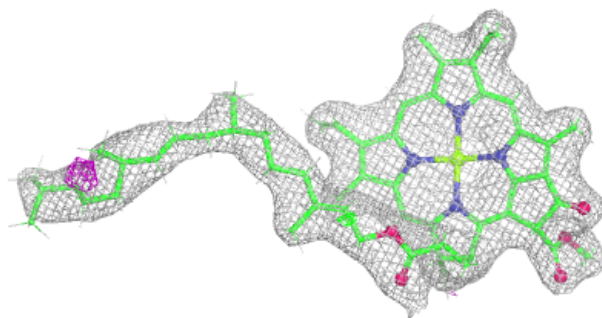


Electron density around CLA d 402:

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

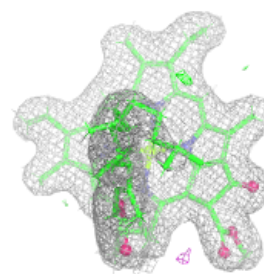
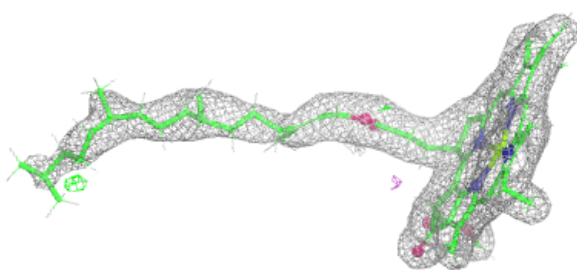
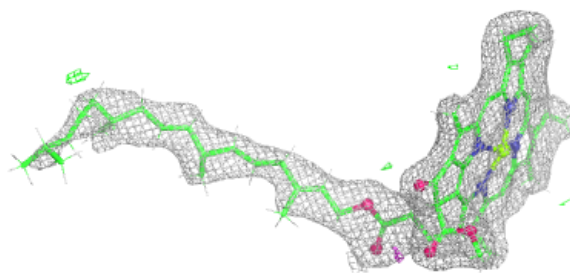
**Electron density around CLA b 603:**

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

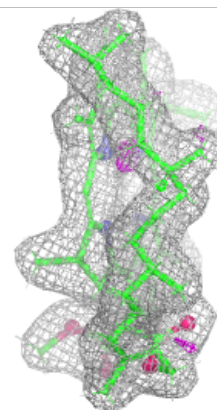
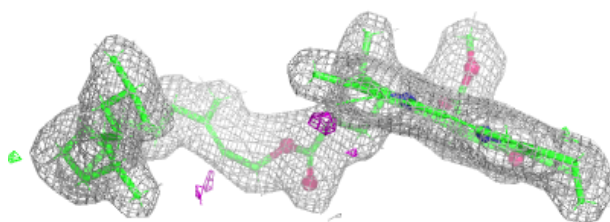
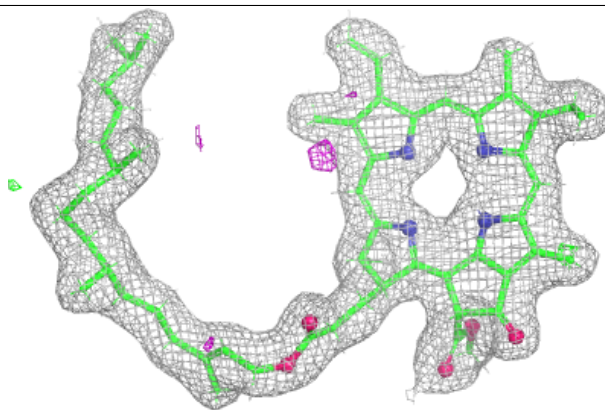


Electron density around CLA b 604:

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

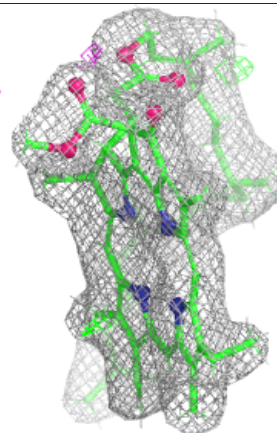
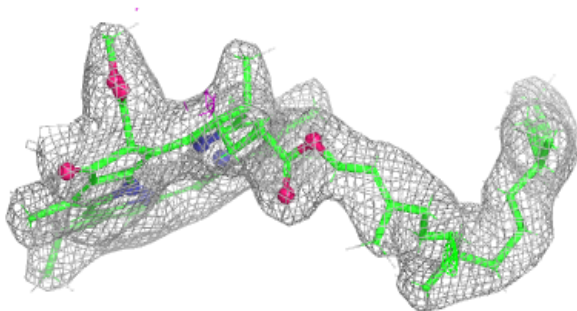
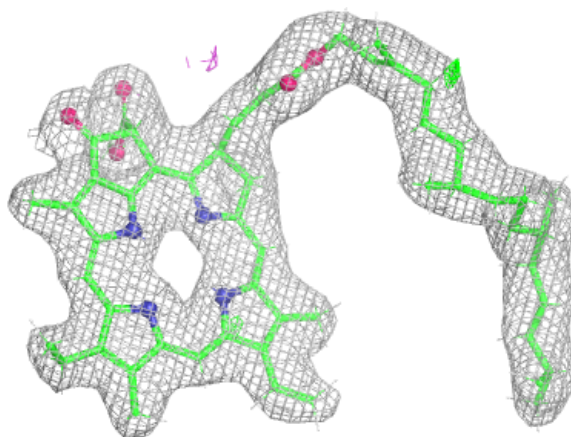
**Electron density around PHO A 605:**

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



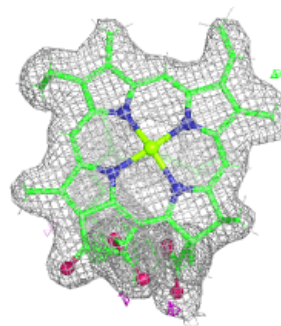
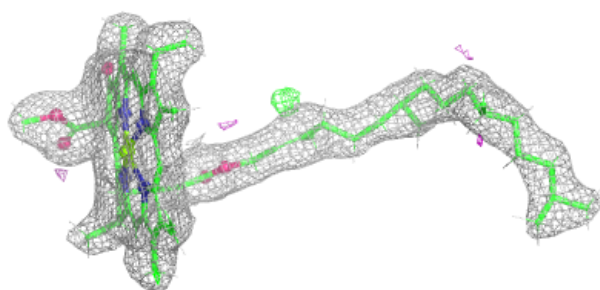
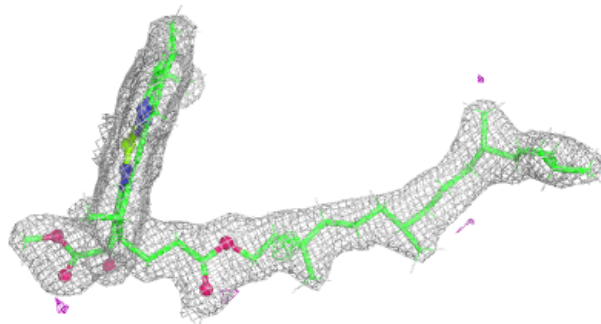
Electron density around PHO A 606:

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

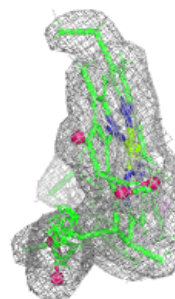
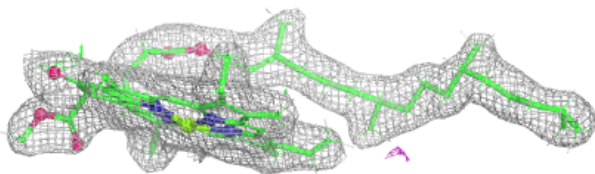
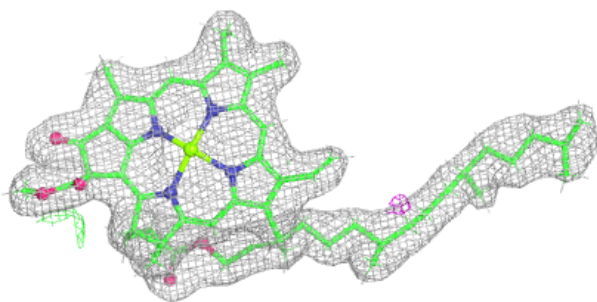


