



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:07 AM UTC

PDB ID : 4TNK / pdb_00004tnk
Title : RT XFEL structure of Photosystem II 250 microsec after the third illumination at 5.2 Å resolution
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2014-06-04
Resolution : 5.20 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

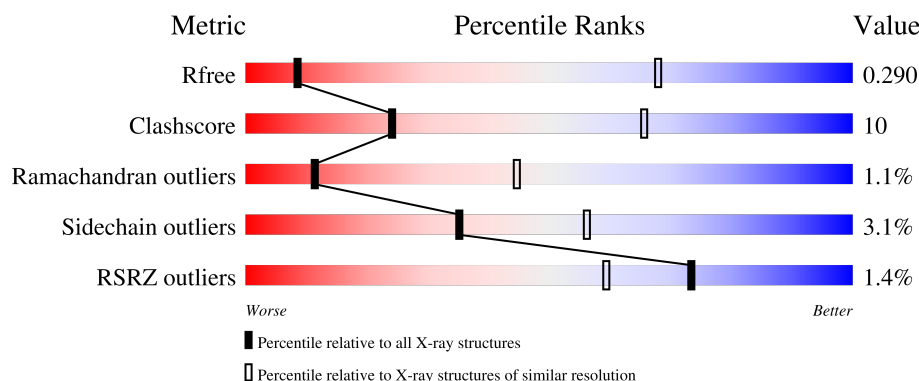
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1011 (6.38-4.00)
Clashscore	190562	1066 (6.38-4.00)
Ramachandran outliers	187476	1004 (6.46-3.94)
Sidechain outliers	187428	1006 (6.46-3.92)
RSRZ outliers	180081	1006 (6.38-4.00)

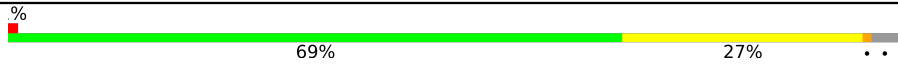
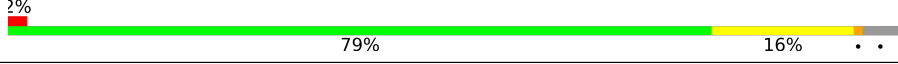
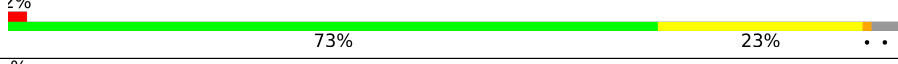
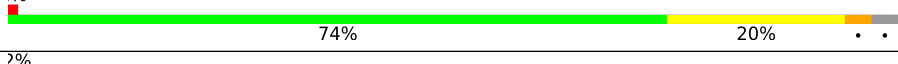
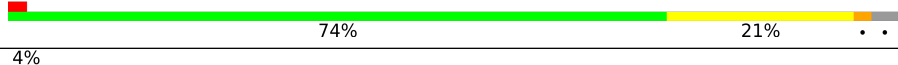
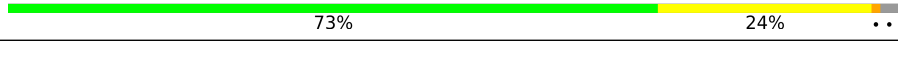
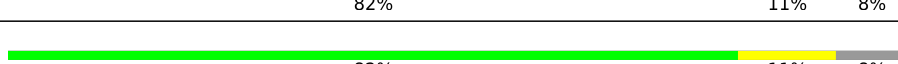
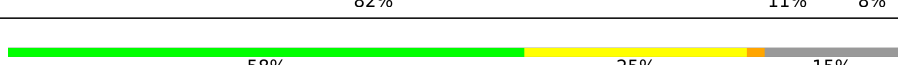
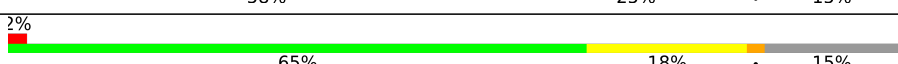
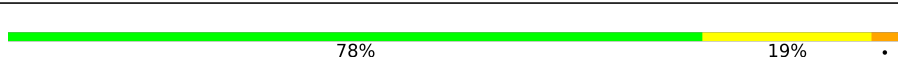
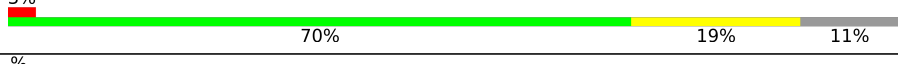
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	344	

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

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Mol	Chain	Length	Quality of chain
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	

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Mol	Chain	Length	Quality of chain
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	519	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	-
22	CLA	b	620	X	-	-	-
22	CLA	c	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	520	X	-	-	-
22	CLA	d	405	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			293	204	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	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	x	37	Total	C	N	O		0	0	0
			270	182	41	47				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	G	28	Total	C	N	O		0	0	0
			140	84	28	28				

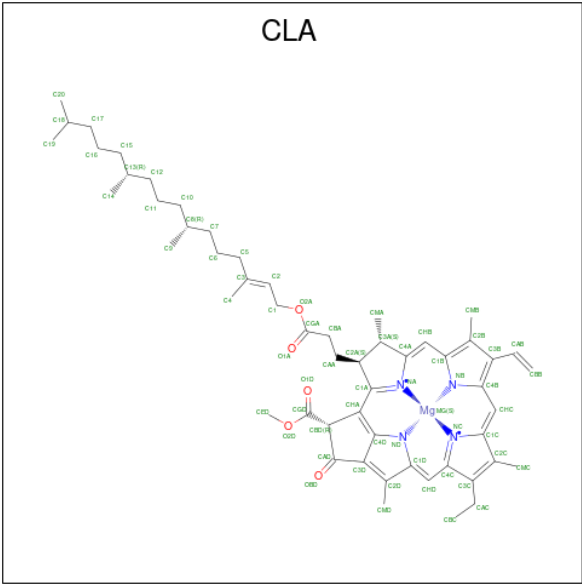
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

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

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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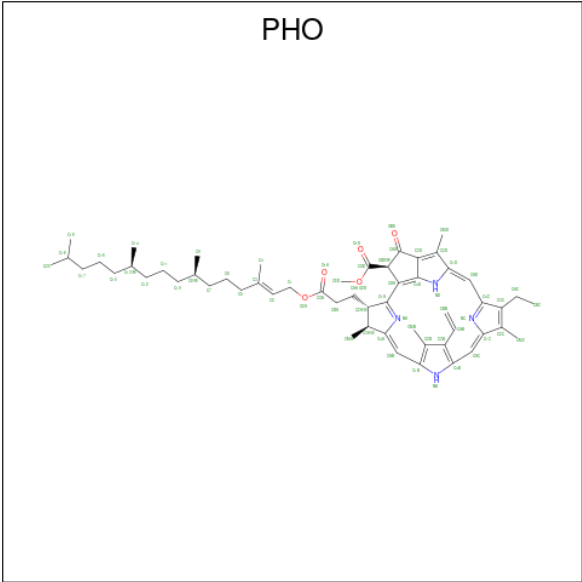
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total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

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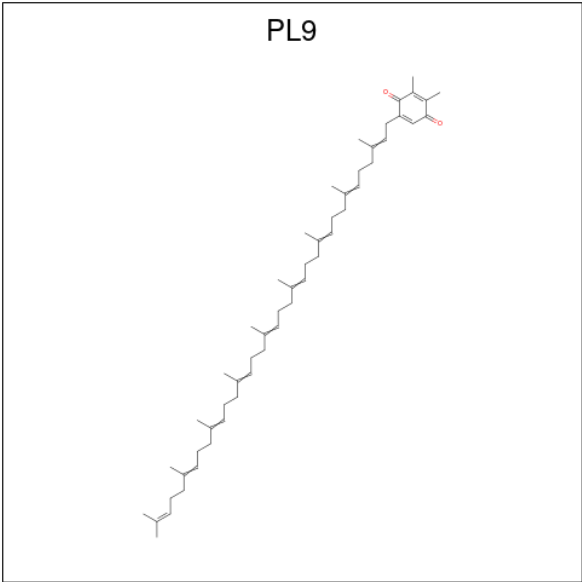
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



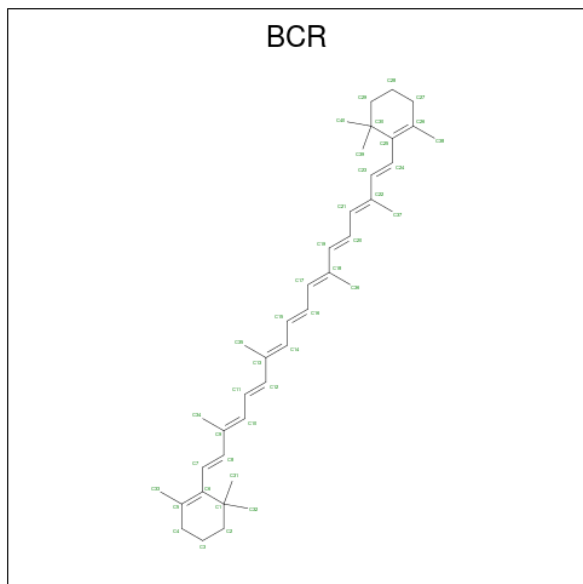
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 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
24	A	1	Total	C	O	0	0
			45	43	2		
24	D	1	Total	C	O	0	0
			55	53	2		
24	J	1	Total	C	O	0	0
			35	33	2		
24	a	1	Total	C	O	0	0
			45	43	2		
24	d	1	Total	C	O	0	0
			55	53	2		
24	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



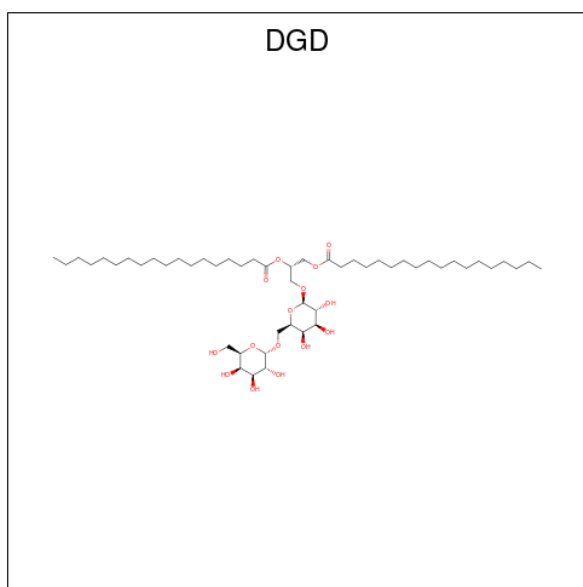
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	1	Total	C	0	0
			40	40		
25	B	1	Total	C	0	0
			40	40		
25	B	1	Total	C	0	0
			40	40		
25	B	1	Total	C	0	0
			40	40		
25	B	1	Total	C	0	0
			40	40		
25	C	1	Total	C	0	0
			40	40		

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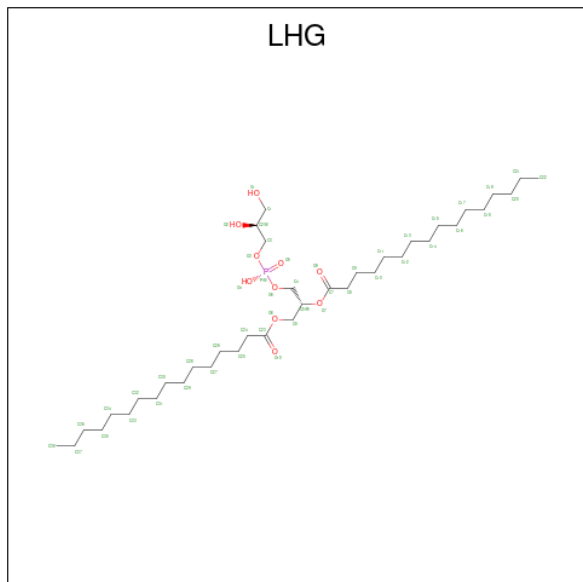
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	f	1	Total C 40 40	0	0
25	i	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	g	1	Total C 40 40	0	0
25	x	1	Total C 40 40	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			56	41	15		
26	B	1	Total	C	O	0	0
			58	43	15		
26	B	1	Total	C	O	0	0
			52	37	15		
26	C	1	Total	C	O	0	0
			53	38	15		
26	C	1	Total	C	O	0	0
			62	47	15		
26	C	1	Total	C	O	0	0
			66	51	15		
26	D	1	Total	C	O	0	0
			63	48	15		
26	a	1	Total	C	O	0	0
			56	41	15		
26	b	1	Total	C	O	0	0
			52	37	15		
26	b	1	Total	C	O	0	0
			58	43	15		
26	c	1	Total	C	O	0	0
			53	38	15		
26	c	1	Total	C	O	0	0
			62	47	15		
26	c	1	Total	C	O	0	0
			66	51	15		
26	d	1	Total	C	O	0	0
			63	48	15		

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

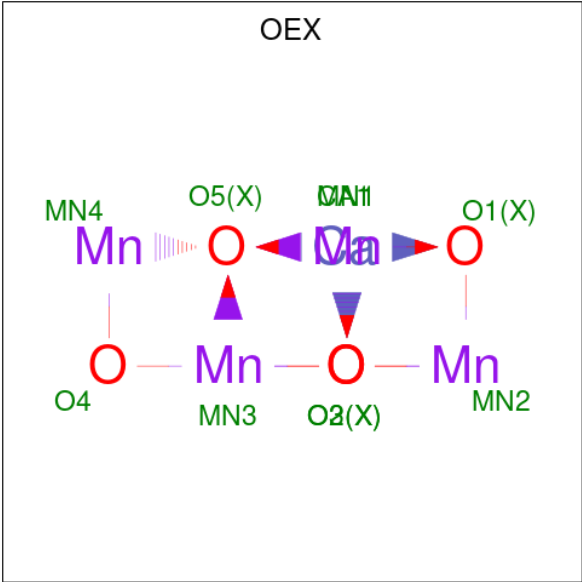


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			39	28	10	1		
27	C	1	Total	C	O	P	0	0
			37	26	10	1		
27	a	1	Total	C	O	P	0	0
			39	28	10	1		
27	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

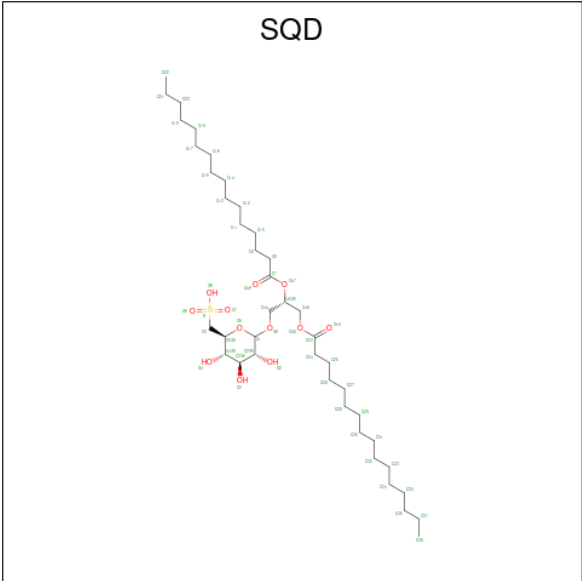
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



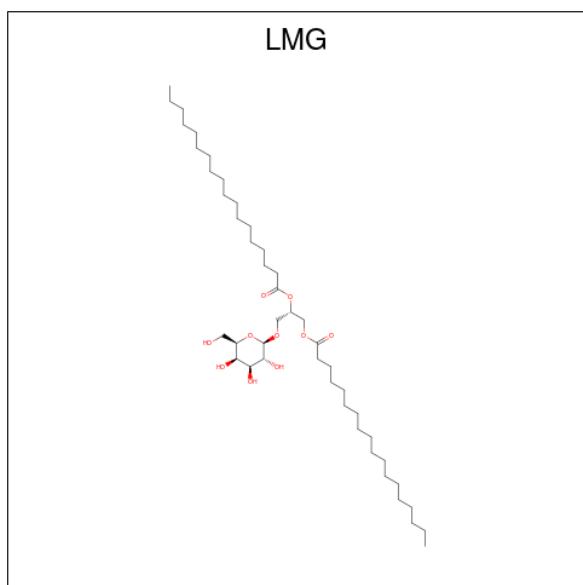
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
30	A	1	51	38	12	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



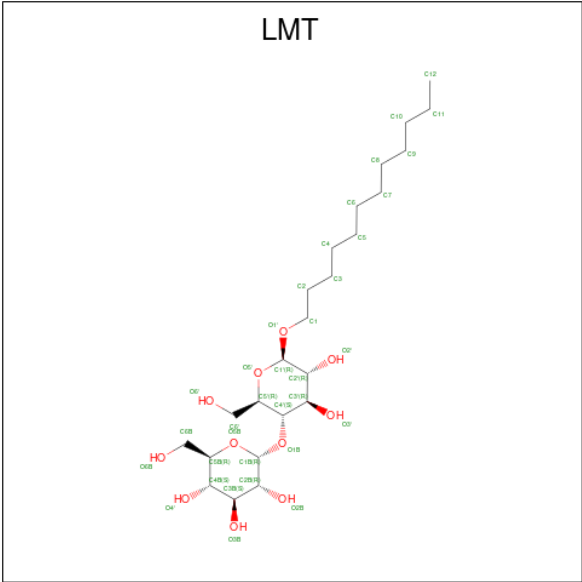
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			49	39	10		
31	B	1	Total	C	O	0	0
			49	39	10		

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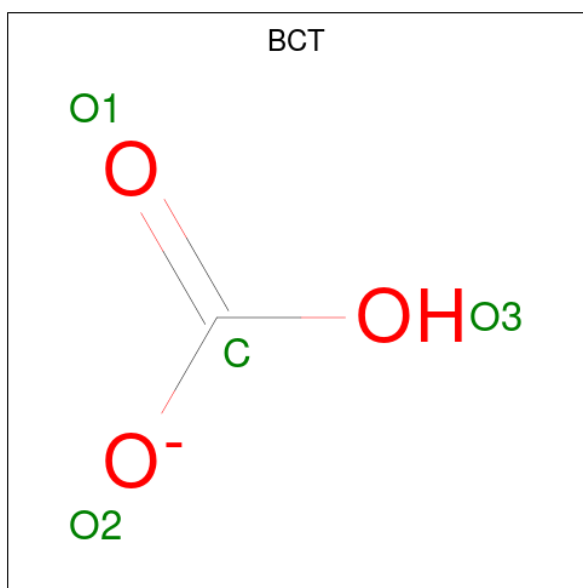
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			45	35	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			46	36	10		
31	E	1	Total	C	O	0	0
			44	34	10		
31	I	1	Total	C	O	0	0
			43	33	10		
31	L	1	Total	C	O	0	0
			51	41	10		
31	M	1	Total	C	O	0	0
			42	32	10		
31	a	1	Total	C	O	0	0
			42	32	10		
31	b	1	Total	C	O	0	0
			49	39	10		
31	b	1	Total	C	O	0	0
			42	32	10		
31	c	1	Total	C	O	0	0
			45	35	10		
31	c	1	Total	C	O	0	0
			48	38	10		
31	d	1	Total	C	O	0	0
			49	39	10		
31	d	1	Total	C	O	0	0
			48	38	10		
31	d	1	Total	C	O	0	0
			46	36	10		
31	e	1	Total	C	O	0	0
			44	34	10		
31	i	1	Total	C	O	0	0
			43	33	10		
31	l	1	Total	C	O	0	0
			51	41	10		
31	m	1	Total	C	O	0	0
			42	32	10		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



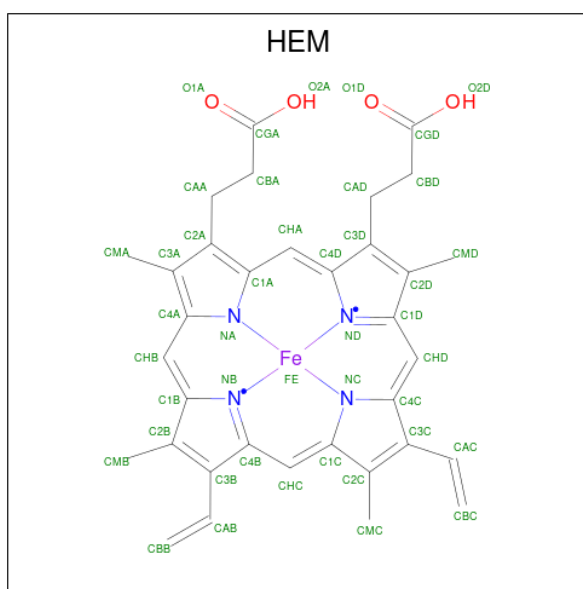
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			31	20	11		
32	I	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	d	1	Total	C	O	0	0
			31	20	11		
32	i	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			4	1	3		
33	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 34 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
34	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

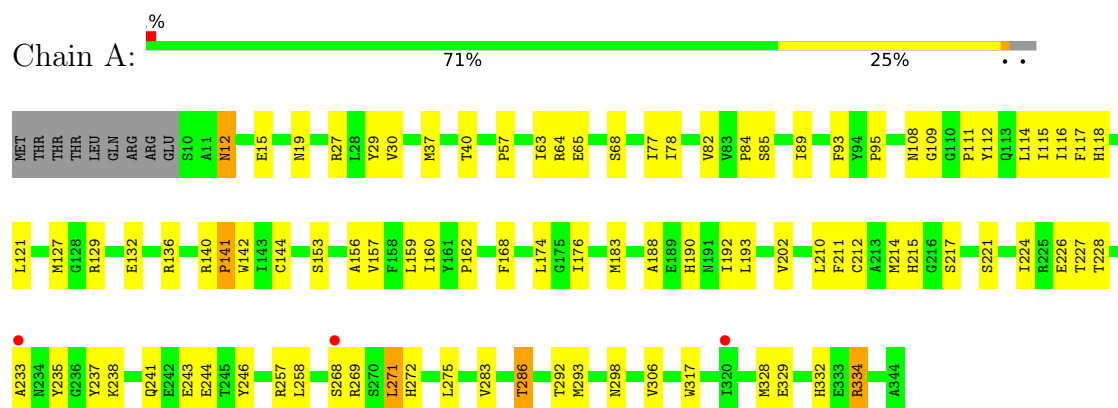
- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	K	1	Total 1	Ca 1	0	0
35	O	1	Total 1	Ca 1	0	0
35	k	1	Total 1	Ca 1	0	0
35	o	1	Total 1	Ca 1	0	0

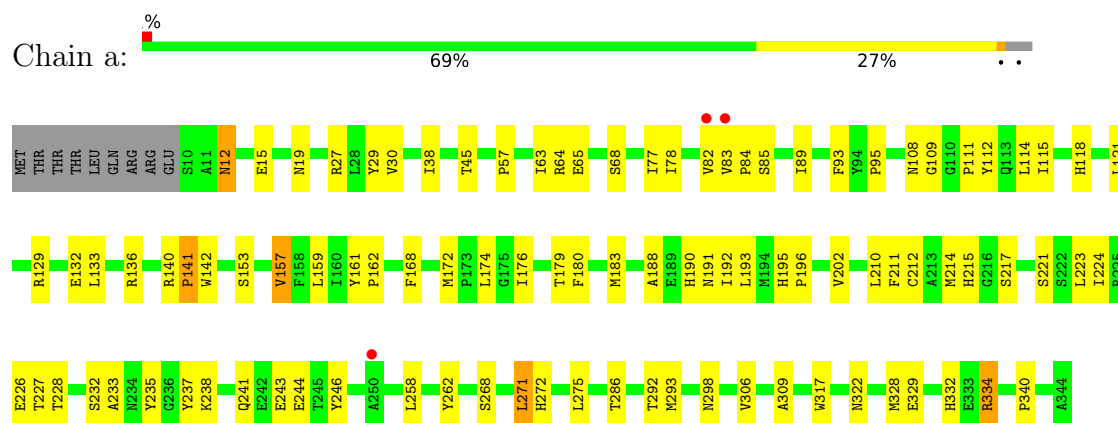
3 Residue-property plots [i](#)

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.

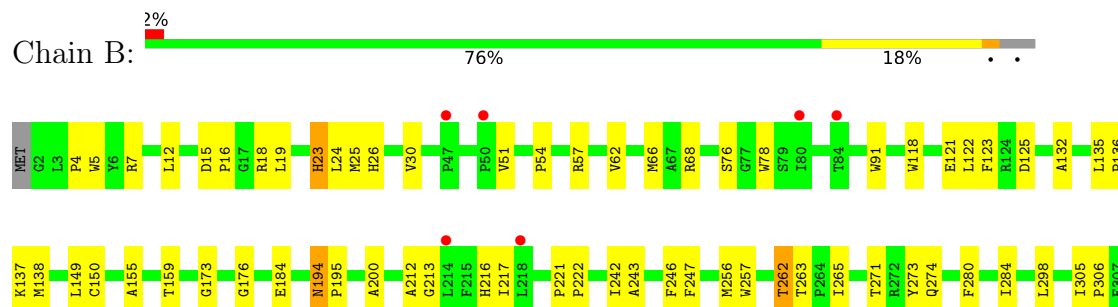
• Molecule 1: Photosystem Q(B) protein 1

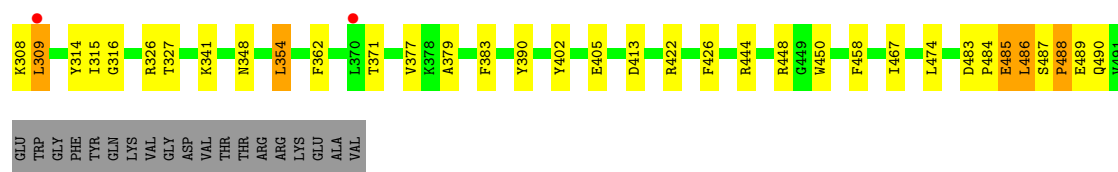


• Molecule 1: Photosystem Q(B) protein 1

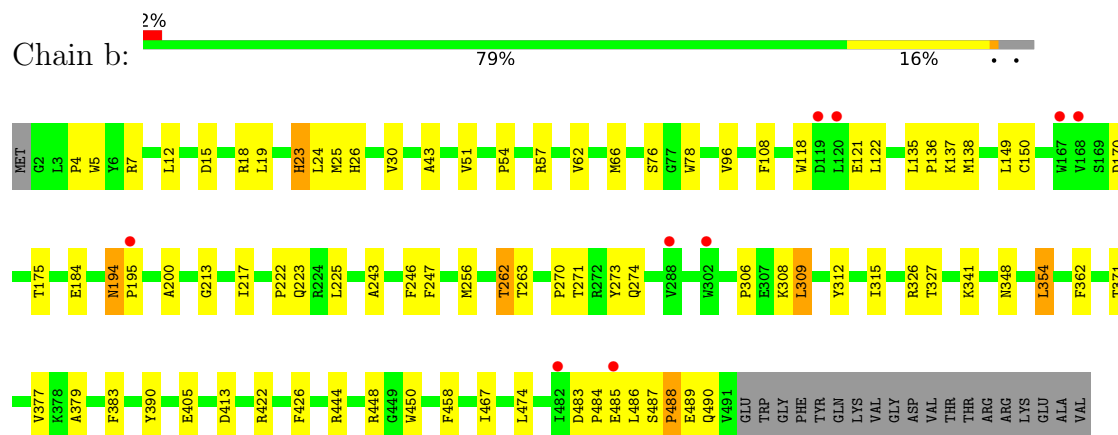


• Molecule 2: Photosystem II core light harvesting protein

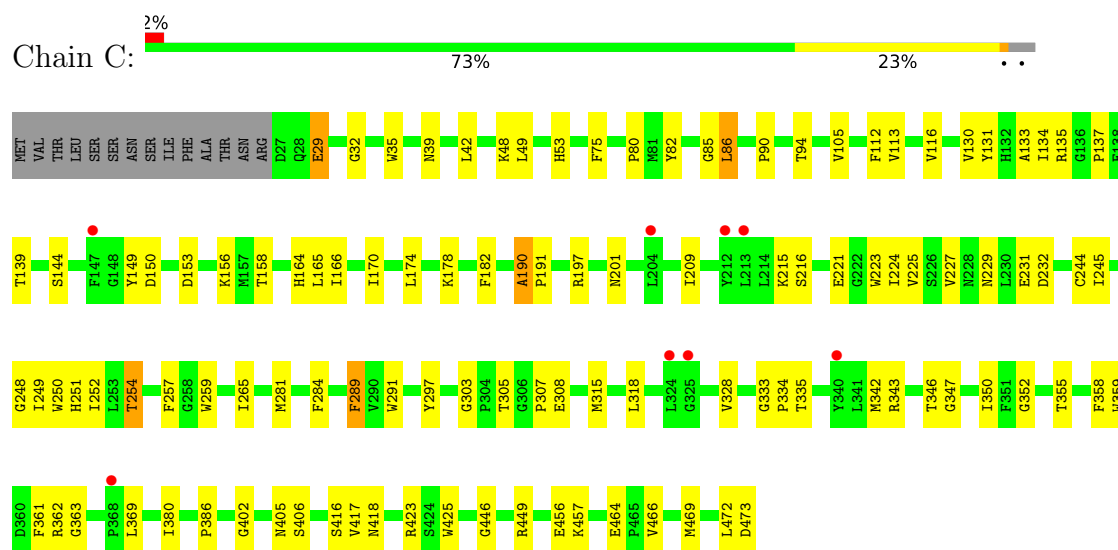




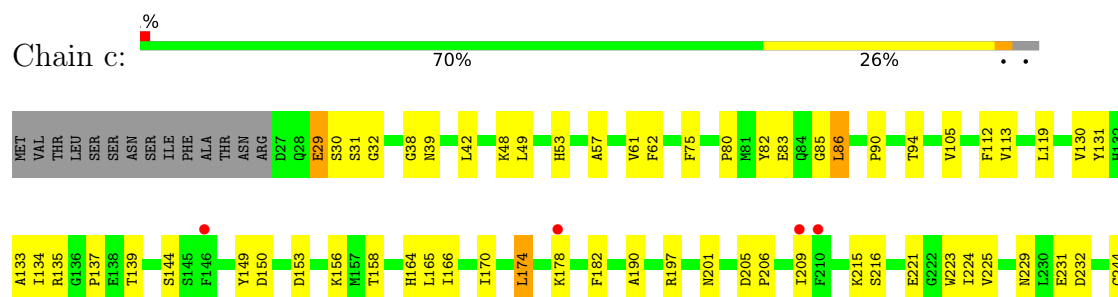
• Molecule 2: Photosystem II core light harvesting protein

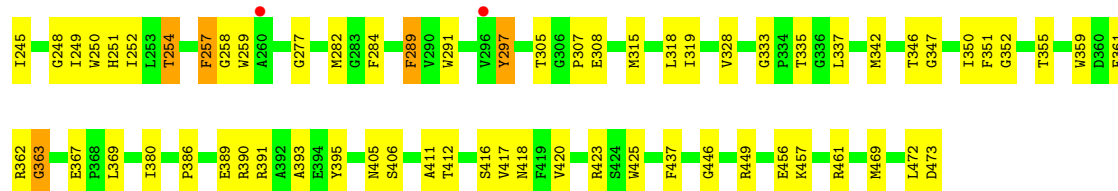


• Molecule 3: Photosystem II CP43 protein

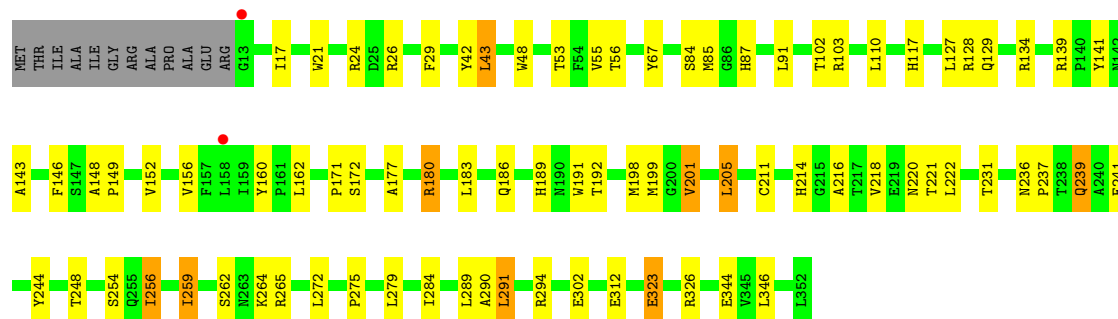
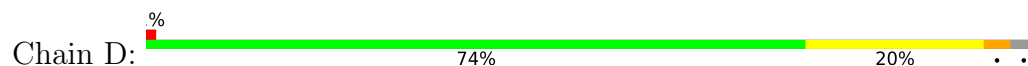


• Molecule 3: Photosystem II CP43 protein

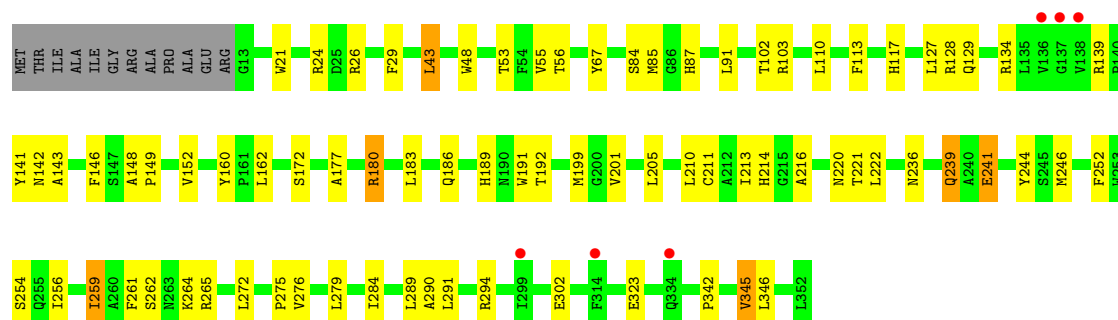
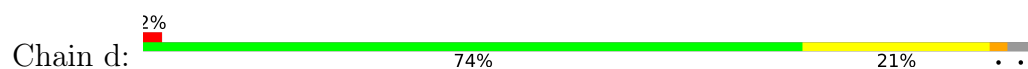




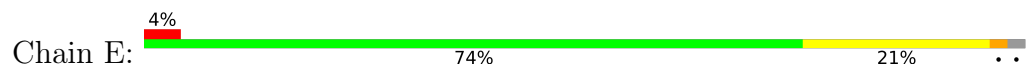
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta

Chain F:  62% 16% 22%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  60% 18% 22%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  5% 70% 27% ..



- Molecule 7: Photosystem II reaction center protein H

Chain h:  6% 77% 18% ..



- Molecule 8: Photosystem II reaction center protein I

Chain I:  82% 11% 8%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  82% 11% 8%

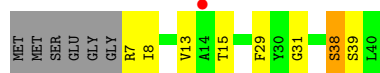


- Molecule 9: Photosystem II reaction center protein J

Chain J:  58% 25% 15%



- Molecule 9: Photosystem II reaction center protein J



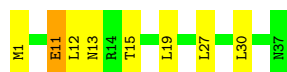
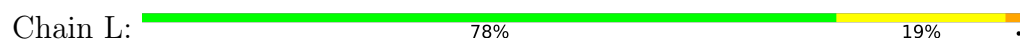
- Molecule 10: Photosystem II reaction center protein K



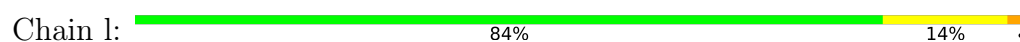
- Molecule 10: Photosystem II reaction center protein K



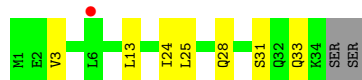
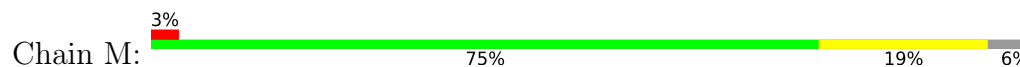
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



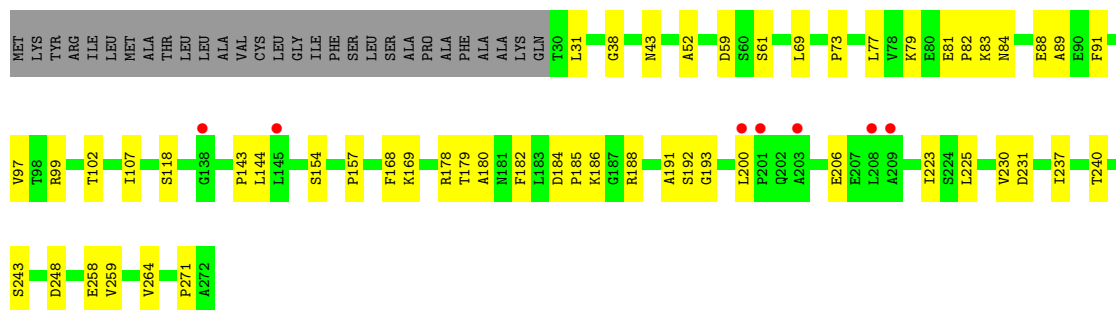
- Molecule 12: Photosystem II reaction center protein M



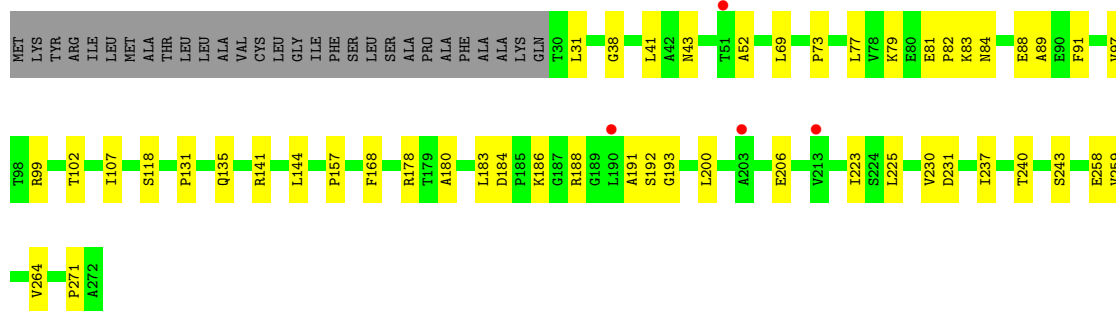
- Molecule 12: Photosystem II reaction center protein M



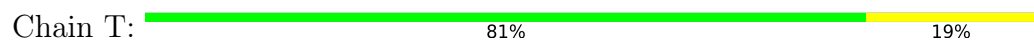
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



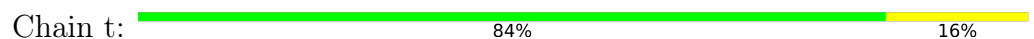
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



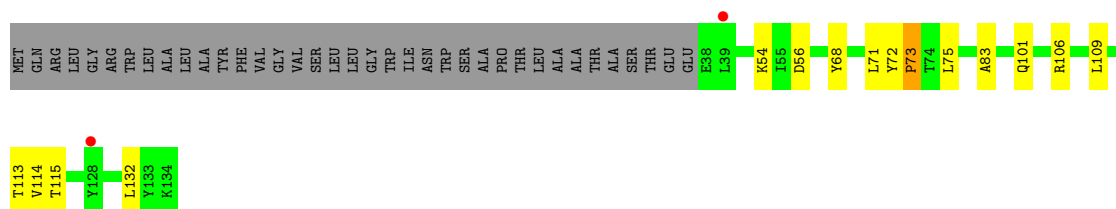
• Molecule 14: Photosystem II reaction center protein T



• Molecule 14: Photosystem II reaction center protein T



• Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 

MET GLN ARG LEU ARG TRP LEU ALA ALA ALA TYR PHE VAL GLY SER LEU LEU TRP ILE ASN THR SER ALA PRO THR LEU ALA THR ALA THR SER THR GLU E38 E54 E55 D56 Y68 L71 Y72 P73 T74 L75 A76 A83 I94 L97 Q101

T113 V114 T115 E116 V117 V122 L132 Y133 K134

- Molecule 16: Cytochrome c-550

Chain V: 

MET LEU LYS CYS VAL TRP LEU VAL VAL ALA LEU CYS LEU CYS TRP LEU GLN PHE THR MET GLY THR ALA LEU ALA A27 L47 Q60 A64 V68 I71 R81 T82 E83 P90 P91 R92 L98 M102 E116 F127 I141 G157 K160

Y163

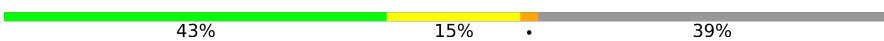
- Molecule 16: Cytochrome c-550

Chain v: 

MET LEU LYS CYS VAL TRP LEU VAL VAL ALA LEU CYS LEU CYS TRP LEU GLN PHE THR MET GLY THR ALA LEU ALA A27 L38 Q60 A64 V68 G69 G70 I71 R81 P90 P91 R92 T95 L98 M102 E116 P119 F127 G157 G158 G159

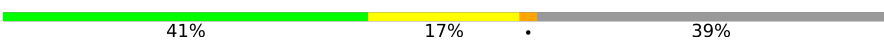
K160 Y161 Y162 Y163

- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 

MET GLY ILE PHE ASN GLY ILE ILE ILE GLU PHE LEU LEU SER ASN ASN PHE PHE GLU VAL I119 M24 I25 I28 A31 I35 I39 R43 L46

- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g: 

MET GLY ILE PHE ASN GLY ILE ILE ILE GLU PHE LEU LEU SER ASN ASN PHE PHE GLU VAL I119 M24 I25 I28 A31 G32 I35 I39 R43 L46

- Molecule 18: Photosystem II reaction center X protein

Chain X: 



- Molecule 18: Photosystem II reaction center X protein

Chain x: 63% 24% 10%



- Molecule 19: Photosystem II reaction center protein Y

Chain Y: 100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

Chain G: 100%

There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 77% 19%



- Molecule 20: Photosystem II reaction center protein Z

Chain z: 85% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.62Å 229.30Å 306.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.41 – 5.20 68.41 – 5.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (68.41-5.20) 97.9 (68.41-5.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.271 , 0.289 0.282 , 0.290	Depositor DCC
R_{free} test set	1753 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	176.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 146.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: CL, LMT, HEM, LHG, CA, BCT, BCR, PL9, DGD, OEX, PHO, SQD, CLA, FE2, LMG

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	0.31	0/2713	0.78	2/3700 (0.1%)
1	a	0.32	0/2713	0.79	2/3700 (0.1%)
2	B	0.31	0/3986	0.81	8/5433 (0.1%)
2	b	0.31	0/3986	0.81	8/5433 (0.1%)
3	C	0.31	0/3556	0.80	8/4842 (0.2%)
3	c	0.31	0/3556	0.81	8/4842 (0.2%)
4	D	0.30	0/2801	0.77	0/3818
4	d	0.30	0/2801	0.77	0/3818
5	E	0.32	0/685	0.84	0/933
5	e	0.33	0/685	0.84	0/933
6	F	0.35	0/291	0.74	0/397
6	f	0.35	0/291	0.76	0/397
7	H	0.33	0/520	0.72	0/709
7	h	0.34	0/520	0.74	0/709
8	I	0.31	0/293	0.78	0/395
8	i	0.30	0/293	0.80	0/395
9	J	0.29	0/255	0.86	0/346
9	j	0.32	0/255	0.84	0/346
10	K	0.44	0/303	0.84	0/416
10	k	0.44	0/303	0.88	0/416
11	L	0.29	0/311	0.71	0/422
11	l	0.29	0/311	0.72	0/422
12	M	0.33	0/270	0.86	0/367
12	m	0.34	0/270	0.87	1/367 (0.3%)
13	O	0.29	0/1876	0.72	2/2548 (0.1%)
13	o	0.28	0/1876	0.72	2/2548 (0.1%)
14	T	0.28	0/284	0.73	0/381
14	t	0.29	0/284	0.74	0/381
15	U	0.30	0/785	0.78	0/1064
15	u	0.30	0/785	0.79	0/1064
16	V	0.30	0/1081	0.76	2/1468 (0.1%)
16	v	0.30	0/1081	0.75	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.35	0/202	0.77	0/272
17	y	0.34	0/202	0.77	0/272
18	X	0.41	0/273	0.82	0/370
18	x	0.39	0/273	0.81	0/370
20	Z	0.32	0/490	0.83	0/669
20	z	0.32	0/490	0.86	0/669
All	All	0.31	0/41950	0.79	43/57100 (0.1%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	483	ASP	CA-C-N	10.68	133.19	119.84
2	B	483	ASP	C-N-CA	10.68	133.19	119.84
2	b	483	ASP	CA-C-N	10.42	132.86	119.84
2	b	483	ASP	C-N-CA	10.42	132.86	119.84
3	c	190	ALA	CA-C-N	6.30	125.79	119.24
3	c	190	ALA	C-N-CA	6.30	125.79	119.24
3	C	190	ALA	CA-C-N	6.28	125.77	119.24
3	C	190	ALA	C-N-CA	6.28	125.77	119.24
2	b	413	ASP	CA-C-N	6.09	126.65	120.38
2	b	413	ASP	C-N-CA	6.09	126.65	120.38
3	c	363	GLY	CA-C-N	6.06	125.54	119.24
3	c	363	GLY	C-N-CA	6.06	125.54	119.24
3	C	363	GLY	CA-C-N	5.92	125.39	119.24
3	C	363	GLY	C-N-CA	5.92	125.39	119.24
2	B	413	ASP	CA-C-N	5.79	126.35	120.38
2	B	413	ASP	C-N-CA	5.79	126.35	120.38
2	b	194	ASN	CA-C-N	5.60	125.27	119.05
2	b	194	ASN	C-N-CA	5.60	125.27	119.05
2	b	15	ASP	CA-C-N	5.55	125.65	119.32
2	b	15	ASP	C-N-CA	5.55	125.65	119.32
13	o	200	LEU	CA-C-N	5.50	125.59	119.32
13	o	200	LEU	C-N-CA	5.50	125.59	119.32
2	B	194	ASN	CA-C-N	5.42	125.06	119.05
2	B	194	ASN	C-N-CA	5.42	125.06	119.05
16	V	127	PHE	CA-C-N	5.38	126.57	119.84
16	V	127	PHE	C-N-CA	5.38	126.57	119.84
2	B	15	ASP	CA-C-N	5.37	125.44	119.32
2	B	15	ASP	C-N-CA	5.37	125.44	119.32
3	c	297	TYR	CA-C-N	5.31	125.56	119.83
3	c	297	TYR	C-N-CA	5.31	125.56	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	333	GLY	CA-C-N	5.29	126.45	119.84
3	C	333	GLY	C-N-CA	5.29	126.45	119.84
1	a	38	ILE	CB-CA-C	-5.26	108.71	113.70
1	A	65	GLU	CA-C-N	5.20	125.50	119.93
1	A	65	GLU	C-N-CA	5.20	125.50	119.93
12	m	17	VAL	CB-CA-C	-5.16	108.79	113.70
13	O	200	LEU	CA-C-N	5.15	125.19	119.32
13	O	200	LEU	C-N-CA	5.15	125.19	119.32
3	c	333	GLY	CA-C-N	5.14	126.27	119.84
3	c	333	GLY	C-N-CA	5.14	126.27	119.84
3	C	464	GLU	CA-C-N	5.05	126.15	119.84
3	C	464	GLU	C-N-CA	5.05	126.15	119.84
1	a	83	VAL	N-CA-C	5.03	112.95	108.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	68	0
1	a	2628	0	2524	73	0
2	B	3850	0	3718	68	0
2	b	3850	0	3718	57	0
3	C	3444	0	3365	74	0
3	c	3444	0	3365	86	0
4	D	2706	0	2608	72	0
4	d	2706	0	2608	60	0
5	E	666	0	651	13	0
5	e	666	0	651	14	0
6	F	282	0	291	6	0
6	f	282	0	291	7	0
7	H	507	0	521	16	0
7	h	507	0	521	14	0
8	I	286	0	308	3	0
8	i	286	0	308	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	249	0	262	8	0
9	j	249	0	262	7	0
10	K	293	0	305	11	0
10	k	293	0	305	13	0
11	L	304	0	316	7	0
11	l	304	0	316	5	0
12	M	267	0	289	7	0
12	m	267	0	289	7	0
13	O	1845	0	1801	30	0
13	o	1845	0	1801	30	0
14	T	275	0	288	4	0
14	t	275	0	288	3	0
15	U	774	0	773	6	0
15	u	774	0	773	9	0
16	V	1060	0	1068	10	0
16	v	1060	0	1068	14	0
17	g	201	0	226	7	0
17	y	201	0	226	5	0
18	X	270	0	299	9	0
18	x	270	0	299	8	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	12	0
20	z	479	0	516	9	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	28	0
22	B	975	0	1080	56	0
22	C	845	0	936	31	0
22	D	130	0	144	13	0
22	H	65	0	72	11	0
22	a	260	0	288	24	0
22	b	1040	0	1152	59	0
22	c	845	0	936	34	0
22	d	130	0	144	11	0
23	A	64	0	74	6	0
23	D	64	0	74	6	0
23	d	128	0	148	11	0
24	A	45	0	61	5	0
24	D	55	0	80	9	0
24	J	35	0	45	0	0
24	a	45	0	61	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	d	55	0	80	6	0
24	j	35	0	45	0	0
25	A	40	0	56	4	0
25	B	160	0	224	14	0
25	C	80	0	112	10	0
25	F	40	0	56	1	0
25	H	40	0	56	2	0
25	J	40	0	56	3	0
25	K	40	0	56	5	0
25	b	160	0	224	10	0
25	c	120	0	168	16	0
25	f	40	0	56	3	0
25	g	40	0	56	11	0
25	i	40	0	56	2	0
25	j	40	0	56	2	0
25	x	40	0	56	1	0
25	y	40	0	56	6	0
26	A	56	0	70	1	0
26	B	110	0	136	4	0
26	C	181	0	245	11	0
26	D	63	0	87	2	0
26	a	56	0	70	2	0
26	b	110	0	136	5	0
26	c	181	0	245	14	0
26	d	63	0	87	3	0
27	A	39	0	51	2	0
27	C	37	0	44	3	0
27	a	39	0	51	1	0
27	c	37	0	44	2	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	6	0
30	B	90	0	111	3	0
30	F	45	0	54	3	0
30	a	105	0	147	8	0
30	b	47	0	61	2	0
30	d	43	0	50	3	0
30	f	45	0	54	3	0
31	B	98	0	136	5	0
31	C	93	0	126	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	D	94	0	128	8	0
31	E	44	0	58	1	0
31	I	43	0	56	1	0
31	L	51	0	72	2	0
31	M	42	0	54	2	0
31	a	42	0	54	0	0
31	b	91	0	122	5	0
31	c	93	0	126	3	0
31	d	143	0	196	10	0
31	e	44	0	58	2	0
31	i	43	0	56	0	0
31	l	51	0	72	2	0
31	m	42	0	54	3	0
32	B	140	0	184	3	0
32	D	31	0	35	0	0
32	I	35	0	46	1	0
32	M	70	0	92	0	0
32	b	140	0	184	6	0
32	d	31	0	35	0	0
32	i	35	0	46	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	4	0
34	v	43	0	30	5	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51374	1012	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1012) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.55	0.87
3:c:39:ASN:HB2	22:c:507:CLA:HBA1	1.57	0.84
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.60	0.83
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.60	0.82
13:o:82:PRO:HG3	13:o:89:ALA:HB2	1.61	0.82
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.80
3:C:362:ARG:H	26:C:514:DGD:HE4	1.47	0.78
4:d:199:MET:HG2	24:d:407:PL9:H322	1.65	0.78
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.67	0.77
3:c:362:ARG:H	26:c:515:DGD:HE4	1.48	0.77
4:D:199:MET:HG2	24:D:405:PL9:H322	1.69	0.74
34:v:201:HEM:HBC2	34:v:201:HEM:HHD	1.68	0.74
22:b:610:CLA:H72	25:b:624:BCR:H311	1.70	0.74
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.53	0.73
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.69	0.73
4:D:29:PHE:O	4:D:128:ARG:NH2	2.22	0.73
10:K:21:LEU:HD13	17:y:24:MET:HE2	1.71	0.72
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.71	0.72
1:a:63:ILE:HB	3:c:335:THR:HG21	1.71	0.72
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.72	0.72
26:C:516:DGD:HAF2	22:C:519:CLA:H202	1.71	0.71
4:D:236:ASN:ND2	4:D:239:GLN:O	2.23	0.71
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.72	0.71
13:o:69:LEU:HB3	13:o:107:ILE:HB	1.72	0.71
22:B:605:CLA:H72	25:B:619:BCR:H311	1.73	0.71
16:v:102:MET:HE3	34:v:201:HEM:HBB2	1.73	0.70
26:c:517:DGD:HAF2	22:c:520:CLA:H202	1.73	0.70
4:D:21:TRP:O	4:D:26:ARG:NH2	2.23	0.70
5:e:60:GLN:OE1	5:e:84:LYS:NZ	2.25	0.69
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.72	0.69
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.73	0.69
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.73	0.69
1:a:129:ARG:HH21	4:d:256:ILE:HD12	1.57	0.69
4:d:189:HIS:HA	4:d:294:ARG:HD2	1.75	0.69
4:d:259:ILE:HG12	31:d:409:LMG:H292	1.73	0.69
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.74	0.68
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.74	0.68
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.75	0.68
2:b:24:LEU:HD21	22:b:620:CLA:HAB	1.74	0.68
4:d:152:VAL:HG21	4:d:279:LEU:HD12	1.76	0.67
12:m:31:SER:HA	31:m:101:LMG:HC1	1.76	0.67
1:a:190:HIS:HB3	1:a:293:MET:HE2	1.76	0.67
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.75	0.67
3:C:297:TYR:O	3:C:423:ARG:NH2	2.28	0.67
3:C:406:SER:O	3:C:418:ASN:ND2	2.28	0.67
1:a:192:ILE:HA	1:a:293:MET:HE1	1.75	0.67
30:d:403:SQD:H171	30:d:403:SQD:H301	1.76	0.67
3:c:297:TYR:O	3:c:423:ARG:NH2	2.28	0.66
6:F:17:THR:HG23	6:F:20:TRP:H	1.60	0.66
22:c:503:CLA:H172	22:c:509:CLA:HBB2	1.75	0.66
4:D:186:GLN:HB2	22:D:403:CLA:HBC1	1.77	0.66
17:y:35:ILE:HG22	20:Z:21:ILE:HG23	1.78	0.66
2:b:474:LEU:O	4:d:134:ARG:NH1	2.29	0.66
10:k:21:LEU:HD13	17:g:24:MET:HE2	1.78	0.66
3:c:165:LEU:HD21	22:c:505:CLA:HAB	1.78	0.66
4:d:21:TRP:O	4:d:26:ARG:NH2	2.25	0.66
22:C:506:CLA:H112	25:C:513:BCR:H362	1.76	0.65
22:a:403:CLA:H122	23:d:401:PHO:H3A	1.77	0.65
3:c:250:TRP:O	3:c:254:THR:OG1	2.13	0.65
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.76	0.65
1:A:63:ILE:HB	3:C:335:THR:HG21	1.79	0.65
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.77	0.65
2:b:271:THR:HG22	2:b:273:TYR:H	1.62	0.65
3:c:291:TRP:O	3:c:305:THR:OG1	2.15	0.65
22:c:507:CLA:HBC3	22:c:509:CLA:H92	1.77	0.65
22:a:403:CLA:H71	22:a:404:CLA:HAB	1.77	0.65
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.80	0.64
1:a:174:LEU:HD22	23:d:401:PHO:H151	1.79	0.64
22:b:612:CLA:H42	4:d:127:LEU:HD11	1.79	0.64
3:c:216:SER:HB3	3:c:221:GLU:HB2	1.80	0.64
30:B:622:SQD:H171	30:B:622:SQD:H301	1.79	0.64
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.80	0.64
2:b:62:VAL:HG12	2:b:66:MET:HE2	1.79	0.64
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.79	0.64
3:C:291:TRP:O	3:C:305:THR:OG1	2.16	0.63
12:M:31:SER:HA	31:M:101:LMG:HC1	1.79	0.63
4:d:29:PHE:O	4:d:128:ARG:NH2	2.31	0.63
22:A:404:CLA:H142	22:D:403:CLA:H151	1.80	0.63
22:B:607:CLA:HBA2	30:B:622:SQD:H101	1.81	0.63
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.80	0.63
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.63
22:a:403:CLA:HHC	22:a:403:CLA:HBB1	1.80	0.63
22:a:405:CLA:H142	22:d:405:CLA:H151	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.80	0.63
4:d:24:ARG:NH2	18:x:44:ASP:O	2.32	0.63
1:A:192:ILE:HA	1:A:293:MET:HE1	1.79	0.62
3:C:49:LEU:O	3:C:53:HIS:ND1	2.30	0.62
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.32	0.62
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.81	0.62
3:C:48:LYS:NZ	3:C:133:ALA:O	2.31	0.62
3:c:342:MET:HE3	3:c:352:GLY:HA2	1.80	0.62
1:a:15:GLU:O	1:a:19:ASN:ND2	2.33	0.62
22:b:607:CLA:H193	7:h:42:LEU:HD12	1.81	0.62
13:o:77:LEU:HB3	13:o:91:PHE:HB3	1.80	0.62
3:c:49:LEU:O	3:c:53:HIS:ND1	2.30	0.62
4:d:186:GLN:HB2	22:d:405:CLA:HBC1	1.80	0.62
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.81	0.62
2:b:121:GLU:O	7:h:12:ARG:NH2	2.31	0.62
3:C:250:TRP:O	3:C:254:THR:OG1	2.13	0.62
30:d:403:SQD:H241	30:d:403:SQD:H111	1.82	0.62
20:z:33:TRP:HA	20:z:36:SER:HB3	1.82	0.62
30:A:414:SQD:H61	22:b:620:CLA:H2	1.82	0.62
3:c:48:LYS:NZ	3:c:133:ALA:O	2.32	0.62
22:B:615:CLA:H2	30:a:401:SQD:H61	1.80	0.61
1:A:140:ARG:NH2	27:A:410:LHG:O5	2.30	0.61
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.65	0.61
4:D:214:HIS:ND1	24:D:405:PL9:O2	2.22	0.61
22:a:404:CLA:H203	23:d:401:PHO:H71	1.82	0.61
30:a:401:SQD:H311	25:i:101:BCR:H342	1.82	0.61
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.65	0.61
15:u:56:ASP:OD2	15:u:115:THR:OG1	2.16	0.61
30:A:413:SQD:H172	27:C:518:LHG:H172	1.83	0.61
1:a:183:MET:HB3	22:a:403:CLA:HBC2	1.83	0.61
2:b:149:LEU:HG	22:b:607:CLA:HBC1	1.82	0.61
26:b:601:DGD:HD1	32:b:603:LMT:H32	1.82	0.61
4:d:216:ALA:O	4:d:220:ASN:ND2	2.31	0.61
9:j:15:THR:HG21	10:k:38:VAL:HG13	1.83	0.61
26:B:620:DGD:HAW2	22:H:101:CLA:H152	1.83	0.60
4:d:214:HIS:ND1	24:d:407:PL9:O2	2.25	0.60
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.83	0.60
6:f:17:THR:HG23	6:f:20:TRP:H	1.65	0.60
1:A:329:GLU:O	1:A:332:HIS:ND1	2.32	0.60
22:A:403:CLA:HED1	24:D:405:PL9:H372	1.83	0.60
11:L:13:ASN:ND2	31:L:101:LMG:O5	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:449:ARG:HE	22:c:504:CLA:HED1	1.67	0.60
1:a:214:MET:HE2	1:a:214:MET:HA	1.84	0.60
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.83	0.60
4:D:259:ILE:HG12	31:D:406:LMG:H292	1.83	0.59
31:D:406:LMG:HO4	31:D:406:LMG:HO5	1.49	0.59
4:d:302:GLU:OE1	13:o:186:LYS:NZ	2.35	0.59
13:o:230:VAL:HG13	13:o:237:ILE:HG22	1.85	0.59
4:D:216:ALA:O	4:D:220:ASN:ND2	2.35	0.59
22:b:612:CLA:HBA2	30:d:403:SQD:H101	1.85	0.59
3:c:150:ASP:HB3	3:c:153:ASP:HB2	1.84	0.59
23:d:402:PHO:H151	22:d:405:CLA:H172	1.83	0.59
1:A:227:THR:HG21	1:A:233:ALA:HA	1.84	0.59
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.84	0.59
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.19	0.59
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.83	0.59
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.84	0.59
1:a:221:SER:HB3	4:d:141:TYR:HB2	1.84	0.59
22:b:607:CLA:C2D	22:b:609:CLA:H2	2.33	0.59
1:A:174:LEU:HD22	23:A:405:PHO:H151	1.85	0.59
4:D:24:ARG:NH2	18:X:44:ASP:O	2.35	0.59
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.59
4:d:236:ASN:ND2	4:d:239:GLN:O	2.36	0.59
1:A:15:GLU:O	1:A:19:ASN:ND2	2.34	0.58
22:B:606:CLA:HBB1	31:B:621:LMG:H341	1.84	0.58
22:b:606:CLA:HAA2	7:h:45:ILE:HD12	1.84	0.58
13:o:83:LYS:HG2	13:o:84:ASN:H	1.67	0.58
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.84	0.58
16:V:102:MET:HE3	34:V:201:HEM:HBB2	1.85	0.58
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.84	0.58
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.37	0.58
13:O:83:LYS:HG2	13:O:84:ASN:H	1.68	0.58
22:a:404:CLA:HED1	24:d:407:PL9:H372	1.84	0.58
4:d:222:LEU:HD23	4:d:244:TYR:HB3	1.86	0.58
22:A:402:CLA:H122	23:A:405:PHO:H3A	1.84	0.58
2:B:327:THR:HG21	31:B:621:LMG:H111	1.85	0.58
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.86	0.58
22:b:611:CLA:HBB1	31:b:626:LMG:H341	1.85	0.57
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.86	0.57
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.84	0.57
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.85	0.57
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.86	0.57
34:v:201:HEM:HBB2	34:v:201:HEM:HMB1	1.86	0.57
1:a:29:TYR:O	1:a:129:ARG:NH1	2.38	0.57
31:D:406:LMG:O6	11:L:15:THR:HG21	2.05	0.57
2:B:487:SER:N	2:B:488:PRO:HD2	2.20	0.57
22:b:615:CLA:H41	22:b:618:CLA:HBC3	1.86	0.57
1:A:214:MET:HA	1:A:214:MET:HE2	1.85	0.57
30:A:413:SQD:H223	26:C:516:DGD:HAE1	1.87	0.56
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.86	0.56
3:c:42:LEU:HD21	22:c:510:CLA:H2A	1.86	0.56
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.30	0.56
1:a:217:SER:HA	4:d:272:LEU:HD12	1.86	0.56
2:B:262:THR:HG22	2:B:263:THR:HG23	1.87	0.56
2:b:487:SER:N	2:b:488:PRO:HD2	2.20	0.56
22:c:506:CLA:H112	25:c:514:BCR:H362	1.88	0.56
22:c:508:CLA:HBD	22:c:508:CLA:H121	1.86	0.56
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.88	0.56
22:A:403:CLA:H203	23:A:405:PHO:H71	1.87	0.56
3:C:361:PHE:HD1	26:C:514:DGD:HE61	1.71	0.56
31:D:409:LMG:H171	25:F:102:BCR:H383	1.86	0.56
27:C:518:LHG:H271	27:C:518:LHG:H101	1.87	0.56
22:B:607:CLA:H151	22:B:608:CLA:H203	1.87	0.56
30:F:103:SQD:H162	18:X:33:THR:HA	1.88	0.56
13:o:240:THR:HG22	13:o:264:VAL:HG12	1.88	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.56
2:B:155:ALA:O	2:B:159:THR:OG1	2.18	0.56
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.71	0.56
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.88	0.56
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.88	0.55
1:a:121:LEU:HD13	26:a:408:DGD:HB92	1.88	0.55
1:a:328:MET:HE1	4:d:183:LEU:HD22	1.87	0.55
2:b:327:THR:HG21	31:b:626:LMG:H111	1.88	0.55
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.87	0.55
1:a:329:GLU:O	1:a:332:HIS:ND1	2.32	0.55
22:b:606:CLA:HBD	22:b:606:CLA:H2	1.88	0.55
13:O:73:PRO:HG2	13:O:102:THR:HB	1.89	0.55
30:a:412:SQD:H311	22:c:507:CLA:H71	1.89	0.55
2:b:262:THR:OG1	22:b:607:CLA:O1D	2.23	0.55
17:g:35:ILE:HG22	20:z:21:ILE:HG23	1.87	0.55
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.06	0.55
25:c:513:BCR:H11C	25:g:101:BCR:H322	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:192:THR:HG23	22:d:405:CLA:HBC2	1.89	0.55
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.72	0.55
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.88	0.55
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.89	0.55
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.37	0.55
1:a:65:GLU:OE2	1:a:334:ARG:NH2	2.40	0.55
12:m:25:LEU:O	12:m:28:GLN:HG3	2.07	0.55
24:d:407:PL9:H352	31:l:101:LMG:H231	1.89	0.55
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.24	0.55
22:H:101:CLA:H2	22:H:101:CLA:HBD	1.88	0.55
30:a:412:SQD:H172	27:c:519:LHG:H172	1.89	0.55
22:A:404:CLA:H93	22:D:403:CLA:H152	1.89	0.55
22:B:605:CLA:H18	22:B:615:CLA:H121	1.89	0.55
22:b:607:CLA:C3D	22:b:609:CLA:H2	2.36	0.55
22:B:613:CLA:H51	25:B:616:BCR:H372	1.87	0.54
22:A:403:CLA:HMA2	24:D:405:PL9:H411	1.90	0.54
26:B:626:DGD:O1B	26:B:626:DGD:O2D	2.25	0.54
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54
31:d:409:LMG:O6	11:l:15:THR:HG21	2.07	0.54
1:A:217:SER:HA	4:D:272:LEU:HD12	1.89	0.54
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.89	0.54
22:D:404:CLA:H42	18:X:26:GLY:HA3	1.89	0.54
3:c:215:LYS:HB3	3:c:223:TRP:HA	1.89	0.54
27:c:519:LHG:H101	27:c:519:LHG:H271	1.89	0.54
34:f:101:HEM:HBC2	34:f:101:HEM:HMC2	1.90	0.54
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.54
1:a:45:THR:HG21	30:a:401:SQD:H201	1.90	0.54
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.90	0.54
5:E:10:PHE:N	31:E:101:LMG:O3	2.40	0.54
3:c:75:PHE:HD1	3:c:86:LEU:HD21	1.72	0.54
3:c:229:ASN:HD22	3:c:231:GLU:HB2	1.72	0.54
20:z:33:TRP:O	20:z:37:LYS:HB2	2.08	0.54
24:D:405:PL9:H352	31:L:101:LMG:H231	1.89	0.54
1:a:227:THR:HG21	1:a:233:ALA:HA	1.89	0.54
22:b:612:CLA:H51	22:b:613:CLA:H101	1.90	0.54
3:c:461:ARG:NH1	4:d:241:GLU:OE1	2.39	0.54
15:u:54:LYS:HD2	15:u:113:THR:HG23	1.89	0.54
2:B:256:MET:O	2:B:448:ARG:NH1	2.35	0.54
25:b:622:BCR:H19C	25:b:623:BCR:H363	1.90	0.54
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.89	0.54
2:B:121:GLU:O	7:H:12:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.44	0.54
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.90	0.53
3:c:305:THR:HG23	3:c:307:PRO:HD2	1.89	0.53
2:b:150:CYS:HA	22:b:607:CLA:HBC2	1.89	0.53
1:A:78:ILE:O	1:A:176:ILE:HB	2.08	0.53
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.53
2:b:122:LEU:O	7:h:15:ASN:ND2	2.39	0.53
22:b:610:CLA:OBD	32:b:628:LMT:O6'	2.20	0.53
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.73	0.53
30:B:627:SQD:H462	30:B:627:SQD:H1	1.90	0.53
12:M:28:GLN:HA	12:m:28:GLN:HA	1.91	0.53
25:A:408:BCR:H321	30:A:414:SQD:H321	1.91	0.53
3:C:158:THR:O	3:C:251:HIS:HB3	2.09	0.53
25:K:101:BCR:H11C	25:y:101:BCR:H322	1.91	0.53
3:c:405:ASN:HB2	26:c:517:DGD:HG31	1.90	0.53
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.89	0.53
30:f:103:SQD:H162	18:x:33:THR:HA	1.90	0.53
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.89	0.53
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.91	0.53
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.90	0.53
26:C:516:DGD:HA22	9:J:29:PHE:HE1	1.73	0.53
1:a:179:THR:HG22	1:a:183:MET:HE2	1.90	0.53
2:b:458:PHE:HB3	22:b:608:CLA:HBC2	1.90	0.53
31:d:409:LMG:O5	31:d:409:LMG:O4	2.25	0.53
17:g:39:LEU:HD21	20:z:25:VAL:HA	1.90	0.53
2:B:271:THR:HB	2:B:274:GLN:HG3	1.91	0.53
4:D:84:SER:HB2	4:D:85:MET:HE2	1.91	0.53
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.73	0.53
26:b:601:DGD:O1B	26:b:601:DGD:O2D	2.26	0.53
22:B:605:CLA:OBD	32:B:623:LMT:O6'	2.24	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
16:v:81:ARG:CZ	16:v:157:GLY:HA3	2.39	0.53
25:A:408:BCR:H342	30:A:414:SQD:H311	1.91	0.52
32:B:628:LMT:H62	8:i:4:LEU:HD22	1.91	0.52
4:d:262:SER:N	31:d:409:LMG:O3	2.38	0.52
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.92	0.52
1:A:193:LEU:HD11	22:A:402:CLA:HMC2	1.92	0.52
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.91	0.52
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.92	0.52
2:b:12:LEU:HB2	22:b:616:CLA:HMC2	1.91	0.52
2:b:341:LYS:HA	2:b:405:GLU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:262:THR:HG22	2:b:263:THR:HG23	1.92	0.52
2:B:371:THR:HG22	2:B:377:VAL:HA	1.92	0.52
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.74	0.52
34:V:201:HEM:HBB2	34:V:201:HEM:HMB2	1.92	0.52
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.74	0.52
22:b:617:CLA:H51	31:d:408:LMG:H231	1.92	0.52
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.92	0.52
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.44	0.52
4:d:279:LEU:HG	23:d:402:PHO:HBC3	1.90	0.52
3:C:85:GLY:N	26:C:515:DGD:HE4	2.24	0.52
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.92	0.52
5:e:57:ALA:HB3	5:e:60:GLN:HB3	1.92	0.52
1:A:210:LEU:HG	23:D:401:PHO:NC	2.25	0.52
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.92	0.52
22:d:406:CLA:H43	18:x:23:LEU:HA	1.91	0.52
22:A:404:CLA:H161	24:A:407:PL9:H253	1.91	0.52
22:b:608:CLA:HBD	22:b:609:CLA:H43	1.92	0.52
31:c:518:LMG:H292	31:c:518:LMG:H111	1.92	0.52
4:d:275:PRO:O	4:d:279:LEU:HD23	2.09	0.52
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.91	0.52
1:A:64:ARG:O	13:O:178:ARG:NH2	2.43	0.52
30:A:413:SQD:H311	22:C:507:CLA:H71	1.92	0.51
26:c:517:DGD:HA22	9:j:29:PHE:HE1	1.74	0.51
22:D:404:CLA:H43	18:X:23:LEU:HA	1.92	0.51
3:c:85:GLY:N	26:c:516:DGD:HE4	2.25	0.51
22:c:504:CLA:HBA1	22:c:504:CLA:HBD	1.92	0.51
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.41	0.51
3:c:158:THR:O	3:c:251:HIS:HB3	2.11	0.51
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.93	0.51
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.45	0.51
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.34	0.51
6:F:45:ARG:NH2	9:J:40:LEU:O	2.42	0.51
2:b:383:PHE:CZ	13:o:193:GLY:HA2	2.46	0.51
10:k:12:PRO:HB2	10:k:15:TYR:HD2	1.75	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.42	0.51
17:y:24:MET:O	17:y:28:ILE:HG23	2.11	0.51
22:b:607:CLA:H2	22:b:609:CLA:H93	1.93	0.51
3:c:29:GLU:HB3	10:k:46:ARG:HH11	1.76	0.51
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.93	0.51
7:h:55:LEU:HB2	7:h:58:VAL:HG12	1.93	0.51
15:u:72:TYR:HB3	15:u:73:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:HA	1:A:109:GLY:HA3	1.92	0.51
1:a:85:SER:HA	1:a:109:GLY:HA3	1.93	0.51
22:a:405:CLA:H161	24:a:407:PL9:H253	1.92	0.51
22:A:403:CLA:CHA	22:A:403:CLA:HBA1	2.41	0.51
1:a:224:ILE:O	4:d:265:ARG:NH2	2.37	0.51
22:b:612:CLA:H151	22:b:613:CLA:H203	1.93	0.51
1:a:190:HIS:O	1:a:298:ASN:HB3	2.11	0.51
4:d:85:MET:HA	5:e:69:ARG:HB3	1.92	0.51
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.46	0.51
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.92	0.50
2:b:4:PRO:HD2	2:b:7:ARG:HD2	1.92	0.50
2:b:222:PRO:HG3	7:h:27:THR:H	1.76	0.50
18:x:11:THR:HG23	18:x:12:ILE:HG22	1.94	0.50
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.93	0.50
22:a:404:CLA:H42	24:d:407:PL9:H162	1.93	0.50
2:b:327:THR:HG22	22:b:611:CLA:H12	1.92	0.50
22:b:613:CLA:HMD1	7:h:27:THR:HB	1.92	0.50
25:B:617:BCR:H19C	25:B:618:BCR:H363	1.92	0.50
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.50
23:D:401:PHO:H151	22:D:403:CLA:H172	1.92	0.50
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.93	0.50
30:b:602:SQD:H1	30:b:602:SQD:H462	1.93	0.50
22:d:406:CLA:H42	18:x:26:GLY:HA3	1.94	0.50
10:K:40:GLN:HA	10:K:43:VAL:HG12	1.94	0.50
25:c:513:BCR:H343	25:c:513:BCR:H311	1.94	0.50
13:o:168:PHE:HB2	13:o:225:LEU:HB2	1.92	0.50
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.27	0.50
1:a:64:ARG:O	13:o:178:ARG:NH2	2.45	0.50
17:g:24:MET:O	17:g:28:ILE:HG23	2.12	0.50
1:A:271:LEU:HD11	24:A:407:PL9:C4	2.42	0.50
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.42	0.50
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.93	0.50
3:c:473:ASP:HB2	14:t:26:PRO:HB3	1.93	0.50
1:A:37:MET:HE1	1:A:129:ARG:CZ	2.42	0.50
2:B:256:MET:HA	2:B:263:THR:HG21	1.93	0.50
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.92	0.50
13:o:73:PRO:HG2	13:o:102:THR:HB	1.93	0.50
22:B:606:CLA:HBC3	25:B:618:BCR:HC8	1.94	0.50
22:C:512:CLA:HAB	25:C:520:BCR:H371	1.94	0.50
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.76	0.50
22:c:501:CLA:C2D	22:c:503:CLA:H2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:412:LMG:H171	25:f:102:BCR:H383	1.94	0.50
1:a:57:PRO:HG3	1:a:68:SER:HB3	1.94	0.49
22:b:606:CLA:H72	7:h:46:LEU:HD13	1.94	0.49
5:e:15:THR:HG23	9:j:8:ILE:O	2.11	0.49
3:c:166:ILE:O	3:c:170:ILE:HG13	2.12	0.49
4:d:221:THR:HG23	4:d:244:TYR:HB2	1.94	0.49
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.49
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.94	0.49
22:b:609:CLA:H202	22:b:613:CLA:HBB2	1.93	0.49
13:o:144:LEU:HD13	13:o:259:VAL:HG11	1.93	0.49
13:o:180:ALA:HB1	13:o:191:ALA:HB2	1.95	0.49
22:C:504:CLA:HBA1	22:C:504:CLA:HBD	1.94	0.49
10:K:26:PRO:O	10:K:29:PRO:HD2	2.12	0.49
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.94	0.49
1:a:78:ILE:O	1:a:176:ILE:HB	2.12	0.49
1:a:153:SER:HB3	22:a:403:CLA:HED1	1.94	0.49
3:c:361:PHE:HD1	26:c:515:DGD:HE61	1.77	0.49
2:B:19:LEU:HG	2:B:23:HIS:CE1	2.48	0.49
13:O:118:SER:HB3	13:O:157:PRO:HA	1.95	0.49
22:a:404:CLA:HBA1	22:a:404:CLA:CHA	2.41	0.49
13:o:118:SER:HB3	13:o:157:PRO:HA	1.95	0.49
27:A:410:LHG:H382	22:C:509:CLA:H93	1.95	0.49
22:B:612:CLA:H171	31:B:625:LMG:H401	1.95	0.49
3:C:223:TRP:CG	3:C:224:ILE:H	2.30	0.49
1:a:132:GLU:O	1:a:136:ARG:HG2	2.13	0.49
30:a:412:SQD:H223	26:c:517:DGD:HAE1	1.95	0.49
2:b:184:GLU:H	2:b:200:ALA:HB2	1.78	0.49
3:c:86:LEU:HB3	3:c:90:PRO:HD3	1.94	0.49
10:k:26:PRO:O	10:k:29:PRO:HD2	2.12	0.49
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.49
2:B:19:LEU:O	2:B:23:HIS:ND1	2.45	0.49
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.95	0.49
31:D:406:LMG:H111	11:L:19:LEU:HD21	1.93	0.49
8:I:4:LEU:HD22	32:b:603:LMT:H62	1.93	0.49
1:a:211:PHE:HA	1:a:214:MET:HB2	1.93	0.49
1:a:244:GLU:HG3	1:a:246:TYR:H	1.78	0.49
3:c:284:PHE:HB3	26:c:515:DGD:HA51	1.94	0.49
31:m:101:LMG:H142	31:m:101:LMG:H311	1.93	0.49
3:c:80:PRO:HB3	3:c:82:TYR:CE1	2.47	0.49
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.94	0.49
4:D:48:TRP:CE2	23:D:401:PHO:H161	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:611:CLA:H102	31:b:626:LMG:H392	1.95	0.49
5:e:23:HIS:NE2	34:f:101:HEM:ND	2.61	0.49
1:A:114:LEU:O	1:A:118:HIS:ND1	2.42	0.48
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.43	0.48
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.95	0.48
22:a:405:CLA:HAB	22:d:405:CLA:H42	1.95	0.48
4:d:84:SER:HB2	4:d:85:MET:HE2	1.95	0.48
1:A:132:GLU:O	1:A:136:ARG:HG2	2.13	0.48
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.94	0.48
2:b:170:ASP:OD1	2:b:175:THR:N	2.42	0.48
22:b:612:CLA:H18	22:b:613:CLA:H192	1.93	0.48
5:e:10:PHE:N	31:e:101:LMG:O3	2.45	0.48
3:C:425:TRP:CE2	22:C:519:CLA:HBA1	2.48	0.48
34:F:101:HEM:HBC2	34:F:101:HEM:HMC2	1.94	0.48
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.94	0.48
4:D:102:THR:OG1	26:D:407:DGD:HD62	2.13	0.48
1:a:183:MET:HE1	22:a:404:CLA:HMD2	1.95	0.48
4:d:55:VAL:HG21	4:d:110:LEU:HD12	1.96	0.48
22:A:404:CLA:HAB	22:D:403:CLA:H72	1.95	0.48
25:B:616:BCR:H333	12:M:13:LEU:HD12	1.96	0.48
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.96	0.48
2:b:326:ARG:HB3	2:b:444:ARG:HG2	1.95	0.48
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.49	0.48
4:D:262:SER:N	31:D:406:LMG:O3	2.42	0.48
2:b:43:ALA:HA	31:b:627:LMG:H112	1.96	0.48
2:b:371:THR:HG22	2:b:377:VAL:HA	1.95	0.48
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.78	0.48
2:b:25:MET:HE3	25:b:621:BCR:H23C	1.95	0.48
22:b:606:CLA:H62	22:b:606:CLA:H41	1.60	0.48
3:c:318:LEU:HG	3:c:328:VAL:HG11	1.96	0.48
26:D:407:DGD:O5E	26:D:407:DGD:O4E	2.24	0.48
13:o:240:THR:HA	13:o:264:VAL:HA	1.95	0.48
3:C:284:PHE:HB3	26:C:514:DGD:HA51	1.96	0.48
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.28	0.48
22:H:101:CLA:H41	22:H:101:CLA:H62	1.56	0.48
13:O:230:VAL:HG12	13:O:231:ASP:H	1.77	0.48
3:c:337:LEU:HA	13:o:131:PRO:HG3	1.96	0.48
23:A:405:PHO:H62	23:A:405:PHO:H41	1.46	0.47
1:a:89:ILE:HG12	13:o:99:ARG:NH2	2.29	0.47
2:b:96:VAL:HG22	22:b:610:CLA:HBA1	1.95	0.47
26:b:601:DGD:HB22	32:b:603:LMT:H72	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:406:SER:O	3:c:418:ASN:ND2	2.42	0.47
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.47	0.47
3:c:346:THR:HG21	13:o:38:GLY:HA2	1.96	0.47
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.44	0.47
22:C:510:CLA:HMB1	25:K:101:BCR:H382	1.96	0.47
22:D:403:CLA:H61	22:D:403:CLA:H41	1.67	0.47
3:c:209:ILE:HG23	25:c:514:BCR:H382	1.95	0.47
1:A:224:ILE:O	4:D:265:ARG:NH2	2.46	0.47
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.97	0.47
3:C:248:GLY:O	3:C:252:ILE:HG12	2.15	0.47
26:d:410:DGD:O5E	26:d:410:DGD:O4E	2.26	0.47
13:o:184:ASP:OD2	13:o:188:ARG:HB2	2.13	0.47
2:B:125:ASP:HB2	2:B:132:ALA:HB3	1.97	0.47
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.48	0.47
3:c:130:VAL:O	3:c:134:ILE:HG12	2.14	0.47
18:x:12:ILE:HG12	18:x:16:LEU:HD12	1.97	0.47
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.96	0.47
2:B:222:PRO:HG3	7:H:27:THR:H	1.79	0.47
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.96	0.47
2:b:18:ARG:HD3	2:b:118:TRP:HB3	1.96	0.47
3:c:113:VAL:HG11	31:c:518:LMG:H132	1.96	0.47
1:A:244:GLU:HG3	1:A:246:TYR:H	1.79	0.47
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.96	0.47
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.50	0.47
3:C:113:VAL:HG11	31:C:517:LMG:H132	1.97	0.47
1:a:210:LEU:HG	23:d:402:PHO:NC	2.30	0.47
3:c:164:HIS:ND1	22:c:506:CLA:OBD	2.36	0.47
3:c:391:ARG:HD2	3:c:395:TYR:CZ	2.50	0.47
26:c:517:DGD:HA22	9:j:29:PHE:CE1	2.50	0.47
13:o:135:GLN:HG2	13:o:141:ARG:HG3	1.97	0.47
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.96	0.47
2:B:68:ARG:HH22	22:B:603:CLA:HED1	1.80	0.47
4:D:275:PRO:O	4:D:279:LEU:HD23	2.15	0.47
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.63	0.47
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.96	0.47
22:b:618:CLA:H51	25:b:621:BCR:H372	1.97	0.47
22:B:603:CLA:H101	22:B:614:CLA:H2	1.97	0.47
25:B:619:BCR:H20C	25:B:619:BCR:H361	1.76	0.47
1:A:298:ASN:ND2	3:C:402:GLY:O	2.48	0.47
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.97	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:30:VAL:HG12	22:b:609:CLA:HHD	1.97	0.47
22:b:611:CLA:H193	11:l:27:LEU:HD11	1.97	0.47
1:A:159:LEU:C	1:A:162:PRO:HD2	2.40	0.46
3:C:315:MET:HE1	3:C:369:LEU:HD12	1.97	0.46
1:a:317:TRP:CZ3	4:d:180:ARG:HD3	2.48	0.46
3:c:319:ILE:HG21	3:c:389:GLU:HG3	1.96	0.46
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.46
17:y:39:LEU:HD21	20:Z:25:VAL:HA	1.97	0.46
2:b:5:TRP:HZ3	22:b:615:CLA:H51	1.80	0.46
3:c:245:ILE:O	3:c:249:ILE:HG12	2.15	0.46
9:j:38:SER:OG	9:j:39:SER:N	2.47	0.46
22:A:402:CLA:H3A	22:A:402:CLA:HBA1	1.53	0.46
2:B:135:LEU:HA	2:B:138:MET:HE3	1.98	0.46
9:J:38:SER:OG	9:J:39:SER:N	2.47	0.46
2:b:270:PRO:HG3	2:b:312:TYR:HD2	1.80	0.46
22:b:606:CLA:H162	22:b:606:CLA:H122	1.52	0.46
3:c:347:GLY:HA3	13:o:43:ASN:HB2	1.97	0.46
22:c:508:CLA:H92	22:c:508:CLA:H62	1.72	0.46
13:o:223:ILE:HG13	13:o:243:SER:HB3	1.98	0.46
2:B:213:GLY:O	2:B:217:ILE:HG13	2.14	0.46
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.80	0.46
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.46
16:V:68:VAL:O	16:V:71:ILE:HG12	2.14	0.46
2:b:121:GLU:HG2	7:h:4:ARG:HA	1.97	0.46
2:b:348:ASN:HB3	2:b:354:LEU:HD21	1.97	0.46
13:o:230:VAL:HG12	13:o:231:ASP:H	1.79	0.46
17:g:32:GLY:O	17:g:35:ILE:HG12	2.15	0.46
1:A:211:PHE:HA	1:A:214:MET:HB2	1.96	0.46
22:A:404:CLA:H161	22:A:404:CLA:H143	1.80	0.46
22:C:512:CLA:H3A	22:C:512:CLA:HBA2	1.70	0.46
2:b:213:GLY:O	2:b:217:ILE:HG13	2.15	0.46
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.81	0.46
22:a:404:CLA:H202	22:a:404:CLA:H162	1.76	0.46
22:a:405:CLA:HAB	22:d:405:CLA:H72	1.97	0.46
3:c:229:ASN:ND2	3:c:232:ASP:OD1	2.41	0.46
4:d:56:THR:HG21	5:e:50:PRO:HD3	1.97	0.46
23:d:401:PHO:H41	23:d:401:PHO:H62	1.48	0.46
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.97	0.46
7:H:46:LEU:HD13	22:H:101:CLA:H72	1.98	0.46
3:c:149:TYR:HA	3:c:156:LYS:HD3	1.97	0.46
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.49	0.46
2:b:315:ILE:HG22	2:b:426:PHE:HB3	1.98	0.46
3:c:197:ARG:NH2	3:c:231:GLU:OE2	2.49	0.46
3:c:223:TRP:CG	3:c:224:ILE:H	2.31	0.46
22:C:510:CLA:H93	22:C:510:CLA:H61	1.80	0.46
2:b:19:LEU:O	2:b:23:HIS:ND1	2.49	0.46
2:b:271:THR:HB	2:b:274:GLN:HG3	1.98	0.46
3:c:131:TYR:HE1	3:c:135:ARG:HD2	1.81	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.49	0.46
3:C:456:GLU:OE1	3:C:456:GLU:N	2.48	0.46
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.46
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.51	0.46
1:a:159:LEU:C	1:a:162:PRO:HD2	2.40	0.46
30:f:103:SQD:H131	18:x:36:VAL:HG11	1.97	0.46
15:u:75:LEU:HD21	15:u:101:GLN:HB3	1.97	0.46
25:y:101:BCR:HC32	20:Z:13:VAL:HG13	1.97	0.45
1:a:140:ARG:NH2	27:a:409:LHG:O5	2.37	0.45
22:b:609:CLA:H62	22:b:609:CLA:H41	1.80	0.45
4:d:43:LEU:HD23	4:d:117:HIS:CE1	2.51	0.45
4:d:102:THR:OG1	26:d:410:DGD:HD62	2.15	0.45
26:C:516:DGD:HA22	9:J:29:PHE:CE1	2.50	0.45
1:a:12:ASN:HB3	1:a:15:GLU:HB3	1.97	0.45
2:b:306:PRO:HG2	2:b:309:LEU:HB2	1.98	0.45
22:B:607:CLA:H18	22:B:608:CLA:H192	1.98	0.45
2:b:135:LEU:HA	2:b:138:MET:HE3	1.98	0.45
3:c:166:ILE:HG23	3:c:245:ILE:HG23	1.99	0.45
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.99	0.45
18:X:40:ILE:HA	18:X:43:ILE:HD12	1.99	0.45
1:a:214:MET:HE1	4:d:142:ASN:HD21	1.80	0.45
20:z:32:ASP:CG	20:z:33:TRP:H	2.23	0.45
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.45
25:C:513:BCR:H15C	25:C:513:BCR:H351	1.83	0.45
22:b:611:CLA:HBC3	25:b:623:BCR:HC8	1.98	0.45
3:c:223:TRP:CD2	3:c:224:ILE:HG13	2.51	0.45
22:c:520:CLA:H141	22:c:520:CLA:H161	1.75	0.45
4:d:244:TYR:OH	4:d:264:LYS:HE3	2.17	0.45
22:A:403:CLA:H62	22:A:403:CLA:H41	1.74	0.45
22:A:403:CLA:HAA1	24:D:405:PL9:H362	1.99	0.45
25:B:618:BCR:H20C	25:B:618:BCR:H361	1.81	0.45
2:b:450:TRP:NE1	22:b:611:CLA:HBA1	2.31	0.45
22:b:617:CLA:H171	31:d:408:LMG:H401	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD21	24:A:407:PL9:HC71	1.97	0.45
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.52	0.45
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.45
25:K:101:BCR:H20C	25:K:101:BCR:H361	1.77	0.45
1:a:27:ARG:NH1	4:d:254:SER:O	2.47	0.45
1:a:29:TYR:CG	1:a:133:LEU:HD13	2.52	0.45
2:b:25:MET:HG2	25:b:621:BCR:H23C	1.99	0.45
3:c:437:PHE:HA	22:c:507:CLA:HMC2	1.99	0.45
16:v:102:MET:HE3	34:v:201:HEM:HMB1	1.99	0.45
2:B:26:HIS:CE1	22:B:611:CLA:HMA2	2.51	0.45
22:B:614:CLA:H92	22:B:614:CLA:H62	1.78	0.45
22:H:101:CLA:H162	22:H:101:CLA:H122	1.55	0.45
22:b:606:CLA:H152	26:b:625:DGD:HAW2	1.97	0.45
31:d:409:LMG:H111	11:l:19:LEU:HD21	1.98	0.45
22:C:509:CLA:H2	22:C:509:CLA:H61	1.73	0.45
22:b:607:CLA:H92	22:b:607:CLA:HBB2	1.98	0.45
3:c:305:THR:HG22	3:c:308:GLU:HB2	1.99	0.45
22:c:508:CLA:H11	22:c:508:CLA:H51	1.82	0.45
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.98	0.45
22:C:501:CLA:H193	22:C:506:CLA:H111	1.99	0.44
4:D:85:MET:HA	5:E:69:ARG:HB3	2.00	0.44
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.99	0.44
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.52	0.44
22:A:403:CLA:H42	24:D:405:PL9:H162	1.98	0.44
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.98	0.44
15:U:54:LYS:HD2	15:U:113:THR:HG23	2.00	0.44
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.47	0.44
25:y:101:BCR:H20C	25:y:101:BCR:H361	1.80	0.44
3:c:137:PRO:HB2	3:c:139:THR:O	2.17	0.44
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.98	0.44
2:B:383:PHE:N	4:D:344:GLU:O	2.37	0.44
31:I:101:LMG:H181	32:I:102:LMT:H42	1.98	0.44
1:a:111:PRO:O	1:a:115:ILE:HG13	2.17	0.44
25:B:616:BCR:H11C	25:B:616:BCR:H341	1.88	0.44
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.00	0.44
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.00	0.44
4:D:279:LEU:HG	23:D:401:PHO:HBC3	2.00	0.44
6:F:22:ALA:O	6:F:25:THR:OG1	2.33	0.44
7:H:3:ARG:NH2	11:L:1:MET:HE1	2.32	0.44
22:H:101:CLA:H62	22:H:101:CLA:H93	1.86	0.44
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:101:BCR:H311	25:K:101:BCR:H343	1.98	0.44
16:V:83:GLU:H	16:V:83:GLU:CD	2.25	0.44
2:b:26:HIS:CE1	22:b:616:CLA:HMA2	2.52	0.44
2:b:247:PHE:HB2	22:b:612:CLA:HBC1	1.99	0.44
3:c:350:ILE:HG21	3:c:359:TRP:HB2	1.99	0.44
26:c:516:DGD:HA91	26:c:516:DGD:HAW2	1.76	0.44
22:d:405:CLA:H92	22:d:405:CLA:H62	1.80	0.44
12:m:3:VAL:HG11	14:t:2:GLU:HG2	2.00	0.44
13:o:79:LYS:HB3	13:o:258:GLU:HB2	2.00	0.44
13:o:81:GLU:HA	13:o:82:PRO:HD3	1.78	0.44
16:v:38:LEU:HD12	16:v:95:ILE:HB	1.99	0.44
30:F:103:SQD:H131	18:X:36:VAL:HG11	2.00	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.81	0.44
1:a:258:LEU:O	4:d:128:ARG:NH1	2.50	0.44
1:a:268:SER:O	1:a:272:HIS:ND1	2.43	0.44
2:b:76:SER:HG	2:b:78:TRP:CD1	2.35	0.44
2:b:135:LEU:HB2	2:b:136:PRO:HD3	1.99	0.44
22:b:620:CLA:H72	22:b:620:CLA:H12	1.98	0.44
25:b:624:BCR:H20C	25:b:624:BCR:H361	1.75	0.44
3:c:90:PRO:O	3:c:94:THR:HG23	2.17	0.44
25:c:521:BCR:H20C	25:c:521:BCR:H361	1.81	0.44
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	2.00	0.44
22:B:614:CLA:H172	22:B:614:CLA:H111	2.00	0.44
26:B:620:DGD:HA71	22:H:101:CLA:H193	2.00	0.44
10:K:37:PHE:HB3	25:y:101:BCR:C40	2.47	0.44
16:V:60:GLN:HA	16:V:64:ALA:HB2	1.99	0.44
18:X:12:ILE:HG12	18:X:16:LEU:HD12	1.98	0.44
3:c:386:PRO:HB3	16:v:116:GLU:HG2	2.00	0.44
7:h:12:ARG:O	7:h:12:ARG:HD3	2.18	0.44
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.52	0.44
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.44
25:K:101:BCR:H353	25:y:101:BCR:H321	1.98	0.44
3:c:318:LEU:HD21	3:c:380:ILE:HG23	2.00	0.44
13:o:135:GLN:HE21	13:o:135:GLN:HB3	1.69	0.44
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.44
22:B:606:CLA:H62	22:B:606:CLA:H41	1.86	0.44
3:C:112:PHE:HE2	25:C:520:BCR:HC31	1.82	0.44
3:C:456:GLU:HG2	3:C:457:LYS:HG3	1.99	0.44
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.44
22:a:405:CLA:H161	22:a:405:CLA:H143	1.87	0.44
15:u:68:TYR:HB2	15:u:71:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.00	0.43
31:M:101:LMG:H142	31:M:101:LMG:H311	1.99	0.43
25:b:624:BCR:H24C	25:b:624:BCR:H371	1.87	0.43
3:c:425:TRP:CE2	22:c:520:CLA:HBA1	2.52	0.43
22:c:501:CLA:H193	22:c:506:CLA:H111	2.00	0.43
25:c:513:BCR:H15C	25:c:513:BCR:H351	1.89	0.43
25:c:513:BCR:H353	25:g:101:BCR:H321	2.00	0.43
22:d:405:CLA:H61	22:d:405:CLA:H41	1.64	0.43
8:i:6:ILE:O	8:i:10:ILE:HG12	2.17	0.43
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.01	0.43
22:B:612:CLA:H51	31:B:625:LMG:H231	1.99	0.43
26:B:620:DGD:HAT2	22:H:101:CLA:H151	2.00	0.43
3:C:209:ILE:HG23	25:C:513:BCR:H382	1.99	0.43
1:a:114:LEU:O	1:a:118:HIS:ND1	2.48	0.43
25:g:101:BCR:H20C	25:g:101:BCR:H361	1.78	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.17	0.43
3:C:137:PRO:HB2	3:C:139:THR:O	2.18	0.43
5:E:42:LEU:O	5:E:46:VAL:HG23	2.17	0.43
10:K:18:PHE:O	10:K:22:VAL:HG23	2.18	0.43
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.54	0.43
20:Z:33:TRP:O	20:Z:33:TRP:CD1	2.72	0.43
1:a:195:HIS:HA	1:a:196:PRO:HD3	1.92	0.43
26:a:408:DGD:HD2	26:a:408:DGD:HG32	1.73	0.43
3:c:456:GLU:OE1	3:c:456:GLU:N	2.48	0.43
20:z:33:TRP:O	20:z:33:TRP:CD1	2.71	0.43
1:A:183:MET:HE1	22:A:403:CLA:HMD2	2.00	0.43
1:A:258:LEU:O	4:D:128:ARG:NH1	2.52	0.43
25:B:616:BCR:H20C	25:B:616:BCR:H361	1.78	0.43
3:C:245:ILE:O	3:C:249:ILE:HG12	2.18	0.43
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.01	0.43
26:C:515:DGD:HA91	26:C:515:DGD:HAW2	1.75	0.43
22:D:403:CLA:H92	22:D:403:CLA:H62	1.83	0.43
1:a:244:GLU:CD	4:d:264:LYS:HZ3	2.27	0.43
3:c:420:VAL:H	26:c:516:DGD:HE62	1.83	0.43
22:c:520:CLA:O2D	31:c:522:LMG:O2	2.35	0.43
16:v:68:VAL:O	16:v:71:ILE:HG12	2.18	0.43
1:A:156:ALA:HA	1:A:160:ILE:HB	1.99	0.43
1:A:238:LYS:O	1:A:241:GLN:HG3	2.18	0.43
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.43
7:H:12:ARG:O	7:H:12:ARG:HD3	2.18	0.43
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:93:PHE:HZ	22:a:406:CLA:HAA1	1.84	0.43
1:a:212:CYS:HB2	4:d:211:CYS:HB2	2.01	0.43
3:c:393:ALA:HB1	34:v:201:HEM:HBC1	2.01	0.43
22:c:504:CLA:H11	25:c:514:BCR:H312	1.99	0.43
22:c:509:CLA:H2	22:c:509:CLA:H61	1.71	0.43
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.82	0.43
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.00	0.43
1:A:269:ARG:NH1	4:D:231:THR:HB	2.33	0.43
22:A:402:CLA:H51	23:A:405:PHO:C3B	2.49	0.43
2:B:25:MET:HE3	25:B:616:BCR:H23C	2.00	0.43
22:B:602:CLA:HBB2	22:B:602:CLA:H92	2.01	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.18	0.43
5:E:15:THR:HG23	9:J:8:ILE:O	2.18	0.43
2:b:108:PHE:HB2	30:b:602:SQD:H223	2.00	0.43
3:c:29:GLU:HB2	3:c:30:SER:H	1.63	0.43
22:c:512:CLA:HAB	25:c:521:BCR:H24C	2.01	0.43
26:c:516:DGD:HA42	22:c:520:CLA:H2	2.00	0.43
10:k:40:GLN:HA	10:k:43:VAL:HG12	2.01	0.43
22:A:406:CLA:HMC1	25:A:408:BCR:H14C	1.99	0.43
23:D:401:PHO:CHB	22:D:403:CLA:H101	2.49	0.43
13:O:192:SER:OG	13:O:193:GLY:N	2.51	0.43
2:b:19:LEU:HG	2:b:23:HIS:CE1	2.54	0.43
22:b:610:CLA:H3A	22:b:610:CLA:HBA2	1.23	0.43
22:c:512:CLA:H3A	22:c:512:CLA:HBA2	1.69	0.43
10:k:12:PRO:HB2	10:k:15:TYR:CD2	2.53	0.43
22:C:507:CLA:H172	26:C:515:DGD:HBW2	2.00	0.43
6:F:16:PHE:HB3	30:F:103:SQD:H241	2.01	0.43
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.27	0.43
31:b:626:LMG:H421	4:d:284:ILE:HD13	1.99	0.43
11:l:13:ASN:ND2	31:l:101:LMG:O5	2.51	0.43
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.54	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.43
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.53	0.43
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.00	0.43
1:a:237:TYR:OH	4:d:246:MET:HG2	2.18	0.43
25:b:621:BCR:H333	12:m:13:LEU:HD12	2.00	0.43
23:d:402:PHO:CHB	22:d:405:CLA:H101	2.48	0.43
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.54	0.43
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.43
3:C:350:ILE:HG21	3:C:359:TRP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:PHE:C	4:D:149:PRO:HD2	2.44	0.43
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.43
25:b:624:BCR:H15C	25:b:624:BCR:H351	1.89	0.43
17:g:28:ILE:O	25:g:101:BCR:H14C	2.19	0.43
17:g:31:ALA:O	17:g:35:ILE:HG23	2.18	0.43
1:A:40:THR:HG21	1:A:121:LEU:HD23	2.01	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.90	0.42
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.00	0.42
22:B:601:CLA:HMB2	25:H:102:BCR:H393	2.01	0.42
22:B:611:CLA:H122	22:B:611:CLA:H162	1.74	0.42
22:a:404:CLA:HMA2	24:d:407:PL9:H411	2.00	0.42
3:c:62:PHE:CE2	10:k:29:PRO:HD3	2.54	0.42
25:c:513:BCR:H371	25:c:513:BCR:H24C	1.79	0.42
6:f:16:PHE:HB3	30:f:103:SQD:H241	2.01	0.42
6:f:17:THR:OG1	6:f:18:VAL:N	2.53	0.42
3:C:35:TRP:CZ2	27:C:518:LHG:H261	2.54	0.42
3:C:405:ASN:HB2	26:C:516:DGD:HG31	2.01	0.42
25:C:513:BCR:H11C	25:C:513:BCR:H341	1.90	0.42
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.19	0.42
13:O:79:LYS:HB3	13:O:258:GLU:HB2	2.02	0.42
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.18	0.42
1:a:322:ASN:OD1	3:c:412:THR:HA	2.19	0.42
22:a:404:CLA:H51	22:a:404:CLA:H11	1.83	0.42
22:b:620:CLA:H111	22:b:620:CLA:H143	1.73	0.42
3:c:363:GLY:O	3:c:367:GLU:HG2	2.18	0.42
3:c:456:GLU:HG2	3:c:457:LYS:HG3	2.01	0.42
10:k:37:PHE:HB3	25:g:101:BCR:C40	2.49	0.42
1:A:127:MET:HG3	1:A:144:CYS:HB2	2.02	0.42
22:A:403:CLA:H162	22:A:403:CLA:H202	1.76	0.42
2:B:485:GLU:HG3	2:B:486:LEU:N	2.34	0.42
22:B:603:CLA:HBD	22:B:604:CLA:H43	2.02	0.42
22:B:605:CLA:H3A	22:B:605:CLA:HBA2	1.23	0.42
3:C:224:ILE:O	3:C:227:VAL:HG23	2.20	0.42
3:C:259:TRP:H	3:C:259:TRP:CD1	2.37	0.42
3:C:303:GLY:O	3:C:423:ARG:NE	2.39	0.42
5:E:81:GLU:C	5:E:83:LEU:H	2.27	0.42
6:F:17:THR:OG1	6:F:18:VAL:N	2.52	0.42
1:A:283:VAL:O	1:A:286:THR:HG22	2.19	0.42
22:B:602:CLA:H192	22:B:602:CLA:H162	1.76	0.42
22:C:512:CLA:HAB	25:C:520:BCR:H24C	2.00	0.42
1:a:157:VAL:HG13	1:a:172:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:406:CLA:H141	22:a:406:CLA:H162	1.68	0.42
24:a:407:PL9:H371	24:a:407:PL9:H351	1.76	0.42
25:c:513:BCR:H391	10:k:36:ALA:HB2	2.01	0.42
5:e:42:LEU:O	5:e:46:VAL:HG23	2.19	0.42
1:A:235:TYR:C	1:A:237:TYR:H	2.27	0.42
1:A:257:ARG:HH22	2:B:488:PRO:C	2.28	0.42
2:B:25:MET:HG2	25:B:616:BCR:H23C	2.00	0.42
2:B:137:LYS:HD2	7:H:14:LEU:O	2.20	0.42
22:B:604:CLA:H202	22:B:608:CLA:HBB2	2.01	0.42
25:C:513:BCR:H20C	25:C:513:BCR:H361	1.85	0.42
13:O:143:PRO:HG2	13:O:248:ASP:HB3	2.00	0.42
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.01	0.42
30:a:412:SQD:H202	26:c:517:DGD:HAH2	2.01	0.42
22:b:618:CLA:H112	22:b:618:CLA:H152	1.78	0.42
25:c:513:BCR:H20C	25:c:513:BCR:H361	1.80	0.42
25:c:521:BCR:H15C	25:c:521:BCR:H351	1.84	0.42
31:d:409:LMG:HC1	31:d:409:LMG:O9	2.20	0.42
16:v:90:PRO:O	16:v:92:ARG:HD3	2.19	0.42
1:A:190:HIS:O	1:A:298:ASN:HB3	2.19	0.42
31:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.00	0.42
7:H:12:ARG:N	7:H:13:PRO:HD2	2.35	0.42
25:H:102:BCR:H20C	25:H:102:BCR:H361	1.79	0.42
13:O:206:GLU:CD	13:O:206:GLU:H	2.27	0.42
1:a:340:PRO:HG3	15:u:133:TYR:CG	2.55	0.42
3:c:318:LEU:HD13	3:c:351:PHE:HE1	1.83	0.42
22:c:506:CLA:H92	22:c:506:CLA:H62	1.77	0.42
13:o:192:SER:OG	13:o:193:GLY:N	2.52	0.42
16:v:60:GLN:HA	16:v:64:ALA:HB2	2.02	0.42
25:g:101:BCR:H323	25:g:101:BCR:HC31	1.68	0.42
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.28	0.42
1:A:221:SER:HB2	4:D:139:ARG:O	2.19	0.42
31:C:517:LMG:H111	31:C:517:LMG:H292	2.00	0.42
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.01	0.42
13:O:154:SER:N	13:O:169:LYS:O	2.51	0.42
16:V:90:PRO:O	16:V:92:ARG:HD3	2.18	0.42
20:Z:5:PHE:CE1	20:Z:54:VAL:HG13	2.55	0.42
15:u:72:TYR:O	15:u:76:ALA:HB3	2.20	0.42
1:A:153:SER:HB2	22:A:402:CLA:H43	2.00	0.42
1:A:268:SER:O	1:A:272:HIS:ND1	2.42	0.42
2:B:327:THR:HG22	22:B:606:CLA:H12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:604:CLA:H62	22:B:604:CLA:H41	1.81	0.42
22:B:615:CLA:H143	22:B:615:CLA:H111	1.78	0.42
25:B:617:BCR:H15C	25:B:617:BCR:H351	1.87	0.42
25:B:618:BCR:H24C	25:B:618:BCR:H371	1.82	0.42
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.54	0.42
1:a:176:ILE:HD12	22:a:404:CLA:HED3	2.01	0.42
1:a:180:PHE:HA	1:a:183:MET:HE3	2.02	0.42
30:a:401:SQD:H321	25:i:101:BCR:H321	2.02	0.42
22:c:510:CLA:H141	20:z:20:VAL:HG13	2.00	0.42
2:B:91:TRP:CH2	22:B:605:CLA:H12	2.55	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.01	0.42
25:C:520:BCR:H371	25:C:520:BCR:H24C	1.84	0.42
4:D:201:VAL:O	4:D:205:LEU:HB2	2.20	0.42
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.42
22:b:616:CLA:H162	22:b:616:CLA:H122	1.75	0.42
22:c:501:CLA:H162	22:c:501:CLA:H141	1.80	0.42
22:B:603:CLA:H11	22:B:604:CLA:H42	2.02	0.42
3:C:166:ILE:O	3:C:170:ILE:HG13	2.19	0.42
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.02	0.42
1:a:191:ASN:HB2	3:c:411:ALA:HB1	2.02	0.42
1:a:271:LEU:HD11	24:a:407:PL9:C4	2.50	0.42
22:b:619:CLA:H172	22:b:619:CLA:H111	2.02	0.42
3:c:38:GLY:HA3	22:c:510:CLA:HMD2	2.02	0.42
3:c:248:GLY:O	3:c:252:ILE:HG12	2.19	0.42
22:c:507:CLA:H172	26:c:516:DGD:HBW2	2.01	0.42
22:c:510:CLA:H171	20:z:20:VAL:HA	2.02	0.42
4:d:53:THR:HG22	4:d:67:TYR:CD2	2.54	0.42
5:e:81:GLU:C	5:e:83:LEU:H	2.28	0.42
10:k:25:LEU:HD22	25:g:101:BCR:H312	2.02	0.42
16:v:158:GLY:HA3	16:v:162:TYR:CD2	2.54	0.42
23:A:405:PHO:H13	23:A:405:PHO:H102	1.86	0.41
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.49	0.41
22:C:501:CLA:H162	22:C:501:CLA:H141	1.77	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.84	0.41
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.41
4:d:146:PHE:C	4:d:149:PRO:HD2	2.44	0.41
4:d:252:PHE:O	4:d:256:ILE:HG22	2.20	0.41
23:d:401:PHO:H102	23:d:401:PHO:H13	1.81	0.41
15:u:94:ILE:HB	15:u:97:LEU:HD11	2.02	0.41
22:A:403:CLA:HED2	4:D:198:MET:SD	2.60	0.41
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.96	0.41
22:D:403:CLA:H3A	22:D:403:CLA:HBA1	1.86	0.41
5:E:60:GLN:HG2	5:E:62:SER:H	1.85	0.41
14:T:7:VAL:HG12	32:b:604:LMT:H122	2.02	0.41
1:a:221:SER:HB2	4:d:139:ARG:O	2.20	0.41
26:b:601:DGD:HG2	32:b:603:LMT:H72	2.01	0.41
22:b:607:CLA:H41	22:b:607:CLA:H61	1.61	0.41
22:b:612:CLA:H143	22:b:612:CLA:H161	1.85	0.41
3:c:80:PRO:HB2	3:c:83:GLU:HG3	2.03	0.41
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.02	0.41
25:j:102:BCR:HC42	25:g:101:BCR:H381	2.03	0.41
1:A:215:HIS:HA	24:A:407:PL9:O1	2.21	0.41
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.02	0.41
3:C:135:ARG:HB2	20:Z:27:TYR:HB3	2.02	0.41
31:C:521:LMG:H112	25:J:102:BCR:H373	2.02	0.41
24:D:405:PL9:H13	31:D:406:LMG:H132	2.02	0.41
13:O:223:ILE:HG13	13:O:243:SER:HB3	2.01	0.41
2:b:256:MET:HA	2:b:263:THR:HG21	2.02	0.41
25:f:102:BCR:H11C	25:f:102:BCR:H341	1.97	0.41
1:A:29:TYR:O	1:A:129:ARG:NH1	2.53	0.41
22:A:406:CLA:H141	22:A:406:CLA:H162	1.68	0.41
25:A:408:BCR:H11C	25:A:408:BCR:H341	1.95	0.41
26:A:409:DGD:HD2	26:A:409:DGD:HG32	1.73	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.93	0.41
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.02	0.41
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.86	0.41
4:D:148:ALA:HB1	4:D:279:LEU:HB2	2.02	0.41
31:D:406:LMG:HC1	31:D:406:LMG:O9	2.20	0.41
1:a:215:HIS:HA	24:a:407:PL9:O1	2.20	0.41
3:c:112:PHE:HE2	25:c:521:BCR:HC31	1.85	0.41
3:c:205:ASP:HA	3:c:206:PRO:HD2	1.93	0.41
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.02	0.41
25:J:102:BCR:H351	25:J:102:BCR:H15C	1.75	0.41
1:a:232:SER:HB3	1:a:235:TYR:HD1	1.84	0.41
22:a:403:CLA:H3A	22:a:403:CLA:HBA1	1.53	0.41
22:b:616:CLA:H171	22:b:617:CLA:HBB2	2.02	0.41
3:c:282:MET:HG2	22:c:501:CLA:H61	2.01	0.41
4:d:113:PHE:O	4:d:117:HIS:HB2	2.20	0.41
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.01	0.41
26:d:410:DGD:HO4E	26:d:410:DGD:HO5E	1.61	0.41
5:e:14:ILE:HG22	9:j:13:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:x:17:LYS:O	18:x:21:ILE:HG13	2.20	0.41
22:B:607:CLA:H51	22:B:608:CLA:H101	2.02	0.41
3:C:265:ILE:HD11	8:I:28:PRO:HB3	2.02	0.41
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.93	0.41
1:a:238:LYS:O	1:a:241:GLN:HG3	2.20	0.41
22:a:403:CLA:H151	23:d:401:PHO:H72	2.03	0.41
2:b:54:PRO:HD2	2:b:57:ARG:HG3	2.01	0.41
2:b:222:PRO:HD2	2:b:225:LEU:HD12	2.02	0.41
22:b:612:CLA:CHA	22:b:612:CLA:HBA1	2.51	0.41
22:b:613:CLA:H11	7:h:35:MET:HE1	2.02	0.41
4:d:129:GLN:OE1	4:d:143:ALA:HA	2.20	0.41
22:B:613:CLA:H91	22:B:613:CLA:H112	1.85	0.41
3:C:116:VAL:HG21	25:C:520:BCR:HC21	2.02	0.41
22:C:505:CLA:H202	22:C:505:CLA:H161	1.90	0.41
4:D:312:GLU:HB2	13:O:185:PRO:CG	2.50	0.41
5:e:10:PHE:HE1	34:f:101:HEM:HBD2	1.86	0.41
25:f:102:BCR:H15C	25:f:102:BCR:H351	1.95	0.41
16:v:158:GLY:HA3	16:v:162:TYR:HD2	1.85	0.41
16:v:160:LYS:HA	16:v:163:TYR:CD2	2.56	0.41
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.02	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD2	1.95	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.41
22:B:609:CLA:H12	22:B:609:CLA:H51	1.88	0.41
1:a:309:ALA:HA	6:f:45:ARG:HB2	2.03	0.41
3:c:259:TRP:CD1	3:c:259:TRP:H	2.38	0.41
4:d:342:PRO:O	4:d:345:VAL:HG12	2.20	0.41
5:e:50:PRO:HB3	5:e:54:SER:O	2.20	0.41
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.21	0.41
25:x:101:BCR:H15C	25:x:101:BCR:H351	1.92	0.41
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.55	0.41
1:A:111:PRO:O	1:A:115:ILE:HG13	2.21	0.41
2:B:76:SER:HG	2:B:78:TRP:CD1	2.39	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.03	0.41
22:B:604:CLA:H161	22:B:604:CLA:H141	1.88	0.41
32:B:624:LMT:H102	7:H:35:MET:SD	2.61	0.41
3:C:334:PRO:HA	13:O:179:THR:OG1	2.21	0.41
4:D:48:TRP:CD2	23:D:401:PHO:H161	2.56	0.41
25:J:102:BCR:H341	25:J:102:BCR:H11C	1.82	0.41
1:a:262:TYR:CZ	31:e:101:LMG:HC5	2.56	0.41
2:b:194:ASN:HA	2:b:195:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:606:CLA:H61	7:h:46:LEU:HB2	2.02	0.41
22:b:614:CLA:H12	22:b:614:CLA:H51	1.86	0.41
3:c:57:ALA:O	3:c:61:VAL:HG23	2.21	0.41
3:c:386:PRO:O	3:c:390:ARG:HG2	2.20	0.41
10:k:31:LEU:HB3	25:g:101:BCR:C15	2.51	0.41
25:g:101:BCR:HC32	20:z:13:VAL:HG13	2.03	0.41
1:A:27:ARG:NH1	4:D:254:SER:O	2.48	0.41
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.03	0.41
22:B:602:CLA:H41	22:B:602:CLA:H61	1.64	0.41
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.03	0.41
16:V:102:MET:HE1	16:V:141:ILE:HD12	2.02	0.41
1:a:334:ARG:NH1	13:o:183:LEU:O	2.54	0.41
3:c:119:LEU:HG	25:c:513:BCR:H10C	2.02	0.41
3:c:315:MET:HE1	3:c:369:LEU:HD12	2.03	0.41
11:l:11:GLU:HG2	11:l:12:LEU:N	2.35	0.41
12:m:19:SER:O	12:m:23:ILE:HG13	2.21	0.41
2:B:474:LEU:O	4:D:134:ARG:NH1	2.54	0.40
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.51	0.40
1:a:223:LEU:HD13	4:d:265:ARG:HD3	2.03	0.40
1:a:235:TYR:C	1:a:237:TYR:H	2.29	0.40
22:b:606:CLA:H41	22:b:606:CLA:H93	2.03	0.40
3:c:29:GLU:OE1	3:c:31:SER:HB2	2.21	0.40
10:k:18:PHE:O	10:k:22:VAL:HG23	2.20	0.40
13:o:41:LEU:HD12	13:o:41:LEU:HA	1.95	0.40
1:A:141:PRO:HG3	3:C:446:GLY:C	2.46	0.40
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.57	0.40
20:Z:33:TRP:O	20:Z:33:TRP:HD1	2.05	0.40
2:b:222:PRO:HG3	7:h:26:GLY:HA3	2.04	0.40
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.57	0.40
3:c:257:PHE:HB3	3:c:258:GLY:H	1.61	0.40
4:d:261:PHE:HA	31:d:409:LMG:O2	2.21	0.40
1:A:116:ILE:HG13	1:A:117:PHE:N	2.35	0.40
2:B:212:ALA:O	2:B:216:HIS:ND1	2.52	0.40
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.03	0.40
10:K:31:LEU:HB3	25:y:101:BCR:C15	2.51	0.40
12:M:24:ILE:HG21	31:m:101:LMG:H322	2.04	0.40
13:O:59:ASP:C	13:O:61:SER:H	2.30	0.40
2:b:137:LYS:HB2	2:b:137:LYS:HE3	1.97	0.40
2:b:256:MET:O	2:b:448:ARG:NH1	2.41	0.40
4:d:48:TRP:CE2	23:d:402:PHO:H161	2.56	0.40
25:j:102:BCR:H15C	25:j:102:BCR:H351	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:101:BCR:H24C	25:g:101:BCR:H371	1.95	0.40
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.36	0.40
22:C:519:CLA:H161	22:C:519:CLA:H141	1.90	0.40
24:D:405:PL9:H372	11:L:30:LEU:HD13	2.03	0.40
3:c:174:LEU:HD13	22:c:502:CLA:H111	2.03	0.40
15:u:117:VAL:HG13	15:u:122:VAL:HG21	2.03	0.40
16:v:81:ARG:NE	16:v:157:GLY:HA3	2.36	0.40
16:v:119:PRO:HA	16:v:127:PHE:CD2	2.57	0.40
22:A:403:CLA:H51	22:A:403:CLA:H11	1.85	0.40
22:A:404:CLA:HAB	22:D:403:CLA:H42	2.03	0.40
24:A:407:PL9:H301	4:D:42:TYR:HA	2.03	0.40
22:B:613:CLA:H112	22:B:613:CLA:H152	1.81	0.40
25:B:616:BCR:H15C	25:B:616:BCR:H351	1.88	0.40
22:C:511:CLA:H13	22:C:511:CLA:H61	2.04	0.40
11:L:11:GLU:HG2	11:L:12:LEU:N	2.35	0.40
13:O:168:PHE:HB2	13:O:225:LEU:HB2	2.02	0.40
15:U:106:ARG:HA	15:U:109:LEU:HG	2.03	0.40
17:y:31:ALA:O	17:y:35:ILE:HG23	2.22	0.40
1:a:141:PRO:HG3	3:c:446:GLY:C	2.47	0.40
1:a:193:LEU:HD11	22:a:403:CLA:HMC2	2.03	0.40
22:b:607:CLA:H141	22:b:607:CLA:H161	1.85	0.40
3:c:131:TYR:CE1	3:c:135:ARG:HD2	2.57	0.40
3:c:277:GLY:C	22:c:504:CLA:HBC2	2.46	0.40
13:o:206:GLU:H	13:o:206:GLU:CD	2.29	0.40
16:v:98:LEU:O	16:v:102:MET:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	10 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	10	42
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	16	52
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	21	58
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	14	49
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	14	49
4	D	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	36	71
4	d	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	36	71
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9	40
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9	40
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	16
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	16
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	21
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	21
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	207 (86%)	31 (13%)	3 (1%)	10	42
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10	42
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	20
14	t	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	3	20
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	28
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	28
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	2	18
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	2	18
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	13
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	13
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	34
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	34
All	All	5138/5618 (92%)	4677 (91%)	406 (8%)	55 (1%)	11	45

