



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:23 PM UTC

PDB ID : 4TNH / pdb_00004tnh
Title : RT XFEL structure of Photosystem II in the dark state at 4.9 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 : 4.90 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)

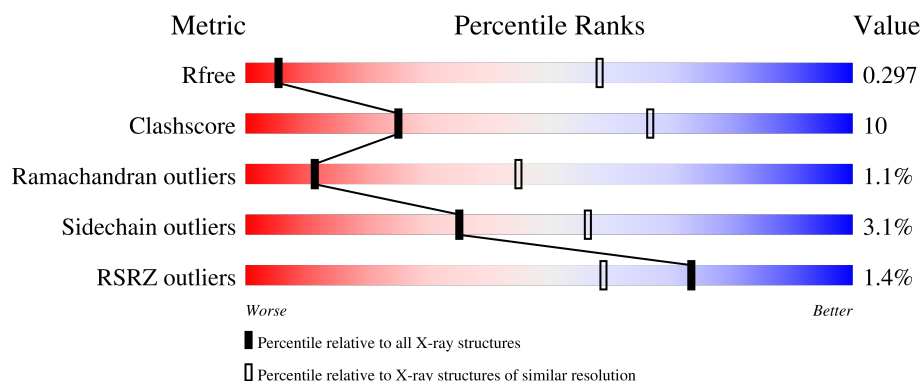
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.90 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	1007 (5.82-3.96)
Clashscore	190562	1020 (5.82-3.98)
Ramachandran outliers	187476	1123 (5.90-3.90)
Sidechain outliers	187428	1103 (5.90-3.90)
RSRZ outliers	180081	1002 (5.82-3.96)

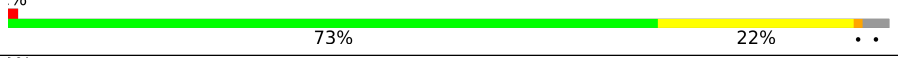
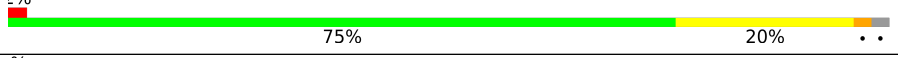
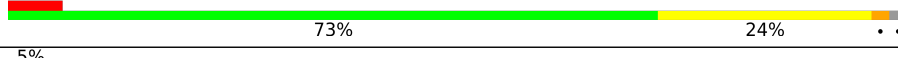
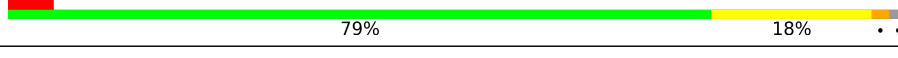
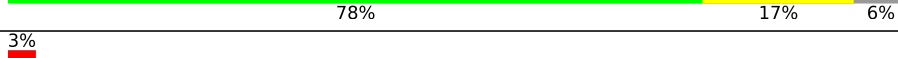
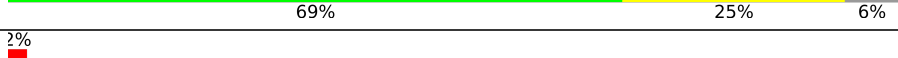
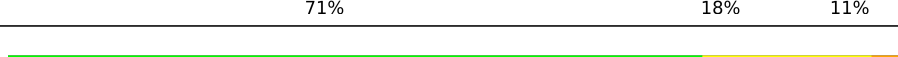
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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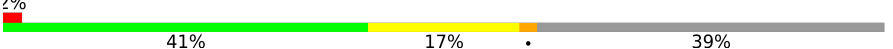
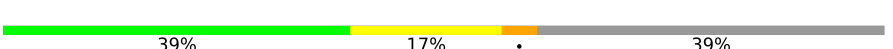
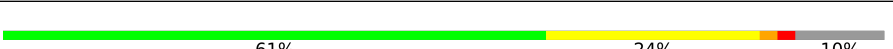
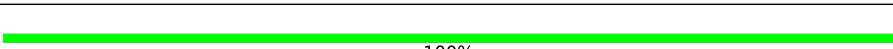
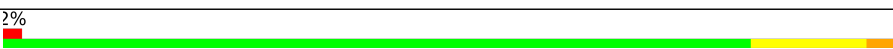
CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
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	
14	T	32	

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Mol	Chain	Length	Quality of chain
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	405	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	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	520	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	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	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	404	X	-	-	-
22	CLA	h	101	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				

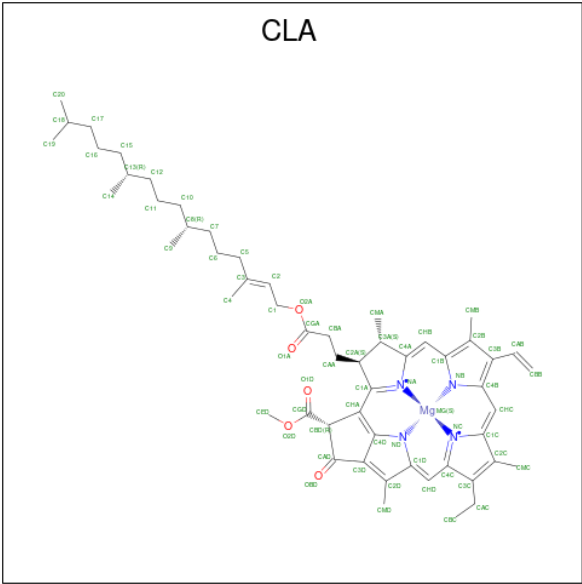
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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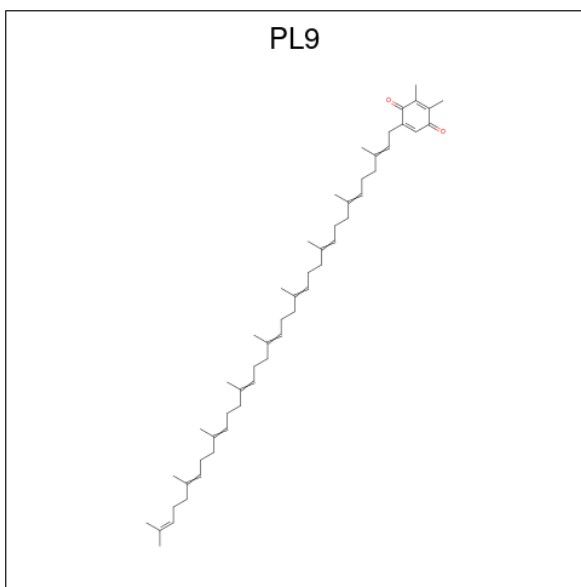
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22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55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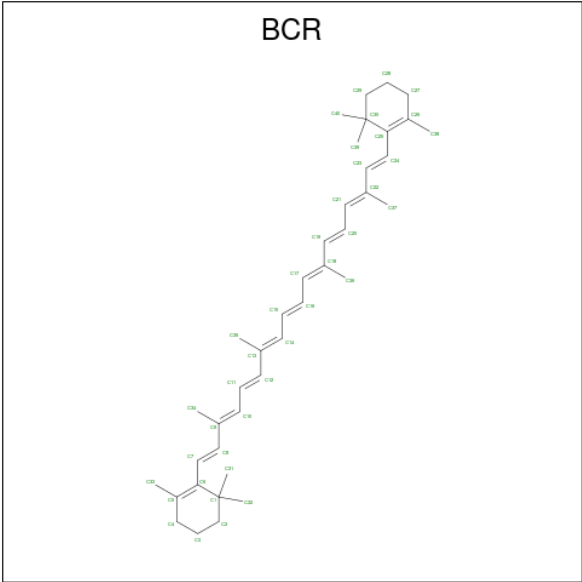
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 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
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	a	1	Total	C	O	0	0
			45	43	2		
23	d	1	Total	C	O	0	0
			55	53	2		
23	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



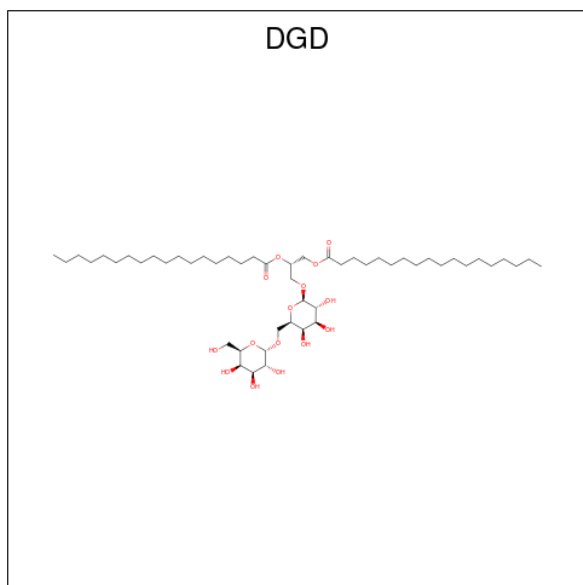
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



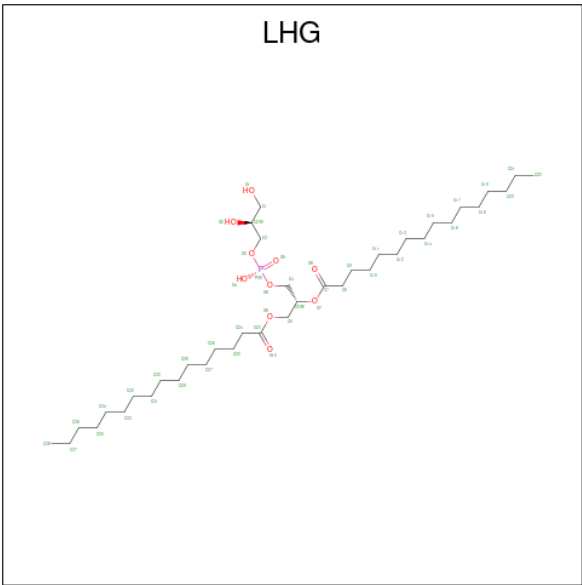
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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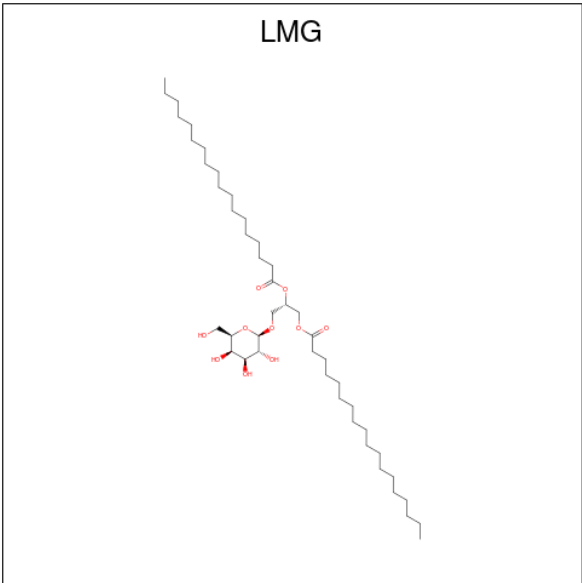
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

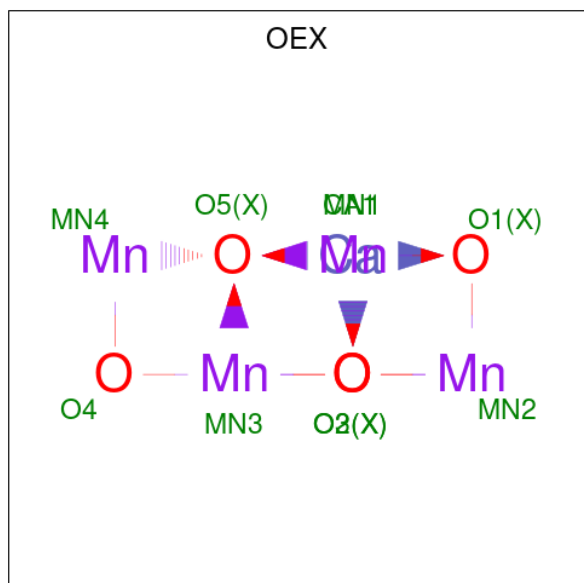


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total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

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

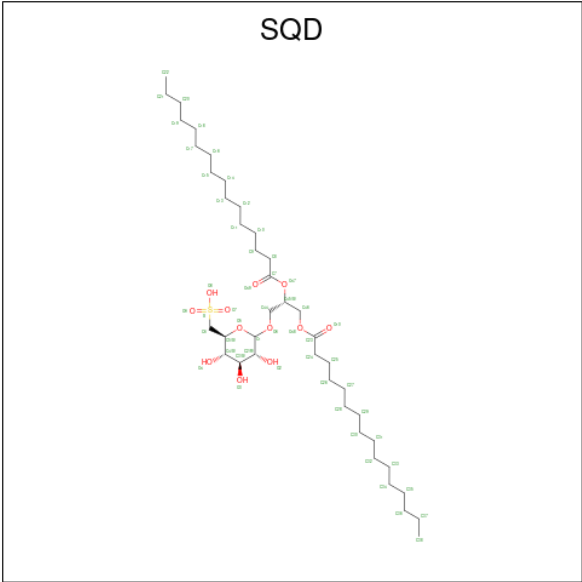
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

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



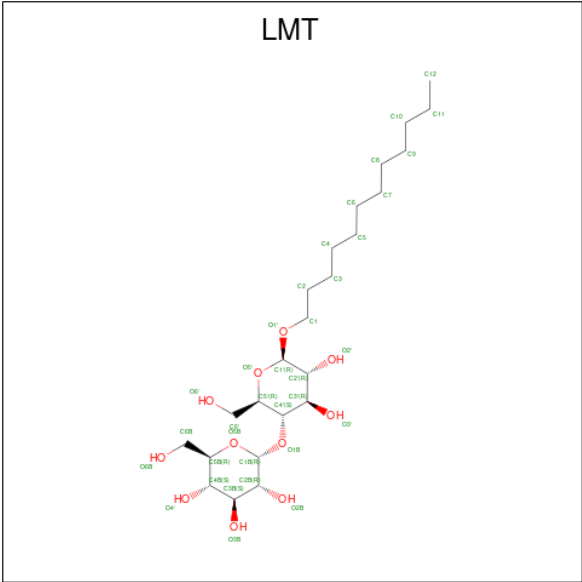
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



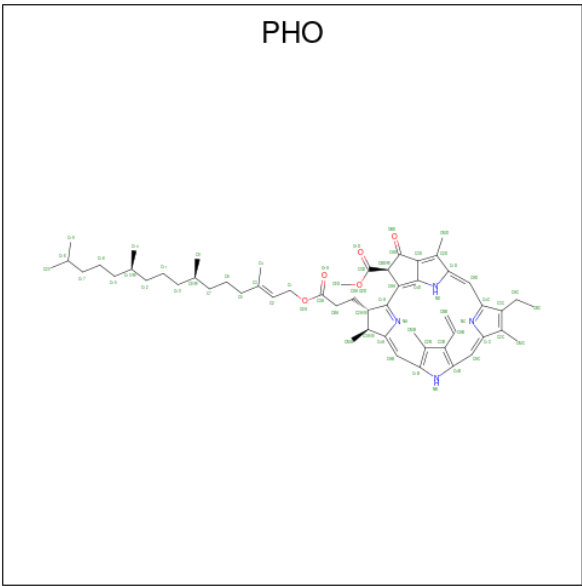
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			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 DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



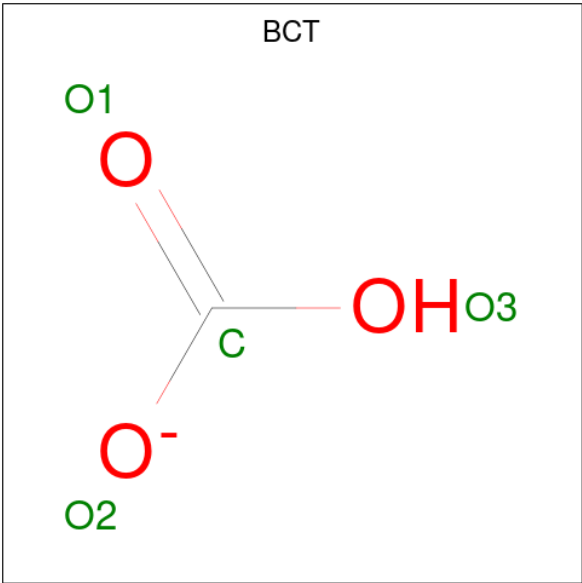
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total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

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



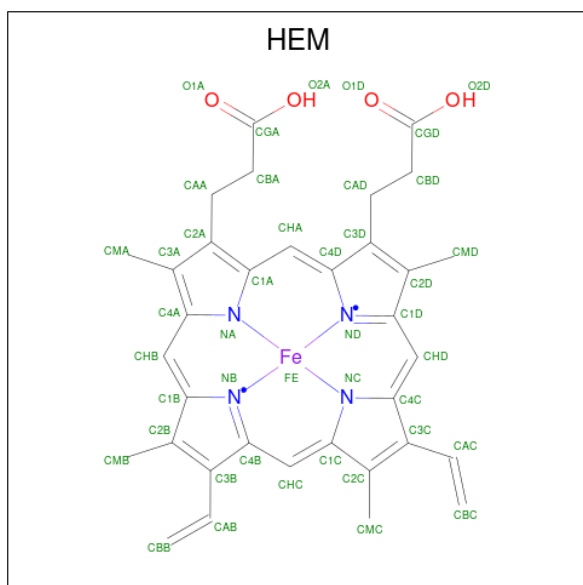
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	F	1	Total C Fe N O 43 34 1 4 4	0	0
34	V	1	Total C Fe N O 43 34 1 4 4	0	0
34	f	1	Total C Fe N O 43 34 1 4 4	0	0
34	v	1	Total C Fe N O 43 34 1 4 4	0	0

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

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

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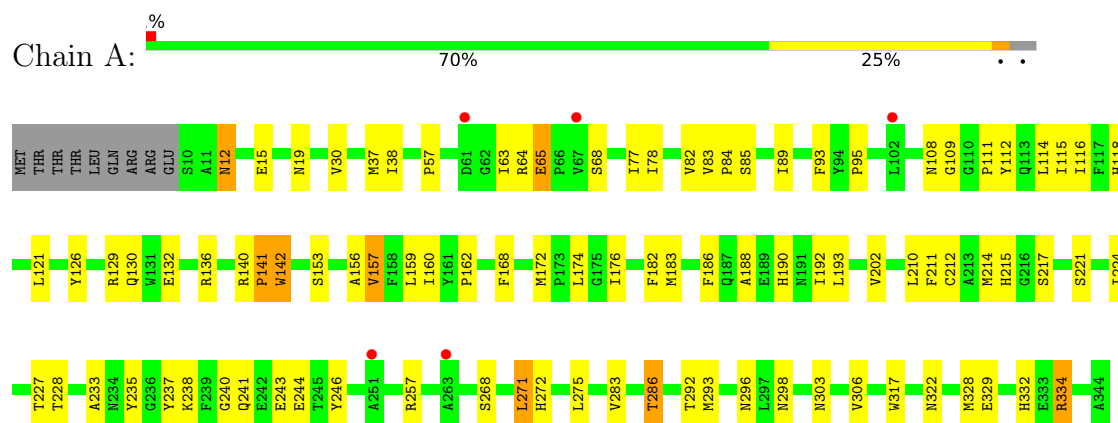
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total	Ca	0	0
			1	1		

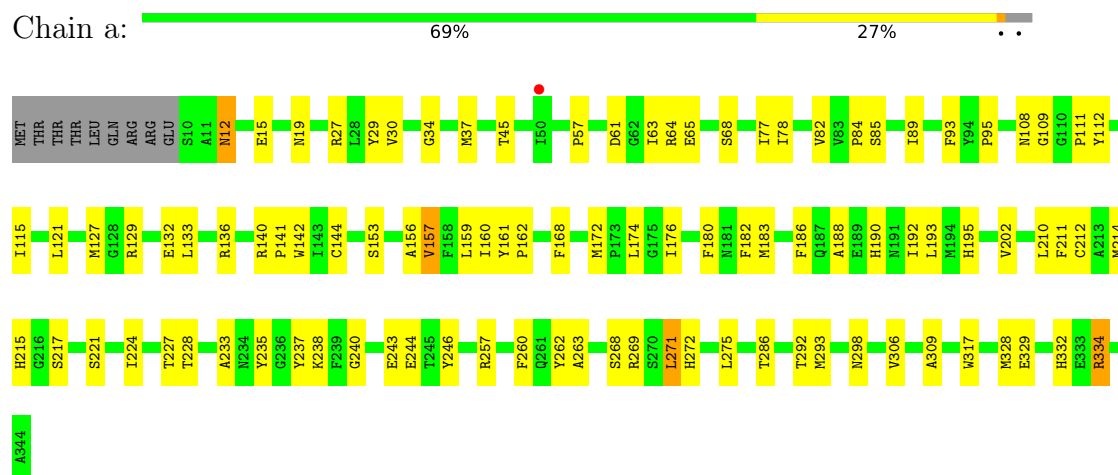
3 Residue-property plots [i](#)

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.

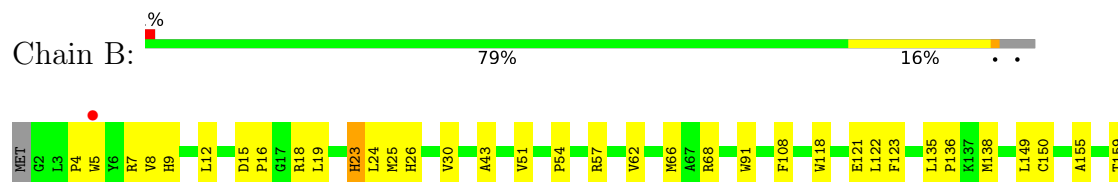
• Molecule 1: Photosystem Q(B) protein 1

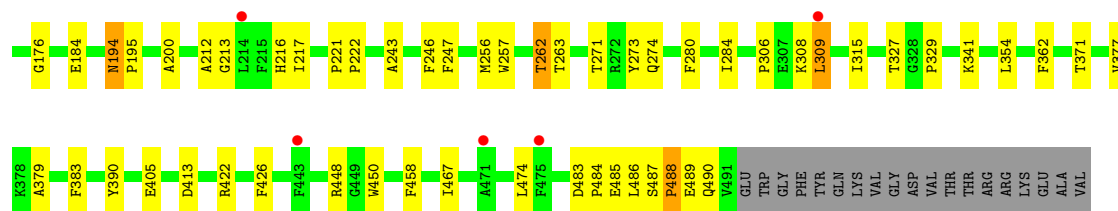


• Molecule 1: Photosystem Q(B) protein 1

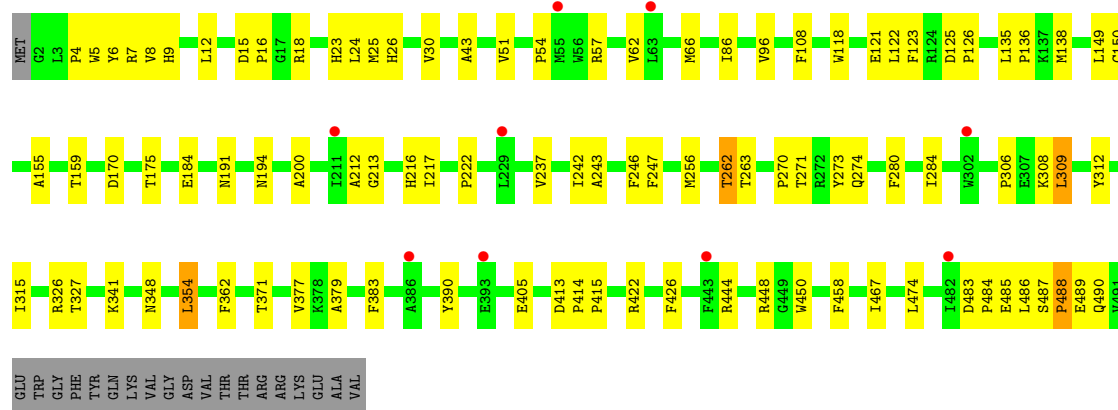
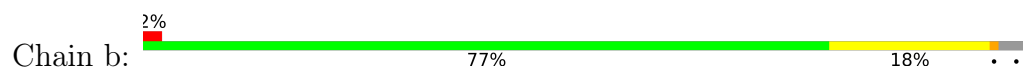


• Molecule 2: Photosystem II core light harvesting protein

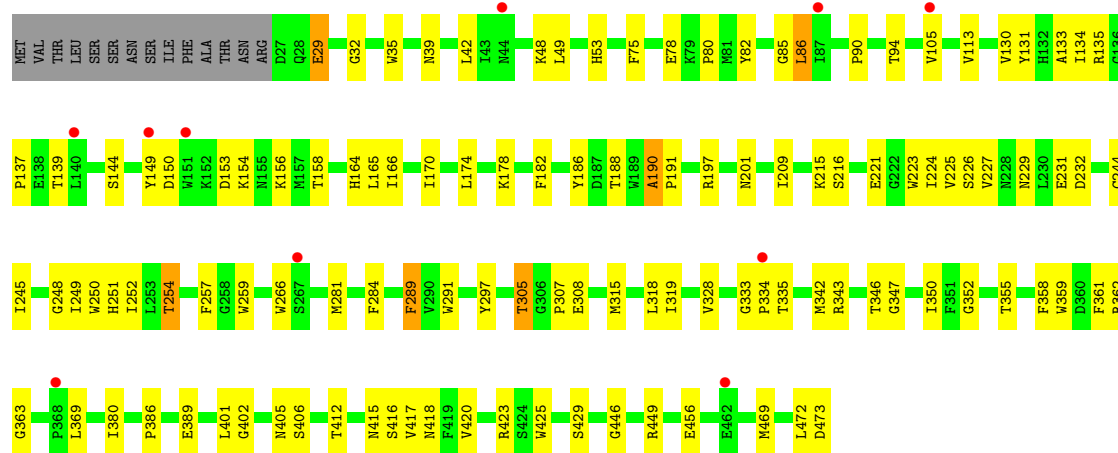




• Molecule 2: Photosystem II core light harvesting protein

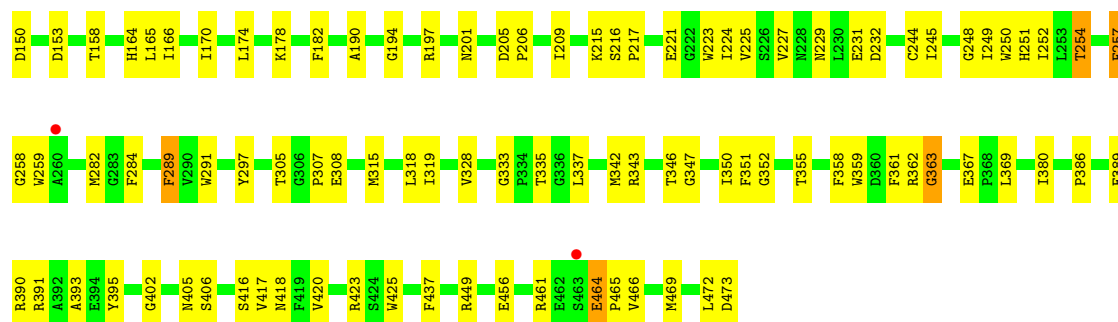


• Molecule 3: Photosystem II CP43 protein

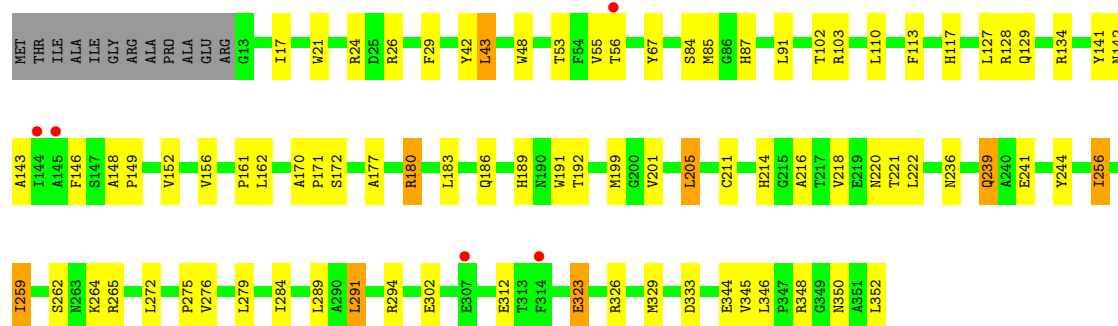
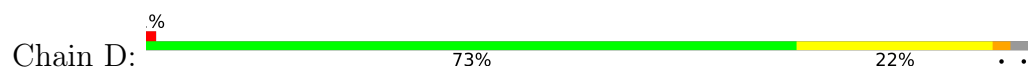


• Molecule 3: Photosystem II CP43 protein

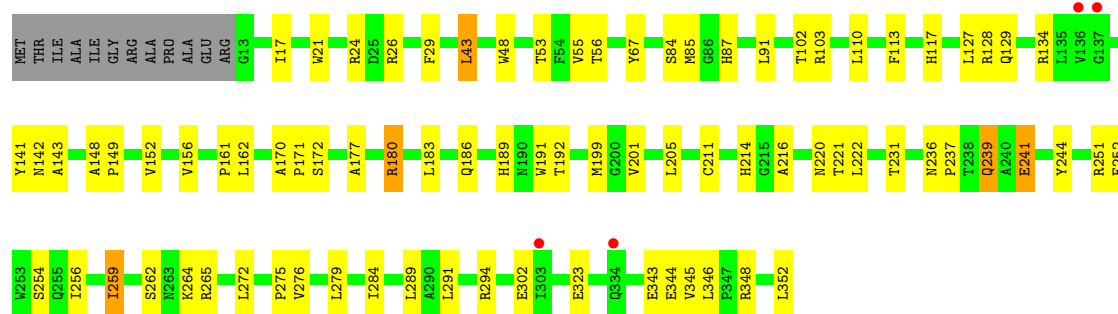
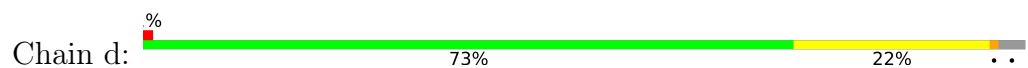




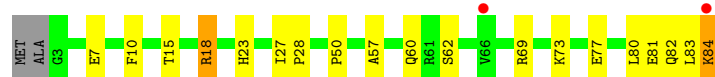
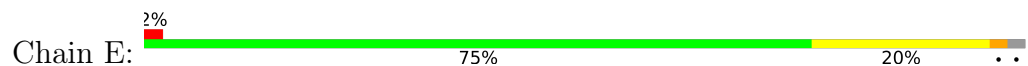
• Molecule 4: Photosystem II D2 protein



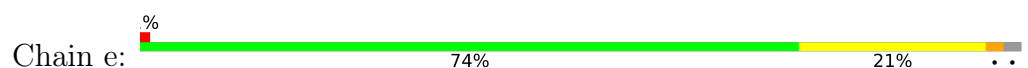
• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha





- Molecule 6: Cytochrome b559 subunit beta



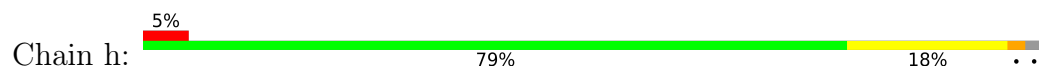
- Molecule 6: Cytochrome b559 subunit beta



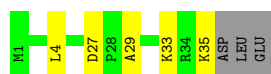
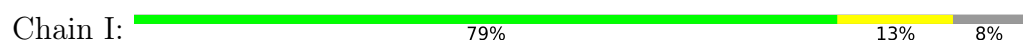
- Molecule 7: Photosystem II reaction center protein H



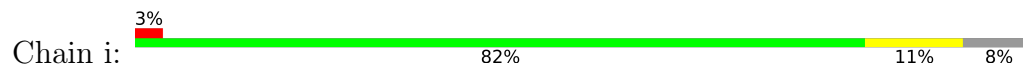
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

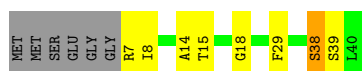


- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





- Molecule 9: Photosystem II reaction center protein J



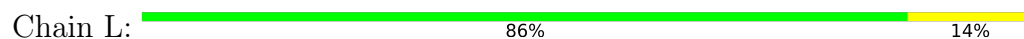
- Molecule 10: Photosystem II reaction center protein K



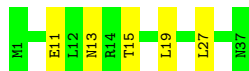
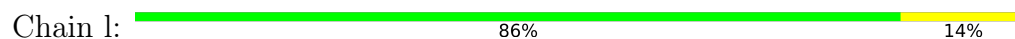
- Molecule 10: Photosystem II reaction center protein K



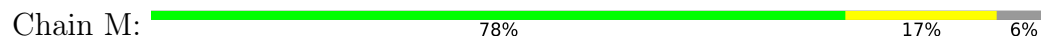
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

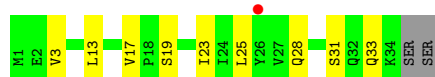


- Molecule 12: Photosystem II reaction center protein M

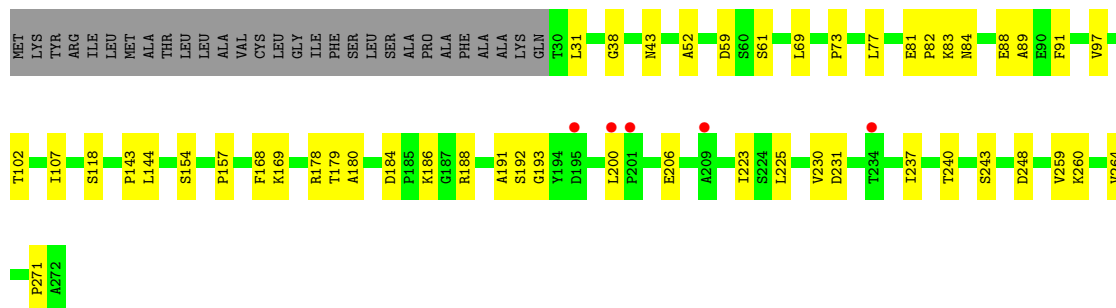


- Molecule 12: Photosystem II reaction center protein M

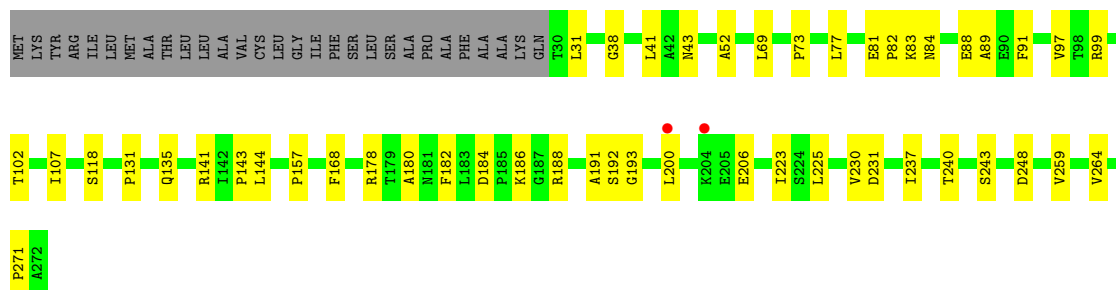




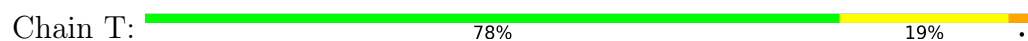
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



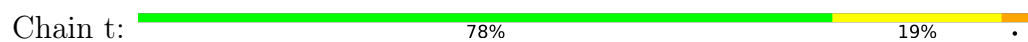
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T

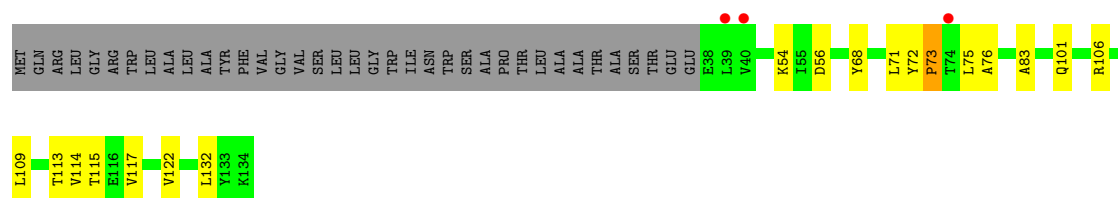


- Molecule 14: Photosystem II reaction center protein T

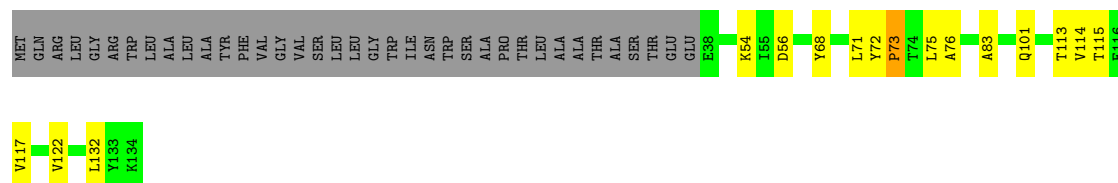


- Molecule 15: Photosystem II 12 kDa extrinsic protein

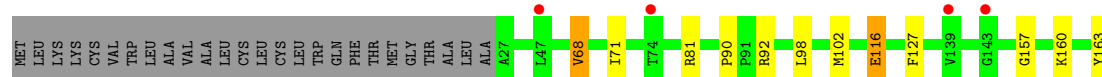
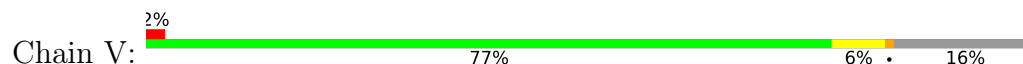




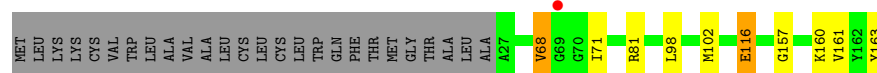
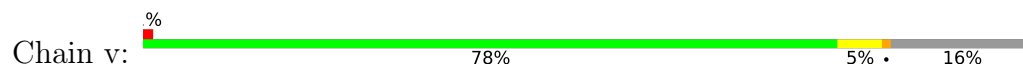
• Molecule 15: Photosystem II 12 kDa extrinsic protein



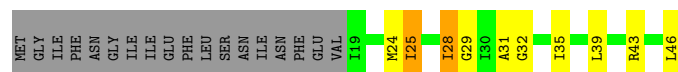
• Molecule 16: Cytochrome c-550



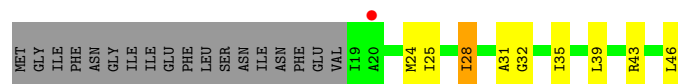
• Molecule 16: Cytochrome c-550



• Molecule 17: Photosystem II reaction center protein Ycf12

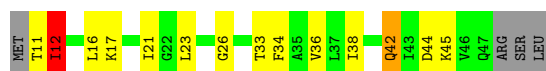


• Molecule 17: Photosystem II reaction center protein Ycf12



• Molecule 18: Photosystem II reaction center X protein





- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Y



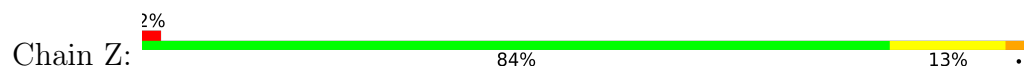
There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

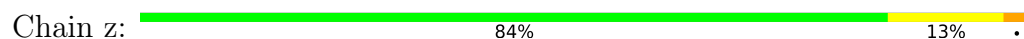


There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.88Å 229.03Å 307.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 4.90 72.93 – 4.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (72.93-4.90) 97.8 (72.93-4.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.281 , 0.292 0.287 , 0.297	Depositor DCC
R_{free} test set	2096 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	173.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 153.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	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)	206.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: OEX, BCT, LMG, CLA, HEM, PHO, CL, FE2, LMT, LHG, BCR, SQD, CA, PL9, DGD

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	0.30	0/2713	0.78	2/3700 (0.1%)
1	a	0.31	0/2713	0.78	2/3700 (0.1%)
2	B	0.30	0/3986	0.81	8/5433 (0.1%)
2	b	0.30	0/3986	0.81	8/5433 (0.1%)
3	C	0.30	0/3556	0.79	6/4842 (0.1%)
3	c	0.30	0/3556	0.80	8/4842 (0.2%)
4	D	0.29	0/2801	0.76	0/3818
4	d	0.30	0/2801	0.76	0/3818
5	E	0.31	0/685	0.83	0/933
5	e	0.32	0/685	0.83	0/933
6	F	0.33	0/291	0.75	0/397
6	f	0.33	0/291	0.73	0/397
7	H	0.33	0/520	0.73	0/709
7	h	0.33	0/520	0.74	0/709
8	I	0.30	0/293	0.77	0/395
8	i	0.29	0/293	0.77	0/395
9	J	0.30	0/255	0.84	0/346
9	j	0.31	0/255	0.84	0/346
10	K	0.45	0/303	0.86	0/416
10	k	0.45	0/303	0.86	0/416
11	L	0.28	0/311	0.71	0/422
11	l	0.28	0/311	0.72	0/422
12	M	0.30	0/270	0.78	0/367
12	m	0.33	0/270	0.85	1/367 (0.3%)
13	O	0.28	0/1876	0.71	2/2548 (0.1%)
13	o	0.27	0/1876	0.71	2/2548 (0.1%)
14	T	0.27	0/284	0.75	0/381
14	t	0.27	0/284	0.74	0/381
15	U	0.29	0/785	0.77	0/1064
15	u	0.29	0/785	0.78	0/1064
16	V	0.29	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	0.32	0/202	0.79	0/272
17	y	0.32	0/202	0.76	0/272
18	X	0.39	0/273	0.80	0/370
18	x	0.37	0/273	0.79	0/370
20	Z	0.31	0/490	0.83	0/669
20	z	0.31	0/490	0.84	0/669
All	All	0.30	0/41950	0.78	41/57100 (0.1%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	483	ASP	CA-C-N	10.63	133.13	119.84
2	b	483	ASP	C-N-CA	10.63	133.13	119.84
2	B	483	ASP	CA-C-N	10.59	133.08	119.84
2	B	483	ASP	C-N-CA	10.59	133.08	119.84
3	c	190	ALA	CA-C-N	6.24	125.73	119.24
3	c	190	ALA	C-N-CA	6.24	125.73	119.24
3	C	190	ALA	CA-C-N	6.20	125.68	119.24
3	C	190	ALA	C-N-CA	6.20	125.68	119.24
3	c	363	GLY	CA-C-N	6.18	125.67	119.24
3	c	363	GLY	C-N-CA	6.18	125.67	119.24
2	b	413	ASP	CA-C-N	5.91	126.47	120.38
2	b	413	ASP	C-N-CA	5.91	126.47	120.38
3	C	363	GLY	CA-C-N	5.85	125.33	119.24
3	C	363	GLY	C-N-CA	5.85	125.33	119.24
2	b	15	ASP	CA-C-N	5.71	125.83	119.32
2	b	15	ASP	C-N-CA	5.71	125.83	119.32
2	B	413	ASP	CA-C-N	5.56	126.11	120.38
2	B	413	ASP	C-N-CA	5.56	126.11	120.38
2	B	194	ASN	CA-C-N	5.45	125.09	119.05
2	B	194	ASN	C-N-CA	5.45	125.09	119.05
2	B	15	ASP	CA-C-N	5.35	125.42	119.32
2	B	15	ASP	C-N-CA	5.35	125.42	119.32
2	b	194	ASN	CA-C-N	5.32	124.96	119.05
2	b	194	ASN	C-N-CA	5.32	124.96	119.05
16	V	127	PHE	CA-C-N	5.28	126.44	119.84
16	V	127	PHE	C-N-CA	5.28	126.44	119.84
1	a	195	HIS	CA-C-N	5.25	125.31	119.32
1	a	195	HIS	C-N-CA	5.25	125.31	119.32
3	c	333	GLY	CA-C-N	5.25	126.41	119.84
3	c	333	GLY	C-N-CA	5.25	126.41	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	200	LEU	CA-C-N	5.23	125.28	119.32
13	o	200	LEU	C-N-CA	5.23	125.28	119.32
3	C	333	GLY	CA-C-N	5.18	126.31	119.84
3	C	333	GLY	C-N-CA	5.18	126.31	119.84
12	m	17	VAL	CB-CA-C	-5.13	108.82	113.70
1	A	65	GLU	CA-C-N	5.10	125.39	119.93
1	A	65	GLU	C-N-CA	5.10	125.39	119.93
3	c	464	GLU	CA-C-N	5.08	126.19	119.84
3	c	464	GLU	C-N-CA	5.08	126.19	119.84
13	O	200	LEU	CA-C-N	5.02	125.05	119.32
13	O	200	LEU	C-N-CA	5.02	125.05	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	75	0
1	a	2628	0	2524	71	0
2	B	3850	0	3718	60	0
2	b	3850	0	3718	64	0
3	C	3444	0	3365	76	0
3	c	3444	0	3365	78	0
4	D	2706	0	2608	66	0
4	d	2706	0	2608	61	0
5	E	666	0	651	13	0
5	e	666	0	651	13	0
6	F	282	0	291	6	0
6	f	282	0	291	6	0
7	H	507	0	521	12	0
7	h	507	0	521	13	0
8	I	286	0	308	3	0
8	i	286	0	308	2	0
9	J	249	0	262	6	0
9	j	249	0	262	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	293	0	305	9	0
10	k	293	0	305	12	0
11	L	304	0	316	4	0
11	l	304	0	316	4	0
12	M	267	0	289	6	0
12	m	267	0	289	8	0
13	O	1845	0	1801	28	0
13	o	1845	0	1801	30	0
14	T	275	0	288	6	0
14	t	275	0	288	6	0
15	U	774	0	773	8	0
15	u	774	0	773	7	0
16	V	1060	0	1068	8	0
16	v	1060	0	1068	8	0
17	g	201	0	226	7	0
17	y	201	0	226	8	0
18	X	270	0	299	10	0
18	x	270	0	299	9	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	8	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	27	0
22	B	975	0	1080	56	0
22	C	845	0	936	29	0
22	D	130	0	144	14	0
22	H	65	0	72	9	0
22	a	260	0	288	26	0
22	b	975	0	1080	50	0
22	c	845	0	936	32	0
22	d	130	0	144	11	0
22	h	65	0	72	10	0
23	A	45	0	61	5	0
23	D	55	0	80	8	0
23	J	35	0	45	0	0
23	a	45	0	61	4	0
23	d	55	0	80	6	0
23	j	35	0	45	0	0
24	A	40	0	56	2	0
24	B	160	0	224	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	80	0	112	10	0
24	F	40	0	56	3	0
24	H	40	0	56	2	0
24	J	40	0	56	2	0
24	K	40	0	56	3	0
24	a	40	0	56	4	0
24	b	160	0	224	12	0
24	c	120	0	168	13	0
24	f	40	0	56	1	0
24	g	40	0	56	5	0
24	j	40	0	56	1	0
24	x	40	0	56	0	0
24	y	40	0	56	6	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	12	0
25	D	63	0	87	1	0
25	a	56	0	70	3	0
25	b	110	0	136	4	0
25	c	181	0	245	11	0
25	d	63	0	87	1	0
26	A	39	0	51	3	0
26	C	37	0	44	3	0
26	a	39	0	51	1	0
26	c	37	0	44	2	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	2	0
27	D	143	0	196	9	0
27	E	44	0	58	1	0
27	I	43	0	56	0	0
27	M	42	0	54	1	0
27	a	42	0	54	1	0
27	b	49	0	68	4	0
27	c	93	0	126	3	0
27	d	143	0	196	10	0
27	e	44	0	58	2	0
27	i	43	0	56	1	0
27	l	51	0	72	2	0
27	m	42	0	54	2	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	8	0
30	B	90	0	111	5	0
30	F	45	0	54	2	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	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	0	0
31	M	70	0	92	0	0
31	b	140	0	183	5	0
31	d	31	0	35	0	0
31	i	35	0	46	1	0
32	D	128	0	148	11	0
32	a	64	0	74	4	0
32	d	64	0	74	5	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	4	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	51373	983	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 (983) 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	1.57	0.86
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.56	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.82
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:362:ARG:H	25:c:515:DGD:HE4	1.46	0.80
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.80
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.63	0.79
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.66	0.78
13:o:82:PRO:HG3	13:o:89:ALA:HB2	1.67	0.77
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.69	0.74
22:b:609:CLA:H72	24:b:623:BCR:H311	1.69	0.73
34:v:201:HEM:HBC2	34:v:201:HEM:HHD	1.69	0.73
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.71	0.73
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.71	0.73
22:B:605:CLA:H72	24:B:619:BCR:H311	1.71	0.73
3:C:362:ARG:H	25:C:515:DGD:HE4	1.53	0.72
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.55	0.72
13:o:69:LEU:HB3	13:o:107:ILE:HB	1.72	0.71
4:d:199:MET:HG2	23:d:406:PL9:H322	1.72	0.71
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.72	0.71
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.73	0.70
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.73	0.70
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.72	0.70
1:a:129:ARG:HH21	4:d:256:ILE:HD12	1.55	0.70
3:c:165:LEU:HD21	22:c:505:CLA:HAB	1.73	0.70
1:a:192:ILE:HA	1:a:293:MET:HE1	1.73	0.69
4:D:29:PHE:O	4:D:128:ARG:NH2	2.25	0.69
4:D:199:MET:HG2	23:D:406:PL9:H322	1.75	0.69
10:K:21:LEU:HD13	17:y:24:MET:HE2	1.74	0.69
1:a:63:ILE:HB	3:c:335:THR:HG21	1.73	0.69
22:C:506:CLA:H112	24:C:514:BCR:H362	1.75	0.69
10:k:21:LEU:HD13	17:g:24:MET:HE2	1.75	0.68
4:D:259:ILE:HG12	27:D:408:LMG:H292	1.76	0.68
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.76	0.68
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.76	0.68
5:e:60:GLN:OE1	5:e:84:LYS:NZ	2.27	0.68
16:v:102:MET:HE3	34:v:201:HEM:HBB2	1.76	0.68
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.76	0.68
25:c:517:DGD:HAF2	22:c:520:CLA:H202	1.76	0.68
4:d:259:ILE:HG12	27:d:408:LMG:H292	1.75	0.67
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.75	0.67
24:b:621:BCR:H19C	24:b:622:BCR:H363	1.77	0.67
17:y:35:ILE:HG22	20:Z:21:ILE:HG23	1.77	0.67
4:d:152:VAL:HG21	4:d:279:LEU:HD12	1.76	0.67
1:A:15:GLU:O	1:A:19:ASN:ND2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.77	0.67
4:d:21:TRP:O	4:d:26:ARG:NH2	2.26	0.67
30:d:402:SQD:H301	30:d:402:SQD:H171	1.77	0.67
1:A:192:ILE:HA	1:A:293:MET:HE1	1.76	0.66
16:V:102:MET:HE3	34:V:201:HEM:HBB2	1.77	0.66
1:a:190:HIS:HB3	1:a:293:MET:HE2	1.76	0.66
4:d:236:ASN:ND2	4:d:239:GLN:O	2.29	0.66
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.76	0.66
2:b:24:LEU:HD21	22:b:619:CLA:HAB	1.76	0.66
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.76	0.66
22:c:507:CLA:HBC3	22:c:509:CLA:H92	1.77	0.66
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.66
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
4:d:189:HIS:HA	4:d:294:ARG:HD2	1.77	0.65
1:A:174:LEU:HD22	32:D:401:PHO:H151	1.79	0.65
1:A:63:ILE:HB	3:C:335:THR:HG21	1.79	0.65
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.30	0.64
30:B:622:SQD:H171	30:B:622:SQD:H301	1.80	0.64
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.78	0.64
32:a:407:PHO:H151	22:d:404:CLA:H172	1.78	0.64
3:C:291:TRP:O	3:C:305:THR:OG1	2.15	0.64
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.80	0.64
2:b:271:THR:HG22	2:b:273:TYR:H	1.63	0.64
4:D:236:ASN:ND2	4:D:239:GLN:O	2.31	0.64
12:m:31:SER:HA	27:m:101:LMG:HC1	1.80	0.64
1:a:174:LEU:HD22	32:d:401:PHO:H151	1.80	0.64
3:c:48:LYS:NZ	3:c:133:ALA:O	2.30	0.63
3:c:216:SER:HB3	3:c:221:GLU:HB2	1.80	0.63
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.79	0.63
3:c:250:TRP:O	3:c:254:THR:OG1	2.16	0.63
22:b:611:CLA:H42	4:d:127:LEU:HD11	1.78	0.63
22:A:404:CLA:H142	22:D:404:CLA:H151	1.80	0.63
3:C:250:TRP:O	3:C:254:THR:OG1	2.12	0.63
4:d:29:PHE:O	4:d:128:ARG:NH2	2.32	0.63
22:B:607:CLA:HBA2	30:B:622:SQD:H101	1.81	0.63
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.64	0.62
2:B:271:THR:HG22	2:B:273:TYR:H	1.64	0.62
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
22:a:404:CLA:HHC	22:a:404:CLA:HBB1	1.81	0.62
22:a:406:CLA:H142	22:d:404:CLA:H151	1.81	0.62
3:c:291:TRP:O	3:c:305:THR:OG1	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:183:MET:HB3	22:a:404:CLA:HBC2	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	2.32	0.62
9:j:15:THR:HG21	10:k:38:VAL:HG13	1.82	0.62
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.82	0.62
3:c:49:LEU:O	3:c:53:HIS:ND1	2.30	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.61
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.81	0.61
3:c:342:MET:HE3	3:c:352:GLY:HA2	1.82	0.61
4:D:24:ARG:NH2	18:X:44:ASP:O	2.33	0.61
4:D:186:GLN:HB2	22:D:404:CLA:HBC1	1.81	0.61
12:M:31:SER:HA	27:M:101:LMG:HC1	1.82	0.61
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.83	0.61
22:B:615:CLA:H2	30:a:401:SQD:H61	1.82	0.61
1:a:15:GLU:O	1:a:19:ASN:ND2	2.34	0.61
2:b:149:LEU:HG	22:b:606:CLA:HBC1	1.83	0.61
22:c:506:CLA:H112	24:c:514:BCR:H362	1.83	0.61
30:A:413:SQD:H172	26:C:519:LHG:H172	1.83	0.60
1:a:214:MET:HE2	1:a:214:MET:HA	1.84	0.60
1:a:221:SER:HB3	4:d:141:TYR:HB2	1.82	0.60
4:d:186:GLN:HB2	22:d:404:CLA:HBC1	1.82	0.60
17:g:35:ILE:HG22	20:z:21:ILE:HG23	1.82	0.60
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.82	0.60
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.82	0.60
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.82	0.60
3:C:406:SER:O	3:C:418:ASN:ND2	2.35	0.60
6:f:17:THR:HG23	6:f:20:TRP:H	1.66	0.60
4:D:216:ALA:O	4:D:220:ASN:ND2	2.33	0.60
22:b:606:CLA:H193	7:h:42:LEU:HD12	1.83	0.60
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.83	0.60
1:a:329:GLU:O	1:a:332:HIS:ND1	2.34	0.60
22:c:503:CLA:H172	22:c:509:CLA:HBB2	1.81	0.60
30:A:414:SQD:H61	22:b:619:CLA:H2	1.83	0.60
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.83	0.60
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.35	0.60
3:c:150:ASP:HB3	3:c:153:ASP:HB2	1.84	0.60
22:a:404:CLA:H122	32:d:401:PHO:H3A	1.83	0.59
4:d:24:ARG:NH2	18:x:44:ASP:O	2.35	0.59
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.67	0.59
4:D:192:THR:HG23	22:D:404:CLA:HBC2	1.85	0.59
22:a:404:CLA:H71	22:a:405:CLA:HAB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.59
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.83	0.58
22:b:611:CLA:HBA2	30:d:402:SQD:H101	1.85	0.58
22:B:605:CLA:OBD	31:B:623:LMT:O6'	2.20	0.58
3:c:449:ARG:HE	22:c:504:CLA:HED1	1.68	0.58
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.84	0.58
2:b:121:GLU:O	7:h:12:ARG:NH2	2.35	0.58
2:b:262:THR:OG1	22:b:606:CLA:O1D	2.21	0.58
34:v:201:HEM:HBB2	34:v:201:HEM:HMB1	1.85	0.58
1:A:214:MET:HA	1:A:214:MET:HE2	1.84	0.58
2:B:121:GLU:O	7:H:12:ARG:NH2	2.36	0.58
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.58
22:b:606:CLA:C2D	22:b:608:CLA:H2	2.34	0.58
1:a:328:MET:HE1	4:d:183:LEU:HD22	1.85	0.58
30:a:415:SQD:H311	22:c:507:CLA:H71	1.86	0.58
13:o:240:THR:HG22	13:o:264:VAL:HG12	1.86	0.58
32:D:402:PHO:H151	22:D:404:CLA:H172	1.85	0.58
1:a:217:SER:HA	4:d:272:LEU:HD12	1.85	0.58
22:h:101:CLA:H2	22:h:101:CLA:HBD	1.86	0.58
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.85	0.58
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.86	0.58
1:a:29:TYR:O	1:a:129:ARG:NH1	2.37	0.58
3:c:406:SER:O	3:c:418:ASN:ND2	2.37	0.58
15:u:56:ASP:OD2	15:u:115:THR:OG1	2.18	0.58
2:b:62:VAL:HG12	2:b:66:MET:HE2	1.86	0.57
30:d:402:SQD:H241	30:d:402:SQD:H111	1.86	0.57
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.34	0.57
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.86	0.57
3:c:284:PHE:HB3	25:c:515:DGD:HA51	1.86	0.57
22:A:403:CLA:H203	32:D:401:PHO:H71	1.85	0.57
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.85	0.57
13:O:83:LYS:HG2	13:O:84:ASN:H	1.69	0.57
22:b:611:CLA:H151	22:b:612:CLA:H203	1.87	0.57
4:d:216:ALA:O	4:d:220:ASN:ND2	2.34	0.57
22:A:403:CLA:HMA2	23:D:406:PL9:H411	1.87	0.57
12:M:28:GLN:HA	12:m:28:GLN:HA	1.87	0.57
1:A:84:PRO:HA	1:A:112:TYR:CG	2.39	0.57
2:b:155:ALA:O	2:b:159:THR:OG1	2.23	0.57
13:o:230:VAL:HG13	13:o:237:ILE:HG22	1.87	0.57
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.87	0.57
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.30	0.56
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.87	0.56
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.70	0.56
26:C:519:LHG:H271	26:C:519:LHG:H101	1.86	0.56
4:D:214:HIS:ND1	23:D:406:PL9:O2	2.26	0.56
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.86	0.56
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.86	0.56
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.88	0.56
27:D:408:LMG:O6	11:L:15:THR:HG21	2.05	0.56
1:a:224:ILE:O	4:d:265:ARG:NH2	2.38	0.56
3:c:42:LEU:HD21	22:c:510:CLA:H2A	1.87	0.56
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.34	0.56
4:d:192:THR:HG23	22:d:404:CLA:HBC2	1.87	0.56
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.88	0.56
12:m:25:LEU:O	12:m:28:GLN:HG3	2.06	0.56
2:B:327:THR:HG21	27:B:621:LMG:H111	1.87	0.56
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.88	0.56
1:A:329:GLU:O	1:A:332:HIS:ND1	2.37	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.24	0.56
2:b:487:SER:N	2:b:488:PRO:HD2	2.21	0.56
2:B:262:THR:HG22	2:B:263:THR:HG23	1.87	0.56
30:a:401:SQD:H311	24:a:410:BCR:H342	1.87	0.56
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.88	0.55
2:B:256:MET:O	2:B:448:ARG:NH1	2.34	0.55
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.36	0.55
22:b:607:CLA:HBD	22:b:608:CLA:H43	1.88	0.55
3:c:229:ASN:HD22	3:c:231:GLU:HB2	1.71	0.55
2:b:12:LEU:HB2	22:b:615:CLA:HMC2	1.88	0.55
27:d:408:LMG:O5	27:d:408:LMG:O4	2.23	0.55
22:b:610:CLA:HBB1	27:b:625:LMG:H341	1.88	0.55
4:d:214:HIS:ND1	23:d:406:PL9:O2	2.28	0.55
17:g:39:LEU:HD21	20:z:25:VAL:HA	1.88	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.55
1:a:84:PRO:HA	1:a:112:TYR:CG	2.41	0.55
22:b:612:CLA:HMD1	7:h:27:THR:HB	1.88	0.55
3:c:297:TYR:O	3:c:423:ARG:NH2	2.40	0.55
30:B:626:SQD:H1	30:B:626:SQD:H462	1.88	0.55
1:a:85:SER:HA	1:a:109:GLY:HA3	1.88	0.55
2:b:474:LEU:O	4:d:134:ARG:NH1	2.40	0.55
3:c:229:ASN:ND2	3:c:232:ASP:OD1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:517:DGD:HA22	9:j:29:PHE:HE1	1.71	0.55
13:o:83:LYS:HG2	13:o:84:ASN:H	1.70	0.55
22:A:404:CLA:H93	22:D:404:CLA:H152	1.89	0.55
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.88	0.55
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.87	0.55
22:b:606:CLA:C3D	22:b:608:CLA:H2	2.36	0.55
30:a:415:SQD:H172	26:c:519:LHG:H172	1.89	0.55
13:o:180:ALA:HB1	13:o:191:ALA:HB2	1.89	0.55
20:z:33:TRP:HA	20:z:36:SER:HB3	1.89	0.55
25:b:601:DGD:HD1	31:b:603:LMT:H32	1.88	0.55
23:d:406:PL9:H352	27:l:101:LMG:H231	1.89	0.55
1:A:64:ARG:O	13:O:178:ARG:NH2	2.40	0.55
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.42	0.55
24:A:407:BCR:H321	30:A:414:SQD:H321	1.89	0.54
2:B:184:GLU:H	2:B:200:ALA:HB2	1.72	0.54
2:b:327:THR:HG21	27:b:625:LMG:H111	1.89	0.54
2:b:458:PHE:HB3	22:b:607:CLA:HBC2	1.89	0.54
3:c:215:LYS:HB3	3:c:223:TRP:HA	1.89	0.54
27:d:408:LMG:O6	11:l:15:THR:HG21	2.07	0.54
1:A:217:SER:HA	4:D:272:LEU:HD12	1.90	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54
22:H:101:CLA:H2	22:H:101:CLA:HBD	1.89	0.54
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.88	0.54
22:a:405:CLA:H203	32:d:401:PHO:H71	1.90	0.54
16:v:81:ARG:CZ	16:v:157:GLY:HA3	2.38	0.54
25:b:601:DGD:O1B	25:b:601:DGD:O2D	2.25	0.54
1:a:57:PRO:HG3	1:a:68:SER:HB3	1.90	0.54
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.54
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.54
20:z:33:TRP:O	20:z:37:LYS:HB2	2.08	0.54
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.90	0.54
4:d:302:GLU:OE1	13:o:186:LYS:NZ	2.40	0.54
34:f:101:HEM:HBC2	34:f:101:HEM:HMC2	1.90	0.54
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.90	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.90	0.54
1:A:268:SER:O	1:A:272:HIS:ND1	2.38	0.54
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.39	0.54
2:B:271:THR:HB	2:B:274:GLN:HG3	1.90	0.54
1:a:64:ARG:O	13:o:178:ARG:NH2	2.40	0.54
22:c:501:CLA:C2D	22:c:503:CLA:H2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:405:CLA:H42	18:X:26:GLY:HA3	1.90	0.54
22:d:405:CLA:H42	18:x:26:GLY:HA3	1.90	0.53
22:D:405:CLA:H43	18:X:23:LEU:HA	1.90	0.53
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.53
1:a:65:GLU:OE2	1:a:334:ARG:NH2	2.40	0.53
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.91	0.53
22:c:508:CLA:HBD	22:c:508:CLA:H121	1.89	0.53
24:A:407:BCR:H342	30:A:414:SQD:H311	1.90	0.53
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.91	0.53
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.89	0.53
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.90	0.53
22:a:405:CLA:HED1	23:d:406:PL9:H372	1.89	0.53
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.91	0.53
4:d:222:LEU:HD23	4:d:244:TYR:HB3	1.91	0.53
13:O:73:PRO:HG2	13:O:102:THR:HB	1.91	0.53
3:c:461:ARG:NH1	4:d:241:GLU:OE1	2.40	0.53
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.91	0.53
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.38	0.53
27:D:408:LMG:HO4	27:D:408:LMG:HO5	1.54	0.53
30:a:415:SQD:H223	25:c:517:DGD:HAE1	1.90	0.53
2:b:184:GLU:H	2:b:200:ALA:HB2	1.74	0.53
22:A:402:CLA:H122	32:D:401:PHO:H3A	1.90	0.53
22:A:403:CLA:HED1	23:D:406:PL9:H372	1.90	0.53
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.91	0.53
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.91	0.53
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.74	0.53
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.90	0.53
22:B:607:CLA:H151	22:B:608:CLA:H203	1.91	0.53
27:A:410:LMG:H231	23:D:406:PL9:H352	1.91	0.52
31:B:627:LMT:H62	8:i:4:LEU:HD22	1.90	0.52
2:b:262:THR:HG22	2:b:263:THR:HG23	1.89	0.52
22:b:608:CLA:H202	22:b:612:CLA:HBB2	1.92	0.52
25:B:625:DGD:O1B	25:B:625:DGD:O2D	2.27	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.42	0.52
2:b:25:MET:HE3	24:b:620:BCR:H23C	1.91	0.52
3:c:85:GLY:N	25:c:516:DGD:HE4	2.24	0.52
3:c:209:ILE:HG23	24:c:514:BCR:H382	1.91	0.52
30:A:413:SQD:H311	22:C:507:CLA:H71	1.92	0.52
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.73	0.52
3:C:85:GLY:N	25:C:516:DGD:HE4	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:507:CLA:H172	25:c:516:DGD:HBW2	1.91	0.52
7:h:45:ILE:HD12	22:h:101:CLA:HAA2	1.92	0.52
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.45	0.52
3:c:305:THR:HG23	3:c:307:PRO:HD2	1.91	0.52
2:b:4:PRO:HD2	2:b:7:ARG:HD2	1.91	0.51
15:u:72:TYR:HB3	15:u:73:PRO:HD3	1.92	0.51
27:A:415:LMG:H112	2:b:43:ALA:HA	1.92	0.51
3:c:197:ARG:NH2	3:c:231:GLU:OE2	2.43	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
1:a:268:SER:O	1:a:272:HIS:ND1	2.38	0.51
2:b:383:PHE:CZ	13:o:193:GLY:HA2	2.46	0.51
3:c:405:ASN:HB2	25:c:517:DGD:HG31	1.92	0.51
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.93	0.51
13:o:73:PRO:HG2	13:o:102:THR:HB	1.92	0.51
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.41	0.51
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.93	0.51
2:B:25:MET:HE3	24:B:616:BCR:H23C	1.91	0.51
2:B:371:THR:HG22	2:B:377:VAL:HA	1.93	0.51
30:b:602:SQD:H1	30:b:602:SQD:H462	1.91	0.51
22:b:614:CLA:H41	22:b:617:CLA:HBC3	1.92	0.51
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.91	0.51
17:y:39:LEU:HD21	20:Z:25:VAL:HA	1.93	0.51
3:c:305:THR:HG22	3:c:308:GLU:HB2	1.93	0.51
4:d:275:PRO:O	4:d:279:LEU:HD23	2.11	0.51
22:b:611:CLA:H51	22:b:612:CLA:H101	1.94	0.50
7:h:55:LEU:HB2	7:h:58:VAL:HG12	1.93	0.50
22:B:612:CLA:H51	27:D:407:LMG:H231	1.93	0.50
1:A:210:LEU:HG	32:D:402:PHO:NC	2.27	0.50
22:C:504:CLA:HBA1	22:C:504:CLA:HBD	1.93	0.50
1:a:132:GLU:O	1:a:136:ARG:HG2	2.11	0.50
3:c:164:HIS:ND1	22:c:506:CLA:OBD	2.31	0.50
1:A:132:GLU:O	1:A:136:ARG:HG2	2.12	0.50
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.93	0.50
1:a:183:MET:HE1	22:a:405:CLA:HMD2	1.93	0.50
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.93	0.50
4:d:17:ILE:HG21	18:x:42:GLN:HG3	1.93	0.50
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.92	0.50
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.94	0.50
2:b:270:PRO:HG3	2:b:312:TYR:HD2	1.76	0.50
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.92	0.50
7:h:45:ILE:HD11	22:h:101:CLA:H42	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.94	0.50
13:o:168:PHE:HB2	13:o:225:LEU:HB2	1.92	0.50
22:A:403:CLA:CHA	22:A:403:CLA:HBA1	2.42	0.50
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.24	0.50
22:c:504:CLA:HBA1	22:c:504:CLA:HBD	1.94	0.50
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.76	0.50
34:F:101:HEM:HBC2	34:F:101:HEM:HMC2	1.93	0.50
1:a:153:SER:HB3	22:a:404:CLA:HED1	1.93	0.50
1:a:211:PHE:HA	1:a:214:MET:HB2	1.93	0.50
25:b:624:DGD:HA71	22:h:101:CLA:H193	1.93	0.50
5:e:57:ALA:HB3	5:e:60:GLN:HB3	1.94	0.50
10:k:12:PRO:HB2	10:k:15:TYR:HD2	1.76	0.50
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.94	0.50
8:I:4:LEU:HD22	31:b:603:LMT:H62	1.93	0.50
17:g:24:MET:O	17:g:28:ILE:HG23	2.12	0.50
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.42	0.49
17:y:24:MET:O	17:y:28:ILE:HG23	2.12	0.49
3:c:29:GLU:HB3	10:k:46:ARG:HH11	1.77	0.49
3:c:75:PHE:HD1	3:c:86:LEU:HD21	1.77	0.49
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.47	0.49
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.44	0.49
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.47	0.49
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.94	0.49
2:b:306:PRO:HG2	2:b:309:LEU:HB2	1.93	0.49
22:d:405:CLA:H43	18:x:23:LEU:HA	1.94	0.49
13:o:118:SER:HB3	13:o:157:PRO:HA	1.95	0.49
13:o:144:LEU:HD13	13:o:259:VAL:HG11	1.93	0.49
15:u:75:LEU:HD21	15:u:101:GLN:HB3	1.94	0.49
1:A:211:PHE:HA	1:A:214:MET:HB2	1.93	0.49
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.49
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.92	0.49
22:b:609:CLA:OBD	31:b:626:LMT:O6'	2.22	0.49
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.49
2:b:122:LEU:O	7:h:15:ASN:ND2	2.42	0.49
10:k:26:PRO:O	10:k:29:PRO:HD2	2.12	0.49
18:x:11:THR:HG23	18:x:12:ILE:HG22	1.95	0.49
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.95	0.49
30:A:413:SQD:H223	25:C:517:DGD:HAE1	1.93	0.49
2:b:327:THR:HG22	22:b:610:CLA:H12	1.94	0.49
3:c:158:THR:O	3:c:251:HIS:HB3	2.13	0.49
27:d:411:LMG:H171	24:f:102:BCR:H383	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.49
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.28	0.49
2:b:150:CYS:HA	22:b:606:CLA:HBC2	1.93	0.49
3:c:166:ILE:O	3:c:170:ILE:HG13	2.13	0.49
22:a:405:CLA:CHA	22:a:405:CLA:HBA1	2.41	0.49
3:c:361:PHE:HD1	25:c:515:DGD:HE61	1.78	0.49
30:F:103:SQD:H162	18:X:33:THR:HA	1.94	0.49
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.76	0.49
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.78	0.49
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.95	0.49
1:a:190:HIS:O	1:a:298:ASN:HB3	2.13	0.49
1:a:227:THR:HG21	1:a:233:ALA:HA	1.94	0.49
22:a:406:CLA:H161	23:a:409:PL9:H253	1.94	0.49
2:B:135:LEU:HA	2:B:138:MET:HE3	1.95	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
1:a:244:GLU:HG3	1:a:246:TYR:H	1.78	0.48
2:b:5:TRP:HZ3	22:b:614:CLA:H51	1.78	0.48
5:e:10:PHE:N	27:e:101:LMG:O3	2.45	0.48
22:a:405:CLA:HMA2	23:d:406:PL9:H411	1.95	0.48
2:b:135:LEU:HA	2:b:138:MET:HE3	1.95	0.48
26:c:519:LHG:H101	26:c:519:LHG:H271	1.95	0.48
4:d:43:LEU:HD23	4:d:117:HIS:CE1	2.47	0.48
27:d:408:LMG:H111	11:l:19:LEU:HD21	1.95	0.48
1:A:78:ILE:O	1:A:176:ILE:HB	2.13	0.48
3:C:158:THR:O	3:C:251:HIS:HB3	2.13	0.48
22:b:618:CLA:H111	22:b:618:CLA:H172	1.95	0.48
25:c:517:DGD:HA22	9:j:29:PHE:CE1	2.49	0.48
32:a:407:PHO:HBC3	4:d:279:LEU:HG	1.95	0.48
22:b:610:CLA:H193	11:l:27:LEU:HD11	1.95	0.48
5:e:15:THR:HG23	9:j:8:ILE:O	2.12	0.48
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.94	0.48
22:a:405:CLA:H42	23:d:406:PL9:H162	1.96	0.48
22:b:617:CLA:H51	24:b:620:BCR:H372	1.95	0.48
22:C:510:CLA:HMB1	24:C:513:BCR:H382	1.95	0.48
30:f:103:SQD:H162	18:x:33:THR:HA	1.95	0.48
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.48
26:A:409:LHG:H382	22:C:509:CLA:H93	1.96	0.48
3:c:86:LEU:HB3	3:c:90:PRO:HD3	1.95	0.48
4:d:102:THR:OG1	25:d:409:DGD:HD62	2.13	0.48
22:A:404:CLA:H161	23:A:406:PL9:H253	1.94	0.48
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.96	0.48
22:A:404:CLA:HAB	22:D:404:CLA:H72	1.96	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.48
32:D:401:PHO:H41	32:D:401:PHO:H62	1.45	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
30:a:401:SQD:H321	24:a:410:BCR:H321	1.96	0.48
2:b:212:ALA:O	2:b:216:HIS:ND1	2.41	0.48
1:A:244:GLU:HG3	1:A:246:TYR:H	1.78	0.48
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.95	0.48
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.49	0.48
1:a:121:LEU:HD13	25:a:411:DGD:HB92	1.96	0.48
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.95	0.48
9:J:14:ALA:O	9:J:18:GLY:N	2.45	0.47
3:c:130:VAL:O	3:c:134:ILE:HG12	2.14	0.47
13:o:240:THR:HA	13:o:264:VAL:HA	1.95	0.47
1:A:224:ILE:O	4:D:265:ARG:NH2	2.46	0.47
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.44	0.47
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.79	0.47
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
22:B:613:CLA:H51	24:B:616:BCR:H372	1.96	0.47
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.38	0.47
2:b:247:PHE:HE1	22:h:101:CLA:H101	1.77	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.45	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.78	0.47
4:D:279:LEU:HG	32:D:402:PHO:HBC3	1.96	0.47
32:d:401:PHO:H41	32:d:401:PHO:H62	1.48	0.47
2:B:474:LEU:O	4:D:134:ARG:NH1	2.47	0.47
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.96	0.47
4:d:85:MET:HA	5:e:69:ARG:HB3	1.95	0.47
15:u:54:LYS:HD2	15:u:113:THR:HG23	1.96	0.47
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.96	0.47
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.96	0.47
3:C:223:TRP:CG	3:C:224:ILE:H	2.32	0.47
22:D:404:CLA:H61	22:D:404:CLA:H41	1.64	0.47
4:d:262:SER:N	27:d:408:LMG:O3	2.42	0.47
15:u:68:TYR:HB2	15:u:71:LEU:HD12	1.95	0.47
22:B:614:CLA:H172	22:B:614:CLA:H111	1.97	0.47
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.95	0.47
5:E:15:THR:HG23	9:J:8:ILE:O	2.14	0.47
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.96	0.47
2:b:271:THR:HB	2:b:274:GLN:HG3	1.97	0.47
13:o:223:ILE:HG13	13:o:243:SER:HB3	1.97	0.47
18:x:12:ILE:HG12	18:x:16:LEU:HD12	1.97	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.47
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.80	0.47
1:a:140:ARG:NH2	26:a:412:LHG:O5	2.36	0.47
1:a:156:ALA:HA	1:a:160:ILE:HB	1.97	0.47
7:h:46:LEU:HD13	22:h:101:CLA:H72	1.96	0.47
9:j:14:ALA:O	9:j:18:GLY:N	2.46	0.47
1:A:193:LEU:HD11	22:A:402:CLA:HMC2	1.97	0.47
2:B:222:PRO:HG3	7:H:27:THR:H	1.80	0.47
22:B:605:CLA:H203	30:a:401:SQD:H332	1.97	0.47
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.79	0.47
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.50	0.47
9:J:38:SER:OG	9:J:39:SER:N	2.47	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.46	0.47
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.47
1:a:210:LEU:HG	32:a:407:PHO:NC	2.30	0.47
22:b:619:CLA:H72	22:b:619:CLA:H12	1.97	0.47
1:A:183:MET:HE1	22:A:403:CLA:HMD2	1.97	0.46
22:B:605:CLA:H18	22:B:615:CLA:H121	1.97	0.46
24:B:616:BCR:H20C	24:B:616:BCR:H361	1.75	0.46
4:D:85:MET:HA	5:E:69:ARG:HB3	1.98	0.46
2:b:315:ILE:HG22	2:b:426:PHE:HB3	1.97	0.46
2:b:450:TRP:NE1	22:b:610:CLA:HBA1	2.30	0.46
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.97	0.46
1:A:215:HIS:ND1	23:A:406:PL9:O1	2.48	0.46
22:A:405:CLA:H162	22:A:405:CLA:H141	1.70	0.46
24:C:513:BCR:H11C	24:y:101:BCR:H322	1.98	0.46
4:D:275:PRO:O	4:D:279:LEU:HD23	2.14	0.46
1:a:78:ILE:O	1:a:176:ILE:HB	2.15	0.46
24:c:513:BCR:H343	24:c:513:BCR:H311	1.97	0.46
13:o:135:GLN:HG2	13:o:141:ARG:HG3	1.97	0.46
22:B:604:CLA:H62	22:B:604:CLA:H41	1.79	0.46
25:B:625:DGD:HD1	31:B:627:LMT:H32	1.97	0.46
4:D:48:TRP:CE2	32:D:402:PHO:H161	2.51	0.46
7:H:46:LEU:HD13	22:H:101:CLA:H72	1.98	0.46
24:y:101:BCR:H20C	24:y:101:BCR:H361	1.80	0.46
3:c:337:LEU:HA	13:o:131:PRO:HG3	1.98	0.46
25:B:620:DGD:HAW2	22:H:101:CLA:H152	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:SER:HB2	4:D:85:MET:HE2	1.98	0.46
4:D:348:ARG:NH2	4:D:352:LEU:O	2.35	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46
27:C:518:LMG:H292	27:C:518:LMG:H111	1.96	0.46
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.64	0.46
3:c:131:TYR:HE1	3:c:135:ARG:HD2	1.80	0.46
1:A:114:LEU:O	1:A:118:HIS:ND1	2.45	0.46
31:B:628:LMT:H122	14:t:7:VAL:HG12	1.96	0.46
3:C:224:ILE:O	3:C:227:VAL:HG23	2.16	0.46
27:D:411:LMG:H171	24:F:102:BCR:H383	1.96	0.46
22:H:101:CLA:H41	22:H:101:CLA:H62	1.57	0.46
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.97	0.46
2:b:18:ARG:HD3	2:b:118:TRP:HB3	1.97	0.46
2:b:341:LYS:HA	2:b:405:GLU:HB2	1.98	0.46
4:d:348:ARG:NH2	4:d:352:LEU:O	2.36	0.46
22:A:402:CLA:H3A	22:A:402:CLA:HBA1	1.53	0.46
13:O:118:SER:HB3	13:O:157:PRO:HA	1.98	0.46
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.98	0.46
6:F:22:ALA:O	6:F:25:THR:OG1	2.31	0.46
22:b:606:CLA:H2	22:b:608:CLA:H93	1.98	0.46
3:c:386:PRO:HB3	16:v:116:GLU:HG2	1.97	0.46
13:o:184:ASP:OD2	13:o:188:ARG:HB2	2.15	0.46
13:o:230:VAL:HG12	13:o:231:ASP:H	1.80	0.46
22:A:403:CLA:H42	23:D:406:PL9:H162	1.96	0.46
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.98	0.46
22:B:607:CLA:H51	22:B:608:CLA:H101	1.97	0.46
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.51	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	1.98	0.46
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.98	0.46
16:v:160:LYS:HA	16:v:163:TYR:CD2	2.51	0.46
17:g:32:GLY:O	17:g:35:ILE:HG12	2.16	0.46
24:B:618:BCR:H20C	24:B:618:BCR:H361	1.82	0.46
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.97	0.46
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.98	0.45
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.98	0.45
1:a:12:ASN:HB3	1:a:15:GLU:HB3	1.97	0.45
22:a:406:CLA:HAB	22:d:404:CLA:H42	1.98	0.45
4:d:221:THR:HG23	4:d:244:TYR:HB2	1.98	0.45
5:e:23:HIS:NE2	34:f:101:HEM:ND	2.64	0.45
14:T:7:VAL:HG12	31:b:604:LMT:H122	1.98	0.45
1:a:159:LEU:C	1:a:162:PRO:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:404:CLA:H3A	22:a:404:CLA:HBA1	1.52	0.45
22:a:408:CLA:H141	22:a:408:CLA:H162	1.67	0.45
3:c:223:TRP:CG	3:c:224:ILE:H	2.32	0.45
9:j:38:SER:OG	9:j:39:SER:N	2.48	0.45
1:a:212:CYS:HB2	4:d:211:CYS:HB2	1.99	0.45
3:c:137:PRO:HB2	3:c:139:THR:O	2.16	0.45
3:c:473:ASP:HB2	14:t:26:PRO:HB3	1.97	0.45
22:h:101:CLA:H162	22:h:101:CLA:H122	1.52	0.45
27:i:101:LMG:H181	31:i:102:LMT:H42	1.97	0.45
2:B:213:GLY:O	2:B:217:ILE:HG13	2.15	0.45
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.52	0.45
22:C:510:CLA:H93	22:C:510:CLA:H61	1.81	0.45
1:a:317:TRP:CZ3	4:d:180:ARG:HD3	2.51	0.45
2:b:326:ARG:HB3	2:b:444:ARG:HG2	1.98	0.45
3:c:223:TRP:CD2	3:c:224:ILE:HG13	2.51	0.45
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.97	0.45
20:z:29:SER:HA	20:z:30:PRO:HD3	1.83	0.45
4:D:262:SER:N	27:D:408:LMG:O3	2.44	0.45
3:c:318:LEU:HG	3:c:328:VAL:HG11	1.99	0.45
24:c:521:BCR:H20C	24:c:521:BCR:H361	1.80	0.45
5:e:60:GLN:HG2	5:e:62:SER:H	1.81	0.45
22:B:611:CLA:H122	22:B:611:CLA:H162	1.75	0.45
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.98	0.45
3:c:425:TRP:CE2	22:c:520:CLA:HBA1	2.51	0.45
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.45
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.99	0.45
25:b:624:DGD:HAW2	22:h:101:CLA:H152	1.98	0.45
22:d:404:CLA:H61	22:d:404:CLA:H41	1.66	0.45
27:d:408:LMG:HC1	27:d:408:LMG:O9	2.17	0.45
2:B:329:PRO:HB3	22:B:606:CLA:HED1	1.99	0.45
22:B:607:CLA:H18	22:B:608:CLA:H192	1.99	0.45
25:B:620:DGD:HA71	22:H:101:CLA:H193	1.99	0.45
3:C:318:LEU:HD21	3:C:380:ILE:HG23	1.99	0.45
2:b:213:GLY:O	2:b:217:ILE:HG13	2.16	0.45
2:b:247:PHE:HB2	22:b:611:CLA:HBC1	1.98	0.45
22:b:608:CLA:H62	22:b:608:CLA:H41	1.78	0.45
22:c:510:CLA:H121	24:c:513:BCR:H21C	1.98	0.45
16:v:102:MET:HE3	34:v:201:HEM:HMB1	1.99	0.45
22:C:509:CLA:H2	22:C:509:CLA:H61	1.72	0.45
3:c:315:MET:HE1	3:c:369:LEU:HD12	1.98	0.45
4:d:84:SER:HB2	4:d:85:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ALA:O	2:B:216:HIS:ND1	2.47	0.45
3:C:113:VAL:HG11	27:C:518:LMG:H132	1.99	0.45
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.98	0.45
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.99	0.45
3:c:80:PRO:HB3	3:c:82:TYR:CE1	2.51	0.45
20:z:32:ASP:CG	20:z:33:TRP:H	2.25	0.45
2:B:150:CYS:HA	22:B:602:CLA:HBC2	2.00	0.44
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.44
3:C:137:PRO:HB2	3:C:139:THR:O	2.17	0.44
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.99	0.44
30:F:103:SQD:H131	18:X:36:VAL:HG11	2.00	0.44
15:U:106:ARG:HA	15:U:109:LEU:HG	1.98	0.44
22:a:406:CLA:HAB	22:d:404:CLA:H72	1.99	0.44
2:b:26:HIS:CE1	22:b:615:CLA:HMA2	2.52	0.44
2:b:96:VAL:HG22	22:b:609:CLA:HBA1	1.98	0.44
24:c:513:BCR:H371	24:c:513:BCR:H24C	1.79	0.44
13:O:240:THR:HA	13:O:264:VAL:HA	1.98	0.44
4:d:244:TYR:OH	4:d:264:LYS:HE3	2.18	0.44
1:A:238:LYS:O	1:A:241:GLN:HG3	2.17	0.44
2:B:327:THR:HG22	22:B:606:CLA:H12	1.99	0.44
2:B:383:PHE:N	4:D:344:GLU:O	2.36	0.44
20:Z:33:TRP:O	20:Z:33:TRP:CD1	2.70	0.44
22:b:619:CLA:H143	22:b:619:CLA:H111	1.74	0.44
3:c:245:ILE:O	3:c:249:ILE:HG12	2.17	0.44
3:c:347:GLY:HA3	13:o:43:ASN:HB2	1.99	0.44
22:c:506:CLA:H92	22:c:506:CLA:H62	1.75	0.44
22:A:402:CLA:H51	32:D:401:PHO:C3B	2.48	0.44
1:a:45:THR:HG21	30:a:401:SQD:H201	1.99	0.44
22:b:616:CLA:H51	27:d:407:LMG:H231	1.99	0.44
22:c:501:CLA:H193	22:c:506:CLA:H111	2.00	0.44
10:k:40:GLN:HA	10:k:43:VAL:HG12	1.99	0.44
4:D:146:PHE:C	4:D:149:PRO:HD2	2.43	0.44
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.44
32:D:401:PHO:H13	32:D:401:PHO:H102	1.82	0.44
24:H:102:BCR:H20C	24:H:102:BCR:H361	1.78	0.44
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.79	0.44
1:a:271:LEU:HD11	23:a:409:PL9:C4	2.48	0.44
22:b:606:CLA:H61	22:b:606:CLA:H41	1.61	0.44
3:c:29:GLU:HB2	3:c:30:SER:H	1.65	0.44
22:c:508:CLA:H11	22:c:508:CLA:H51	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:43:LEU:HD23	4:d:117:HIS:HE1	1.82	0.44
13:o:143:PRO:HG2	13:o:248:ASP:HB3	1.98	0.44
22:B:602:CLA:H192	22:B:602:CLA:H162	1.76	0.44
22:B:613:CLA:H91	22:B:613:CLA:H112	1.82	0.44
24:C:514:BCR:H20C	24:C:514:BCR:H361	1.84	0.44
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.17	0.44
16:V:102:MET:HE3	34:V:201:HEM:HMB1	1.98	0.44
11:l:13:ASN:ND2	27:l:101:LMG:O5	2.50	0.44
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.44
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.75	0.44
24:y:101:BCR:H15C	24:y:101:BCR:H351	1.88	0.44
1:a:157:VAL:HG13	1:a:172:MET:HB3	2.00	0.44
3:c:343:ARG:NH1	3:c:347:GLY:O	2.51	0.44
22:h:101:CLA:H62	22:h:101:CLA:H41	1.57	0.44
1:A:159:LEU:C	1:A:162:PRO:HD2	2.43	0.44
1:A:303:ASN:O	3:C:415:ASN:ND2	2.40	0.44
22:a:406:CLA:H161	22:a:406:CLA:H143	1.86	0.44
25:a:411:DGD:HD2	25:a:411:DGD:HG32	1.72	0.44
25:a:411:DGD:HA32	3:c:217:PRO:HD3	1.98	0.44
2:b:135:LEU:HD22	2:b:237:VAL:HG21	1.99	0.44
22:b:610:CLA:H102	27:b:625:LMG:H392	2.00	0.44
32:d:401:PHO:H102	32:d:401:PHO:H13	1.84	0.44
13:o:81:GLU:HA	13:o:82:PRO:HD3	1.78	0.44
22:A:403:CLA:H51	22:A:403:CLA:H11	1.82	0.44
22:B:612:CLA:H171	27:D:407:LMG:H401	2.00	0.44
24:B:616:BCR:H11C	24:B:616:BCR:H341	1.90	0.44
3:C:343:ARG:NH1	3:C:347:GLY:O	2.50	0.44
4:D:102:THR:OG1	25:D:409:DGD:HD62	2.18	0.44
27:D:408:LMG:H111	11:L:19:LEU:HD21	1.99	0.44
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.99	0.44
24:b:623:BCR:H15C	24:b:623:BCR:H351	1.89	0.44
5:e:27:ILE:HB	5:e:28:PRO:HD3	2.00	0.44
2:B:26:HIS:CE1	22:B:611:CLA:HMA2	2.52	0.43
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.43
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.53	0.43
1:a:111:PRO:O	1:a:115:ILE:HG13	2.17	0.43
24:b:623:BCR:H24C	24:b:623:BCR:H371	1.88	0.43
16:v:68:VAL:O	16:v:71:ILE:HG12	2.18	0.43
24:C:514:BCR:H15C	24:C:514:BCR:H351	1.83	0.43
24:a:410:BCR:H24C	24:a:410:BCR:H371	1.82	0.43
2:b:25:MET:HG2	24:b:620:BCR:H23C	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:170:ASP:OD1	2:b:175:THR:N	2.47	0.43
13:o:192:SER:OG	13:o:193:GLY:N	2.51	0.43
20:z:33:TRP:O	20:z:33:TRP:CD1	2.71	0.43
3:C:315:MET:HE1	3:C:369:LEU:HD12	2.00	0.43
3:c:90:PRO:O	3:c:94:THR:HG23	2.18	0.43
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.83	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.00	0.43
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.49	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
4:d:55:VAL:HG21	4:d:110:LEU:HD12	2.00	0.43
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.53	0.43
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.54	0.43
6:f:17:THR:OG1	6:f:18:VAL:N	2.52	0.43
15:u:72:TYR:O	15:u:76:ALA:HB3	2.19	0.43
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.00	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.77	0.43
15:U:54:LYS:HD2	15:U:113:THR:HG23	2.01	0.43
2:b:256:MET:O	2:b:448:ARG:NH1	2.37	0.43
22:b:611:CLA:H18	22:b:612:CLA:H192	2.00	0.43
4:d:56:THR:HG21	5:e:50:PRO:HD3	2.01	0.43
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.43
30:A:414:SQD:H332	22:b:609:CLA:H203	2.01	0.43
22:B:605:CLA:H3A	22:B:605:CLA:HBA2	1.25	0.43
22:C:512:CLA:HAB	24:K:102:BCR:H371	2.01	0.43
22:D:404:CLA:H3A	22:D:404:CLA:HBA1	1.84	0.43
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.27	0.43
22:a:406:CLA:H93	22:d:404:CLA:H152	2.00	0.43
24:b:620:BCR:H333	12:m:13:LEU:HD12	2.00	0.43
22:c:512:CLA:H3A	22:c:512:CLA:HBA2	1.69	0.43
24:c:513:BCR:H15C	24:c:513:BCR:H351	1.88	0.43
17:g:28:ILE:O	24:g:101:BCR:H14C	2.18	0.43
3:C:456:GLU:OE1	3:C:456:GLU:N	2.51	0.43
6:F:17:THR:OG1	6:F:18:VAL:N	2.52	0.43
16:V:90:PRO:O	16:V:92:ARG:HD3	2.18	0.43
22:a:405:CLA:H51	22:a:405:CLA:H11	1.82	0.43
2:b:30:VAL:HG12	22:b:608:CLA:HHD	2.01	0.43
3:c:113:VAL:HG11	27:c:518:LMG:H132	1.99	0.43
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.01	0.43
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.54	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:222:PRO:HG3	7:h:27:THR:H	1.84	0.43
2:b:348:ASN:HB3	2:b:354:LEU:HD21	2.00	0.43
22:b:615:CLA:H171	22:b:616:CLA:HBB2	2.00	0.43
27:c:518:LMG:H292	27:c:518:LMG:H111	2.01	0.43
24:j:102:BCR:H15C	24:j:102:BCR:H351	1.77	0.43
10:k:12:PRO:HB2	10:k:15:TYR:CD2	2.54	0.43
13:o:135:GLN:HE21	13:o:135:GLN:HB3	1.71	0.43
15:u:117:VAL:HG13	15:u:122:VAL:HG21	2.00	0.43
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.54	0.43
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.01	0.43
22:C:512:CLA:H3A	22:C:512:CLA:HBA2	1.75	0.43
5:E:81:GLU:C	5:E:83:LEU:H	2.27	0.43
24:J:102:BCR:H341	24:J:102:BCR:H11C	1.80	0.43
2:b:86:ILE:H	2:b:86:ILE:HG13	1.73	0.43
22:b:615:CLA:H162	22:b:615:CLA:H122	1.72	0.43
3:c:437:PHE:HA	22:c:507:CLA:HMC2	2.00	0.43
22:c:504:CLA:H11	24:c:514:BCR:H312	2.01	0.43
22:c:510:CLA:H141	20:z:20:VAL:HG13	2.01	0.43
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.01	0.43
1:A:37:MET:HE1	1:A:129:ARG:CZ	2.49	0.42
22:B:615:CLA:H12	22:B:615:CLA:H72	2.01	0.42
13:O:192:SER:OG	13:O:193:GLY:N	2.51	0.42
3:c:224:ILE:O	3:c:227:VAL:HG23	2.19	0.42
22:c:501:CLA:H162	22:c:501:CLA:H141	1.79	0.42
24:g:101:BCR:H20C	24:g:101:BCR:H361	1.80	0.42
1:A:38:ILE:HD13	30:A:414:SQD:H121	2.01	0.42
22:A:404:CLA:H161	22:A:404:CLA:H143	1.85	0.42
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.54	0.42
22:B:601:CLA:HMB2	24:H:102:BCR:H393	2.01	0.42
22:B:613:CLA:H112	22:B:613:CLA:H152	1.85	0.42
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.42
10:K:37:PHE:HB3	24:y:101:BCR:C40	2.49	0.42
1:a:176:ILE:HD12	22:a:405:CLA:HED3	2.00	0.42
3:c:363:GLY:O	3:c:367:GLU:HG2	2.18	0.42
3:c:464:GLU:HA	3:c:465:PRO:HD2	1.78	0.42
24:c:513:BCR:H361	24:c:513:BCR:H20C	1.80	0.42
25:c:516:DGD:HA91	25:c:516:DGD:HAW2	1.75	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.42
27:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
31:B:628:LMT:H1B	31:B:628:LMT:H3'	1.53	0.42
3:C:245:ILE:O	3:C:249:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:406:PL9:H401	23:D:406:PL9:H421	1.85	0.42
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.76	0.42
13:O:143:PRO:HG2	13:O:248:ASP:HB3	2.00	0.42
13:O:223:ILE:HG13	13:O:243:SER:HB3	2.00	0.42
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.01	0.42
22:b:611:CLA:CHA	22:b:611:CLA:HBA1	2.50	0.42
3:c:205:ASP:HA	3:c:206:PRO:HD2	1.93	0.42
3:c:248:GLY:O	3:c:252:ILE:HG12	2.19	0.42
4:d:129:GLN:OE1	4:d:143:ALA:HA	2.19	0.42
9:j:9:PRO:HB2	9:j:12:ILE:HG13	2.00	0.42
1:A:271:LEU:HD21	23:A:406:PL9:HC71	2.01	0.42
22:A:402:CLA:H62	22:A:402:CLA:H102	1.88	0.42
22:B:614:CLA:H12	22:B:614:CLA:H52	1.85	0.42
30:B:622:SQD:H241	30:B:622:SQD:H111	2.02	0.42
3:C:223:TRP:O	3:C:226:SER:OG	2.33	0.42
22:H:101:CLA:H162	22:H:101:CLA:H122	1.51	0.42
32:a:407:PHO:H161	4:d:48:TRP:CE2	2.54	0.42
2:b:54:PRO:HD2	2:b:57:ARG:HG3	2.00	0.42
3:c:391:ARG:HD2	3:c:395:TYR:CZ	2.54	0.42
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.55	0.42
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.02	0.42
3:C:248:GLY:O	3:C:252:ILE:HG12	2.20	0.42
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.19	0.42
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.20	0.42
1:a:61:ASP:HB2	1:a:63:ILE:HG12	2.02	0.42
1:a:309:ALA:HA	6:f:45:ARG:HB2	2.01	0.42
23:a:409:PL9:H371	23:a:409:PL9:H351	1.79	0.42
22:b:616:CLA:H171	27:d:407:LMG:H401	2.00	0.42
3:c:319:ILE:HG21	3:c:389:GLU:HG3	2.01	0.42
22:c:510:CLA:H122	10:k:32:PHE:HE1	1.84	0.42
4:d:53:THR:HG22	4:d:67:TYR:CD2	2.53	0.42
1:A:111:PRO:O	1:A:115:ILE:HG13	2.20	0.42
1:A:141:PRO:HG3	3:C:446:GLY:C	2.44	0.42
24:C:513:BCR:H353	24:y:101:BCR:H321	2.01	0.42
7:H:12:ARG:O	7:H:12:ARG:HD3	2.20	0.42
17:y:28:ILE:O	24:y:101:BCR:H14C	2.20	0.42
1:a:34:GLY:HA2	1:a:37:MET:HB3	2.02	0.42
1:a:262:TYR:HB3	27:e:101:LMG:H112	2.01	0.42
24:c:513:BCR:H11C	24:g:101:BCR:H322	2.02	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.92	0.42
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.02	0.42
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.42
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.83	0.42
18:X:34:PHE:O	18:X:38:ILE:HG12	2.20	0.42
1:a:214:MET:HE1	4:d:142:ASN:HD21	1.84	0.42
18:x:17:LYS:O	18:x:21:ILE:HG13	2.18	0.42
22:A:403:CLA:H162	22:A:403:CLA:H202	1.75	0.42
2:B:280:PHE:O	2:B:284:ILE:HG13	2.19	0.42
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.02	0.42
22:D:404:CLA:H92	22:D:404:CLA:H62	1.81	0.42
13:O:59:ASP:C	13:O:61:SER:H	2.28	0.42
1:a:153:SER:HB2	22:a:404:CLA:H43	2.01	0.42
1:a:238:LYS:HD2	14:t:32:LYS:HB3	2.01	0.42
2:b:6:TYR:OH	27:d:407:LMG:HC5	2.20	0.42
3:c:259:TRP:CD1	3:c:259:TRP:H	2.38	0.42
3:c:282:MET:HG2	22:c:501:CLA:H61	2.01	0.42
3:c:318:LEU:HD21	3:c:380:ILE:HG23	2.02	0.42
3:c:346:THR:HG21	13:o:38:GLY:HA2	2.01	0.42
4:d:236:ASN:HA	4:d:237:PRO:HD2	1.94	0.42
1:A:156:ALA:HA	1:A:160:ILE:HB	2.01	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.01	0.42
24:C:513:BCR:H311	24:C:513:BCR:H343	2.00	0.42
27:D:408:LMG:HC1	27:D:408:LMG:O9	2.20	0.42
5:E:60:GLN:HG2	5:E:62:SER:H	1.85	0.42
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.42
1:a:257:ARG:HH22	2:b:488:PRO:C	2.28	0.42
2:b:371:THR:HG22	2:b:377:VAL:HA	2.01	0.42
3:c:466:VAL:HG13	4:d:251:ARG:HD2	2.01	0.42
22:c:509:CLA:H61	22:c:509:CLA:H2	1.70	0.42
22:c:520:CLA:H141	22:c:520:CLA:H161	1.81	0.42
4:d:113:PHE:O	4:d:117:HIS:HB2	2.19	0.42
8:i:29:ALA:HA	8:i:35:LYS:HB2	2.02	0.42
22:B:604:CLA:H202	22:B:608:CLA:HBB2	2.02	0.42
24:B:616:BCR:H15C	24:B:616:BCR:H351	1.86	0.42
22:C:505:CLA:H161	22:C:505:CLA:H202	1.86	0.42
22:C:512:CLA:HAB	24:K:102:BCR:H24C	2.02	0.42
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.42
1:a:93:PHE:HZ	22:a:408:CLA:HAA1	1.85	0.42
22:b:609:CLA:H3A	22:b:609:CLA:HBA2	1.24	0.42
13:o:178:ARG:HD2	13:o:182:PHE:CD1	2.55	0.42
1:A:141:PRO:HB2	1:A:142:TRP:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.85	0.41
1:a:127:MET:HG3	1:a:144:CYS:HB2	2.02	0.41
2:b:256:MET:HA	2:b:263:THR:HG21	2.02	0.41
24:b:620:BCR:H24C	24:b:620:BCR:H371	1.91	0.41
24:b:623:BCR:H20C	24:b:623:BCR:H361	1.76	0.41
3:c:456:GLU:OE1	3:c:456:GLU:N	2.50	0.41
24:c:513:BCR:H391	10:k:36:ALA:HB2	2.01	0.41
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.02	0.41
4:d:252:PHE:O	4:d:256:ILE:HG22	2.20	0.41
30:f:103:SQD:H131	18:x:36:VAL:HG11	2.02	0.41
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.41
22:B:604:CLA:H202	22:B:604:CLA:H162	1.86	0.41
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.84	0.41
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.03	0.41
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.02	0.41
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.41
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.21	0.41
22:D:405:CLA:H41	22:D:405:CLA:H61	1.87	0.41
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.02	0.41
31:b:604:LMT:H3'	31:b:604:LMT:H1B	1.53	0.41
22:b:611:CLA:H143	22:b:611:CLA:H161	1.87	0.41
3:c:318:LEU:HD13	3:c:351:PHE:HE1	1.84	0.41
1:A:140:ARG:HH22	26:A:409:LHG:P	2.43	0.41
22:B:606:CLA:HBC3	24:B:618:BCR:HC8	2.01	0.41
3:C:90:PRO:O	3:C:94:THR:HG23	2.19	0.41
22:C:511:CLA:H13	22:C:511:CLA:H61	2.02	0.41
1:a:27:ARG:NH1	4:d:254:SER:O	2.49	0.41
1:a:298:ASN:ND2	3:c:402:GLY:O	2.53	0.41
2:b:135:LEU:HB2	2:b:136:PRO:HD3	2.01	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.55	0.41
22:b:608:CLA:H141	22:b:608:CLA:H161	1.87	0.41
22:c:520:CLA:H142	22:c:520:CLA:H112	1.77	0.41
5:e:18:ARG:NH1	34:f:101:HEM:O1A	2.53	0.41
5:e:42:LEU:O	5:e:46:VAL:HG23	2.20	0.41
16:v:98:LEU:O	16:v:102:MET:HG3	2.21	0.41
1:A:183:MET:HA	22:A:402:CLA:HMD2	2.02	0.41
2:B:68:ARG:HH22	22:B:603:CLA:HED1	1.85	0.41
2:B:108:PHE:HB2	30:B:626:SQD:H223	2.02	0.41
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.01	0.41
3:C:429:SER:HB3	25:C:516:DGD:HA81	2.02	0.41
5:E:7:GLU:H	5:E:7:GLU:CD	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:182:PHE:O	1:a:186:PHE:HB2	2.21	0.41
22:a:405:CLA:H202	22:a:405:CLA:H162	1.78	0.41
2:b:16:PRO:HB2	2:b:123:PHE:CG	2.55	0.41
4:d:87:HIS:CD2	4:d:162:LEU:HD23	2.55	0.41
1:A:121:LEU:HD13	25:A:408:DGD:HB92	2.03	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.93	0.41
22:B:602:CLA:H61	22:B:602:CLA:H41	1.66	0.41
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.89	0.41
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.41
22:b:607:CLA:H202	22:b:607:CLA:H161	1.84	0.41
22:d:404:CLA:H92	22:d:404:CLA:H62	1.80	0.41
13:o:41:LEU:HD12	13:o:41:LEU:HA	1.94	0.41
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.41
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.89	0.41
4:D:350:ASN:O	4:D:352:LEU:N	2.49	0.41
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.03	0.41
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.01	0.41
1:a:240:GLY:HA3	14:t:29:ILE:HG22	2.03	0.41
7:h:12:ARG:O	7:h:12:ARG:HD3	2.20	0.41
13:o:206:GLU:H	13:o:206:GLU:CD	2.28	0.41
3:C:259:TRP:H	3:C:259:TRP:CD1	2.38	0.41
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.03	0.41
15:U:72:TYR:O	15:U:76:ALA:HB3	2.20	0.41
1:a:235:TYR:C	1:a:237:TYR:H	2.29	0.41
4:d:343:GLU:HG2	16:v:161:VAL:HG11	2.02	0.41
12:m:19:SER:O	12:m:23:ILE:HG13	2.21	0.41
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.29	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.85	0.41
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.35	0.41
7:H:12:ARG:N	7:H:13:PRO:HD2	2.36	0.41
2:b:383:PHE:N	4:d:344:GLU:O	2.39	0.41
22:c:508:CLA:H142	22:c:508:CLA:H112	1.83	0.41
4:d:156:VAL:HG12	4:d:171:PRO:HG3	2.01	0.41
1:A:235:TYR:C	1:A:237:TYR:H	2.28	0.41
1:A:240:GLY:HA3	14:T:29:ILE:HG22	2.02	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.21	0.41
2:B:19:LEU:O	2:B:23:HIS:ND1	2.53	0.41
2:B:25:MET:HG2	24:B:616:BCR:H23C	2.02	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
22:B:605:CLA:C3D	31:B:623:LMT:H11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:506:CLA:H92	22:C:506:CLA:H62	1.75	0.41
13:O:206:GLU:CD	13:O:206:GLU:H	2.28	0.41
16:V:98:LEU:O	16:V:102:MET:HG3	2.21	0.41
17:y:25:ILE:O	17:y:29:GLY:N	2.53	0.41
17:y:31:ALA:O	17:y:35:ILE:HG23	2.21	0.41
17:y:32:GLY:O	17:y:35:ILE:HG12	2.20	0.41
1:a:269:ARG:NH1	4:d:231:THR:HB	2.36	0.41
2:b:125:ASP:HA	2:b:126:PRO:HD3	1.98	0.41
24:b:622:BCR:H15C	24:b:622:BCR:H351	1.85	0.41
3:c:386:PRO:O	3:c:390:ARG:HG2	2.21	0.41
6:f:16:PHE:HB3	30:f:103:SQD:H241	2.03	0.41
10:k:31:LEU:HB3	24:g:101:BCR:C15	2.51	0.41
10:k:37:PHE:HB3	24:g:101:BCR:C40	2.50	0.41
12:m:31:SER:HA	27:m:101:LMG:HC5	2.03	0.41
1:A:238:LYS:HD2	14:T:32:LYS:HB3	2.03	0.41
2:B:43:ALA:HA	27:a:402:LMG:H112	2.02	0.41
3:C:334:PRO:HA	13:O:179:THR:OG1	2.21	0.41
32:D:402:PHO:CHB	22:D:404:CLA:H101	2.51	0.41
24:F:102:BCR:H11C	24:F:102:BCR:H341	1.94	0.41
10:K:24:VAL:O	10:K:27:VAL:HG12	2.21	0.41
2:b:191:ASN:HB2	7:h:58:VAL:HG23	2.03	0.41
2:b:280:PHE:O	2:b:284:ILE:HG13	2.20	0.41
3:c:402:GLY:HA3	3:c:420:VAL:HG22	2.02	0.41
3:c:425:TRP:CZ2	22:c:520:CLA:HBA1	2.57	0.41
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.51	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.90	0.40
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.50	0.40
3:C:78:GLU:H	3:C:78:GLU:CD	2.29	0.40
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.02	0.40
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.95	0.40
1:a:180:PHE:HA	1:a:183:MET:HE3	2.03	0.40
24:a:410:BCR:H20C	24:a:410:BCR:H361	1.82	0.40
2:b:108:PHE:HB2	30:b:602:SQD:H223	2.02	0.40
22:b:613:CLA:H12	22:b:613:CLA:H51	1.87	0.40
24:b:622:BCR:H11C	24:b:622:BCR:H341	1.88	0.40
3:c:257:PHE:HB3	3:c:258:GLY:H	1.62	0.40
22:c:512:CLA:HAB	24:c:521:BCR:H24C	2.03	0.40
24:c:521:BCR:H15C	24:c:521:BCR:H351	1.85	0.40
5:e:81:GLU:C	5:e:83:LEU:H	2.29	0.40
7:h:46:LEU:HB2	22:h:101:CLA:H61	2.02	0.40
1:A:182:PHE:O	1:A:186:PHE:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:ND2	3:C:402:GLY:O	2.55	0.40
22:B:602:CLA:HBB	22:H:101:CLA:O1D	2.21	0.40
24:B:618:BCR:H24C	24:B:618:BCR:H371	1.81	0.40
22:C:520:CLA:H112	22:C:520:CLA:H142	1.76	0.40
6:F:21:VAL:O	6:F:25:THR:HG23	2.22	0.40
24:F:102:BCR:H361	24:F:102:BCR:H20C	1.81	0.40
1:a:183:MET:HA	22:a:404:CLA:HMD2	2.03	0.40
1:a:260:PHE:CZ	1:a:263:ALA:HB2	2.56	0.40
27:b:625:LMG:H421	4:d:284:ILE:HD13	2.02	0.40
3:c:307:PRO:HB3	3:c:358:PHE:HB3	2.03	0.40
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.98	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.40
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.02	0.40
1:A:257:ARG:HH22	2:B:488:PRO:C	2.30	0.40
22:A:403:CLA:HAA1	23:D:406:PL9:H362	2.03	0.40
1:a:89:ILE:HG12	13:o:99:ARG:NH2	2.37	0.40
1:a:193:LEU:HD11	22:a:404:CLA:HMC2	2.03	0.40
1:a:215:HIS:ND1	23:a:409:PL9:O1	2.54	0.40
1:A:322:ASN:OD1	3:C:412:THR:HA	2.22	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
2:B:91:TRP:CH2	22:B:605:CLA:H12	2.56	0.40
22:B:607:CLA:H172	22:D:405:CLA:H3A	2.03	0.40
3:C:35:TRP:CZ2	26:C:519:LHG:H261	2.56	0.40
4:D:329:MET:HG2	4:D:333:ASP:HB2	2.04	0.40
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.40
1:a:29:TYR:CG	1:a:133:LEU:HD13	2.55	0.40
2:b:242:ILE:HG12	22:b:614:CLA:HBB1	2.04	0.40
2:b:414:PRO:HB2	2:b:415:PRO:HD3	2.02	0.40
3:c:350:ILE:HG21	3:c:359:TRP:HB2	2.03	0.40
23:A:406:PL9:H301	4:D:42:TYR:HA	2.03	0.40
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.56	0.40
4:D:294:ARG:H	4:D:294:ARG:HG2	1.64	0.40
3:c:393:ALA:HB1	34:v:201:HEM:HBC1	2.04	0.40
27:c:522:LMG:H322	10:k:27:VAL:HG23	2.03	0.40
17:g:31:ALA:O	17:g:35:ILE:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	312 (94%)	17 (5%)	4 (1%)	10	42
1	a	333/344 (97%)	310 (93%)	19 (6%)	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%)	406 (91%)	35 (8%)	4 (1%)	14	49
3	c	445/461 (96%)	405 (91%)	35 (8%)	5 (1%)	11	45
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	36	71
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	36	71
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	41
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9	41
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%)	208 (86%)	30 (12%)	3 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	27 (90%)	2 (7%)	1 (3%)	3	20
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	29
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	29
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2	19
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2	19
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	14
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	14
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	35
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	35
All	All	5138/5618 (92%)	4678 (91%)	404 (8%)	56 (1%)	11	45