Electron density around CLA b 605:

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

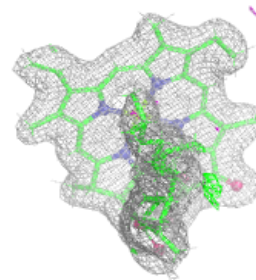
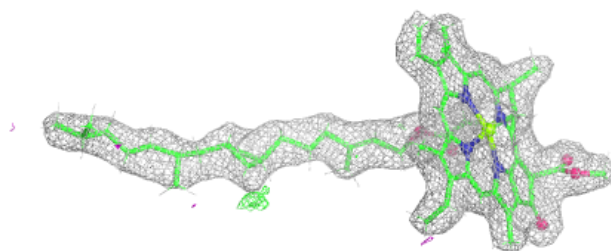
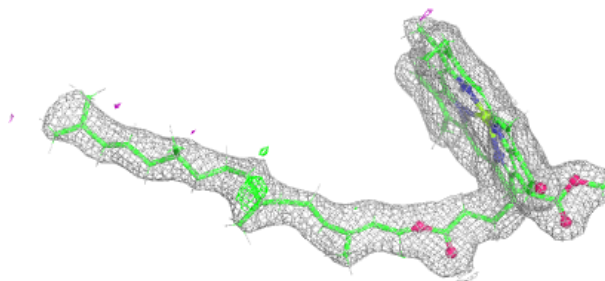
**Electron density around CLA C 501:**

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

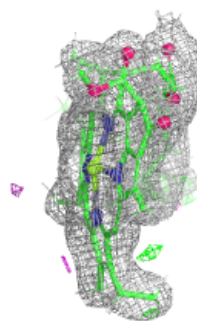
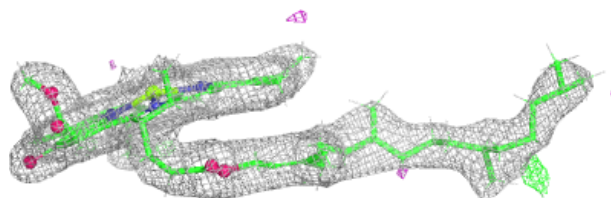
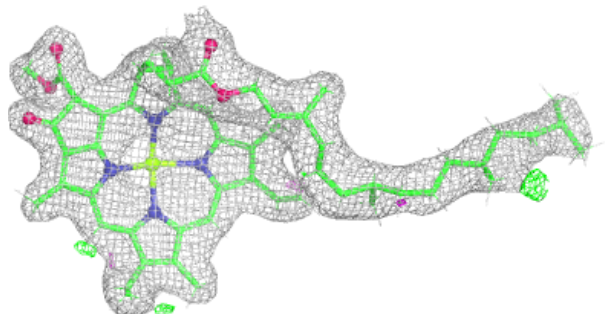


Electron density around CLA b 607:

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

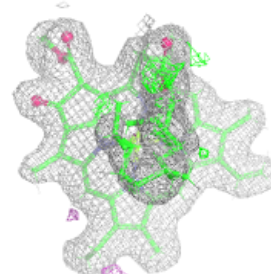
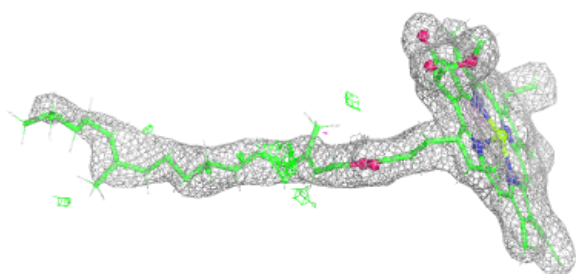
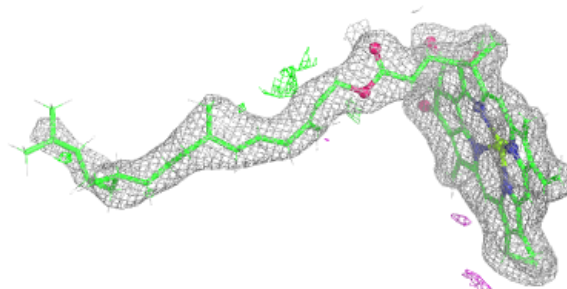
**Electron density around CLA B 603:**