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
14	T	30	THR
17	y	43	ARG
18	X	12	ILE
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
13	o	52	ALA
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
2	B	489	GLU
3	C	32	GLY
4	D	239	GLN

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Mol	Chain	Res	Type
7	H	26	GLY
9	J	38	SER
13	O	88	GLU
13	O	271	PRO
2	b	489	GLU
3	c	32	GLY
4	d	239	GLN
5	e	82	GLN
9	j	38	SER
13	o	88	GLU
1	A	142	TRP
1	A	334	ARG
5	E	82	GLN
1	a	334	ARG
13	o	271	PRO
15	u	73	PRO
7	H	16	SER
15	U	73	PRO
3	c	144	SER
7	h	16	SER
7	h	26	GLY
3	C	144	SER
15	U	83	ALA
1	a	142	TRP
15	u	83	ALA
2	B	176	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	260 (96%)	11 (4%)	27	48
1	a	271/280 (97%)	260 (96%)	11 (4%)	27	48
2	B	390/407 (96%)	380 (97%)	10 (3%)	40	61
2	b	390/407 (96%)	379 (97%)	11 (3%)	38	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	347/362 (96%)	336 (97%)	11 (3%)	34	55
3	c	347/362 (96%)	336 (97%)	11 (3%)	34	55
4	D	275/283 (97%)	264 (96%)	11 (4%)	28	49
4	d	275/283 (97%)	264 (96%)	11 (4%)	28	49
5	E	72/73 (99%)	68 (94%)	4 (6%)	19	40
5	e	72/73 (99%)	68 (94%)	4 (6%)	19	40
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	51 (96%)	2 (4%)	29	50
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	50
8	I	32/35 (91%)	31 (97%)	1 (3%)	35	56
8	i	32/35 (91%)	31 (97%)	1 (3%)	35	56
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	48
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	48
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	58
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	58
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	68	77
13	o	202/228 (89%)	200 (99%)	2 (1%)	68	77
14	T	29/29 (100%)	28 (97%)	1 (3%)	32	54
14	t	29/29 (100%)	28 (97%)	1 (3%)	32	54
15	U	84/112 (75%)	82 (98%)	2 (2%)	43	63
15	u	84/112 (75%)	82 (98%)	2 (2%)	43	63
16	V	116/138 (84%)	114 (98%)	2 (2%)	53	68
16	v	116/138 (84%)	114 (98%)	2 (2%)	53	68
17	g	20/37 (54%)	17 (85%)	3 (15%)	3	13
17	y	20/37 (54%)	17 (85%)	3 (15%)	3	13
18	X	30/34 (88%)	28 (93%)	2 (7%)	15	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	x	30/34 (88%)	29 (97%)	1 (3%)	33	55
20	Z	52/52 (100%)	50 (96%)	2 (4%)	29	50
20	z	52/52 (100%)	50 (96%)	2 (4%)	29	50
All	All	4244/4594 (92%)	4112 (97%)	132 (3%)	35	56

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	157	VAL
1	A	202	VAL
1	A	226	GLU
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	275	LEU
1	A	286	THR
1	A	292	THR
1	A	306	VAL
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	354	LEU
2	B	362	PHE
2	B	422	ARG
2	B	467	ILE
2	B	485	GLU
2	B	486	LEU
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	174	LEU
3	C	201	ASN
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	417	VAL
3	C	469	MET
3	C	472	LEU
4	D	43	LEU

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Mol	Chain	Res	Type
4	D	91	LEU
4	D	180	ARG
4	D	201	VAL
4	D	205	LEU
4	D	241	GLU
4	D	256	ILE
4	D	259	ILE
4	D	291	LEU
4	D	323	GLU
4	D	346	LEU
5	E	18	ARG
5	E	77	GLU
5	E	80	LEU
5	E	84	LYS
7	H	27	THR
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	11	GLU
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	114	VAL
15	U	132	LEU
16	V	68	VAL
16	V	116	GLU
17	y	25	ILE
17	y	28	ILE
17	y	46	LEU
18	X	12	ILE
18	X	42	GLN
20	Z	33	TRP
20	Z	62	VAL
1	a	30	VAL
1	a	157	VAL
1	a	202	VAL
1	a	226	GLU
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	275	LEU
1	a	286	THR

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Mol	Chain	Res	Type
1	a	292	THR
1	a	306	VAL
2	b	23	HIS
2	b	223	GLN
2	b	262	THR
2	b	309	LEU
2	b	354	LEU
2	b	362	PHE
2	b	422	ARG
2	b	467	ILE
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	174	LEU
3	c	201	ASN
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	417	VAL
3	c	469	MET
3	c	472	LEU
4	d	43	LEU
4	d	91	LEU
4	d	180	ARG
4	d	201	VAL
4	d	205	LEU
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	323	GLU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	77	GLU
5	e	80	LEU
5	e	84	LYS
7	h	27	THR
7	h	60	VAL
8	i	33	LYS

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Mol	Chain	Res	Type
9	j	7	ARG
11	l	11	GLU
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	114	VAL
15	u	132	LEU
16	v	68	VAL
16	v	116	GLU
17	g	25	ILE
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
20	z	33	TRP
20	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	337	HIS
2	B	26	HIS
2	B	223	GLN
2	B	374	ASN
3	C	44	ASN
3	C	56	HIS
3	C	441	HIS
4	D	117	HIS
4	D	186	GLN
4	D	239	GLN
4	D	250	ASN
4	D	322	ASN
12	M	32	GLN
12	M	33	GLN
13	O	150	ASN
13	O	173	ASN
13	O	257	HIS
15	U	93	ASN
15	U	108	ASN
15	U	111	HIS
1	a	247	ASN
1	a	337	HIS

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Mol	Chain	Res	Type
2	b	26	HIS
2	b	223	GLN
2	b	282	GLN
2	b	331	ASN
3	c	44	ASN
3	c	56	HIS
4	d	117	HIS
4	d	142	ASN
4	d	186	GLN
4	d	239	GLN
4	d	250	ASN
4	d	255	GLN
4	d	301	GLN
4	d	322	ASN
12	m	32	GLN
12	m	33	GLN
13	o	150	ASN
13	o	173	ASN
15	u	111	HIS
20	z	31	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	605	-	69,73,73	1.21	8 (11%)	82,113,113	1.27	6 (7%)
34	HEM	F	101	5,6	50,50,50	1.93	8 (16%)	67,82,82	1.26	5 (7%)
24	PL9	D	405	-	55,55,55	1.14	4 (7%)	68,69,69	1.52	14 (20%)
26	DGD	B	620	-	59,59,67	0.94	1 (1%)	73,73,81	1.35	7 (9%)
30	SQD	A	413	-	49,51,54	0.96	3 (6%)	59,62,65	1.71	10 (16%)
32	LMT	D	408	-	32,32,36	1.15	3 (9%)	43,43,47	1.04	2 (4%)
26	DGD	C	515	-	63,63,67	0.92	2 (3%)	77,77,81	1.41	11 (14%)
30	SQD	d	403	-	41,43,54	1.05	2 (4%)	51,54,65	1.70	11 (21%)
24	PL9	j	101	-	35,35,55	1.06	2 (5%)	44,45,69	1.60	9 (20%)
31	LMG	d	409	-	48,48,55	0.77	0	56,56,63	1.41	5 (8%)
25	BCR	c	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	8 (14%)
32	LMT	B	624	-	36,36,36	1.08	3 (8%)	47,47,47	1.02	2 (4%)
22	CLA	b	616	-	69,73,73	1.17	6 (8%)	82,113,113	1.28	5 (6%)
25	BCR	C	513	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	8 (14%)
22	CLA	c	508	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	b	619	-	69,73,73	1.18	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	C	505	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
22	CLA	A	402	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
27	LHG	a	409	-	38,38,48	0.69	1 (2%)	41,44,54	1.24	3 (7%)
30	SQD	A	414	-	52,54,54	0.95	4 (7%)	62,65,65	1.50	9 (14%)
22	CLA	A	404	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
30	SQD	f	103	-	43,45,54	1.02	2 (4%)	53,56,65	1.62	11 (20%)
27	LHG	c	519	-	36,36,48	0.77	2 (5%)	39,42,54	1.30	4 (10%)
22	CLA	A	406	-	69,73,73	1.19	6 (8%)	82,113,113	1.23	4 (4%)
22	CLA	B	604	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	4 (4%)
31	LMG	C	517	-	45,45,55	0.76	0	53,53,63	1.31	6 (11%)
22	CLA	c	520	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
30	SQD	B	627	-	45,47,54	1.01	3 (6%)	55,58,65	1.76	10 (18%)
30	SQD	a	401	-	52,54,54	0.95	3 (5%)	62,65,65	1.51	10 (16%)
22	CLA	d	406	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	4 (4%)
25	BCR	J	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.61	13 (23%)
25	BCR	b	623	-	41,41,41	1.14	2 (4%)	56,56,56	1.42	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCT	d	404	21	3,3,3	1.11	0	2,3,3	4.40	2 (100%)
25	BCR	c	514	-	41,41,41	1.12	3 (7%)	56,56,56	1.32	8 (14%)
29	OEX	A	412	3,1	0,15,15	-	-	-		
32	LMT	B	629	-	36,36,36	1.12	5 (13%)	47,47,47	1.04	1 (2%)
30	SQD	a	412	-	49,51,54	0.96	3 (6%)	59,62,65	1.70	11 (18%)
27	LHG	C	518	-	36,36,48	0.72	1 (2%)	39,42,54	1.31	4 (10%)
31	LMG	i	102	-	43,43,55	0.83	0	51,51,63	1.25	4 (7%)
32	LMT	M	102	-	36,36,36	1.12	4 (11%)	47,47,47	1.03	2 (4%)
22	CLA	c	506	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	C	502	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	6 (7%)
22	CLA	B	614	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
22	CLA	c	509	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
25	BCR	C	520	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	9 (16%)
22	CLA	B	607	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	C	503	-	69,73,73	1.19	6 (8%)	82,113,113	1.31	5 (6%)
26	DGD	a	408	-	57,57,67	0.96	0	71,71,81	1.39	9 (12%)
22	CLA	b	608	-	69,73,73	1.18	7 (10%)	82,113,113	1.34	7 (8%)
26	DGD	c	516	-	63,63,67	0.93	2 (3%)	77,77,81	1.42	11 (14%)
32	LMT	B	628	-	36,36,36	1.10	4 (11%)	47,47,47	1.02	1 (2%)
22	CLA	B	606	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
25	BCR	y	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	8 (14%)
22	CLA	A	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	5 (6%)
25	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.38	9 (16%)
32	LMT	i	103	-	36,36,36	1.07	4 (11%)	47,47,47	1.03	2 (4%)
22	CLA	C	509	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
22	CLA	b	613	-	69,73,73	1.20	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	C	510	3	69,73,73	1.19	5 (7%)	82,113,113	1.32	5 (6%)
31	LMG	D	409	-	46,46,55	0.79	1 (2%)	54,54,63	1.32	6 (11%)
26	DGD	B	626	-	53,53,67	1.05	3 (5%)	67,67,81	1.32	7 (10%)
26	DGD	D	407	-	64,64,67	0.97	3 (4%)	78,78,81	1.33	8 (10%)
31	LMG	b	627	-	42,42,55	0.86	1 (2%)	50,50,63	1.24	4 (8%)
24	PL9	J	101	-	35,35,55	1.02	3 (8%)	44,45,69	1.64	9 (20%)
32	LMT	b	604	-	36,36,36	1.11	5 (13%)	47,47,47	1.05	1 (2%)
22	CLA	b	618	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
22	CLA	B	613	-	69,73,73	1.17	6 (8%)	82,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	602	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
25	BCR	f	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	7 (12%)
22	CLA	c	507	-	69,73,73	1.19	7 (10%)	82,113,113	1.32	7 (8%)
22	CLA	D	404	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	C	501	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
22	CLA	C	504	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	7 (8%)
22	CLA	B	605	-	69,73,73	1.17	7 (10%)	82,113,113	1.33	5 (6%)
22	CLA	c	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
25	BCR	b	621	-	41,41,41	1.14	3 (7%)	56,56,56	1.24	7 (12%)
22	CLA	b	609	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	4 (4%)
22	CLA	b	614	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	b	607	-	69,73,73	1.19	6 (8%)	82,113,113	1.21	7 (8%)
26	DGD	b	601	-	53,53,67	1.04	4 (7%)	67,67,81	1.33	7 (10%)
22	CLA	c	505	-	69,73,73	1.19	7 (10%)	82,113,113	1.29	5 (6%)
23	PHO	d	401	-	58,69,69	2.12	11 (18%)	55,99,99	1.43	6 (10%)
22	CLA	b	620	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
31	LMG	d	412	-	46,46,55	0.80	1 (2%)	54,54,63	1.30	5 (9%)
22	CLA	a	406	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
26	DGD	d	410	-	64,64,67	0.95	2 (3%)	78,78,81	1.36	9 (11%)
31	LMG	b	626	-	49,49,55	0.80	1 (2%)	57,57,63	1.33	7 (12%)
22	CLA	b	610	-	69,73,73	1.17	5 (7%)	82,113,113	1.29	5 (6%)
22	CLA	b	606	-	69,73,73	1.19	8 (11%)	82,113,113	1.23	4 (4%)
25	BCR	b	624	-	41,41,41	1.15	2 (4%)	56,56,56	1.34	9 (16%)
25	BCR	j	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.55	13 (23%)
25	BCR	B	616	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	8 (14%)
26	DGD	A	409	-	57,57,67	0.96	0	71,71,81	1.43	8 (11%)
31	LMG	B	621	-	49,49,55	0.78	1 (2%)	57,57,63	1.32	7 (12%)
31	LMG	a	402	-	42,42,55	0.87	2 (4%)	50,50,63	1.23	4 (8%)
22	CLA	b	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.22	5 (6%)
32	LMT	b	603	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	1 (2%)
34	HEM	v	201	16	50,50,50	2.01	11 (22%)	67,82,82	1.26	3 (4%)
30	SQD	B	622	-	41,43,54	1.05	2 (4%)	51,54,65	1.74	11 (21%)
26	DGD	C	516	-	67,67,67	0.87	0	81,81,81	1.42	9 (11%)
22	CLA	a	404	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
25	BCR	K	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	510	3	69,73,73	1.21	5 (7%)	82,113,113	1.27	6 (7%)
25	BCR	b	622	-	41,41,41	1.10	2 (4%)	56,56,56	1.37	10 (17%)
31	LMG	B	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.34	7 (12%)
22	CLA	B	609	-	69,73,73	1.19	7 (10%)	82,113,113	1.28	5 (6%)
24	PL9	d	407	-	55,55,55	1.08	5 (9%)	68,69,69	1.52	12 (17%)
26	DGD	c	515	-	54,54,67	0.96	1 (1%)	68,68,81	1.29	5 (7%)
34	HEM	f	101	5,6	50,50,50	1.92	8 (16%)	67,82,82	1.32	5 (7%)
24	PL9	A	407	-	45,45,55	1.00	4 (8%)	56,57,69	1.54	10 (17%)
22	CLA	a	405	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
25	BCR	B	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.43	10 (17%)
32	LMT	d	411	-	32,32,36	1.15	5 (15%)	43,43,47	1.03	2 (4%)
22	CLA	C	506	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
22	CLA	B	608	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	5 (6%)
25	BCR	c	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.37	10 (17%)
32	LMT	b	628	-	36,36,36	1.10	4 (11%)	47,47,47	1.01	1 (2%)
22	CLA	b	612	-	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	H	101	-	69,73,73	1.20	6 (8%)	82,113,113	1.24	5 (6%)
31	LMG	I	101	-	43,43,55	0.84	1 (2%)	51,51,63	1.26	4 (7%)
26	DGD	c	517	-	67,67,67	0.89	0	81,81,81	1.39	8 (9%)
25	BCR	F	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	7 (12%)
25	BCR	H	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	6 (10%)
31	LMG	e	101	-	44,44,55	0.76	0	52,52,63	1.29	4 (7%)
22	CLA	B	615	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	4 (4%)
22	CLA	c	504	-	69,73,73	1.18	8 (11%)	82,113,113	1.31	7 (8%)
22	CLA	d	405	-	69,73,73	1.18	7 (10%)	82,113,113	1.22	5 (6%)
32	LMT	M	103	-	36,36,36	1.11	4 (11%)	47,47,47	1.01	2 (4%)
22	CLA	C	508	-	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
27	LHG	A	410	-	38,38,48	0.71	1 (2%)	41,44,54	1.23	3 (7%)
30	SQD	b	602	-	45,47,54	1.02	3 (6%)	55,58,65	1.78	10 (18%)
31	LMG	L	101	-	51,51,55	0.76	0	59,59,63	1.35	5 (8%)
32	LMT	B	623	-	36,36,36	1.11	4 (11%)	47,47,47	1.02	1 (2%)
26	DGD	b	625	-	59,59,67	0.92	1 (1%)	73,73,81	1.37	8 (10%)
23	PHO	D	401	-	58,69,69	2.18	9 (15%)	55,99,99	1.41	5 (9%)
29	OEX	a	411	3,1	0,15,15	-	-	-	-	-
31	LMG	l	101	-	51,51,55	0.74	1 (1%)	59,59,63	1.33	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	601	-	69,73,73	1.21	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.32	6 (7%)
22	CLA	C	512	-	69,73,73	1.19	6 (8%)	82,113,113	1.30	6 (7%)
24	PL9	a	407	-	45,45,55	1.03	3 (6%)	56,57,69	1.56	11 (19%)
25	BCR	x	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	4 (7%)
22	CLA	b	617	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	7 (8%)
22	CLA	C	507	-	69,73,73	1.19	6 (8%)	82,113,113	1.32	7 (8%)
22	CLA	B	610	-	69,73,73	1.24	6 (8%)	82,113,113	1.39	8 (9%)
31	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.30	6 (11%)
31	LMG	m	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.24	4 (8%)
22	CLA	c	503	-	69,73,73	1.20	7 (10%)	82,113,113	1.31	5 (6%)
31	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.30	4 (7%)
33	BCT	D	402	21	3,3,3	1.10	0	2,3,3	4.37	2 (100%)
22	CLA	C	519	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
25	BCR	i	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)
31	LMG	d	408	-	49,49,55	0.77	1 (2%)	57,57,63	1.34	7 (12%)
30	SQD	F	103	-	43,45,54	1.04	2 (4%)	53,56,65	1.62	11 (20%)
22	CLA	c	512	-	69,73,73	1.20	6 (8%)	82,113,113	1.26	4 (4%)
32	LMT	I	102	-	36,36,36	1.09	4 (11%)	47,47,47	1.06	2 (4%)
31	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.29	5 (8%)
22	CLA	B	612	-	69,73,73	1.17	6 (8%)	82,113,113	1.26	8 (9%)
34	HEM	V	201	16	50,50,50	1.94	9 (18%)	67,82,82	1.16	1 (1%)
25	BCR	g	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	8 (14%)
32	LMT	b	629	-	36,36,36	1.08	3 (8%)	47,47,47	1.04	2 (4%)
22	CLA	b	615	-	69,73,73	1.24	6 (8%)	82,113,113	1.36	7 (8%)
31	LMG	C	521	-	48,48,55	0.76	0	56,56,63	1.31	5 (8%)
31	LMG	D	406	-	48,48,55	0.76	0	56,56,63	1.39	4 (7%)
22	CLA	c	502	-	69,73,73	1.20	9 (13%)	82,113,113	1.25	4 (4%)
22	CLA	D	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.21	5 (6%)
22	CLA	a	403	-	69,73,73	1.19	7 (10%)	82,113,113	1.29	5 (6%)
25	BCR	A	408	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	7 (12%)
26	DGD	C	514	-	54,54,67	0.97	2 (3%)	68,68,81	1.26	4 (5%)
31	LMG	M	101	-	42,42,55	0.86	0	50,50,63	1.23	4 (8%)
22	CLA	c	501	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	C	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PHO	d	402	-	58,69,69	2.18	9 (15%)	55,99,99	1.41	5 (9%)
25	BCR	B	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)
23	PHO	A	405	-	58,69,69	2.15	9 (15%)	55,99,99	1.39	6 (10%)
22	CLA	B	603	-	69,73,73	1.20	7 (10%)	82,113,113	1.34	7 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	605	-	1/1/15/20	15/39/115/115	-
34	HEM	F	101	5,6	-	2/14/54/54	-
24	PL9	D	405	-	-	12/53/73/73	0/1/1/1
26	DGD	B	620	-	-	18/47/87/95	0/2/2/2
30	SQD	A	413	-	-	19/46/66/69	0/1/1/1
32	LMT	D	408	-	-	2/17/57/61	0/2/2/2
26	DGD	C	515	-	-	20/51/91/95	0/2/2/2
30	SQD	d	403	-	-	17/38/58/69	0/1/1/1
24	PL9	j	101	-	-	8/29/49/73	0/1/1/1
31	LMG	d	409	-	-	21/43/63/70	0/1/1/1
25	BCR	c	521	-	-	4/29/63/63	0/2/2/2
32	LMT	B	624	-	-	3/21/61/61	0/2/2/2
22	CLA	b	616	-	1/1/15/20	10/39/115/115	-
25	BCR	C	513	-	-	4/29/63/63	0/2/2/2
22	CLA	c	508	-	1/1/15/20	18/39/115/115	-
22	CLA	b	619	-	1/1/15/20	10/39/115/115	-
22	CLA	C	505	-	1/1/15/20	16/39/115/115	-
22	CLA	A	402	-	1/1/15/20	7/39/115/115	-
27	LHG	a	409	-	-	10/43/43/53	-
30	SQD	A	414	-	-	14/49/69/69	0/1/1/1
22	CLA	A	404	-	1/1/15/20	10/39/115/115	-
30	SQD	f	103	-	-	10/40/60/69	0/1/1/1
27	LHG	c	519	-	-	16/41/41/53	-
22	CLA	A	406	-	1/1/15/20	8/39/115/115	-
22	CLA	B	604	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	C	517	-	-	22/40/60/70	0/1/1/1
22	CLA	c	520	-	1/1/15/20	12/39/115/115	-
30	SQD	B	627	-	-	15/42/62/69	0/1/1/1
30	SQD	a	401	-	-	14/49/69/69	0/1/1/1
22	CLA	d	406	-	-	8/39/115/115	-
25	BCR	J	102	-	-	6/29/63/63	0/2/2/2
25	BCR	b	623	-	-	0/29/63/63	0/2/2/2
25	BCR	c	514	-	-	4/29/63/63	0/2/2/2
32	LMT	B	629	-	-	4/21/61/61	0/2/2/2
30	SQD	a	412	-	-	20/46/66/69	0/1/1/1
27	LHG	C	518	-	-	14/41/41/53	-
31	LMG	i	102	-	-	18/38/58/70	0/1/1/1
32	LMT	M	102	-	-	0/21/61/61	0/2/2/2
22	CLA	c	506	-	1/1/15/20	10/39/115/115	-
22	CLA	C	502	-	1/1/15/20	10/39/115/115	-
22	CLA	B	614	-	1/1/15/20	10/39/115/115	-
22	CLA	c	509	-	1/1/15/20	15/39/115/115	-
25	BCR	C	520	-	-	3/29/63/63	0/2/2/2
22	CLA	B	607	-	1/1/15/20	12/39/115/115	-
22	CLA	C	503	-	1/1/15/20	12/39/115/115	-
26	DGD	a	408	-	-	14/45/85/95	0/2/2/2
22	CLA	b	608	-	1/1/15/20	5/39/115/115	-
26	DGD	c	516	-	-	20/51/91/95	0/2/2/2
32	LMT	B	628	-	-	2/21/61/61	0/2/2/2
22	CLA	B	606	-	1/1/15/20	10/39/115/115	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	A	403	-	1/1/15/20	13/39/115/115	-
25	BCR	B	617	-	-	7/29/63/63	0/2/2/2
32	LMT	i	103	-	-	4/21/61/61	0/2/2/2
22	CLA	C	509	-	1/1/15/20	12/39/115/115	-
22	CLA	b	613	-	1/1/15/20	10/39/115/115	-
22	CLA	C	510	3	1/1/15/20	15/39/115/115	-
31	LMG	D	409	-	-	15/41/61/70	0/1/1/1
26	DGD	B	626	-	-	18/41/81/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DGD	D	407	-	-	36/52/92/95	0/2/2/2
31	LMG	b	627	-	-	15/37/57/70	0/1/1/1
24	PL9	J	101	-	-	9/29/49/73	0/1/1/1
32	LMT	b	604	-	-	5/21/61/61	0/2/2/2
22	CLA	b	618	-	1/1/15/20	13/39/115/115	-
22	CLA	B	613	-	1/1/15/20	14/39/115/115	-
22	CLA	B	602	-	1/1/15/20	13/39/115/115	-
25	BCR	f	102	-	-	4/29/63/63	0/2/2/2
22	CLA	c	507	-	1/1/15/20	12/39/115/115	-
22	CLA	D	404	-	-	6/39/115/115	-
22	CLA	C	501	-	1/1/15/20	15/39/115/115	-
22	CLA	C	504	-	1/1/15/20	17/39/115/115	-
22	CLA	B	605	-	1/1/15/20	18/39/115/115	-
22	CLA	c	511	-	1/1/15/20	17/39/115/115	-
25	BCR	b	621	-	-	2/29/63/63	0/2/2/2
22	CLA	b	609	-	1/1/15/20	15/39/115/115	-
22	CLA	b	614	-	1/1/15/20	18/39/115/115	-
22	CLA	b	607	-	1/1/15/20	13/39/115/115	-
26	DGD	b	601	-	-	18/41/81/95	0/2/2/2
22	CLA	c	505	-	1/1/15/20	15/39/115/115	-
23	PHO	d	401	-	-	8/37/103/103	0/5/6/6
22	CLA	b	620	-	1/1/15/20	19/39/115/115	-
31	LMG	d	412	-	-	15/41/61/70	0/1/1/1
22	CLA	a	406	-	1/1/15/20	9/39/115/115	-
26	DGD	d	410	-	-	36/52/92/95	0/2/2/2
31	LMG	b	626	-	-	14/44/64/70	0/1/1/1
22	CLA	b	610	-	1/1/15/20	14/39/115/115	-
22	CLA	b	606	-	1/1/15/20	14/39/115/115	-
25	BCR	b	624	-	-	5/29/63/63	0/2/2/2
25	BCR	j	102	-	-	7/29/63/63	0/2/2/2
25	BCR	B	616	-	-	2/29/63/63	0/2/2/2
26	DGD	A	409	-	-	16/45/85/95	0/2/2/2
31	LMG	B	621	-	-	15/44/64/70	0/1/1/1
31	LMG	a	402	-	-	16/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	611	-	1/1/15/20	10/39/115/115	-
32	LMT	b	603	-	-	3/21/61/61	0/2/2/2
34	HEM	v	201	16	-	5/14/54/54	-
30	SQD	B	622	-	-	15/38/58/69	0/1/1/1
26	DGD	C	516	-	-	21/55/95/95	0/2/2/2
22	CLA	a	404	-	1/1/15/20	14/39/115/115	-
25	BCR	K	101	-	-	5/29/63/63	0/2/2/2
22	CLA	c	510	3	1/1/15/20	13/39/115/115	-
25	BCR	b	622	-	-	6/29/63/63	0/2/2/2
31	LMG	B	625	-	-	24/44/64/70	0/1/1/1
22	CLA	B	609	-	1/1/15/20	19/39/115/115	-
24	PL9	d	407	-	-	11/53/73/73	0/1/1/1
26	DGD	c	515	-	-	19/42/82/95	0/2/2/2
34	HEM	f	101	5,6	-	2/14/54/54	-
24	PL9	A	407	-	-	19/41/61/73	0/1/1/1
22	CLA	a	405	-	1/1/15/20	8/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	LMT	d	411	-	-	1/17/57/61	0/2/2/2
22	CLA	C	506	-	1/1/15/20	11/39/115/115	-
22	CLA	B	608	-	1/1/15/20	10/39/115/115	-
25	BCR	c	513	-	-	5/29/63/63	0/2/2/2
32	LMT	b	628	-	-	3/21/61/61	0/2/2/2
22	CLA	b	612	-	1/1/15/20	13/39/115/115	-
22	CLA	H	101	-	1/1/15/20	15/39/115/115	-
31	LMG	I	101	-	-	20/38/58/70	0/1/1/1
26	DGD	c	517	-	-	21/55/95/95	0/2/2/2
25	BCR	F	102	-	-	4/29/63/63	0/2/2/2
25	BCR	H	102	-	-	7/29/63/63	0/2/2/2
31	LMG	e	101	-	-	20/39/59/70	0/1/1/1
22	CLA	B	615	-	1/1/15/20	19/39/115/115	-
22	CLA	c	504	-	1/1/15/20	20/39/115/115	-
22	CLA	d	405	-	1/1/15/20	12/39/115/115	-
32	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	C	508	-	1/1/15/20	18/39/115/115	-
27	LHG	A	410	-	-	11/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	b	602	-	-	14/42/62/69	0/1/1/1
31	LMG	L	101	-	-	27/46/66/70	0/1/1/1
32	LMT	B	623	-	-	2/21/61/61	0/2/2/2
26	DGD	b	625	-	-	18/47/87/95	0/2/2/2
23	PHO	D	401	-	-	9/37/103/103	0/5/6/6
31	LMG	l	101	-	-	27/46/66/70	0/1/1/1
22	CLA	B	601	-	1/1/15/20	15/39/115/115	-
22	CLA	B	611	-	1/1/15/20	9/39/115/115	-
22	CLA	C	512	-	1/1/15/20	16/39/115/115	-
24	PL9	a	407	-	-	18/41/61/73	0/1/1/1
25	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	b	617	-	1/1/15/20	15/39/115/115	-
22	CLA	C	507	-	1/1/15/20	13/39/115/115	-
22	CLA	B	610	-	1/1/15/20	11/39/115/115	-
31	LMG	c	518	-	-	22/40/60/70	0/1/1/1
31	LMG	m	101	-	-	17/37/57/70	0/1/1/1
22	CLA	c	503	-	1/1/15/20	13/39/115/115	-
31	LMG	E	101	-	-	16/39/59/70	0/1/1/1
22	CLA	C	519	-	1/1/15/20	13/39/115/115	-
25	BCR	i	101	-	-	4/29/63/63	0/2/2/2
31	LMG	d	408	-	-	25/44/64/70	0/1/1/1
30	SQD	F	103	-	-	11/40/60/69	0/1/1/1
22	CLA	c	512	-	1/1/15/20	16/39/115/115	-
32	LMT	I	102	-	-	3/21/61/61	0/2/2/2
31	LMG	c	522	-	-	19/43/63/70	0/1/1/1
22	CLA	B	612	-	1/1/15/20	15/39/115/115	-
34	HEM	V	201	16	-	5/14/54/54	-
25	BCR	g	101	-	-	5/29/63/63	0/2/2/2
32	LMT	b	629	-	-	3/21/61/61	0/2/2/2
22	CLA	b	615	-	1/1/15/20	13/39/115/115	-
31	LMG	C	521	-	-	20/43/63/70	0/1/1/1
31	LMG	D	406	-	-	22/43/63/70	0/1/1/1
22	CLA	c	502	-	1/1/15/20	10/39/115/115	-
22	CLA	D	403	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	403	-	1/1/15/20	8/39/115/115	-
25	BCR	A	408	-	-	4/29/63/63	0/2/2/2
26	DGD	C	514	-	-	18/42/82/95	0/2/2/2
31	LMG	M	101	-	-	17/37/57/70	0/1/1/1
22	CLA	c	501	-	1/1/15/20	14/39/115/115	-
22	CLA	C	511	-	1/1/15/20	17/39/115/115	-
23	PHO	d	402	-	-	13/37/103/103	0/5/6/6
25	BCR	B	619	-	-	4/29/63/63	0/2/2/2
23	PHO	A	405	-	-	10/37/103/103	0/5/6/6
22	CLA	B	603	-	1/1/15/20	10/39/115/115	-

All (750) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	401	PHO	C1B-C2B	9.54	1.50	1.39
23	A	405	PHO	C1B-C2B	9.52	1.50	1.39
23	d	402	PHO	C1B-C2B	9.50	1.49	1.39
23	d	401	PHO	C1B-C2B	9.32	1.49	1.39
23	D	401	PHO	C3B-C4B	8.81	1.50	1.41
23	d	402	PHO	C3B-C4B	8.77	1.50	1.41
23	A	405	PHO	C3B-C4B	8.35	1.49	1.41
23	d	401	PHO	C3B-C4B	8.33	1.49	1.41
34	v	201	HEM	C3D-C2D	8.14	1.54	1.36
34	V	201	HEM	C3D-C2D	8.12	1.54	1.36
34	F	101	HEM	C3D-C2D	7.91	1.53	1.36
34	f	101	HEM	C3D-C2D	7.78	1.53	1.36
34	F	101	HEM	FE-ND	5.33	2.11	1.94
34	v	201	HEM	FE-ND	5.24	2.11	1.94
34	V	201	HEM	FE-ND	5.14	2.10	1.94
34	f	101	HEM	FE-ND	5.07	2.10	1.94
34	v	201	HEM	FE-NB	4.68	2.09	1.94
23	d	402	PHO	C1D-C2D	4.38	1.44	1.39
34	f	101	HEM	FE-NB	4.22	2.07	1.94
34	V	201	HEM	FE-NB	4.21	2.07	1.94
23	A	405	PHO	C1D-C2D	4.12	1.44	1.39
34	v	201	HEM	FE-NA	4.09	2.08	1.95
23	D	401	PHO	C1D-C2D	4.08	1.44	1.39
25	F	102	BCR	C1-C6	-3.88	1.48	1.53
22	c	510	CLA	C1D-ND	3.87	1.42	1.37
25	H	102	BCR	C1-C6	-3.87	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	101	HEM	FE-NA	3.85	2.07	1.95
22	B	608	CLA	C1D-ND	3.84	1.42	1.37
23	D	401	PHO	C4D-CHA	3.83	1.45	1.39
22	b	609	CLA	C1D-ND	3.82	1.42	1.37
25	x	101	BCR	C1-C6	-3.82	1.48	1.53
23	A	405	PHO	C4D-CHA	3.82	1.45	1.39
22	c	501	CLA	C1D-ND	3.81	1.42	1.37
25	f	102	BCR	C1-C6	-3.80	1.48	1.53
22	C	510	CLA	C1D-ND	3.80	1.42	1.37
22	C	501	CLA	C1D-ND	3.79	1.42	1.37
23	d	402	PHO	C4D-CHA	3.79	1.45	1.39
22	a	406	CLA	C1D-ND	3.78	1.42	1.37
22	d	406	CLA	C1D-ND	3.78	1.42	1.37
23	d	401	PHO	C1D-C2D	3.77	1.43	1.39
22	B	601	CLA	C1D-ND	3.77	1.42	1.37
22	C	512	CLA	C1D-ND	3.76	1.42	1.37
22	C	503	CLA	C1D-ND	3.76	1.42	1.37
22	c	503	CLA	C1D-ND	3.76	1.42	1.37
23	d	401	PHO	C4D-CHA	3.75	1.45	1.39
22	H	101	CLA	C1D-ND	3.74	1.42	1.37
22	b	606	CLA	C1D-ND	3.74	1.42	1.37
22	b	605	CLA	C1D-ND	3.74	1.42	1.37
22	b	613	CLA	C1D-ND	3.73	1.42	1.37
22	c	506	CLA	C1D-ND	3.73	1.42	1.37
22	c	512	CLA	C1D-ND	3.72	1.42	1.37
22	A	406	CLA	C1D-ND	3.71	1.42	1.37
22	B	604	CLA	C1D-ND	3.70	1.42	1.37
22	C	506	CLA	C1D-ND	3.69	1.42	1.37
34	F	101	HEM	FE-NB	3.69	2.06	1.94
25	B	616	BCR	C1-C6	-3.69	1.49	1.53
25	g	101	BCR	C30-C25	-3.68	1.49	1.53
22	A	403	CLA	C1D-ND	3.68	1.42	1.37
22	D	404	CLA	C1D-ND	3.67	1.42	1.37
22	B	603	CLA	C1D-ND	3.67	1.42	1.37
22	B	602	CLA	C1D-ND	3.66	1.42	1.37
22	c	508	CLA	C1D-ND	3.66	1.42	1.37
22	C	511	CLA	C1D-ND	3.65	1.42	1.37
22	b	607	CLA	C1D-ND	3.65	1.42	1.37
22	c	505	CLA	C1D-ND	3.65	1.42	1.37
22	b	618	CLA	C1D-ND	3.65	1.42	1.37
22	B	613	CLA	C1D-ND	3.64	1.42	1.37
22	B	607	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	101	BCR	C1-C6	-3.63	1.49	1.53
22	b	610	CLA	C1D-ND	3.63	1.42	1.37
22	c	502	CLA	C1D-ND	3.63	1.42	1.37
22	c	504	CLA	C1D-ND	3.63	1.42	1.37
25	b	621	BCR	C1-C6	-3.63	1.49	1.53
22	b	619	CLA	C1D-ND	3.62	1.42	1.37
22	C	519	CLA	C1D-ND	3.62	1.42	1.37
22	b	608	CLA	C1D-ND	3.61	1.42	1.37
22	c	511	CLA	C1D-ND	3.61	1.42	1.37
22	b	612	CLA	C1D-ND	3.60	1.42	1.37
22	b	614	CLA	C1D-ND	3.60	1.42	1.37
22	C	504	CLA	C1D-ND	3.59	1.42	1.37
22	c	520	CLA	C1D-ND	3.59	1.42	1.37
25	C	513	BCR	C1-C6	-3.59	1.49	1.53
22	C	502	CLA	C1D-ND	3.58	1.42	1.37
22	B	614	CLA	C1D-ND	3.58	1.42	1.37
22	B	605	CLA	C1D-ND	3.58	1.42	1.37
22	a	405	CLA	C1D-ND	3.58	1.42	1.37
22	C	505	CLA	C1D-ND	3.57	1.42	1.37
22	B	612	CLA	C1D-ND	3.57	1.42	1.37
25	c	514	BCR	C1-C6	-3.56	1.49	1.53
22	b	617	CLA	C1D-ND	3.56	1.42	1.37
22	c	507	CLA	C1D-ND	3.56	1.42	1.37
25	b	623	BCR	C30-C25	-3.55	1.49	1.53
25	J	102	BCR	C30-C25	-3.55	1.49	1.53
25	y	101	BCR	C30-C25	-3.55	1.49	1.53
22	a	404	CLA	C1D-ND	3.55	1.42	1.37
22	C	507	CLA	C1D-ND	3.54	1.42	1.37
22	b	611	CLA	C1D-ND	3.54	1.42	1.37
25	g	101	BCR	C1-C6	-3.54	1.49	1.53
22	B	615	CLA	C1D-ND	3.53	1.42	1.37
22	d	405	CLA	C1D-ND	3.53	1.42	1.37
22	a	403	CLA	C1D-ND	3.53	1.42	1.37
22	B	606	CLA	C1D-ND	3.52	1.42	1.37
22	B	609	CLA	C1D-ND	3.52	1.42	1.37
25	b	622	BCR	C1-C6	-3.52	1.49	1.53
22	D	403	CLA	C1D-ND	3.51	1.42	1.37
22	A	404	CLA	C1D-ND	3.51	1.42	1.37
25	B	618	BCR	C30-C25	-3.50	1.49	1.53
22	b	620	CLA	C1D-ND	3.49	1.42	1.37
25	j	102	BCR	C30-C25	-3.49	1.49	1.53
22	A	402	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	C1D-ND	3.49	1.42	1.37
25	c	513	BCR	C1-C6	-3.48	1.49	1.53
22	c	509	CLA	C1D-ND	3.48	1.42	1.37
22	b	615	CLA	C1D-ND	3.48	1.42	1.37
25	b	624	BCR	C30-C25	-3.48	1.49	1.53
25	C	520	BCR	C30-C25	-3.47	1.49	1.53
25	K	101	BCR	C1-C6	-3.47	1.49	1.53
25	B	619	BCR	C30-C25	-3.42	1.49	1.53
25	F	102	BCR	C30-C25	-3.42	1.49	1.53
22	C	509	CLA	C1D-ND	3.41	1.42	1.37
22	B	610	CLA	C1D-ND	3.40	1.42	1.37
34	f	101	HEM	FE-NA	3.40	2.06	1.95
22	c	509	CLA	C4B-NB	3.40	1.42	1.37
25	B	616	BCR	C30-C25	-3.38	1.49	1.53
25	i	101	BCR	C1-C6	-3.37	1.49	1.53
25	A	408	BCR	C30-C25	-3.35	1.49	1.53
25	b	624	BCR	C1-C6	-3.35	1.49	1.53
25	c	521	BCR	C30-C25	-3.34	1.49	1.53
25	i	101	BCR	C30-C25	-3.33	1.49	1.53
25	B	617	BCR	C1-C6	-3.32	1.49	1.53
25	f	102	BCR	C30-C25	-3.32	1.49	1.53
22	A	402	CLA	C4B-NB	3.30	1.42	1.37
22	a	403	CLA	C4B-NB	3.30	1.42	1.37
25	B	619	BCR	C1-C6	-3.30	1.49	1.53
22	B	601	CLA	C4B-NB	3.29	1.42	1.37
30	b	602	SQD	O48-C23	3.29	1.43	1.33
25	B	618	BCR	C1-C6	-3.29	1.49	1.53
25	b	621	BCR	C30-C25	-3.29	1.49	1.53
22	b	605	CLA	C4B-NB	3.29	1.42	1.37
25	A	408	BCR	C1-C6	-3.28	1.49	1.53
25	b	623	BCR	C1-C6	-3.28	1.49	1.53
22	c	508	CLA	C4B-NB	3.28	1.42	1.37
22	C	508	CLA	C4B-NB	3.28	1.42	1.37
22	b	616	CLA	C1D-ND	3.26	1.42	1.37
22	B	614	CLA	C4B-NB	3.26	1.42	1.37
22	c	512	CLA	C4B-NB	3.26	1.42	1.37
25	C	513	BCR	C30-C25	-3.25	1.49	1.53
34	f	101	HEM	FE-NC	3.24	2.05	1.95
22	b	620	CLA	C4B-NB	3.24	1.42	1.37
22	C	509	CLA	C4B-NB	3.24	1.42	1.37
22	b	615	CLA	CMB-C2B	-3.23	1.44	1.50
22	B	610	CLA	CMB-C2B	-3.23	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	FE-NA	3.22	2.05	1.95
22	B	615	CLA	C4B-NB	3.22	1.42	1.37
22	c	511	CLA	C4B-NB	3.21	1.42	1.37
30	B	622	SQD	O48-C23	3.21	1.42	1.33
25	K	101	BCR	C30-C25	-3.21	1.49	1.53
22	c	505	CLA	C4B-NB	3.20	1.42	1.37
30	B	627	SQD	O48-C23	3.20	1.42	1.33
22	c	503	CLA	C4B-NB	3.20	1.42	1.37
22	d	406	CLA	C4B-NB	3.20	1.42	1.37
22	C	507	CLA	C4B-NB	3.20	1.42	1.37
22	B	610	CLA	C4B-NB	3.19	1.42	1.37
25	C	520	BCR	C1-C6	-3.19	1.49	1.53
22	c	510	CLA	C4B-NB	3.19	1.42	1.37
22	c	507	CLA	C4B-NB	3.18	1.42	1.37
22	b	615	CLA	C4B-NB	3.18	1.42	1.37
22	B	608	CLA	C4B-NB	3.17	1.42	1.37
30	a	401	SQD	O48-C23	3.16	1.42	1.33
22	c	520	CLA	C4B-NB	3.16	1.42	1.37
22	b	616	CLA	C4B-NB	3.16	1.42	1.37
24	D	405	PL9	C7-C3	-3.15	1.47	1.51
22	C	511	CLA	C4B-NB	3.14	1.42	1.37
22	H	101	CLA	C4B-NB	3.14	1.42	1.37
30	F	103	SQD	O48-C23	3.14	1.42	1.33
30	A	414	SQD	O48-C23	3.14	1.42	1.33
22	A	403	CLA	C4B-NB	3.13	1.42	1.37
22	B	604	CLA	C4B-NB	3.13	1.42	1.37
22	a	405	CLA	C4B-NB	3.13	1.42	1.37
22	A	406	CLA	C4B-NB	3.13	1.42	1.37
34	v	201	HEM	FE-NC	3.13	2.05	1.95
30	f	103	SQD	O48-C23	3.12	1.42	1.33
22	c	501	CLA	C4B-NB	3.12	1.42	1.37
30	a	412	SQD	O48-C23	3.12	1.42	1.33
22	b	611	CLA	C4B-NB	3.12	1.42	1.37
22	B	611	CLA	C1D-ND	3.12	1.42	1.37
22	b	619	CLA	C4B-NB	3.11	1.42	1.37
34	f	101	HEM	CAC-C3C	3.11	1.55	1.47
22	C	505	CLA	C4B-NB	3.11	1.41	1.37
22	b	613	CLA	C4B-NB	3.10	1.41	1.37
25	c	521	BCR	C1-C6	-3.10	1.49	1.53
25	c	514	BCR	C30-C25	-3.10	1.49	1.53
25	H	102	BCR	C30-C25	-3.10	1.49	1.53
24	D	405	PL9	C3-C4	-3.10	1.44	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	C4B-NB	3.09	1.41	1.37
34	V	201	HEM	CAB-C3B	3.09	1.55	1.47
22	d	405	CLA	C4B-NB	3.09	1.41	1.37
22	b	610	CLA	C4B-NB	3.08	1.41	1.37
30	d	403	SQD	O48-C23	3.08	1.42	1.33
25	x	101	BCR	C30-C25	-3.08	1.49	1.53
22	B	611	CLA	C4B-NB	3.08	1.41	1.37
22	C	512	CLA	C4B-NB	3.07	1.41	1.37
34	v	201	HEM	CAB-C3B	3.07	1.55	1.47
25	c	513	BCR	C30-C25	-3.06	1.49	1.53
22	b	612	CLA	C4B-NB	3.06	1.41	1.37
22	C	503	CLA	C4B-NB	3.06	1.41	1.37
22	C	510	CLA	C4B-NB	3.06	1.41	1.37
30	A	413	SQD	O48-C23	3.05	1.42	1.33
22	C	501	CLA	C4B-NB	3.05	1.41	1.37
22	b	617	CLA	C4B-NB	3.05	1.41	1.37
34	F	101	HEM	CAC-C3C	3.04	1.55	1.47
22	B	603	CLA	C4B-NB	3.04	1.41	1.37
22	c	504	CLA	C4B-NB	3.03	1.41	1.37
22	b	609	CLA	C4B-NB	3.03	1.41	1.37
22	b	614	CLA	C4B-NB	3.03	1.41	1.37
34	V	201	HEM	CAC-C3C	3.02	1.55	1.47
34	v	201	HEM	CAC-C3C	3.02	1.55	1.47
22	D	403	CLA	C4B-NB	3.01	1.41	1.37
22	C	502	CLA	C4B-NB	3.00	1.41	1.37
22	c	502	CLA	C4B-NB	2.99	1.41	1.37
22	a	404	CLA	C4B-NB	2.99	1.41	1.37
22	a	406	CLA	C4B-NB	2.99	1.41	1.37
22	b	608	CLA	C4B-NB	2.98	1.41	1.37
22	B	606	CLA	C4B-NB	2.98	1.41	1.37
22	c	506	CLA	C4B-NB	2.97	1.41	1.37
22	b	620	CLA	C1B-C2B	2.96	1.50	1.43
22	A	404	CLA	C4B-NB	2.95	1.41	1.37
22	B	609	CLA	C4B-NB	2.95	1.41	1.37
22	C	506	CLA	C4B-NB	2.95	1.41	1.37
22	B	605	CLA	C4B-NB	2.95	1.41	1.37
22	d	405	CLA	C1B-C2B	2.94	1.50	1.43
30	B	622	SQD	O47-C7	2.94	1.42	1.34
22	c	501	CLA	C1B-C2B	2.94	1.50	1.43
22	b	618	CLA	C4B-NB	2.94	1.41	1.37
25	B	617	BCR	C30-C25	-2.94	1.50	1.53
22	C	519	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	C4B-NB	2.93	1.41	1.37
26	C	514	DGD	O2G-C2G	-2.91	1.39	1.46
25	b	622	BCR	C30-C25	-2.91	1.50	1.53
30	d	403	SQD	O47-C7	2.91	1.42	1.34
22	C	501	CLA	C1B-C2B	2.91	1.50	1.43
34	f	101	HEM	CAB-C3B	2.91	1.55	1.47
22	B	612	CLA	C4B-NB	2.90	1.41	1.37
22	C	504	CLA	C4B-NB	2.90	1.41	1.37
25	j	102	BCR	C1-C6	-2.90	1.50	1.53
30	a	412	SQD	O47-C7	2.89	1.42	1.34
30	A	414	SQD	O47-C7	2.89	1.42	1.34
30	a	401	SQD	O47-C7	2.89	1.42	1.34
22	B	615	CLA	C1B-C2B	2.89	1.49	1.43
22	B	614	CLA	C1B-C2B	2.88	1.49	1.43
22	c	504	CLA	C1B-C2B	2.88	1.49	1.43
25	J	102	BCR	C1-C6	-2.88	1.50	1.53
22	b	616	CLA	C1B-C2B	2.88	1.49	1.43
22	c	511	CLA	C1B-C2B	2.88	1.49	1.43
22	b	606	CLA	C4B-NB	2.88	1.41	1.37
22	b	610	CLA	C1B-C2B	2.87	1.49	1.43
30	A	413	SQD	O47-C7	2.87	1.42	1.34
30	F	103	SQD	O47-C7	2.87	1.42	1.34
22	B	602	CLA	C4B-NB	2.87	1.41	1.37
30	B	627	SQD	O47-C7	2.87	1.42	1.34
22	c	503	CLA	C1B-C2B	2.86	1.49	1.43
22	B	603	CLA	C1B-C2B	2.86	1.49	1.43
22	b	607	CLA	C4B-NB	2.86	1.41	1.37
22	B	613	CLA	C4B-NB	2.86	1.41	1.37
22	c	510	CLA	C1B-C2B	2.85	1.49	1.43
30	b	602	SQD	O47-C7	2.85	1.42	1.34
22	C	504	CLA	C1B-C2B	2.85	1.49	1.43
22	b	608	CLA	C1B-C2B	2.85	1.49	1.43
24	d	407	PL9	C7-C3	-2.84	1.47	1.51
34	F	101	HEM	CAB-C3B	2.84	1.55	1.47
22	H	101	CLA	C1B-C2B	2.84	1.49	1.43
22	D	403	CLA	C1B-C2B	2.83	1.49	1.43
22	C	511	CLA	C1B-C2B	2.83	1.49	1.43
24	j	101	PL9	C7-C3	-2.83	1.47	1.51
22	B	611	CLA	C1B-C2B	2.82	1.49	1.43
24	d	407	PL9	C3-C4	-2.82	1.45	1.49
26	b	601	DGD	C1E-C2E	2.81	1.60	1.52
22	b	617	CLA	C1B-C2B	2.81	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	619	CLA	C1B-C2B	2.81	1.49	1.43
22	a	405	CLA	C1B-C2B	2.80	1.49	1.43
22	c	512	CLA	C1B-C2B	2.79	1.49	1.43
22	C	510	CLA	C1B-C2B	2.79	1.49	1.43
22	C	503	CLA	C1B-C2B	2.78	1.49	1.43
22	B	604	CLA	C1B-C2B	2.78	1.49	1.43
26	B	626	DGD	C1E-C2E	2.78	1.60	1.52
22	d	406	CLA	C1B-C2B	2.77	1.49	1.43
22	c	502	CLA	C1B-C2B	2.77	1.49	1.43
30	f	103	SQD	O47-C7	2.77	1.42	1.34
22	c	520	CLA	C1B-C2B	2.76	1.49	1.43
22	C	512	CLA	C1B-C2B	2.76	1.49	1.43
22	b	605	CLA	C1B-C2B	2.76	1.49	1.43
22	B	613	CLA	C1B-C2B	2.74	1.49	1.43
22	A	404	CLA	C1B-C2B	2.74	1.49	1.43
22	C	502	CLA	C1B-C2B	2.74	1.49	1.43
22	B	601	CLA	C1B-C2B	2.74	1.49	1.43
22	B	608	CLA	C1B-C2B	2.74	1.49	1.43
22	C	506	CLA	C1B-C2B	2.73	1.49	1.43
22	b	618	CLA	C1B-C2B	2.73	1.49	1.43
22	b	607	CLA	C1B-C2B	2.73	1.49	1.43
22	c	509	CLA	C1B-C2B	2.73	1.49	1.43
22	C	507	CLA	C1B-C2B	2.72	1.49	1.43
22	A	406	CLA	C1B-C2B	2.72	1.49	1.43
22	b	611	CLA	C1B-C2B	2.72	1.49	1.43
22	B	605	CLA	C1B-C2B	2.72	1.49	1.43
22	C	509	CLA	C1B-C2B	2.72	1.49	1.43
22	B	612	CLA	C1B-C2B	2.71	1.49	1.43
22	D	404	CLA	C1B-C2B	2.71	1.49	1.43
22	C	505	CLA	C1B-C2B	2.71	1.49	1.43
22	b	609	CLA	C1B-C2B	2.70	1.49	1.43
22	c	505	CLA	C1B-C2B	2.70	1.49	1.43
22	B	602	CLA	C1B-C2B	2.70	1.49	1.43
22	b	613	CLA	C1B-C2B	2.69	1.49	1.43
22	A	402	CLA	C1B-C2B	2.68	1.49	1.43
22	B	606	CLA	C1B-C2B	2.68	1.49	1.43
22	a	406	CLA	C1B-C2B	2.67	1.49	1.43
22	C	508	CLA	C1B-C2B	2.67	1.49	1.43
22	A	403	CLA	C1B-C2B	2.67	1.49	1.43
22	c	506	CLA	C1B-C2B	2.66	1.49	1.43
22	b	606	CLA	C1B-C2B	2.66	1.49	1.43
34	F	101	HEM	FE-NC	2.65	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	C1B-C2B	2.64	1.49	1.43
22	b	612	CLA	C1B-C2B	2.64	1.49	1.43
24	A	407	PL9	C3-C4	-2.64	1.45	1.49
22	b	614	CLA	C1B-C2B	2.64	1.49	1.43
22	C	519	CLA	C1B-C2B	2.63	1.49	1.43
24	a	407	PL9	C3-C4	-2.63	1.45	1.49
22	a	403	CLA	C1B-C2B	2.62	1.49	1.43
23	d	401	PHO	CMC-C2C	-2.62	1.46	1.50
23	D	401	PHO	CMC-C2C	-2.62	1.46	1.50
22	c	508	CLA	C1B-C2B	2.61	1.49	1.43
22	A	402	CLA	C3B-C4B	2.61	1.50	1.42
22	c	507	CLA	C1B-C2B	2.60	1.49	1.43
34	V	201	HEM	FE-NC	2.59	2.03	1.95
22	B	608	CLA	CHC-C1C	2.59	1.43	1.38
22	a	403	CLA	C3B-C4B	2.58	1.50	1.42
23	d	402	PHO	CMC-C2C	-2.58	1.46	1.50
23	d	402	PHO	C3D-C4D	2.58	1.44	1.41
22	B	610	CLA	MG-NB	-2.57	2.00	2.05
23	d	401	PHO	C3D-C4D	2.57	1.44	1.41
23	D	401	PHO	C3D-C4D	2.57	1.44	1.41
22	B	609	CLA	C1B-C2B	2.56	1.49	1.43
22	B	607	CLA	C1B-C2B	2.55	1.49	1.43
23	A	405	PHO	CMC-C2C	-2.55	1.46	1.50
22	b	615	CLA	MG-NB	-2.54	2.00	2.05
23	A	405	PHO	C3D-C4D	2.53	1.44	1.41
24	D	405	PL9	C6-C1	-2.52	1.44	1.48
24	j	101	PL9	C3-C4	-2.52	1.45	1.49
22	b	613	CLA	CHC-C1C	2.51	1.43	1.38
23	d	401	PHO	CMB-C2B	-2.49	1.46	1.51
22	c	508	CLA	C3B-C4B	2.49	1.50	1.42
22	b	606	CLA	CHC-C1C	2.48	1.43	1.38
32	b	629	LMT	O3'-C3'	-2.47	1.36	1.43
22	b	612	CLA	CHC-C1C	2.47	1.43	1.38
23	D	401	PHO	CAC-C3C	-2.47	1.47	1.51
22	B	613	CLA	CHC-C1C	2.46	1.43	1.38
23	D	401	PHO	CMD-C2D	-2.46	1.46	1.51
23	d	401	PHO	CAC-C3C	-2.45	1.47	1.51
23	d	401	PHO	CMD-C2D	-2.45	1.46	1.51
23	A	405	PHO	CMB-C2B	-2.45	1.46	1.51
22	A	403	CLA	C3B-C4B	2.45	1.49	1.42
24	a	407	PL9	C7-C3	-2.44	1.48	1.51
22	B	611	CLA	CMD-C2D	-2.44	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	PHO	CMD-C2D	-2.44	1.46	1.51
31	b	626	LMG	C4-C5	2.43	1.58	1.53
31	D	409	LMG	O7-C8	-2.43	1.40	1.46
23	d	402	PHO	CMD-C2D	-2.43	1.46	1.51
32	b	603	LMT	O3'-C3'	-2.43	1.36	1.43
32	d	411	LMT	O3'-C3'	-2.43	1.36	1.43
22	H	101	CLA	CHC-C1C	2.43	1.43	1.38
32	M	103	LMT	O3'-C3'	-2.43	1.36	1.43
26	B	626	DGD	C4D-C5D	2.42	1.58	1.53
22	B	613	CLA	C3B-C4B	2.42	1.49	1.42
22	c	512	CLA	C3B-C4B	2.42	1.49	1.42
22	c	509	CLA	C3B-C4B	2.42	1.49	1.42
22	b	612	CLA	C3B-C4B	2.42	1.49	1.42
22	c	511	CLA	C3B-C4B	2.42	1.49	1.42
22	c	512	CLA	CHC-C1C	2.42	1.43	1.38
32	b	628	LMT	O3'-C3'	-2.42	1.37	1.43
32	B	624	LMT	O3'-C3'	-2.41	1.37	1.43
22	B	607	CLA	CHC-C1C	2.41	1.43	1.38
23	d	402	PHO	CMB-C2B	-2.41	1.46	1.51
24	J	101	PL9	C7-C3	-2.41	1.48	1.51
23	D	401	PHO	CMB-C2B	-2.41	1.46	1.51
22	b	607	CLA	CHC-C1C	2.40	1.43	1.38
32	B	623	LMT	O3'-C3'	-2.40	1.37	1.43
22	c	505	CLA	C3B-C4B	2.40	1.49	1.42
22	B	610	CLA	C1B-NB	-2.40	1.34	1.37
22	b	605	CLA	C3B-C4B	2.39	1.49	1.42
22	b	616	CLA	C3B-C4B	2.39	1.49	1.42
32	M	102	LMT	O3'-C3'	-2.39	1.37	1.43
32	D	408	LMT	O3'-C3'	-2.39	1.37	1.43
22	a	405	CLA	C3B-C4B	2.39	1.49	1.42
22	C	508	CLA	C3B-C4B	2.38	1.49	1.42
22	d	406	CLA	CHC-C1C	2.38	1.43	1.38
32	I	102	LMT	O3'-C3'	-2.38	1.37	1.43
22	c	502	CLA	CHC-C1C	2.38	1.43	1.38
22	b	613	CLA	C3B-C4B	2.38	1.49	1.42
22	c	510	CLA	C3B-C4B	2.37	1.49	1.42
22	B	608	CLA	C3B-C4B	2.37	1.49	1.42
22	H	101	CLA	C3B-C4B	2.37	1.49	1.42
22	b	620	CLA	C3B-C4B	2.37	1.49	1.42
22	b	618	CLA	CHC-C1C	2.37	1.43	1.38
22	C	519	CLA	C3B-C4B	2.37	1.49	1.42
22	C	511	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	628	LMT	O3'-C3'	-2.36	1.37	1.43
22	C	511	CLA	CHC-C1C	2.36	1.43	1.38
22	B	612	CLA	C3B-C4B	2.36	1.49	1.42
22	c	511	CLA	CHC-C1C	2.36	1.43	1.38
22	D	404	CLA	C3B-C4B	2.36	1.49	1.42
22	B	601	CLA	C3B-C4B	2.36	1.49	1.42
32	i	103	LMT	O3'-C3'	-2.35	1.37	1.43
22	b	606	CLA	C3B-C4B	2.35	1.49	1.42
22	B	607	CLA	C3B-C4B	2.35	1.49	1.42
22	d	406	CLA	C3B-C4B	2.35	1.49	1.42
23	A	405	PHO	CAC-C3C	-2.34	1.47	1.51
22	b	607	CLA	C3B-C4B	2.34	1.49	1.42
22	a	405	CLA	CHC-C1C	2.34	1.43	1.38
22	c	520	CLA	C3B-C4B	2.34	1.49	1.42
22	a	404	CLA	C3B-C4B	2.34	1.49	1.42
22	B	615	CLA	C3B-C4B	2.33	1.49	1.42
22	B	614	CLA	C3B-C4B	2.33	1.49	1.42
22	c	507	CLA	C3B-C4B	2.33	1.49	1.42
22	C	505	CLA	C3B-C4B	2.33	1.49	1.42
22	b	619	CLA	C3B-C4B	2.33	1.49	1.42
22	c	509	CLA	CHC-C1C	2.33	1.43	1.38
22	B	603	CLA	CHC-C1C	2.33	1.43	1.38
24	d	407	PL9	C6-C1	-2.32	1.44	1.48
22	b	616	CLA	CMD-C2D	-2.32	1.46	1.50
22	A	404	CLA	C3B-C4B	2.32	1.49	1.42
22	C	509	CLA	C3B-C4B	2.32	1.49	1.42
22	C	507	CLA	C3B-C4B	2.31	1.49	1.42
22	C	510	CLA	C3B-C4B	2.31	1.49	1.42
27	a	409	LHG	O7-C5	-2.31	1.41	1.46
22	B	611	CLA	C3B-C4B	2.31	1.49	1.42
22	b	610	CLA	C3B-C4B	2.30	1.49	1.42
22	b	608	CLA	CHC-C1C	2.30	1.43	1.38
22	b	615	CLA	C1B-NB	-2.30	1.34	1.37
22	c	507	CLA	CHC-C1C	2.30	1.43	1.38
31	B	621	LMG	C4-C5	2.30	1.57	1.53
22	c	505	CLA	CHC-C1C	2.30	1.43	1.38
22	b	617	CLA	C3B-C4B	2.30	1.49	1.42
22	B	602	CLA	CHC-C1C	2.29	1.43	1.38
22	D	404	CLA	CHC-C1C	2.29	1.43	1.38
22	b	618	CLA	C3B-C4B	2.29	1.49	1.42
22	c	506	CLA	CHC-C1C	2.29	1.43	1.38
22	B	604	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	CLA	CHC-C1C	2.29	1.43	1.38
27	c	519	LHG	O7-C5	-2.28	1.41	1.46
22	c	506	CLA	C3B-C4B	2.28	1.49	1.42
22	D	403	CLA	C3B-C4B	2.28	1.49	1.42
22	C	502	CLA	CHC-C1C	2.28	1.43	1.38
22	a	406	CLA	CHC-C1C	2.28	1.43	1.38
22	c	501	CLA	C3B-C4B	2.28	1.49	1.42
22	B	612	CLA	CHC-C1C	2.28	1.43	1.38
24	a	407	PL9	C53-C6	-2.27	1.46	1.50
22	C	512	CLA	CHC-C1C	2.27	1.43	1.38
25	g	101	BCR	C33-C5	-2.27	1.47	1.50
32	B	629	LMT	O3'-C3'	-2.27	1.37	1.43
32	b	604	LMT	O3'-C3'	-2.27	1.37	1.43
31	I	101	LMG	C4-C5	2.27	1.57	1.53
22	d	405	CLA	C3B-C4B	2.27	1.49	1.42
23	d	402	PHO	CAC-C3C	-2.27	1.47	1.51
22	c	510	CLA	CHC-C1C	2.27	1.43	1.38
22	c	503	CLA	CHC-C1C	2.27	1.43	1.38
22	b	614	CLA	C3B-C4B	2.26	1.49	1.42
31	b	627	LMG	C4-C5	2.26	1.57	1.53
26	c	515	DGD	O2G-C2G	-2.26	1.41	1.46
22	C	509	CLA	CHC-C1C	2.26	1.43	1.38
22	b	614	CLA	MG-NB	-2.26	2.01	2.05
22	c	504	CLA	CMD-C2D	-2.26	1.46	1.50
22	c	502	CLA	C3B-C4B	2.26	1.49	1.42
22	a	406	CLA	C3B-C4B	2.26	1.49	1.42
26	b	601	DGD	C4D-C5D	2.26	1.57	1.53
22	A	404	CLA	CHC-C1C	2.26	1.43	1.38
26	c	516	DGD	O2G-C2G	-2.25	1.41	1.46
22	c	508	CLA	CHC-C1C	2.25	1.43	1.38
22	B	606	CLA	C3B-C4B	2.25	1.49	1.42
22	c	503	CLA	C3B-C4B	2.25	1.49	1.42
22	b	617	CLA	CHC-C1C	2.25	1.43	1.38
22	A	406	CLA	C3B-C4B	2.25	1.49	1.42
32	I	102	LMT	O2'-C2'	-2.25	1.37	1.43
22	c	509	CLA	CMD-C2D	-2.25	1.46	1.50
22	B	602	CLA	C3B-C4B	2.25	1.49	1.42
22	b	608	CLA	C3B-C4B	2.25	1.49	1.42
22	B	614	CLA	CHC-C1C	2.25	1.43	1.38
22	B	604	CLA	CHC-C1C	2.25	1.43	1.38
22	A	403	CLA	CHC-C1C	2.25	1.43	1.38
22	c	501	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	407	DGD	O5D-C6D	-2.25	1.39	1.43
22	C	502	CLA	C3B-C4B	2.25	1.49	1.42
22	b	616	CLA	CHC-C1C	2.24	1.43	1.38
22	C	507	CLA	CMB-C2B	-2.24	1.46	1.50
22	C	505	CLA	CHC-C1C	2.24	1.43	1.38
22	b	609	CLA	C3B-C4B	2.24	1.49	1.42
22	B	605	CLA	CHC-C1C	2.24	1.43	1.38
22	B	609	CLA	CHC-C1C	2.24	1.43	1.38
22	C	512	CLA	C3B-C4B	2.24	1.49	1.42
22	C	519	CLA	CHC-C1C	2.24	1.43	1.38
22	D	403	CLA	CHC-C1C	2.23	1.43	1.38
22	b	619	CLA	CHC-C1C	2.23	1.43	1.38
22	b	611	CLA	C3B-C4B	2.23	1.49	1.42
22	C	506	CLA	C3B-C4B	2.23	1.49	1.42
22	B	609	CLA	C3B-C4B	2.23	1.49	1.42
31	a	402	LMG	O7-C8	-2.22	1.41	1.46
22	C	503	CLA	C3B-C4B	2.22	1.49	1.42
32	M	102	LMT	O1'-C1'	-2.22	1.36	1.40
22	a	403	CLA	CHC-C1C	2.21	1.42	1.38
22	C	504	CLA	CMD-C2D	-2.21	1.46	1.50
22	c	507	CLA	CMB-C2B	-2.21	1.46	1.50
24	A	407	PL9	C6-C1	-2.21	1.44	1.48
22	A	406	CLA	CHC-C1C	2.21	1.42	1.38
22	B	606	CLA	CHC-C1C	2.21	1.42	1.38
22	B	603	CLA	C3B-C4B	2.20	1.49	1.42
22	B	609	CLA	MG-NB	-2.20	2.01	2.05
25	y	101	BCR	C33-C5	-2.20	1.47	1.50
22	C	501	CLA	CHC-C1C	2.20	1.42	1.38
22	C	501	CLA	C3B-C4B	2.20	1.49	1.42
22	b	610	CLA	CHC-C1C	2.20	1.42	1.38
22	b	614	CLA	CHC-C1C	2.20	1.42	1.38
32	B	629	LMT	O3B-C3B	-2.20	1.37	1.43
22	B	605	CLA	C3B-C4B	2.20	1.49	1.42
22	C	510	CLA	CHC-C1C	2.19	1.42	1.38
22	C	508	CLA	CHC-C1C	2.19	1.42	1.38
27	c	519	LHG	P-O6	2.19	1.68	1.59
24	A	407	PL9	C7-C3	-2.19	1.48	1.51
26	C	515	DGD	O2G-C2G	-2.19	1.41	1.46
22	C	509	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	612	CLA	CMD-C2D	-2.19	1.46	1.50
24	A	407	PL9	C53-C6	-2.19	1.46	1.50
22	C	503	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	407	PL9	C31-C29	-2.18	1.46	1.51
26	c	516	DGD	O5D-C6D	-2.18	1.40	1.43
32	D	408	LMT	O3B-C3B	-2.18	1.37	1.43
22	b	605	CLA	CHC-C1C	2.18	1.42	1.38
32	b	604	LMT	O3B-C3B	-2.18	1.37	1.43
22	C	519	CLA	MG-NB	-2.18	2.01	2.05
22	c	520	CLA	CHC-C1C	2.17	1.42	1.38
32	M	103	LMT	O3B-C3B	-2.17	1.37	1.43
32	b	629	LMT	O3B-C3B	-2.17	1.37	1.43
32	i	103	LMT	O2'-C2'	-2.17	1.37	1.43
26	C	514	DGD	O1G-C1G	-2.17	1.40	1.45
22	C	507	CLA	CHC-C1C	2.17	1.42	1.38
22	B	607	CLA	CMD-C2D	-2.17	1.46	1.50
22	A	402	CLA	CHC-C1C	2.17	1.42	1.38
27	A	410	LHG	O7-C5	-2.16	1.41	1.46
31	d	412	LMG	O7-C8	-2.16	1.41	1.46
32	B	623	LMT	O2'-C2'	-2.16	1.37	1.43
31	a	402	LMG	C4-C5	2.16	1.57	1.53
22	b	611	CLA	CHC-C1C	2.16	1.42	1.38
22	B	606	CLA	MG-NB	-2.15	2.01	2.05
22	C	506	CLA	CHC-C1C	2.15	1.42	1.38
32	b	603	LMT	O3B-C3B	-2.15	1.37	1.43
22	b	609	CLA	CHC-C1C	2.15	1.42	1.38
32	B	629	LMT	O2'-C2'	-2.15	1.37	1.43
22	B	601	CLA	CHC-C1C	2.15	1.42	1.38
22	B	607	CLA	CMB-C2B	-2.15	1.46	1.50
26	d	410	DGD	O5D-C6D	-2.15	1.40	1.43
22	a	404	CLA	MG-NB	-2.14	2.01	2.05
32	B	628	LMT	O2B-C2B	-2.14	1.37	1.43
22	c	504	CLA	CHC-C1C	2.14	1.42	1.38
22	B	603	CLA	CMD-C2D	-2.14	1.46	1.50
22	b	615	CLA	C1B-C2B	2.14	1.48	1.43
26	d	410	DGD	C1D-C2D	2.14	1.58	1.52
32	b	628	LMT	O3B-C3B	-2.14	1.37	1.43
22	D	403	CLA	CMD-C2D	-2.13	1.46	1.50
24	J	101	PL9	C3-C4	-2.13	1.46	1.49
22	C	504	CLA	CHC-C1C	2.13	1.42	1.38
22	B	602	CLA	MG-NB	-2.13	2.01	2.05
32	I	102	LMT	O3B-C3B	-2.13	1.37	1.43
32	B	624	LMT	O3B-C3B	-2.13	1.37	1.43
32	b	603	LMT	O2'-C2'	-2.13	1.37	1.43
22	B	603	CLA	CMB-C2B	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	411	LMT	O3B-C3B	-2.13	1.37	1.43
22	B	615	CLA	CHC-C1C	2.13	1.42	1.38
22	a	403	CLA	CMB-C2B	-2.12	1.46	1.50
32	M	102	LMT	O3B-C3B	-2.12	1.37	1.43
32	b	628	LMT	O2'-C2'	-2.12	1.37	1.43
22	d	405	CLA	CMD-C2D	-2.12	1.46	1.50
32	B	628	LMT	O3B-C3B	-2.12	1.37	1.43
22	B	607	CLA	MG-NB	-2.12	2.01	2.05
31	d	408	LMG	O7-C8	-2.12	1.41	1.46
22	b	607	CLA	MG-NB	-2.12	2.01	2.05
22	C	504	CLA	C3B-C4B	2.11	1.48	1.42
22	b	606	CLA	MG-NB	-2.11	2.01	2.05
32	i	103	LMT	O2B-C2B	-2.11	1.37	1.43
31	m	101	LMG	C4-C5	2.11	1.57	1.53
32	i	103	LMT	O3B-C3B	-2.11	1.37	1.43
22	c	504	CLA	C3B-C4B	2.11	1.48	1.42
22	b	612	CLA	CMB-C2B	-2.11	1.46	1.50
34	V	201	HEM	CMB-C2B	2.11	1.55	1.50
22	B	612	CLA	MG-NB	-2.11	2.01	2.05
22	A	404	CLA	CMD-C2D	-2.10	1.46	1.50
22	a	403	CLA	CMD-C2D	-2.10	1.46	1.50
34	f	101	HEM	CMC-C2C	2.10	1.55	1.50
22	A	403	CLA	CMB-C2B	-2.10	1.46	1.50
26	B	620	DGD	O2G-C2G	-2.10	1.41	1.46
22	b	620	CLA	CHC-C1C	2.10	1.42	1.38
32	I	102	LMT	O2B-C2B	-2.10	1.37	1.43
32	b	628	LMT	O2B-C2B	-2.10	1.37	1.43
32	M	102	LMT	O2'-C2'	-2.10	1.37	1.43
22	A	406	CLA	CMB-C2B	-2.09	1.46	1.50
22	b	608	CLA	CMD-C2D	-2.09	1.46	1.50
32	B	624	LMT	O2'-C2'	-2.09	1.37	1.43
32	b	629	LMT	O2'-C2'	-2.09	1.37	1.43
32	b	604	LMT	O2'-C2'	-2.09	1.37	1.43
22	b	618	CLA	MG-NB	-2.09	2.01	2.05
22	C	501	CLA	CMB-C2B	-2.09	1.46	1.50
22	B	611	CLA	CHC-C1C	2.09	1.42	1.38
32	B	629	LMT	O1'-C1'	-2.09	1.36	1.40
34	v	201	HEM	CMB-C2B	2.09	1.55	1.50
32	B	623	LMT	O3B-C3B	-2.09	1.37	1.43
26	b	625	DGD	O2G-C2G	-2.08	1.41	1.46
22	b	609	CLA	CMB-C2B	-2.08	1.46	1.50
22	A	404	CLA	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	615	CLA	CMC-C2C	-2.08	1.46	1.50
22	C	504	CLA	CMB-C2B	-2.08	1.46	1.50
22	D	403	CLA	MG-NB	-2.08	2.01	2.05
22	C	502	CLA	MG-NB	-2.08	2.01	2.05
34	v	201	HEM	CMD-C2D	2.08	1.55	1.50
22	C	509	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	610	CLA	C1B-C2B	2.08	1.48	1.43
22	c	506	CLA	MG-NB	-2.08	2.01	2.05
34	V	201	HEM	CMD-C2D	2.08	1.55	1.50
32	D	408	LMT	O2B-C2B	-2.08	1.37	1.43
22	A	402	CLA	CMD-C2D	-2.08	1.46	1.50
22	a	406	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	611	CLA	MG-NB	-2.07	2.01	2.05
26	B	626	DGD	C3G-C2G	2.07	1.57	1.50
22	B	605	CLA	CMB-C2B	-2.07	1.46	1.50
22	b	620	CLA	CMC-C2C	-2.07	1.46	1.50
32	M	103	LMT	O2'-C2'	-2.07	1.37	1.43
22	a	405	CLA	CMD-C2D	-2.07	1.46	1.50
22	H	101	CLA	CMB-C2B	-2.07	1.46	1.50
32	B	629	LMT	O2B-C2B	-2.07	1.37	1.43
22	C	508	CLA	CMD-C2D	-2.07	1.46	1.50
22	C	512	CLA	CMB-C2B	-2.07	1.46	1.50
22	a	404	CLA	CMD-C2D	-2.07	1.46	1.50
22	C	503	CLA	CMB-C2B	-2.07	1.46	1.50
22	C	508	CLA	MG-NB	-2.07	2.01	2.05
22	b	620	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	606	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	605	CLA	MG-NB	-2.06	2.01	2.05
32	b	603	LMT	O2B-C2B	-2.06	1.37	1.43
22	C	506	CLA	MG-NB	-2.06	2.01	2.05
22	C	502	CLA	CMB-C2B	-2.06	1.46	1.50
34	F	101	HEM	CMC-C2C	2.06	1.55	1.50
22	A	402	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	601	CLA	CMB-C2B	-2.06	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.06	1.46	1.50
24	d	407	PL9	C53-C6	-2.06	1.46	1.50
32	B	628	LMT	O2'-C2'	-2.06	1.37	1.43
22	c	504	CLA	CMB-C2B	-2.06	1.46	1.50
34	v	201	HEM	CMA-C3A	2.06	1.55	1.50
22	a	404	CLA	CMB-C2B	-2.06	1.46	1.50
30	b	602	SQD	O2-C2	-2.06	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C4D-ND	-2.06	1.35	1.38
22	B	601	CLA	CMD-C2D	-2.05	1.46	1.50
22	b	614	CLA	CMB-C2B	-2.05	1.46	1.50
25	C	513	BCR	C38-C26	-2.05	1.47	1.50
22	c	501	CLA	CMB-C2B	-2.05	1.46	1.50
22	c	520	CLA	CMB-C2B	-2.05	1.46	1.50
22	c	502	CLA	MG-NB	-2.05	2.01	2.05
22	B	614	CLA	CMD-C2D	-2.05	1.46	1.50
22	C	502	CLA	CMC-C2C	-2.05	1.46	1.50
22	b	618	CLA	CMB-C2B	-2.05	1.46	1.50
22	B	615	CLA	CMD-C2D	-2.05	1.46	1.50
22	b	605	CLA	CMB-C2B	-2.05	1.46	1.50
22	c	502	CLA	CMB-C2B	-2.05	1.46	1.50
22	c	503	CLA	CMD-C2D	-2.05	1.46	1.50
22	b	611	CLA	CMB-C2B	-2.05	1.46	1.50
32	M	103	LMT	O2B-C2B	-2.05	1.37	1.43
22	C	508	CLA	CMB-C2B	-2.05	1.46	1.50
32	B	623	LMT	O2B-C2B	-2.05	1.37	1.43
22	b	608	CLA	CMB-C2B	-2.04	1.46	1.50
32	b	604	LMT	O1'-C1'	-2.04	1.36	1.40
22	C	519	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	617	CLA	MG-NB	-2.04	2.01	2.05
27	C	518	LHG	O7-C5	-2.04	1.41	1.46
26	b	601	DGD	C3G-C2G	2.04	1.57	1.50
22	B	604	CLA	CMD-C2D	-2.04	1.46	1.50
31	l	101	LMG	C7-C8	2.04	1.57	1.50
22	b	611	CLA	MG-NB	-2.04	2.01	2.05
22	A	403	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	606	CLA	CMB-C2B	-2.04	1.46	1.50
30	a	401	SQD	O47-C45	-2.04	1.41	1.46
22	B	602	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	606	CLA	CMC-C2C	-2.04	1.46	1.50
25	c	514	BCR	C38-C26	-2.04	1.47	1.50
22	b	613	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	608	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	617	CLA	CMD-C2D	-2.03	1.46	1.50
22	c	505	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	613	CLA	MG-NB	-2.03	2.01	2.05
22	b	611	CLA	CMD-C2D	-2.03	1.46	1.50
24	J	101	PL9	C6-C1	-2.03	1.45	1.48
26	C	515	DGD	O5D-C6D	-2.03	1.40	1.43
22	B	604	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	411	LMT	O2B-C2B	-2.03	1.37	1.43
22	b	606	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	613	CLA	CMB-C2B	-2.03	1.46	1.50
22	c	505	CLA	CMD-C2D	-2.03	1.46	1.50
22	c	509	CLA	CMB-C2B	-2.03	1.46	1.50
22	c	508	CLA	CMD-C2D	-2.03	1.46	1.50
30	B	627	SQD	O2-C2	-2.03	1.37	1.43
22	C	509	CLA	MG-NB	-2.03	2.01	2.05
22	b	612	CLA	MG-NB	-2.02	2.01	2.05
25	B	616	BCR	C33-C5	-2.02	1.47	1.50
25	J	102	BCR	C38-C26	-2.02	1.47	1.50
26	D	407	DGD	C1G-C2G	2.02	1.57	1.50
22	c	503	CLA	CMB-C2B	-2.02	1.46	1.50
30	a	412	SQD	O2-C2	-2.02	1.38	1.43
22	c	508	CLA	CMB-C2B	-2.02	1.46	1.50
30	A	413	SQD	O2-C2	-2.02	1.38	1.43
22	d	406	CLA	CMB-C2B	-2.02	1.46	1.50
25	b	621	BCR	C33-C5	-2.02	1.47	1.50
22	C	505	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	605	CLA	CMC-C2C	-2.02	1.46	1.50
30	A	414	SQD	O47-C45	-2.02	1.41	1.46
32	b	604	LMT	O2B-C2B	-2.02	1.38	1.43
32	b	603	LMT	O1'-C1'	-2.02	1.36	1.40
22	c	507	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	504	CLA	MG-NB	-2.01	2.01	2.05
34	v	201	HEM	CMC-C2C	2.01	1.54	1.50
22	C	505	CLA	CMD-C2D	-2.01	1.46	1.50
22	c	502	CLA	CMC-C2C	-2.01	1.46	1.50
22	C	511	CLA	CMD-C2D	-2.01	1.46	1.50
23	d	401	PHO	C3B-C2B	-2.01	1.37	1.40
25	j	102	BCR	C38-C26	-2.01	1.47	1.50
22	B	608	CLA	CMD-C2D	-2.01	1.46	1.50
22	D	404	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	511	CLA	CMD-C2D	-2.01	1.46	1.50
22	c	512	CLA	CMB-C2B	-2.01	1.46	1.50
26	D	407	DGD	C1D-C2D	2.01	1.58	1.52
22	D	404	CLA	MG-NB	-2.01	2.01	2.05
25	F	102	BCR	C33-C5	-2.01	1.47	1.50
22	c	502	CLA	CMD-C2D	-2.01	1.46	1.50
31	B	625	LMG	O7-C8	-2.01	1.41	1.46
32	d	411	LMT	O4'-C4B	-2.01	1.38	1.43
24	D	405	PL9	C53-C6	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	619	CLA	CMD-C2D	-2.01	1.46	1.50
22	d	405	CLA	CMC-C2C	-2.01	1.46	1.50
22	C	506	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	404	CLA	CMB-C2B	-2.00	1.46	1.50
32	d	411	LMT	O2'-C2'	-2.00	1.38	1.43
22	C	502	CLA	CMD-C2D	-2.00	1.46	1.50
22	C	504	CLA	MG-NB	-2.00	2.01	2.05
30	A	414	SQD	O3-C3	-2.00	1.38	1.43
26	b	601	DGD	C1G-C2G	2.00	1.57	1.50