All (56) 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
9	J	38	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

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Mol	Chain	Res	Type
3	c	257	PHE
3	c	416	SER
9	j	38	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
4	D	239	GLN
7	H	26	GLY
13	O	88	GLU
2	b	489	GLU
4	d	239	GLN
7	h	26	GLY
13	o	88	GLU
1	A	142	TRP
1	A	334	ARG
2	B	489	GLU
3	C	32	GLY
5	E	82	GLN
13	O	271	PRO
1	a	334	ARG
3	c	32	GLY
5	e	82	GLN
13	o	271	PRO
7	H	16	SER
15	U	73	PRO
1	a	142	TRP
3	c	144	SER
7	h	16	SER
15	u	73	PRO
3	C	144	SER
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY
3	c	194	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%)	261 (96%)	10 (4%)	30	51
1	a	271/280 (97%)	261 (96%)	10 (4%)	30	51
2	B	390/407 (96%)	380 (97%)	10 (3%)	40	61
2	b	390/407 (96%)	380 (97%)	10 (3%)	40	61
3	C	347/362 (96%)	335 (96%)	12 (4%)	32	53
3	c	347/362 (96%)	336 (97%)	11 (3%)	34	55
4	D	275/283 (97%)	263 (96%)	12 (4%)	25	47
4	d	275/283 (97%)	264 (96%)	11 (4%)	28	49
5	E	72/73 (99%)	68 (94%)	4 (6%)	19	41
5	e	72/73 (99%)	68 (94%)	4 (6%)	19	41
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%)	50 (94%)	3 (6%)	18	40
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	51
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	76
13	o	202/228 (89%)	200 (99%)	2 (1%)	68	76
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	37
18	x	30/34 (88%)	28 (93%)	2 (7%)	15	37
20	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
20	z	52/52 (100%)	50 (96%)	2 (4%)	29	51
All	All	4244/4594 (92%)	4111 (97%)	133 (3%)	35	56

All (133) 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	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

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Mol	Chain	Res	Type
3	C	254	THR
3	C	289	PHE
3	C	305	THR
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	256	ILE
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	56	ASP
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

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Mol	Chain	Res	Type
20	Z	62	VAL
1	a	30	VAL
1	a	157	VAL
1	a	202	VAL
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
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

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Mol	Chain	Res	Type
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	g	25	ILE
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
18	x	42	GLN
20	z	33	TRP
20	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
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	250	ASN
12	M	33	GLN
13	O	150	ASN
13	O	173	ASN
15	U	93	ASN
15	U	111	HIS

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Mol	Chain	Res	Type
1	a	241	GLN
1	a	337	HIS
2	b	26	HIS
2	b	223	GLN
2	b	282	GLN
2	b	374	ASN
3	c	44	ASN
3	c	56	HIS
3	c	229	ASN
3	c	441	HIS
4	d	117	HIS
4	d	186	GLN
4	d	250	ASN
4	d	255	GLN
4	d	322	ASN
12	m	33	GLN
13	o	130	GLN
13	o	150	ASN
13	o	173	ASN
15	u	111	HIS

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
30	SQD	B	622	-	41,43,54	1.05	2 (4%)	51,54,65	1.70	11 (21%)
31	LMT	b	603	-	36,36,36	1.11	4 (11%)	47,47,47	0.96	1 (2%)
23	PL9	A	406	-	45,45,55	0.99	3 (6%)	56,57,69	1.55	10 (17%)
24	BCR	b	622	-	41,41,41	1.13	2 (4%)	56,56,56	1.39	10 (17%)
24	BCR	g	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.31	8 (14%)
25	DGD	B	620	-	59,59,67	0.92	1 (1%)	73,73,81	1.34	8 (10%)
24	BCR	x	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	5 (8%)
23	PL9	j	101	-	35,35,55	0.97	2 (5%)	44,45,69	1.59	9 (20%)
27	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.29	3 (5%)
22	CLA	c	512	-	69,73,73	1.19	5 (7%)	82,113,113	1.27	5 (6%)
22	CLA	B	606	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
30	SQD	A	413	-	49,51,54	0.96	2 (4%)	59,62,65	1.69	10 (16%)
22	CLA	B	605	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
24	BCR	K	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	9 (16%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.29	6 (11%)
22	CLA	b	617	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
22	CLA	d	404	-	69,73,73	1.19	7 (10%)	82,113,113	1.21	6 (7%)
27	LMG	m	101	-	42,42,55	0.85	1 (2%)	50,50,63	1.25	4 (8%)
34	HEM	v	201	16	50,50,50	2.00	10 (20%)	67,82,82	1.25	4 (5%)
22	CLA	b	618	-	69,73,73	1.19	5 (7%)	82,113,113	1.27	5 (6%)
25	DGD	a	411	-	57,57,67	0.92	1 (1%)	71,71,81	1.40	8 (11%)
22	CLA	B	612	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	7 (8%)
24	BCR	H	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	6 (10%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	a	404	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	6 (7%)
25	DGD	C	515	-	54,54,67	0.96	2 (3%)	68,68,81	1.26	5 (7%)
33	BCT	d	403	21	3,3,3	1.11	0	2,3,3	4.23	2 (100%)
25	DGD	d	409	-	64,64,67	0.93	1 (1%)	78,78,81	1.34	9 (11%)
25	DGD	D	409	-	64,64,67	0.92	0	78,78,81	1.33	9 (11%)
22	CLA	B	601	-	69,73,73	1.20	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	B	610	-	69,73,73	1.24	7 (10%)	82,113,113	1.34	7 (8%)
22	CLA	b	614	-	69,73,73	1.24	7 (10%)	82,113,113	1.34	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	501	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	c	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
27	LMG	C	521	-	48,48,55	0.76	1 (2%)	56,56,63	1.30	5 (8%)
22	CLA	b	609	-	69,73,73	1.17	6 (8%)	82,113,113	1.28	5 (6%)
27	LMG	D	407	-	49,49,55	0.76	1 (2%)	57,57,63	1.31	5 (8%)
34	HEM	V	201	16	50,50,50	1.98	10 (20%)	67,82,82	1.21	3 (4%)
24	BCR	y	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.29	7 (12%)
22	CLA	C	509	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
31	LMT	i	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.01	2 (4%)
31	LMT	B	628	-	36,36,36	1.13	5 (13%)	47,47,47	1.05	1 (2%)
32	PHO	D	401	-	58,69,69	2.15	9 (15%)	55,99,99	1.40	6 (10%)
24	BCR	b	621	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	8 (14%)
27	LMG	d	411	-	46,46,55	0.78	1 (2%)	54,54,63	1.30	6 (11%)
22	CLA	b	605	-	69,73,73	1.21	7 (10%)	82,113,113	1.26	6 (7%)
27	LMG	A	410	-	51,51,55	0.75	0	59,59,63	1.36	7 (11%)
22	CLA	A	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.29	4 (7%)
27	LMG	l	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.34	6 (10%)
22	CLA	A	404	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
30	SQD	b	602	-	45,47,54	1.02	3 (6%)	55,58,65	1.72	10 (18%)
22	CLA	B	607	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
22	CLA	d	405	-	69,73,73	1.19	5 (7%)	82,113,113	1.25	5 (6%)
22	CLA	c	505	-	69,73,73	1.20	6 (8%)	82,113,113	1.28	4 (4%)
22	CLA	C	512	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
31	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	0.98	1 (2%)
22	CLA	B	614	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.31	7 (10%)
27	LMG	A	415	-	42,42,55	0.83	1 (2%)	50,50,63	1.26	5 (10%)
24	BCR	b	623	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	9 (16%)
25	DGD	b	601	-	53,53,67	1.05	2 (3%)	67,67,81	1.33	7 (10%)
31	LMT	D	410	-	32,32,36	1.17	4 (12%)	43,43,47	1.01	2 (4%)
24	BCR	a	410	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	7 (12%)
22	CLA	B	608	-	69,73,73	1.20	6 (8%)	82,113,113	1.24	5 (6%)
22	CLA	C	507	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	6 (7%)
25	DGD	c	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.42	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
31	LMT	d	410	-	32,32,36	1.16	4 (12%)	43,43,47	1.01	2 (4%)
25	DGD	c	517	-	67,67,67	0.87	0	81,81,81	1.39	9 (11%)
22	CLA	b	616	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	7 (8%)
22	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
32	PHO	D	402	-	58,69,69	2.18	9 (15%)	55,99,99	1.39	5 (9%)
22	CLA	B	615	-	69,73,73	1.18	9 (13%)	82,113,113	1.26	5 (6%)
22	CLA	D	405	-	69,73,73	1.18	6 (8%)	82,113,113	1.25	5 (6%)
24	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
22	CLA	b	612	-	69,73,73	1.20	6 (8%)	82,113,113	1.23	5 (6%)
24	BCR	c	521	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	8 (14%)
31	LMT	b	626	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	1 (2%)
22	CLA	b	619	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	c	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	c	503	-	69,73,73	1.20	6 (8%)	82,113,113	1.28	5 (6%)
22	CLA	b	606	-	69,73,73	1.19	6 (8%)	82,113,113	1.24	7 (8%)
24	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.38	9 (16%)
27	LMG	M	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.22	4 (8%)
30	SQD	d	402	-	41,43,54	1.05	2 (4%)	51,54,65	1.71	11 (21%)
22	CLA	h	101	-	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
31	LMT	b	604	-	36,36,36	1.12	4 (11%)	47,47,47	1.04	1 (2%)
22	CLA	B	604	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
22	CLA	C	508	-	69,73,73	1.19	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	b	615	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
27	LMG	D	408	-	48,48,55	0.75	0	56,56,63	1.38	4 (7%)
27	LMG	d	407	-	49,49,55	0.76	1 (2%)	57,57,63	1.30	5 (8%)
22	CLA	C	505	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
29	OEX	a	414	1,3	0,15,15	-	-	-	-	-
26	LHG	c	519	-	36,36,48	0.74	2 (5%)	39,42,54	1.28	4 (10%)
22	CLA	C	503	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	5 (6%)
34	HEM	F	101	6,5	50,50,50	1.96	9 (18%)	67,82,82	1.31	4 (5%)
24	BCR	J	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.59	13 (23%)
26	LHG	A	409	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	3 (7%)
22	CLA	b	607	-	69,73,73	1.19	7 (10%)	82,113,113	1.33	7 (8%)
22	CLA	c	502	-	69,73,73	1.20	8 (11%)	82,113,113	1.25	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	520	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
25	DGD	C	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.43	12 (15%)
22	CLA	a	405	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
24	BCR	A	407	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	7 (12%)
24	BCR	f	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	5 (8%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.27	5 (7%)
24	BCR	F	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
27	LMG	d	408	-	48,48,55	0.75	0	56,56,63	1.37	4 (7%)
30	SQD	F	103	-	43,45,54	1.03	2 (4%)	53,56,65	1.58	10 (18%)
30	SQD	a	401	-	52,54,54	0.96	3 (5%)	62,65,65	1.48	9 (14%)
31	LMT	M	102	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
30	SQD	B	626	-	45,47,54	1.02	3 (6%)	55,58,65	1.72	10 (18%)
25	DGD	A	408	-	57,57,67	0.92	0	71,71,81	1.41	9 (12%)
24	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	8 (14%)
24	BCR	B	618	-	41,41,41	1.13	2 (4%)	56,56,56	1.40	9 (16%)
24	BCR	B	616	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	8 (14%)
22	CLA	b	608	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
22	CLA	B	603	-	69,73,73	1.19	8 (11%)	82,113,113	1.34	7 (8%)
22	CLA	c	510	3	69,73,73	1.20	5 (7%)	82,113,113	1.27	5 (6%)
25	DGD	b	624	-	59,59,67	0.90	1 (1%)	73,73,81	1.35	6 (8%)
22	CLA	C	502	-	69,73,73	1.19	9 (13%)	82,113,113	1.26	5 (6%)
22	CLA	C	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	C	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
22	CLA	B	613	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
22	CLA	A	405	-	69,73,73	1.19	8 (11%)	82,113,113	1.22	4 (4%)
27	LMG	B	621	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	7 (12%)
27	LMG	a	402	-	42,42,55	0.82	1 (2%)	50,50,63	1.26	4 (8%)
22	CLA	b	610	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
34	HEM	f	101	6,5	50,50,50	1.96	8 (16%)	67,82,82	1.32	4 (5%)
31	LMT	I	102	-	36,36,36	1.09	4 (11%)	47,47,47	1.03	2 (4%)
30	SQD	f	103	-	43,45,54	1.03	2 (4%)	53,56,65	1.58	10 (18%)
22	CLA	D	404	-	69,73,73	1.19	8 (11%)	82,113,113	1.20	5 (6%)
32	PHO	d	401	-	58,69,69	2.14	9 (15%)	55,99,99	1.41	7 (12%)
22	CLA	C	510	3	69,73,73	1.19	6 (8%)	82,113,113	1.30	6 (7%)
33	BCT	D	403	21	3,3,3	1.10	0	2,3,3	4.25	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	402	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	B	609	-	69,73,73	1.19	8 (11%)	82,113,113	1.28	5 (6%)
23	PL9	D	406	-	55,55,55	1.05	3 (5%)	68,69,69	1.49	13 (19%)
30	SQD	a	415	-	49,51,54	0.96	2 (4%)	59,62,65	1.69	9 (15%)
24	BCR	j	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.58	13 (23%)
26	LHG	a	412	-	38,38,48	0.71	1 (2%)	41,44,54	1.23	3 (7%)
24	BCR	c	514	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	8 (14%)
24	BCR	C	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.37	9 (16%)
31	LMT	B	624	-	36,36,36	1.09	3 (8%)	47,47,47	1.01	2 (4%)
31	LMT	b	627	-	36,36,36	1.08	3 (8%)	47,47,47	1.01	2 (4%)
22	CLA	C	501	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
30	SQD	A	414	-	52,54,54	0.96	2 (3%)	62,65,65	1.49	9 (14%)
22	CLA	b	613	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	C	520	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.29	5 (9%)
26	LHG	C	519	-	36,36,48	0.71	1 (2%)	39,42,54	1.29	4 (10%)
29	OEX	A	412	1,3	0,15,15	-	-	-	-	-
22	CLA	B	602	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
22	CLA	H	101	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	c	504	-	69,73,73	1.18	6 (8%)	82,113,113	1.31	7 (8%)
27	LMG	i	101	-	43,43,55	0.81	0	51,51,63	1.27	5 (9%)
23	PL9	a	409	-	45,45,55	1.05	4 (8%)	56,57,69	1.55	11 (19%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.26	4 (7%)
23	PL9	d	406	-	55,55,55	1.03	3 (5%)	68,69,69	1.51	13 (19%)
23	PL9	J	101	-	35,35,55	1.00	2 (5%)	44,45,69	1.59	8 (18%)
31	LMT	B	627	-	36,36,36	1.11	4 (11%)	47,47,47	0.97	1 (2%)
22	CLA	a	408	-	69,73,73	1.18	6 (8%)	82,113,113	1.25	4 (4%)
27	LMG	D	411	-	46,46,55	0.76	1 (2%)	54,54,63	1.31	5 (9%)
22	CLA	c	508	-	69,73,73	1.19	7 (10%)	82,113,113	1.24	5 (6%)
32	PHO	a	407	-	58,69,69	2.18	9 (15%)	55,99,99	1.39	5 (9%)
22	CLA	b	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
31	LMT	M	103	-	36,36,36	1.12	4 (11%)	47,47,47	1.00	2 (4%)
22	CLA	a	406	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
22	CLA	C	504	-	69,73,73	1.18	7 (10%)	82,113,113	1.31	7 (8%)
22	CLA	c	509	-	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DGD	C	517	-	67,67,67	0.88	1 (1%)	81,81,81	1.39	10 (12%)
22	CLA	c	507	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	7 (8%)
24	BCR	C	514	-	41,41,41	1.14	3 (7%)	56,56,56	1.30	9 (16%)
24	BCR	b	620	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	5 (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
30	SQD	B	622	-	-	15/38/58/69	0/1/1/1
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	BCR	g	101	-	-	4/29/63/63	0/2/2/2
25	DGD	B	620	-	-	18/47/87/95	0/2/2/2
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
27	LMG	E	101	-	-	17/39/59/70	0/1/1/1
22	CLA	c	512	-	1/1/15/20	16/39/115/115	-
22	CLA	B	606	-	1/1/15/20	9/39/115/115	-
30	SQD	A	413	-	-	18/46/66/69	0/1/1/1
22	CLA	B	605	-	1/1/15/20	14/39/115/115	-
24	BCR	K	102	-	-	4/29/63/63	0/2/2/2
27	LMG	c	518	-	-	22/40/60/70	0/1/1/1
22	CLA	b	617	-	1/1/15/20	13/39/115/115	-
22	CLA	d	404	-	1/1/15/20	11/39/115/115	-
27	LMG	m	101	-	-	16/37/57/70	0/1/1/1
34	HEM	v	201	16	-	5/14/54/54	-
22	CLA	b	618	-	1/1/15/20	9/39/115/115	-
25	DGD	a	411	-	-	14/45/85/95	0/2/2/2
22	CLA	B	612	-	1/1/15/20	16/39/115/115	-
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
22	CLA	a	404	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
25	DGD	d	409	-	-	34/52/92/95	0/2/2/2
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2
22	CLA	B	601	-	1/1/15/20	15/39/115/115	-
22	CLA	B	610	-	1/1/15/20	11/39/115/115	-
22	CLA	b	614	-	1/1/15/20	11/39/115/115	-
22	CLA	c	501	-	1/1/15/20	14/39/115/115	-
22	CLA	c	506	-	1/1/15/20	11/39/115/115	-
27	LMG	C	521	-	-	19/43/63/70	0/1/1/1
22	CLA	b	609	-	1/1/15/20	18/39/115/115	-
27	LMG	D	407	-	-	24/44/64/70	0/1/1/1
34	HEM	V	201	16	-	5/14/54/54	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	C	509	-	1/1/15/20	15/39/115/115	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
32	PHO	D	401	-	-	10/37/103/103	0/5/6/6
24	BCR	b	621	-	-	7/29/63/63	0/2/2/2
27	LMG	d	411	-	-	16/41/61/70	0/1/1/1
22	CLA	b	605	-	1/1/15/20	16/39/115/115	-
27	LMG	A	410	-	-	28/46/66/70	0/1/1/1
22	CLA	A	403	-	1/1/15/20	13/39/115/115	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
27	LMG	l	101	-	-	25/46/66/70	0/1/1/1
22	CLA	A	404	-	1/1/15/20	8/39/115/115	-
30	SQD	b	602	-	-	13/42/62/69	0/1/1/1
22	CLA	B	607	-	1/1/15/20	12/39/115/115	-
22	CLA	d	405	-	-	8/39/115/115	-
22	CLA	c	505	-	1/1/15/20	16/39/115/115	-
22	CLA	C	512	-	1/1/15/20	14/39/115/115	-
31	LMT	B	623	-	-	3/21/61/61	0/2/2/2
22	CLA	B	614	-	1/1/15/20	10/39/115/115	-
25	DGD	B	625	-	-	19/41/81/95	0/2/2/2
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	623	-	-	5/29/63/63	0/2/2/2
25	DGD	b	601	-	-	19/41/81/95	0/2/2/2
31	LMT	D	410	-	-	2/17/57/61	0/2/2/2
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
22	CLA	B	608	-	1/1/15/20	9/39/115/115	-
22	CLA	C	507	-	1/1/15/20	13/39/115/115	-
25	DGD	c	516	-	-	19/51/91/95	0/2/2/2
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
31	LMT	d	410	-	-	1/17/57/61	0/2/2/2
25	DGD	c	517	-	-	19/55/95/95	0/2/2/2
22	CLA	b	616	-	1/1/15/20	15/39/115/115	-
22	CLA	B	611	-	1/1/15/20	9/39/115/115	-
32	PHO	D	402	-	-	11/37/103/103	0/5/6/6
22	CLA	B	615	-	1/1/15/20	19/39/115/115	-
22	CLA	D	405	-	1/1/15/20	8/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
22	CLA	b	612	-	1/1/15/20	10/39/115/115	-
24	BCR	c	521	-	-	4/29/63/63	0/2/2/2
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
22	CLA	b	619	-	1/1/15/20	19/39/115/115	-
22	CLA	c	511	-	1/1/15/20	17/39/115/115	-
22	CLA	c	503	-	1/1/15/20	12/39/115/115	-
22	CLA	b	606	-	1/1/15/20	14/39/115/115	-
24	BCR	c	513	-	-	5/29/63/63	0/2/2/2
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
30	SQD	d	402	-	-	15/38/58/69	0/1/1/1
22	CLA	h	101	-	1/1/15/20	14/39/115/115	-
31	LMT	b	604	-	-	5/21/61/61	0/2/2/2
22	CLA	B	604	-	1/1/15/20	15/39/115/115	-
22	CLA	C	508	-	1/1/15/20	19/39/115/115	-
22	CLA	b	615	-	1/1/15/20	10/39/115/115	-
27	LMG	D	408	-	-	21/43/63/70	0/1/1/1
27	LMG	d	407	-	-	24/44/64/70	0/1/1/1
22	CLA	C	505	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	c	519	-	-	17/41/41/53	-
22	CLA	C	503	-	1/1/15/20	12/39/115/115	-
34	HEM	F	101	6,5	-	2/14/54/54	-
24	BCR	J	102	-	-	7/29/63/63	0/2/2/2
26	LHG	A	409	-	-	11/43/43/53	-
22	CLA	b	607	-	1/1/15/20	8/39/115/115	-
22	CLA	c	502	-	1/1/15/20	10/39/115/115	-
22	CLA	c	520	-	1/1/15/20	12/39/115/115	-
25	DGD	C	516	-	-	19/51/91/95	0/2/2/2
22	CLA	a	405	-	1/1/15/20	12/39/115/115	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
24	BCR	f	102	-	-	5/29/63/63	0/2/2/2
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
24	BCR	F	102	-	-	5/29/63/63	0/2/2/2
27	LMG	d	408	-	-	21/43/63/70	0/1/1/1
30	SQD	F	103	-	-	12/40/60/69	0/1/1/1
30	SQD	a	401	-	-	13/49/69/69	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
30	SQD	B	626	-	-	13/42/62/69	0/1/1/1
25	DGD	A	408	-	-	13/45/85/95	0/2/2/2
24	BCR	B	617	-	-	6/29/63/63	0/2/2/2
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/15/20	15/39/115/115	-
22	CLA	B	603	-	1/1/15/20	8/39/115/115	-
22	CLA	c	510	3	1/1/15/20	15/39/115/115	-
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
22	CLA	C	502	-	1/1/15/20	10/39/115/115	-
22	CLA	C	511	-	1/1/15/20	17/39/115/115	-
22	CLA	C	506	-	1/1/15/20	12/39/115/115	-
22	CLA	B	613	-	1/1/15/20	12/39/115/115	-
22	CLA	A	405	-	1/1/15/20	8/39/115/115	-
27	LMG	B	621	-	-	14/44/64/70	0/1/1/1
27	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	610	-	1/1/15/20	9/39/115/115	-
34	HEM	f	101	6,5	-	2/14/54/54	-
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
22	CLA	D	404	-	1/1/15/20	14/39/115/115	-
32	PHO	d	401	-	-	10/37/103/103	0/5/6/6
22	CLA	C	510	3	1/1/15/20	15/39/115/115	-
22	CLA	A	402	-	1/1/15/20	8/39/115/115	-
22	CLA	B	609	-	1/1/15/20	18/39/115/115	-
23	PL9	D	406	-	-	12/53/73/73	0/1/1/1
30	SQD	a	415	-	-	18/46/66/69	0/1/1/1
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
26	LHG	a	412	-	-	11/43/43/53	-
24	BCR	c	514	-	-	4/29/63/63	0/2/2/2
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
31	LMT	B	624	-	-	3/21/61/61	0/2/2/2
31	LMT	b	627	-	-	3/21/61/61	0/2/2/2
22	CLA	C	501	-	1/1/15/20	15/39/115/115	-
30	SQD	A	414	-	-	11/49/69/69	0/1/1/1
22	CLA	b	613	-	1/1/15/20	17/39/115/115	-
22	CLA	C	520	-	1/1/15/20	13/39/115/115	-
27	LMG	C	518	-	-	22/40/60/70	0/1/1/1
26	LHG	C	519	-	-	16/41/41/53	-
22	CLA	B	602	-	1/1/15/20	14/39/115/115	-
22	CLA	H	101	-	1/1/15/20	15/39/115/115	-
22	CLA	c	504	-	1/1/15/20	18/39/115/115	-
27	LMG	i	101	-	-	19/38/58/70	0/1/1/1
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
27	LMG	I	101	-	-	19/38/58/70	0/1/1/1
23	PL9	d	406	-	-	12/53/73/73	0/1/1/1
23	PL9	J	101	-	-	9/29/49/73	0/1/1/1
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
22	CLA	a	408	-	1/1/15/20	8/39/115/115	-
27	LMG	D	411	-	-	15/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	508	-	1/1/15/20	19/39/115/115	-
32	PHO	a	407	-	-	11/37/103/103	0/5/6/6
22	CLA	b	611	-	1/1/15/20	13/39/115/115	-
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	a	406	-	1/1/15/20	8/39/115/115	-
22	CLA	C	504	-	1/1/15/20	17/39/115/115	-
22	CLA	c	509	-	1/1/15/20	17/39/115/115	-
25	DGD	C	517	-	-	20/55/95/95	0/2/2/2
22	CLA	c	507	-	1/1/15/20	13/39/115/115	-
24	BCR	C	514	-	-	4/29/63/63	0/2/2/2
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2

All (736) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	402	PHO	C1B-C2B	9.63	1.50	1.39
32	D	401	PHO	C1B-C2B	9.55	1.50	1.39
32	d	401	PHO	C1B-C2B	9.52	1.50	1.39
32	a	407	PHO	C1B-C2B	9.52	1.50	1.39
32	a	407	PHO	C3B-C4B	8.72	1.50	1.41
32	D	402	PHO	C3B-C4B	8.69	1.50	1.41
32	d	401	PHO	C3B-C4B	8.42	1.50	1.41
32	D	401	PHO	C3B-C4B	8.40	1.50	1.41
34	v	201	HEM	C3D-C2D	8.17	1.54	1.36
34	V	201	HEM	C3D-C2D	8.15	1.54	1.36
34	f	101	HEM	C3D-C2D	7.91	1.53	1.36
34	F	101	HEM	C3D-C2D	7.90	1.53	1.36
34	f	101	HEM	FE-ND	5.35	2.11	1.94
34	F	101	HEM	FE-ND	5.28	2.11	1.94
34	V	201	HEM	FE-ND	5.13	2.10	1.94
34	v	201	HEM	FE-ND	5.08	2.10	1.94
34	v	201	HEM	FE-NB	4.60	2.09	1.94
34	f	101	HEM	FE-NB	4.42	2.08	1.94
34	F	101	HEM	FE-NB	4.41	2.08	1.94
34	V	201	HEM	FE-NB	4.33	2.08	1.94
32	a	407	PHO	C1D-C2D	4.32	1.44	1.39
32	D	402	PHO	C1D-C2D	4.29	1.44	1.39
32	D	401	PHO	C1D-C2D	4.11	1.44	1.39
24	g	101	BCR	C1-C6	-4.04	1.48	1.53
24	y	101	BCR	C1-C6	-3.98	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	401	PHO	C1D-C2D	3.98	1.43	1.39
24	H	102	BCR	C1-C6	-3.91	1.48	1.53
24	x	101	BCR	C1-C6	-3.90	1.48	1.53
24	F	102	BCR	C1-C6	-3.86	1.48	1.53
24	f	102	BCR	C1-C6	-3.84	1.48	1.53
34	v	201	HEM	FE-NA	3.84	2.07	1.95
32	D	401	PHO	C4D-CHA	3.81	1.45	1.39
22	c	503	CLA	C1D-ND	3.79	1.42	1.37
22	C	501	CLA	C1D-ND	3.79	1.42	1.37
22	C	503	CLA	C1D-ND	3.78	1.42	1.37
22	c	501	CLA	C1D-ND	3.77	1.42	1.37
22	b	608	CLA	C1D-ND	3.77	1.42	1.37
22	b	605	CLA	C1D-ND	3.77	1.42	1.37
22	c	505	CLA	C1D-ND	3.76	1.42	1.37
22	B	608	CLA	C1D-ND	3.76	1.42	1.37
22	d	405	CLA	C1D-ND	3.75	1.42	1.37
32	a	407	PHO	C4D-CHA	3.75	1.45	1.39
22	c	510	CLA	C1D-ND	3.75	1.42	1.37
34	F	101	HEM	FE-NA	3.74	2.07	1.95
22	B	601	CLA	C1D-ND	3.73	1.42	1.37
32	D	402	PHO	C4D-CHA	3.72	1.45	1.39
22	c	512	CLA	C1D-ND	3.72	1.42	1.37
22	a	408	CLA	C1D-ND	3.72	1.42	1.37
22	A	403	CLA	C1D-ND	3.72	1.42	1.37
22	d	404	CLA	C1D-ND	3.72	1.42	1.37
22	C	510	CLA	C1D-ND	3.71	1.42	1.37
22	D	404	CLA	C1D-ND	3.71	1.42	1.37
22	B	604	CLA	C1D-ND	3.71	1.42	1.37
22	h	101	CLA	C1D-ND	3.71	1.42	1.37
22	C	512	CLA	C1D-ND	3.70	1.42	1.37
22	H	101	CLA	C1D-ND	3.70	1.42	1.37
32	d	401	PHO	C4D-CHA	3.70	1.45	1.39
22	b	612	CLA	C1D-ND	3.69	1.42	1.37
22	c	506	CLA	C1D-ND	3.69	1.42	1.37
22	b	618	CLA	C1D-ND	3.69	1.42	1.37
22	b	606	CLA	C1D-ND	3.68	1.42	1.37
22	D	405	CLA	C1D-ND	3.68	1.42	1.37
22	A	405	CLA	C1D-ND	3.67	1.42	1.37
22	C	505	CLA	C1D-ND	3.66	1.42	1.37
22	b	609	CLA	C1D-ND	3.66	1.42	1.37
22	b	613	CLA	C1D-ND	3.65	1.42	1.37
22	C	506	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	C1D-ND	3.64	1.42	1.37
34	V	201	HEM	FE-NA	3.63	2.07	1.95
34	f	101	HEM	FE-NA	3.63	2.07	1.95
22	C	511	CLA	C1D-ND	3.63	1.42	1.37
22	c	502	CLA	C1D-ND	3.63	1.42	1.37
22	B	602	CLA	C1D-ND	3.63	1.42	1.37
22	a	405	CLA	C1D-ND	3.62	1.42	1.37
22	c	504	CLA	C1D-ND	3.62	1.42	1.37
22	c	508	CLA	C1D-ND	3.62	1.42	1.37
22	B	605	CLA	C1D-ND	3.62	1.42	1.37
22	C	504	CLA	C1D-ND	3.61	1.42	1.37
22	B	607	CLA	C1D-ND	3.61	1.42	1.37
22	b	607	CLA	C1D-ND	3.60	1.42	1.37
22	C	520	CLA	C1D-ND	3.60	1.42	1.37
22	B	614	CLA	C1D-ND	3.60	1.42	1.37
24	C	514	BCR	C1-C6	-3.60	1.49	1.53
24	c	514	BCR	C1-C6	-3.60	1.49	1.53
22	B	613	CLA	C1D-ND	3.59	1.42	1.37
22	B	612	CLA	C1D-ND	3.58	1.42	1.37
24	b	620	BCR	C1-C6	-3.58	1.49	1.53
24	B	616	BCR	C1-C6	-3.58	1.49	1.53
22	a	406	CLA	C1D-ND	3.58	1.42	1.37
22	b	610	CLA	C1D-ND	3.57	1.42	1.37
22	c	520	CLA	C1D-ND	3.57	1.42	1.37
22	a	404	CLA	C1D-ND	3.56	1.42	1.37
22	c	511	CLA	C1D-ND	3.56	1.42	1.37
22	b	617	CLA	C1D-ND	3.56	1.42	1.37
22	B	606	CLA	C1D-ND	3.56	1.42	1.37
22	c	507	CLA	C1D-ND	3.56	1.42	1.37
22	B	609	CLA	C1D-ND	3.56	1.42	1.37
22	b	616	CLA	C1D-ND	3.55	1.42	1.37
22	b	611	CLA	C1D-ND	3.55	1.42	1.37
22	A	404	CLA	C1D-ND	3.54	1.42	1.37
22	C	502	CLA	C1D-ND	3.53	1.42	1.37
22	A	402	CLA	C1D-ND	3.51	1.42	1.37
22	C	508	CLA	C1D-ND	3.50	1.42	1.37
24	g	101	BCR	C30-C25	-3.49	1.49	1.53
24	y	101	BCR	C30-C25	-3.48	1.49	1.53
24	J	102	BCR	C30-C25	-3.48	1.49	1.53
22	B	615	CLA	C1D-ND	3.47	1.42	1.37
24	j	102	BCR	C30-C25	-3.47	1.49	1.53
22	C	507	CLA	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	619	CLA	C1D-ND	3.46	1.42	1.37
24	b	622	BCR	C30-C25	-3.45	1.49	1.53
24	C	513	BCR	C1-C6	-3.44	1.49	1.53
24	b	621	BCR	C1-C6	-3.44	1.49	1.53
22	C	509	CLA	C1D-ND	3.43	1.42	1.37
22	c	509	CLA	C1D-ND	3.43	1.42	1.37
34	v	201	HEM	FE-NC	3.43	2.06	1.95
24	B	617	BCR	C1-C6	-3.43	1.49	1.53
22	b	614	CLA	C1D-ND	3.43	1.42	1.37
24	F	102	BCR	C30-C25	-3.42	1.49	1.53
22	B	610	CLA	C1D-ND	3.41	1.42	1.37
24	c	513	BCR	C1-C6	-3.41	1.49	1.53
24	B	618	BCR	C30-C25	-3.41	1.49	1.53
24	K	102	BCR	C30-C25	-3.39	1.49	1.53
24	b	623	BCR	C30-C25	-3.38	1.49	1.53
24	B	619	BCR	C30-C25	-3.37	1.49	1.53
24	f	102	BCR	C30-C25	-3.36	1.49	1.53
24	c	521	BCR	C30-C25	-3.34	1.49	1.53
24	a	410	BCR	C30-C25	-3.33	1.49	1.53
24	B	618	BCR	C1-C6	-3.33	1.49	1.53
24	A	407	BCR	C30-C25	-3.32	1.49	1.53
24	b	623	BCR	C1-C6	-3.32	1.49	1.53
24	b	620	BCR	C30-C25	-3.32	1.49	1.53
24	B	619	BCR	C1-C6	-3.31	1.49	1.53
24	b	622	BCR	C1-C6	-3.30	1.49	1.53
22	b	614	CLA	CMB-C2B	-3.30	1.44	1.50
24	a	410	BCR	C1-C6	-3.29	1.49	1.53
22	b	605	CLA	C4B-NB	3.29	1.42	1.37
22	A	402	CLA	C4B-NB	3.29	1.42	1.37
22	c	509	CLA	C4B-NB	3.28	1.42	1.37
22	a	404	CLA	C4B-NB	3.28	1.42	1.37
24	B	616	BCR	C30-C25	-3.28	1.49	1.53
24	A	407	BCR	C1-C6	-3.25	1.49	1.53
22	b	615	CLA	C1D-ND	3.25	1.42	1.37
24	K	102	BCR	C1-C6	-3.23	1.49	1.53
22	B	610	CLA	CMB-C2B	-3.23	1.44	1.50
22	c	508	CLA	C4B-NB	3.22	1.42	1.37
22	C	508	CLA	C4B-NB	3.22	1.42	1.37
24	H	102	BCR	C30-C25	-3.21	1.49	1.53
24	C	513	BCR	C30-C25	-3.21	1.49	1.53
22	c	512	CLA	C4B-NB	3.20	1.42	1.37
24	C	514	BCR	C30-C25	-3.20	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	C4B-NB	3.19	1.42	1.37
22	B	601	CLA	C4B-NB	3.19	1.42	1.37
22	B	610	CLA	C4B-NB	3.19	1.42	1.37
34	V	201	HEM	FE-NC	3.18	2.05	1.95
22	B	615	CLA	C4B-NB	3.18	1.42	1.37
22	C	509	CLA	C4B-NB	3.18	1.42	1.37
22	B	611	CLA	C1D-ND	3.18	1.42	1.37
22	c	511	CLA	C4B-NB	3.18	1.42	1.37
24	x	101	BCR	C30-C25	-3.18	1.49	1.53
24	c	521	BCR	C1-C6	-3.17	1.49	1.53
22	c	503	CLA	C4B-NB	3.17	1.42	1.37
30	B	626	SQD	O48-C23	3.16	1.42	1.33
22	b	619	CLA	C4B-NB	3.16	1.42	1.37
22	C	505	CLA	C4B-NB	3.16	1.42	1.37
30	b	602	SQD	O48-C23	3.16	1.42	1.33
22	B	608	CLA	C4B-NB	3.15	1.42	1.37
30	a	401	SQD	O48-C23	3.15	1.42	1.33
34	F	101	HEM	FE-NC	3.15	2.05	1.95
24	c	514	BCR	C30-C25	-3.15	1.49	1.53
22	b	614	CLA	C4B-NB	3.15	1.42	1.37
22	c	504	CLA	C4B-NB	3.15	1.42	1.37
22	b	612	CLA	C4B-NB	3.15	1.42	1.37
30	A	414	SQD	O48-C23	3.14	1.42	1.33
30	d	402	SQD	O48-C23	3.14	1.42	1.33
22	b	618	CLA	C4B-NB	3.14	1.42	1.37
30	B	622	SQD	O48-C23	3.14	1.42	1.33
22	B	604	CLA	C4B-NB	3.14	1.42	1.37
22	c	520	CLA	C4B-NB	3.13	1.42	1.37
30	f	103	SQD	O48-C23	3.13	1.42	1.33
22	d	405	CLA	C4B-NB	3.13	1.42	1.37
22	B	614	CLA	C4B-NB	3.13	1.42	1.37
22	c	510	CLA	C4B-NB	3.12	1.42	1.37
30	F	103	SQD	O48-C23	3.12	1.42	1.33
22	A	405	CLA	C4B-NB	3.12	1.42	1.37
34	f	101	HEM	CAC-C3C	3.11	1.55	1.47
22	C	507	CLA	C4B-NB	3.11	1.41	1.37
22	B	611	CLA	C4B-NB	3.11	1.41	1.37
34	V	201	HEM	CAB-C3B	3.11	1.55	1.47
22	b	610	CLA	C4B-NB	3.10	1.41	1.37
22	a	405	CLA	C4B-NB	3.10	1.41	1.37
34	f	101	HEM	FE-NC	3.09	2.05	1.95
22	H	101	CLA	C4B-NB	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	CAB-C3B	3.09	1.55	1.47
22	a	406	CLA	C4B-NB	3.09	1.41	1.37
30	a	415	SQD	O48-C23	3.09	1.42	1.33
22	C	511	CLA	C4B-NB	3.09	1.41	1.37
22	A	403	CLA	C4B-NB	3.08	1.41	1.37
22	c	507	CLA	C4B-NB	3.08	1.41	1.37
22	B	609	CLA	C4B-NB	3.07	1.41	1.37
22	a	408	CLA	C4B-NB	3.07	1.41	1.37
22	B	606	CLA	C4B-NB	3.07	1.41	1.37
22	b	611	CLA	C4B-NB	3.07	1.41	1.37
22	D	405	CLA	C4B-NB	3.07	1.41	1.37
22	b	615	CLA	C4B-NB	3.07	1.41	1.37
34	F	101	HEM	CAC-C3C	3.07	1.55	1.47
22	C	504	CLA	C4B-NB	3.06	1.41	1.37
22	b	609	CLA	C4B-NB	3.06	1.41	1.37
22	b	607	CLA	C4B-NB	3.06	1.41	1.37
30	A	413	SQD	O48-C23	3.05	1.42	1.33
22	C	512	CLA	C4B-NB	3.05	1.41	1.37
22	d	404	CLA	C4B-NB	3.04	1.41	1.37
34	v	201	HEM	CAC-C3C	3.04	1.55	1.47
22	C	520	CLA	C4B-NB	3.03	1.41	1.37
22	h	101	CLA	C4B-NB	3.03	1.41	1.37
22	C	510	CLA	C4B-NB	3.03	1.41	1.37
22	b	608	CLA	C4B-NB	3.03	1.41	1.37
22	c	502	CLA	C4B-NB	3.03	1.41	1.37
24	c	513	BCR	C30-C25	-3.03	1.49	1.53
22	c	501	CLA	C4B-NB	3.03	1.41	1.37
34	V	201	HEM	CAC-C3C	3.02	1.55	1.47
22	b	616	CLA	C4B-NB	3.02	1.41	1.37
22	D	404	CLA	C4B-NB	3.01	1.41	1.37
22	b	617	CLA	C4B-NB	3.01	1.41	1.37
22	B	605	CLA	C4B-NB	3.00	1.41	1.37
22	b	606	CLA	C4B-NB	3.00	1.41	1.37
22	C	501	CLA	C4B-NB	3.00	1.41	1.37
22	b	613	CLA	C4B-NB	2.99	1.41	1.37
22	B	603	CLA	C4B-NB	2.99	1.41	1.37
22	C	503	CLA	C4B-NB	2.99	1.41	1.37
22	A	404	CLA	C4B-NB	2.99	1.41	1.37
22	B	612	CLA	C4B-NB	2.99	1.41	1.37
22	B	607	CLA	C4B-NB	2.99	1.41	1.37
22	C	502	CLA	C4B-NB	2.99	1.41	1.37
24	J	102	BCR	C1-C6	-2.98	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	506	CLA	C4B-NB	2.98	1.41	1.37
24	j	102	BCR	C1-C6	-2.97	1.50	1.53
24	b	621	BCR	C30-C25	-2.97	1.50	1.53
22	B	613	CLA	C4B-NB	2.96	1.41	1.37
24	B	617	BCR	C30-C25	-2.96	1.50	1.53
22	C	506	CLA	C4B-NB	2.95	1.41	1.37
30	A	414	SQD	O47-C7	2.94	1.42	1.34
22	c	504	CLA	C1B-C2B	2.93	1.50	1.43
30	d	402	SQD	O47-C7	2.93	1.42	1.34
22	B	602	CLA	C4B-NB	2.92	1.41	1.37
23	D	406	PL9	C3-C4	-2.92	1.45	1.49
34	F	101	HEM	CAB-C3B	2.90	1.55	1.47
25	b	601	DGD	C1E-C2E	2.90	1.61	1.52
30	A	413	SQD	O47-C7	2.90	1.42	1.34
23	a	409	PL9	C3-C4	-2.89	1.45	1.49
34	f	101	HEM	CAB-C3B	2.89	1.55	1.47
30	a	401	SQD	O47-C7	2.89	1.42	1.34
22	C	501	CLA	C1B-C2B	2.88	1.49	1.43
30	F	103	SQD	O47-C7	2.88	1.42	1.34
30	B	622	SQD	O47-C7	2.88	1.42	1.34
22	C	504	CLA	C1B-C2B	2.88	1.49	1.43
22	b	607	CLA	C1B-C2B	2.87	1.49	1.43
30	a	415	SQD	O47-C7	2.86	1.42	1.34
22	c	501	CLA	C1B-C2B	2.86	1.49	1.43
30	B	626	SQD	O47-C7	2.86	1.42	1.34
22	d	404	CLA	C1B-C2B	2.86	1.49	1.43
22	b	619	CLA	C1B-C2B	2.85	1.49	1.43
30	b	602	SQD	O47-C7	2.85	1.42	1.34
22	c	503	CLA	C1B-C2B	2.84	1.49	1.43
22	B	603	CLA	C1B-C2B	2.84	1.49	1.43
22	c	511	CLA	C1B-C2B	2.83	1.49	1.43
22	c	510	CLA	C1B-C2B	2.83	1.49	1.43
22	b	609	CLA	C1B-C2B	2.83	1.49	1.43
22	D	404	CLA	C1B-C2B	2.83	1.49	1.43
30	f	103	SQD	O47-C7	2.82	1.42	1.34
22	h	101	CLA	C1B-C2B	2.82	1.49	1.43
22	B	615	CLA	C1B-C2B	2.82	1.49	1.43
22	H	101	CLA	C1B-C2B	2.82	1.49	1.43
22	b	605	CLA	C1B-C2B	2.81	1.49	1.43
22	b	618	CLA	C1B-C2B	2.81	1.49	1.43
22	B	611	CLA	C1B-C2B	2.81	1.49	1.43
22	B	604	CLA	C1B-C2B	2.80	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	625	DGD	C1E-C2E	2.80	1.60	1.52
22	B	614	CLA	C1B-C2B	2.80	1.49	1.43
22	a	406	CLA	C1B-C2B	2.79	1.49	1.43
23	d	406	PL9	C7-C3	-2.79	1.47	1.51
22	B	613	CLA	C1B-C2B	2.79	1.49	1.43
22	b	617	CLA	C1B-C2B	2.79	1.49	1.43
22	C	511	CLA	C1B-C2B	2.78	1.49	1.43
22	c	512	CLA	C1B-C2B	2.78	1.49	1.43
22	b	612	CLA	C1B-C2B	2.78	1.49	1.43
22	B	608	CLA	C1B-C2B	2.78	1.49	1.43
22	B	612	CLA	C1B-C2B	2.77	1.49	1.43
22	b	606	CLA	C1B-C2B	2.77	1.49	1.43
22	C	510	CLA	C1B-C2B	2.77	1.49	1.43
22	B	605	CLA	C1B-C2B	2.77	1.49	1.43
22	c	502	CLA	C1B-C2B	2.77	1.49	1.43
22	b	616	CLA	C1B-C2B	2.76	1.49	1.43
22	A	405	CLA	C1B-C2B	2.76	1.49	1.43
22	C	502	CLA	C1B-C2B	2.76	1.49	1.43
22	b	615	CLA	C1B-C2B	2.76	1.49	1.43
23	d	406	PL9	C3-C4	-2.76	1.45	1.49
22	c	520	CLA	C1B-C2B	2.75	1.49	1.43
22	B	602	CLA	C1B-C2B	2.75	1.49	1.43
22	D	405	CLA	C1B-C2B	2.74	1.49	1.43
22	b	608	CLA	C1B-C2B	2.74	1.49	1.43
22	B	601	CLA	C1B-C2B	2.73	1.49	1.43
22	d	405	CLA	C1B-C2B	2.73	1.49	1.43
22	B	606	CLA	C1B-C2B	2.73	1.49	1.43
22	C	503	CLA	C1B-C2B	2.72	1.49	1.43
22	c	505	CLA	C1B-C2B	2.72	1.49	1.43
22	b	610	CLA	C1B-C2B	2.72	1.49	1.43
22	c	509	CLA	C1B-C2B	2.72	1.49	1.43
22	c	506	CLA	C1B-C2B	2.72	1.49	1.43
22	B	607	CLA	C1B-C2B	2.72	1.49	1.43
22	C	505	CLA	C1B-C2B	2.72	1.49	1.43
22	A	404	CLA	C1B-C2B	2.72	1.49	1.43
22	C	512	CLA	C1B-C2B	2.72	1.49	1.43
22	C	509	CLA	C1B-C2B	2.71	1.49	1.43
22	a	408	CLA	C1B-C2B	2.71	1.49	1.43
22	C	506	CLA	C1B-C2B	2.70	1.49	1.43
22	c	508	CLA	C1B-C2B	2.69	1.49	1.43
22	C	508	CLA	C1B-C2B	2.69	1.49	1.43
23	a	409	PL9	C7-C3	-2.69	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	611	CLA	C1B-C2B	2.69	1.49	1.43
22	B	609	CLA	C1B-C2B	2.69	1.49	1.43
22	C	520	CLA	C1B-C2B	2.68	1.49	1.43
22	a	404	CLA	C3B-C4B	2.66	1.50	1.42
22	b	613	CLA	C1B-C2B	2.66	1.49	1.43
22	a	405	CLA	C1B-C2B	2.65	1.49	1.43
22	C	507	CLA	C1B-C2B	2.65	1.49	1.43
23	A	406	PL9	C3-C4	-2.65	1.45	1.49
22	A	403	CLA	C1B-C2B	2.65	1.49	1.43
22	A	402	CLA	C3B-C4B	2.63	1.50	1.42
22	b	614	CLA	MG-NB	-2.63	2.00	2.05
22	A	402	CLA	C1B-C2B	2.62	1.49	1.43
23	D	406	PL9	C7-C3	-2.62	1.47	1.51
32	D	402	PHO	CMC-C2C	-2.60	1.46	1.50
25	C	515	DGD	O2G-C2G	-2.60	1.40	1.46
32	d	401	PHO	CMC-C2C	-2.59	1.46	1.50
22	B	610	CLA	MG-NB	-2.59	2.00	2.05
32	a	407	PHO	CMC-C2C	-2.58	1.46	1.50
22	c	507	CLA	C1B-C2B	2.57	1.49	1.43
22	a	404	CLA	C1B-C2B	2.56	1.49	1.43
32	a	407	PHO	C3D-C4D	2.56	1.44	1.41
32	D	401	PHO	CMC-C2C	-2.54	1.46	1.50
32	D	401	PHO	C3D-C4D	2.52	1.44	1.41
32	d	401	PHO	C3D-C4D	2.52	1.44	1.41
32	D	402	PHO	C3D-C4D	2.50	1.44	1.41
23	J	101	PL9	C7-C3	-2.48	1.48	1.51
31	d	410	LMT	O3'-C3'	-2.48	1.36	1.43
32	d	401	PHO	CMD-C2D	-2.48	1.46	1.51
31	b	627	LMT	O3'-C3'	-2.48	1.36	1.43
32	D	402	PHO	CMD-C2D	-2.47	1.46	1.51
31	D	410	LMT	O3'-C3'	-2.47	1.36	1.43
22	c	508	CLA	C3B-C4B	2.46	1.49	1.42
31	M	102	LMT	O3'-C3'	-2.46	1.36	1.43
32	D	401	PHO	CMD-C2D	-2.46	1.46	1.51
31	B	624	LMT	O3'-C3'	-2.46	1.36	1.43
32	a	407	PHO	CMD-C2D	-2.46	1.46	1.51
32	D	401	PHO	CMB-C2B	-2.45	1.46	1.51
32	d	401	PHO	CMB-C2B	-2.45	1.46	1.51
31	M	103	LMT	O3'-C3'	-2.45	1.36	1.43
31	b	603	LMT	O3'-C3'	-2.44	1.36	1.43
22	a	405	CLA	C3B-C4B	2.43	1.49	1.42
22	b	612	CLA	CHC-C1C	2.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	C3B-C4B	2.43	1.49	1.42
31	b	626	LMT	O3'-C3'	-2.43	1.36	1.43
25	c	515	DGD	O2G-C2G	-2.43	1.40	1.46
31	i	102	LMT	O3'-C3'	-2.43	1.36	1.43
31	I	102	LMT	O3'-C3'	-2.43	1.36	1.43
22	B	608	CLA	CHC-C1C	2.42	1.43	1.38
23	A	406	PL9	C7-C3	-2.42	1.48	1.51
32	D	402	PHO	CAC-C3C	-2.42	1.47	1.51
22	A	403	CLA	C3B-C4B	2.41	1.49	1.42
32	d	401	PHO	CAC-C3C	-2.41	1.47	1.51
31	B	627	LMT	O3'-C3'	-2.41	1.37	1.43
23	j	101	PL9	C7-C3	-2.40	1.48	1.51
22	B	613	CLA	CHC-C1C	2.40	1.43	1.38
32	a	407	PHO	CMB-C2B	-2.40	1.46	1.51
32	D	402	PHO	CMB-C2B	-2.40	1.46	1.51
25	B	625	DGD	C4D-C5D	2.40	1.58	1.53
31	B	623	LMT	O3'-C3'	-2.39	1.37	1.43
22	b	605	CLA	C3B-C4B	2.39	1.49	1.42
22	b	611	CLA	CHC-C1C	2.38	1.43	1.38
22	b	612	CLA	C3B-C4B	2.38	1.49	1.42
22	B	601	CLA	C3B-C4B	2.38	1.49	1.42
22	C	520	CLA	C3B-C4B	2.38	1.49	1.42
22	c	505	CLA	C3B-C4B	2.38	1.49	1.42
22	b	611	CLA	C3B-C4B	2.38	1.49	1.42
31	b	604	LMT	O3'-C3'	-2.38	1.37	1.43
22	c	509	CLA	C3B-C4B	2.38	1.49	1.42
22	H	101	CLA	CHC-C1C	2.37	1.43	1.38
22	B	611	CLA	CMD-C2D	-2.37	1.45	1.50
22	C	505	CLA	C3B-C4B	2.37	1.49	1.42
22	c	512	CLA	C3B-C4B	2.37	1.49	1.42
22	B	613	CLA	C3B-C4B	2.37	1.49	1.42
22	c	511	CLA	C3B-C4B	2.37	1.49	1.42
22	C	511	CLA	C3B-C4B	2.37	1.49	1.42
22	b	606	CLA	C3B-C4B	2.36	1.49	1.42
22	b	617	CLA	CHC-C1C	2.36	1.43	1.38
22	c	502	CLA	CHC-C1C	2.36	1.43	1.38
22	c	512	CLA	CHC-C1C	2.35	1.43	1.38
22	c	510	CLA	C3B-C4B	2.35	1.49	1.42
22	d	405	CLA	C3B-C4B	2.35	1.49	1.42
22	h	101	CLA	CHC-C1C	2.35	1.43	1.38
22	B	608	CLA	C3B-C4B	2.35	1.49	1.42
22	c	520	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	101	CLA	C3B-C4B	2.35	1.49	1.42
22	b	618	CLA	C3B-C4B	2.34	1.49	1.42
32	D	401	PHO	CAC-C3C	-2.34	1.47	1.51
22	b	606	CLA	CHC-C1C	2.34	1.43	1.38
22	D	405	CLA	C3B-C4B	2.34	1.49	1.42
22	B	612	CLA	C3B-C4B	2.34	1.49	1.42
32	a	407	PHO	CAC-C3C	-2.34	1.47	1.51
31	B	628	LMT	O3'-C3'	-2.33	1.37	1.43
23	D	406	PL9	C6-C1	-2.33	1.44	1.48
22	a	406	CLA	C3B-C4B	2.33	1.49	1.42
22	b	615	CLA	C3B-C4B	2.33	1.49	1.42
22	b	619	CLA	C3B-C4B	2.33	1.49	1.42
26	a	412	LHG	O7-C5	-2.32	1.41	1.46
22	C	511	CLA	CHC-C1C	2.32	1.43	1.38
22	h	101	CLA	C3B-C4B	2.32	1.49	1.42
22	B	614	CLA	C3B-C4B	2.32	1.49	1.42
27	D	411	LMG	O7-C8	-2.32	1.41	1.46
23	a	409	PL9	C53-C6	-2.31	1.46	1.50
22	c	507	CLA	C3B-C4B	2.31	1.49	1.42
22	a	404	CLA	CHC-C1C	2.31	1.43	1.38
22	C	509	CLA	C3B-C4B	2.31	1.49	1.42
22	b	609	CLA	C3B-C4B	2.31	1.49	1.42
22	c	505	CLA	CHC-C1C	2.31	1.43	1.38
22	c	511	CLA	CHC-C1C	2.31	1.43	1.38
22	C	510	CLA	C3B-C4B	2.31	1.49	1.42
22	c	503	CLA	C3B-C4B	2.31	1.49	1.42
22	b	615	CLA	CMD-C2D	-2.30	1.46	1.50
22	B	609	CLA	C3B-C4B	2.30	1.49	1.42
22	B	607	CLA	CHC-C1C	2.30	1.43	1.38
22	B	607	CLA	C3B-C4B	2.30	1.49	1.42
22	b	617	CLA	C3B-C4B	2.30	1.49	1.42
22	a	408	CLA	C3B-C4B	2.30	1.49	1.42
22	B	611	CLA	C3B-C4B	2.30	1.49	1.42
22	c	502	CLA	C3B-C4B	2.30	1.49	1.42
22	A	404	CLA	C3B-C4B	2.29	1.49	1.42
22	b	616	CLA	C3B-C4B	2.29	1.49	1.42
22	B	615	CLA	C3B-C4B	2.29	1.49	1.42
22	d	404	CLA	CHC-C1C	2.29	1.43	1.38
25	c	516	DGD	O2G-C2G	-2.29	1.41	1.46
22	C	507	CLA	C3B-C4B	2.29	1.49	1.42
22	c	509	CLA	CHC-C1C	2.29	1.43	1.38
22	A	405	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	CHC-C1C	2.29	1.43	1.38
22	b	618	CLA	CHC-C1C	2.29	1.43	1.38
22	B	602	CLA	C3B-C4B	2.28	1.49	1.42
22	B	605	CLA	C3B-C4B	2.28	1.49	1.42
22	B	602	CLA	CHC-C1C	2.28	1.43	1.38
22	B	603	CLA	CHC-C1C	2.28	1.43	1.38
22	B	609	CLA	CHC-C1C	2.28	1.43	1.38
22	B	604	CLA	C3B-C4B	2.28	1.49	1.42
22	C	512	CLA	C3B-C4B	2.28	1.49	1.42
22	c	507	CLA	CHC-C1C	2.28	1.43	1.38
22	b	613	CLA	C3B-C4B	2.28	1.49	1.42
22	B	606	CLA	C3B-C4B	2.28	1.49	1.42
22	a	408	CLA	CHC-C1C	2.27	1.43	1.38
22	d	405	CLA	CHC-C1C	2.27	1.43	1.38
22	b	608	CLA	C3B-C4B	2.27	1.49	1.42
22	D	404	CLA	CHC-C1C	2.27	1.43	1.38
22	b	616	CLA	CHC-C1C	2.27	1.43	1.38
22	c	506	CLA	C3B-C4B	2.27	1.49	1.42
22	C	506	CLA	C3B-C4B	2.26	1.49	1.42
22	d	404	CLA	C3B-C4B	2.26	1.49	1.42
22	a	406	CLA	CHC-C1C	2.26	1.43	1.38
22	b	607	CLA	CHC-C1C	2.26	1.43	1.38
22	c	508	CLA	CHC-C1C	2.26	1.43	1.38
22	C	505	CLA	CHC-C1C	2.26	1.43	1.38
22	C	520	CLA	CHC-C1C	2.26	1.43	1.38
22	c	503	CLA	CHC-C1C	2.26	1.43	1.38
22	C	508	CLA	CHC-C1C	2.26	1.43	1.38
22	B	614	CLA	CHC-C1C	2.26	1.43	1.38
22	D	404	CLA	C3B-C4B	2.25	1.49	1.42
31	I	102	LMT	O2B-C2B	-2.25	1.37	1.43
22	A	404	CLA	CHC-C1C	2.25	1.43	1.38
22	C	509	CLA	CHC-C1C	2.24	1.43	1.38
22	C	503	CLA	C3B-C4B	2.24	1.49	1.42
22	c	504	CLA	CHC-C1C	2.24	1.43	1.38
22	C	502	CLA	C3B-C4B	2.24	1.49	1.42
22	b	610	CLA	C3B-C4B	2.24	1.49	1.42
22	c	501	CLA	C3B-C4B	2.24	1.49	1.42
25	C	516	DGD	O2G-C2G	-2.24	1.41	1.46
22	c	504	CLA	C3B-C4B	2.24	1.49	1.42
22	c	510	CLA	CHC-C1C	2.24	1.43	1.38
22	b	614	CLA	C1B-NB	-2.24	1.34	1.37
22	C	503	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	CHC-C1C	2.23	1.43	1.38
22	C	504	CLA	CHC-C1C	2.23	1.43	1.38
31	I	102	LMT	O2'-C2'	-2.23	1.37	1.43
22	b	607	CLA	C3B-C4B	2.23	1.49	1.42
22	C	510	CLA	CHC-C1C	2.23	1.43	1.38
22	b	605	CLA	CHC-C1C	2.23	1.42	1.38
22	B	603	CLA	C3B-C4B	2.23	1.49	1.42
22	A	403	CLA	CHC-C1C	2.22	1.42	1.38
22	b	608	CLA	CHC-C1C	2.22	1.42	1.38
22	b	613	CLA	CHC-C1C	2.22	1.42	1.38
22	C	502	CLA	CHC-C1C	2.22	1.42	1.38
22	C	504	CLA	C3B-C4B	2.22	1.49	1.42
26	c	519	LHG	P-O6	2.22	1.68	1.59
22	c	504	CLA	CMD-C2D	-2.22	1.46	1.50
22	B	604	CLA	CHC-C1C	2.22	1.42	1.38
22	B	612	CLA	CHC-C1C	2.22	1.42	1.38
22	C	506	CLA	CHC-C1C	2.21	1.42	1.38
22	C	507	CLA	CMB-C2B	-2.21	1.46	1.50
22	C	501	CLA	C3B-C4B	2.21	1.49	1.42
31	i	102	LMT	O2B-C2B	-2.21	1.37	1.43
22	b	609	CLA	CHC-C1C	2.21	1.42	1.38
22	c	506	CLA	CHC-C1C	2.21	1.42	1.38
22	B	610	CLA	C1B-NB	-2.20	1.35	1.37
22	c	520	CLA	CHC-C1C	2.19	1.42	1.38
22	B	601	CLA	CHC-C1C	2.19	1.42	1.38
27	B	621	LMG	C4-C5	2.19	1.57	1.53
22	c	501	CLA	CHC-C1C	2.19	1.42	1.38
27	b	625	LMG	C4-C5	2.19	1.57	1.53
22	b	613	CLA	MG-NB	-2.19	2.01	2.05
22	C	504	CLA	CMD-C2D	-2.19	1.46	1.50
22	A	402	CLA	CHC-C1C	2.19	1.42	1.38
22	B	605	CLA	CHC-C1C	2.19	1.42	1.38
22	D	405	CLA	CHC-C1C	2.19	1.42	1.38
31	i	102	LMT	O2'-C2'	-2.19	1.37	1.43
22	c	509	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	615	CLA	CHC-C1C	2.18	1.42	1.38
25	B	620	DGD	O2G-C2G	-2.18	1.41	1.46
22	c	507	CLA	CMB-C2B	-2.18	1.46	1.50
22	b	610	CLA	CHC-C1C	2.18	1.42	1.38
27	M	101	LMG	C4-C5	2.18	1.57	1.53
22	A	405	CLA	CHC-C1C	2.18	1.42	1.38
31	M	103	LMT	O3B-C3B	-2.18	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	409	LHG	O7-C5	-2.17	1.41	1.46
22	C	501	CLA	CHC-C1C	2.17	1.42	1.38
23	J	101	PL9	C3-C4	-2.17	1.46	1.49
31	b	604	LMT	O3B-C3B	-2.17	1.37	1.43
31	b	626	LMT	O2'-C2'	-2.17	1.37	1.43
25	d	409	DGD	C1D-C2D	2.16	1.58	1.52
31	M	102	LMT	O1'-C1'	-2.16	1.36	1.40
31	I	102	LMT	O3B-C3B	-2.16	1.37	1.43
22	C	507	CLA	CHC-C1C	2.16	1.42	1.38
31	b	627	LMT	O3B-C3B	-2.16	1.37	1.43
27	d	411	LMG	O7-C8	-2.16	1.41	1.46
22	b	619	CLA	CHC-C1C	2.16	1.42	1.38
25	b	624	DGD	O2G-C2G	-2.16	1.41	1.46
22	b	611	CLA	CMD-C2D	-2.16	1.46	1.50
31	B	628	LMT	O3B-C3B	-2.16	1.37	1.43
31	b	603	LMT	O3B-C3B	-2.15	1.37	1.43
25	C	515	DGD	O1G-C1G	-2.15	1.40	1.45
25	b	601	DGD	C4D-C5D	2.15	1.57	1.53
23	A	406	PL9	C53-C6	-2.15	1.46	1.50
24	g	101	BCR	C33-C5	-2.15	1.47	1.50
31	B	627	LMT	O2B-C2B	-2.15	1.37	1.43
31	B	623	LMT	O2'-C2'	-2.15	1.37	1.43
22	C	502	CLA	MG-NB	-2.15	2.01	2.05
31	D	410	LMT	O3B-C3B	-2.15	1.37	1.43
22	B	611	CLA	CHC-C1C	2.14	1.42	1.38
31	M	103	LMT	O2'-C2'	-2.14	1.37	1.43
31	M	102	LMT	O3B-C3B	-2.14	1.37	1.43
22	B	610	CLA	C1B-C2B	2.14	1.48	1.43
31	B	628	LMT	O2'-C2'	-2.14	1.37	1.43
31	B	624	LMT	O3B-C3B	-2.14	1.37	1.43
31	b	603	LMT	O2'-C2'	-2.14	1.37	1.43
22	C	509	CLA	CMD-C2D	-2.13	1.46	1.50
23	j	101	PL9	C3-C4	-2.13	1.46	1.49
31	M	102	LMT	O2'-C2'	-2.13	1.37	1.43
31	i	102	LMT	O3B-C3B	-2.13	1.37	1.43
31	B	627	LMT	O2'-C2'	-2.13	1.37	1.43
22	B	602	CLA	MG-NB	-2.13	2.01	2.05
31	b	603	LMT	O2B-C2B	-2.13	1.37	1.43
22	B	603	CLA	CMD-C2D	-2.13	1.46	1.50
34	f	101	HEM	CMC-C2C	2.13	1.55	1.50
31	B	628	LMT	O2B-C2B	-2.13	1.37	1.43
31	d	410	LMT	O3B-C3B	-2.13	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	101	BCR	C33-C5	-2.12	1.47	1.50
25	B	625	DGD	C3G-C2G	2.12	1.57	1.50
31	B	623	LMT	O3B-C3B	-2.12	1.37	1.43
22	B	615	CLA	CHC-C1C	2.12	1.42	1.38
22	A	402	CLA	CMD-C2D	-2.12	1.46	1.50
27	d	407	LMG	O7-C8	-2.12	1.41	1.46
31	B	627	LMT	O3B-C3B	-2.12	1.37	1.43
22	c	507	CLA	MG-NB	-2.12	2.01	2.05
34	F	101	HEM	CMC-C2C	2.11	1.55	1.50
31	M	103	LMT	O2B-C2B	-2.11	1.37	1.43
22	A	404	CLA	MG-NB	-2.11	2.01	2.05
31	b	626	LMT	O3B-C3B	-2.11	1.37	1.43
31	B	624	LMT	O2'-C2'	-2.11	1.37	1.43
22	B	607	CLA	CMD-C2D	-2.11	1.46	1.50
22	a	404	CLA	CMB-C2B	-2.11	1.46	1.50
22	a	405	CLA	CHC-C1C	2.11	1.42	1.38
22	a	406	CLA	CMD-C2D	-2.11	1.46	1.50
34	V	201	HEM	CMB-C2B	2.10	1.55	1.50
22	b	614	CLA	C1B-C2B	2.10	1.48	1.43
31	D	410	LMT	O2B-C2B	-2.10	1.37	1.43
31	M	102	LMT	O2B-C2B	-2.10	1.37	1.43
22	B	607	CLA	MG-NB	-2.09	2.01	2.05
31	b	604	LMT	O2'-C2'	-2.09	1.37	1.43
27	a	402	LMG	O7-C8	-2.09	1.41	1.46
31	D	410	LMT	O2'-C2'	-2.09	1.37	1.43
22	C	509	CLA	CMB-C2B	-2.09	1.46	1.50
22	C	506	CLA	MG-NB	-2.09	2.01	2.05
27	m	101	LMG	C4-C5	2.09	1.57	1.53
31	b	626	LMT	O2B-C2B	-2.09	1.37	1.43
22	b	606	CLA	MG-NB	-2.09	2.01	2.05
22	b	611	CLA	MG-NB	-2.09	2.01	2.05
25	a	411	DGD	O1G-C1G	-2.09	1.40	1.45
27	A	415	LMG	O7-C8	-2.09	1.41	1.46
22	a	404	CLA	CMD-C2D	-2.09	1.46	1.50
22	b	607	CLA	CMD-C2D	-2.08	1.46	1.50
23	d	406	PL9	C6-C1	-2.08	1.45	1.48
30	B	626	SQD	O2-C2	-2.08	1.37	1.43
23	a	409	PL9	C6-C1	-2.08	1.45	1.48
22	C	507	CLA	MG-NB	-2.08	2.01	2.05
22	B	605	CLA	MG-NB	-2.08	2.01	2.05
31	d	410	LMT	O2B-C2B	-2.08	1.37	1.43
30	b	602	SQD	O2-C2	-2.08	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	MG-NB	-2.08	2.01	2.05
22	c	509	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	612	CLA	MG-NB	-2.08	2.01	2.05
26	C	519	LHG	O7-C5	-2.08	1.41	1.46
22	A	403	CLA	CMB-C2B	-2.08	1.46	1.50
22	A	404	CLA	CMD-C2D	-2.07	1.46	1.50
34	v	201	HEM	CMB-C2B	2.07	1.55	1.50
31	b	627	LMT	O2'-C2'	-2.07	1.37	1.43
31	b	604	LMT	O2B-C2B	-2.07	1.37	1.43
34	V	201	HEM	CMD-C2D	2.07	1.55	1.50
24	C	514	BCR	C38-C26	-2.07	1.47	1.50
22	B	603	CLA	CMB-C2B	-2.07	1.46	1.50
22	C	520	CLA	MG-NB	-2.07	2.01	2.05
22	c	502	CLA	MG-NB	-2.07	2.01	2.05
22	b	619	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	607	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	615	CLA	CMD-C2D	-2.07	1.46	1.50
34	v	201	HEM	CMD-C2D	2.06	1.55	1.50
24	c	514	BCR	C38-C26	-2.06	1.47	1.50
22	B	606	CLA	MG-NB	-2.06	2.01	2.05
22	D	405	CLA	MG-NB	-2.06	2.01	2.05
22	B	601	CLA	CMB-C2B	-2.06	1.46	1.50
22	c	506	CLA	MG-NB	-2.06	2.01	2.05
22	a	405	CLA	CMB-C2B	-2.06	1.46	1.50
22	b	610	CLA	MG-NB	-2.06	2.01	2.05
22	b	619	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	402	CLA	CMB-C2B	-2.05	1.46	1.50
22	B	609	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	505	CLA	CMB-C2B	-2.05	1.46	1.50
27	D	407	LMG	O7-C8	-2.05	1.41	1.46
31	B	623	LMT	O2B-C2B	-2.05	1.37	1.43
22	b	616	CLA	MG-NB	-2.05	2.01	2.05
22	C	502	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	602	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	609	CLA	MG-NB	-2.05	2.01	2.05
22	b	607	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	508	CLA	CMD-C2D	-2.05	1.46	1.50
22	A	404	CLA	CMB-C2B	-2.05	1.46	1.50
22	b	617	CLA	MG-NB	-2.05	2.01	2.05
31	d	410	LMT	O2'-C2'	-2.04	1.37	1.43
22	B	603	CLA	MG-NB	-2.04	2.01	2.05
22	C	501	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	MG-NB	-2.04	2.01	2.05
22	h	101	CLA	MG-NB	-2.04	2.01	2.05
22	b	610	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	614	CLA	MG-ND	-2.04	2.01	2.05
22	A	403	CLA	CMD-C2D	-2.04	1.46	1.50
22	C	502	CLA	CMC-C2C	-2.04	1.46	1.50
22	b	613	CLA	CMB-C2B	-2.04	1.46	1.50
22	c	505	CLA	CMB-C2B	-2.04	1.46	1.50
22	c	520	CLA	CMB-C2B	-2.04	1.46	1.50
22	d	404	CLA	CMB-C2B	-2.04	1.46	1.50
22	a	405	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	613	CLA	MG-NB	-2.04	2.01	2.05
22	C	520	CLA	CMB-C2B	-2.04	1.46	1.50
22	D	404	CLA	MG-NB	-2.04	2.01	2.05
22	C	508	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	610	CLA	MG-ND	-2.04	2.01	2.05
22	b	610	CLA	CMD-C2D	-2.04	1.46	1.50
22	C	505	CLA	CMD-C2D	-2.03	1.46	1.50
22	D	404	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	605	CLA	CMB-C2B	-2.03	1.46	1.50
22	a	408	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	611	CLA	CMB-C2B	-2.03	1.46	1.50
22	C	509	CLA	MG-NB	-2.03	2.01	2.05
31	B	628	LMT	O1'-C1'	-2.03	1.36	1.40
22	B	615	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	604	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	606	CLA	CMD-C2D	-2.03	1.46	1.50
22	D	404	CLA	CMB-C2B	-2.03	1.46	1.50
22	H	101	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	606	CLA	CMB-C2B	-2.03	1.46	1.50
22	h	101	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	605	CLA	CMB-C2B	-2.03	1.46	1.50
22	C	512	CLA	CMB-C2B	-2.03	1.46	1.50
22	A	405	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	405	CLA	MG-NB	-2.02	2.01	2.05
26	c	519	LHG	O7-C5	-2.02	1.41	1.46
22	b	616	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	502	CLA	CMB-C2B	-2.02	1.46	1.50
22	c	508	CLA	CMB-C2B	-2.02	1.46	1.50
22	c	508	CLA	CMD-C2D	-2.02	1.46	1.50
24	j	102	BCR	C38-C26	-2.02	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	CMA-C3A	2.02	1.54	1.50
22	C	503	CLA	CMB-C2B	-2.02	1.46	1.50
27	C	521	LMG	O7-C8	-2.02	1.41	1.46
22	A	405	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	614	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	604	CLA	CMB-C2B	-2.02	1.46	1.50
22	c	501	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	601	CLA	CMD-C2D	-2.01	1.46	1.50
34	F	101	HEM	CMA-C3A	2.01	1.54	1.50
22	c	502	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	615	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	616	CLA	CMB-C2B	-2.01	1.46	1.50
22	b	608	CLA	CMB-C2B	-2.01	1.46	1.50
22	a	406	CLA	MG-NB	-2.01	2.01	2.05
22	H	101	CLA	CMD-C2D	-2.01	1.46	1.50
22	c	511	CLA	CMD-C2D	-2.01	1.46	1.50
22	C	512	CLA	MG-NB	-2.01	2.01	2.05
22	b	609	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	611	CLA	MG-NB	-2.01	2.01	2.05
22	B	608	CLA	CMB-C2B	-2.01	1.46	1.50
22	b	615	CLA	CMC-C2C	-2.01	1.46	1.50
22	C	511	CLA	MG-NB	-2.01	2.01	2.05
22	B	605	CLA	CMD-C2D	-2.01	1.46	1.50
22	C	510	CLA	CMB-C2B	-2.01	1.46	1.50
34	V	201	HEM	CMA-C3A	2.01	1.54	1.50
22	C	502	CLA	CMB-C2B	-2.01	1.46	1.50
22	C	520	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	401	SQD	O3-C3	-2.01	1.38	1.43
22	a	405	CLA	MG-NB	-2.00	2.01	2.05
25	C	517	DGD	C1G-C2G	2.00	1.57	1.50
22	B	609	CLA	CMD-C2D	-2.00	1.46	1.50
22	c	503	CLA	CMD-C2D	-2.00	1.46	1.50
22	C	504	CLA	CMB-C2B	-2.00	1.46	1.50
27	l	101	LMG	C7-C8	2.00	1.57	1.50
22	d	404	CLA	CMD-C2D	-2.00	1.46	1.50
22	b	612	CLA	CMD-C2D	-2.00	1.46	1.50
22	c	520	CLA	CMD-C2D	-2.00	1.46	1.50
22	B	615	CLA	MG-NB	-2.00	2.01	2.05
22	c	520	CLA	MG-NB	-2.00	2.01	2.05