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

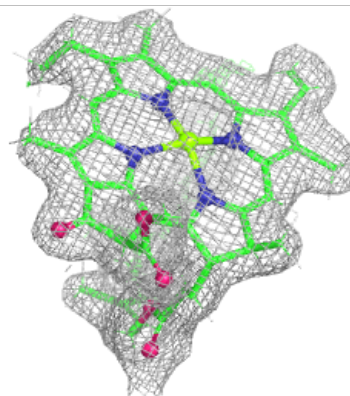
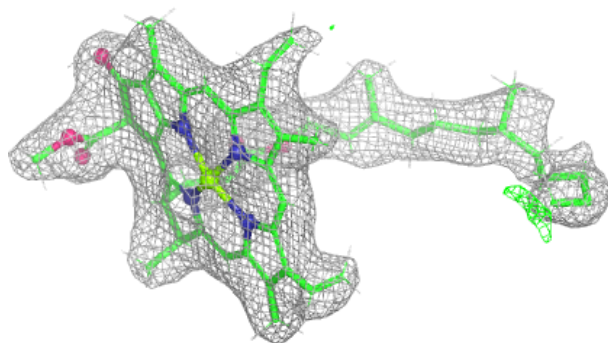
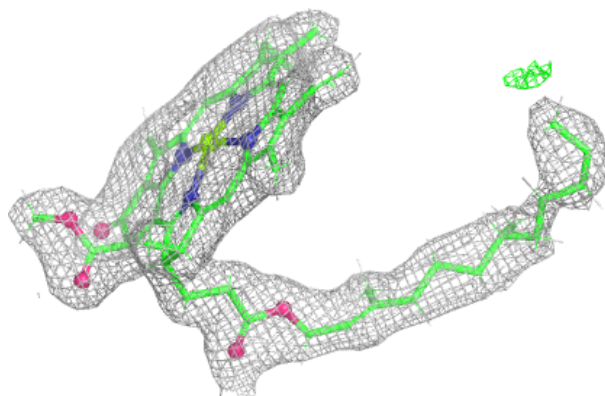


Electron density around CLA B 604:

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

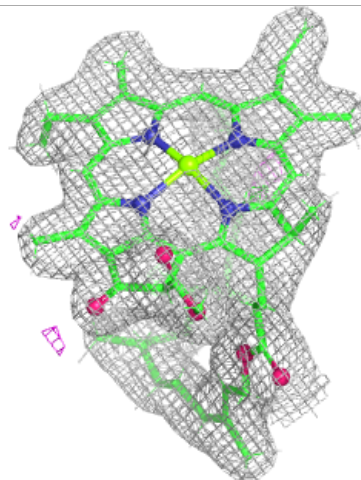
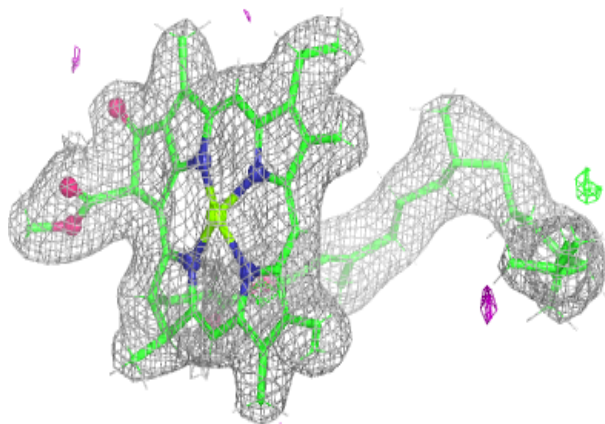
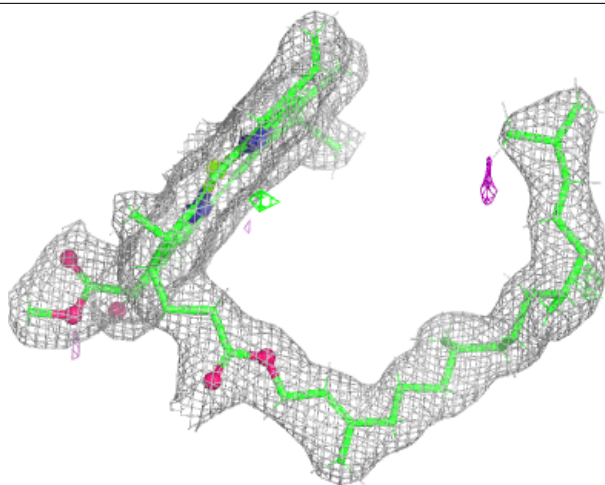
**Electron density around CLA C 504:**