All (1047) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.55	110.12	106.68
22	B	611	CLA	C4A-NA-C1A	7.50	110.10	106.68
22	B	605	CLA	C4A-NA-C1A	7.34	110.03	106.68
22	b	608	CLA	C4A-NA-C1A	7.30	110.01	106.68
22	C	501	CLA	C4A-NA-C1A	7.18	109.96	106.68
22	b	610	CLA	C4A-NA-C1A	7.18	109.95	106.68
22	C	503	CLA	C4A-NA-C1A	7.17	109.95	106.68
22	b	616	CLA	C4A-NA-C1A	7.15	109.94	106.68
22	B	603	CLA	C4A-NA-C1A	7.15	109.94	106.68
22	C	511	CLA	C4A-NA-C1A	7.15	109.94	106.68
22	c	503	CLA	C4A-NA-C1A	7.14	109.94	106.68
22	B	615	CLA	C4A-NA-C1A	7.10	109.92	106.68
22	c	501	CLA	C4A-NA-C1A	7.09	109.91	106.68
22	C	510	CLA	C4A-NA-C1A	7.09	109.91	106.68
22	C	507	CLA	C4A-NA-C1A	7.02	109.88	106.68
22	B	604	CLA	C4A-NA-C1A	7.00	109.87	106.68
22	c	504	CLA	C4A-NA-C1A	6.99	109.87	106.68
22	C	512	CLA	C4A-NA-C1A	6.96	109.85	106.68
22	A	403	CLA	C4A-NA-C1A	6.92	109.83	106.68
22	C	506	CLA	C4A-NA-C1A	6.90	109.83	106.68
22	B	614	CLA	C4A-NA-C1A	6.89	109.82	106.68
22	b	609	CLA	C4A-NA-C1A	6.88	109.82	106.68
22	c	520	CLA	C4A-NA-C1A	6.85	109.81	106.68
22	a	406	CLA	C4A-NA-C1A	6.83	109.80	106.68
22	c	511	CLA	C4A-NA-C1A	6.83	109.79	106.68
22	d	405	CLA	C4A-NA-C1A	6.82	109.79	106.68
22	c	507	CLA	C4A-NA-C1A	6.79	109.78	106.68
22	b	619	CLA	C4A-NA-C1A	6.79	109.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	620	CLA	C4A-NA-C1A	6.78	109.77	106.68
22	d	406	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	b	617	CLA	C4A-NA-C1A	6.68	109.73	106.68
22	c	512	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	A	406	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	B	613	CLA	C4A-NA-C1A	6.64	109.71	106.68
22	H	101	CLA	C4A-NA-C1A	6.63	109.71	106.68
22	c	505	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	B	612	CLA	C4A-NA-C1A	6.57	109.68	106.68
22	c	508	CLA	C4A-NA-C1A	6.56	109.67	106.68
22	C	519	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	a	404	CLA	C4A-NA-C1A	6.52	109.66	106.68
22	b	618	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	c	509	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	c	502	CLA	C4A-NA-C1A	6.48	109.64	106.68
22	B	606	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	A	404	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	C	508	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	D	403	CLA	C4A-NA-C1A	6.37	109.59	106.68
22	b	612	CLA	C4A-NA-C1A	6.37	109.59	106.68
22	a	403	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	b	606	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	c	510	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	B	608	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	B	607	CLA	C4A-NA-C1A	6.32	109.56	106.68
30	b	602	SQD	O6-C1-C2	6.32	117.87	108.27
22	C	509	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	c	506	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	A	402	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	B	602	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	a	405	CLA	C4A-NA-C1A	6.27	109.54	106.68
22	B	609	CLA	C4A-NA-C1A	6.24	109.53	106.68
22	b	611	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	C	505	CLA	C4A-NA-C1A	6.21	109.51	106.68
22	D	404	CLA	C4A-NA-C1A	6.19	109.50	106.68
22	C	502	CLA	C4A-NA-C1A	6.09	109.46	106.68
23	d	401	PHO	C4D-CHA-CBD	-6.09	105.53	108.45
22	b	605	CLA	C4A-NA-C1A	6.05	109.44	106.68
30	B	627	SQD	O6-C1-C2	6.05	117.45	108.27
22	B	601	CLA	C4A-NA-C1A	6.01	109.42	106.68
23	d	402	PHO	C4D-CHA-CBD	-5.98	105.58	108.45
22	b	613	CLA	C4A-NA-C1A	5.98	109.41	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	PHO	C4D-CHA-CBD	-5.88	105.63	108.45
22	b	607	CLA	C4A-NA-C1A	5.87	109.36	106.68
33	d	404	BCT	O2-C-O1	5.82	134.56	119.68
22	b	614	CLA	C4A-NA-C1A	5.78	109.32	106.68
33	D	402	BCT	O2-C-O1	5.76	134.42	119.68
24	J	101	PL9	C7-C3-C4	5.76	121.66	116.91
23	A	405	PHO	C4D-CHA-CBD	-5.71	105.72	108.45
30	A	413	SQD	O6-C1-C2	5.66	116.86	108.27
22	b	615	CLA	C4A-NA-C1A	5.66	109.26	106.68
30	a	412	SQD	O6-C1-C2	5.65	116.86	108.27
34	v	201	HEM	C4D-ND-C1D	5.49	111.70	105.21
22	B	610	CLA	C4A-NA-C1A	5.41	109.15	106.68
24	j	101	PL9	C7-C3-C4	5.35	121.32	116.91
24	a	407	PL9	C7-C3-C4	5.31	121.28	116.91
24	A	407	PL9	C7-C3-C4	5.28	121.26	116.91
24	d	407	PL9	C7-C3-C4	5.24	121.22	116.91
24	D	405	PL9	C7-C3-C4	5.11	121.12	116.91
34	f	101	HEM	C4D-ND-C1D	5.08	111.23	105.21
34	F	101	HEM	C4D-ND-C1D	4.97	111.09	105.21
34	V	201	HEM	C4D-ND-C1D	4.94	111.06	105.21
26	A	409	DGD	O3G-C3G-C2G	-4.53	99.80	110.82
27	C	518	LHG	O4-P-O5	4.47	133.25	112.44
27	a	409	LHG	O4-P-O5	4.46	133.17	112.44
27	c	519	LHG	O4-P-O5	4.45	133.13	112.44
27	A	410	LHG	O4-P-O5	4.43	133.06	112.44
26	a	408	DGD	O3G-C3G-C2G	-4.38	100.16	110.82
24	J	101	PL9	C7-C3-C2	-4.38	118.23	123.39
30	d	403	SQD	O5-C5-C4	4.32	117.49	109.70
30	B	622	SQD	O5-C5-C4	4.30	117.45	109.70
30	A	413	SQD	O9-S-C6	4.28	113.15	106.76
26	C	516	DGD	O3G-C3G-C2G	-4.26	100.45	110.82
24	j	101	PL9	C7-C3-C2	-4.26	118.37	123.39
30	B	622	SQD	O6-C1-C2	4.21	114.67	108.27
24	d	407	PL9	C7-C3-C2	-4.11	118.54	123.39
30	f	103	SQD	O9-S-O7	-4.11	100.46	113.82
30	d	403	SQD	O9-S-O7	-4.10	100.50	113.82
31	d	409	LMG	C1-C2-C3	-4.07	101.45	110.01
30	F	103	SQD	O9-S-O7	-4.06	100.61	113.82
25	c	513	BCR	C2-C1-C6	4.05	116.33	110.44
25	j	102	BCR	C2-C1-C6	4.05	116.32	110.44
25	K	101	BCR	C2-C1-C6	4.04	116.31	110.44
24	D	405	PL9	C7-C3-C2	-4.04	118.63	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	622	SQD	O9-S-O7	-4.03	100.72	113.82
24	a	407	PL9	C7-C3-C2	-4.03	118.64	123.39
31	D	406	LMG	C1-C2-C3	-4.03	101.54	110.01
30	a	412	SQD	O9-S-O7	-4.00	100.80	113.82
30	A	413	SQD	O9-S-O7	-3.97	100.90	113.82
26	c	517	DGD	O3G-C3G-C2G	-3.97	101.16	110.82
30	a	401	SQD	O9-S-O7	-3.96	100.95	113.82
25	J	102	BCR	C2-C1-C6	3.95	116.18	110.44
30	b	602	SQD	O9-S-O7	-3.93	101.04	113.82
30	a	412	SQD	O9-S-C6	3.92	112.61	106.76
24	A	407	PL9	C7-C3-C2	-3.91	118.78	123.39
30	d	403	SQD	O6-C1-C2	3.90	114.20	108.27
30	A	414	SQD	O5-C5-C4	3.90	116.72	109.70
30	B	627	SQD	O9-S-O7	-3.90	101.15	113.82
30	A	414	SQD	O9-S-O7	-3.89	101.17	113.82
30	B	622	SQD	O7-S-C6	3.89	112.56	106.76
25	J	102	BCR	C11-C10-C9	-3.86	121.86	127.28
30	A	413	SQD	O47-C7-C8	3.86	119.82	111.48
30	F	103	SQD	O5-C5-C4	3.84	116.62	109.70
30	b	602	SQD	O47-C7-C8	3.82	119.75	111.48
30	f	103	SQD	O5-C5-C4	3.81	116.56	109.70
30	B	627	SQD	O5-C5-C4	3.80	116.55	109.70
30	b	602	SQD	O5-C5-C4	3.76	116.48	109.70
30	f	103	SQD	O7-S-C6	3.76	112.36	106.76
30	a	401	SQD	O5-C5-C4	3.74	116.44	109.70
30	a	412	SQD	O47-C7-C8	3.74	119.57	111.48
30	a	412	SQD	O5-C5-C4	3.72	116.41	109.70
30	B	627	SQD	O47-C7-C8	3.72	119.53	111.48
30	A	413	SQD	O5-C5-C4	3.69	116.35	109.70
26	d	410	DGD	O6D-C1D-O3G	-3.69	101.33	110.04
30	a	401	SQD	O7-S-C6	3.62	112.16	106.76
26	D	407	DGD	O6D-C1D-O3G	-3.61	101.52	110.04
30	F	103	SQD	O6-C1-C2	3.59	113.73	108.27
25	j	102	BCR	C11-C10-C9	-3.58	122.26	127.28
22	B	610	CLA	CMB-C2B-C1B	-3.57	119.98	125.42
26	c	516	DGD	O3G-C3G-C2G	-3.57	102.14	110.82
26	C	515	DGD	O3G-C3G-C2G	-3.57	102.15	110.82
25	A	408	BCR	C2-C1-C6	3.56	115.61	110.44
23	A	405	PHO	C2B-C1B-NB	-3.54	106.87	109.43
30	F	103	SQD	O7-S-C6	3.51	112.00	106.76
30	B	622	SQD	O47-C7-C8	3.49	119.04	111.48
26	b	625	DGD	O3G-C3G-C2G	-3.46	102.40	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	414	SQD	O7-S-C6	3.45	111.91	106.76
30	f	103	SQD	O6-C1-C2	3.44	113.50	108.27
22	c	503	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
30	d	403	SQD	O47-C7-C8	3.43	118.90	111.48
30	B	627	SQD	O9-S-C6	3.43	111.87	106.76
22	b	615	CLA	CMB-C2B-C1B	-3.43	120.20	125.42
23	D	401	PHO	C2B-C1B-NB	-3.41	106.96	109.43
30	F	103	SQD	O47-C7-C8	3.41	118.85	111.48
22	b	618	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
26	c	515	DGD	O3G-C3G-C2G	-3.39	102.58	110.82
25	B	617	BCR	C15-C16-C17	-3.38	116.61	123.52
26	b	625	DGD	O6D-C1D-O3G	-3.38	102.06	110.04
26	B	620	DGD	O3G-C3G-C2G	-3.38	102.61	110.82
25	B	618	BCR	C2-C1-C6	3.37	115.33	110.44
23	d	402	PHO	C2B-C1B-NB	-3.37	107.00	109.43
30	b	602	SQD	O7-S-C6	3.37	111.78	106.76
25	j	102	BCR	C7-C8-C9	-3.35	121.28	126.23
30	A	414	SQD	O47-C7-C8	3.35	118.72	111.48
30	d	403	SQD	O7-S-C6	3.34	111.74	106.76
30	b	602	SQD	O9-S-C6	3.33	111.73	106.76
30	a	401	SQD	C44-O6-C1	3.32	120.92	113.80
23	d	401	PHO	C2B-C1B-NB	-3.32	107.03	109.43
26	B	620	DGD	O6D-C1D-O3G	-3.29	102.26	110.04
25	i	101	BCR	C2-C1-C6	3.29	115.22	110.44
22	C	503	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
22	B	603	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
22	B	613	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
26	C	514	DGD	O3G-C3G-C2G	-3.26	102.90	110.82
25	b	622	BCR	C15-C16-C17	-3.25	116.87	123.52
22	c	504	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
25	b	623	BCR	C2-C1-C6	3.23	115.14	110.44
25	J	102	BCR	C7-C8-C9	-3.23	121.45	126.23
26	c	516	DGD	O6D-C1D-O3G	-3.23	102.42	110.04
25	J	102	BCR	C24-C23-C22	-3.23	121.46	126.23
24	J	101	PL9	C7-C8-C9	-3.19	121.33	126.83
30	a	401	SQD	O47-C7-C8	3.19	118.38	111.48
30	f	103	SQD	O47-C7-C8	3.18	118.37	111.48
30	B	627	SQD	C3-C4-C5	3.18	116.00	110.23
22	C	502	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
25	b	623	BCR	C24-C23-C22	-3.17	121.55	126.23
32	b	604	LMT	C1'-O5'-C5'	-3.16	107.55	113.72
26	c	516	DGD	O5D-C6D-C5D	-3.15	102.31	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	627	SQD	O7-S-C6	3.15	111.46	106.76
22	C	507	CLA	O2D-CGD-O1D	-3.15	117.73	123.85
25	B	617	BCR	C33-C5-C6	-3.14	121.06	124.48
32	B	629	LMT	C1'-O5'-C5'	-3.13	107.60	113.72
23	d	402	PHO	O1D-CGD-CBD	3.13	129.48	124.72
24	j	101	PL9	C7-C8-C9	-3.13	121.45	126.83
22	B	604	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	b	622	BCR	C33-C5-C6	-3.12	121.08	124.48
22	C	504	CLA	O2D-CGD-O1D	-3.11	117.78	123.85
26	A	409	DGD	O6D-C1D-O3G	-3.11	102.69	110.04
22	a	403	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
22	B	605	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
22	b	613	CLA	C3B-C4B-NB	-3.11	107.76	110.53
25	x	101	BCR	C33-C5-C6	-3.10	121.10	124.48
32	i	103	LMT	O1'-C1'-C2'	3.09	112.97	108.27
25	J	102	BCR	C27-C26-C25	3.09	126.88	122.70
31	B	625	LMG	O6-C1-O1	-3.09	102.75	110.04
26	C	515	DGD	O5D-C6D-C5D	-3.08	102.47	109.42
22	B	608	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
30	a	412	SQD	O7-S-C6	3.08	111.35	106.76
22	B	606	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
30	A	414	SQD	C44-O6-C1	3.08	120.39	113.80
22	B	607	CLA	C3B-C4B-NB	-3.07	107.79	110.53
25	j	102	BCR	C27-C26-C25	3.07	126.85	122.70
22	c	507	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	D	401	PHO	O1D-CGD-CBD	3.06	129.37	124.72
22	B	608	CLA	C3B-C4B-NB	-3.06	107.80	110.53
22	a	405	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
25	c	521	BCR	C15-C16-C17	-3.05	117.27	123.52
25	F	102	BCR	C33-C5-C6	-3.05	121.15	124.48
26	C	515	DGD	O6D-C1D-O3G	-3.05	102.83	110.04
22	b	607	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
22	c	510	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
22	a	403	CLA	C3B-C4B-NB	-3.04	107.81	110.53
25	H	102	BCR	C33-C5-C6	-3.04	121.16	124.48
25	b	624	BCR	C2-C1-C6	3.04	114.86	110.44
26	c	515	DGD	O6D-C1D-O3G	-3.04	102.86	110.04
25	j	102	BCR	C24-C23-C22	-3.04	121.74	126.23
22	B	609	CLA	C3B-C4B-NB	-3.04	107.82	110.53
23	d	401	PHO	O1D-CGD-CBD	3.04	129.33	124.72
25	F	102	BCR	C29-C30-C25	3.04	114.85	110.44
30	d	403	SQD	C3-C4-C5	3.03	115.73	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	619	BCR	C2-C1-C6	3.03	114.85	110.44
26	B	626	DGD	O5D-C1E-C2E	3.03	112.88	108.27
22	C	519	CLA	C3B-C4B-NB	-3.03	107.83	110.53
22	b	614	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
25	g	101	BCR	C27-C26-C25	3.02	126.79	122.70
25	C	513	BCR	C15-C16-C17	-3.02	117.34	123.52
22	b	613	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
22	B	602	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
25	f	102	BCR	C29-C30-C25	3.01	114.81	110.44
22	b	612	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
22	A	402	CLA	C3B-C4B-NB	-3.01	107.84	110.53
30	d	403	SQD	O9-S-C6	3.01	111.25	106.76
25	f	102	BCR	C33-C5-C6	-3.01	121.20	124.48
30	A	413	SQD	O7-S-C6	3.01	111.25	106.76
22	A	403	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
22	C	505	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
25	g	101	BCR	C38-C26-C25	-3.00	121.21	124.48
25	y	101	BCR	C27-C26-C25	3.00	126.76	122.70
22	C	501	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
25	B	618	BCR	C24-C23-C22	-3.00	121.80	126.23
22	b	605	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
22	c	520	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
30	B	622	SQD	C3-C4-C5	2.99	115.66	110.23
22	A	402	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
22	c	505	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
26	C	516	DGD	CDB-CCB-CBB	-2.99	99.27	114.37
34	f	101	HEM	C3B-C2B-C1B	2.98	108.65	106.41
26	d	410	DGD	O3G-C3G-C2G	-2.98	103.56	110.82
31	d	408	LMG	O6-C1-O1	-2.98	103.00	110.04
32	I	102	LMT	O1'-C1'-C2'	2.98	112.80	108.27
32	b	629	LMT	C3'-C4'-C5'	-2.98	104.32	110.93
22	b	608	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
32	B	624	LMT	C3'-C4'-C5'	-2.98	104.33	110.93
22	b	610	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	b	624	BCR	C7-C8-C9	-2.98	121.83	126.23
26	b	601	DGD	O5D-C1E-C2E	2.97	112.79	108.27
22	c	508	CLA	C3B-C4B-NB	-2.97	107.88	110.53
22	c	502	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
23	A	405	PHO	O1D-CGD-CBD	2.97	129.22	124.72
26	c	517	DGD	CDB-CCB-CBB	-2.96	99.40	114.37
22	B	601	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
30	F	103	SQD	O9-S-C6	2.96	111.17	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
32	M	102	LMT	C1'-O5'-C5'	-2.96	107.95	113.72
22	C	502	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	b	614	CLA	C3B-C4B-NB	-2.95	107.89	110.53
22	A	404	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
22	c	506	CLA	C3B-C4B-NB	-2.95	107.90	110.53
25	c	521	BCR	C2-C1-C6	2.95	114.72	110.44
27	a	409	LHG	O8-C23-C24	2.94	120.81	111.83
22	b	612	CLA	C3B-C4B-NB	-2.94	107.91	110.53
30	b	602	SQD	C4-C3-C2	2.94	115.99	110.83
30	F	103	SQD	O8-S-C6	2.94	111.64	105.97
30	f	103	SQD	O8-S-C6	2.93	111.64	105.97
22	b	618	CLA	C3B-C4B-NB	-2.93	107.91	110.53
26	a	408	DGD	O6D-C1D-O3G	-2.93	103.12	110.04
22	B	613	CLA	C3B-C4B-NB	-2.93	107.92	110.53
30	a	412	SQD	C3-C4-C5	2.92	115.53	110.23
26	C	514	DGD	O6D-C1D-O3G	-2.92	103.15	110.04
22	C	508	CLA	C3B-C4B-NB	-2.92	107.92	110.53
22	B	609	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	c	501	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	d	407	PL9	C7-C8-C9	-2.91	121.81	126.83
27	A	410	LHG	O8-C23-C24	2.91	120.72	111.83
26	D	407	DGD	O3G-C3G-C2G	-2.91	103.75	110.82
25	J	102	BCR	C15-C14-C13	-2.91	123.20	127.28
30	A	414	SQD	O9-S-C6	2.91	111.10	106.76
22	B	610	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	b	601	DGD	O3G-C3G-C2G	-2.90	103.77	110.82
22	C	510	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
22	b	609	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
22	c	511	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
22	C	506	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
25	B	619	BCR	C7-C8-C9	-2.88	121.97	126.23
22	b	611	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	c	506	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
22	c	502	CLA	C3B-C4B-NB	-2.88	107.96	110.53
25	b	623	BCR	C29-C30-C25	2.87	114.61	110.44
26	d	410	DGD	C3D-C4D-C5D	-2.87	105.03	110.23
25	C	520	BCR	C2-C1-C6	2.87	114.61	110.44
25	y	101	BCR	C38-C26-C25	-2.87	121.36	124.48
22	B	607	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
30	a	401	SQD	O9-S-C6	2.86	111.03	106.76
24	A	407	PL9	C22-C23-C24	-2.86	121.09	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	516	DGD	CDB-CCB-CBB	-2.85	99.94	114.37
22	b	608	CLA	C1-C2-C3	-2.85	121.53	126.20
22	d	406	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
24	d	407	PL9	C40-C39-C41	2.85	120.17	115.23
25	b	623	BCR	C15-C16-C17	-2.84	117.70	123.52
22	b	619	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
26	d	410	DGD	CDB-CCB-CBB	-2.84	100.02	114.37
26	c	517	DGD	C1D-O6D-C5D	-2.84	108.18	113.72
22	C	509	CLA	C3B-C4B-NB	-2.84	108.00	110.53
25	B	618	BCR	C11-C10-C9	-2.84	123.30	127.28
25	b	624	BCR	C3-C4-C5	-2.83	109.00	114.06
25	g	101	BCR	C7-C8-C9	-2.83	122.05	126.23
31	i	102	LMG	O6-C1-O1	-2.83	103.36	110.04
22	C	512	CLA	C3B-C4B-NB	-2.83	108.00	110.53
25	K	101	BCR	C24-C23-C22	-2.83	122.05	126.23
32	B	628	LMT	C1'-O5'-C5'	-2.83	108.20	113.72
25	b	621	BCR	C33-C5-C6	-2.83	121.40	124.48
26	B	626	DGD	O3G-C3G-C2G	-2.83	103.95	110.82
30	B	622	SQD	C44-O6-C1	2.82	119.85	113.80
22	C	519	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
24	a	407	PL9	C22-C23-C24	-2.82	121.16	127.62
30	F	103	SQD	C44-O6-C1	2.82	119.85	113.80
30	f	103	SQD	C44-O6-C1	2.82	119.84	113.80
22	A	404	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	b	607	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	b	606	CLA	C3B-C4B-NB	-2.82	108.02	110.53
26	D	407	DGD	CDB-CCB-CBB	-2.81	100.14	114.37
26	C	515	DGD	CDB-CCB-CBB	-2.81	100.14	114.37
22	C	511	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
22	b	617	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
30	B	627	SQD	C4-C3-C2	2.81	115.76	110.83
22	c	509	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	B	614	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	D	405	PL9	C7-C8-C9	-2.80	122.00	126.83
26	C	516	DGD	C1D-C2D-C3D	-2.80	104.11	110.01
30	b	602	SQD	C3-C4-C5	2.80	115.31	110.23
34	f	101	HEM	C3B-C4B-NB	-2.80	107.46	109.47
23	D	401	PHO	O2D-CGD-O1D	-2.80	118.41	123.85
31	C	517	LMG	O6-C1-O1	-2.79	103.45	110.04
22	c	512	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	B	616	BCR	C33-C5-C6	-2.79	121.44	124.48
25	B	617	BCR	C15-C14-C13	-2.79	123.37	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	CHB-C4A-NA	2.79	128.42	124.40
23	d	402	PHO	CMB-C2B-C3B	2.79	130.25	124.68
22	B	612	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
22	C	512	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
30	f	103	SQD	O9-S-C6	2.78	110.91	106.76
25	C	513	BCR	C29-C30-C25	2.78	114.48	110.44
23	d	401	PHO	O2D-CGD-O1D	-2.78	118.44	123.85
22	b	615	CLA	C1-C2-C3	-2.77	121.65	126.20
25	B	617	BCR	C28-C27-C26	-2.77	109.11	114.06
31	c	518	LMG	O6-C1-O1	-2.77	103.49	110.04
22	c	503	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	b	615	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
22	a	404	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
23	D	401	PHO	CMB-C2B-C3B	2.76	130.20	124.68
25	C	520	BCR	C27-C26-C25	2.76	126.43	122.70
22	B	602	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	B	619	BCR	C3-C4-C5	-2.76	109.14	114.06
22	H	101	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
32	b	628	LMT	C1'-O5'-C5'	-2.76	108.33	113.72
25	c	514	BCR	C15-C16-C17	-2.75	117.89	123.52
22	b	619	CLA	C3B-C4B-NB	-2.75	108.08	110.53
25	y	101	BCR	C7-C8-C9	-2.75	122.17	126.23
25	b	622	BCR	C28-C27-C26	-2.75	109.16	114.06
22	C	511	CLA	C3B-C4B-NB	-2.74	108.08	110.53
34	F	101	HEM	C3B-C4B-NB	-2.74	107.50	109.47
22	D	404	CLA	C3B-C4B-NB	-2.74	108.08	110.53
22	B	603	CLA	C1-C2-C3	-2.74	121.72	126.20
23	A	405	PHO	O2D-CGD-O1D	-2.73	118.53	123.85
22	b	608	CLA	CHB-C4A-NA	2.73	128.34	124.40
22	a	405	CLA	C3B-C4B-NB	-2.73	108.09	110.53
30	A	413	SQD	C3-C4-C5	2.72	115.17	110.23
31	I	101	LMG	O6-C1-O1	-2.72	103.61	110.04
22	C	510	CLA	CHB-C4A-NA	2.72	128.33	124.40
22	D	404	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
25	c	514	BCR	C29-C30-C25	2.72	114.38	110.44
32	d	411	LMT	C3'-C4'-C5'	-2.71	104.92	110.93
22	C	503	CLA	C3B-C4B-NB	-2.71	108.11	110.53
25	B	618	BCR	C15-C16-C17	-2.71	117.97	123.52
22	c	509	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	B	605	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	B	626	DGD	C3G-C2G-C1G	-2.71	105.47	111.78
22	c	511	CLA	C3B-C4B-NB	-2.71	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	601	DGD	C3G-C2G-C1G	-2.70	105.48	111.78
25	B	618	BCR	C29-C30-C25	2.70	114.36	110.44
25	C	520	BCR	C15-C16-C17	-2.70	117.99	123.52
25	c	514	BCR	C11-C10-C9	-2.70	123.49	127.28
30	d	403	SQD	O8-S-C6	2.70	111.18	105.97
32	B	623	LMT	C1'-O5'-C5'	-2.70	108.45	113.72
22	B	604	CLA	CHB-C4A-NA	2.70	128.29	124.40
27	c	519	LHG	O8-C23-C24	2.70	120.06	111.83
24	d	407	PL9	C22-C23-C24	-2.70	121.45	127.62
32	D	408	LMT	C3'-C4'-C5'	-2.70	104.95	110.93
22	B	605	CLA	CHB-C4A-NA	2.70	128.29	124.40
30	B	622	SQD	O9-S-C6	2.69	110.78	106.76
22	B	610	CLA	C1-C2-C3	-2.69	121.79	126.20
34	F	101	HEM	C3B-C2B-C1B	2.69	108.43	106.41
25	b	623	BCR	C11-C10-C9	-2.69	123.50	127.28
24	D	405	PL9	C22-C23-C24	-2.69	121.47	127.62
25	b	622	BCR	C15-C14-C13	-2.69	123.51	127.28
22	b	616	CLA	C3B-C4B-NB	-2.69	108.13	110.53
25	J	102	BCR	C3-C4-C5	-2.68	109.27	114.06
22	c	520	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	B	603	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	b	606	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
22	D	403	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
22	b	608	CLA	C3B-C4B-NB	-2.67	108.14	110.53
26	c	517	DGD	O5D-C6D-C5D	-2.67	103.40	109.42
27	C	518	LHG	O8-C23-C24	2.67	119.97	111.83
22	A	403	CLA	CHB-C4A-NA	2.67	128.25	124.40
25	c	521	BCR	C27-C26-C25	2.67	126.31	122.70
22	c	510	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	c	507	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	b	610	CLA	C3B-C4B-NB	-2.66	108.15	110.53
30	d	403	SQD	C44-O6-C1	2.65	119.49	113.80
22	C	501	CLA	CHB-C4A-NA	2.65	128.23	124.40
24	D	405	PL9	C40-C39-C41	2.65	119.83	115.23
24	J	101	PL9	C22-C23-C24	-2.65	121.55	127.62
25	J	102	BCR	C15-C16-C17	-2.65	118.09	123.52
22	C	511	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	b	601	DGD	C1D-C2D-C3D	-2.65	104.44	110.01
22	c	508	CLA	CHB-C4A-NA	2.65	128.22	124.40
22	C	506	CLA	CHB-C4A-NA	2.65	128.22	124.40
24	j	101	PL9	C22-C23-C24	-2.65	121.57	127.62
22	b	609	CLA	C3B-C4B-NB	-2.64	108.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C15-C14-C13	-2.64	123.57	127.28
23	d	401	PHO	CMB-C2B-C3B	2.64	129.96	124.68
22	B	603	CLA	CHB-C4A-NA	2.64	128.21	124.40
22	b	610	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	B	619	BCR	C27-C26-C25	2.64	126.27	122.70
22	A	403	CLA	C3B-C4B-NB	-2.64	108.18	110.53
25	b	624	BCR	C27-C26-C25	2.63	126.26	122.70
22	B	611	CLA	C3B-C4B-NB	-2.63	108.18	110.53
26	c	517	DGD	C1D-C2D-C3D	-2.63	104.48	110.01
26	d	410	DGD	CFB-CEB-CDB	-2.63	101.08	114.37
22	D	404	CLA	C1-C2-C3	-2.63	121.89	126.20
25	J	102	BCR	C38-C26-C25	-2.62	121.62	124.48
25	i	101	BCR	C27-C26-C25	2.62	126.25	122.70
22	a	406	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	c	501	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	D	407	DGD	CFB-CEB-CDB	-2.62	101.13	114.37
22	c	506	CLA	CHB-C4A-NA	2.62	128.18	124.40
22	b	611	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	c	511	CLA	CHB-C4A-NA	2.61	128.17	124.40
25	c	513	BCR	C24-C23-C22	-2.61	122.37	126.23
31	D	409	LMG	C38-C37-C36	-2.61	101.18	114.37
25	j	102	BCR	C38-C26-C25	-2.61	121.64	124.48
25	A	408	BCR	C27-C26-C25	2.61	126.23	122.70
25	c	521	BCR	C15-C14-C13	-2.61	123.62	127.28
24	A	407	PL9	C41-C39-C40	2.61	120.58	114.59
26	C	516	DGD	O5D-C6D-C5D	-2.60	103.55	109.42
26	A	409	DGD	CBB-CAB-C9B	-2.60	101.20	114.37
24	d	407	PL9	C37-C38-C39	-2.60	121.67	127.62
22	B	613	CLA	CHB-C4A-NA	2.60	128.15	124.40
22	A	406	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
26	C	516	DGD	C1D-O6D-C5D	-2.60	108.64	113.72
22	a	404	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	C	506	CLA	C3B-C4B-NB	-2.59	108.21	110.53
30	a	412	SQD	O48-C23-C24	2.59	119.74	111.83
25	c	513	BCR	C7-C8-C9	-2.59	122.40	126.23
25	b	621	BCR	C2-C1-C6	2.59	114.20	110.44
22	b	619	CLA	CHB-C4A-NA	2.59	128.13	124.40
22	d	406	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	c	512	CLA	CHB-C4A-NA	2.58	128.13	124.40
25	c	514	BCR	C28-C27-C26	-2.58	109.45	114.06
23	d	402	PHO	O2D-CGD-O1D	-2.58	118.82	123.85
22	a	406	CLA	CHB-C4A-NA	2.58	128.12	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	612	CLA	CHB-C4A-NA	2.58	128.12	124.40
22	C	504	CLA	CHB-C4A-NA	2.58	128.12	124.40
25	B	616	BCR	C11-C10-C9	-2.58	123.67	127.28
22	b	606	CLA	CHB-C4A-NA	2.57	128.12	124.40
25	B	617	BCR	C29-C30-C25	2.57	114.18	110.44
25	B	616	BCR	C7-C8-C9	-2.57	122.43	126.23
22	B	601	CLA	C3B-C4B-NB	-2.57	108.24	110.53
25	c	514	BCR	C15-C14-C13	-2.57	123.68	127.28
22	C	503	CLA	CHB-C4A-NA	2.57	128.10	124.40
25	B	616	BCR	C2-C1-C6	2.56	114.16	110.44
22	a	406	CLA	C3B-C4B-NB	-2.56	108.24	110.53
22	d	405	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
22	C	519	CLA	CHB-C4A-NA	2.56	128.10	124.40
31	d	412	LMG	C38-C37-C36	-2.56	101.42	114.37
25	J	102	BCR	C35-C13-C14	-2.56	118.67	122.82
25	C	513	BCR	C28-C27-C26	-2.56	109.49	114.06
22	c	505	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	d	406	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	c	514	BCR	C33-C5-C6	-2.56	121.70	124.48
22	b	605	CLA	C3B-C4B-NB	-2.55	108.25	110.53
22	C	501	CLA	C3B-C4B-NB	-2.55	108.25	110.53
26	C	515	DGD	O6E-C1E-O5D	-2.55	104.02	110.04
26	c	516	DGD	C3G-C2G-C1G	-2.55	105.84	111.78
26	b	625	DGD	CBB-CAB-C9B	-2.55	101.49	114.37
22	B	608	CLA	CHB-C4A-NA	2.55	128.08	124.40
26	B	626	DGD	C1D-C2D-C3D	-2.54	104.66	110.01
22	C	509	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
31	d	408	LMG	C38-C37-C36	-2.54	101.52	114.37
22	B	606	CLA	C3B-C4B-NB	-2.54	108.26	110.53
22	A	404	CLA	CHB-C4A-NA	2.54	128.07	124.40
23	A	405	PHO	CMB-C2B-C3B	2.54	129.76	124.68
26	A	409	DGD	O5D-C6D-C5D	-2.54	103.69	109.42
26	C	516	DGD	CFB-CEB-CDB	-2.54	101.53	114.37
22	a	404	CLA	CHB-C4A-NA	2.54	128.06	124.40
22	c	508	CLA	O2D-CGD-O1D	-2.53	118.91	123.85
22	b	620	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
31	b	627	LMG	O6-C1-O1	-2.53	104.07	110.04
31	a	402	LMG	O6-C1-O1	-2.53	104.07	110.04
22	c	507	CLA	CHB-C4A-NA	2.53	128.05	124.40
22	c	520	CLA	CHB-C4A-NA	2.53	128.05	124.40
22	D	403	CLA	C3B-C4B-NB	-2.53	108.28	110.53
25	C	513	BCR	C33-C5-C6	-2.53	121.73	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	408	DGD	CBB-CAB-C9B	-2.53	101.60	114.37
25	b	622	BCR	C29-C30-C25	2.53	114.11	110.44
22	c	505	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	C	513	BCR	C15-C14-C13	-2.52	123.74	127.28
25	K	101	BCR	C11-C10-C9	-2.52	123.74	127.28
31	d	409	LMG	C38-C37-C36	-2.52	101.62	114.37
22	C	508	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	b	620	CLA	C3B-C4B-NB	-2.52	108.28	110.53
30	d	403	SQD	O48-C23-C24	2.52	119.52	111.83
25	j	102	BCR	C3-C4-C5	-2.52	109.57	114.06
25	i	101	BCR	C15-C16-C17	-2.52	118.37	123.52
22	B	608	CLA	C1-C2-C3	-2.52	122.07	126.20
32	M	103	LMT	C1'-O5'-C5'	-2.52	108.81	113.72
22	B	612	CLA	C3B-C4B-NB	-2.51	108.29	110.53
22	B	609	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	b	603	LMT	C1'-O5'-C5'	-2.51	108.82	113.72
32	i	103	LMT	C1'-O5'-C5'	-2.51	108.83	113.72
22	C	512	CLA	CHB-C4A-NA	2.51	128.02	124.40
26	C	515	DGD	C3G-C2G-C1G	-2.51	105.94	111.78
25	c	513	BCR	C15-C16-C17	-2.50	118.39	123.52
30	A	413	SQD	O48-C23-C24	2.50	119.47	111.83
22	c	503	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	D	404	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	c	516	DGD	O6E-C1E-O5D	-2.50	104.13	110.04
27	C	518	LHG	C11-C10-C9	-2.50	101.73	114.37
22	B	607	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	B	622	SQD	O8-S-C6	2.50	110.80	105.97
22	c	504	CLA	C3B-C4B-NB	-2.50	108.30	110.53
22	B	615	CLA	C3B-C4B-NB	-2.49	108.30	110.53
30	a	401	SQD	O8-S-C6	2.49	110.79	105.97
26	c	517	DGD	CFB-CEB-CDB	-2.49	101.76	114.37
31	B	625	LMG	C38-C37-C36	-2.49	101.77	114.37
22	c	509	CLA	CHB-C4A-NA	2.49	128.00	124.40
24	D	405	PL9	C37-C38-C39	-2.49	121.92	127.62
25	B	616	BCR	C27-C26-C25	2.49	126.07	122.70
22	C	510	CLA	C3B-C4B-NB	-2.49	108.31	110.53
22	B	611	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	C	507	CLA	CHB-C4A-NA	2.49	127.99	124.40
34	f	101	HEM	C1B-NB-C4B	2.49	108.15	105.21
30	B	627	SQD	O48-C23-C24	2.49	119.42	111.83
22	b	616	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	C	511	CLA	O2A-CGA-O1A	-2.48	117.42	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	CLA	CHB-C4A-NA	2.48	127.98	124.40
31	L	101	LMG	C40-C39-C38	-2.48	101.83	114.37
22	B	614	CLA	C3B-C4B-NB	-2.48	108.32	110.53
25	b	621	BCR	C27-C26-C25	2.48	126.05	122.70
22	B	606	CLA	C1-C2-C3	-2.48	122.14	126.20
22	C	505	CLA	C3B-C4B-NB	-2.48	108.32	110.53
25	C	513	BCR	C11-C10-C9	-2.47	123.81	127.28
22	c	502	CLA	CHB-C4A-NA	2.47	127.97	124.40
30	B	627	SQD	O8-S-C6	2.47	110.75	105.97
25	b	624	BCR	C11-C10-C9	-2.47	123.81	127.28
25	b	623	BCR	C15-C14-C13	-2.47	123.81	127.28
24	a	407	PL9	C41-C39-C40	2.47	120.28	114.59
31	E	101	LMG	C1-C2-C3	-2.47	104.81	110.01
31	D	406	LMG	C38-C37-C36	-2.47	101.88	114.37
25	K	101	BCR	C15-C16-C17	-2.47	118.47	123.52
22	H	101	CLA	C3B-C4B-NB	-2.47	108.33	110.53
25	y	101	BCR	C1-C6-C5	-2.47	119.26	122.64
32	b	629	LMT	C1'-O5'-C5'	-2.47	108.90	113.72
22	C	505	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	d	407	PL9	C32-C33-C34	-2.46	121.99	127.62
22	b	613	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	a	403	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	b	612	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	j	102	BCR	C15-C16-C17	-2.46	118.48	123.52
30	A	413	SQD	C44-O6-C1	2.46	119.07	113.80
32	M	103	LMT	C3'-C4'-C5'	-2.46	105.48	110.93
22	B	606	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	C	508	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
26	B	620	DGD	CBB-CAB-C9B	-2.46	101.94	114.37
22	B	614	CLA	CHB-C4A-NA	2.46	127.94	124.40
25	b	621	BCR	C15-C14-C13	-2.46	123.83	127.28
24	a	407	PL9	C27-C28-C29	-2.46	122.00	127.62
22	H	101	CLA	CHB-C4A-NA	2.45	127.94	124.40
22	c	501	CLA	C3B-C4B-NB	-2.45	108.34	110.53
24	D	405	PL9	C20-C19-C21	2.45	119.49	115.23
22	B	603	CLA	O1D-CGD-CBD	2.45	129.36	124.52
22	c	511	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
22	B	602	CLA	CHB-C4A-NA	2.45	127.94	124.40
31	c	522	LMG	C40-C39-C38	-2.45	101.98	114.37
25	K	101	BCR	C7-C8-C9	-2.45	122.62	126.23
25	x	101	BCR	C29-C30-C25	2.44	113.99	110.44
24	D	405	PL9	C32-C33-C34	-2.44	122.04	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	101	PL9	O2-C1-C6	2.44	124.36	120.48
31	b	626	LMG	C40-C39-C38	-2.44	102.05	114.37
26	c	515	DGD	C3G-C2G-C1G	-2.44	106.11	111.78
24	D	405	PL9	C27-C28-C29	-2.43	122.06	127.62
24	a	407	PL9	C7-C8-C9	-2.43	122.65	126.83
25	c	513	BCR	C11-C10-C9	-2.43	123.87	127.28
24	a	407	PL9	O2-C1-C6	2.43	124.34	120.48
22	B	615	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	c	503	CLA	O2D-CGD-CBD	2.43	115.47	111.23
30	a	401	SQD	C1-O5-C5	2.42	118.45	113.72
31	l	101	LMG	C40-C39-C38	-2.42	102.13	114.37
25	B	618	BCR	C7-C8-C9	-2.42	122.66	126.23
27	c	519	LHG	C11-C10-C9	-2.42	102.14	114.37
30	F	103	SQD	C1-O5-C5	2.42	118.44	113.72
26	d	410	DGD	C3G-C2G-C1G	-2.42	106.14	111.78
25	i	101	BCR	C33-C5-C6	-2.42	121.84	124.48
24	A	407	PL9	C7-C8-C9	-2.42	122.67	126.83
22	B	604	CLA	C3B-C4B-NB	-2.42	108.37	110.53
30	B	622	SQD	O48-C23-C24	2.41	119.19	111.83
22	B	610	CLA	C3B-C4B-NB	-2.41	108.38	110.53
25	A	408	BCR	C15-C14-C13	-2.41	123.90	127.28
25	A	408	BCR	C33-C5-C6	-2.41	121.86	124.48
25	g	101	BCR	C1-C6-C5	-2.41	119.35	122.64
22	c	510	CLA	CHB-C4A-NA	2.41	127.87	124.40
24	D	405	PL9	O1-C4-C3	-2.41	118.19	120.73
25	b	623	BCR	C7-C8-C9	-2.41	122.68	126.23
22	a	405	CLA	CHB-C4A-NA	2.40	127.86	124.40
22	b	620	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	B	620	DGD	C3G-C2G-C1G	-2.40	106.20	111.78
26	b	625	DGD	C3G-C2G-C1G	-2.40	106.20	111.78
22	B	610	CLA	CHB-C1B-NB	2.40	127.64	124.05
31	C	521	LMG	C40-C39-C38	-2.39	102.26	114.37
24	d	407	PL9	C27-C28-C29	-2.39	122.14	127.62
25	F	102	BCR	C15-C16-C17	-2.39	118.62	123.52
22	b	616	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
22	b	611	CLA	CHB-C4A-NA	2.39	127.85	124.40
30	A	414	SQD	O48-C23-C24	2.39	119.11	111.83
25	j	102	BCR	C15-C14-C13	-2.39	123.93	127.28
22	B	615	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
31	D	406	LMG	O6-C1-C2	-2.38	105.47	110.37
22	b	613	CLA	C1-C2-C3	-2.38	122.30	126.20
31	b	626	LMG	O6-C1-O1	-2.38	104.42	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	402	CLA	CHB-C4A-NA	2.38	127.83	124.40
26	c	516	DGD	CFB-CEB-CDB	-2.38	102.35	114.37
22	b	617	CLA	C3B-C4B-NB	-2.38	108.41	110.53
25	b	624	BCR	C38-C26-C25	-2.37	121.89	124.48
31	d	412	LMG	O6-C1-O1	-2.37	104.43	110.04
25	c	513	BCR	C27-C26-C25	2.37	125.91	122.70
26	B	620	DGD	C4E-C3E-C2E	-2.37	106.66	110.83
22	b	617	CLA	CHB-C4A-NA	2.37	127.83	124.40
31	L	101	LMG	C38-C37-C36	-2.37	102.37	114.37
31	C	517	LMG	C38-C37-C36	-2.37	102.41	114.37
30	a	401	SQD	O48-C23-C24	2.37	119.05	111.83
22	c	504	CLA	CHB-C4A-NA	2.36	127.81	124.40
22	b	618	CLA	O2D-CGD-CBD	2.36	115.36	111.23
25	H	102	BCR	C29-C30-C25	2.36	113.87	110.44
22	A	406	CLA	CHB-C4A-NA	2.36	127.81	124.40
32	I	102	LMT	C1'-O5'-C5'	-2.36	109.11	113.72
22	C	509	CLA	CHB-C4A-NA	2.36	127.80	124.40
22	B	611	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
25	B	619	BCR	C38-C26-C25	-2.35	121.92	124.48
31	d	409	LMG	O6-C1-C2	-2.35	105.54	110.37
25	g	101	BCR	C15-C16-C17	-2.35	118.71	123.52
30	a	412	SQD	O8-S-C6	2.35	110.51	105.97
25	C	520	BCR	C11-C10-C9	-2.35	123.98	127.28
31	d	408	LMG	O2-C2-C1	-2.35	104.48	110.08
22	b	607	CLA	CHB-C4A-NA	2.35	127.79	124.40
31	e	101	LMG	O6-C1-O1	-2.34	104.50	110.04
24	d	407	PL9	C20-C19-C21	2.34	119.29	115.23
26	b	601	DGD	O6D-C1D-O3G	-2.34	104.51	110.04
24	A	407	PL9	O2-C1-C6	2.34	124.21	120.48
22	C	502	CLA	CHB-C4A-NA	2.34	127.78	124.40
34	F	101	HEM	C1B-NB-C4B	2.34	107.98	105.21
22	b	608	CLA	O1D-CGD-CBD	2.34	129.13	124.52
25	b	623	BCR	C27-C26-C25	2.34	125.86	122.70
22	b	615	CLA	CHB-C1B-NB	2.34	127.56	124.05
31	B	621	LMG	C40-C39-C38	-2.34	102.56	114.37
24	J	101	PL9	O2-C1-C6	2.34	124.20	120.48
24	d	407	PL9	O2-C1-C6	2.34	124.19	120.48
25	b	621	BCR	C15-C16-C17	-2.33	118.75	123.52
22	c	507	CLA	C1-C2-C3	-2.33	122.38	126.20
26	a	408	DGD	C3G-C2G-C1G	-2.33	106.35	111.78
25	K	101	BCR	C27-C26-C25	2.33	125.85	122.70
31	B	625	LMG	O3-C3-C2	-2.33	104.89	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	j	102	BCR	C35-C13-C14	-2.33	119.05	122.82
31	L	101	LMG	C1-C2-C3	-2.33	105.12	110.01
31	m	101	LMG	C1-O6-C5	-2.33	109.18	113.72
22	B	605	CLA	O1D-CGD-CBD	2.32	129.10	124.52
26	B	626	DGD	O6D-C1D-O3G	-2.32	104.55	110.04
25	c	513	BCR	C15-C14-C13	-2.32	124.02	127.28
31	l	101	LMG	C38-C37-C36	-2.32	102.64	114.37
22	C	503	CLA	O2D-CGD-CBD	2.32	115.29	111.23
22	b	614	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	F	102	BCR	C27-C26-C25	2.32	125.84	122.70
30	B	622	SQD	C4-C3-C2	2.32	114.90	110.83
31	B	625	LMG	O2-C2-C1	-2.32	104.56	110.08
22	b	615	CLA	C3B-C4B-NB	-2.32	108.46	110.53
26	C	515	DGD	CFB-CEB-CDB	-2.31	102.68	114.37
25	C	520	BCR	C24-C23-C22	-2.31	122.81	126.23
31	c	522	LMG	C38-C37-C36	-2.31	102.69	114.37
31	c	518	LMG	C38-C37-C36	-2.31	102.69	114.37
25	C	513	BCR	C24-C23-C22	-2.31	122.82	126.23
31	M	101	LMG	C1-O6-C5	-2.31	109.21	113.72
25	H	102	BCR	C16-C15-C14	-2.31	118.80	123.52
31	b	626	LMG	C38-C37-C36	-2.30	102.72	114.37
31	D	409	LMG	C1-C2-C3	-2.30	105.16	110.01
25	C	513	BCR	C38-C26-C25	-2.30	121.97	124.48
25	f	102	BCR	C15-C16-C17	-2.30	118.81	123.52
30	A	413	SQD	O8-S-C6	2.30	110.42	105.97
22	d	405	CLA	C3B-C4B-NB	-2.30	108.47	110.53
24	a	407	PL9	C20-C19-C21	2.30	119.22	115.23
25	y	101	BCR	C33-C5-C6	-2.30	121.97	124.48
25	b	624	BCR	C24-C23-C22	-2.30	122.83	126.23
30	A	414	SQD	C1-O5-C5	2.30	118.21	113.72
25	c	514	BCR	C38-C26-C25	-2.30	121.98	124.48
32	D	408	LMT	C1'-O5'-C5'	-2.29	109.24	113.72
22	c	504	CLA	O1D-CGD-CBD	2.29	129.04	124.52
24	J	101	PL9	C20-C19-C21	2.29	119.20	115.23
31	B	621	LMG	O6-C1-O1	-2.28	104.65	110.04
22	c	509	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
31	m	101	LMG	O2-C2-C1	-2.28	104.64	110.08
31	L	101	LMG	O7-C10-O9	-2.28	118.37	123.70
22	b	605	CLA	C1-C2-C3	-2.28	122.46	126.20
30	F	103	SQD	C3-C4-C5	2.28	114.37	110.23
31	b	626	LMG	O2-C2-C1	-2.28	104.65	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	C1-C2-C3	-2.28	122.47	126.20
22	C	504	CLA	C3B-C4B-NB	-2.28	108.50	110.53
31	E	101	LMG	O6-C1-O1	-2.27	104.67	110.04
31	B	621	LMG	C1-C2-C3	-2.27	105.23	110.01
30	b	602	SQD	O8-S-C6	2.27	110.36	105.97
30	A	414	SQD	O8-S-C6	2.27	110.35	105.97
25	c	521	BCR	C33-C5-C6	-2.27	122.01	124.48
31	D	409	LMG	O3-C3-C2	-2.27	105.03	110.38
30	d	403	SQD	C4-C3-C2	2.26	114.81	110.83
31	D	406	LMG	O6-C1-O1	-2.26	104.69	110.04
24	D	405	PL9	O2-C1-C6	2.26	124.08	120.48
25	C	520	BCR	C33-C5-C6	-2.26	122.01	124.48
31	C	521	LMG	O6-C1-O1	-2.26	104.69	110.04
22	C	504	CLA	O1D-CGD-CBD	2.26	128.98	124.52
31	C	521	LMG	C38-C37-C36	-2.26	102.94	114.37
22	b	619	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
22	B	611	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
25	c	521	BCR	C24-C23-C22	-2.26	122.89	126.23
31	I	101	LMG	O7-C10-O9	-2.26	118.42	123.70
25	A	408	BCR	C38-C26-C25	-2.26	122.02	124.48
25	F	102	BCR	C11-C10-C9	-2.26	124.11	127.28
24	A	407	PL9	C20-C19-C21	2.26	119.15	115.23
30	b	602	SQD	O48-C23-C24	2.26	118.72	111.83
31	c	522	LMG	O6-C1-O1	-2.26	104.71	110.04
31	C	517	LMG	O7-C10-O9	-2.26	118.43	123.70
31	b	626	LMG	C1-C2-C3	-2.26	105.27	110.01
25	b	624	BCR	C15-C16-C17	-2.25	118.91	123.52
22	D	403	CLA	CHB-C4A-NA	2.25	127.65	124.40
31	d	408	LMG	O3-C3-C2	-2.25	105.06	110.38
32	B	624	LMT	C1'-O5'-C5'	-2.25	109.32	113.72
26	A	409	DGD	C3G-C2G-C1G	-2.25	106.54	111.78
24	d	407	PL9	O1-C4-C3	-2.25	118.36	120.73
25	H	102	BCR	C27-C26-C25	2.25	125.74	122.70
24	A	407	PL9	C27-C28-C29	-2.25	122.48	127.62
30	f	103	SQD	C1-O5-C5	2.25	118.11	113.72
31	B	621	LMG	C38-C37-C36	-2.25	103.00	114.37
22	b	616	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
33	D	402	BCT	O3-C-O1	-2.25	113.93	119.68
25	f	102	BCR	C27-C26-C25	2.25	125.74	122.70
30	f	103	SQD	C3-C4-C5	2.25	114.30	110.23
26	b	601	DGD	CBB-CAB-C9B	-2.24	103.04	114.37
25	x	101	BCR	C15-C16-C17	-2.24	118.94	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	412	LMG	O3-C3-C2	-2.24	105.10	110.38
22	c	507	CLA	O2D-CGD-CBD	2.24	115.14	111.23
25	A	408	BCR	C15-C16-C17	-2.24	118.94	123.52
31	C	521	LMG	O2-C2-C1	-2.23	104.75	110.08
31	L	101	LMG	O3-C3-C2	-2.23	105.11	110.38
26	c	516	DGD	C3D-C4D-C5D	-2.23	106.19	110.23
25	F	102	BCR	C7-C8-C9	-2.23	122.93	126.23
25	j	102	BCR	C29-C30-C25	2.23	113.68	110.44
32	M	102	LMT	C3'-C4'-C5'	-2.23	105.99	110.93
31	c	518	LMG	O2-C2-C1	-2.23	104.76	110.08
26	b	601	DGD	CAB-C9B-C8B	-2.23	103.10	114.37
25	C	520	BCR	C7-C8-C9	-2.23	122.94	126.23
25	J	102	BCR	C20-C21-C22	-2.23	124.15	127.28
22	A	406	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	i	101	BCR	C38-C26-C25	-2.23	122.05	124.48
25	J	102	BCR	C29-C30-C25	2.23	113.67	110.44
31	I	101	LMG	O2-C2-C1	-2.23	104.77	110.08
22	b	610	CLA	O1D-CGD-CBD	2.23	128.91	124.52
22	C	504	CLA	C1-C2-C3	-2.23	122.55	126.20
26	a	408	DGD	CAB-C9B-C8B	-2.23	103.12	114.37
22	B	601	CLA	CHB-C4A-NA	2.23	127.61	124.40
31	l	101	LMG	O3-C3-C2	-2.22	105.13	110.38
33	d	404	BCT	O3-C-O1	-2.22	113.99	119.68
31	D	409	LMG	O7-C10-O9	-2.22	118.51	123.70
31	c	518	LMG	O7-C10-O9	-2.22	118.51	123.70
22	d	405	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
22	c	507	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
31	l	101	LMG	C1-C2-C3	-2.22	105.34	110.01
25	B	618	BCR	C27-C26-C25	2.22	125.70	122.70
24	j	101	PL9	O1-C4-C3	-2.22	118.39	120.73
31	d	409	LMG	O6-C1-O1	-2.22	104.80	110.04
31	m	101	LMG	C1-C2-C3	-2.22	105.35	110.01
25	g	101	BCR	C33-C5-C6	-2.21	122.07	124.48
25	B	619	BCR	C24-C23-C22	-2.21	122.96	126.23
30	a	412	SQD	C44-O6-C1	2.21	118.54	113.80
31	c	522	LMG	O2-C2-C1	-2.21	104.80	110.08
31	l	101	LMG	O7-C10-O9	-2.21	118.54	123.70
31	b	627	LMG	O7-C10-O9	-2.21	118.55	123.70
26	c	516	DGD	CBB-CAB-C9B	-2.21	103.22	114.37
25	B	617	BCR	C24-C23-C22	-2.20	122.98	126.23
26	A	409	DGD	CAB-C9B-C8B	-2.20	103.25	114.37
25	f	102	BCR	C11-C10-C9	-2.20	124.19	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	M	101	LMG	O2-C2-C1	-2.19	104.86	110.08
31	B	621	LMG	O7-C10-O9	-2.19	118.59	123.70
24	j	101	PL9	O2-C1-C2	-2.19	116.86	121.83
32	d	411	LMT	C1'-O5'-C5'	-2.19	109.45	113.72
31	e	101	LMG	C1-C2-C3	-2.18	105.42	110.01
25	b	623	BCR	C33-C5-C6	-2.18	122.10	124.48
22	b	605	CLA	CHB-C4A-NA	2.18	127.55	124.40
25	g	101	BCR	C3-C2-C1	-2.18	106.71	114.43
31	i	102	LMG	O2-C2-C1	-2.18	104.88	110.08
26	B	626	DGD	CAB-C9B-C8B	-2.18	103.35	114.37
26	C	515	DGD	CBB-CAB-C9B	-2.18	103.35	114.37
22	H	101	CLA	C1-C2-C3	-2.18	122.63	126.20
24	d	407	PL9	O2-C1-C2	-2.18	116.88	121.83
25	B	616	BCR	C38-C26-C25	-2.18	122.11	124.48
26	c	516	DGD	O3D-C3D-C4D	-2.18	105.24	110.38
25	K	101	BCR	C15-C14-C13	-2.18	124.22	127.28
26	A	409	DGD	CDB-CCB-CBB	-2.18	98.65	113.36
31	e	101	LMG	O3-C3-C2	-2.18	105.25	110.38
22	B	612	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
22	B	602	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
30	F	103	SQD	O48-C23-C24	2.17	118.46	111.83
30	f	103	SQD	O48-C23-C24	2.17	118.45	111.83
31	B	621	LMG	O2-C2-C1	-2.17	104.90	110.08
22	D	403	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
31	B	621	LMG	O3-C3-C2	-2.17	105.27	110.38
26	C	516	DGD	CBB-CAB-C9B	-2.17	103.41	114.37
22	b	607	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
24	D	405	PL9	O2-C1-C2	-2.17	116.91	121.83
31	C	517	LMG	O2-C2-C1	-2.16	104.92	110.08
34	v	201	HEM	C1B-NB-C4B	2.16	107.77	105.21
31	c	518	LMG	O1-C7-C8	-2.16	105.56	110.82
24	j	101	PL9	C20-C19-C21	2.16	118.98	115.23
22	c	508	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
25	i	101	BCR	C15-C14-C13	-2.16	124.25	127.28
25	b	622	BCR	C24-C23-C22	-2.16	123.04	126.23
22	B	613	CLA	O2D-CGD-CBD	2.16	115.01	111.23
25	y	101	BCR	C15-C16-C17	-2.16	119.10	123.52
25	c	513	BCR	C8-C7-C6	-2.16	121.23	127.00
25	g	101	BCR	C24-C23-C22	-2.16	123.04	126.23
31	C	521	LMG	O3-C3-C2	-2.16	105.29	110.38
22	b	617	CLA	C1-C2-C3	-2.15	122.67	126.20
27	a	409	LHG	C27-C26-C25	-2.15	103.48	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	410	LHG	C27-C26-C25	-2.15	103.48	114.37
31	M	101	LMG	C1-C2-C3	-2.15	105.48	110.01
24	a	407	PL9	O2-C1-C2	-2.15	116.94	121.83
31	a	402	LMG	O3-C3-C2	-2.15	105.31	110.38
25	b	622	BCR	C35-C13-C14	-2.15	119.33	122.82
25	J	102	BCR	C33-C5-C6	-2.15	122.14	124.48
22	B	611	CLA	C1-C2-C3	-2.15	122.68	126.20
22	b	617	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
31	i	102	LMG	O3-C3-C2	-2.14	105.32	110.38
24	J	101	PL9	O2-C1-C2	-2.14	116.95	121.83
26	a	408	DGD	CDB-CCB-CBB	-2.14	98.89	113.36
31	d	412	LMG	O7-C10-O9	-2.14	118.71	123.70
25	A	408	BCR	C24-C23-C22	-2.14	123.07	126.23
25	H	102	BCR	C15-C16-C17	-2.14	119.15	123.52
26	d	410	DGD	CAB-C9B-C8B	-2.14	103.57	114.37
24	A	407	PL9	O2-C1-C2	-2.13	116.97	121.83
22	B	603	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
25	C	520	BCR	C38-C26-C25	-2.13	122.16	124.48
22	C	519	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
26	B	626	DGD	CBB-CAB-C9B	-2.13	103.58	114.37
22	C	507	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
26	C	514	DGD	C5B-C4B-C3B	-2.13	103.59	114.37
22	b	617	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
34	v	201	HEM	C2A-C1A-NA	-2.13	107.79	110.15
22	C	512	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
25	B	619	BCR	C11-C10-C9	-2.13	124.29	127.28
22	C	501	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
31	b	626	LMG	O3-C3-C2	-2.13	105.36	110.38
22	B	602	CLA	C1-C2-C3	-2.13	122.71	126.20
22	B	614	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
25	B	619	BCR	C33-C5-C6	-2.13	122.16	124.48
22	C	508	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
26	c	516	DGD	CAB-C9B-C8B	-2.13	103.62	114.37
31	d	408	LMG	O1-C1-C2	-2.12	105.05	108.27
22	d	405	CLA	CHB-C4A-NA	2.12	127.47	124.40
26	b	625	DGD	CAB-C9B-C8B	-2.12	103.63	114.37
22	A	402	CLA	O1D-CGD-CBD	2.12	128.71	124.52
22	C	504	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
26	C	514	DGD	C3G-C2G-C1G	-2.12	106.84	111.78
22	c	506	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	j	102	BCR	C20-C21-C22	-2.12	124.31	127.28
22	c	504	CLA	CBA-CAA-C2A	2.12	120.10	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	616	BCR	C15-C16-C17	-2.12	119.19	123.52
26	c	515	DGD	C1D-C2D-C3D	-2.12	105.56	110.01
22	B	601	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	B	606	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	C	506	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
31	C	517	LMG	O3-C3-C2	-2.12	105.39	110.38
31	c	518	LMG	O3-C3-C2	-2.11	105.39	110.38
25	K	101	BCR	C8-C7-C6	-2.11	121.35	127.00
22	C	507	CLA	O2D-CGD-CBD	2.11	114.92	111.23
22	a	404	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
31	d	408	LMG	O7-C10-O9	-2.11	118.77	123.70
25	b	623	BCR	C20-C21-C22	-2.11	124.32	127.28
31	a	402	LMG	O1-C7-C8	-2.11	105.69	110.82
26	c	515	DGD	C5B-C4B-C3B	-2.11	103.71	114.37
22	C	505	CLA	C1-C2-C3	-2.11	122.74	126.20
26	b	625	DGD	C1D-C2D-C3D	-2.11	105.58	110.01
31	c	522	LMG	O3-C3-C2	-2.11	105.41	110.38
31	I	101	LMG	O3-C3-C2	-2.11	105.41	110.38
26	C	515	DGD	CAB-C9B-C8B	-2.10	103.74	114.37
26	c	517	DGD	CBB-CAB-C9B	-2.10	103.74	114.37
31	d	412	LMG	C1-C2-C3	-2.10	105.59	110.01
22	C	512	CLA	O1D-CGD-CBD	2.10	128.66	124.52
25	K	101	BCR	C3-C4-C5	-2.10	110.31	114.06
31	b	627	LMG	O1-C7-C8	-2.10	105.72	110.82
22	B	612	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
22	a	405	CLA	C1-C2-C3	-2.10	122.76	126.20
25	b	624	BCR	C33-C5-C6	-2.10	122.20	124.48
25	C	520	BCR	C15-C14-C13	-2.09	124.34	127.28
22	c	520	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
22	C	502	CLA	O2D-CGD-CBD	2.09	114.89	111.23
25	B	617	BCR	C8-C7-C6	-2.09	121.41	127.00
25	b	621	BCR	C11-C10-C9	-2.09	124.34	127.28
22	B	610	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
24	A	407	PL9	O1-C4-C3	-2.09	118.53	120.73
31	B	625	LMG	O7-C10-O9	-2.09	118.82	123.70
26	D	407	DGD	CAB-C9B-C8B	-2.09	103.81	114.37
25	B	616	BCR	C15-C14-C13	-2.09	124.35	127.28
31	b	626	LMG	O7-C10-O9	-2.09	118.82	123.70
25	B	618	BCR	C33-C5-C6	-2.09	122.21	124.48
22	A	404	CLA	C1-C2-C3	-2.09	122.78	126.20
30	a	412	SQD	C4-C3-C2	2.09	114.49	110.83
25	x	101	BCR	C27-C26-C25	2.09	125.52	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	PL9	O1-C4-C3	-2.09	118.53	120.73
22	B	610	CLA	CHB-C4A-NA	2.08	127.41	124.40
31	E	101	LMG	O3-C3-C2	-2.08	105.47	110.38
25	c	521	BCR	C11-C10-C9	-2.08	124.36	127.28
31	C	517	LMG	O1-C7-C8	-2.08	105.76	110.82
22	a	403	CLA	O1D-CGD-CBD	2.08	128.62	124.52
26	C	515	DGD	C5B-C4B-C3B	-2.08	103.86	114.37
24	J	101	PL9	C8-C7-C3	2.08	117.40	112.03
22	c	501	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
27	c	519	LHG	C27-C26-C25	-2.07	103.89	114.37
34	F	101	HEM	CHB-C1B-NB	2.07	126.93	124.37
34	f	101	HEM	CHB-C1B-NB	2.07	126.93	124.37
22	A	403	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	D	407	DGD	C3D-C4D-C5D	-2.07	106.47	110.23
31	b	627	LMG	O3-C3-C2	-2.07	105.49	110.38
24	j	101	PL9	C12-C13-C14	-2.07	122.88	127.62
26	C	515	DGD	O3D-C3D-C4D	-2.07	105.50	110.38
25	b	622	BCR	C7-C8-C9	-2.07	123.17	126.23
26	C	516	DGD	CAB-C9B-C8B	-2.07	103.91	114.37
23	d	401	PHO	O2A-CGA-O1A	-2.07	118.46	123.63
22	b	620	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
22	C	510	CLA	C1-C2-C3	-2.07	122.81	126.20
25	B	618	BCR	C29-C28-C27	2.06	115.82	111.28
25	f	102	BCR	C24-C23-C22	-2.06	123.18	126.23
22	b	614	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
26	d	410	DGD	C5B-C4B-C3B	-2.06	103.94	114.37
22	C	502	CLA	C1-C2-C3	-2.06	122.82	126.20
24	a	407	PL9	C32-C33-C34	-2.06	122.90	127.62
27	C	518	LHG	C27-C26-C25	-2.06	103.94	114.37
24	J	101	PL9	C12-C13-C14	-2.06	122.91	127.62
26	D	407	DGD	C5B-C4B-C3B	-2.06	103.95	114.37
26	a	408	DGD	O5D-C6D-C5D	-2.06	104.78	109.42
22	B	612	CLA	C1-C2-C3	-2.06	122.83	126.20
25	y	101	BCR	C3-C2-C1	-2.05	107.16	114.43
26	D	407	DGD	CBB-CAB-C9B	-2.05	103.99	114.37
25	c	514	BCR	C24-C23-C22	-2.05	123.20	126.23
25	f	102	BCR	C38-C26-C25	-2.05	122.25	124.48
31	i	102	LMG	O7-C10-O9	-2.05	118.91	123.70
22	b	608	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
23	A	405	PHO	O2A-CGA-O1A	-2.05	118.50	123.63
22	B	607	CLA	O1D-CGD-CBD	2.05	128.56	124.52
22	b	615	CLA	CHB-C4A-NA	2.05	127.36	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	521	BCR	C38-C26-C25	-2.05	122.25	124.48
25	b	623	BCR	C29-C28-C27	2.05	115.78	111.28
26	d	410	DGD	CBB-CAB-C9B	-2.05	104.03	114.37
31	a	402	LMG	O7-C10-O9	-2.05	118.92	123.70
31	D	409	LMG	O2-C2-C1	-2.05	105.20	110.08
24	D	405	PL9	C42-C43-C44	-2.04	122.94	127.62
22	c	510	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
25	b	622	BCR	C8-C7-C6	-2.04	121.54	127.00
22	a	405	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
31	M	101	LMG	O3-C3-C2	-2.04	105.57	110.38
25	c	513	BCR	C3-C4-C5	-2.04	110.42	114.06
25	H	102	BCR	C38-C26-C25	-2.04	122.26	124.48
31	l	101	LMG	O6-C1-O1	-2.04	105.23	110.04
31	e	101	LMG	O7-C10-O9	-2.03	118.95	123.70
31	D	409	LMG	O6-C1-O1	-2.03	105.24	110.04
25	F	102	BCR	C38-C26-C25	-2.03	122.27	124.48
25	b	622	BCR	C38-C26-C25	-2.03	122.27	124.48
25	j	102	BCR	C33-C5-C6	-2.03	122.27	124.48
31	d	408	LMG	C22-C21-C20	-2.03	104.11	114.37
22	c	505	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	b	621	BCR	C38-C26-C25	-2.03	122.27	124.48
31	d	409	LMG	C4-C3-C2	-2.03	107.27	110.83
26	a	408	DGD	C5B-C4B-C3B	-2.03	104.11	114.37
22	b	611	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
26	A	409	DGD	C5B-C4B-C3B	-2.03	104.12	114.37
22	b	605	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
25	B	617	BCR	C7-C8-C9	-2.03	123.24	126.23
26	c	517	DGD	CAB-C9B-C8B	-2.03	104.13	114.37
30	a	401	SQD	C4-C3-C2	2.03	114.39	110.83
22	b	607	CLA	O2D-CGD-CBD	2.02	114.77	111.23
31	l	101	LMG	O2-C2-C1	-2.02	105.25	110.08
22	B	607	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
31	E	101	LMG	O2-C2-C1	-2.02	105.26	110.08
22	b	612	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	C	516	DGD	C5B-C4B-C3B	-2.02	104.16	114.37
25	y	101	BCR	C24-C23-C22	-2.02	123.25	126.23
22	B	609	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
26	a	408	DGD	C1D-C2D-C3D	-2.01	105.77	110.01
31	B	625	LMG	C22-C21-C20	-2.01	104.20	114.37
22	B	612	CLA	CMB-C2B-C3B	2.01	131.28	126.55
22	c	504	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
26	B	620	DGD	CAB-C9B-C8B	-2.01	104.21	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	625	LMG	O1-C1-C2	-2.01	105.22	108.27
25	c	513	BCR	C33-C5-C6	-2.01	122.29	124.48
22	A	404	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
31	m	101	LMG	O3-C3-C2	-2.01	105.65	110.38
22	c	510	CLA	O1D-CGD-CBD	2.01	128.47	124.52
22	b	607	CLA	C1-C2-C3	-2.00	122.91	126.20
26	b	625	DGD	CDB-CCB-CBB	-2.00	99.83	113.36
24	D	405	PL9	C12-C13-C14	-2.00	123.04	127.62
26	b	625	DGD	C5B-C4B-C3B	-2.00	104.24	114.37
25	B	617	BCR	C35-C13-C14	-2.00	119.57	122.82
26	B	620	DGD	C5B-C4B-C3B	-2.00	104.26	114.37

All (68) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	404	CLA	ND
22	A	406	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	609	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	C	501	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	519	CLA	ND
22	D	403	CLA	ND
22	H	101	CLA	ND
22	a	403	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	406	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	b	617	CLA	ND
22	b	618	CLA	ND
22	b	619	CLA	ND
22	b	620	CLA	ND
22	c	501	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	520	CLA	ND
22	d	405	CLA	ND

All (2097) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	404	CLA	C4B-C3B-CAB-CBB
22	B	601	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	C4-C3-C5-C6
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C2B-C3B-CAB-CBB
22	B	605	CLA	C4B-C3B-CAB-CBB
22	B	606	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C4B-C3B-CAB-CBB
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C2B-C3B-CAB-CBB
22	B	608	CLA	C4B-C3B-CAB-CBB
22	B	609	CLA	C2B-C3B-CAB-CBB
22	B	609	CLA	C4B-C3B-CAB-CBB
22	B	609	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	C2B-C3B-CAB-CBB
22	B	610	CLA	C4B-C3B-CAB-CBB
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	C2B-C3B-CAB-CBB
22	B	615	CLA	C4B-C3B-CAB-CBB
22	B	615	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	C2B-C3B-CAB-CBB
22	C	509	CLA	C4B-C3B-CAB-CBB
22	C	511	CLA	C1A-C2A-CAA-CBA
22	D	403	CLA	C4-C3-C5-C6
22	H	101	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C6-C7-C8-C9
22	a	403	CLA	CBD-CGD-O2D-CED
22	a	404	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C3A-C2A-CAA-CBA
22	a	405	CLA	C4B-C3B-CAB-CBB
22	b	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	C1A-C2A-CAA-CBA
22	b	606	CLA	C2-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
22	b	606	CLA	C6-C7-C8-C9
22	b	607	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C1A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C2B-C3B-CAB-CBB
22	b	611	CLA	C4B-C3B-CAB-CBB
22	b	612	CLA	C1A-C2A-CAA-CBA
22	b	613	CLA	C2B-C3B-CAB-CBB
22	b	613	CLA	C4B-C3B-CAB-CBB
22	b	614	CLA	C2B-C3B-CAB-CBB
22	b	614	CLA	C4B-C3B-CAB-CBB
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	C2B-C3B-CAB-CBB
22	b	615	CLA	C4B-C3B-CAB-CBB
22	b	617	CLA	CBD-CGD-O2D-CED
22	b	618	CLA	CAD-CBD-CGD-O1D
22	b	618	CLA	CAD-CBD-CGD-O2D
22	b	620	CLA	C1A-C2A-CAA-CBA
22	b	620	CLA	C3A-C2A-CAA-CBA
22	b	620	CLA	C2B-C3B-CAB-CBB
22	b	620	CLA	C4B-C3B-CAB-CBB
22	b	620	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	C1A-C2A-CAA-CBA
22	c	504	CLA	C3A-C2A-CAA-CBA
22	c	504	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	C2B-C3B-CAB-CBB
22	c	509	CLA	C4B-C3B-CAB-CBB
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	C6-C7-C8-C9
22	d	405	CLA	C4-C3-C5-C6
24	A	407	PL9	C7-C8-C9-C10
24	A	407	PL9	C7-C8-C9-C11
24	A	407	PL9	C12-C13-C14-C15
24	A	407	PL9	C12-C13-C14-C16
24	A	407	PL9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
24	A	407	PL9	C22-C23-C24-C25
24	A	407	PL9	C27-C28-C29-C30
24	A	407	PL9	C27-C28-C29-C31
24	A	407	PL9	C37-C38-C39-C41
24	D	405	PL9	C27-C28-C29-C31
24	D	405	PL9	C34-C36-C37-C38
24	J	101	PL9	C7-C8-C9-C10
24	J	101	PL9	C12-C13-C14-C16
24	J	101	PL9	C22-C23-C24-C25
24	J	101	PL9	C22-C23-C24-C26
24	a	407	PL9	C7-C8-C9-C11
24	a	407	PL9	C12-C13-C14-C15
24	a	407	PL9	C12-C13-C14-C16
24	a	407	PL9	C22-C23-C24-C25
24	a	407	PL9	C27-C28-C29-C30
24	a	407	PL9	C27-C28-C29-C31
24	a	407	PL9	C37-C38-C39-C40
24	a	407	PL9	C37-C38-C39-C41
24	d	407	PL9	C27-C28-C29-C31
24	d	407	PL9	C34-C36-C37-C38
24	j	101	PL9	C7-C8-C9-C11
24	j	101	PL9	C12-C13-C14-C16
24	j	101	PL9	C22-C23-C24-C25
24	j	101	PL9	C22-C23-C24-C26
25	B	617	BCR	C7-C8-C9-C10
25	B	617	BCR	C21-C22-C23-C24
25	B	617	BCR	C23-C24-C25-C26
25	B	617	BCR	C23-C24-C25-C30
25	C	520	BCR	C7-C8-C9-C10
25	C	520	BCR	C7-C8-C9-C34
25	F	102	BCR	C7-C8-C9-C10
25	H	102	BCR	C21-C22-C23-C24
25	J	102	BCR	C21-C22-C23-C24
25	K	101	BCR	C6-C7-C8-C9
25	y	101	BCR	C7-C8-C9-C10
25	b	622	BCR	C21-C22-C23-C24
25	b	622	BCR	C23-C24-C25-C26
25	c	513	BCR	C6-C7-C8-C9
25	c	521	BCR	C7-C8-C9-C10
25	c	521	BCR	C7-C8-C9-C34
25	f	102	BCR	C7-C8-C9-C10
25	j	102	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	g	101	BCR	C7-C8-C9-C10
25	x	101	BCR	C7-C8-C9-C34
25	x	101	BCR	C21-C22-C23-C24
26	A	409	DGD	C2D-C1D-O3G-C3G
26	B	620	DGD	C2E-C1E-O5D-C6D
26	B	626	DGD	O1B-C1B-O2G-C2G
26	B	626	DGD	O2G-C2G-C3G-O3G
26	B	626	DGD	C2E-C1E-O5D-C6D
26	B	626	DGD	O6E-C1E-O5D-C6D
26	C	514	DGD	C2B-C1B-O2G-C2G
26	C	514	DGD	O1B-C1B-O2G-C2G
26	C	515	DGD	C2B-C1B-O2G-C2G
26	C	515	DGD	O1B-C1B-O2G-C2G
26	C	516	DGD	O6D-C1D-O3G-C3G
26	D	407	DGD	O1B-C1B-O2G-C2G
26	D	407	DGD	O6D-C1D-O3G-C3G
26	a	408	DGD	C2D-C1D-O3G-C3G
26	b	601	DGD	O1B-C1B-O2G-C2G
26	b	601	DGD	O2G-C2G-C3G-O3G
26	b	601	DGD	C2E-C1E-O5D-C6D
26	b	601	DGD	O6E-C1E-O5D-C6D
26	c	515	DGD	C2B-C1B-O2G-C2G
26	c	515	DGD	O1B-C1B-O2G-C2G
26	c	515	DGD	C2E-C1E-O5D-C6D
26	c	516	DGD	O1B-C1B-O2G-C2G
26	c	516	DGD	C2D-C1D-O3G-C3G
26	c	517	DGD	O6D-C1D-O3G-C3G
26	d	410	DGD	O6D-C1D-O3G-C3G
27	A	410	LHG	C1-C2-C3-O3
27	C	518	LHG	C3-O3-P-O6
27	C	518	LHG	C4-O6-P-O3
27	C	518	LHG	C4-O6-P-O4
27	C	518	LHG	C4-O6-P-O5
27	a	409	LHG	C1-C2-C3-O3
27	c	519	LHG	C3-O3-P-O6
27	c	519	LHG	C4-O6-P-O3
27	c	519	LHG	C4-O6-P-O4
27	c	519	LHG	C4-O6-P-O5
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	C5-C6-S-O7
30	A	413	SQD	C5-C6-S-O8
30	A	413	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
30	A	414	SQD	O10-C23-O48-C46
30	A	414	SQD	C24-C23-O48-C46
30	B	622	SQD	C2-C1-O6-C44
30	B	622	SQD	O5-C1-O6-C44
30	B	622	SQD	O49-C7-O47-C45
30	B	622	SQD	C8-C7-O47-C45
30	B	627	SQD	O5-C5-C6-S
30	a	401	SQD	C24-C23-O48-C46
30	a	412	SQD	C5-C6-S-O7
30	a	412	SQD	C5-C6-S-O8
30	a	412	SQD	C5-C6-S-O9
30	b	602	SQD	O5-C5-C6-S
30	d	403	SQD	C2-C1-O6-C44
30	d	403	SQD	O49-C7-O47-C45
30	d	403	SQD	C8-C7-O47-C45
31	B	621	LMG	C11-C10-O7-C8
31	B	625	LMG	O1-C7-C8-O7
31	B	625	LMG	C11-C10-O7-C8
31	C	517	LMG	C9-C8-O7-C10
31	C	517	LMG	O9-C10-O7-C8
31	C	517	LMG	C11-C10-O7-C8
31	D	406	LMG	O6-C1-O1-C7
31	D	409	LMG	O9-C10-O7-C8
31	D	409	LMG	C11-C10-O7-C8
31	M	101	LMG	O9-C10-O7-C8
31	b	626	LMG	C11-C10-O7-C8
31	c	518	LMG	C9-C8-O7-C10
31	c	518	LMG	O9-C10-O7-C8
31	c	518	LMG	C11-C10-O7-C8
31	c	518	LMG	O10-C28-O8-C9
31	c	522	LMG	C2-C1-O1-C7
31	d	408	LMG	O1-C7-C8-O7
31	d	408	LMG	C11-C10-O7-C8
31	d	409	LMG	O6-C1-O1-C7
31	d	412	LMG	O9-C10-O7-C8
31	d	412	LMG	C11-C10-O7-C8
31	e	101	LMG	C7-C8-O7-C10
31	m	101	LMG	O9-C10-O7-C8
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	b	620	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
32	B	629	LMT	C3'-C4'-O1B-C1B
32	b	604	LMT	C3'-C4'-O1B-C1B
22	A	402	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	a	403	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	519	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	b	611	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	520	CLA	CBD-CGD-O2D-CED
30	a	401	SQD	O10-C23-O48-C46
31	d	408	LMG	O10-C28-O8-C9
26	b	625	DGD	C4D-C5D-C6D-O5D
24	A	407	PL9	C37-C38-C39-C40
30	F	103	SQD	C24-C23-O48-C46
30	f	103	SQD	C24-C23-O48-C46
31	d	409	LMG	C29-C28-O8-C9
31	l	101	LMG	C29-C28-O8-C9
30	F	103	SQD	O10-C23-O48-C46
30	f	103	SQD	O10-C23-O48-C46
31	B	625	LMG	O10-C28-O8-C9
31	C	517	LMG	O10-C28-O8-C9
31	D	406	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
31	E	101	LMG	O10-C28-O8-C9
31	L	101	LMG	O10-C28-O8-C9
31	d	409	LMG	O10-C28-O8-C9
31	e	101	LMG	O10-C28-O8-C9
31	l	101	LMG	O10-C28-O8-C9
22	B	601	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
32	b	603	LMT	C3'-C4'-O1B-C1B
22	B	604	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
26	D	407	DGD	O1A-C1A-O1G-C1G
26	d	410	DGD	O1B-C1B-O2G-C2G
31	B	621	LMG	O9-C10-O7-C8
31	B	625	LMG	O9-C10-O7-C8
31	I	101	LMG	O9-C10-O7-C8
31	a	402	LMG	O9-C10-O7-C8
31	b	626	LMG	O9-C10-O7-C8
31	b	627	LMG	O9-C10-O7-C8
31	d	408	LMG	O9-C10-O7-C8
31	d	409	LMG	O9-C10-O7-C8
31	i	102	LMG	O9-C10-O7-C8
22	b	607	CLA	O1D-CGD-O2D-CED
26	C	515	DGD	C4E-C5E-C6E-O5E
22	A	404	CLA	C3-C5-C6-C7
22	B	607	CLA	C3-C5-C6-C7
22	B	613	CLA	C3-C5-C6-C7
22	a	405	CLA	C3-C5-C6-C7
22	b	612	CLA	C3-C5-C6-C7
22	b	618	CLA	C3-C5-C6-C7
32	B	628	LMT	C3'-C4'-O1B-C1B
22	b	614	CLA	O1D-CGD-O2D-CED
31	C	517	LMG	C29-C28-O8-C9
31	D	406	LMG	C29-C28-O8-C9
31	L	101	LMG	C29-C28-O8-C9
31	c	518	LMG	C29-C28-O8-C9
22	B	605	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	b	618	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
23	d	402	PHO	CBD-CGD-O2D-CED
26	B	626	DGD	C2B-C1B-O2G-C2G
26	b	601	DGD	C2B-C1B-O2G-C2G
26	c	516	DGD	C2B-C1B-O2G-C2G
30	F	103	SQD	C8-C7-O47-C45
31	M	101	LMG	C11-C10-O7-C8
31	m	101	LMG	C11-C10-O7-C8
22	B	612	CLA	O1D-CGD-O2D-CED
22	C	519	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	C4-C3-C5-C6
22	H	101	CLA	C4-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
22	b	609	CLA	C4-C3-C5-C6
24	A	407	PL9	C30-C29-C31-C32
24	a	407	PL9	C30-C29-C31-C32
22	B	602	CLA	C2-C3-C5-C6
22	B	604	CLA	C2-C3-C5-C6
22	D	403	CLA	C2-C3-C5-C6
22	H	101	CLA	C2-C3-C5-C6
22	b	607	CLA	C2-C3-C5-C6
22	b	609	CLA	C2-C3-C5-C6
22	d	405	CLA	C2-C3-C5-C6
32	i	103	LMT	C3'-C4'-O1B-C1B
22	B	607	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	C2A-CAA-CBA-CGA
22	b	611	CLA	C2A-CAA-CBA-CGA
32	I	102	LMT	C3'-C4'-O1B-C1B
31	B	625	LMG	C29-C28-O8-C9
31	E	101	LMG	C29-C28-O8-C9
31	d	408	LMG	C29-C28-O8-C9
24	A	407	PL9	C17-C18-C19-C20
24	a	407	PL9	C7-C8-C9-C10
24	a	407	PL9	C17-C18-C19-C20
24	j	101	PL9	C7-C8-C9-C10
26	B	620	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
24	A	407	PL9	C22-C23-C24-C26
24	J	101	PL9	C7-C8-C9-C11
24	a	407	PL9	C17-C18-C19-C21
24	a	407	PL9	C22-C23-C24-C26
26	B	620	DGD	O6E-C5E-C6E-O5E
31	i	102	LMG	O6-C5-C6-O5
26	d	410	DGD	O1A-C1A-O1G-C1G
31	c	522	LMG	O10-C28-O8-C9
31	c	522	LMG	O9-C10-O7-C8
22	b	611	CLA	O1D-CGD-O2D-CED
26	c	516	DGD	C4E-C5E-C6E-O5E
22	c	501	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	C3-C5-C6-C7
22	H	101	CLA	C3-C5-C6-C7
23	A	405	PHO	C3-C5-C6-C7
23	d	401	PHO	C3-C5-C6-C7
23	D	401	PHO	CBD-CGD-O2D-CED
27	A	410	LHG	O2-C2-C3-O3
27	a	409	LHG	O2-C2-C3-O3
22	B	608	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	c	505	CLA	O1D-CGD-O2D-CED
23	A	405	PHO	CBA-CGA-O2A-C1
26	d	410	DGD	C2A-C1A-O1G-C1G
31	C	521	LMG	C29-C28-O8-C9
31	c	522	LMG	C29-C28-O8-C9
31	e	101	LMG	C29-C28-O8-C9
26	A	409	DGD	O6E-C5E-C6E-O5E
26	C	514	DGD	O6E-C5E-C6E-O5E
26	a	408	DGD	O6E-C5E-C6E-O5E
26	c	515	DGD	O6E-C5E-C6E-O5E
31	I	101	LMG	O6-C5-C6-O5
31	d	408	LMG	C4-C5-C6-O5
22	c	520	CLA	O1D-CGD-O2D-CED
26	b	625	DGD	O6E-C5E-C6E-O5E
26	D	407	DGD	C2B-C1B-O2G-C2G
26	d	410	DGD	C2B-C1B-O2G-C2G
30	f	103	SQD	C8-C7-O47-C45
31	a	402	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
31	b	627	LMG	C11-C10-O7-C8
31	d	409	LMG	C11-C10-O7-C8
31	B	625	LMG	O6-C5-C6-O5
26	C	514	DGD	C4E-C5E-C6E-O5E
24	J	101	PL9	C27-C28-C29-C31
24	j	101	PL9	C27-C28-C29-C31
22	C	501	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	C3-C5-C6-C7
26	C	515	DGD	O6E-C5E-C6E-O5E
22	c	508	CLA	O1D-CGD-O2D-CED
26	D	407	DGD	C2A-C1A-O1G-C1G
23	A	405	PHO	C4-C3-C5-C6
23	d	401	PHO	C4-C3-C5-C6
23	A	405	PHO	C2-C3-C5-C6
23	d	401	PHO	C2-C3-C5-C6
31	C	521	LMG	O10-C28-O8-C9
31	D	406	LMG	O9-C10-O7-C8
31	e	101	LMG	O9-C10-O7-C8
31	C	517	LMG	O6-C5-C6-O5
24	A	407	PL9	C24-C26-C27-C28
24	a	407	PL9	C24-C26-C27-C28
26	b	625	DGD	C4E-C5E-C6E-O5E
31	I	101	LMG	C4-C5-C6-O5
31	i	102	LMG	C4-C5-C6-O5
22	c	512	CLA	CBD-CGD-O2D-CED
34	V	201	HEM	C2D-C3D-CAD-CBD
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	610	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
26	C	515	DGD	O6D-C1D-O3G-C3G
26	b	625	DGD	O6E-C1E-O5D-C6D
26	c	515	DGD	O6E-C1E-O5D-C6D
26	c	516	DGD	O6D-C1D-O3G-C3G
30	d	403	SQD	O5-C1-O6-C44
31	C	517	LMG	O6-C1-O1-C7
31	C	521	LMG	O6-C1-O1-C7
31	E	101	LMG	O6-C1-O1-C7
31	a	402	LMG	O6-C1-O1-C7
31	b	627	LMG	O6-C1-O1-C7
31	c	518	LMG	O6-C1-O1-C7
31	c	522	LMG	O6-C1-O1-C7
31	e	101	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
26	B	620	DGD	C4E-C5E-C6E-O5E
22	B	611	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CBD-CGD-O2D-CED
23	A	405	PHO	O1A-CGA-O2A-C1
26	c	516	DGD	O6E-C5E-C6E-O5E
31	c	518	LMG	O6-C5-C6-O5
31	d	408	LMG	O6-C5-C6-O5
22	b	612	CLA	CBD-CGD-O2D-CED
31	D	406	LMG	C11-C10-O7-C8
26	c	515	DGD	C4E-C5E-C6E-O5E
34	V	201	HEM	C4D-C3D-CAD-CBD
22	B	615	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
22	b	620	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
23	d	401	PHO	CBA-CGA-O2A-C1
31	c	522	LMG	O6-C5-C6-O5
22	B	615	CLA	O1A-CGA-O2A-C1
22	C	509	CLA	CBD-CGD-O2D-CED
22	B	607	CLA	C6-C7-C8-C9
22	B	609	CLA	C14-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C9
22	C	510	CLA	C6-C7-C8-C9
22	b	612	CLA	C6-C7-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9
31	c	518	LMG	C4-C5-C6-O5
22	c	511	CLA	O1D-CGD-O2D-CED
23	d	402	PHO	O1D-CGD-O2D-CED
31	C	517	LMG	C8-C9-O8-C28
26	C	514	DGD	C2E-C1E-O5D-C6D
26	C	515	DGD	C2D-C1D-O3G-C3G
26	C	516	DGD	C2D-C1D-O3G-C3G
26	b	625	DGD	C2E-C1E-O5D-C6D
26	c	517	DGD	C2D-C1D-O3G-C3G
30	a	412	SQD	C2-C1-O6-C44
31	C	517	LMG	C2-C1-O1-C7
31	C	521	LMG	C2-C1-O1-C7
31	D	406	LMG	C2-C1-O1-C7
31	E	101	LMG	C2-C1-O1-C7
31	c	518	LMG	C2-C1-O1-C7
31	d	409	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
31	e	101	LMG	C2-C1-O1-C7
22	B	605	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
22	b	618	CLA	O1D-CGD-O2D-CED
26	A	409	DGD	C4E-C5E-C6E-O5E
26	a	408	DGD	C4E-C5E-C6E-O5E
31	c	522	LMG	C4-C5-C6-O5
22	B	606	CLA	O1D-CGD-O2D-CED
25	H	102	BCR	C7-C8-C9-C34
25	H	102	BCR	C37-C22-C23-C24
25	J	102	BCR	C37-C22-C23-C24
25	y	101	BCR	C7-C8-C9-C34
25	j	102	BCR	C37-C22-C23-C24
25	g	101	BCR	C7-C8-C9-C34
25	x	101	BCR	C37-C22-C23-C24
25	b	622	BCR	C7-C8-C9-C10
22	c	507	CLA	C2A-CAA-CBA-CGA
23	d	401	PHO	O1A-CGA-O2A-C1
22	A	402	CLA	C3-C5-C6-C7
22	a	403	CLA	C3-C5-C6-C7
31	C	521	LMG	C11-C10-O7-C8
31	c	522	LMG	C11-C10-O7-C8
26	C	515	DGD	O2G-C2G-C3G-O3G
26	c	516	DGD	O2G-C2G-C3G-O3G
30	A	414	SQD	O6-C44-C45-O47
31	C	517	LMG	C4-C5-C6-O5
22	c	511	CLA	CBA-CGA-O2A-C1
22	A	404	CLA	C10-C11-C12-C13
22	b	613	CLA	C13-C15-C16-C17
22	B	615	CLA	C5-C6-C7-C8
22	C	508	CLA	C5-C6-C7-C8
31	c	518	LMG	C28-C29-C30-C31
22	B	606	CLA	C15-C16-C17-C18
22	b	616	CLA	C5-C6-C7-C8
22	c	505	CLA	C5-C6-C7-C8
23	D	401	PHO	C15-C16-C17-C18
26	D	407	DGD	C1B-C2B-C3B-C4B
31	C	521	LMG	C10-C11-C12-C13
31	c	522	LMG	C10-C11-C12-C13
30	b	602	SQD	O10-C23-O48-C46
26	C	516	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
24	D	405	PL9	C29-C31-C32-C33
24	d	407	PL9	C29-C31-C32-C33
22	B	608	CLA	C13-C15-C16-C17
22	C	505	CLA	C15-C16-C17-C18
22	b	616	CLA	C13-C15-C16-C17
23	d	402	PHO	C15-C16-C17-C18
26	c	515	DGD	C1B-C2B-C3B-C4B
31	C	517	LMG	C10-C11-C12-C13
31	C	517	LMG	C28-C29-C30-C31
31	b	627	LMG	C28-C29-C30-C31
31	d	412	LMG	C10-C11-C12-C13
22	C	512	CLA	O1A-CGA-O2A-C1
31	I	101	LMG	C11-C10-O7-C8
22	C	512	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	CBA-CGA-O2A-C1
22	B	609	CLA	C8-C10-C11-C12
22	C	503	CLA	C10-C11-C12-C13
22	D	403	CLA	C15-C16-C17-C18
22	a	405	CLA	C10-C11-C12-C13
22	b	611	CLA	C15-C16-C17-C18
22	b	620	CLA	C5-C6-C7-C8
22	c	501	CLA	C15-C16-C17-C18
22	c	509	CLA	C15-C16-C17-C18
22	c	520	CLA	C15-C16-C17-C18
22	C	507	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
22	A	403	CLA	C15-C16-C17-C18
22	B	601	CLA	C13-C15-C16-C17
22	B	610	CLA	C15-C16-C17-C18
22	C	509	CLA	C15-C16-C17-C18
22	b	614	CLA	C8-C10-C11-C12
22	c	503	CLA	C10-C11-C12-C13
22	c	504	CLA	C10-C11-C12-C13
22	c	505	CLA	C15-C16-C17-C18
22	c	508	CLA	C5-C6-C7-C8
22	d	405	CLA	C13-C15-C16-C17
26	C	514	DGD	C1B-C2B-C3B-C4B
31	D	409	LMG	C10-C11-C12-C13
31	c	518	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	O1A-CGA-O2A-C1
26	B	620	DGD	O6E-C1E-O5D-C6D
26	C	514	DGD	O6E-C1E-O5D-C6D
30	A	413	SQD	O5-C1-O6-C44
30	a	412	SQD	O5-C1-O6-C44
31	I	101	LMG	O6-C1-O1-C7
31	i	102	LMG	O6-C1-O1-C7
22	B	603	CLA	C13-C15-C16-C17
22	B	606	CLA	C13-C15-C16-C17
22	B	611	CLA	C5-C6-C7-C8
22	B	615	CLA	C10-C11-C12-C13
22	C	519	CLA	C13-C15-C16-C17
22	C	519	CLA	C15-C16-C17-C18
22	D	403	CLA	C13-C15-C16-C17
22	b	605	CLA	C13-C15-C16-C17
22	b	608	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
22	b	620	CLA	C10-C11-C12-C13
22	c	507	CLA	C15-C16-C17-C18
22	d	405	CLA	C15-C16-C17-C18
31	i	102	LMG	C29-C28-O8-C9
22	b	620	CLA	O1A-CGA-O2A-C1
26	b	625	DGD	C1B-C2B-C3B-C4B
22	A	404	CLA	C15-C16-C17-C18
22	B	607	CLA	C15-C16-C17-C18
22	c	501	CLA	C8-C10-C11-C12
22	c	505	CLA	C13-C15-C16-C17
22	c	520	CLA	C13-C15-C16-C17
31	E	101	LMG	O9-C10-O7-C8
32	B	629	LMT	O1'-C1-C2-C3
22	b	606	CLA	C3-C5-C6-C7
22	B	607	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	C5-C6-C7-C8
22	C	501	CLA	C10-C11-C12-C13
22	C	501	CLA	C15-C16-C17-C18
22	C	505	CLA	C13-C15-C16-C17
22	C	506	CLA	C5-C6-C7-C8
22	C	507	CLA	C10-C11-C12-C13
22	c	507	CLA	C10-C11-C12-C13
31	c	518	LMG	C8-C9-O8-C28
26	d	410	DGD	C1B-C2B-C3B-C4B
22	a	405	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C5-C6-C7-C8
22	B	604	CLA	CBA-CGA-O2A-C1
22	C	511	CLA	CBA-CGA-O2A-C1
31	i	102	LMG	C11-C10-O7-C8
23	D	401	PHO	O1D-CGD-O2D-CED
31	a	402	LMG	C28-C29-C30-C31
22	C	512	CLA	C15-C16-C17-C18
26	c	517	DGD	O1B-C1B-O2G-C2G
22	B	601	CLA	C2A-CAA-CBA-CGA
30	B	627	SQD	C24-C23-O48-C46
22	A	406	CLA	C10-C11-C12-C13
22	B	614	CLA	C13-C15-C16-C17
22	C	501	CLA	C8-C10-C11-C12
22	C	504	CLA	C10-C11-C12-C13
22	C	507	CLA	C15-C16-C17-C18
22	C	510	CLA	C5-C6-C7-C8
22	b	615	CLA	C15-C16-C17-C18
22	b	619	CLA	C13-C15-C16-C17
22	b	620	CLA	C13-C15-C16-C17
22	c	510	CLA	C5-C6-C7-C8
26	b	625	DGD	O6D-C5D-C6D-O5D
22	c	511	CLA	O1A-CGA-O2A-C1
22	B	615	CLA	C3-C5-C6-C7
22	b	612	CLA	C15-C16-C17-C18
31	C	521	LMG	C4-C5-C6-O5
31	d	412	LMG	O6-C5-C6-O5
22	B	611	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
22	b	617	CLA	C5-C6-C7-C8
22	c	501	CLA	C10-C11-C12-C13
22	c	520	CLA	CBA-CGA-O2A-C1
30	b	602	SQD	C24-C23-O48-C46
31	C	521	LMG	O6-C5-C6-O5
31	M	101	LMG	O6-C5-C6-O5
26	B	620	DGD	C1B-C2B-C3B-C4B
22	B	607	CLA	C5-C6-C7-C8
22	c	512	CLA	C15-C16-C17-C18
24	D	405	PL9	C27-C28-C29-C30
30	F	103	SQD	O49-C7-O47-C45
31	C	521	LMG	O9-C10-O7-C8
26	D	407	DGD	C2D-C1D-O3G-C3G
26	D	407	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
26	d	410	DGD	C2D-C1D-O3G-C3G
26	d	410	DGD	C2E-C1E-O5D-C6D
31	I	101	LMG	C2-C1-O1-C7
31	d	408	LMG	C2-C1-O1-C7
31	i	102	LMG	C2-C1-O1-C7
22	c	503	CLA	C5-C6-C7-C8
26	a	408	DGD	C1B-C2B-C3B-C4B
31	I	101	LMG	C29-C28-O8-C9
25	B	617	BCR	C7-C8-C9-C34
25	F	102	BCR	C37-C22-C23-C24
25	b	622	BCR	C7-C8-C9-C34
25	b	622	BCR	C37-C22-C23-C24
32	b	604	LMT	O1'-C1-C2-C3
22	b	609	CLA	O1A-CGA-O2A-C1
22	b	610	CLA	C2A-CAA-CBA-CGA
22	C	519	CLA	C10-C11-C12-C13
32	b	628	LMT	O1'-C1-C2-C3
31	L	101	LMG	C4-C5-C6-O5
22	b	620	CLA	C3-C5-C6-C7
22	b	606	CLA	C5-C6-C7-C8
25	H	102	BCR	C11-C10-C9-C8
25	J	102	BCR	C20-C21-C22-C23
25	j	102	BCR	C20-C21-C22-C23
25	x	101	BCR	C11-C10-C9-C8
26	D	407	DGD	O6E-C1E-O5D-C6D
31	B	625	LMG	O6-C1-O1-C7
31	d	408	LMG	O6-C1-O1-C7
31	E	101	LMG	C28-C29-C30-C31
22	c	520	CLA	C10-C11-C12-C13
24	a	407	PL9	C33-C34-C36-C37
22	b	616	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	C5-C6-C7-C8
22	c	509	CLA	CBD-CGD-O2D-CED
31	D	409	LMG	O6-C5-C6-O5
30	B	627	SQD	O10-C23-O48-C46
22	B	603	CLA	C8-C10-C11-C12
22	c	512	CLA	O1D-CGD-O2D-CED
26	B	620	DGD	C3B-C4B-C5B-C6B
26	B	626	DGD	C5B-C6B-C7B-C8B
26	C	515	DGD	C2A-C3A-C4A-C5A
26	b	625	DGD	C3B-C4B-C5B-C6B
30	f	103	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	B	621	LMG	C31-C32-C33-C34
31	c	518	LMG	C29-C30-C31-C32
26	c	515	DGD	C3B-C4B-C5B-C6B
26	c	516	DGD	C2A-C3A-C4A-C5A
30	F	103	SQD	C12-C13-C14-C15
30	a	412	SQD	C14-C15-C16-C17
31	C	517	LMG	C29-C30-C31-C32
31	L	101	LMG	C34-C35-C36-C37
31	i	102	LMG	C12-C13-C14-C15
32	i	103	LMT	C6-C7-C8-C9
26	B	626	DGD	C9B-CAB-CBB-CCB
26	D	407	DGD	CCB-CDB-CEB-CFB
26	b	601	DGD	C5B-C6B-C7B-C8B
26	b	601	DGD	C9B-CAB-CBB-CCB
26	d	410	DGD	CEB-CFB-CGB-CHB
31	b	626	LMG	C31-C32-C33-C34
22	B	604	CLA	O1A-CGA-O2A-C1
27	C	518	LHG	C24-C23-O8-C6
32	B	623	LMT	C1-C2-C3-C4
32	b	628	LMT	C1-C2-C3-C4
26	D	407	DGD	C4B-C5B-C6B-C7B
26	D	407	DGD	C5B-C6B-C7B-C8B
26	d	410	DGD	CCB-CDB-CEB-CFB
26	C	514	DGD	C3A-C4A-C5A-C6A
26	C	514	DGD	C2B-C3B-C4B-C5B
26	C	514	DGD	C3B-C4B-C5B-C6B
26	c	515	DGD	C3A-C4A-C5A-C6A
31	B	625	LMG	C18-C19-C20-C21
31	I	101	LMG	C12-C13-C14-C15
31	a	402	LMG	C30-C31-C32-C33
31	l	101	LMG	C33-C34-C35-C36
32	I	102	LMT	C6-C7-C8-C9
22	C	501	CLA	C4B-C3B-CAB-CBB
22	C	504	CLA	C4B-C3B-CAB-CBB
22	b	610	CLA	C4B-C3B-CAB-CBB
22	c	501	CLA	C4B-C3B-CAB-CBB
22	c	504	CLA	C4B-C3B-CAB-CBB
30	A	413	SQD	C7-C8-C9-C10
26	C	516	DGD	CBA-CCA-CDA-CEA
26	b	625	DGD	C6B-C7B-C8B-C9B
22	C	511	CLA	O1A-CGA-O2A-C1
26	B	620	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
26	d	410	DGD	C4B-C5B-C6B-C7B
26	d	410	DGD	C5B-C6B-C7B-C8B
22	C	503	CLA	C5-C6-C7-C8
22	a	404	CLA	C15-C16-C17-C18
22	b	608	CLA	C8-C10-C11-C12
30	B	627	SQD	C8-C7-O47-C45
31	d	408	LMG	C18-C19-C20-C21
26	D	407	DGD	CEB-CFB-CGB-CHB
26	C	514	DGD	C1A-C2A-C3A-C4A
26	C	516	DGD	C1A-C2A-C3A-C4A
30	a	412	SQD	C7-C8-C9-C10
31	B	621	LMG	C10-C11-C12-C13
31	b	627	LMG	O6-C5-C6-O5
30	A	413	SQD	C14-C15-C16-C17
30	B	627	SQD	C9-C10-C11-C12
31	I	101	LMG	C14-C15-C16-C17
31	L	101	LMG	C33-C34-C35-C36
31	b	627	LMG	C30-C31-C32-C33
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	C3A-C2A-CAA-CBA
22	C	506	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	C3A-C2A-CAA-CBA
22	H	101	CLA	C3A-C2A-CAA-CBA
22	b	606	CLA	C3A-C2A-CAA-CBA
22	b	612	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C3A-C2A-CAA-CBA
26	c	516	DGD	C4A-C5A-C6A-C7A
30	a	412	SQD	C27-C28-C29-C30
31	D	406	LMG	C14-C15-C16-C17
31	i	102	LMG	C16-C17-C18-C19
31	l	101	LMG	C34-C35-C36-C37
31	b	627	LMG	C15-C16-C17-C18
22	B	615	CLA	C13-C15-C16-C17
22	H	101	CLA	C5-C6-C7-C8
26	c	517	DGD	CBA-CCA-CDA-CEA
22	b	615	CLA	CBA-CGA-O2A-C1
22	d	406	CLA	CBA-CGA-O2A-C1
26	A	409	DGD	C1G-C2G-C3G-O3G
26	B	620	DGD	C7A-C8A-C9A-CAA
26	D	407	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
31	l	101	LMG	C30-C31-C32-C33
31	d	408	LMG	C28-C29-C30-C31
26	c	515	DGD	C2B-C3B-C4B-C5B
26	d	410	DGD	C7B-C8B-C9B-CAB
31	L	101	LMG	C31-C32-C33-C34
22	c	520	CLA	O1A-CGA-O2A-C1
30	A	413	SQD	C27-C28-C29-C30
31	d	409	LMG	C14-C15-C16-C17
22	B	611	CLA	O1D-CGD-O2D-CED
31	L	101	LMG	O6-C5-C6-O5
26	b	625	DGD	C4B-C5B-C6B-C7B
30	b	602	SQD	C9-C10-C11-C12
31	B	625	LMG	C31-C32-C33-C34
31	C	521	LMG	C12-C13-C14-C15
31	D	409	LMG	C17-C18-C19-C20
31	b	627	LMG	C18-C19-C20-C21
31	b	627	LMG	C32-C33-C34-C35
31	c	522	LMG	C12-C13-C14-C15
31	d	408	LMG	C31-C32-C33-C34
26	C	515	DGD	C1A-C2A-C3A-C4A
26	b	601	DGD	C1A-C2A-C3A-C4A
22	A	404	CLA	C2B-C3B-CAB-CBB
22	B	606	CLA	C2B-C3B-CAB-CBB
22	a	405	CLA	C2B-C3B-CAB-CBB
25	C	513	BCR	C23-C24-C25-C26
25	C	513	BCR	C23-C24-C25-C30
25	H	102	BCR	C1-C6-C7-C8
25	H	102	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
25	b	622	BCR	C23-C24-C25-C30
25	c	514	BCR	C23-C24-C25-C26
25	c	514	BCR	C23-C24-C25-C30
25	g	101	BCR	C23-C24-C25-C26
25	g	101	BCR	C23-C24-C25-C30
25	x	101	BCR	C1-C6-C7-C8
25	x	101	BCR	C5-C6-C7-C8
26	C	514	DGD	C4A-C5A-C6A-C7A
26	c	517	DGD	C2B-C1B-O2G-C2G
30	b	602	SQD	C8-C7-O47-C45
26	C	515	DGD	C4A-C5A-C6A-C7A
30	F	103	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	I	101	LMG	C16-C17-C18-C19
31	L	101	LMG	C30-C31-C32-C33
26	A	409	DGD	C8B-C9B-CAB-CBB
26	a	408	DGD	C8B-C9B-CAB-CBB
30	f	103	SQD	C11-C12-C13-C14
31	D	406	LMG	C13-C14-C15-C16
22	A	402	CLA	C2A-CAA-CBA-CGA
31	B	625	LMG	C28-C29-C30-C31
31	e	101	LMG	C28-C29-C30-C31
24	A	407	PL9	C4-C3-C7-C8
26	a	408	DGD	C5B-C6B-C7B-C8B
26	c	517	DGD	C9B-CAB-CBB-CCB
31	m	101	LMG	C29-C30-C31-C32
30	f	103	SQD	O49-C7-O47-C45
24	d	407	PL9	C20-C19-C21-C22
31	a	402	LMG	C15-C16-C17-C18
25	j	102	BCR	C18-C19-C20-C21
31	m	101	LMG	O6-C5-C6-O5
26	b	601	DGD	C2B-C3B-C4B-C5B
22	B	610	CLA	CBA-CGA-O2A-C1
22	C	519	CLA	CBA-CGA-O2A-C1
22	D	404	CLA	CBA-CGA-O2A-C1
31	m	101	LMG	C29-C28-O8-C9
22	A	402	CLA	C11-C12-C13-C14
22	a	404	CLA	C6-C7-C8-C9
22	b	613	CLA	C6-C7-C8-C9
31	a	402	LMG	C18-C19-C20-C21
31	c	518	LMG	C34-C35-C36-C37
31	i	102	LMG	C14-C15-C16-C17
31	l	101	LMG	C14-C15-C16-C17
26	d	410	DGD	O6E-C1E-O5D-C6D
26	C	516	DGD	C9B-CAB-CBB-CCB
30	B	627	SQD	C11-C10-C9-C8
30	b	602	SQD	C11-C10-C9-C8
31	d	408	LMG	C36-C37-C38-C39
31	i	102	LMG	C13-C14-C15-C16
22	H	101	CLA	C13-C15-C16-C17
26	A	409	DGD	C5B-C6B-C7B-C8B
26	C	516	DGD	CAB-CBB-CCB-CDB
26	b	625	DGD	C7A-C8A-C9A-CAA
26	c	515	DGD	C4A-C5A-C6A-C7A
31	I	101	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	D	406	LMG	C15-C16-C17-C18
31	a	402	LMG	C32-C33-C34-C35
31	d	408	LMG	C30-C31-C32-C33
31	d	409	LMG	C19-C20-C21-C22
26	B	620	DGD	O6D-C5D-C6D-O5D
26	b	601	DGD	C4A-C5A-C6A-C7A
26	c	517	DGD	CAB-CBB-CCB-CDB
27	A	410	LHG	C25-C26-C27-C28
31	B	625	LMG	C36-C37-C38-C39
31	b	627	LMG	C31-C32-C33-C34
31	c	518	LMG	C12-C13-C14-C15
22	C	509	CLA	C3-C5-C6-C7
22	B	612	CLA	C16-C17-C18-C19
26	C	516	DGD	C2B-C1B-O2G-C2G
27	A	410	LHG	C8-C7-O7-C5
27	a	409	LHG	C8-C7-O7-C5
31	E	101	LMG	C11-C10-O7-C8
31	e	101	LMG	C11-C10-O7-C8
31	c	518	LMG	C36-C37-C38-C39
22	C	505	CLA	C10-C11-C12-C13
22	d	406	CLA	C15-C16-C17-C18
27	A	410	LHG	O9-C7-O7-C5
23	A	405	PHO	CBD-CGD-O2D-CED
25	B	619	BCR	C7-C8-C9-C34
25	f	102	BCR	C37-C22-C23-C24
26	B	620	DGD	C5B-C6B-C7B-C8B
26	c	517	DGD	C1A-C2A-C3A-C4A
32	B	629	LMT	C7-C8-C9-C10
32	b	604	LMT	C7-C8-C9-C10
22	A	403	CLA	C3-C5-C6-C7
22	c	509	CLA	C3-C5-C6-C7
25	x	101	BCR	C7-C8-C9-C10
31	D	406	LMG	C8-C7-O1-C1
31	d	409	LMG	C8-C7-O1-C1
31	l	101	LMG	C4-C5-C6-O5
26	D	407	DGD	C3A-C4A-C5A-C6A
22	B	603	CLA	C15-C16-C17-C18
22	c	520	CLA	C2A-CAA-CBA-CGA
22	B	612	CLA	C16-C17-C18-C20
22	b	617	CLA	C16-C17-C18-C19
26	B	626	DGD	C4A-C5A-C6A-C7A
26	B	626	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C4-C3-C5-C6
22	b	606	CLA	C13-C15-C16-C17
24	D	405	PL9	C47-C48-C49-C51
26	D	407	DGD	C6B-C7B-C8B-C9B
31	M	101	LMG	C29-C30-C31-C32
32	B	623	LMT	O1'-C1-C2-C3
22	b	615	CLA	O1A-CGA-O2A-C1
22	d	406	CLA	O1A-CGA-O2A-C1
22	a	406	CLA	C5-C6-C7-C8
22	b	609	CLA	C15-C16-C17-C18
26	B	620	DGD	C4B-C5B-C6B-C7B
31	d	409	LMG	C13-C14-C15-C16
31	l	101	LMG	C31-C32-C33-C34
31	M	101	LMG	C29-C28-O8-C9
26	A	409	DGD	C1B-C2B-C3B-C4B
27	a	409	LHG	C23-C24-C25-C26
27	a	409	LHG	O9-C7-O7-C5
31	e	101	LMG	O6-C5-C6-O5
31	D	406	LMG	C19-C20-C21-C22
22	B	601	CLA	C10-C11-C12-C13
22	C	511	CLA	C13-C15-C16-C17
22	b	617	CLA	C16-C17-C18-C20
26	d	410	DGD	C5A-C6A-C7A-C8A
31	d	412	LMG	C17-C18-C19-C20
31	e	101	LMG	C15-C16-C17-C18
31	i	102	LMG	O10-C28-O8-C9
31	C	517	LMG	C34-C35-C36-C37
26	c	515	DGD	C1A-C2A-C3A-C4A
31	b	626	LMG	C10-C11-C12-C13
22	C	512	CLA	C13-C15-C16-C17
22	b	612	CLA	O1D-CGD-O2D-CED
30	A	413	SQD	O47-C45-C46-O48
30	a	401	SQD	O6-C44-C45-O47
30	a	412	SQD	O47-C45-C46-O48
31	I	101	LMG	O1-C7-C8-O7
31	M	101	LMG	O1-C7-C8-O7
31	i	102	LMG	O1-C7-C8-O7
31	m	101	LMG	O1-C7-C8-O7
31	L	101	LMG	C14-C15-C16-C17
26	D	407	DGD	C5A-C6A-C7A-C8A
27	a	409	LHG	C25-C26-C27-C28
31	B	621	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
31	d	409	LMG	C15-C16-C17-C18
30	F	103	SQD	C10-C11-C12-C13
31	d	412	LMG	C34-C35-C36-C37
26	b	625	DGD	C5B-C6B-C7B-C8B
31	D	406	LMG	C32-C33-C34-C35
31	d	409	LMG	C32-C33-C34-C35
22	A	406	CLA	C5-C6-C7-C8
31	a	402	LMG	C31-C32-C33-C34
22	C	512	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
24	a	407	PL9	C35-C34-C36-C37
22	C	502	CLA	C13-C15-C16-C17
30	B	622	SQD	C9-C10-C11-C12
31	E	101	LMG	C15-C16-C17-C18
31	b	626	LMG	C34-C35-C36-C37
22	B	605	CLA	C2A-CAA-CBA-CGA
22	a	403	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
24	d	407	PL9	C27-C28-C29-C30
22	a	406	CLA	C10-C11-C12-C13
31	l	101	LMG	C11-C10-O7-C8
30	a	412	SQD	C17-C18-C19-C20
30	b	602	SQD	C12-C13-C14-C15
31	C	517	LMG	C12-C13-C14-C15
31	C	517	LMG	C36-C37-C38-C39
22	B	601	CLA	C16-C17-C18-C20
22	D	404	CLA	C15-C16-C17-C18
22	C	502	CLA	C3-C5-C6-C7
27	A	410	LHG	C30-C31-C32-C33
27	c	519	LHG	C25-C26-C27-C28
31	L	101	LMG	C15-C16-C17-C18
22	B	615	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	D	403	CLA	C1A-C2A-CAA-CBA
22	c	501	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
31	a	402	LMG	O6-C5-C6-O5
27	c	519	LHG	C24-C23-O8-C6
22	c	511	CLA	C13-C15-C16-C17
26	A	409	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
26	D	407	DGD	C8B-C9B-CAB-CBB
31	d	412	LMG	C31-C32-C33-C34
31	B	625	LMG	C4-C5-C6-O5
32	I	102	LMT	C5'-C4'-O1B-C1B
22	C	519	CLA	O1A-CGA-O2A-C1
26	C	516	DGD	C3B-C4B-C5B-C6B
30	d	403	SQD	C9-C10-C11-C12
31	B	625	LMG	C30-C31-C32-C33
26	c	516	DGD	CAB-CBB-CCB-CDB
32	b	629	LMT	C2B-C1B-O1B-C4'
22	B	602	CLA	C6-C7-C8-C10
22	B	614	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C10-C8-C7
22	C	503	CLA	C11-C12-C13-C15
22	C	504	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C10-C8-C7
22	D	403	CLA	C12-C13-C15-C16
22	H	101	CLA	C6-C7-C8-C10
22	a	405	CLA	C6-C7-C8-C10
22	b	606	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C12-C13-C15
22	b	619	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C12-C13-C15
22	c	504	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	510	CLA	C12-C13-C15-C16
22	d	405	CLA	C12-C13-C15-C16
23	D	401	PHO	C12-C13-C15-C16
22	C	511	CLA	C16-C17-C18-C20
22	C	503	CLA	C8-C10-C11-C12
22	D	404	CLA	O1A-CGA-O2A-C1
31	B	625	LMG	C17-C18-C19-C20
31	L	101	LMG	C8-C9-O8-C28
22	a	406	CLA	C13-C15-C16-C17
26	B	626	DGD	C1A-C2A-C3A-C4A
26	c	516	DGD	C1A-C2A-C3A-C4A
22	C	509	CLA	C4-C3-C5-C6
22	C	509	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C2-C3-C5-C6
32	i	103	LMT	C5'-C4'-O1B-C1B
26	C	514	DGD	C2A-C3A-C4A-C5A
26	d	410	DGD	C6B-C7B-C8B-C9B
30	f	103	SQD	C10-C11-C12-C13
22	A	406	CLA	C13-C15-C16-C17
22	C	501	CLA	C2A-CAA-CBA-CGA
22	A	403	CLA	C6-C7-C8-C9
22	B	602	CLA	C6-C7-C8-C9
22	B	605	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C9
22	C	502	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	504	CLA	C14-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C9
22	b	607	CLA	C11-C12-C13-C14
22	b	610	CLA	C14-C13-C15-C16
22	c	502	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	c	504	CLA	C6-C7-C8-C9
22	c	505	CLA	C14-C13-C15-C16
27	a	409	LHG	C30-C31-C32-C33
26	d	410	DGD	C1A-C2A-C3A-C4A
31	b	627	LMG	C17-C18-C19-C20
31	d	408	LMG	C17-C18-C19-C20
26	C	514	DGD	C4B-C5B-C6B-C7B
31	E	101	LMG	O6-C5-C6-O5
22	C	509	CLA	O1D-CGD-O2D-CED
26	d	410	DGD	CAB-CBB-CCB-CDB
26	c	515	DGD	C2A-C3A-C4A-C5A
31	D	409	LMG	C34-C35-C36-C37
26	a	408	DGD	C1G-C2G-C3G-O3G
30	A	413	SQD	C44-C45-C46-O48
30	A	414	SQD	O6-C44-C45-C46
30	B	627	SQD	C44-C45-C46-O48
30	a	412	SQD	C44-C45-C46-O48
30	b	602	SQD	C44-C45-C46-O48
31	B	621	LMG	C7-C8-C9-O8
31	B	625	LMG	O1-C7-C8-C9
31	M	101	LMG	C7-C8-C9-O8
31	b	626	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
31	c	522	LMG	C7-C8-C9-O8
31	d	408	LMG	O1-C7-C8-C9
31	i	102	LMG	O1-C7-C8-C9
31	m	101	LMG	C7-C8-C9-O8
26	D	407	DGD	CAB-CBB-CCB-CDB
27	C	518	LHG	C24-C25-C26-C27
31	B	625	LMG	C32-C33-C34-C35
32	B	624	LMT	C2B-C1B-O1B-C4'
22	C	508	CLA	CBA-CGA-O2A-C1
22	B	601	CLA	C16-C17-C18-C19
26	d	410	DGD	C2A-C3A-C4A-C5A
26	c	516	DGD	O6D-C5D-C6D-O5D
22	c	502	CLA	C3-C5-C6-C7
22	B	610	CLA	O1A-CGA-O2A-C1
22	c	509	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
22	B	613	CLA	C5-C6-C7-C8
22	B	615	CLA	C15-C16-C17-C18
22	c	502	CLA	C13-C15-C16-C17
27	c	519	LHG	C24-C25-C26-C27
31	i	102	LMG	C17-C18-C19-C20
22	C	504	CLA	C15-C16-C17-C18
22	c	512	CLA	C2A-CAA-CBA-CGA
22	a	404	CLA	C3-C5-C6-C7
22	B	615	CLA	C8-C10-C11-C12
22	b	608	CLA	C15-C16-C17-C18
26	C	515	DGD	CAB-CBB-CCB-CDB
26	D	407	DGD	C2A-C3A-C4A-C5A
30	B	627	SQD	C12-C13-C14-C15
31	C	521	LMG	C16-C17-C18-C19
22	C	504	CLA	CBA-CGA-O2A-C1
22	c	508	CLA	CBA-CGA-O2A-C1
26	D	407	DGD	C1G-C2G-O2G-C1B
26	d	410	DGD	C1G-C2G-O2G-C1B
31	E	101	LMG	C7-C8-O7-C10
26	A	409	DGD	C4B-C5B-C6B-C7B
27	c	519	LHG	C11-C10-C9-C8
31	D	409	LMG	C31-C32-C33-C34
26	B	626	DGD	O6D-C5D-C6D-O5D
22	c	504	CLA	C15-C16-C17-C18
22	c	505	CLA	C10-C11-C12-C13
26	D	407	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
26	a	408	DGD	C4B-C5B-C6B-C7B
22	C	511	CLA	C16-C17-C18-C19
31	b	626	LMG	C28-C29-C30-C31
26	c	516	DGD	C4D-C5D-C6D-O5D
26	c	515	DGD	C4B-C5B-C6B-C7B
34	v	201	HEM	C4D-C3D-CAD-CBD
27	C	518	LHG	O6-C4-C5-O7
30	b	602	SQD	C11-C12-C13-C14
22	B	614	CLA	CBA-CGA-O2A-C1
27	C	518	LHG	C25-C26-C27-C28
22	B	613	CLA	C16-C17-C18-C20
26	c	517	DGD	C3B-C4B-C5B-C6B
30	a	412	SQD	C10-C11-C12-C13
31	c	522	LMG	C16-C17-C18-C19
31	l	101	LMG	C15-C16-C17-C18
26	C	515	DGD	O6D-C5D-C6D-O5D
26	B	626	DGD	C5A-C6A-C7A-C8A
26	a	408	DGD	C3B-C4B-C5B-C6B
31	I	101	LMG	C18-C19-C20-C21
31	e	101	LMG	C18-C19-C20-C21
26	C	514	DGD	O2G-C2G-C3G-O3G
31	L	101	LMG	O1-C7-C8-O7
31	c	518	LMG	O1-C7-C8-O7
31	l	101	LMG	O1-C7-C8-O7
30	a	401	SQD	C10-C11-C12-C13
31	d	408	LMG	C32-C33-C34-C35
26	c	517	DGD	CFA-CGA-CHA-CIA
34	v	201	HEM	C2D-C3D-CAD-CBD
30	B	627	SQD	C11-C12-C13-C14
30	A	414	SQD	C10-C11-C12-C13
31	B	621	LMG	C13-C14-C15-C16
30	b	602	SQD	C17-C18-C19-C20
22	b	614	CLA	C16-C17-C18-C20
26	C	516	DGD	CDB-CEB-CFB-CGB
26	d	410	DGD	C3A-C4A-C5A-C6A
31	C	521	LMG	C17-C18-C19-C20
30	A	413	SQD	C17-C18-C19-C20
31	i	102	LMG	C18-C19-C20-C21
31	L	101	LMG	C11-C10-O7-C8
26	D	407	DGD	CBA-CCA-CDA-CEA
30	A	413	SQD	C10-C11-C12-C13
22	b	618	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	C8-C10-C11-C12
27	c	519	LHG	O10-C23-O8-C6
22	c	511	CLA	C3-C5-C6-C7
27	A	410	LHG	C23-C24-C25-C26
26	d	410	DGD	C8B-C9B-CAB-CBB
22	c	504	CLA	C4-C3-C5-C6
24	D	405	PL9	C15-C14-C16-C17
24	D	405	PL9	C35-C34-C36-C37
22	b	614	CLA	CBA-CGA-O2A-C1
26	b	601	DGD	C5A-C6A-C7A-C8A
31	l	101	LMG	O6-C5-C6-O5
31	b	626	LMG	C13-C14-C15-C16
22	B	608	CLA	C6-C7-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C14
22	C	503	CLA	C11-C12-C13-C14
22	C	504	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	D	403	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C12-C13-C14
22	a	405	CLA	C6-C7-C8-C9
22	b	613	CLA	C14-C13-C15-C16
22	b	619	CLA	C11-C10-C8-C9
22	b	619	CLA	C14-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C14
22	c	504	CLA	C14-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C9
22	c	510	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C14
22	d	405	CLA	C14-C13-C15-C16
23	D	401	PHO	C14-C13-C15-C16
23	d	402	PHO	C14-C13-C15-C16
22	b	605	CLA	C10-C11-C12-C13
26	d	410	DGD	CBA-CCA-CDA-CEA
31	d	408	LMG	C13-C14-C15-C16
22	B	604	CLA	C5-C6-C7-C8
22	b	620	CLA	C8-C10-C11-C12
22	c	512	CLA	C13-C15-C16-C17
24	D	405	PL9	C32-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
26	d	410	DGD	C3B-C4B-C5B-C6B
27	c	519	LHG	O6-C4-C5-C6
26	c	516	DGD	C3A-C4A-C5A-C6A
31	I	101	LMG	C17-C18-C19-C20
22	B	605	CLA	C12-C13-C15-C16
22	B	608	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	C	504	CLA	C12-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C12-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C15
22	b	607	CLA	C6-C7-C8-C10
22	b	610	CLA	C12-C13-C15-C16
22	b	612	CLA	C6-C7-C8-C10
22	b	613	CLA	C12-C13-C15-C16
22	b	619	CLA	C11-C10-C8-C7
22	b	620	CLA	C12-C13-C15-C16
22	c	502	CLA	C12-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C10
22	c	505	CLA	C12-C13-C15-C16
22	c	507	CLA	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
22	c	511	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16
23	d	402	PHO	C12-C13-C15-C16
23	D	401	PHO	C10-C11-C12-C13
31	D	406	LMG	C29-C30-C31-C32
31	I	101	LMG	C31-C32-C33-C34
31	C	521	LMG	C34-C35-C36-C37
26	C	515	DGD	C4D-C5D-C6D-O5D
22	A	402	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	C4-C3-C5-C6
22	a	403	CLA	C3A-C2A-CAA-CBA
24	d	407	PL9	C15-C14-C16-C17
31	a	402	LMG	C17-C18-C19-C20
22	C	508	CLA	O1A-CGA-O2A-C1
31	E	101	LMG	C18-C19-C20-C21
31	d	408	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C16-C17-C18-C20
25	b	624	BCR	C7-C8-C9-C34
32	B	628	LMT	C5'-C4'-O1B-C1B
31	E	101	LMG	C19-C20-C21-C22
22	c	508	CLA	O1A-CGA-O2A-C1
31	d	409	LMG	C28-C29-C30-C31
26	d	410	DGD	CDB-CEB-CFB-CGB
22	C	519	CLA	C2A-CAA-CBA-CGA
22	c	504	CLA	CBA-CGA-O2A-C1
31	B	625	LMG	C15-C16-C17-C18
26	B	626	DGD	C1G-C2G-C3G-O3G
26	C	515	DGD	C1G-C2G-C3G-O3G
26	D	407	DGD	C1G-C2G-C3G-O3G
26	c	516	DGD	C1G-C2G-C3G-O3G
26	c	517	DGD	O1G-C1G-C2G-C3G
30	a	401	SQD	O6-C44-C45-C46
31	C	517	LMG	O1-C7-C8-C9
31	C	521	LMG	C7-C8-C9-O8
31	D	406	LMG	O1-C7-C8-C9
31	I	101	LMG	O1-C7-C8-C9
31	L	101	LMG	O1-C7-C8-C9
31	c	518	LMG	O1-C7-C8-C9
31	d	409	LMG	O1-C7-C8-C9
31	l	101	LMG	O1-C7-C8-C9
31	m	101	LMG	O1-C7-C8-C9
31	d	412	LMG	C19-C20-C21-C22
22	C	511	CLA	C3-C5-C6-C7
22	B	609	CLA	C16-C17-C18-C20
22	B	613	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C19
31	B	621	LMG	C17-C18-C19-C20
31	B	625	LMG	C19-C20-C21-C22
31	D	409	LMG	C19-C20-C21-C22
31	B	625	LMG	C13-C14-C15-C16
31	E	101	LMG	C17-C18-C19-C20
31	b	627	LMG	C11-C12-C13-C14
26	c	517	DGD	CDB-CEB-CFB-CGB
22	A	403	CLA	C4-C3-C5-C6
24	J	101	PL9	C15-C14-C16-C17
31	b	626	LMG	C17-C18-C19-C20
31	c	522	LMG	C17-C18-C19-C20
31	E	101	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	C2-C3-C5-C6
22	b	605	CLA	C16-C17-C18-C20
27	c	519	LHG	O6-C4-C5-O7
24	J	101	PL9	C27-C28-C29-C30
24	j	101	PL9	C27-C28-C29-C30
25	B	616	BCR	C1-C6-C7-C8
25	F	102	BCR	C1-C6-C7-C8
25	J	102	BCR	C1-C6-C7-C8
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C23-C24-C25-C30
25	b	621	BCR	C1-C6-C7-C8
25	b	624	BCR	C23-C24-C25-C30
25	c	513	BCR	C1-C6-C7-C8
25	f	102	BCR	C1-C6-C7-C8
25	j	102	BCR	C1-C6-C7-C8
22	B	604	CLA	C10-C11-C12-C13
22	b	618	CLA	C15-C16-C17-C18
26	D	407	DGD	C3B-C4B-C5B-C6B
22	b	609	CLA	C10-C11-C12-C13
31	d	408	LMG	C15-C16-C17-C18
22	b	618	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C19
26	C	516	DGD	O1G-C1G-C2G-O2G
26	c	515	DGD	O2G-C2G-C3G-O3G
26	c	517	DGD	O1G-C1G-C2G-O2G
30	B	622	SQD	O6-C44-C45-O47
30	B	627	SQD	O47-C45-C46-O48
30	b	602	SQD	O47-C45-C46-O48
30	d	403	SQD	O6-C44-C45-O47
31	C	517	LMG	O1-C7-C8-O7
31	c	522	LMG	O7-C8-C9-O8
31	I	101	LMG	O10-C28-O8-C9
24	a	407	PL9	C4-C3-C7-C8
31	e	101	LMG	C19-C20-C21-C22
30	b	602	SQD	C10-C11-C12-C13
22	A	403	CLA	C5-C6-C7-C8
22	C	504	CLA	C2-C3-C5-C6
26	c	516	DGD	C4B-C5B-C6B-C7B
31	b	626	LMG	C12-C13-C14-C15
27	C	518	LHG	C11-C10-C9-C8
22	C	504	CLA	O1A-CGA-O2A-C1
22	A	403	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C11-C10-C8-C9
22	B	608	CLA	C14-C13-C15-C16
22	C	507	CLA	C14-C13-C15-C16
22	D	403	CLA	C6-C7-C8-C9
22	b	620	CLA	C11-C12-C13-C14
22	c	501	CLA	C11-C12-C13-C14
31	D	409	LMG	C38-C39-C40-C41
32	B	624	LMT	O5B-C1B-O1B-C4'
31	a	402	LMG	C11-C12-C13-C14
26	D	407	DGD	C4E-C5E-C6E-O5E
30	A	413	SQD	C31-C32-C33-C34
22	c	509	CLA	O1D-CGD-O2D-CED
31	i	102	LMG	C31-C32-C33-C34
22	B	614	CLA	O1A-CGA-O2A-C1
24	D	405	PL9	C24-C26-C27-C28
26	D	407	DGD	C1A-C2A-C3A-C4A
22	C	510	CLA	CBA-CGA-O2A-C1
32	b	603	LMT	C5'-C4'-O1B-C1B
22	B	609	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C19
31	L	101	LMG	C20-C21-C22-C23
31	D	406	LMG	C28-C29-C30-C31
31	d	412	LMG	C38-C39-C40-C41
26	C	516	DGD	CFA-CGA-CHA-CIA
30	F	103	SQD	C29-C30-C31-C32
22	B	613	CLA	C15-C16-C17-C18
32	b	629	LMT	O5B-C1B-O1B-C4'
31	e	101	LMG	C17-C18-C19-C20
25	H	102	BCR	C16-C17-C18-C36
25	g	101	BCR	C20-C21-C22-C37
22	B	605	CLA	CBA-CGA-O2A-C1
22	B	609	CLA	C5-C6-C7-C8
22	a	404	CLA	C5-C6-C7-C8
27	C	518	LHG	O6-C4-C5-C6
22	b	618	CLA	C16-C17-C18-C19
26	d	410	DGD	C4A-C5A-C6A-C7A
22	A	403	CLA	C12-C13-C15-C16
22	A	406	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C10-C8-C7
22	B	607	CLA	C6-C7-C8-C10
22	B	609	CLA	C11-C12-C13-C15
22	B	609	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	610	CLA	C11-C10-C8-C7
22	B	612	CLA	C11-C12-C13-C15
22	B	615	CLA	C11-C10-C8-C7
22	C	501	CLA	C11-C12-C13-C15
22	C	508	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	C	511	CLA	C12-C13-C15-C16
22	a	404	CLA	C12-C13-C15-C16
22	b	609	CLA	C11-C10-C8-C7
22	b	615	CLA	C11-C10-C8-C7
22	b	617	CLA	C11-C12-C13-C15
22	b	620	CLA	C11-C10-C8-C7
22	c	501	CLA	C11-C12-C13-C15
30	a	412	SQD	C31-C32-C33-C34
31	B	625	LMG	C20-C21-C22-C23
22	b	610	CLA	C13-C15-C16-C17
22	b	616	CLA	C10-C11-C12-C13
25	J	102	BCR	C7-C8-C9-C10
25	c	514	BCR	C7-C8-C9-C10
31	B	621	LMG	C29-C28-O8-C9
22	b	614	CLA	O1A-CGA-O2A-C1
30	B	622	SQD	C45-C44-O6-C1
30	B	622	SQD	C5-C6-S-O8
30	d	403	SQD	C45-C44-O6-C1
30	d	403	SQD	C5-C6-S-O8
31	L	101	LMG	C8-C7-O1-C1
31	l	101	LMG	C8-C7-O1-C1
22	C	511	CLA	C5-C6-C7-C8
23	A	405	PHO	O1D-CGD-O2D-CED
30	B	627	SQD	O49-C7-O47-C45
30	b	602	SQD	O49-C7-O47-C45
26	D	407	DGD	C4A-C5A-C6A-C7A
24	d	407	PL9	C35-C34-C36-C37
22	c	504	CLA	O1A-CGA-O2A-C1
31	C	517	LMG	C13-C14-C15-C16
26	c	517	DGD	C3G-C2G-O2G-C1B
27	C	518	LHG	O10-C23-O8-C6
26	D	407	DGD	CAA-CBA-CCA-CDA
22	b	614	CLA	C5-C6-C7-C8
22	b	614	CLA	C10-C11-C12-C13
31	M	101	LMG	O6-C1-O1-C7
26	C	516	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
26	b	601	DGD	C1G-C2G-C3G-O3G
26	d	410	DGD	C1G-C2G-C3G-O3G
34	F	101	HEM	C4B-C3B-CAB-CBB
34	V	201	HEM	C4C-C3C-CAC-CBC
34	f	101	HEM	C4B-C3B-CAB-CBB
34	v	201	HEM	C4C-C3C-CAC-CBC
31	d	409	LMG	C29-C30-C31-C32
22	c	510	CLA	C2A-CAA-CBA-CGA
26	b	625	DGD	CCA-CDA-CEA-CFA
30	A	413	SQD	C15-C16-C17-C18
30	F	103	SQD	C24-C25-C26-C27
31	C	521	LMG	O7-C8-C9-O8
31	M	101	LMG	O7-C8-C9-O8
31	m	101	LMG	O7-C8-C9-O8
22	B	609	CLA	C10-C11-C12-C13
22	a	405	CLA	C5-C6-C7-C8
22	B	612	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C10-C8-C9
22	C	511	CLA	C14-C13-C15-C16
22	b	609	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C10-C8-C9
23	D	401	PHO	C11-C10-C8-C9
23	d	401	PHO	C6-C7-C8-C9
26	C	515	DGD	C4B-C5B-C6B-C7B
22	C	510	CLA	O1A-CGA-O2A-C1
26	c	515	DGD	C5B-C6B-C7B-C8B
30	B	627	SQD	C10-C11-C12-C13
22	c	508	CLA	C15-C16-C17-C18
32	D	408	LMT	O5'-C5'-C6'-O6'
26	c	516	DGD	C6A-C7A-C8A-C9A
30	A	414	SQD	C9-C10-C11-C12
31	m	101	LMG	C30-C31-C32-C33
23	d	402	PHO	C10-C11-C12-C13
22	C	508	CLA	C2-C1-O2A-CGA
22	c	508	CLA	C2-C1-O2A-CGA
31	B	625	LMG	C2-C1-O1-C7
22	b	619	CLA	CBA-CGA-O2A-C1
22	b	620	CLA	C15-C16-C17-C18
30	B	627	SQD	C17-C18-C19-C20
30	A	414	SQD	C32-C33-C34-C35
26	b	601	DGD	O6D-C5D-C6D-O5D
22	b	616	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	j	101	PL9	C15-C14-C16-C17
22	B	604	CLA	C15-C16-C17-C18
30	f	103	SQD	C29-C30-C31-C32
26	C	515	DGD	C3A-C4A-C5A-C6A
22	B	613	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
23	d	401	PHO	C5-C6-C7-C8
26	B	620	DGD	O1A-C1A-O1G-C1G
26	d	410	DGD	C4E-C5E-C6E-O5E
30	f	103	SQD	C24-C25-C26-C27
22	B	605	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	C3-C5-C6-C7
22	A	402	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C4B-C3B-CAB-CBB
22	C	508	CLA	C4B-C3B-CAB-CBB
22	C	519	CLA	C4B-C3B-CAB-CBB
22	a	403	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C4B-C3B-CAB-CBB
22	c	520	CLA	C4B-C3B-CAB-CBB
26	d	410	DGD	CAA-CBA-CCA-CDA
25	j	102	BCR	C7-C8-C9-C10
22	c	509	CLA	C16-C17-C18-C19
31	B	621	LMG	C28-C29-C30-C31
26	D	407	DGD	C2B-C3B-C4B-C5B
23	A	405	PHO	C5-C6-C7-C8
26	d	410	DGD	C2B-C3B-C4B-C5B
22	B	607	CLA	C11-C12-C13-C15
22	B	612	CLA	C11-C10-C8-C7
22	C	507	CLA	C11-C12-C13-C15
22	C	509	CLA	C6-C7-C8-C10
22	D	404	CLA	C11-C10-C8-C7
22	b	605	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C7
22	b	612	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C12-C13-C15
22	b	614	CLA	C12-C13-C15-C16
22	b	617	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C12-C13-C15
22	c	508	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
22	c	520	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	C11-C10-C8-C7
22	d	406	CLA	C11-C10-C8-C7
23	d	402	PHO	C6-C7-C8-C10
23	d	402	PHO	C11-C10-C8-C7
22	b	607	CLA	C16-C17-C18-C19
26	A	409	DGD	C2A-C3A-C4A-C5A
26	b	625	DGD	C5A-C6A-C7A-C8A
26	c	515	DGD	C5A-C6A-C7A-C8A
22	b	609	CLA	C5-C6-C7-C8
22	C	506	CLA	C3-C5-C6-C7
22	A	404	CLA	C5-C6-C7-C8
27	A	410	LHG	C2-C3-O3-P
31	c	522	LMG	C35-C36-C37-C38
22	c	512	CLA	C3A-C2A-CAA-CBA
24	d	407	PL9	C47-C48-C49-C51
22	C	508	CLA	C2A-CAA-CBA-CGA
22	b	618	CLA	C2A-CAA-CBA-CGA
22	A	406	CLA	C11-C10-C8-C9
22	B	610	CLA	C11-C10-C8-C9
22	C	501	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C12-C13-C14
22	C	508	CLA	C11-C10-C8-C9
22	a	404	CLA	C14-C13-C15-C16
22	b	617	CLA	C11-C12-C13-C14
22	b	620	CLA	C11-C10-C8-C9
22	b	620	CLA	C14-C13-C15-C16
22	d	405	CLA	C6-C7-C8-C9
23	d	402	PHO	C11-C10-C8-C9
22	C	508	CLA	C15-C16-C17-C18
31	d	408	LMG	C20-C21-C22-C23
30	d	403	SQD	O5-C5-C6-S
30	d	403	SQD	C10-C11-C12-C13
31	C	521	LMG	C35-C36-C37-C38
31	c	522	LMG	C34-C35-C36-C37
22	b	619	CLA	O1A-CGA-O2A-C1
26	A	409	DGD	O2G-C2G-C3G-O3G
26	D	407	DGD	O2G-C2G-C3G-O3G
26	a	408	DGD	O2G-C2G-C3G-O3G
26	d	410	DGD	O2G-C2G-C3G-O3G
31	D	406	LMG	O1-C7-C8-O7
31	d	409	LMG	O1-C7-C8-O7
23	d	402	PHO	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	b	627	LMG	C12-C13-C14-C15
30	d	403	SQD	O6-C44-C45-C46
31	B	621	LMG	C12-C13-C14-C15
22	B	608	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	CAD-CBD-CGD-O2D
31	b	626	LMG	C29-C28-O8-C9
22	B	612	CLA	C10-C11-C12-C13
31	C	517	LMG	C32-C33-C34-C35
27	c	519	LHG	C7-C8-C9-C10
22	a	406	CLA	C16-C17-C18-C19
30	A	413	SQD	C11-C10-C9-C8
30	B	622	SQD	C10-C11-C12-C13
22	c	506	CLA	C3-C5-C6-C7
22	c	508	CLA	C2A-CAA-CBA-CGA
32	b	603	LMT	C4'-C5'-C6'-O6'
22	B	608	CLA	CAD-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O1D
27	A	410	LHG	C3-O3-P-O5
27	C	518	LHG	C3-O3-P-O5
27	c	519	LHG	C3-O3-P-O5
31	L	101	LMG	C11-C12-C13-C14
30	a	412	SQD	C12-C13-C14-C15
31	l	101	LMG	C16-C17-C18-C19
22	B	611	CLA	C4-C3-C5-C6
22	C	501	CLA	C2B-C3B-CAB-CBB
22	C	504	CLA	C2B-C3B-CAB-CBB
22	C	519	CLA	C2B-C3B-CAB-CBB
22	b	610	CLA	C2B-C3B-CAB-CBB
22	c	501	CLA	C2B-C3B-CAB-CBB
22	c	504	CLA	C2B-C3B-CAB-CBB
25	i	101	BCR	C1-C6-C7-C8
22	b	616	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	d	407	PL9	C13-C14-C16-C17
22	c	511	CLA	C5-C6-C7-C8
27	a	409	LHG	C2-C3-O3-P
30	a	401	SQD	C26-C27-C28-C29
30	a	412	SQD	C15-C16-C17-C18
31	a	402	LMG	C16-C17-C18-C19
31	l	101	LMG	C35-C36-C37-C38
26	B	620	DGD	C5A-C6A-C7A-C8A
31	l	101	LMG	C10-C11-C12-C13
32	b	604	LMT	C2-C3-C4-C5
26	C	516	DGD	C3G-C2G-O2G-C1B
27	A	410	LHG	C6-C5-O7-C7
22	B	602	CLA	C15-C16-C17-C18
22	C	508	CLA	C10-C11-C12-C13
22	c	501	CLA	C13-C15-C16-C17
22	b	607	CLA	C16-C17-C18-C20
31	L	101	LMG	C29-C30-C31-C32
22	A	404	CLA	C6-C7-C8-C9
22	B	609	CLA	C11-C12-C13-C14
22	B	612	CLA	C11-C10-C8-C9
22	B	615	CLA	C14-C13-C15-C16
22	C	509	CLA	C6-C7-C8-C9
22	b	617	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	c	507	CLA	C14-C13-C15-C16
22	c	510	CLA	C11-C10-C8-C9
22	c	511	CLA	C14-C13-C15-C16
23	A	405	PHO	C6-C7-C8-C9
22	A	404	CLA	C6-C7-C8-C10
22	H	101	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
23	D	401	PHO	C11-C10-C8-C7
22	B	604	CLA	C8-C10-C11-C12
31	c	518	LMG	C32-C33-C34-C35
31	L	101	LMG	C38-C39-C40-C41
31	e	101	LMG	C31-C32-C33-C34
22	B	602	CLA	C16-C17-C18-C19
22	c	509	CLA	C16-C17-C18-C20
31	d	409	LMG	C34-C35-C36-C37
22	a	404	CLA	C4-C3-C5-C6
26	C	516	DGD	C8B-C9B-CAB-CBB
26	d	410	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
31	B	621	LMG	O7-C8-C9-O8
31	b	626	LMG	O7-C8-C9-O8
23	D	401	PHO	C13-C15-C16-C17
22	B	613	CLA	C2C-C3C-CAC-CBC
26	C	516	DGD	C1B-C2B-C3B-C4B
22	A	406	CLA	C16-C17-C18-C19
34	F	101	HEM	C3D-CAD-CBD-CGD
31	C	521	LMG	C30-C31-C32-C33
31	e	101	LMG	O7-C10-C11-C12
26	C	514	DGD	C5B-C6B-C7B-C8B
22	b	610	CLA	C16-C17-C18-C20
22	C	511	CLA	CAA-CBA-CGA-O2A
31	L	101	LMG	C16-C17-C18-C19
24	d	407	PL9	C24-C26-C27-C28
30	B	622	SQD	O6-C44-C45-C46
31	M	101	LMG	O1-C7-C8-C9
31	D	409	LMG	C32-C33-C34-C35
30	a	401	SQD	C32-C33-C34-C35
30	f	103	SQD	C9-C10-C11-C12
31	B	625	LMG	C16-C17-C18-C19
31	d	409	LMG	C31-C32-C33-C34
22	a	406	CLA	C16-C17-C18-C20
26	C	515	DGD	C7B-C8B-C9B-CAB
31	B	625	LMG	C10-C11-C12-C13
26	B	626	DGD	C2G-C3G-O3G-C1D
26	b	601	DGD	C2G-C3G-O3G-C1D
31	D	409	LMG	C8-C7-O1-C1
31	l	101	LMG	C11-C12-C13-C14
27	c	519	LHG	O2-C2-C3-O3
31	l	101	LMG	C20-C21-C22-C23
22	b	615	CLA	C4-C3-C5-C6
24	D	405	PL9	C40-C39-C41-C42
22	c	511	CLA	CAA-CBA-CGA-O2A
31	d	409	LMG	C36-C37-C38-C39
22	B	607	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
22	c	505	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	d	406	CLA	C11-C10-C8-C9
22	b	606	CLA	CBA-CGA-O2A-C1
26	D	407	DGD	C8A-C9A-CAA-CBA
34	f	101	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	CBA-CGA-O2A-C1
22	b	617	CLA	C10-C11-C12-C13
22	c	504	CLA	C8-C10-C11-C12
22	B	610	CLA	C4-C3-C5-C6
24	D	405	PL9	C13-C14-C16-C17
22	c	510	CLA	C11-C10-C8-C7
22	C	507	CLA	C5-C6-C7-C8
22	b	606	CLA	O1A-CGA-O2A-C1
22	A	406	CLA	C16-C17-C18-C20
22	B	602	CLA	C16-C17-C18-C20
22	b	610	CLA	C16-C17-C18-C19
31	l	101	LMG	C17-C18-C19-C20
22	b	618	CLA	C2C-C3C-CAC-CBC
22	B	609	CLA	O1A-CGA-O2A-C1
31	B	621	LMG	O1-C7-C8-O7
22	C	512	CLA	C3A-C2A-CAA-CBA
31	D	406	LMG	C31-C32-C33-C34
22	A	403	CLA	C2-C3-C5-C6
31	D	409	LMG	C16-C17-C18-C19
32	b	629	LMT	O5'-C5'-C6'-O6'
26	c	515	DGD	O6D-C1D-O3G-C3G
30	a	401	SQD	C9-C10-C11-C12
31	M	101	LMG	C30-C31-C32-C33
22	B	607	CLA	C13-C15-C16-C17
22	c	502	CLA	C5-C6-C7-C8
22	B	605	CLA	C13-C15-C16-C17
31	b	627	LMG	C16-C17-C18-C19
22	B	612	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
22	b	617	CLA	C2-C1-O2A-CGA
23	A	405	PHO	C2-C1-O2A-CGA
31	L	101	LMG	C35-C36-C37-C38
31	d	408	LMG	C16-C17-C18-C19
22	c	510	CLA	C4-C3-C5-C6
24	A	407	PL9	C35-C34-C36-C37
22	B	611	CLA	C2-C3-C5-C6
22	b	617	CLA	C8-C10-C11-C12
31	c	518	LMG	C13-C14-C15-C16
31	D	406	LMG	C11-C12-C13-C14
31	d	412	LMG	O1-C7-C8-C9
31	e	101	LMG	O1-C7-C8-C9
30	A	414	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	e	101	LMG	C30-C31-C32-C33
22	B	601	CLA	C6-C7-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	B	602	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C12-C13-C14
22	C	510	CLA	C11-C10-C8-C9
22	D	404	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
31	B	621	LMG	C15-C16-C17-C18
27	a	409	LHG	C6-C5-O7-C7
31	M	101	LMG	C9-C8-O7-C10
31	m	101	LMG	C9-C8-O7-C10
31	d	412	LMG	C16-C17-C18-C19
30	F	103	SQD	C9-C10-C11-C12
30	a	401	SQD	C12-C13-C14-C15
22	c	512	CLA	C1A-C2A-CAA-CBA
31	D	406	LMG	C36-C37-C38-C39
22	B	612	CLA	C8-C10-C11-C12
22	B	601	CLA	C2B-C3B-CAB-CBB
22	C	508	CLA	C2B-C3B-CAB-CBB
22	b	605	CLA	C2B-C3B-CAB-CBB
22	c	520	CLA	C2B-C3B-CAB-CBB
22	d	406	CLA	C2B-C3B-CAB-CBB
25	A	408	BCR	C1-C6-C7-C8
25	A	408	BCR	C23-C24-C25-C30
25	B	616	BCR	C5-C6-C7-C8
25	B	619	BCR	C1-C6-C7-C8
25	B	619	BCR	C23-C24-C25-C30
25	F	102	BCR	C5-C6-C7-C8
25	J	102	BCR	C5-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C23-C24-C25-C26
25	b	621	BCR	C5-C6-C7-C8
25	b	624	BCR	C1-C6-C7-C8
25	b	624	BCR	C23-C24-C25-C26
25	c	513	BCR	C5-C6-C7-C8
25	c	513	BCR	C23-C24-C25-C30
25	f	102	BCR	C5-C6-C7-C8
25	i	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	i	101	BCR	C23-C24-C25-C30
31	L	101	LMG	C10-C11-C12-C13
31	l	101	LMG	C29-C30-C31-C32
22	C	510	CLA	C4-C3-C5-C6
22	b	615	CLA	C2-C3-C5-C6
32	B	629	LMT	C2-C3-C4-C5
22	b	609	CLA	C8-C10-C11-C12
32	i	103	LMT	C7-C8-C9-C10
32	D	408	LMT	O5B-C5B-C6B-O6B
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C12-C13-C15-C16
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	B	605	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C10-C8-C7
22	C	519	CLA	C6-C7-C8-C10
22	a	406	CLA	C11-C10-C8-C7
22	b	605	CLA	C6-C7-C8-C10
22	b	606	CLA	C12-C13-C15-C16
22	b	609	CLA	C11-C12-C13-C15
22	C	502	CLA	C5-C6-C7-C8
22	c	509	CLA	C13-C15-C16-C17
30	a	412	SQD	C16-C17-C18-C19
22	b	607	CLA	C15-C16-C17-C18
22	B	603	CLA	CBA-CGA-O2A-C1
22	c	502	CLA	CBA-CGA-O2A-C1
31	b	626	LMG	C15-C16-C17-C18
27	c	519	LHG	C1-C2-C3-O3
26	B	626	DGD	C2A-C3A-C4A-C5A
25	B	617	BCR	C37-C22-C23-C24
24	d	407	PL9	C42-C43-C44-C46
22	C	504	CLA	C8-C10-C11-C12
22	B	610	CLA	C2-C3-C5-C6
22	c	510	CLA	C2-C3-C5-C6
26	B	620	DGD	C7B-C8B-C9B-CAB
26	C	514	DGD	C5A-C6A-C7A-C8A
22	C	506	CLA	C11-C10-C8-C9
31	L	101	LMG	C13-C14-C15-C16
31	l	101	LMG	C39-C40-C41-C42
31	c	518	LMG	C17-C18-C19-C20
22	B	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	D	406	LMG	C34-C35-C36-C37
31	m	101	LMG	C17-C18-C19-C20
24	D	405	PL9	C20-C19-C21-C22
22	b	607	CLA	C8-C10-C11-C12
22	B	613	CLA	C4C-C3C-CAC-CBC
22	c	502	CLA	O1A-CGA-O2A-C1
22	D	404	CLA	C2A-CAA-CBA-CGA
26	d	410	DGD	C8A-C9A-CAA-CBA
22	c	507	CLA	C5-C6-C7-C8
22	B	603	CLA	O1A-CGA-O2A-C1
30	a	401	SQD	C17-C18-C19-C20
26	c	517	DGD	C5B-C6B-C7B-C8B
22	A	406	CLA	C4-C3-C5-C6
22	B	606	CLA	C4-C3-C5-C6
22	b	612	CLA	C4-C3-C5-C6
27	C	518	LHG	C7-C8-C9-C10
26	b	601	DGD	C2A-C3A-C4A-C5A
30	F	103	SQD	C15-C16-C17-C18
31	c	522	LMG	C30-C31-C32-C33
31	C	517	LMG	C17-C18-C19-C20
22	B	614	CLA	C4B-C3B-CAB-CBB
22	b	619	CLA	C4B-C3B-CAB-CBB
22	d	406	CLA	C4B-C3B-CAB-CBB
31	M	101	LMG	C17-C18-C19-C20
30	A	413	SQD	C16-C17-C18-C19
26	B	620	DGD	CCA-CDA-CEA-CFA
23	d	402	PHO	CHA-CBD-CGD-O1D
26	b	601	DGD	C4E-C5E-C6E-O5E
30	A	414	SQD	C26-C27-C28-C29
31	e	101	LMG	C14-C15-C16-C17
22	b	618	CLA	C4C-C3C-CAC-CBC
22	b	611	CLA	C4-C3-C5-C6
22	B	611	CLA	C10-C11-C12-C13
22	b	617	CLA	C13-C15-C16-C17
26	b	625	DGD	C4A-C5A-C6A-C7A
26	C	515	DGD	O6E-C1E-O5D-C6D
26	D	407	DGD	O6E-C5E-C6E-O5E
22	b	605	CLA	C11-C12-C13-C15
31	M	101	LMG	C31-C32-C33-C34
22	B	609	CLA	C13-C15-C16-C17
31	m	101	LMG	C31-C32-C33-C34
31	D	409	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
34	V	201	HEM	CAA-CBA-CGA-O2A
22	C	505	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	C	512	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
26	a	408	DGD	C2A-C3A-C4A-C5A
31	d	412	LMG	C8-C7-O1-C1
31	m	101	LMG	C11-C12-C13-C14
22	C	507	CLA	C2-C1-O2A-CGA
22	a	403	CLA	C2-C1-O2A-CGA
22	b	614	CLA	C2-C1-O2A-CGA
23	d	401	PHO	C2-C1-O2A-CGA
22	C	510	CLA	C3-C5-C6-C7
22	B	605	CLA	C16-C17-C18-C20
26	d	410	DGD	O6E-C5E-C6E-O5E
22	C	519	CLA	C3A-C2A-CAA-CBA
22	D	403	CLA	C3A-C2A-CAA-CBA
26	B	626	DGD	CAB-CBB-CCB-CDB
26	c	516	DGD	C7B-C8B-C9B-CAB
31	E	101	LMG	C31-C32-C33-C34
27	A	410	LHG	C4-C5-O7-C7
27	a	409	LHG	C4-C5-O7-C7
26	c	517	DGD	C8B-C9B-CAB-CBB
31	e	101	LMG	C11-C12-C13-C14
31	d	408	LMG	C29-C30-C31-C32
22	B	603	CLA	C2C-C3C-CAC-CBC
30	a	412	SQD	C11-C10-C9-C8
26	c	517	DGD	CBB-CCB-CDB-CEB
31	m	101	LMG	C16-C17-C18-C19
26	A	409	DGD	O6D-C5D-C6D-O5D
22	b	615	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C20
22	C	506	CLA	O1D-CGD-O2D-CED
26	b	601	DGD	O6D-C1D-O3G-C3G
31	l	101	LMG	C38-C39-C40-C41
26	C	514	DGD	C1G-C2G-C3G-O3G
31	C	517	LMG	C7-C8-C9-O8
31	D	409	LMG	O1-C7-C8-C9
31	E	101	LMG	O1-C7-C8-C9
31	I	101	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
31	c	518	LMG	C7-C8-C9-O8
31	d	408	LMG	C7-C8-C9-O8
26	b	625	DGD	CAB-CBB-CCB-CDB
26	C	515	DGD	C6A-C7A-C8A-C9A
22	a	404	CLA	C2-C3-C5-C6
31	B	625	LMG	C29-C30-C31-C32
31	c	522	LMG	C32-C33-C34-C35
26	B	626	DGD	C4E-C5E-C6E-O5E
31	M	101	LMG	C16-C17-C18-C19
27	C	518	LHG	O7-C7-C8-C9
30	A	413	SQD	C12-C13-C14-C15
31	b	626	LMG	O1-C7-C8-O7
31	d	412	LMG	O1-C7-C8-O7
22	B	614	CLA	C6-C7-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	612	CLA	C11-C12-C13-C14
22	b	619	CLA	C6-C7-C8-C9
22	c	520	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C10-C8-C9
23	d	402	PHO	C6-C7-C8-C9
22	d	405	CLA	CAA-CBA-CGA-O2A
27	c	519	LHG	O7-C7-C8-C9
31	L	101	LMG	O7-C10-C11-C12
30	d	403	SQD	C7-C8-C9-C10
25	C	513	BCR	C7-C8-C9-C10
26	c	516	DGD	CEB-CFB-CGB-CHB
26	C	516	DGD	O1A-C1A-O1G-C1G
22	B	612	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
34	v	201	HEM	CAA-CBA-CGA-O2A
22	B	601	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C10-C8-C7
22	C	505	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	H	101	CLA	C12-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C7
22	c	512	CLA	C11-C10-C8-C7
22	c	512	CLA	C11-C12-C13-C15
22	c	512	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	A	409	DGD	O1A-C1A-O1G-C1G
31	M	101	LMG	O10-C28-O8-C9
22	c	504	CLA	C3-C5-C6-C7
22	B	603	CLA	C4C-C3C-CAC-CBC
34	V	201	HEM	CAA-CBA-CGA-O1A
22	B	604	CLA	C2B-C3B-CAB-CBB
22	B	614	CLA	C2B-C3B-CAB-CBB
22	b	619	CLA	C2B-C3B-CAB-CBB
25	A	408	BCR	C5-C6-C7-C8
25	A	408	BCR	C23-C24-C25-C26
25	B	617	BCR	C1-C6-C7-C8
25	B	619	BCR	C5-C6-C7-C8
25	C	513	BCR	C1-C6-C7-C8
25	C	520	BCR	C23-C24-C25-C30
25	b	624	BCR	C5-C6-C7-C8
25	c	513	BCR	C23-C24-C25-C26
25	c	514	BCR	C1-C6-C7-C8
25	c	521	BCR	C23-C24-C25-C26
25	c	521	BCR	C23-C24-C25-C30
25	i	101	BCR	C23-C24-C25-C26
25	j	102	BCR	C5-C6-C7-C8
26	D	407	DGD	CBB-CCB-CDB-CEB
22	B	609	CLA	C2-C1-O2A-CGA
22	C	502	CLA	C16-C17-C18-C20
26	A	409	DGD	C4D-C5D-C6D-O5D
30	a	412	SQD	C32-C33-C34-C35
22	B	611	CLA	CAA-CBA-CGA-O2A
31	d	408	LMG	C12-C13-C14-C15
31	B	621	LMG	C35-C36-C37-C38
31	C	521	LMG	C32-C33-C34-C35
26	B	620	DGD	CAB-CBB-CCB-CDB
26	c	517	DGD	O1G-C1A-C2A-C3A
22	C	510	CLA	C2-C3-C5-C6
22	C	510	CLA	C2A-CAA-CBA-CGA
22	H	101	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
22	d	406	CLA	C2A-CAA-CBA-CGA
30	A	413	SQD	C8-C7-O47-C45
30	a	412	SQD	C8-C7-O47-C45
22	C	501	CLA	C13-C15-C16-C17
22	c	503	CLA	C15-C16-C17-C18
22	C	506	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	b	627	LMG	O7-C10-C11-C12
31	l	101	LMG	O7-C10-C11-C12
26	b	601	DGD	CAB-CBB-CCB-CDB
30	a	401	SQD	C23-C24-C25-C26
24	A	407	PL9	C28-C29-C31-C32
24	a	407	PL9	C28-C29-C31-C32
26	D	407	DGD	C9B-CAB-CBB-CCB
32	d	411	LMT	C1-C2-C3-C4
26	D	407	DGD	C6A-C7A-C8A-C9A
22	c	501	CLA	CAA-CBA-CGA-O2A
22	A	404	CLA	O1A-CGA-O2A-C1
22	B	605	CLA	C6-C7-C8-C9
22	C	519	CLA	C6-C7-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	b	606	CLA	C11-C10-C8-C9
22	b	609	CLA	C11-C12-C13-C14
30	a	412	SQD	C24-C25-C26-C27
31	C	521	LMG	O8-C28-C29-C30
26	c	515	DGD	C1G-C2G-C3G-O3G
22	B	605	CLA	C16-C17-C18-C19
22	A	403	CLA	C4B-C3B-CAB-CBB
22	B	604	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C4B-C3B-CAB-CBB
22	b	609	CLA	C4B-C3B-CAB-CBB
22	c	508	CLA	C4B-C3B-CAB-CBB
26	A	409	DGD	O6E-C1E-O5D-C6D
26	B	626	DGD	O6D-C1D-O3G-C3G
26	a	408	DGD	O6E-C1E-O5D-C6D
26	c	516	DGD	O6E-C1E-O5D-C6D
31	L	101	LMG	O6-C1-O1-C7
31	m	101	LMG	O6-C1-O1-C7
22	C	501	CLA	CAA-CBA-CGA-O2A
22	c	509	CLA	CAA-CBA-CGA-O2A
30	A	414	SQD	O47-C7-C8-C9
31	a	402	LMG	O7-C10-C11-C12
22	B	605	CLA	C15-C16-C17-C18
26	d	410	DGD	C9B-CAB-CBB-CCB
26	C	516	DGD	O1G-C1A-C2A-C3A
26	c	517	DGD	O2G-C1B-C2B-C3B
30	a	401	SQD	O47-C7-C8-C9
22	C	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	d	403	SQD	C12-C13-C14-C15
22	A	403	CLA	C2A-CAA-CBA-CGA
30	B	627	SQD	C15-C16-C17-C18
26	b	625	DGD	O1A-C1A-O1G-C1G
22	c	506	CLA	CAA-CBA-CGA-O2A
31	c	522	LMG	O8-C28-C29-C30
34	v	201	HEM	CAA-CBA-CGA-O1A
30	A	414	SQD	C5-C6-S-O9
30	B	622	SQD	C5-C6-S-O9
30	d	403	SQD	C5-C6-S-O9
30	A	414	SQD	C18-C19-C20-C21
22	A	403	CLA	C2-C1-O2A-CGA
26	c	517	DGD	C4A-C5A-C6A-C7A
31	a	402	LMG	C12-C13-C14-C15
22	D	403	CLA	C11-C10-C8-C7
22	a	406	CLA	C6-C7-C8-C10
22	b	610	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C10-C8-C7
22	c	505	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C12-C13-C15
22	c	507	CLA	C11-C12-C13-C15
22	A	404	CLA	CBA-CGA-O2A-C1
24	A	407	PL9	C33-C34-C36-C37
22	b	615	CLA	C16-C17-C18-C20
30	B	622	SQD	C7-C8-C9-C10
26	b	625	DGD	C7B-C8B-C9B-CAB
30	a	401	SQD	C25-C26-C27-C28
22	b	616	CLA	CAA-CBA-CGA-O2A
32	B	624	LMT	C6-C7-C8-C9
30	B	622	SQD	O49-C7-C8-C9
22	a	404	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C8-C10-C11-C12
22	c	506	CLA	O1D-CGD-O2D-CED
22	C	503	CLA	C15-C16-C17-C18
31	M	101	LMG	C11-C12-C13-C14
30	B	627	SQD	C19-C20-C21-C22
22	a	406	CLA	C4-C3-C5-C6
31	m	101	LMG	O10-C28-O8-C9
26	a	408	DGD	O6D-C5D-C6D-O5D
22	D	403	CLA	CAA-CBA-CGA-O2A
26	C	516	DGD	O2G-C1B-C2B-C3B
32	b	628	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	b	617	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
22	H	101	CLA	O1A-CGA-O2A-C1
22	H	101	CLA	CBA-CGA-O2A-C1
24	A	407	PL9	C2-C3-C7-C8
24	J	101	PL9	C2-C3-C7-C8
31	l	101	LMG	O6-C1-O1-C7
26	C	516	DGD	C4B-C5B-C6B-C7B
30	d	403	SQD	O47-C7-C8-C9
22	B	612	CLA	CAA-CBA-CGA-O1A
22	B	602	CLA	C2A-CAA-CBA-CGA
22	a	404	CLA	C2C-C3C-CAC-CBC
22	B	601	CLA	C14-C13-C15-C16
22	B	604	CLA	C11-C12-C13-C14
22	C	505	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C12-C13-C14
22	C	512	CLA	C11-C12-C13-C14
22	D	403	CLA	C11-C10-C8-C9
22	a	406	CLA	C11-C10-C8-C9
22	b	610	CLA	C6-C7-C8-C9
31	d	412	LMG	O9-C10-C11-C12
30	d	403	SQD	C11-C10-C9-C8
22	C	509	CLA	C13-C15-C16-C17
26	d	410	DGD	C6A-C7A-C8A-C9A
30	A	413	SQD	C9-C10-C11-C12
30	b	602	SQD	C15-C16-C17-C18
22	C	501	CLA	CAA-CBA-CGA-O1A
22	d	405	CLA	CAA-CBA-CGA-O1A
30	B	622	SQD	O5-C5-C6-S
22	b	616	CLA	CAA-CBA-CGA-O1A
31	l	101	LMG	O9-C10-C11-C12
22	B	605	CLA	C3-C5-C6-C7
22	B	613	CLA	O1A-CGA-O2A-C1
31	d	409	LMG	O7-C10-C11-C12
31	L	101	LMG	C39-C40-C41-C42
22	C	506	CLA	CAA-CBA-CGA-O1A
30	A	414	SQD	O49-C7-C8-C9
31	D	409	LMG	O9-C10-C11-C12
31	d	409	LMG	O9-C10-C11-C12
30	A	414	SQD	C25-C26-C27-C28
32	b	604	LMT	C11-C10-C9-C8
22	b	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	A	409	DGD	C5D-C6D-O5D-C1E
26	a	408	DGD	C5D-C6D-O5D-C1E
31	I	101	LMG	C8-C7-O1-C1
31	i	102	LMG	C8-C7-O1-C1
31	e	101	LMG	O1-C7-C8-O7
26	c	517	DGD	C4B-C5B-C6B-C7B
26	C	515	DGD	C2E-C1E-O5D-C6D
22	B	611	CLA	CAA-CBA-CGA-O1A
30	d	403	SQD	O49-C7-C8-C9
22	C	509	CLA	CAA-CBA-CGA-O2A
31	d	412	LMG	C11-C12-C13-C14
31	L	101	LMG	C7-C8-C9-O8
22	c	501	CLA	CAA-CBA-CGA-O1A
31	C	521	LMG	O10-C28-C29-C30
31	a	402	LMG	O9-C10-C11-C12
26	B	620	DGD	O2G-C1B-C2B-C3B
22	b	616	CLA	C3-C5-C6-C7
22	d	405	CLA	C3-C5-C6-C7
22	B	603	CLA	CAD-CBD-CGD-O2D
22	C	501	CLA	CAD-CBD-CGD-O2D
23	d	402	PHO	CAD-CBD-CGD-O2D
22	b	618	CLA	CAA-CBA-CGA-O2A
30	B	622	SQD	O47-C7-C8-C9
22	C	502	CLA	O1A-CGA-O2A-C1
22	C	502	CLA	CBA-CGA-O2A-C1
22	c	507	CLA	C2-C1-O2A-CGA
22	B	609	CLA	CAA-CBA-CGA-O2A
31	I	101	LMG	O7-C10-C11-C12
31	l	101	LMG	C8-C9-O8-C28
22	c	503	CLA	C2A-CAA-CBA-CGA
31	D	406	LMG	C12-C13-C14-C15
22	b	614	CLA	CAA-CBA-CGA-O2A
22	c	508	CLA	CAA-CBA-CGA-O2A
22	c	509	CLA	CAA-CBA-CGA-O1A
26	C	516	DGD	O1A-C1A-C2A-C3A
30	a	401	SQD	O49-C7-C8-C9
22	B	613	CLA	CAA-CBA-CGA-O2A
31	D	406	LMG	O9-C10-C11-C12