All (1041) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.26	109.99	106.68
22	B	611	CLA	C4A-NA-C1A	7.22	109.97	106.68
22	c	504	CLA	C4A-NA-C1A	7.21	109.97	106.68
22	b	615	CLA	C4A-NA-C1A	7.12	109.93	106.68
22	B	603	CLA	C4A-NA-C1A	7.07	109.91	106.68
22	b	607	CLA	C4A-NA-C1A	7.04	109.89	106.68
22	b	609	CLA	C4A-NA-C1A	6.93	109.84	106.68
22	C	510	CLA	C4A-NA-C1A	6.91	109.83	106.68
22	A	403	CLA	C4A-NA-C1A	6.90	109.83	106.68
22	C	503	CLA	C4A-NA-C1A	6.90	109.83	106.68
22	B	605	CLA	C4A-NA-C1A	6.86	109.81	106.68
22	b	618	CLA	C4A-NA-C1A	6.81	109.79	106.68
22	c	503	CLA	C4A-NA-C1A	6.79	109.78	106.68
22	C	501	CLA	C4A-NA-C1A	6.76	109.76	106.68
22	C	520	CLA	C4A-NA-C1A	6.73	109.75	106.68
22	C	511	CLA	C4A-NA-C1A	6.72	109.74	106.68
22	c	511	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	a	405	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	B	615	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	c	520	CLA	C4A-NA-C1A	6.67	109.72	106.68
22	c	501	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	B	604	CLA	C4A-NA-C1A	6.63	109.70	106.68
22	b	616	CLA	C4A-NA-C1A	6.63	109.70	106.68
22	c	506	CLA	C4A-NA-C1A	6.59	109.69	106.68
22	c	512	CLA	C4A-NA-C1A	6.59	109.69	106.68
22	b	608	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	C	506	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	a	408	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	B	614	CLA	C4A-NA-C1A	6.57	109.68	106.68
22	C	507	CLA	C4A-NA-C1A	6.56	109.67	106.68
22	b	617	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	B	607	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	c	505	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	H	101	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	c	510	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	B	612	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	C	512	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	B	609	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	b	619	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	c	507	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	A	405	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	h	101	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	B	606	CLA	C4A-NA-C1A	6.37	109.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	d	404	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	B	613	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	a	406	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	C	505	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	C	508	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	B	608	CLA	C4A-NA-C1A	6.30	109.56	106.68
22	c	508	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	b	611	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	b	610	CLA	C4A-NA-C1A	6.24	109.52	106.68
22	B	601	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	d	405	CLA	C4A-NA-C1A	6.20	109.51	106.68
22	c	502	CLA	C4A-NA-C1A	6.19	109.50	106.68
22	b	605	CLA	C4A-NA-C1A	6.18	109.50	106.68
22	b	612	CLA	C4A-NA-C1A	6.18	109.50	106.68
22	c	509	CLA	C4A-NA-C1A	6.14	109.48	106.68
22	A	404	CLA	C4A-NA-C1A	6.13	109.47	106.68
22	b	606	CLA	C4A-NA-C1A	6.13	109.47	106.68
22	D	404	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	a	404	CLA	C4A-NA-C1A	6.10	109.46	106.68
22	D	405	CLA	C4A-NA-C1A	6.09	109.46	106.68
22	C	509	CLA	C4A-NA-C1A	6.09	109.46	106.68
22	C	502	CLA	C4A-NA-C1A	6.01	109.42	106.68
22	A	402	CLA	C4A-NA-C1A	6.00	109.42	106.68
22	b	613	CLA	C4A-NA-C1A	5.98	109.41	106.68
30	a	415	SQD	O6-C1-C2	5.82	117.11	108.27
32	a	407	PHO	C4D-CHA-CBD	-5.81	105.67	108.45
30	A	413	SQD	O6-C1-C2	5.71	116.95	108.27
32	d	401	PHO	C4D-CHA-CBD	-5.70	105.72	108.45
30	b	602	SQD	O6-C1-C2	5.65	116.86	108.27
32	D	401	PHO	C4D-CHA-CBD	-5.65	105.75	108.45
33	D	403	BCT	O2-C-O1	5.63	134.07	119.68
33	d	403	BCT	O2-C-O1	5.61	134.03	119.68
30	B	626	SQD	O6-C1-C2	5.60	116.78	108.27
23	j	101	PL9	C7-C3-C4	5.58	121.50	116.91
23	J	101	PL9	C7-C3-C4	5.54	121.48	116.91
32	D	402	PHO	C4D-CHA-CBD	-5.54	105.80	108.45
34	v	201	HEM	C4D-ND-C1D	5.44	111.65	105.21
22	b	614	CLA	C4A-NA-C1A	5.38	109.14	106.68
23	A	406	PL9	C7-C3-C4	5.33	121.30	116.91
34	V	201	HEM	C4D-ND-C1D	5.23	111.40	105.21
34	f	101	HEM	C4D-ND-C1D	5.18	111.34	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	406	PL9	C7-C3-C4	5.18	121.17	116.91
22	B	610	CLA	C4A-NA-C1A	5.18	109.04	106.68
34	F	101	HEM	C4D-ND-C1D	5.17	111.33	105.21
23	a	409	PL9	C7-C3-C4	5.08	121.09	116.91
23	D	406	PL9	C7-C3-C4	5.05	121.07	116.91
25	a	411	DGD	O3G-C3G-C2G	-4.64	99.54	110.82
25	A	408	DGD	O3G-C3G-C2G	-4.59	99.65	110.82
30	B	622	SQD	O5-C5-C4	4.49	117.78	109.70
30	d	402	SQD	O6-C1-C2	4.46	115.05	108.27
30	d	402	SQD	O5-C5-C4	4.43	117.68	109.70
26	C	519	LHG	O4-P-O5	4.41	132.97	112.44
30	B	622	SQD	O6-C1-C2	4.41	114.97	108.27
26	a	412	LHG	O4-P-O5	4.40	132.92	112.44
26	c	519	LHG	O4-P-O5	4.39	132.88	112.44
26	A	409	LHG	O4-P-O5	4.39	132.87	112.44
23	j	101	PL9	C7-C3-C2	-4.29	118.34	123.39
30	A	413	SQD	O9-S-C6	4.28	113.15	106.76
23	J	101	PL9	C7-C3-C2	-4.28	118.35	123.39
30	a	415	SQD	O9-S-C6	4.25	113.10	106.76
25	C	517	DGD	O3G-C3G-C2G	-4.20	100.61	110.82
24	C	513	BCR	C2-C1-C6	4.10	116.39	110.44
23	d	406	PL9	C7-C3-C2	-4.08	118.58	123.39
24	c	513	BCR	C2-C1-C6	4.07	116.35	110.44
30	F	103	SQD	O9-S-O7	-4.05	100.64	113.82
30	f	103	SQD	O9-S-O7	-4.05	100.64	113.82
25	c	517	DGD	O3G-C3G-C2G	-4.05	100.97	110.82
23	A	406	PL9	C7-C3-C2	-4.04	118.63	123.39
30	d	402	SQD	O9-S-O7	-4.00	100.81	113.82
30	A	413	SQD	O9-S-O7	-3.99	100.85	113.82
24	J	102	BCR	C11-C10-C9	-3.97	121.72	127.28
30	A	414	SQD	O5-C5-C4	3.96	116.84	109.70
30	a	415	SQD	O9-S-O7	-3.96	100.93	113.82
30	B	622	SQD	O9-S-O7	-3.95	100.96	113.82
30	a	401	SQD	O9-S-O7	-3.93	101.03	113.82
23	D	406	PL9	C7-C3-C2	-3.93	118.76	123.39
23	a	409	PL9	C7-C3-C2	-3.93	118.76	123.39
30	b	602	SQD	O5-C5-C4	3.93	116.78	109.70
30	B	626	SQD	O9-S-O7	-3.90	101.12	113.82
30	b	602	SQD	O9-S-O7	-3.89	101.16	113.82
30	B	626	SQD	O5-C5-C4	3.89	116.71	109.70
30	A	414	SQD	O9-S-O7	-3.85	101.29	113.82
27	d	408	LMG	C1-C2-C3	-3.83	101.95	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	102	BCR	C11-C10-C9	-3.83	121.91	127.28
27	D	408	LMG	C1-C2-C3	-3.82	101.97	110.01
30	A	413	SQD	O47-C7-C8	3.82	119.74	111.48
30	a	401	SQD	O5-C5-C4	3.81	116.57	109.70
30	f	103	SQD	O5-C5-C4	3.76	116.47	109.70
30	a	415	SQD	O5-C5-C4	3.73	116.43	109.70
24	j	102	BCR	C2-C1-C6	3.73	115.86	110.44
30	a	415	SQD	O47-C7-C8	3.71	119.51	111.48
24	J	102	BCR	C2-C1-C6	3.71	115.82	110.44
25	d	409	DGD	O6D-C1D-O3G	-3.70	101.31	110.04
25	D	409	DGD	O6D-C1D-O3G	-3.65	101.41	110.04
30	F	103	SQD	O5-C5-C4	3.63	116.25	109.70
32	D	401	PHO	C2B-C1B-NB	-3.62	106.81	109.43
30	b	602	SQD	O47-C7-C8	3.61	119.29	111.48
30	B	626	SQD	O47-C7-C8	3.60	119.27	111.48
30	A	413	SQD	O5-C5-C4	3.60	116.19	109.70
25	c	516	DGD	O3G-C3G-C2G	-3.59	102.08	110.82
25	C	516	DGD	O3G-C3G-C2G	-3.57	102.14	110.82
30	F	103	SQD	O6-C1-C2	3.56	113.68	108.27
30	f	103	SQD	O7-S-C6	3.54	112.05	106.76
32	d	401	PHO	C2B-C1B-NB	-3.52	106.89	109.43
24	A	407	BCR	C2-C1-C6	3.51	115.53	110.44
30	a	401	SQD	O7-S-C6	3.49	111.97	106.76
32	D	402	PHO	C2B-C1B-NB	-3.48	106.92	109.43
30	A	414	SQD	O47-C7-C8	3.47	118.98	111.48
30	F	103	SQD	O7-S-C6	3.46	111.92	106.76
30	B	626	SQD	O9-S-C6	3.43	111.88	106.76
30	F	103	SQD	O47-C7-C8	3.43	118.89	111.48
24	a	410	BCR	C2-C1-C6	3.43	115.42	110.44
30	A	414	SQD	O7-S-C6	3.39	111.81	106.76
30	d	402	SQD	O47-C7-C8	3.38	118.80	111.48
30	B	622	SQD	O47-C7-C8	3.37	118.77	111.48
32	a	407	PHO	C2B-C1B-NB	-3.36	107.00	109.43
30	f	103	SQD	O6-C1-C2	3.34	113.34	108.27
30	b	602	SQD	O7-S-C6	3.31	111.70	106.76
25	b	624	DGD	O3G-C3G-C2G	-3.31	102.77	110.82
22	b	614	CLA	CMB-C2B-C1B	-3.30	120.39	125.42
22	c	503	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
25	c	515	DGD	O3G-C3G-C2G	-3.29	102.81	110.82
30	f	103	SQD	O47-C7-C8	3.29	118.60	111.48
25	C	515	DGD	O3G-C3G-C2G	-3.29	102.82	110.82
30	b	602	SQD	O9-S-C6	3.29	111.67	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	BCR	C15-C16-C17	-3.28	116.80	123.52
24	B	618	BCR	C2-C1-C6	3.28	115.20	110.44
22	B	613	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
25	c	516	DGD	O5D-C6D-C5D	-3.24	102.11	109.42
22	B	603	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
30	a	401	SQD	O47-C7-C8	3.23	118.47	111.48
22	a	404	CLA	C3B-C4B-NB	-3.23	107.65	110.53
22	B	605	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
22	B	610	CLA	CMB-C2B-C1B	-3.22	120.52	125.42
25	b	624	DGD	O6D-C1D-O3G	-3.22	102.44	110.04
24	J	102	BCR	C24-C23-C22	-3.21	121.48	126.23
25	B	620	DGD	O3G-C3G-C2G	-3.21	103.01	110.82
22	C	503	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
24	b	622	BCR	C2-C1-C6	3.20	115.09	110.44
25	B	620	DGD	O6D-C1D-O3G	-3.20	102.49	110.04
30	B	622	SQD	O7-S-C6	3.19	111.52	106.76
25	C	516	DGD	O5D-C6D-C5D	-3.19	102.22	109.42
22	b	617	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
22	A	402	CLA	C3B-C4B-NB	-3.17	107.70	110.53
22	b	606	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
24	J	102	BCR	C3-C4-C5	-3.16	108.42	114.06
24	j	102	BCR	C24-C23-C22	-3.15	121.57	126.23
22	b	609	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
30	a	401	SQD	C44-O6-C1	3.14	120.54	113.80
24	B	617	BCR	C33-C5-C6	-3.14	121.06	124.48
22	c	507	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
24	b	622	BCR	C24-C23-C22	-3.14	121.59	126.23
25	c	516	DGD	O6D-C1D-O3G	-3.14	102.62	110.04
30	A	413	SQD	O7-S-C6	3.14	111.44	106.76
22	B	608	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
31	B	628	LMT	C1'-O5'-C5'	-3.14	107.59	113.72
24	j	102	BCR	C3-C4-C5	-3.13	108.47	114.06
25	C	516	DGD	O6D-C1D-O3G	-3.13	102.64	110.04
25	D	409	DGD	O3G-C3G-C2G	-3.13	103.20	110.82
32	a	407	PHO	O1D-CGD-CBD	3.12	129.46	124.72
32	D	402	PHO	O1D-CGD-CBD	3.12	129.45	124.72
24	b	621	BCR	C15-C16-C17	-3.12	117.14	123.52
22	c	504	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
30	B	626	SQD	O7-S-C6	3.11	111.40	106.76
22	C	504	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
30	d	402	SQD	O7-S-C6	3.10	111.38	106.76
30	B	626	SQD	C3-C4-C5	3.09	115.84	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	521	BCR	C2-C1-C6	3.09	114.93	110.44
24	b	623	BCR	C2-C1-C6	3.09	114.93	110.44
30	b	602	SQD	C3-C4-C5	3.09	115.83	110.23
25	d	409	DGD	O3G-C3G-C2G	-3.09	103.31	110.82
30	d	402	SQD	C3-C4-C5	3.09	115.83	110.23
22	c	505	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
22	b	607	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
22	C	502	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
30	a	415	SQD	O7-S-C6	3.07	111.34	106.76
22	b	613	CLA	C3B-C4B-NB	-3.06	107.80	110.53
24	J	102	BCR	C27-C26-C25	3.06	126.84	122.70
24	b	621	BCR	C33-C5-C6	-3.05	121.15	124.48
24	B	619	BCR	C2-C1-C6	3.05	114.88	110.44
22	C	505	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
22	b	612	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
31	b	604	LMT	C1'-O5'-C5'	-3.04	107.79	113.72
22	B	606	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
22	B	604	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
32	d	401	PHO	O1D-CGD-CBD	3.03	129.32	124.72
30	d	402	SQD	O9-S-C6	3.03	111.28	106.76
24	j	102	BCR	C27-C26-C25	3.03	126.79	122.70
25	A	408	DGD	O6D-C1D-O3G	-3.03	102.89	110.04
24	f	102	BCR	C29-C30-C25	3.03	114.83	110.44
22	c	502	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
30	B	622	SQD	O9-S-C6	3.02	111.26	106.76
22	a	404	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
25	a	411	DGD	O6D-C1D-O3G	-3.01	102.92	110.04
22	b	610	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
34	f	101	HEM	C3B-C4B-NB	-3.01	107.31	109.47
22	b	605	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
32	D	401	PHO	O1D-CGD-CBD	3.00	129.27	124.72
22	a	406	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
24	x	101	BCR	C33-C5-C6	-3.00	121.22	124.48
24	F	102	BCR	C29-C30-C25	2.99	114.78	110.44
24	j	102	BCR	C7-C8-C9	-2.99	121.81	126.23
22	b	611	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
22	b	613	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	F	102	BCR	C33-C5-C6	-2.99	121.22	124.48
24	f	102	BCR	C33-C5-C6	-2.99	121.23	124.48
22	b	611	CLA	C3B-C4B-NB	-2.98	107.87	110.53
30	B	622	SQD	C3-C4-C5	2.98	115.64	110.23
22	b	608	CLA	O2D-CGD-O1D	-2.98	118.05	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
24	y	101	BCR	C27-C26-C25	2.97	126.72	122.70
31	I	102	LMT	O1'-C1'-C2'	2.97	112.78	108.27
22	c	512	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
31	B	624	LMT	C3'-C4'-C5'	-2.97	104.34	110.93
25	B	625	DGD	O5D-C1E-C2E	2.97	112.78	108.27
27	D	407	LMG	O6-C1-O1	-2.97	103.03	110.04
22	A	402	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
22	C	508	CLA	C3B-C4B-NB	-2.97	107.88	110.53
24	K	102	BCR	C2-C1-C6	2.97	114.75	110.44
30	A	414	SQD	C44-O6-C1	2.96	120.15	113.80
30	a	401	SQD	O9-S-C6	2.96	111.18	106.76
26	a	412	LHG	O8-C23-C24	2.96	120.86	111.83
27	d	407	LMG	O6-C1-O1	-2.96	103.05	110.04
22	B	609	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	c	508	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	C	506	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	C	512	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	b	612	CLA	C3B-C4B-NB	-2.96	107.89	110.53
25	C	515	DGD	O6D-C1D-O3G	-2.96	103.06	110.04
34	F	101	HEM	C3B-C4B-NB	-2.96	107.34	109.47
22	C	507	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	c	510	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
24	H	102	BCR	C33-C5-C6	-2.95	121.26	124.48
24	g	101	BCR	C27-C26-C25	2.95	126.69	122.70
24	J	102	BCR	C7-C8-C9	-2.95	121.87	126.23
22	c	520	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
25	c	515	DGD	O6D-C1D-O3G	-2.94	103.10	110.04
22	c	502	CLA	C3B-C4B-NB	-2.93	107.91	110.53
22	C	501	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	A	403	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	B	613	CLA	C3B-C4B-NB	-2.93	107.91	110.53
22	B	609	CLA	C3B-C4B-NB	-2.93	107.92	110.53
30	A	413	SQD	C3-C4-C5	2.93	115.54	110.23
22	c	511	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	h	101	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	C	520	CLA	C3B-C4B-NB	-2.92	107.92	110.53
25	C	517	DGD	CDB-CCB-CBB	-2.91	99.64	114.37
31	i	102	LMT	O1'-C1'-C2'	2.91	112.69	108.27
22	b	617	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	B	612	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
22	H	101	CLA	O2D-CGD-O1D	-2.91	118.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	517	DGD	CDB-CCB-CBB	-2.91	99.68	114.37
25	b	601	DGD	O5D-C1E-C2E	2.90	112.68	108.27
22	d	405	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	A	409	LHG	O8-C23-C24	2.90	120.68	111.83
22	D	404	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	B	607	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	c	506	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
22	A	404	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
22	C	512	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
22	b	616	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
22	C	510	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	C	514	BCR	C15-C16-C17	-2.89	117.61	123.52
23	A	406	PL9	C22-C23-C24	-2.89	121.02	127.62
22	C	520	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
30	a	415	SQD	C3-C4-C5	2.88	115.45	110.23
25	c	517	DGD	C1D-C2D-C3D	-2.88	103.95	110.01
22	C	502	CLA	C3B-C4B-NB	-2.88	107.96	110.53
24	B	618	BCR	C24-C23-C22	-2.88	121.98	126.23
24	c	521	BCR	C15-C16-C17	-2.87	117.64	123.52
22	c	501	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	B	601	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
22	D	405	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	C	503	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	d	404	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
30	A	414	SQD	O9-S-C6	2.85	111.02	106.76
25	c	516	DGD	CDB-CCB-CBB	-2.85	99.95	114.37
22	B	605	CLA	C3B-C4B-NB	-2.85	107.99	110.53
22	c	512	CLA	C3B-C4B-NB	-2.85	107.99	110.53
23	a	409	PL9	C22-C23-C24	-2.85	121.11	127.62
24	B	618	BCR	C11-C10-C9	-2.85	123.29	127.28
25	b	601	DGD	C1D-C2D-C3D	-2.84	104.03	110.01
31	b	627	LMT	C3'-C4'-C5'	-2.84	104.64	110.93
25	C	516	DGD	CDB-CCB-CBB	-2.84	100.04	114.37
22	B	610	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
22	a	408	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
32	D	402	PHO	O2D-CGD-O1D	-2.83	118.33	123.85
22	c	509	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	B	607	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	b	618	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
22	A	404	CLA	C3B-C4B-NB	-2.83	108.01	110.53
30	F	103	SQD	O8-S-C6	2.82	111.42	105.97
22	b	607	CLA	C1-C2-C3	-2.82	121.58	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	BCR	C15-C14-C13	-2.82	123.33	127.28
24	B	618	BCR	C29-C30-C25	2.81	114.53	110.44
24	b	622	BCR	C29-C30-C25	2.81	114.52	110.44
25	b	601	DGD	C3G-C2G-C1G	-2.81	105.24	111.78
23	j	101	PL9	C7-C8-C9	-2.81	121.99	126.83
23	d	406	PL9	C40-C39-C41	2.80	120.09	115.23
30	f	103	SQD	O9-S-C6	2.80	110.93	106.76
27	C	518	LMG	O6-C1-O1	-2.80	103.44	110.04
23	D	406	PL9	C22-C23-C24	-2.80	121.23	127.62
24	b	623	BCR	C3-C4-C5	-2.79	109.08	114.06
22	b	615	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	D	405	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	B	614	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	C	506	CLA	C3B-C4B-NB	-2.79	108.04	110.53
24	B	619	BCR	C3-C4-C5	-2.79	109.08	114.06
22	c	507	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	C	509	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	b	601	DGD	O3G-C3G-C2G	-2.78	104.05	110.82
22	C	511	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	C	511	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
22	c	520	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	d	401	PHO	O2D-CGD-O1D	-2.78	118.45	123.85
22	b	609	CLA	C3B-C4B-NB	-2.77	108.05	110.53
22	a	405	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
24	g	101	BCR	C7-C8-C9	-2.77	122.14	126.23
22	d	405	CLA	C3B-C4B-NB	-2.77	108.06	110.53
24	c	514	BCR	C11-C10-C9	-2.77	123.39	127.28
23	J	101	PL9	C7-C8-C9	-2.77	122.06	126.83
22	A	405	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	g	101	BCR	C33-C5-C6	-2.77	121.46	124.48
25	D	409	DGD	CDB-CCB-CBB	-2.77	100.38	114.37
34	f	101	HEM	C3B-C2B-C1B	2.76	108.48	106.41
22	c	503	CLA	C3B-C4B-NB	-2.76	108.06	110.53
22	C	509	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
34	F	101	HEM	C3B-C2B-C1B	2.76	108.48	106.41
25	d	409	DGD	CDB-CCB-CBB	-2.76	100.43	114.37
24	y	101	BCR	C7-C8-C9	-2.75	122.17	126.23
30	b	602	SQD	C4-C3-C2	2.75	115.66	110.83
22	B	602	CLA	C3B-C4B-NB	-2.75	108.08	110.53
24	K	102	BCR	C15-C16-C17	-2.75	117.90	123.52
24	J	102	BCR	C15-C14-C13	-2.75	123.43	127.28
24	y	101	BCR	C38-C26-C25	-2.74	121.49	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	101	BCR	C38-C26-C25	-2.74	121.49	124.48
24	j	102	BCR	C15-C14-C13	-2.74	123.44	127.28
22	c	506	CLA	C3B-C4B-NB	-2.74	108.08	110.53
32	a	407	PHO	CMB-C2B-C3B	2.74	130.16	124.68
23	d	406	PL9	C22-C23-C24	-2.74	121.36	127.62
22	c	511	CLA	C3B-C4B-NB	-2.74	108.09	110.53
23	D	406	PL9	C40-C39-C41	2.74	119.98	115.23
24	B	617	BCR	C15-C14-C13	-2.74	123.44	127.28
24	C	514	BCR	C29-C30-C25	2.73	114.41	110.44
22	b	606	CLA	C3B-C4B-NB	-2.73	108.09	110.53
27	i	101	LMG	O6-C1-O1	-2.73	103.59	110.04
30	F	103	SQD	O9-S-C6	2.73	110.83	106.76
22	b	608	CLA	C3B-C4B-NB	-2.73	108.09	110.53
27	I	101	LMG	O6-C1-O1	-2.73	103.60	110.04
27	c	518	LMG	O6-C1-O1	-2.72	103.61	110.04
23	d	406	PL9	C7-C8-C9	-2.72	122.14	126.83
24	B	617	BCR	C28-C27-C26	-2.72	109.20	114.06
22	b	614	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
24	b	620	BCR	C33-C5-C6	-2.72	121.52	124.48
22	a	406	CLA	C3B-C4B-NB	-2.72	108.11	110.53
32	D	401	PHO	O2D-CGD-O1D	-2.71	118.56	123.85
22	c	509	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
30	f	103	SQD	O8-S-C6	2.71	111.20	105.97
32	D	402	PHO	CMB-C2B-C3B	2.71	130.09	124.68
24	B	616	BCR	C33-C5-C6	-2.71	121.53	124.48
22	B	611	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	c	514	BCR	C29-C30-C25	2.70	114.37	110.44
22	B	603	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	B	608	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	C	517	DGD	C1D-C2D-C3D	-2.70	104.33	110.01
24	b	621	BCR	C28-C27-C26	-2.69	109.25	114.06
22	b	619	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	A	403	CLA	CHB-C4A-NA	2.69	128.28	124.40
32	a	407	PHO	O2D-CGD-O1D	-2.68	118.62	123.85
25	B	625	DGD	O3G-C3G-C2G	-2.68	104.30	110.82
22	A	403	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	b	618	CLA	C3B-C4B-NB	-2.68	108.14	110.53
31	M	102	LMT	C1'-O5'-C5'	-2.68	108.48	113.72
26	c	519	LHG	O8-C23-C24	2.68	120.01	111.83
24	c	514	BCR	C15-C16-C17	-2.67	118.05	123.52
22	B	614	CLA	C3B-C4B-NB	-2.67	108.15	110.53
25	c	517	DGD	C1D-O6D-C5D	-2.67	108.51	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	101	PL9	C22-C23-C24	-2.66	121.53	127.62
24	y	101	BCR	C33-C5-C6	-2.66	121.58	124.48
22	b	607	CLA	C3B-C4B-NB	-2.66	108.16	110.53
25	B	625	DGD	C1D-C2D-C3D	-2.65	104.42	110.01
24	c	513	BCR	C7-C8-C9	-2.65	122.31	126.23
24	C	513	BCR	C24-C23-C22	-2.65	122.32	126.23
24	B	618	BCR	C15-C16-C17	-2.65	118.10	123.52
24	K	102	BCR	C27-C26-C25	2.64	126.28	122.70
24	c	521	BCR	C27-C26-C25	2.64	126.28	122.70
22	b	607	CLA	CHB-C4A-NA	2.64	128.21	124.40
24	b	622	BCR	C15-C16-C17	-2.63	118.13	123.52
22	C	510	CLA	C3B-C4B-NB	-2.63	108.18	110.53
22	a	405	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	b	622	BCR	C11-C10-C9	-2.63	123.59	127.28
23	j	101	PL9	C22-C23-C24	-2.63	121.61	127.62
24	b	623	BCR	C27-C26-C25	2.63	126.25	122.70
22	C	506	CLA	CHB-C4A-NA	2.63	128.19	124.40
26	C	519	LHG	O8-C23-C24	2.63	119.84	111.83
24	c	514	BCR	C28-C27-C26	-2.62	109.38	114.06
22	B	603	CLA	CHB-C4A-NA	2.62	128.19	124.40
22	B	603	CLA	C1-C2-C3	-2.62	121.90	126.20
22	b	610	CLA	C3B-C4B-NB	-2.62	108.19	110.53
22	C	510	CLA	CHB-C4A-NA	2.62	128.18	124.40
24	B	618	BCR	C15-C14-C13	-2.62	123.61	127.28
22	c	508	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
23	D	406	PL9	C7-C8-C9	-2.61	122.33	126.83
22	b	619	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
25	B	625	DGD	C3G-C2G-C1G	-2.61	105.70	111.78
22	C	501	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	c	501	CLA	C3B-C4B-NB	-2.60	108.21	110.53
30	d	402	SQD	O8-S-C6	2.60	111.00	105.97
22	C	507	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	b	608	CLA	CHB-C4A-NA	2.60	128.15	124.40
22	b	609	CLA	CHB-C4A-NA	2.60	128.15	124.40
30	B	626	SQD	C4-C3-C2	2.60	115.39	110.83
22	c	510	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	c	506	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	B	605	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	a	405	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	B	615	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
22	B	615	CLA	C3B-C4B-NB	-2.59	108.22	110.53
31	B	623	LMT	C1'-O5'-C5'	-2.59	108.67	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	C3B-C4B-NB	-2.59	108.22	110.53
24	C	514	BCR	C15-C14-C13	-2.58	123.65	127.28
24	C	513	BCR	C15-C16-C17	-2.58	118.23	123.52
24	b	621	BCR	C29-C30-C25	2.58	114.18	110.44
22	B	610	CLA	C1-C2-C3	-2.58	121.98	126.20
22	c	511	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	D	404	CLA	C3B-C4B-NB	-2.57	108.23	110.53
22	C	503	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	B	619	BCR	C27-C26-C25	2.57	126.17	122.70
32	d	401	PHO	CMB-C2B-C3B	2.57	129.81	124.68
22	b	618	CLA	CHB-C4A-NA	2.57	128.10	124.40
24	C	514	BCR	C28-C27-C26	-2.56	109.48	114.06
22	C	520	CLA	CHB-C4A-NA	2.56	128.10	124.40
22	C	511	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	B	616	BCR	C2-C1-C6	2.56	114.16	110.44
24	c	513	BCR	C24-C23-C22	-2.56	122.45	126.23
24	b	620	BCR	C2-C1-C6	2.56	114.15	110.44
25	D	409	DGD	CFB-CEB-CDB	-2.56	101.44	114.37
22	c	505	CLA	CHB-C4A-NA	2.55	128.09	124.40
30	d	402	SQD	C44-O6-C1	2.55	119.27	113.80
24	A	407	BCR	C27-C26-C25	2.55	126.15	122.70
24	a	410	BCR	C27-C26-C25	2.55	126.15	122.70
25	C	517	DGD	C1D-O6D-C5D	-2.55	108.74	113.72
22	h	101	CLA	C3B-C4B-NB	-2.55	108.26	110.53
24	B	617	BCR	C29-C30-C25	2.55	114.14	110.44
22	b	615	CLA	CHB-C4A-NA	2.54	128.07	124.40
22	a	408	CLA	C3B-C4B-NB	-2.54	108.26	110.53
22	c	512	CLA	CHB-C4A-NA	2.54	128.07	124.40
24	C	514	BCR	C33-C5-C6	-2.54	121.71	124.48
24	c	514	BCR	C33-C5-C6	-2.54	121.71	124.48
24	y	101	BCR	C1-C6-C5	-2.54	119.17	122.64
22	b	614	CLA	C3B-C4B-NB	-2.54	108.27	110.53
22	B	610	CLA	C3B-C4B-NB	-2.53	108.27	110.53
24	b	623	BCR	C7-C8-C9	-2.53	122.49	126.23
22	c	504	CLA	C3B-C4B-NB	-2.53	108.27	110.53
31	d	410	LMT	C3'-C4'-C5'	-2.53	105.32	110.93
22	B	601	CLA	C3B-C4B-NB	-2.53	108.27	110.53
32	D	401	PHO	CMB-C2B-C3B	2.53	129.74	124.68
31	M	103	LMT	C3'-C4'-C5'	-2.53	105.32	110.93
25	d	409	DGD	CFB-CEB-CDB	-2.53	101.58	114.37
27	A	415	LMG	O6-C1-O1	-2.53	104.07	110.04
24	c	513	BCR	C15-C16-C17	-2.53	118.35	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	622	BCR	C15-C14-C13	-2.53	123.73	127.28
34	f	101	HEM	C1B-NB-C4B	2.53	108.20	105.21
27	a	402	LMG	O6-C1-O1	-2.53	104.08	110.04
22	c	501	CLA	CHB-C4A-NA	2.53	128.04	124.40
31	M	103	LMT	C1'-O5'-C5'	-2.52	108.79	113.72
22	b	614	CLA	C1-C2-C3	-2.52	122.06	126.20
22	H	101	CLA	C3B-C4B-NB	-2.52	108.28	110.53
23	a	409	PL9	C7-C8-C9	-2.52	122.49	126.83
22	B	608	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	C	504	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	c	508	CLA	CHB-C4A-NA	2.51	128.03	124.40
30	B	622	SQD	C44-O6-C1	2.51	119.18	113.80
22	b	615	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
22	a	408	CLA	CHB-C4A-NA	2.51	128.02	124.40
22	C	512	CLA	CHB-C4A-NA	2.51	128.02	124.40
22	B	604	CLA	C3B-C4B-NB	-2.51	108.29	110.53
22	b	605	CLA	C3B-C4B-NB	-2.51	108.29	110.53
23	D	406	PL9	C27-C28-C29	-2.51	121.89	127.62
22	C	501	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	C	513	BCR	C15-C14-C13	-2.50	123.77	127.28
22	c	505	CLA	C3B-C4B-NB	-2.50	108.29	110.53
25	d	409	DGD	C3G-C2G-C1G	-2.50	105.94	111.78
24	c	513	BCR	C15-C14-C13	-2.50	123.77	127.28
22	B	609	CLA	CHB-C4A-NA	2.50	128.01	124.40
27	D	411	LMG	C38-C37-C36	-2.50	101.72	114.37
30	B	622	SQD	O8-S-C6	2.50	110.80	105.97
25	C	516	DGD	O6E-C1E-O5D	-2.50	104.14	110.04
24	J	102	BCR	C15-C16-C17	-2.50	118.41	123.52
24	c	514	BCR	C15-C14-C13	-2.50	123.78	127.28
24	B	616	BCR	C27-C26-C25	2.50	126.08	122.70
23	a	409	PL9	C41-C39-C40	2.50	120.33	114.59
22	B	604	CLA	CHB-C4A-NA	2.50	128.00	124.40
22	c	520	CLA	CHB-C4A-NA	2.50	128.00	124.40
31	D	410	LMT	C3'-C4'-C5'	-2.50	105.40	110.93
27	d	411	LMG	C38-C37-C36	-2.49	101.77	114.37
22	C	508	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	c	504	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	a	404	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	j	102	BCR	C38-C26-C25	-2.49	121.77	124.48
22	C	508	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
24	A	407	BCR	C15-C14-C13	-2.49	123.79	127.28
24	g	101	BCR	C1-C6-C5	-2.49	119.24	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	CHB-C1B-NB	2.48	127.78	124.05
25	A	408	DGD	CBB-CAB-C9B	-2.48	101.83	114.37
27	d	408	LMG	C38-C37-C36	-2.48	101.83	114.37
24	C	514	BCR	C11-C10-C9	-2.48	123.80	127.28
22	C	505	CLA	C3B-C4B-NB	-2.48	108.32	110.53
23	a	409	PL9	C20-C19-C21	2.48	119.53	115.23
34	F	101	HEM	C1B-NB-C4B	2.48	108.14	105.21
22	C	505	CLA	CHB-C4A-NA	2.48	127.97	124.40
22	c	503	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	b	620	BCR	C27-C26-C25	2.48	126.05	122.70
30	a	415	SQD	O48-C23-C24	2.47	119.38	111.83
27	E	101	LMG	C1-C2-C3	-2.47	104.81	110.01
24	j	102	BCR	C15-C16-C17	-2.47	118.46	123.52
27	b	625	LMG	C1-C2-C3	-2.47	104.81	110.01
31	b	626	LMT	C1'-O5'-C5'	-2.47	108.90	113.72
25	c	516	DGD	O6E-C1E-O5D	-2.47	104.21	110.04
22	B	607	CLA	CHB-C4A-NA	2.47	127.96	124.40
22	B	614	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	b	617	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	J	102	BCR	C38-C26-C25	-2.46	121.80	124.48
30	A	413	SQD	O48-C23-C24	2.46	119.34	111.83
22	a	406	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	c	517	DGD	O5D-C6D-C5D	-2.46	103.87	109.42
22	b	612	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	a	411	DGD	CBB-CAB-C9B	-2.46	101.94	114.37
22	B	611	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	d	405	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	C	513	BCR	C7-C8-C9	-2.46	122.60	126.23
27	B	621	LMG	C1-C2-C3	-2.46	104.84	110.01
22	C	511	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
27	A	410	LMG	C40-C39-C38	-2.46	101.96	114.37
22	c	511	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
25	B	620	DGD	CBB-CAB-C9B	-2.45	101.97	114.37
27	l	101	LMG	C40-C39-C38	-2.45	101.97	114.37
22	B	612	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	f	103	SQD	C44-O6-C1	2.45	119.05	113.80
22	B	613	CLA	CHB-C4A-NA	2.45	127.94	124.40
31	M	102	LMT	C3'-C4'-C5'	-2.45	105.50	110.93
24	b	623	BCR	C11-C10-C9	-2.45	123.84	127.28
22	B	610	CLA	CHB-C1B-NB	2.45	127.72	124.05
24	c	521	BCR	C15-C14-C13	-2.45	123.84	127.28
25	b	624	DGD	CBB-CAB-C9B	-2.45	101.99	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	102	BCR	C35-C13-C14	-2.44	118.86	122.82
22	B	612	CLA	C3B-C4B-NB	-2.44	108.35	110.53
25	C	517	DGD	CFB-CEB-CDB	-2.44	102.05	114.37
27	D	408	LMG	C38-C37-C36	-2.44	102.06	114.37
25	c	516	DGD	C3G-C2G-C1G	-2.44	106.11	111.78
22	b	611	CLA	CHB-C4A-NA	2.43	127.91	124.40
27	D	407	LMG	C38-C37-C36	-2.43	102.08	114.37
23	A	406	PL9	C41-C39-C40	2.43	120.18	114.59
23	a	409	PL9	C27-C28-C29	-2.43	122.06	127.62
22	D	405	CLA	CHB-C4A-NA	2.43	127.91	124.40
30	a	401	SQD	O48-C23-C24	2.43	119.24	111.83
27	D	408	LMG	O6-C1-C2	-2.43	105.38	110.37
22	h	101	CLA	CHB-C4A-NA	2.43	127.90	124.40
30	B	622	SQD	O48-C23-C24	2.43	119.23	111.83
23	j	101	PL9	O2-C1-C6	2.43	124.34	120.48
30	d	402	SQD	O48-C23-C24	2.42	119.23	111.83
24	B	619	BCR	C7-C8-C9	-2.42	122.65	126.23
22	C	504	CLA	C3B-C4B-NB	-2.42	108.37	110.53
22	A	404	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	c	507	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	c	510	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	c	502	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	C	517	DGD	O5D-C6D-C5D	-2.42	103.97	109.42
25	c	515	DGD	C3G-C2G-C1G	-2.42	106.14	111.78
26	C	519	LHG	C11-C10-C9	-2.42	102.14	114.37
22	B	606	CLA	CHB-C4A-NA	2.42	127.89	124.40
23	A	406	PL9	C7-C8-C9	-2.42	122.67	126.83
24	A	407	BCR	C15-C16-C17	-2.41	118.58	123.52
24	j	102	BCR	C35-C13-C14	-2.41	118.91	122.82
27	d	407	LMG	C38-C37-C36	-2.41	102.17	114.37
27	c	522	LMG	O6-C1-O1	-2.41	104.35	110.04
24	K	102	BCR	C11-C10-C9	-2.41	123.90	127.28
22	d	404	CLA	C3B-C4B-NB	-2.41	108.38	110.53
23	d	406	PL9	C27-C28-C29	-2.41	122.11	127.62
24	c	513	BCR	C11-C10-C9	-2.41	123.90	127.28
27	c	522	LMG	C40-C39-C38	-2.40	102.22	114.37
25	c	517	DGD	CFB-CEB-CDB	-2.40	102.23	114.37
23	A	406	PL9	C27-C28-C29	-2.40	122.13	127.62
25	C	515	DGD	C3G-C2G-C1G	-2.40	106.19	111.78
26	c	519	LHG	C11-C10-C9	-2.40	102.25	114.37
25	C	516	DGD	C3G-C2G-C1G	-2.40	106.19	111.78
22	B	611	CLA	O2D-CGD-O1D	-2.40	119.18	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	101	CLA	CHB-C4A-NA	2.39	127.86	124.40
22	B	615	CLA	CHB-C4A-NA	2.39	127.86	124.40
22	b	616	CLA	CHB-C4A-NA	2.39	127.86	124.40
31	D	410	LMT	C1'-O5'-C5'	-2.39	109.05	113.72
22	B	603	CLA	O1D-CGD-CBD	2.39	129.24	124.52
22	C	507	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	B	602	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	b	610	CLA	CHB-C4A-NA	2.39	127.85	124.40
27	e	101	LMG	O6-C1-O1	-2.39	104.40	110.04
25	c	516	DGD	CFB-CEB-CDB	-2.39	102.29	114.37
24	x	101	BCR	C29-C30-C25	2.39	113.91	110.44
23	a	409	PL9	O2-C1-C6	2.39	124.28	120.48
23	A	406	PL9	O2-C1-C6	2.38	124.27	120.48
22	B	608	CLA	C1-C2-C3	-2.38	122.29	126.20
23	D	406	PL9	C37-C38-C39	-2.38	122.17	127.62
23	J	101	PL9	O2-C1-C6	2.38	124.27	120.48
30	A	414	SQD	O48-C23-C24	2.38	119.10	111.83
27	B	621	LMG	O6-C1-O1	-2.38	104.42	110.04
27	C	521	LMG	C40-C39-C38	-2.38	102.33	114.37
22	A	402	CLA	CHB-C4A-NA	2.38	127.84	124.40
25	D	409	DGD	C3G-C2G-C1G	-2.38	106.24	111.78
24	b	620	BCR	C11-C10-C9	-2.38	123.94	127.28
24	c	513	BCR	C27-C26-C25	2.38	125.92	122.70
22	b	616	CLA	C3B-C4B-NB	-2.37	108.41	110.53
22	b	613	CLA	CHB-C4A-NA	2.37	127.82	124.40
30	b	602	SQD	O48-C23-C24	2.37	119.07	111.83
22	A	405	CLA	C3B-C4B-NB	-2.37	108.41	110.53
23	d	406	PL9	O2-C1-C6	2.37	124.25	120.48
22	C	507	CLA	C1-C2-C3	-2.37	122.32	126.20
23	d	406	PL9	C37-C38-C39	-2.37	122.21	127.62
22	b	606	CLA	CHB-C4A-NA	2.36	127.81	124.40
30	B	626	SQD	O48-C23-C24	2.36	119.03	111.83
30	a	401	SQD	C1-O5-C5	2.36	118.33	113.72
31	B	627	LMT	C1'-O5'-C5'	-2.36	109.11	113.72
24	a	410	BCR	C33-C5-C6	-2.36	121.91	124.48
27	C	518	LMG	C38-C37-C36	-2.36	102.45	114.37
22	A	405	CLA	CHB-C4A-NA	2.36	127.80	124.40
30	F	103	SQD	C44-O6-C1	2.35	118.84	113.80
24	f	102	BCR	C27-C26-C25	2.35	125.88	122.70
24	K	102	BCR	C15-C14-C13	-2.35	123.98	127.28
27	A	410	LMG	C38-C37-C36	-2.35	102.50	114.37
27	b	625	LMG	C40-C39-C38	-2.35	102.50	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	101	LMG	C1-C2-C3	-2.34	105.08	110.01
25	A	408	DGD	O5D-C6D-C5D	-2.34	104.14	109.42
24	j	102	BCR	C29-C30-C25	2.34	113.84	110.44
24	J	102	BCR	C29-C30-C25	2.34	113.84	110.44
25	C	516	DGD	CFB-CEB-CDB	-2.34	102.54	114.37
22	D	404	CLA	O1D-CGD-CBD	2.34	129.13	124.52
31	b	603	LMT	C1'-O5'-C5'	-2.34	109.16	113.72
22	c	509	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	l	101	LMG	C38-C37-C36	-2.33	102.56	114.37
24	C	513	BCR	C27-C26-C25	2.33	125.86	122.70
23	D	406	PL9	C32-C33-C34	-2.33	122.28	127.62
27	D	411	LMG	C1-C2-C3	-2.33	105.10	110.01
22	C	502	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	g	101	BCR	C15-C16-C17	-2.33	118.75	123.52
24	K	102	BCR	C24-C23-C22	-2.33	122.79	126.23
22	b	619	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	a	410	BCR	C15-C16-C17	-2.32	118.76	123.52
22	c	507	CLA	C1-C2-C3	-2.32	122.39	126.20
22	B	601	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	D	406	PL9	O1-C4-C3	-2.32	118.28	120.73
24	F	102	BCR	C11-C10-C9	-2.32	124.02	127.28
23	D	406	PL9	C20-C19-C21	2.32	119.25	115.23
24	y	101	BCR	C3-C2-C1	-2.32	106.22	114.43
24	B	618	BCR	C7-C8-C9	-2.32	122.81	126.23
22	D	405	CLA	C1-C2-C3	-2.32	122.40	126.20
27	E	101	LMG	O6-C1-O1	-2.32	104.57	110.04
27	A	410	LMG	O3-C3-C2	-2.32	104.92	110.38
27	c	518	LMG	C38-C37-C36	-2.32	102.66	114.37
31	i	102	LMT	C1'-O5'-C5'	-2.31	109.20	113.72
27	C	521	LMG	O6-C1-O1	-2.31	104.58	110.04
32	d	401	PHO	C1-C2-C3	-2.31	122.41	126.20
24	H	102	BCR	C29-C30-C25	2.31	113.80	110.44
24	B	616	BCR	C11-C10-C9	-2.31	124.03	127.28
27	B	621	LMG	C40-C39-C38	-2.31	102.68	114.37
23	d	406	PL9	C32-C33-C34	-2.31	122.33	127.62
27	d	411	LMG	O6-C1-O1	-2.31	104.58	110.04
27	m	101	LMG	C1-C2-C3	-2.31	105.15	110.01
30	B	626	SQD	O8-S-C6	2.31	110.43	105.97
25	a	411	DGD	C3G-C2G-C1G	-2.31	106.40	111.78
25	A	408	DGD	C3G-C2G-C1G	-2.31	106.41	111.78
23	d	406	PL9	C20-C19-C21	2.30	119.22	115.23
22	b	607	CLA	O1D-CGD-CBD	2.30	129.06	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	601	DGD	O6D-C1D-O3G	-2.30	104.62	110.04
23	D	406	PL9	O2-C1-C6	2.29	124.13	120.48
24	b	621	BCR	C11-C10-C9	-2.29	124.06	127.28
24	K	102	BCR	C33-C5-C6	-2.29	121.98	124.48
24	g	101	BCR	C3-C2-C1	-2.29	106.31	114.43
24	f	102	BCR	C15-C16-C17	-2.29	118.83	123.52
24	A	407	BCR	C33-C5-C6	-2.29	121.99	124.48
22	C	509	CLA	CHB-C4A-NA	2.29	127.70	124.40
22	B	605	CLA	O1D-CGD-CBD	2.28	129.02	124.52
24	B	616	BCR	C15-C14-C13	-2.28	124.08	127.28
24	B	619	BCR	C24-C23-C22	-2.28	122.86	126.23
23	J	101	PL9	C20-C19-C21	2.28	119.19	115.23
22	d	404	CLA	O1D-CGD-CBD	2.28	129.01	124.52
24	F	102	BCR	C15-C16-C17	-2.28	118.86	123.52
31	d	410	LMT	C1'-O5'-C5'	-2.28	109.28	113.72
23	d	406	PL9	O1-C4-C3	-2.27	118.33	120.73
24	y	101	BCR	C15-C16-C17	-2.27	118.86	123.52
24	F	102	BCR	C27-C26-C25	2.27	125.78	122.70
27	m	101	LMG	O2-C2-C1	-2.27	104.66	110.08
23	A	406	PL9	C20-C19-C21	2.27	119.17	115.23
24	b	620	BCR	C15-C14-C13	-2.27	124.09	127.28
27	b	625	LMG	C38-C37-C36	-2.27	102.89	114.37
24	C	513	BCR	C3-C4-C5	-2.27	110.01	114.06
24	B	619	BCR	C38-C26-C25	-2.27	122.01	124.48
27	e	101	LMG	C1-C2-C3	-2.27	105.24	110.01
27	C	521	LMG	C38-C37-C36	-2.27	102.92	114.37
30	A	414	SQD	C1-O5-C5	2.27	118.14	113.72
24	B	619	BCR	C11-C10-C9	-2.26	124.10	127.28
24	c	521	BCR	C24-C23-C22	-2.26	122.89	126.23
24	b	623	BCR	C38-C26-C25	-2.26	122.02	124.48
27	A	410	LMG	C1-C2-C3	-2.26	105.25	110.01
25	B	625	DGD	O6D-C1D-O3G	-2.26	104.70	110.04
24	c	521	BCR	C33-C5-C6	-2.26	122.02	124.48
22	c	507	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
24	c	513	BCR	C3-C4-C5	-2.25	110.03	114.06
22	b	605	CLA	C1-C2-C3	-2.25	122.50	126.20
22	b	605	CLA	CHB-C4A-NA	2.25	127.65	124.40
24	c	513	BCR	C8-C7-C6	-2.25	120.98	127.00
24	C	513	BCR	C11-C10-C9	-2.25	124.12	127.28
27	c	518	LMG	O7-C10-O9	-2.25	118.44	123.70
27	c	522	LMG	C38-C37-C36	-2.25	102.99	114.37
27	d	411	LMG	C1-C2-C3	-2.25	105.28	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	l	101	LMG	C1-C2-C3	-2.25	105.28	110.01
27	b	625	LMG	O6-C1-O1	-2.25	104.73	110.04
22	B	606	CLA	C1-C2-C3	-2.25	122.52	126.20
22	c	503	CLA	O2D-CGD-CBD	2.25	115.16	111.23
27	m	101	LMG	C1-O6-C5	-2.24	109.34	113.72
22	C	502	CLA	C1-C2-C3	-2.24	122.52	126.20
24	c	521	BCR	C11-C10-C9	-2.24	124.13	127.28
27	A	410	LMG	O7-C10-O9	-2.24	118.46	123.70
25	b	624	DGD	C1D-C2D-C3D	-2.24	105.30	110.01
25	d	409	DGD	C3D-C4D-C5D	-2.24	106.18	110.23
27	B	621	LMG	C38-C37-C36	-2.23	103.08	114.37
27	C	518	LMG	O7-C10-O9	-2.23	118.49	123.70
23	j	101	PL9	C20-C19-C21	2.23	119.10	115.23
24	f	102	BCR	C11-C10-C9	-2.23	124.16	127.28
24	j	102	BCR	C20-C21-C22	-2.23	124.16	127.28
27	D	411	LMG	O3-C3-C2	-2.22	105.13	110.38
22	c	507	CLA	O2D-CGD-CBD	2.22	115.12	111.23
30	f	103	SQD	C3-C4-C5	2.22	114.26	110.23
24	b	622	BCR	C27-C26-C25	2.22	125.70	122.70
25	c	516	DGD	O3D-C3D-C4D	-2.22	105.14	110.38
27	D	408	LMG	O6-C1-O1	-2.22	104.80	110.04
22	C	507	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
27	c	522	LMG	O2-C2-C1	-2.22	104.79	110.08
24	a	410	BCR	C15-C14-C13	-2.22	124.17	127.28
30	d	402	SQD	C4-C3-C2	2.22	114.72	110.83
23	j	101	PL9	O2-C1-C2	-2.21	116.79	121.83
22	b	615	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
24	C	513	BCR	C8-C7-C6	-2.21	121.09	127.00
27	d	408	LMG	O6-C1-C2	-2.21	105.83	110.37
25	B	620	DGD	C3G-C2G-C1G	-2.21	106.63	111.78
24	J	102	BCR	C20-C21-C22	-2.21	124.18	127.28
24	b	622	BCR	C7-C8-C9	-2.21	122.97	126.23
22	d	405	CLA	C1-C2-C3	-2.21	122.58	126.20
22	H	101	CLA	C1-C2-C3	-2.21	122.58	126.20
30	a	415	SQD	C4-C3-C2	2.21	114.70	110.83
27	d	408	LMG	O6-C1-O1	-2.21	104.83	110.04
27	D	407	LMG	O2-C2-C1	-2.20	104.82	110.08
30	A	414	SQD	O8-S-C6	2.20	110.23	105.97
23	d	406	PL9	O2-C1-C2	-2.20	116.82	121.83
22	D	404	CLA	CHB-C4A-NA	2.20	127.58	124.40
31	B	624	LMT	C1'-O5'-C5'	-2.20	109.42	113.72
25	C	516	DGD	CBB-CAB-C9B	-2.20	103.24	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I	102	LMT	C1'-O5'-C5'	-2.20	109.43	113.72
27	l	101	LMG	O7-C10-O9	-2.20	118.56	123.70
22	b	609	CLA	O1D-CGD-CBD	2.20	128.85	124.52
24	C	514	BCR	C38-C26-C25	-2.20	122.09	124.48
27	D	411	LMG	O6-C1-O1	-2.20	104.86	110.04
25	C	515	DGD	C1D-C2D-C3D	-2.20	105.39	110.01
24	b	623	BCR	C24-C23-C22	-2.20	122.99	126.23
25	a	411	DGD	O5D-C6D-C5D	-2.20	104.47	109.42
25	b	624	DGD	C3G-C2G-C1G	-2.19	106.67	111.78
22	d	404	CLA	CHB-C4A-NA	2.19	127.57	124.40
27	A	415	LMG	O1-C7-C8	-2.19	105.48	110.82
25	A	408	DGD	CAB-C9B-C8B	-2.19	103.29	114.37
30	f	103	SQD	O48-C23-C24	2.19	118.51	111.83
27	I	101	LMG	O7-C10-O9	-2.19	118.59	123.70
27	i	101	LMG	O2-C2-C1	-2.19	104.86	110.08
22	b	606	CLA	C1-C2-C3	-2.19	122.61	126.20
23	J	101	PL9	O2-C1-C2	-2.19	116.86	121.83
25	c	516	DGD	CBB-CAB-C9B	-2.18	103.33	114.37
22	B	611	CLA	C1-C2-C3	-2.18	122.62	126.20
25	B	620	DGD	C4E-C3E-C2E	-2.18	107.00	110.83
24	b	621	BCR	C7-C8-C9	-2.18	123.01	126.23
24	K	102	BCR	C7-C8-C9	-2.18	123.01	126.23
30	a	401	SQD	O8-S-C6	2.18	110.18	105.97
27	M	101	LMG	O2-C2-C1	-2.18	104.88	110.08
25	a	411	DGD	CAB-C9B-C8B	-2.18	103.35	114.37
27	d	407	LMG	O2-C2-C1	-2.18	104.88	110.08
24	B	617	BCR	C11-C10-C9	-2.18	124.23	127.28
24	A	407	BCR	C24-C23-C22	-2.18	123.02	126.23
22	b	618	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
27	b	625	LMG	O2-C2-C1	-2.17	104.90	110.08
27	I	101	LMG	O2-C2-C1	-2.17	104.90	110.08
22	B	603	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
22	c	504	CLA	O1D-CGD-CBD	2.17	128.80	124.52
22	a	406	CLA	C1-C2-C3	-2.17	122.65	126.20
27	d	407	LMG	O3-C3-C2	-2.17	105.27	110.38
24	g	101	BCR	C24-C23-C22	-2.17	123.03	126.23
23	a	409	PL9	O1-C4-C3	-2.17	118.45	120.73
25	C	517	DGD	CBB-CAB-C9B	-2.16	103.43	114.37
27	D	407	LMG	O3-C3-C2	-2.16	105.28	110.38
27	e	101	LMG	O3-C3-C2	-2.16	105.28	110.38
25	b	601	DGD	CBB-CAB-C9B	-2.16	103.43	114.37
25	a	411	DGD	C1D-C2D-C3D	-2.16	105.46	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	102	BCR	C16-C15-C14	-2.16	119.09	123.52
22	C	506	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
24	B	618	BCR	C27-C26-C25	2.16	125.62	122.70
30	A	413	SQD	C4-C3-C2	2.16	114.62	110.83
26	a	412	LHG	C27-C26-C25	-2.16	103.46	114.37
22	C	504	CLA	O1D-CGD-CBD	2.16	128.78	124.52
22	C	503	CLA	O2D-CGD-CBD	2.16	115.00	111.23
24	H	102	BCR	C27-C26-C25	2.16	125.62	122.70
25	B	625	DGD	CBB-CAB-C9B	-2.16	103.46	114.37
24	C	514	BCR	C24-C23-C22	-2.16	123.04	126.23
30	b	602	SQD	O8-S-C6	2.16	110.13	105.97
25	c	517	DGD	CBB-CAB-C9B	-2.15	103.48	114.37
23	A	406	PL9	O2-C1-C2	-2.15	116.93	121.83
24	c	514	BCR	C38-C26-C25	-2.15	122.14	124.48
27	b	625	LMG	O3-C3-C2	-2.15	105.30	110.38
25	c	516	DGD	C3D-C4D-C5D	-2.15	106.33	110.23
30	F	103	SQD	C3-C4-C5	2.15	114.13	110.23
24	b	622	BCR	C33-C5-C6	-2.15	122.14	124.48
31	b	627	LMT	C1'-O5'-C5'	-2.15	109.52	113.72
22	b	612	CLA	C1-C2-C3	-2.15	122.67	126.20
27	I	101	LMG	O3-C3-C2	-2.15	105.31	110.38
27	C	521	LMG	O2-C2-C1	-2.15	104.95	110.08
22	b	616	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
26	A	409	LHG	C27-C26-C25	-2.15	103.51	114.37
22	B	612	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
23	D	406	PL9	O2-C1-C2	-2.15	116.95	121.83
27	d	411	LMG	O3-C3-C2	-2.15	105.32	110.38
27	A	415	LMG	O7-C10-O9	-2.14	118.69	123.70
24	J	102	BCR	C33-C5-C6	-2.14	122.14	124.48
22	c	509	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
25	C	516	DGD	C3D-C4D-C5D	-2.14	106.35	110.23
24	A	407	BCR	C38-C26-C25	-2.14	122.15	124.48
27	d	411	LMG	O7-C10-O9	-2.14	118.70	123.70
22	c	506	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
27	c	518	LMG	O2-C2-C1	-2.14	104.98	110.08
27	B	621	LMG	O3-C3-C2	-2.14	105.33	110.38
24	B	616	BCR	C15-C16-C17	-2.14	119.14	123.52
27	C	518	LMG	O3-C3-C2	-2.14	105.34	110.38
25	C	516	DGD	CAB-C9B-C8B	-2.14	103.56	114.37
24	a	410	BCR	C24-C23-C22	-2.14	123.07	126.23
25	d	409	DGD	C5B-C4B-C3B	-2.14	103.57	114.37
24	F	102	BCR	C7-C8-C9	-2.14	123.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
25	C	516	DGD	O3D-C3D-C4D	-2.14	105.34	110.38
27	l	101	LMG	O3-C3-C2	-2.13	105.34	110.38
22	c	512	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
25	b	601	DGD	CAB-C9B-C8B	-2.13	103.61	114.37
25	B	625	DGD	CAB-C9B-C8B	-2.13	103.62	114.37
23	a	409	PL9	O2-C1-C2	-2.12	117.00	121.83
22	B	611	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
30	F	103	SQD	O48-C23-C24	2.12	118.31	111.83
22	B	602	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
22	c	510	CLA	C1-C2-C3	-2.12	122.72	126.20
27	a	402	LMG	O1-C7-C8	-2.12	105.66	110.82
27	D	411	LMG	O7-C10-O9	-2.12	118.75	123.70
22	B	601	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
24	b	622	BCR	C20-C21-C22	-2.12	124.31	127.28
34	v	201	HEM	C1B-NB-C4B	2.12	107.71	105.21
22	C	510	CLA	C1-C2-C3	-2.11	122.73	126.20
22	c	508	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
25	c	515	DGD	C1D-C2D-C3D	-2.11	105.56	110.01
34	v	201	HEM	C2A-C1A-NA	-2.11	107.81	110.15
33	D	403	BCT	O3-C-O1	-2.11	114.27	119.68
27	a	402	LMG	O3-C3-C2	-2.11	105.40	110.38
22	A	404	CLA	C1-C2-C3	-2.11	122.74	126.20
22	c	501	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
24	c	514	BCR	C24-C23-C22	-2.10	123.12	126.23
23	A	406	PL9	O1-C4-C3	-2.10	118.52	120.73
25	c	517	DGD	CAB-C9B-C8B	-2.10	103.75	114.37
24	a	410	BCR	C38-C26-C25	-2.10	122.19	124.48
22	B	612	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
24	c	521	BCR	C7-C8-C9	-2.10	123.13	126.23
25	D	409	DGD	C3D-C4D-C5D	-2.10	106.43	110.23
24	B	617	BCR	C24-C23-C22	-2.10	123.13	126.23
27	c	518	LMG	O3-C3-C2	-2.10	105.43	110.38
27	c	522	LMG	O3-C3-C2	-2.10	105.43	110.38
30	B	622	SQD	C4-C3-C2	2.10	114.51	110.83
22	B	606	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
24	x	101	BCR	C15-C16-C17	-2.10	119.23	123.52
33	d	403	BCT	O3-C-O1	-2.10	114.32	119.68
22	B	614	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
22	b	615	CLA	C1-C2-C3	-2.09	122.77	126.20
24	B	618	BCR	C33-C5-C6	-2.09	122.20	124.48
24	j	102	BCR	C33-C5-C6	-2.09	122.20	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	625	LMG	O7-C10-O9	-2.09	118.81	123.70
22	b	616	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
25	B	620	DGD	C1D-C2D-C3D	-2.09	105.61	110.01
22	b	610	CLA	C1-C2-C3	-2.09	122.77	126.20
27	B	621	LMG	O2-C2-C1	-2.09	105.10	110.08
22	C	501	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
25	D	409	DGD	C5B-C4B-C3B	-2.09	103.82	114.37
24	B	619	BCR	C33-C5-C6	-2.09	122.21	124.48
27	i	101	LMG	O3-C3-C2	-2.09	105.46	110.38
30	A	413	SQD	O8-S-C6	2.09	110.00	105.97
27	E	101	LMG	O3-C3-C2	-2.09	105.46	110.38
22	C	508	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
25	D	409	DGD	CAB-C9B-C8B	-2.08	103.83	114.37
24	b	623	BCR	C33-C5-C6	-2.08	122.21	124.48
26	C	519	LHG	C27-C26-C25	-2.08	103.84	114.37
27	C	518	LMG	O2-C2-C1	-2.08	105.11	110.08
22	c	502	CLA	C1-C2-C3	-2.08	122.78	126.20
22	C	504	CLA	C1-C2-C3	-2.08	122.78	126.20
22	b	610	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	C	517	DGD	CAB-C9B-C8B	-2.08	103.85	114.37
26	c	519	LHG	C27-C26-C25	-2.08	103.85	114.37
22	C	520	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
24	H	102	BCR	C15-C16-C17	-2.08	119.26	123.52
24	b	621	BCR	C35-C13-C14	-2.08	119.45	122.82
22	b	606	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
24	x	101	BCR	C27-C26-C25	2.08	125.51	122.70
27	A	415	LMG	O3-C3-C2	-2.08	105.48	110.38
24	b	623	BCR	C15-C16-C17	-2.08	119.27	123.52
27	i	101	LMG	O7-C10-O9	-2.08	118.85	123.70
25	c	516	DGD	CAB-C9B-C8B	-2.08	103.87	114.37
25	A	408	DGD	CDB-CCB-CBB	-2.08	99.34	113.36
22	B	612	CLA	C1-C2-C3	-2.08	122.80	126.20
27	C	521	LMG	O3-C3-C2	-2.08	105.48	110.38
25	a	411	DGD	CDB-CCB-CBB	-2.07	99.35	113.36
27	l	101	LMG	O2-C2-C1	-2.07	105.14	110.08
22	A	402	CLA	O1D-CGD-CBD	2.07	128.60	124.52
22	c	520	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
22	B	607	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
32	D	401	PHO	O2A-CGA-O1A	-2.06	118.47	123.63
27	A	410	LMG	O2-C2-C1	-2.06	105.16	110.08
25	d	409	DGD	CAB-C9B-C8B	-2.06	103.95	114.37
22	a	404	CLA	O1D-CGD-CBD	2.06	128.58	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	607	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
22	a	406	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
22	b	616	CLA	C1-C2-C3	-2.06	122.83	126.20
23	d	406	PL9	C12-C13-C14	-2.06	122.91	127.62
27	B	621	LMG	O7-C10-O9	-2.06	118.89	123.70
22	B	607	CLA	C1-C2-C3	-2.06	122.83	126.20
23	J	101	PL9	C12-C13-C14	-2.06	122.92	127.62
22	C	509	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
25	D	409	DGD	CBB-CAB-C9B	-2.05	103.98	114.37
23	D	406	PL9	C12-C13-C14	-2.05	122.93	127.62
25	C	515	DGD	C5B-C4B-C3B	-2.05	104.00	114.37
25	d	409	DGD	CBB-CAB-C9B	-2.05	104.00	114.37
25	A	408	DGD	C5B-C4B-C3B	-2.05	104.00	114.37
27	i	101	LMG	O1-C7-C8	-2.05	105.83	110.82
23	j	101	PL9	C12-C13-C14	-2.05	122.93	127.62
22	b	619	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	a	405	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	A	403	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
24	B	617	BCR	C7-C8-C9	-2.05	123.21	126.23
27	M	101	LMG	C1-O6-C5	-2.04	109.73	113.72
22	C	510	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
27	m	101	LMG	O3-C3-C2	-2.04	105.56	110.38
25	c	515	DGD	C5B-C4B-C3B	-2.04	104.05	114.37
25	b	624	DGD	CAB-C9B-C8B	-2.04	104.06	114.37
27	a	402	LMG	O2-C2-C1	-2.04	105.21	110.08
22	d	404	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	b	613	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
24	H	102	BCR	C7-C8-C9	-2.04	123.22	126.23
27	A	410	LMG	O1-C1-C2	-2.04	105.18	108.27
27	e	101	LMG	O7-C10-O9	-2.04	118.94	123.70
24	x	101	BCR	C16-C15-C14	-2.04	119.35	123.52
25	A	408	DGD	C1D-C2D-C3D	-2.04	105.73	110.01
22	B	613	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
22	B	602	CLA	C1-C2-C3	-2.03	122.86	126.20
23	a	409	PL9	C32-C33-C34	-2.03	122.98	127.62
22	b	611	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
27	d	411	LMG	O2-C2-C1	-2.03	105.24	110.08
22	A	404	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
27	M	101	LMG	O3-C3-C2	-2.03	105.59	110.38
25	c	516	DGD	O2D-C2D-C1D	-2.03	105.24	110.08
34	V	201	HEM	C3B-C2B-C1B	2.03	107.93	106.41
22	C	512	CLA	O1D-CGD-CBD	2.03	128.51	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	518	LMG	O1-C7-C8	-2.02	105.89	110.82
22	b	614	CLA	O1D-CGD-CBD	2.02	128.51	124.52
25	C	516	DGD	C5B-C4B-C3B	-2.02	104.14	114.37
22	C	505	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	C	517	DGD	C5B-C4B-C3B	-2.02	104.16	114.37
25	B	620	DGD	C5B-C4B-C3B	-2.02	104.17	114.37
24	B	616	BCR	C7-C8-C9	-2.02	123.25	126.23
27	A	415	LMG	O2-C2-C1	-2.02	105.27	110.08
22	B	601	CLA	C1-C2-C3	-2.02	122.89	126.20
22	B	613	CLA	O2D-CGD-CBD	2.02	114.75	111.23
22	c	504	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
27	d	407	LMG	O7-C10-O9	-2.01	119.00	123.70
25	C	517	DGD	C3G-O3G-C1D	2.01	118.11	113.80
22	b	605	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
32	d	401	PHO	O2A-CGA-O1A	-2.01	118.59	123.63
22	c	504	CLA	C1-C2-C3	-2.01	122.90	126.20
24	B	616	BCR	C38-C26-C25	-2.01	122.29	124.48
22	a	404	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
34	v	201	HEM	C3B-C2B-C1B	2.01	107.92	106.41
22	b	606	CLA	O2D-CGD-CBD	2.01	114.75	111.23
22	B	609	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
23	j	101	PL9	O1-C4-C3	-2.01	118.61	120.73
22	C	504	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
25	B	620	DGD	CAB-C9B-C8B	-2.01	104.21	114.37
22	B	610	CLA	O1D-CGD-CBD	2.01	128.48	124.52
22	h	101	CLA	C1-C2-C3	-2.01	122.91	126.20
24	K	102	BCR	C38-C26-C25	-2.01	122.30	124.48
24	C	514	BCR	C7-C8-C9	-2.01	123.27	126.23
27	D	407	LMG	O7-C10-O9	-2.00	119.02	123.70
34	V	201	HEM	C1B-NB-C4B	2.00	107.58	105.21
25	c	517	DGD	C5B-C4B-C3B	-2.00	104.25	114.37
22	B	615	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (69) 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	405	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND

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Mol	Chain	Res	Type	Atom
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
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	404	CLA	ND
22	D	405	CLA	ND
22	H	101	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	406	CLA	ND
22	a	408	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

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Mol	Chain	Res	Type	Atom
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	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	404	CLA	ND
22	h	101	CLA	ND

All (2084) 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	C2B-C3B-CAB-CBB
22	A	404	CLA	C4B-C3B-CAB-CBB
22	B	601	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	CBD-CGD-O2D-CED
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C3A-C2A-CAA-CBA
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

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Mol	Chain	Res	Type	Atoms
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	510	CLA	C6-C7-C8-C9
22	C	511	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C3A-C2A-CAA-CBA
22	H	101	CLA	C4-C3-C5-C6
22	H	101	CLA	C6-C7-C8-C9
22	a	404	CLA	CBD-CGD-O2D-CED
22	a	405	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	C3A-C2A-CAA-CBA
22	a	406	CLA	C4B-C3B-CAB-CBB
22	b	605	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	C4-C3-C5-C6
22	b	609	CLA	C1A-C2A-CAA-CBA
22	b	609	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C2B-C3B-CAB-CBB
22	b	610	CLA	C4B-C3B-CAB-CBB
22	b	611	CLA	C1A-C2A-CAA-CBA
22	b	612	CLA	C2B-C3B-CAB-CBB
22	b	612	CLA	C4B-C3B-CAB-CBB
22	b	613	CLA	C2B-C3B-CAB-CBB
22	b	613	CLA	C4B-C3B-CAB-CBB
22	b	614	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C4B-C3B-CAB-CBB
22	b	616	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CAD-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O2D
22	b	619	CLA	C3A-C2A-CAA-CBA
22	b	619	CLA	C2B-C3B-CAB-CBB
22	b	619	CLA	C4B-C3B-CAB-CBB
22	b	619	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	d	404	CLA	C2-C3-C5-C6
22	d	404	CLA	C4-C3-C5-C6
22	h	101	CLA	C1A-C2A-CAA-CBA
22	h	101	CLA	C4-C3-C5-C6
22	h	101	CLA	C6-C7-C8-C9
23	A	406	PL9	C7-C8-C9-C10
23	A	406	PL9	C7-C8-C9-C11
23	A	406	PL9	C12-C13-C14-C15
23	A	406	PL9	C12-C13-C14-C16
23	A	406	PL9	C17-C18-C19-C20
23	A	406	PL9	C17-C18-C19-C21
23	A	406	PL9	C22-C23-C24-C25
23	A	406	PL9	C27-C28-C29-C30
23	A	406	PL9	C27-C28-C29-C31
23	A	406	PL9	C37-C38-C39-C41
23	D	406	PL9	C27-C28-C29-C31
23	D	406	PL9	C34-C36-C37-C38
23	J	101	PL9	C12-C13-C14-C16
23	J	101	PL9	C22-C23-C24-C25
23	J	101	PL9	C22-C23-C24-C26
23	a	409	PL9	C7-C8-C9-C10
23	a	409	PL9	C7-C8-C9-C11
23	a	409	PL9	C12-C13-C14-C15
23	a	409	PL9	C12-C13-C14-C16
23	a	409	PL9	C17-C18-C19-C20
23	a	409	PL9	C17-C18-C19-C21
23	a	409	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
23	a	409	PL9	C27-C28-C29-C30
23	a	409	PL9	C27-C28-C29-C31
23	a	409	PL9	C37-C38-C39-C41
23	d	406	PL9	C27-C28-C29-C31
23	d	406	PL9	C34-C36-C37-C38
23	j	101	PL9	C12-C13-C14-C16
23	j	101	PL9	C22-C23-C24-C25
23	j	101	PL9	C22-C23-C24-C26
24	B	617	BCR	C21-C22-C23-C24
24	B	617	BCR	C23-C24-C25-C26
24	C	513	BCR	C6-C7-C8-C9
24	F	102	BCR	C7-C8-C9-C10
24	H	102	BCR	C21-C22-C23-C24
24	J	102	BCR	C21-C22-C23-C24
24	K	102	BCR	C7-C8-C9-C10
24	K	102	BCR	C7-C8-C9-C34
24	y	101	BCR	C7-C8-C9-C10
24	b	621	BCR	C21-C22-C23-C24
24	b	621	BCR	C23-C24-C25-C26
24	c	513	BCR	C6-C7-C8-C9
24	c	521	BCR	C7-C8-C9-C34
24	f	102	BCR	C7-C8-C9-C10
24	j	102	BCR	C21-C22-C23-C24
24	g	101	BCR	C7-C8-C9-C10
24	x	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C21-C22-C23-C24
25	A	408	DGD	C2D-C1D-O3G-C3G
25	B	620	DGD	C2E-C1E-O5D-C6D
25	B	625	DGD	O1B-C1B-O2G-C2G
25	B	625	DGD	O2G-C2G-C3G-O3G
25	B	625	DGD	C2E-C1E-O5D-C6D
25	B	625	DGD	O6E-C1E-O5D-C6D
25	C	515	DGD	C2B-C1B-O2G-C2G
25	C	515	DGD	O1B-C1B-O2G-C2G
25	C	515	DGD	C2E-C1E-O5D-C6D
25	C	516	DGD	O1B-C1B-O2G-C2G
25	C	516	DGD	C2D-C1D-O3G-C3G
25	C	517	DGD	C2D-C1D-O3G-C3G
25	C	517	DGD	O6D-C1D-O3G-C3G
25	D	409	DGD	O6D-C1D-O3G-C3G
25	a	411	DGD	C2D-C1D-O3G-C3G
25	b	601	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
25	b	601	DGD	O2G-C2G-C3G-O3G
25	b	601	DGD	C2E-C1E-O5D-C6D
25	b	601	DGD	O6E-C1E-O5D-C6D
25	c	515	DGD	C2B-C1B-O2G-C2G
25	c	515	DGD	O1B-C1B-O2G-C2G
25	c	515	DGD	C2E-C1E-O5D-C6D
25	c	516	DGD	O1B-C1B-O2G-C2G
25	c	516	DGD	O2G-C2G-C3G-O3G
25	c	516	DGD	C2D-C1D-O3G-C3G
25	c	517	DGD	O6D-C1D-O3G-C3G
25	d	409	DGD	O6D-C1D-O3G-C3G
26	A	409	LHG	C1-C2-C3-O3
26	C	519	LHG	C3-O3-P-O6
26	C	519	LHG	C4-O6-P-O3
26	C	519	LHG	C4-O6-P-O4
26	a	412	LHG	C1-C2-C3-O3
26	c	519	LHG	C3-O3-P-O6
26	c	519	LHG	C4-O6-P-O3
26	c	519	LHG	C4-O6-P-O4
27	B	621	LMG	C11-C10-O7-C8
27	C	518	LMG	C9-C8-O7-C10
27	C	518	LMG	O9-C10-O7-C8
27	C	518	LMG	C11-C10-O7-C8
27	D	407	LMG	O1-C7-C8-O7
27	D	407	LMG	C11-C10-O7-C8
27	D	408	LMG	O6-C1-O1-C7
27	D	411	LMG	O9-C10-O7-C8
27	D	411	LMG	C11-C10-O7-C8
27	M	101	LMG	O9-C10-O7-C8
27	b	625	LMG	C11-C10-O7-C8
27	c	518	LMG	O9-C10-O7-C8
27	c	518	LMG	C11-C10-O7-C8
27	c	518	LMG	O10-C28-O8-C9
27	d	407	LMG	O1-C7-C8-O7
27	d	407	LMG	C11-C10-O7-C8
27	d	408	LMG	O6-C1-O1-C7
27	d	411	LMG	O9-C10-O7-C8
27	d	411	LMG	C11-C10-O7-C8
27	e	101	LMG	C7-C8-O7-C10
27	m	101	LMG	O9-C10-O7-C8
30	A	413	SQD	C5-C6-S-O7
30	A	413	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
30	A	413	SQD	C5-C6-S-O9
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	626	SQD	O5-C5-C6-S
30	a	401	SQD	C24-C23-O48-C46
30	a	415	SQD	C5-C6-S-O7
30	a	415	SQD	C5-C6-S-O8
30	a	415	SQD	C5-C6-S-O9
30	b	602	SQD	O5-C5-C6-S
30	d	402	SQD	C2-C1-O6-C44
30	d	402	SQD	O49-C7-O47-C45
30	d	402	SQD	C8-C7-O47-C45
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	O1D-CGD-O2D-CED
22	a	404	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
31	B	628	LMT	C3'-C4'-O1B-C1B
31	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	b	619	CLA	O1D-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	520	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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
27	E	101	LMG	O10-C28-O8-C9
30	A	414	SQD	O10-C23-O48-C46
30	a	401	SQD	O10-C23-O48-C46
25	b	624	DGD	C4D-C5D-C6D-O5D
23	A	406	PL9	C37-C38-C39-C40
23	a	409	PL9	C37-C38-C39-C40
27	l	101	LMG	C29-C28-O8-C9
30	F	103	SQD	C24-C23-O48-C46
30	f	103	SQD	C24-C23-O48-C46
22	B	608	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	O10-C28-O8-C9
27	C	518	LMG	O10-C28-O8-C9
27	D	407	LMG	O10-C28-O8-C9
27	D	408	LMG	O10-C28-O8-C9
27	d	407	LMG	O10-C28-O8-C9
27	d	408	LMG	O10-C28-O8-C9
27	e	101	LMG	O10-C28-O8-C9
27	l	101	LMG	O10-C28-O8-C9
30	F	103	SQD	O10-C23-O48-C46
30	f	103	SQD	O10-C23-O48-C46
22	C	510	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
31	B	627	LMT	C3'-C4'-O1B-C1B
22	B	601	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
31	b	603	LMT	C3'-C4'-O1B-C1B
25	D	409	DGD	O1B-C1B-O2G-C2G
25	d	409	DGD	O1B-C1B-O2G-C2G
27	A	415	LMG	O9-C10-O7-C8
27	B	621	LMG	O9-C10-O7-C8
27	D	407	LMG	O9-C10-O7-C8
27	I	101	LMG	O9-C10-O7-C8
27	a	402	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
27	b	625	LMG	O9-C10-O7-C8
27	d	407	LMG	O9-C10-O7-C8
27	i	101	LMG	O9-C10-O7-C8
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	406	CLA	C3-C5-C6-C7
22	b	611	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
22	B	612	CLA	O1D-CGD-O2D-CED
27	A	410	LMG	C29-C28-O8-C9
27	C	518	LMG	C29-C28-O8-C9
27	D	408	LMG	C29-C28-O8-C9
27	c	518	LMG	C29-C28-O8-C9
27	d	408	LMG	C29-C28-O8-C9
22	B	605	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
32	a	407	PHO	CBD-CGD-O2D-CED
25	B	625	DGD	C2B-C1B-O2G-C2G
25	C	516	DGD	C2B-C1B-O2G-C2G
25	b	601	DGD	C2B-C1B-O2G-C2G
25	c	516	DGD	C2B-C1B-O2G-C2G
27	M	101	LMG	C11-C10-O7-C8
27	m	101	LMG	C11-C10-O7-C8
22	B	602	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	b	616	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	C4-C3-C5-C6
22	D	404	CLA	C4-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
23	A	406	PL9	C30-C29-C31-C32
23	a	409	PL9	C30-C29-C31-C32
22	B	602	CLA	C2-C3-C5-C6
22	D	404	CLA	C2-C3-C5-C6
22	H	101	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
22	b	608	CLA	C2-C3-C5-C6
22	h	101	CLA	C2-C3-C5-C6
31	i	102	LMT	C3'-C4'-O1B-C1B
22	C	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED
22	C	520	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
27	I	101	LMG	O6-C5-C6-O5
27	i	101	LMG	O6-C5-C6-O5
22	b	610	CLA	C2A-CAA-CBA-CGA
32	d	401	PHO	C3-C5-C6-C7
31	I	102	LMT	C3'-C4'-O1B-C1B
25	D	409	DGD	C2A-C1A-O1G-C1G
27	C	521	LMG	C29-C28-O8-C9
27	D	407	LMG	C29-C28-O8-C9
27	c	522	LMG	C29-C28-O8-C9
27	d	407	LMG	C29-C28-O8-C9
23	J	101	PL9	C7-C8-C9-C10
23	j	101	PL9	C7-C8-C9-C10
25	B	620	DGD	C4D-C5D-C6D-O5D
23	A	406	PL9	C22-C23-C24-C26
23	J	101	PL9	C7-C8-C9-C11
23	a	409	PL9	C22-C23-C24-C26
23	j	101	PL9	C7-C8-C9-C11
25	A	408	DGD	O6E-C5E-C6E-O5E
25	B	620	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	O6E-C5E-C6E-O5E
25	D	409	DGD	O1A-C1A-O1G-C1G
25	d	409	DGD	O1A-C1A-O1G-C1G
27	e	101	LMG	O9-C10-O7-C8
25	a	411	DGD	O6E-C5E-C6E-O5E
25	C	516	DGD	C4E-C5E-C6E-O5E
25	c	516	DGD	C4E-C5E-C6E-O5E
22	c	505	CLA	O1D-CGD-O2D-CED
23	J	101	PL9	C27-C28-C29-C31
23	j	101	PL9	C27-C28-C29-C31
22	C	508	CLA	C3-C5-C6-C7
32	D	401	PHO	C3-C5-C6-C7
22	B	607	CLA	CBD-CGD-O2D-CED
32	D	402	PHO	CBD-CGD-O2D-CED
27	C	518	LMG	C8-C9-O8-C28
26	A	409	LHG	O2-C2-C3-O3
26	a	412	LHG	O2-C2-C3-O3
22	C	508	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
25	d	409	DGD	C2A-C1A-O1G-C1G
27	E	101	LMG	C29-C28-O8-C9
27	e	101	LMG	C29-C28-O8-C9
25	c	515	DGD	O6E-C5E-C6E-O5E
27	d	407	LMG	O6-C5-C6-O5
27	C	521	LMG	O10-C28-O8-C9
27	c	522	LMG	O10-C28-O8-C9
27	I	101	LMG	C4-C5-C6-O5
22	C	501	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	c	520	CLA	O1D-CGD-O2D-CED
25	b	624	DGD	C4E-C5E-C6E-O5E
27	i	101	LMG	C4-C5-C6-O5
25	D	409	DGD	C2B-C1B-O2G-C2G
25	d	409	DGD	C2B-C1B-O2G-C2G
27	A	415	LMG	C11-C10-O7-C8
27	D	408	LMG	C11-C10-O7-C8
27	a	402	LMG	C11-C10-O7-C8
27	d	408	LMG	C11-C10-O7-C8
30	F	103	SQD	C8-C7-O47-C45
30	f	103	SQD	C8-C7-O47-C45
22	B	613	CLA	O1D-CGD-O2D-CED
25	C	515	DGD	O6E-C5E-C6E-O5E
27	D	407	LMG	O6-C5-C6-O5
22	b	614	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	C3-C5-C6-C7
27	c	518	LMG	C8-C9-O8-C28
22	c	512	CLA	CBD-CGD-O2D-CED
25	B	620	DGD	C4E-C5E-C6E-O5E
22	B	610	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
32	D	401	PHO	CBA-CGA-O2A-C1
22	B	604	CLA	C4-C3-C5-C6
32	D	401	PHO	C4-C3-C5-C6
32	d	401	PHO	C4-C3-C5-C6
32	D	401	PHO	C2-C3-C5-C6
32	d	401	PHO	C2-C3-C5-C6
27	D	408	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
23	A	406	PL9	C24-C26-C27-C28
23	a	409	PL9	C24-C26-C27-C28
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	C2A-CAA-CBA-CGA
25	B	620	DGD	O6E-C1E-O5D-C6D
25	C	516	DGD	O6D-C1D-O3G-C3G
25	c	515	DGD	O6E-C1E-O5D-C6D
25	c	516	DGD	O6D-C1D-O3G-C3G
27	C	518	LMG	O6-C1-O1-C7
27	C	521	LMG	O6-C1-O1-C7
27	E	101	LMG	O6-C1-O1-C7
27	c	518	LMG	O6-C1-O1-C7
27	c	522	LMG	O6-C1-O1-C7
27	e	101	LMG	O6-C1-O1-C7
30	d	402	SQD	O5-C1-O6-C44
22	B	608	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
32	d	401	PHO	CBA-CGA-O2A-C1
22	B	611	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
25	C	516	DGD	O6E-C5E-C6E-O5E
27	c	518	LMG	O6-C5-C6-O5
32	D	401	PHO	O1A-CGA-O2A-C1
25	c	516	DGD	O6E-C5E-C6E-O5E
27	C	518	LMG	O6-C5-C6-O5
25	A	408	DGD	C4E-C5E-C6E-O5E
22	b	611	CLA	CBD-CGD-O2D-CED
27	i	101	LMG	C11-C10-O7-C8
25	a	411	DGD	C4E-C5E-C6E-O5E
25	c	515	DGD	C4E-C5E-C6E-O5E
22	B	615	CLA	O1A-CGA-O2A-C1
32	d	401	PHO	O1A-CGA-O2A-C1
22	b	619	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
27	C	518	LMG	C4-C5-C6-O5
22	B	606	CLA	O1D-CGD-O2D-CED
25	C	515	DGD	C4E-C5E-C6E-O5E
27	c	518	LMG	C4-C5-C6-O5
22	B	604	CLA	C2-C3-C5-C6
22	C	509	CLA	CBD-CGD-O2D-CED
22	B	607	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C14-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	b	613	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9
22	c	510	CLA	C6-C7-C8-C9
25	b	624	DGD	C2E-C1E-O5D-C6D
25	c	517	DGD	C2D-C1D-O3G-C3G
27	C	518	LMG	C2-C1-O1-C7
27	C	521	LMG	C2-C1-O1-C7
27	D	408	LMG	C2-C1-O1-C7
27	E	101	LMG	C2-C1-O1-C7
27	c	518	LMG	C2-C1-O1-C7
27	c	522	LMG	C2-C1-O1-C7
27	d	408	LMG	C2-C1-O1-C7
27	e	101	LMG	C2-C1-O1-C7
30	A	413	SQD	C2-C1-O6-C44
30	a	415	SQD	C2-C1-O6-C44
30	b	602	SQD	O10-C23-O48-C46
27	d	407	LMG	C4-C5-C6-O5
22	B	605	CLA	O1D-CGD-O2D-CED
24	H	102	BCR	C7-C8-C9-C34
24	H	102	BCR	C37-C22-C23-C24
24	y	101	BCR	C7-C8-C9-C34
24	g	101	BCR	C7-C8-C9-C34
24	B	617	BCR	C7-C8-C9-C10
24	b	621	BCR	C7-C8-C9-C10
22	b	605	CLA	C2A-CAA-CBA-CGA
27	C	518	LMG	C10-C11-C12-C13
22	b	619	CLA	O1A-CGA-O2A-C1
27	c	522	LMG	O6-C5-C6-O5
27	E	101	LMG	O9-C10-O7-C8
27	d	408	LMG	O9-C10-O7-C8
27	C	521	LMG	C11-C10-O7-C8
27	I	101	LMG	C11-C10-O7-C8
27	c	522	LMG	C11-C10-O7-C8
25	C	516	DGD	O2G-C2G-C3G-O3G
22	B	615	CLA	C5-C6-C7-C8
22	b	609	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	C15-C16-C17-C18
22	B	608	CLA	C13-C15-C16-C17
22	B	611	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	508	CLA	C5-C6-C7-C8
22	b	615	CLA	C5-C6-C7-C8
22	b	619	CLA	C5-C6-C7-C8
22	H	101	CLA	C3-C5-C6-C7
22	h	101	CLA	C3-C5-C6-C7
22	B	604	CLA	CBA-CGA-O2A-C1
22	b	612	CLA	C13-C15-C16-C17
25	d	409	DGD	C1B-C2B-C3B-C4B
27	A	415	LMG	C28-C29-C30-C31
32	a	407	PHO	O1D-CGD-O2D-CED
23	D	406	PL9	C29-C31-C32-C33
23	d	406	PL9	C29-C31-C32-C33
22	A	402	CLA	C3-C5-C6-C7
22	a	404	CLA	C3-C5-C6-C7
22	b	610	CLA	C15-C16-C17-C18
25	C	515	DGD	C1B-C2B-C3B-C4B
25	c	515	DGD	C1B-C2B-C3B-C4B
27	C	518	LMG	C28-C29-C30-C31
27	D	411	LMG	C10-C11-C12-C13
27	c	518	LMG	C10-C11-C12-C13
27	d	411	LMG	C10-C11-C12-C13
22	B	603	CLA	C13-C15-C16-C17
22	B	611	CLA	C13-C15-C16-C17
22	b	610	CLA	C13-C15-C16-C17
22	b	619	CLA	C10-C11-C12-C13
22	c	501	CLA	C15-C16-C17-C18
22	c	504	CLA	C10-C11-C12-C13
22	c	505	CLA	C5-C6-C7-C8
22	c	507	CLA	C10-C11-C12-C13
22	c	509	CLA	C15-C16-C17-C18
32	D	402	PHO	C15-C16-C17-C18
32	a	407	PHO	C15-C16-C17-C18
34	V	201	HEM	C2D-C3D-CAD-CBD
27	c	522	LMG	C4-C5-C6-O5
22	C	507	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
22	A	404	CLA	C10-C11-C12-C13
22	B	601	CLA	C13-C15-C16-C17
22	B	609	CLA	C8-C10-C11-C12
22	C	505	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	613	CLA	C8-C10-C11-C12
22	b	615	CLA	C13-C15-C16-C17
22	c	508	CLA	C5-C6-C7-C8
22	d	404	CLA	C13-C15-C16-C17
25	D	409	DGD	C1B-C2B-C3B-C4B
27	C	521	LMG	C10-C11-C12-C13
27	c	518	LMG	C28-C29-C30-C31
27	c	522	LMG	C10-C11-C12-C13
22	C	512	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	O1A-CGA-O2A-C1
25	C	515	DGD	O6E-C1E-O5D-C6D
25	b	624	DGD	O6E-C1E-O5D-C6D
27	A	415	LMG	O6-C1-O1-C7
27	I	101	LMG	O6-C1-O1-C7
27	a	402	LMG	O6-C1-O1-C7
27	i	101	LMG	O6-C1-O1-C7
30	A	413	SQD	O5-C1-O6-C44
30	a	415	SQD	O5-C1-O6-C44
22	B	606	CLA	C13-C15-C16-C17
22	B	615	CLA	C10-C11-C12-C13
22	C	503	CLA	C10-C11-C12-C13
22	C	505	CLA	C13-C15-C16-C17
22	C	509	CLA	C15-C16-C17-C18
22	C	520	CLA	C13-C15-C16-C17
22	D	404	CLA	C13-C15-C16-C17
22	D	404	CLA	C15-C16-C17-C18
22	b	607	CLA	C13-C15-C16-C17
22	c	503	CLA	C10-C11-C12-C13
22	c	507	CLA	C15-C16-C17-C18
22	c	520	CLA	C13-C15-C16-C17
22	c	520	CLA	C15-C16-C17-C18
22	d	404	CLA	C15-C16-C17-C18
27	i	101	LMG	C29-C28-O8-C9
22	C	512	CLA	O1A-CGA-O2A-C1
30	B	626	SQD	O10-C23-O48-C46
22	C	520	CLA	C15-C16-C17-C18
22	b	605	CLA	C13-C15-C16-C17
25	C	517	DGD	O1B-C1B-O2G-C2G
27	c	522	LMG	O9-C10-O7-C8
27	C	521	LMG	C4-C5-C6-O5
22	B	607	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	O1D-CGD-O2D-CED
22	A	404	CLA	C15-C16-C17-C18
22	C	501	CLA	C8-C10-C11-C12
22	C	501	CLA	C15-C16-C17-C18
22	a	406	CLA	C15-C16-C17-C18
22	b	614	CLA	C15-C16-C17-C18
22	c	501	CLA	C10-C11-C12-C13
22	c	505	CLA	C13-C15-C16-C17
27	C	521	LMG	O6-C5-C6-O5
27	D	407	LMG	C4-C5-C6-O5
27	B	621	LMG	C10-C11-C12-C13
27	a	402	LMG	C28-C29-C30-C31
27	b	625	LMG	C10-C11-C12-C13
22	A	403	CLA	C15-C16-C17-C18
22	B	610	CLA	C15-C16-C17-C18
22	C	506	CLA	C5-C6-C7-C8
22	C	507	CLA	C10-C11-C12-C13
22	C	507	CLA	C15-C16-C17-C18
22	a	405	CLA	C15-C16-C17-C18
22	c	506	CLA	C5-C6-C7-C8
22	C	511	CLA	CBA-CGA-O2A-C1
22	b	608	CLA	CBA-CGA-O2A-C1
30	b	602	SQD	C24-C23-O48-C46
22	c	509	CLA	CBD-CGD-O2D-CED
25	b	624	DGD	C1B-C2B-C3B-C4B
22	C	504	CLA	C10-C11-C12-C13
25	c	517	DGD	O1B-C1B-O2G-C2G
22	B	601	CLA	C2A-CAA-CBA-CGA
22	b	613	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	CBA-CGA-O2A-C1
22	c	520	CLA	CBA-CGA-O2A-C1
30	B	626	SQD	C24-C23-O48-C46
22	B	607	CLA	C5-C6-C7-C8
22	C	510	CLA	C5-C6-C7-C8
22	a	406	CLA	C10-C11-C12-C13
22	b	611	CLA	C5-C6-C7-C8
22	b	611	CLA	C15-C16-C17-C18
22	b	618	CLA	C13-C15-C16-C17
22	c	501	CLA	C8-C10-C11-C12
22	c	505	CLA	C15-C16-C17-C18
22	c	510	CLA	C5-C6-C7-C8
22	c	512	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	D	402	PHO	O1D-CGD-O2D-CED
22	C	512	CLA	C15-C16-C17-C18
22	b	619	CLA	C13-C15-C16-C17
27	D	411	LMG	O6-C5-C6-O5
22	B	607	CLA	C15-C16-C17-C18
22	B	612	CLA	C5-C6-C7-C8
22	B	614	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
23	j	101	PL9	C15-C14-C16-C17
22	c	512	CLA	O1D-CGD-O2D-CED
23	D	406	PL9	C27-C28-C29-C30
27	C	521	LMG	O9-C10-O7-C8
30	F	103	SQD	O49-C7-O47-C45
30	f	103	SQD	O49-C7-O47-C45
25	D	409	DGD	C2D-C1D-O3G-C3G
25	D	409	DGD	C2E-C1E-O5D-C6D
25	d	409	DGD	C2D-C1D-O3G-C3G
25	d	409	DGD	C2E-C1E-O5D-C6D
27	I	101	LMG	C2-C1-O1-C7
27	i	101	LMG	C2-C1-O1-C7
22	c	520	CLA	C10-C11-C12-C13
25	B	620	DGD	C1B-C2B-C3B-C4B
30	a	415	SQD	C7-C8-C9-C10
24	B	617	BCR	C7-C8-C9-C34
24	F	102	BCR	C37-C22-C23-C24
24	J	102	BCR	C37-C22-C23-C24
24	b	621	BCR	C7-C8-C9-C34
24	b	621	BCR	C37-C22-C23-C24
24	x	101	BCR	C37-C22-C23-C24
27	M	101	LMG	O6-C5-C6-O5
24	c	521	BCR	C7-C8-C9-C10
22	B	604	CLA	O1A-CGA-O2A-C1
22	A	402	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
22	c	520	CLA	C2A-CAA-CBA-CGA
22	C	501	CLA	C10-C11-C12-C13
22	b	616	CLA	C5-C6-C7-C8
27	c	518	LMG	C9-C8-O7-C10
22	B	615	CLA	C3-C5-C6-C7
22	b	619	CLA	C3-C5-C6-C7
22	C	520	CLA	C10-C11-C12-C13
24	H	102	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	J	102	BCR	C20-C21-C22-C23
24	j	102	BCR	C20-C21-C22-C23
24	x	101	BCR	C11-C10-C9-C8
25	D	409	DGD	O6E-C1E-O5D-C6D
27	D	407	LMG	O6-C1-O1-C7
27	d	407	LMG	O6-C1-O1-C7
25	b	624	DGD	O6D-C5D-C6D-O5D
22	C	520	CLA	CBA-CGA-O2A-C1
27	I	101	LMG	C29-C28-O8-C9
22	B	615	CLA	C13-C15-C16-C17
22	H	101	CLA	C5-C6-C7-C8
31	B	628	LMT	O1'-C1-C2-C3
22	c	508	CLA	C2-C1-O2A-CGA
22	b	616	CLA	C16-C17-C18-C19
22	b	608	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	O1A-CGA-O2A-C1
25	B	625	DGD	C5B-C6B-C7B-C8B
25	D	409	DGD	CCB-CDB-CEB-CFB
27	c	518	LMG	C29-C30-C31-C32
31	B	623	LMT	C1-C2-C3-C4
25	C	516	DGD	C2A-C3A-C4A-C5A
25	b	601	DGD	C5B-C6B-C7B-C8B
25	b	624	DGD	C3B-C4B-C5B-C6B
27	B	621	LMG	C31-C32-C33-C34
27	C	518	LMG	C29-C30-C31-C32
27	b	625	LMG	C31-C32-C33-C34
27	i	101	LMG	C12-C13-C14-C15
30	f	103	SQD	C12-C13-C14-C15
31	I	102	LMT	C6-C7-C8-C9
27	d	411	LMG	O6-C5-C6-O5
22	c	503	CLA	C5-C6-C7-C8
25	C	515	DGD	C3B-C4B-C5B-C6B
25	c	516	DGD	C4A-C5A-C6A-C7A
25	d	409	DGD	CCB-CDB-CEB-CFB
27	A	415	LMG	C30-C31-C32-C33
27	I	101	LMG	C12-C13-C14-C15
27	a	402	LMG	C30-C31-C32-C33
30	F	103	SQD	C12-C13-C14-C15
31	i	102	LMT	C6-C7-C8-C9
31	b	626	LMT	C1-C2-C3-C4
25	B	620	DGD	C3B-C4B-C5B-C6B
25	D	409	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
25	b	601	DGD	C9B-CAB-CBB-CCB
25	c	516	DGD	C2A-C3A-C4A-C5A
25	d	409	DGD	C4B-C5B-C6B-C7B
25	d	409	DGD	C5B-C6B-C7B-C8B
25	d	409	DGD	CEB-CFB-CGB-CHB
27	I	101	LMG	C14-C15-C16-C17
27	l	101	LMG	C33-C34-C35-C36
27	l	101	LMG	C34-C35-C36-C37
25	D	409	DGD	C5B-C6B-C7B-C8B
27	A	410	LMG	C33-C34-C35-C36
27	c	522	LMG	C12-C13-C14-C15
22	B	605	CLA	C4B-C3B-CAB-CBB
22	C	501	CLA	C4B-C3B-CAB-CBB
22	C	504	CLA	C4B-C3B-CAB-CBB
22	b	609	CLA	C4B-C3B-CAB-CBB
22	c	501	CLA	C4B-C3B-CAB-CBB
22	c	504	CLA	C4B-C3B-CAB-CBB
25	B	625	DGD	C9B-CAB-CBB-CCB
25	C	515	DGD	C2B-C3B-C4B-C5B
25	D	409	DGD	CEB-CFB-CGB-CHB
25	c	515	DGD	C3B-C4B-C5B-C6B
27	A	410	LMG	C34-C35-C36-C37
25	A	408	DGD	C8B-C9B-CAB-CBB
25	B	620	DGD	C7A-C8A-C9A-CAA
22	A	405	CLA	C10-C11-C12-C13
30	B	626	SQD	C8-C7-O47-C45
30	b	602	SQD	C8-C7-O47-C45
25	C	515	DGD	C3A-C4A-C5A-C6A
22	C	502	CLA	C11-C12-C13-C15
22	D	404	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
25	b	624	DGD	C6B-C7B-C8B-C9B
25	c	515	DGD	C3A-C4A-C5A-C6A
25	C	515	DGD	C1A-C2A-C3A-C4A
22	d	405	CLA	CBA-CGA-O2A-C1
22	C	503	CLA	C5-C6-C7-C8
25	B	620	DGD	C6B-C7B-C8B-C9B
27	A	415	LMG	C15-C16-C17-C18
30	B	626	SQD	C9-C10-C11-C12
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	C3A-C2A-CAA-CBA
22	b	611	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	611	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
27	D	407	LMG	C18-C19-C20-C21
27	d	407	LMG	C18-C19-C20-C21
27	i	101	LMG	C16-C17-C18-C19
31	b	604	LMT	O1'-C1-C2-C3
30	a	415	SQD	C14-C15-C16-C17
22	H	101	CLA	C13-C15-C16-C17
22	h	101	CLA	C5-C6-C7-C8
27	E	101	LMG	C28-C29-C30-C31
22	C	511	CLA	O1A-CGA-O2A-C1
22	c	520	CLA	O1A-CGA-O2A-C1
30	A	413	SQD	C14-C15-C16-C17
34	V	201	HEM	C4D-C3D-CAD-CBD
25	a	411	DGD	C8B-C9B-CAB-CBB
26	C	519	LHG	C24-C23-O8-C6
25	D	409	DGD	C7B-C8B-C9B-CAB
25	b	624	DGD	C7A-C8A-C9A-CAA
25	c	515	DGD	C2B-C3B-C4B-C5B
27	C	521	LMG	C12-C13-C14-C15
27	a	402	LMG	C18-C19-C20-C21
27	a	402	LMG	C32-C33-C34-C35
27	d	408	LMG	C14-C15-C16-C17
30	b	602	SQD	C11-C10-C9-C8
25	C	517	DGD	CBA-CCA-CDA-CEA
25	c	517	DGD	CBA-CCA-CDA-CEA
25	d	409	DGD	C7B-C8B-C9B-CAB
27	A	415	LMG	C18-C19-C20-C21
27	D	408	LMG	C14-C15-C16-C17
27	i	101	LMG	C14-C15-C16-C17
30	b	602	SQD	C9-C10-C11-C12
27	l	101	LMG	C4-C5-C6-O5
27	A	410	LMG	C30-C31-C32-C33
30	a	415	SQD	C27-C28-C29-C30
25	B	620	DGD	O6D-C5D-C6D-O5D
22	b	607	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	C	516	DGD	C4A-C5A-C6A-C7A
27	a	402	LMG	C15-C16-C17-C18
23	d	406	PL9	C27-C28-C29-C30
22	B	612	CLA	C16-C17-C18-C19
25	b	601	DGD	C1A-C2A-C3A-C4A
27	D	407	LMG	C28-C29-C30-C31
22	B	606	CLA	C2B-C3B-CAB-CBB
22	C	501	CLA	C2B-C3B-CAB-CBB
22	a	406	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C23-C24-C25-C30
24	C	514	BCR	C23-C24-C25-C26
24	C	514	BCR	C23-C24-C25-C30
24	H	102	BCR	C1-C6-C7-C8
24	H	102	BCR	C5-C6-C7-C8
24	y	101	BCR	C23-C24-C25-C26
24	y	101	BCR	C23-C24-C25-C30
24	b	621	BCR	C23-C24-C25-C30
24	c	514	BCR	C23-C24-C25-C26
24	c	514	BCR	C23-C24-C25-C30
24	g	101	BCR	C23-C24-C25-C26
24	g	101	BCR	C23-C24-C25-C30
24	x	101	BCR	C1-C6-C7-C8
24	x	101	BCR	C5-C6-C7-C8
25	c	517	DGD	C2B-C1B-O2G-C2G
27	m	101	LMG	C29-C28-O8-C9
22	B	603	CLA	C8-C10-C11-C12
22	C	511	CLA	C13-C15-C16-C17
22	A	403	CLA	C3-C5-C6-C7
27	A	415	LMG	C32-C33-C34-C35
27	A	410	LMG	C31-C32-C33-C34
27	D	407	LMG	C31-C32-C33-C34
27	I	101	LMG	C16-C17-C18-C19
27	l	101	LMG	C30-C31-C32-C33
30	B	626	SQD	C11-C10-C9-C8
22	B	605	CLA	C2A-CAA-CBA-CGA
22	a	404	CLA	C2A-CAA-CBA-CGA
25	c	517	DGD	C1A-C2A-C3A-C4A
26	a	412	LHG	C23-C24-C25-C26
27	d	407	LMG	C28-C29-C30-C31
27	e	101	LMG	C28-C29-C30-C31
30	A	413	SQD	C7-C8-C9-C10
30	A	413	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
30	F	103	SQD	C11-C12-C13-C14
22	C	520	CLA	O1A-CGA-O2A-C1
27	d	407	LMG	C31-C32-C33-C34
30	f	103	SQD	C11-C12-C13-C14
23	A	406	PL9	C33-C34-C36-C37
23	a	409	PL9	C33-C34-C36-C37
25	c	517	DGD	CAB-CBB-CCB-CDB
27	c	518	LMG	C34-C35-C36-C37
25	a	411	DGD	C1B-C2B-C3B-C4B
22	A	402	CLA	C11-C12-C13-C14
22	a	405	CLA	C6-C7-C8-C9
22	b	612	CLA	C6-C7-C8-C9
25	C	517	DGD	C9B-CAB-CBB-CCB
27	d	408	LMG	C19-C20-C21-C22
27	l	101	LMG	C31-C32-C33-C34
25	A	408	DGD	C5B-C6B-C7B-C8B
25	C	515	DGD	C4A-C5A-C6A-C7A
25	a	411	DGD	C5B-C6B-C7B-C8B
25	c	517	DGD	C9B-CAB-CBB-CCB
27	D	408	LMG	C19-C20-C21-C22
25	d	409	DGD	O6E-C1E-O5D-C6D
25	c	515	DGD	C4A-C5A-C6A-C7A
25	b	601	DGD	C2B-C3B-C4B-C5B
25	C	517	DGD	C1A-C2A-C3A-C4A
25	c	515	DGD	C1A-C2A-C3A-C4A
25	C	517	DGD	CAB-CBB-CCB-CDB
27	I	101	LMG	C13-C14-C15-C16
27	l	101	LMG	C14-C15-C16-C17
27	m	101	LMG	C29-C30-C31-C32
25	b	624	DGD	C4B-C5B-C6B-C7B
25	C	517	DGD	C2B-C1B-O2G-C2G
26	A	409	LHG	C8-C7-O7-C5
26	a	412	LHG	C8-C7-O7-C5
27	E	101	LMG	C11-C10-O7-C8
27	e	101	LMG	C11-C10-O7-C8
25	A	408	DGD	C1B-C2B-C3B-C4B
25	B	625	DGD	C1A-C2A-C3A-C4A
26	a	412	LHG	O9-C7-O7-C5
31	b	626	LMT	O1'-C1-C2-C3
27	C	518	LMG	C34-C35-C36-C37
27	D	411	LMG	C17-C18-C19-C20
22	d	405	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	j	102	BCR	C37-C22-C23-C24
25	b	601	DGD	C4A-C5A-C6A-C7A
27	D	408	LMG	C8-C7-O1-C1
27	d	408	LMG	C8-C7-O1-C1
22	C	520	CLA	C2A-CAA-CBA-CGA
22	B	601	CLA	C16-C17-C18-C20
22	B	612	CLA	C16-C17-C18-C20
22	b	616	CLA	C16-C17-C18-C20
25	B	625	DGD	C4A-C5A-C6A-C7A
27	c	518	LMG	C12-C13-C14-C15
27	c	518	LMG	C36-C37-C38-C39
27	d	408	LMG	C32-C33-C34-C35
31	B	628	LMT	C7-C8-C9-C10
22	c	512	CLA	C4-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
27	A	410	LMG	C14-C15-C16-C17
27	i	101	LMG	C13-C14-C15-C16
22	a	408	CLA	C10-C11-C12-C13
22	C	502	CLA	C3-C5-C6-C7
22	d	405	CLA	C15-C16-C17-C18
22	h	101	CLA	C13-C15-C16-C17
27	d	407	LMG	C30-C31-C32-C33
25	D	409	DGD	C3A-C4A-C5A-C6A
26	A	409	LHG	O9-C7-O7-C5
25	B	620	DGD	C4B-C5B-C6B-C7B
25	B	625	DGD	C2B-C3B-C4B-C5B
26	A	409	LHG	C25-C26-C27-C28
27	D	408	LMG	C13-C14-C15-C16
30	b	602	SQD	C11-C12-C13-C14
25	D	409	DGD	C6B-C7B-C8B-C9B
27	d	407	LMG	C36-C37-C38-C39
27	C	518	LMG	C12-C13-C14-C15
27	D	407	LMG	C36-C37-C38-C39
30	F	103	SQD	C10-C11-C12-C13
31	b	604	LMT	C7-C8-C9-C10
25	C	516	DGD	C1A-C2A-C3A-C4A
22	C	505	CLA	C10-C11-C12-C13
22	C	512	CLA	C13-C15-C16-C17
27	E	101	LMG	C15-C16-C17-C18
31	B	623	LMT	O1'-C1-C2-C3
27	I	101	LMG	O1-C7-C8-O7
27	M	101	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
27	i	101	LMG	O1-C7-C8-O7
27	m	101	LMG	O1-C7-C8-O7
30	A	413	SQD	O47-C45-C46-O48
30	A	414	SQD	O6-C44-C45-O47
30	a	401	SQD	O6-C44-C45-O47
30	a	415	SQD	O47-C45-C46-O48
25	d	409	DGD	C5A-C6A-C7A-C8A
26	a	412	LHG	C25-C26-C27-C28
27	D	408	LMG	C15-C16-C17-C18
25	C	515	DGD	C2A-C3A-C4A-C5A
25	b	624	DGD	C5B-C6B-C7B-C8B
25	d	409	DGD	C6B-C7B-C8B-C9B
27	B	621	LMG	C34-C35-C36-C37
27	M	101	LMG	C29-C30-C31-C32
27	d	411	LMG	C17-C18-C19-C20
30	B	622	SQD	C9-C10-C11-C12
22	D	405	CLA	C15-C16-C17-C18
27	E	101	LMG	O6-C5-C6-O5
25	B	620	DGD	C5B-C6B-C7B-C8B
27	D	408	LMG	C32-C33-C34-C35
27	D	411	LMG	C34-C35-C36-C37
27	e	101	LMG	C15-C16-C17-C18
30	B	626	SQD	C11-C12-C13-C14
25	c	516	DGD	CAB-CBB-CCB-CDB
27	D	407	LMG	C30-C31-C32-C33
30	d	402	SQD	C9-C10-C11-C12
27	e	101	LMG	O6-C5-C6-O5
27	l	101	LMG	O6-C5-C6-O5
27	m	101	LMG	O6-C5-C6-O5
23	d	406	PL9	C47-C48-C49-C51
25	D	409	DGD	C5A-C6A-C7A-C8A
27	d	408	LMG	C15-C16-C17-C18
22	C	509	CLA	C4-C3-C5-C6
22	c	509	CLA	C3-C5-C6-C7
25	C	516	DGD	CAB-CBB-CCB-CDB
22	c	501	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED
31	b	627	LMT	C2B-C1B-O1B-C4'
27	A	415	LMG	C31-C32-C33-C34
27	d	411	LMG	C34-C35-C36-C37
22	b	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C13-C15-C16-C17
27	d	408	LMG	C13-C14-C15-C16
31	I	102	LMT	C5'-C4'-O1B-C1B
26	A	409	LHG	C30-C31-C32-C33
22	c	505	CLA	C10-C11-C12-C13
22	C	509	CLA	C3-C5-C6-C7
22	c	502	CLA	C3-C5-C6-C7
26	a	412	LHG	C30-C31-C32-C33
27	C	518	LMG	C36-C37-C38-C39
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	b	619	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
22	c	512	CLA	C13-C15-C16-C17
27	A	410	LMG	C15-C16-C17-C18
26	C	519	LHG	C24-C25-C26-C27
25	D	409	DGD	C2A-C3A-C4A-C5A
25	d	409	DGD	C3A-C4A-C5A-C6A
27	D	407	LMG	C17-C18-C19-C20
25	c	516	DGD	C1A-C2A-C3A-C4A
22	B	605	CLA	C12-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7
22	C	503	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C10-C8-C7
22	H	101	CLA	C6-C7-C8-C10
22	b	606	CLA	C6-C7-C8-C10
22	b	618	CLA	C11-C10-C8-C7
22	b	618	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C10-C8-C7
22	c	510	CLA	C6-C7-C8-C10
22	d	404	CLA	C12-C13-C15-C16
22	h	101	CLA	C6-C7-C8-C10
32	D	402	PHO	C12-C13-C15-C16
32	a	407	PHO	C12-C13-C15-C16
22	b	605	CLA	C16-C17-C18-C20
22	B	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	625	DGD	O6D-C5D-C6D-O5D
25	c	515	DGD	C2A-C3A-C4A-C5A
22	c	509	CLA	C4-C3-C5-C6
23	a	409	PL9	C35-C34-C36-C37
22	c	509	CLA	C2-C3-C5-C6
23	D	406	PL9	C47-C48-C49-C51
31	B	624	LMT	C2B-C1B-O1B-C4'
25	d	409	DGD	CAB-CBB-CCB-CDB
26	c	519	LHG	C24-C25-C26-C27
30	b	602	SQD	C12-C13-C14-C15
22	A	405	CLA	C5-C6-C7-C8
22	a	408	CLA	C13-C15-C16-C17
22	b	605	CLA	C10-C11-C12-C13
22	a	405	CLA	C3-C5-C6-C7
22	C	501	CLA	C2A-CAA-CBA-CGA
22	B	602	CLA	C6-C7-C8-C9
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	C	510	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	b	609	CLA	C14-C13-C15-C16
22	c	502	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C9
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	d	404	CLA	C14-C13-C15-C16
31	i	102	LMT	C5'-C4'-O1B-C1B
25	D	409	DGD	CAB-CBB-CCB-CDB
25	d	409	DGD	C2A-C3A-C4A-C5A
25	A	408	DGD	C3B-C4B-C5B-C6B
30	f	103	SQD	C10-C11-C12-C13
22	C	509	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	CBA-CGA-O2A-C1
22	b	614	CLA	CBA-CGA-O2A-C1
22	c	508	CLA	CBA-CGA-O2A-C1
26	c	519	LHG	C24-C23-O8-C6
34	v	201	HEM	C4D-C3D-CAD-CBD
27	d	407	LMG	C2-C1-O1-C7
25	A	408	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
25	C	517	DGD	O1G-C1G-C2G-C3G
25	c	517	DGD	O1G-C1G-C2G-C3G
27	B	621	LMG	C7-C8-C9-O8
27	C	521	LMG	C7-C8-C9-O8
27	D	407	LMG	O1-C7-C8-C9
27	D	408	LMG	O1-C7-C8-C9
27	I	101	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
27	b	625	LMG	C7-C8-C9-O8
27	c	522	LMG	C7-C8-C9-O8
27	d	407	LMG	O1-C7-C8-C9
27	d	408	LMG	O1-C7-C8-C9
27	i	101	LMG	O1-C7-C8-C9
27	m	101	LMG	C7-C8-C9-O8
30	B	626	SQD	C44-C45-C46-O48
30	b	602	SQD	C44-C45-C46-O48
25	D	409	DGD	C8B-C9B-CAB-CBB
25	d	409	DGD	C8B-C9B-CAB-CBB
32	D	401	PHO	CBD-CGD-O2D-CED
27	d	407	LMG	C17-C18-C19-C20
30	B	626	SQD	C12-C13-C14-C15
26	c	519	LHG	O2-C2-C3-O3
27	d	411	LMG	C31-C32-C33-C34
22	C	508	CLA	CBA-CGA-O2A-C1
22	D	405	CLA	CBA-CGA-O2A-C1
22	c	504	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C29-C28-O8-C9
22	B	601	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C19
27	a	402	LMG	C31-C32-C33-C34
25	C	515	DGD	C4B-C5B-C6B-C7B
22	b	607	CLA	C15-C16-C17-C18
26	c	519	LHG	O10-C23-O8-C6
27	B	621	LMG	C13-C14-C15-C16
22	C	509	CLA	C2-C3-C5-C6
22	C	512	CLA	C2-C3-C5-C6
22	a	408	CLA	C5-C6-C7-C8
22	b	608	CLA	C15-C16-C17-C18
22	B	613	CLA	C16-C17-C18-C20
27	l	101	LMG	C15-C16-C17-C18
34	v	201	HEM	C2D-C3D-CAD-CBD
22	C	503	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	C8-C10-C11-C12
27	A	415	LMG	C17-C18-C19-C20
27	D	411	LMG	C31-C32-C33-C34
27	b	625	LMG	C34-C35-C36-C37
27	A	415	LMG	O6-C5-C6-O5
27	a	402	LMG	O6-C5-C6-O5
22	B	615	CLA	C15-C16-C17-C18
22	c	502	CLA	C13-C15-C16-C17
27	d	408	LMG	C28-C29-C30-C31
22	c	508	CLA	O1A-CGA-O2A-C1
22	C	504	CLA	CBA-CGA-O2A-C1
22	b	613	CLA	CBA-CGA-O2A-C1
25	D	409	DGD	C1G-C2G-O2G-C1B
25	d	409	DGD	C1G-C2G-O2G-C1B
27	E	101	LMG	C7-C8-O7-C10
27	C	521	LMG	C16-C17-C18-C19
27	c	522	LMG	C16-C17-C18-C19
25	C	516	DGD	O6D-C5D-C6D-O5D
25	c	516	DGD	O6D-C5D-C6D-O5D
25	A	408	DGD	C4B-C5B-C6B-C7B
25	c	515	DGD	C4B-C5B-C6B-C7B
25	a	411	DGD	C3B-C4B-C5B-C6B
25	a	411	DGD	C4B-C5B-C6B-C7B
25	c	517	DGD	C3B-C4B-C5B-C6B
25	D	409	DGD	CAA-CBA-CCA-CDA
25	C	517	DGD	C3B-C4B-C5B-C6B
27	D	407	LMG	C32-C33-C34-C35
30	a	415	SQD	C17-C18-C19-C20
23	D	406	PL9	C35-C34-C36-C37
23	d	406	PL9	C35-C34-C36-C37
25	B	625	DGD	C5A-C6A-C7A-C8A
22	C	511	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20
27	a	402	LMG	C17-C18-C19-C20
30	A	413	SQD	C17-C18-C19-C20
30	A	414	SQD	C10-C11-C12-C13
30	a	401	SQD	C10-C11-C12-C13
27	b	625	LMG	C28-C29-C30-C31
26	c	519	LHG	C25-C26-C27-C28
27	I	101	LMG	C18-C19-C20-C21
25	C	515	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
25	C	517	DGD	O1G-C1G-C2G-O2G
25	c	517	DGD	O1G-C1G-C2G-O2G
27	A	410	LMG	O1-C7-C8-O7
27	C	518	LMG	O1-C7-C8-O7
27	c	518	LMG	O1-C7-C8-O7
27	l	101	LMG	O1-C7-C8-O7
27	D	407	LMG	C15-C16-C17-C18
27	b	625	LMG	C13-C14-C15-C16
27	A	415	LMG	C11-C12-C13-C14
27	i	101	LMG	C18-C19-C20-C21
22	C	508	CLA	C2-C1-O2A-CGA
25	d	409	DGD	CDB-CEB-CFB-CGB
25	C	516	DGD	C4D-C5D-C6D-O5D
25	c	516	DGD	C4D-C5D-C6D-O5D
26	C	519	LHG	C11-C10-C9-C8
30	A	413	SQD	C10-C11-C12-C13
27	d	407	LMG	C32-C33-C34-C35
22	C	502	CLA	C13-C15-C16-C17
26	c	519	LHG	C11-C10-C9-C8
27	A	410	LMG	C4-C5-C6-O5
22	B	609	CLA	C16-C17-C18-C20
22	b	617	CLA	C16-C17-C18-C20
22	C	504	CLA	C4-C3-C5-C6
22	C	512	CLA	C4-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
23	A	406	PL9	C35-C34-C36-C37
23	D	406	PL9	C15-C14-C16-C17
23	d	406	PL9	C15-C14-C16-C17
23	d	406	PL9	C20-C19-C21-C22
25	d	409	DGD	CBA-CCA-CDA-CEA
27	b	625	LMG	C29-C28-O8-C9
22	B	601	CLA	C10-C11-C12-C13
22	c	504	CLA	C15-C16-C17-C18
25	D	409	DGD	CBA-CCA-CDA-CEA
22	A	403	CLA	C6-C7-C8-C9
22	B	605	CLA	C14-C13-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