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



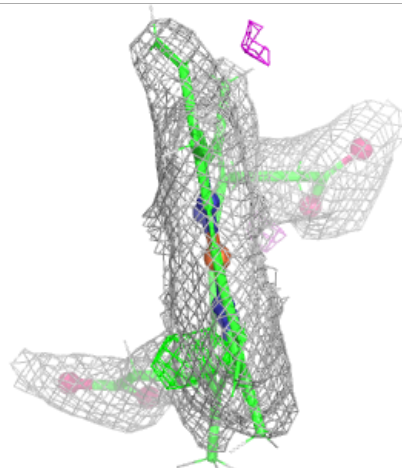
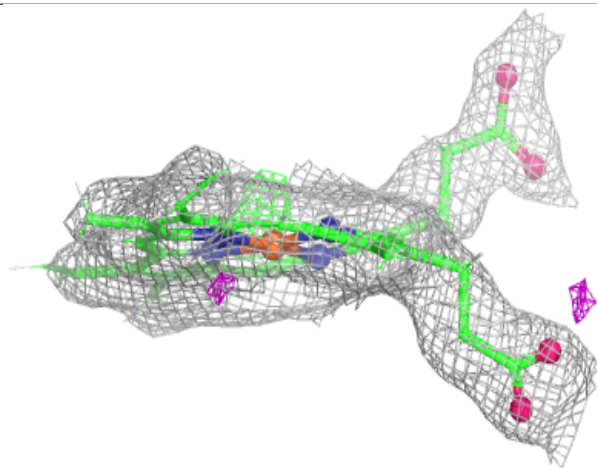
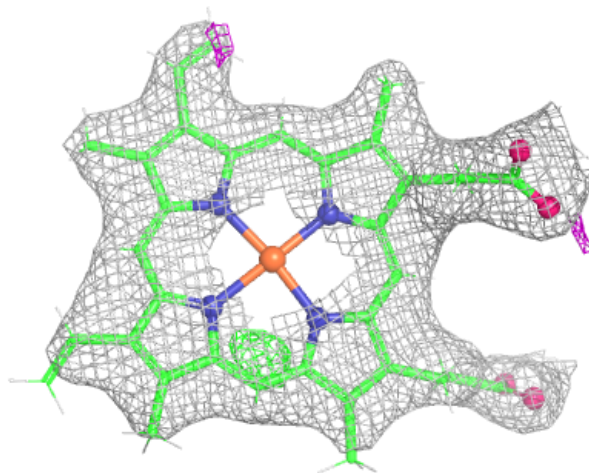
Electron density around CLA b 611:

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



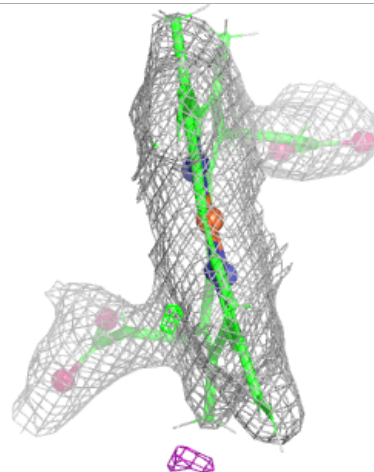
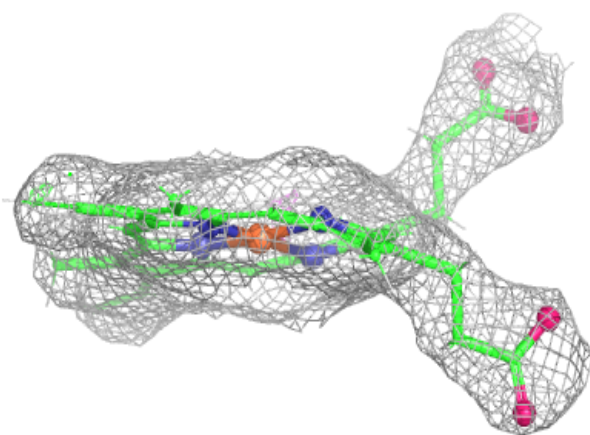
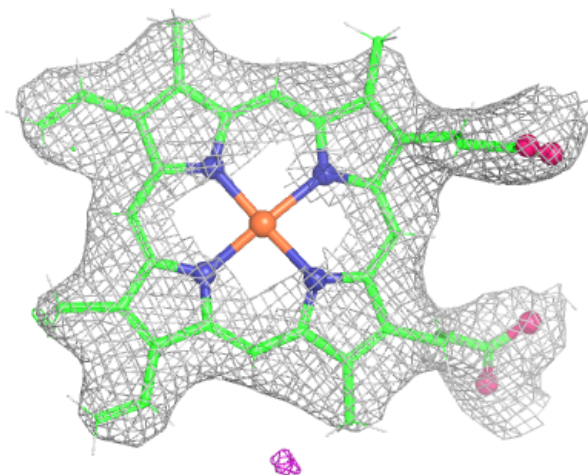
Electron density around HEM F 102:

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



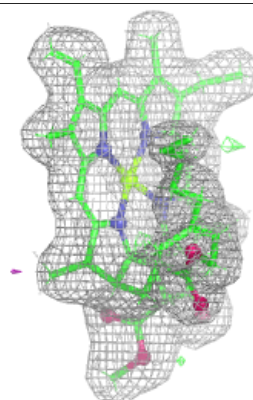
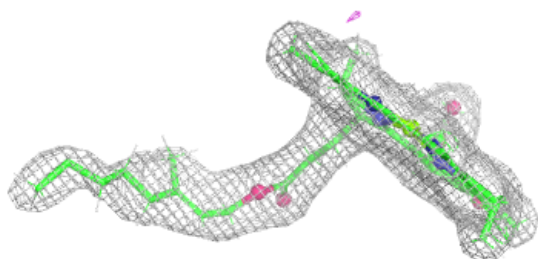
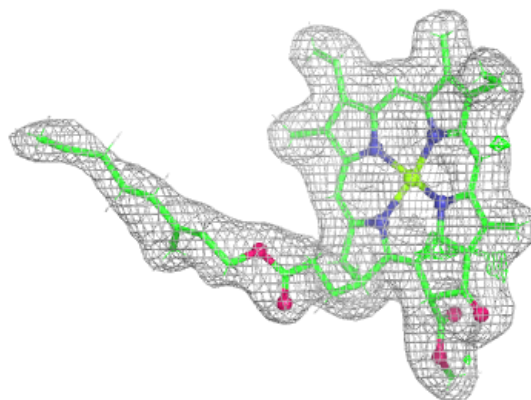
Electron density around HEM f 102:

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



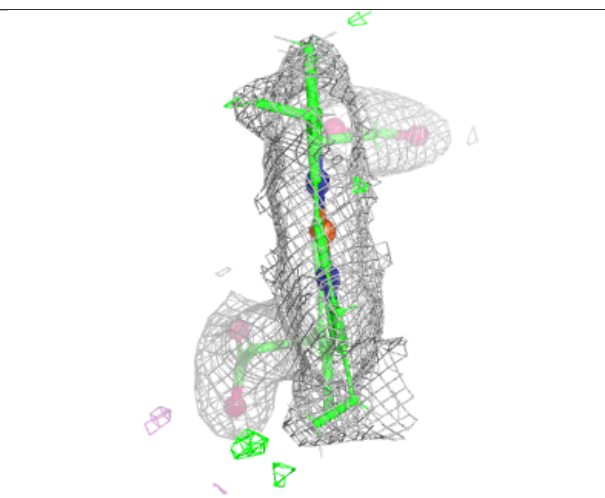
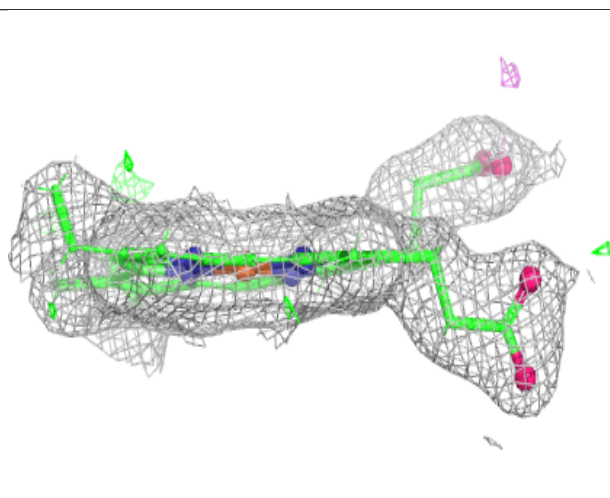
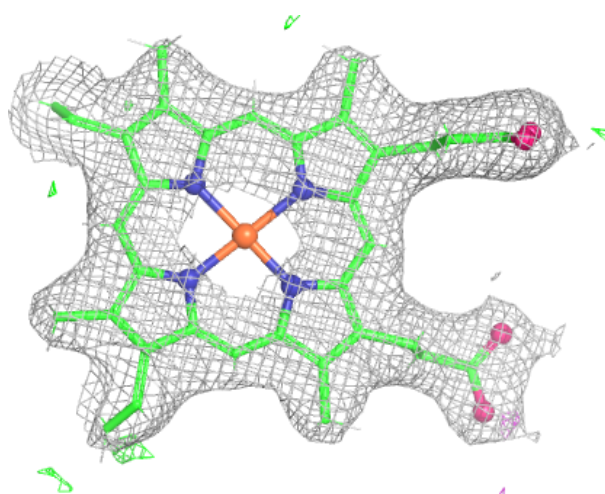
Electron density around CLA A 607:

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



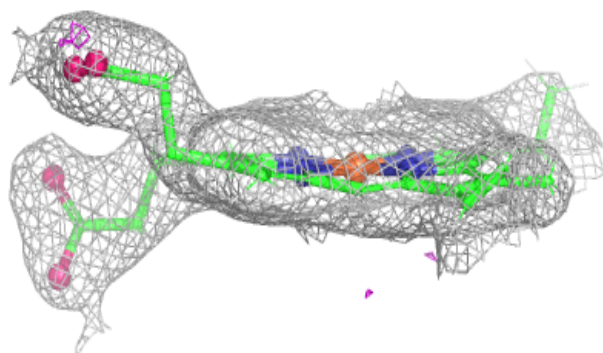
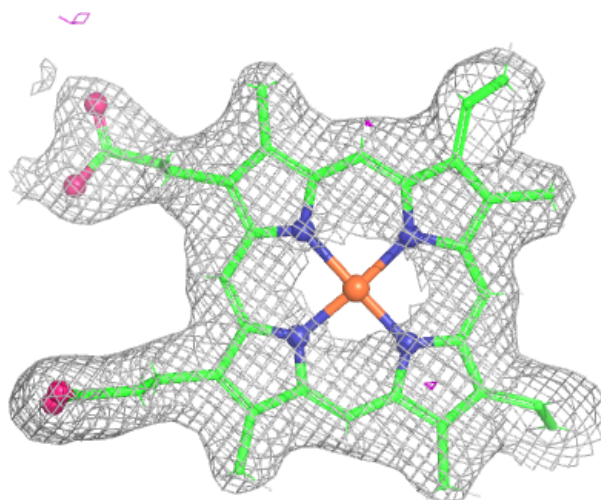
Electron density around HEC v 201:

$2mF_o-DF_c$ (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.