There are no ring outliers.

158 monomers are involved in 464 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	F	101	HEM	4	0
24	D	405	PL9	9	0
26	B	620	DGD	3	0
30	A	413	SQD	3	0
26	C	515	DGD	3	0
30	d	403	SQD	3	0
31	d	409	LMG	7	0
25	c	521	BCR	4	0
32	B	624	LMT	1	0
22	b	616	CLA	4	0
25	C	513	BCR	5	0
22	c	508	CLA	3	0
22	b	619	CLA	1	0
22	C	505	CLA	2	0
22	A	402	CLA	9	0
27	a	409	LHG	1	0
30	A	414	SQD	3	0
22	A	404	CLA	6	0
30	f	103	SQD	3	0
27	c	519	LHG	2	0
22	A	406	CLA	2	0
22	B	604	CLA	9	0
31	C	517	LMG	2	0
22	c	520	CLA	5	0
30	B	627	SQD	1	0
30	a	401	SQD	4	0
22	d	406	CLA	2	0
25	J	102	BCR	3	0
25	b	623	BCR	2	0
25	c	514	BCR	4	0
30	a	412	SQD	4	0
27	C	518	LHG	3	0
22	c	506	CLA	4	0
22	B	614	CLA	3	0
22	c	509	CLA	3	0
25	C	520	BCR	5	0
22	B	607	CLA	7	0
22	C	503	CLA	2	0
26	a	408	DGD	2	0
22	b	608	CLA	2	0
26	c	516	DGD	5	0
32	B	628	LMT	1	0
22	B	606	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	y	101	BCR	6	0
22	A	403	CLA	12	0
25	B	617	BCR	2	0
22	C	509	CLA	4	0
22	b	613	CLA	6	0
22	C	510	CLA	5	0
31	D	409	LMG	1	0
26	B	626	DGD	1	0
26	D	407	DGD	2	0
31	b	627	LMG	1	0
32	b	604	LMT	1	0
22	b	618	CLA	3	0
22	B	613	CLA	4	0
22	B	602	CLA	10	0
25	f	102	BCR	3	0
22	c	507	CLA	5	0
22	D	404	CLA	2	0
22	C	501	CLA	3	0
22	C	504	CLA	3	0
22	B	605	CLA	5	0
25	b	621	BCR	4	0
22	b	609	CLA	7	0
22	b	614	CLA	1	0
22	b	607	CLA	10	0
26	b	601	DGD	4	0
22	c	505	CLA	1	0
23	d	401	PHO	6	0
22	b	620	CLA	4	0
31	d	412	LMG	1	0
22	a	406	CLA	2	0
26	d	410	DGD	3	0
31	b	626	LMG	4	0
22	b	610	CLA	4	0
22	b	606	CLA	8	0
25	b	624	BCR	4	0
25	j	102	BCR	2	0
25	B	616	BCR	7	0
26	A	409	DGD	1	0
31	B	621	LMG	3	0
22	b	611	CLA	6	0
32	b	603	LMT	4	0
34	v	201	HEM	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	622	SQD	2	0
26	C	516	DGD	5	0
22	a	404	CLA	10	0
25	K	101	BCR	5	0
22	c	510	CLA	4	0
25	b	622	BCR	1	0
31	B	625	LMG	2	0
22	B	609	CLA	1	0
24	d	407	PL9	6	0
26	c	515	DGD	3	0
34	f	101	HEM	4	0
24	A	407	PL9	5	0
22	a	405	CLA	5	0
25	B	618	BCR	4	0
22	C	506	CLA	4	0
22	B	608	CLA	5	0
25	c	513	BCR	8	0
32	b	628	LMT	1	0
22	b	612	CLA	8	0
22	H	101	CLA	11	0
31	I	101	LMG	1	0
26	c	517	DGD	6	0
25	F	102	BCR	1	0
25	H	102	BCR	2	0
31	e	101	LMG	2	0
22	B	615	CLA	4	0
22	c	504	CLA	4	0
22	d	405	CLA	9	0
22	C	508	CLA	1	0
27	A	410	LHG	2	0
30	b	602	SQD	2	0
31	L	101	LMG	2	0
32	B	623	LMT	1	0
26	b	625	DGD	1	0
23	D	401	PHO	6	0
31	l	101	LMG	2	0
22	B	601	CLA	1	0
22	B	611	CLA	3	0
22	C	512	CLA	3	0
24	a	407	PL9	4	0
25	x	101	BCR	1	0
22	b	617	CLA	3	0

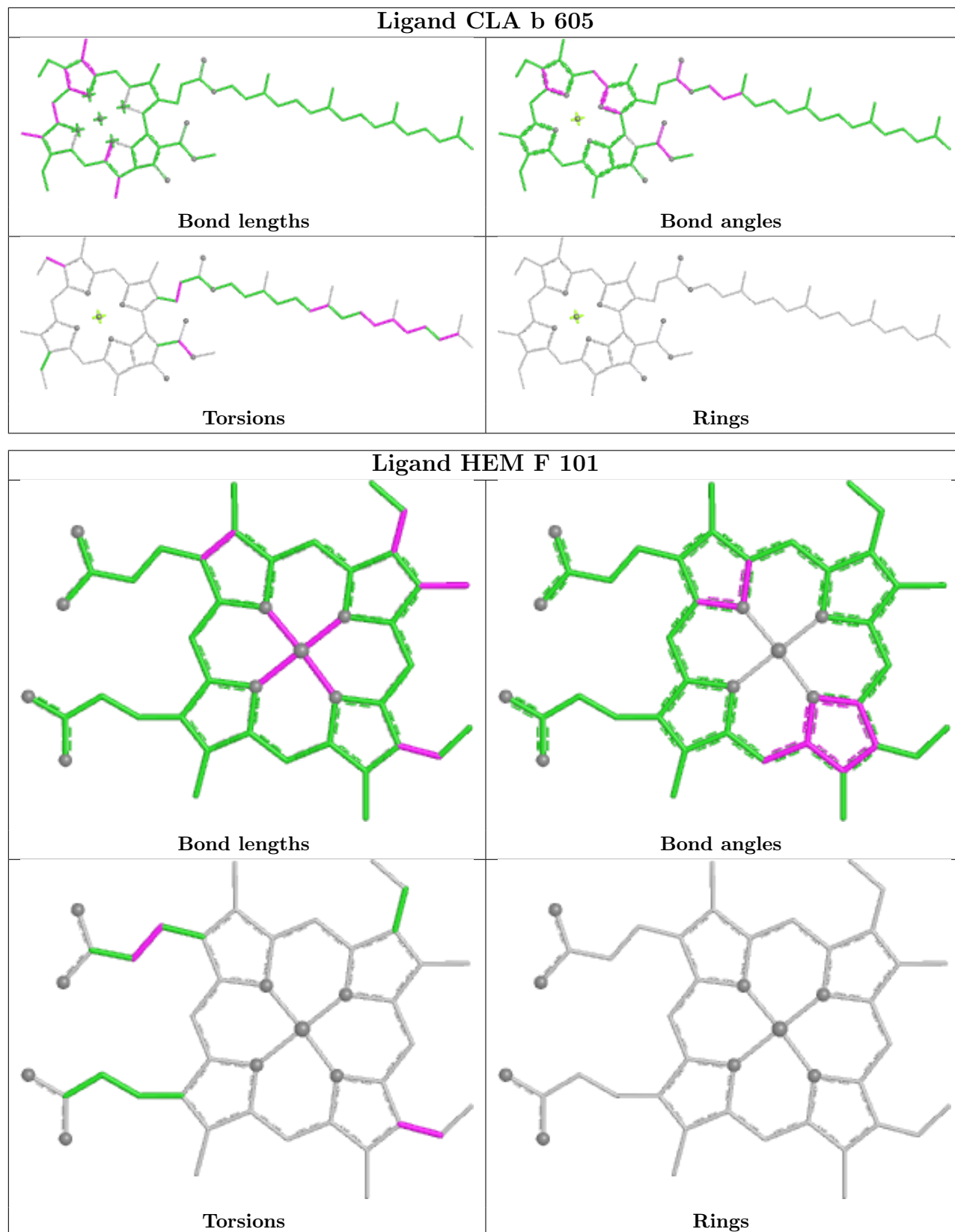
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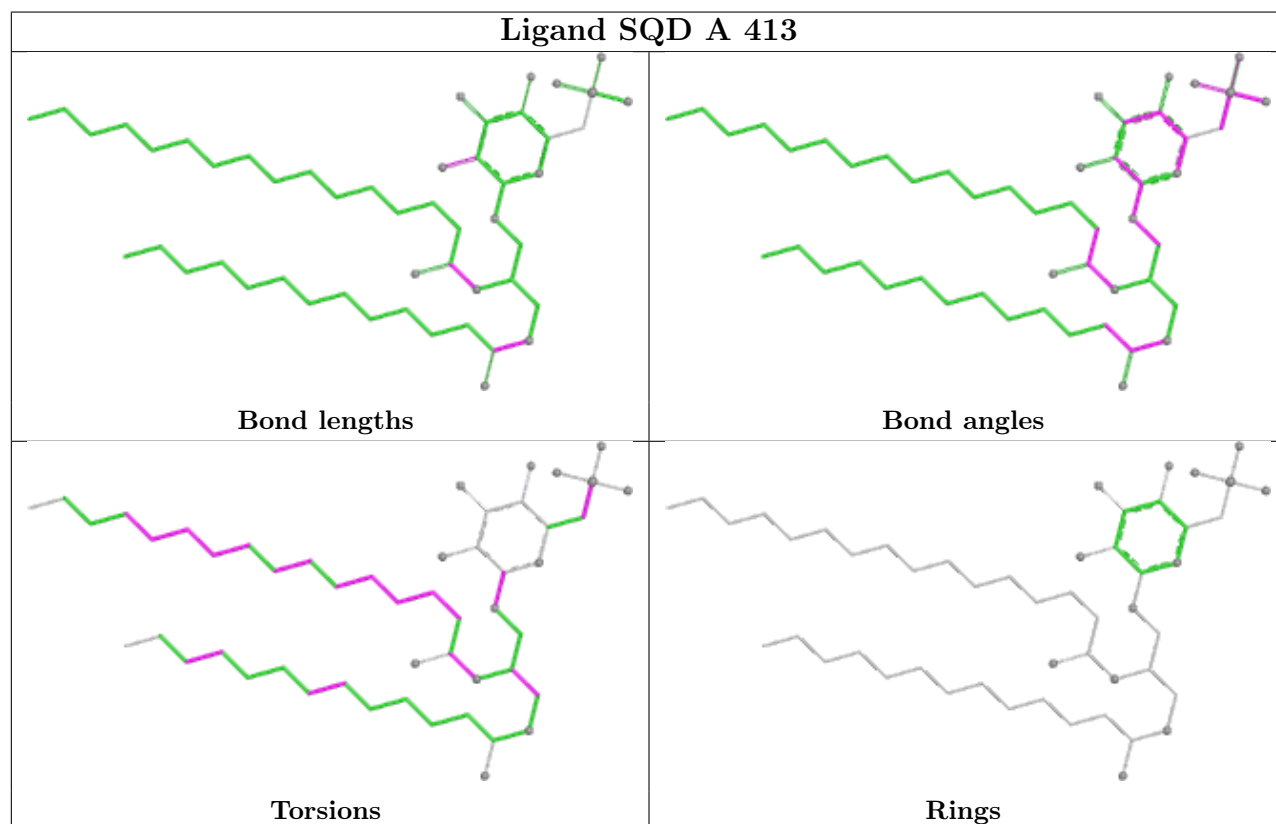
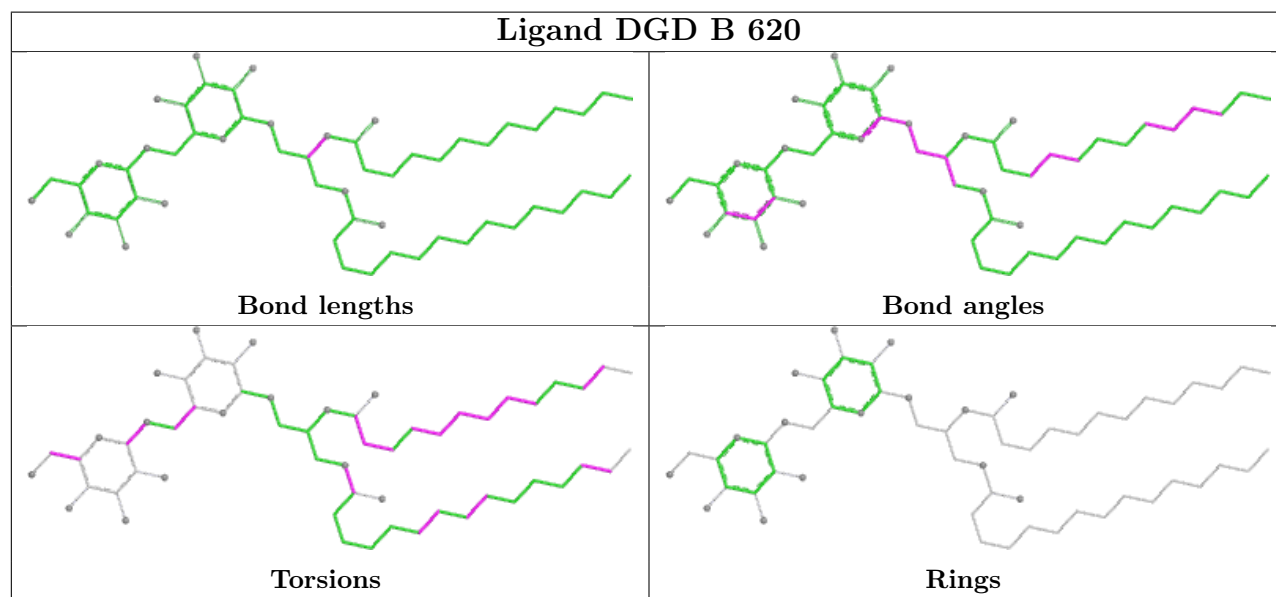
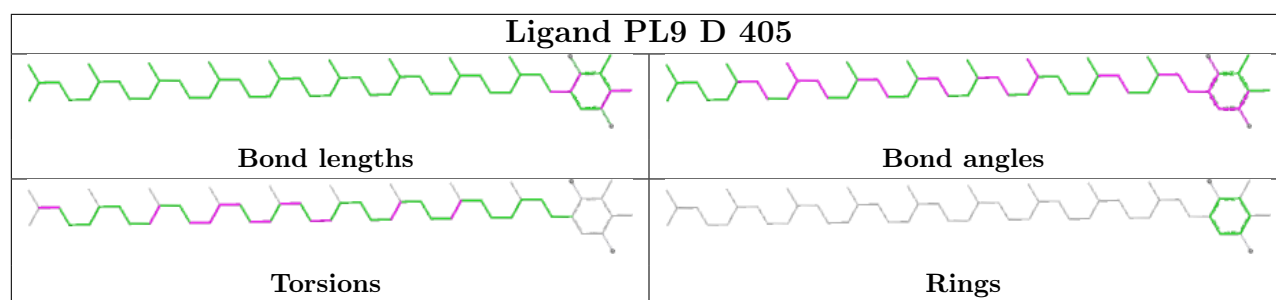
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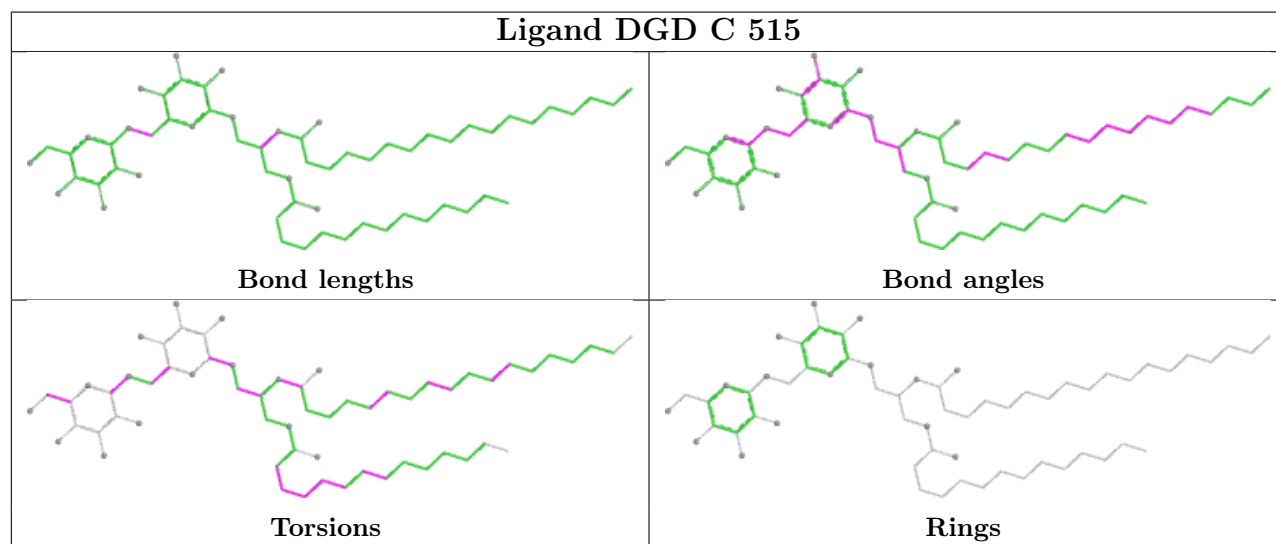
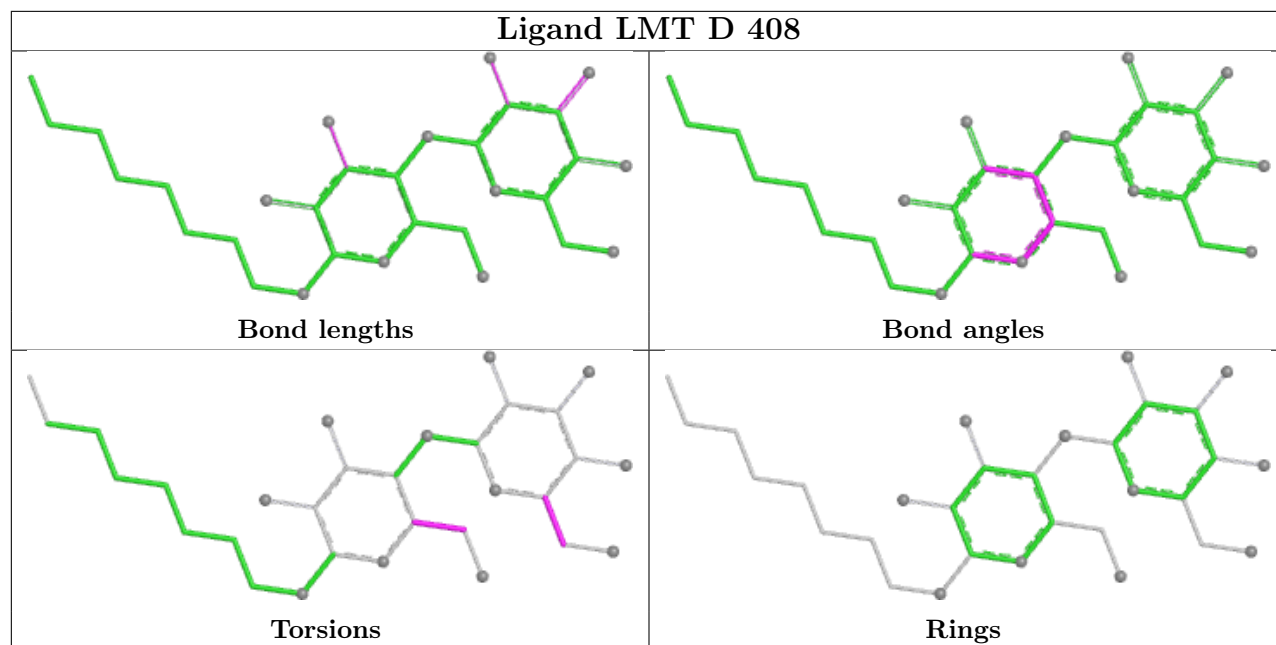
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	507	CLA	4	0
22	B	610	CLA	3	0
31	c	518	LMG	2	0
31	m	101	LMG	3	0
22	c	503	CLA	2	0
31	E	101	LMG	1	0
22	C	519	CLA	3	0
25	i	101	BCR	2	0
31	d	408	LMG	2	0
30	F	103	SQD	3	0
22	c	512	CLA	2	0
32	I	102	LMT	1	0
31	c	522	LMG	1	0
22	B	612	CLA	2	0
34	V	201	HEM	3	0
25	g	101	BCR	11	0
22	b	615	CLA	2	0
31	C	521	LMG	1	0
31	D	406	LMG	7	0
22	c	502	CLA	1	0
22	D	403	CLA	11	0
22	a	403	CLA	8	0
25	A	408	BCR	4	0
26	C	514	DGD	3	0
31	M	101	LMG	2	0
22	c	501	CLA	4	0
22	C	511	CLA	1	0
23	d	402	PHO	5	0
25	B	619	BCR	2	0
23	A	405	PHO	6	0
22	B	603	CLA	5	0

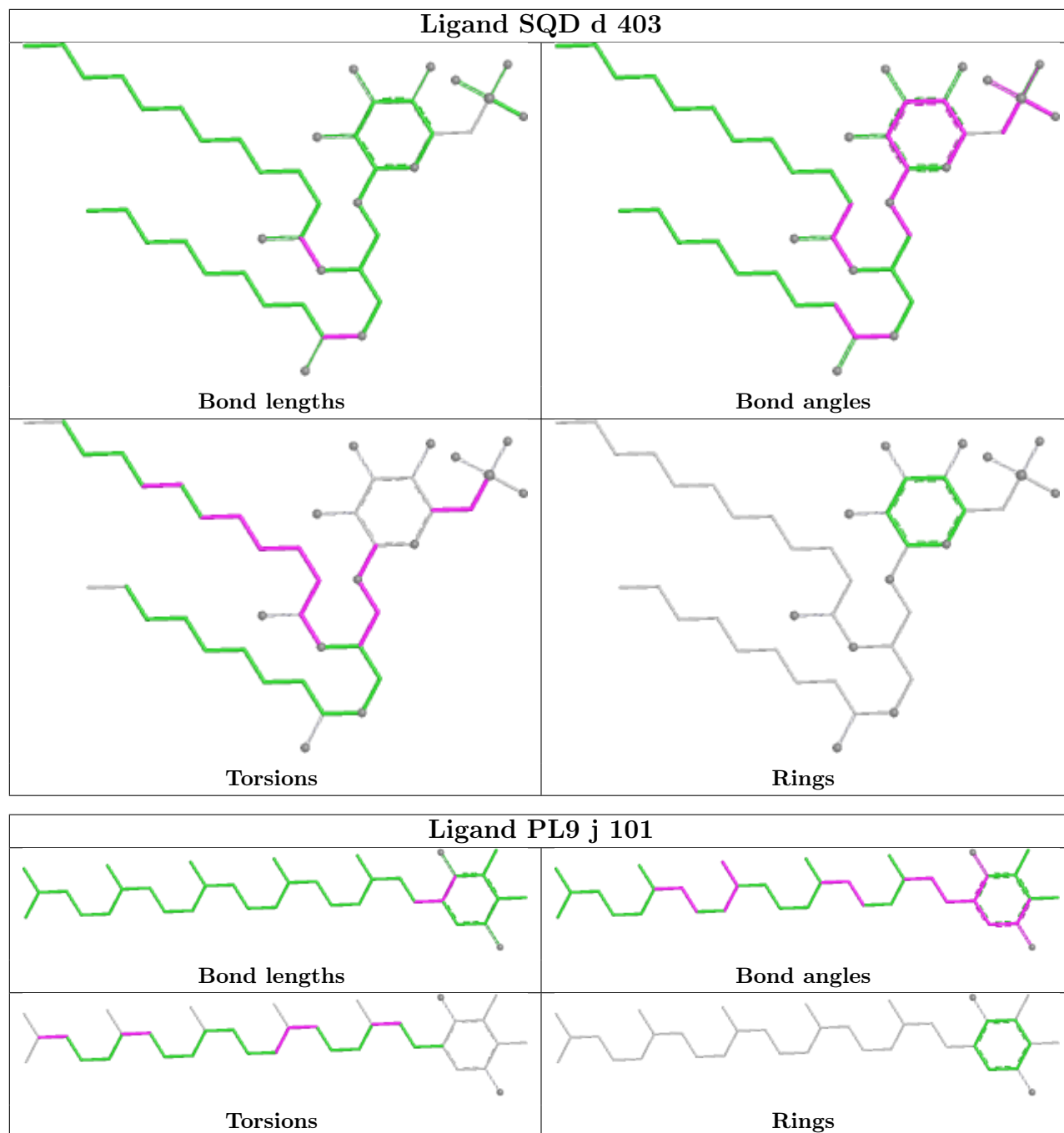
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

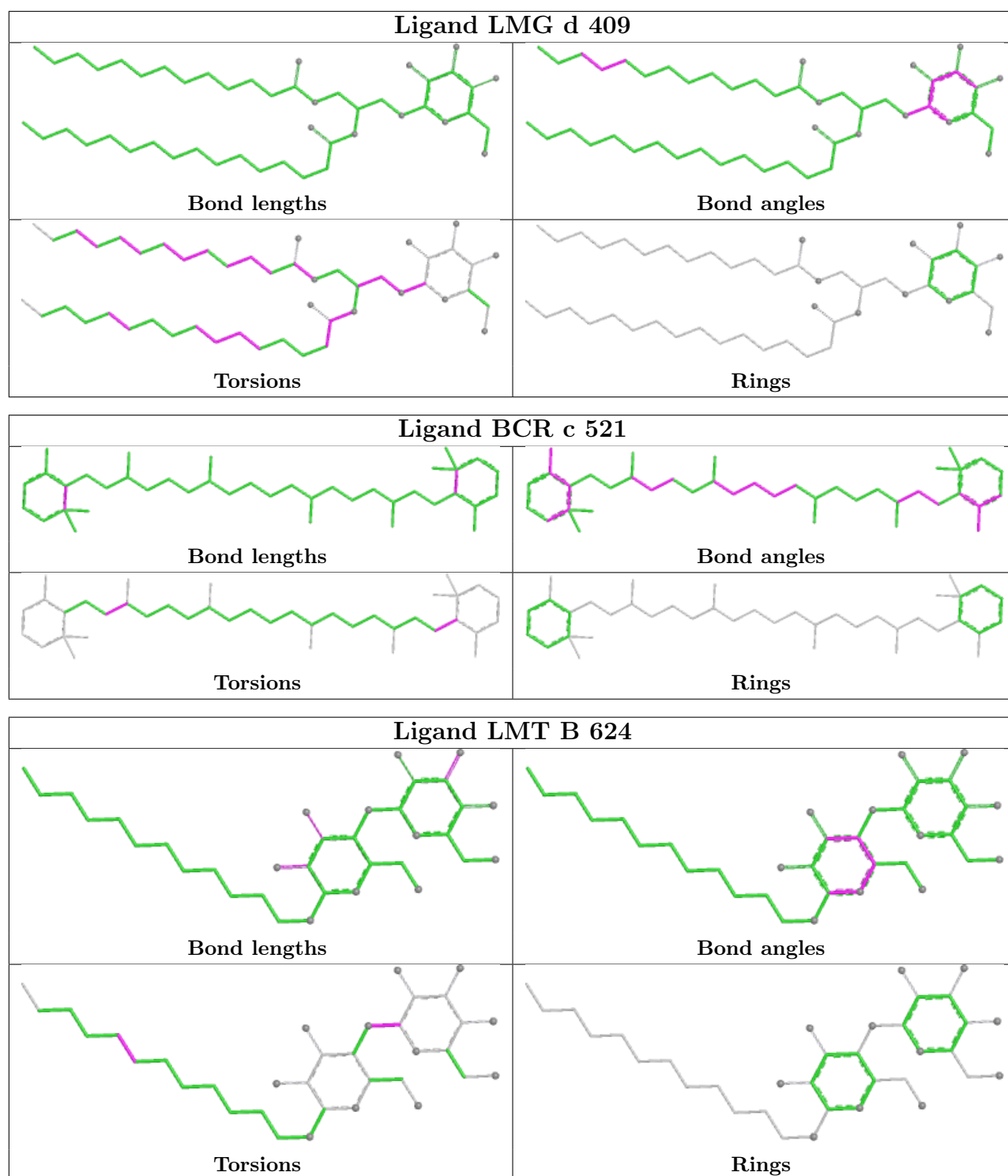
equivalents in the CSD to analyse the geometry.

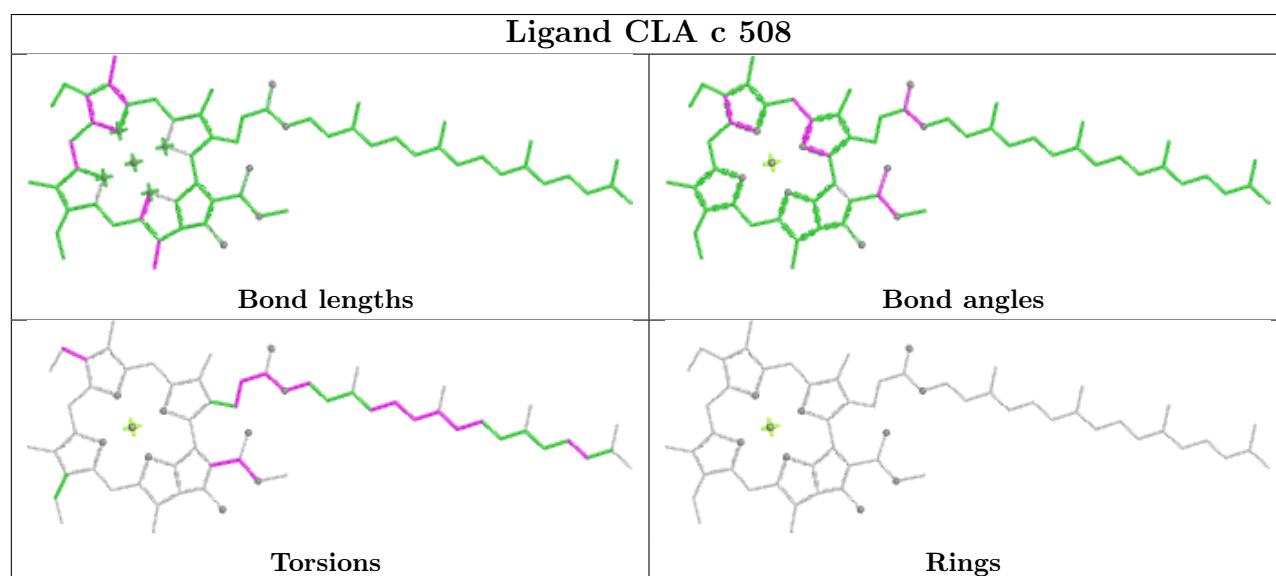
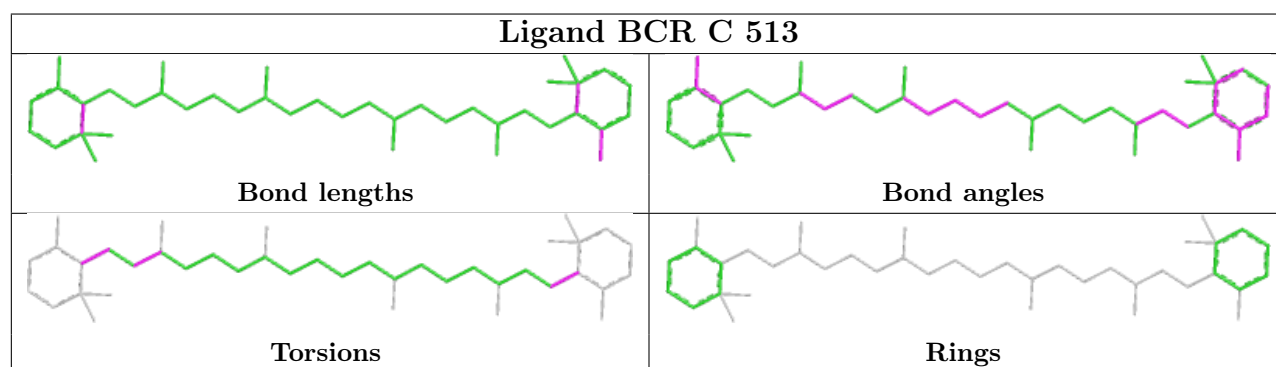
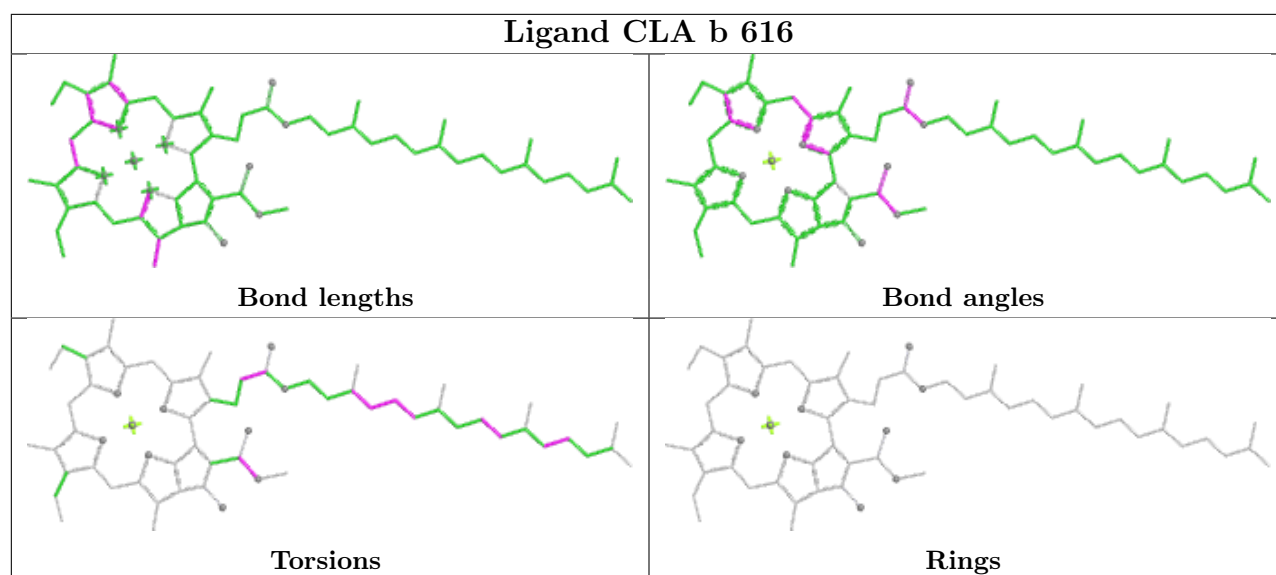




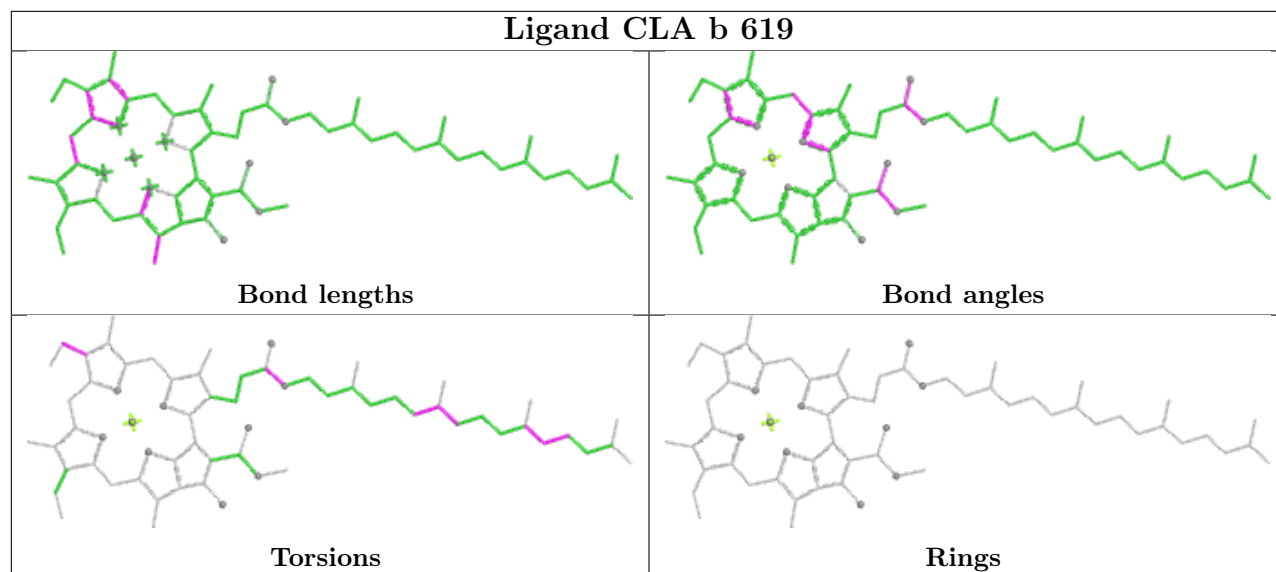




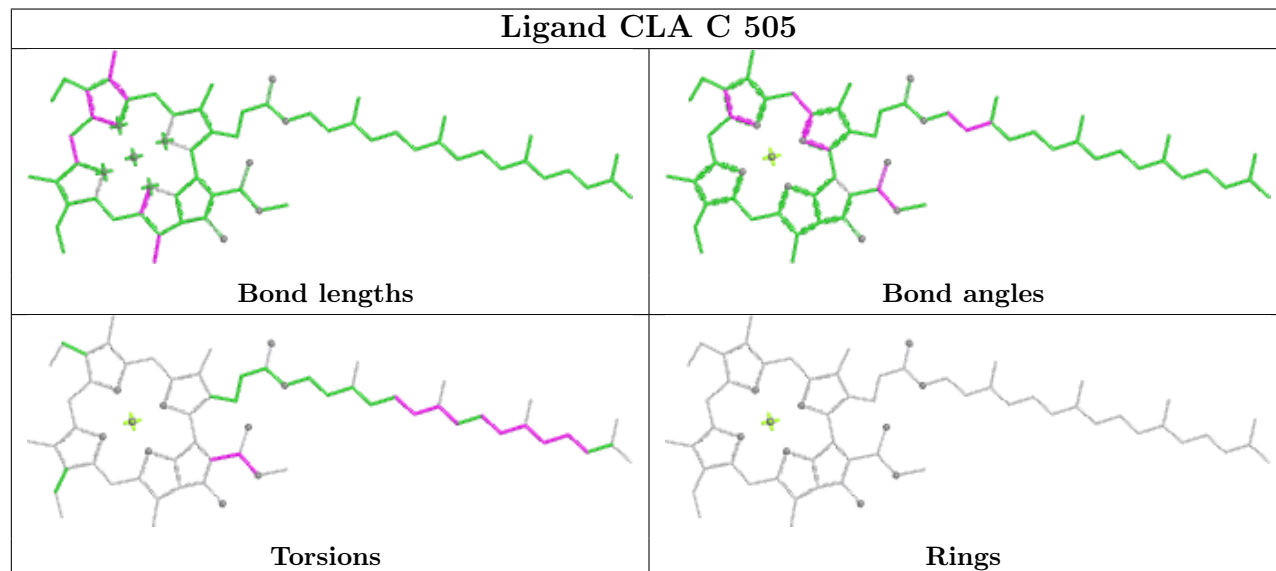




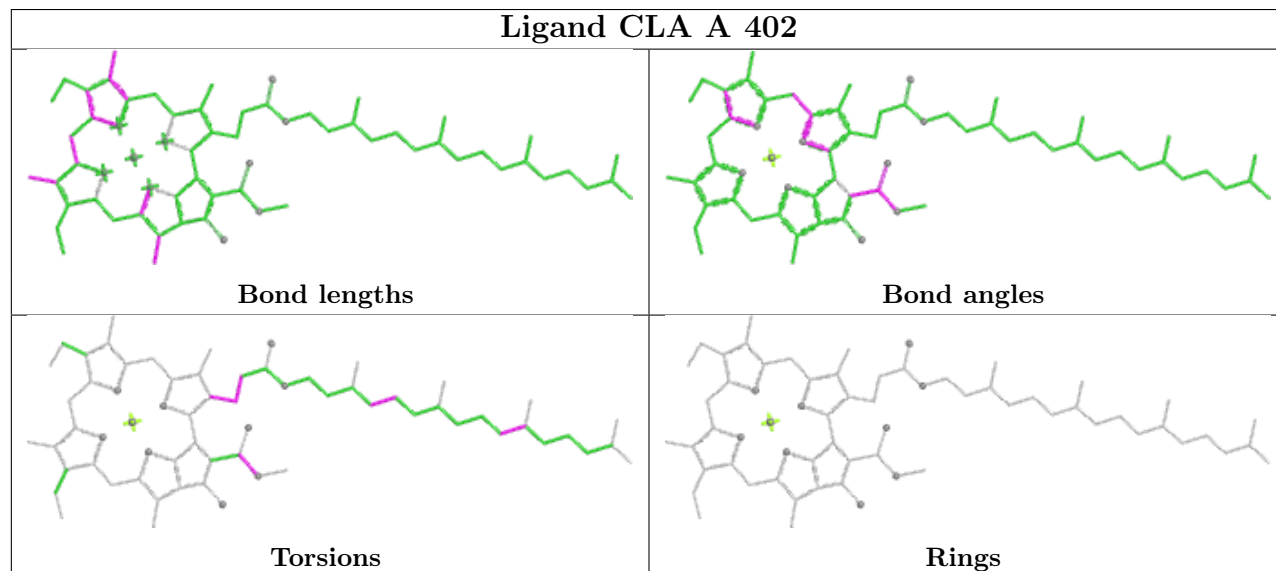
Ligand CLA b 619

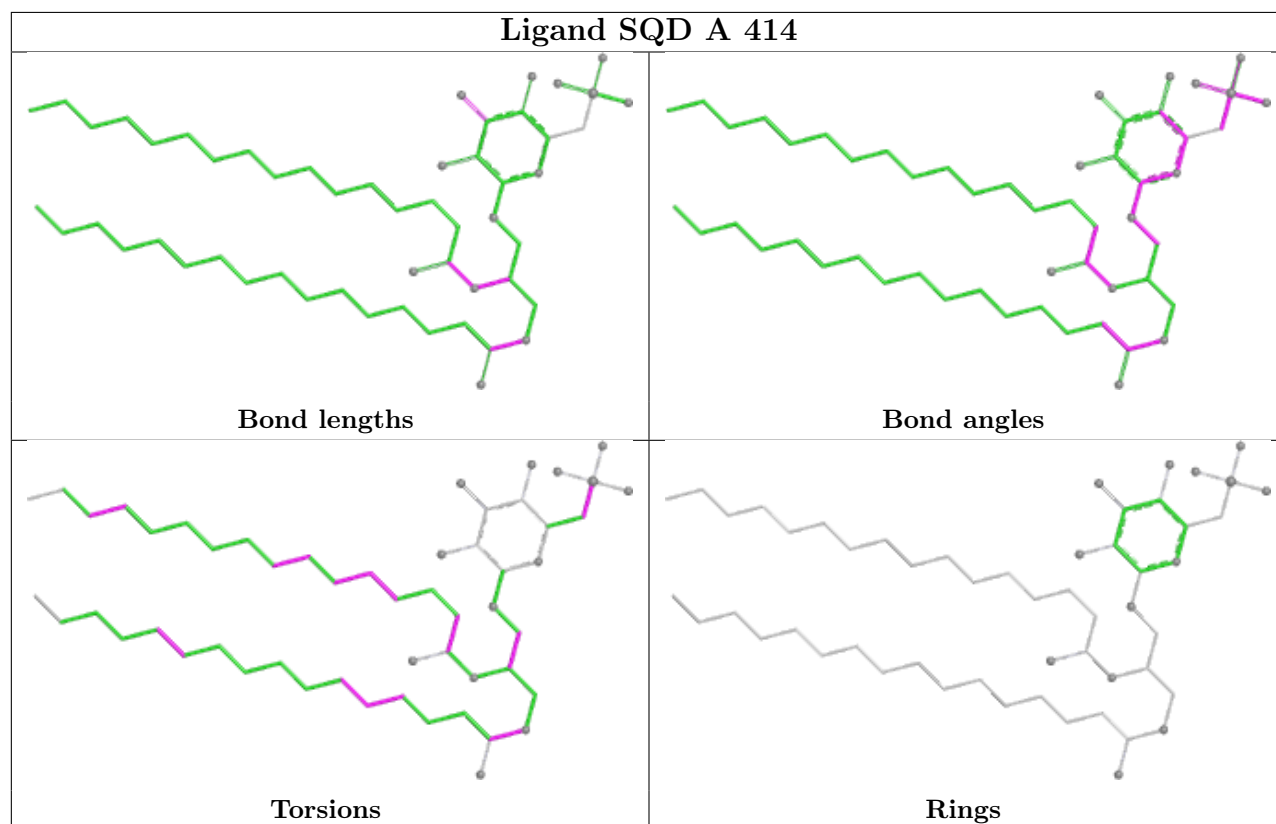
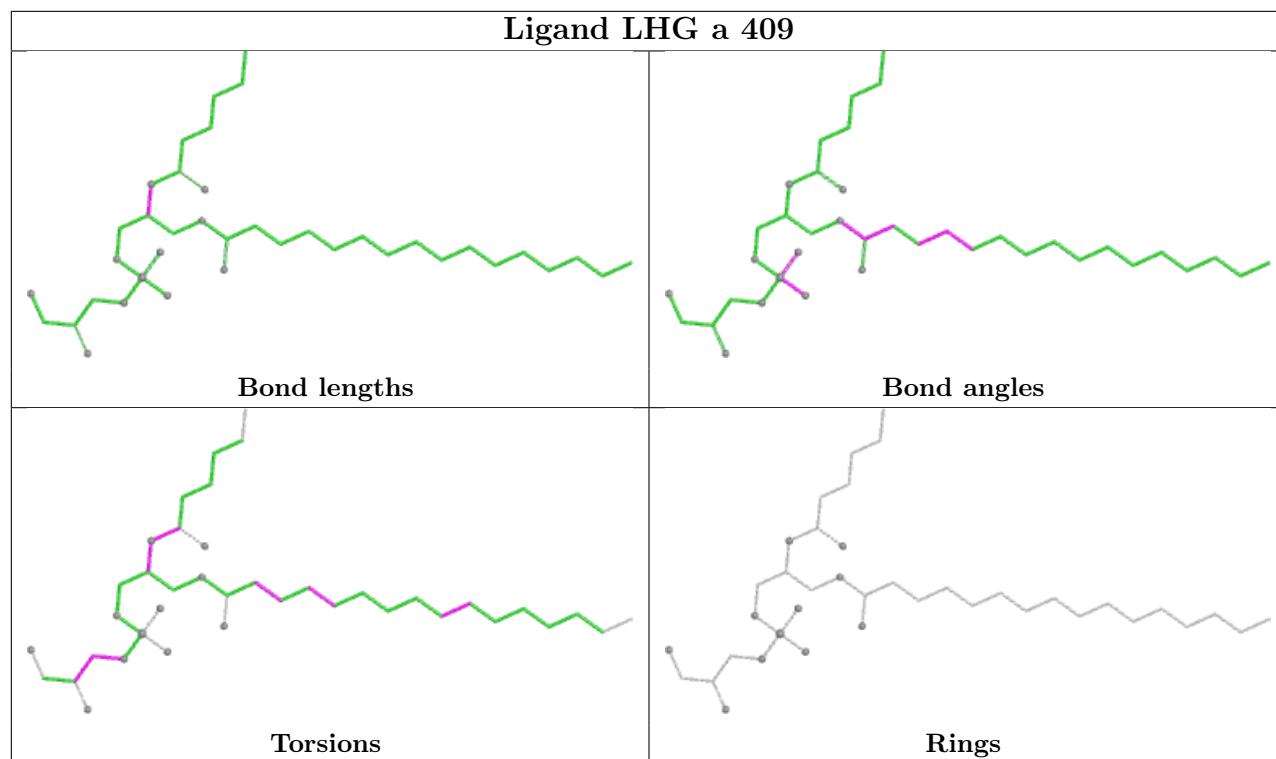


Ligand CLA C 505

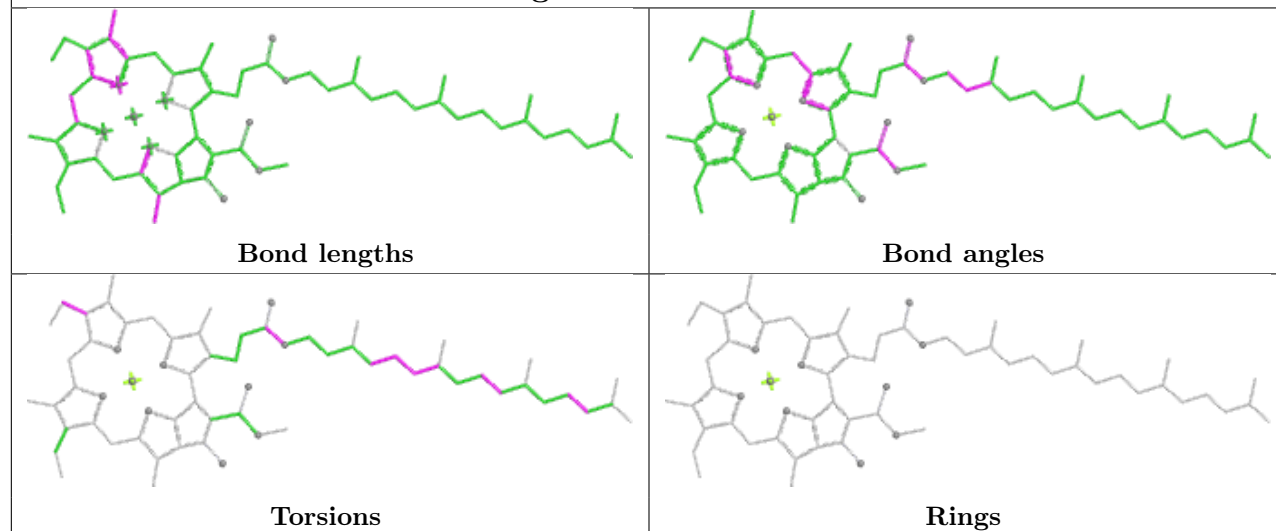


Ligand CLA A 402

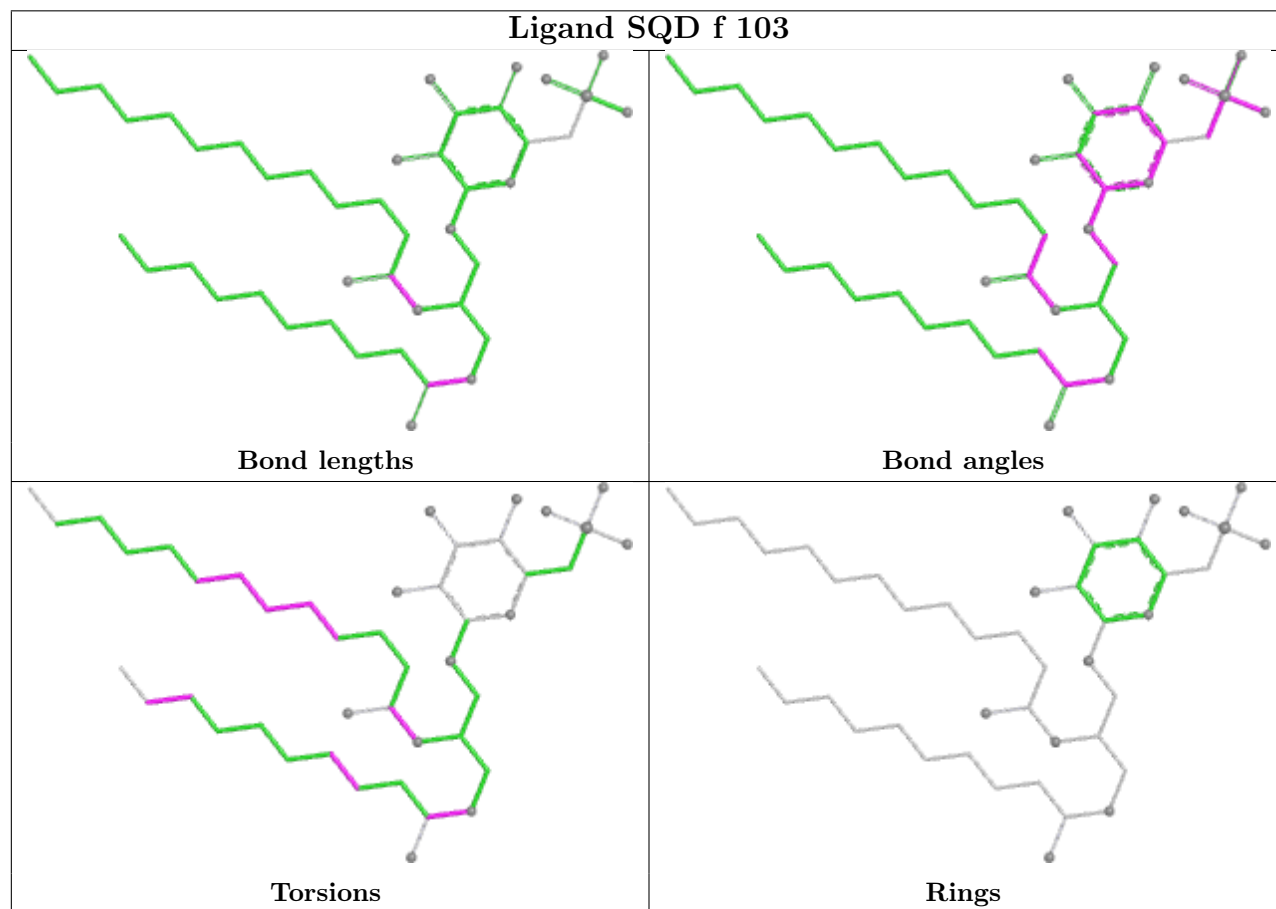


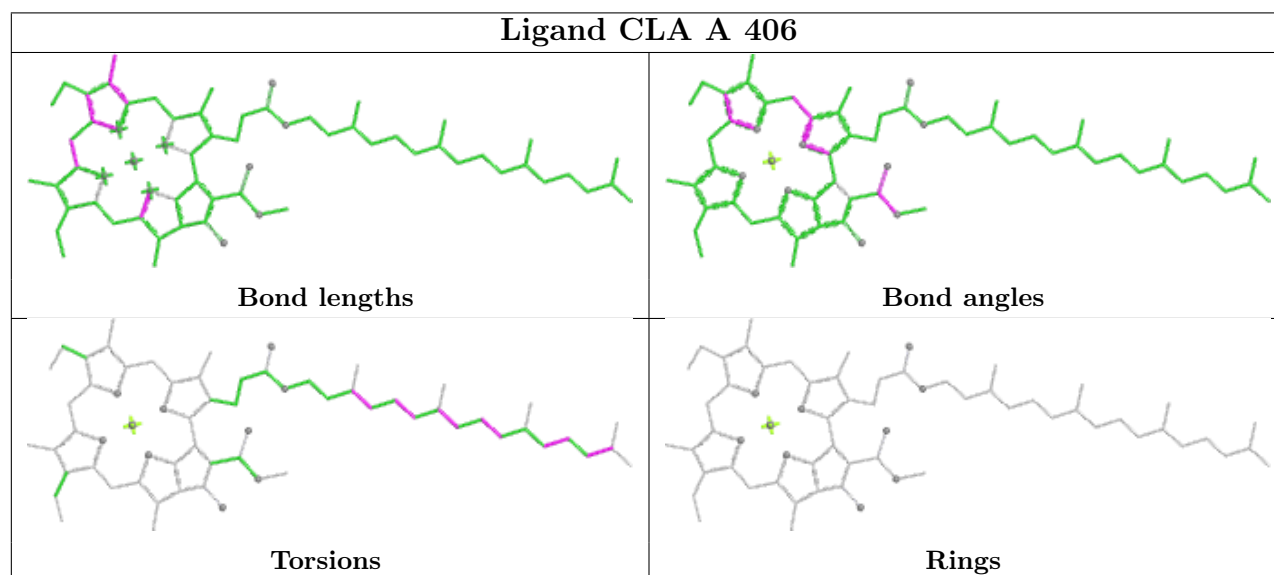
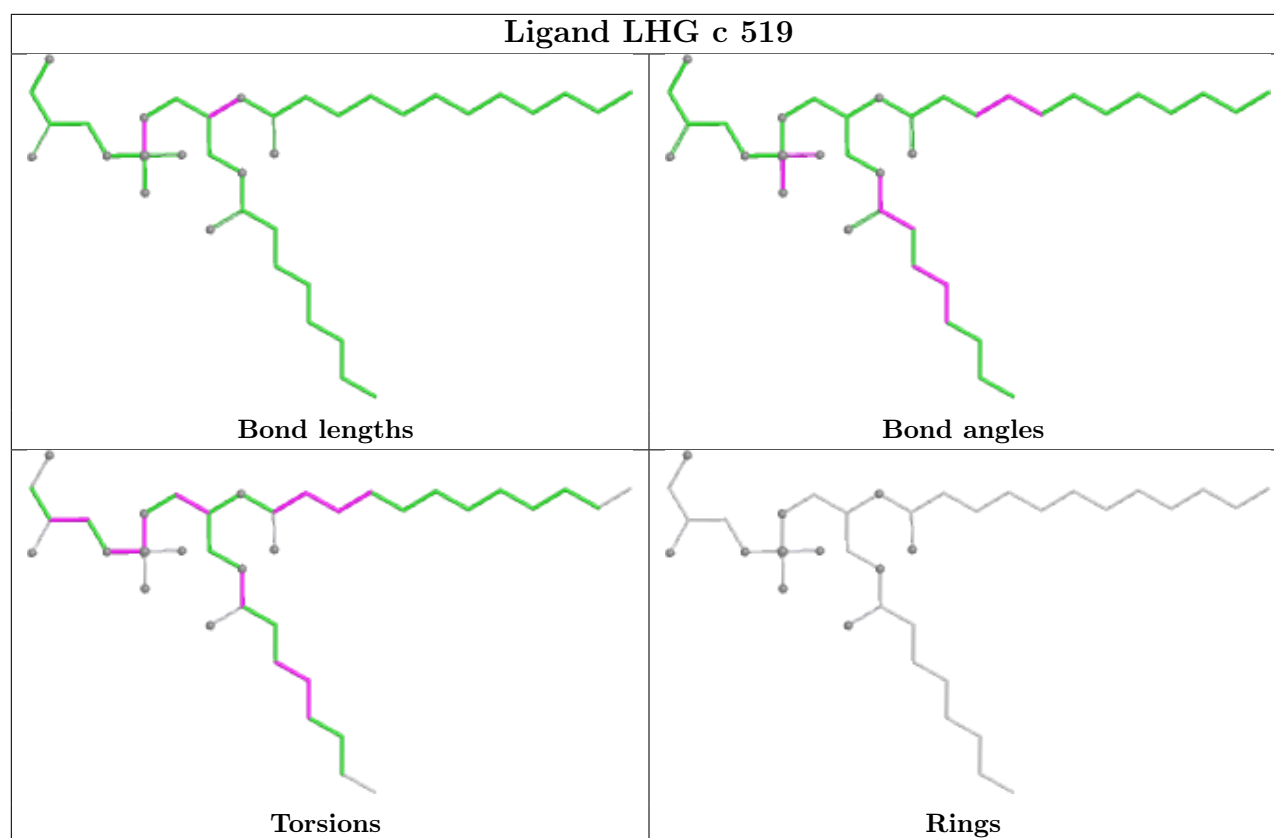


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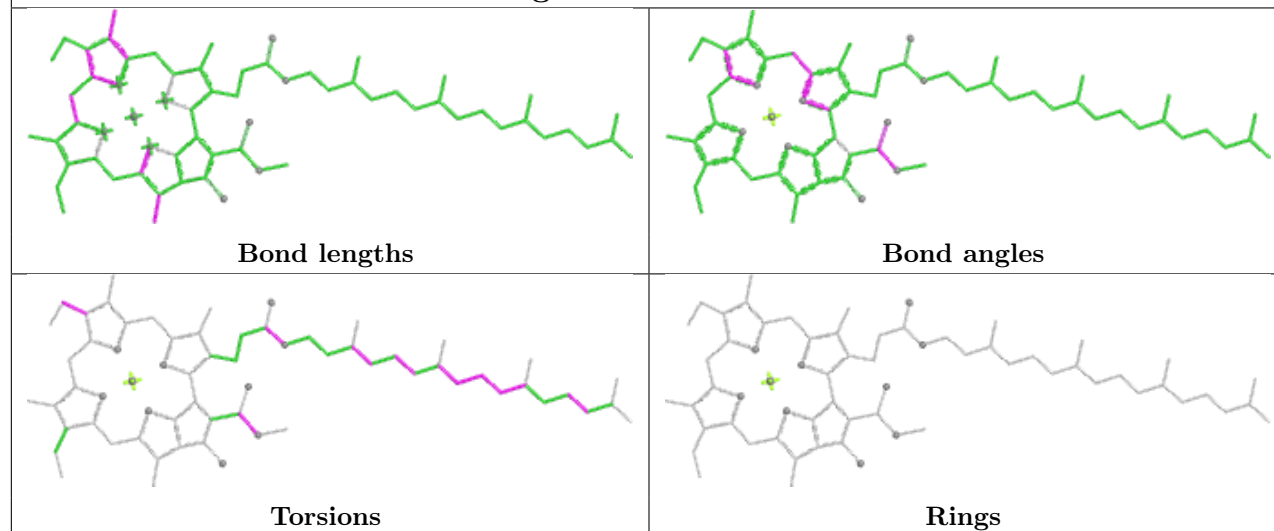


Ligand SQD f 103

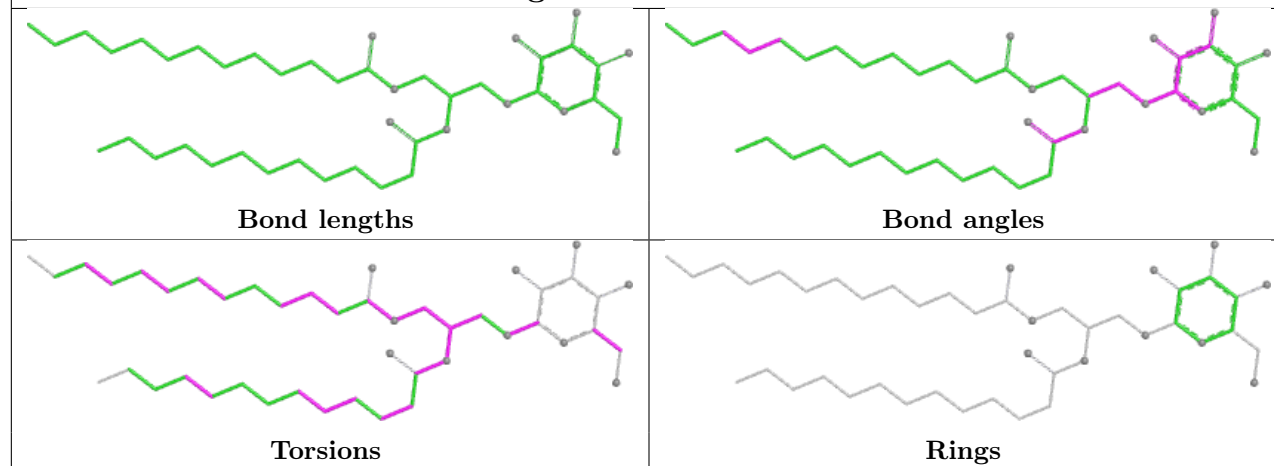




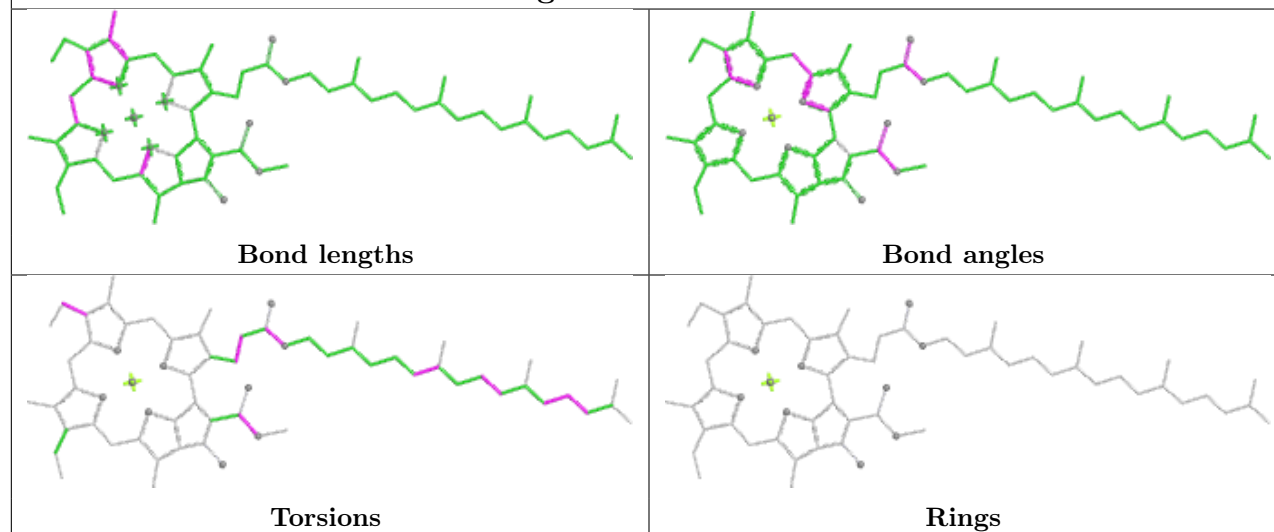
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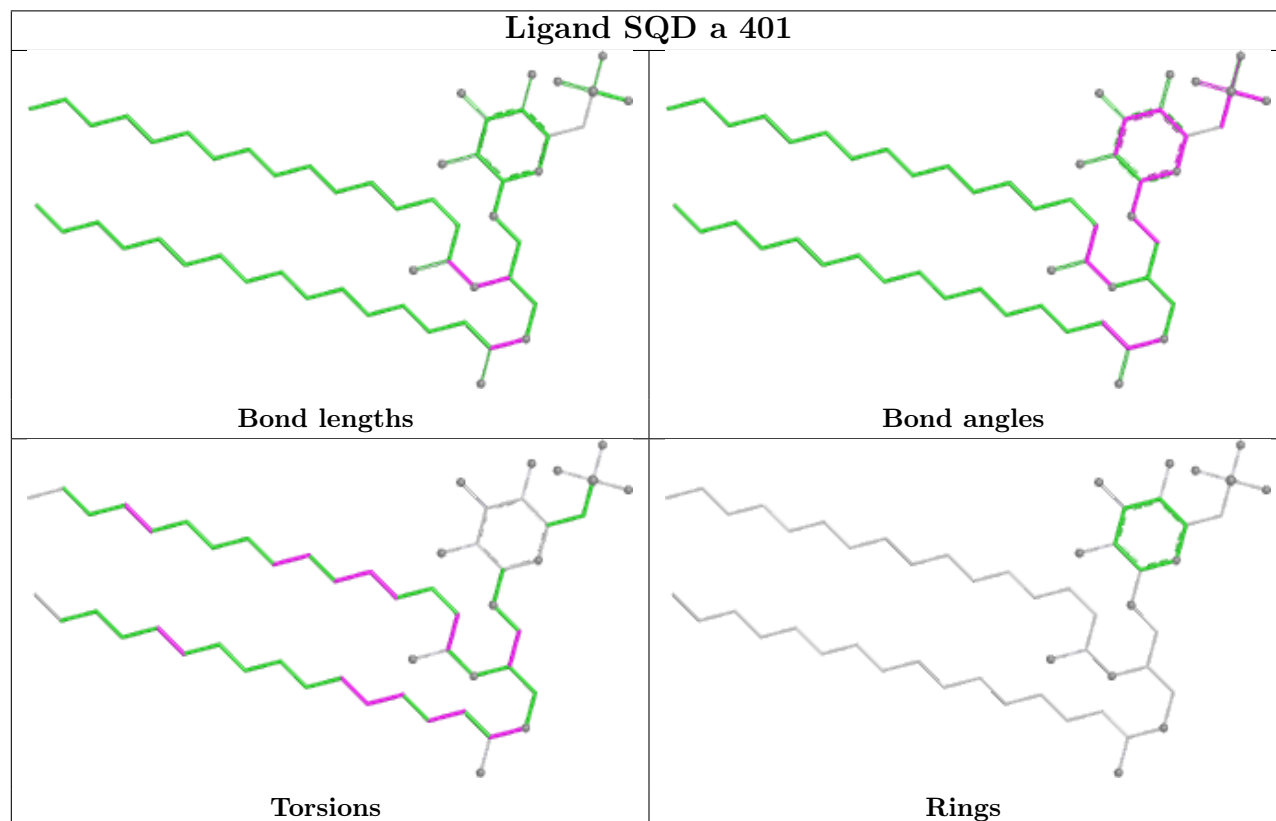
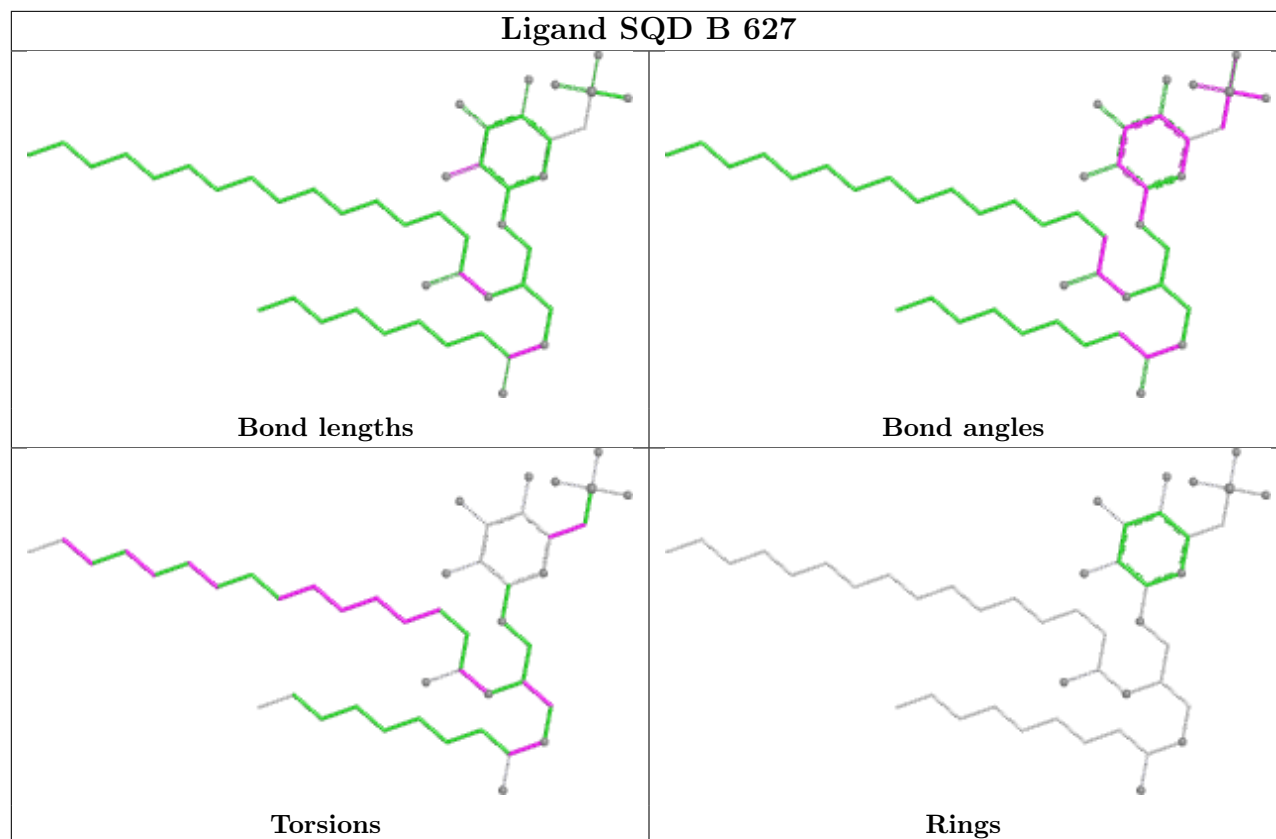


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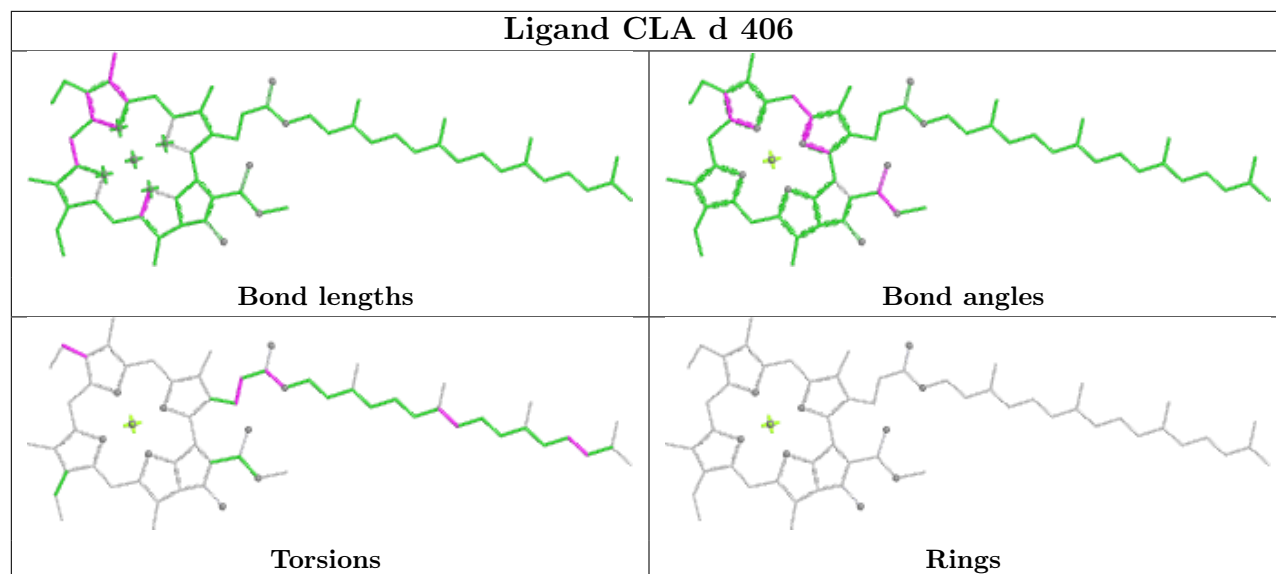


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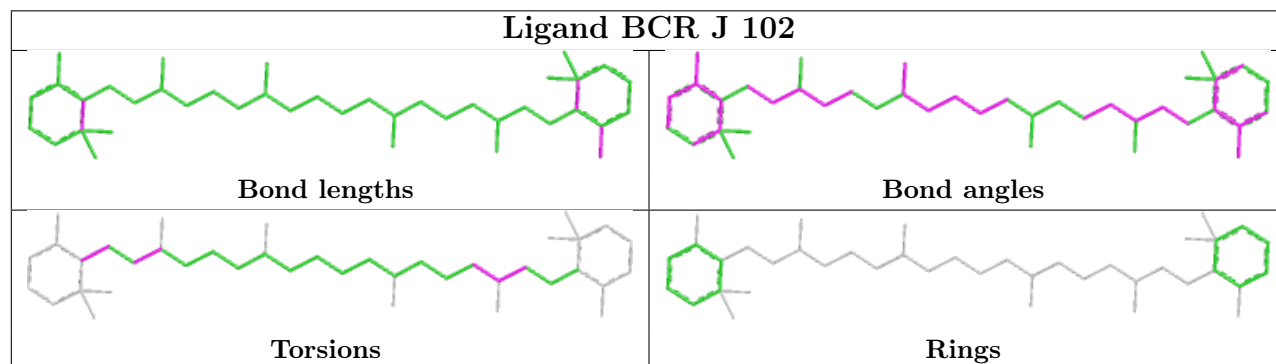




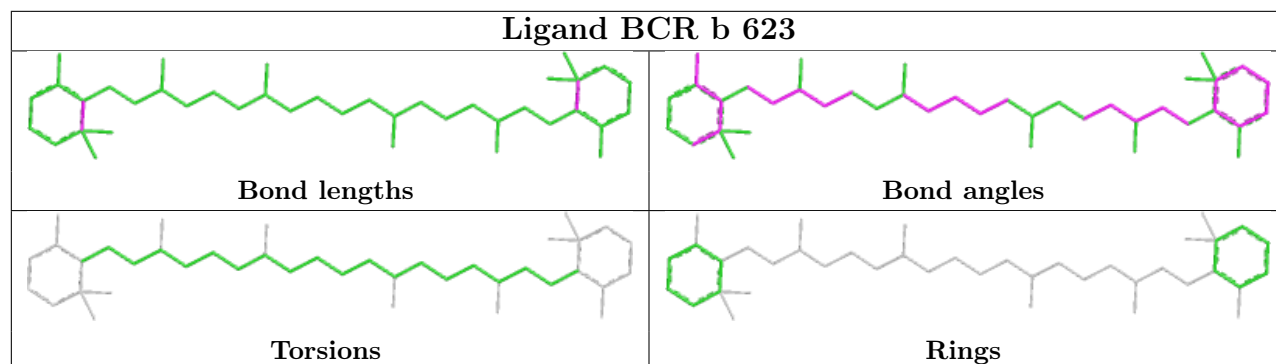
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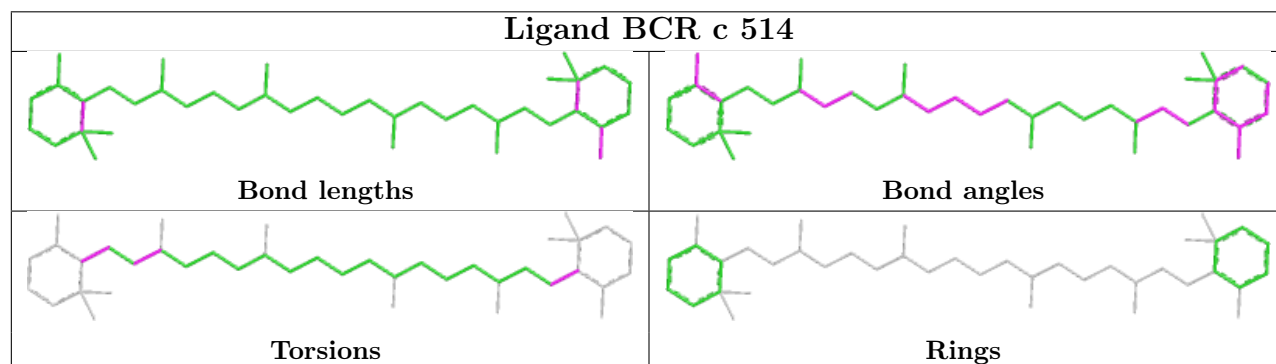
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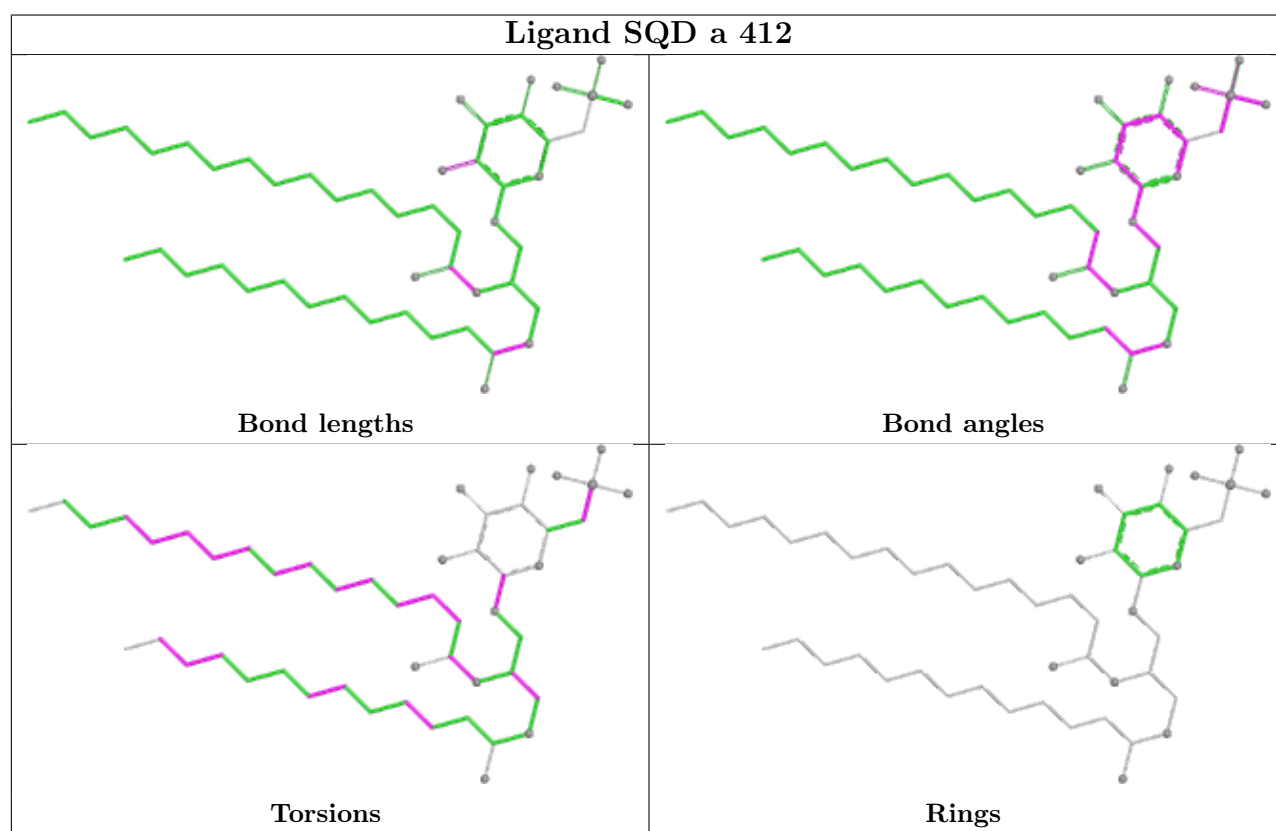
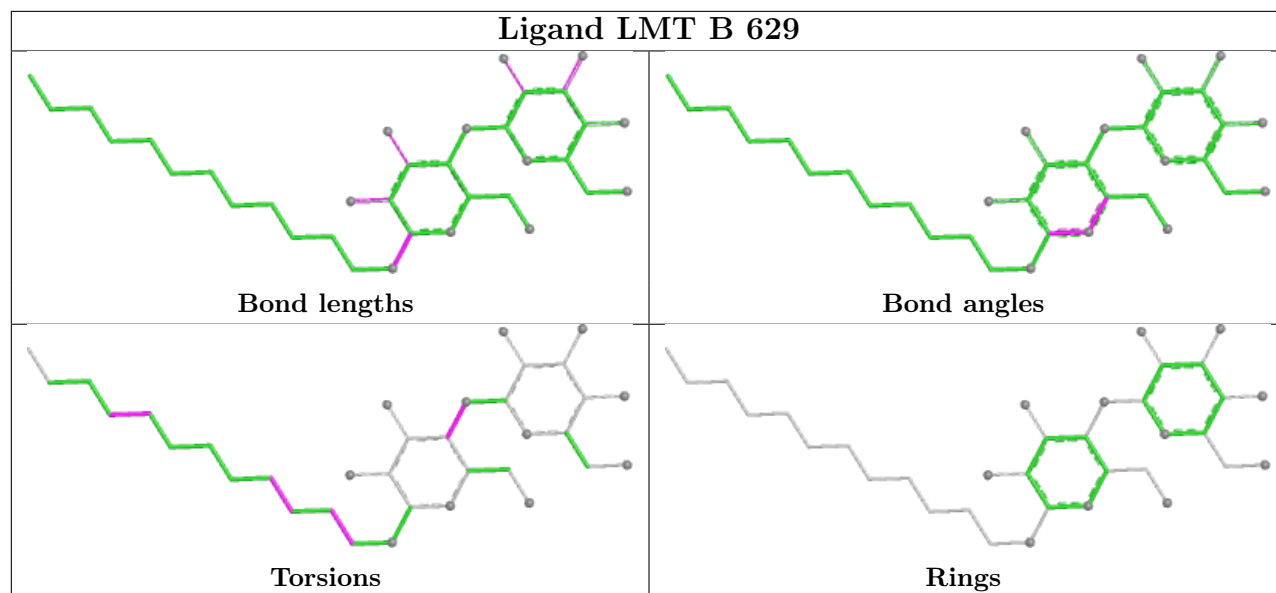


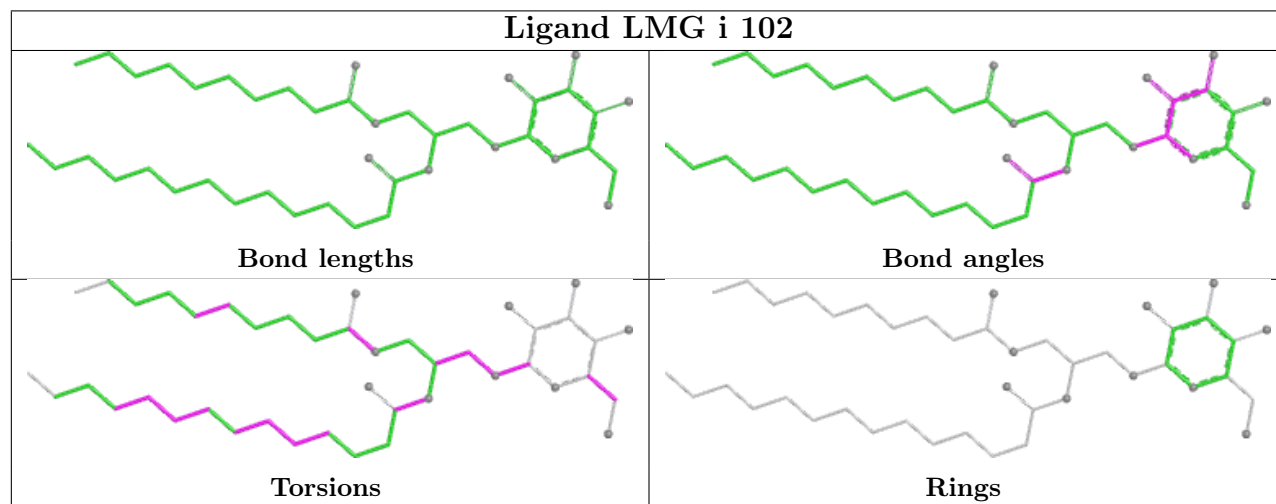
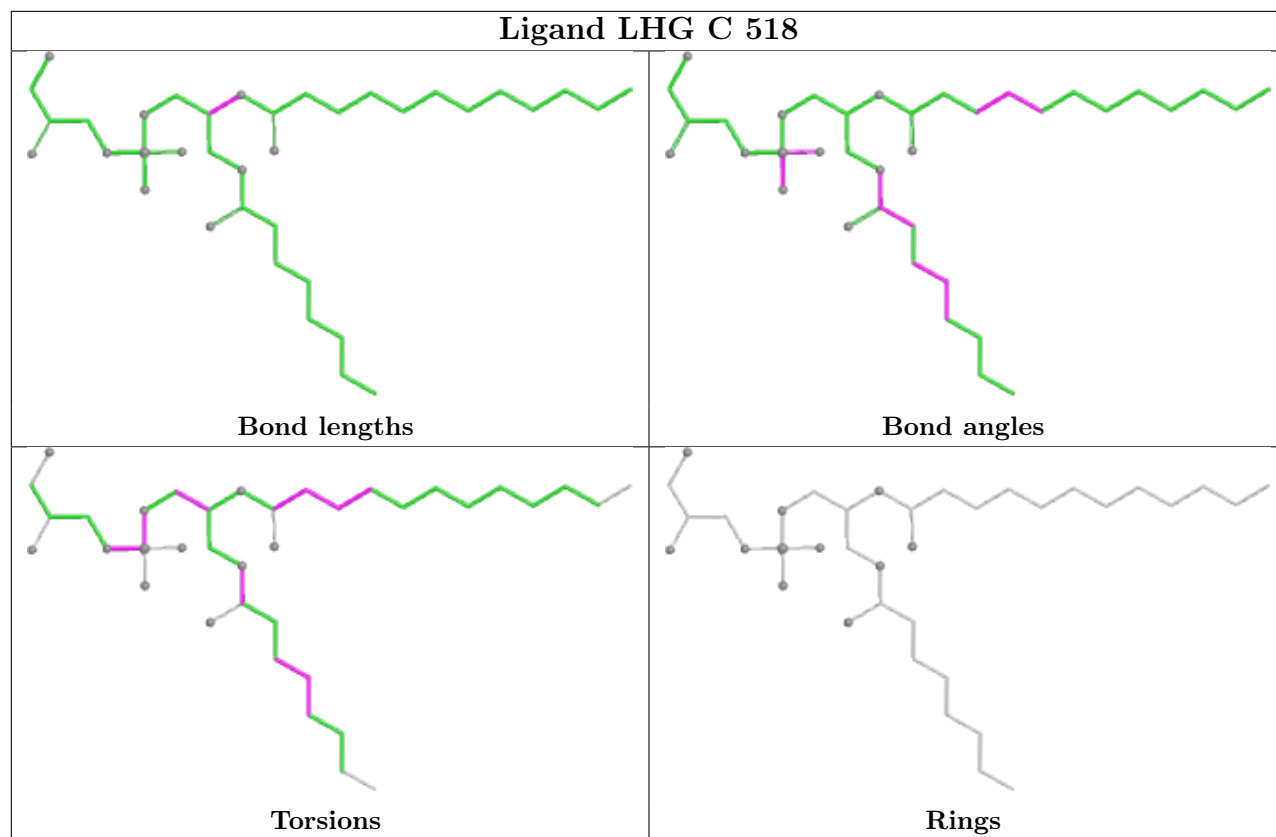
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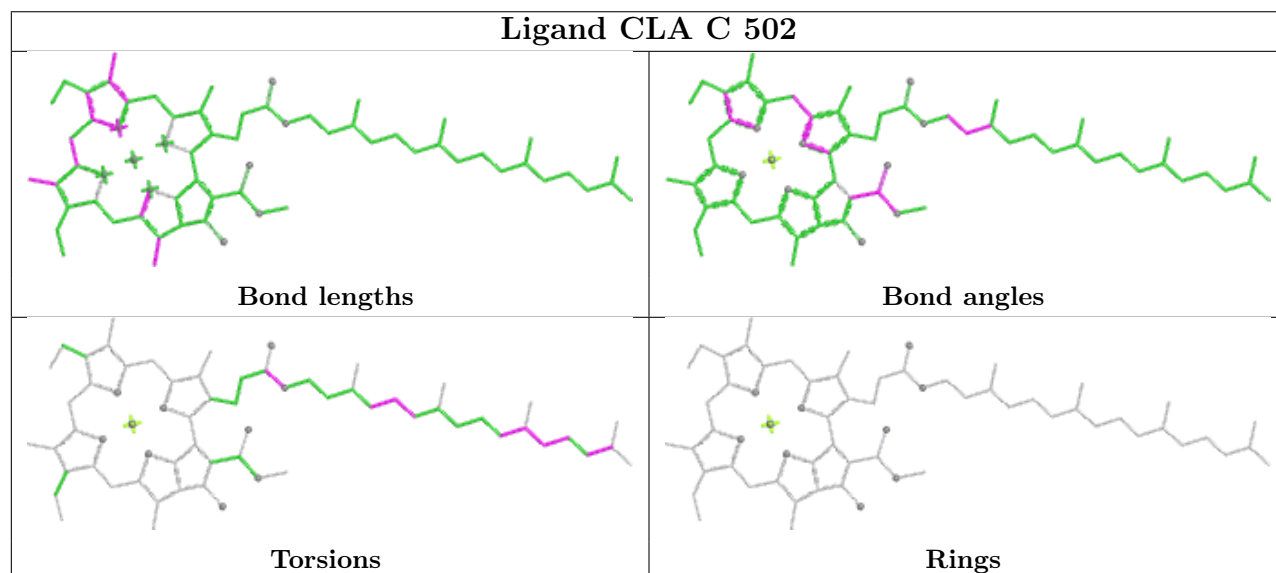
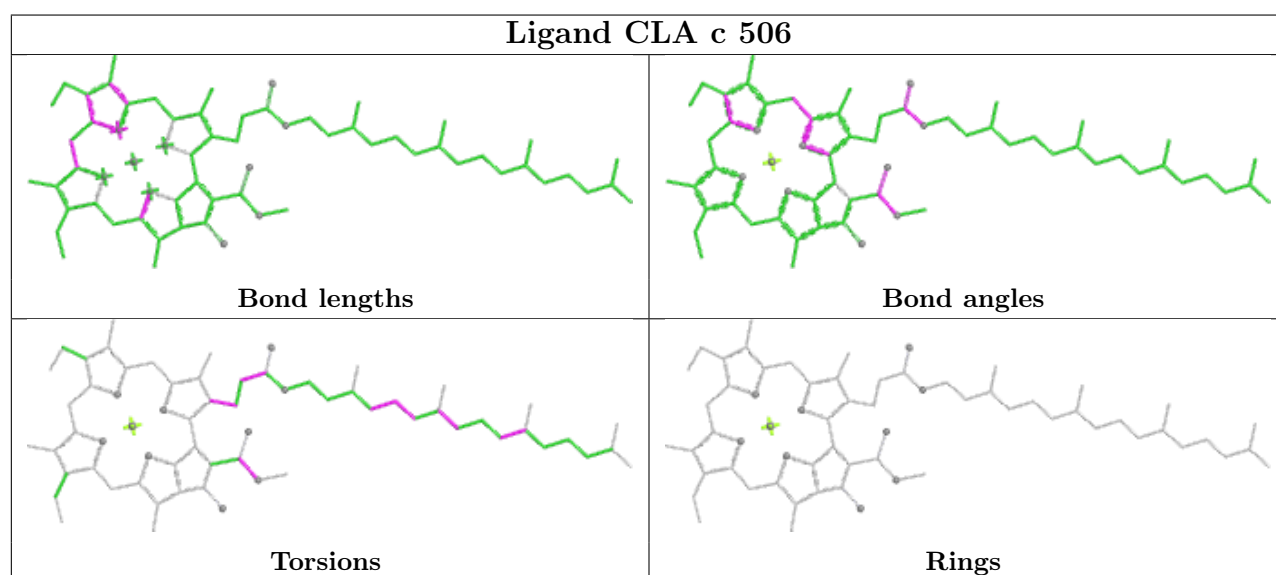
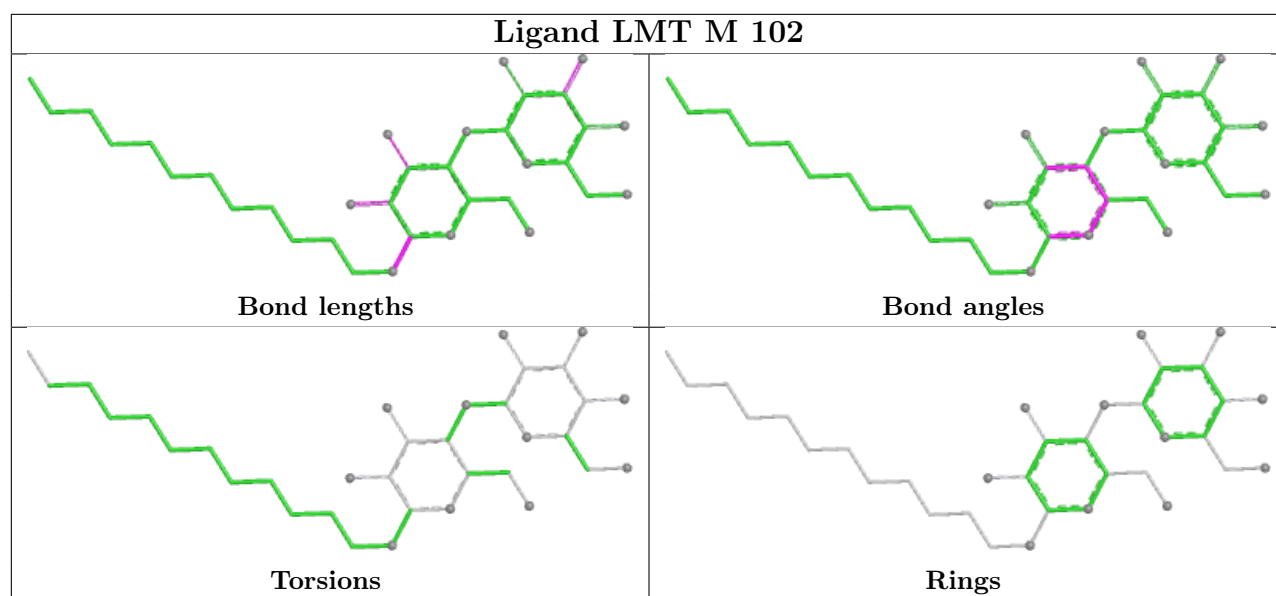


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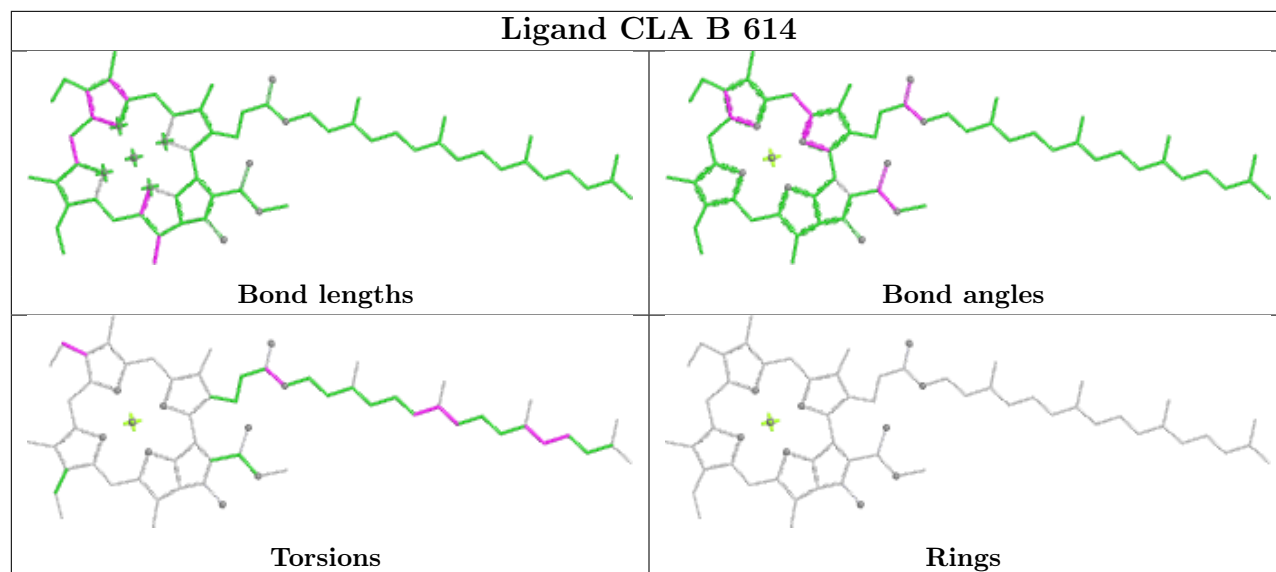