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	C11-C10-C8-C9
22	D	404	CLA	C14-C13-C15-C16
22	a	404	CLA	C11-C12-C13-C14
22	b	606	CLA	C6-C7-C8-C9
22	b	618	CLA	C11-C10-C8-C9
22	b	618	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	C14-C13-C15-C16
22	c	510	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C14
32	D	402	PHO	C14-C13-C15-C16
32	a	407	PHO	C14-C13-C15-C16
25	D	409	DGD	CDB-CEB-CFB-CGB
22	b	617	CLA	C5-C6-C7-C8
22	b	614	CLA	O1A-CGA-O2A-C1
22	d	405	CLA	C4B-C3B-CAB-CBB
27	C	521	LMG	C17-C18-C19-C20
22	C	504	CLA	C15-C16-C17-C18
22	C	512	CLA	C2A-CAA-CBA-CGA
27	C	521	LMG	C34-C35-C36-C37
22	c	509	CLA	O1D-CGD-O2D-CED
27	D	407	LMG	C2-C1-O1-C7
27	e	101	LMG	C18-C19-C20-C21
27	i	101	LMG	C17-C18-C19-C20
22	C	511	CLA	C3-C5-C6-C7
27	l	101	LMG	C11-C10-O7-C8
27	D	407	LMG	C19-C20-C21-C22
27	E	101	LMG	C17-C18-C19-C20
27	I	101	LMG	C31-C32-C33-C34
27	E	101	LMG	O7-C10-C11-C12
22	B	602	CLA	C6-C7-C8-C10
22	B	607	CLA	C6-C7-C8-C10
22	B	609	CLA	C11-C12-C13-C15
22	B	612	CLA	C11-C12-C13-C15
22	C	502	CLA	C12-C13-C15-C16
22	C	504	CLA	C6-C7-C8-C10
22	C	504	CLA	C12-C13-C15-C16
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	509	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
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	C	511	CLA	C12-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C7
22	b	609	CLA	C12-C13-C15-C16
22	b	611	CLA	C6-C7-C8-C10
22	b	619	CLA	C12-C13-C15-C16
22	c	502	CLA	C12-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C10
22	c	504	CLA	C12-C13-C15-C16
22	c	505	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	510	CLA	C12-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C15
22	A	405	CLA	C13-C15-C16-C17
22	B	613	CLA	C15-C16-C17-C18
22	B	615	CLA	C8-C10-C11-C12
22	b	619	CLA	C15-C16-C17-C18
27	E	101	LMG	C19-C20-C21-C22
22	B	613	CLA	C16-C17-C18-C19
25	c	517	DGD	CFA-CGA-CHA-CIA
22	D	405	CLA	O1A-CGA-O2A-C1
30	b	602	SQD	C17-C18-C19-C20
22	A	402	CLA	C3A-C2A-CAA-CBA
22	a	404	CLA	C3A-C2A-CAA-CBA
27	d	411	LMG	C38-C39-C40-C41
27	d	407	LMG	C19-C20-C21-C22
27	d	407	LMG	C15-C16-C17-C18
22	B	610	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	O1A-CGA-O2A-C1
27	i	101	LMG	O10-C28-O8-C9
22	C	510	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	CBA-CGA-O2A-C1
22	B	609	CLA	C16-C17-C18-C19
22	b	613	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C19
22	b	608	CLA	C10-C11-C12-C13
24	B	617	BCR	C37-C22-C23-C24
27	D	411	LMG	C38-C39-C40-C41
27	e	101	LMG	C19-C20-C21-C22
22	c	504	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	c	522	LMG	C34-C35-C36-C37
31	B	624	LMT	O5B-C1B-O1B-C4'
22	b	619	CLA	C8-C10-C11-C12
23	J	101	PL9	C27-C28-C29-C30
31	b	603	LMT	C5'-C4'-O1B-C1B
25	B	625	DGD	C1G-C2G-C3G-O3G
25	C	516	DGD	C1G-C2G-C3G-O3G
25	D	409	DGD	C1G-C2G-C3G-O3G
25	c	516	DGD	C1G-C2G-C3G-O3G
25	d	409	DGD	C1G-C2G-C3G-O3G
27	A	410	LMG	O1-C7-C8-C9
27	C	518	LMG	O1-C7-C8-C9
27	c	518	LMG	O1-C7-C8-C9
27	l	101	LMG	O1-C7-C8-C9
27	m	101	LMG	O1-C7-C8-C9
30	A	413	SQD	C44-C45-C46-O48
30	A	414	SQD	O6-C44-C45-C46
30	a	401	SQD	O6-C44-C45-C46
22	c	511	CLA	C3-C5-C6-C7
27	a	402	LMG	C11-C12-C13-C14
27	c	522	LMG	C17-C18-C19-C20
22	C	511	CLA	C16-C17-C18-C19
22	B	613	CLA	C5-C6-C7-C8
22	b	617	CLA	C15-C16-C17-C18
25	c	516	DGD	C3A-C4A-C5A-C6A
25	d	409	DGD	C3B-C4B-C5B-C6B
22	c	508	CLA	C15-C16-C17-C18
27	d	407	LMG	C13-C14-C15-C16
30	a	415	SQD	C10-C11-C12-C13
25	b	601	DGD	O6D-C5D-C6D-O5D
27	D	411	LMG	C19-C20-C21-C22
22	c	504	CLA	C2-C3-C5-C6
22	b	613	CLA	O1A-CGA-O2A-C1
30	a	415	SQD	C31-C32-C33-C34
27	D	408	LMG	C28-C29-C30-C31
27	I	101	LMG	O10-C28-O8-C9
25	C	517	DGD	CFA-CGA-CHA-CIA
24	B	616	BCR	C1-C6-C7-C8
24	C	513	BCR	C1-C6-C7-C8
24	F	102	BCR	C1-C6-C7-C8
24	J	102	BCR	C1-C6-C7-C8
24	b	620	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	b	623	BCR	C23-C24-C25-C30
24	c	513	BCR	C1-C6-C7-C8
24	f	102	BCR	C1-C6-C7-C8
24	j	102	BCR	C1-C6-C7-C8
27	D	408	LMG	C29-C30-C31-C32
31	B	628	LMT	C2-C3-C4-C5
22	B	604	CLA	C5-C6-C7-C8
27	d	411	LMG	C19-C20-C21-C22
25	C	517	DGD	CDB-CEB-CFB-CGB
27	B	621	LMG	C17-C18-C19-C20
27	E	101	LMG	C18-C19-C20-C21
27	i	101	LMG	C31-C32-C33-C34
23	j	101	PL9	C27-C28-C29-C30
27	I	101	LMG	C17-C18-C19-C20
31	B	627	LMT	C5'-C4'-O1B-C1B
25	c	515	DGD	O2G-C2G-C3G-O3G
27	C	521	LMG	O7-C8-C9-O8
27	c	522	LMG	O7-C8-C9-O8
27	m	101	LMG	O7-C8-C9-O8
30	B	622	SQD	O6-C44-C45-O47
30	b	602	SQD	O47-C45-C46-O48
22	C	504	CLA	O1A-CGA-O2A-C1
23	A	406	PL9	C4-C3-C7-C8
23	a	409	PL9	C4-C3-C7-C8
22	C	504	CLA	C2-C3-C5-C6
25	D	409	DGD	C3B-C4B-C5B-C6B
22	B	608	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
22	b	612	CLA	C14-C13-C15-C16
32	d	401	PHO	C6-C7-C8-C9
26	C	519	LHG	C25-C26-C27-C28
30	A	413	SQD	C31-C32-C33-C34
31	b	627	LMT	O5B-C1B-O1B-C4'
30	B	626	SQD	C17-C18-C19-C20
25	d	409	DGD	CAA-CBA-CCA-CDA
27	b	625	LMG	C17-C18-C19-C20
22	b	617	CLA	C16-C17-C18-C19
27	C	518	LMG	C13-C14-C15-C16
27	d	408	LMG	C29-C30-C31-C32
27	e	101	LMG	C17-C18-C19-C20
25	C	516	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
25	d	409	DGD	C1A-C2A-C3A-C4A
26	A	409	LHG	C23-C24-C25-C26
27	A	410	LMG	C11-C10-O7-C8
22	B	604	CLA	C15-C16-C17-C18
22	B	609	CLA	C10-C11-C12-C13
22	C	508	CLA	C15-C16-C17-C18
30	A	413	SQD	C15-C16-C17-C18
22	C	510	CLA	O1A-CGA-O2A-C1
22	a	405	CLA	C5-C6-C7-C8
25	c	516	DGD	C4B-C5B-C6B-C7B
22	A	403	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	608	CLA	C12-C13-C15-C16
22	B	610	CLA	C11-C10-C8-C7
22	B	615	CLA	C11-C10-C8-C7
22	B	615	CLA	C12-C13-C15-C16
22	C	501	CLA	C11-C12-C13-C15
22	H	101	CLA	C11-C10-C8-C7
22	a	405	CLA	C12-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C10
22	b	606	CLA	C11-C12-C13-C15
22	b	612	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C7
22	b	616	CLA	C11-C12-C13-C15
22	b	619	CLA	C11-C10-C8-C7
22	c	501	CLA	C11-C12-C13-C15
22	c	507	CLA	C12-C13-C15-C16
22	c	511	CLA	C12-C13-C15-C16
30	b	602	SQD	C10-C11-C12-C13
25	C	516	DGD	C4B-C5B-C6B-C7B
24	J	102	BCR	C7-C8-C9-C10
24	c	514	BCR	C7-C8-C9-C10
27	A	410	LMG	C8-C7-O1-C1
27	l	101	LMG	C8-C7-O1-C1
30	B	622	SQD	C45-C44-O6-C1
30	B	622	SQD	C5-C6-S-O8
30	d	402	SQD	C45-C44-O6-C1
30	d	402	SQD	C5-C6-S-O8
22	B	604	CLA	C10-C11-C12-C13
22	C	511	CLA	C5-C6-C7-C8
32	d	401	PHO	C5-C6-C7-C8
22	B	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	d	408	LMG	C36-C37-C38-C39
30	A	414	SQD	C32-C33-C34-C35
23	D	406	PL9	C20-C19-C21-C22
22	c	510	CLA	O1A-CGA-O2A-C1
26	C	519	LHG	O10-C23-O8-C6
27	A	410	LMG	C8-C9-O8-C28
30	a	415	SQD	C15-C16-C17-C18
30	F	103	SQD	C29-C30-C31-C32
27	c	518	LMG	C13-C14-C15-C16
32	d	401	PHO	CBD-CGD-O2D-CED
25	b	601	DGD	C4E-C5E-C6E-O5E
25	c	517	DGD	CDB-CEB-CFB-CGB
22	c	501	CLA	C13-C15-C16-C17
25	b	601	DGD	C5A-C6A-C7A-C8A
30	b	602	SQD	O49-C7-O47-C45
27	D	407	LMG	C13-C14-C15-C16
22	C	506	CLA	O1D-CGD-O2D-CED
25	a	411	DGD	C1G-C2G-C3G-O3G
25	b	601	DGD	C1G-C2G-C3G-O3G
27	M	101	LMG	O1-C7-C8-C9
30	a	415	SQD	C44-C45-C46-O48
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
30	f	103	SQD	C29-C30-C31-C32
22	b	608	CLA	C5-C6-C7-C8
27	e	101	LMG	O7-C10-C11-C12
25	d	409	DGD	C2B-C3B-C4B-C5B
25	D	409	DGD	C4E-C5E-C6E-O5E
27	A	410	LMG	C20-C21-C22-C23
25	A	408	DGD	O2G-C2G-C3G-O3G
27	B	621	LMG	O7-C8-C9-O8
27	M	101	LMG	O7-C8-C9-O8
30	B	626	SQD	O47-C45-C46-O48
30	d	402	SQD	O6-C44-C45-O47
22	A	403	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
22	C	501	CLA	C11-C12-C13-C14
22	C	507	CLA	C14-C13-C15-C16
22	C	511	CLA	C14-C13-C15-C16
22	D	404	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	C11-C12-C13-C14
22	b	616	CLA	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
22	B	603	CLA	CBA-CGA-O2A-C1
25	C	515	DGD	C5A-C6A-C7A-C8A
25	d	409	DGD	C4A-C5A-C6A-C7A
27	D	407	LMG	C20-C21-C22-C23
27	d	407	LMG	C20-C21-C22-C23
27	m	101	LMG	C30-C31-C32-C33
27	A	410	LMG	O6-C5-C6-O5
22	c	507	CLA	C5-C6-C7-C8
22	c	511	CLA	C5-C6-C7-C8
22	b	613	CLA	C10-C11-C12-C13
32	D	401	PHO	C5-C6-C7-C8
31	b	604	LMT	C2-C3-C4-C5
26	c	519	LHG	C1-C2-C3-O3
22	b	615	CLA	C10-C11-C12-C13
22	a	406	CLA	C5-C6-C7-C8
22	c	506	CLA	O1D-CGD-O2D-CED
27	B	621	LMG	C28-C29-C30-C31
27	C	521	LMG	C35-C36-C37-C38
22	c	506	CLA	C3-C5-C6-C7
24	j	102	BCR	C18-C19-C20-C21
32	D	401	PHO	O1D-CGD-O2D-CED
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	520	CLA	C4B-C3B-CAB-CBB
22	D	404	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C4B-C3B-CAB-CBB
22	c	508	CLA	C4B-C3B-CAB-CBB
22	c	520	CLA	C4B-C3B-CAB-CBB
22	B	614	CLA	CBA-CGA-O2A-C1
27	l	101	LMG	C20-C21-C22-C23
23	J	101	PL9	C15-C14-C16-C17
22	A	404	CLA	C5-C6-C7-C8
24	C	514	BCR	C7-C8-C9-C10
24	x	101	BCR	C7-C8-C9-C10
27	C	518	LMG	C32-C33-C34-C35
30	B	626	SQD	C10-C11-C12-C13
26	C	519	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
30	A	414	SQD	C9-C10-C11-C12
30	B	626	SQD	O49-C7-O47-C45
22	b	609	CLA	C13-C15-C16-C17
22	A	405	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	B	609	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	C	505	CLA	C11-C12-C13-C15
22	C	508	CLA	C6-C7-C8-C10
22	C	520	CLA	C6-C7-C8-C10
22	D	405	CLA	C11-C10-C8-C7
22	b	611	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C12-C13-C15
22	b	613	CLA	C12-C13-C15-C16
22	b	616	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
22	c	520	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C10-C8-C7
22	h	101	CLA	C11-C10-C8-C7
32	a	407	PHO	C6-C7-C8-C10
25	b	624	DGD	C5A-C6A-C7A-C8A
22	A	403	CLA	C5-C6-C7-C8
22	B	609	CLA	C5-C6-C7-C8
22	b	618	CLA	CBA-CGA-O2A-C1
25	c	515	DGD	C5B-C6B-C7B-C8B
25	D	409	DGD	C2B-C3B-C4B-C5B
22	B	611	CLA	C4-C3-C5-C6
22	b	615	CLA	C4-C3-C5-C6
23	d	406	PL9	C13-C14-C16-C17
26	C	519	LHG	O6-C4-C5-O7
26	c	519	LHG	O6-C4-C5-O7
22	B	604	CLA	C11-C10-C8-C9
22	B	610	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	a	405	CLA	C14-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	b	619	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	C11-C12-C13-C14
25	D	409	DGD	C1A-C2A-C3A-C4A
25	c	515	DGD	C5A-C6A-C7A-C8A
30	d	402	SQD	C10-C11-C12-C13
30	d	402	SQD	O5-C5-C6-S
27	A	410	LMG	C38-C39-C40-C41
32	D	402	PHO	C10-C11-C12-C13
30	a	401	SQD	C32-C33-C34-C35
22	B	603	CLA	O1A-CGA-O2A-C1
25	D	409	DGD	O2G-C2G-C3G-O3G
25	a	411	DGD	O2G-C2G-C3G-O3G
25	d	409	DGD	O2G-C2G-C3G-O3G
27	e	101	LMG	O1-C7-C8-C9
30	B	622	SQD	O6-C44-C45-C46
32	D	402	PHO	C13-C15-C16-C17
25	B	625	DGD	C4E-C5E-C6E-O5E
25	D	409	DGD	C4A-C5A-C6A-C7A
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	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	C5-C6-C7-C8
32	a	407	PHO	C13-C15-C16-C17
27	A	415	LMG	C12-C13-C14-C15
22	B	614	CLA	O1A-CGA-O2A-C1
25	B	620	DGD	O1A-C1A-O1G-C1G
22	B	611	CLA	C10-C11-C12-C13
22	C	508	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	C2A-CAA-CBA-CGA
27	b	625	LMG	C12-C13-C14-C15
25	B	620	DGD	C5A-C6A-C7A-C8A
22	B	608	CLA	CAD-CBD-CGD-O1D
22	B	612	CLA	CHA-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	612	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
26	A	409	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
26	C	519	LHG	C3-O3-P-O5
26	C	519	LHG	C4-O6-P-O5
26	a	412	LHG	C3-O3-P-O5
26	c	519	LHG	C3-O3-P-O5
26	c	519	LHG	C4-O6-P-O5
27	d	408	LMG	C31-C32-C33-C34
22	b	618	CLA	O1A-CGA-O2A-C1
22	B	610	CLA	C4-C3-C5-C6
22	a	405	CLA	C4-C3-C5-C6
22	B	601	CLA	C2B-C3B-CAB-CBB
22	B	605	CLA	C2B-C3B-CAB-CBB
22	C	504	CLA	C2B-C3B-CAB-CBB
22	C	520	CLA	C2B-C3B-CAB-CBB
22	b	605	CLA	C2B-C3B-CAB-CBB
22	b	609	CLA	C2B-C3B-CAB-CBB
22	c	501	CLA	C2B-C3B-CAB-CBB
22	c	504	CLA	C2B-C3B-CAB-CBB
22	c	520	CLA	C2B-C3B-CAB-CBB
30	a	415	SQD	C11-C10-C9-C8
24	b	623	BCR	C7-C8-C9-C34
26	A	409	LHG	C2-C3-O3-P
27	l	101	LMG	C16-C17-C18-C19
22	C	506	CLA	C3-C5-C6-C7
25	c	516	DGD	C6A-C7A-C8A-C9A
27	D	408	LMG	C31-C32-C33-C34
27	c	522	LMG	C35-C36-C37-C38
27	A	410	LMG	C29-C30-C31-C32
25	C	517	DGD	C3G-C2G-O2G-C1B
25	c	517	DGD	C3G-C2G-O2G-C1B
26	a	412	LHG	C6-C5-O7-C7
27	m	101	LMG	C9-C8-O7-C10
27	l	101	LMG	C29-C30-C31-C32
30	a	401	SQD	C9-C10-C11-C12
22	c	504	CLA	C8-C10-C11-C12
23	D	406	PL9	C13-C14-C16-C17
25	d	409	DGD	C4E-C5E-C6E-O5E
27	c	518	LMG	C32-C33-C34-C35
22	A	405	CLA	C16-C17-C18-C19
22	a	408	CLA	C16-C17-C18-C19
22	B	612	CLA	C10-C11-C12-C13
32	a	407	PHO	C10-C11-C12-C13
26	c	519	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	C11-C12-C13-C14
22	B	607	CLA	C11-C12-C13-C14
22	B	609	CLA	C11-C12-C13-C14
22	B	614	CLA	C6-C7-C8-C9
22	b	605	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	c	507	CLA	C14-C13-C15-C16
22	c	510	CLA	C11-C10-C8-C9
22	d	404	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C15
22	b	605	CLA	C6-C7-C8-C10
26	c	519	LHG	C7-C8-C9-C10
27	B	621	LMG	C12-C13-C14-C15
22	b	616	CLA	C10-C11-C12-C13
27	b	625	LMG	C15-C16-C17-C18
27	A	410	LMG	C35-C36-C37-C38
22	B	605	CLA	O1A-CGA-O2A-C1
26	a	412	LHG	C2-C3-O3-P
27	D	408	LMG	O1-C7-C8-O7
27	b	625	LMG	O7-C8-C9-O8
27	d	408	LMG	O1-C7-C8-O7
22	C	511	CLA	CAA-CBA-CGA-O2A
22	c	511	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	CBA-CGA-O2A-C1
22	h	101	CLA	CBA-CGA-O2A-C1
27	a	402	LMG	C16-C17-C18-C19
30	d	402	SQD	O6-C44-C45-C46
31	b	603	LMT	C4'-C5'-C6'-O6'
22	c	510	CLA	C3-C5-C6-C7
30	f	103	SQD	C24-C25-C26-C27
24	B	619	BCR	C7-C8-C9-C34
22	B	602	CLA	C16-C17-C18-C19
30	a	401	SQD	C12-C13-C14-C15
24	j	102	BCR	C7-C8-C9-C10
25	B	625	DGD	C2G-C3G-O3G-C1D
25	b	601	DGD	C2G-C3G-O3G-C1D
27	D	411	LMG	C8-C7-O1-C1
32	d	401	PHO	O1D-CGD-O2D-CED
25	B	620	DGD	CAB-CBB-CCB-CDB
22	b	609	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	l	101	LMG	C10-C11-C12-C13
27	l	101	LMG	C11-C12-C13-C14
22	A	403	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
30	a	401	SQD	C26-C27-C28-C29
22	A	404	CLA	C6-C7-C8-C9
22	A	405	CLA	C11-C10-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	615	CLA	C14-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C14
22	C	510	CLA	C11-C10-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	b	619	CLA	C14-C13-C15-C16
22	c	505	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	c	520	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C10-C8-C9
32	D	402	PHO	C11-C10-C8-C9
32	a	407	PHO	C11-C10-C8-C9
22	B	609	CLA	O1A-CGA-O2A-C1
27	D	407	LMG	C16-C17-C18-C19
30	B	622	SQD	C10-C11-C12-C13
22	A	403	CLA	C4B-C3B-CAB-CBB
25	c	516	DGD	C7B-C8B-C9B-CAB
34	F	101	HEM	C3D-CAD-CBD-CGD
34	f	101	HEM	C3D-CAD-CBD-CGD
22	b	606	CLA	C16-C17-C18-C19
22	b	607	CLA	CBA-CGA-O2A-C1
31	b	627	LMT	O5'-C5'-C6'-O6'
22	h	101	CLA	O1A-CGA-O2A-C1
27	M	101	LMG	C31-C32-C33-C34
22	B	610	CLA	C2-C3-C5-C6
25	B	625	DGD	C2A-C3A-C4A-C5A
22	A	405	CLA	C16-C17-C18-C20
27	A	415	LMG	C16-C17-C18-C19
30	F	103	SQD	C24-C25-C26-C27
22	C	506	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C10-C8-C7
22	H	101	CLA	C12-C13-C15-C16
22	c	505	CLA	C11-C10-C8-C7
25	b	624	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
27	D	411	LMG	C16-C17-C18-C19
25	c	517	DGD	C8B-C9B-CAB-CBB
22	a	408	CLA	C16-C17-C18-C20
22	b	607	CLA	O1A-CGA-O2A-C1
22	C	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
27	A	410	LMG	C11-C12-C13-C14
27	A	410	LMG	C16-C17-C18-C19
27	E	101	LMG	C31-C32-C33-C34
27	l	101	LMG	C35-C36-C37-C38
22	B	611	CLA	C2-C3-C5-C6
22	b	615	CLA	C2-C3-C5-C6
23	D	406	PL9	C32-C33-C34-C36
24	b	621	BCR	C20-C21-C22-C37
25	c	515	DGD	O6D-C1D-O3G-C3G
27	A	410	LMG	O6-C1-O1-C7
22	B	602	CLA	C15-C16-C17-C18
25	b	601	DGD	O6E-C5E-C6E-O5E
27	c	522	LMG	C32-C33-C34-C35
27	e	101	LMG	C31-C32-C33-C34
27	c	522	LMG	C30-C31-C32-C33
22	a	405	CLA	C2-C1-O2A-CGA
24	f	102	BCR	C7-C8-C9-C34
22	C	507	CLA	C5-C6-C7-C8
22	b	616	CLA	C8-C10-C11-C12
31	D	410	LMT	O5'-C5'-C6'-O6'
27	d	407	LMG	C16-C17-C18-C19
22	b	617	CLA	C2C-C3C-CAC-CBC
27	l	101	LMG	C8-C9-O8-C28
27	d	411	LMG	O1-C7-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	C	506	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	b	618	CLA	C6-C7-C8-C9
22	b	619	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C10-C8-C9
32	D	401	PHO	C6-C7-C8-C9
22	c	509	CLA	C16-C17-C18-C19
30	A	414	SQD	C12-C13-C14-C15
25	C	516	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
25	b	624	DGD	CAB-CBB-CCB-CDB
26	A	409	LHG	C6-C5-O7-C7
26	a	412	LHG	C4-C5-O7-C7
27	M	101	LMG	C9-C8-O7-C10
22	B	605	CLA	C13-C15-C16-C17
25	C	517	DGD	C4A-C5A-C6A-C7A
22	B	612	CLA	C13-C15-C16-C17
25	C	515	DGD	C5B-C6B-C7B-C8B
25	C	517	DGD	C8B-C9B-CAB-CBB
27	D	407	LMG	C29-C30-C31-C32
27	d	407	LMG	C29-C30-C31-C32
30	A	413	SQD	C11-C10-C9-C8
22	B	612	CLA	C8-C10-C11-C12
22	b	606	CLA	C15-C16-C17-C18
22	c	512	CLA	C1A-C2A-CAA-CBA
27	C	521	LMG	C30-C31-C32-C33
31	D	410	LMT	O5B-C5B-C6B-O6B
27	D	408	LMG	C18-C19-C20-C21
27	D	408	LMG	C36-C37-C38-C39
22	B	604	CLA	C2B-C3B-CAB-CBB
22	C	508	CLA	C2B-C3B-CAB-CBB
22	c	508	CLA	C2B-C3B-CAB-CBB
22	d	405	CLA	C2B-C3B-CAB-CBB
24	A	407	BCR	C1-C6-C7-C8
24	B	616	BCR	C5-C6-C7-C8
24	B	619	BCR	C1-C6-C7-C8
24	B	619	BCR	C23-C24-C25-C30
24	C	513	BCR	C5-C6-C7-C8
24	C	513	BCR	C23-C24-C25-C30
24	F	102	BCR	C5-C6-C7-C8
24	J	102	BCR	C5-C6-C7-C8
24	a	410	BCR	C1-C6-C7-C8
24	a	410	BCR	C23-C24-C25-C30
24	b	620	BCR	C5-C6-C7-C8
24	b	623	BCR	C1-C6-C7-C8
24	b	623	BCR	C23-C24-C25-C26
24	c	513	BCR	C5-C6-C7-C8
24	c	513	BCR	C23-C24-C25-C30
24	f	102	BCR	C5-C6-C7-C8
24	j	102	BCR	C5-C6-C7-C8
25	b	601	DGD	C2A-C3A-C4A-C5A
22	C	510	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	D	406	PL9	C40-C39-C41-C42
22	b	614	CLA	C2-C3-C5-C6
27	A	410	LMG	C10-C11-C12-C13
22	A	404	CLA	C6-C7-C8-C10
22	B	601	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C12-C13-C15
22	D	404	CLA	C11-C10-C8-C7
22	a	408	CLA	C11-C10-C8-C7
22	b	605	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C12-C13-C15
22	c	508	CLA	C6-C7-C8-C10
22	c	510	CLA	C11-C10-C8-C7
22	d	404	CLA	C11-C10-C8-C7
22	h	101	CLA	C12-C13-C15-C16
32	D	402	PHO	C6-C7-C8-C10
32	D	402	PHO	C11-C10-C8-C7
32	a	407	PHO	C11-C10-C8-C7
27	D	411	LMG	C36-C37-C38-C39
30	A	413	SQD	C16-C17-C18-C19
22	B	602	CLA	C16-C17-C18-C20
23	D	406	PL9	C24-C26-C27-C28
23	d	406	PL9	C24-C26-C27-C28
22	c	503	CLA	C15-C16-C17-C18
25	d	409	DGD	CBB-CCB-CDB-CEB
27	M	101	LMG	C30-C31-C32-C33
22	H	101	CLA	CBA-CGA-O2A-C1
27	d	411	LMG	C16-C17-C18-C19
25	D	409	DGD	CBB-CCB-CDB-CEB
22	B	607	CLA	C13-C15-C16-C17
22	C	504	CLA	C8-C10-C11-C12
32	d	401	PHO	C2-C1-O2A-CGA
22	C	501	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C19
27	B	621	LMG	C29-C28-O8-C9
25	A	408	DGD	C2A-C3A-C4A-C5A
30	F	103	SQD	C9-C10-C11-C12
22	B	601	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
30	a	415	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	a	402	LMG	C12-C13-C14-C15
22	B	604	CLA	C8-C10-C11-C12
22	c	510	CLA	C4-C3-C5-C6
22	c	510	CLA	C2-C3-C5-C6
27	l	101	LMG	C38-C39-C40-C41
27	m	101	LMG	C31-C32-C33-C34
27	D	408	LMG	C34-C35-C36-C37
27	m	101	LMG	C17-C18-C19-C20
27	D	411	LMG	O1-C7-C8-C9
22	H	101	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	C2A-CAA-CBA-CGA
25	d	409	DGD	C8A-C9A-CAA-CBA
27	B	621	LMG	C15-C16-C17-C18
30	a	401	SQD	C17-C18-C19-C20
31	B	624	LMT	C6-C7-C8-C9
22	B	604	CLA	C4B-C3B-CAB-CBB
22	B	614	CLA	C4B-C3B-CAB-CBB
22	D	405	CLA	C4B-C3B-CAB-CBB
25	B	620	DGD	C7B-C8B-C9B-CAB
25	D	409	DGD	C8A-C9A-CAA-CBA
22	b	606	CLA	C16-C17-C18-C20
22	c	509	CLA	C16-C17-C18-C20
25	B	625	DGD	CAB-CBB-CCB-CDB
25	b	624	DGD	O1A-C1A-O1G-C1G
22	b	617	CLA	C4C-C3C-CAC-CBC
22	B	613	CLA	C2C-C3C-CAC-CBC
27	b	625	LMG	O1-C7-C8-O7
27	d	411	LMG	O1-C7-C8-O7
27	D	407	LMG	C10-C11-C12-C13
22	B	601	CLA	C12-C13-C15-C16
22	b	608	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C10-C8-C7
27	M	101	LMG	C16-C17-C18-C19
22	A	403	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	a	405	CLA	C11-C10-C8-C9
22	b	611	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C12-C13-C14
22	c	509	CLA	C11-C10-C8-C9
32	a	407	PHO	C6-C7-C8-C9
25	B	620	DGD	CCA-CDA-CEA-CFA
27	d	411	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA
22	b	613	CLA	C2-C1-O2A-CGA
22	b	616	CLA	C2-C1-O2A-CGA
32	D	401	PHO	C2-C1-O2A-CGA
23	d	406	PL9	C32-C33-C34-C36
22	C	501	CLA	C16-C17-C18-C19
22	C	520	CLA	C3A-C2A-CAA-CBA
22	D	404	CLA	C3A-C2A-CAA-CBA
34	v	201	HEM	CAA-CBA-CGA-O2A
22	C	510	CLA	C2-C3-C5-C6
22	a	405	CLA	C2-C3-C5-C6
27	e	101	LMG	C30-C31-C32-C33
27	C	518	LMG	C17-C18-C19-C20
27	C	521	LMG	C32-C33-C34-C35
26	A	409	LHG	C4-C5-O7-C7
27	d	411	LMG	C11-C12-C13-C14
24	J	102	BCR	C18-C19-C20-C21
25	a	411	DGD	C2A-C3A-C4A-C5A
22	b	609	CLA	CBA-CGA-O2A-C1
25	c	517	DGD	CBB-CCB-CDB-CEB
22	C	509	CLA	C16-C17-C18-C19
25	b	601	DGD	O6D-C1D-O3G-C3G
22	c	502	CLA	CBA-CGA-O2A-C1
25	C	515	DGD	C1G-C2G-C3G-O3G
27	C	518	LMG	C7-C8-C9-O8
27	E	101	LMG	O1-C7-C8-C9
27	c	518	LMG	C7-C8-C9-O8
25	D	409	DGD	O6E-C5E-C6E-O5E
22	c	502	CLA	O1A-CGA-O2A-C1
27	m	101	LMG	O10-C28-O8-C9
30	a	415	SQD	C16-C17-C18-C19
22	A	405	CLA	C4-C3-C5-C6
22	D	405	CLA	C2A-CAA-CBA-CGA
22	d	405	CLA	C2A-CAA-CBA-CGA
26	C	519	LHG	O7-C7-C8-C9
22	b	611	CLA	C13-C15-C16-C17
22	b	616	CLA	C13-C15-C16-C17
22	b	609	CLA	O1A-CGA-O2A-C1
25	B	625	DGD	O6E-C5E-C6E-O5E
22	d	404	CLA	CAA-CBA-CGA-O2A
26	c	519	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	B	621	LMG	O1-C7-C8-O7
27	e	101	LMG	O1-C7-C8-O7
22	C	512	CLA	C14-C13-C15-C16
22	C	520	CLA	C6-C7-C8-C9
22	H	101	CLA	C11-C12-C13-C14
22	h	101	CLA	C11-C10-C8-C9
24	F	102	BCR	C21-C22-C23-C24
24	H	102	BCR	C7-C8-C9-C10
27	A	410	LMG	C17-C18-C19-C20
22	C	508	CLA	C10-C11-C12-C13
22	B	612	CLA	CAA-CBA-CGA-O2A
27	l	101	LMG	O7-C10-C11-C12
22	B	601	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C12-C13-C15
22	c	509	CLA	C11-C10-C8-C7
22	c	512	CLA	C11-C10-C8-C7
22	c	512	CLA	C12-C13-C15-C16
30	f	103	SQD	C9-C10-C11-C12
22	B	614	CLA	C2B-C3B-CAB-CBB
22	D	405	CLA	C2B-C3B-CAB-CBB
22	b	608	CLA	C2B-C3B-CAB-CBB
24	A	407	BCR	C5-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C26
24	A	407	BCR	C23-C24-C25-C30
24	B	619	BCR	C5-C6-C7-C8
24	C	513	BCR	C23-C24-C25-C26
24	C	514	BCR	C1-C6-C7-C8
24	K	102	BCR	C1-C6-C7-C8
24	K	102	BCR	C23-C24-C25-C30
24	a	410	BCR	C5-C6-C7-C8
24	a	410	BCR	C23-C24-C25-C26
24	b	623	BCR	C5-C6-C7-C8
24	c	513	BCR	C23-C24-C25-C26
24	c	514	BCR	C1-C6-C7-C8
24	c	521	BCR	C1-C6-C7-C8
24	c	521	BCR	C23-C24-C25-C30
22	b	616	CLA	CAA-CBA-CGA-O2A
22	A	402	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
25	C	516	DGD	C6A-C7A-C8A-C9A
27	A	410	LMG	O7-C10-C11-C12
25	C	516	DGD	O6E-C1E-O5D-C6D
25	a	411	DGD	O6E-C1E-O5D-C6D
27	m	101	LMG	O6-C1-O1-C7
27	E	101	LMG	C30-C31-C32-C33
22	B	605	CLA	C16-C17-C18-C20
22	C	510	CLA	C3-C5-C6-C7
22	C	506	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
22	A	403	CLA	C2-C3-C5-C6
34	v	201	HEM	CAA-CBA-CGA-O1A
26	C	519	LHG	C11-C12-C13-C14
22	B	613	CLA	C4C-C3C-CAC-CBC
30	a	415	SQD	C8-C7-O47-C45
30	A	413	SQD	C12-C13-C14-C15
22	c	508	CLA	C8-C10-C11-C12
25	C	517	DGD	O1G-C1A-C2A-C3A
22	a	408	CLA	C4-C3-C5-C6
22	c	501	CLA	CAA-CBA-CGA-O2A
27	A	415	LMG	O7-C10-C11-C12
27	C	521	LMG	O8-C28-C29-C30
30	f	103	SQD	C14-C15-C16-C17
25	d	409	DGD	C9B-CAB-CBB-CCB
30	B	622	SQD	C7-C8-C9-C10
22	C	510	CLA	C2A-CAA-CBA-CGA
27	a	402	LMG	O7-C10-C11-C12
30	A	414	SQD	C26-C27-C28-C29
22	C	507	CLA	C11-C12-C13-C14
22	b	605	CLA	C14-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C9
25	b	601	DGD	CAB-CBB-CCB-CDB
30	A	414	SQD	O47-C7-C8-C9
26	C	519	LHG	O2-C2-C3-O3
25	c	515	DGD	C1G-C2G-C3G-O3G
27	I	101	LMG	C7-C8-C9-O8
27	d	407	LMG	C7-C8-C9-O8
22	b	607	CLA	C4B-C3B-CAB-CBB
22	b	608	CLA	C4B-C3B-CAB-CBB
22	b	618	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C13-C14-C15-C16
23	d	406	PL9	C40-C39-C41-C42
25	B	625	DGD	O6D-C1D-O3G-C3G
25	C	515	DGD	O6D-C1D-O3G-C3G
25	c	516	DGD	O6E-C1E-O5D-C6D
27	M	101	LMG	O6-C1-O1-C7
22	C	501	CLA	CAA-CBA-CGA-O2A
22	C	509	CLA	CAA-CBA-CGA-O2A
22	c	509	CLA	CAA-CBA-CGA-O2A
27	c	522	LMG	O8-C28-C29-C30
25	C	517	DGD	C4B-C5B-C6B-C7B
24	f	102	BCR	C21-C22-C23-C24
22	C	509	CLA	C13-C15-C16-C17
22	b	608	CLA	C8-C10-C11-C12
31	b	604	LMT	C6-C7-C8-C9
22	C	509	CLA	C16-C17-C18-C20
22	C	502	CLA	CBA-CGA-O2A-C1
22	C	503	CLA	C15-C16-C17-C18
25	c	517	DGD	O1G-C1A-C2A-C3A
30	a	401	SQD	O47-C7-C8-C9
25	c	517	DGD	C4A-C5A-C6A-C7A
34	V	201	HEM	CAA-CBA-CGA-O2A
22	C	502	CLA	O1A-CGA-O2A-C1
30	a	401	SQD	C23-C24-C25-C26
30	d	402	SQD	C7-C8-C9-C10
22	c	502	CLA	C16-C17-C18-C20
22	D	404	CLA	CAA-CBA-CGA-O2A
30	B	622	SQD	C5-C6-S-O9
30	d	402	SQD	C5-C6-S-O9
22	A	403	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
22	c	506	CLA	CAA-CBA-CGA-O2A
22	B	602	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C10-C8-C7
22	b	609	CLA	C6-C7-C8-C10
22	c	507	CLA	C11-C12-C13-C15
22	c	512	CLA	C11-C12-C13-C15
27	D	411	LMG	C32-C33-C34-C35
22	C	502	CLA	C16-C17-C18-C20
30	f	103	SQD	C15-C16-C17-C18
27	M	101	LMG	C7-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
27	m	101	LMG	C16-C17-C18-C19
22	B	611	CLA	CAA-CBA-CGA-O2A
25	C	517	DGD	CBB-CCB-CDB-CEB
25	b	624	DGD	C4A-C5A-C6A-C7A
27	d	408	LMG	C18-C19-C20-C21
22	b	606	CLA	C8-C10-C11-C12
22	B	602	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
22	c	509	CLA	C13-C15-C16-C17
25	A	408	DGD	O6D-C5D-C6D-O5D
25	C	517	DGD	O2G-C1B-C2B-C3B
25	c	517	DGD	O2G-C1B-C2B-C3B
26	C	519	LHG	C7-C8-C9-C10
26	c	519	LHG	C11-C12-C13-C14
22	B	605	CLA	C15-C16-C17-C18
22	c	509	CLA	CAA-CBA-CGA-O1A
30	B	622	SQD	O47-C7-C8-C9
30	d	402	SQD	O47-C7-C8-C9
22	B	601	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	C	506	CLA	C11-C12-C13-C14
22	D	404	CLA	C11-C10-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	a	408	CLA	C11-C10-C8-C9
22	b	609	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C12-C13-C14
22	d	404	CLA	C11-C10-C8-C9
32	D	402	PHO	C6-C7-C8-C9
27	c	522	LMG	O10-C28-C29-C30
30	F	103	SQD	C15-C16-C17-C18
31	B	623	LMT	C4-C5-C6-C7
27	M	101	LMG	O10-C28-O8-C9
22	b	611	CLA	C4-C3-C5-C6
30	B	622	SQD	O49-C7-C8-C9
31	B	627	LMT	C4'-C5'-C6'-O6'
27	D	408	LMG	O7-C10-C11-C12
30	B	622	SQD	O5-C5-C6-S
30	A	413	SQD	C9-C10-C11-C12
30	F	103	SQD	C14-C15-C16-C17
22	B	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	d	411	LMG	O9-C10-C11-C12
30	A	414	SQD	O49-C7-C8-C9
30	d	402	SQD	O49-C7-C8-C9
25	b	624	DGD	O2G-C1B-C2B-C3B
27	d	408	LMG	O7-C10-C11-C12
22	C	506	CLA	CAA-CBA-CGA-O1A
22	b	615	CLA	CAA-CBA-CGA-O1A
22	b	616	CLA	CAA-CBA-CGA-O1A
22	d	404	CLA	CAA-CBA-CGA-O1A
27	D	411	LMG	O9-C10-C11-C12
22	c	502	CLA	C5-C6-C7-C8
27	e	101	LMG	C14-C15-C16-C17
25	A	408	DGD	C5D-C6D-O5D-C1E
25	a	411	DGD	C5D-C6D-O5D-C1E
27	I	101	LMG	C8-C7-O1-C1
27	i	101	LMG	C8-C7-O1-C1
22	B	603	CLA	C4C-C3C-CAC-CBC
22	B	611	CLA	CAA-CBA-CGA-O1A
22	C	501	CLA	CAA-CBA-CGA-O1A
27	M	101	LMG	O8-C28-C29-C30
22	D	404	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
27	l	101	LMG	O9-C10-C11-C12
22	C	502	CLA	C5-C6-C7-C8
27	i	101	LMG	O7-C10-C11-C12
22	D	404	CLA	C3-C5-C6-C7
34	V	201	HEM	CAA-CBA-CGA-O1A
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
25	a	411	DGD	O6D-C5D-C6D-O5D
27	a	402	LMG	O9-C10-C11-C12
30	a	401	SQD	O49-C7-C8-C9
27	A	410	LMG	C39-C40-C41-C42
27	A	410	LMG	O9-C10-C11-C12
22	C	508	CLA	C8-C10-C11-C12
27	d	411	LMG	C12-C13-C14-C15
22	B	609	CLA	CAA-CBA-CGA-O2A
22	b	605	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
25	B	620	DGD	O2G-C1B-C2B-C3B
22	c	501	CLA	CAA-CBA-CGA-O1A
22	b	615	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	J	101	PL9	C2-C3-C7-C8
22	b	609	CLA	C15-C16-C17-C18
22	c	508	CLA	C10-C11-C12-C13
27	M	101	LMG	C17-C18-C19-C20
27	c	518	LMG	C17-C18-C19-C20
31	d	410	LMT	O5'-C5'-C6'-O6'
22	C	509	CLA	CAA-CBA-CGA-O1A
27	d	408	LMG	O9-C10-C11-C12
27	l	101	LMG	C17-C18-C19-C20

There are no ring outliers.

155 monomers are involved in 449 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	622	SQD	3	0
31	b	603	LMT	2	0
23	A	406	PL9	5	0
24	b	622	BCR	3	0
24	g	101	BCR	5	0
25	B	620	DGD	2	0
27	E	101	LMG	1	0
22	c	512	CLA	2	0
22	B	606	CLA	7	0
30	A	413	SQD	3	0
22	B	605	CLA	7	0
24	K	102	BCR	3	0
27	c	518	LMG	2	0
22	b	617	CLA	2	0
22	d	404	CLA	9	0
27	m	101	LMG	2	0
34	v	201	HEM	5	0
22	b	618	CLA	1	0
25	a	411	DGD	3	0
22	B	612	CLA	2	0
24	H	102	BCR	2	0
27	b	625	LMG	4	0
22	a	404	CLA	9	0
25	C	515	DGD	3	0
25	d	409	DGD	1	0
25	D	409	DGD	1	0
22	B	601	CLA	1	0
22	B	610	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	614	CLA	3	0
22	c	501	CLA	4	0
22	c	506	CLA	4	0
22	b	609	CLA	5	0
27	D	407	LMG	2	0
34	V	201	HEM	4	0
24	y	101	BCR	6	0
22	C	509	CLA	4	0
31	i	102	LMT	1	0
31	B	628	LMT	2	0
32	D	401	PHO	6	0
24	b	621	BCR	1	0
27	d	411	LMG	1	0
27	A	410	LMG	2	0
22	A	403	CLA	12	0
27	e	101	LMG	2	0
27	l	101	LMG	2	0
22	A	404	CLA	5	0
30	b	602	SQD	2	0
22	B	607	CLA	8	0
22	d	405	CLA	2	0
22	c	505	CLA	1	0
22	C	512	CLA	3	0
31	B	623	LMT	2	0
22	B	614	CLA	2	0
25	B	625	DGD	2	0
27	A	415	LMG	1	0
24	b	623	BCR	4	0
25	b	601	DGD	2	0
24	a	410	BCR	4	0
22	B	608	CLA	5	0
22	C	507	CLA	4	0
25	c	516	DGD	3	0
27	c	522	LMG	1	0
25	c	517	DGD	5	0
22	b	616	CLA	3	0
22	B	611	CLA	3	0
32	D	402	PHO	5	0
22	B	615	CLA	4	0
22	D	405	CLA	4	0
24	B	619	BCR	1	0
22	b	612	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	521	BCR	3	0
31	b	626	LMT	1	0
22	b	619	CLA	4	0
22	c	503	CLA	2	0
22	b	606	CLA	8	0
24	c	513	BCR	7	0
27	M	101	LMG	1	0
30	d	402	SQD	3	0
22	h	101	CLA	10	0
31	b	604	LMT	2	0
22	B	604	CLA	8	0
22	C	508	CLA	1	0
22	b	615	CLA	4	0
27	D	408	LMG	6	0
27	d	407	LMG	3	0
22	C	505	CLA	2	0
26	c	519	LHG	2	0
22	C	503	CLA	3	0
34	F	101	HEM	4	0
24	J	102	BCR	2	0
26	A	409	LHG	3	0
22	b	607	CLA	3	0
22	c	520	CLA	5	0
25	C	516	DGD	4	0
22	a	405	CLA	10	0
24	A	407	BCR	2	0
24	f	102	BCR	1	0
25	c	515	DGD	3	0
24	F	102	BCR	3	0
27	d	408	LMG	6	0
30	F	103	SQD	2	0
30	a	401	SQD	5	0
30	B	626	SQD	2	0
25	A	408	DGD	1	0
24	B	617	BCR	2	0
24	B	618	BCR	4	0
24	B	616	BCR	7	0
22	b	608	CLA	8	0
22	B	603	CLA	3	0
22	c	510	CLA	4	0
25	b	624	DGD	2	0
22	C	511	CLA	1	0

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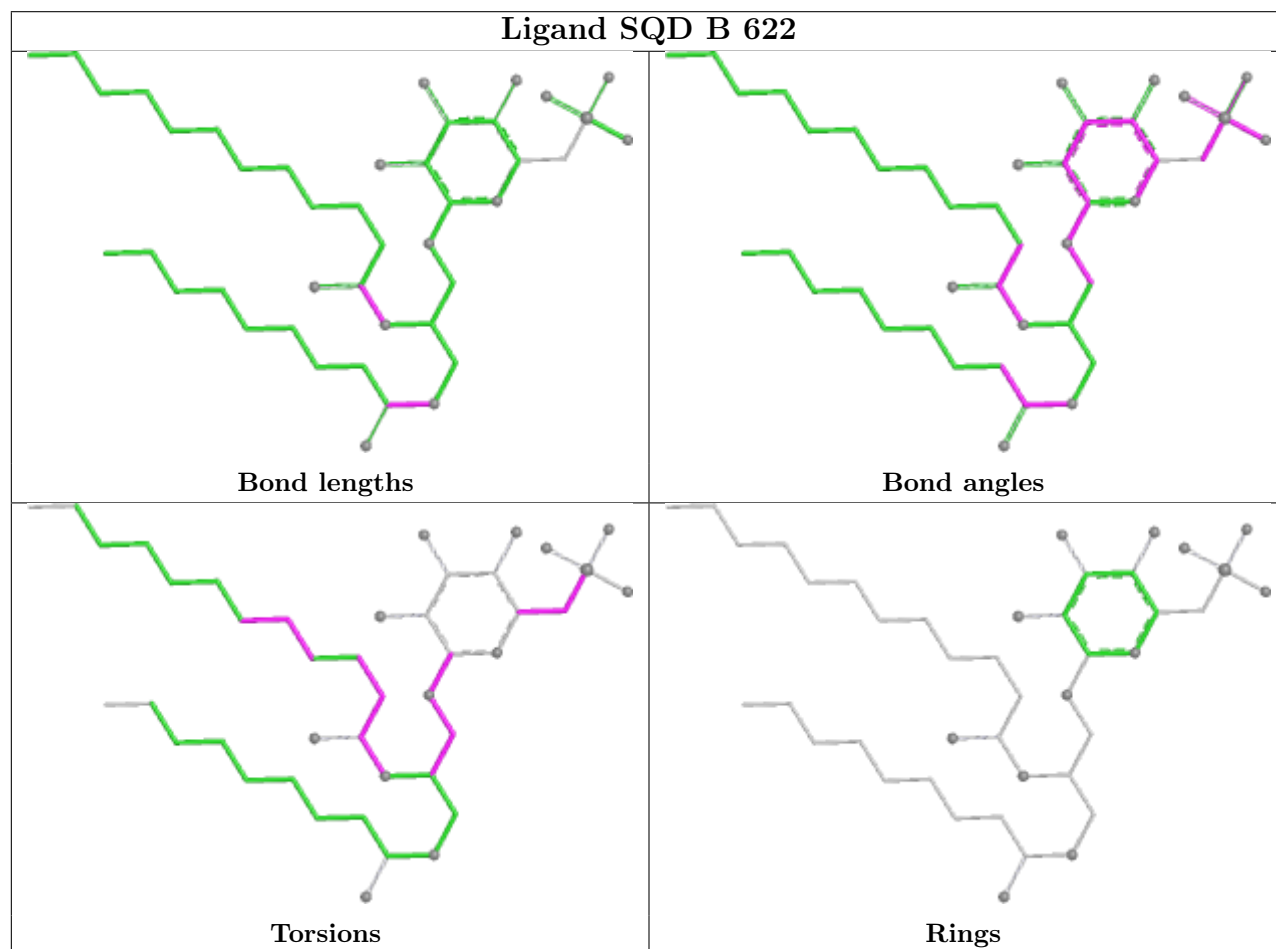
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	506	CLA	3	0
22	B	613	CLA	4	0
22	A	405	CLA	1	0
27	B	621	LMG	3	0
27	a	402	LMG	1	0
22	b	610	CLA	5	0
34	f	101	HEM	4	0
30	f	103	SQD	3	0
22	D	404	CLA	10	0
32	d	401	PHO	5	0
22	C	510	CLA	4	0
22	A	402	CLA	11	0
23	D	406	PL9	8	0
30	a	415	SQD	3	0
24	j	102	BCR	1	0
26	a	412	LHG	1	0
24	c	514	BCR	3	0
24	C	513	BCR	5	0
22	C	501	CLA	2	0
30	A	414	SQD	5	0
22	b	613	CLA	1	0
22	C	520	CLA	3	0
27	C	518	LMG	2	0
26	C	519	LHG	3	0
22	B	602	CLA	10	0
22	H	101	CLA	9	0
22	c	504	CLA	3	0
27	i	101	LMG	1	0
23	a	409	PL9	4	0
23	d	406	PL9	6	0
31	B	627	LMT	2	0
22	a	408	CLA	2	0
27	D	411	LMG	1	0
22	c	508	CLA	3	0
32	a	407	PHO	4	0
22	b	611	CLA	8	0
22	a	406	CLA	6	0
22	C	504	CLA	3	0
22	c	509	CLA	3	0
25	C	517	DGD	5	0
22	c	507	CLA	5	0
24	C	514	BCR	5	0

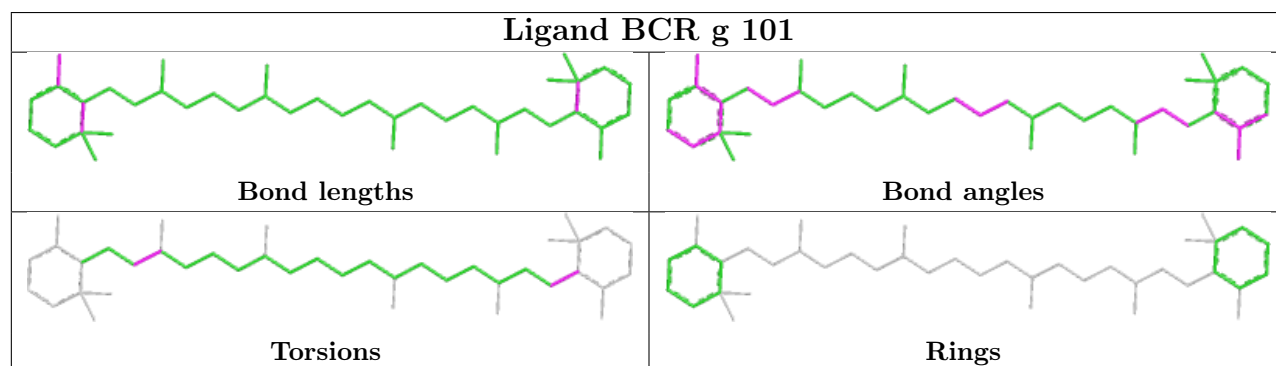
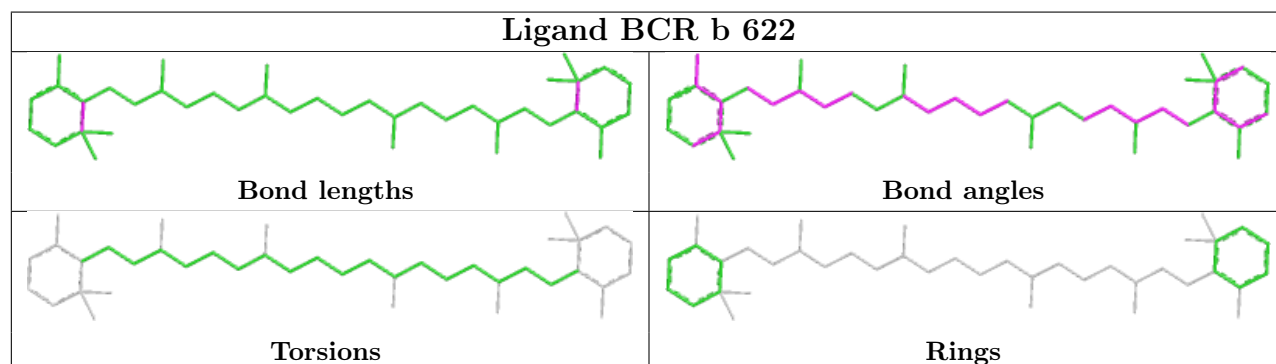
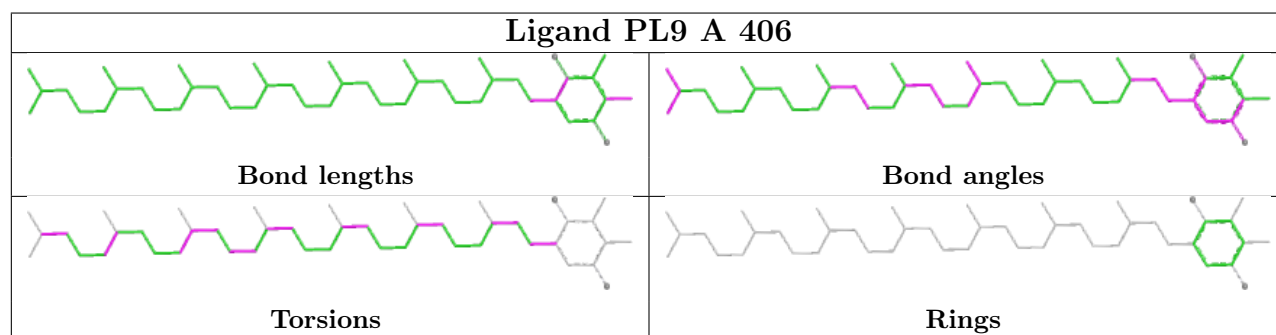
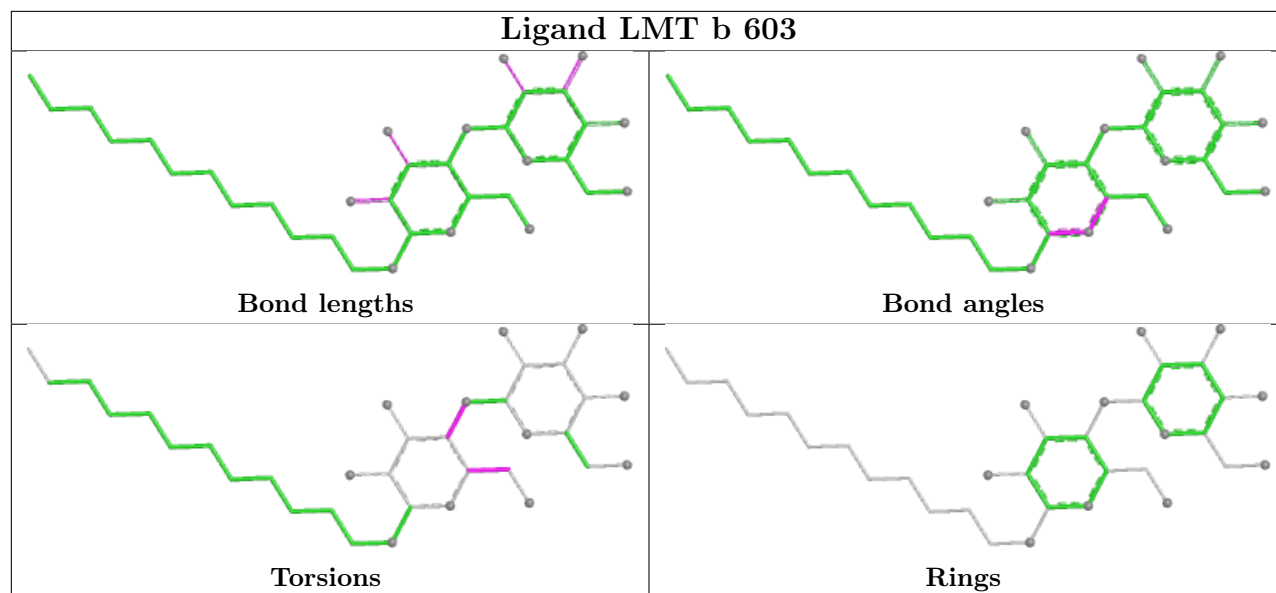
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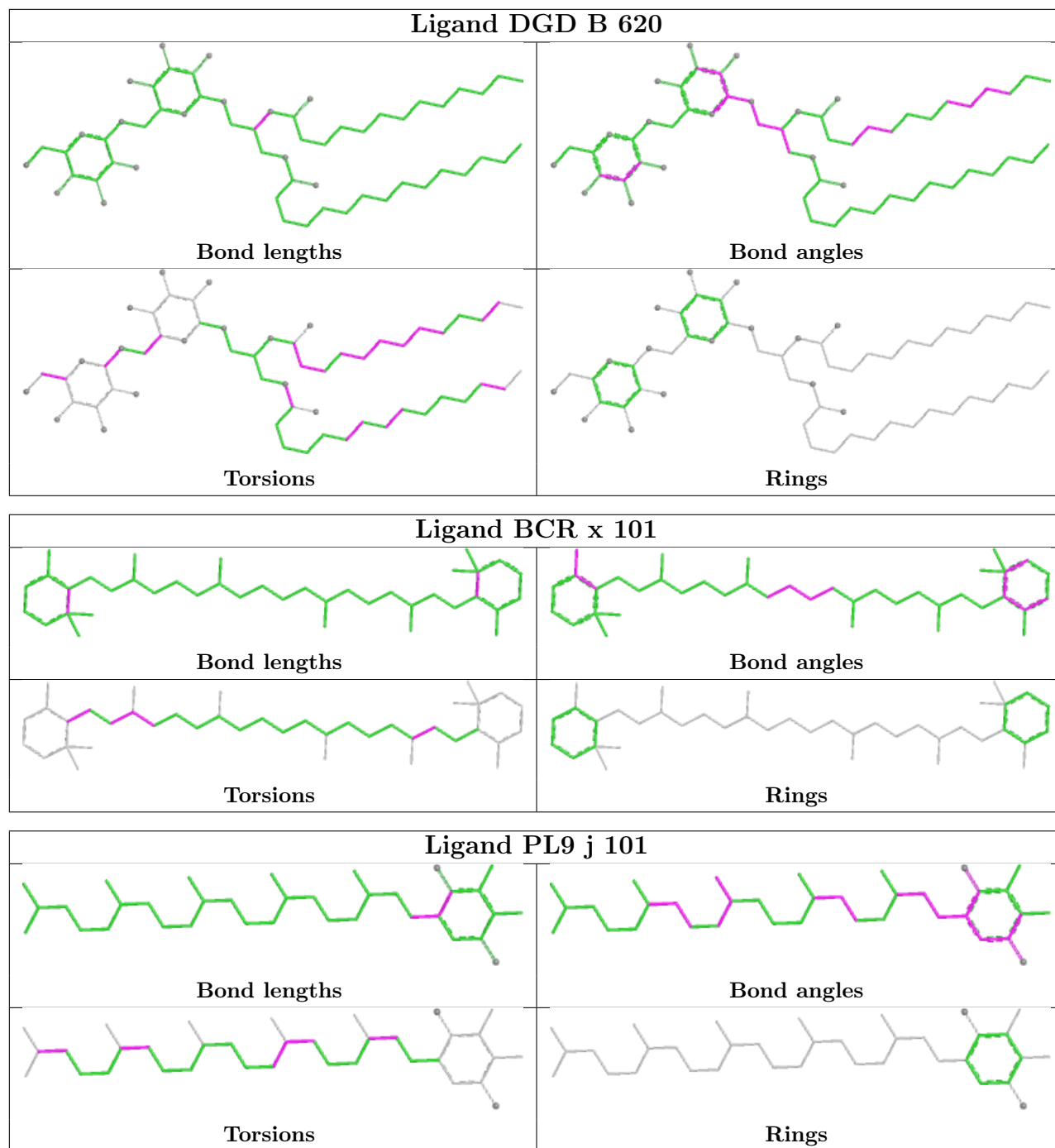
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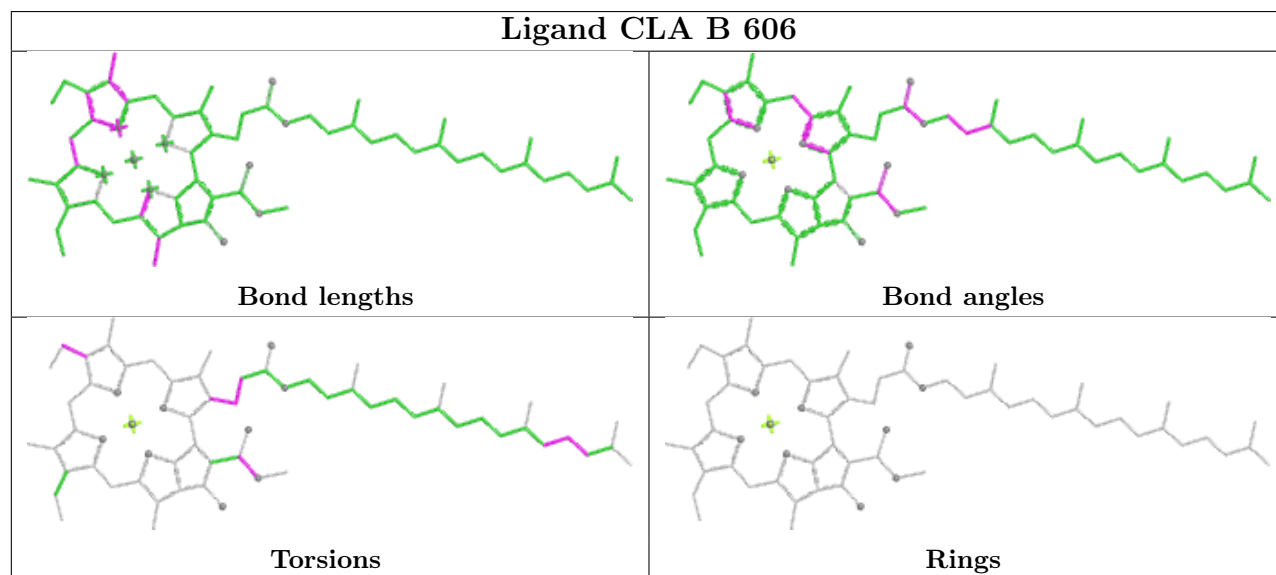
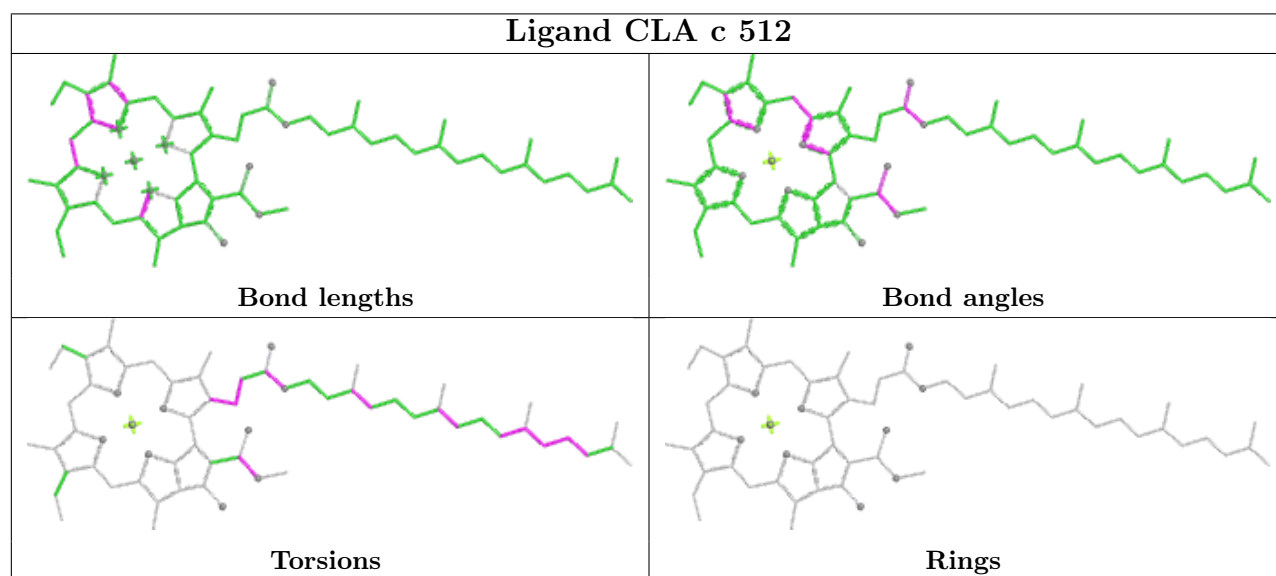
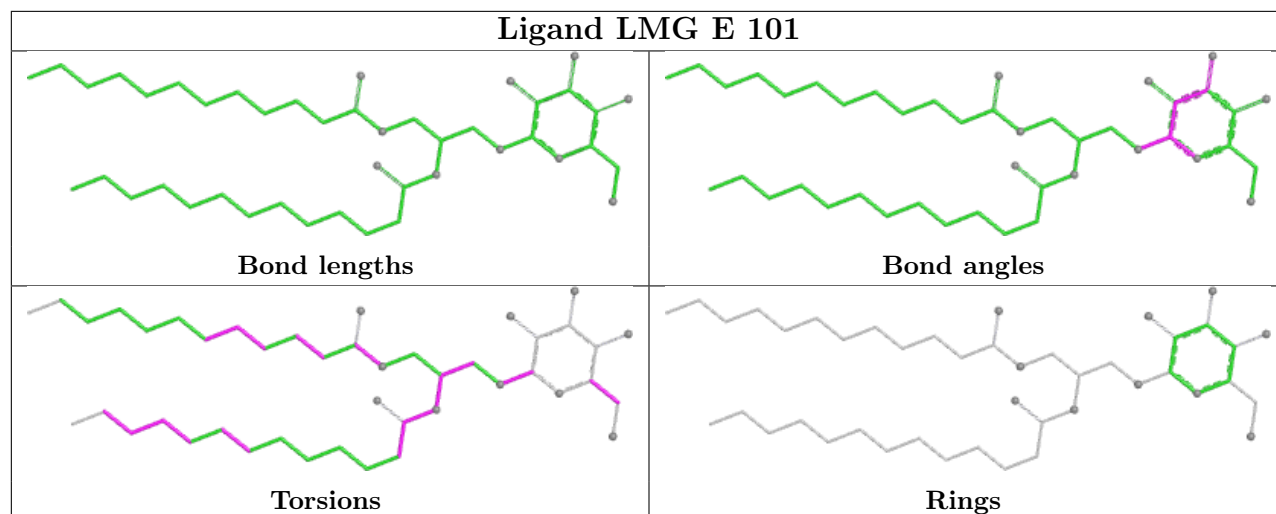
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	620	BCR	5	0

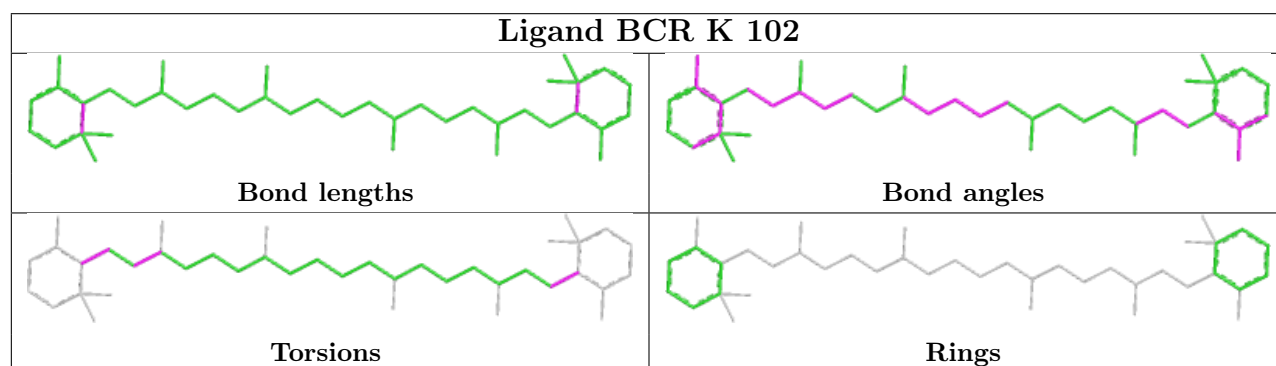
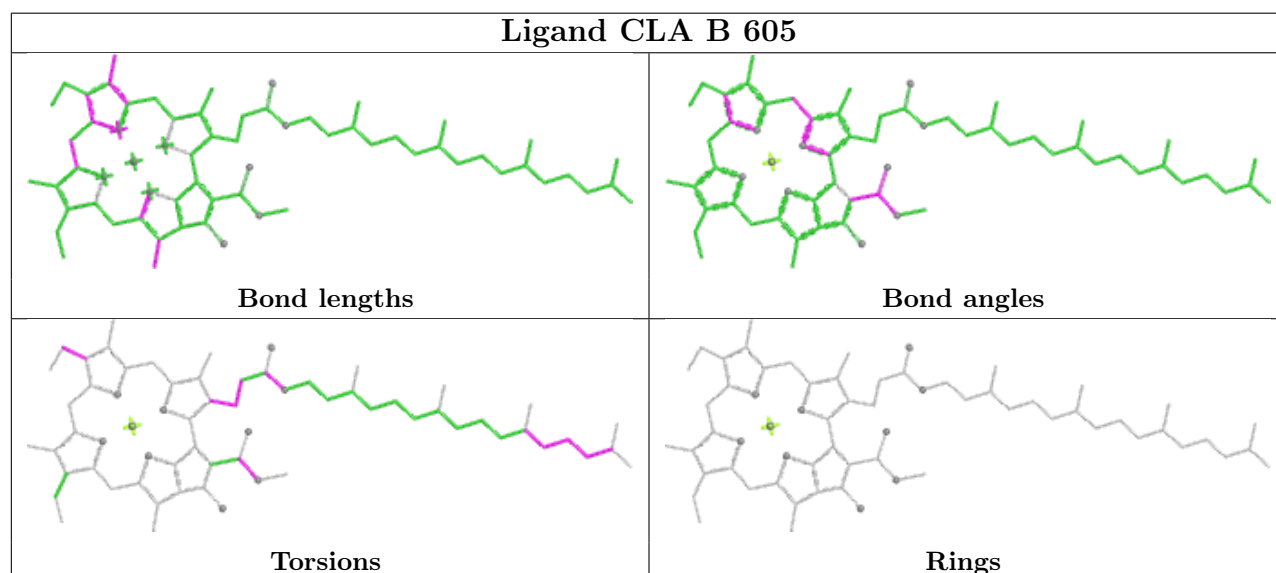
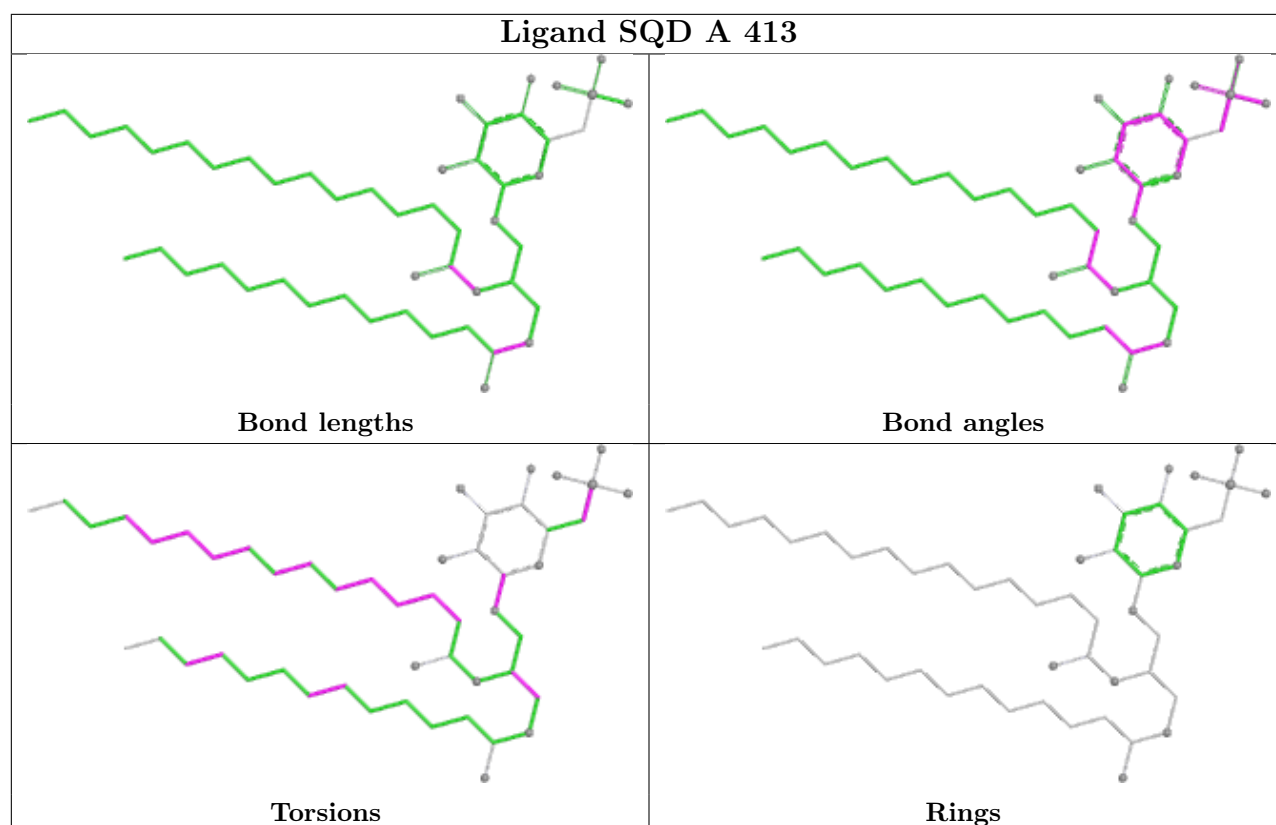
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

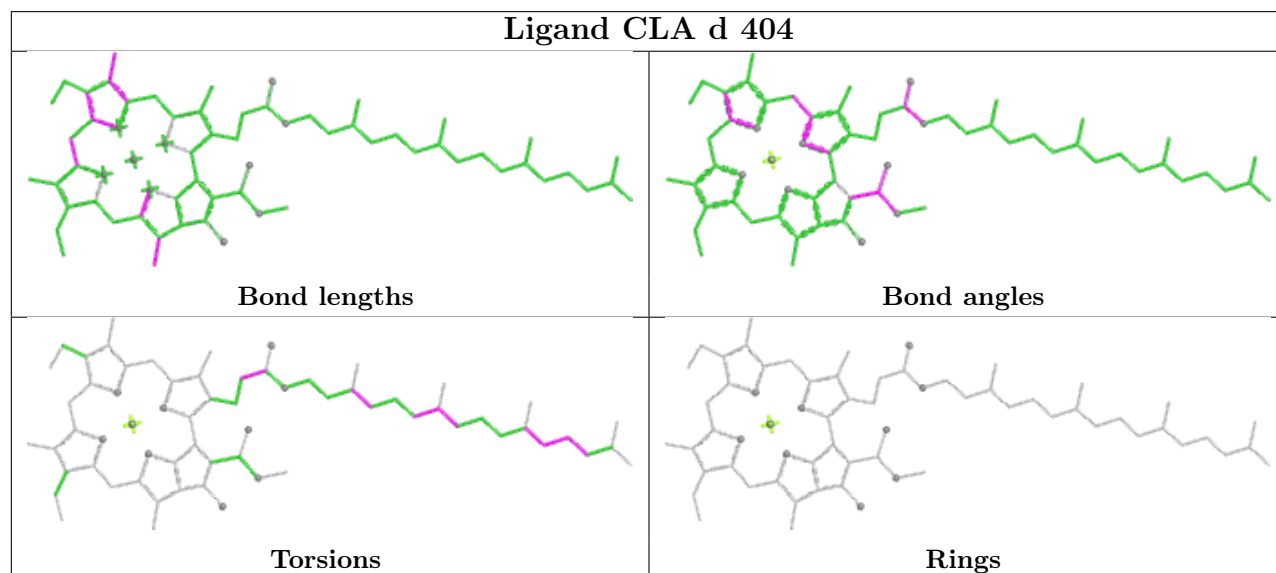
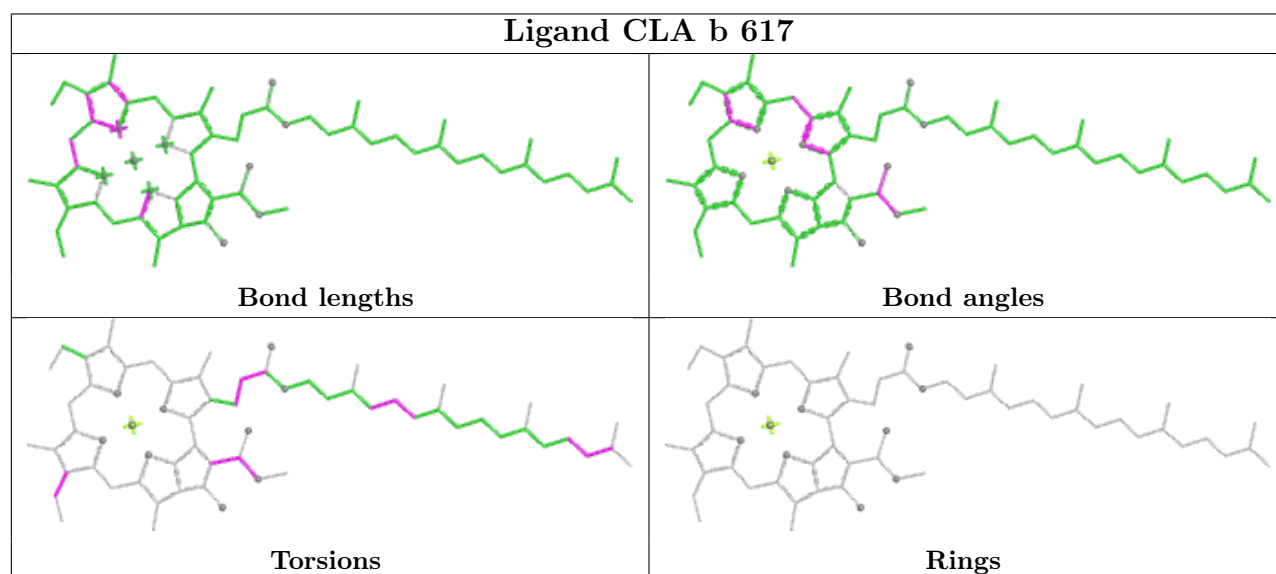
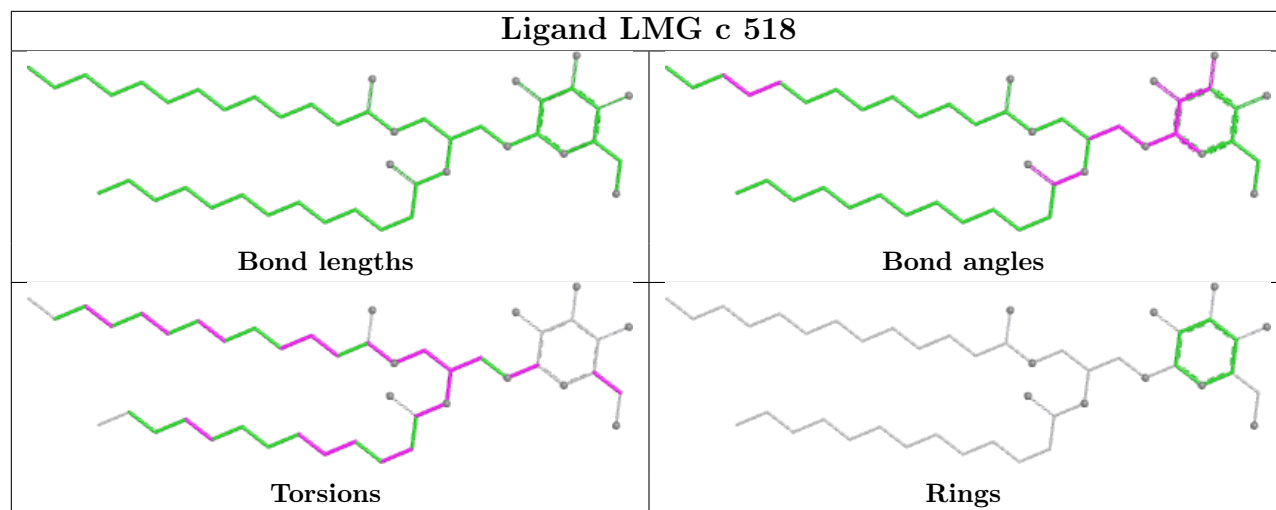


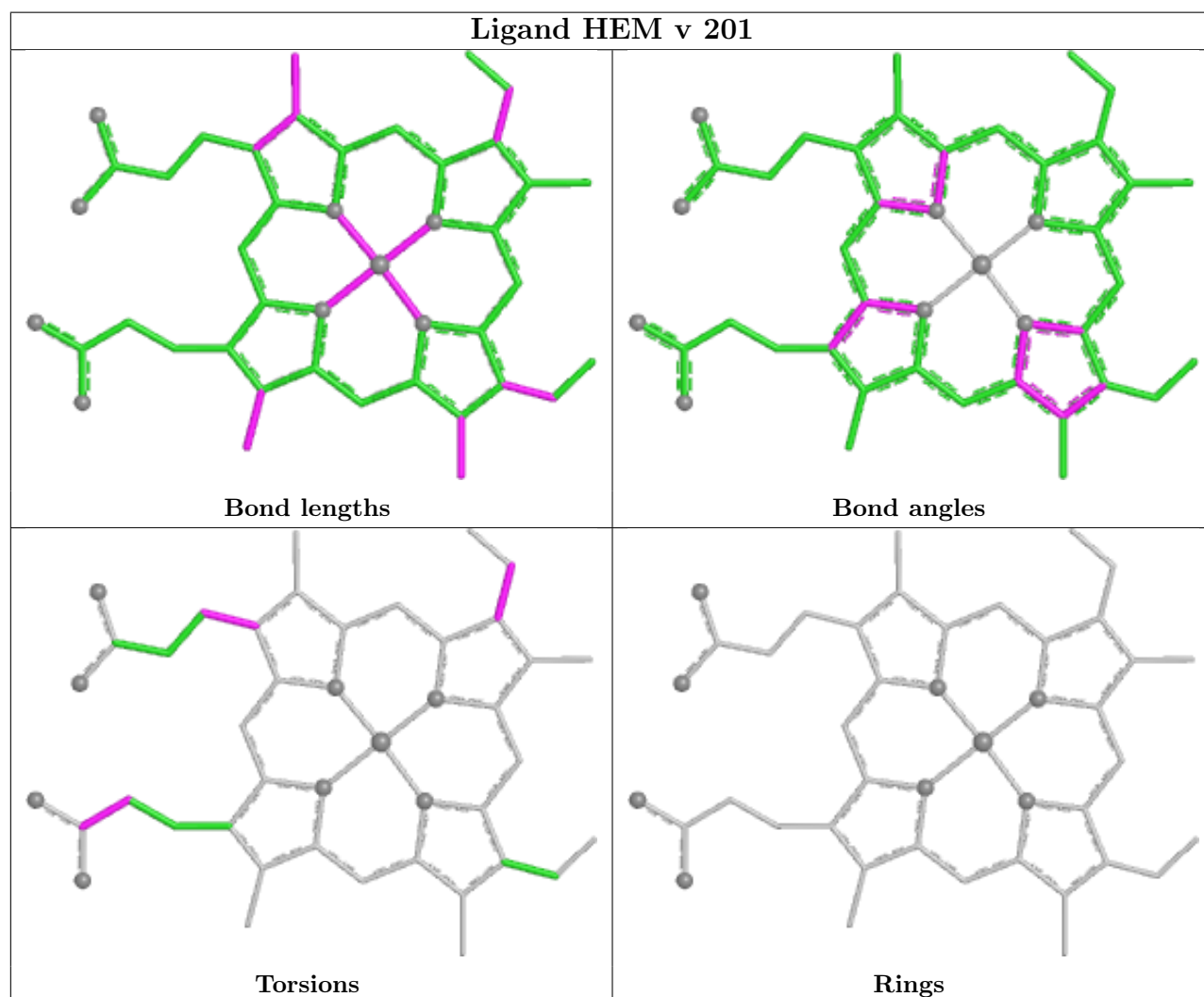
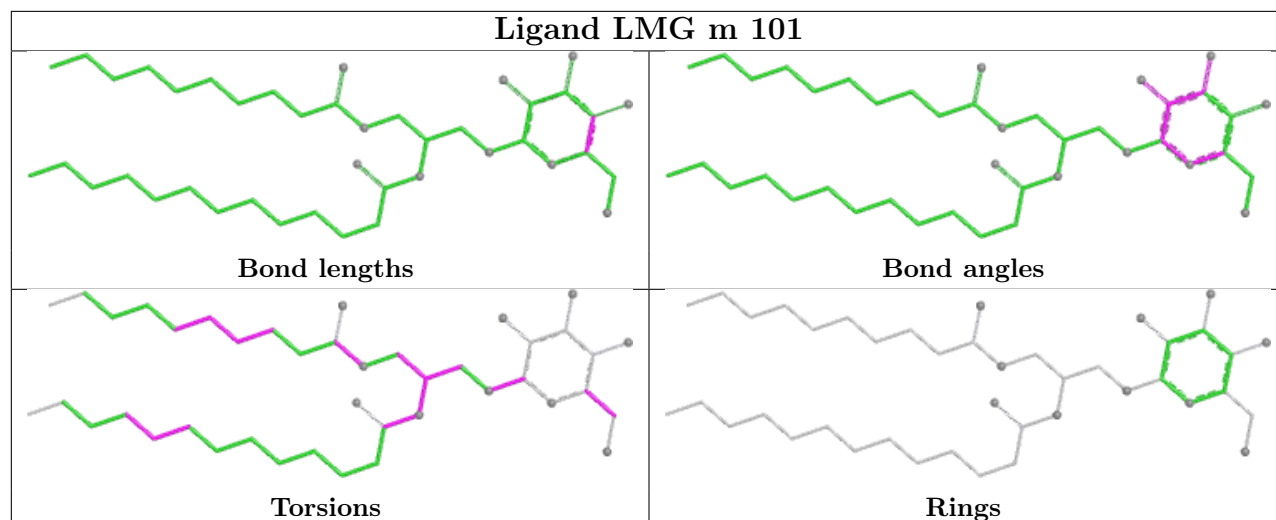




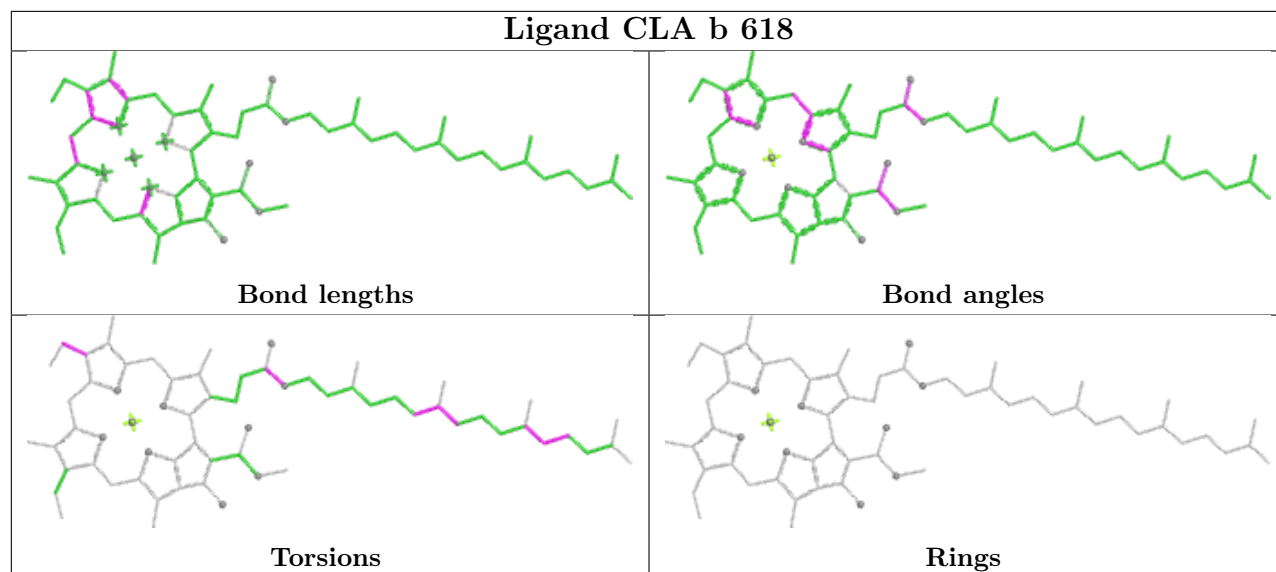




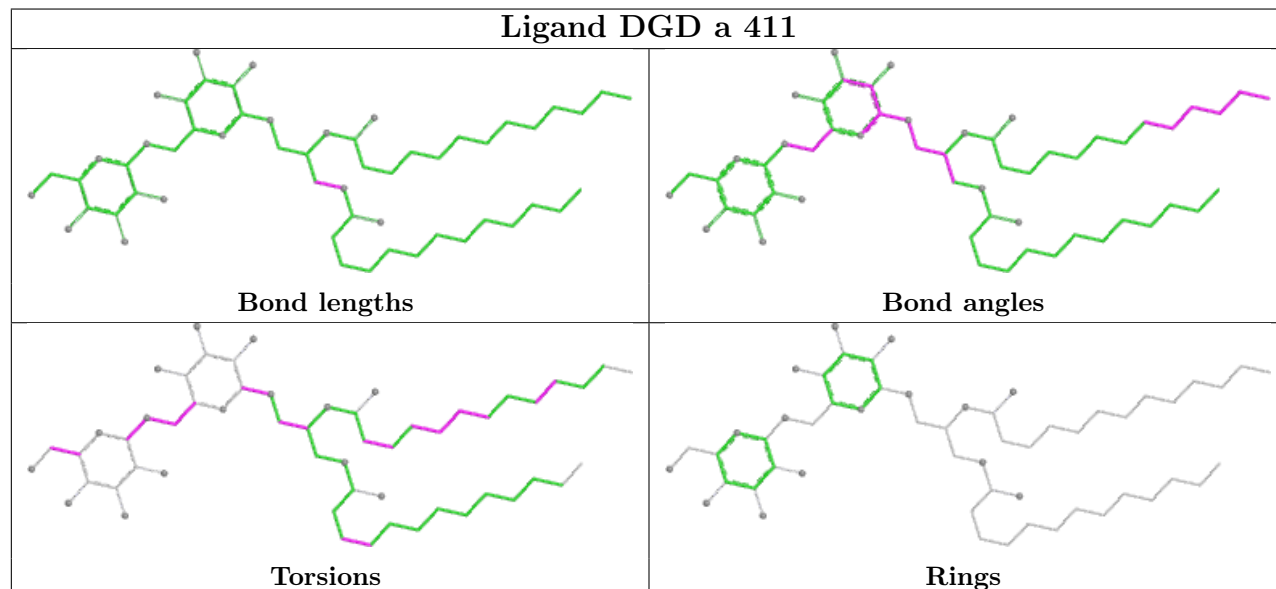




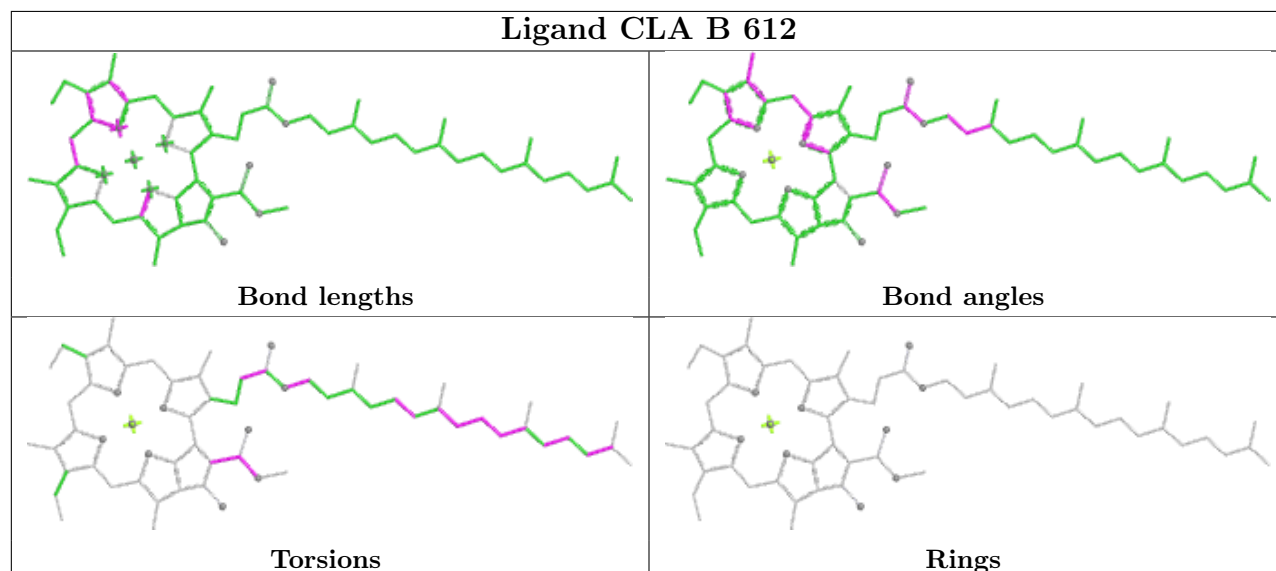
Ligand CLA b 618

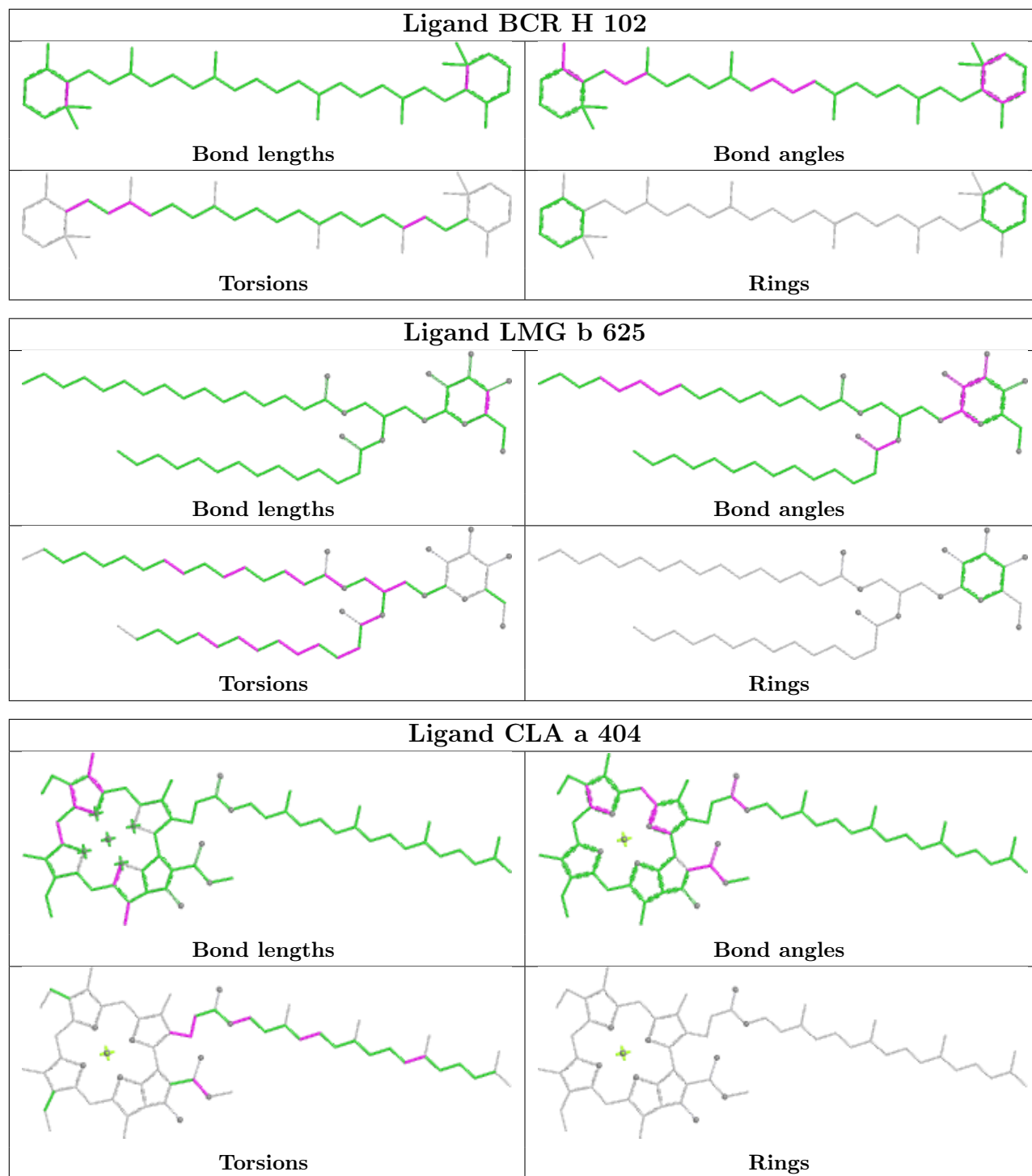


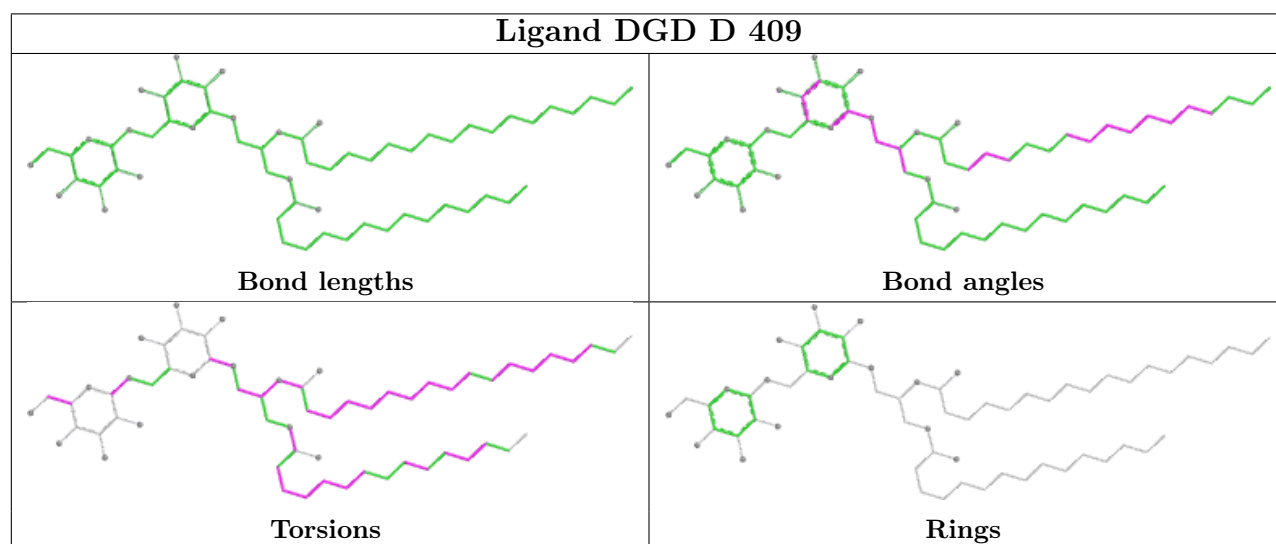
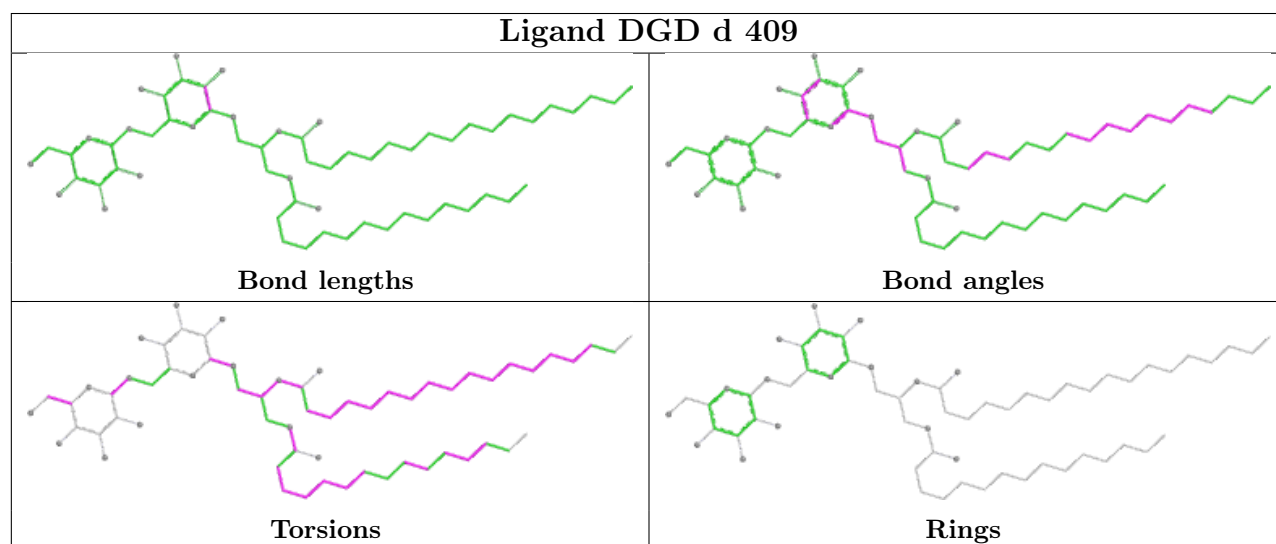
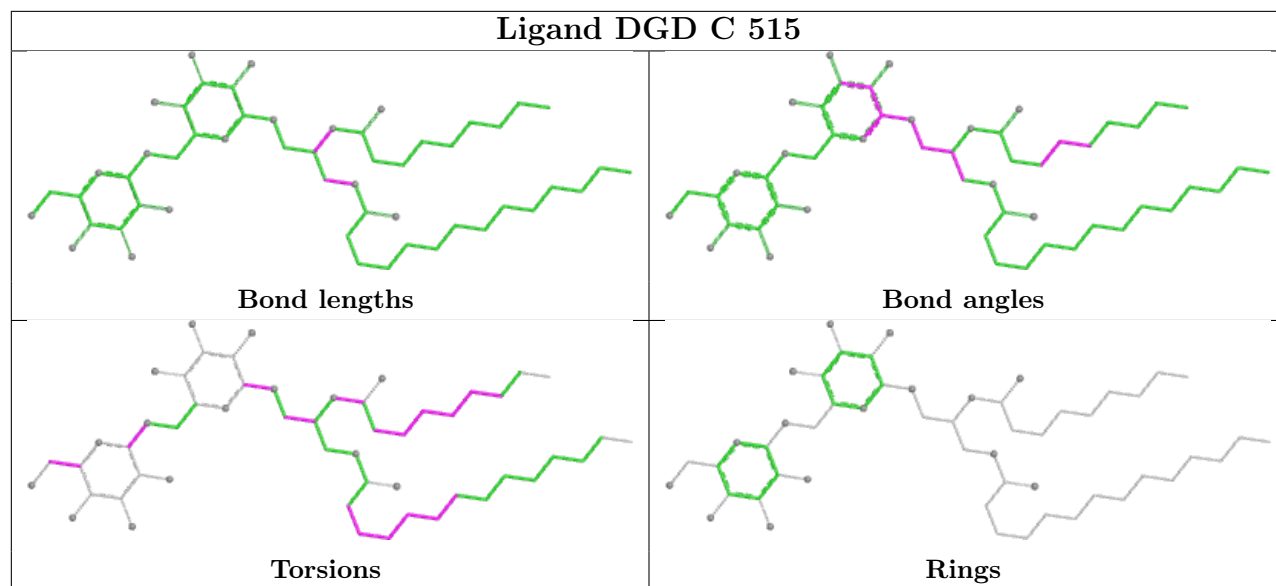
Ligand DGD a 411