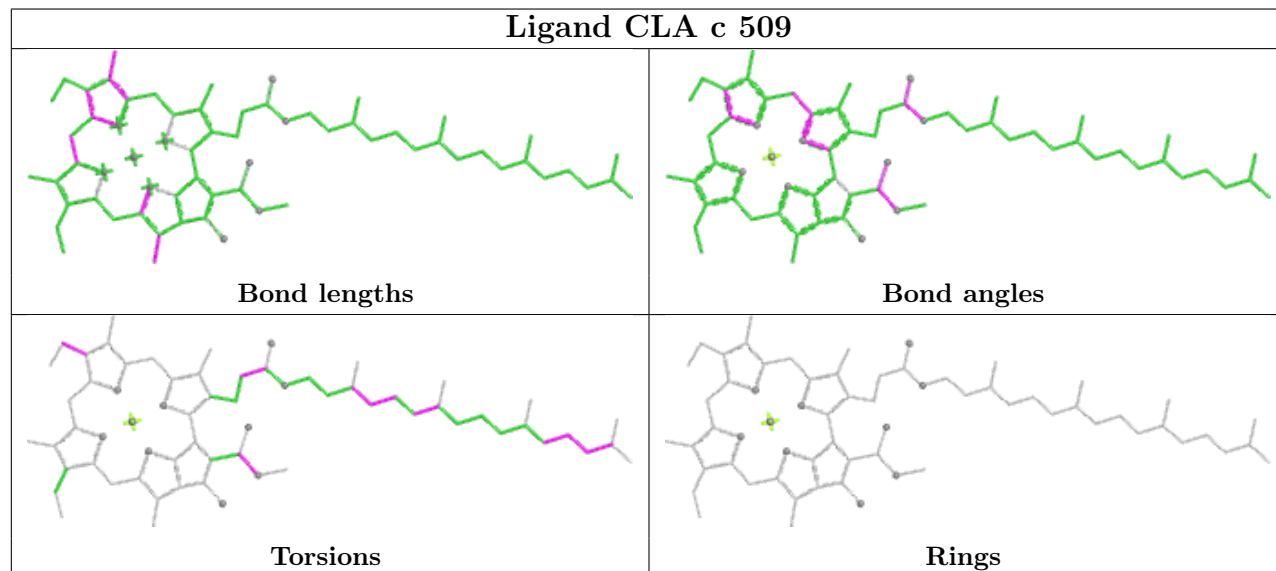




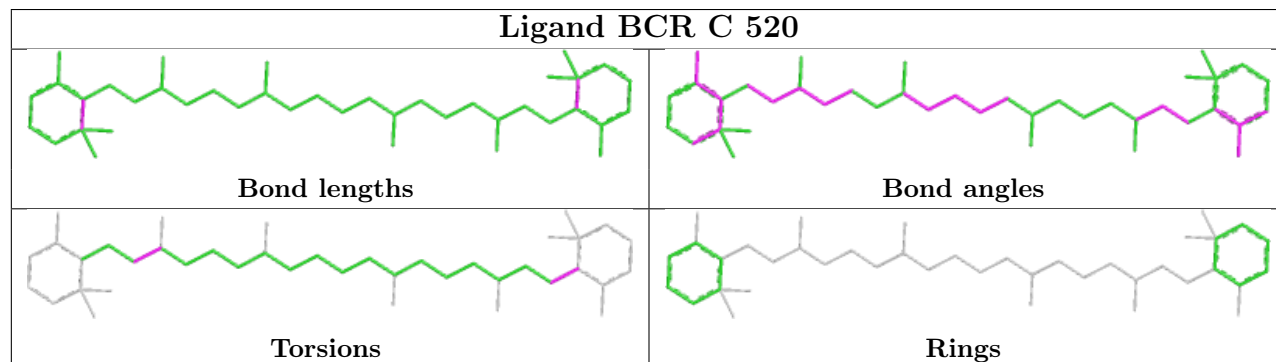
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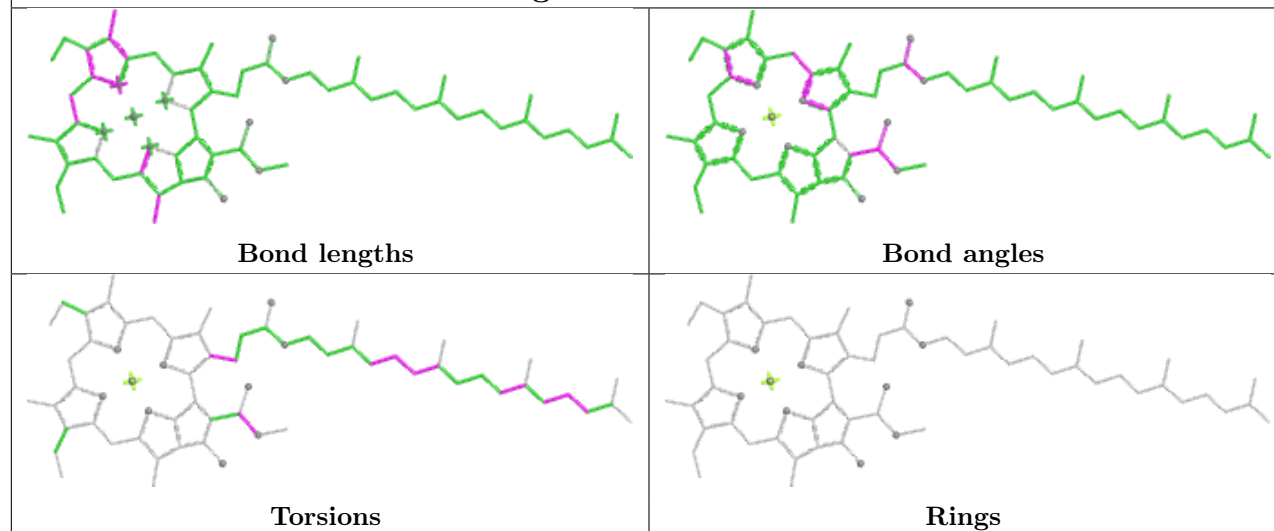
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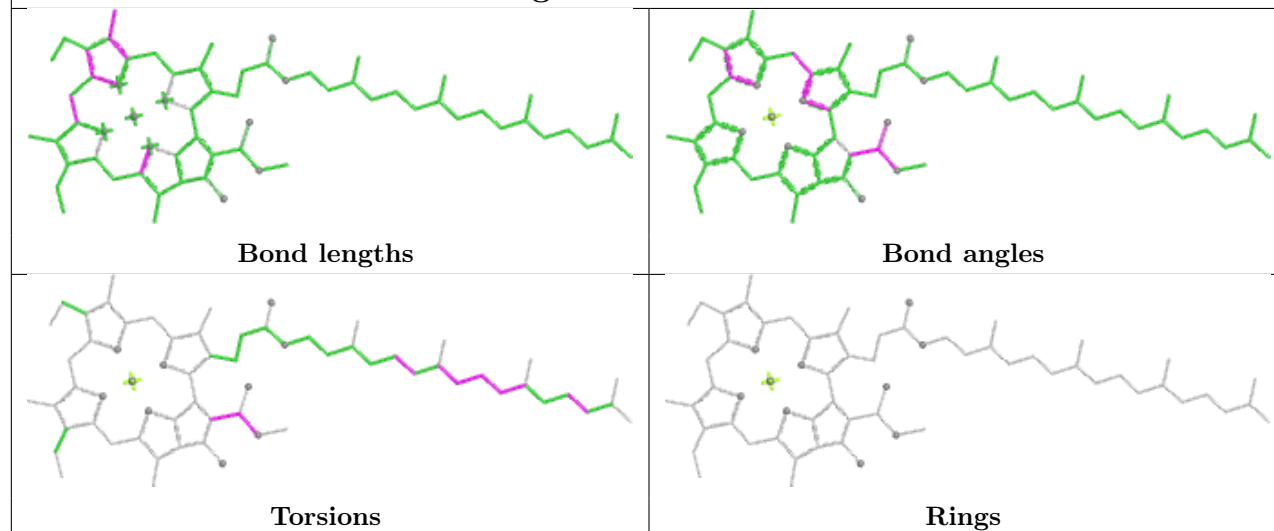
Ligand BCR C 520



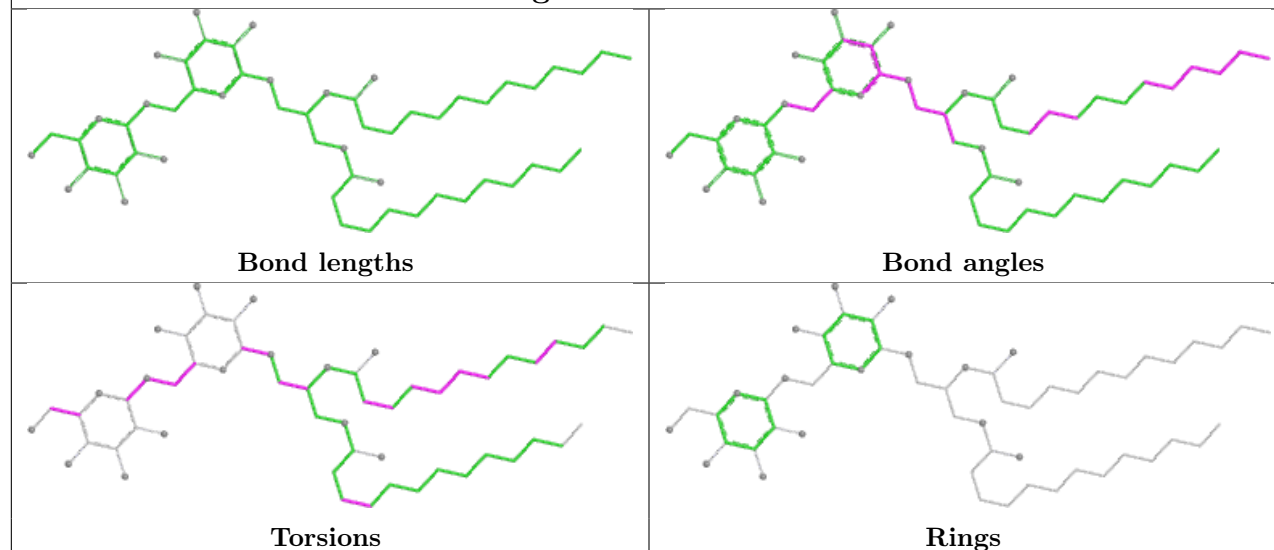
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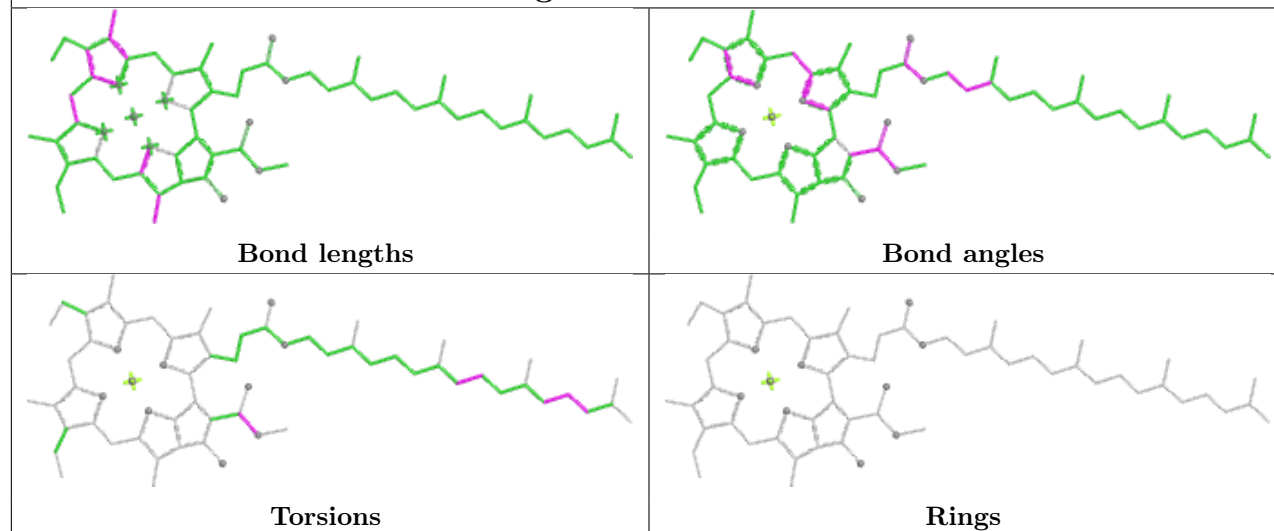
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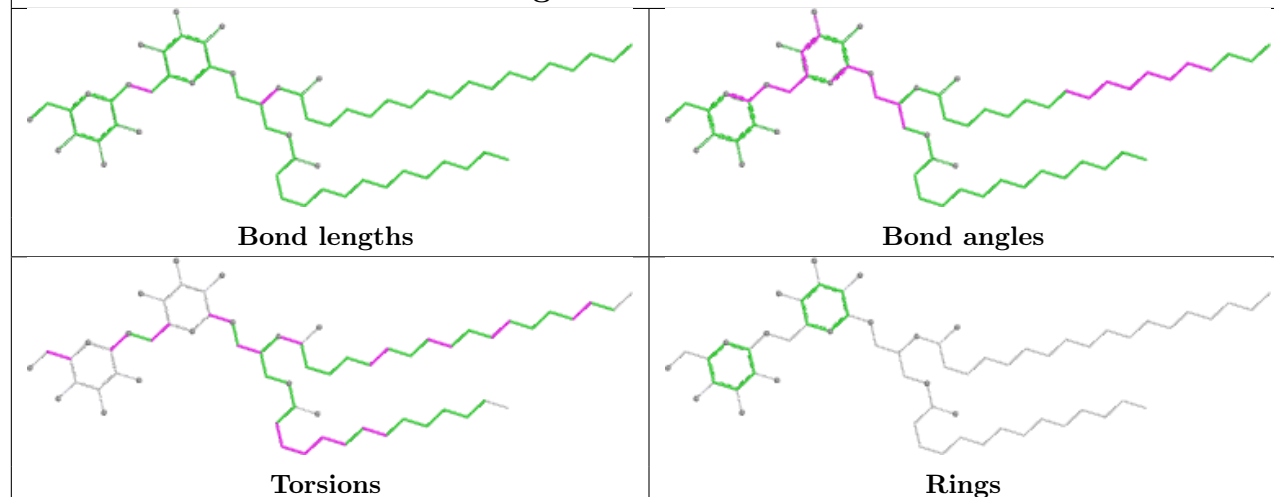
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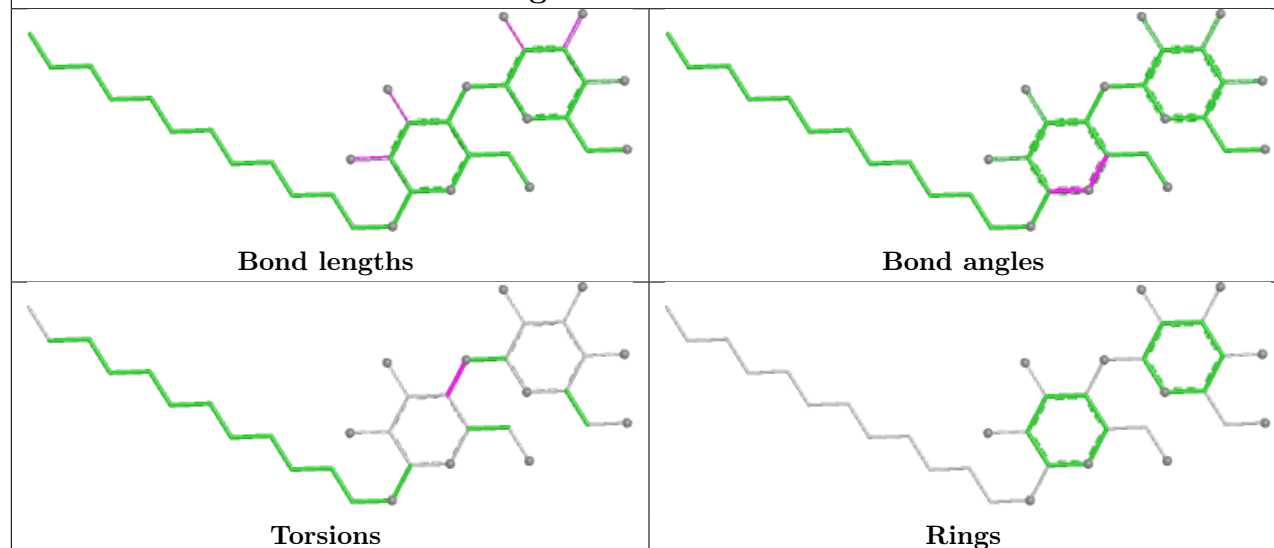
Ligand CLA b 608



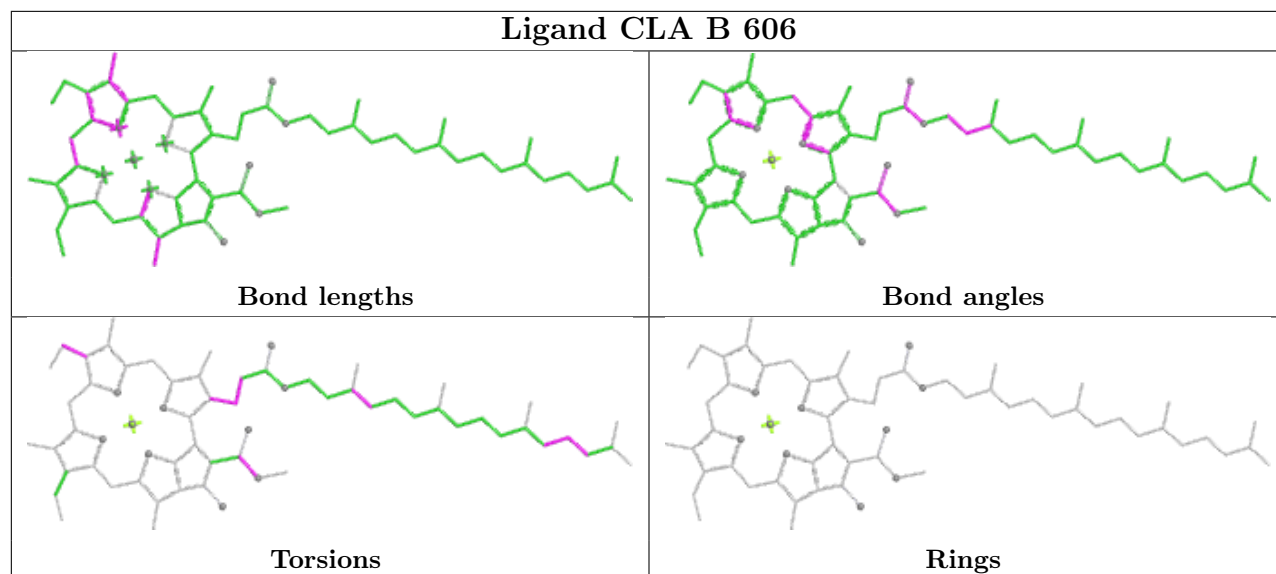
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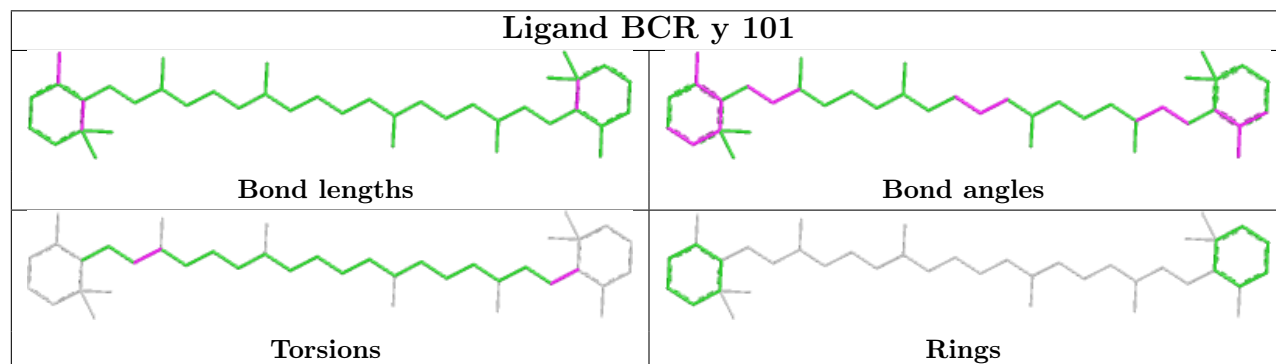
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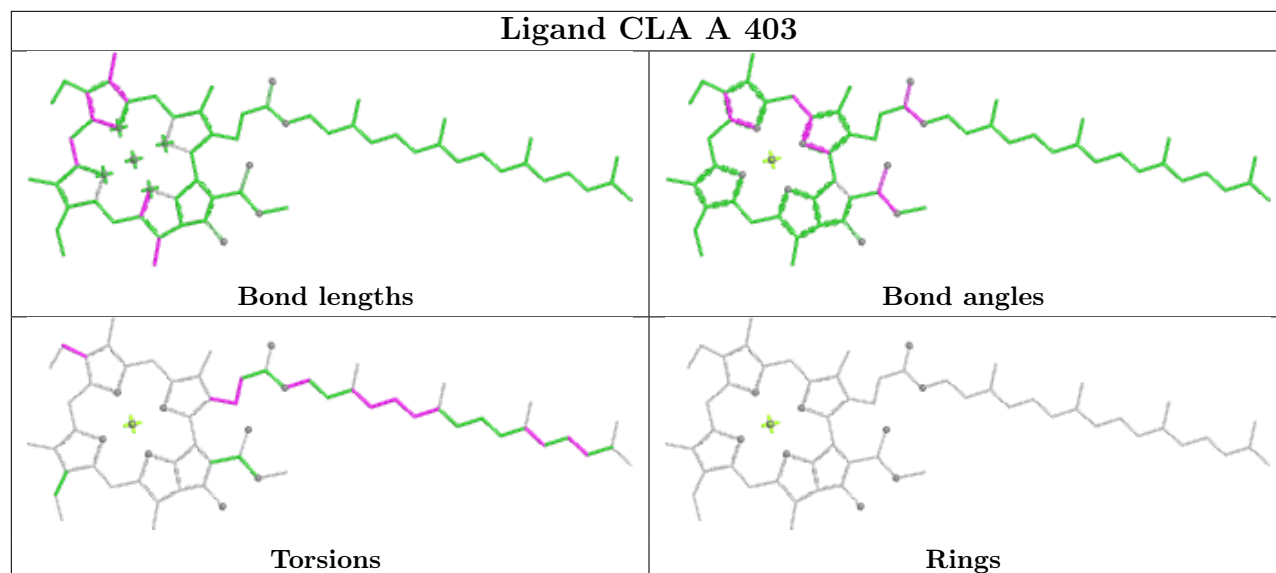
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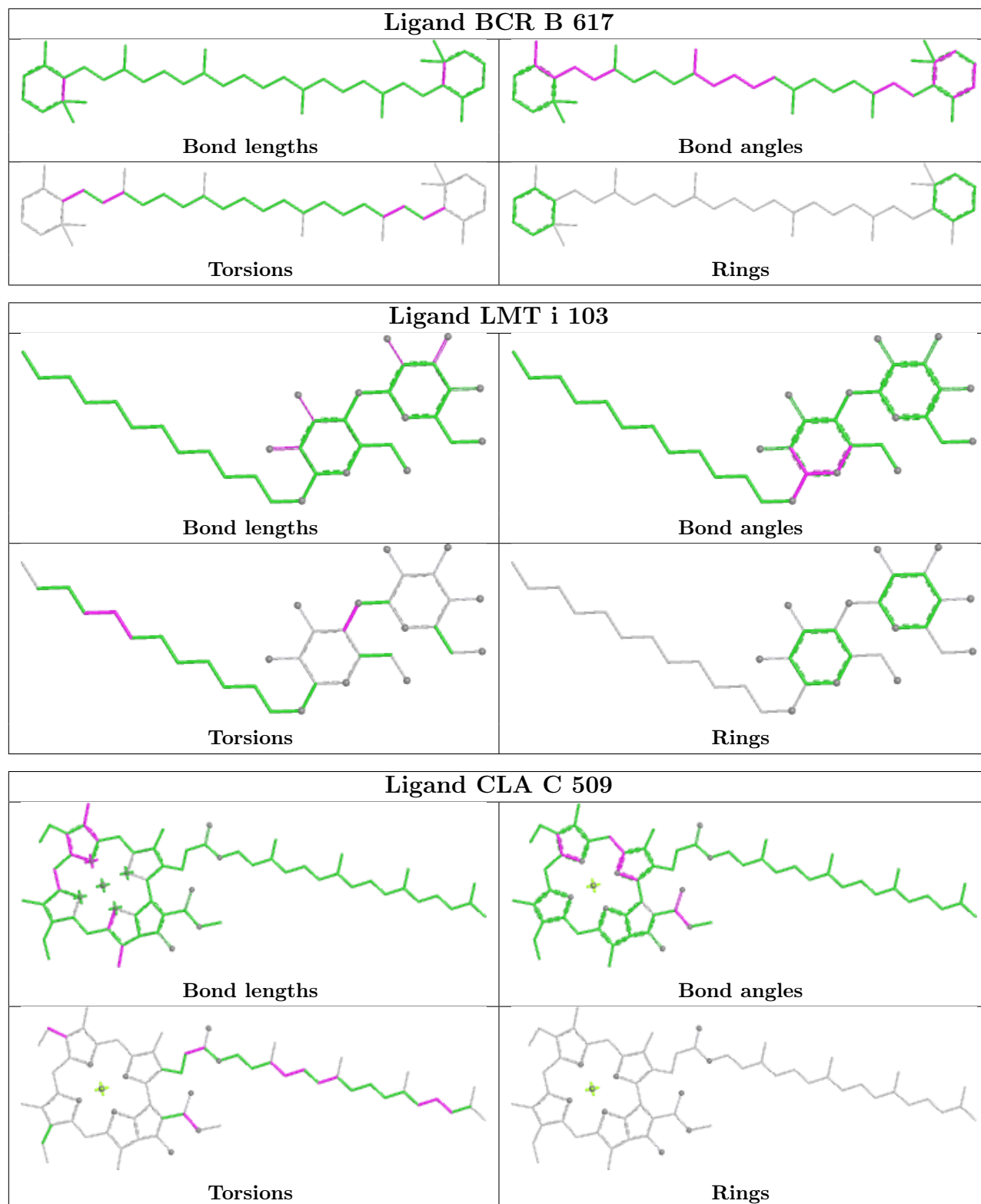


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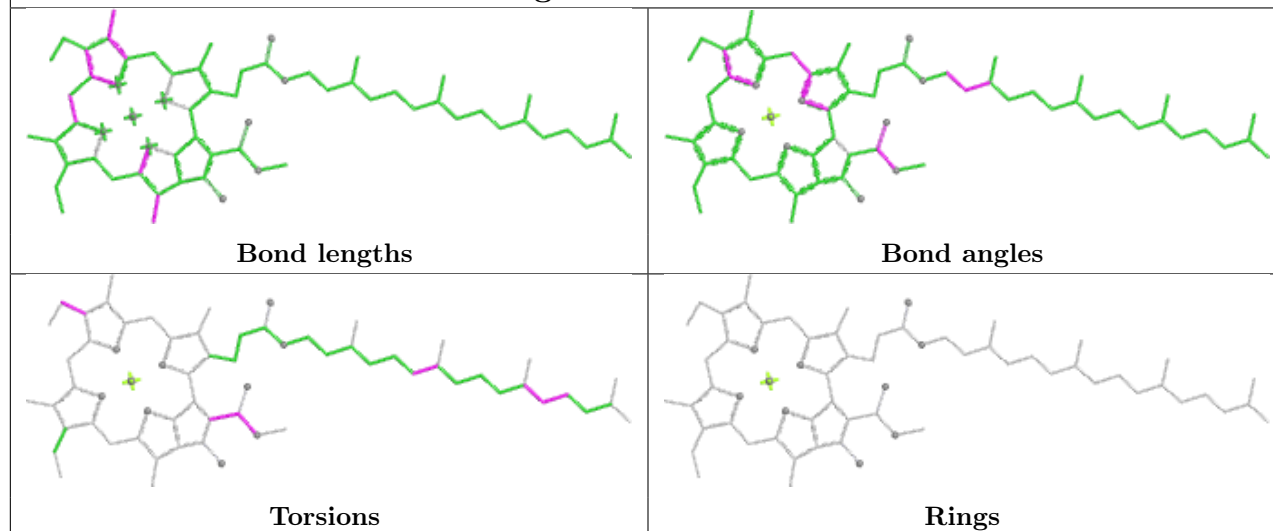


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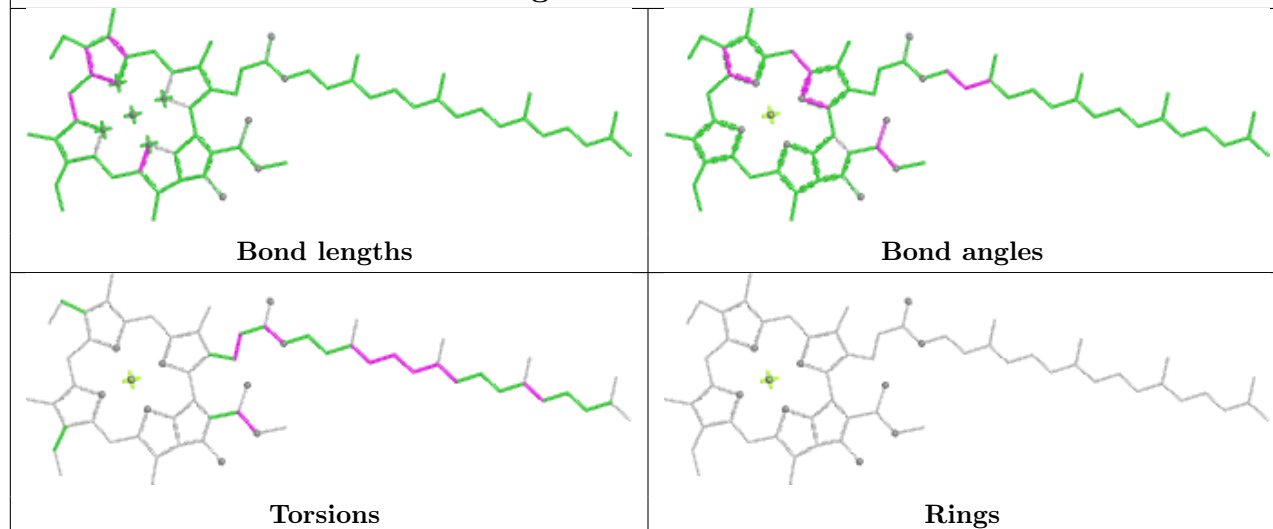




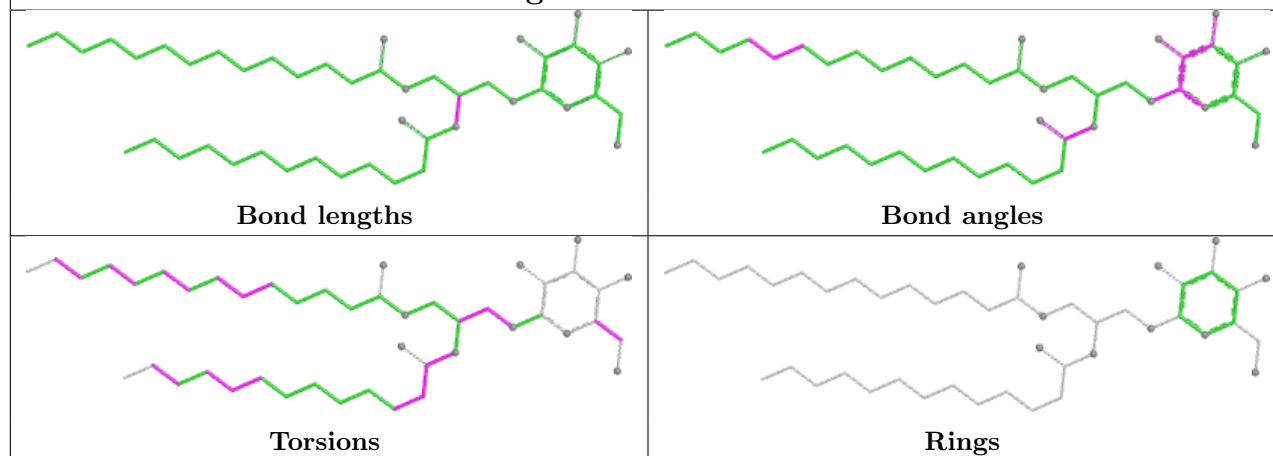
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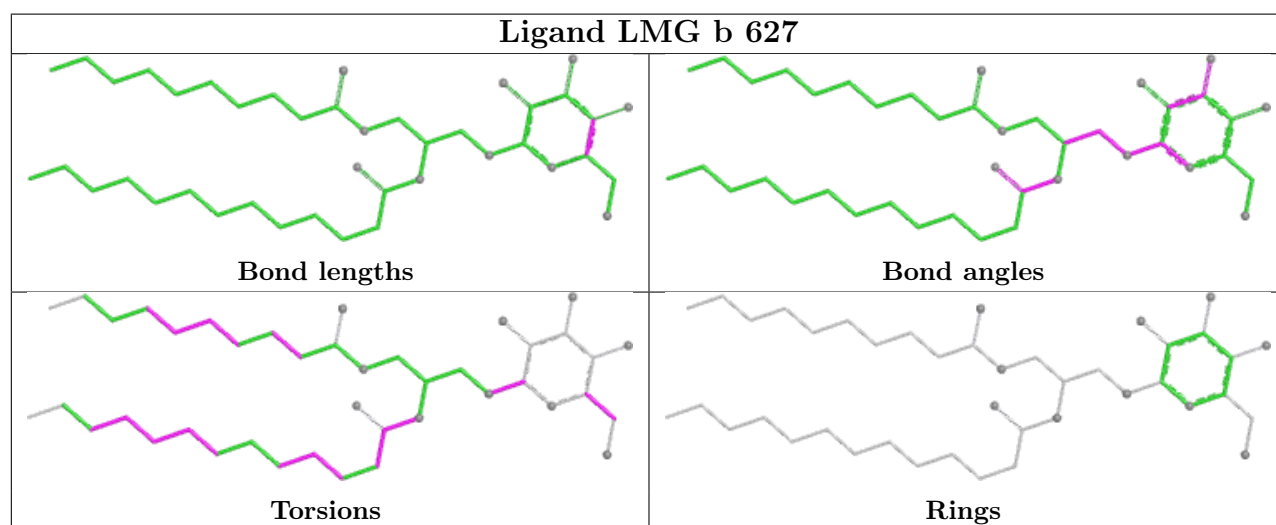
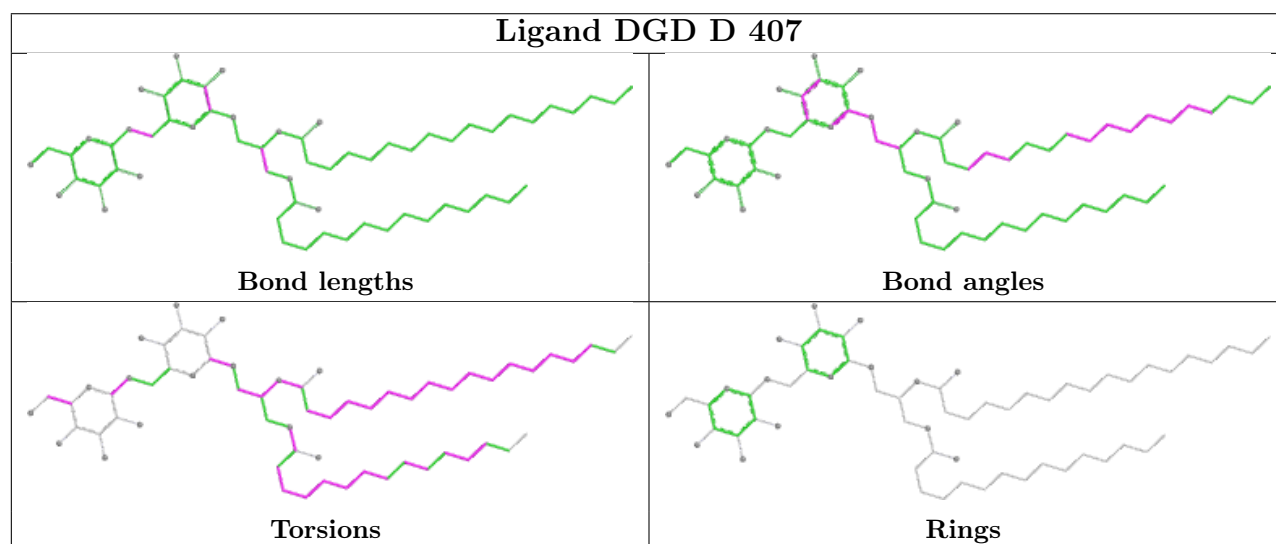
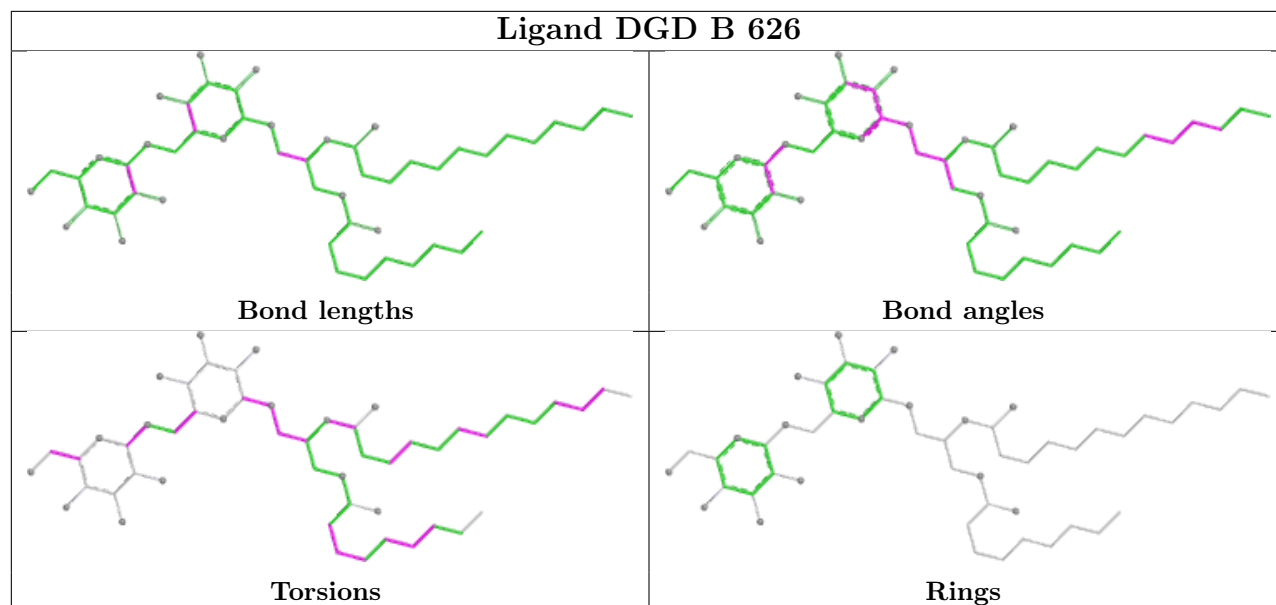


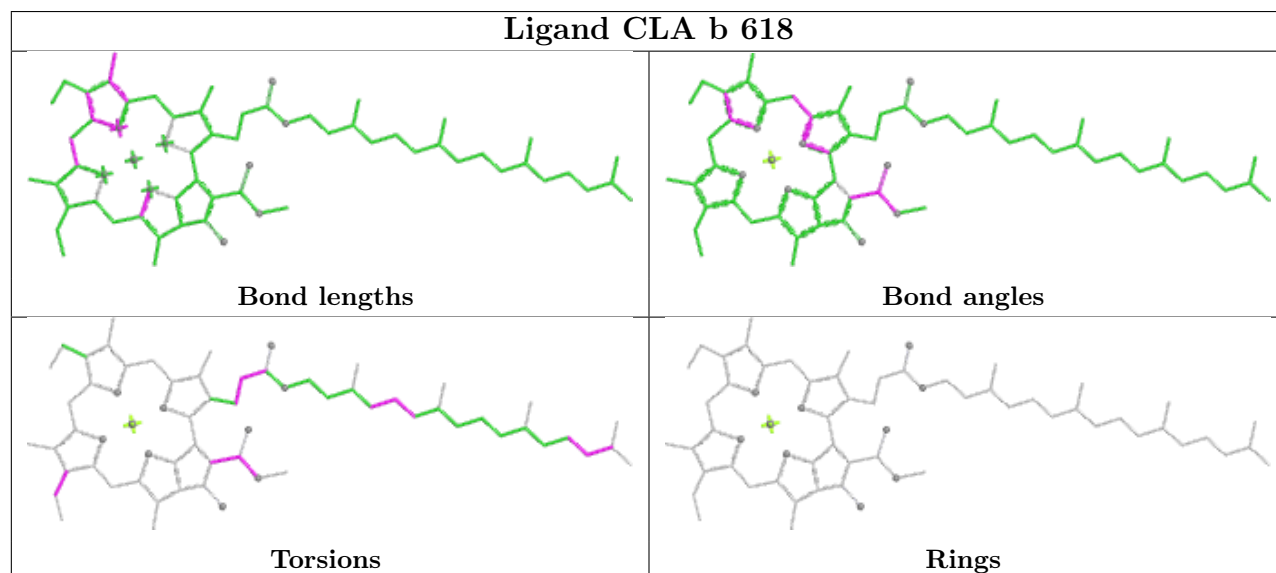
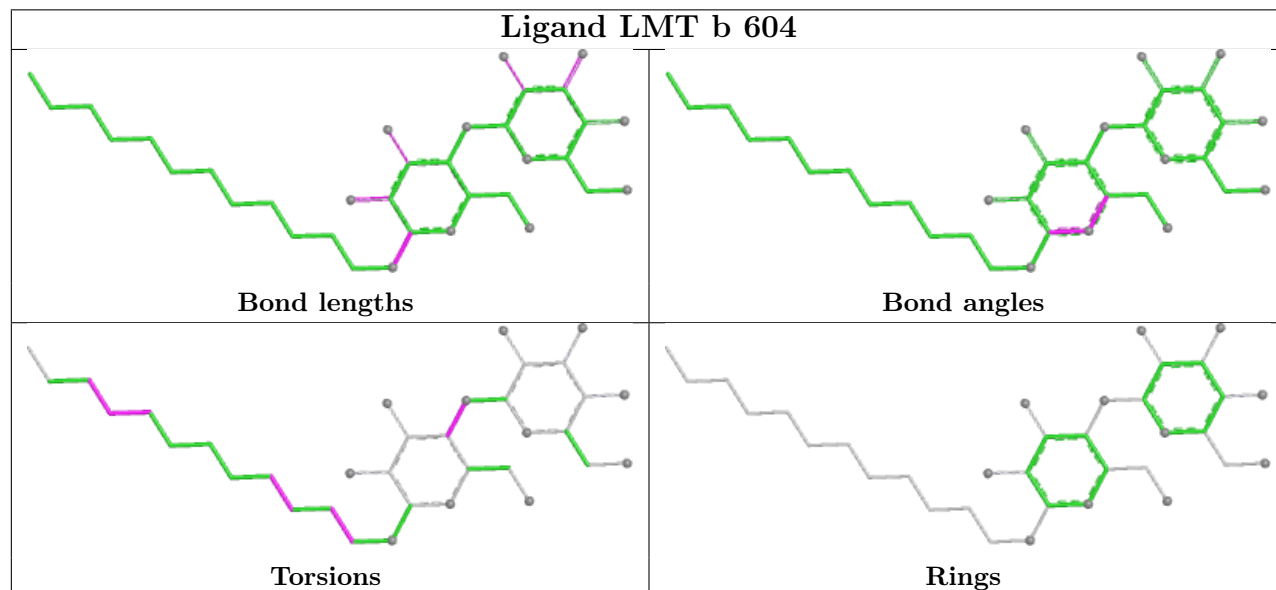
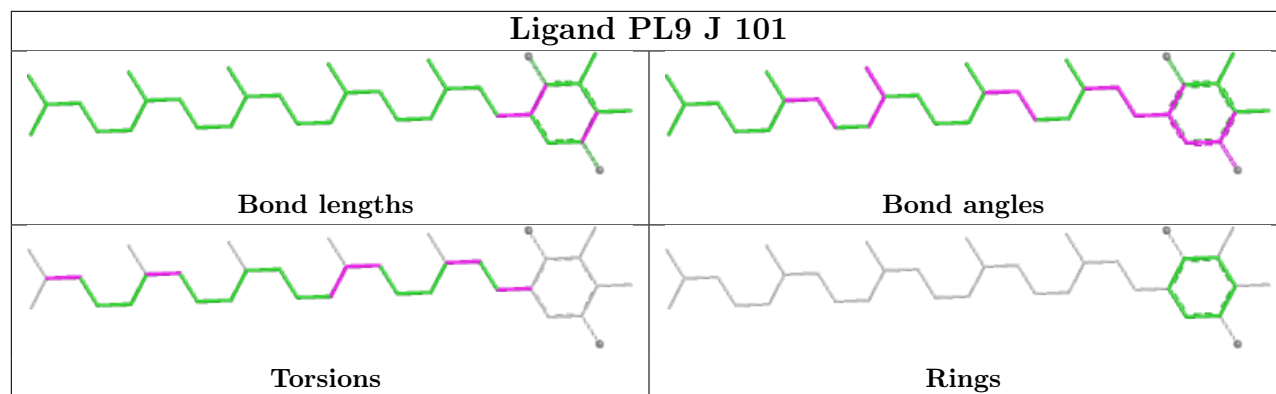
Ligand CLA C 510



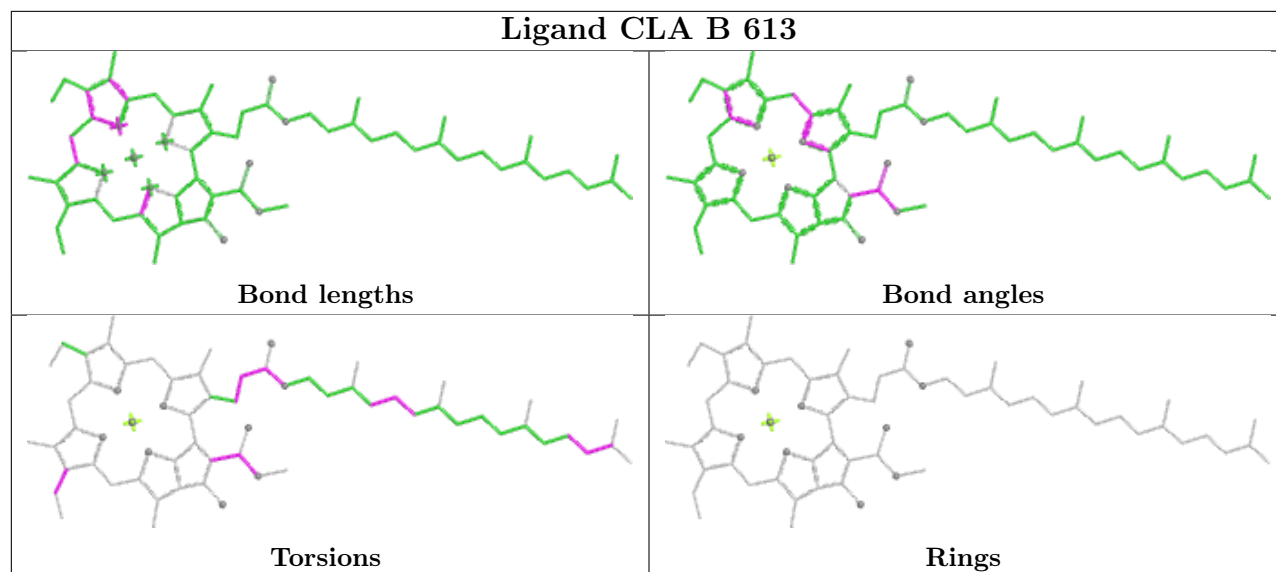
Ligand LMG D 409



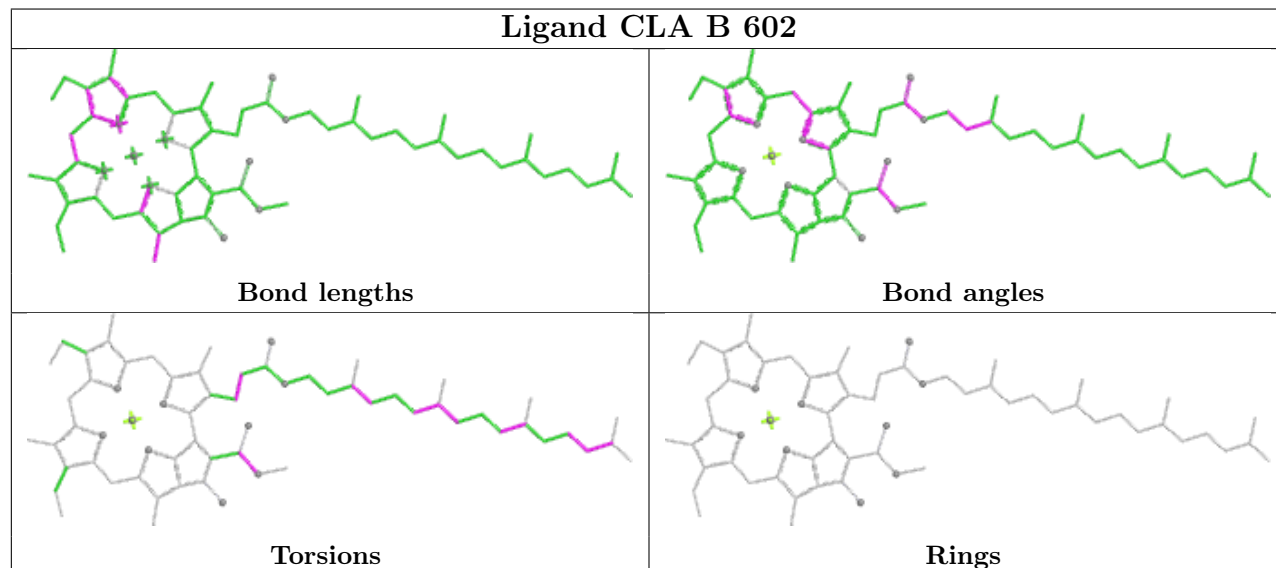




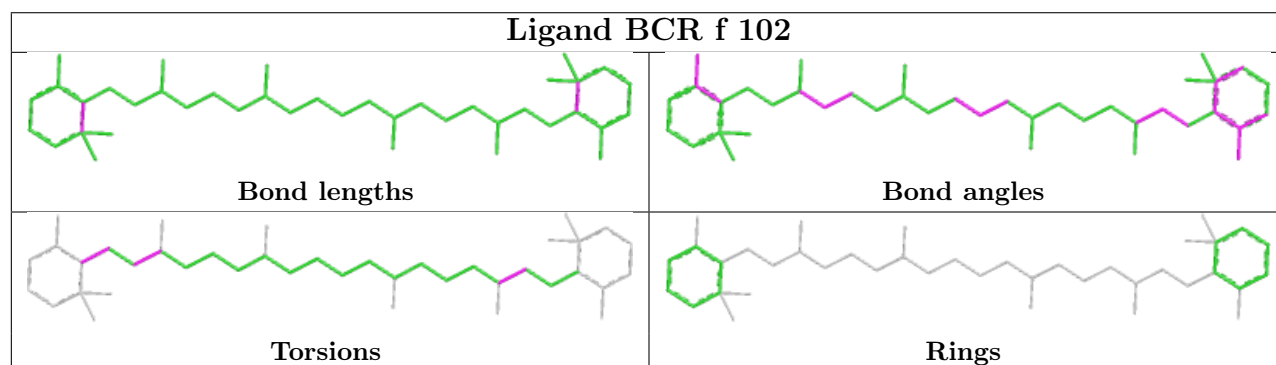
Ligand CLA B 613



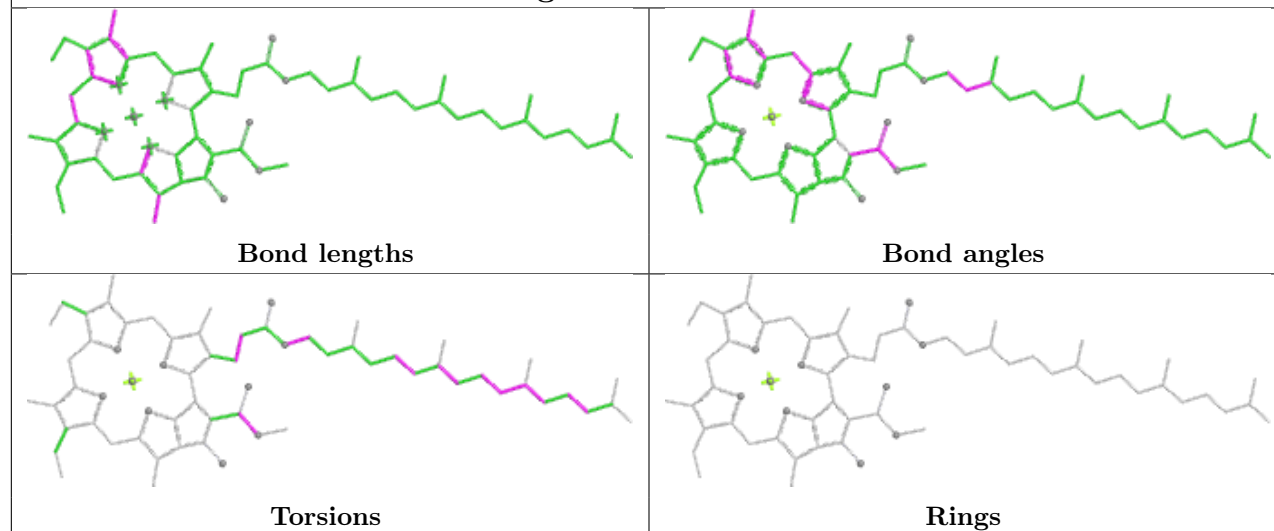
Ligand CLA B 602



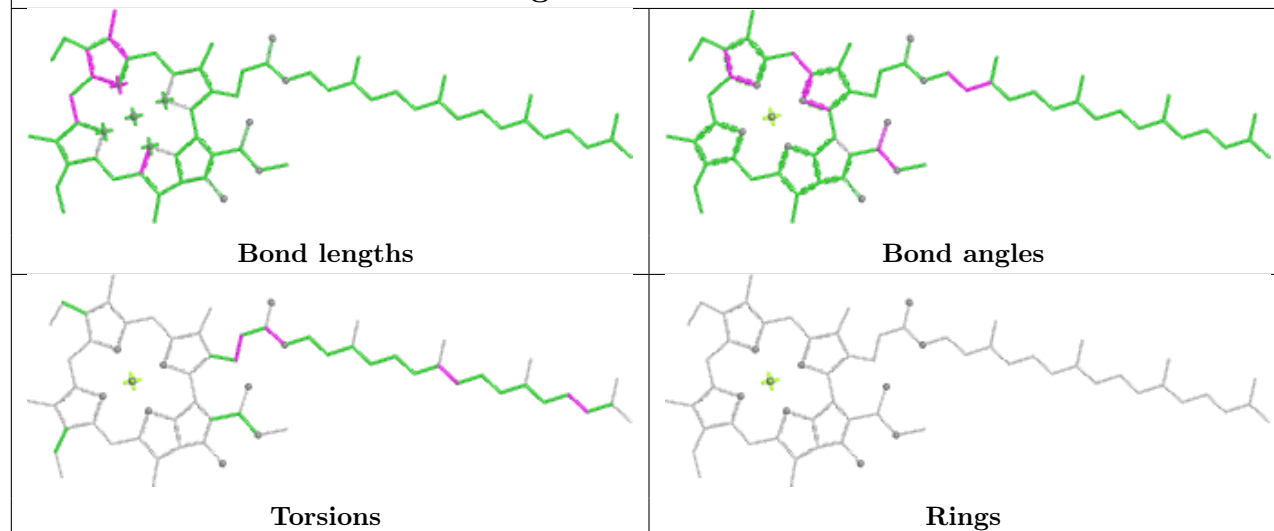
Ligand BCR f 102



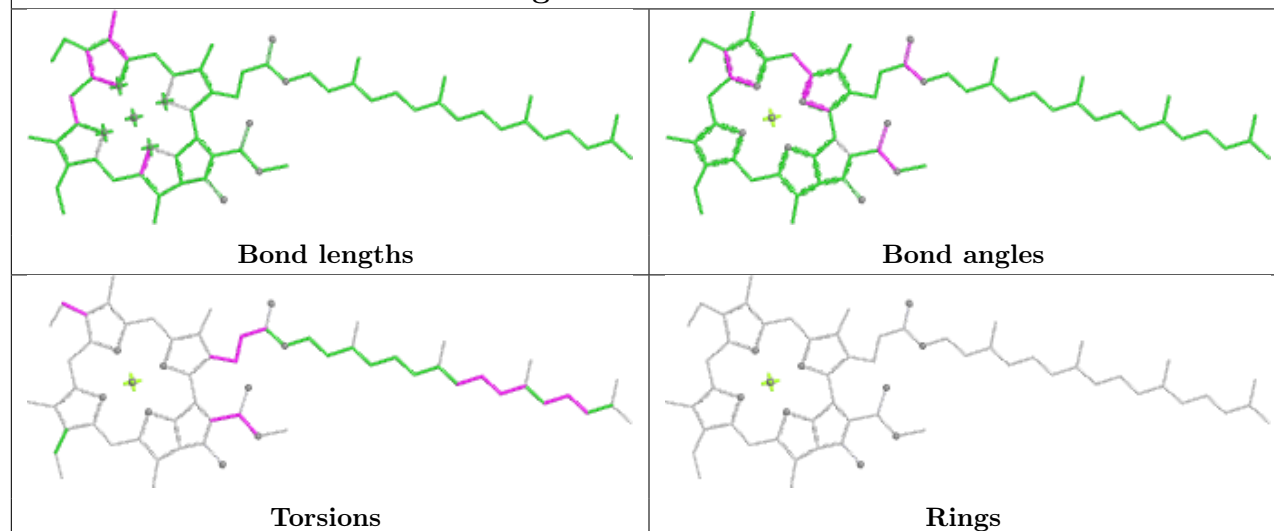
Ligand CLA c 507



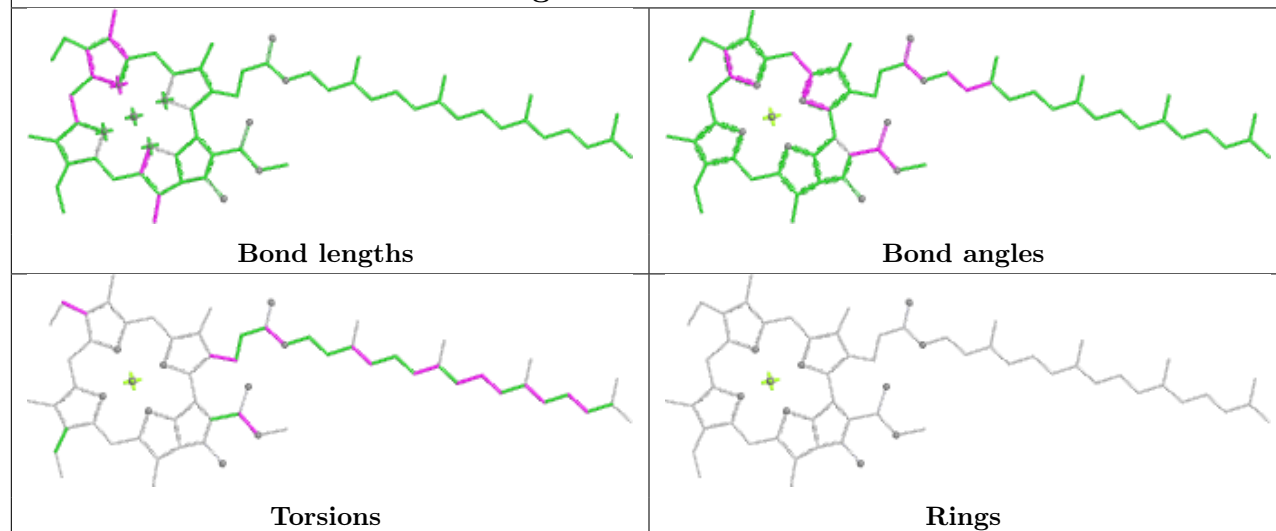
Ligand CLA D 404



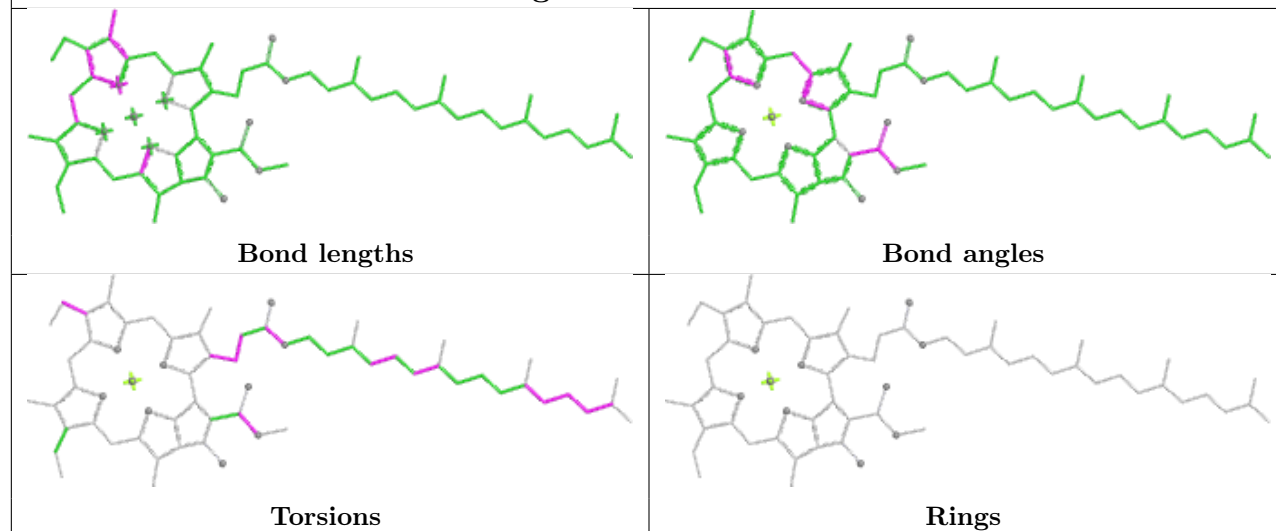
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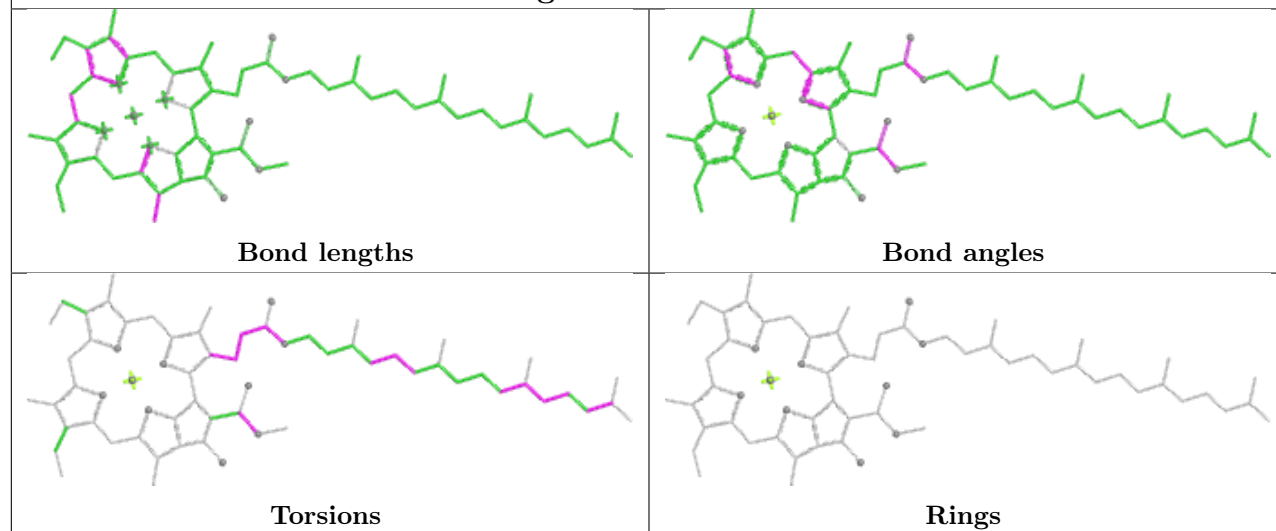
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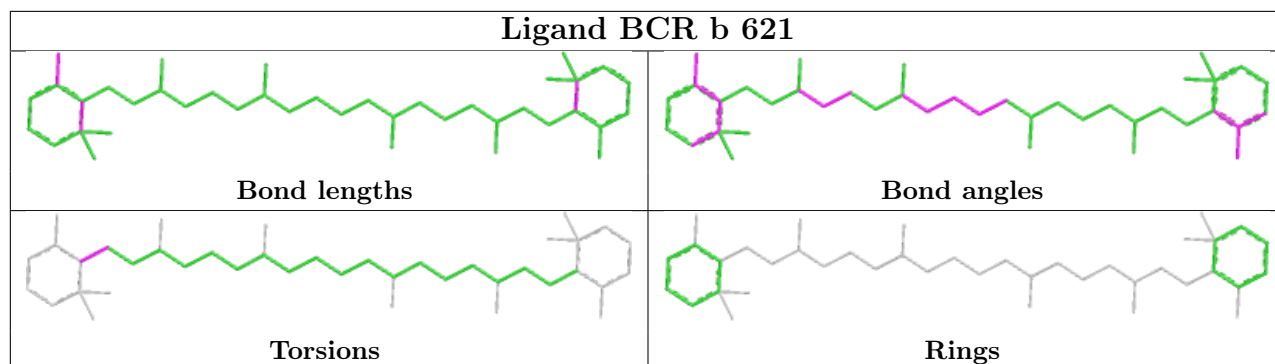
Ligand CLA B 605



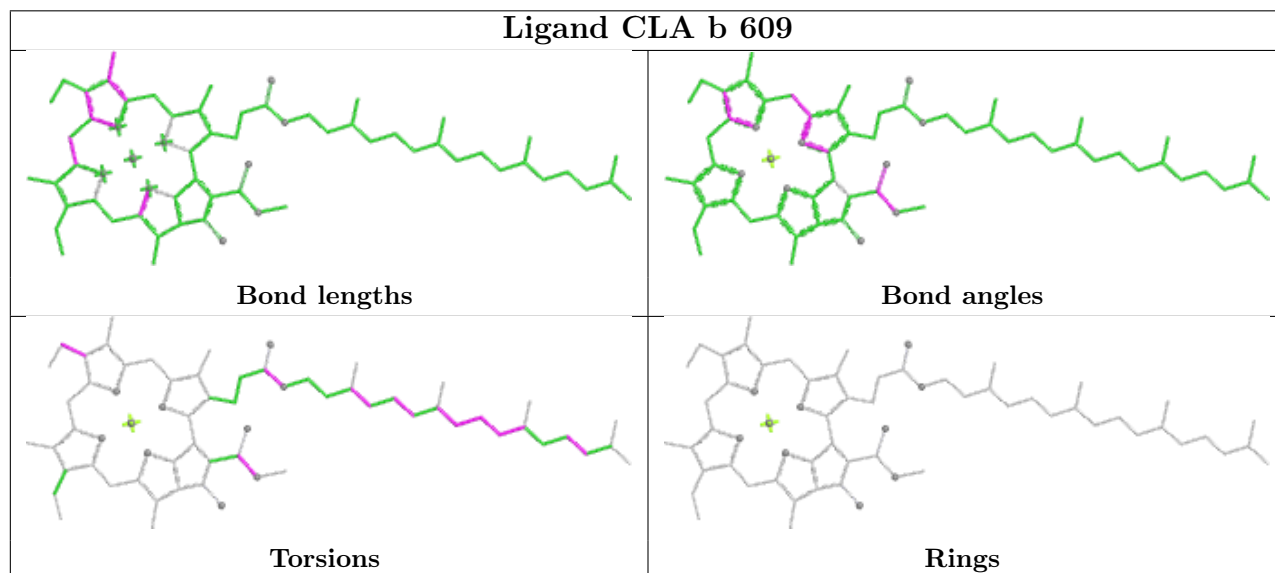
Ligand CLA c 511



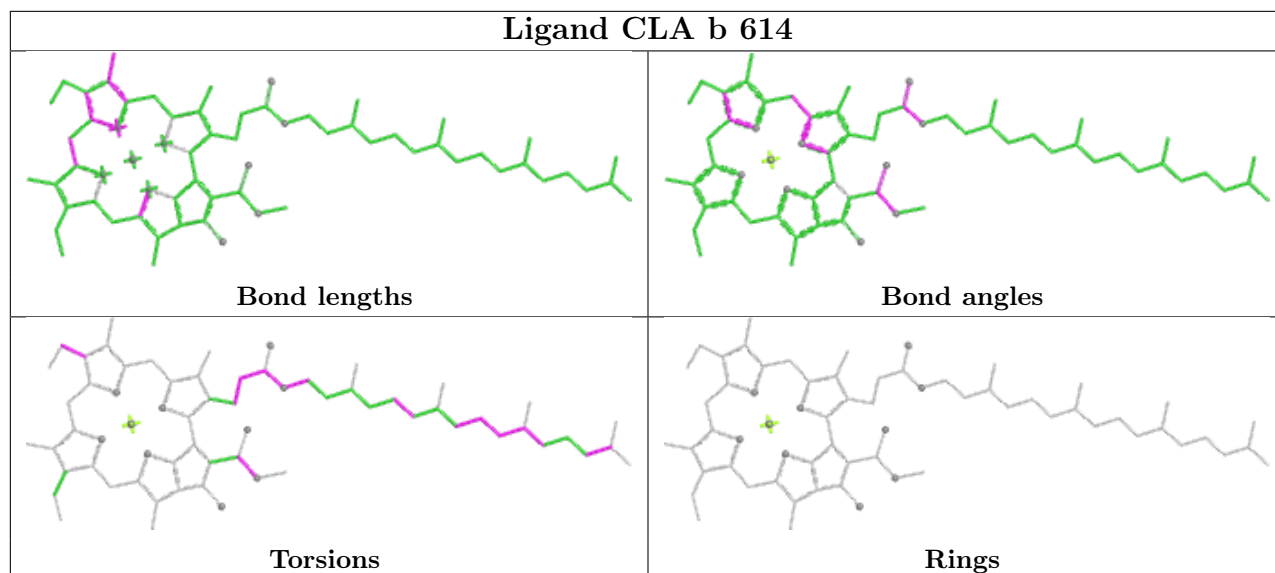
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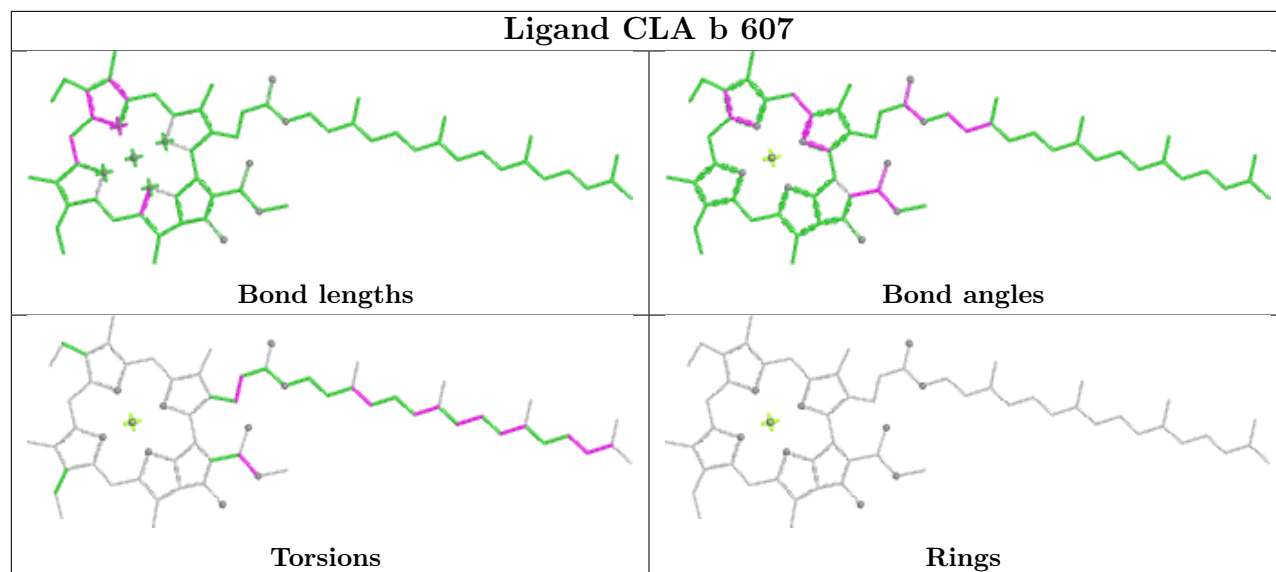
Ligand CLA b 609



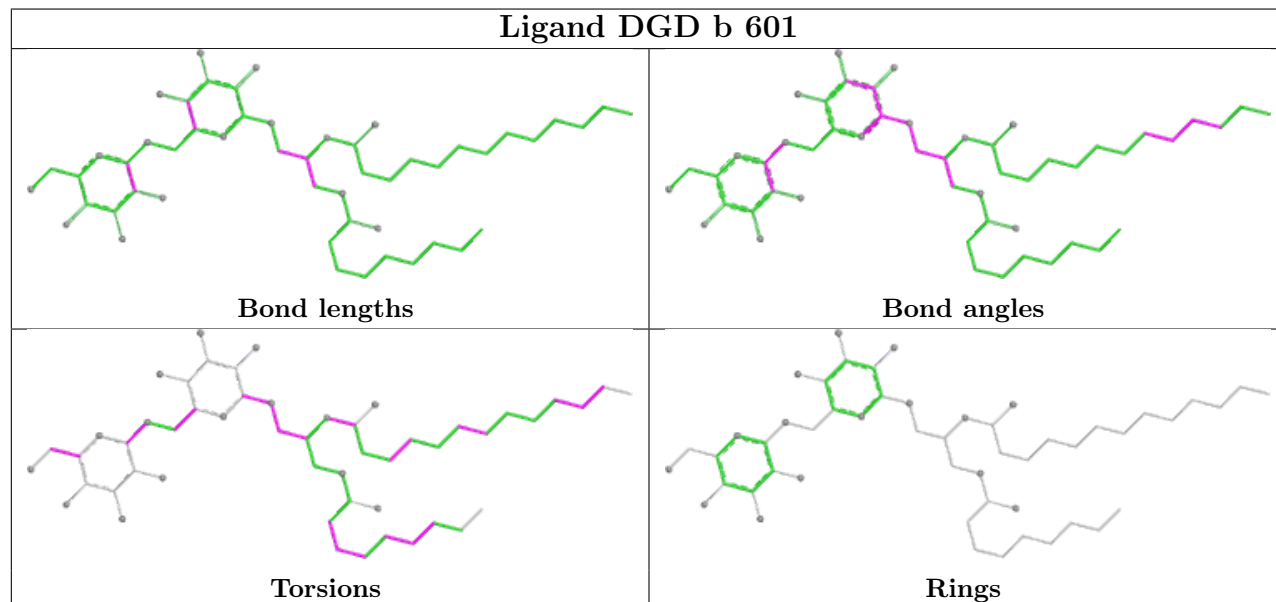
Ligand CLA b 614



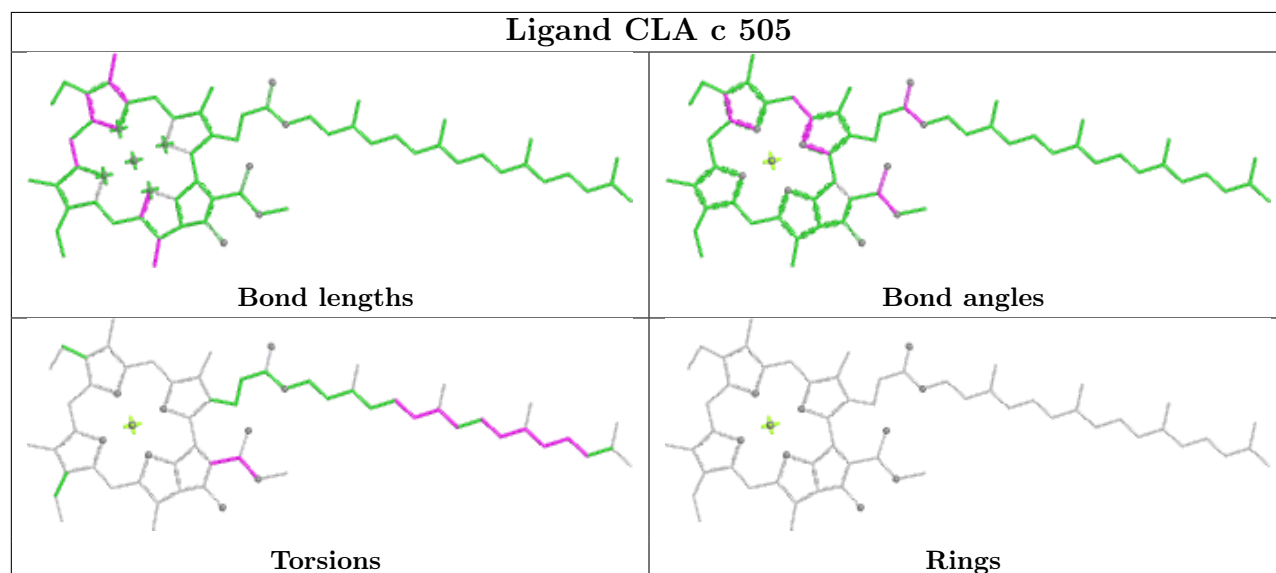
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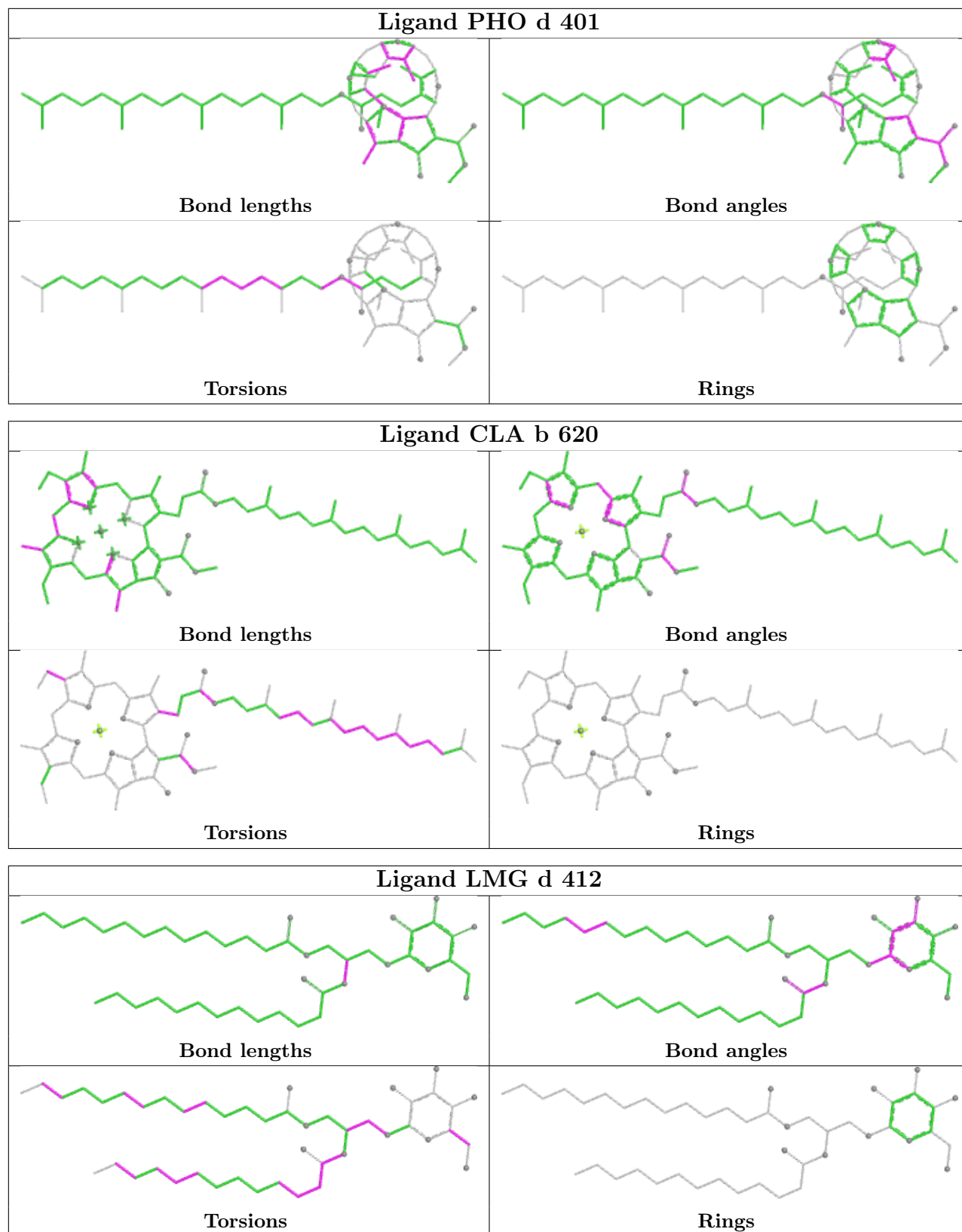


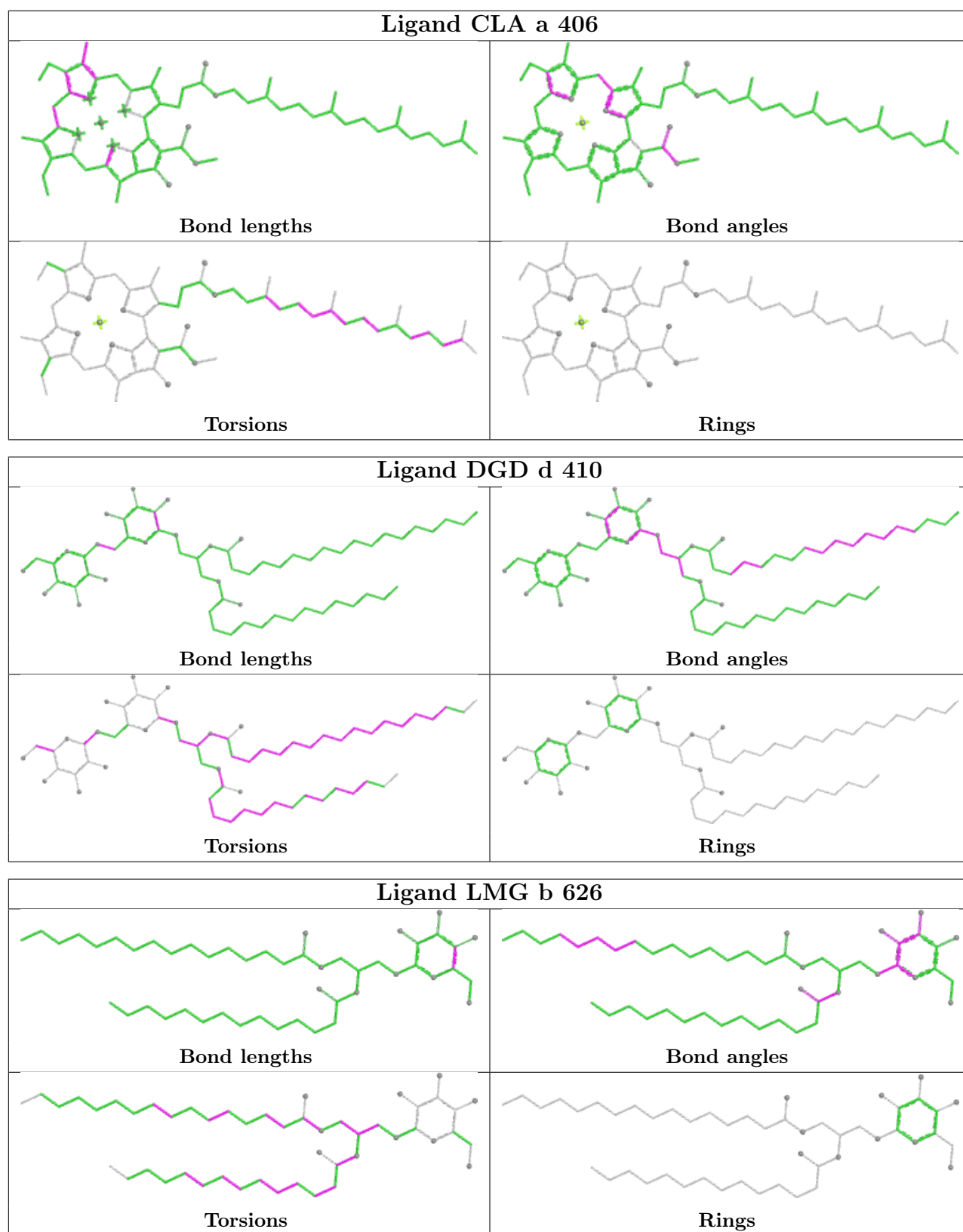
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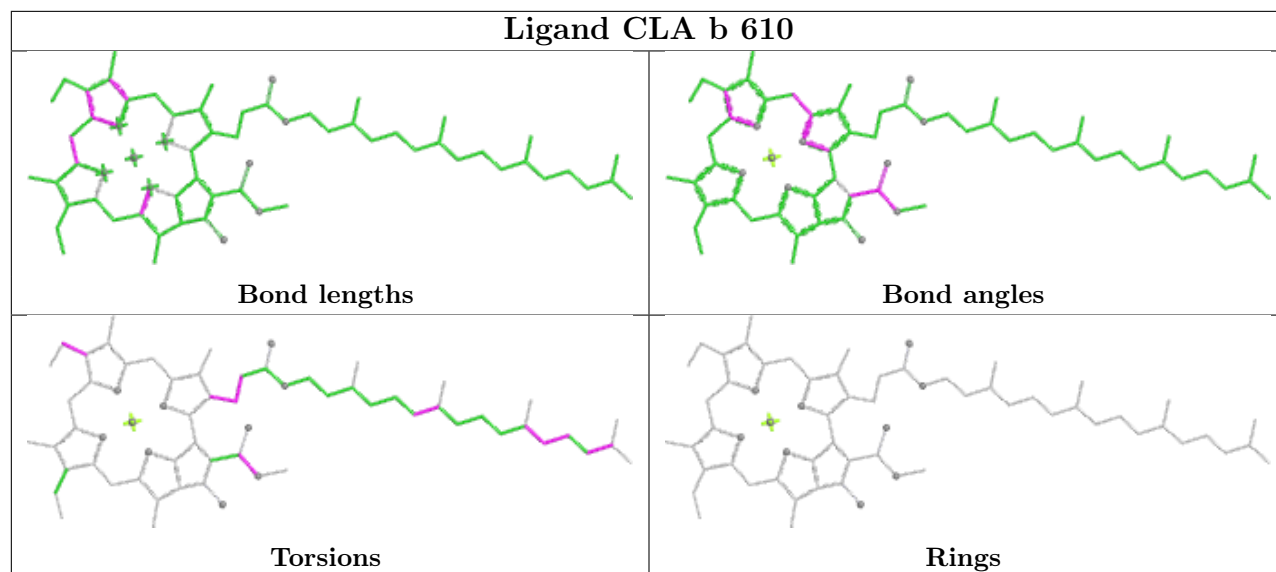
Ligand CLA c 505



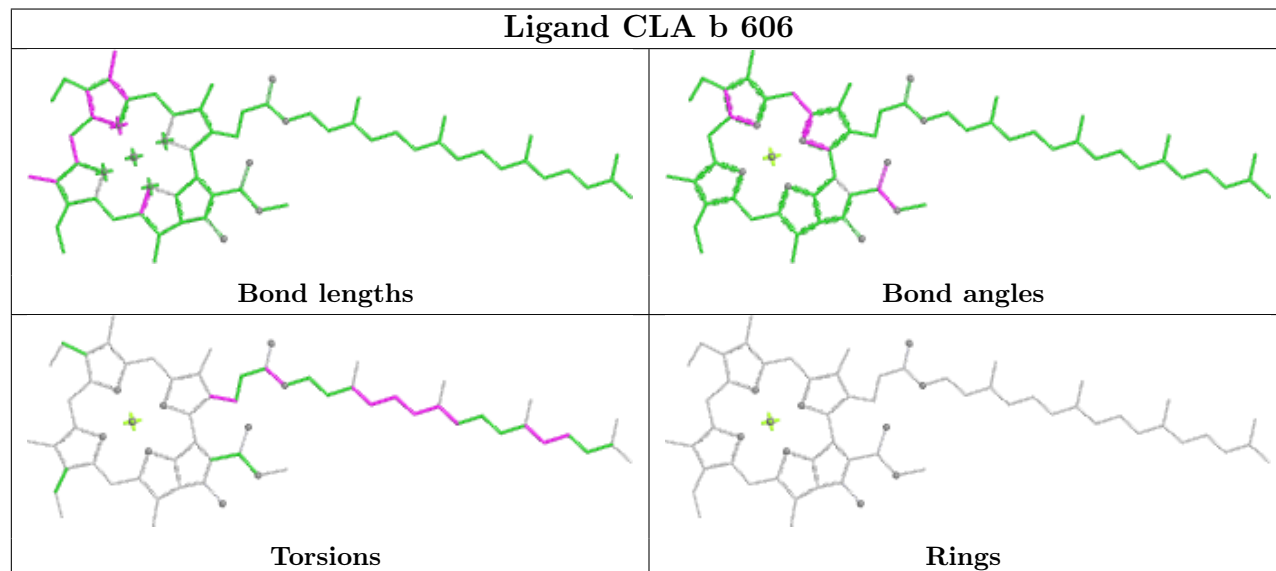




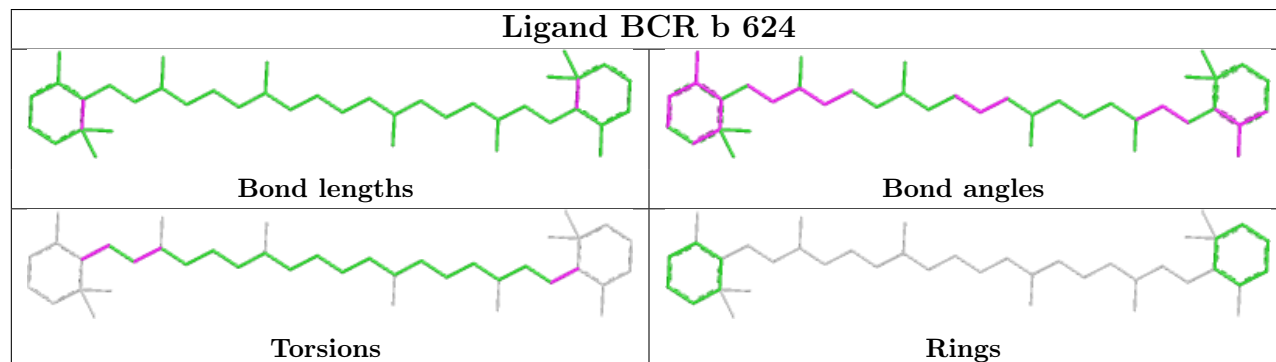
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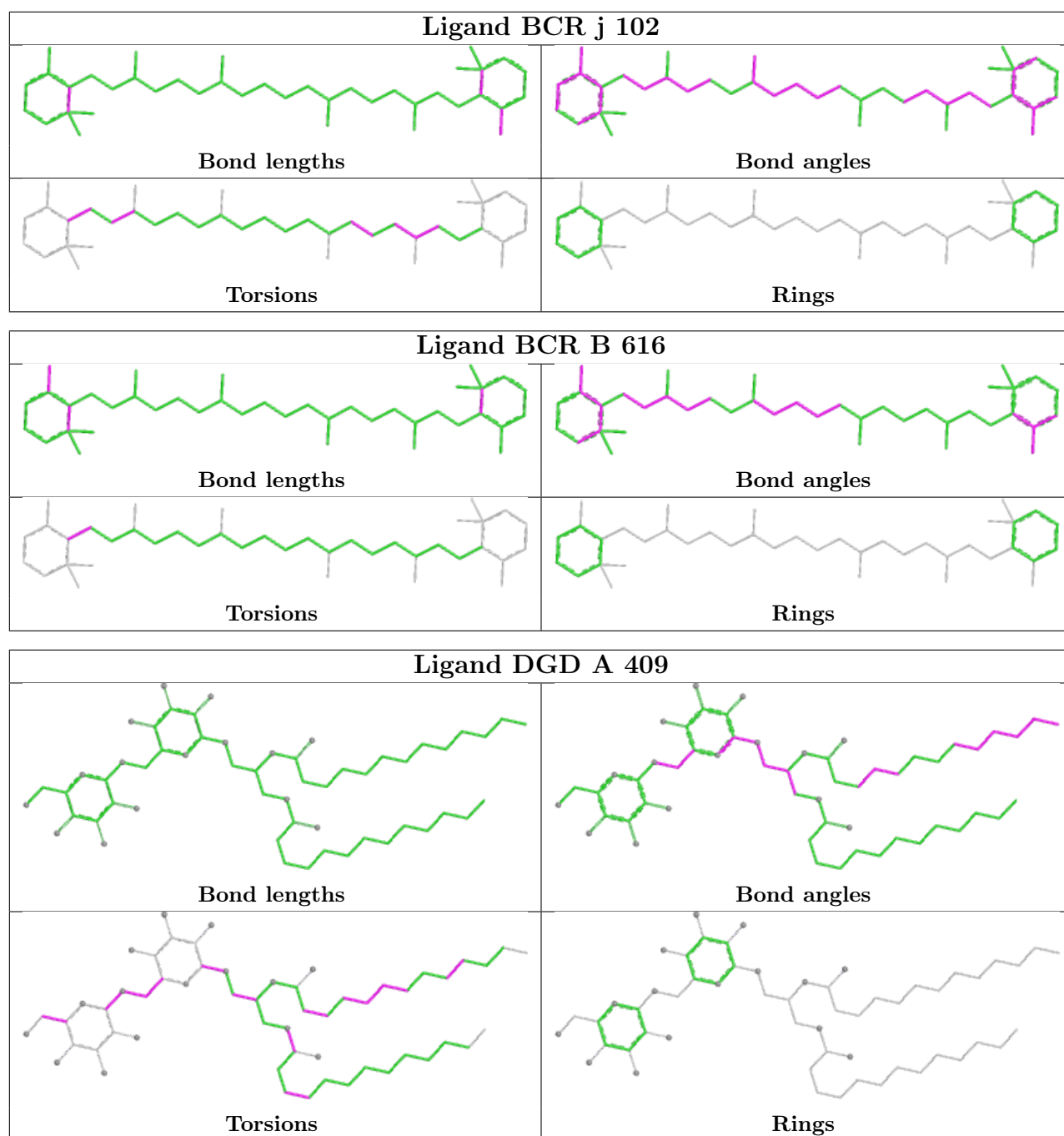


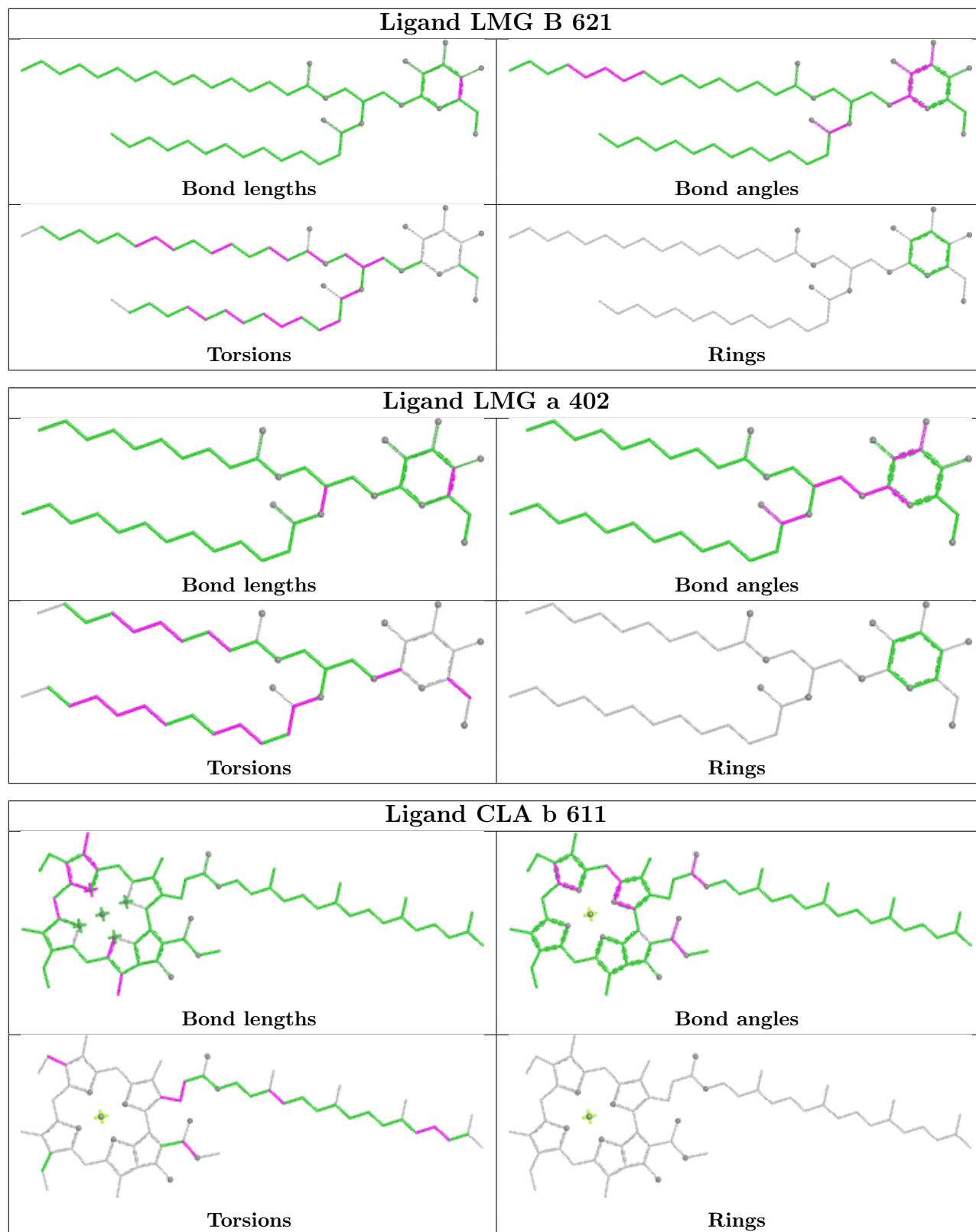
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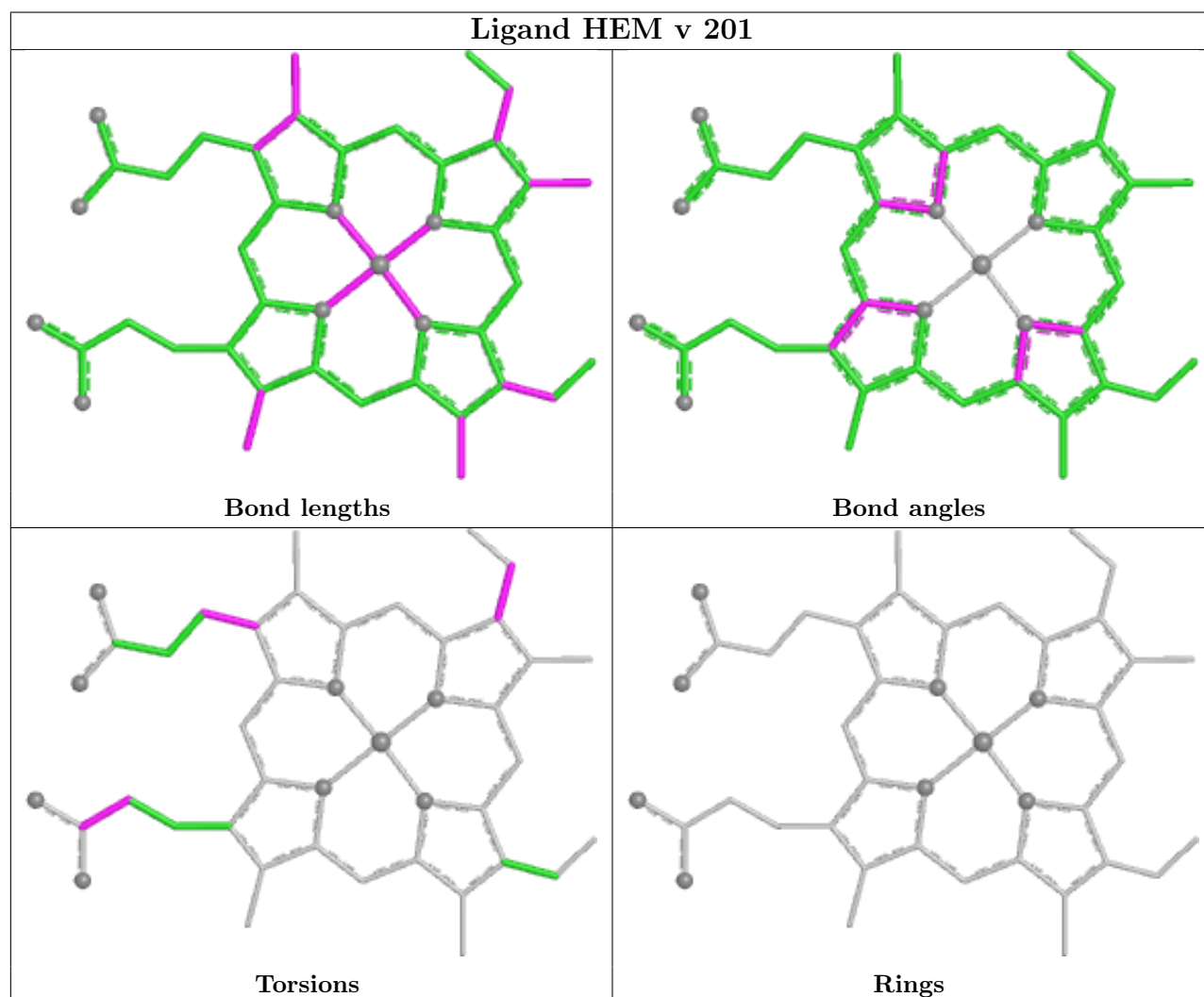
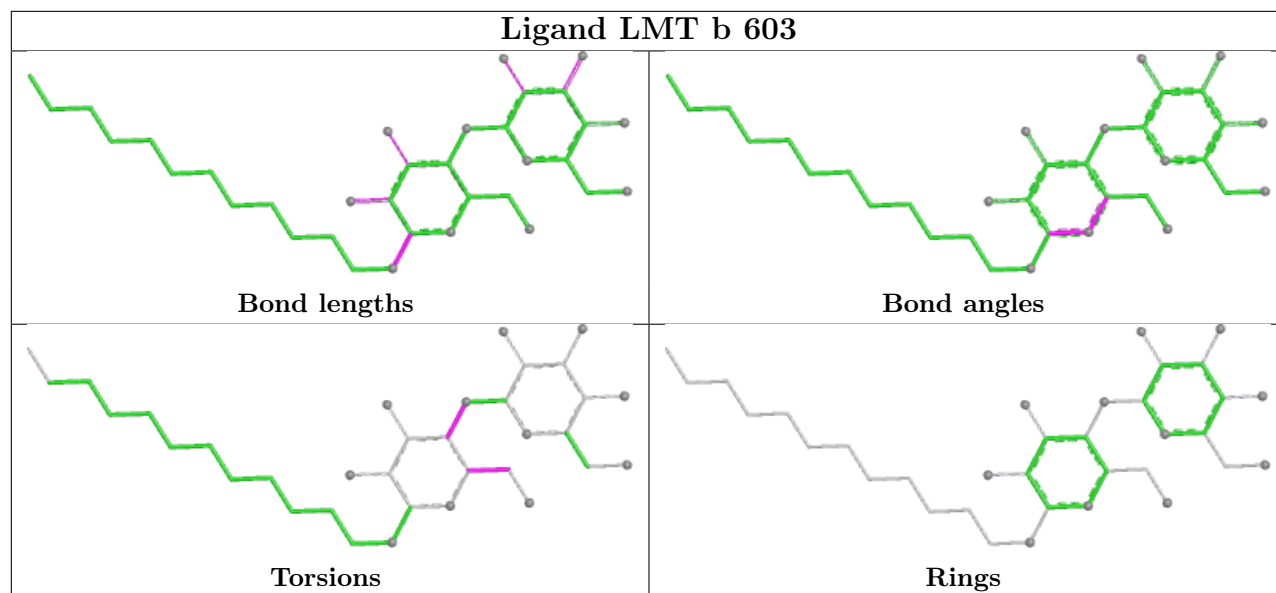


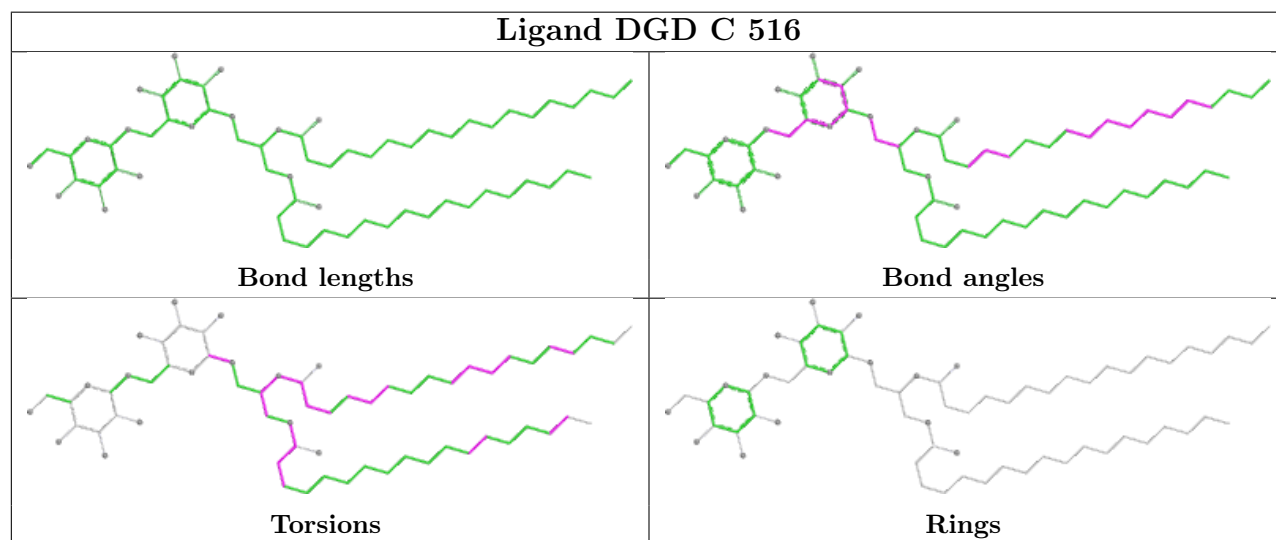
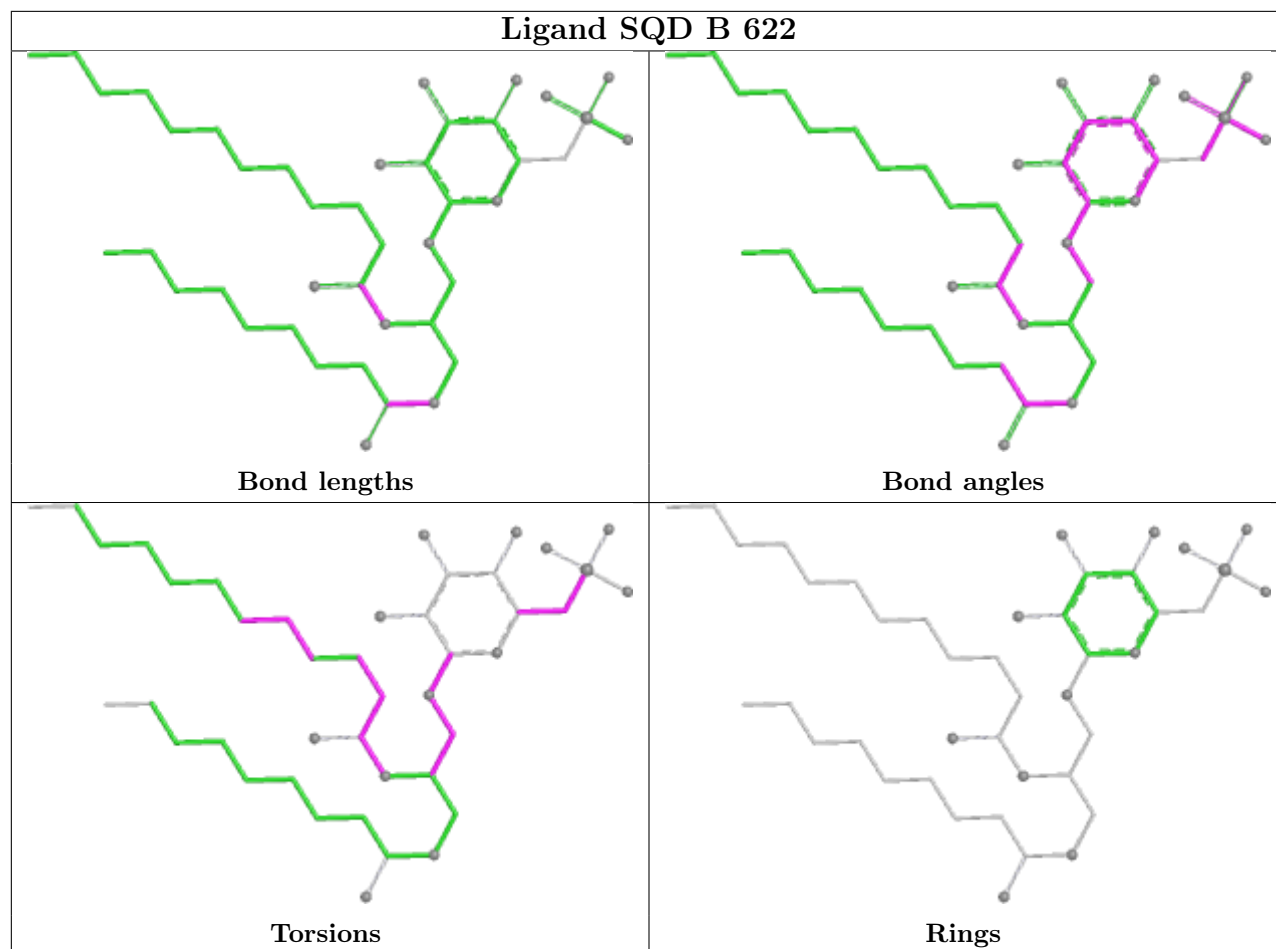
Ligand BCR b 624



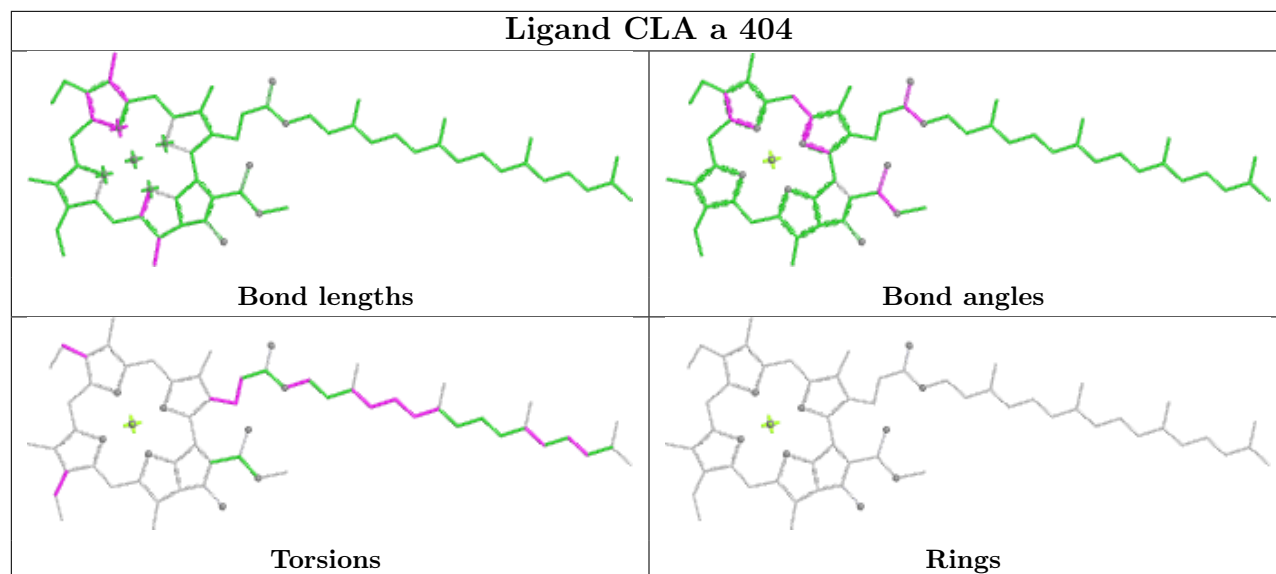




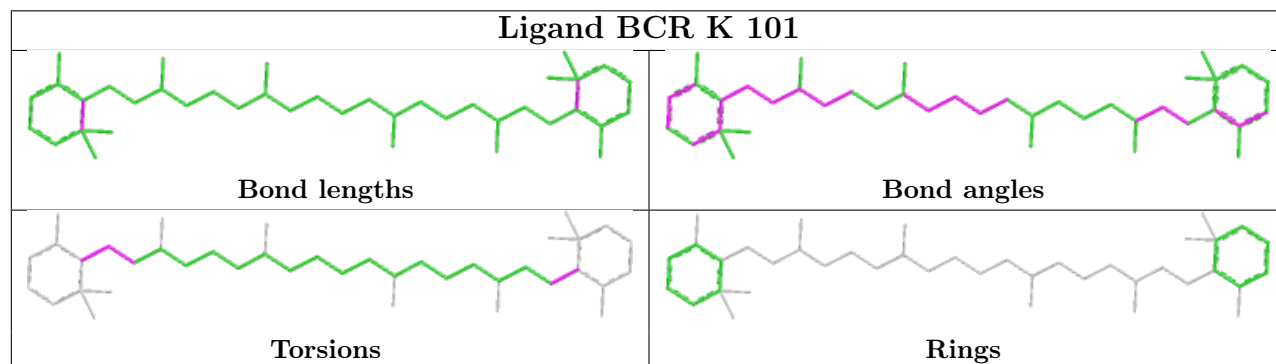




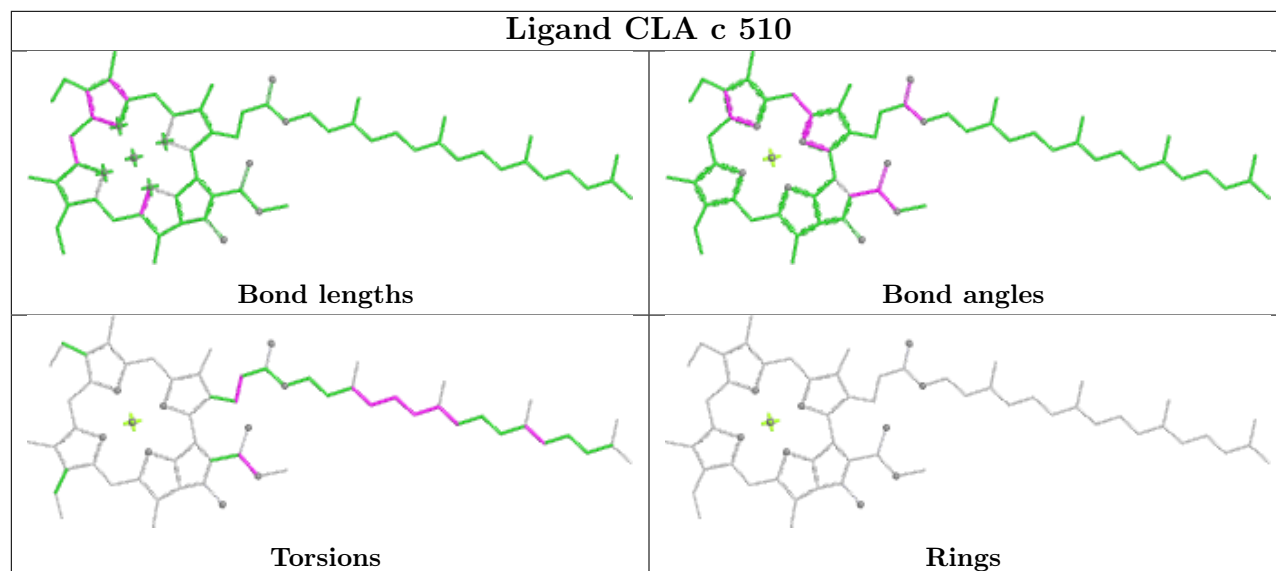
Ligand CLA a 404

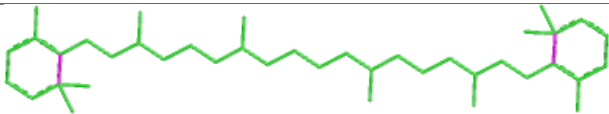
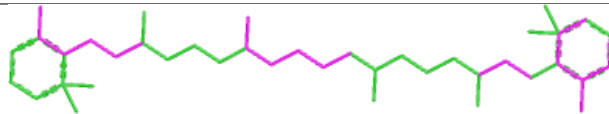
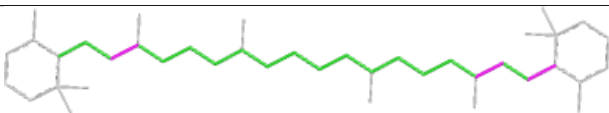
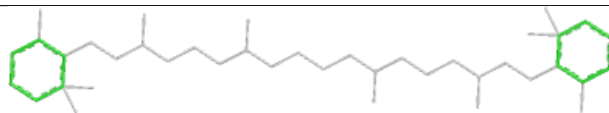