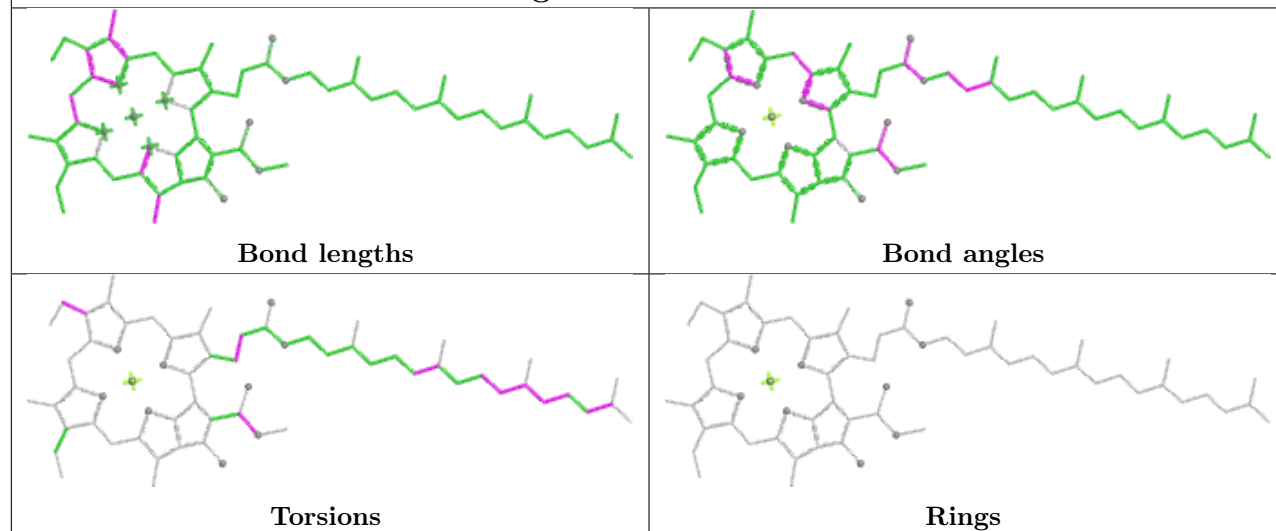
Ligand CLA B 612



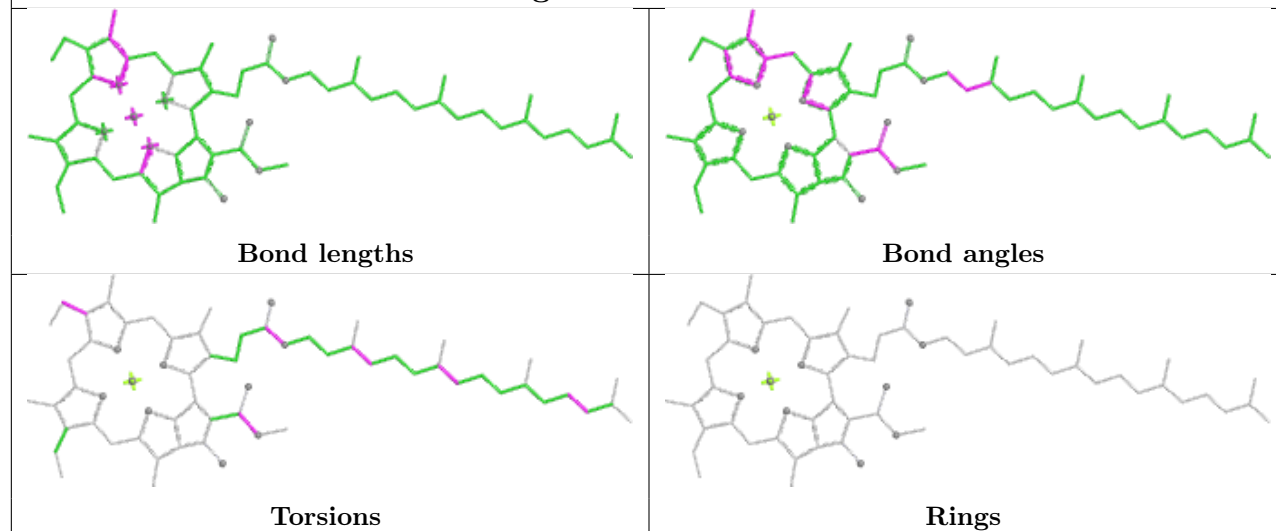




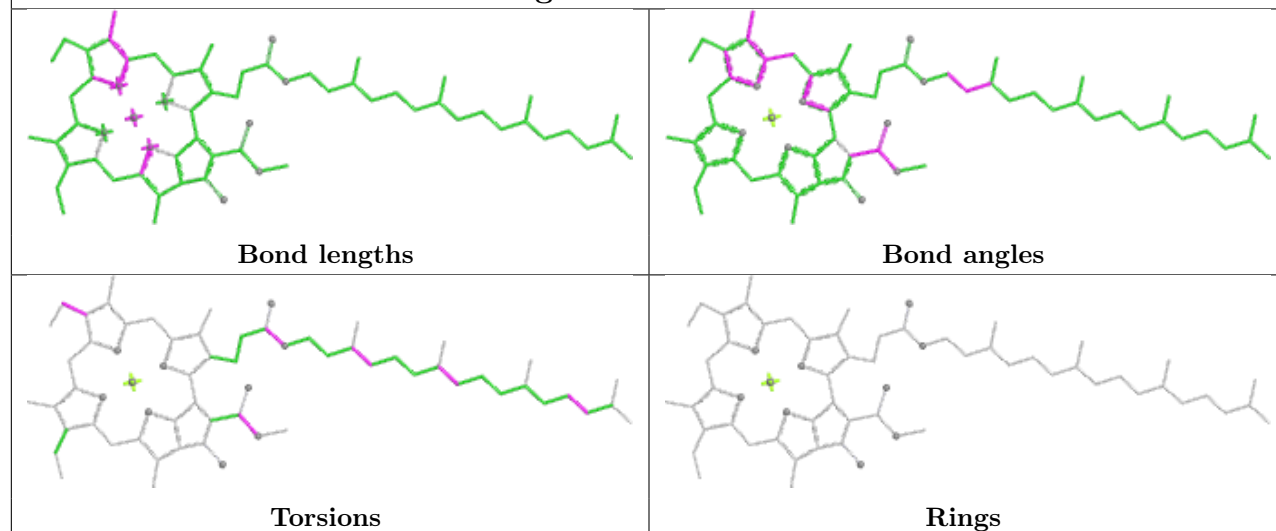
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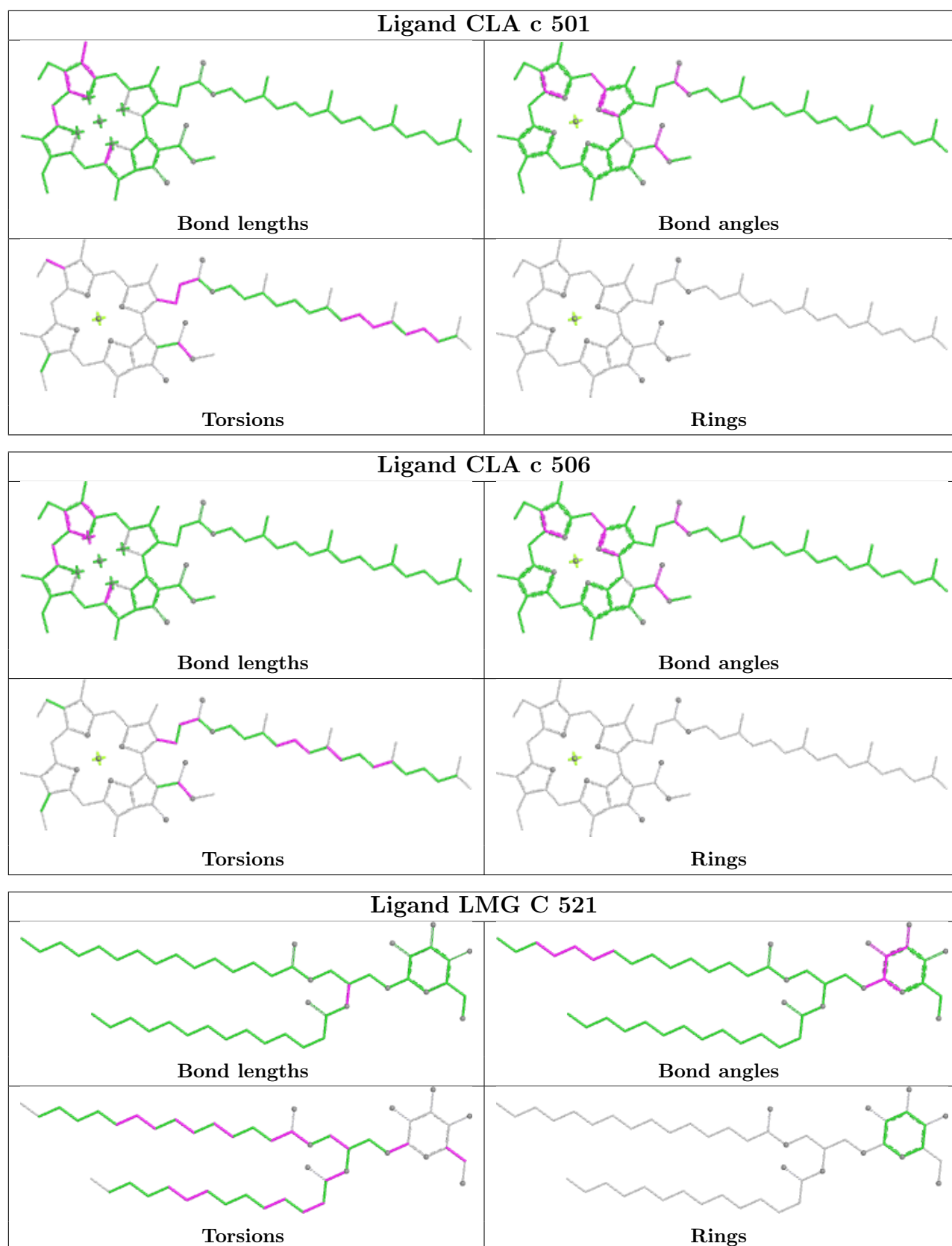


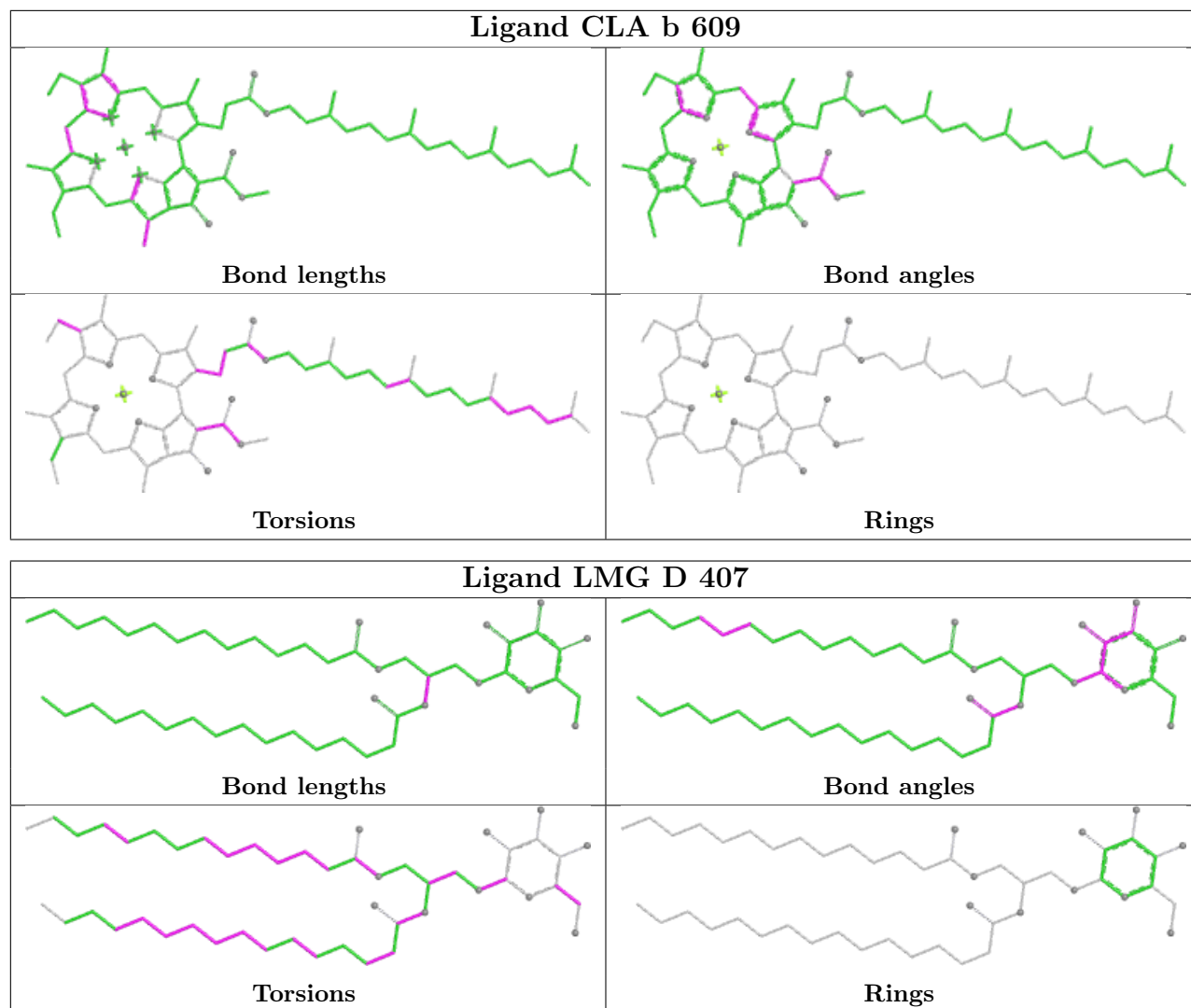
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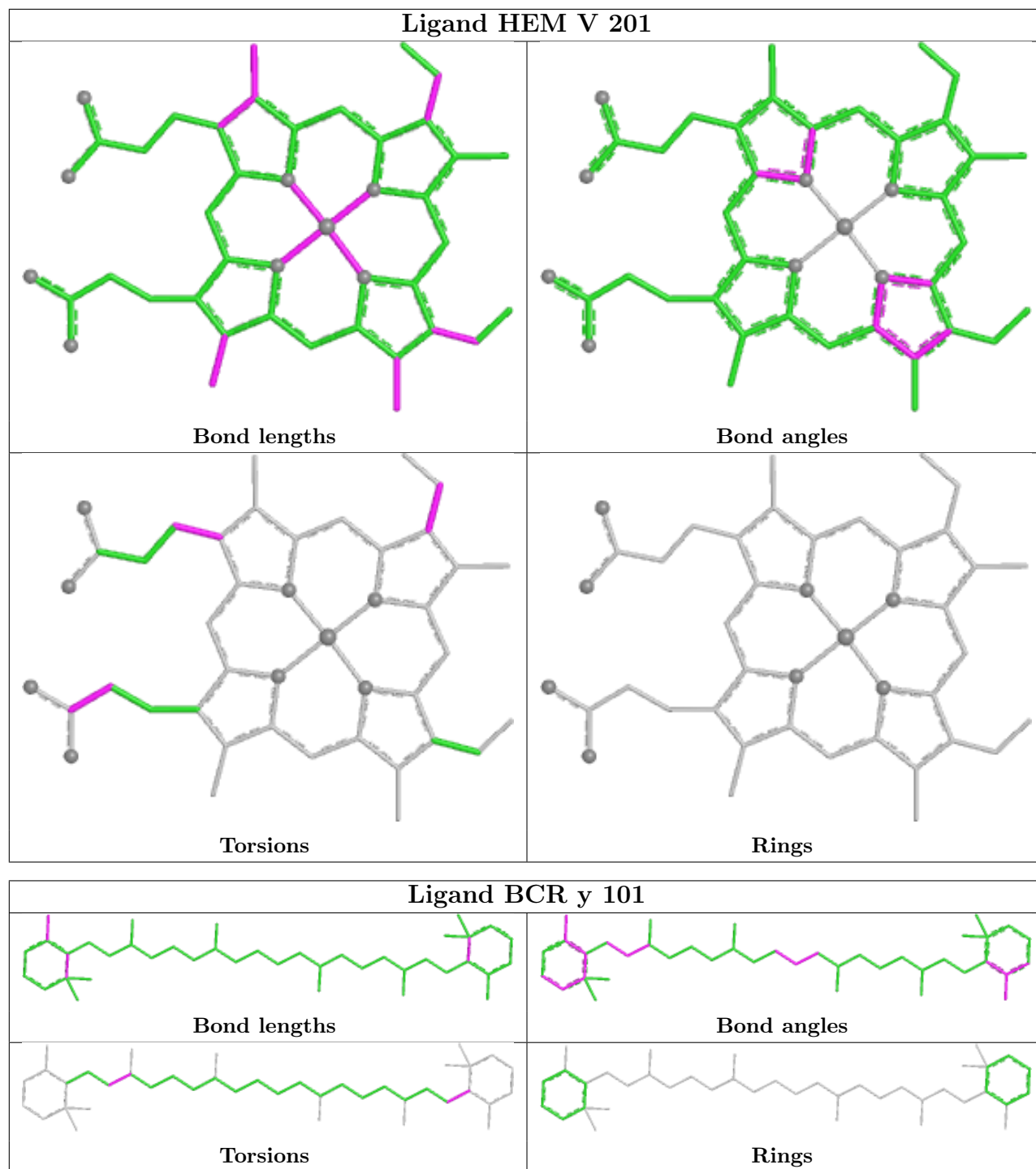


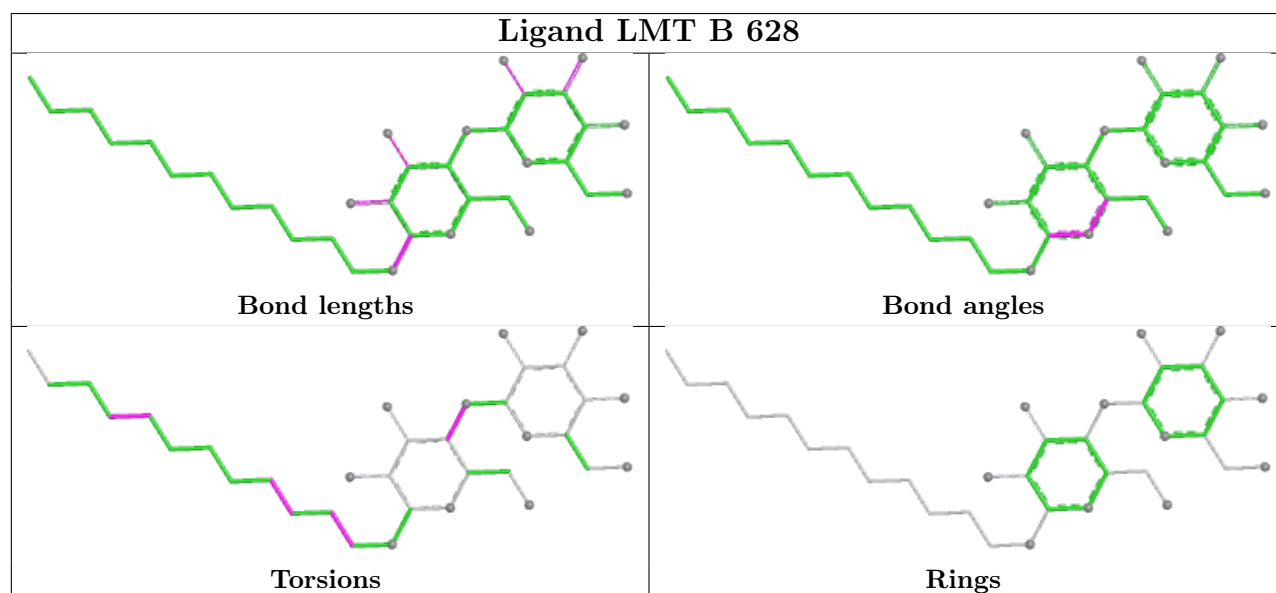
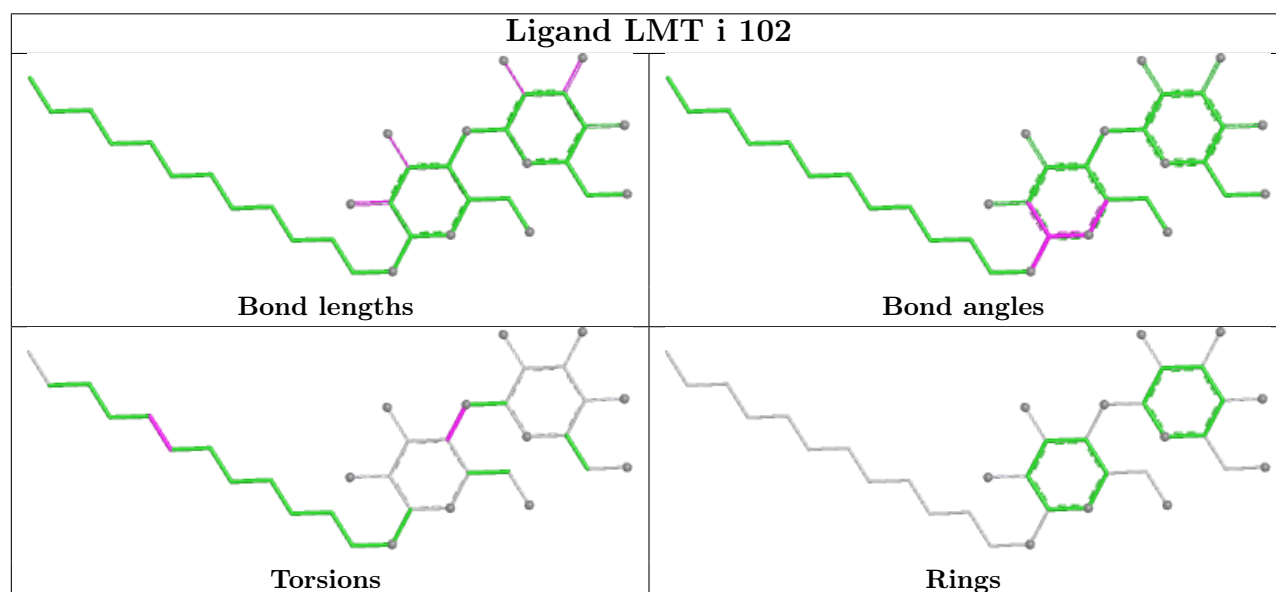
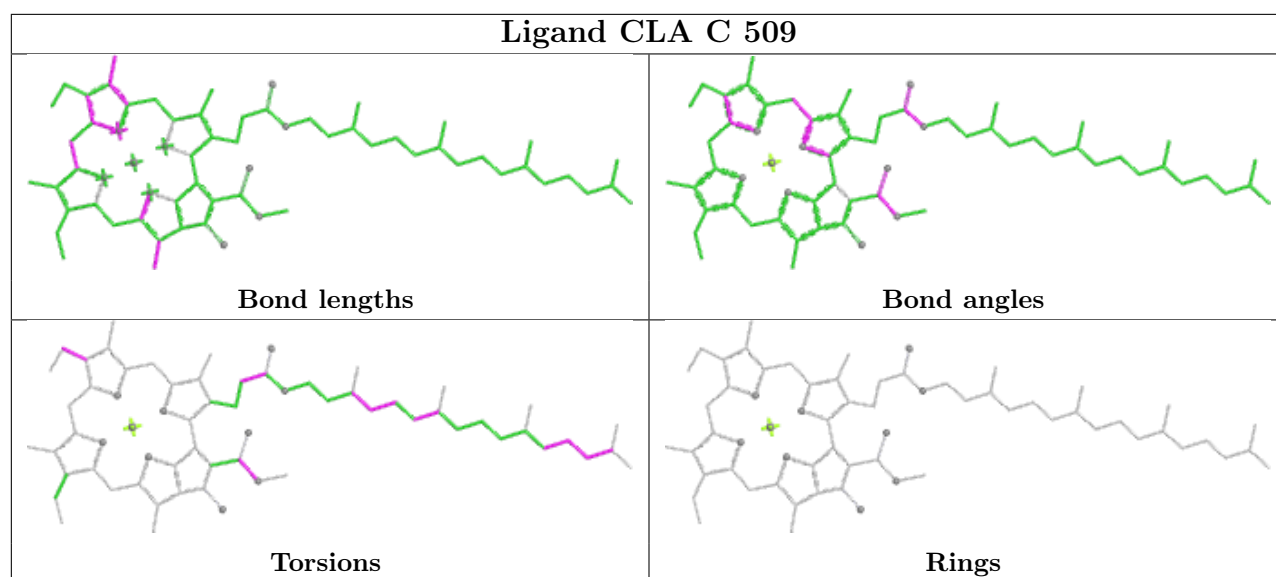
Ligand CLA b 614

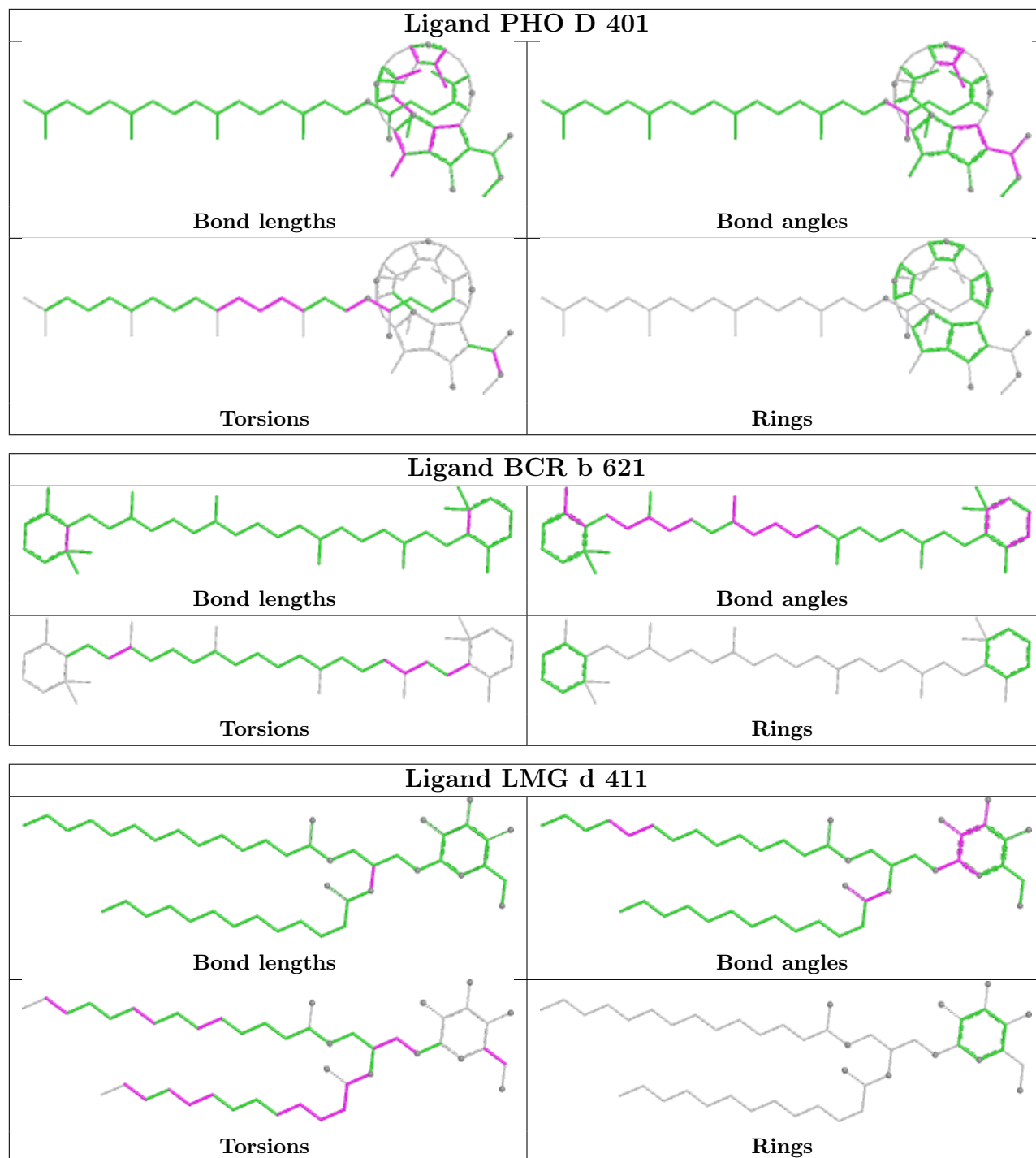




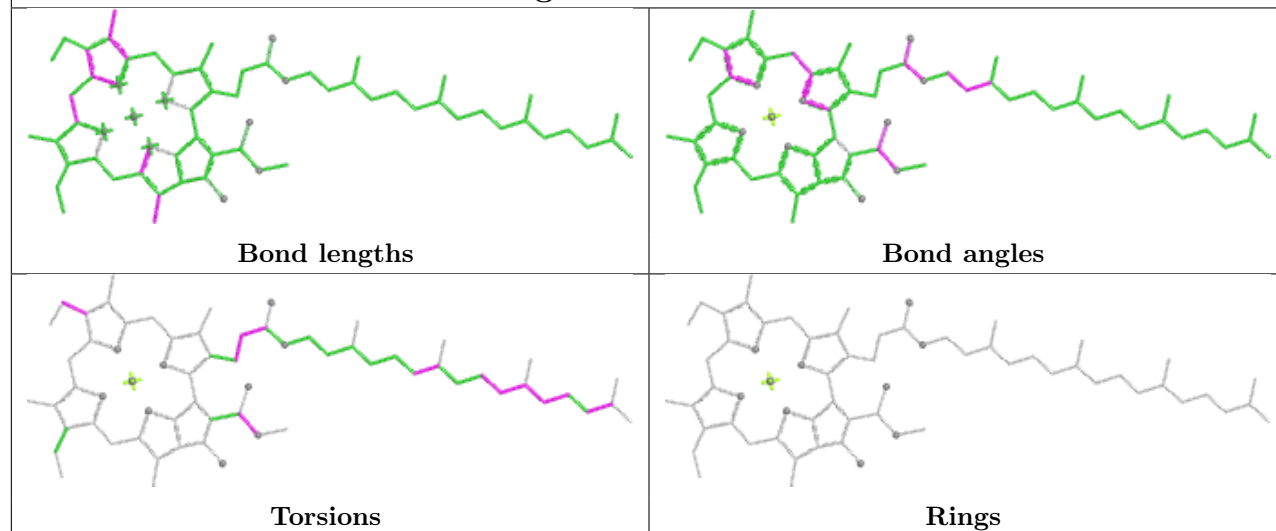




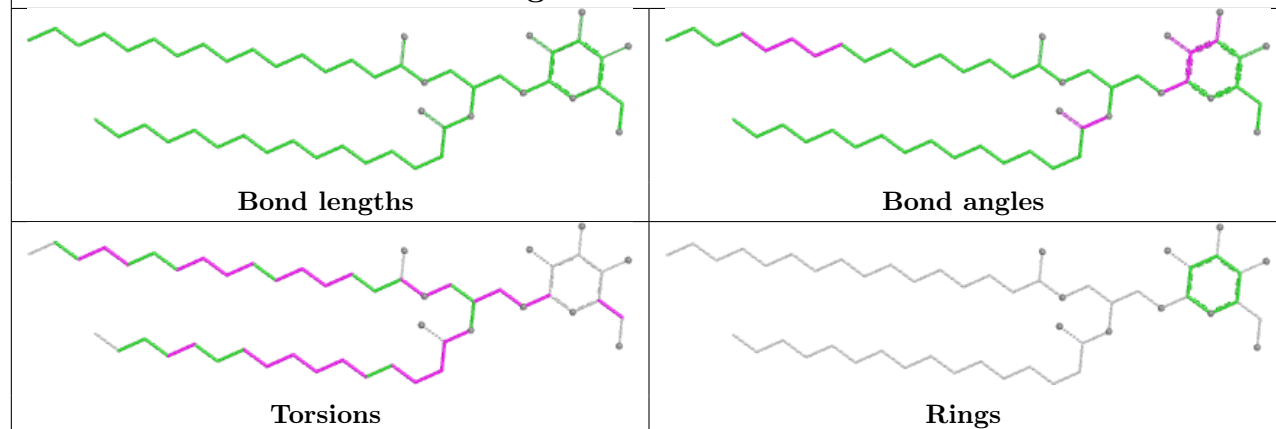




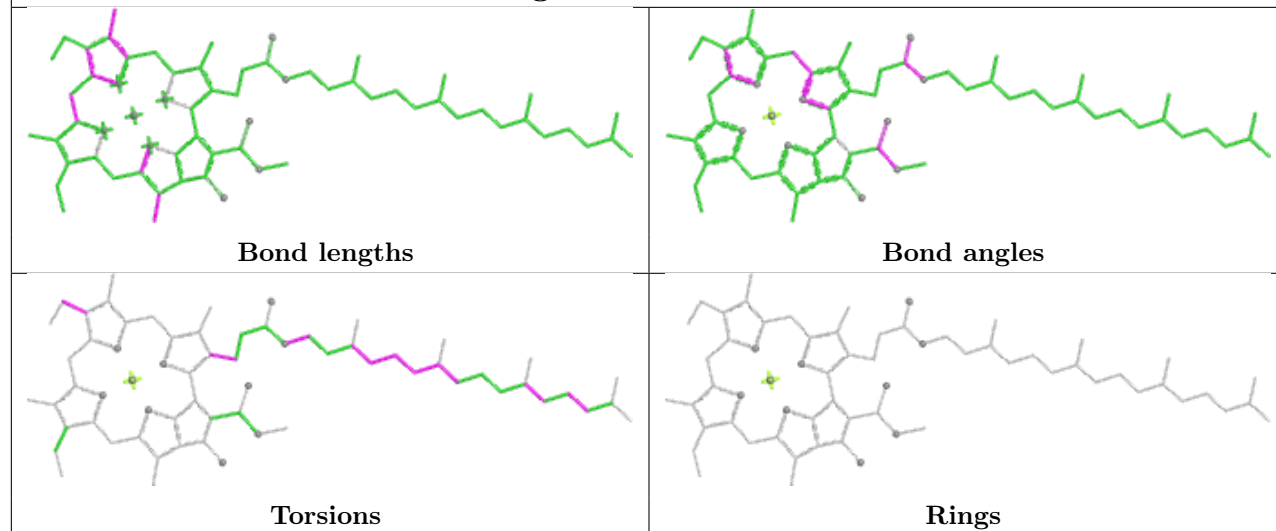
Ligand CLA b 605

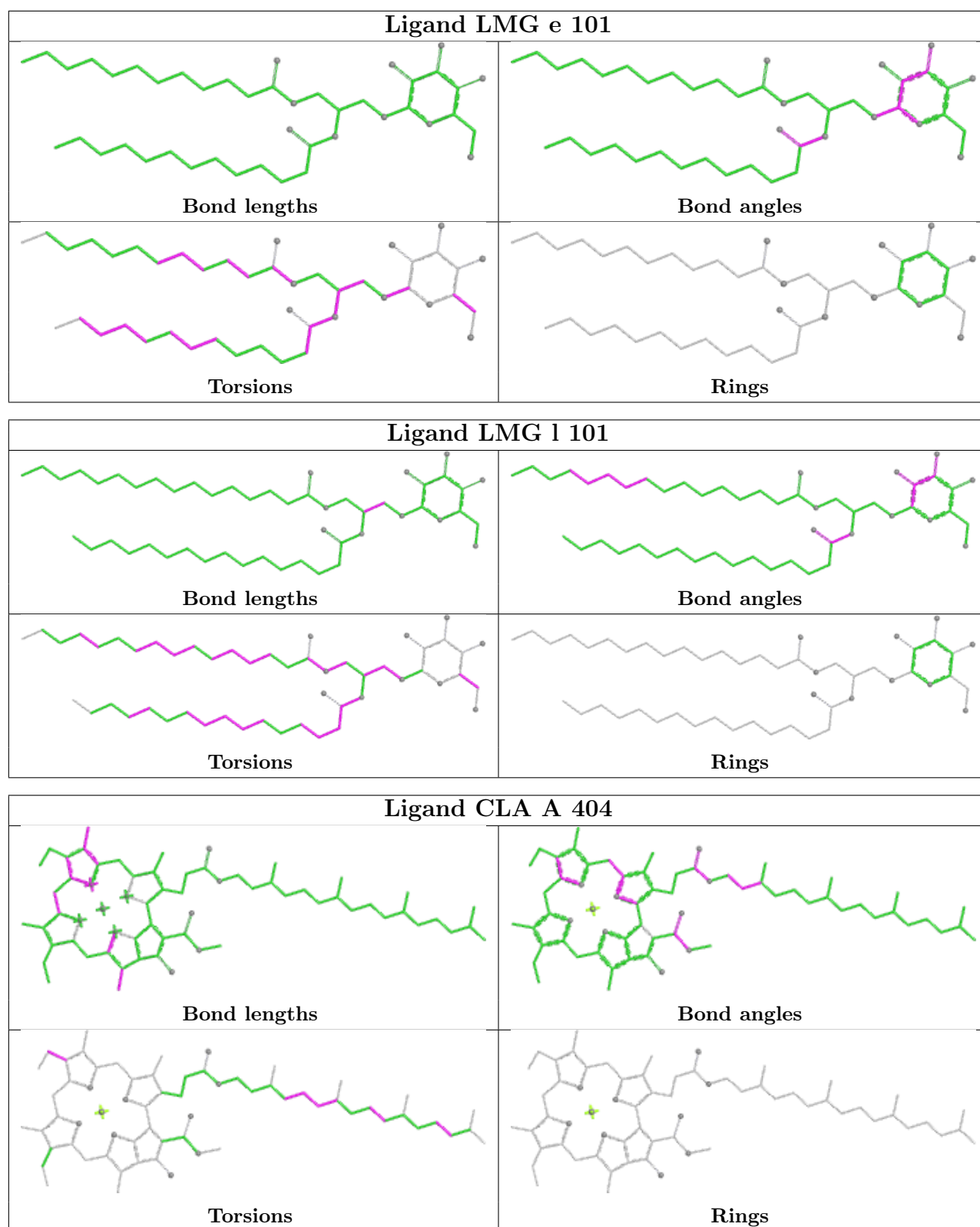


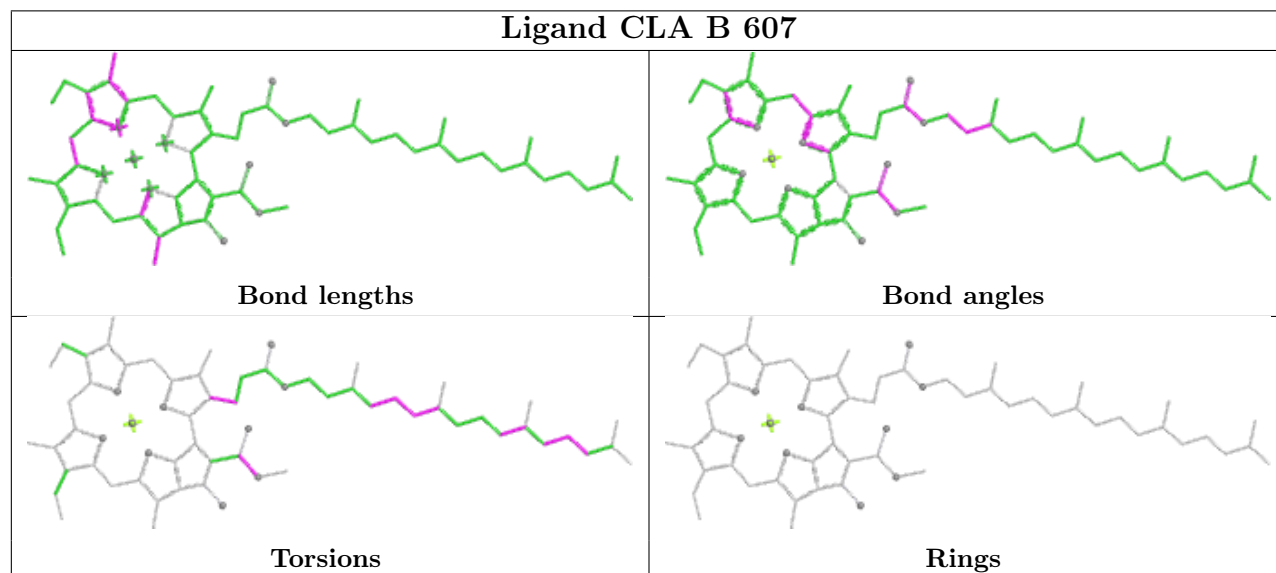
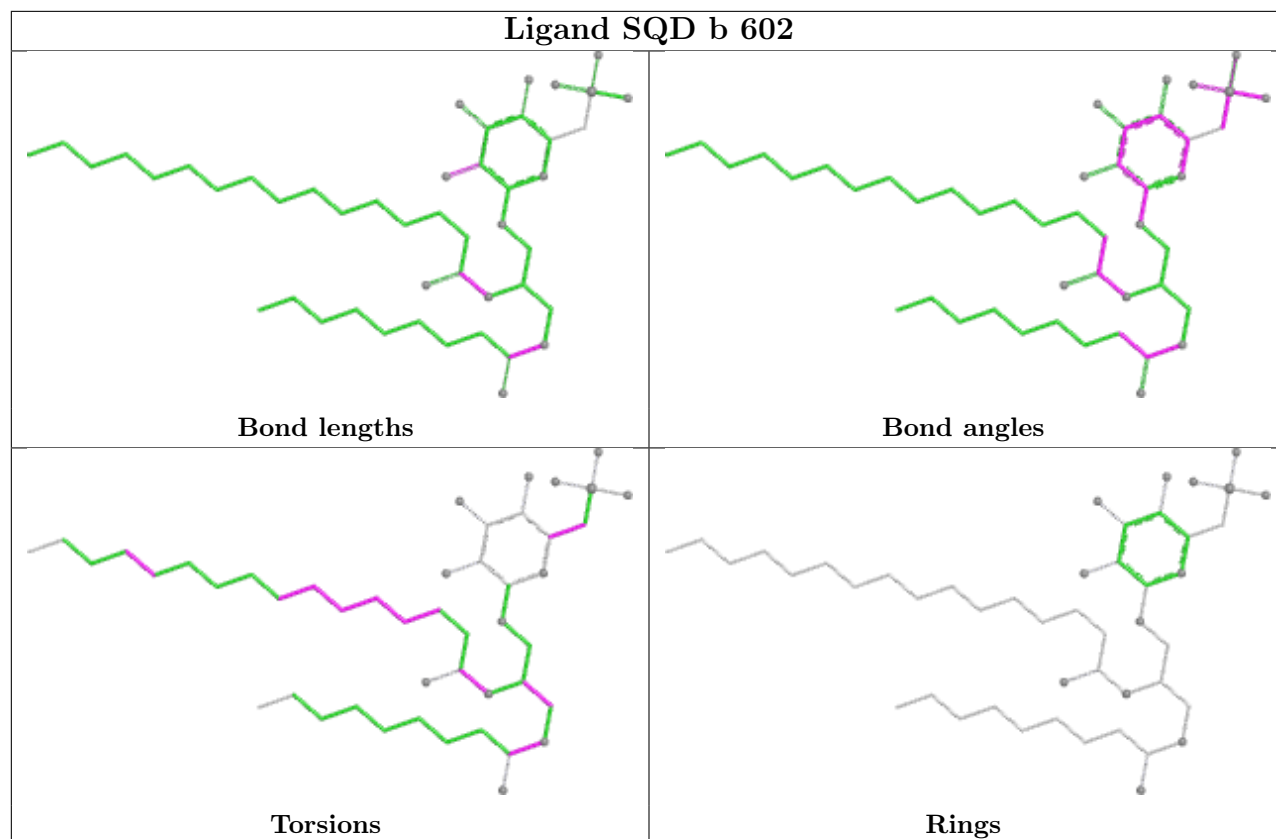
Ligand LMG A 410



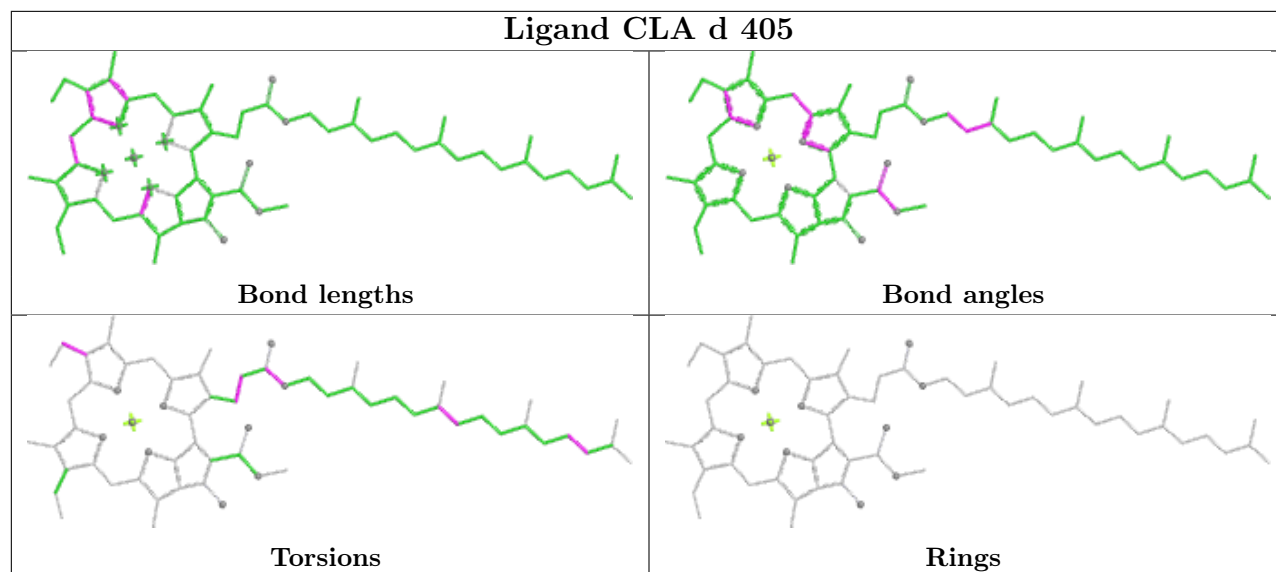
Ligand CLA A 403



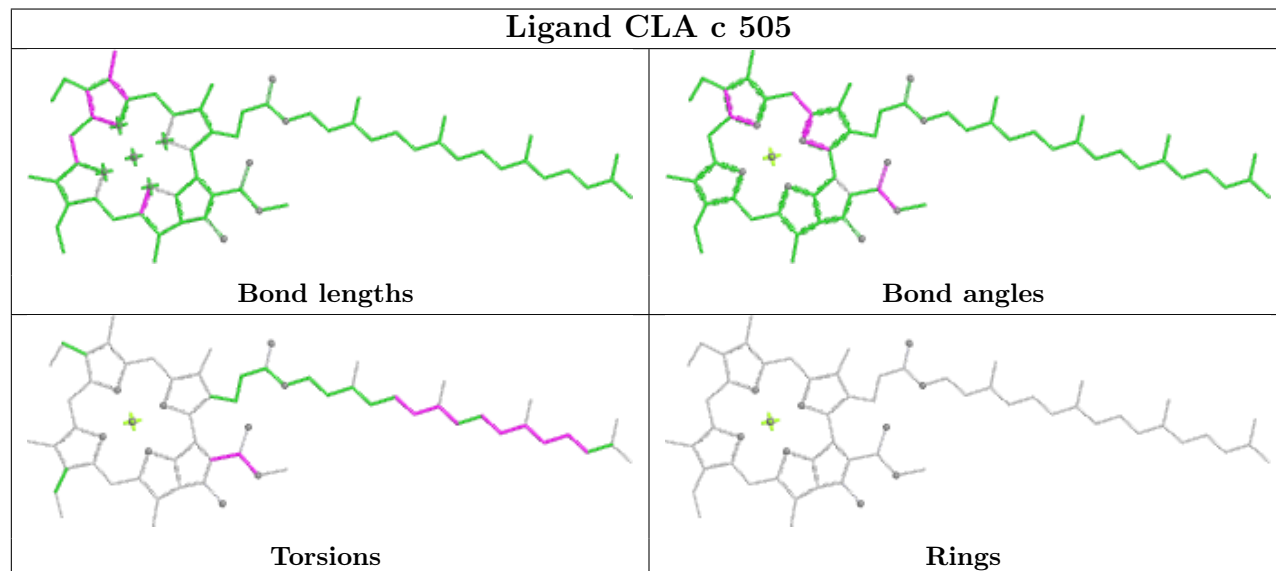




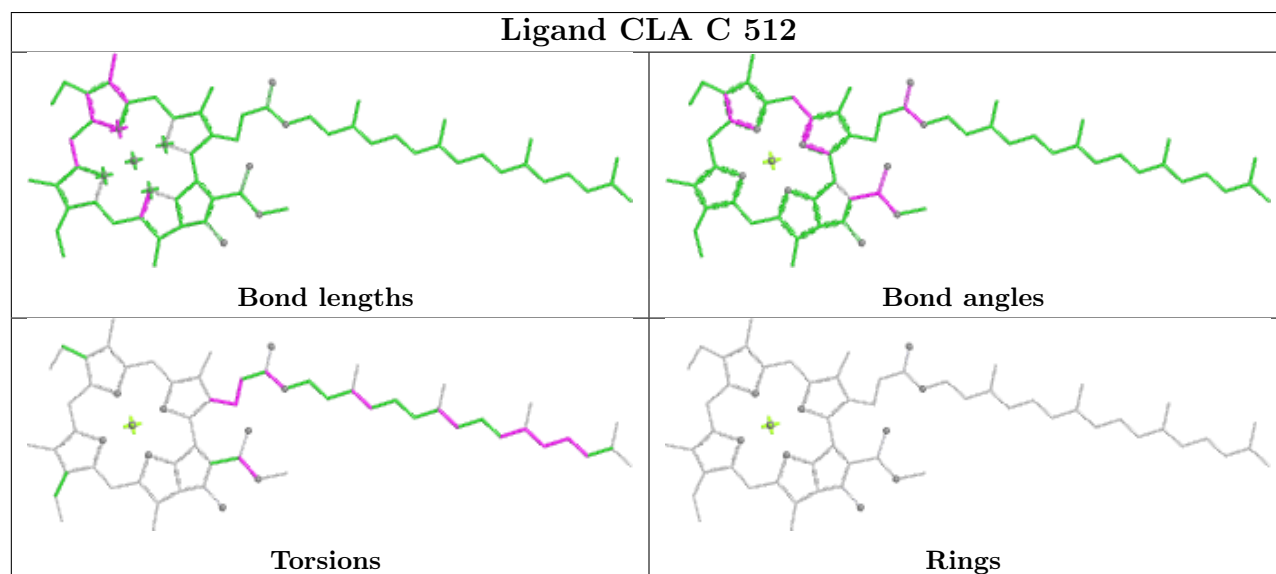
Ligand CLA d 405

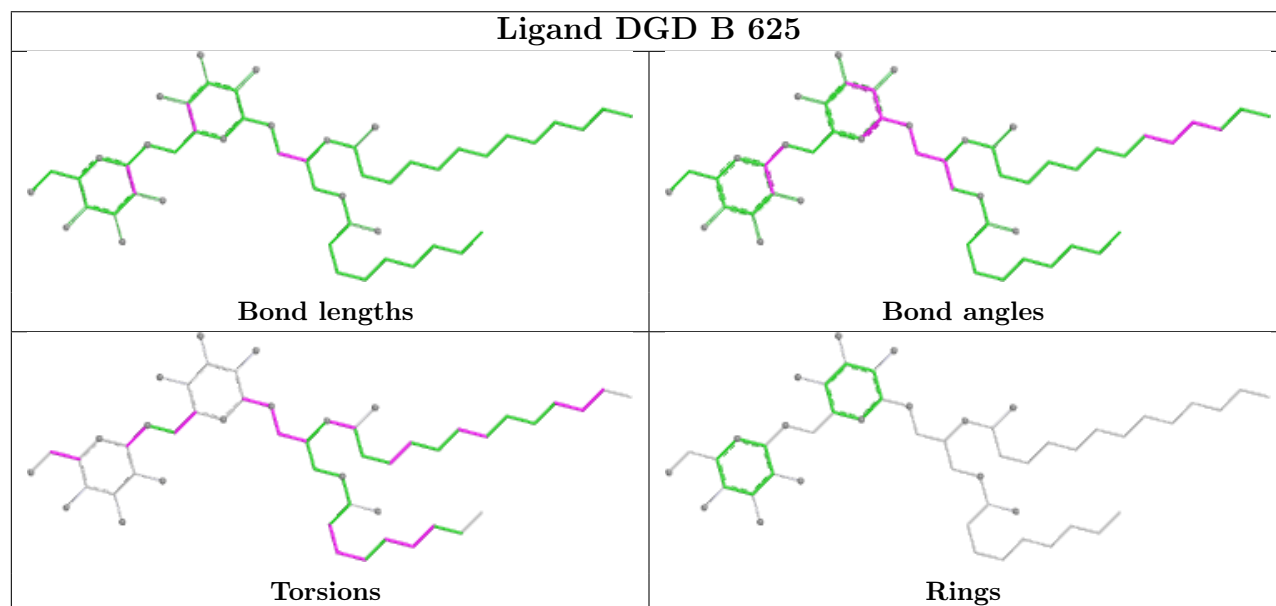
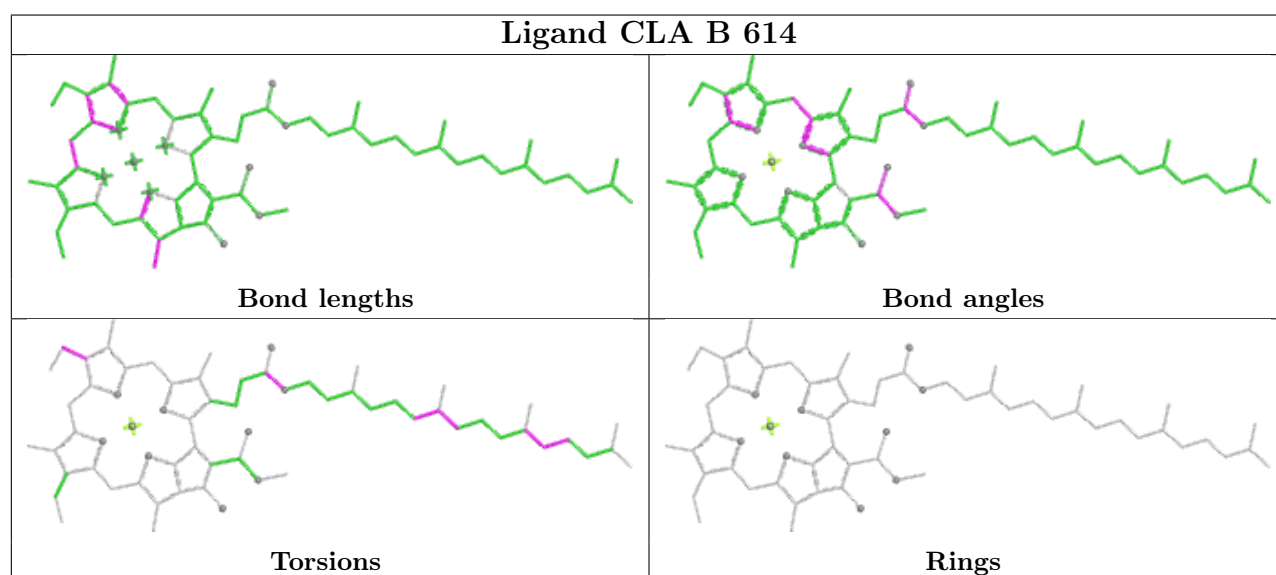
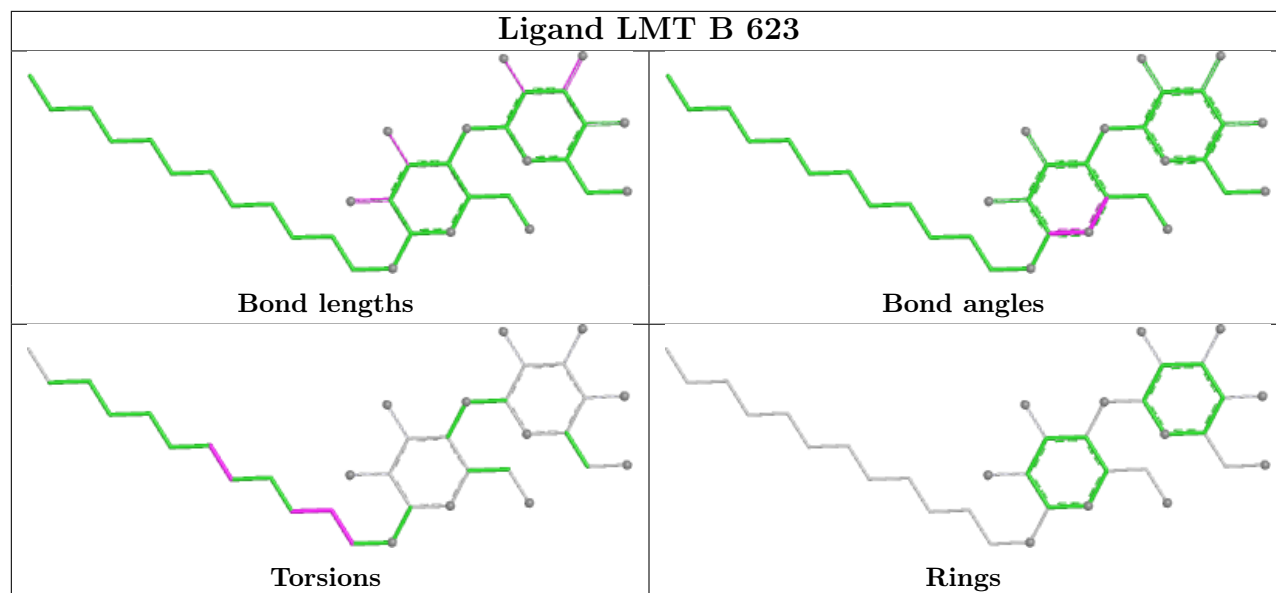


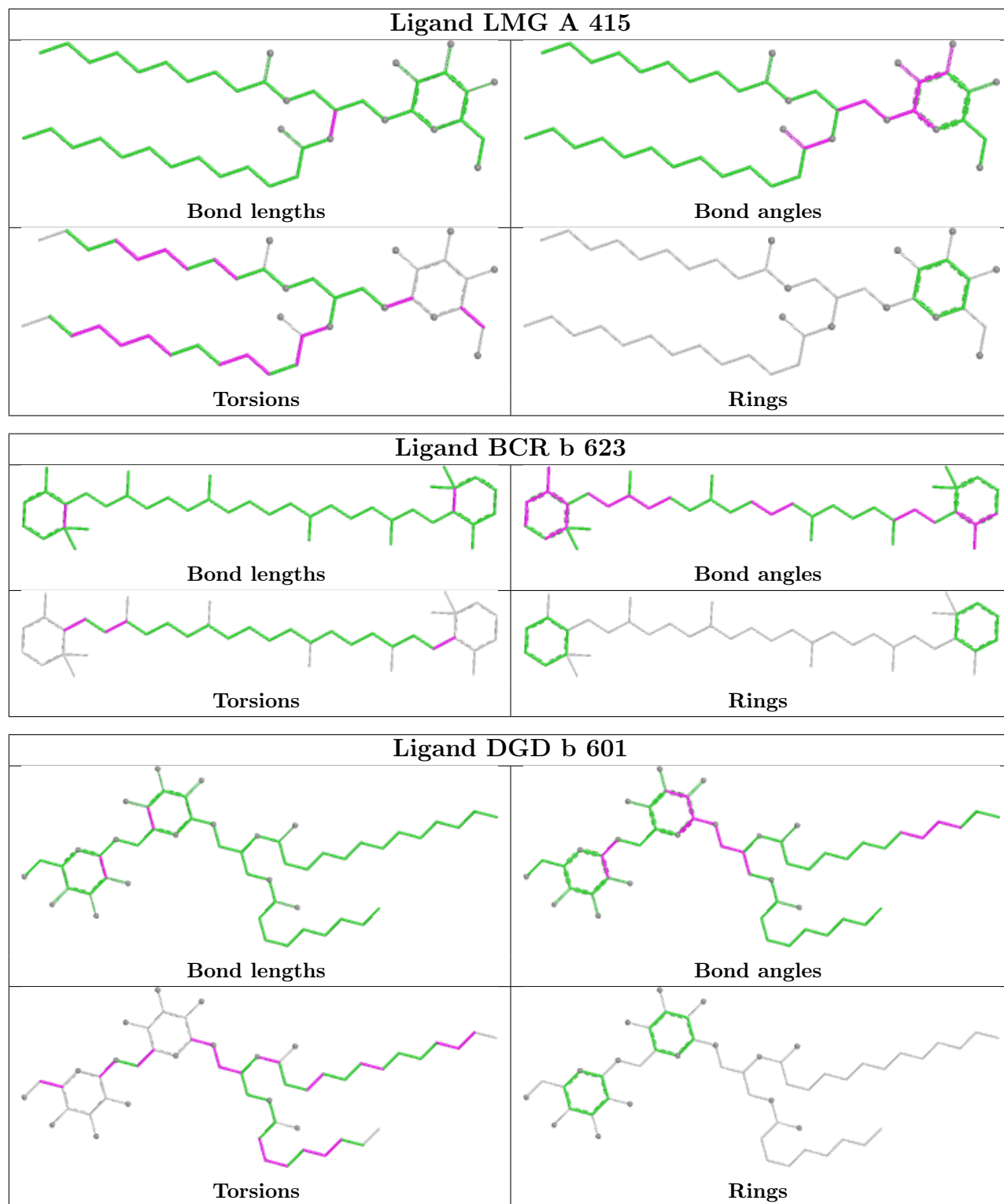
Ligand CLA c 505

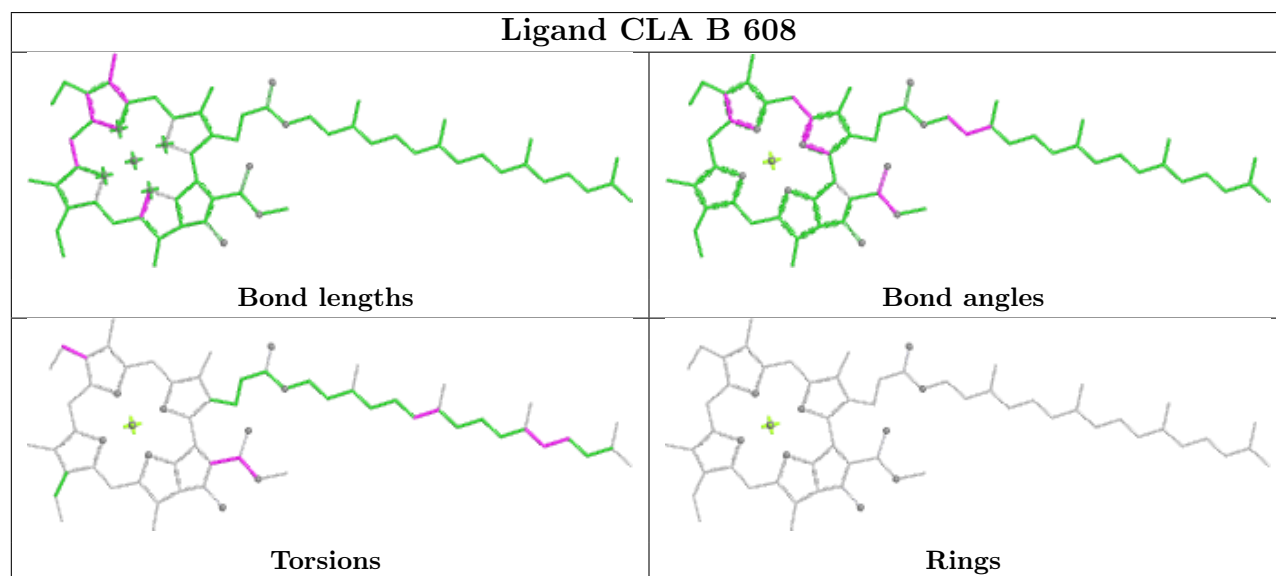
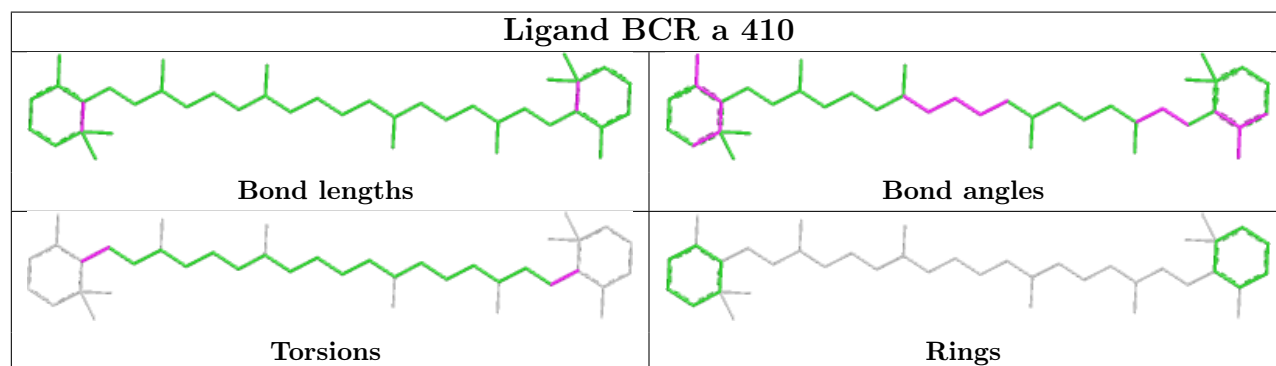
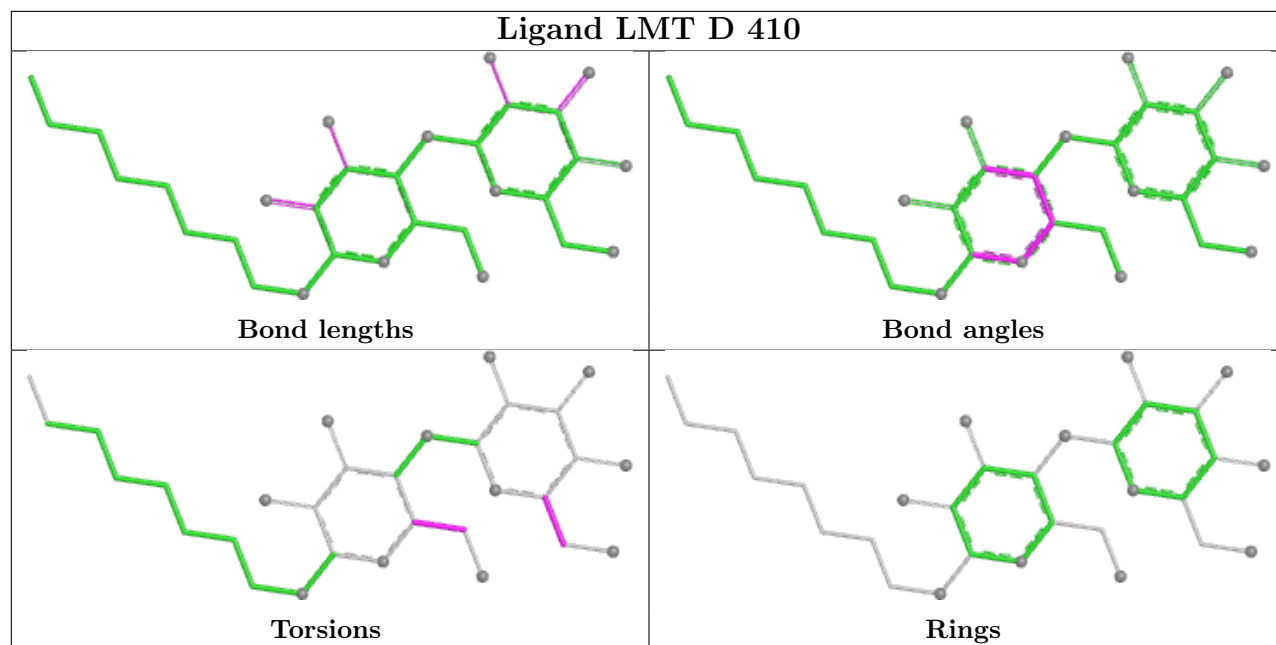


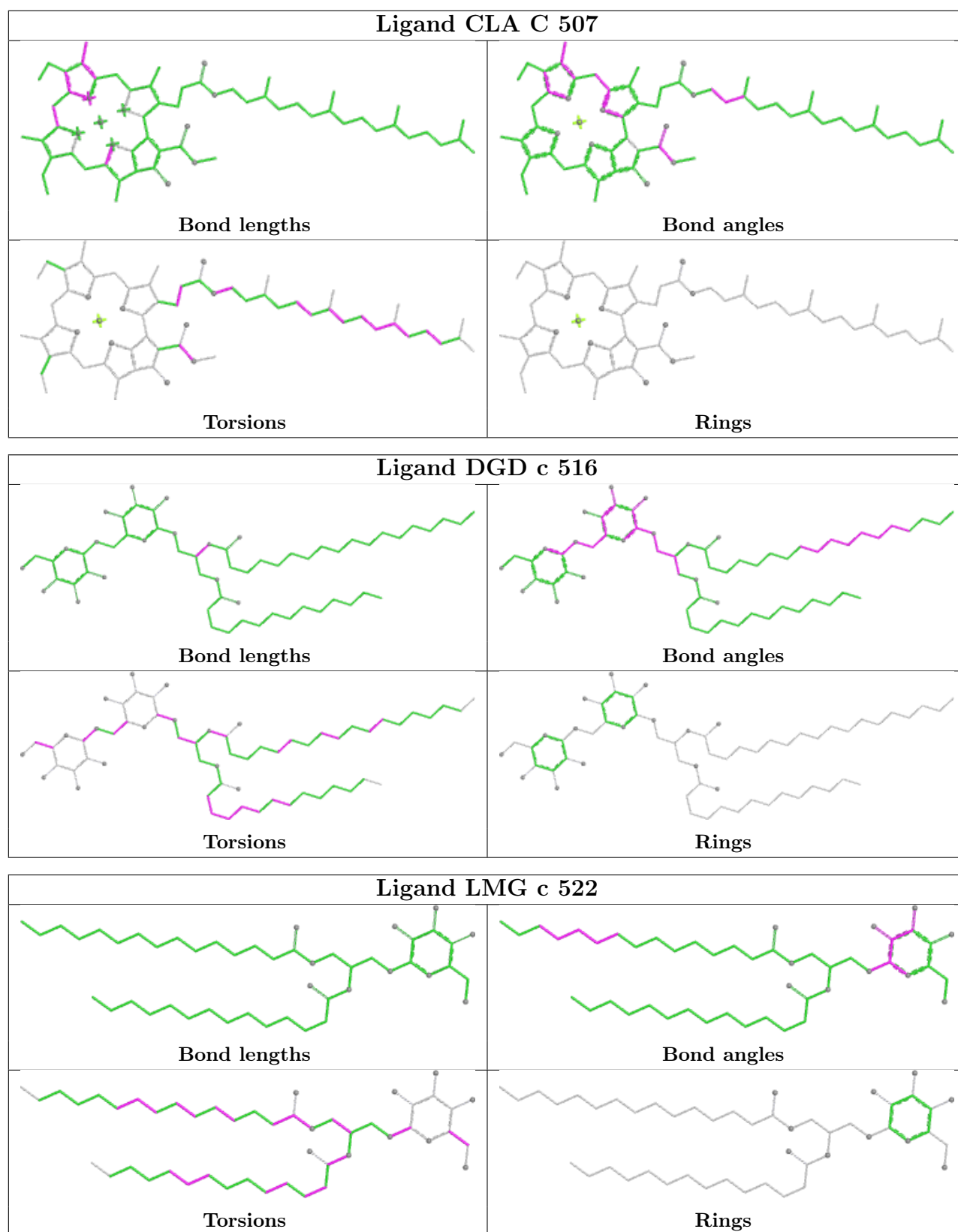
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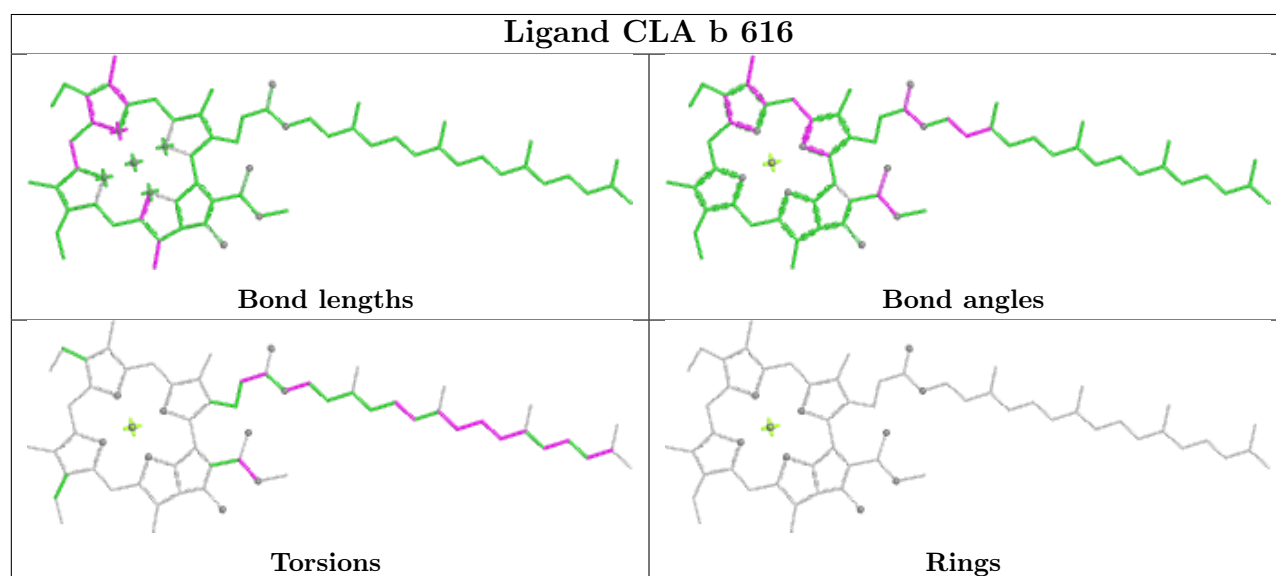
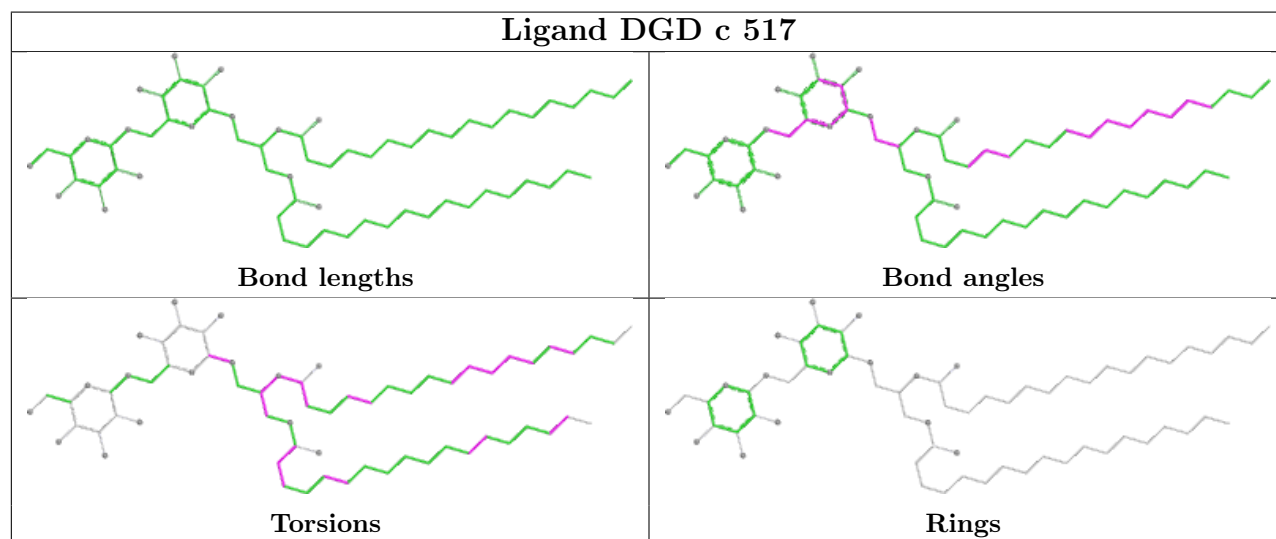
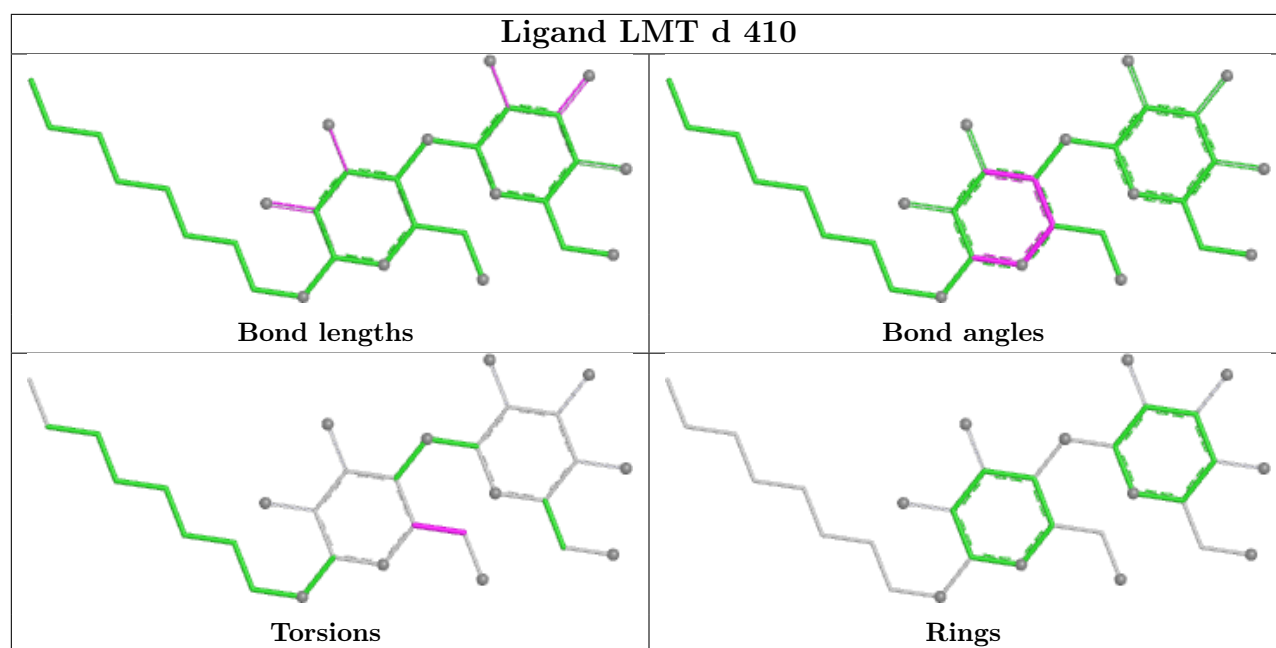




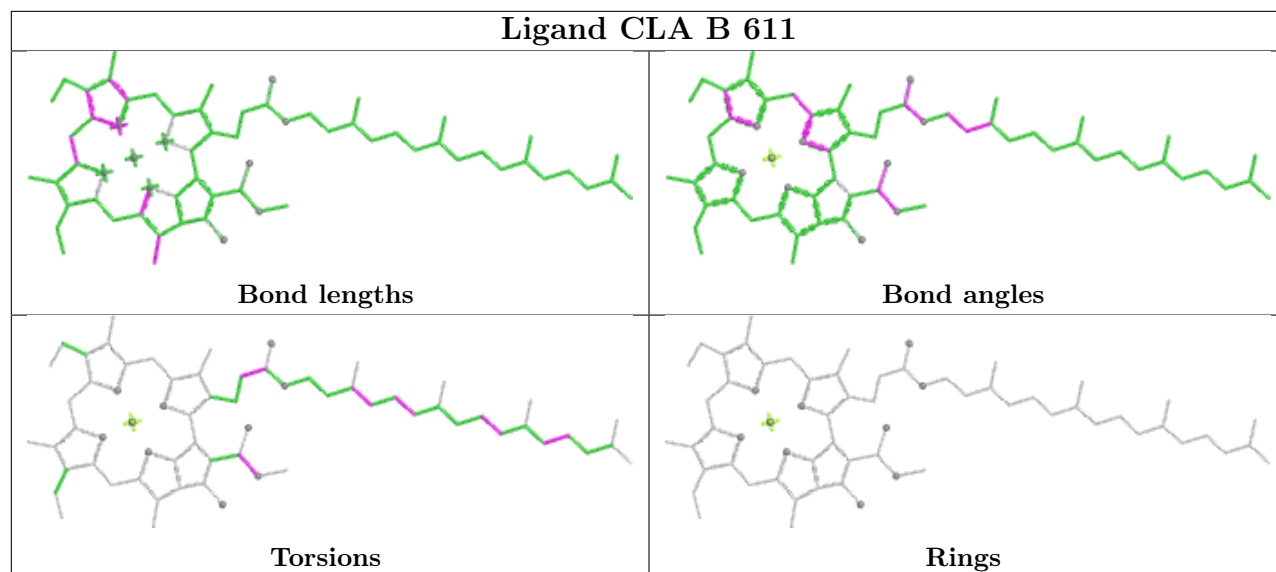




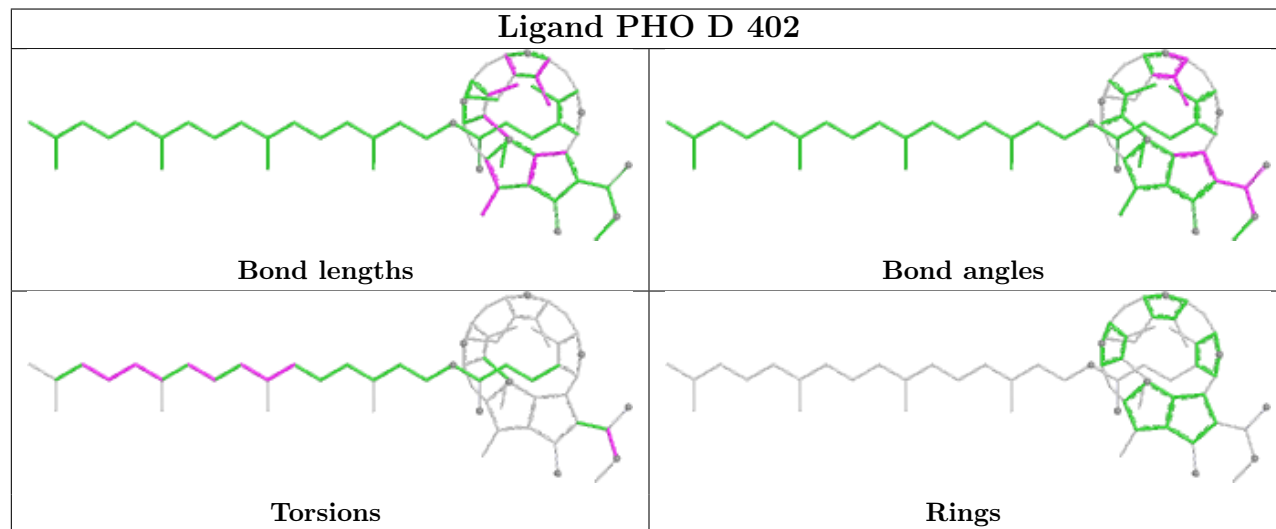




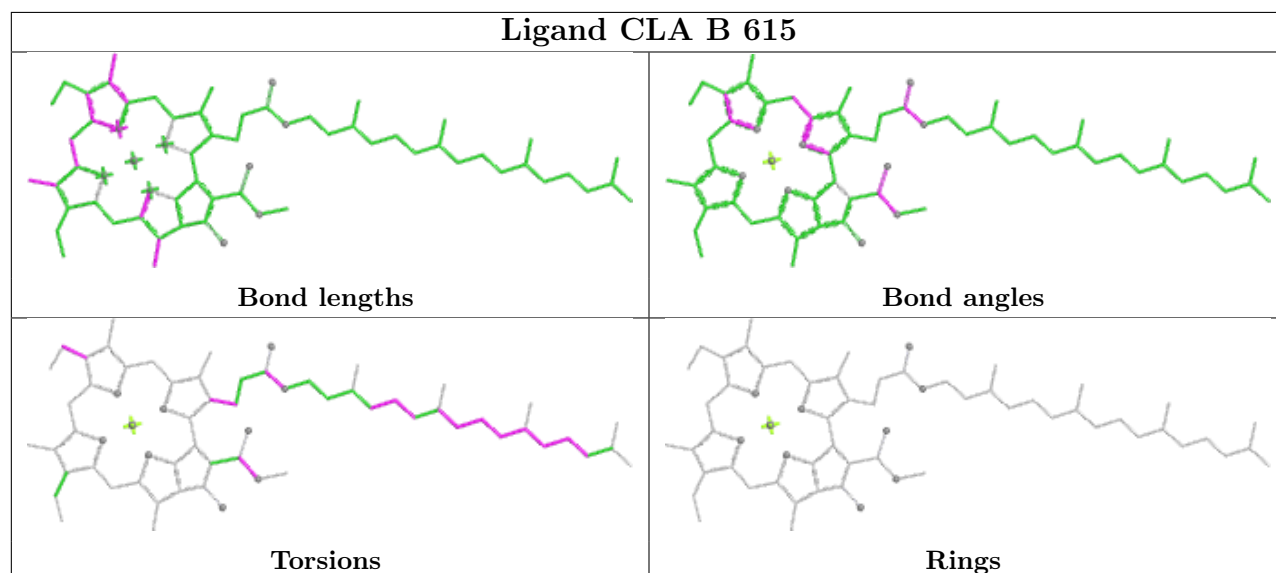
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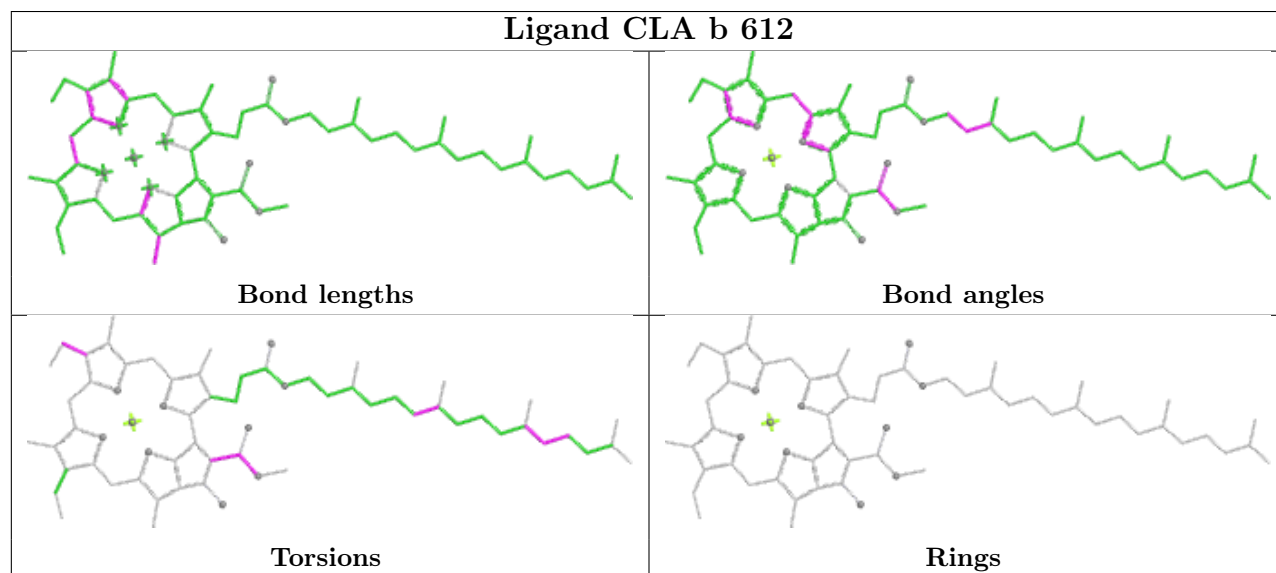
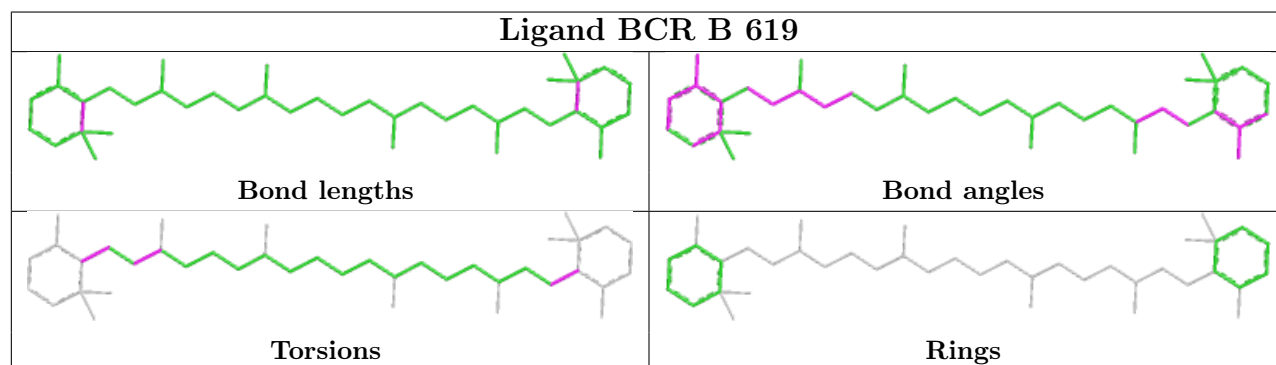
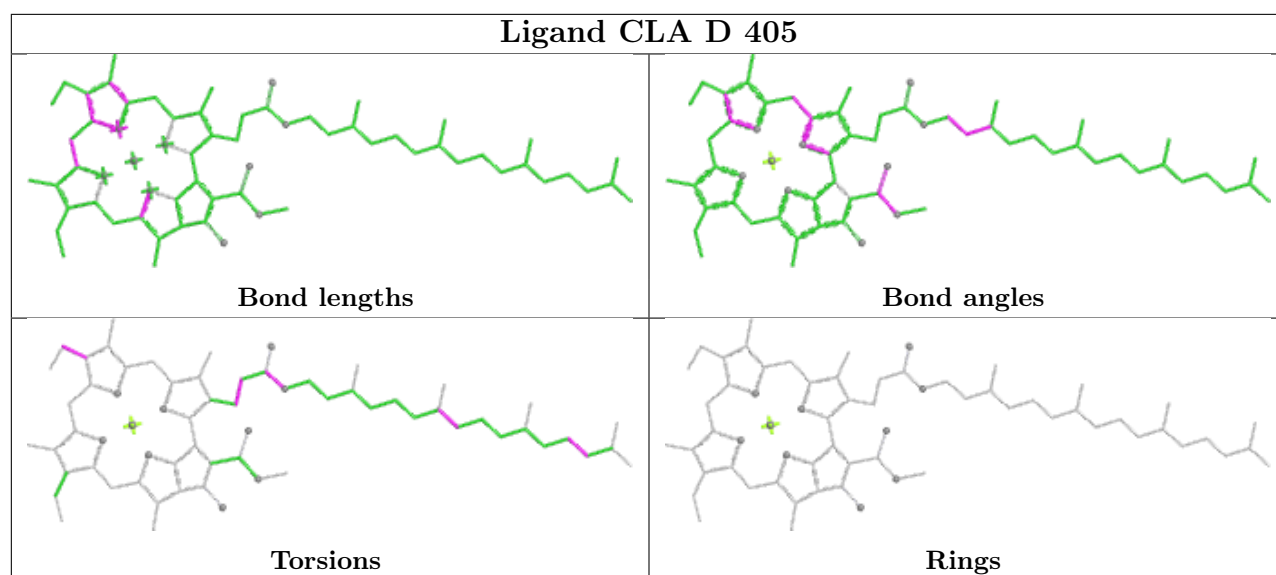


Ligand PHO D 402

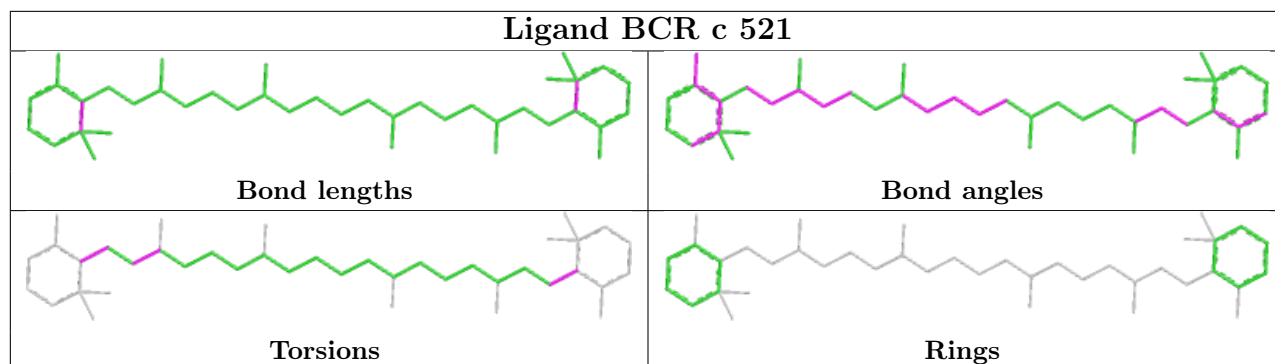


Ligand CLA B 615

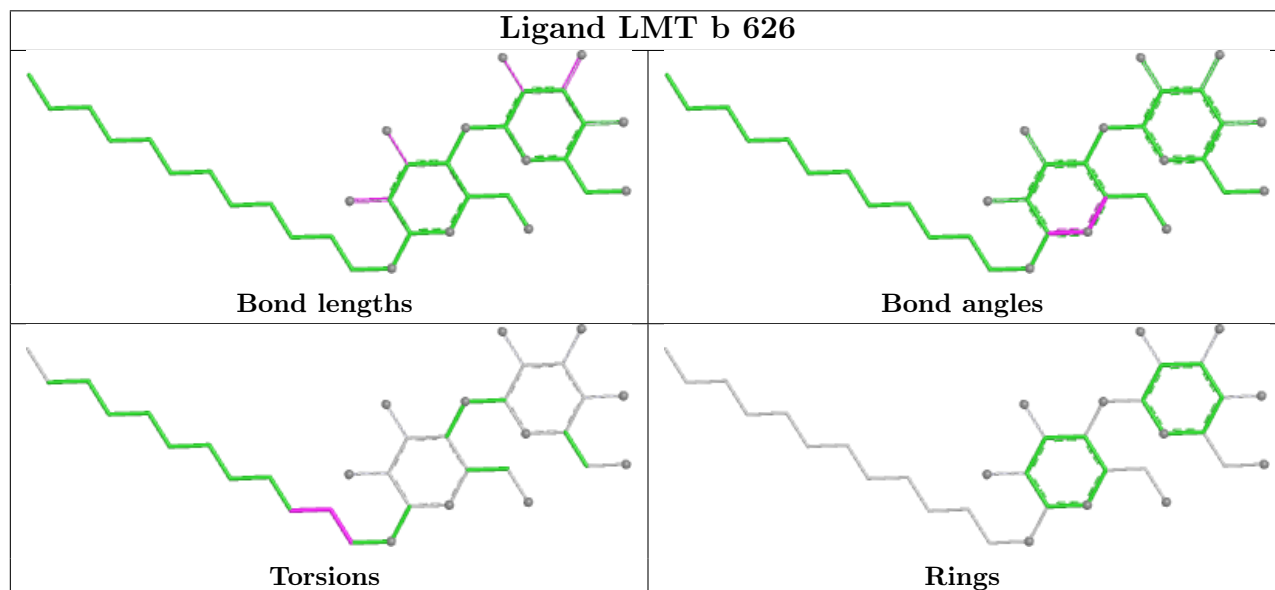




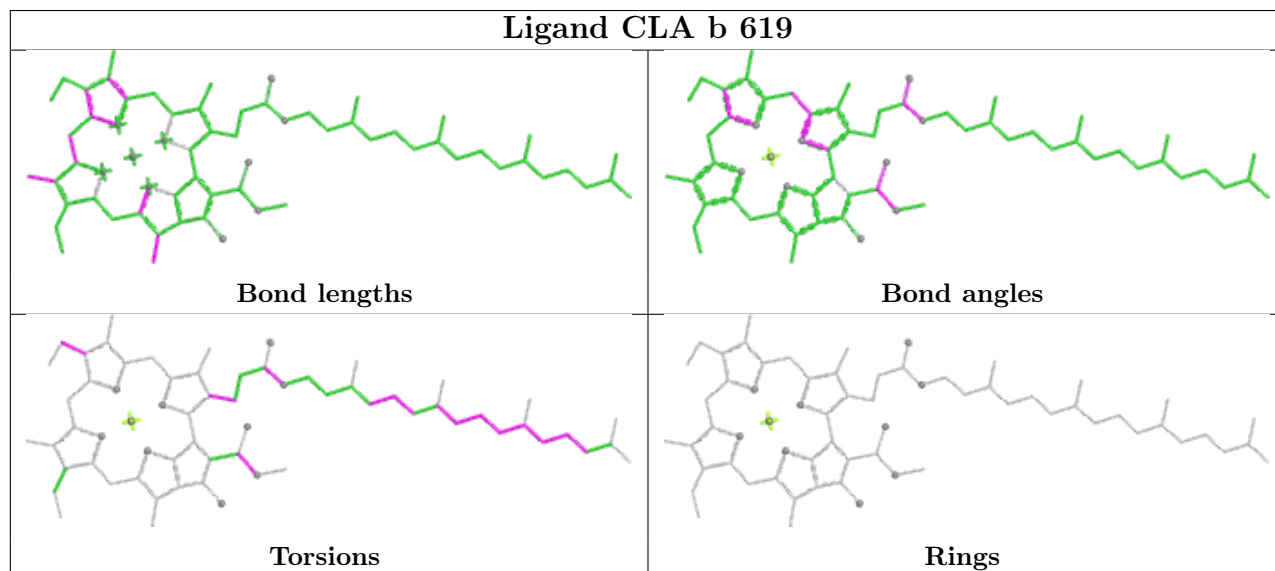
Ligand BCR c 521



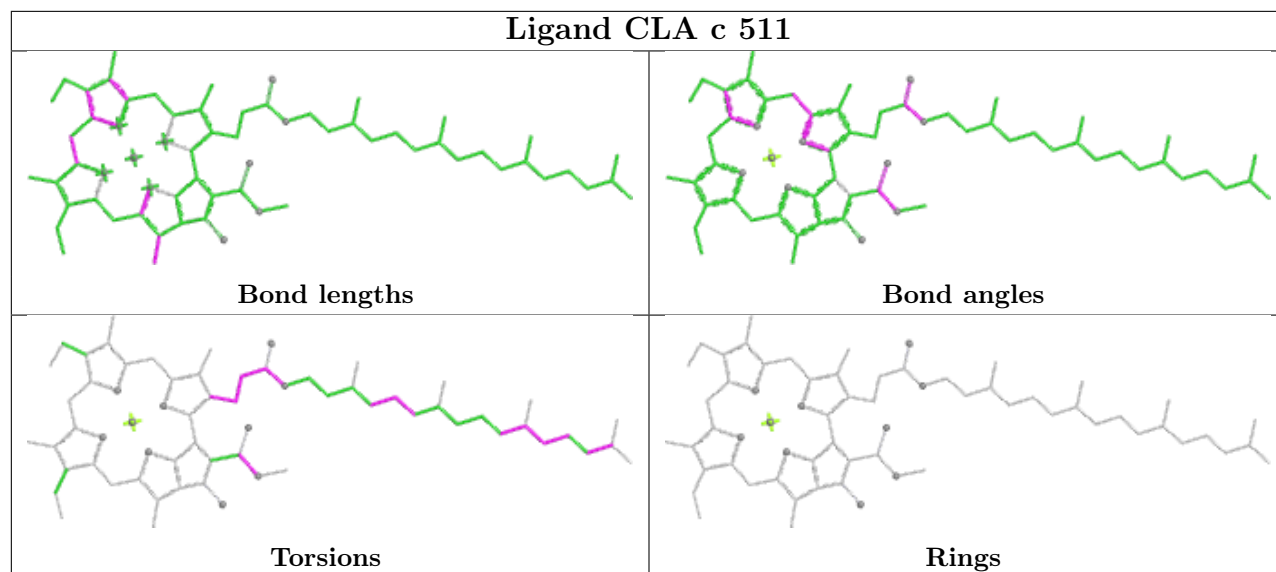
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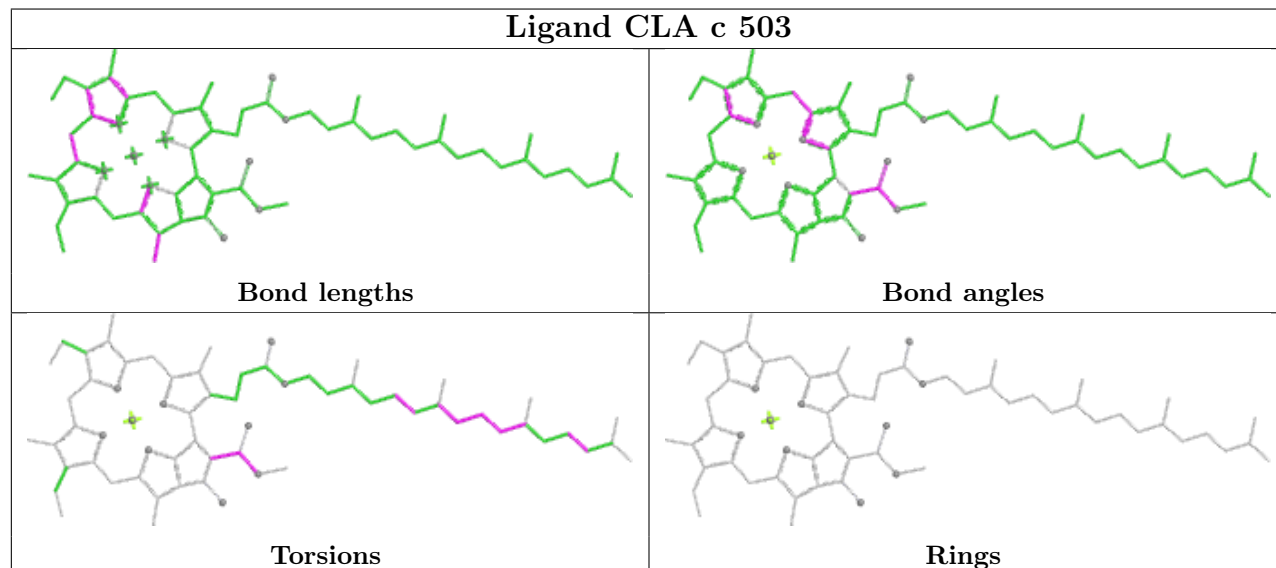
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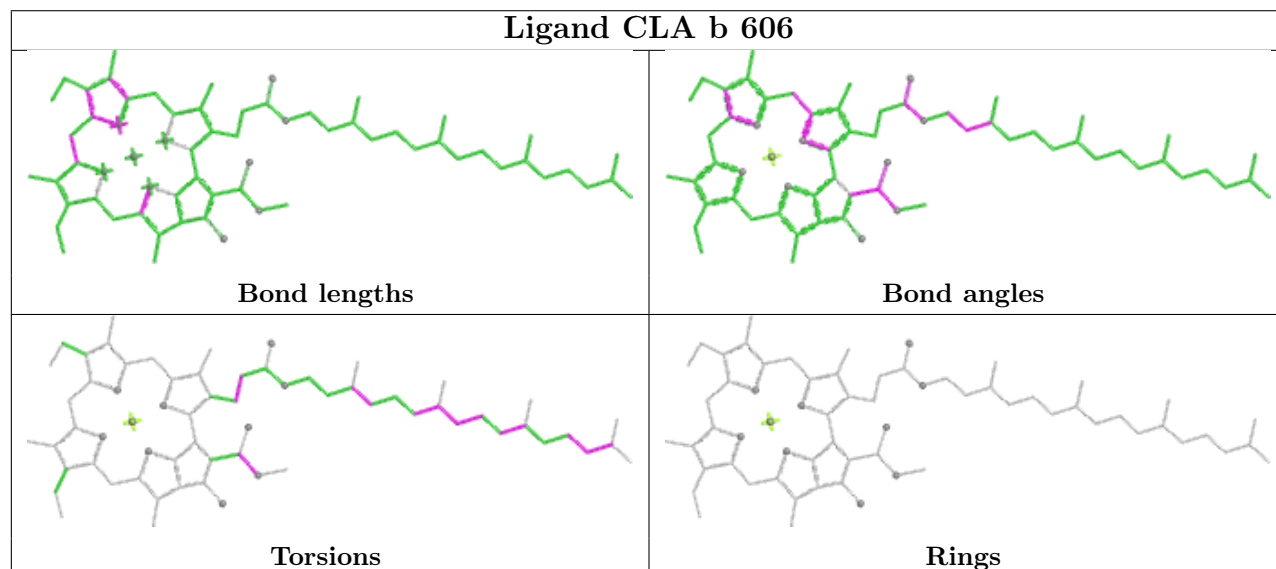
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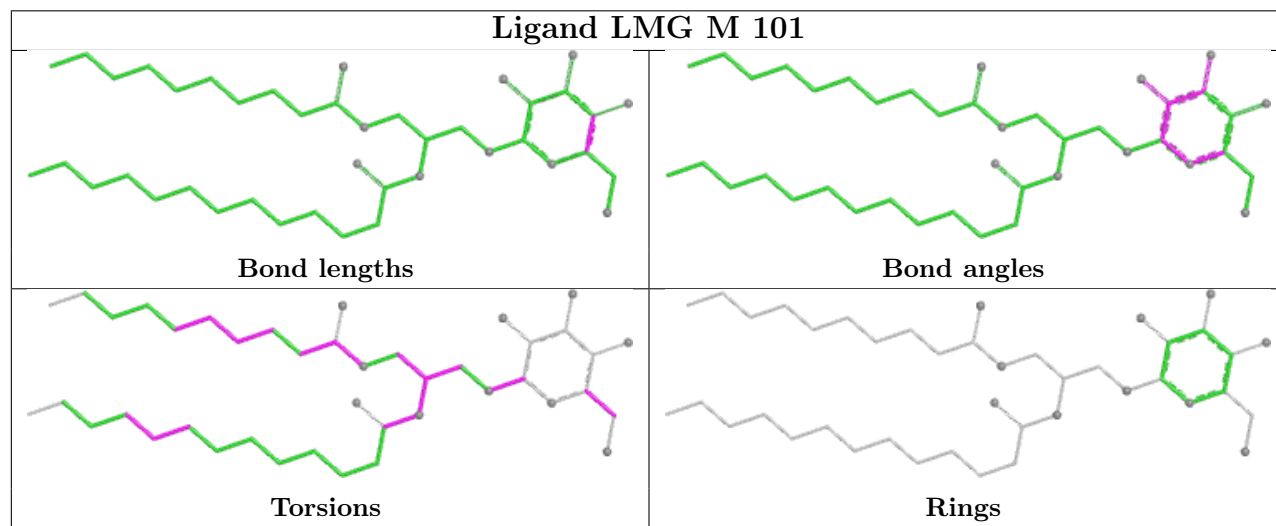
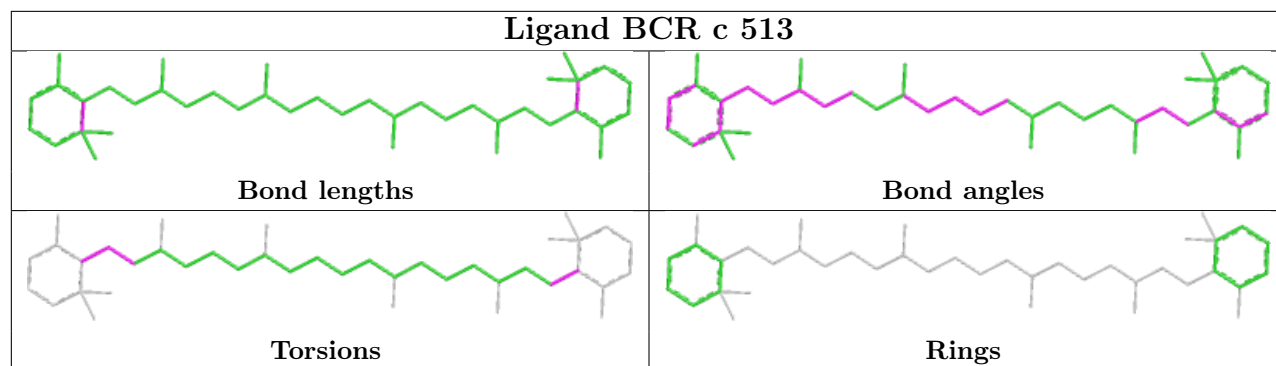


Ligand CLA c 503

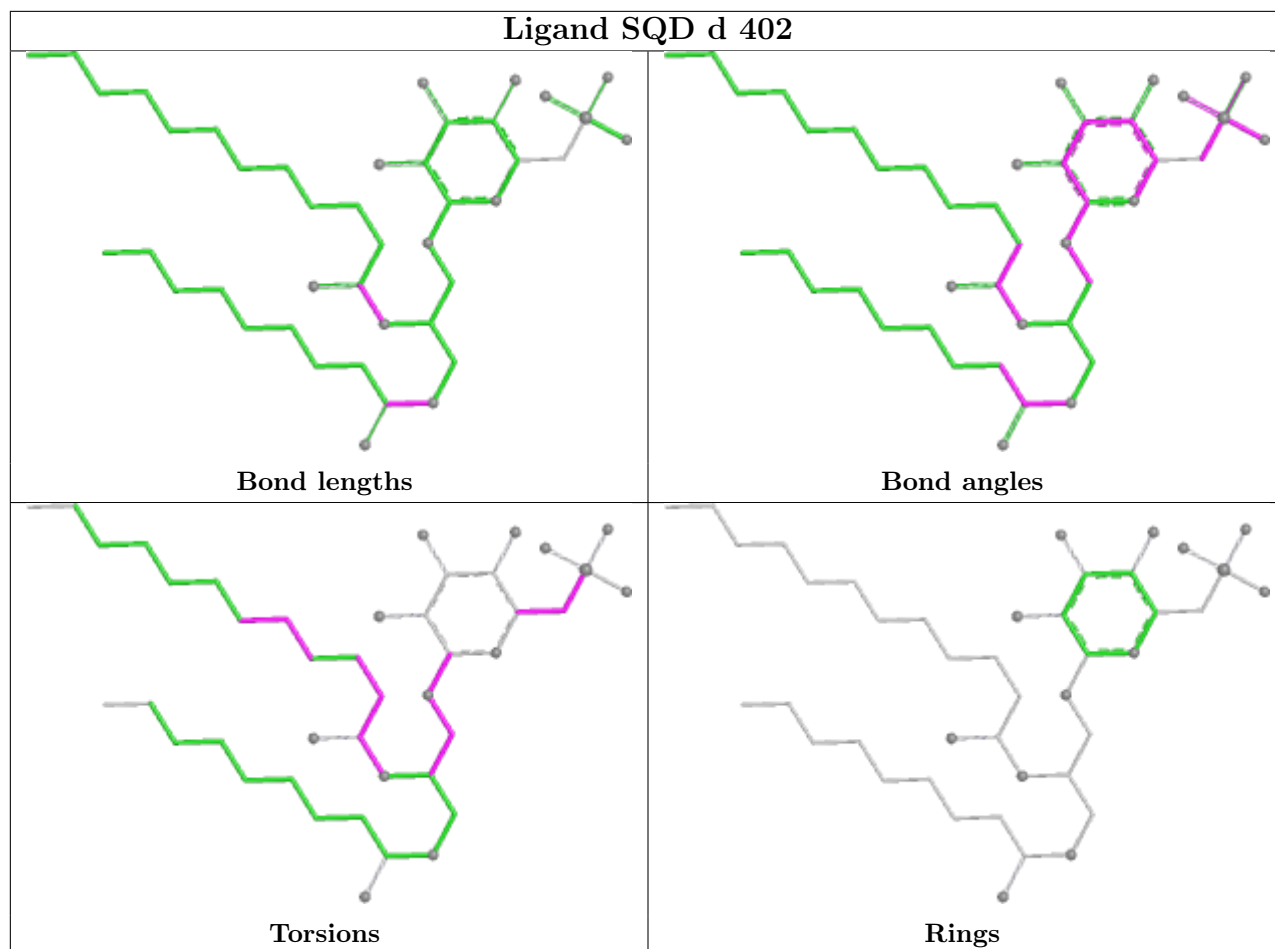


Ligand CLA b 606

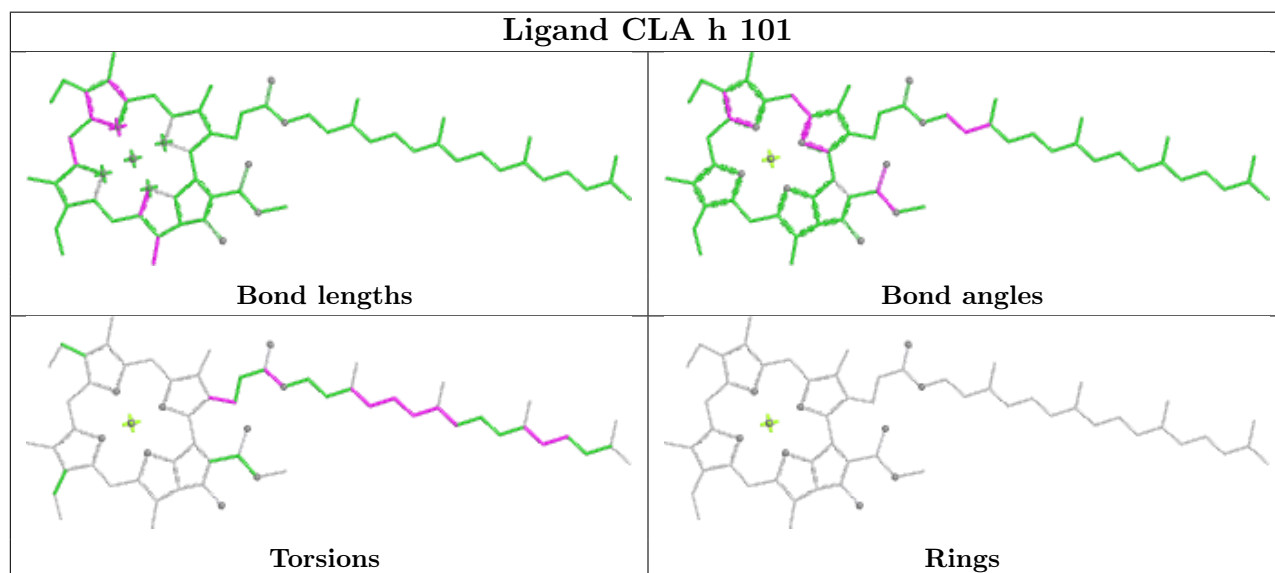


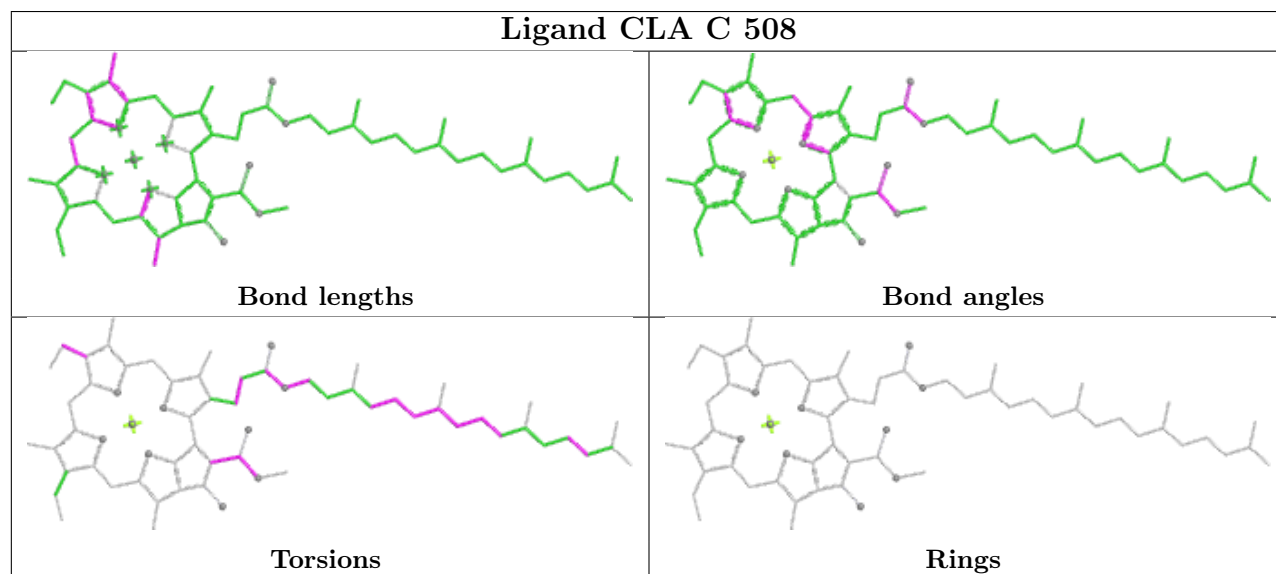
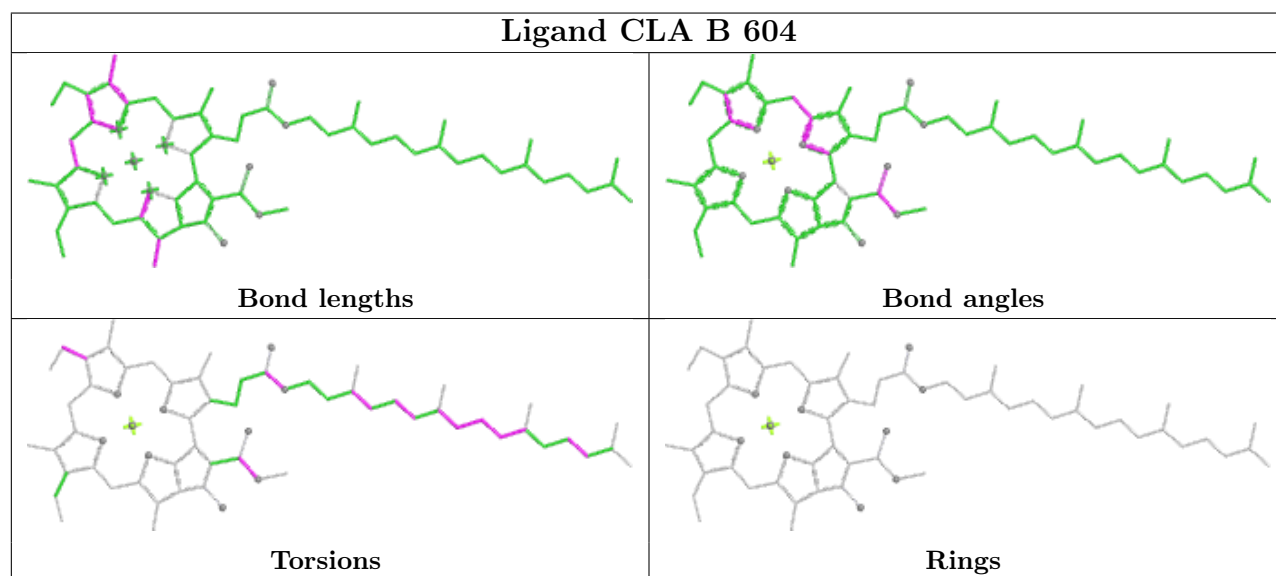
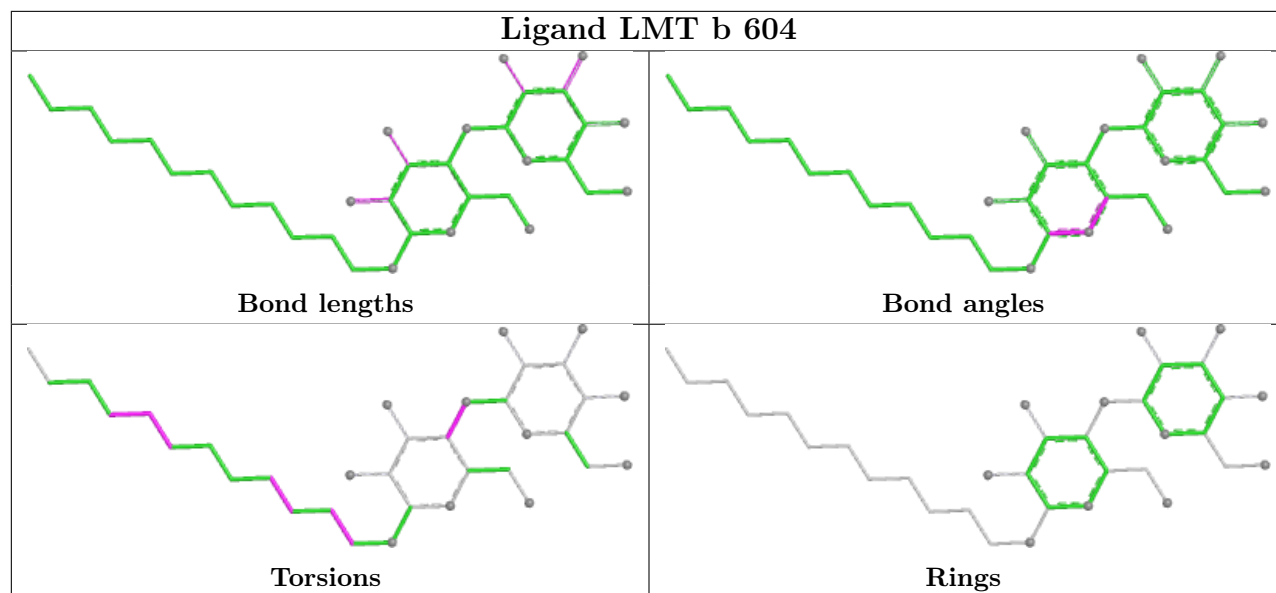


Ligand SQD d 402

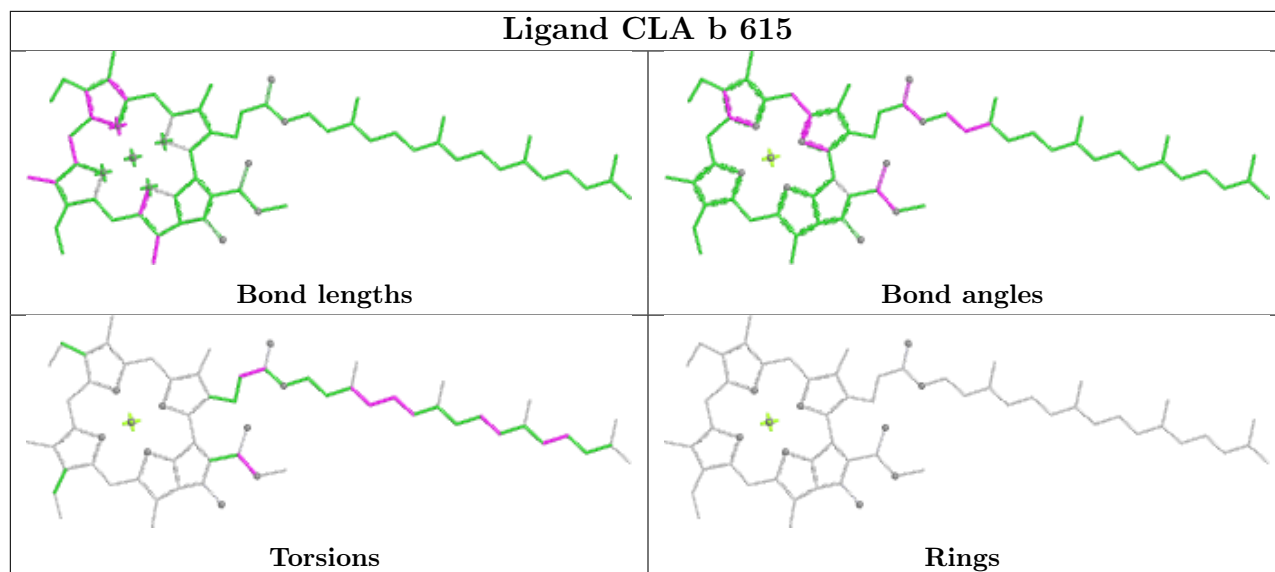


Ligand CLA h 101

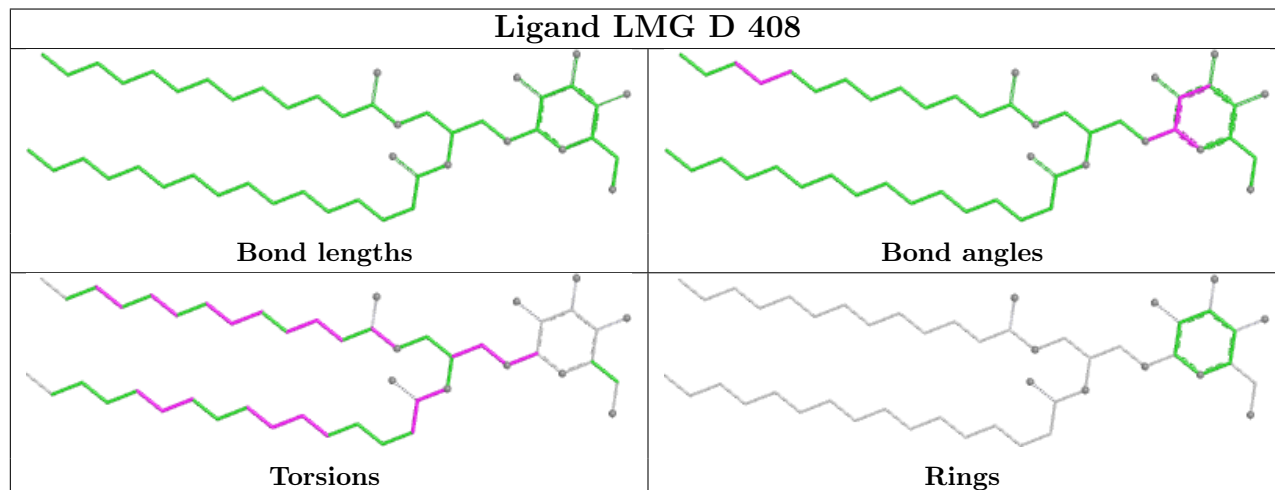




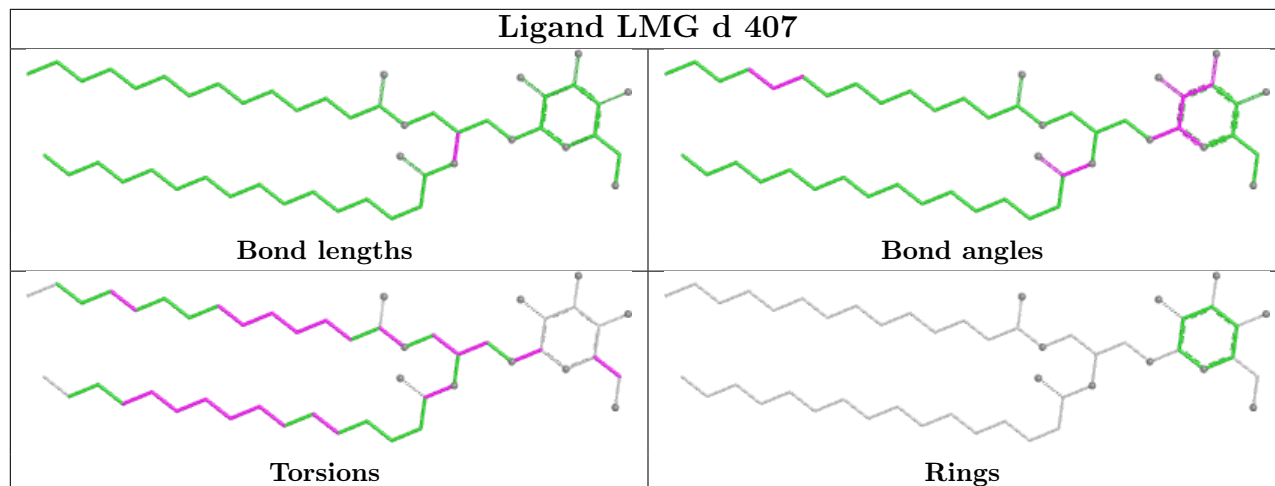
Ligand CLA b 615



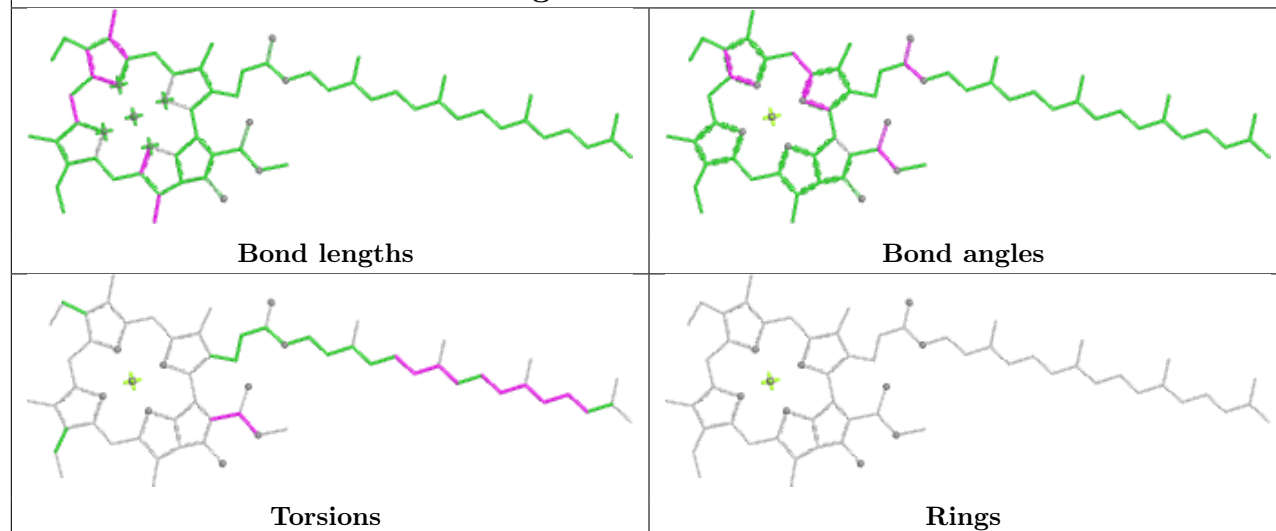
Ligand LMG D 408



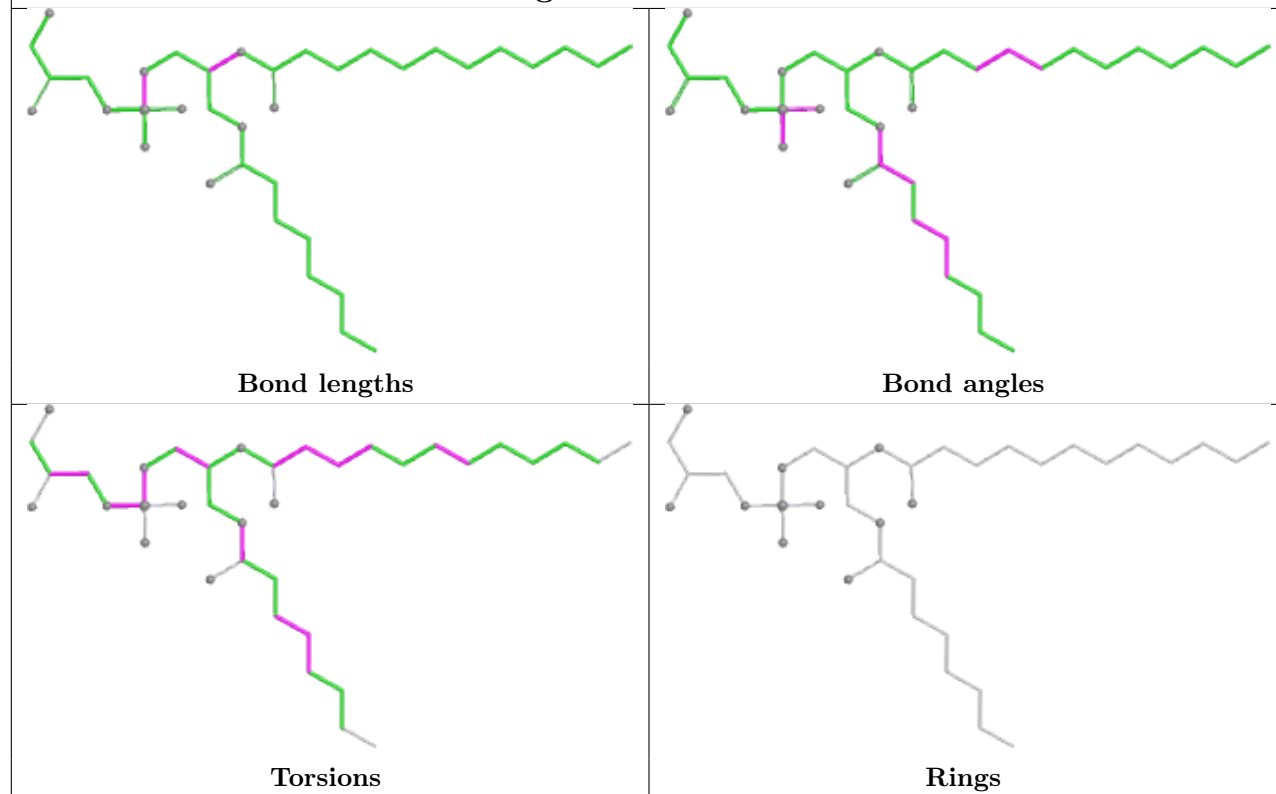
Ligand LMG d 407



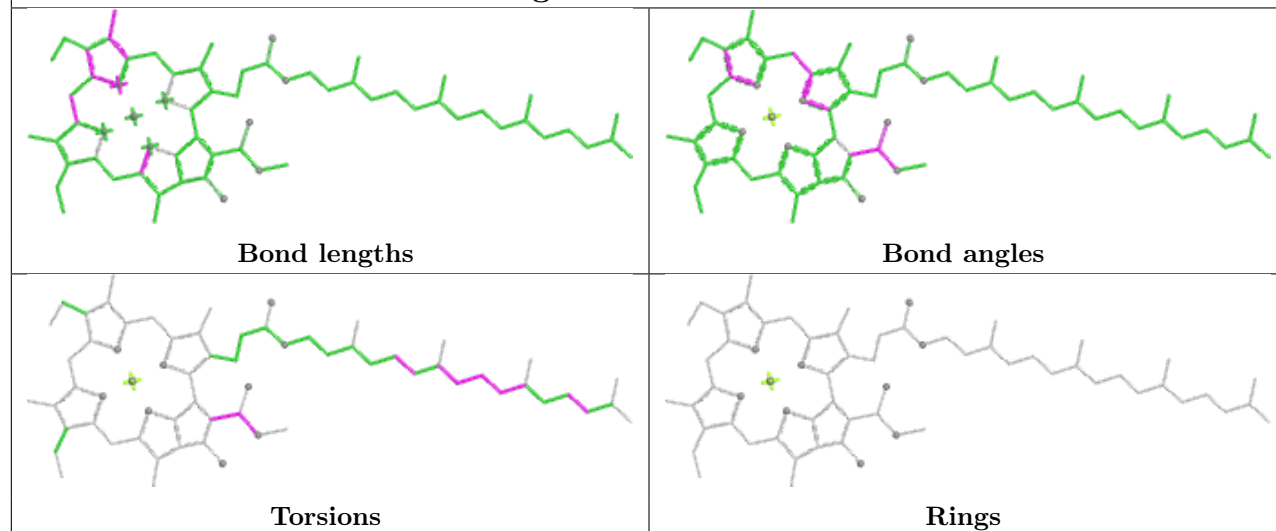
Ligand CLA C 505



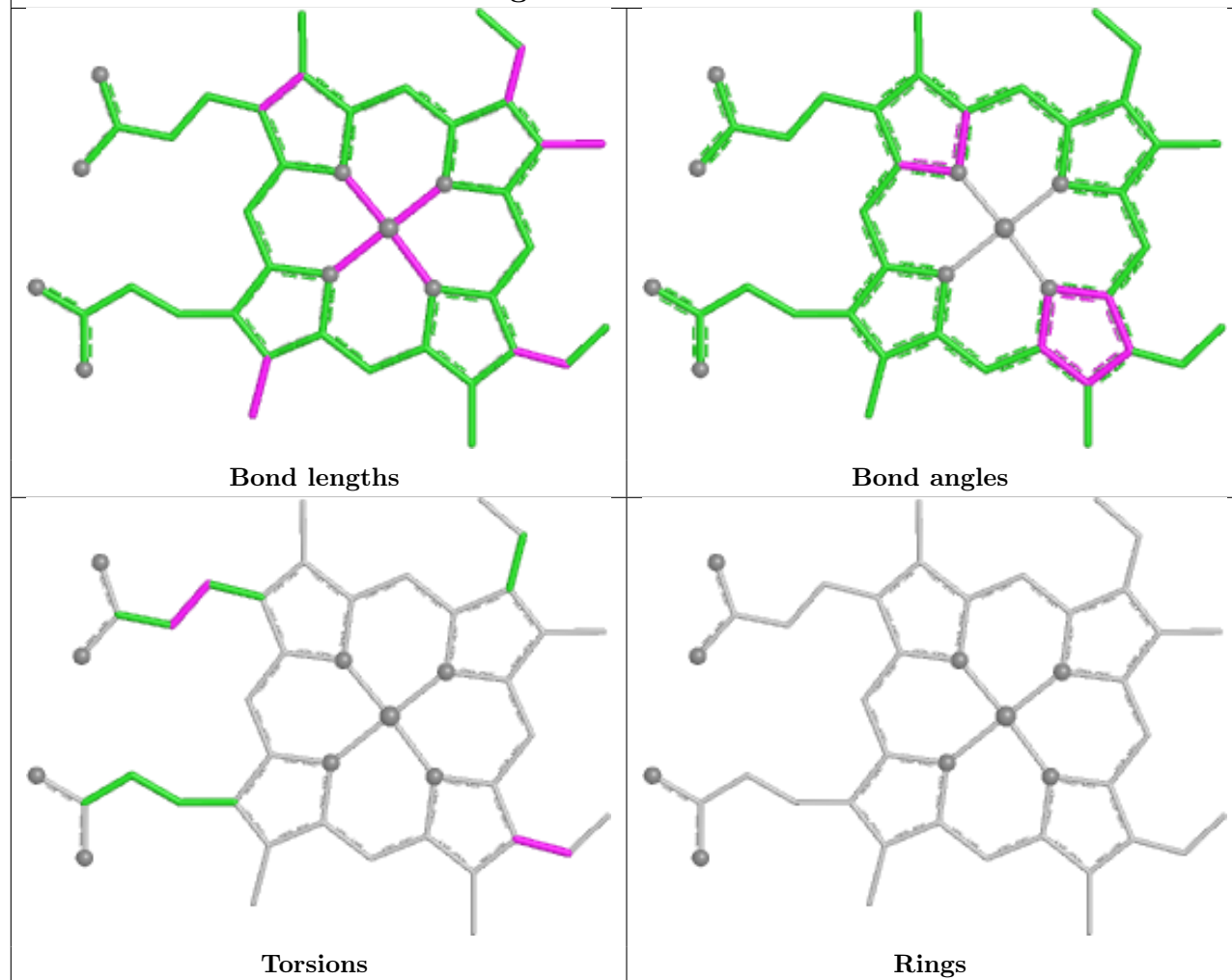
Ligand LHG c 519



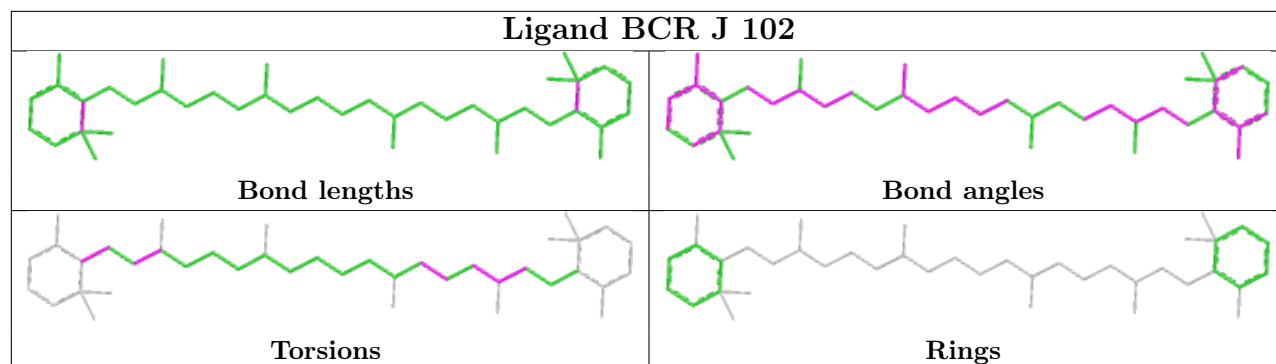
Ligand CLA C 503



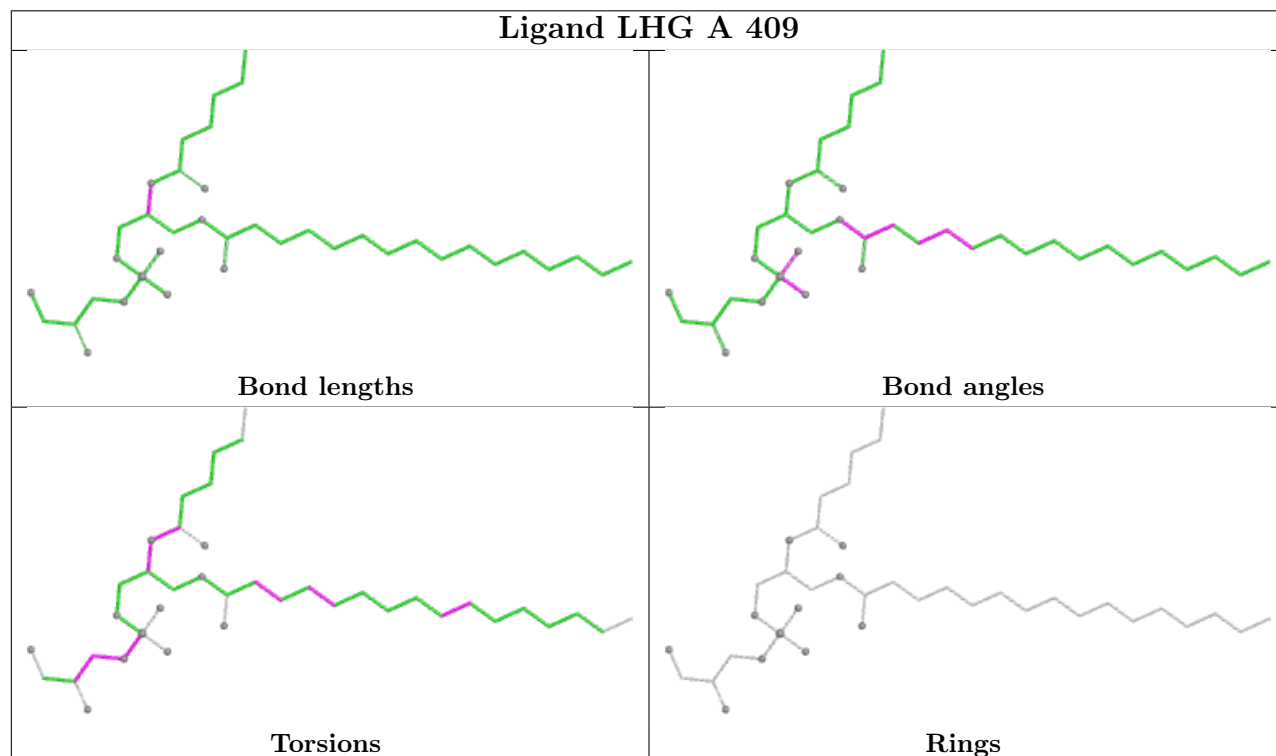
Ligand HEM F 101



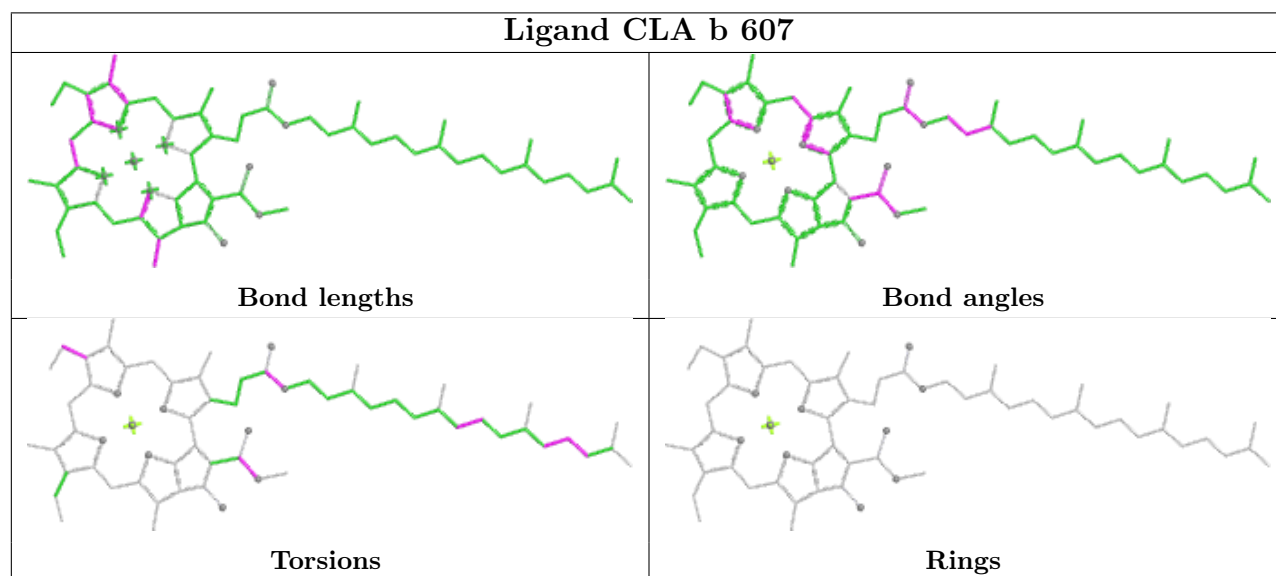
Ligand BCR J 102



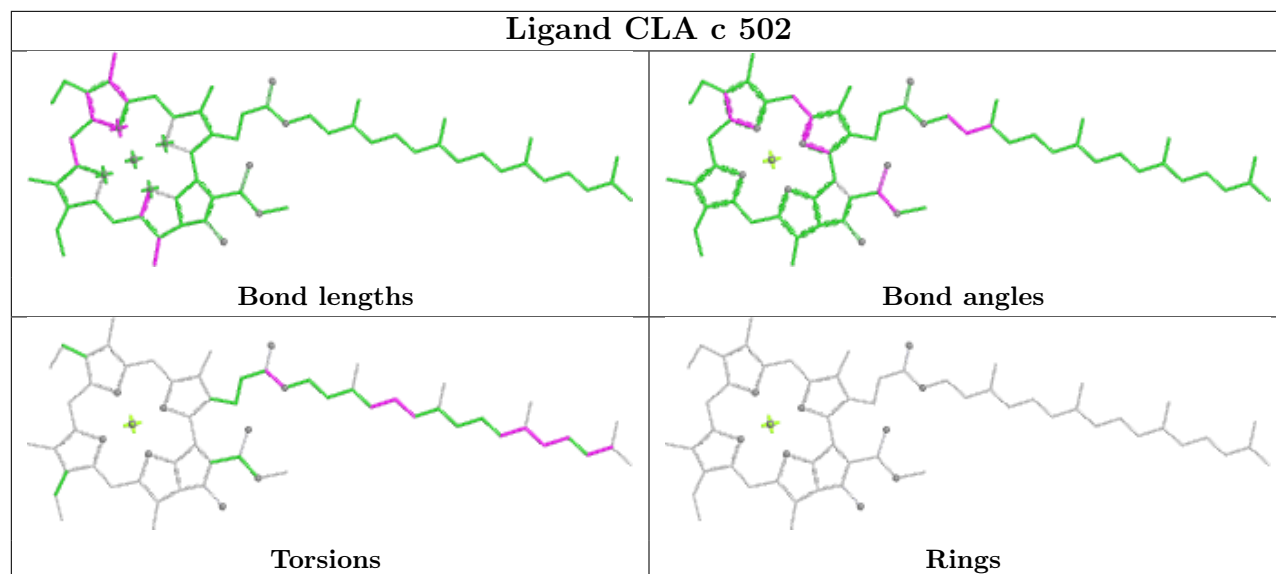
Ligand LHG A 409



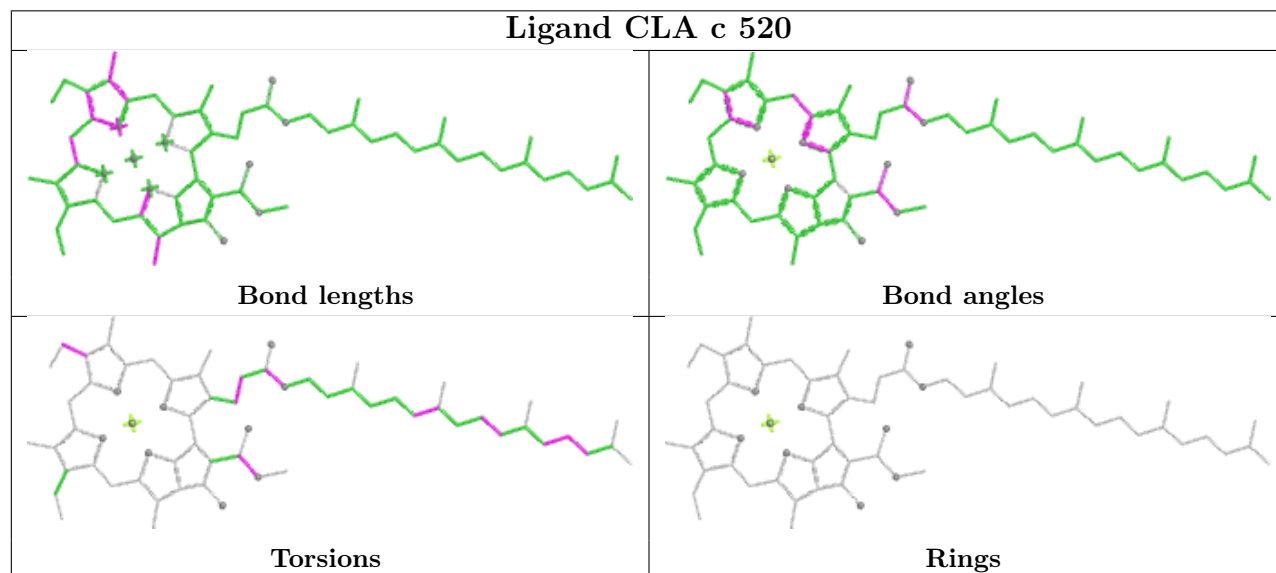
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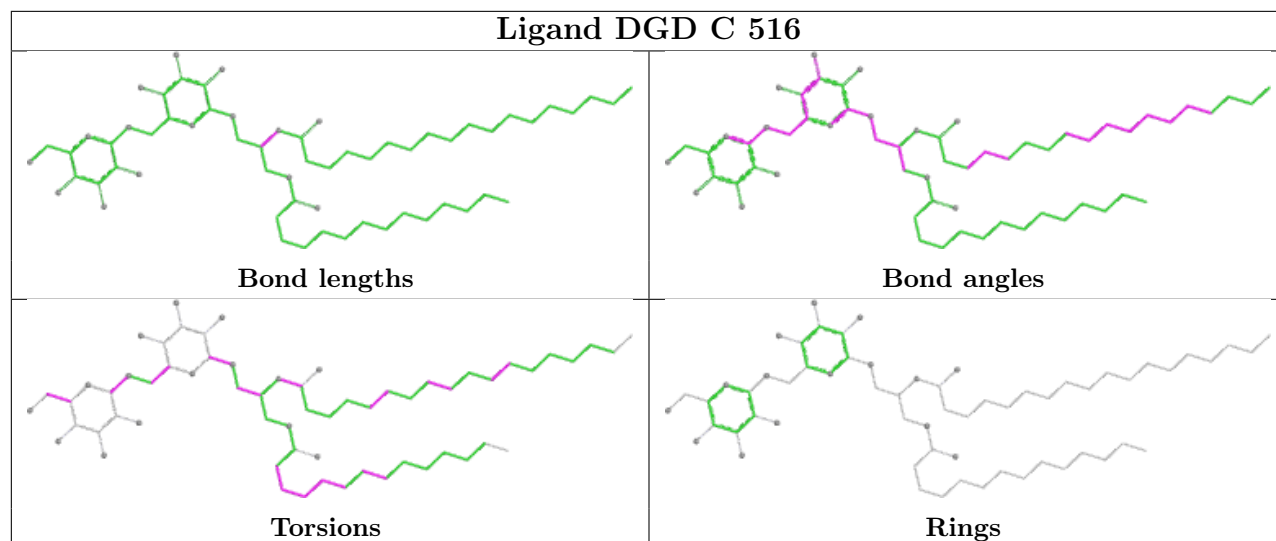
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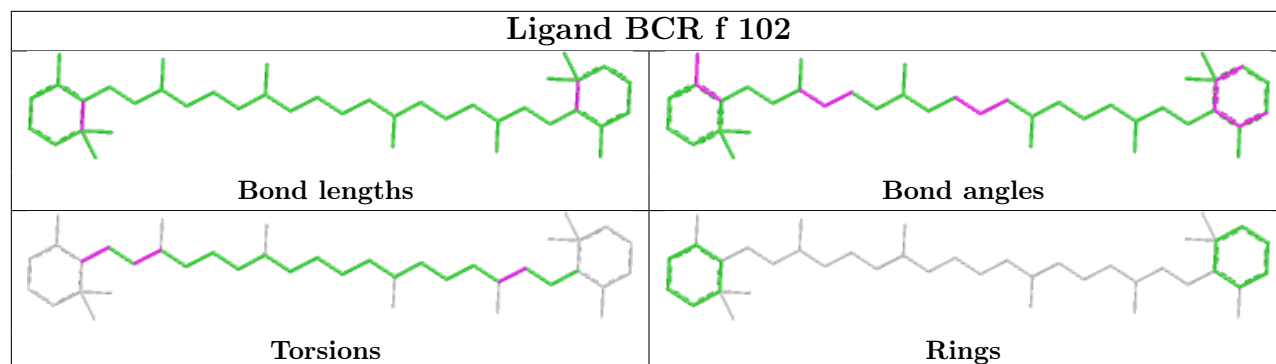
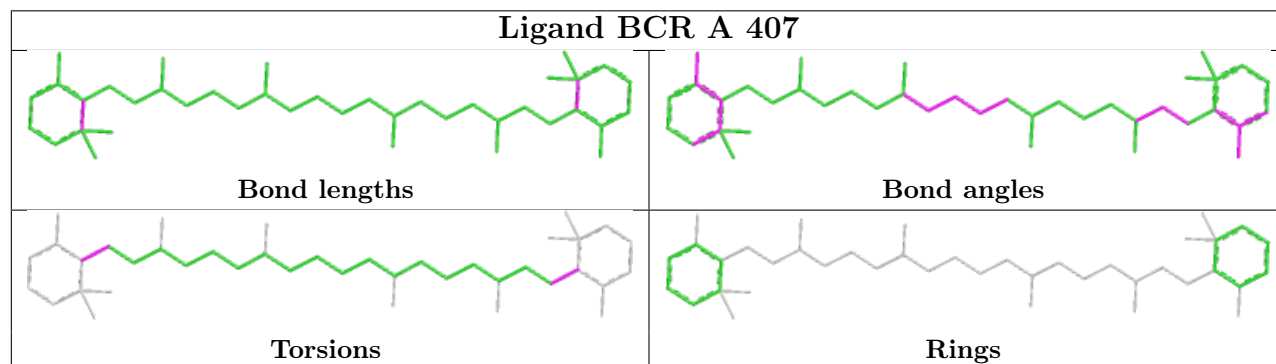
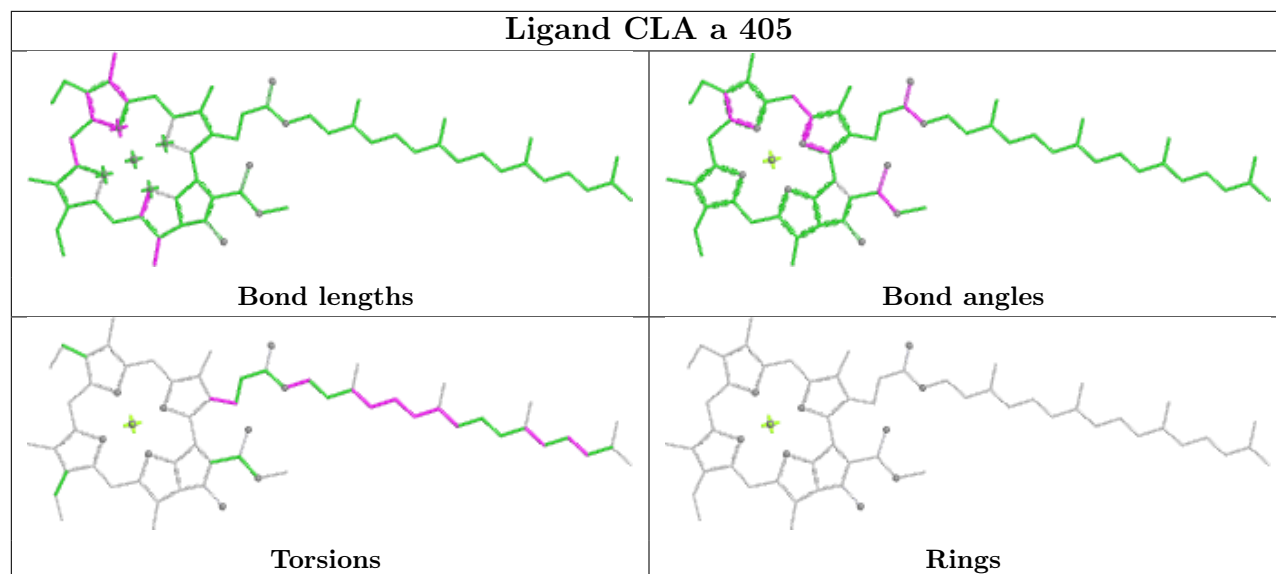