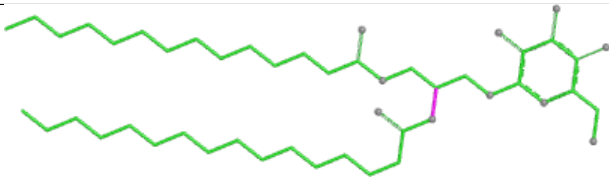
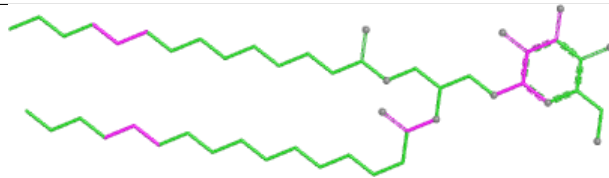
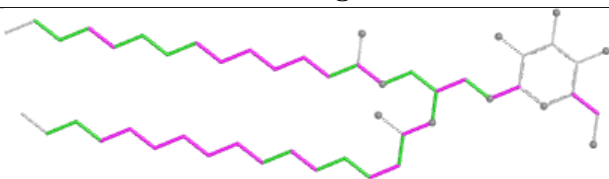
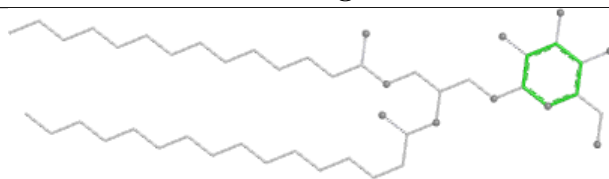
Ligand BCR K 101

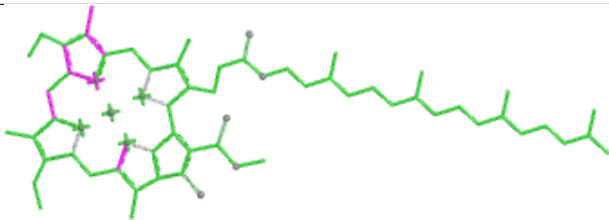
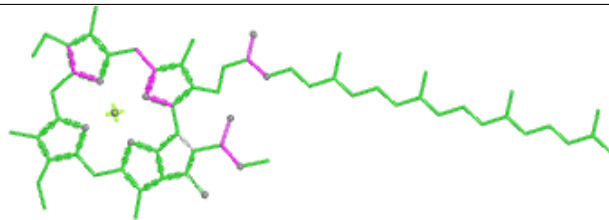
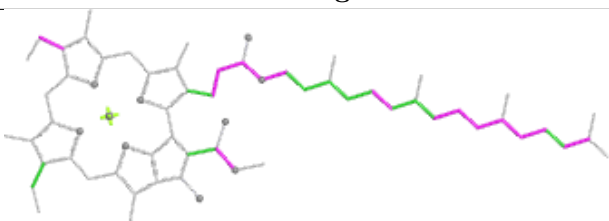
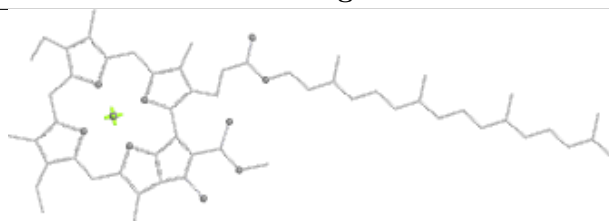


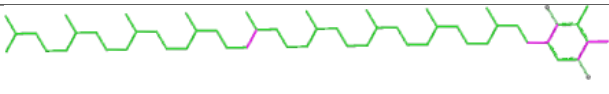
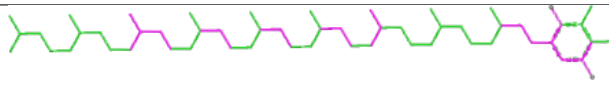
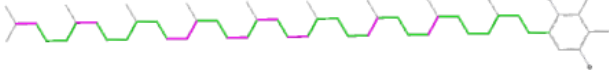
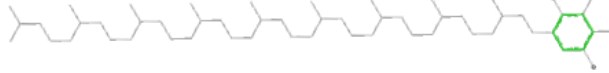
Ligand CLA c 510



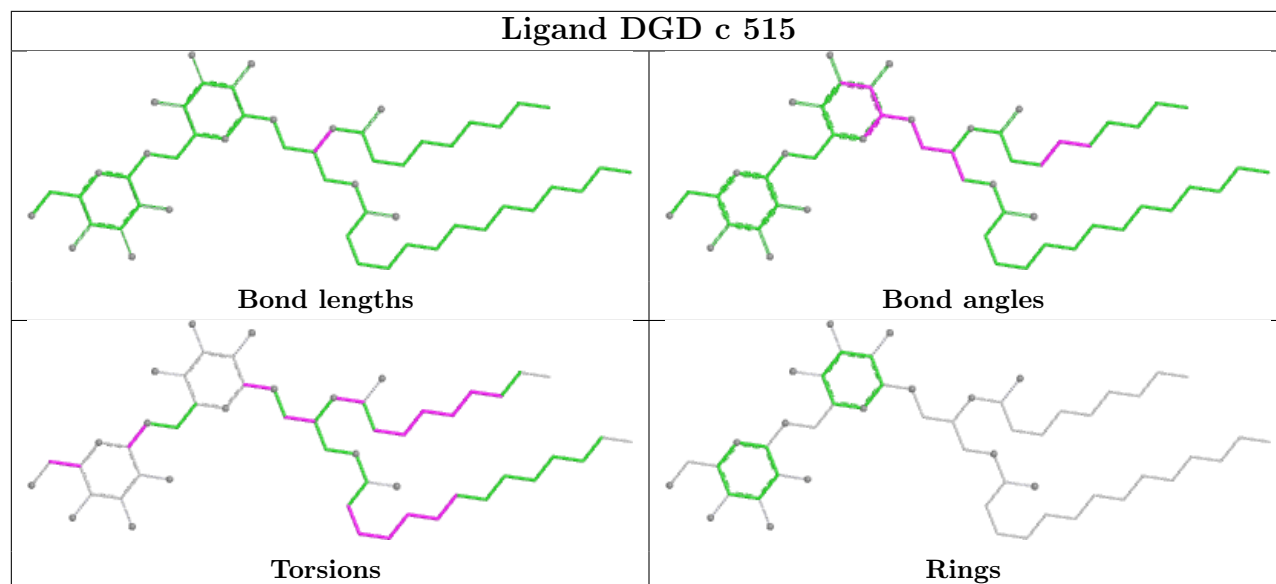
Ligand BCR b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

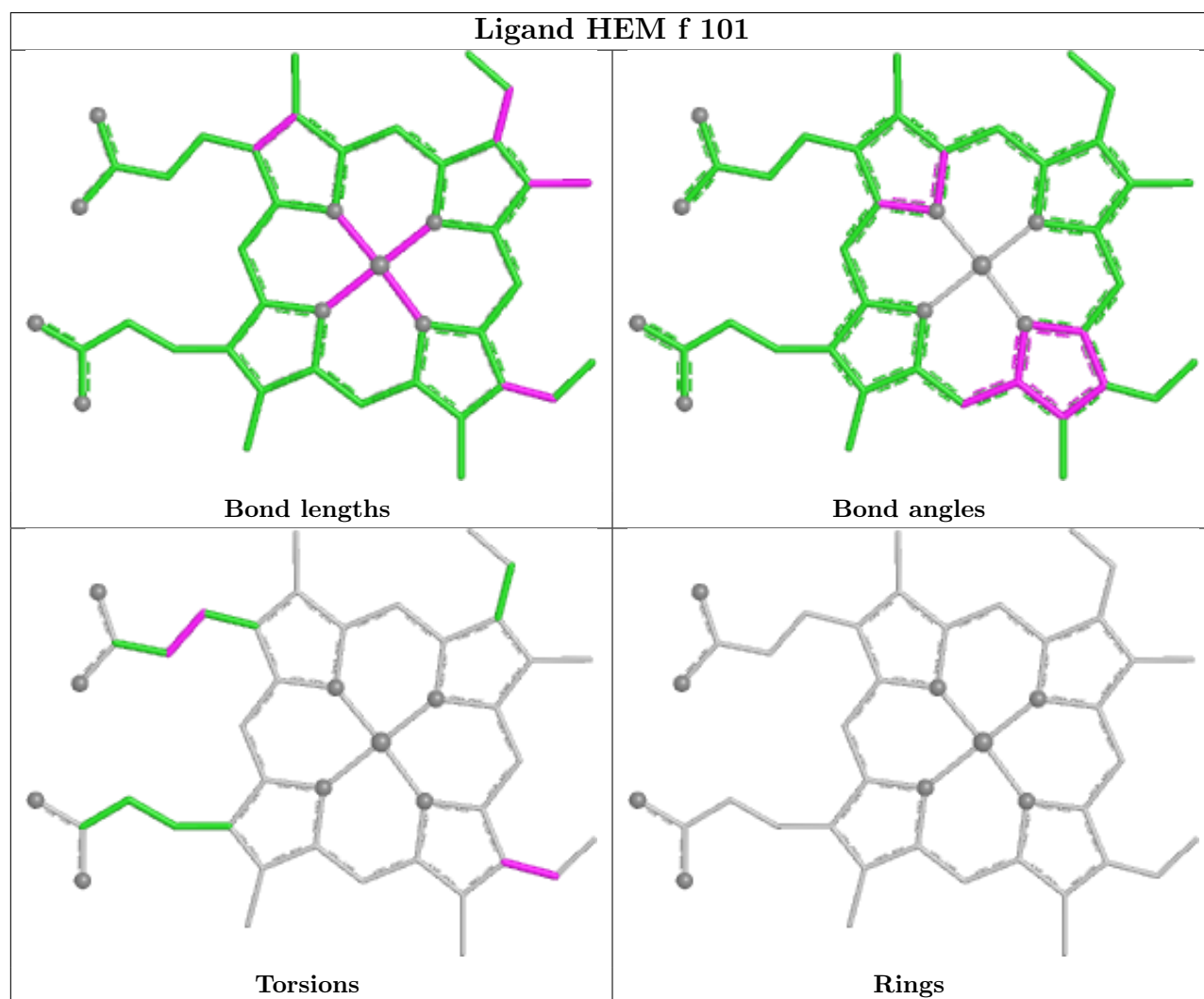
Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

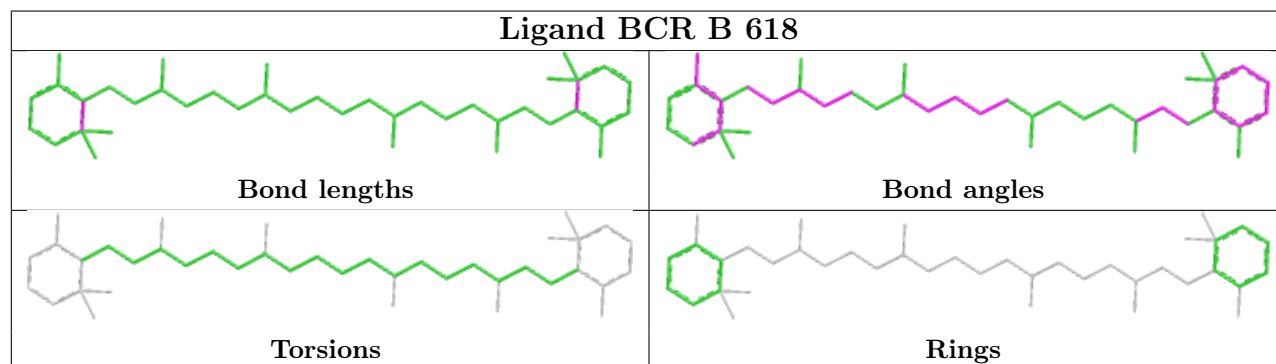
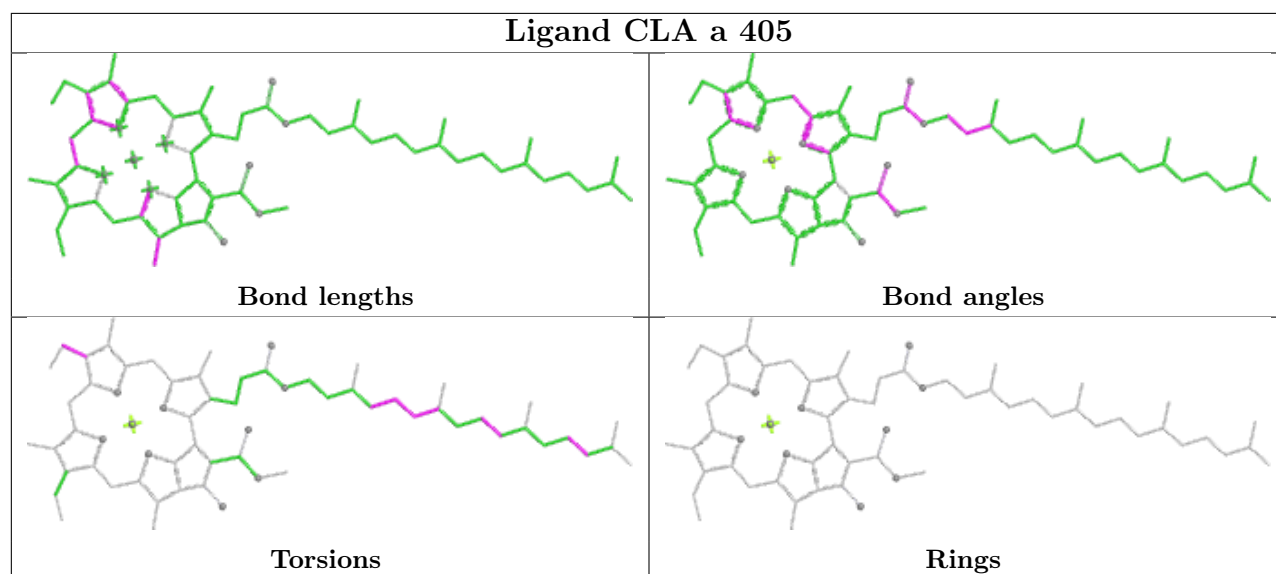
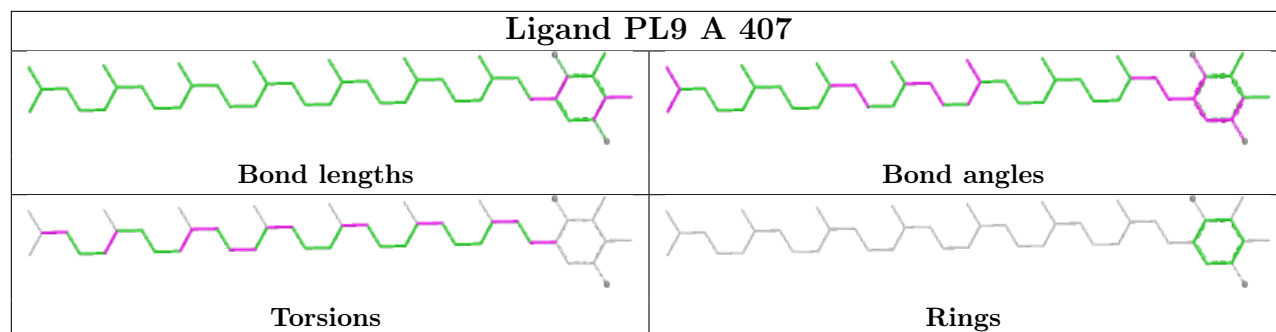
Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

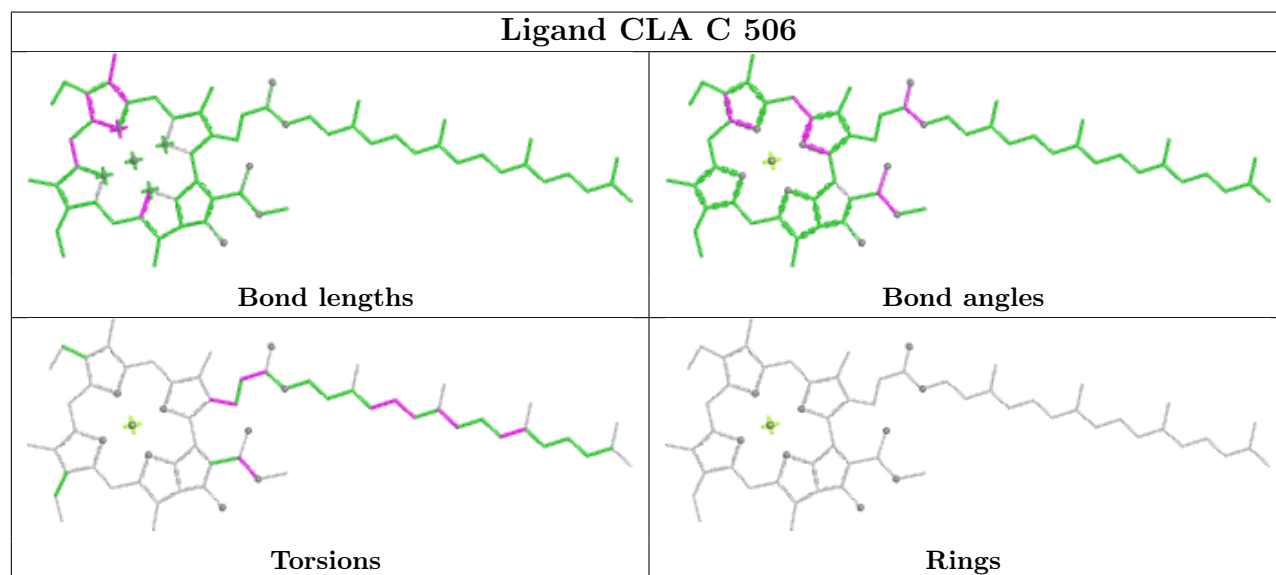
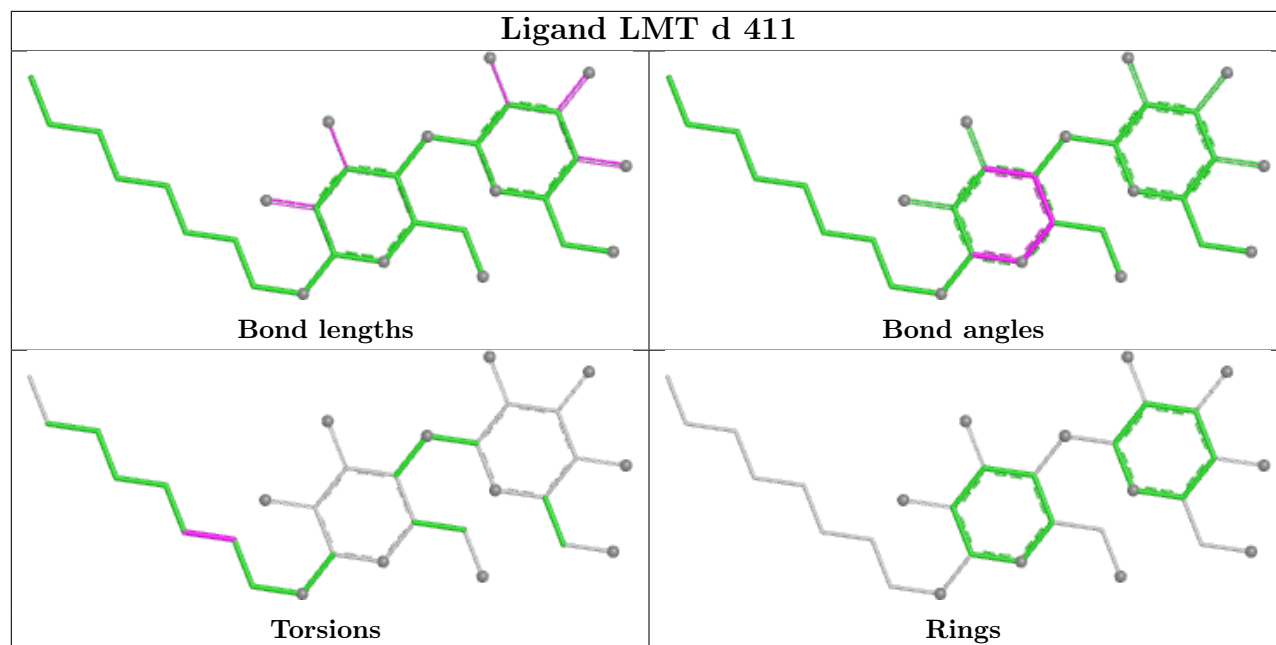
Ligand DGD c 515

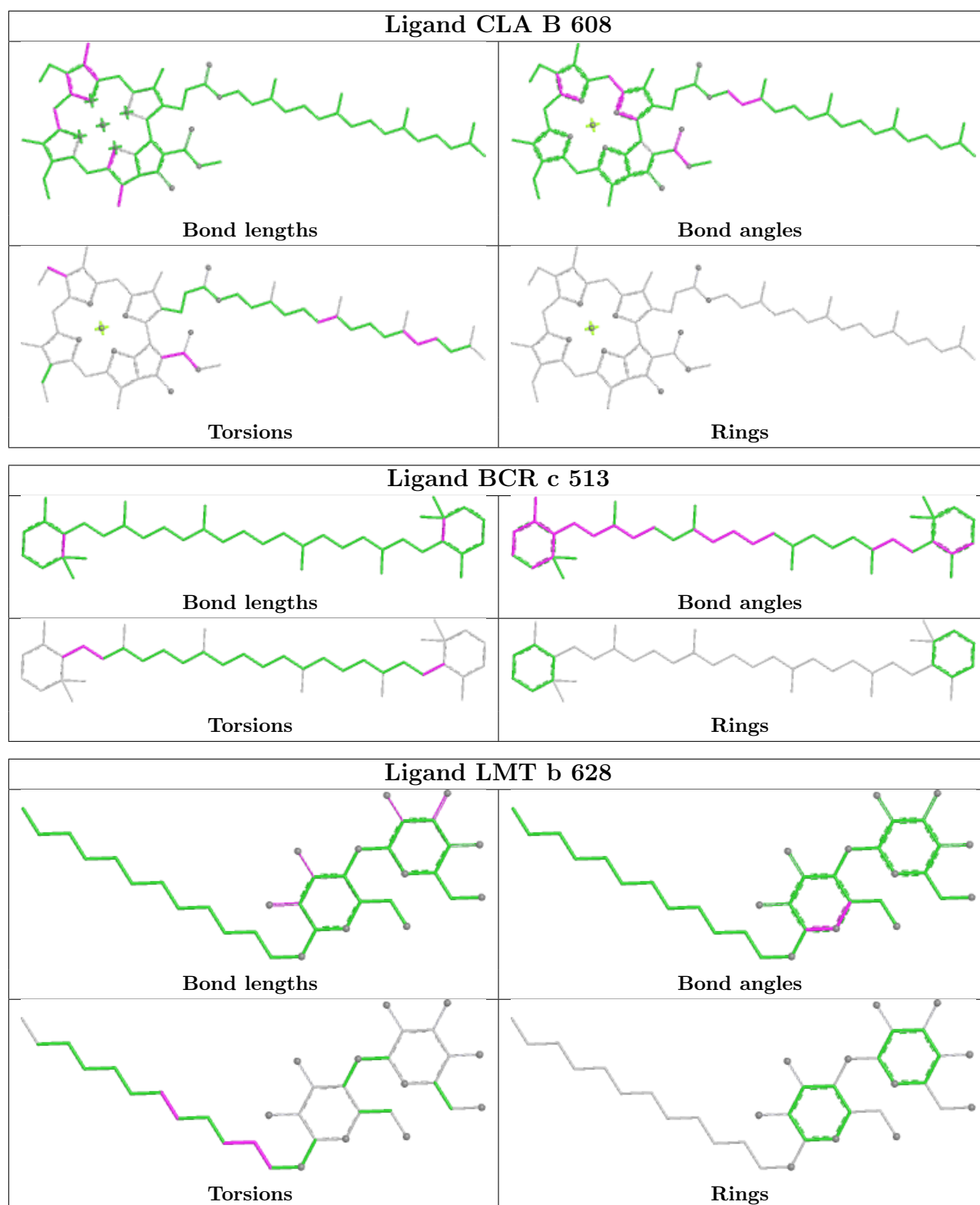


Ligand HEM f 101

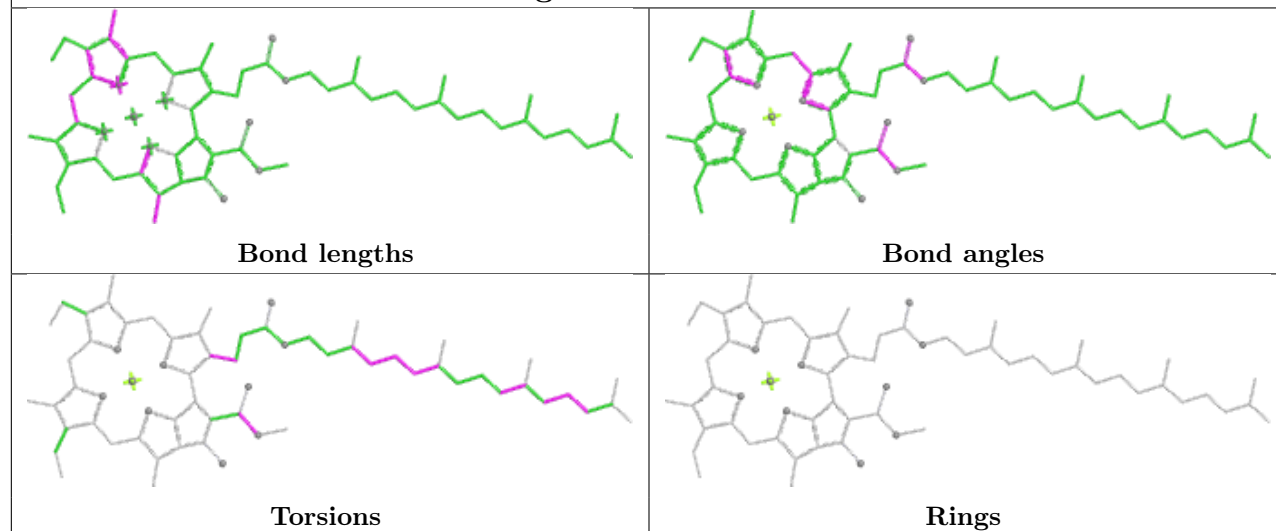




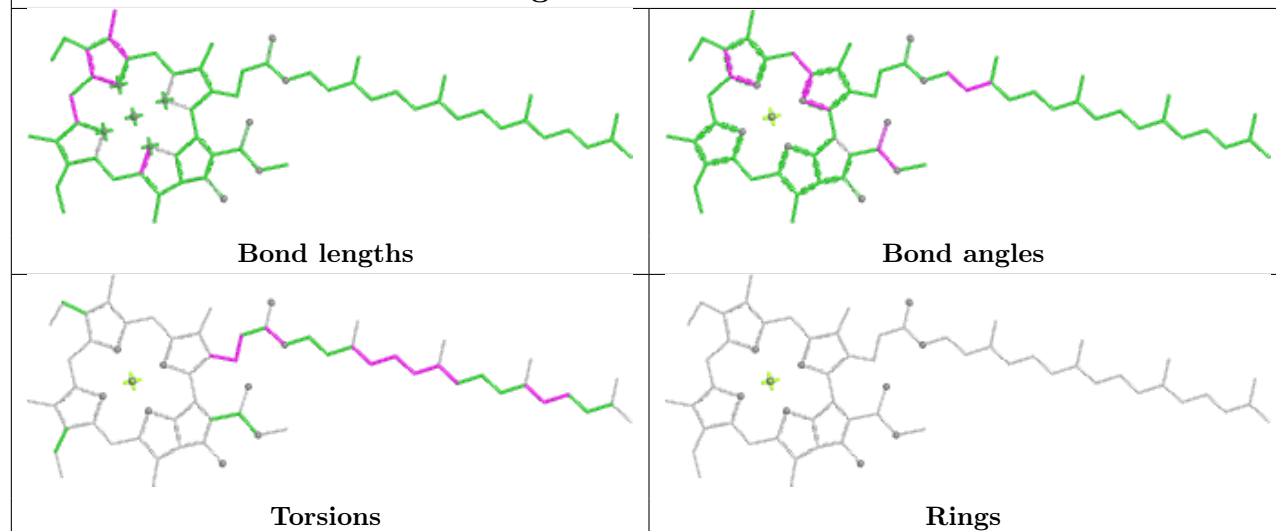




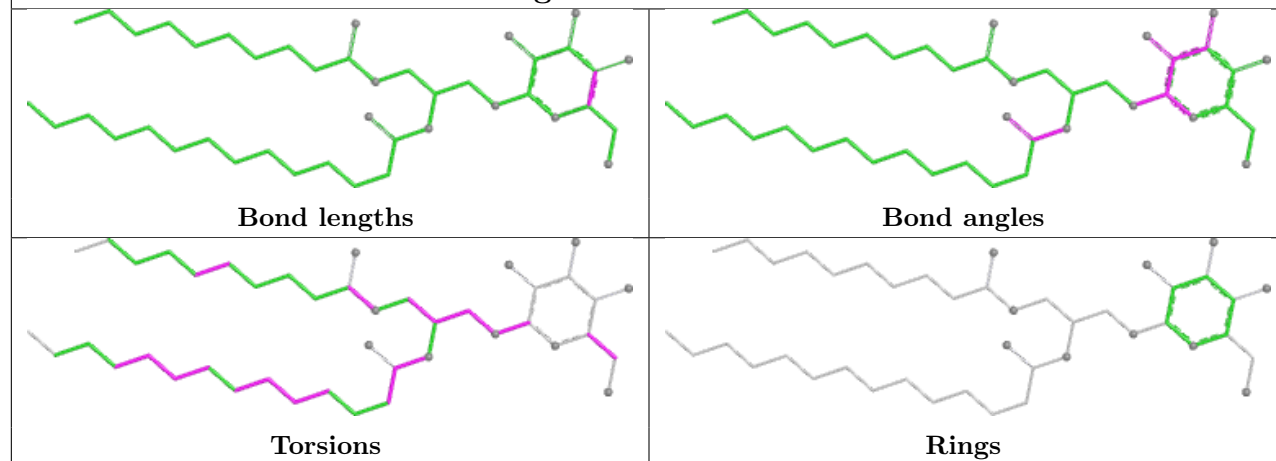
Ligand CLA b 612

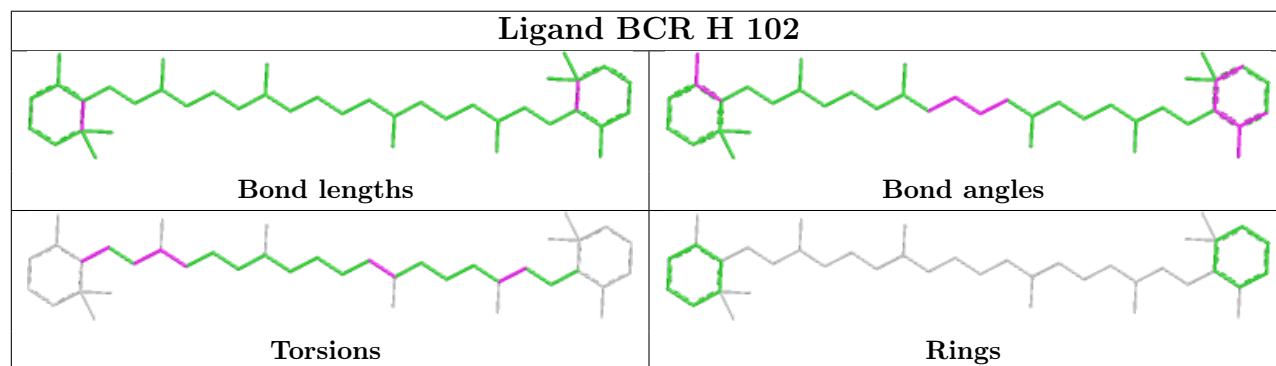
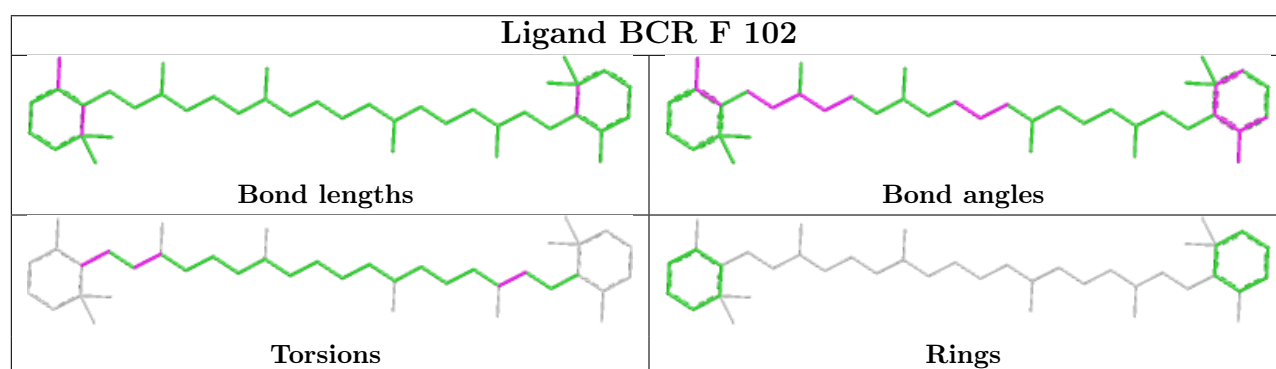
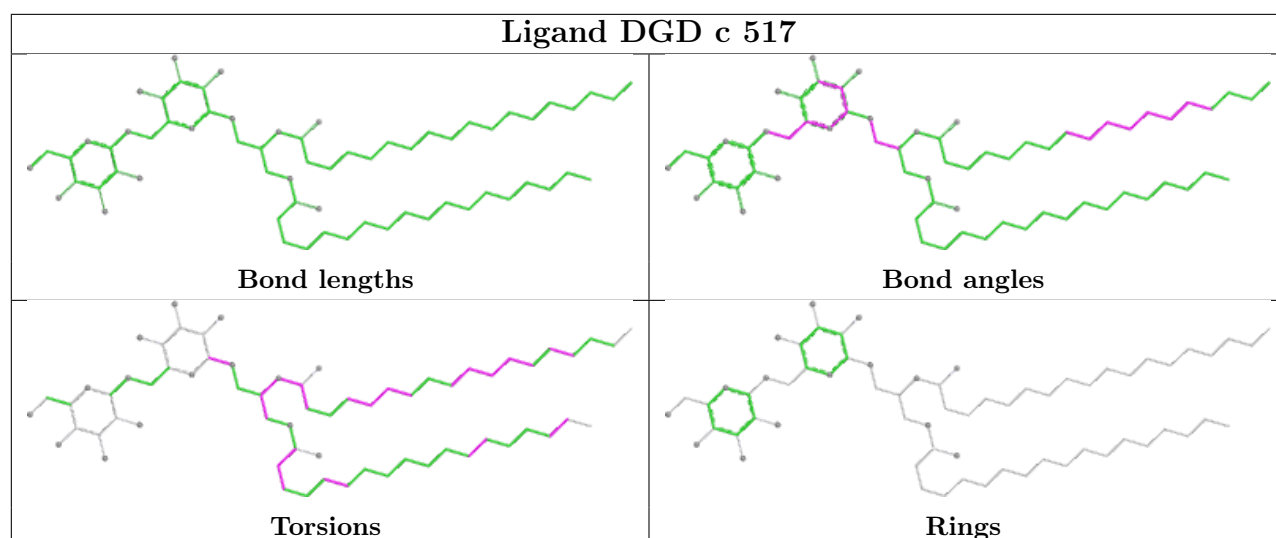


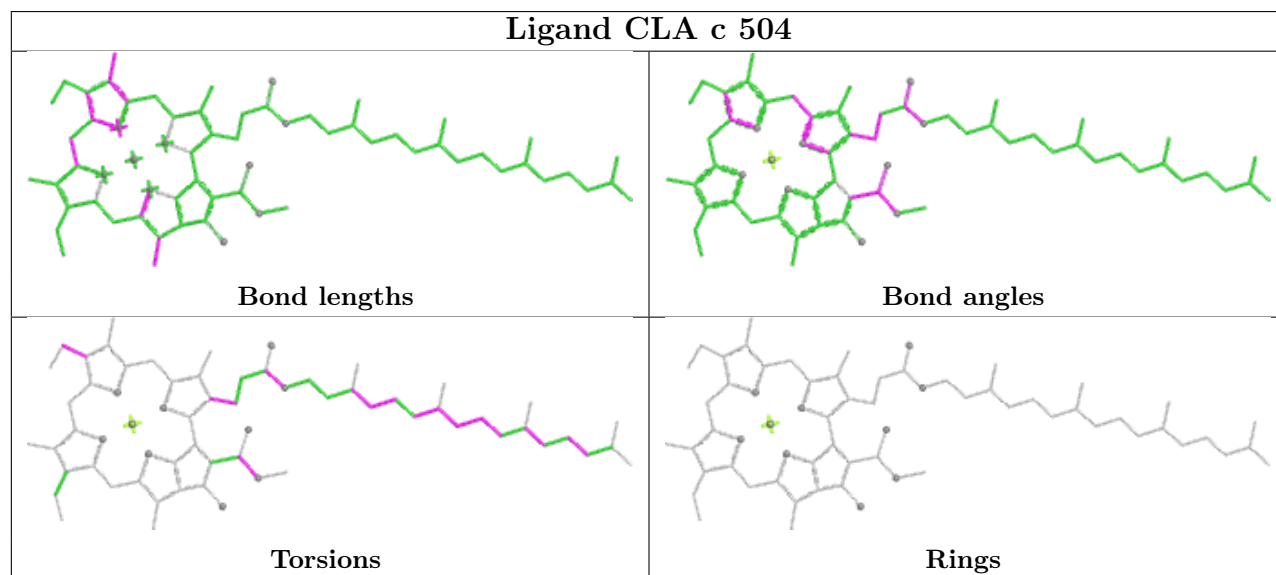
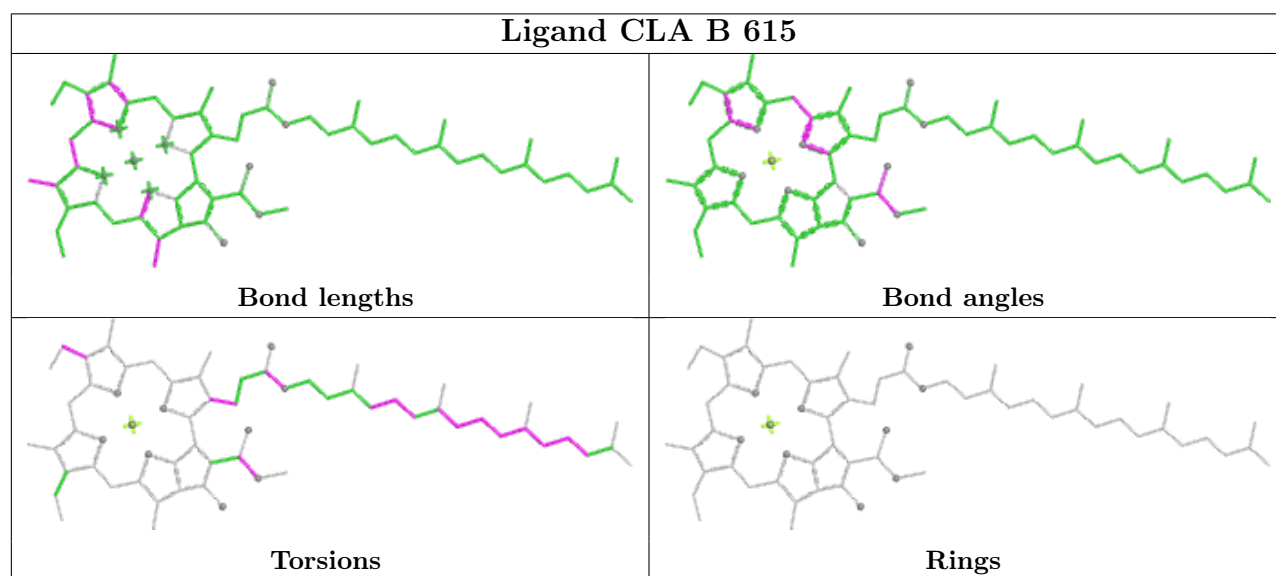
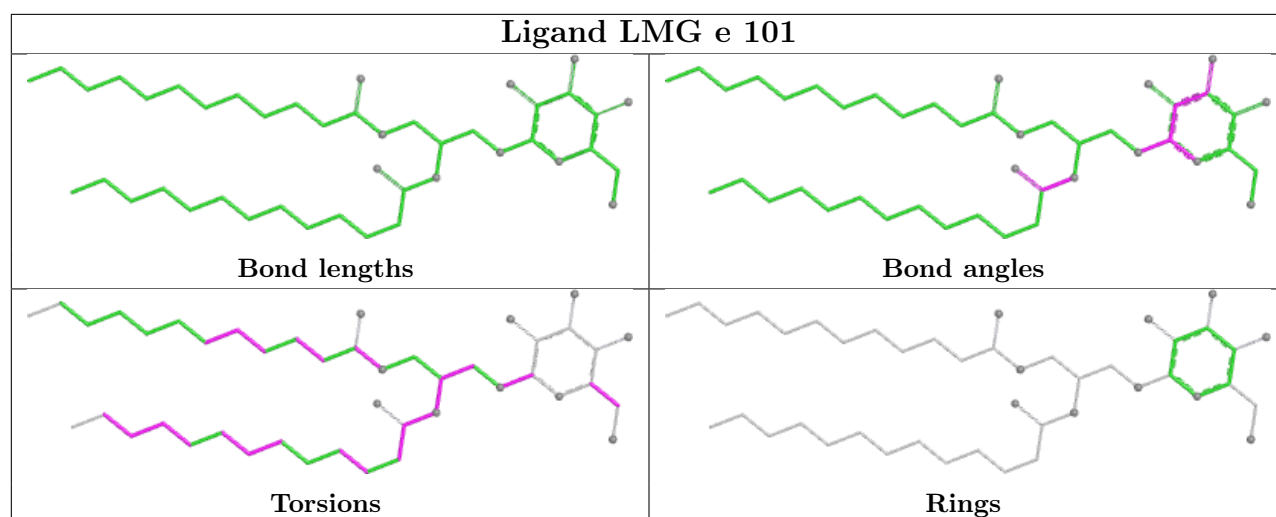
Ligand CLA H 101



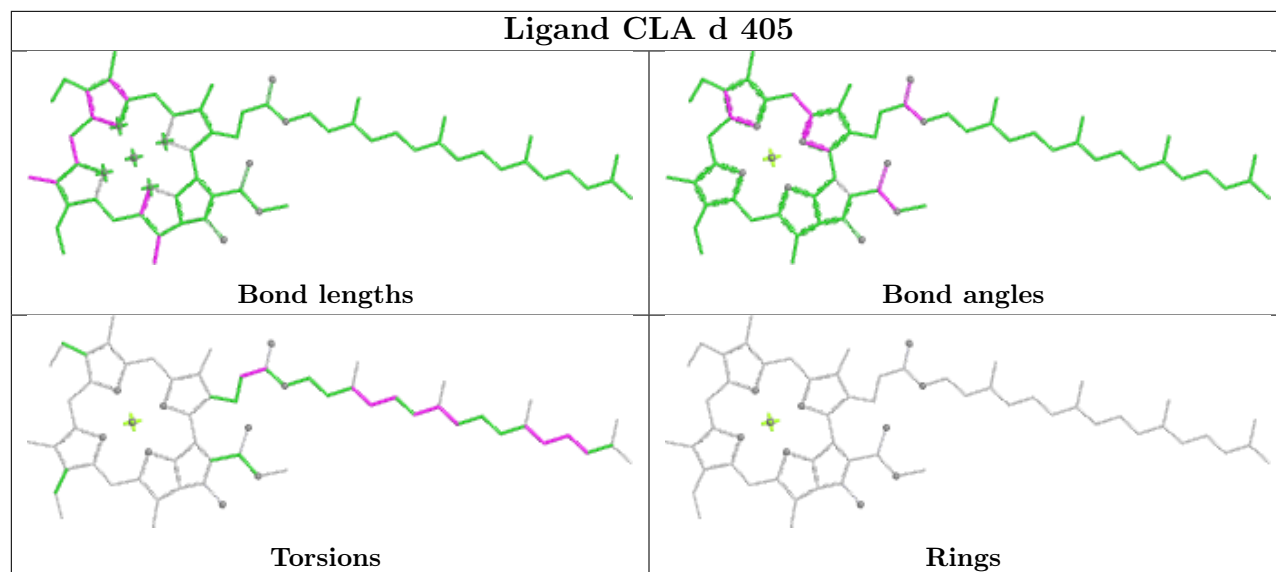
Ligand LMG I 101



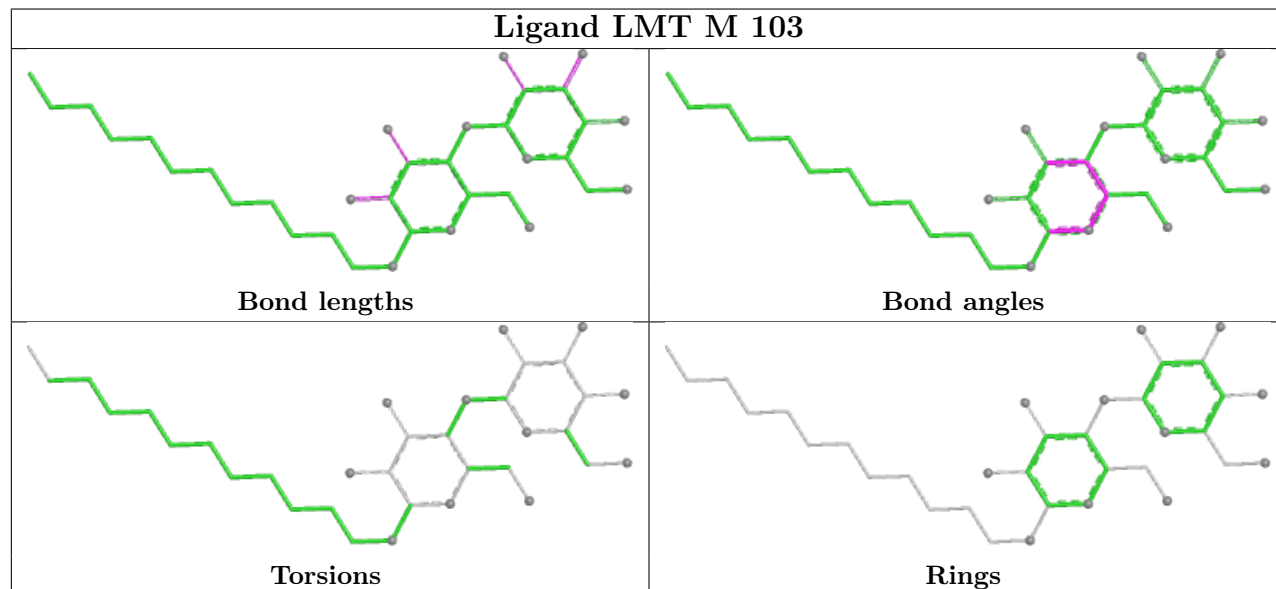




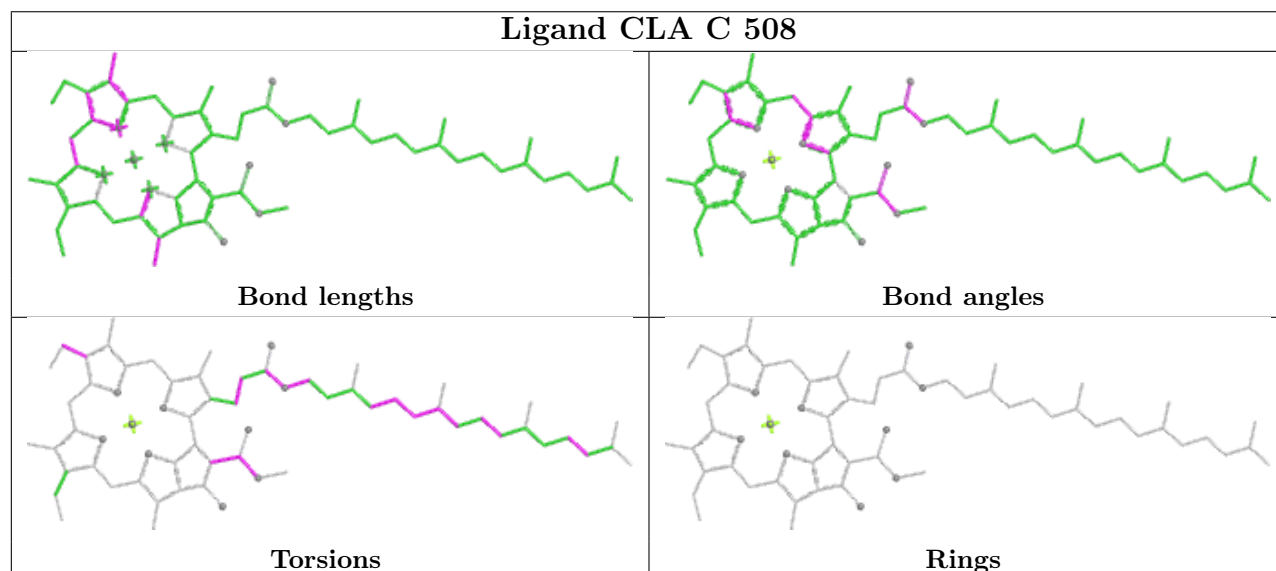
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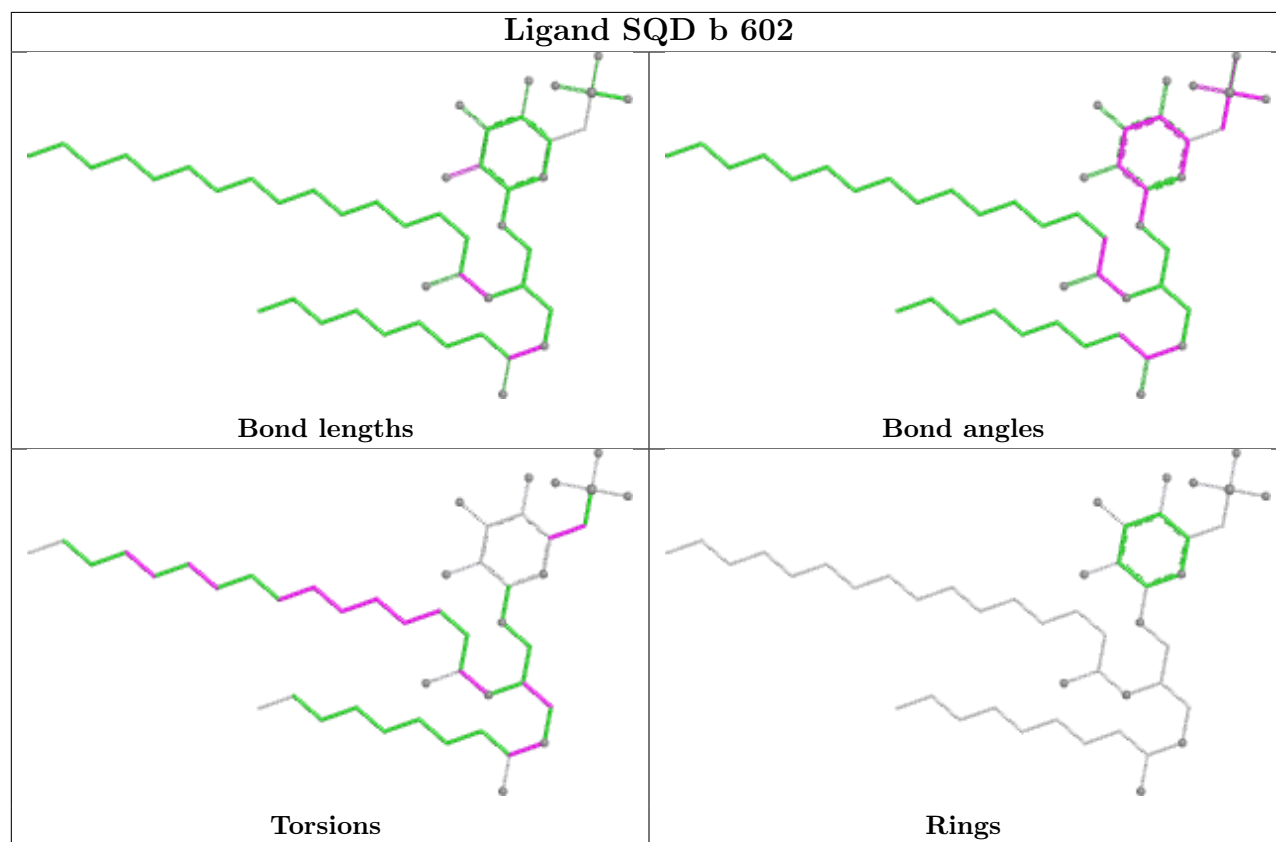
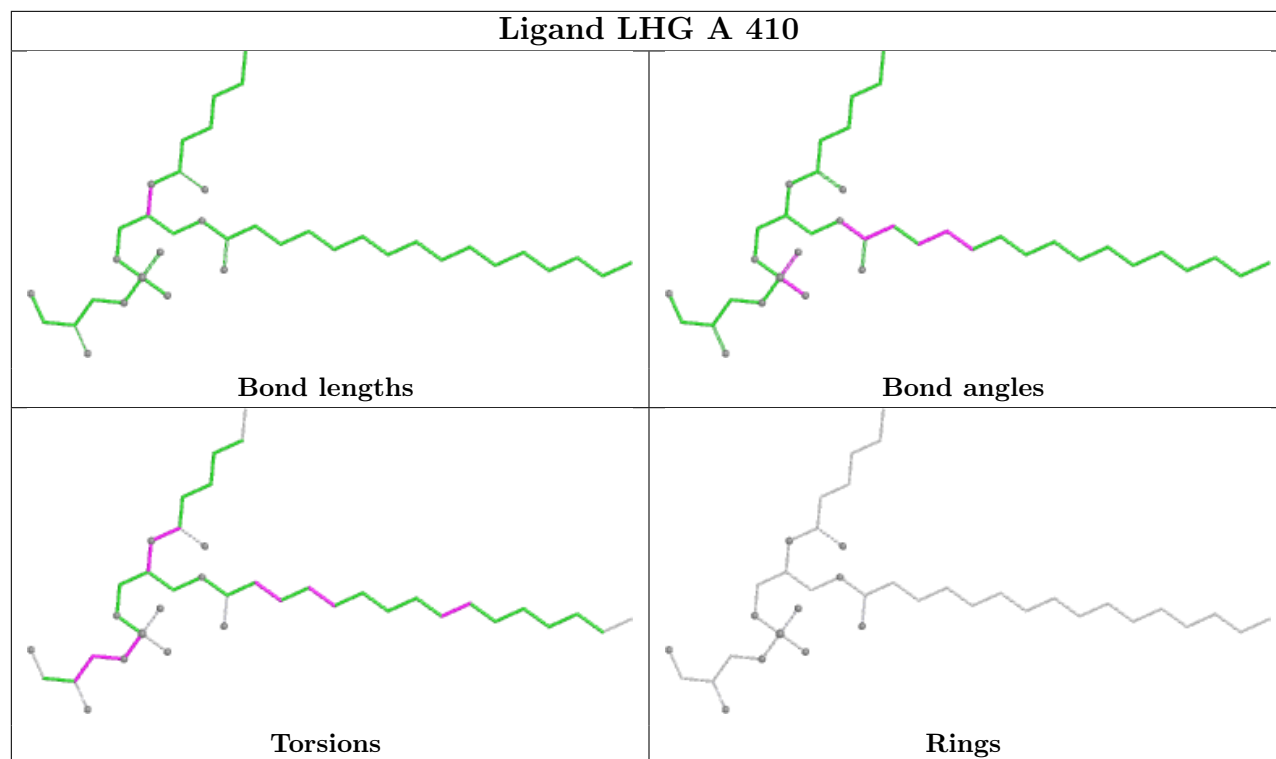


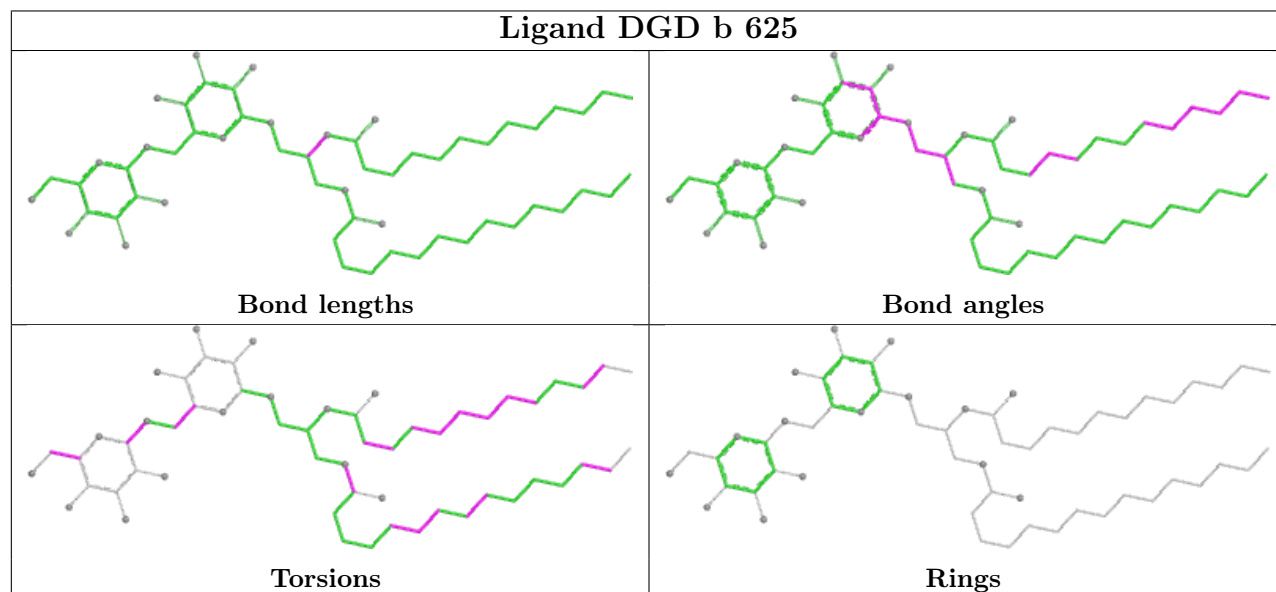
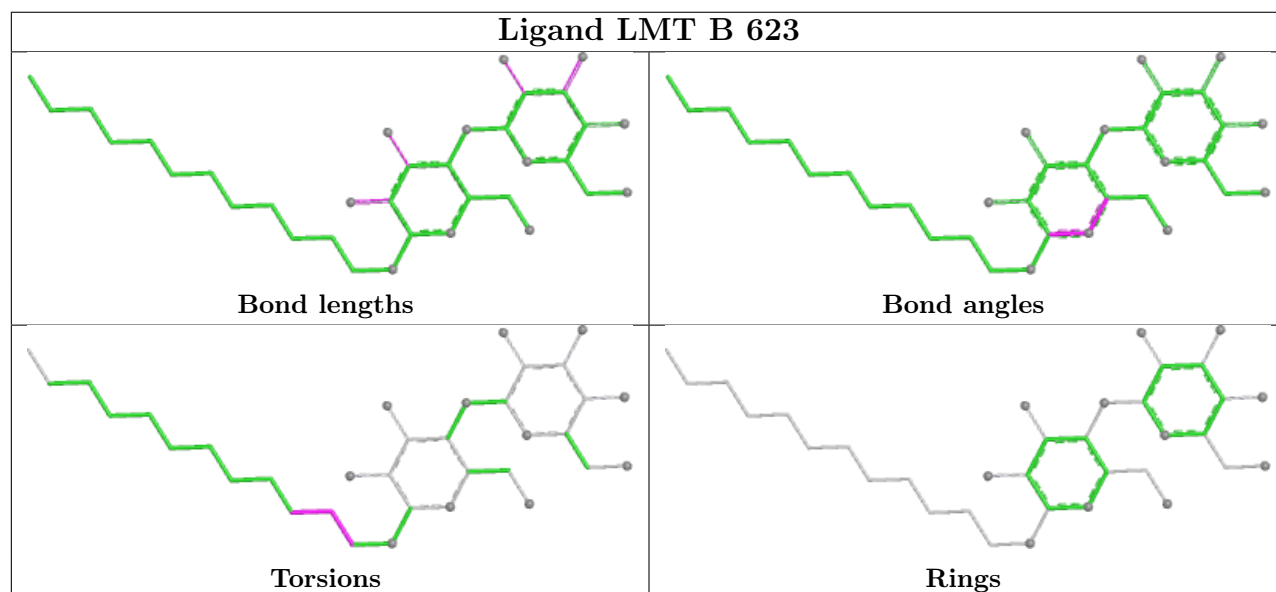
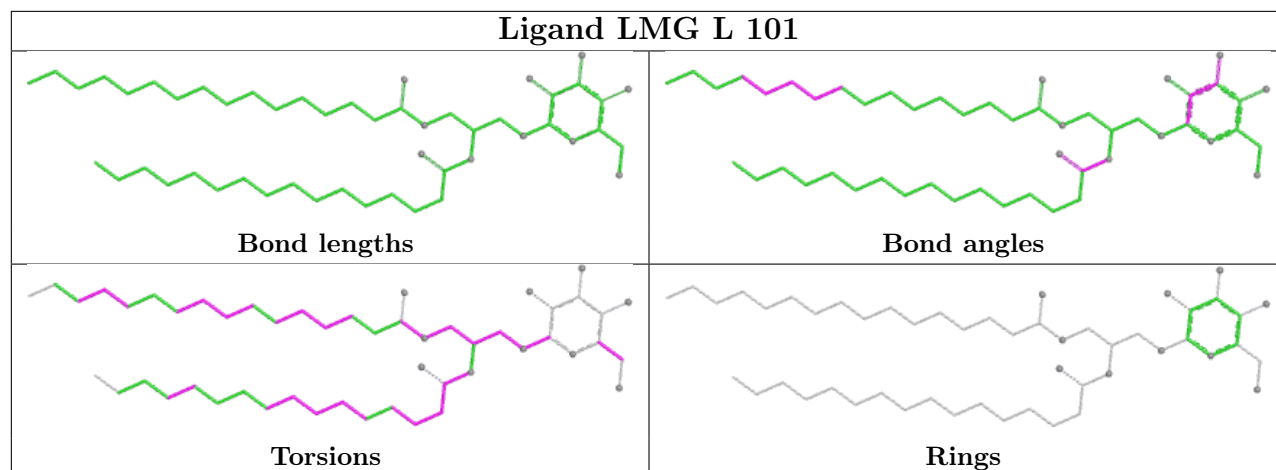
Ligand LMT M 103

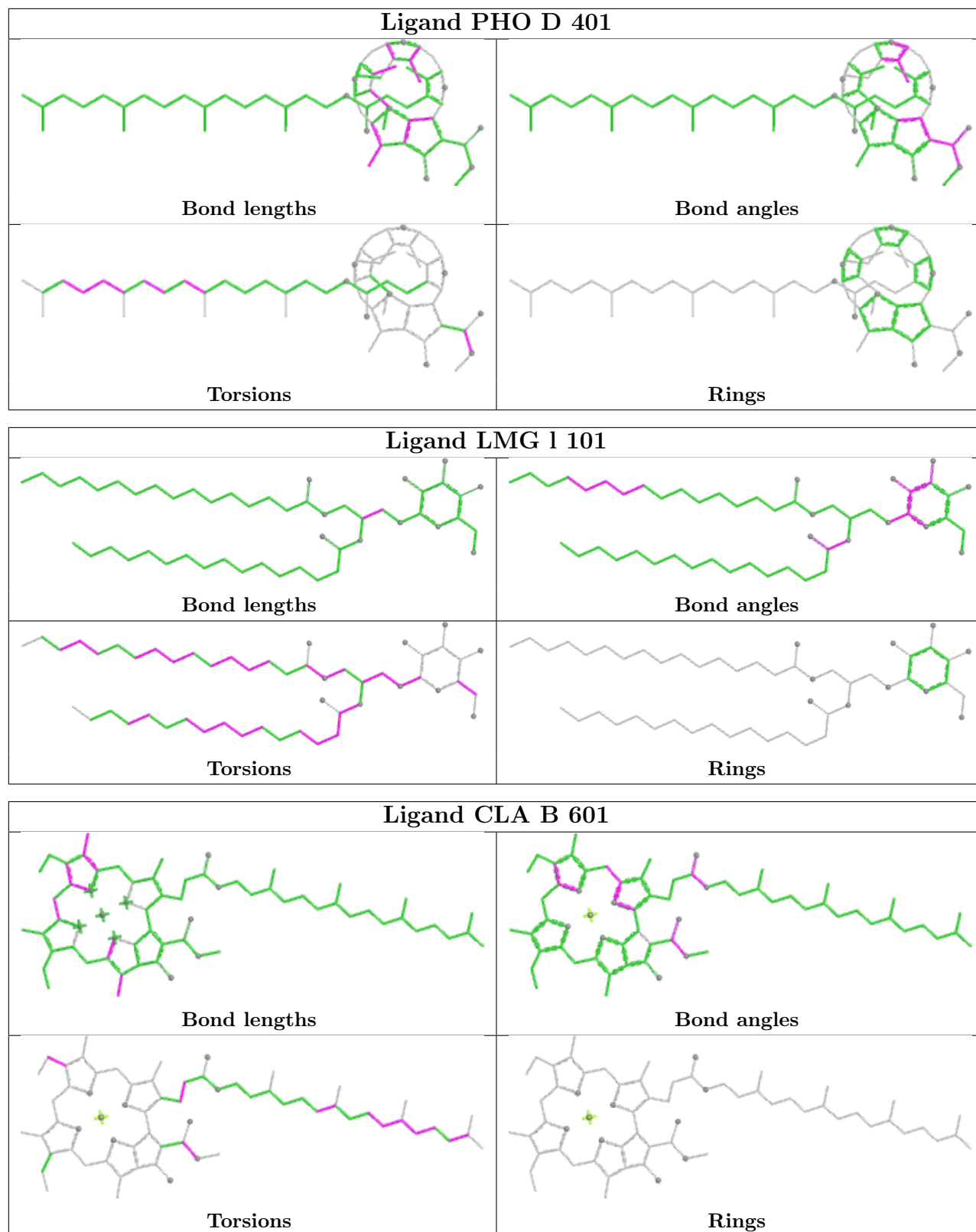


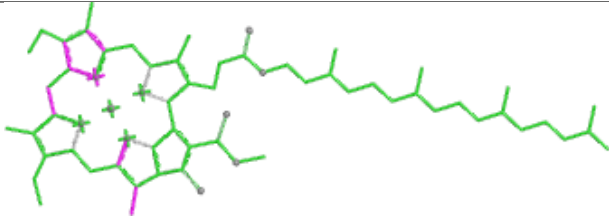
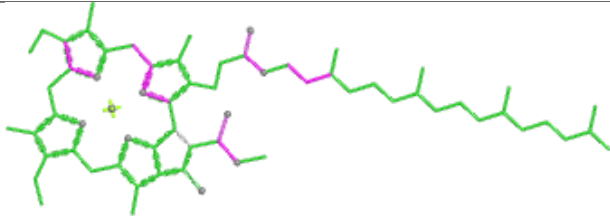
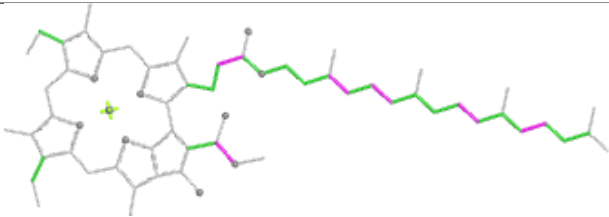
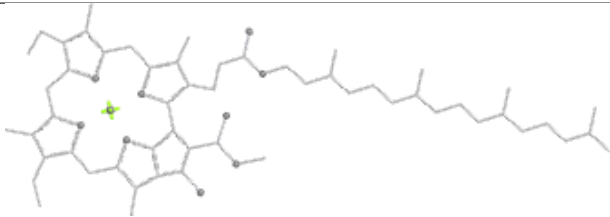
Ligand CLA C 508

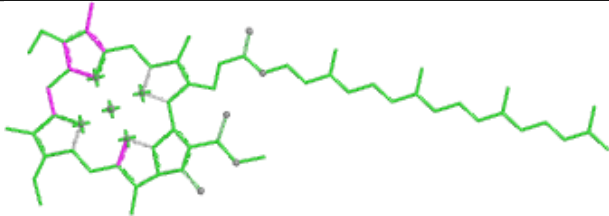
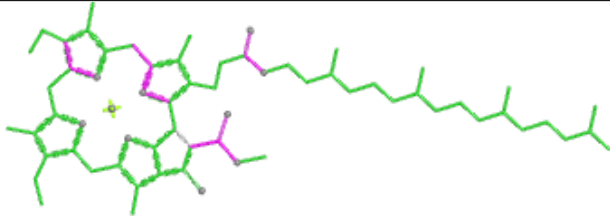
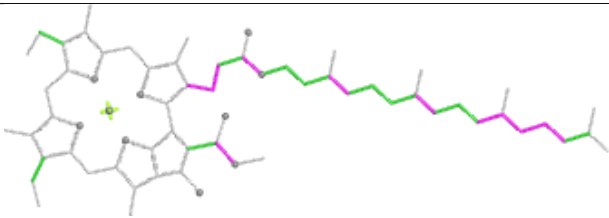
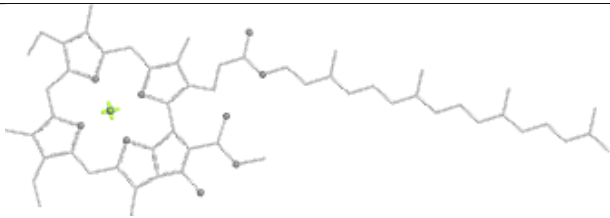


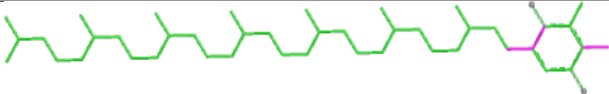
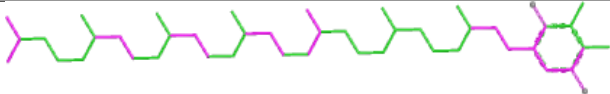
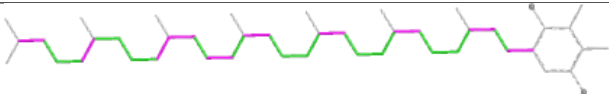
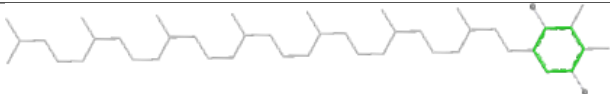




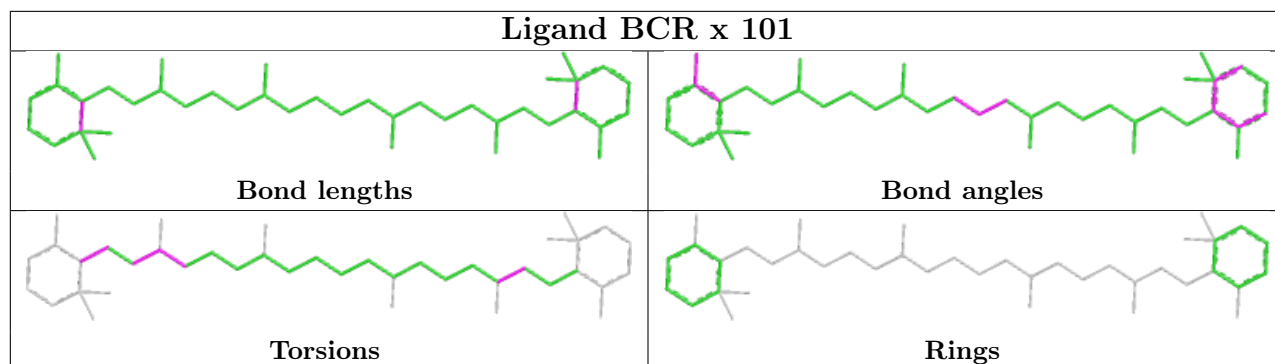


Ligand CLA B 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

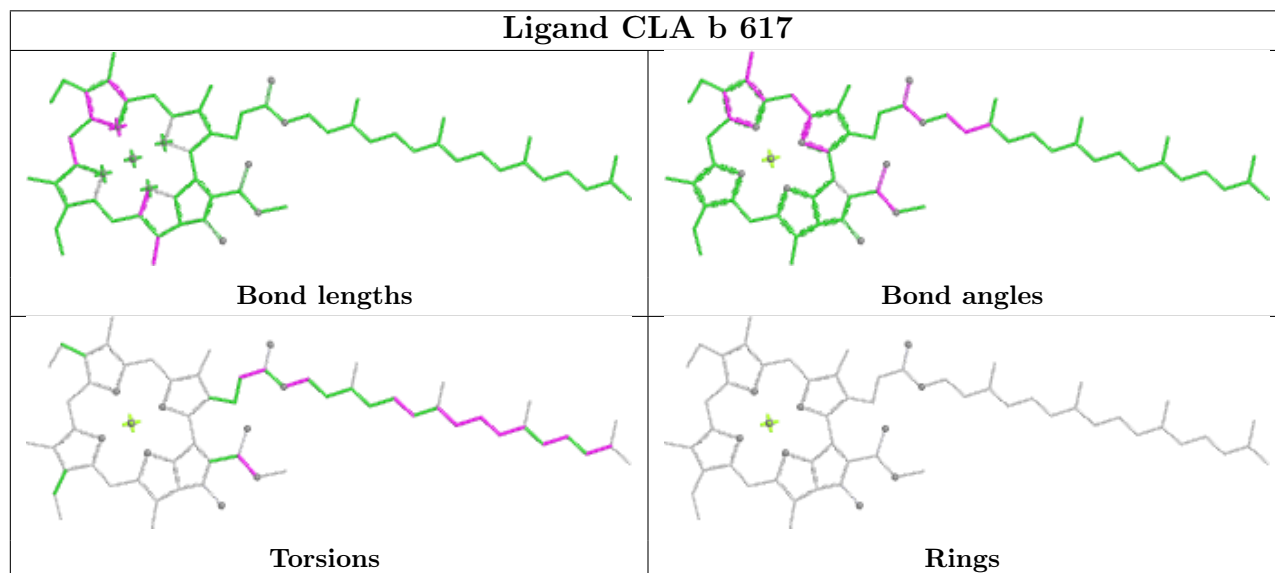
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

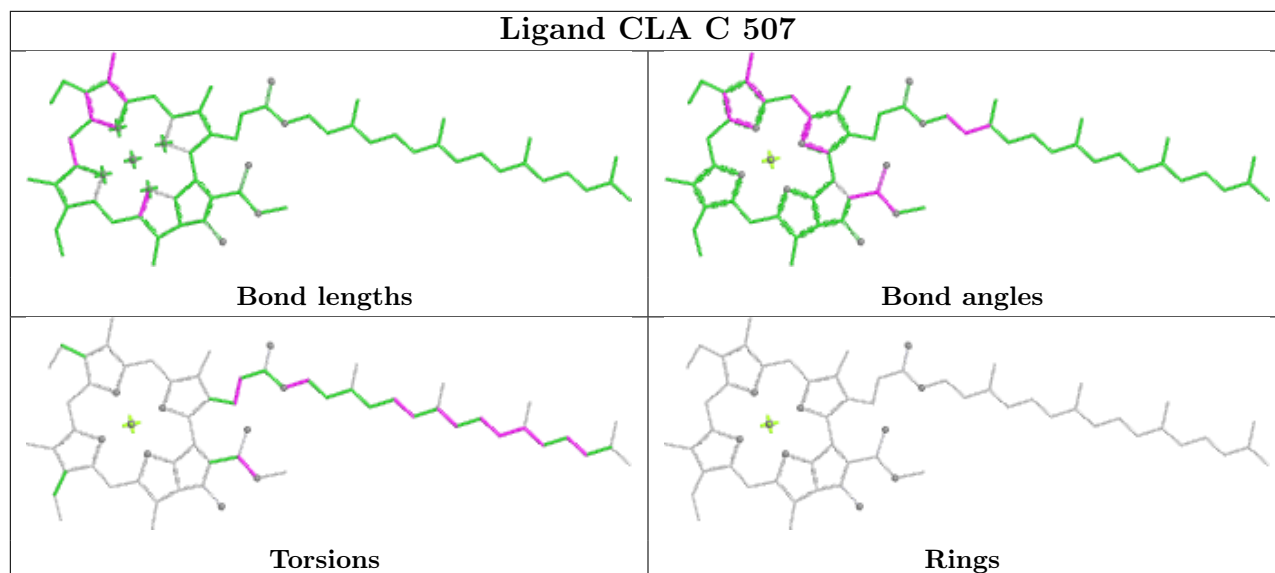
Ligand BCR x 101

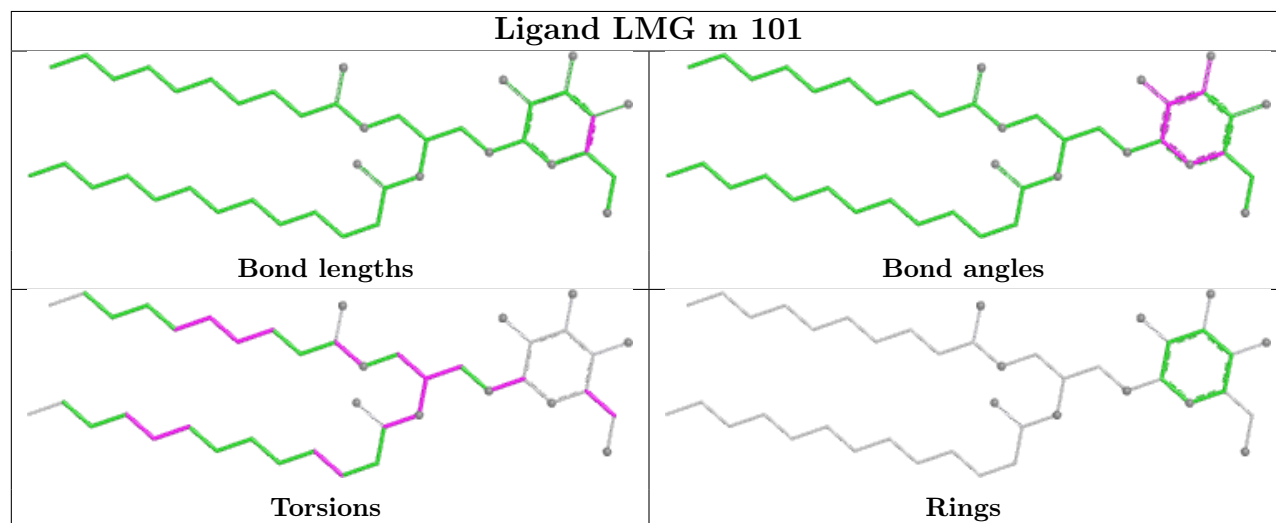
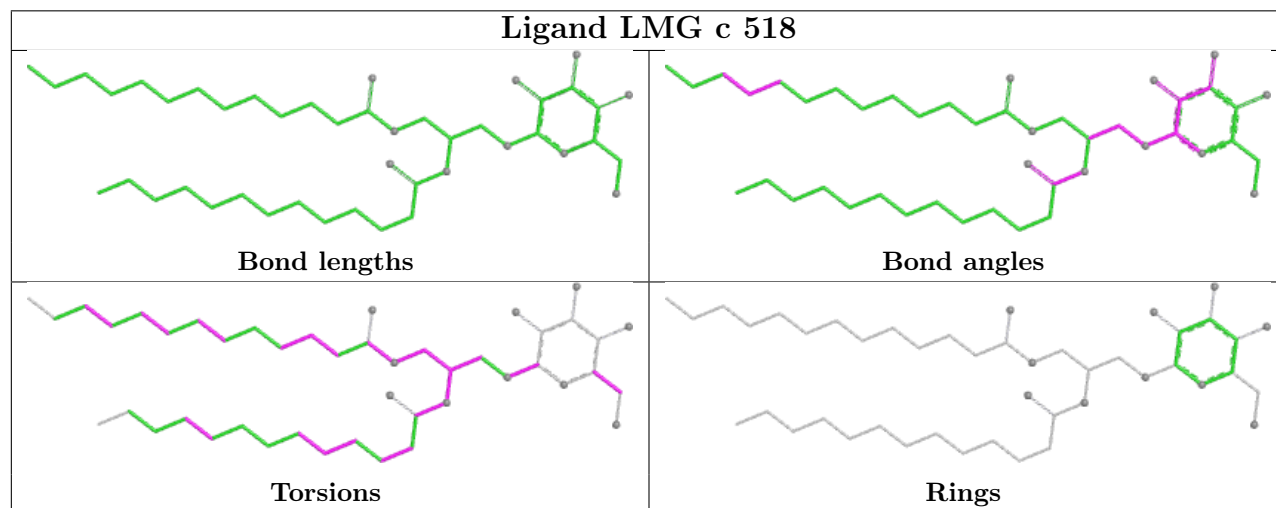
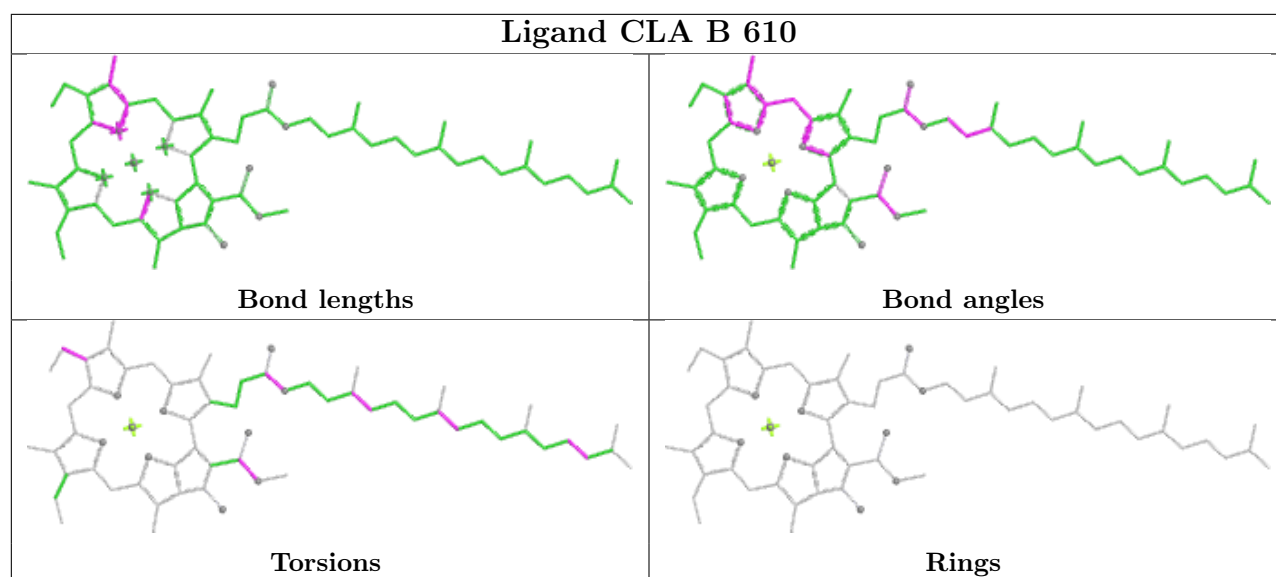


Ligand CLA b 617

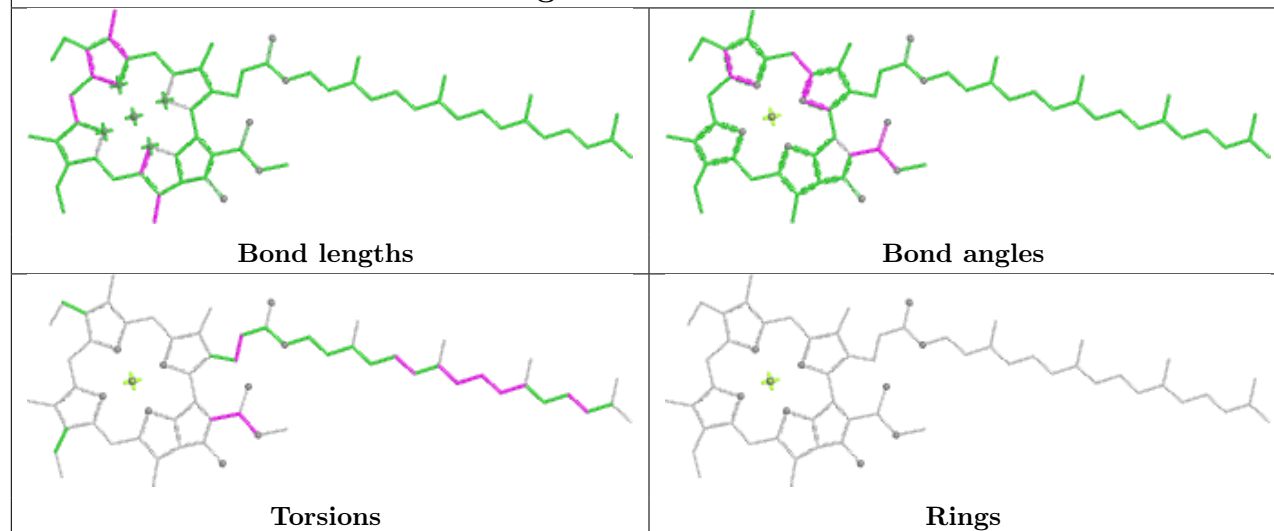


Ligand CLA C 507

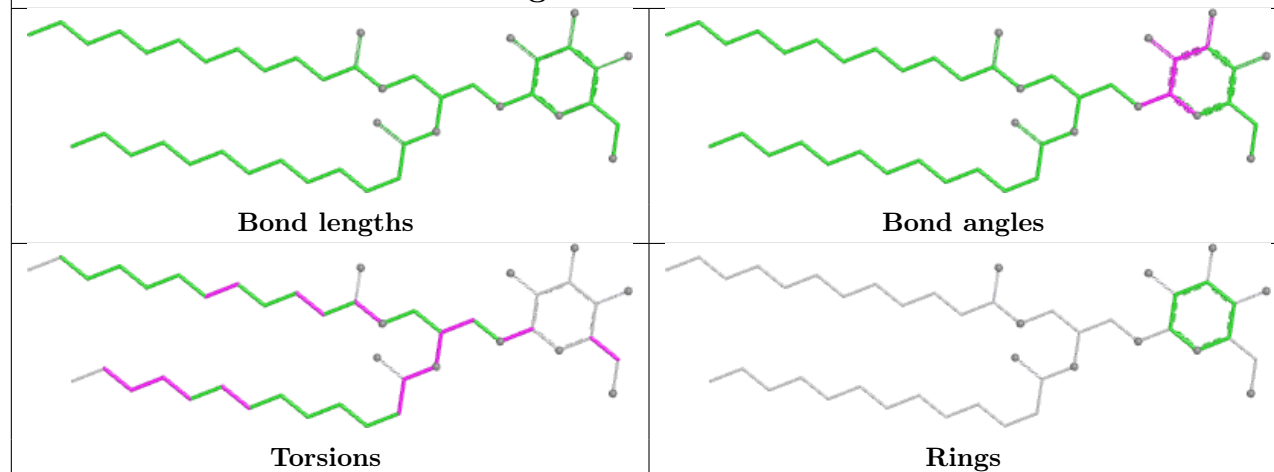




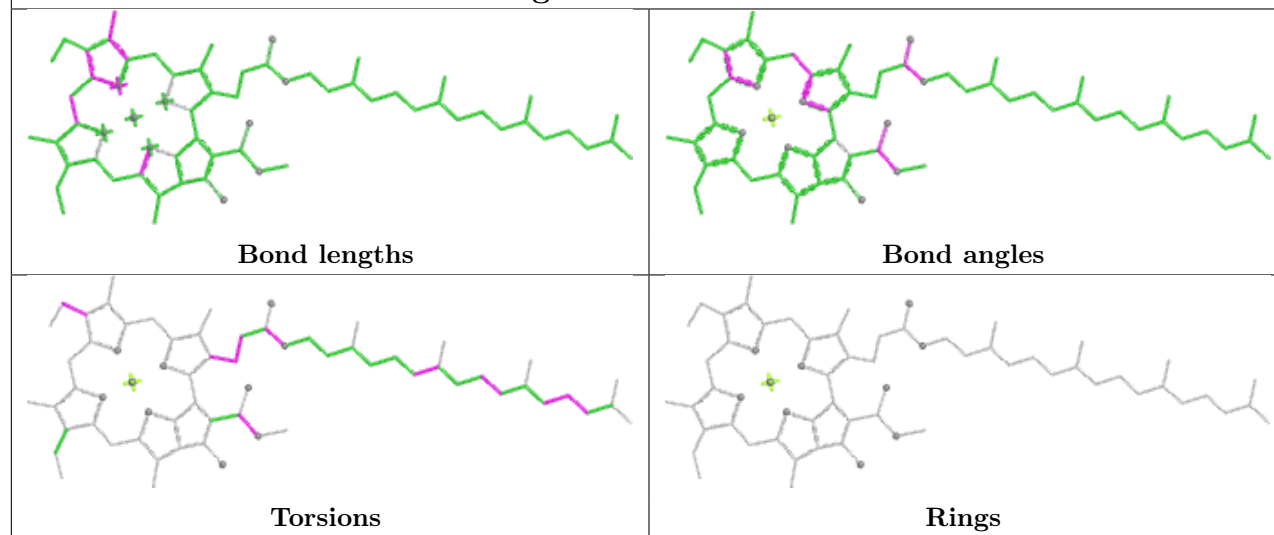
Ligand CLA c 503



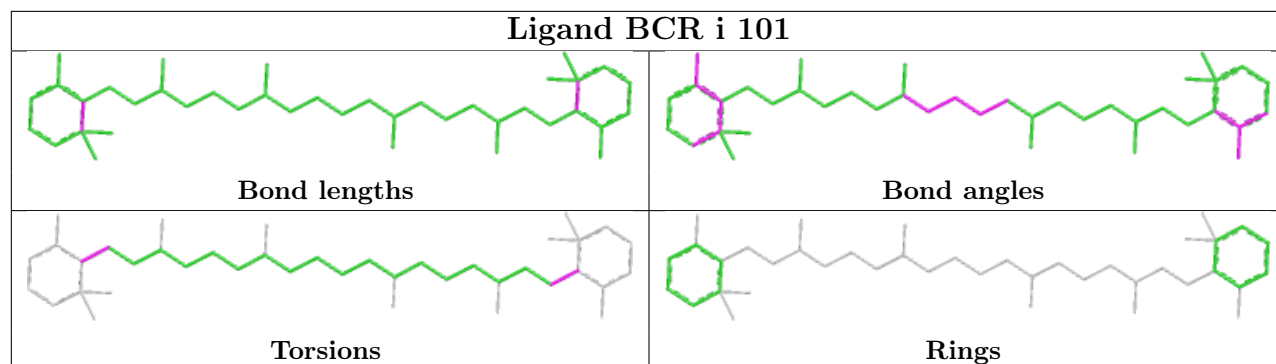
Ligand LMG E 101



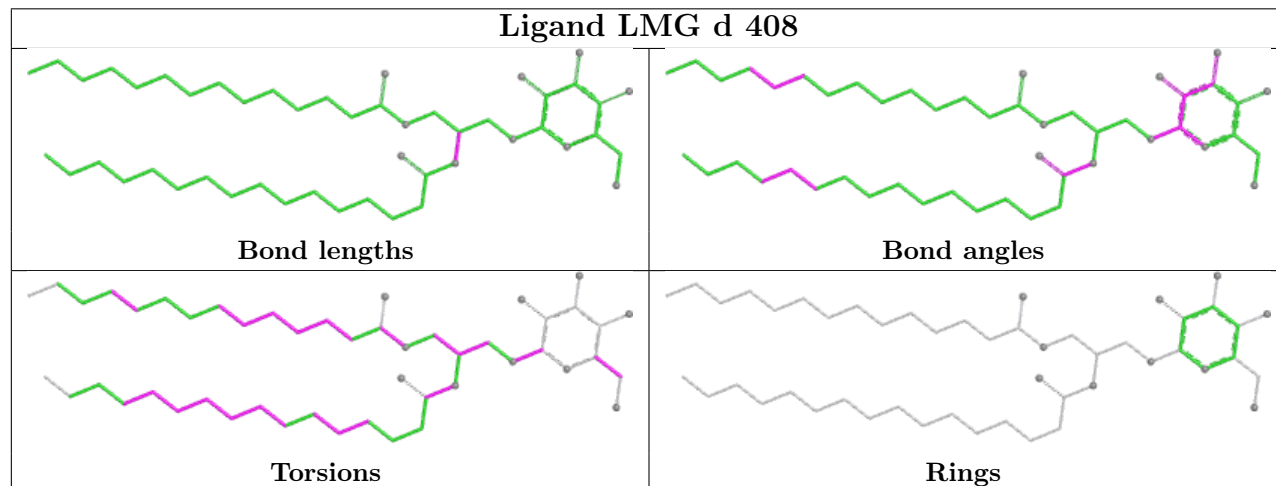
Ligand CLA C 519



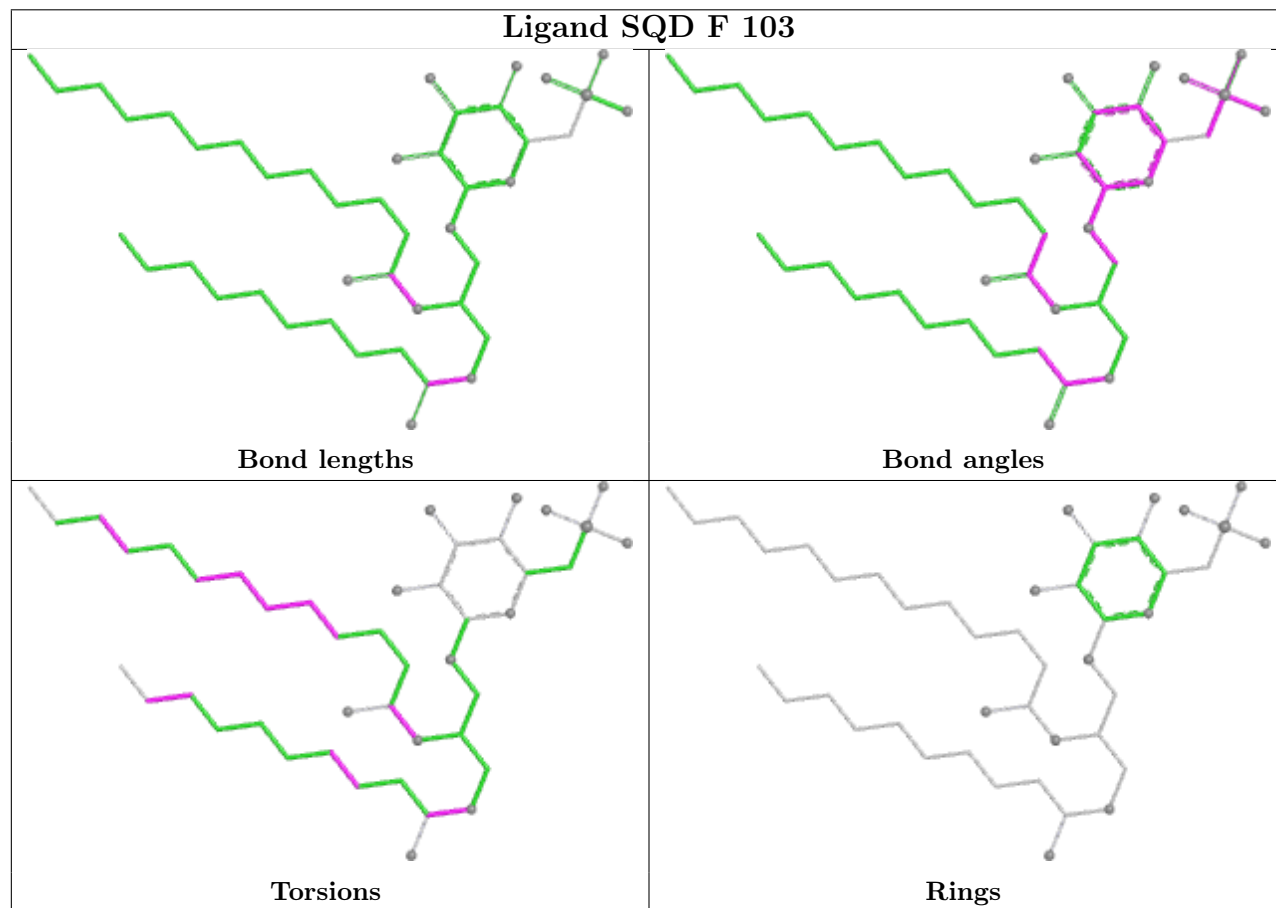
Ligand BCR i 101



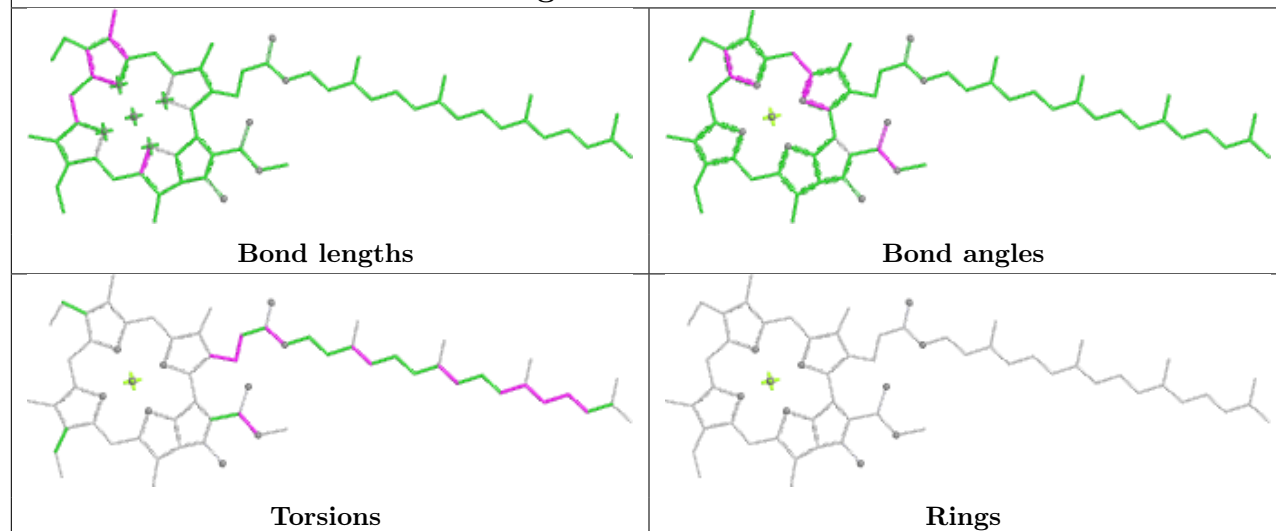
Ligand LMG d 408



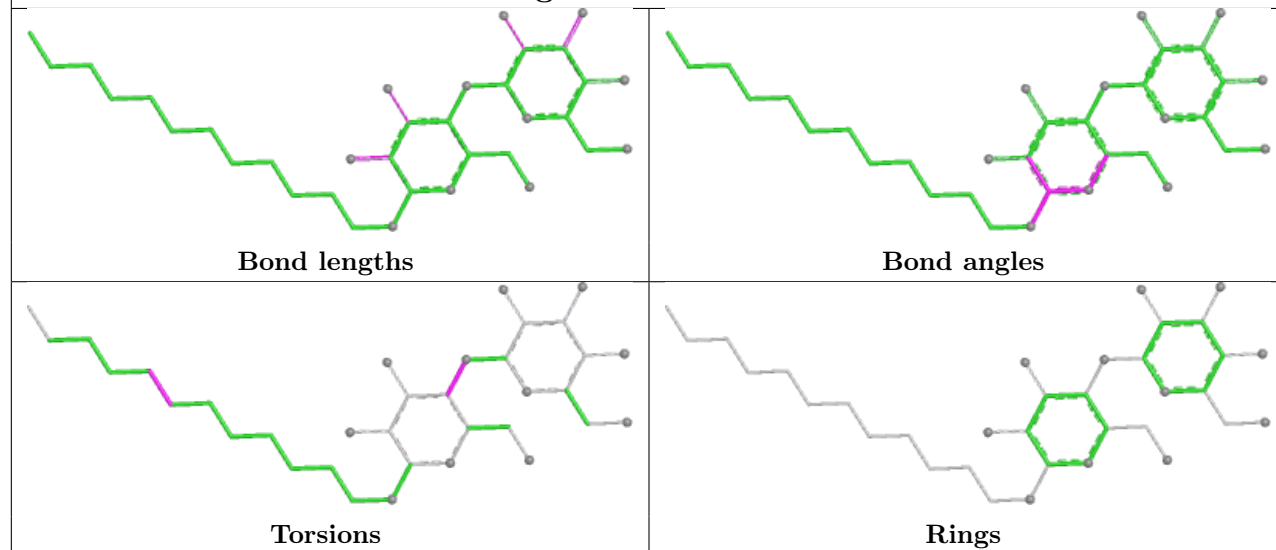
Ligand SQD F 103



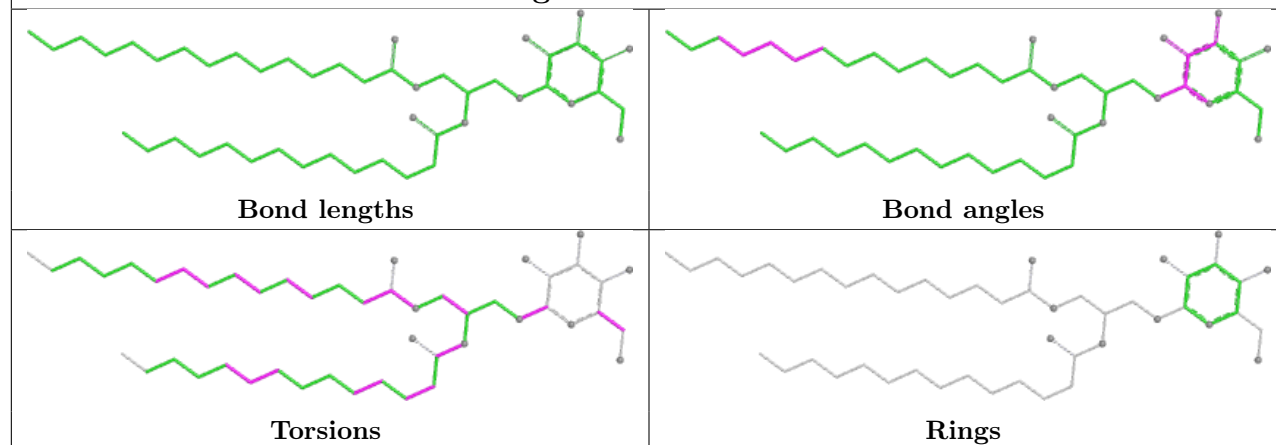
Ligand CLA c 512



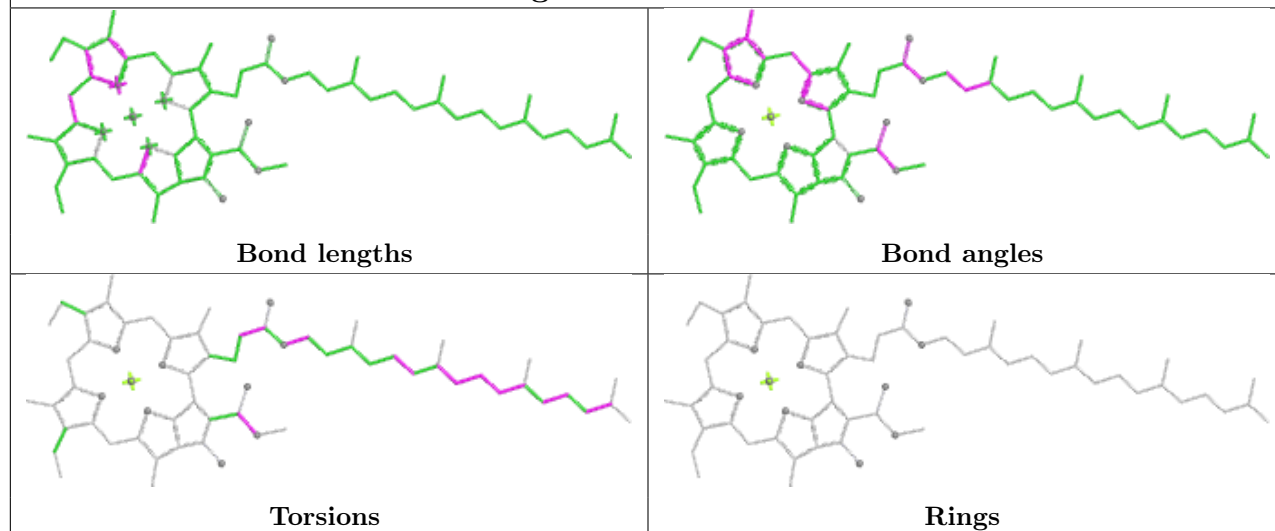
Ligand LMT I 102



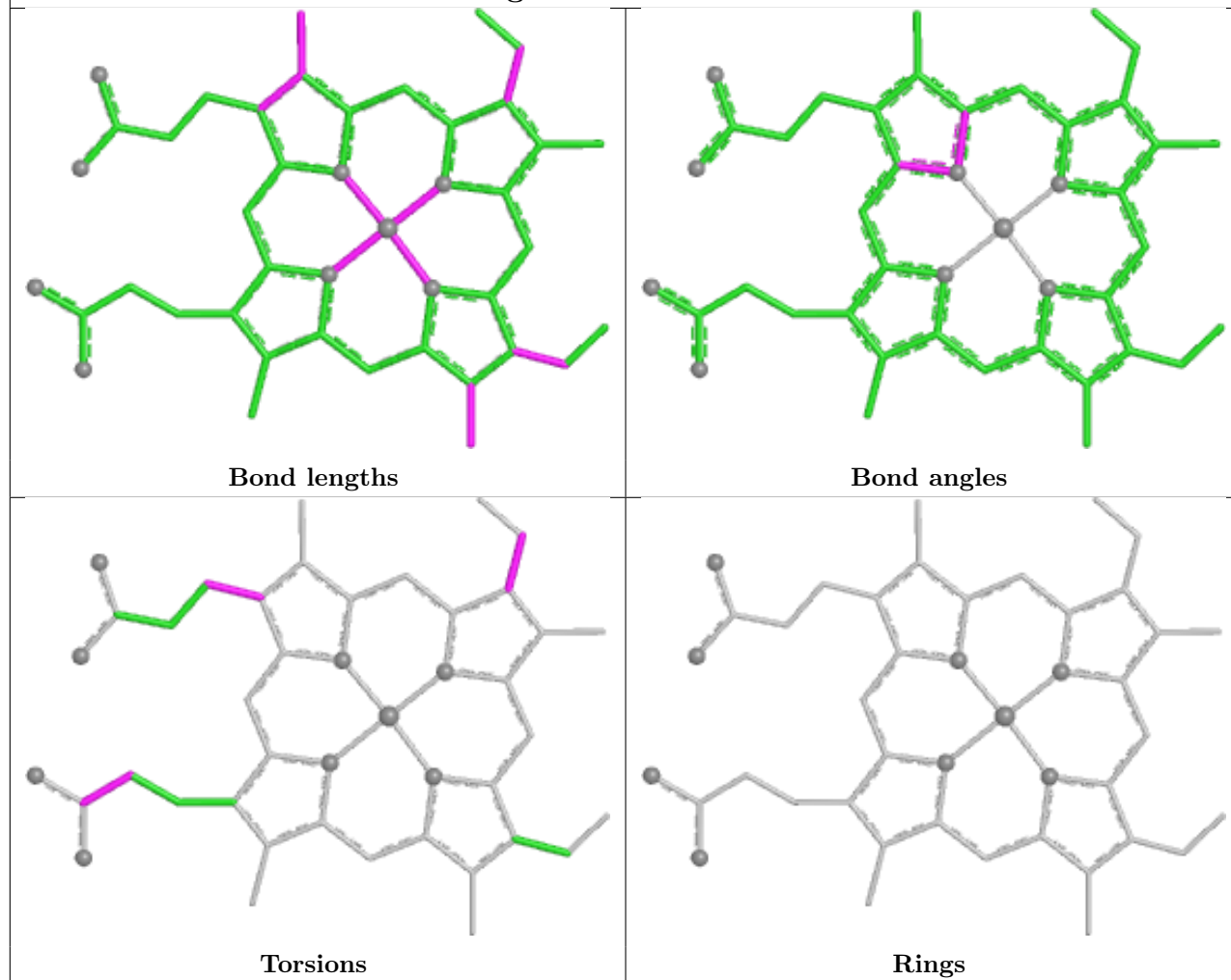
Ligand LMG c 522

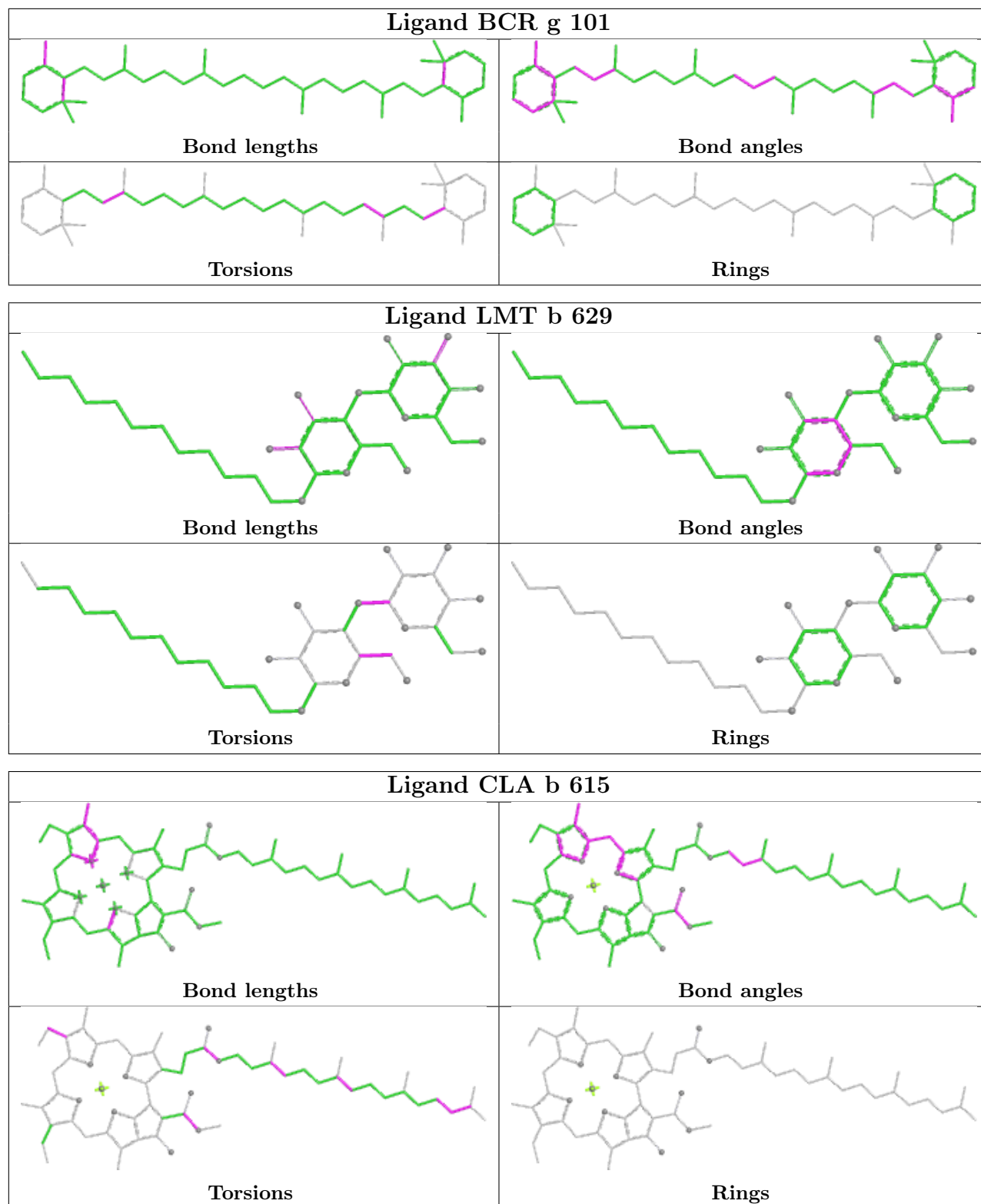


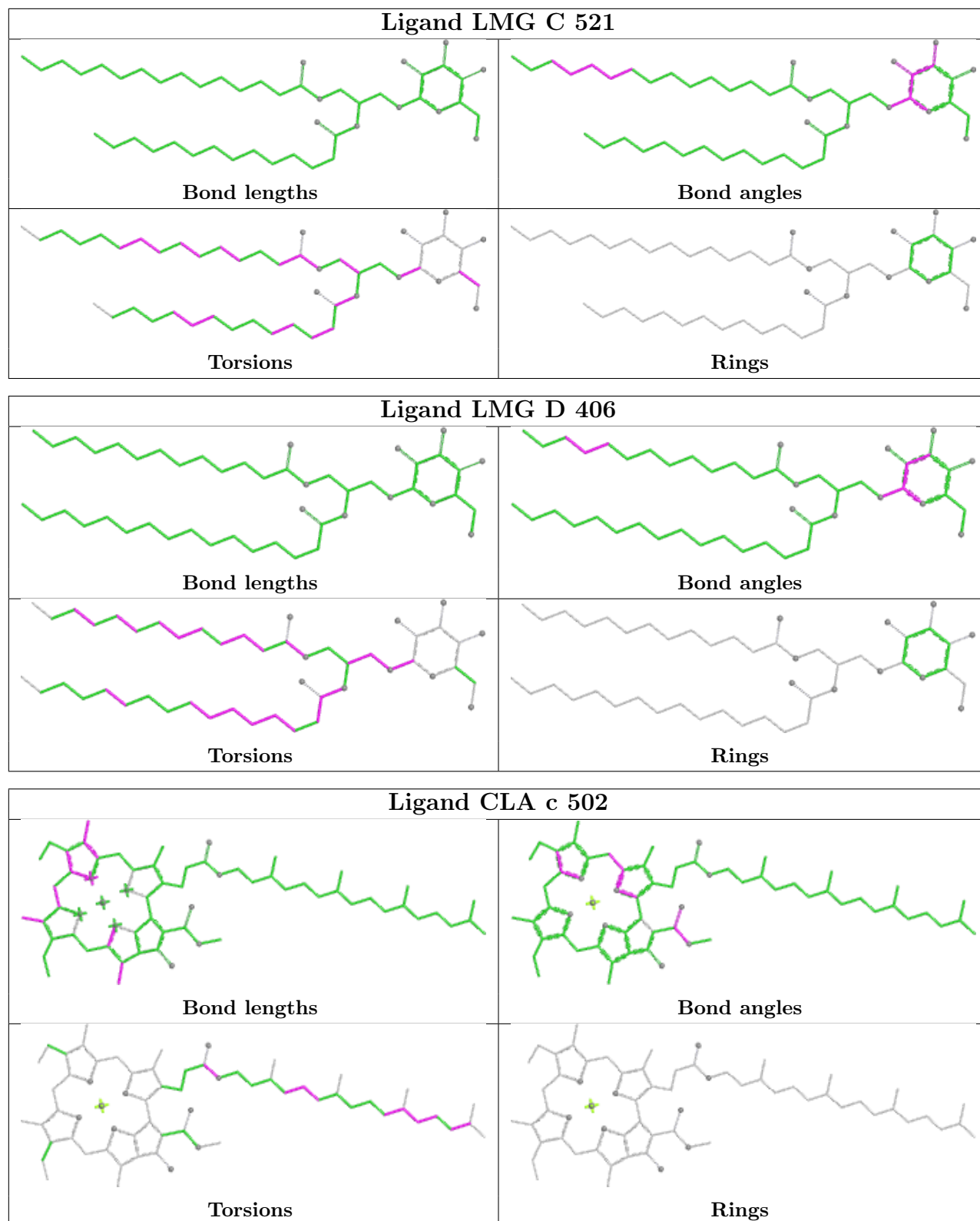
Ligand CLA B 612



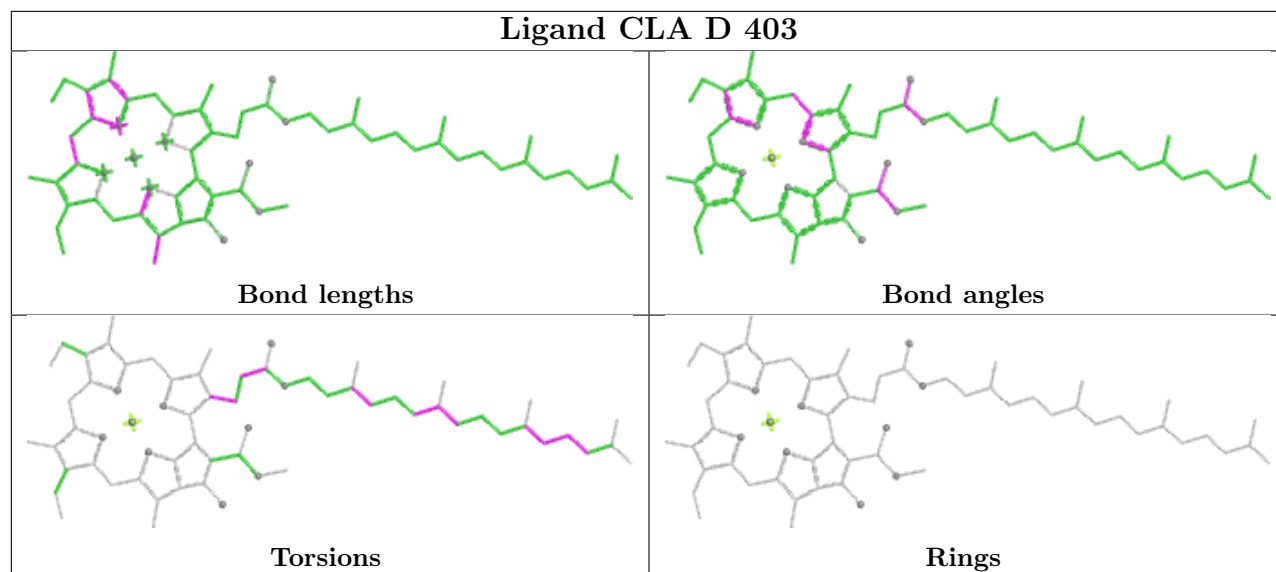
Ligand HEM V 201



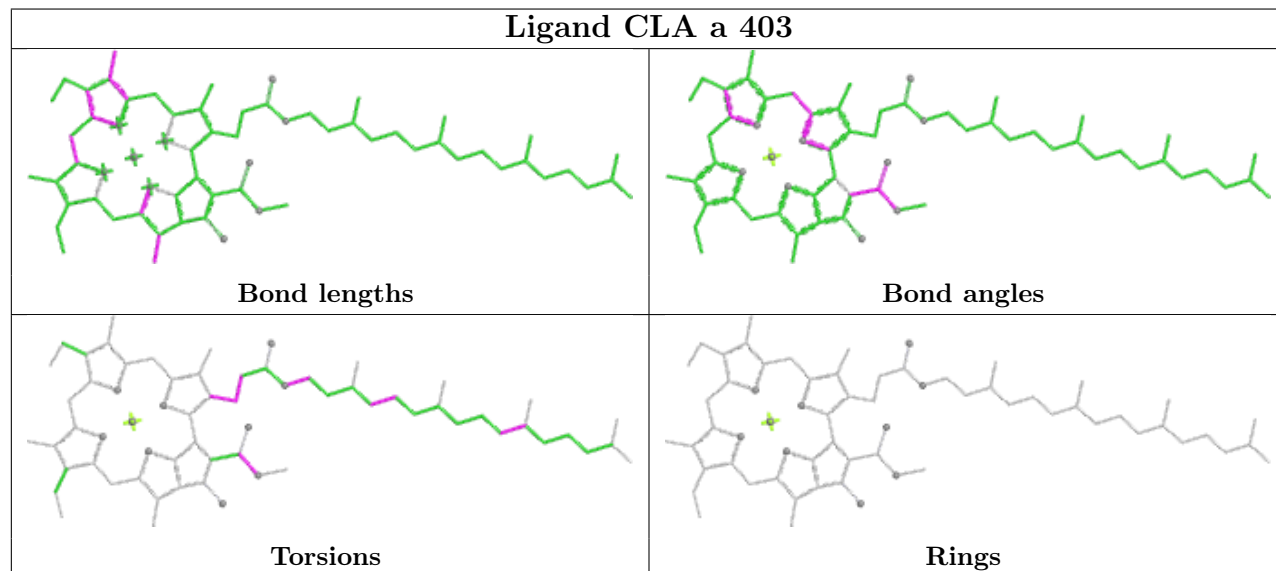




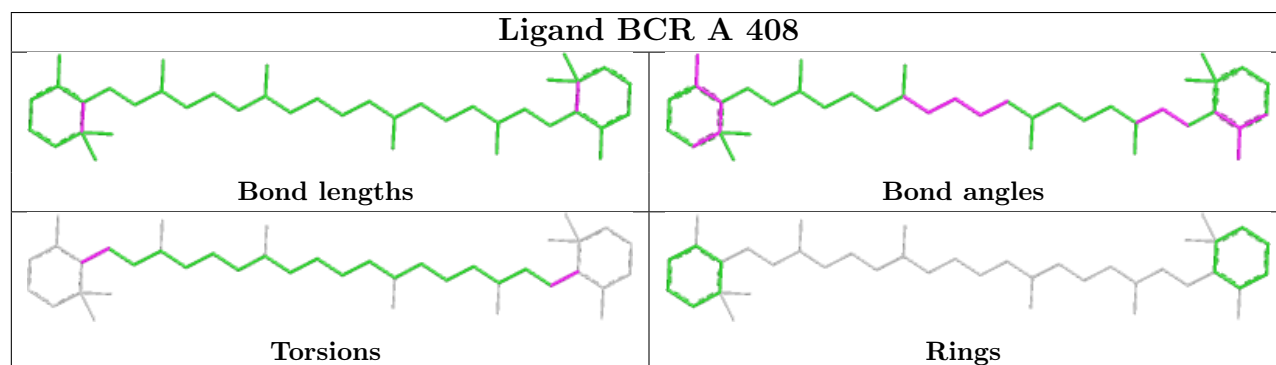
Ligand CLA D 403

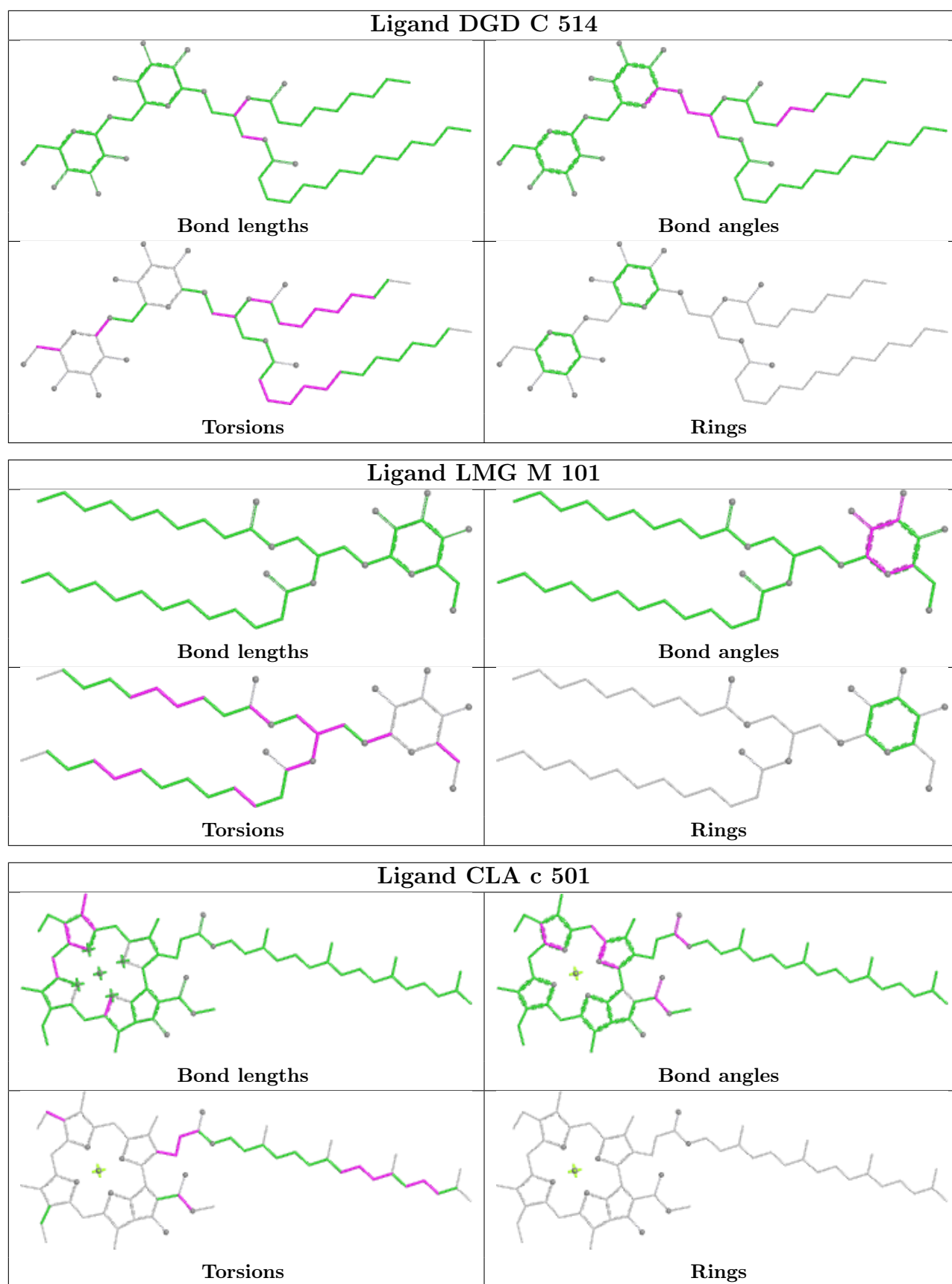


Ligand CLA a 403

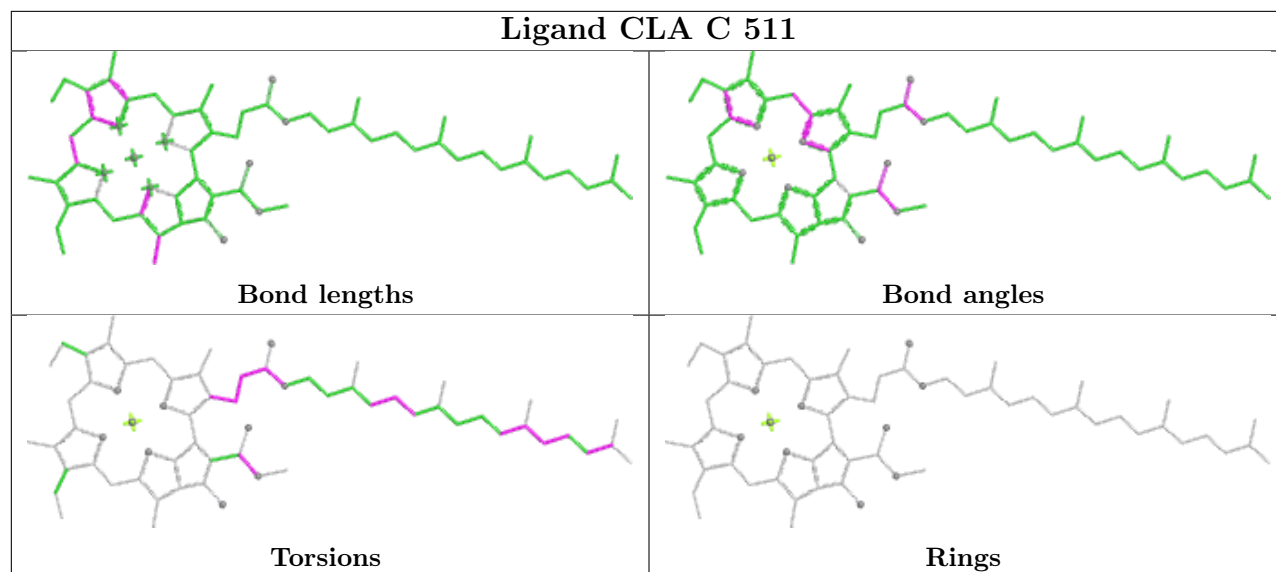


Ligand BCR A 408

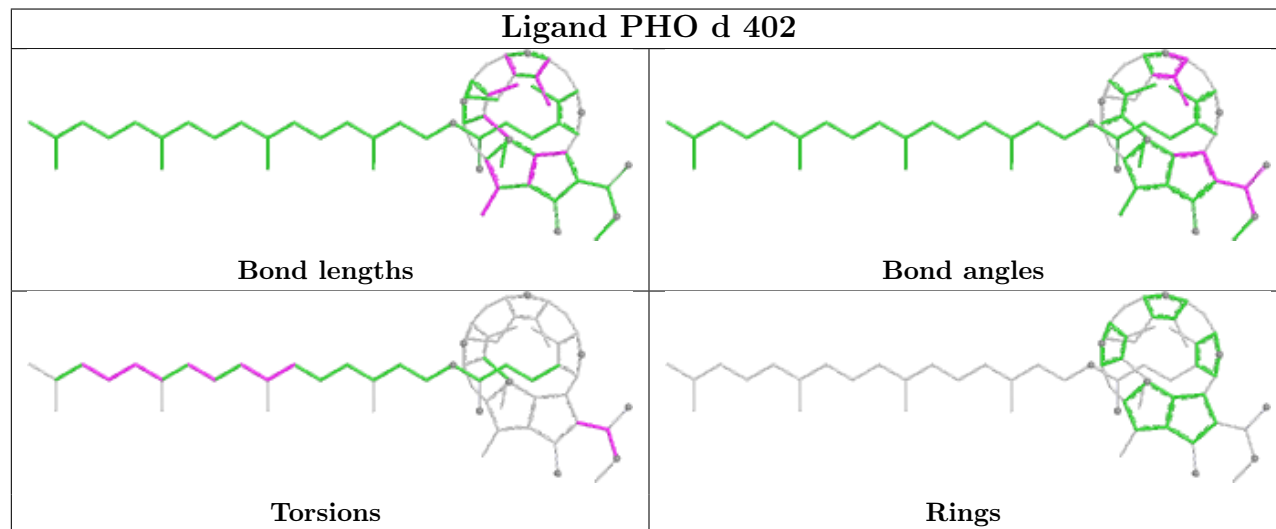




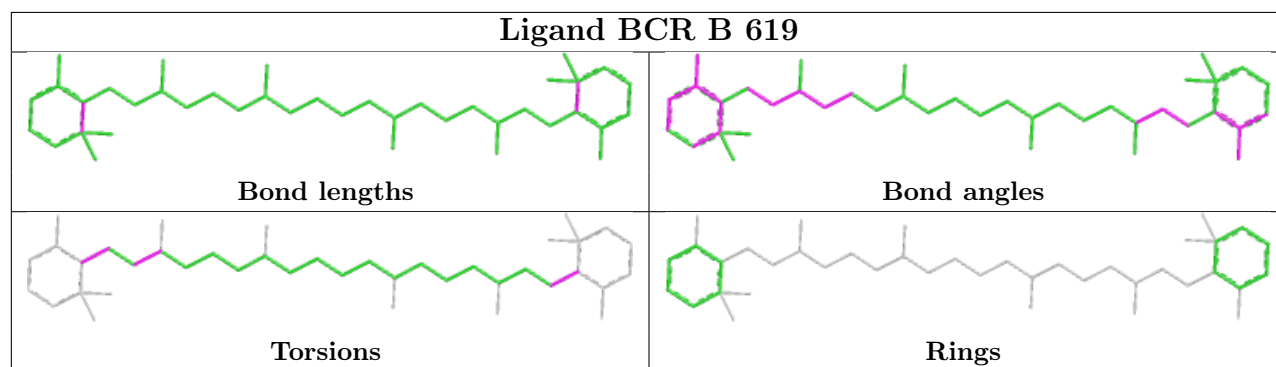
Ligand CLA C 511

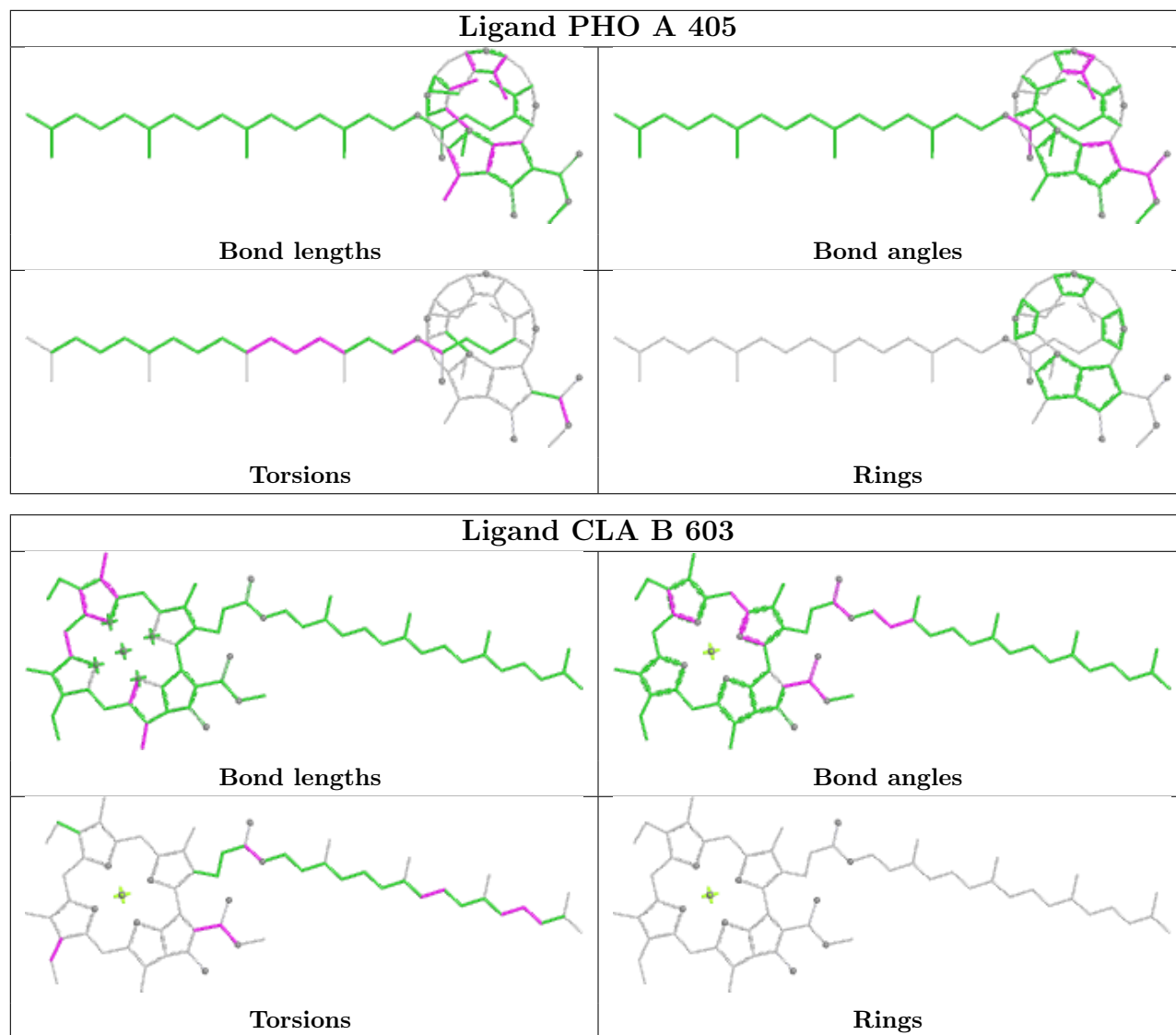


Ligand PHO d 402



Ligand BCR B 619





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	335/344 (97%)	-0.19	3 (0%) 81 67	206, 208, 208, 209	0
1	a	335/344 (97%)	-0.26	3 (0%) 81 67	206, 208, 209, 209	0
2	B	490/510 (96%)	-0.20	8 (1%) 70 57	206, 207, 209, 210	0
2	b	490/510 (96%)	-0.20	9 (1%) 67 55	206, 208, 209, 210	0
3	C	447/461 (96%)	-0.18	8 (1%) 67 55	206, 208, 209, 209	0
3	c	447/461 (96%)	-0.19	6 (1%) 75 61	205, 208, 209, 210	0
4	D	340/352 (96%)	-0.24	2 (0%) 85 73	205, 207, 208, 210	0
4	d	340/352 (96%)	-0.28	6 (1%) 67 55	206, 208, 209, 209	0
5	E	82/84 (97%)	-0.16	3 (3%) 45 40	206, 208, 209, 209	0
5	e	82/84 (97%)	-0.20	0 100 100	207, 208, 209, 209	0
6	F	35/45 (77%)	-0.24	0 100 100	207, 207, 208, 209	0
6	f	35/45 (77%)	-0.35	0 100 100	207, 208, 209, 209	0
7	H	65/66 (98%)	0.29	3 (4%) 37 35	206, 208, 209, 209	0
7	h	65/66 (98%)	0.28	4 (6%) 26 29	206, 208, 209, 209	0
8	I	35/38 (92%)	-0.27	0 100 100	207, 208, 209, 209	0
8	i	35/38 (92%)	-0.33	0 100 100	206, 207, 209, 210	0
9	J	34/40 (85%)	-0.25	0 100 100	207, 208, 208, 209	0
9	j	34/40 (85%)	-0.22	1 (2%) 53 44	206, 208, 209, 209	0
10	K	37/46 (80%)	-0.30	2 (5%) 31 31	207, 208, 209, 209	0
10	k	37/46 (80%)	-0.33	0 100 100	207, 208, 209, 209	0
11	L	37/37 (100%)	-0.32	0 100 100	207, 208, 209, 209	0
11	l	37/37 (100%)	-0.42	0 100 100	206, 208, 209, 210	0
12	M	34/36 (94%)	-0.10	1 (2%) 53 44	206, 207, 208, 209	0
12	m	34/36 (94%)	-0.27	0 100 100	207, 207, 208, 209	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	-0.08	7 (2%) 53 44	205, 208, 209, 210	0
13	o	243/272 (89%)	-0.11	4 (1%) 70 57	206, 208, 209, 210	0
14	T	32/32 (100%)	-0.27	0 100 100	206, 208, 208, 209	0
14	t	32/32 (100%)	-0.18	0 100 100	206, 207, 209, 209	0
15	U	97/134 (72%)	-0.30	2 (2%) 63 51	206, 207, 208, 209	0
15	u	97/134 (72%)	-0.01	0 100 100	206, 207, 208, 209	0
16	V	137/163 (84%)	-0.05	1 (0%) 84 71	206, 207, 208, 209	0
16	v	137/163 (84%)	-0.15	1 (0%) 84 71	206, 208, 209, 209	0
17	g	28/46 (60%)	0.14	0 100 100	207, 208, 209, 209	0
17	y	28/46 (60%)	-0.31	0 100 100	206, 208, 209, 209	0
18	X	37/41 (90%)	0.03	1 (2%) 56 46	206, 208, 209, 210	0
18	x	37/41 (90%)	-0.04	0 100 100	207, 208, 208, 209	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	-0.42	0 100 100	206, 207, 208, 209	0
20	z	62/62 (100%)	-0.22	0 100 100	207, 208, 209, 210	0
All	All	5214/5674 (91%)	-0.18	75 (1%) 73 59	205, 208, 209, 210	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	250	ALA	5.2
2	B	218	LEU	4.9
3	C	324	LEU	4.8
2	B	214	LEU	4.4
2	B	50	PRO	4.2
7	h	27	THR	3.9
13	o	51	THR	3.8
3	c	209	ILE	3.7
7	h	11	LEU	3.6
4	D	158	LEU	3.6
2	b	288	VAL	3.6
4	d	136	VAL	3.6
3	C	213	LEU	3.3
10	K	42	ALA	3.3
13	O	200	LEU	3.3
13	O	201	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	13	GLY	3.2
3	c	210	PHE	3.2
16	V	47	LEU	3.2
2	b	195	PRO	3.1
12	M	6	LEU	3.0
15	U	128	TYR	3.0
2	B	309	LEU	3.0
5	E	84	LYS	2.9
3	C	204	LEU	2.9
1	a	83	VAL	2.9
7	H	27	THR	2.8
3	c	260	ALA	2.8
2	B	84	THR	2.8
4	d	138	VAL	2.7
2	b	168	VAL	2.7
2	b	302	TRP	2.7
13	O	208	LEU	2.7
2	b	482	ILE	2.6
3	C	147	PHE	2.6
3	C	212	TYR	2.6
7	h	14	LEU	2.6
3	C	368	PRO	2.6
4	d	334	GLN	2.6
2	B	47	PRO	2.6
13	o	213	VAL	2.5
10	K	41	ALA	2.5
4	d	299	ILE	2.5
3	C	325	GLY	2.5
13	O	209	ALA	2.5
2	b	119	ASP	2.4
2	b	485	GLU	2.4
13	O	203	ALA	2.3
13	O	138	GLY	2.3
15	U	39	LEU	2.3
7	h	7	LEU	2.3
4	d	137	GLY	2.3
2	b	167	TRP	2.3
4	d	314	PHE	2.3
7	H	10	ILE	2.3
16	v	69	GLY	2.3
1	A	268	SER	2.2
3	C	340	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
7	H	30	LEU	2.2
18	X	13	THR	2.2
3	c	146	PHE	2.2
1	a	82	VAL	2.2
1	A	233	ALA	2.2
5	E	3	GLY	2.2
9	j	14	ALA	2.2
3	c	178	LYS	2.2
13	o	190	LEU	2.2
2	B	80	ILE	2.1
2	b	120	LEU	2.1
1	A	320	ILE	2.1
3	c	296	VAL	2.1
2	B	370	LEU	2.0
5	E	17	VAL	2.0
13	o	203	ALA	2.0
13	O	145	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMT	I	102	35/35	0.49	0.17	206,208,210,210	0
32	LMT	d	411	31/35	0.51	0.16	206,209,210,211	0
22	CLA	b	620	65/65	0.61	0.16	206,208,209,210	0
32	LMT	D	408	31/35	0.61	0.14	207,208,210,210	0
22	CLA	B	601	65/65	0.65	0.17	205,208,209,209	0
35	CA	O	301	1/1	0.65	0.11	208,208,208,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	605	65/65	0.66	0.21	206,208,210,210	0
32	LMT	b	629	35/35	0.67	0.14	206,208,209,210	0
32	LMT	b	628	35/35	0.68	0.13	206,208,210,210	0
32	LMT	B	628	35/35	0.68	0.13	206,208,210,211	0
32	LMT	i	103	35/35	0.69	0.15	206,209,210,210	0
32	LMT	M	102	35/35	0.71	0.19	205,208,209,209	0
31	LMG	I	101	43/55	0.72	0.20	205,208,210,211	0
25	BCR	H	102	40/40	0.73	0.22	206,207,209,210	0
32	LMT	b	603	35/35	0.74	0.13	206,208,210,210	0
30	SQD	B	627	47/54	0.77	0.14	206,208,210,212	0
26	DGD	B	626	52/66	0.77	0.18	206,208,210,211	0
31	LMG	C	517	45/55	0.78	0.17	206,207,209,210	0
27	LHG	c	519	37/49	0.78	0.17	204,207,210,213	0
25	BCR	j	102	40/40	0.79	0.25	206,208,209,210	0
31	LMG	b	627	42/55	0.79	0.21	204,207,211,211	0
26	DGD	d	410	63/66	0.80	0.18	206,208,210,211	0
26	DGD	C	516	66/66	0.80	0.20	205,207,208,208	0
26	DGD	b	601	52/66	0.81	0.17	204,208,209,210	0
35	CA	K	102	1/1	0.81	0.12	210,210,210,210	0
31	LMG	e	101	44/55	0.81	0.22	205,208,209,211	0
32	LMT	b	604	35/35	0.82	0.13	207,208,210,210	0
27	LHG	C	518	37/49	0.83	0.12	205,208,210,211	0
22	CLA	C	512	65/65	0.83	0.15	205,207,209,211	0
32	LMT	B	623	35/35	0.83	0.10	206,208,210,210	0
26	DGD	a	408	56/66	0.83	0.18	206,208,210,211	0
32	LMT	B	629	35/35	0.83	0.14	206,208,209,210	0
26	DGD	A	409	56/66	0.83	0.20	206,208,210,211	0
22	CLA	C	506	65/65	0.83	0.16	206,207,208,209	0
31	LMG	b	626	49/55	0.83	0.18	205,207,209,209	0
32	LMT	B	624	35/35	0.84	0.14	206,207,211,212	0
31	LMG	i	102	43/55	0.84	0.16	205,207,209,210	0
26	DGD	D	407	63/66	0.85	0.17	206,208,209,210	0
25	BCR	b	624	40/40	0.85	0.14	205,206,207,208	0
25	BCR	c	521	40/40	0.85	0.20	206,208,209,209	0
31	LMG	B	621	49/55	0.85	0.16	206,207,208,209	0
24	PL9	A	407	45/55	0.85	0.23	206,207,208,210	0
31	LMG	m	101	42/55	0.85	0.20	205,207,209,210	0
31	LMG	E	101	44/55	0.85	0.16	204,208,209,210	0
25	BCR	g	101	40/40	0.86	0.16	205,207,208,209	0
22	CLA	c	512	65/65	0.86	0.15	206,207,209,210	0
24	PL9	d	407	55/55	0.86	0.15	205,207,208,208	0
31	LMG	a	402	42/55	0.86	0.18	204,207,209,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	J	102	40/40	0.87	0.23	205,207,209,209	0
27	LHG	a	409	39/49	0.87	0.16	206,207,209,209	0
22	CLA	C	508	65/65	0.87	0.14	205,207,208,209	0
30	SQD	A	413	51/54	0.87	0.16	204,207,209,209	0
26	DGD	b	625	58/66	0.87	0.17	206,207,208,209	0
24	PL9	J	101	35/55	0.87	0.21	206,207,210,210	0
35	CA	k	101	1/1	0.87	0.05	208,208,208,208	0
22	CLA	b	607	65/65	0.88	0.13	205,207,208,208	0
30	SQD	b	602	47/54	0.88	0.14	205,208,209,212	0
26	DGD	C	515	62/66	0.88	0.12	205,207,209,210	0
22	CLA	a	405	65/65	0.88	0.18	205,207,209,209	0
33	BCT	d	404	4/4	0.88	0.17	206,207,208,208	0
25	BCR	b	621	40/40	0.88	0.22	206,207,208,208	0
25	BCR	C	513	40/40	0.88	0.18	205,207,208,208	0
26	DGD	B	620	58/66	0.88	0.16	205,207,209,209	0
35	CA	o	301	1/1	0.88	0.08	209,209,209,209	0
30	SQD	d	403	43/54	0.89	0.13	205,208,209,209	0
25	BCR	B	616	40/40	0.89	0.15	205,207,208,209	0
25	BCR	i	101	40/40	0.89	0.22	206,207,208,208	0
22	CLA	a	406	65/65	0.89	0.14	206,208,208,209	0
26	DGD	c	516	62/66	0.89	0.13	206,208,208,209	0
31	LMG	M	101	42/55	0.89	0.14	205,208,209,210	0
25	BCR	C	520	40/40	0.89	0.19	206,207,209,210	0
23	PHO	A	405	64/64	0.89	0.12	205,207,208,209	0
22	CLA	b	619	65/65	0.89	0.12	206,208,209,209	0
22	CLA	C	511	65/65	0.89	0.14	206,207,208,209	0
25	BCR	b	622	40/40	0.89	0.15	205,207,208,208	0
30	SQD	A	414	54/54	0.89	0.15	205,207,209,210	0
30	SQD	B	622	43/54	0.89	0.17	205,208,209,212	0
22	CLA	c	510	65/65	0.89	0.10	206,208,209,211	0
25	BCR	c	514	40/40	0.89	0.18	206,208,208,209	0
24	PL9	j	101	35/55	0.90	0.20	205,208,209,210	0
22	CLA	B	615	65/65	0.90	0.12	206,207,209,209	0
31	LMG	c	518	45/55	0.90	0.13	206,208,209,210	0
31	LMG	C	521	48/55	0.90	0.16	206,207,208,209	0
27	LHG	A	410	39/49	0.90	0.16	206,207,209,210	0
22	CLA	A	406	65/65	0.90	0.13	206,208,209,209	0
23	PHO	d	401	64/64	0.90	0.11	206,207,208,208	0
25	BCR	b	623	40/40	0.90	0.17	205,206,207,207	0
32	LMT	M	103	35/35	0.91	0.11	206,208,209,209	0
31	LMG	c	522	48/55	0.91	0.17	205,207,209,210	0
24	PL9	a	407	45/55	0.91	0.18	205,207,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CLA	b	606	65/65	0.91	0.17	205,207,209,210	0
31	LMG	D	406	48/55	0.91	0.14	204,207,208,209	0
22	CLA	D	404	65/65	0.91	0.14	205,207,208,208	0
30	SQD	F	103	45/54	0.91	0.16	205,208,209,210	0
30	SQD	a	401	54/54	0.91	0.14	205,208,210,213	0
30	SQD	a	412	51/54	0.91	0.16	205,207,208,209	0
22	CLA	c	508	65/65	0.91	0.11	205,208,209,209	0
25	BCR	y	101	40/40	0.91	0.17	206,207,208,208	0
25	BCR	B	619	40/40	0.91	0.13	205,207,208,208	0
25	BCR	F	102	40/40	0.92	0.17	205,207,208,208	0
25	BCR	x	101	40/40	0.92	0.14	206,207,209,209	0
22	CLA	C	505	65/65	0.92	0.14	206,207,209,210	0
22	CLA	C	519	65/65	0.92	0.13	205,207,209,209	0
22	CLA	c	502	65/65	0.92	0.13	206,207,208,209	0
22	CLA	c	503	65/65	0.92	0.10	206,207,208,209	0
22	CLA	c	505	65/65	0.92	0.15	205,207,208,209	0
22	CLA	C	509	65/65	0.92	0.11	205,207,208,208	0
25	BCR	A	408	40/40	0.92	0.16	206,207,208,208	0
22	CLA	A	404	65/65	0.92	0.15	204,207,208,209	0
22	CLA	c	511	65/65	0.92	0.13	206,208,209,209	0
31	LMG	d	408	49/55	0.92	0.13	205,207,208,209	0
22	CLA	b	610	65/65	0.92	0.11	206,207,209,209	0
26	DGD	c	517	66/66	0.92	0.12	206,207,209,209	0
30	SQD	f	103	45/54	0.92	0.14	205,208,210,210	0
22	CLA	b	614	65/65	0.92	0.12	206,207,209,210	0
31	LMG	B	625	49/55	0.92	0.14	205,207,208,208	0
22	CLA	b	611	65/65	0.93	0.12	206,207,208,209	0
22	CLA	a	404	65/65	0.93	0.14	204,207,208,208	0
31	LMG	d	409	48/55	0.93	0.12	206,207,209,210	0
22	CLA	C	510	65/65	0.93	0.09	206,207,209,209	0
26	DGD	c	515	53/66	0.93	0.14	205,207,209,210	0
31	LMG	l	101	51/55	0.93	0.12	206,207,209,209	0
22	CLA	B	609	65/65	0.93	0.10	206,207,209,210	0
22	CLA	B	613	65/65	0.93	0.11	206,207,208,209	0
22	CLA	B	607	65/65	0.93	0.10	206,207,208,209	0
26	DGD	C	514	53/66	0.93	0.14	205,206,208,209	0
24	PL9	D	405	55/55	0.93	0.12	205,207,208,208	0
22	CLA	D	403	65/65	0.93	0.10	205,207,208,208	0
22	CLA	C	501	65/65	0.93	0.12	206,208,209,209	0
28	CL	a	410	1/1	0.94	0.21	205,205,205,205	0
22	CLA	C	507	65/65	0.94	0.14	206,207,208,208	0
31	LMG	L	101	51/55	0.94	0.13	205,207,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	c	506	65/65	0.94	0.10	206,208,209,209	0
22	CLA	B	610	65/65	0.94	0.10	205,207,208,208	0
22	CLA	b	616	65/65	0.94	0.08	206,207,208,209	0
25	BCR	c	513	40/40	0.94	0.11	206,207,208,209	0
22	CLA	b	618	65/65	0.94	0.13	206,207,209,210	0
21	FE2	A	401	1/1	0.94	0.11	209,209,209,209	0
25	BCR	f	102	40/40	0.94	0.14	206,207,208,209	0
22	CLA	d	405	65/65	0.94	0.15	205,207,208,208	0
22	CLA	b	608	65/65	0.94	0.10	205,207,208,209	0
23	PHO	D	401	64/64	0.94	0.09	205,207,208,209	0
22	CLA	c	501	65/65	0.94	0.09	206,207,209,209	0
23	PHO	d	402	64/64	0.94	0.09	206,207,209,209	0
22	CLA	b	609	65/65	0.94	0.09	206,207,208,209	0
22	CLA	B	605	65/65	0.94	0.10	206,207,208,209	0
22	CLA	C	502	65/65	0.95	0.14	206,207,208,208	0
22	CLA	c	520	65/65	0.95	0.12	206,207,208,209	0
22	CLA	b	612	65/65	0.95	0.10	205,207,209,209	0
22	CLA	d	406	65/65	0.95	0.11	206,207,209,209	0
22	CLA	b	613	65/65	0.95	0.10	205,207,208,209	0
25	BCR	B	617	40/40	0.95	0.11	205,207,208,209	0
31	LMG	d	412	46/55	0.95	0.12	205,207,208,209	0
22	CLA	H	101	65/65	0.95	0.15	206,207,208,209	0
22	CLA	a	403	65/65	0.95	0.09	205,207,208,210	0
31	LMG	D	409	46/55	0.95	0.12	205,207,208,209	0
33	BCT	D	402	4/4	0.95	0.06	208,208,208,208	0
22	CLA	C	503	65/65	0.95	0.12	206,207,208,209	0
22	CLA	c	509	65/65	0.95	0.08	206,207,209,209	0
22	CLA	B	608	65/65	0.95	0.10	205,207,209,210	0
22	CLA	B	614	65/65	0.95	0.10	205,207,208,209	0
25	BCR	K	101	40/40	0.95	0.10	206,207,208,209	0
22	CLA	B	612	65/65	0.96	0.12	203,207,208,209	0
22	CLA	A	403	65/65	0.96	0.10	205,207,208,208	0
22	CLA	B	606	65/65	0.96	0.12	205,207,208,209	0
22	CLA	A	402	65/65	0.96	0.11	206,207,208,209	0
22	CLA	B	602	65/65	0.96	0.10	205,207,208,209	0
22	CLA	c	504	65/65	0.96	0.11	205,207,208,209	0
22	CLA	B	603	65/65	0.96	0.09	205,207,208,208	0
22	CLA	B	604	65/65	0.96	0.09	206,207,208,209	0
25	BCR	B	618	40/40	0.96	0.13	205,206,208,208	0
34	HEM	V	201	43/43	0.96	0.14	201,207,208,209	0
34	HEM	f	101	43/43	0.96	0.09	206,207,209,209	0
34	HEM	v	201	43/43	0.96	0.10	206,207,208,209	0

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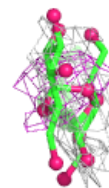
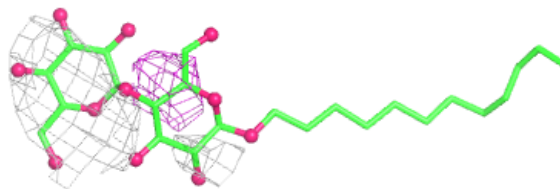
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	c	507	65/65	0.96	0.10	206,207,209,209	0
22	CLA	C	504	65/65	0.96	0.11	205,207,208,209	0
28	CL	A	411	1/1	0.96	0.06	204,204,204,204	0
22	CLA	B	611	65/65	0.96	0.10	205,207,208,208	0
34	HEM	F	101	43/43	0.97	0.08	206,207,208,210	0
22	CLA	b	615	65/65	0.97	0.09	205,207,208,209	0
21	FE2	a	413	1/1	0.97	0.05	206,206,206,206	0
22	CLA	b	617	65/65	0.97	0.10	206,207,208,209	0
29	OEX	a	411	10/10	0.98	0.07	200,204,205,206	0
29	OEX	A	412	10/10	0.99	0.07	197,202,205,206	0

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

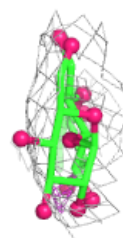
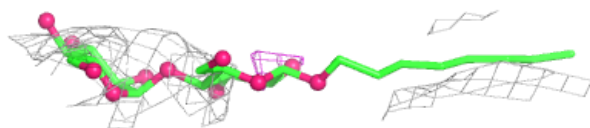
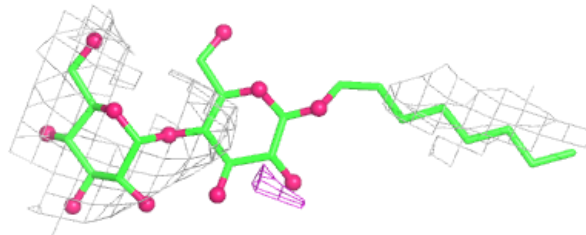
Electron density around LMT I 102:

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



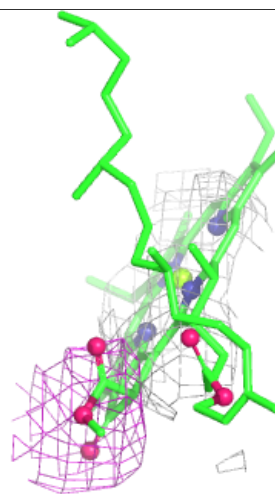
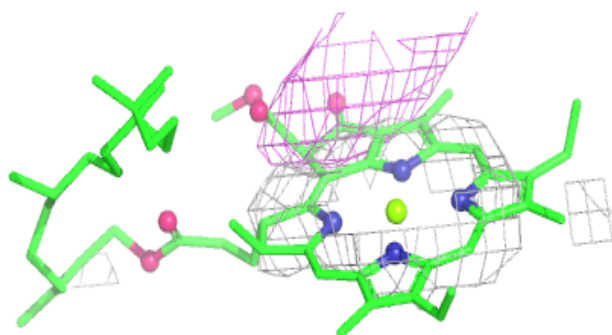
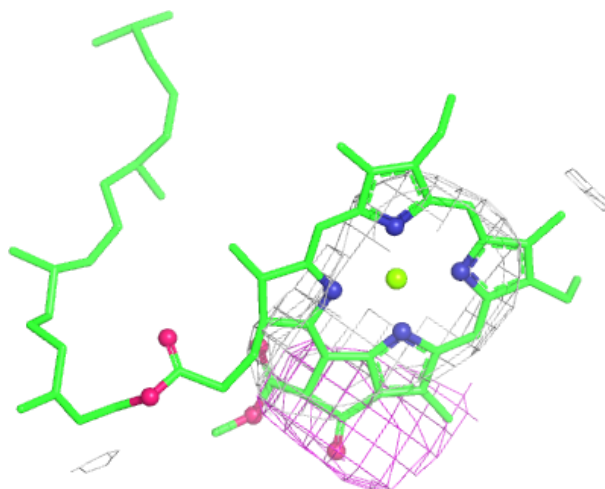
Electron density around LMT d 411:

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



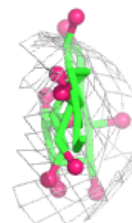
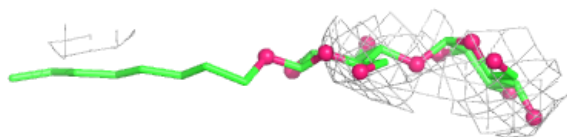
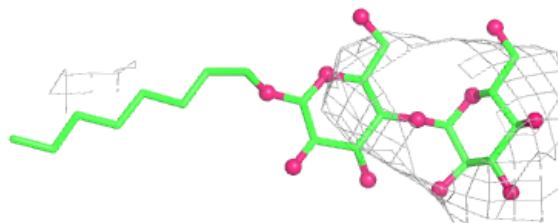
Electron density around CLA b 620:

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



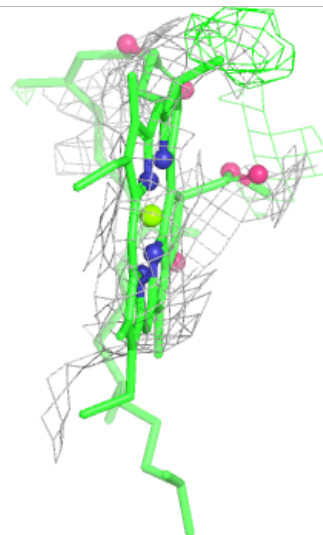
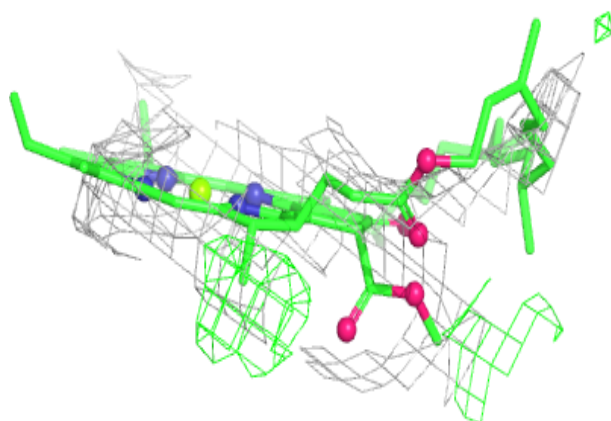
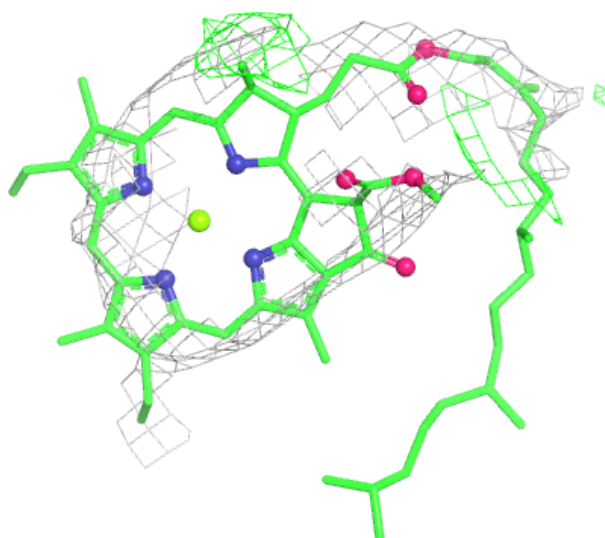
Electron density around LMT D 408:

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



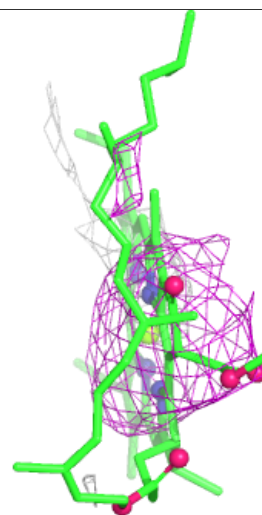
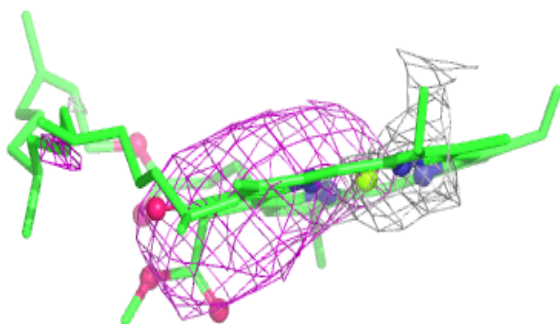
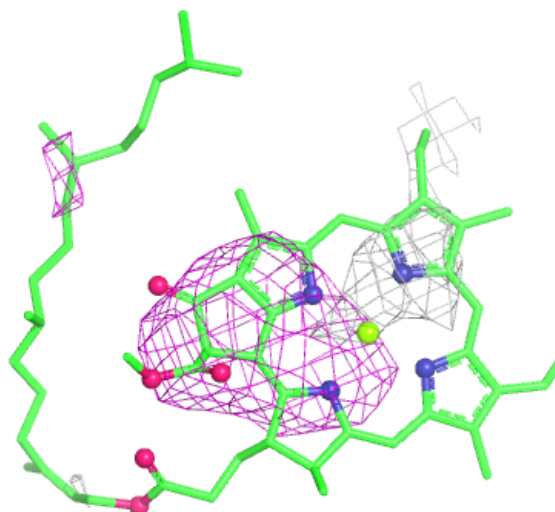
Electron density around CLA B 601:

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



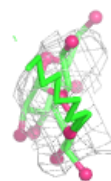
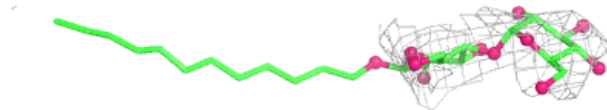
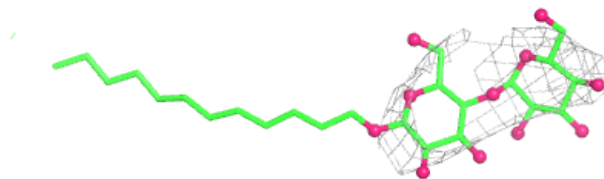
Electron density around CLA b 605:

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

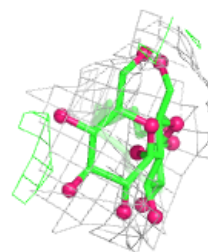
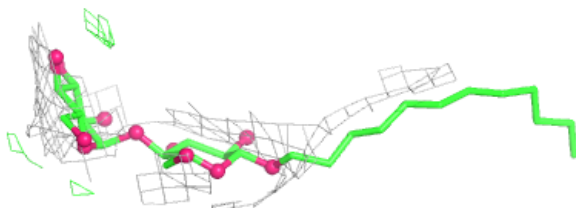
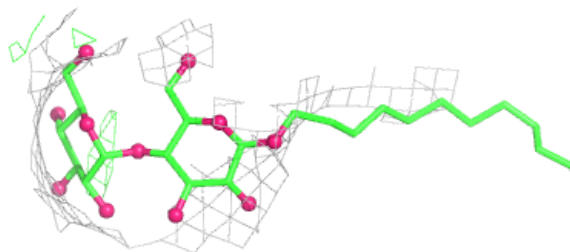


Electron density around LMT b 629:

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

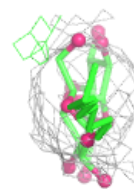
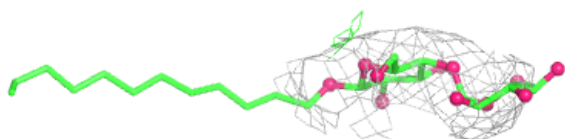
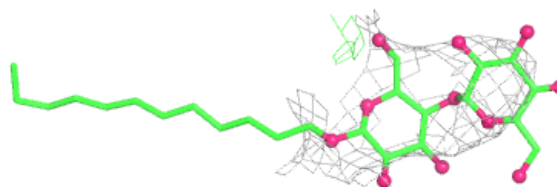
**Electron density around LMT b 628:**

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

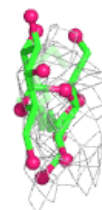
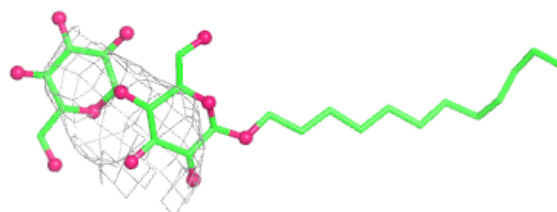


Electron density around LMT B 628:

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

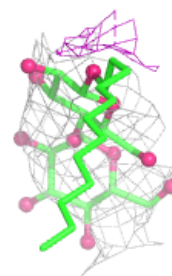
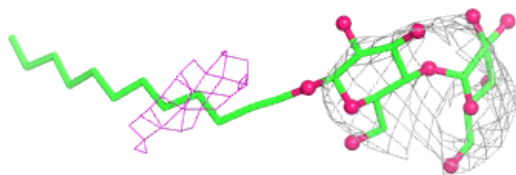
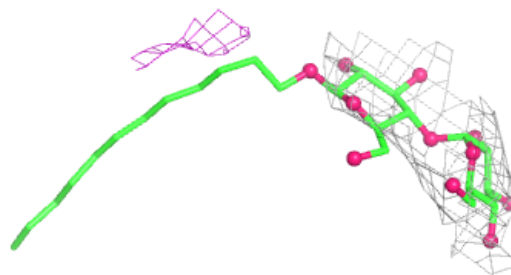
**Electron density around LMT i 103:**

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

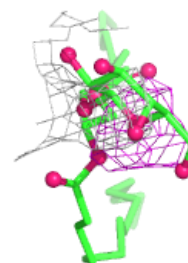
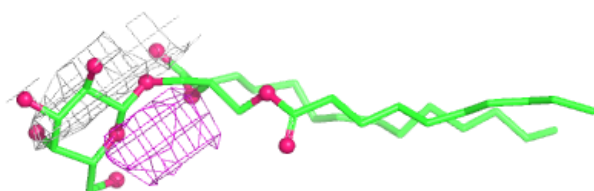
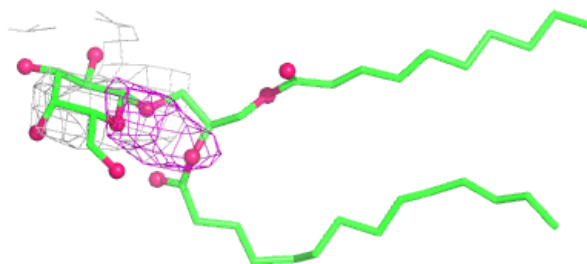


Electron density around LMT M 102:

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

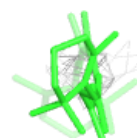
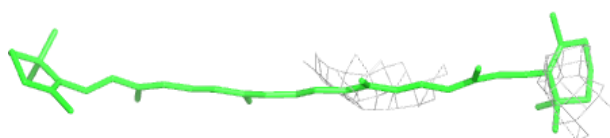
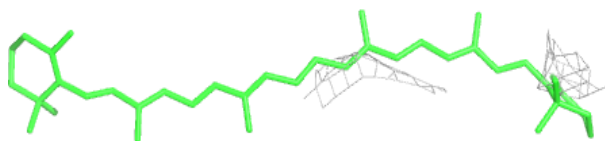
**Electron density around LMG I 101:**

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

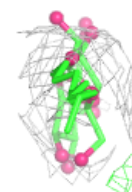
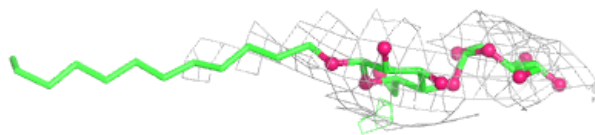
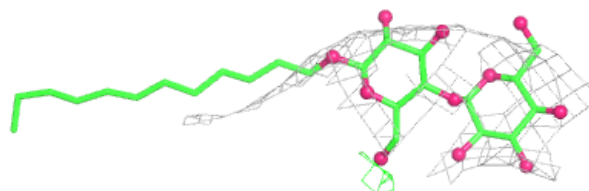


Electron density around BCR H 102:

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

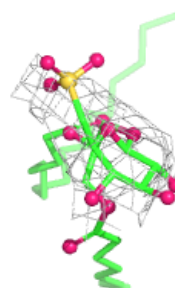
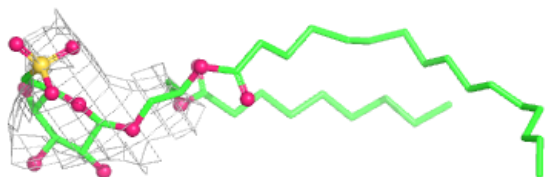
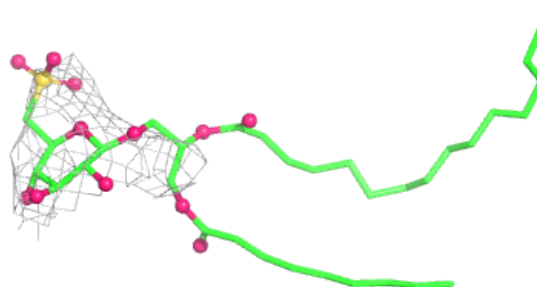
**Electron density around LMT b 603:**

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

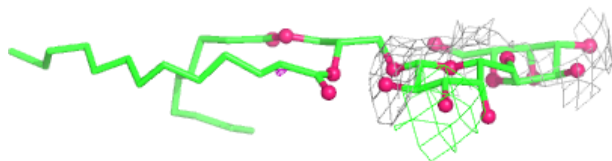
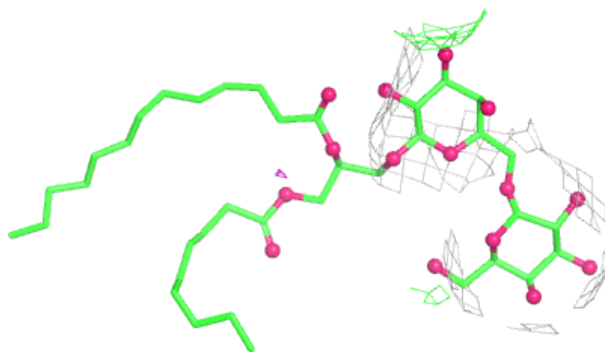


Electron density around SQD B 627:

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

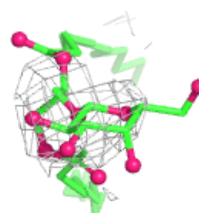
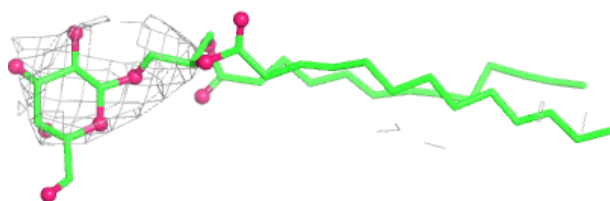
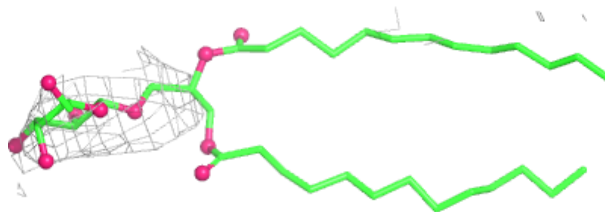
**Electron density around DGD B 626:**

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

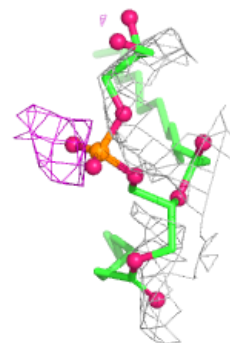
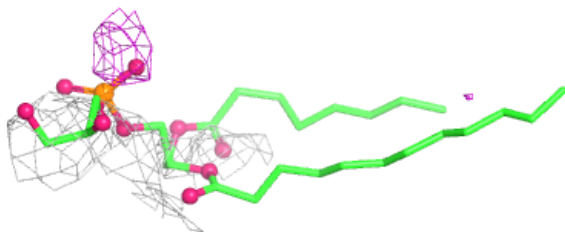
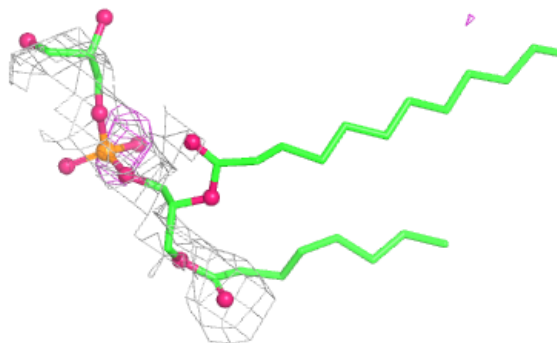


Electron density around LMG C 517:

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

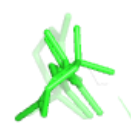
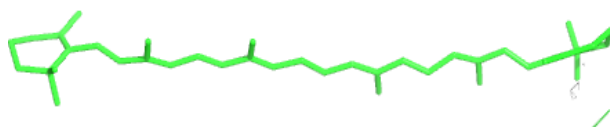
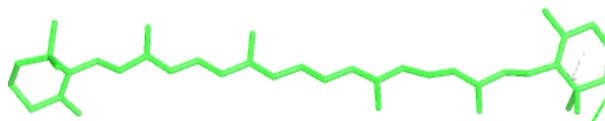
**Electron density around LHG c 519:**

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

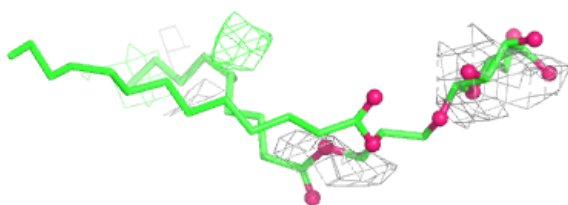
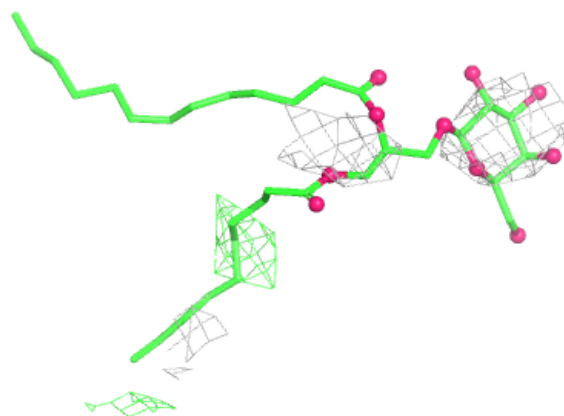


Electron density around BCR j 102:

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

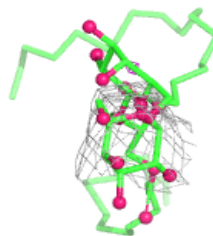
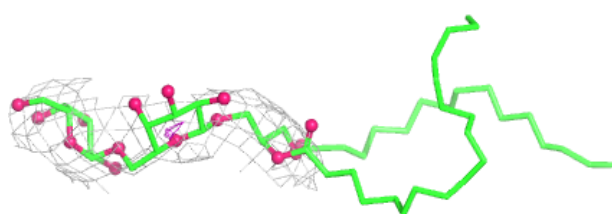
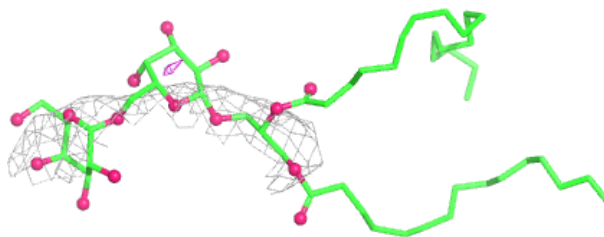
**Electron density around LMG b 627:**

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

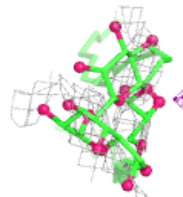
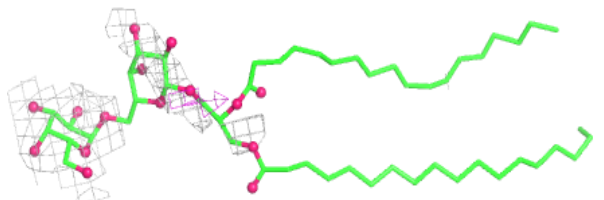


Electron density around DGD d 410:

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

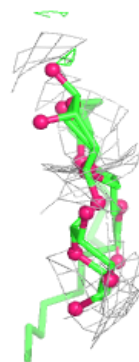
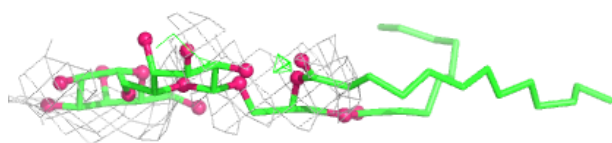
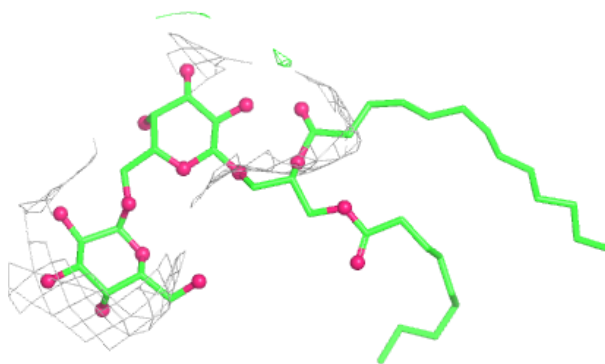
**Electron density around DGD C 516:**

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

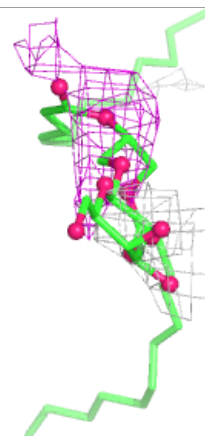
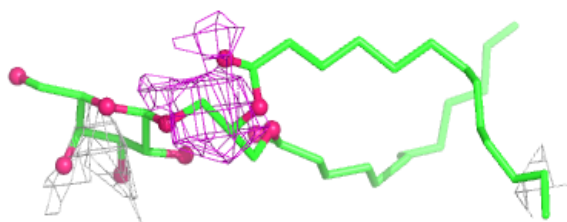
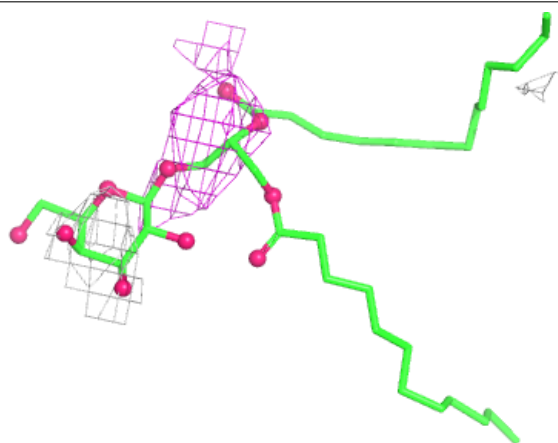


Electron density around DGD b 601:

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

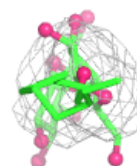
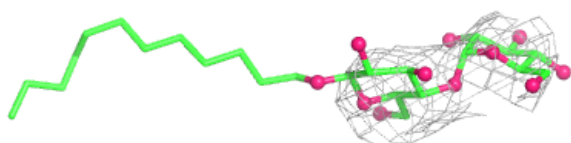
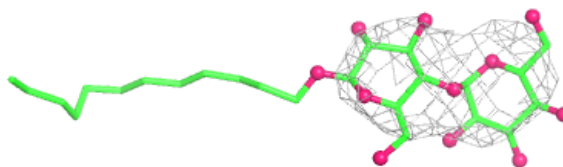
**Electron density around LMG e 101:**

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

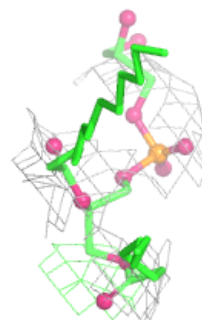
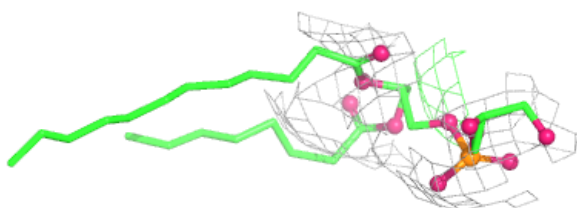


Electron density around LMT b 604:

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

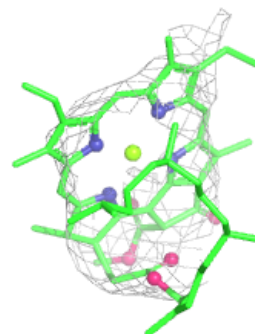
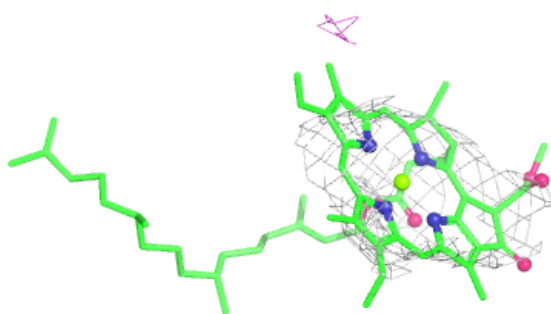
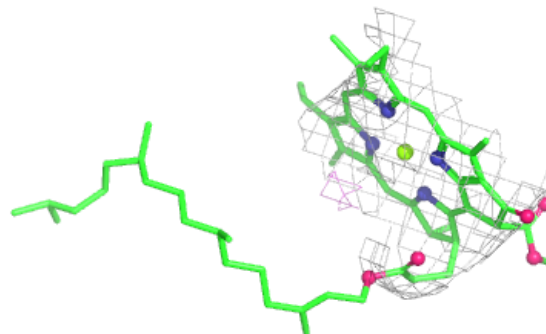
**Electron density around LHG C 518:**

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

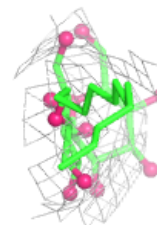
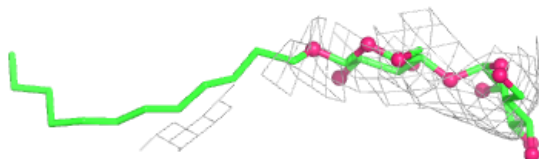
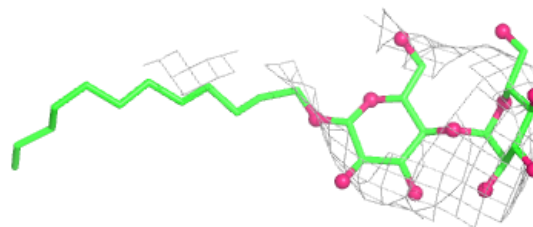


Electron density around CLA C 512:

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

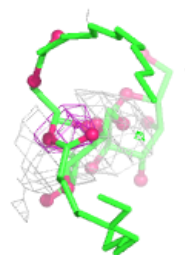
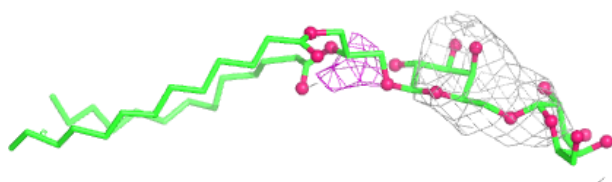
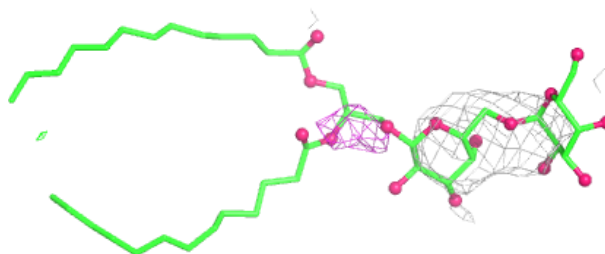
**Electron density around LMT B 623:**

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

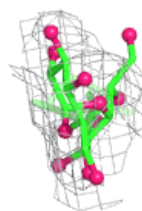
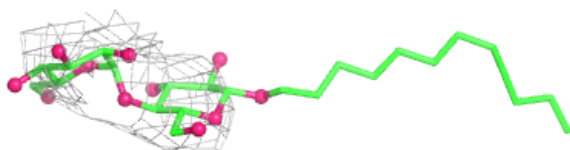
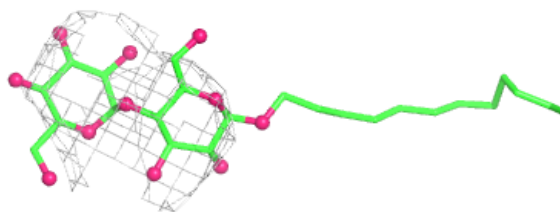


Electron density around DGD a 408:

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

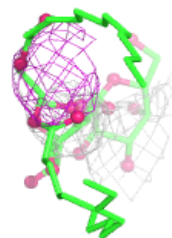
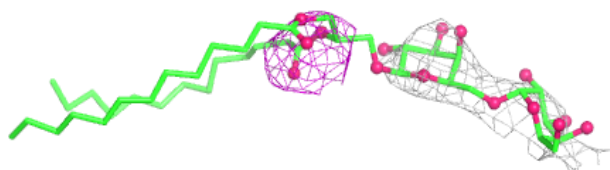
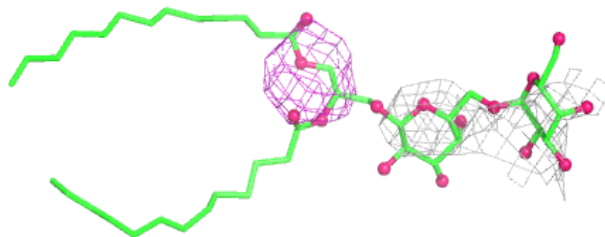
**Electron density around LMT B 629:**

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

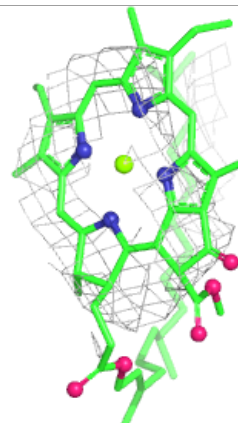
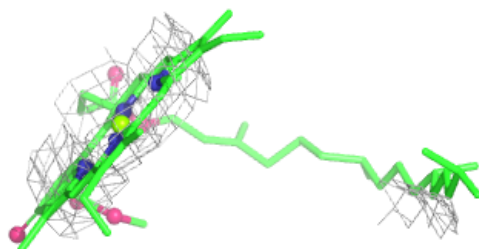
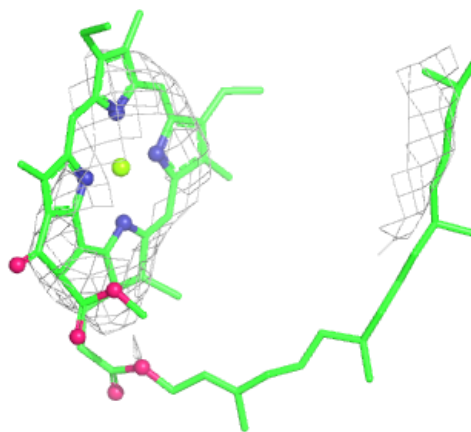


Electron density around DGD A 409:

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

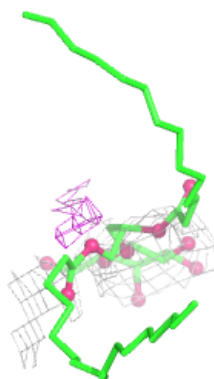
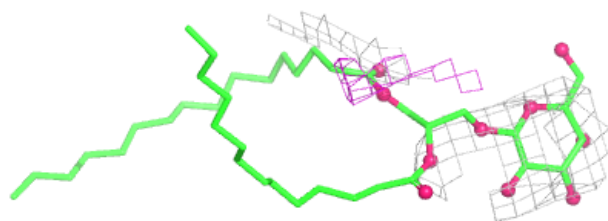
**Electron density around CLA C 506:**

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

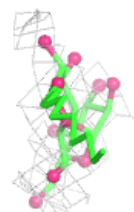
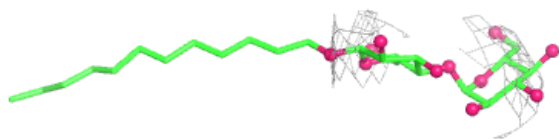
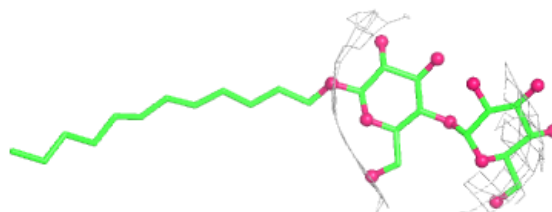


Electron density around LMG b 626:

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

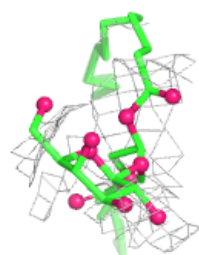
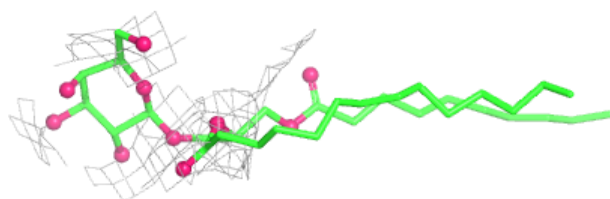
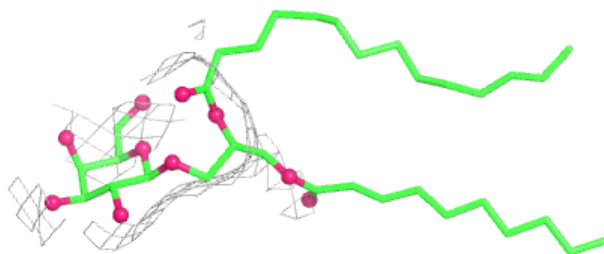
**Electron density around LMT B 624:**

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

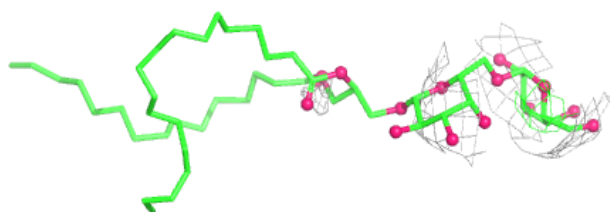
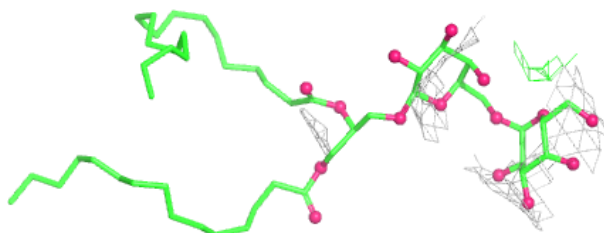


Electron density around LMG i 102:

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

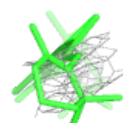
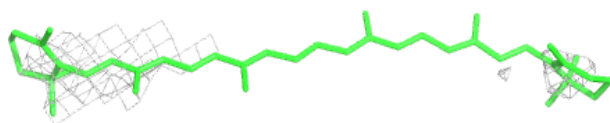
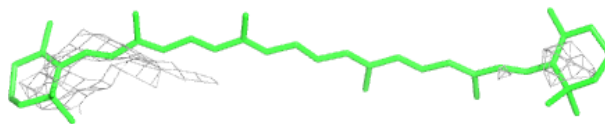
**Electron density around DGD D 407:**

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

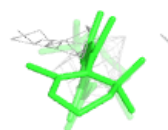
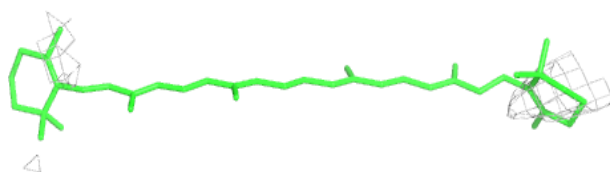
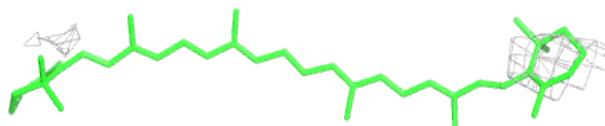


Electron density around BCR b 624:

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

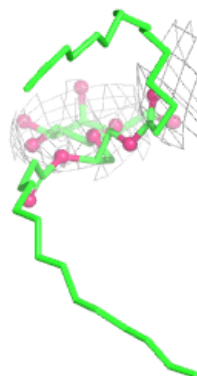
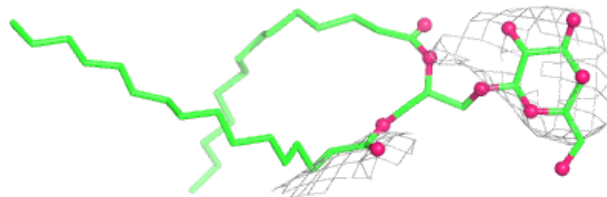
**Electron density around BCR c 521:**

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

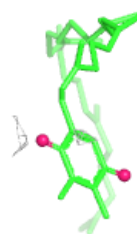
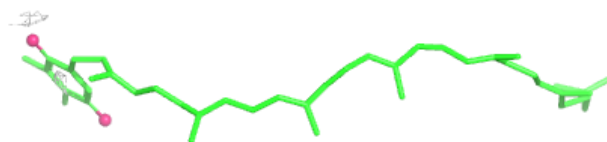
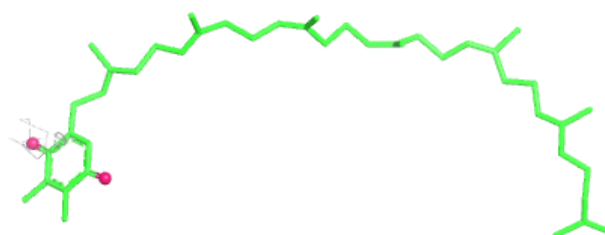


Electron density around LMG B 621:

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

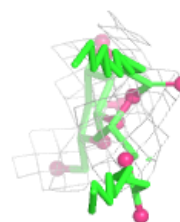
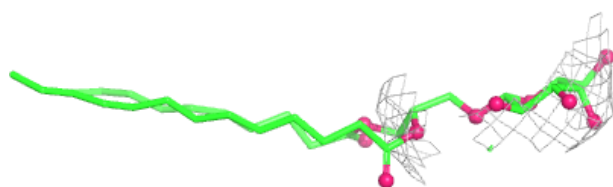
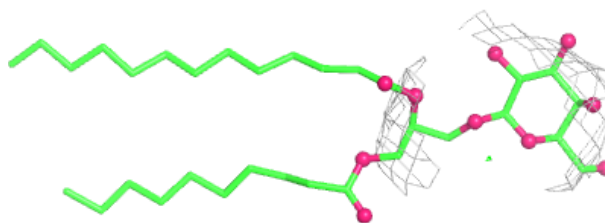
**Electron density around PL9 A 407:**

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

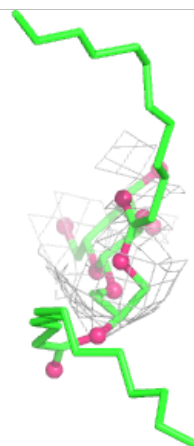
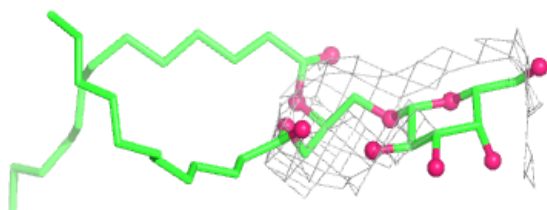
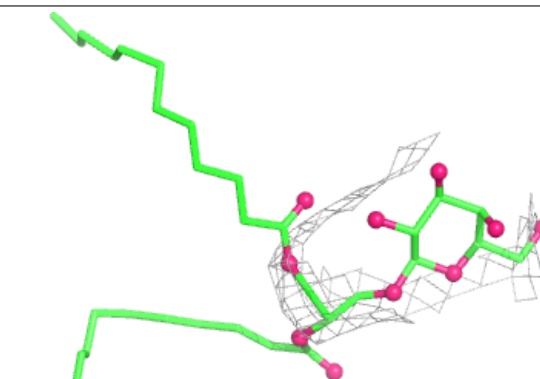


Electron density around LMG m 101:

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

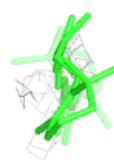
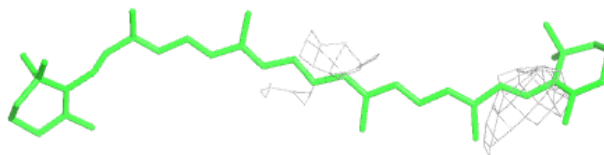
**Electron density around LMG E 101:**

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

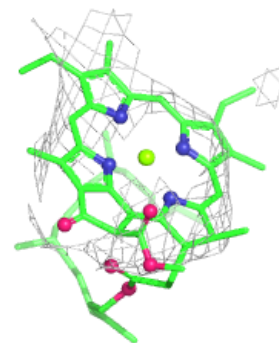
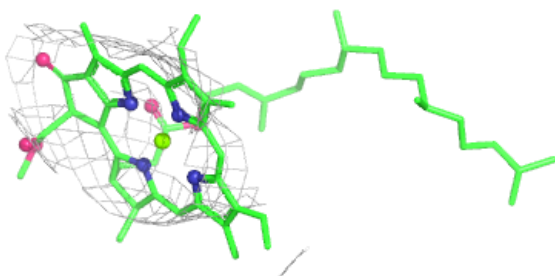
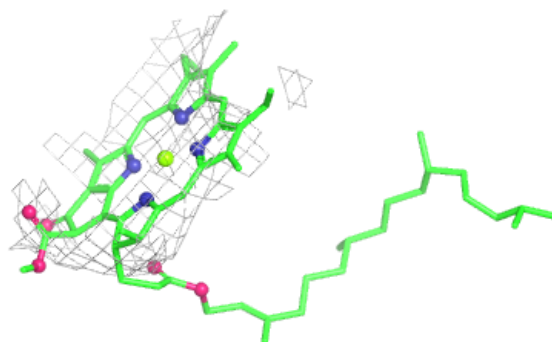


Electron density around BCR g 101:

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

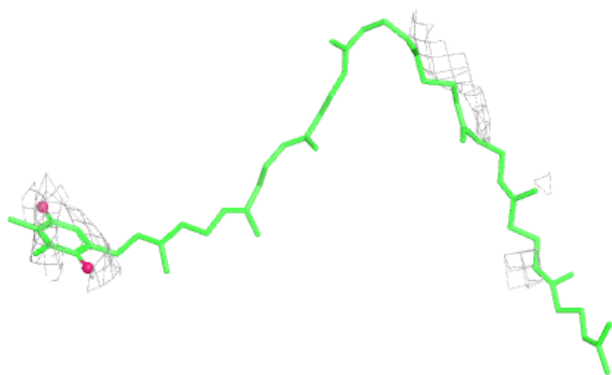
**Electron density around CLA c 512:**

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

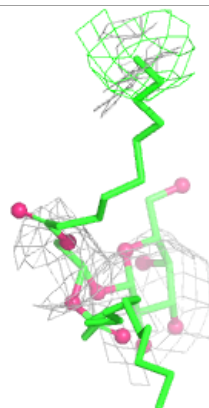
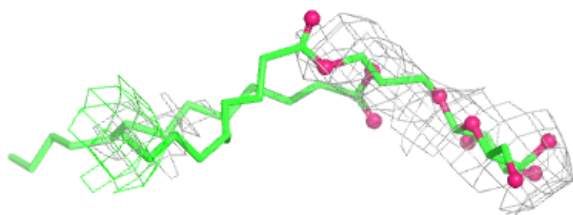
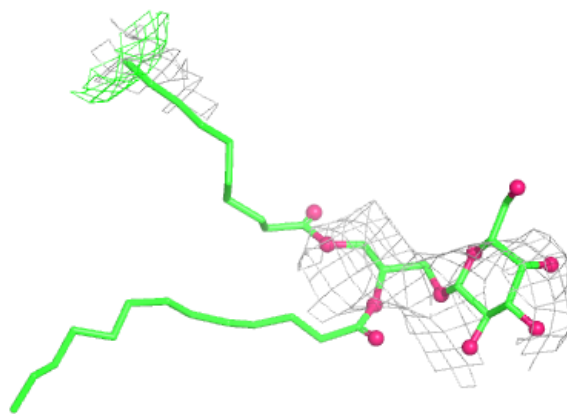


Electron density around PL9 d 407:

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

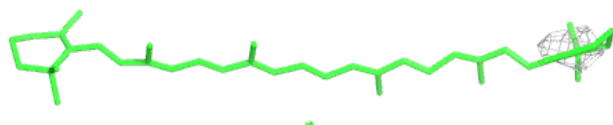
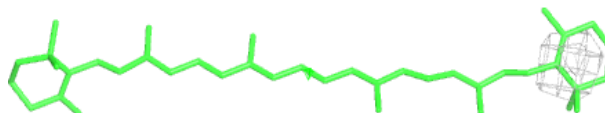
**Electron density around LMG a 402:**

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

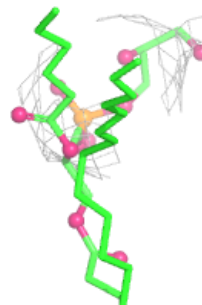
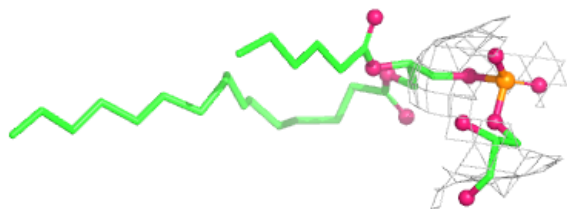
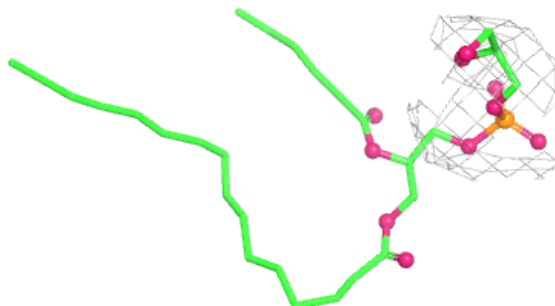


Electron density around BCR J 102:

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

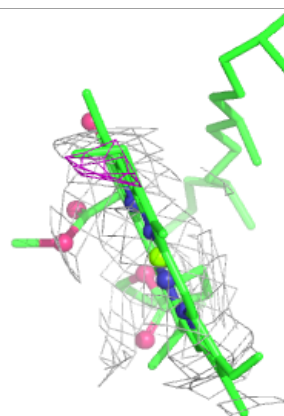
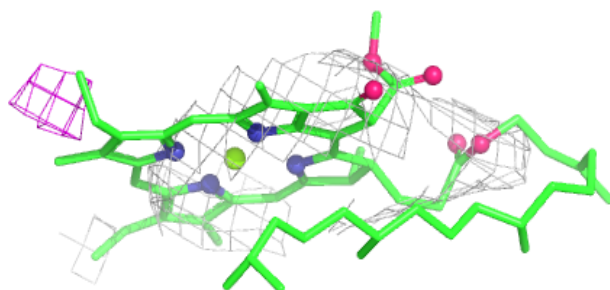
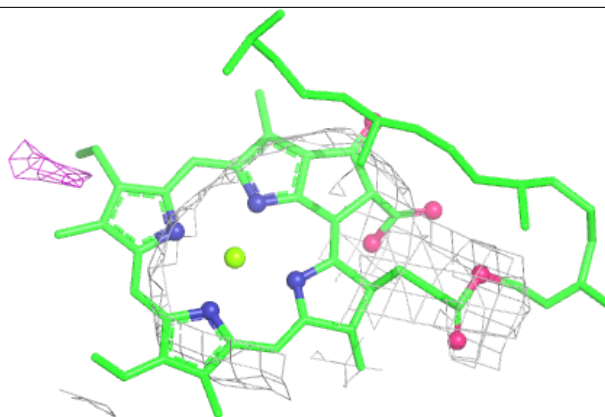
**Electron density around LHG a 409:**

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

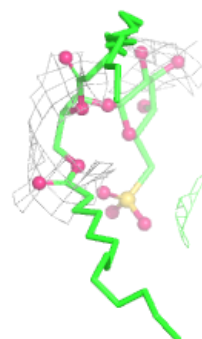
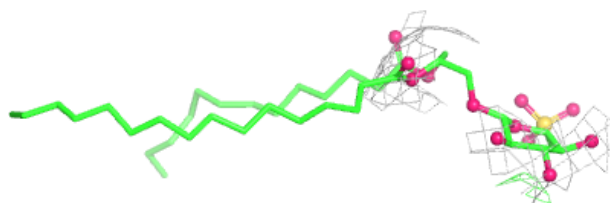
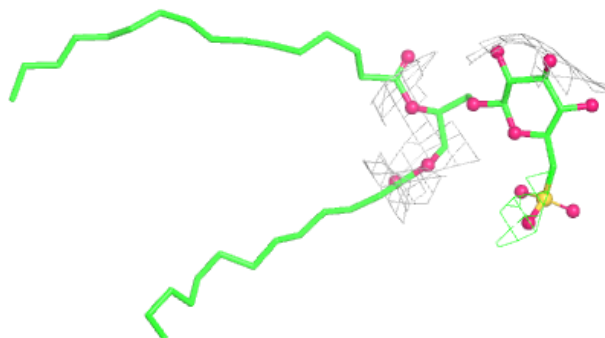


Electron density around CLA C 508:

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

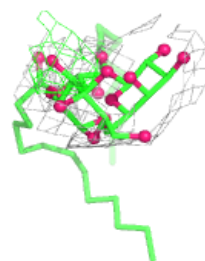
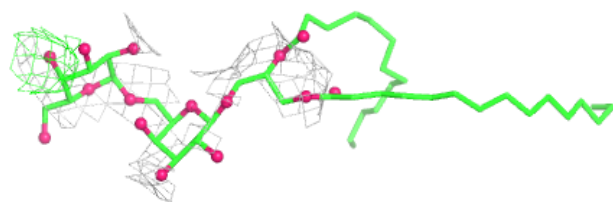
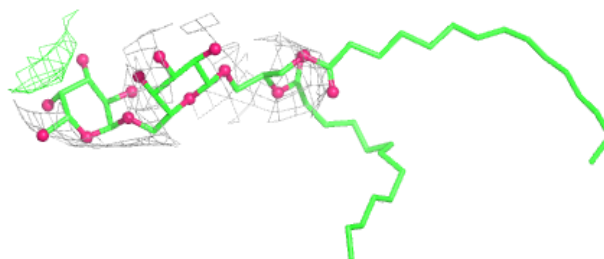
**Electron density around SQD A 413:**

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

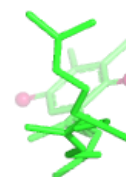
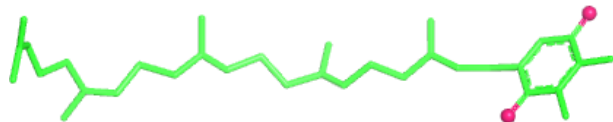
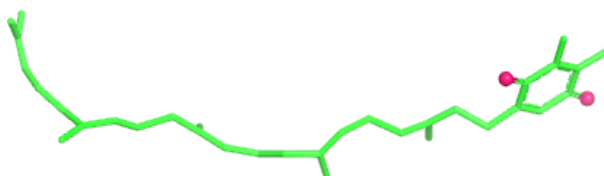


Electron density around DGD b 625:

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

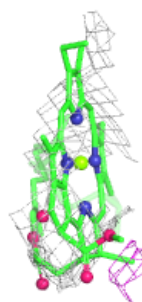
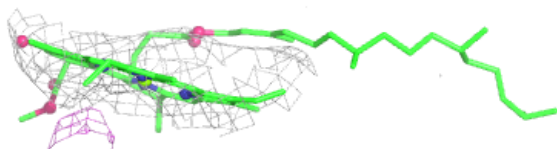
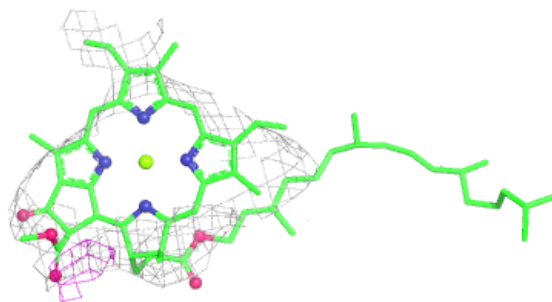
**Electron density around PL9 J 101:**

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

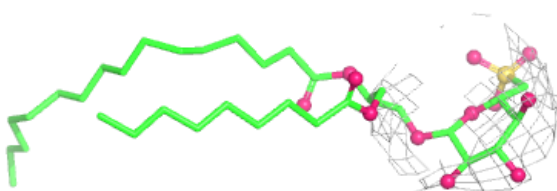
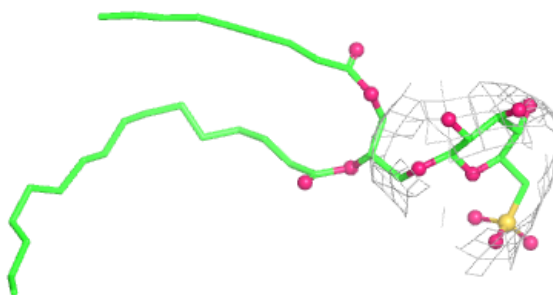


Electron density around CLA b 607:

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

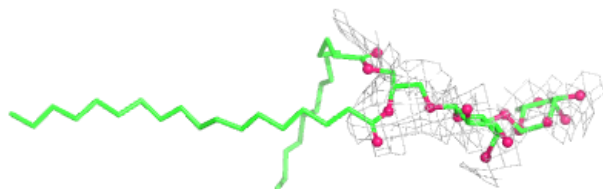
**Electron density around SQD b 602:**

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

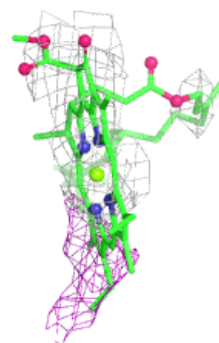
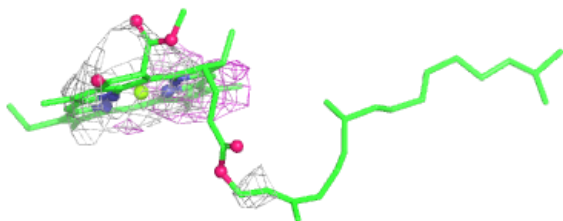
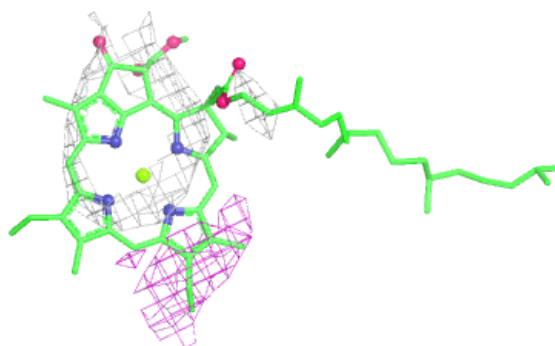


Electron density around DGD C 515:

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

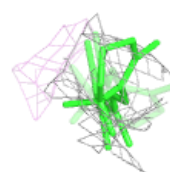
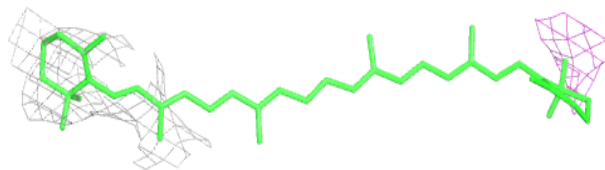
**Electron density around CLA a 405:**

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

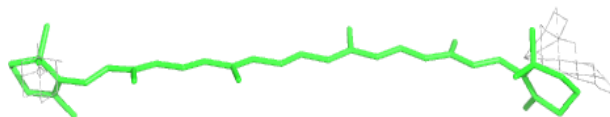
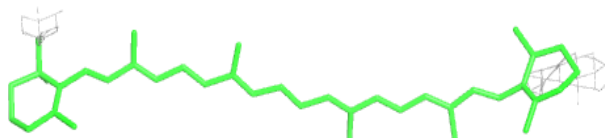


Electron density around BCR b 621:

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

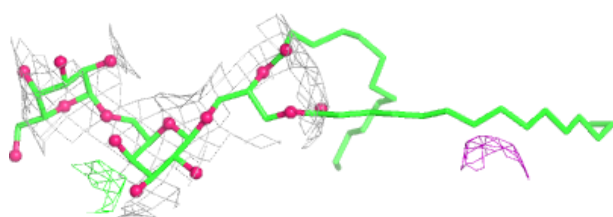
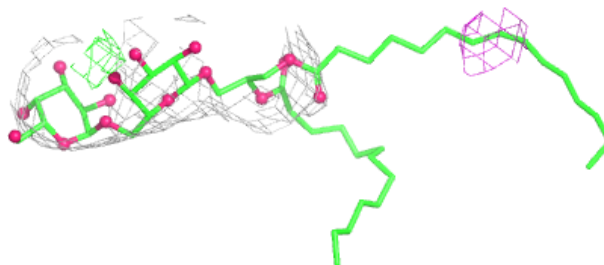
**Electron density around BCR C 513:**

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

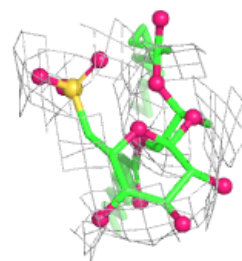
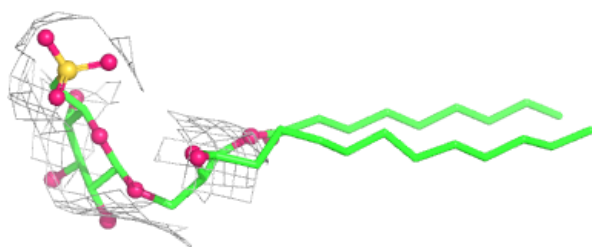
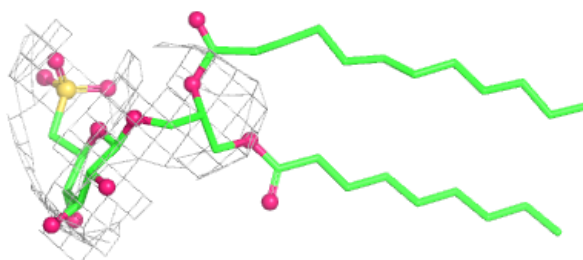


Electron density around DGD B 620:

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

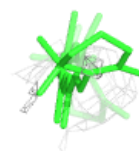
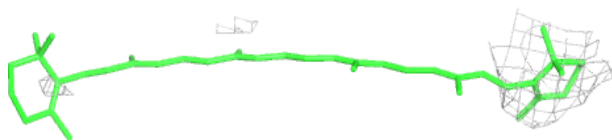
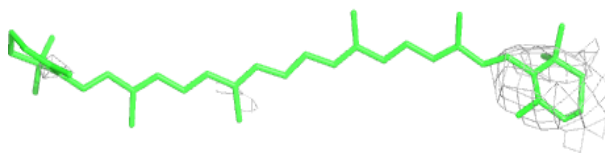
**Electron density around SQD d 403:**

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

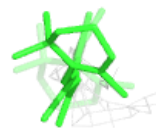
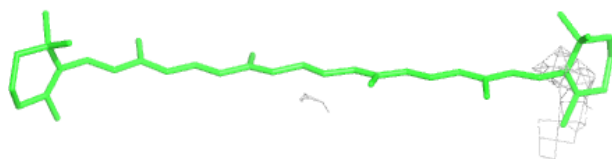
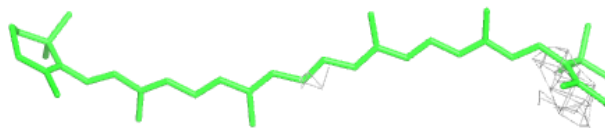


Electron density around BCR B 616:

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

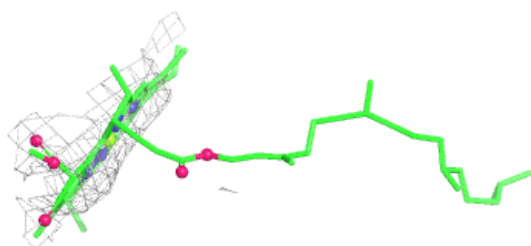
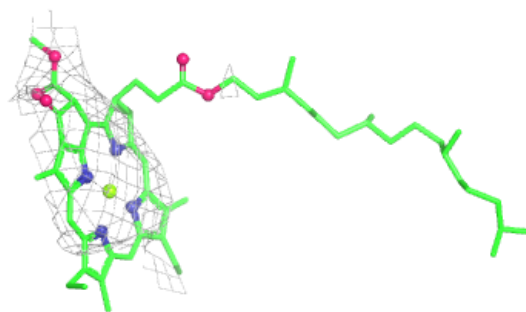
**Electron density around BCR i 101:**

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

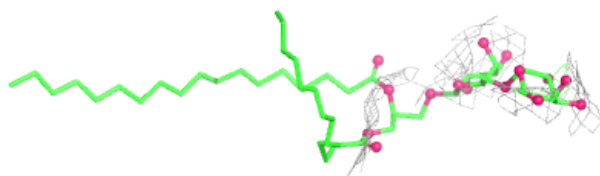


Electron density around CLA a 406:

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

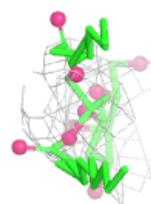
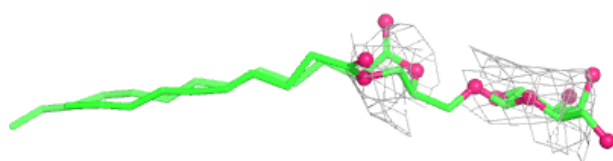
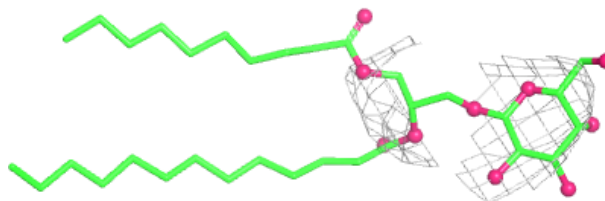
**Electron density around DGD c 516:**

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

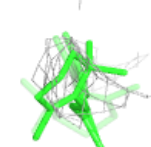
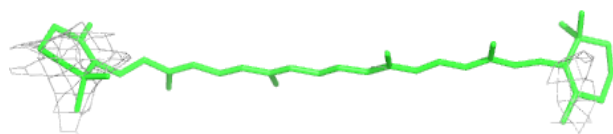
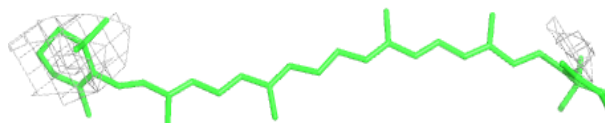


Electron density around LMG M 101:

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

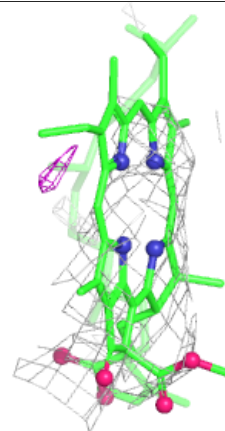
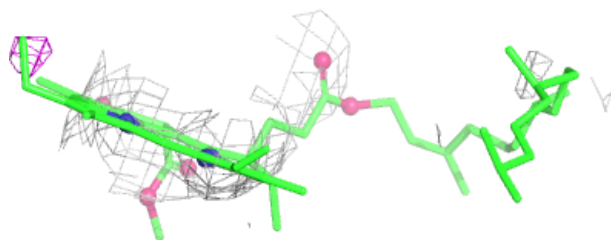
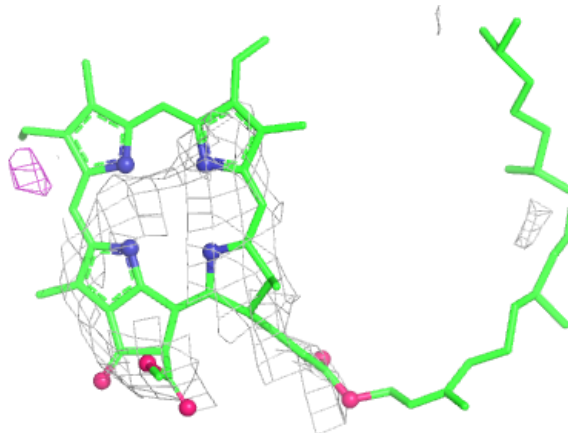
**Electron density around BCR C 520:**

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



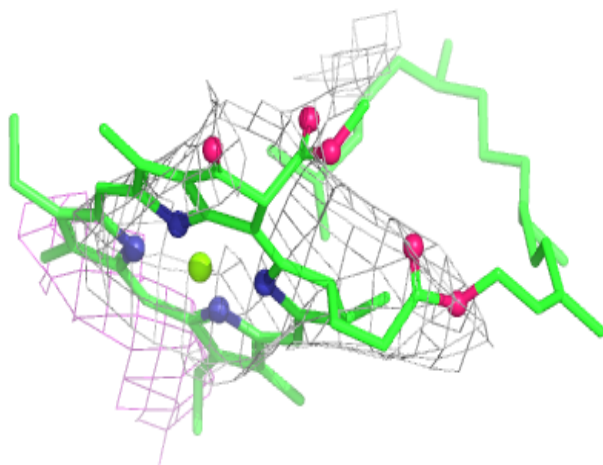
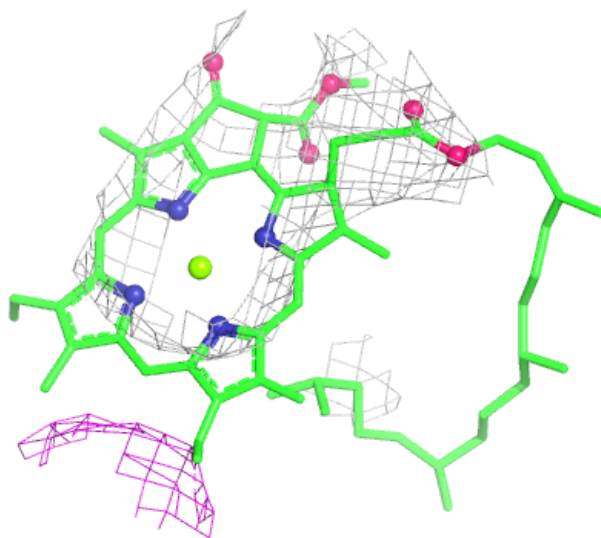
Electron density around PHO A 405:

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



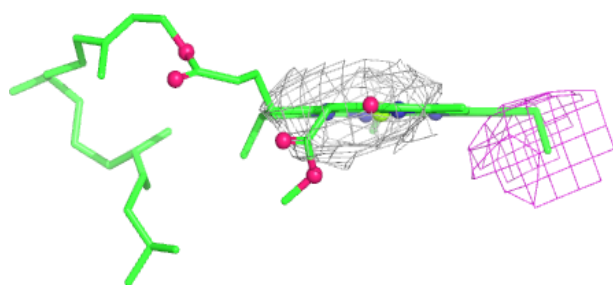
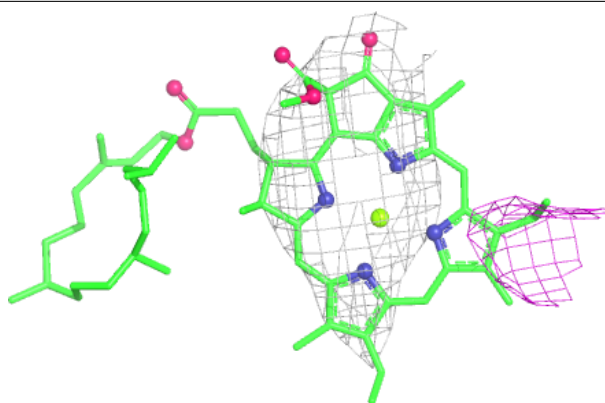
Electron density around CLA b 619:

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

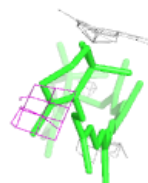
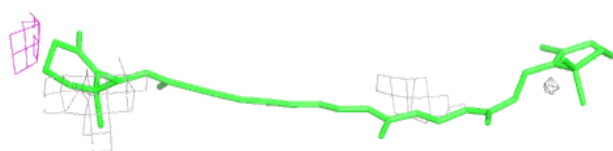
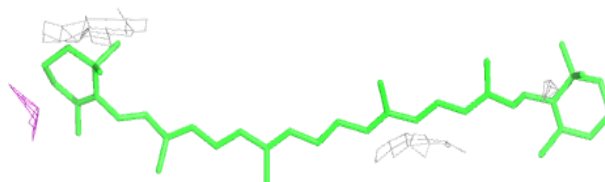


Electron density around CLA C 511:

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

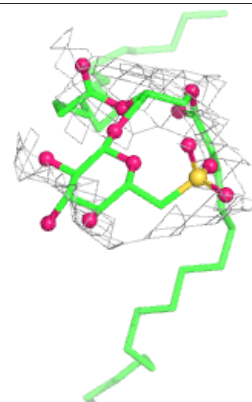
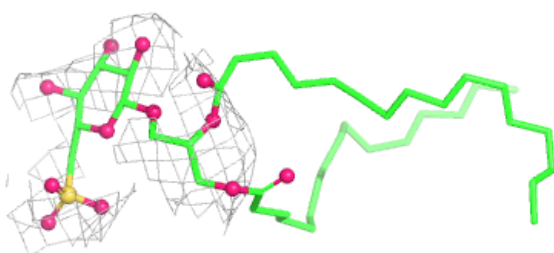
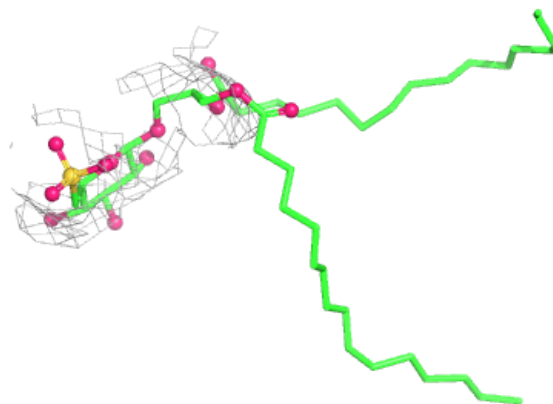
**Electron density around BCR b 622:**

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

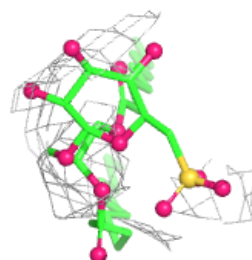
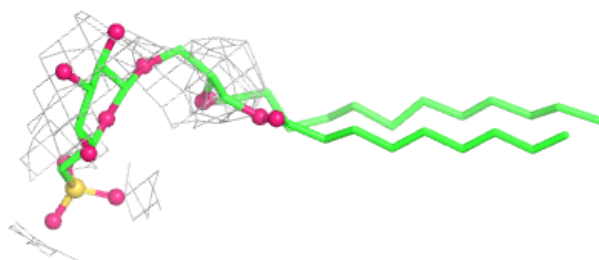
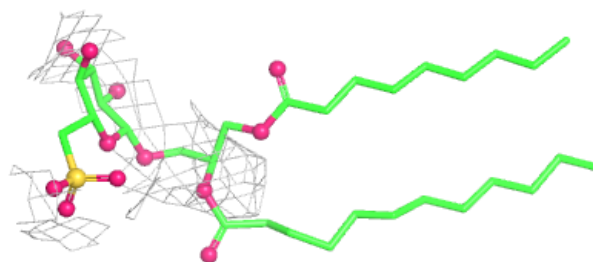


Electron density around SQD A 414:

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

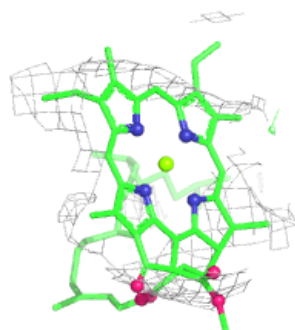
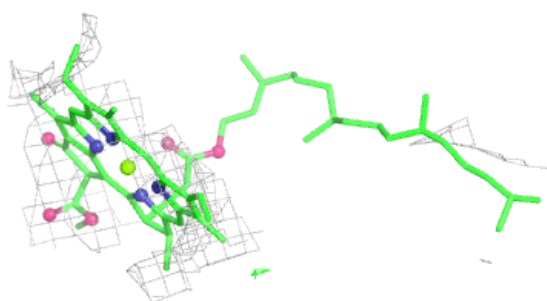
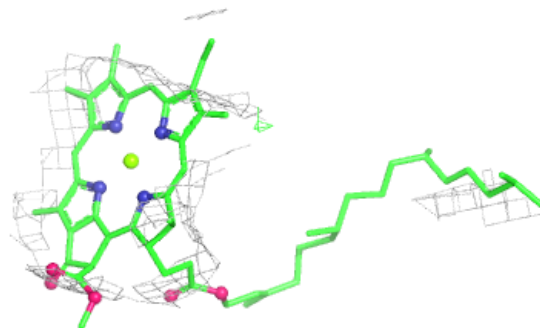
**Electron density around SQD B 622:**

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

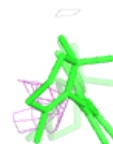
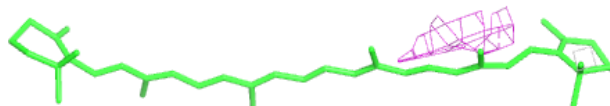
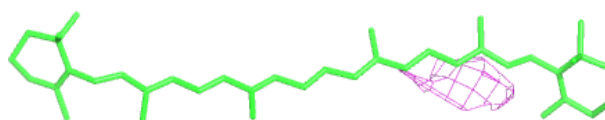


Electron density around CLA c 510:

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

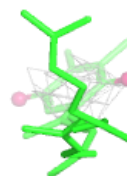
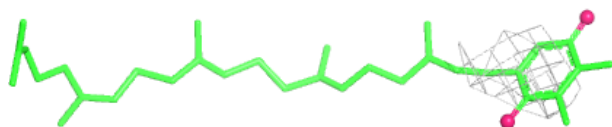
**Electron density around BCR c 514:**

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



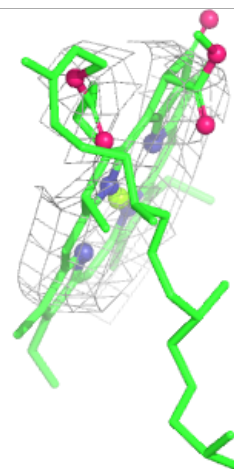
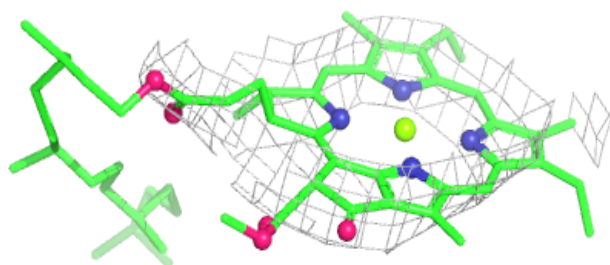
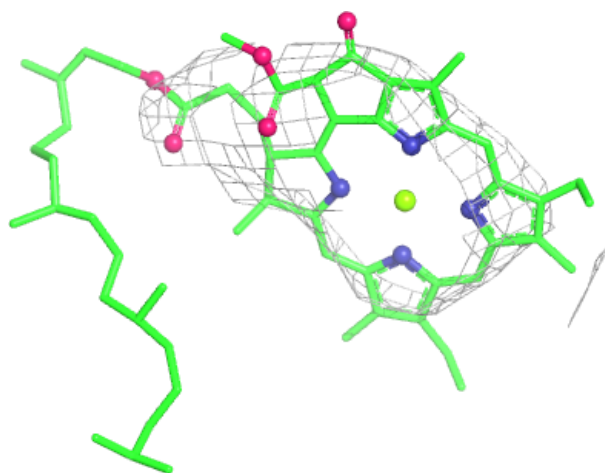
Electron density around PL9 j 101:

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



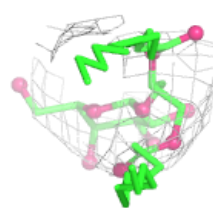
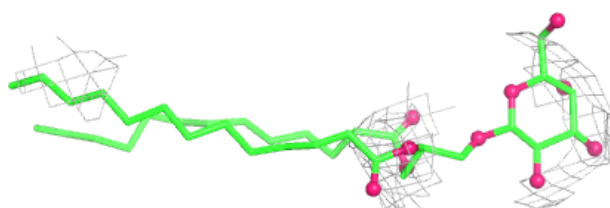
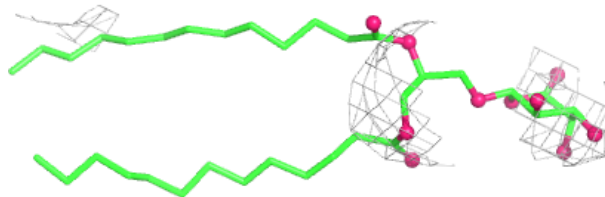
Electron density around CLA B 615:

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

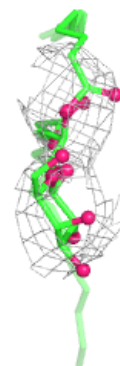
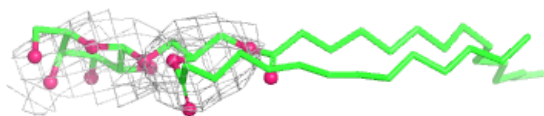
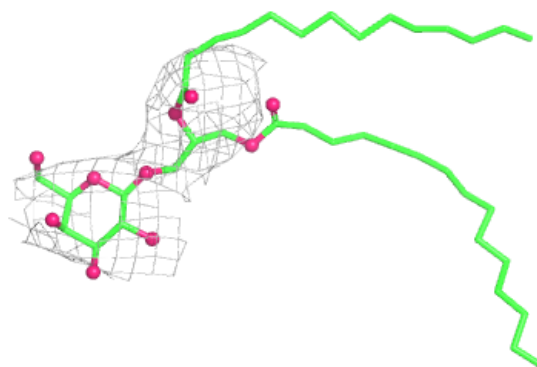


Electron density around LMG c 518:

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

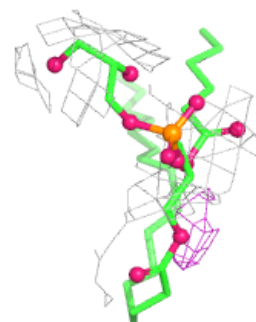
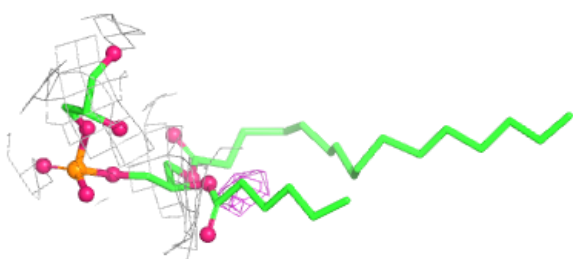
**Electron density around LMG C 521:**

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

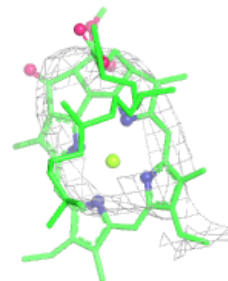
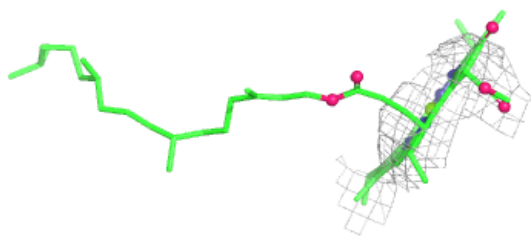
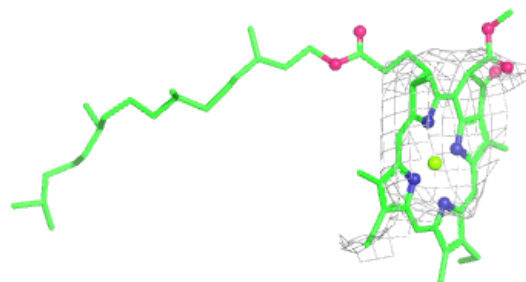


Electron density around LHG A 410:

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

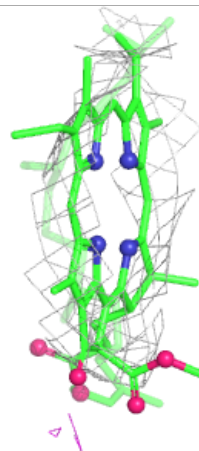
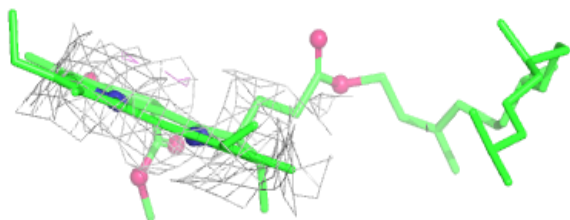
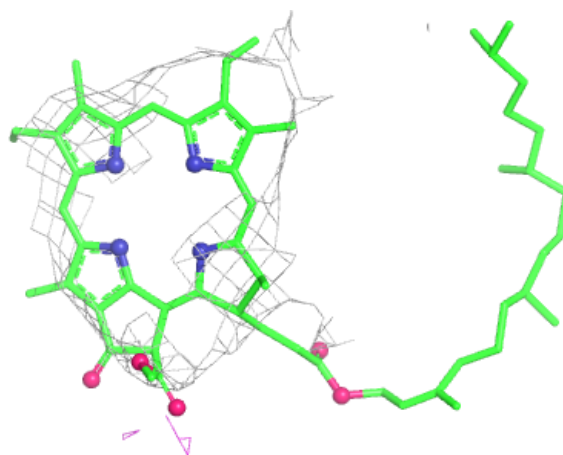
**Electron density around CLA A 406:**

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



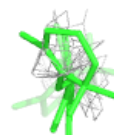
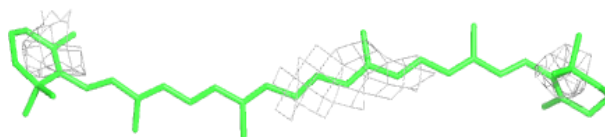
Electron density around PHO d 401:

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

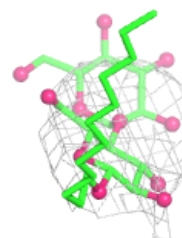
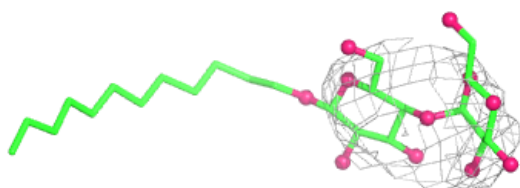
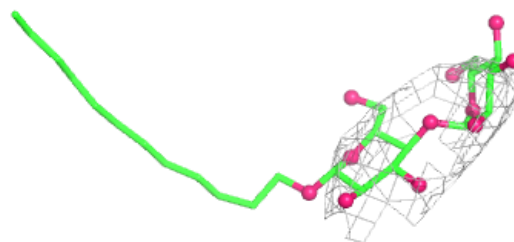


Electron density around BCR b 623:

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

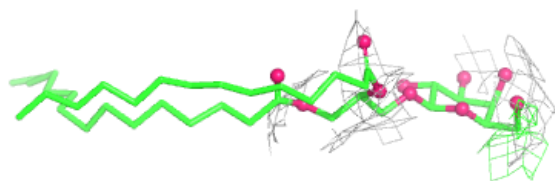
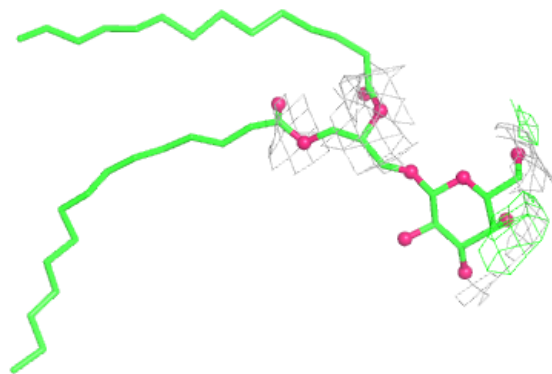
**Electron density around LMT M 103:**

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

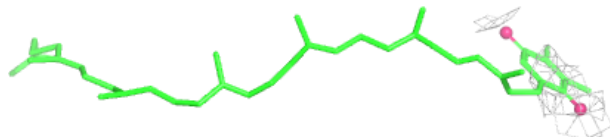
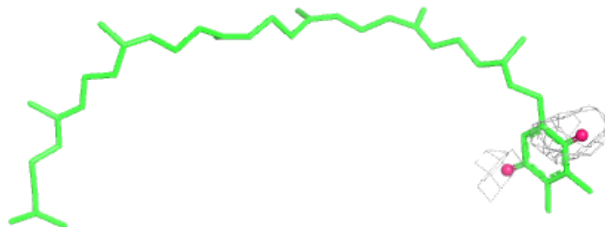


Electron density around LMG c 522:

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

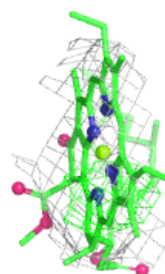
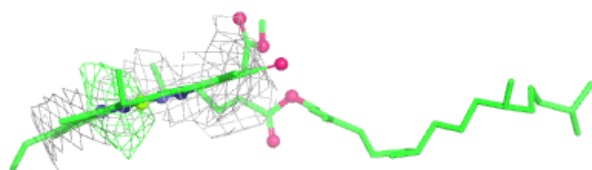
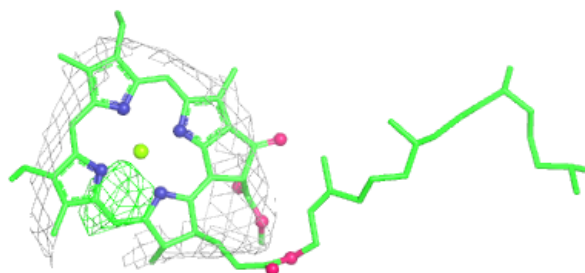
**Electron density around PL9 a 407:**

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

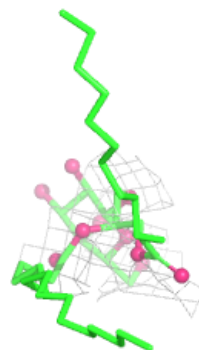
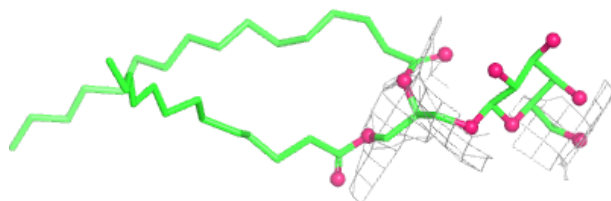
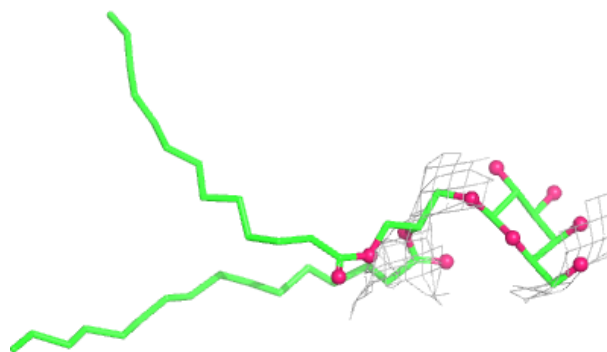


Electron density around CLA b 606:

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

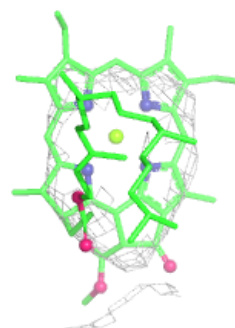
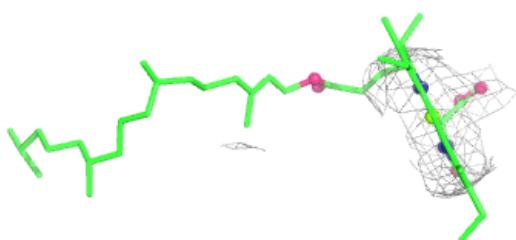
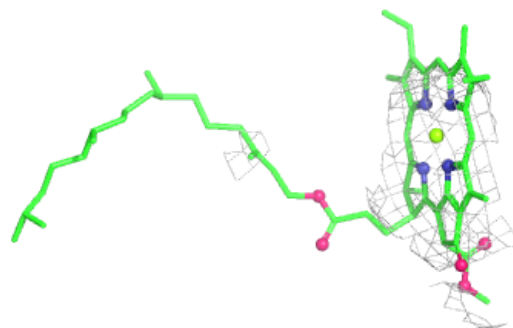
**Electron density around LMG D 406:**

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

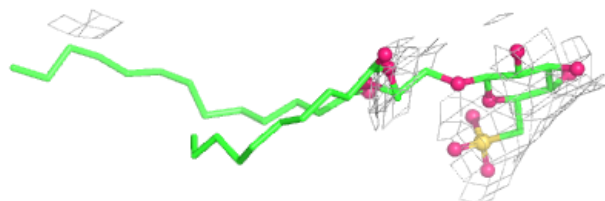
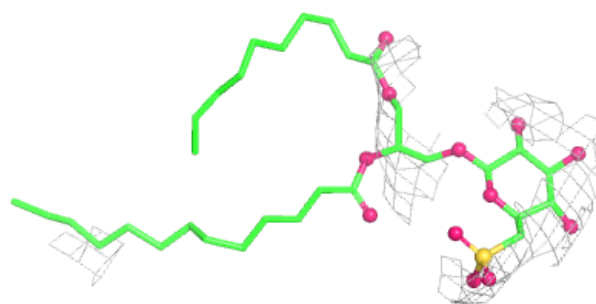


Electron density around CLA D 404:

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

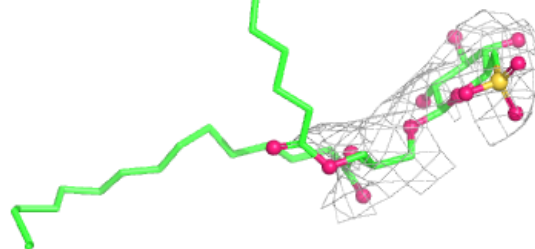
**Electron density around SQD F 103:**

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

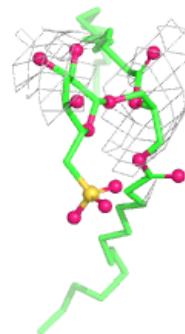
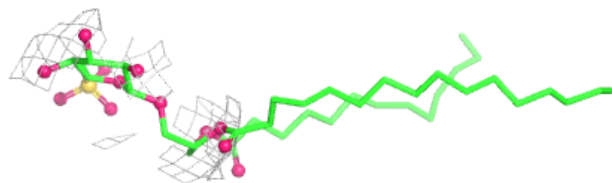


Electron density around SQD a 401:

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

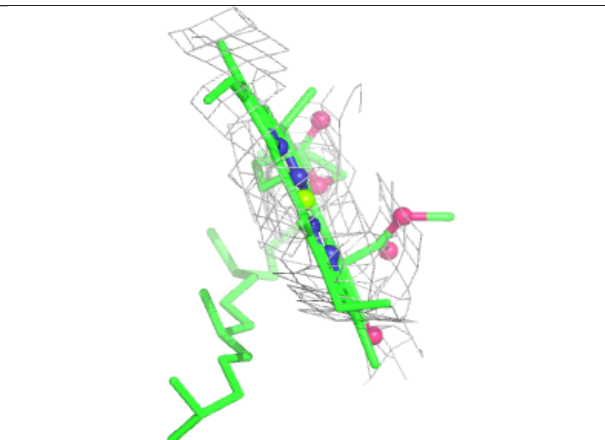
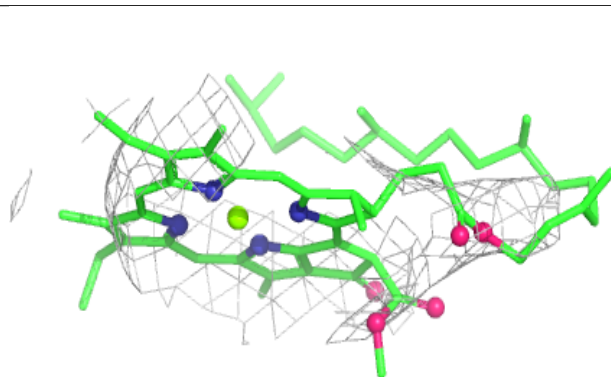
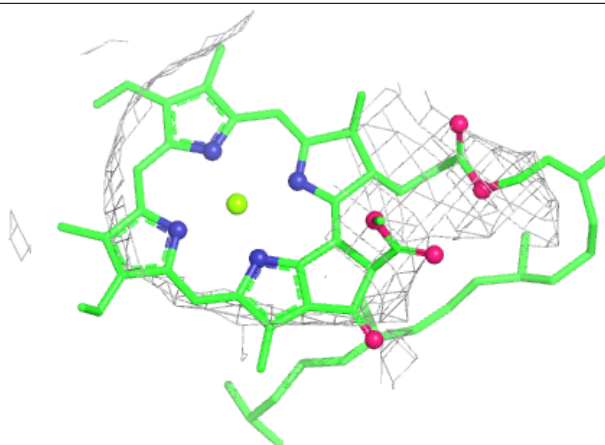
**Electron density around SQD a 412:**

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

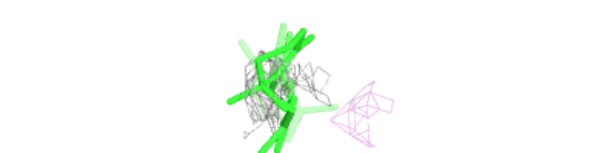
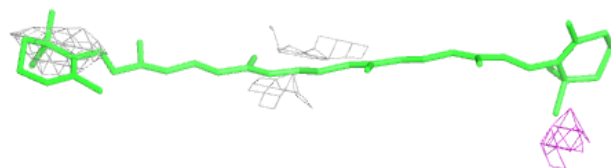


Electron density around CLA c 508:

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

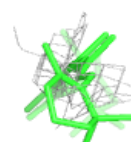
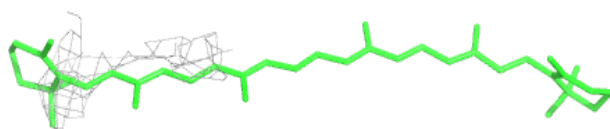
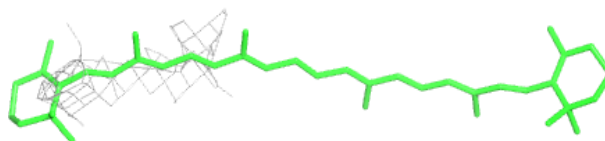
**Electron density around BCR y 101:**

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

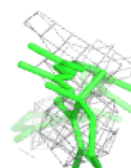
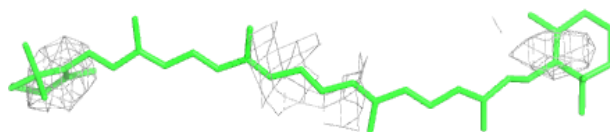
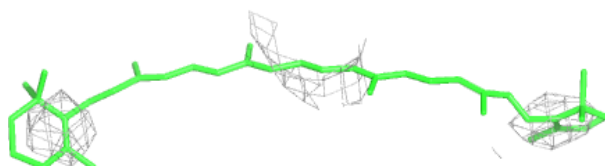


Electron density around BCR B 619:

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

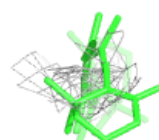
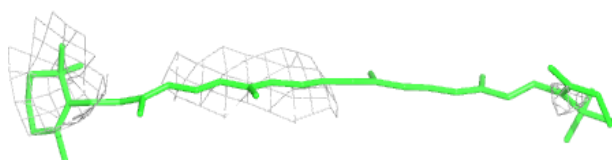
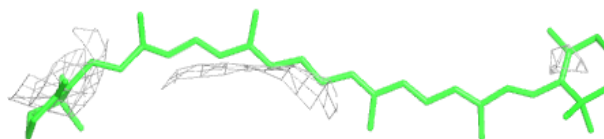
**Electron density around BCR F 102:**

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

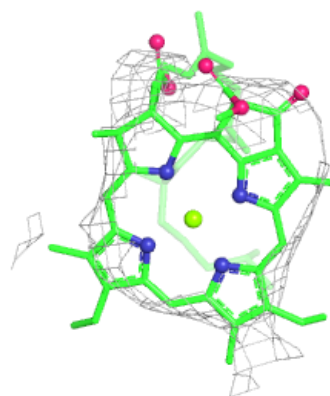
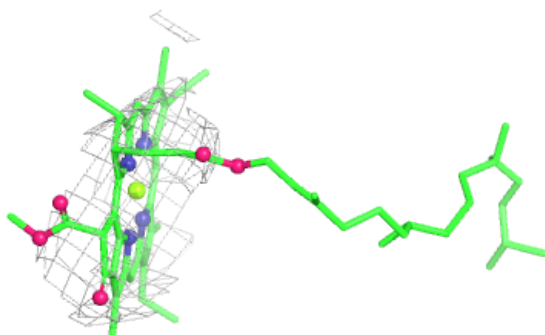
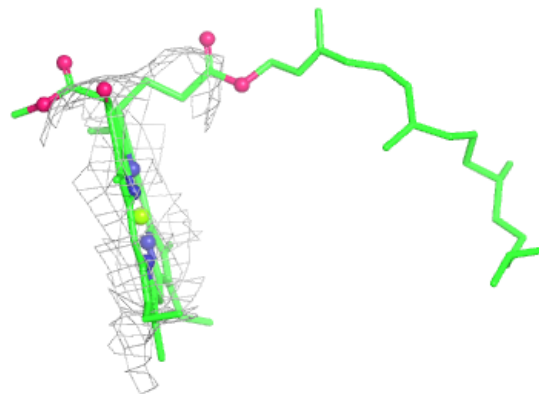


Electron density around BCR x 101:

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

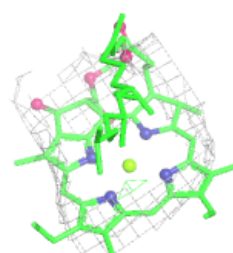
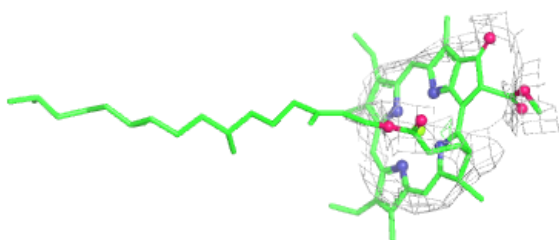
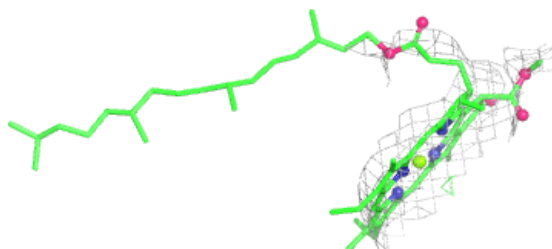
**Electron density around CLA C 505:**

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

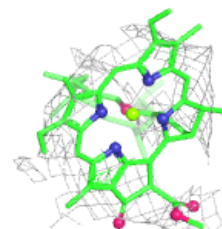
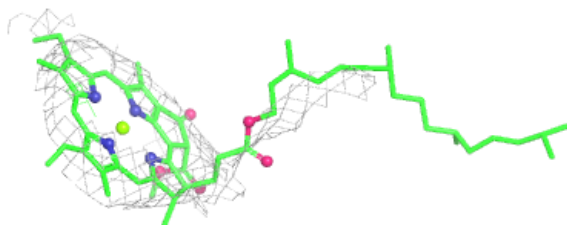
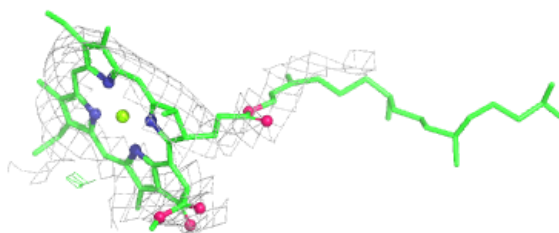


Electron density around CLA C 519:

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

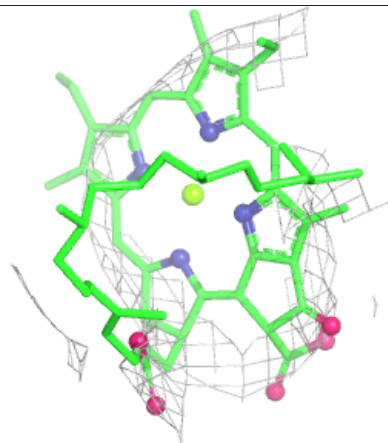
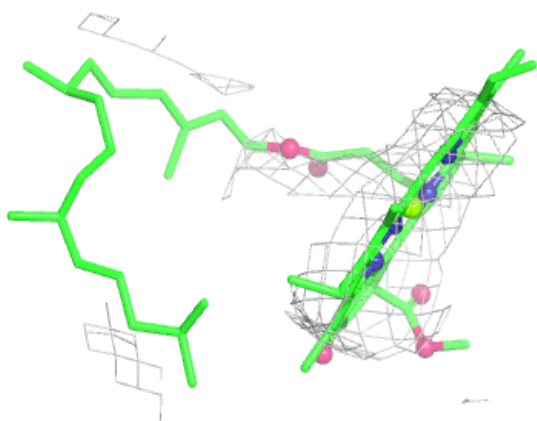
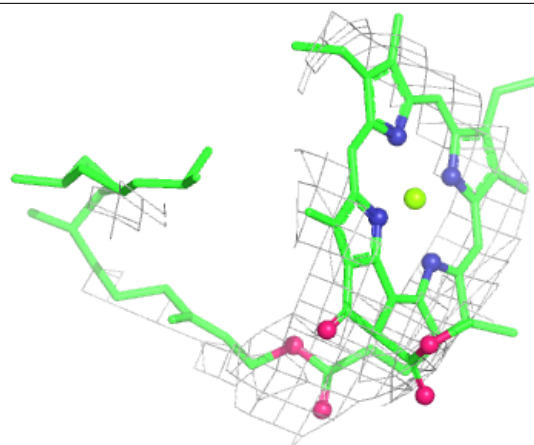
**Electron density around CLA c 502:**

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



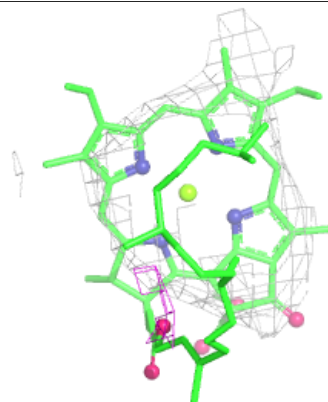
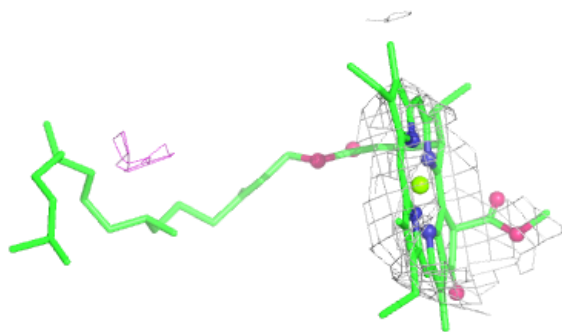
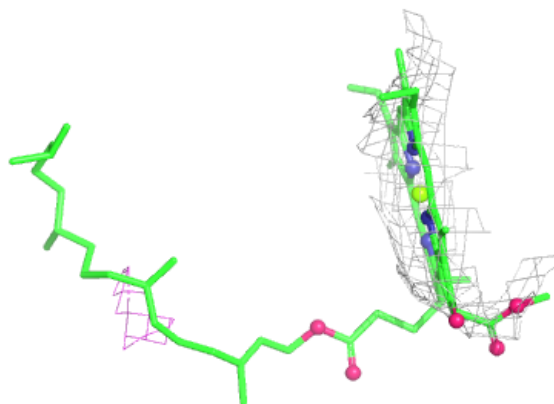
Electron density around CLA c 503:

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



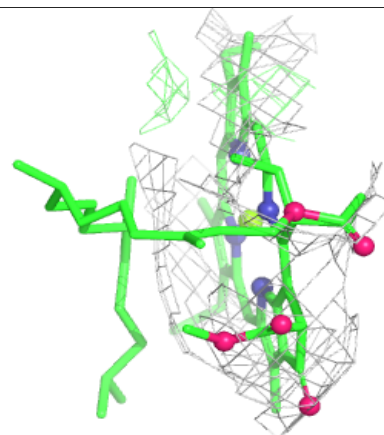
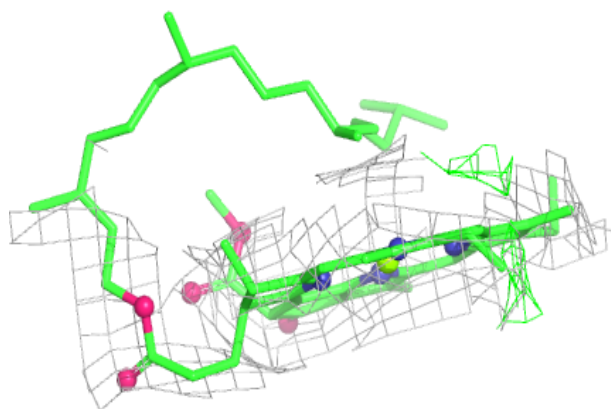
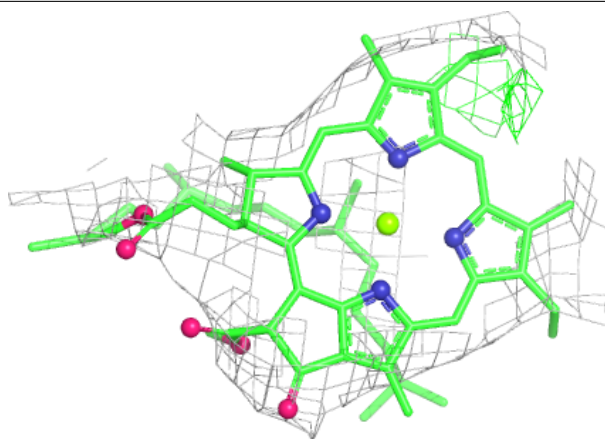
Electron density around CLA c 505:

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

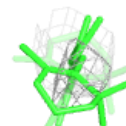
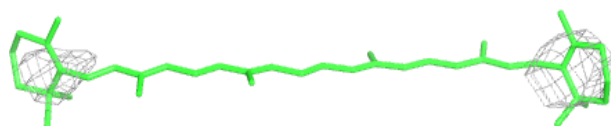
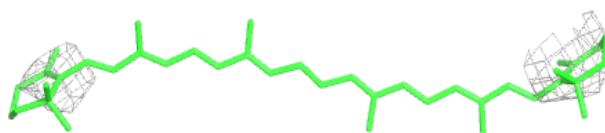


Electron density around CLA C 509:

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

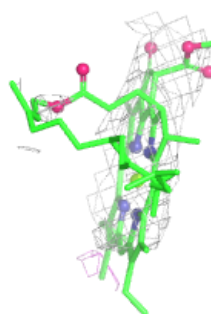
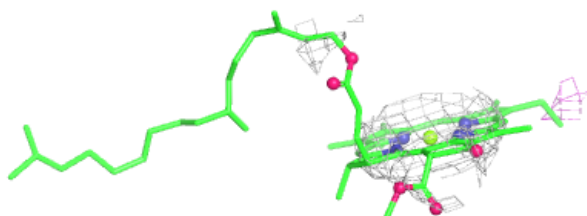
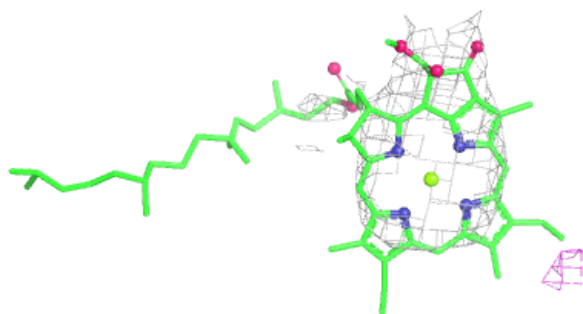
**Electron density around BCR A 408:**

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



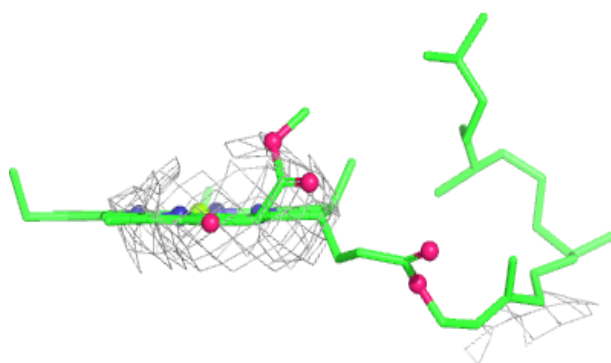
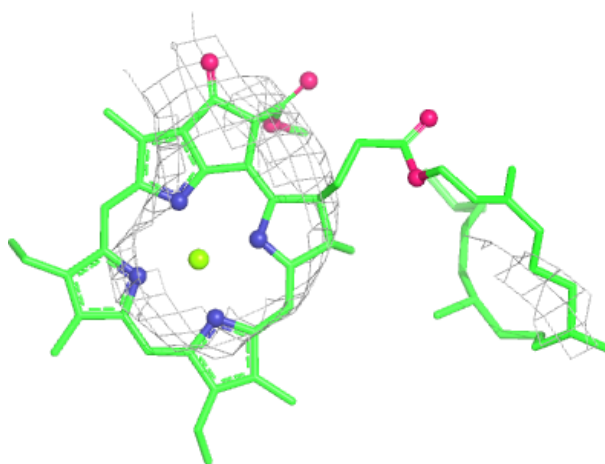
Electron density around CLA A 404:

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



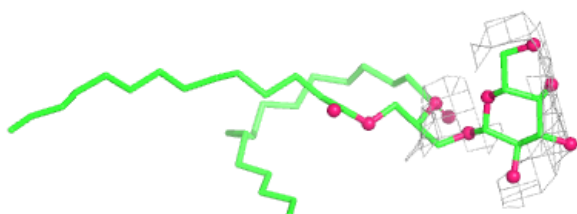
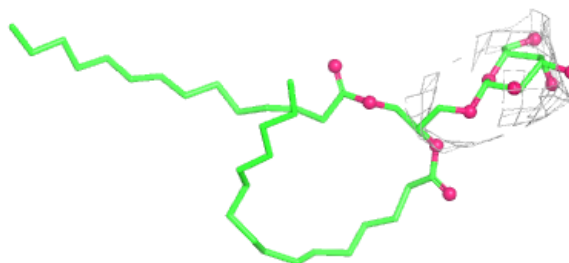
Electron density around CLA c 511:

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

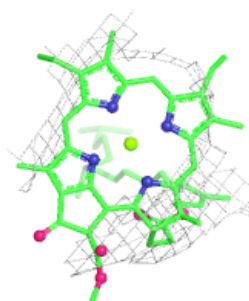
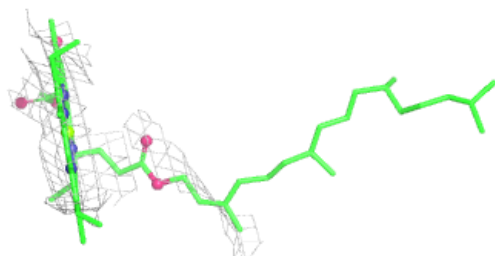
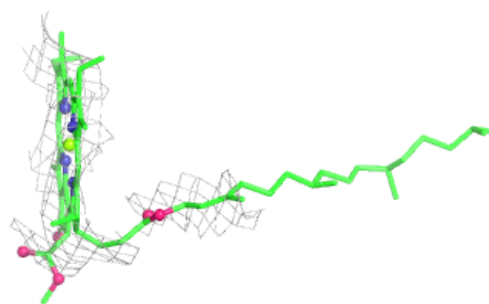


Electron density around LMG d 408:

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

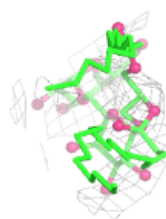
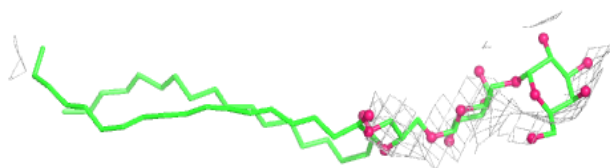
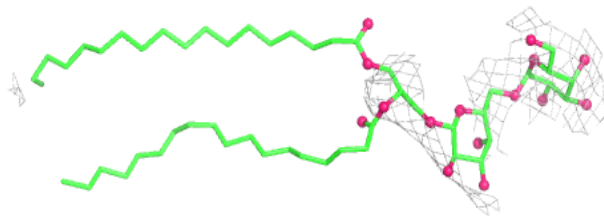
**Electron density around CLA b 610:**

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

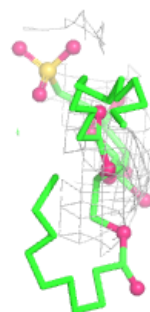
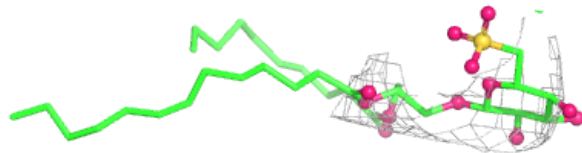
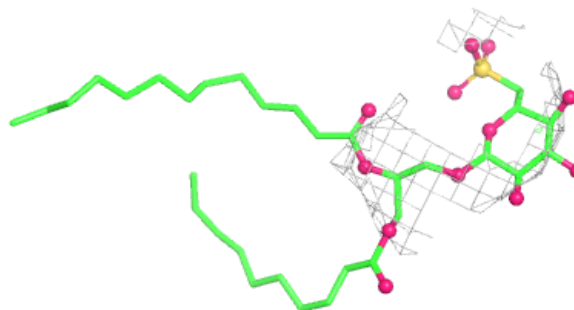


Electron density around DGD c 517:

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

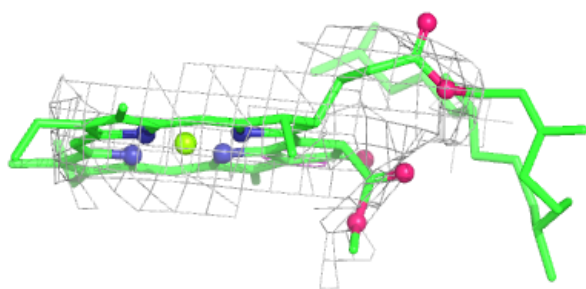
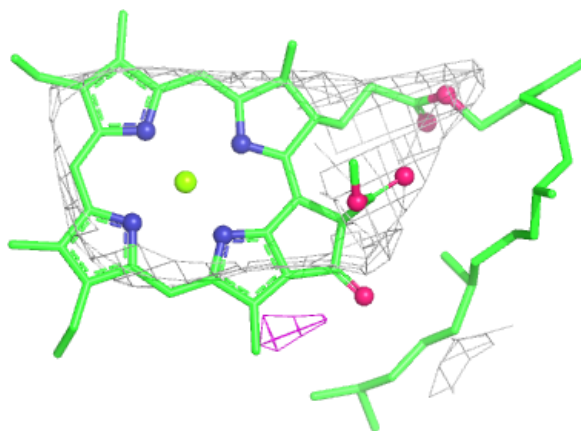
**Electron density around SQD f 103:**

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

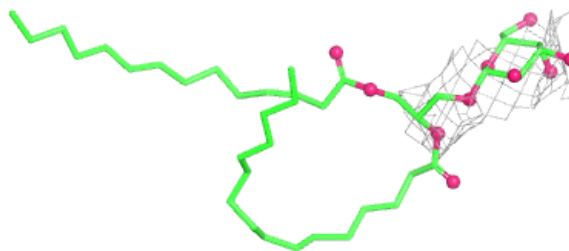


Electron density around CLA b 614:

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

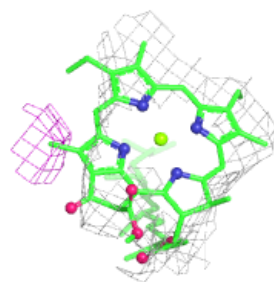
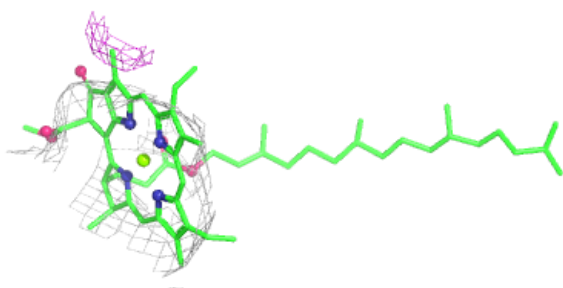
**Electron density around LMG B 625:**

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

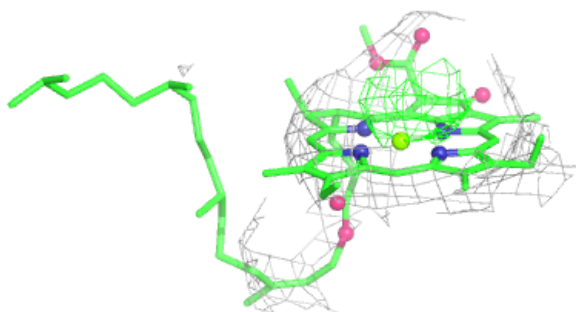
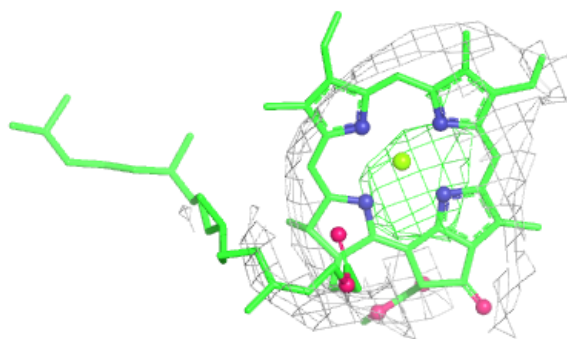


Electron density around CLA b 611:

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

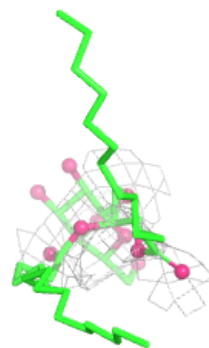
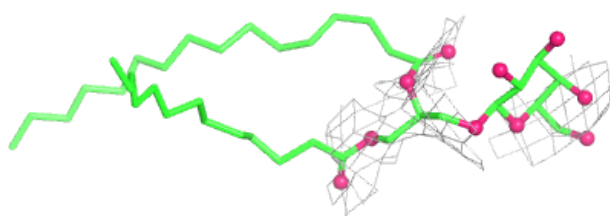
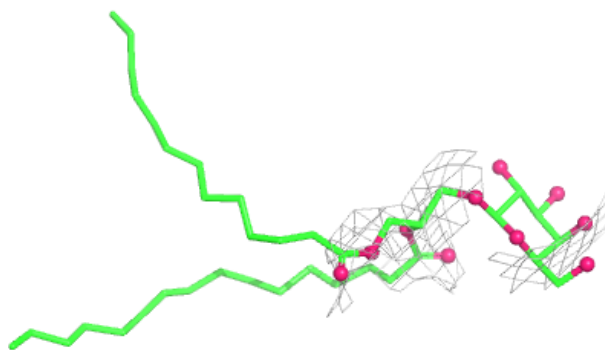
**Electron density around CLA a 404:**

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

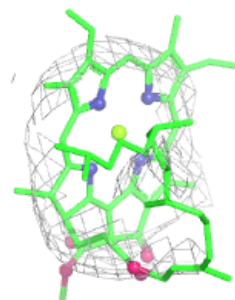
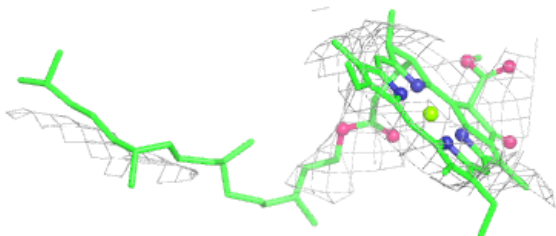
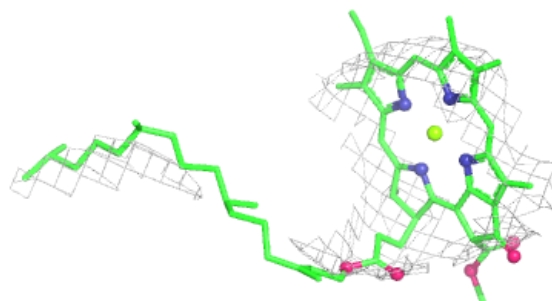


Electron density around LMG d 409:

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

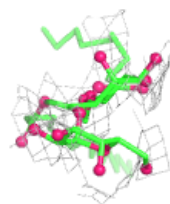
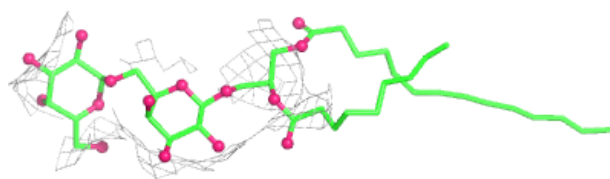
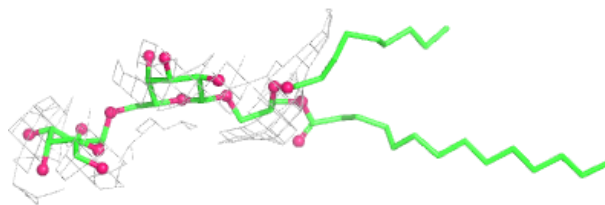
**Electron density around CLA C 510:**

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



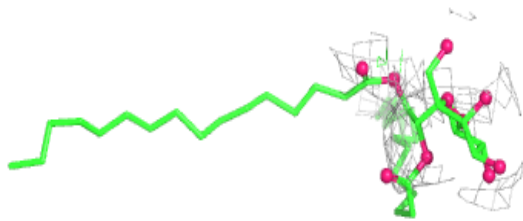
Electron density around DGD c 515:

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



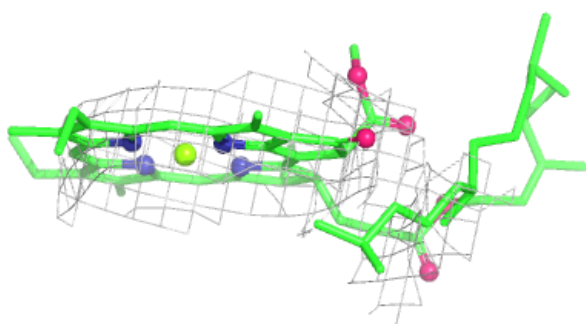
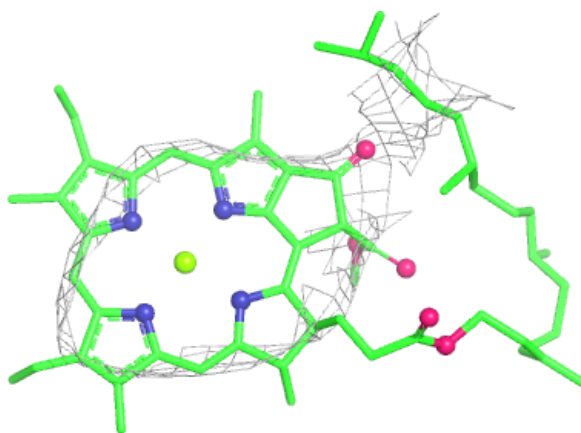
Electron density around LMG 1 101:

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

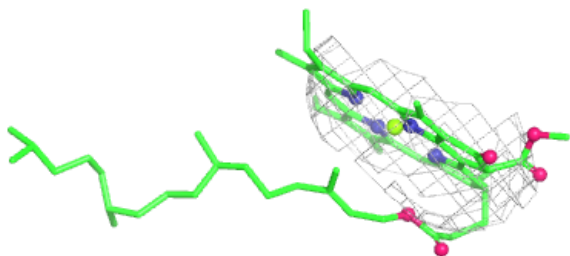
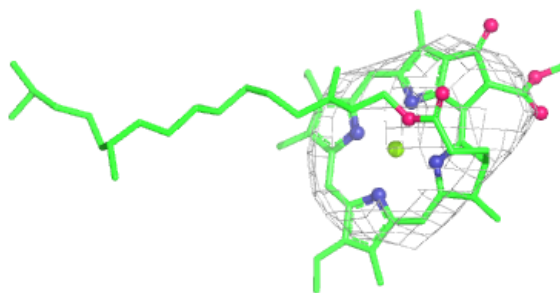


Electron density around CLA B 609:

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

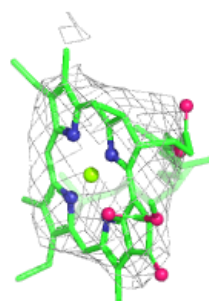
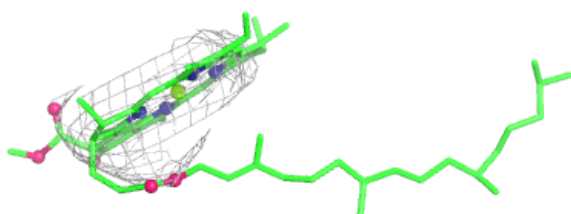
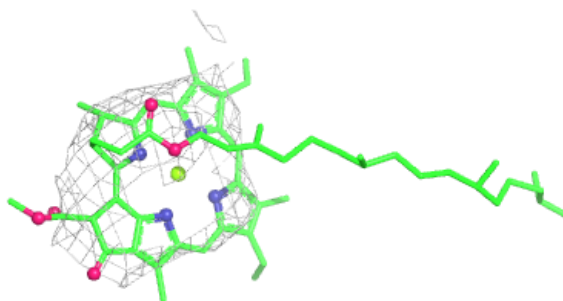
**Electron density around CLA B 613:**

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

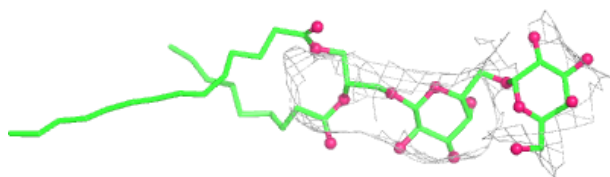
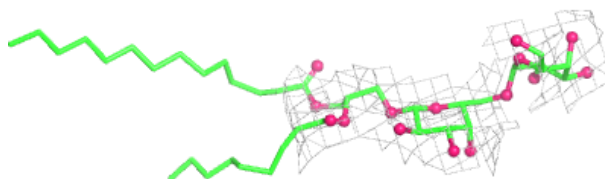


Electron density around CLA B 607:

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

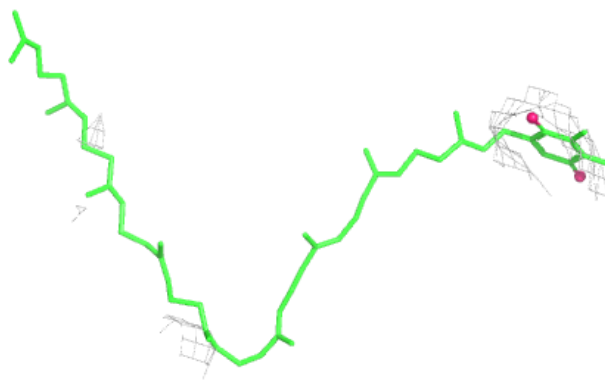
**Electron density around DGD C 514:**

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

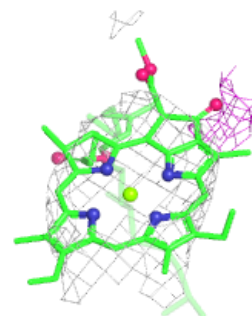
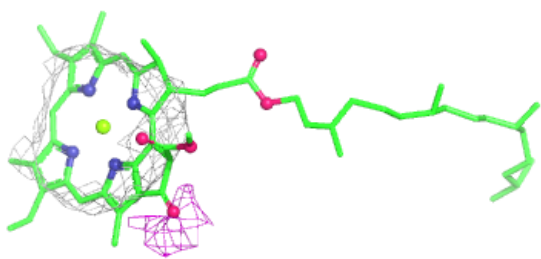
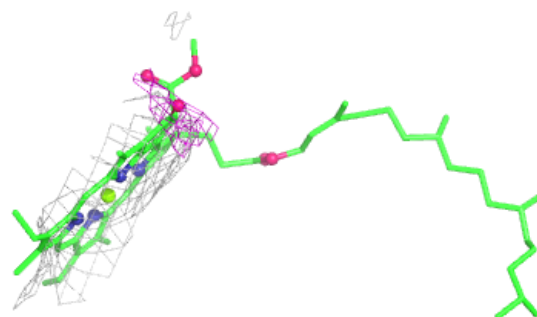


Electron density around PL9 D 405:

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

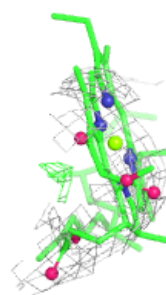
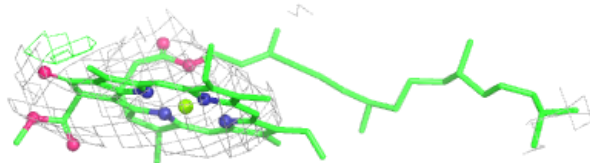
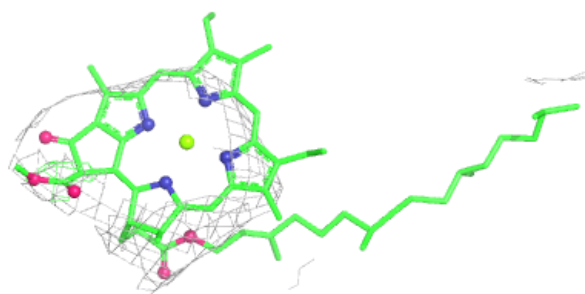
**Electron density around CLA D 403:**

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

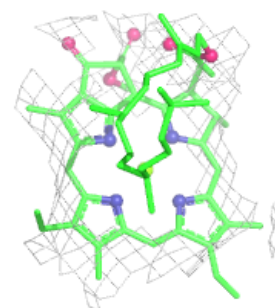
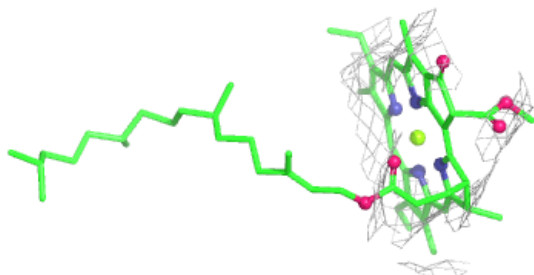
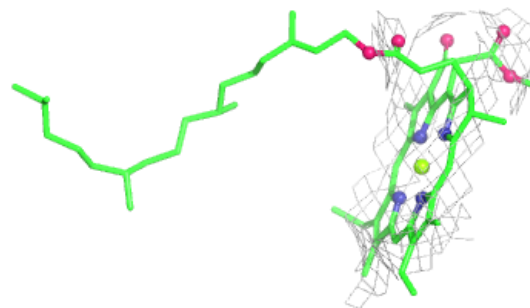


Electron density around CLA C 501:

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

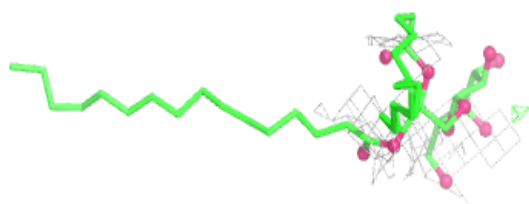
**Electron density around CLA C 507:**

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



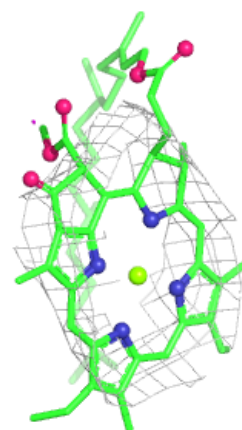
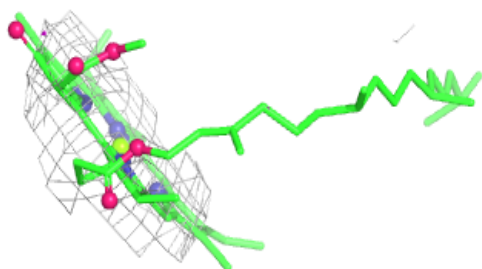
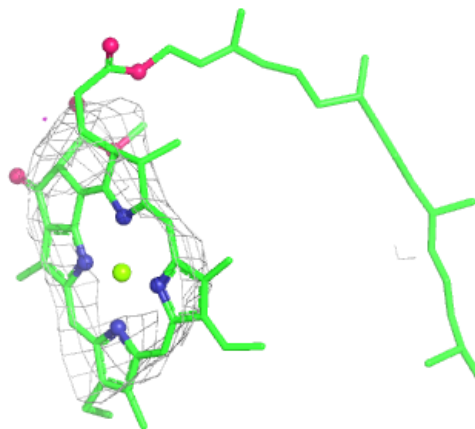
Electron density around LMG L 101:

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



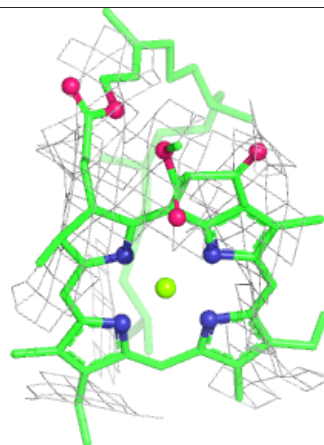
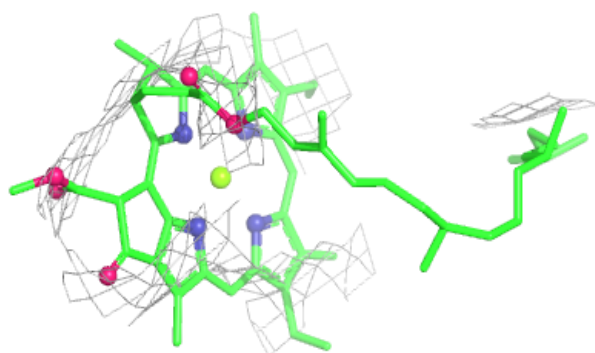
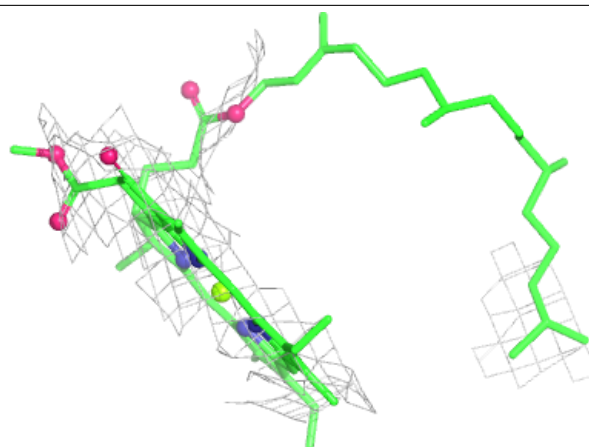
Electron density around CLA c 506:

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

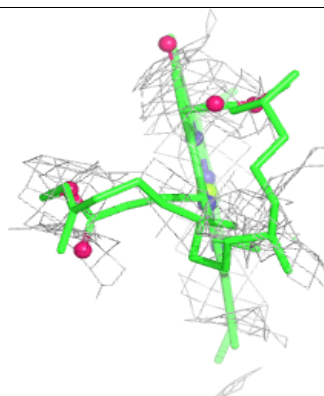
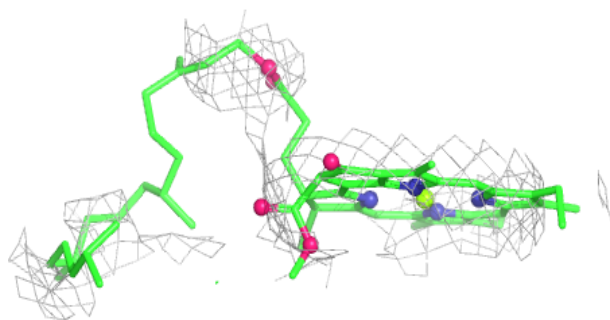
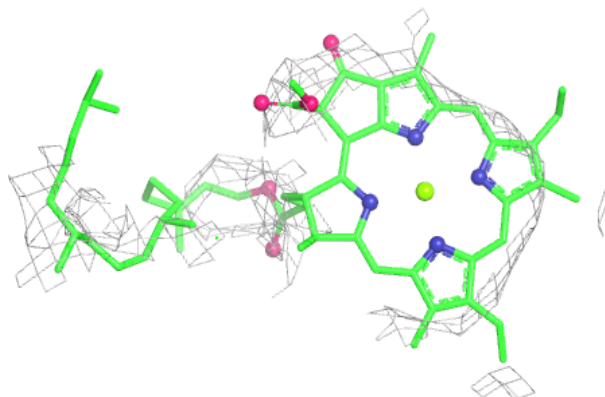


Electron density around CLA B 610:

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

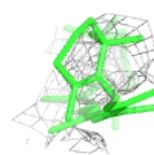
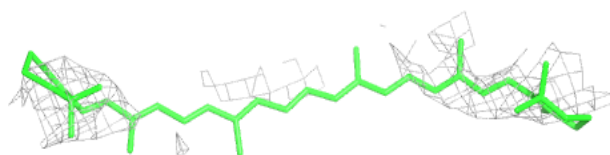
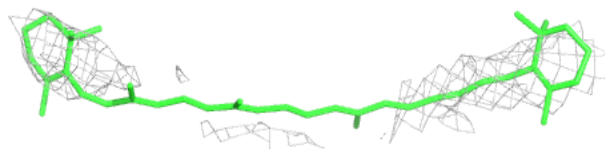
**Electron density around CLA b 616:**

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

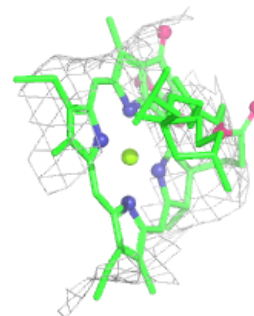
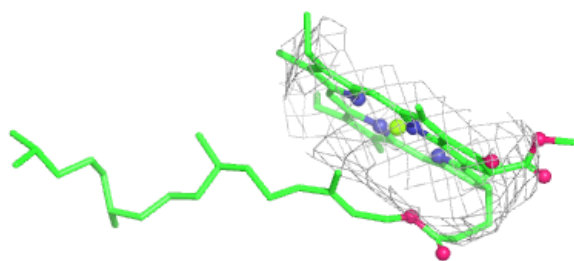
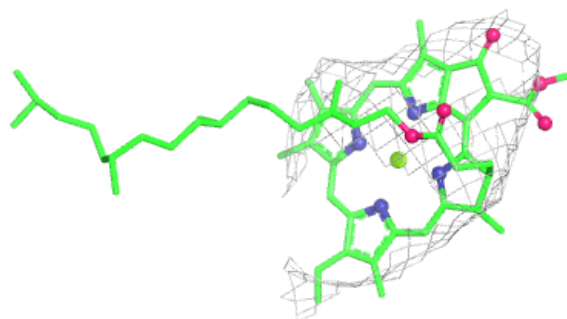


Electron density around BCR c 513:

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

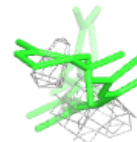
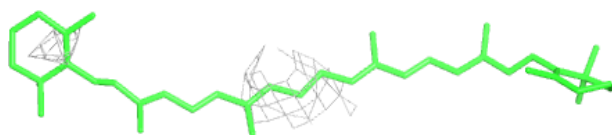
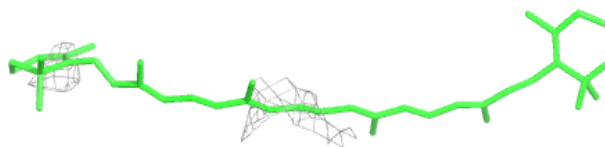
**Electron density around CLA b 618:**

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

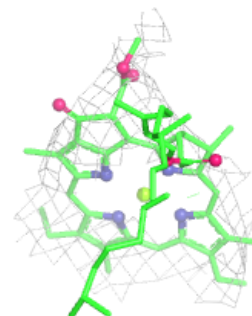
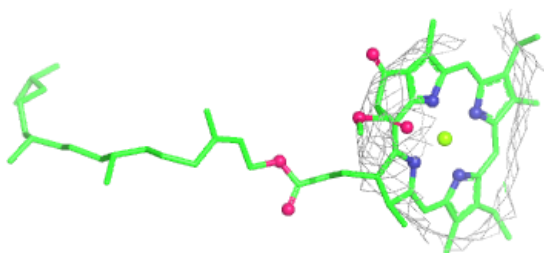
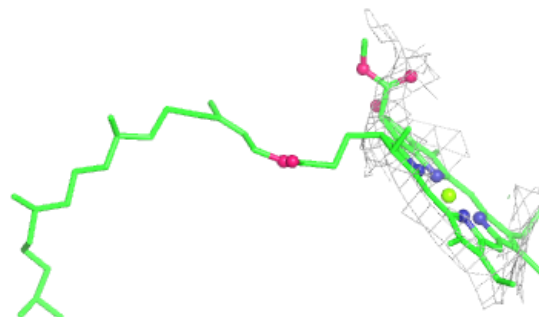


Electron density around BCR f 102:

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

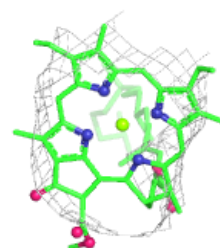
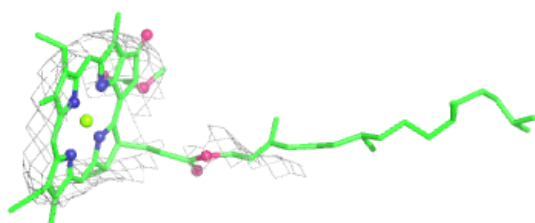
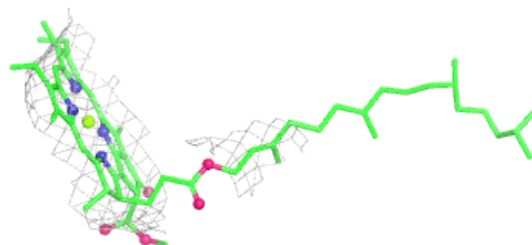
**Electron density around CLA d 405:**

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

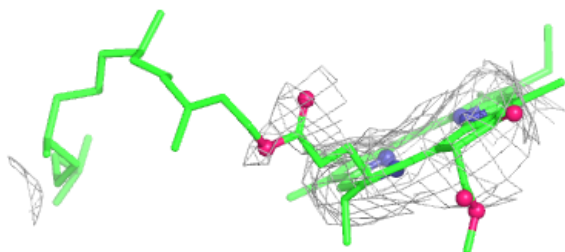
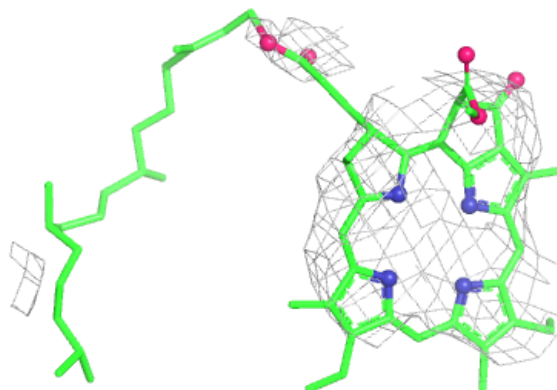


Electron density around CLA b 608:

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

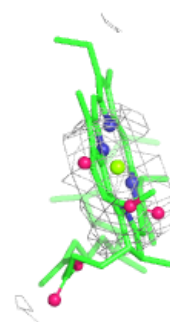
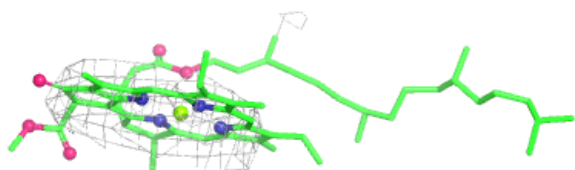
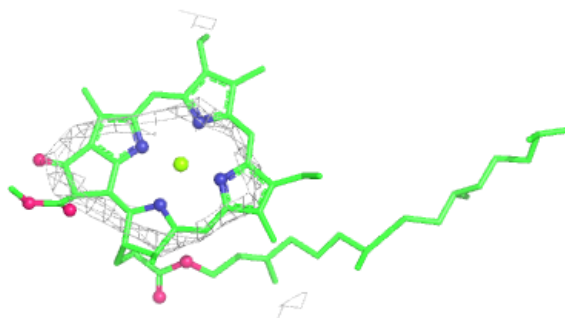
**Electron density around PHO D 401:**

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

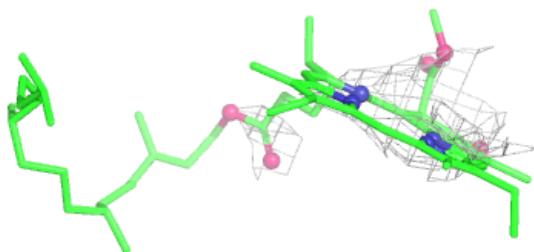
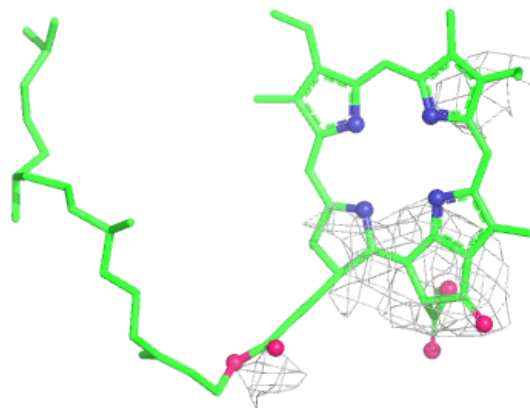


Electron density around CLA c 501:

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

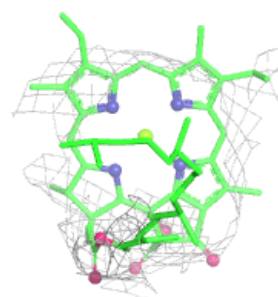
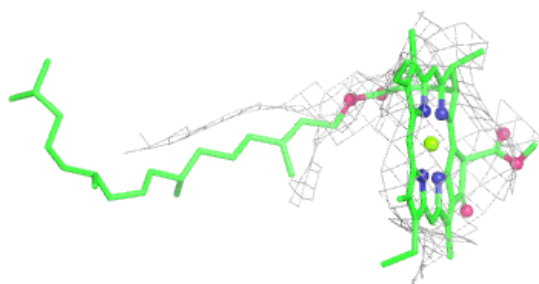
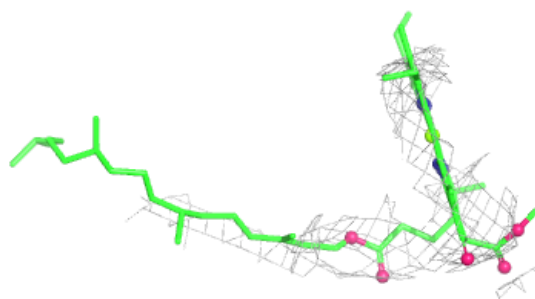
**Electron density around PHO d 402:**

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

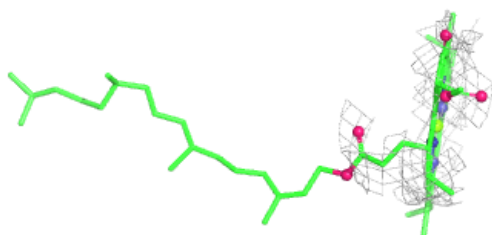
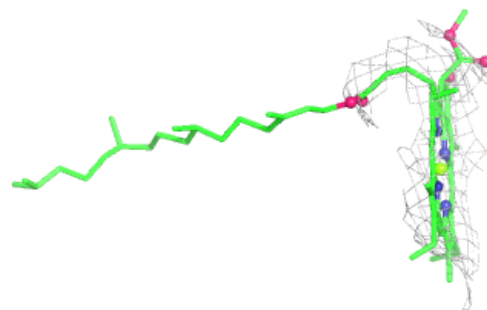


Electron density around CLA b 609:

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

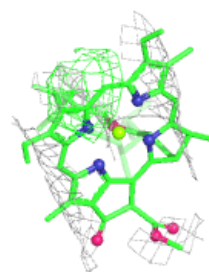
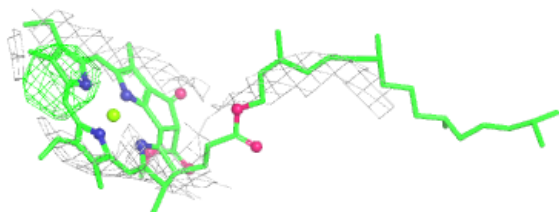
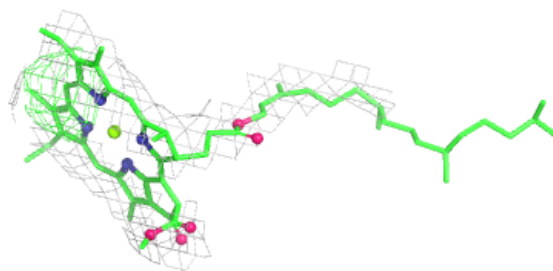
**Electron density around CLA B 605:**

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

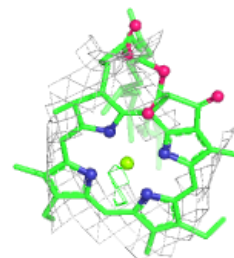
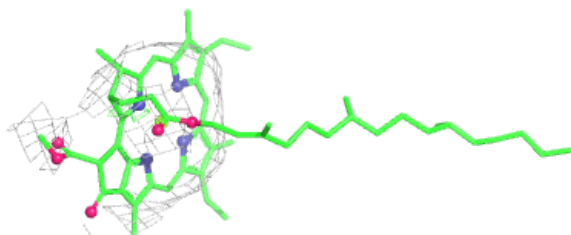
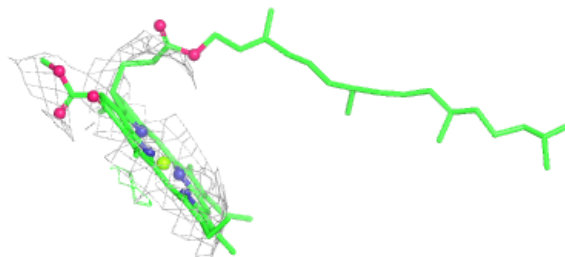


Electron density around CLA C 502:

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

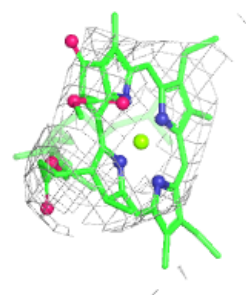
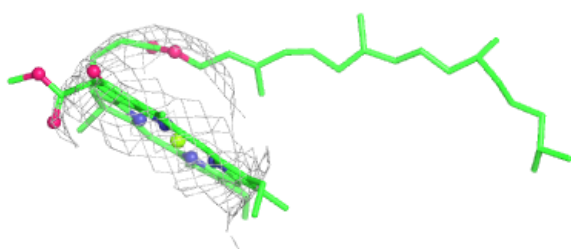
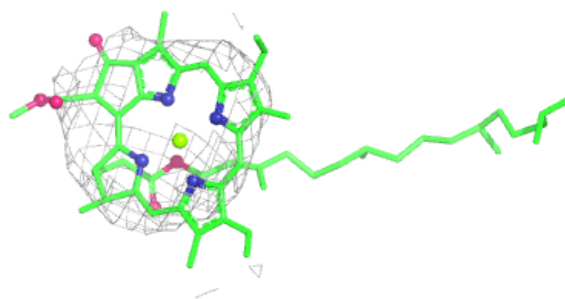
**Electron density around CLA c 520:**

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

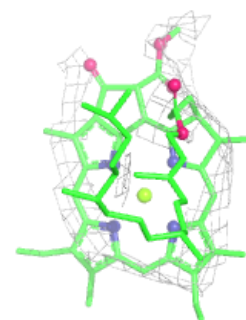
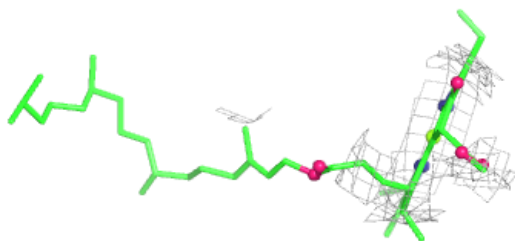
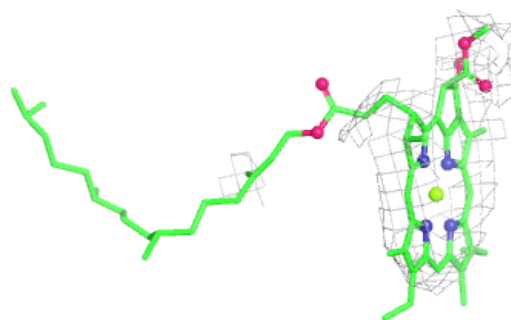


Electron density around CLA b 612:

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

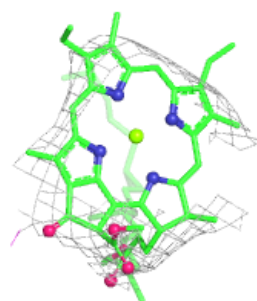
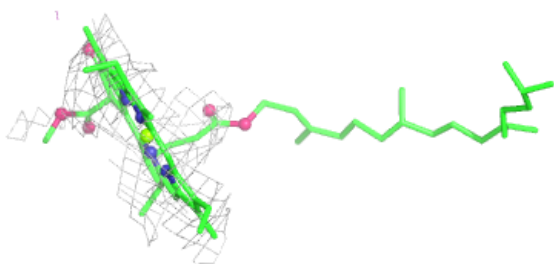
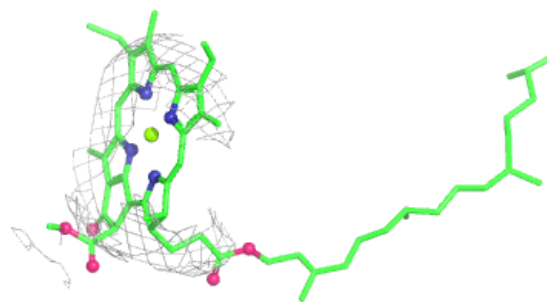
**Electron density around CLA d 406:**

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

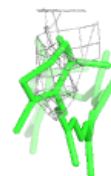
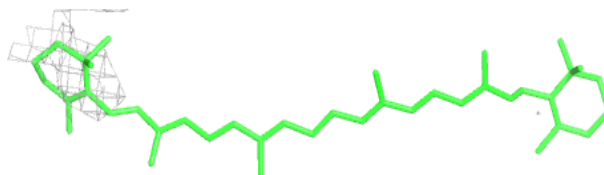


Electron density around CLA b 613:

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

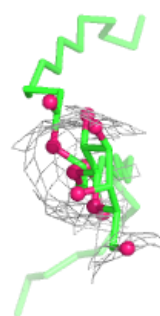
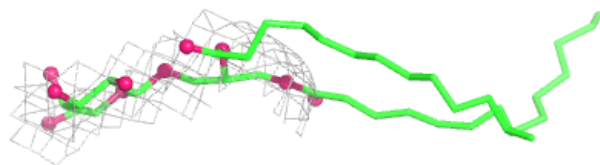
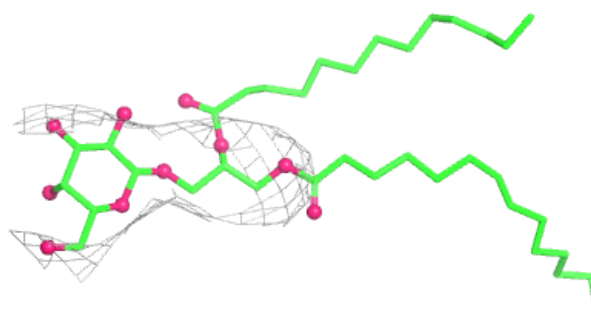
**Electron density around BCR B 617:**

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

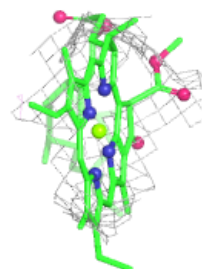
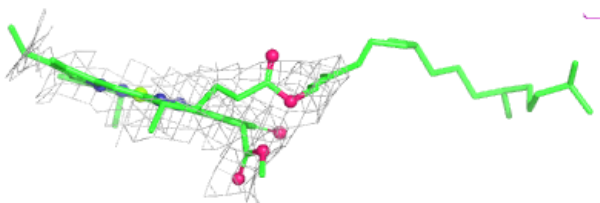


Electron density around LMG d 412:

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

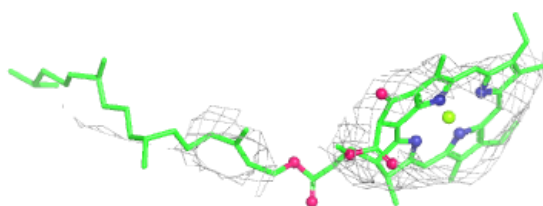
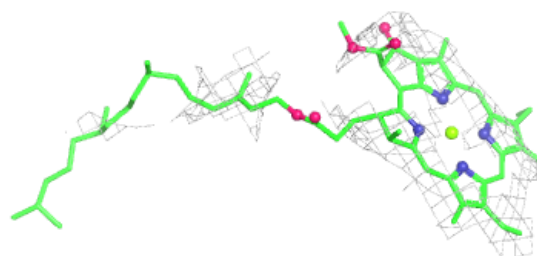
**Electron density around CLA H 101:**

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

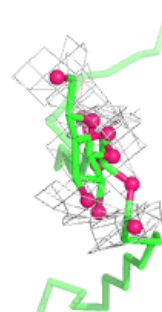
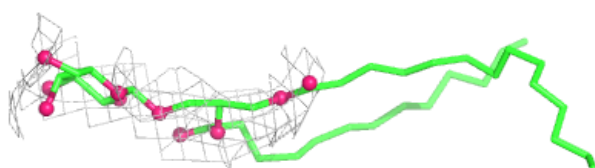
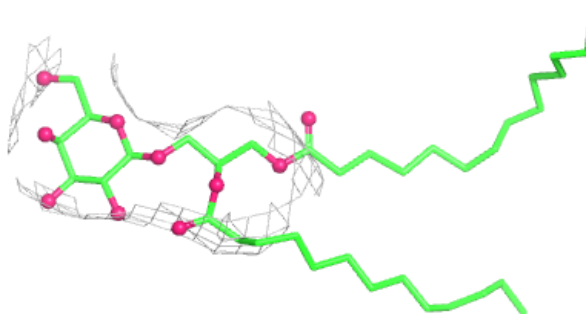


Electron density around CLA a 403:

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

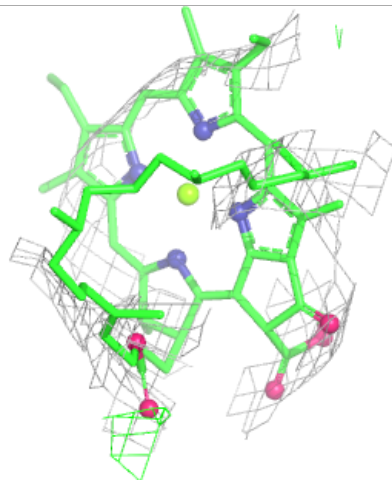
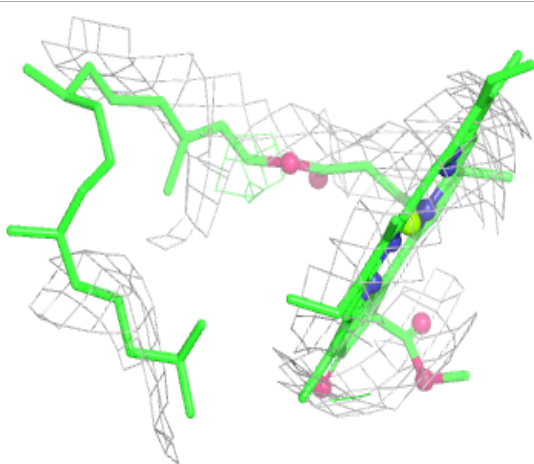
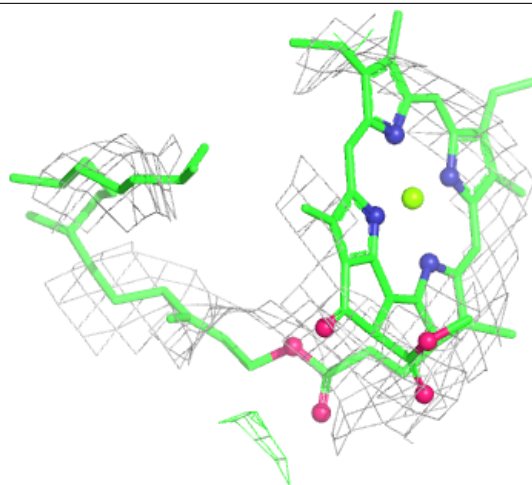
**Electron density around LMG D 409:**

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



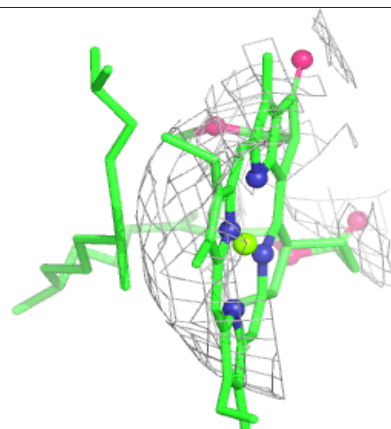
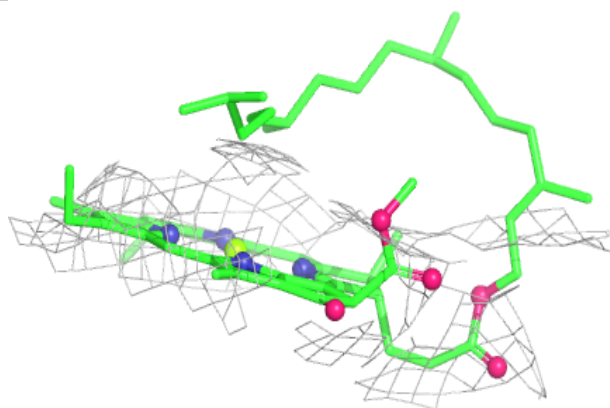
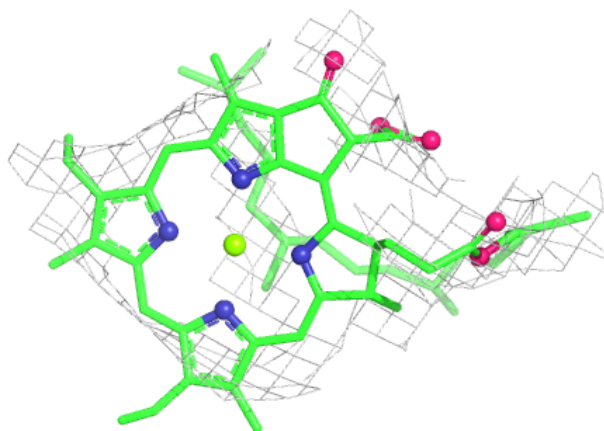
Electron density around CLA C 503:

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

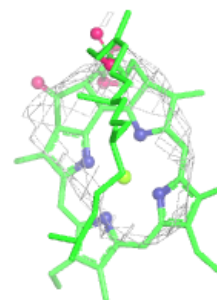
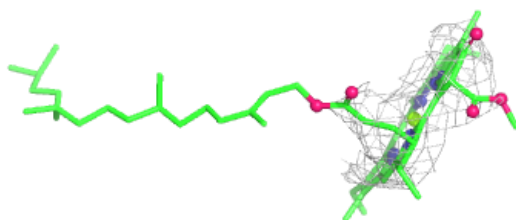
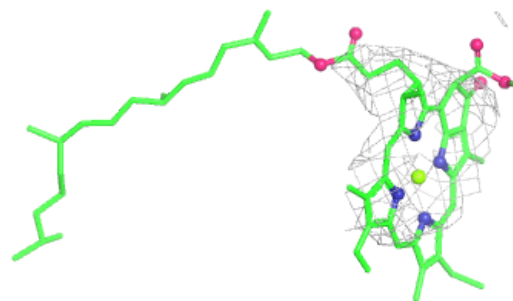


Electron density around CLA c 509:

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

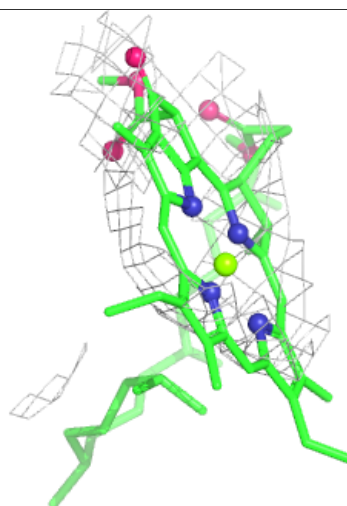
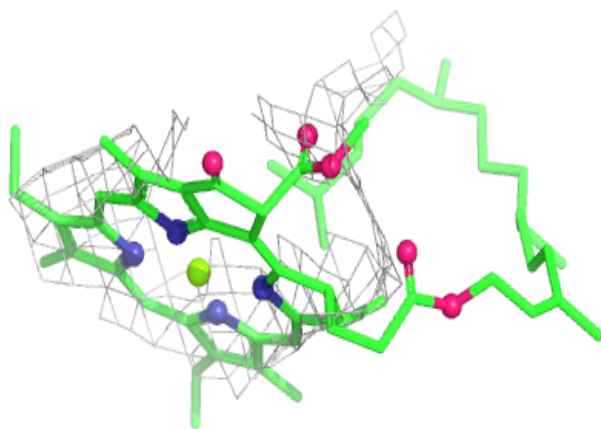
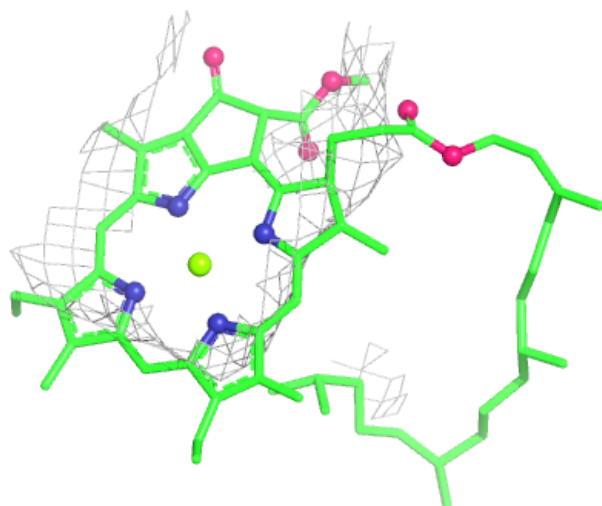
**Electron density around CLA B 608:**

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



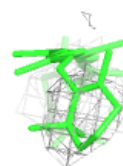
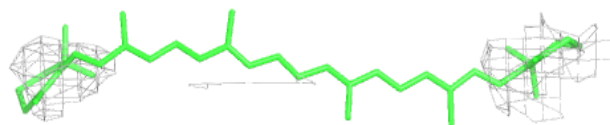
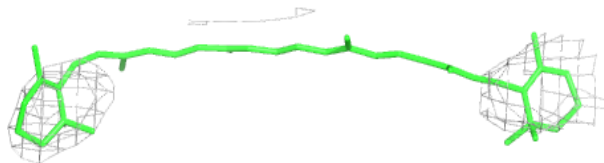
Electron density around CLA B 614:

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



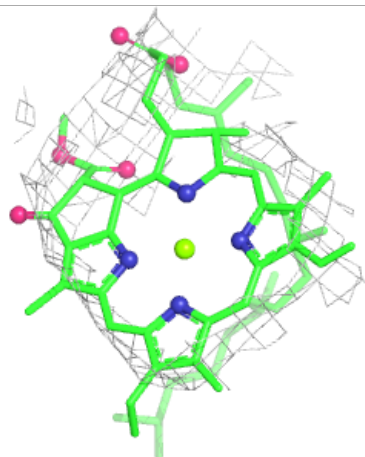
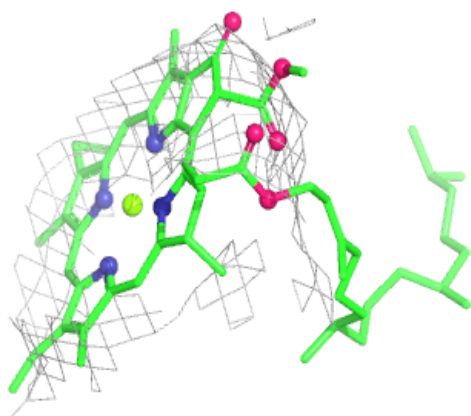
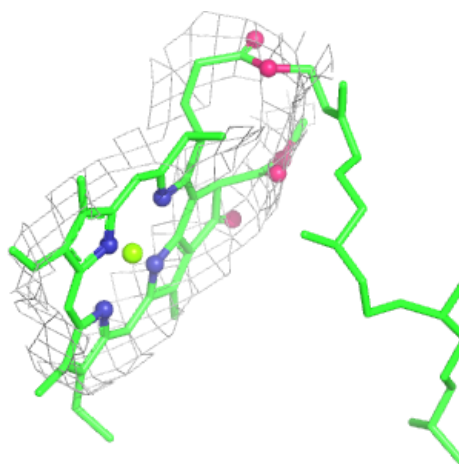
Electron density around BCR K 101:

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



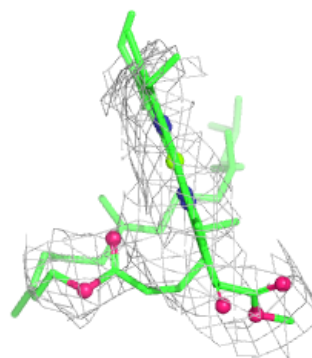
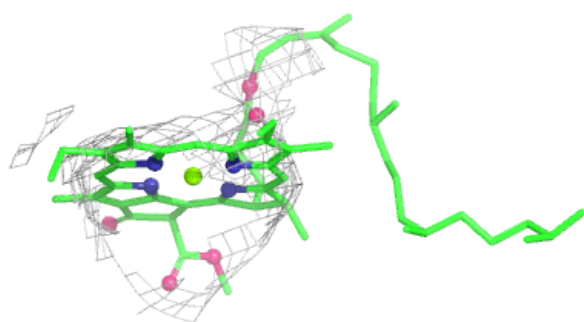
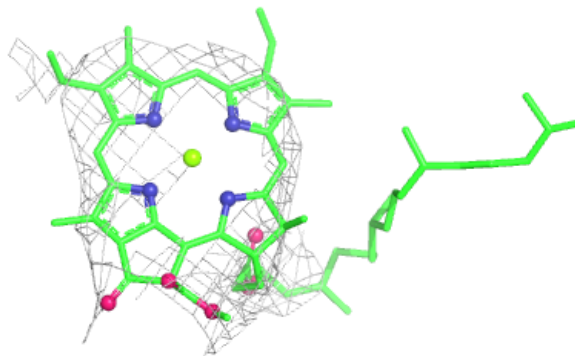
Electron density around CLA B 612:

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

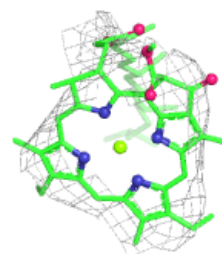
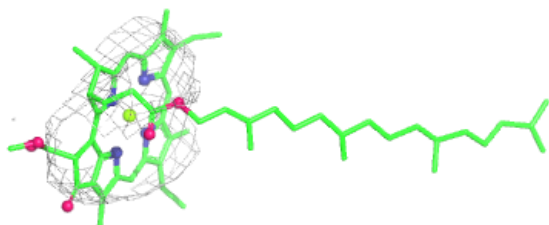
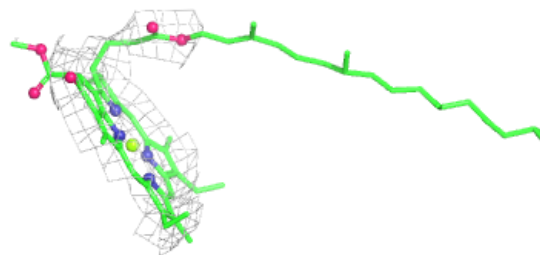


Electron density around CLA A 403:

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

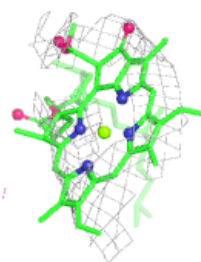
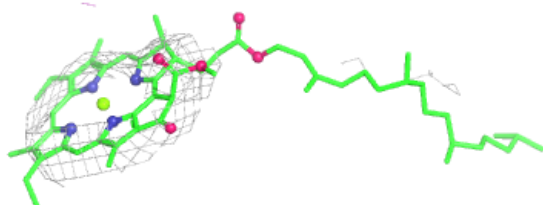
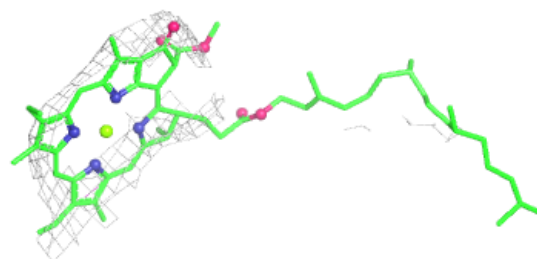
**Electron density around CLA B 606:**

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

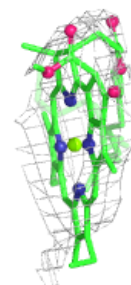
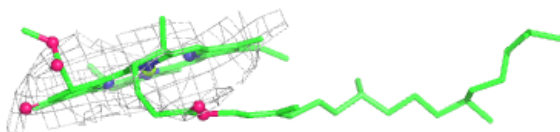
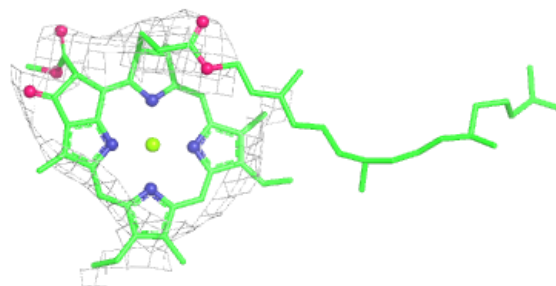


Electron density around CLA A 402:

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

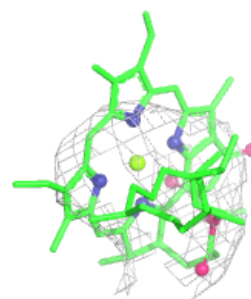
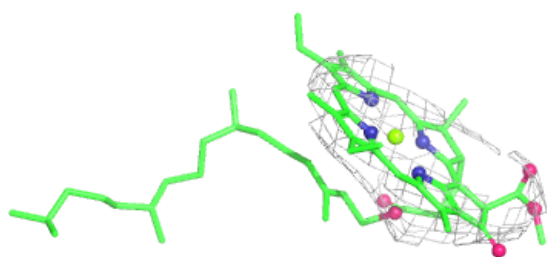
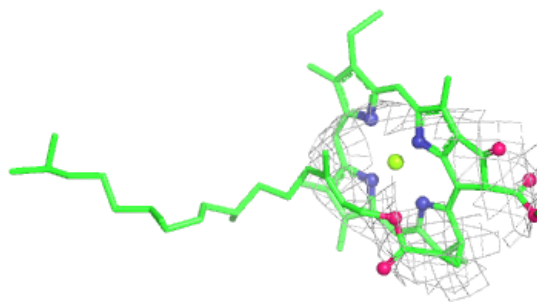
**Electron density around CLA B 602:**

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

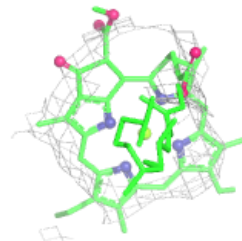
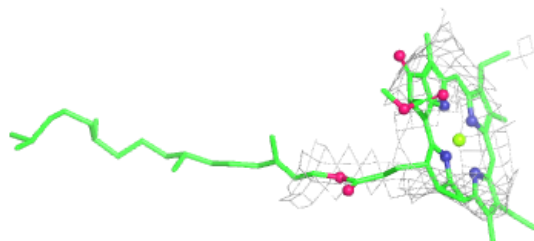
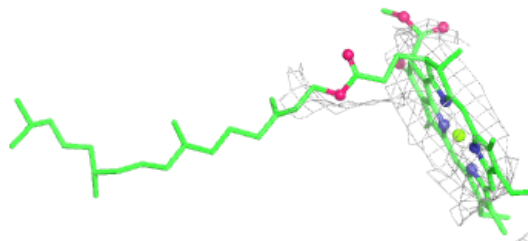


Electron density around CLA c 504:

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

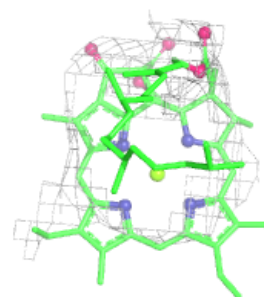
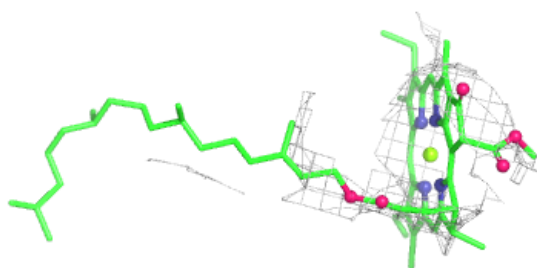
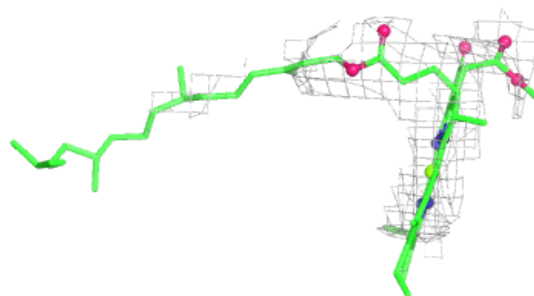
**Electron density around CLA B 603:**

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

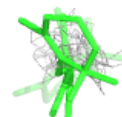
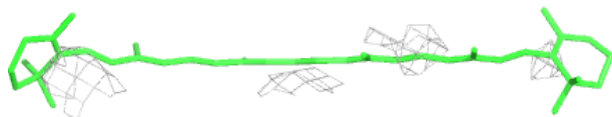
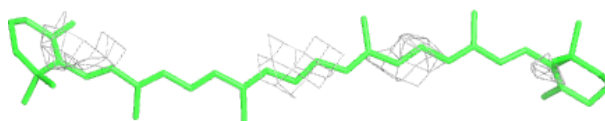


Electron density around CLA B 604:

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

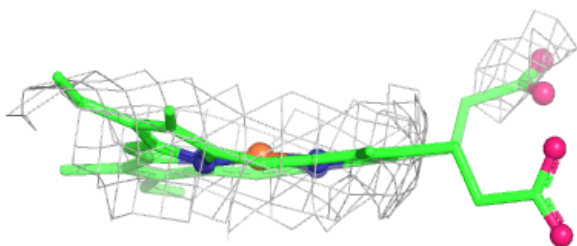
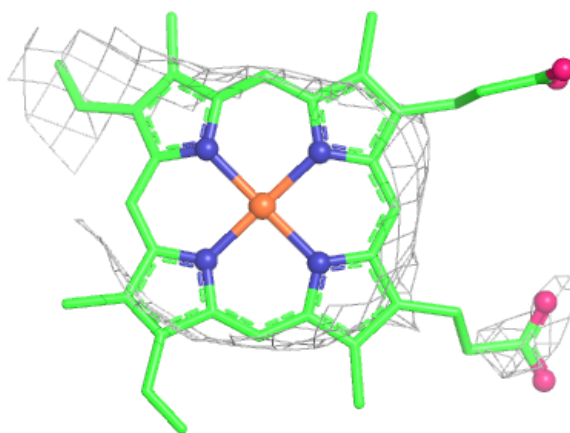
**Electron density around BCR B 618:**

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



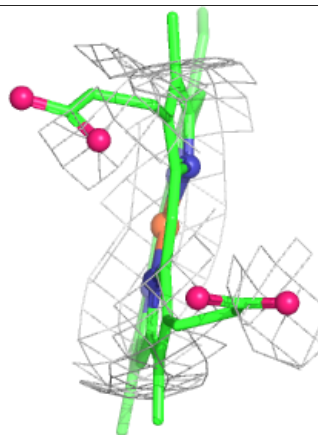
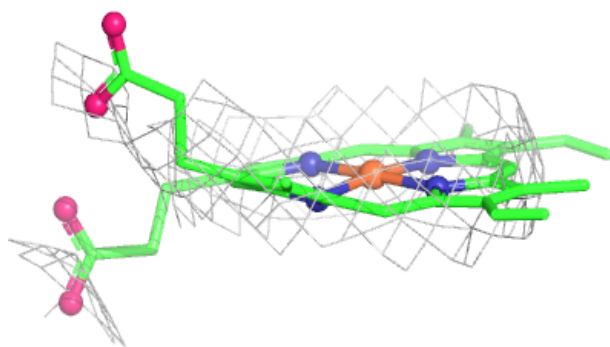
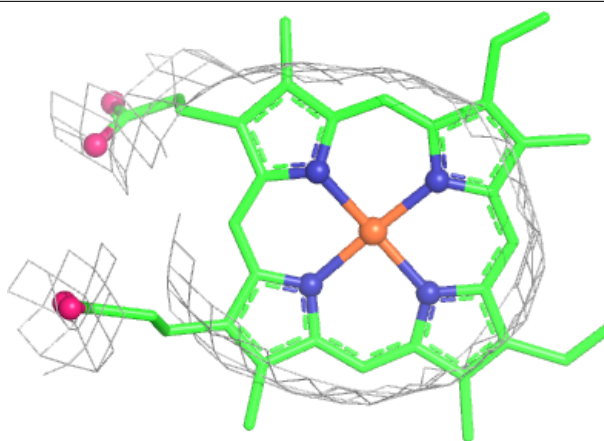
Electron density around HEM V 201:

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



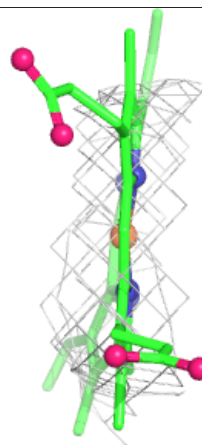
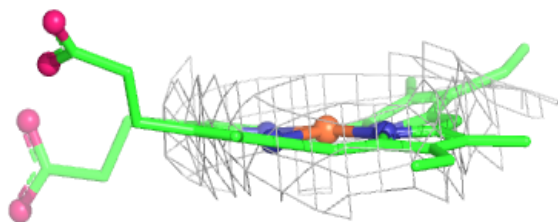
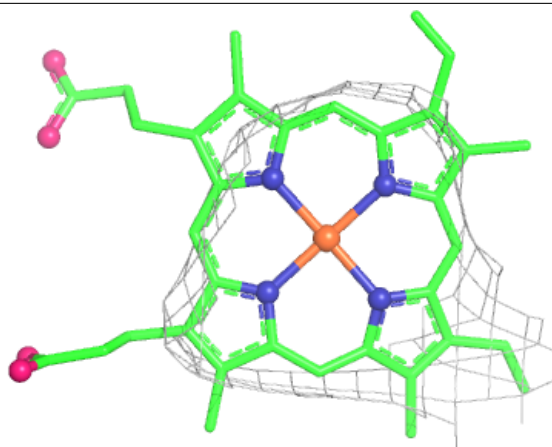
Electron density around HEM f 101:

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



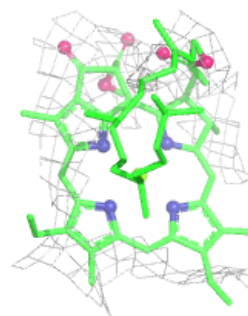
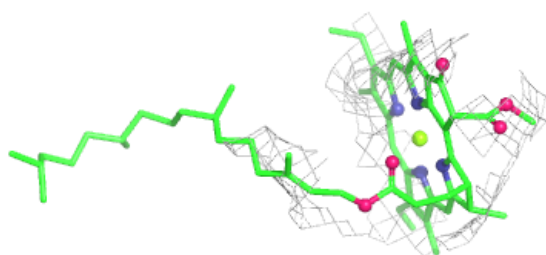
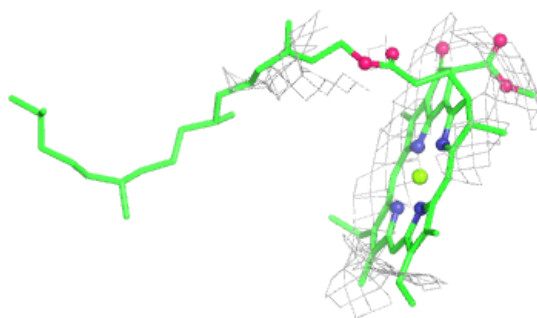
Electron density around HEM v 201:

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

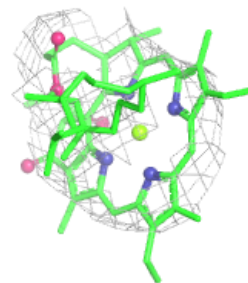
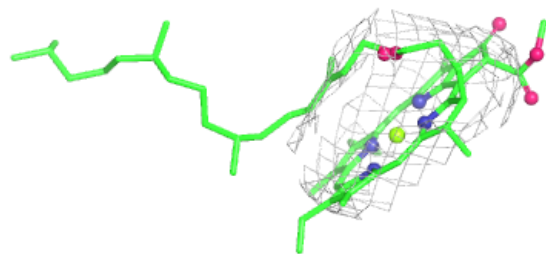
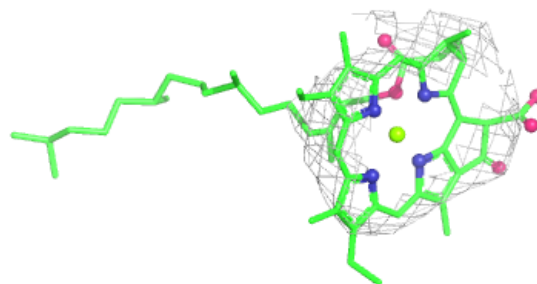


Electron density around CLA c 507:

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

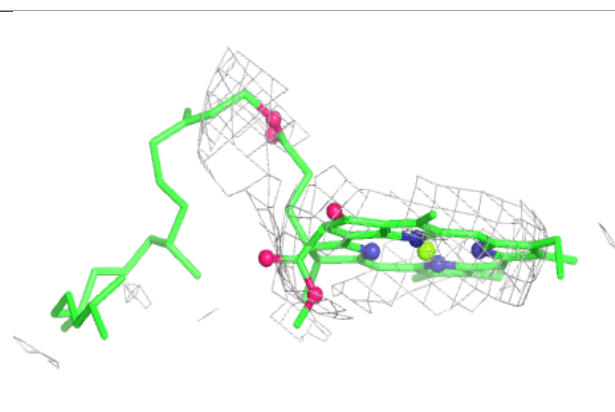
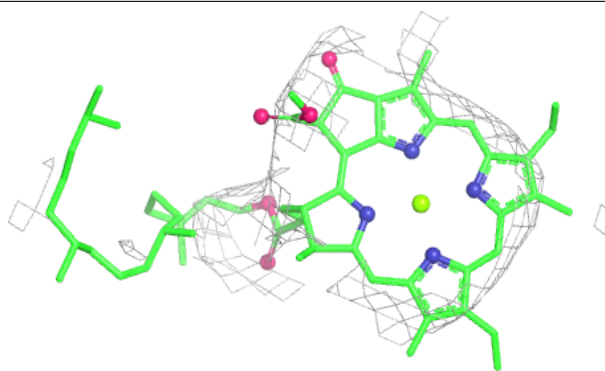
**Electron density around CLA C 504:**

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

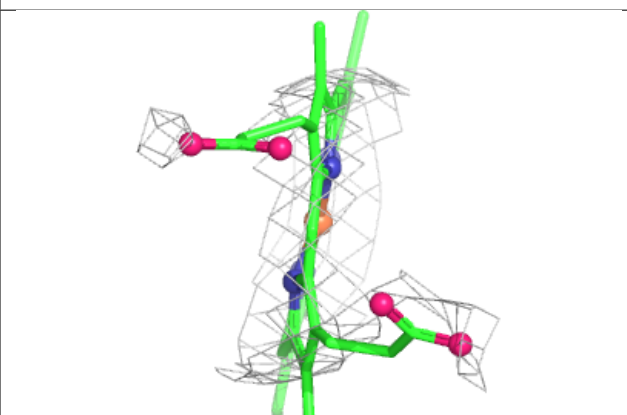
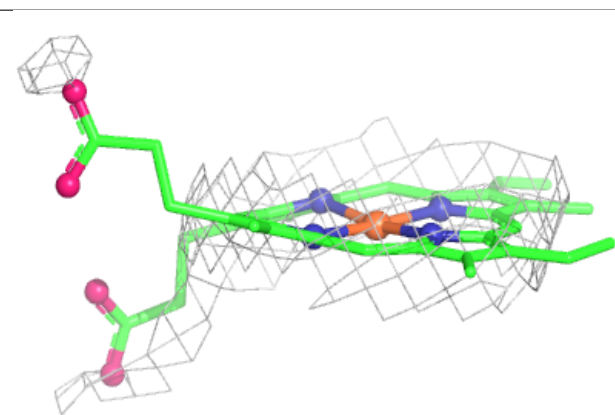
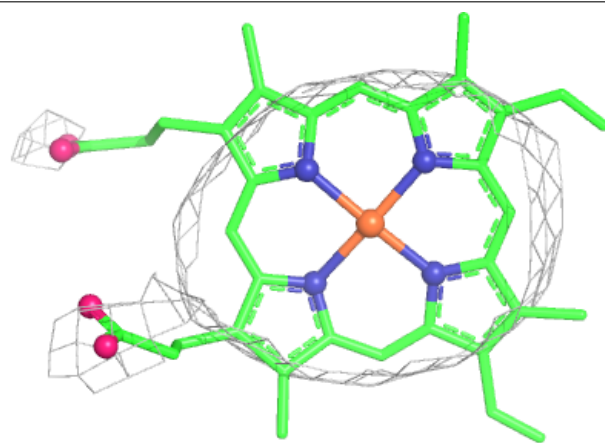


Electron density around CLA B 611:

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

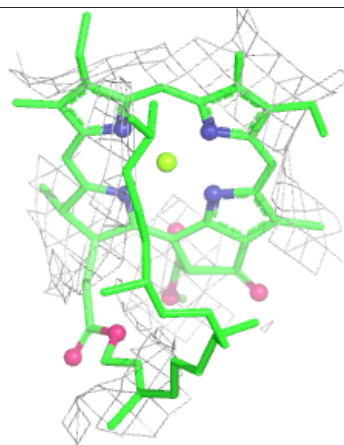
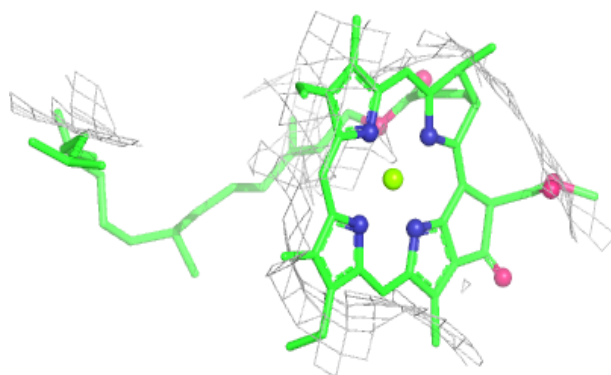
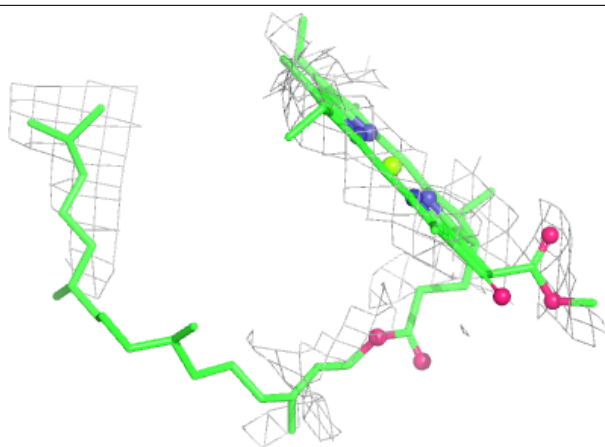
**Electron density around HEM F 101:**

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



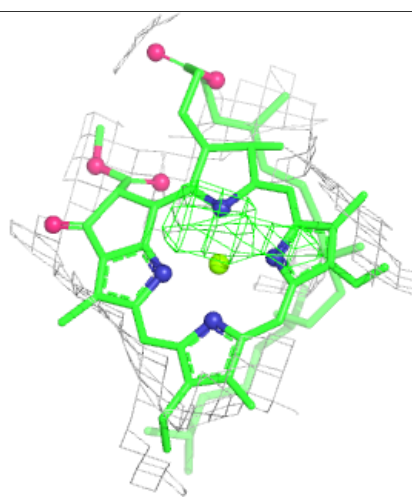
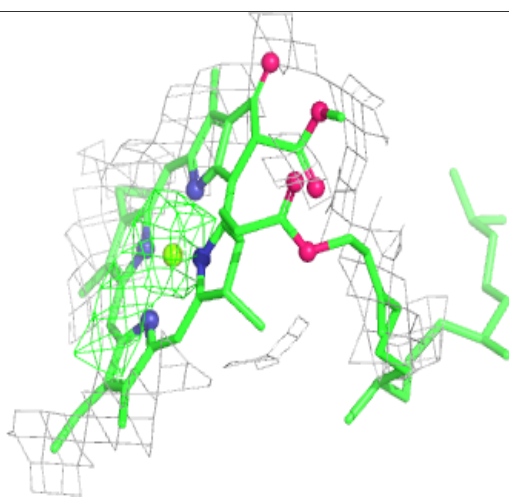
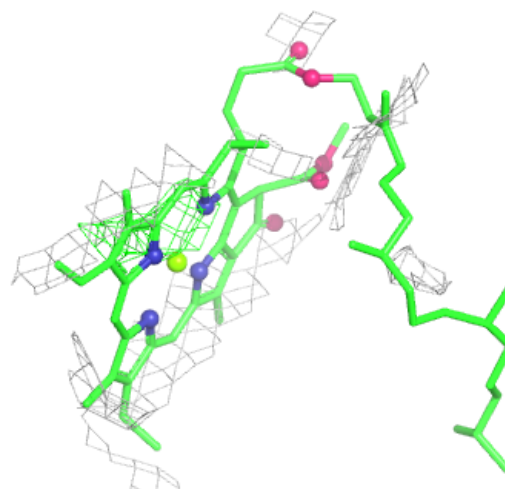
Electron density around CLA b 615:

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



Electron density around CLA b 617:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.