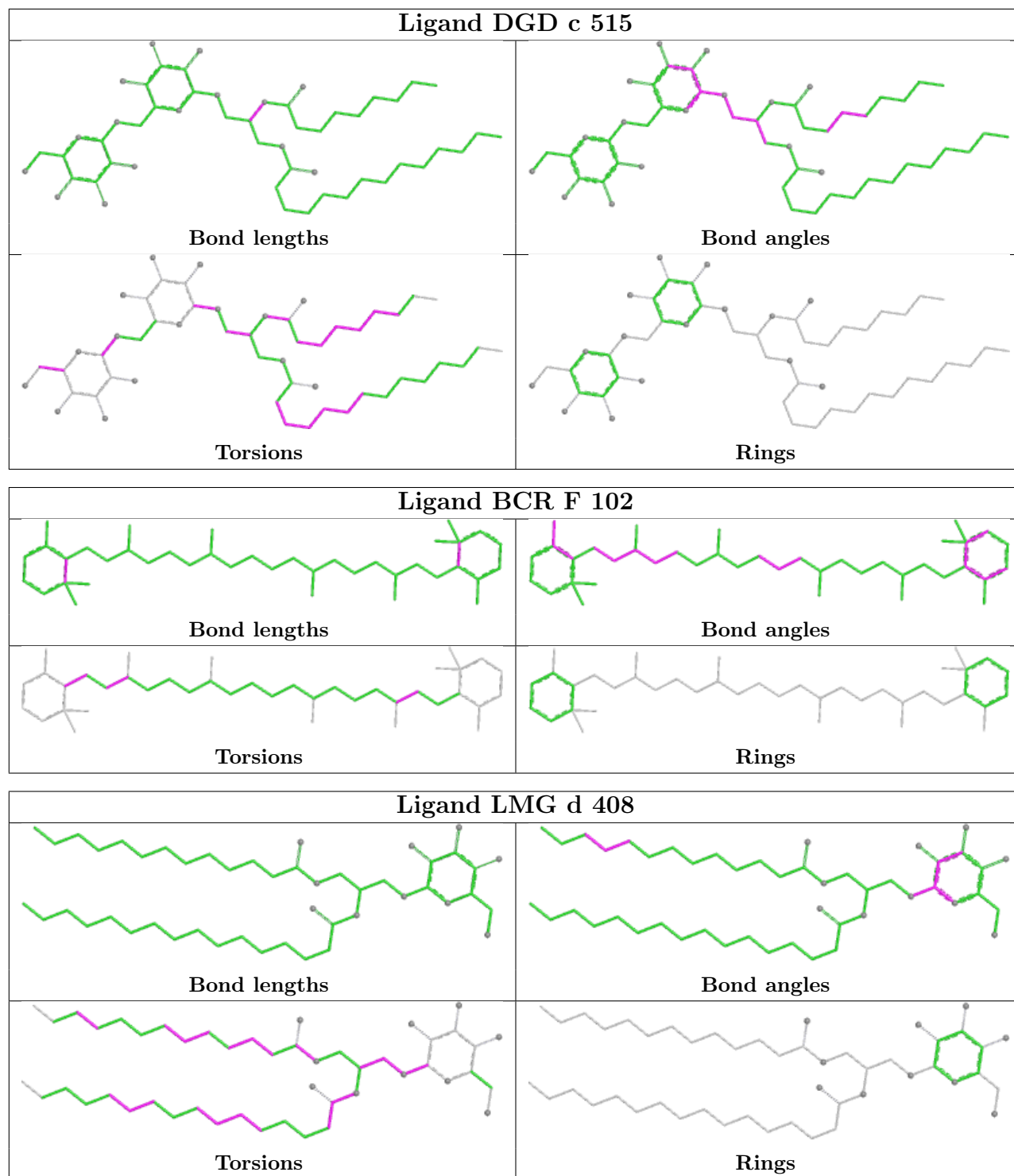
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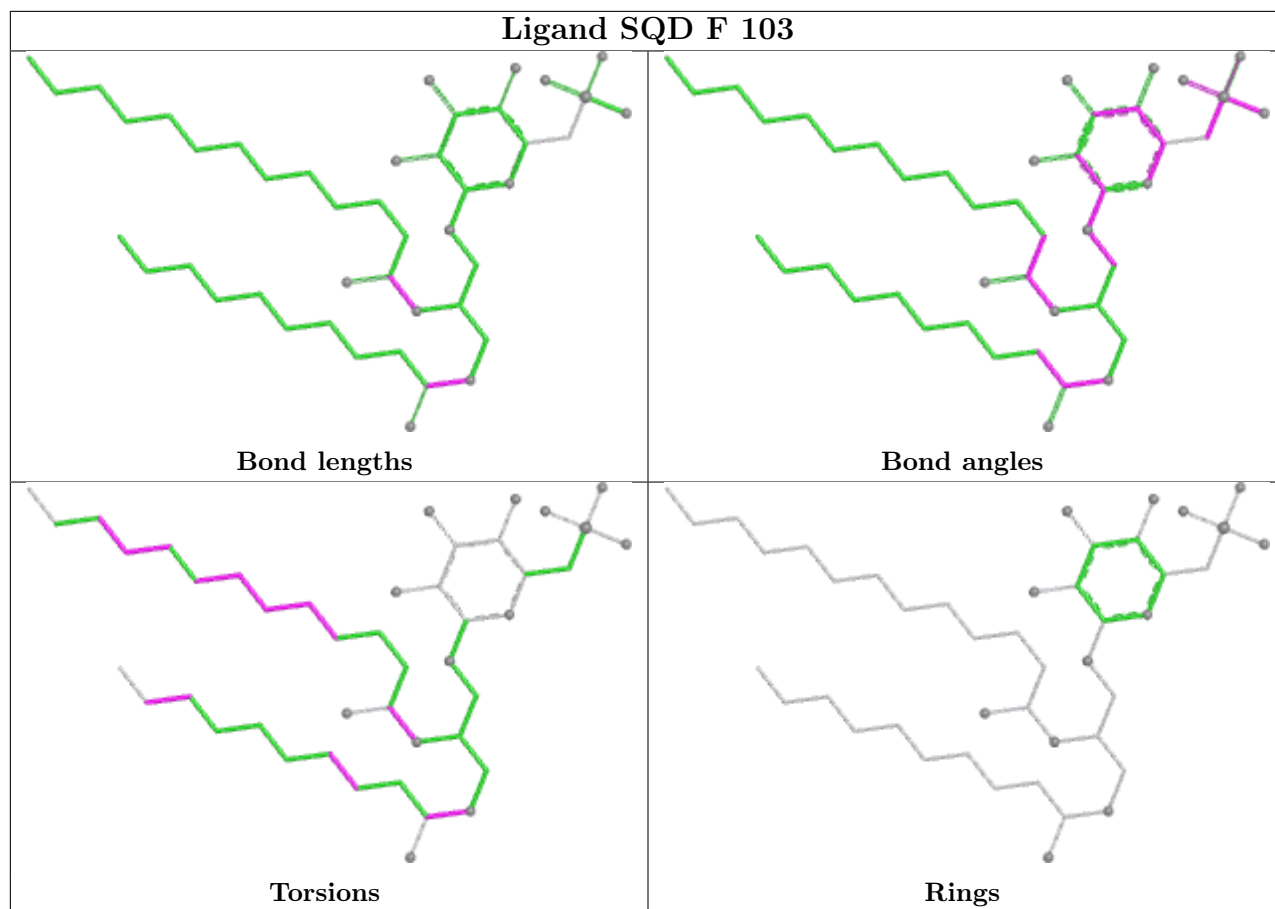
Ligand DGD C 516



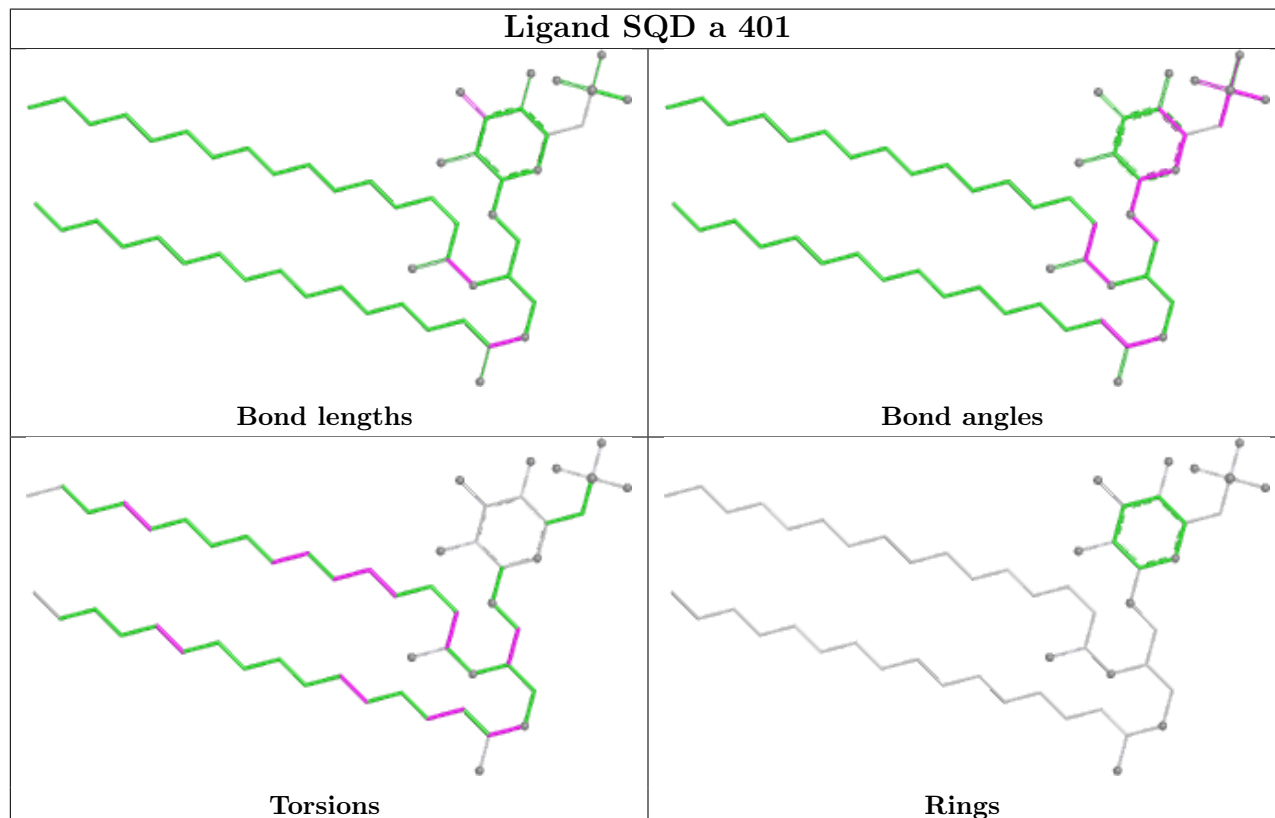


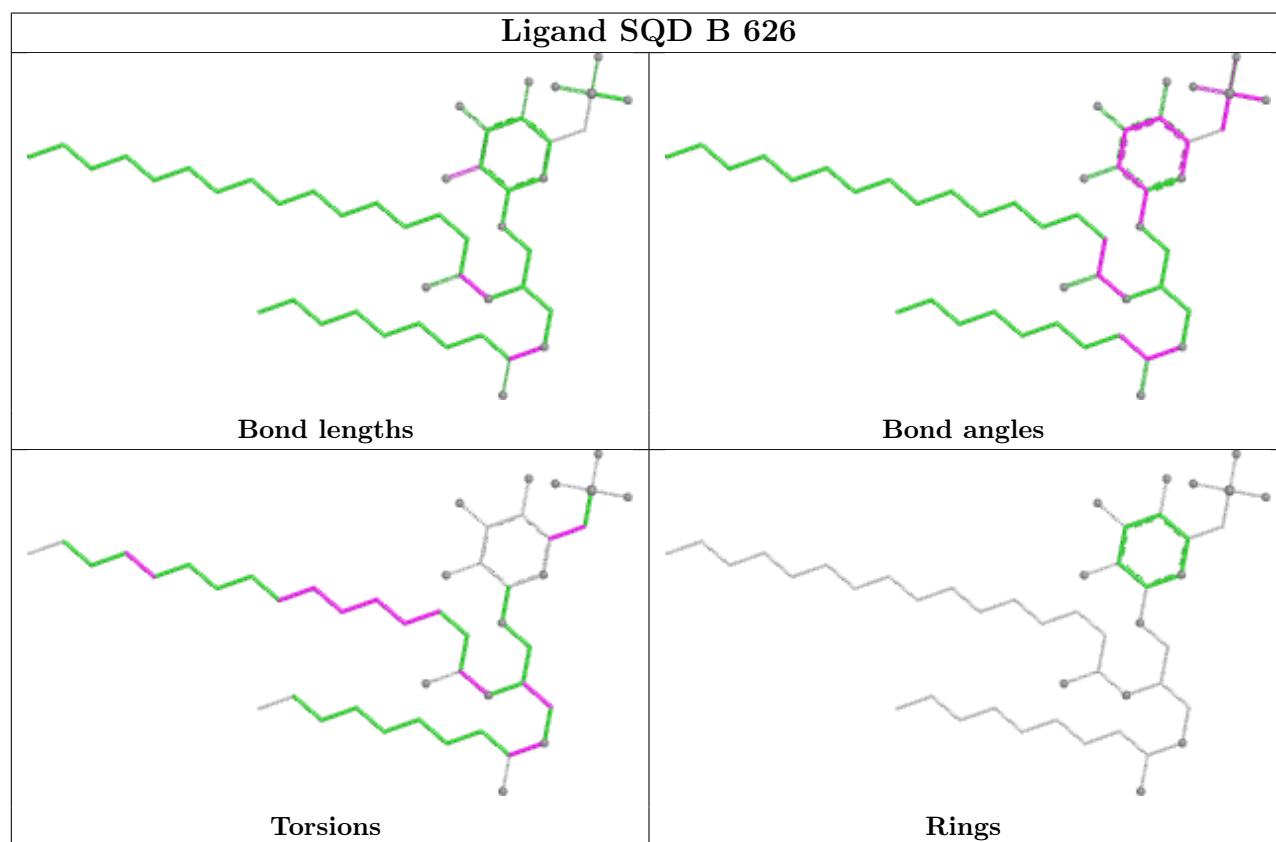
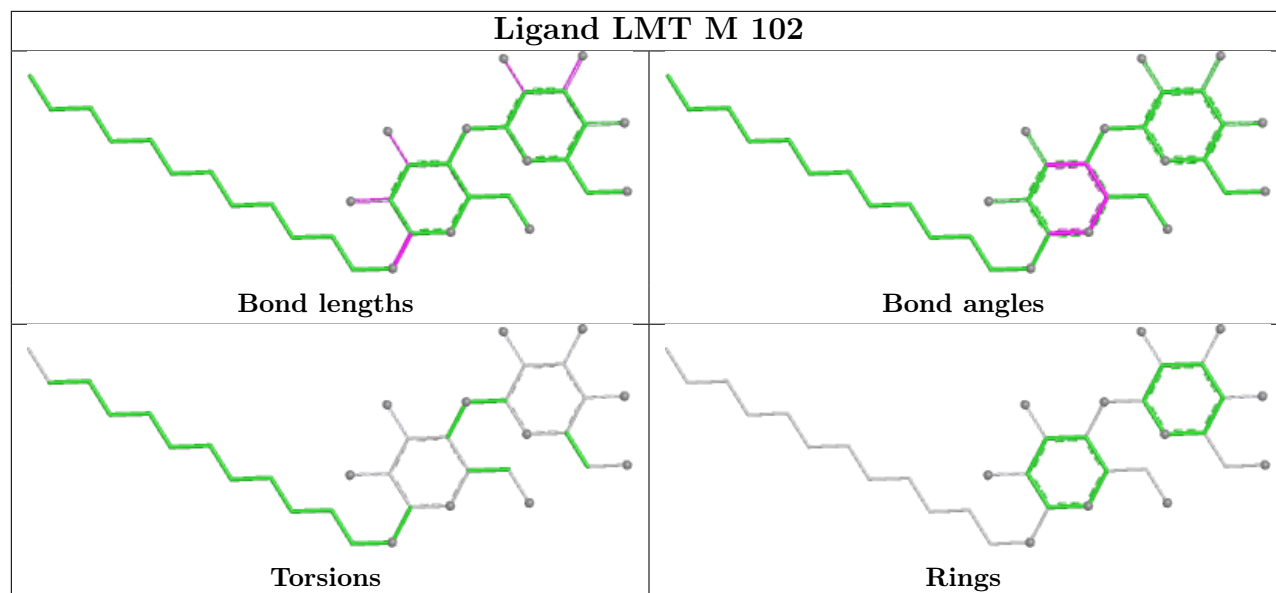


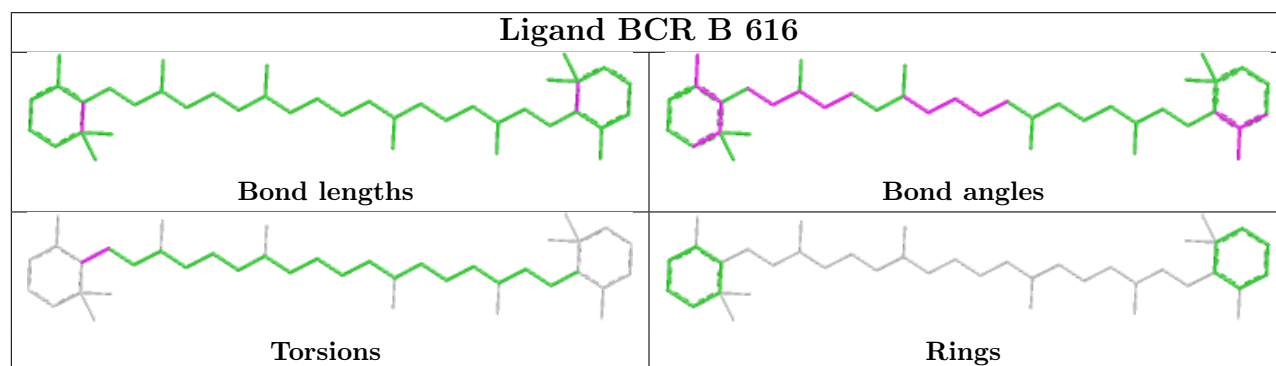
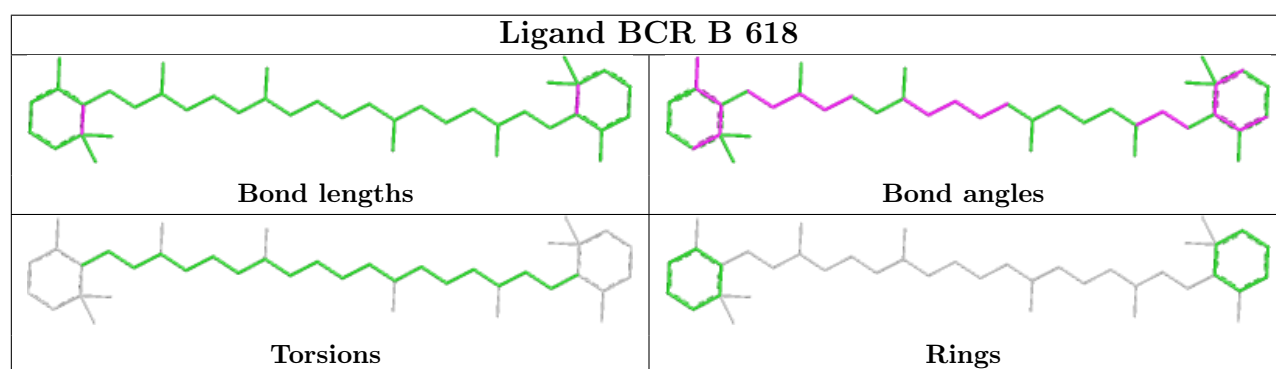
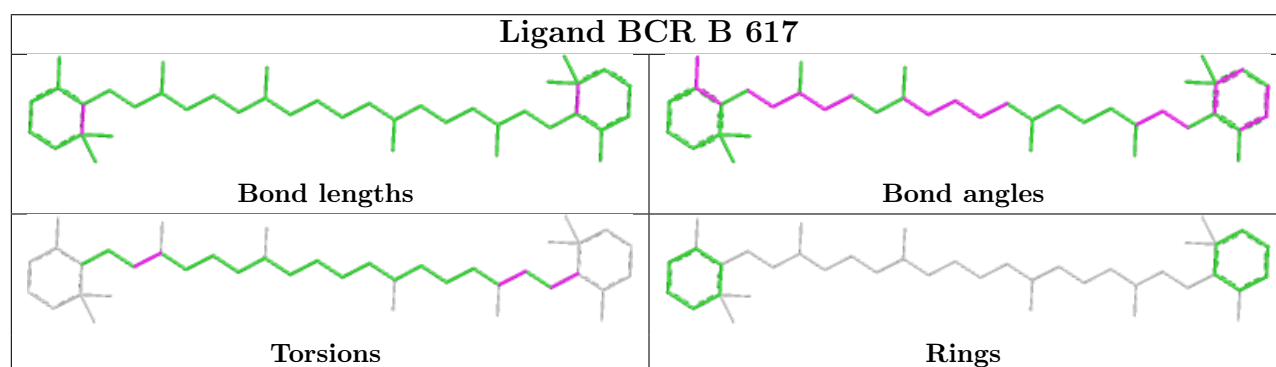
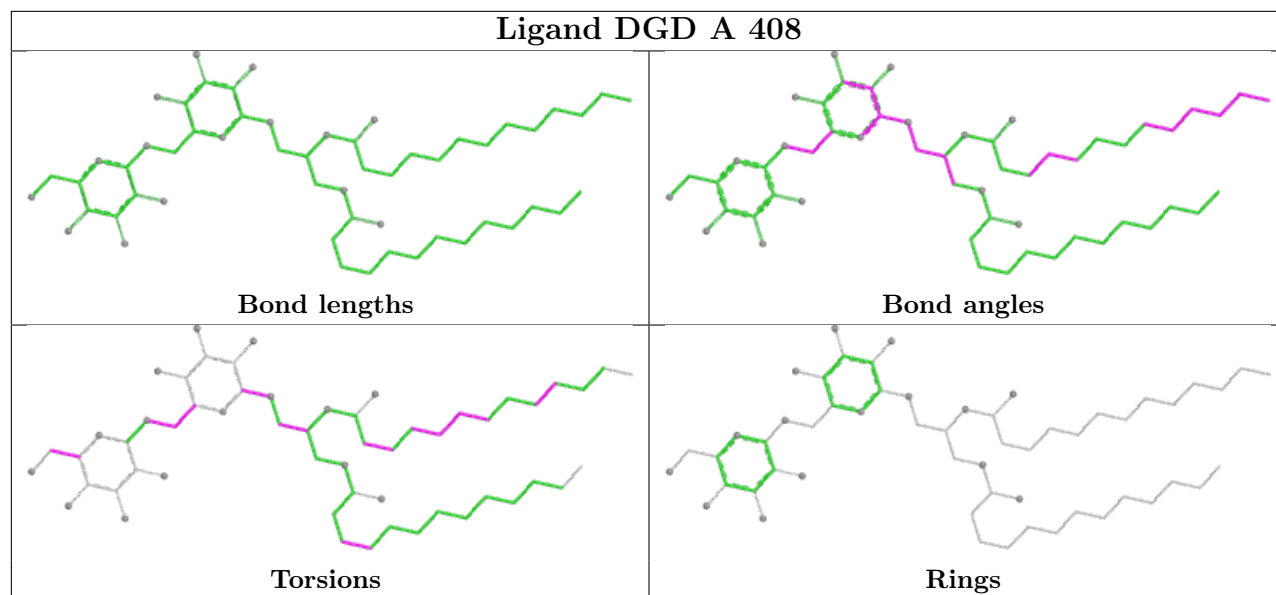
Ligand SQD F 103



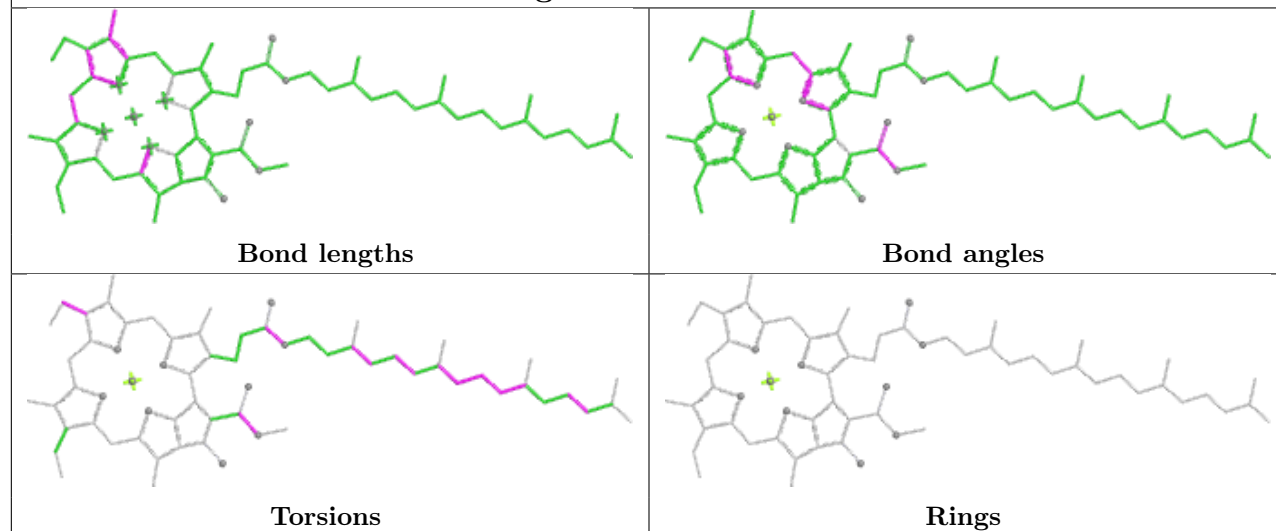
Ligand SQD a 401



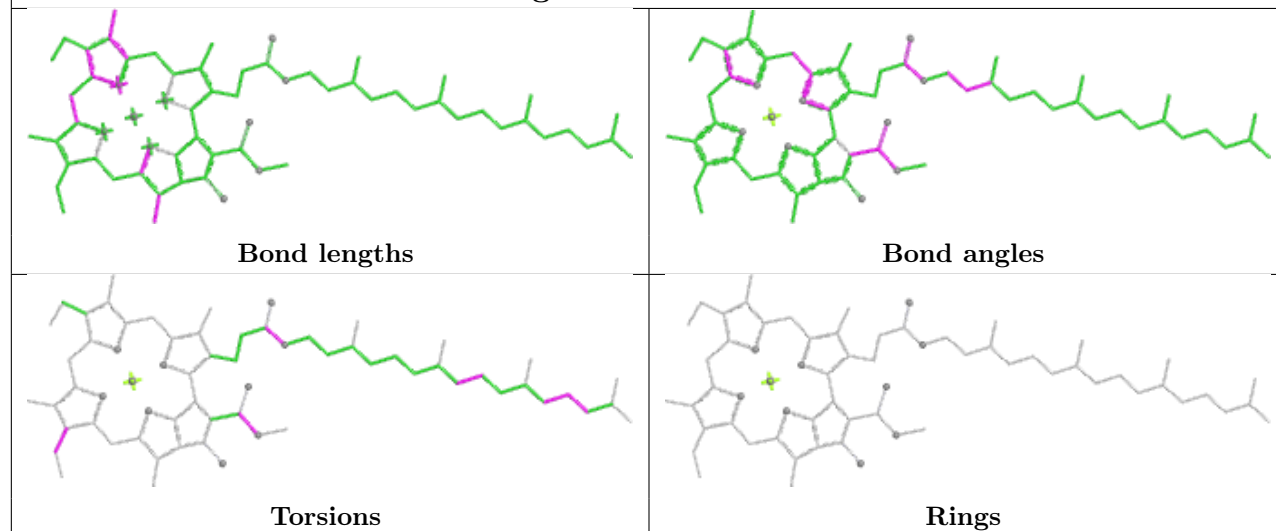




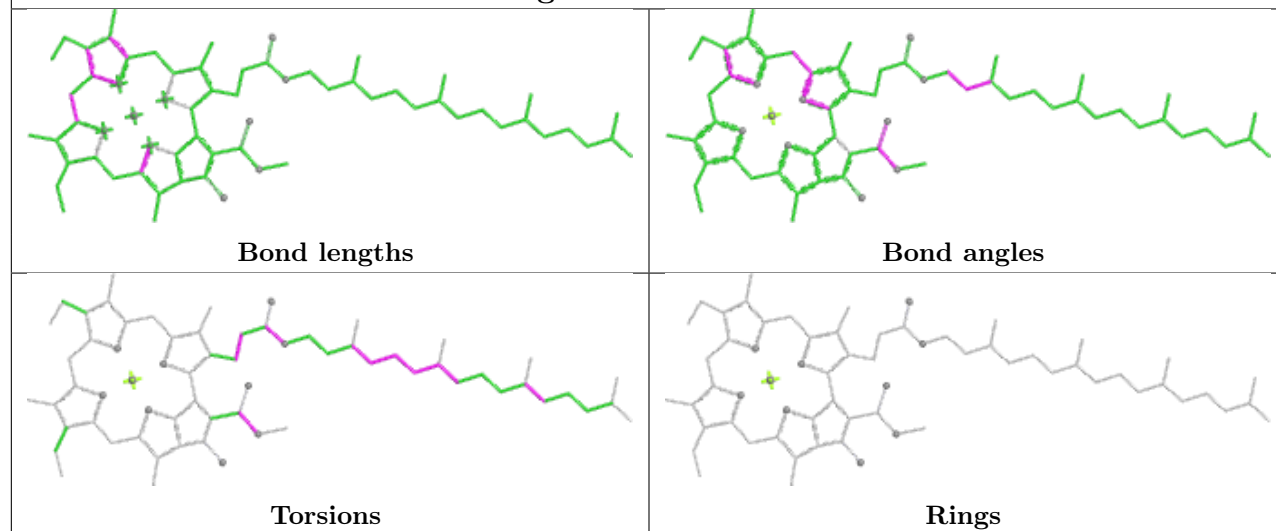
Ligand CLA b 608

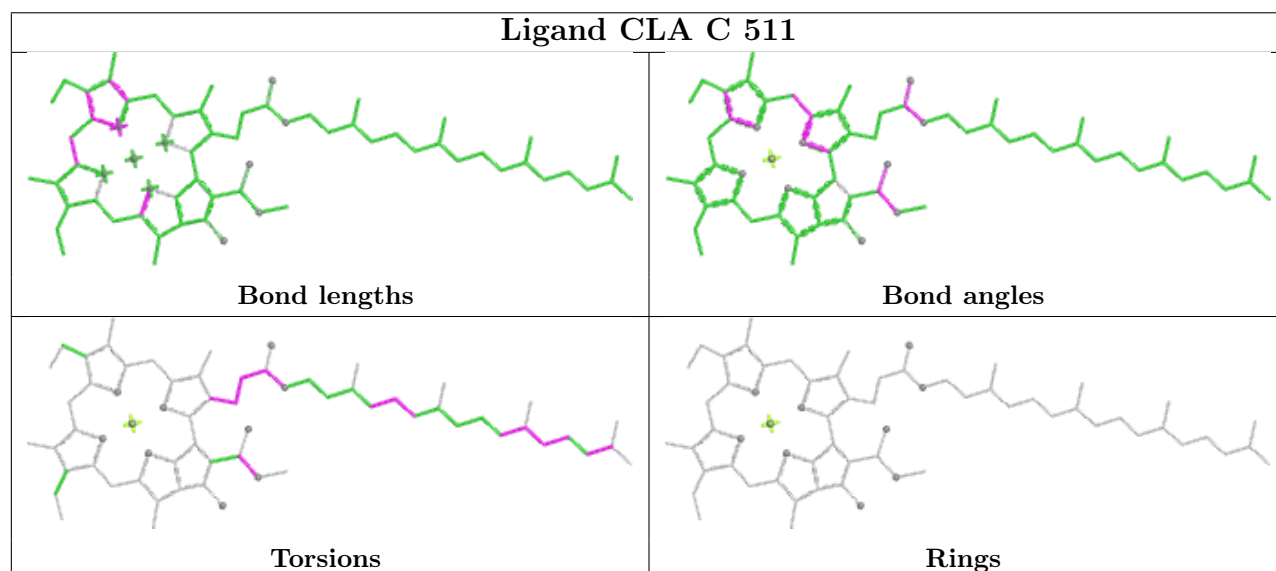
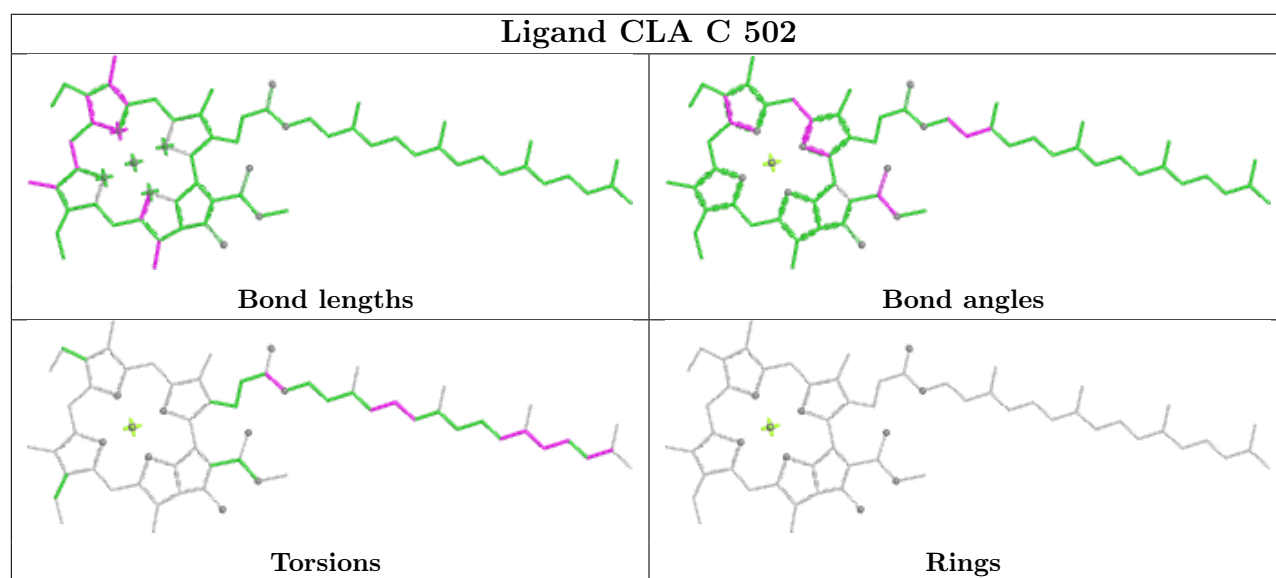
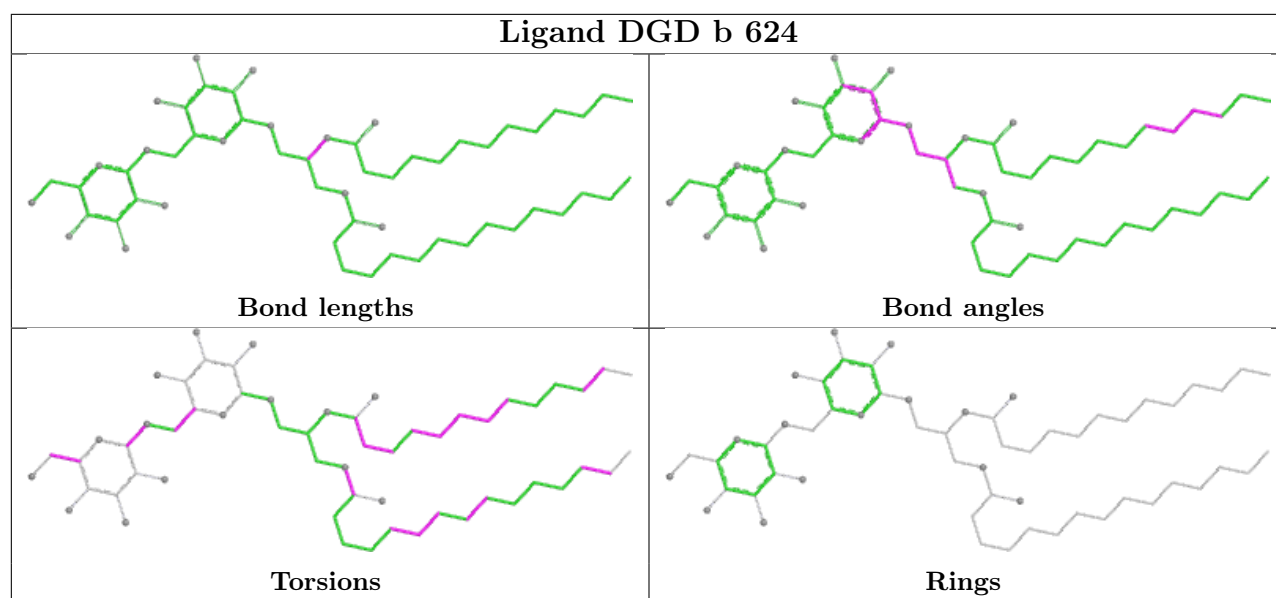


Ligand CLA B 603

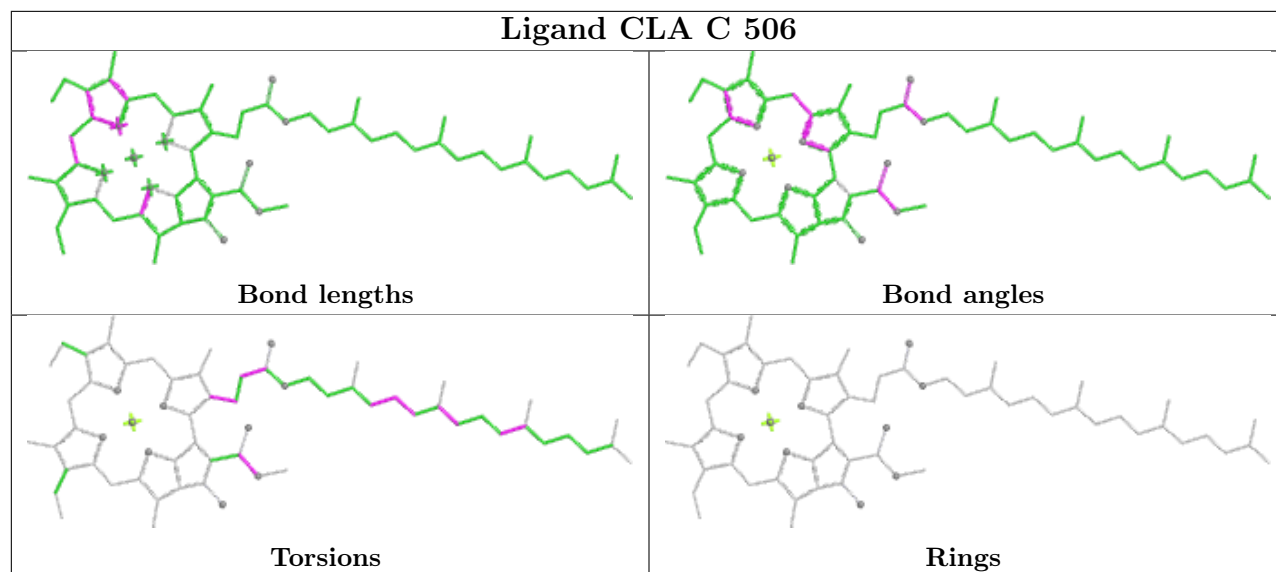


Ligand CLA c 510

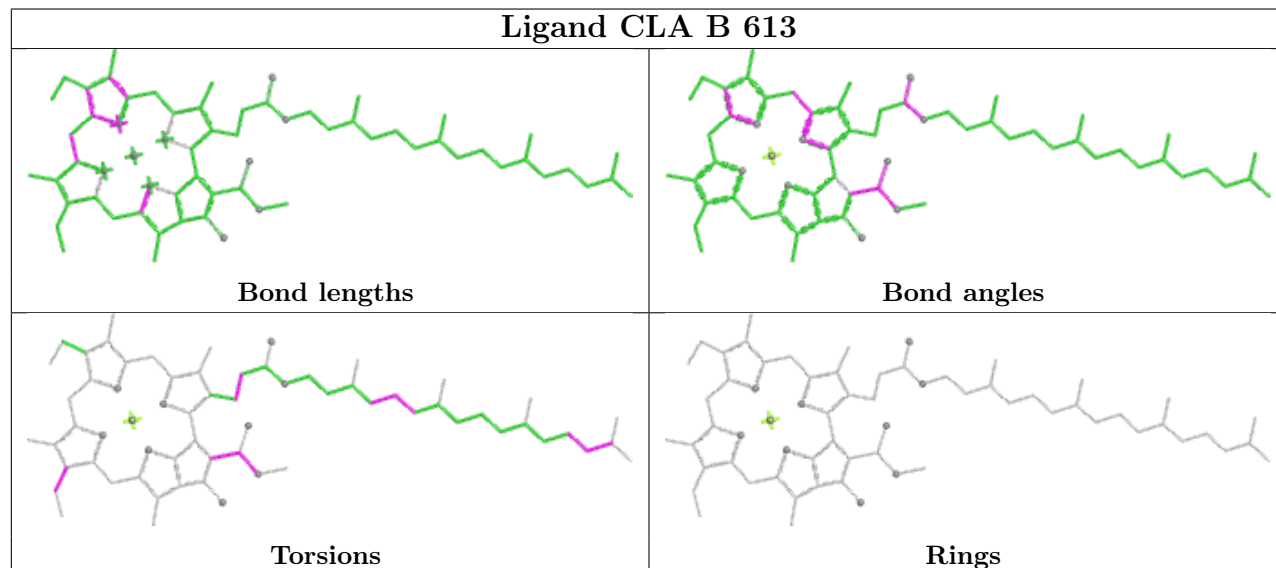




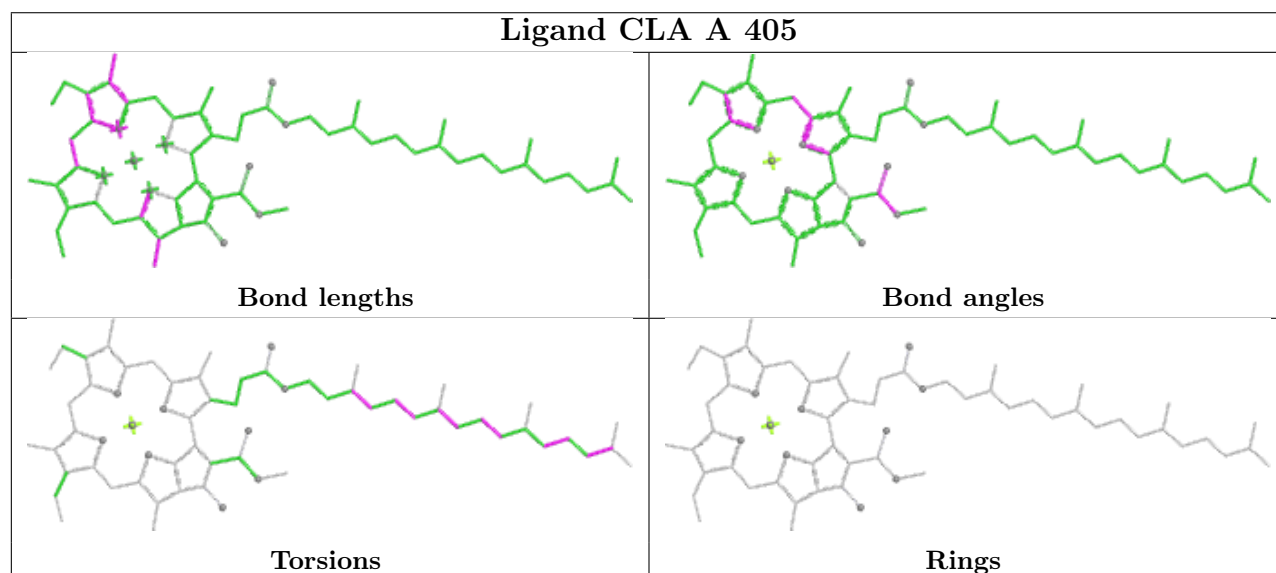
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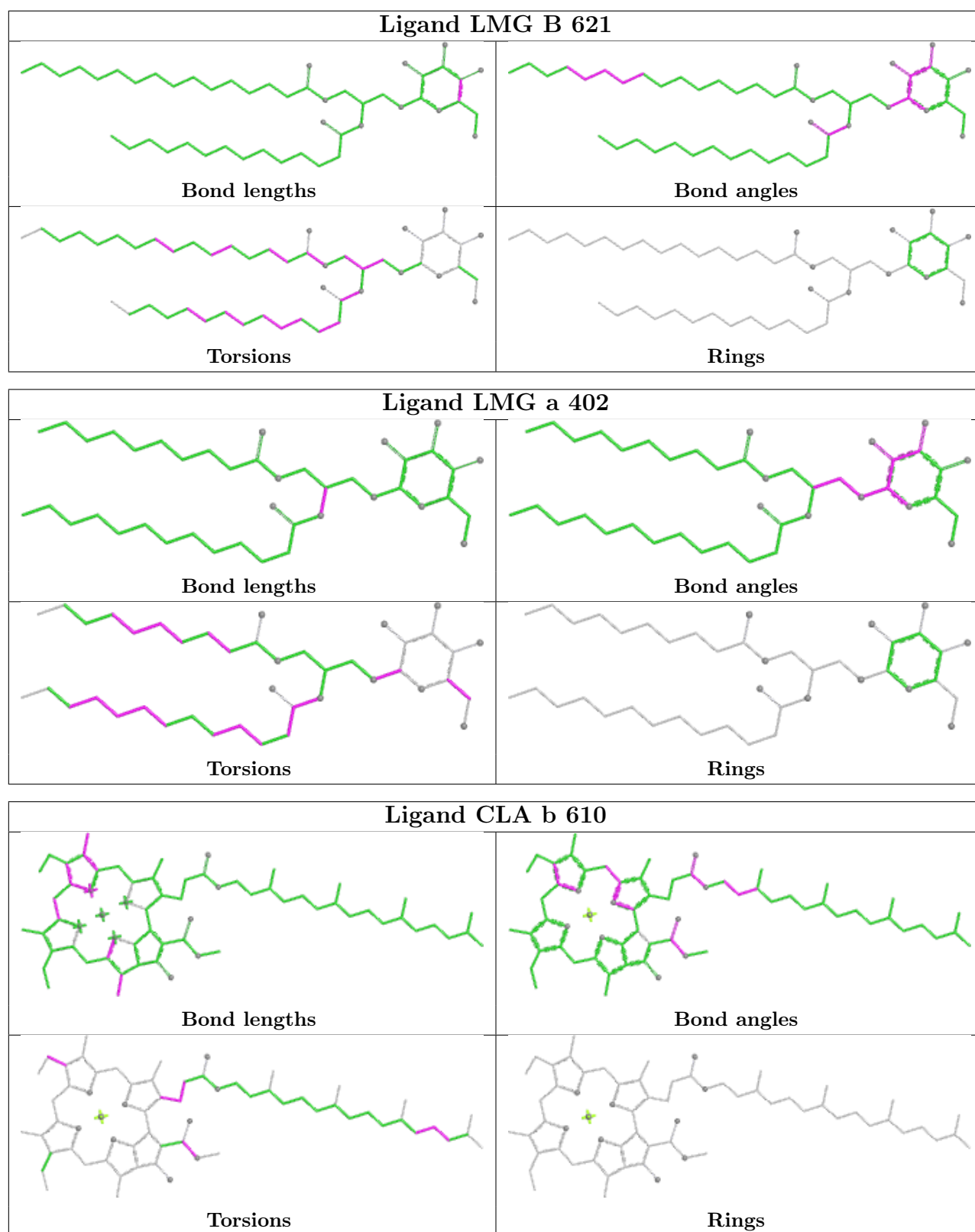


Ligand CLA B 613

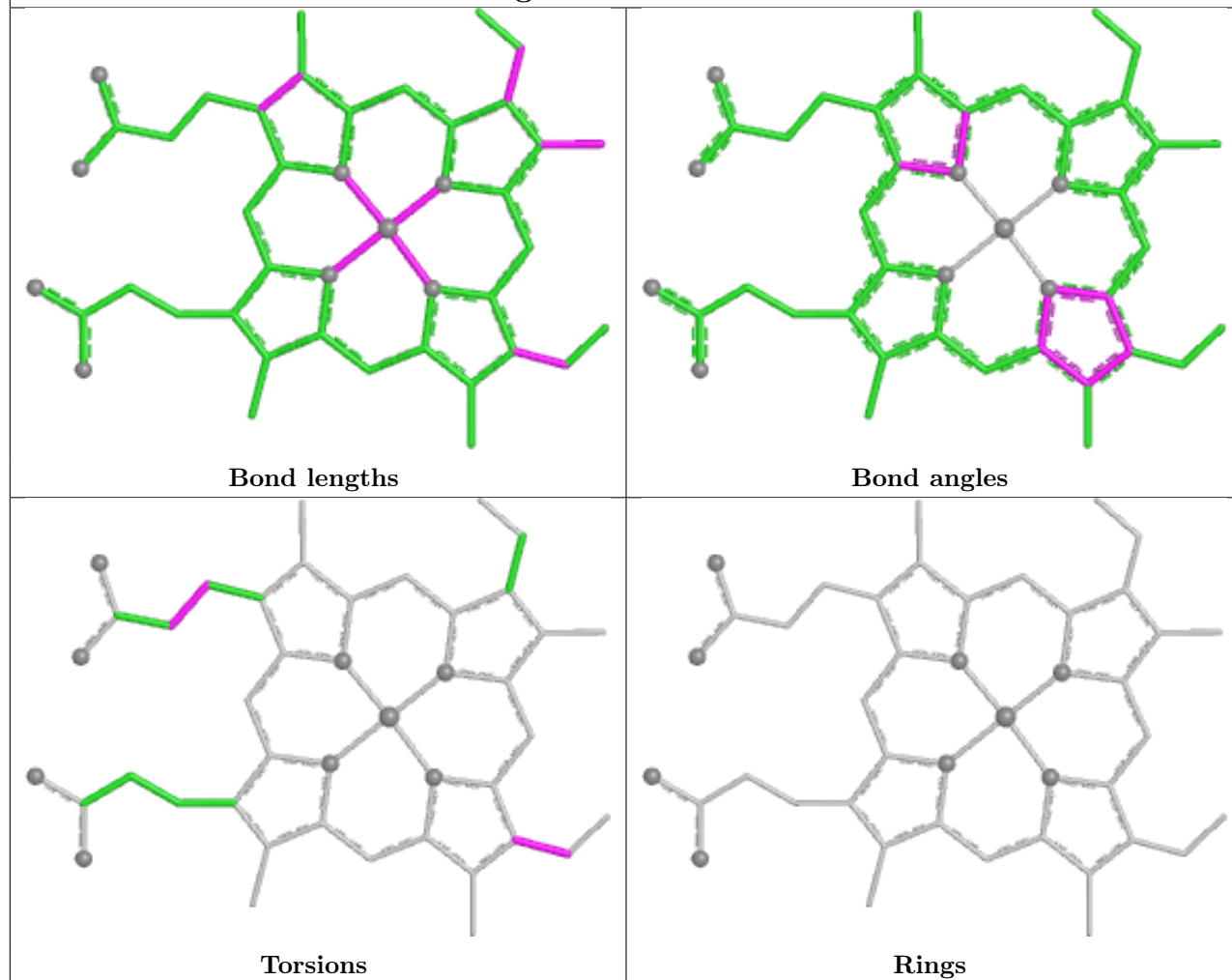


Ligand CLA A 405

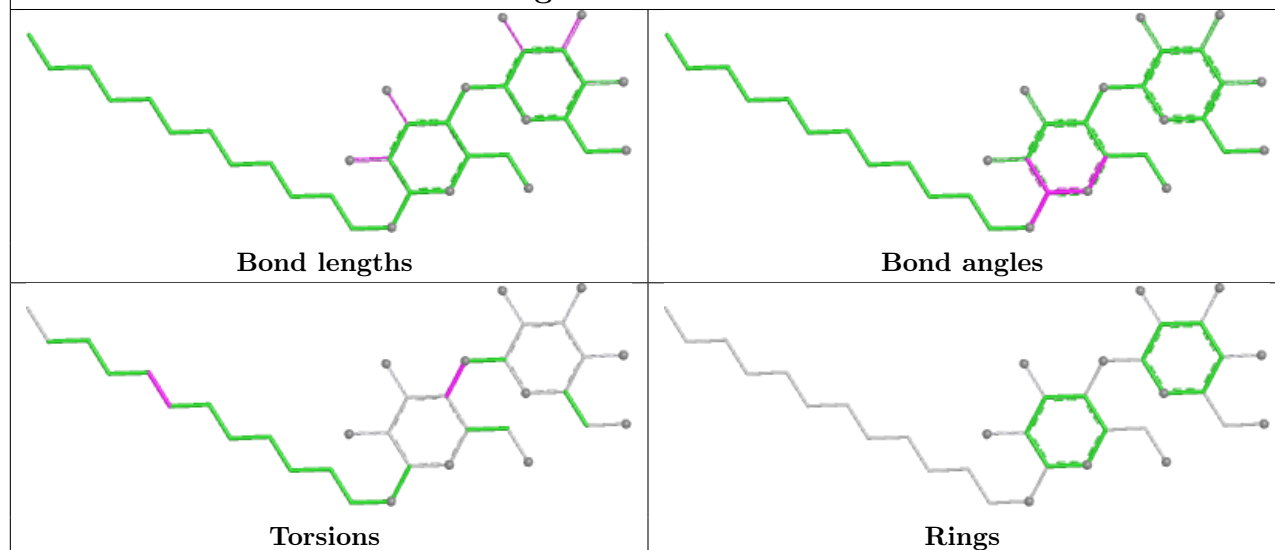


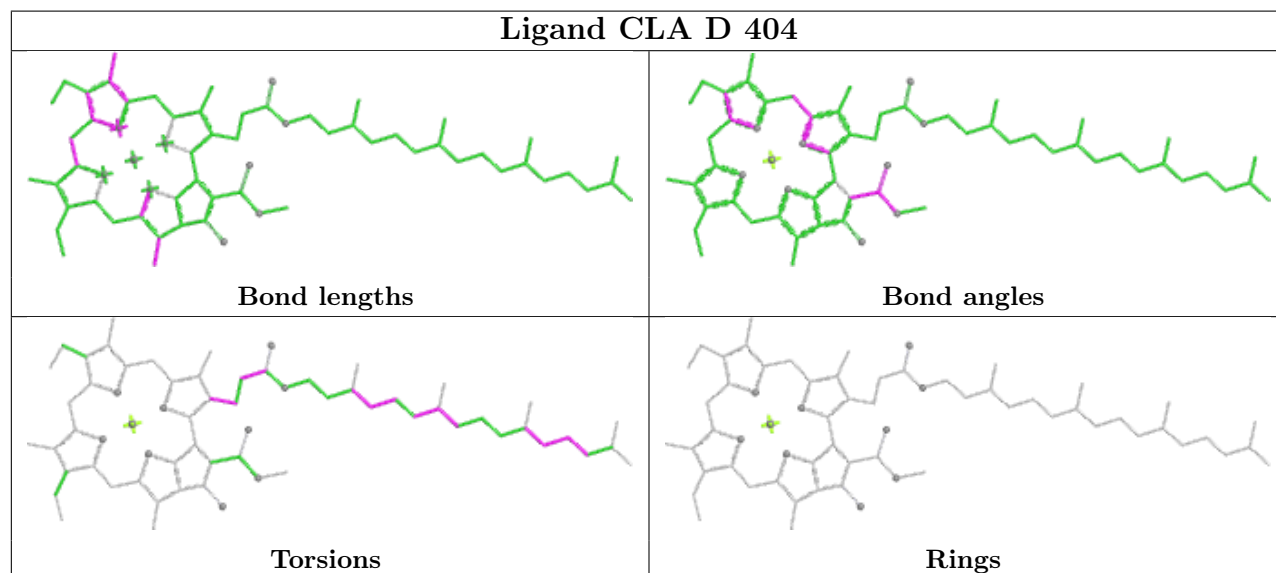
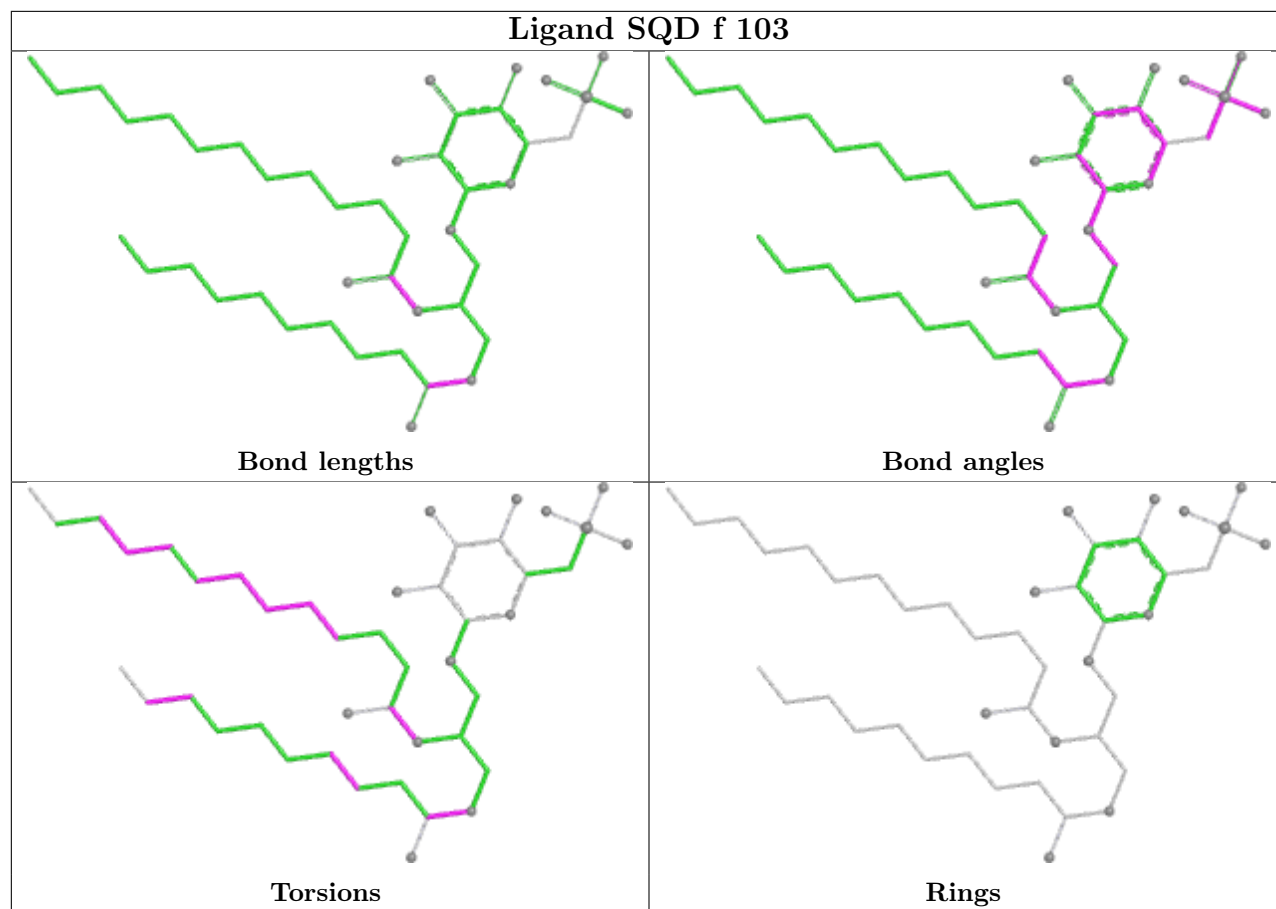


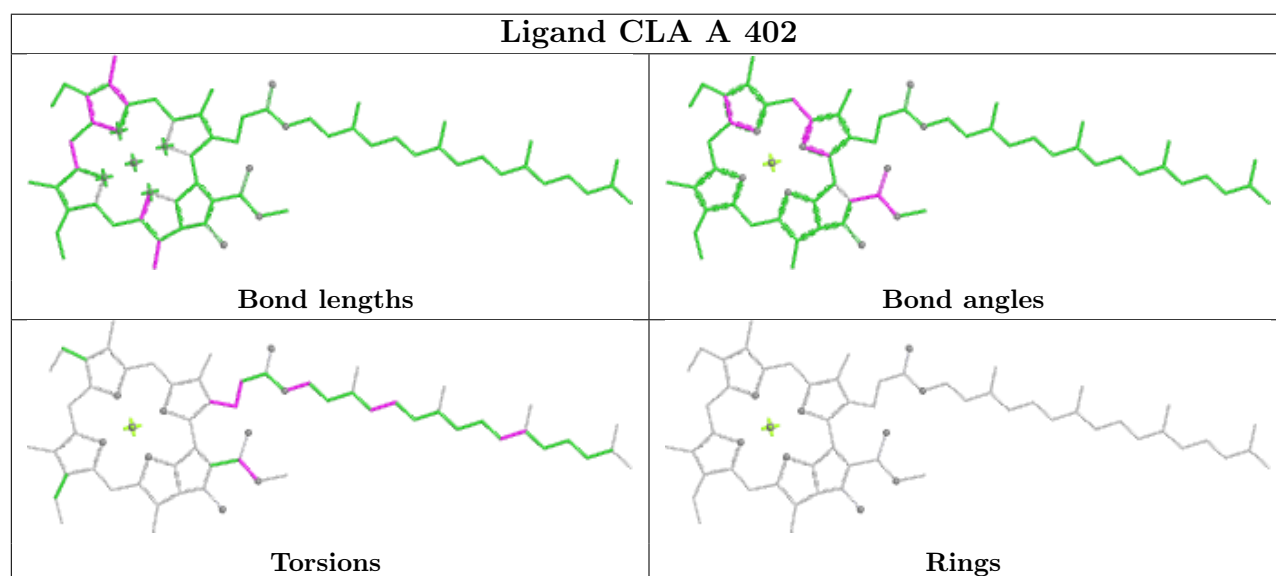
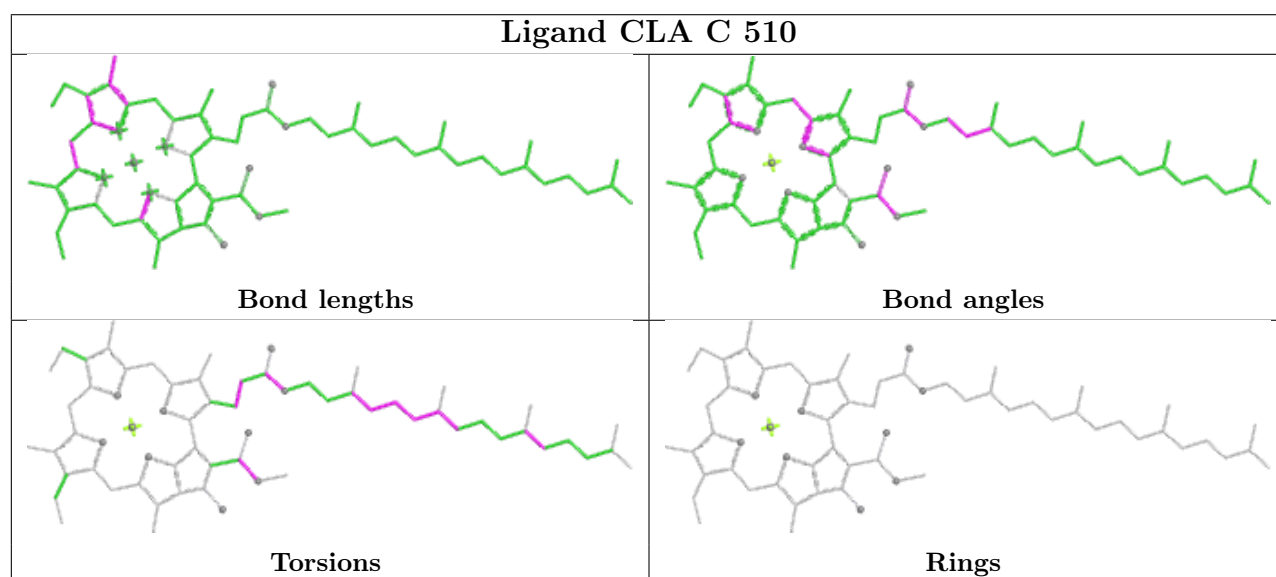
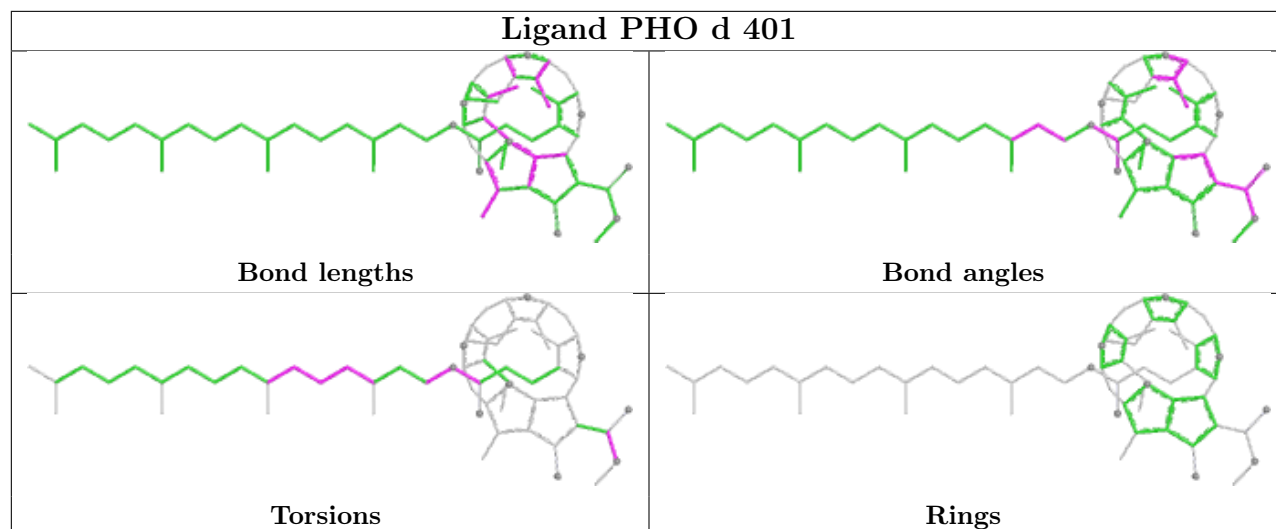
Ligand HEM f 101



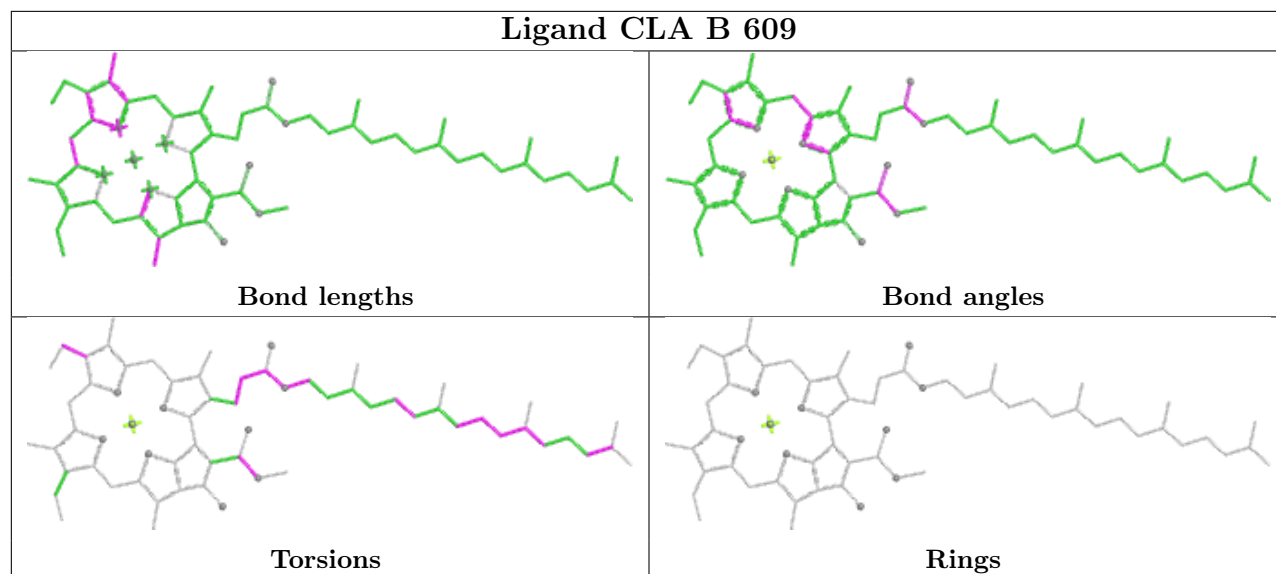
Ligand LMT I 102



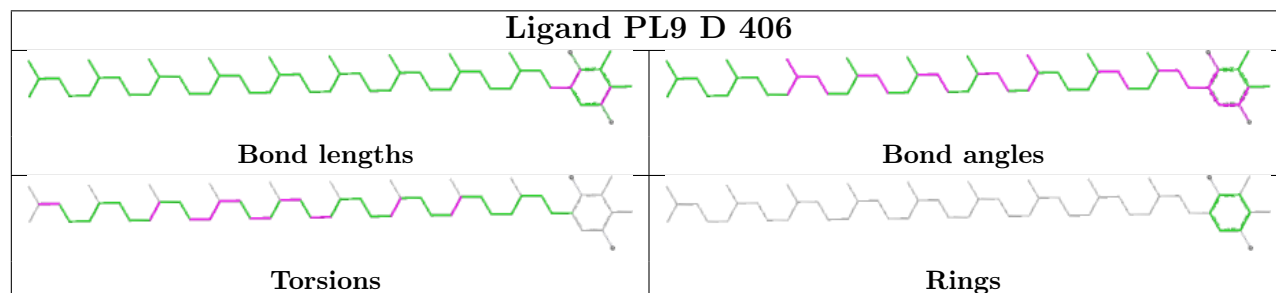




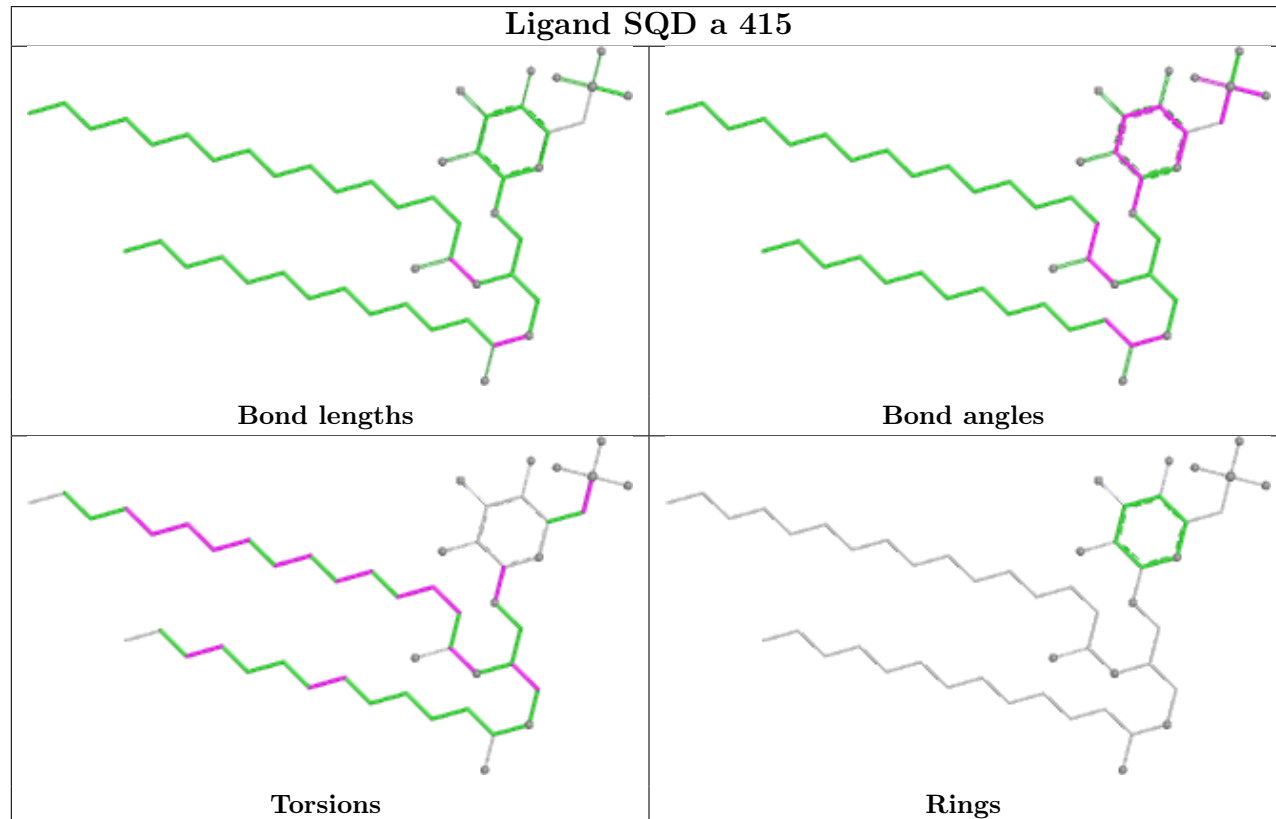
Ligand CLA B 609



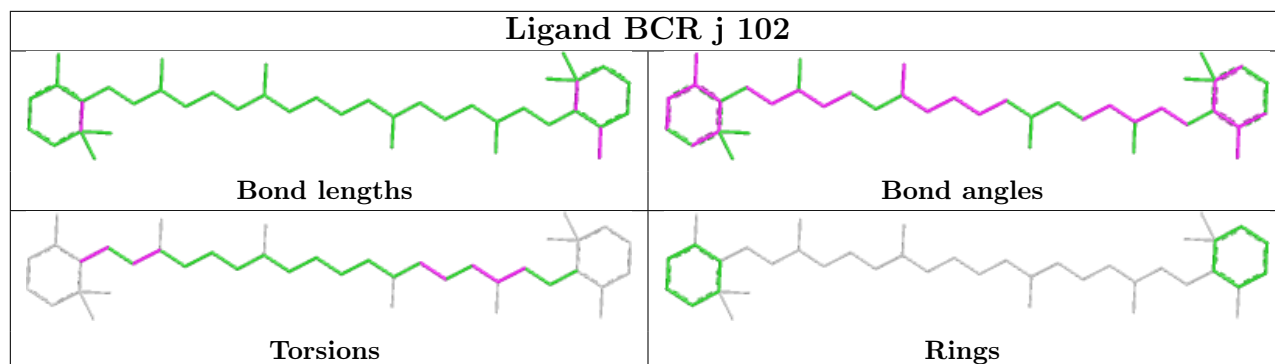
Ligand PL9 D 406



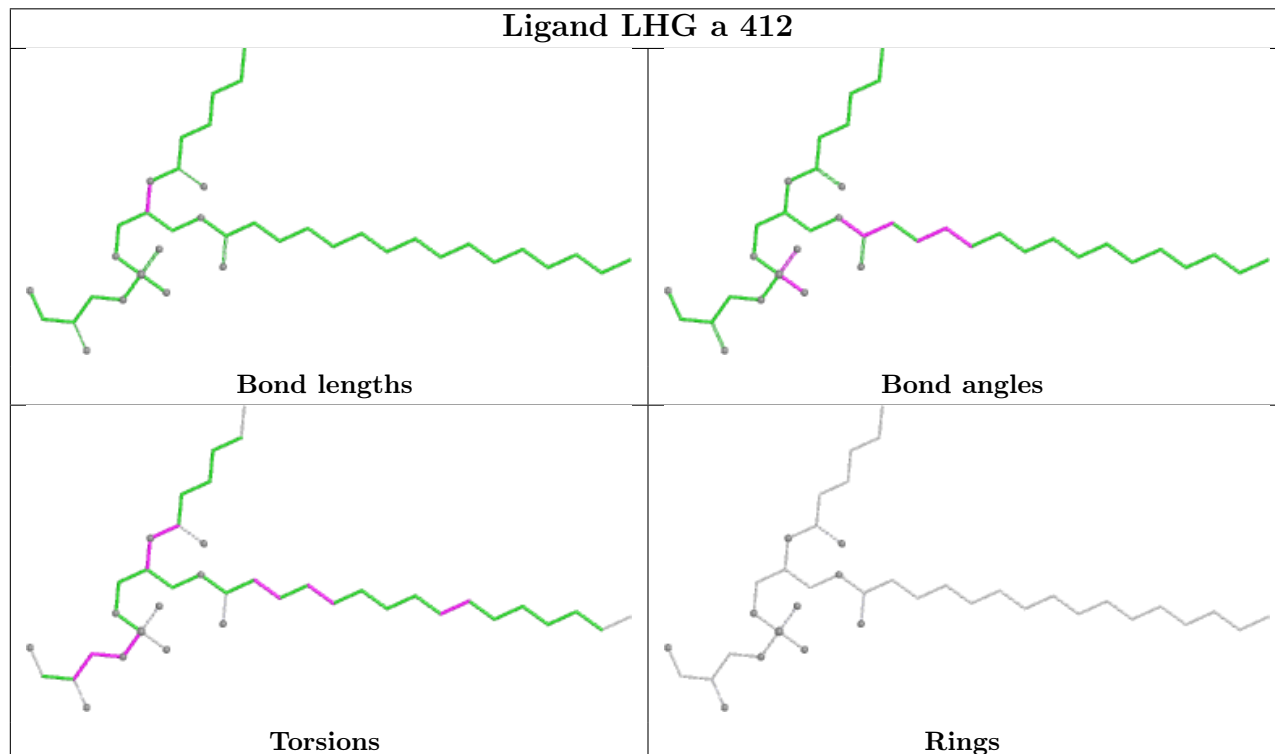
Ligand SQD a 415



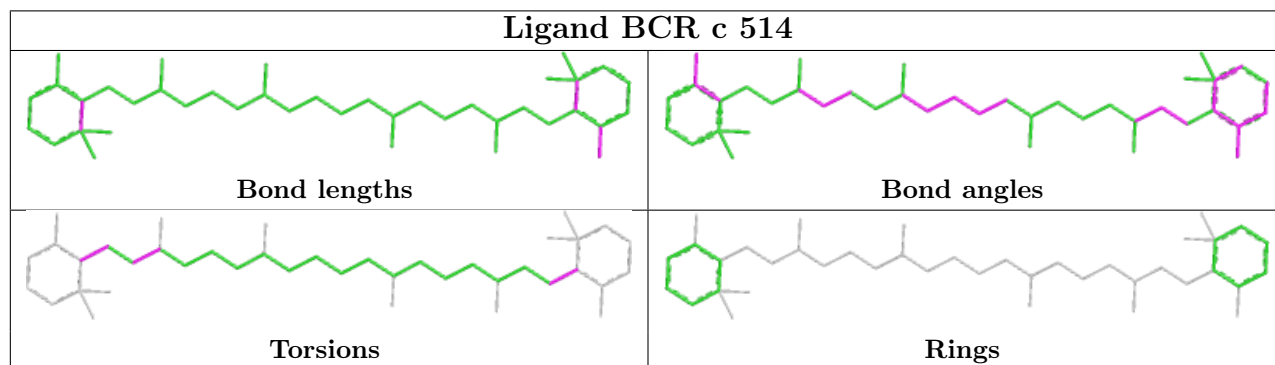
Ligand BCR j 102

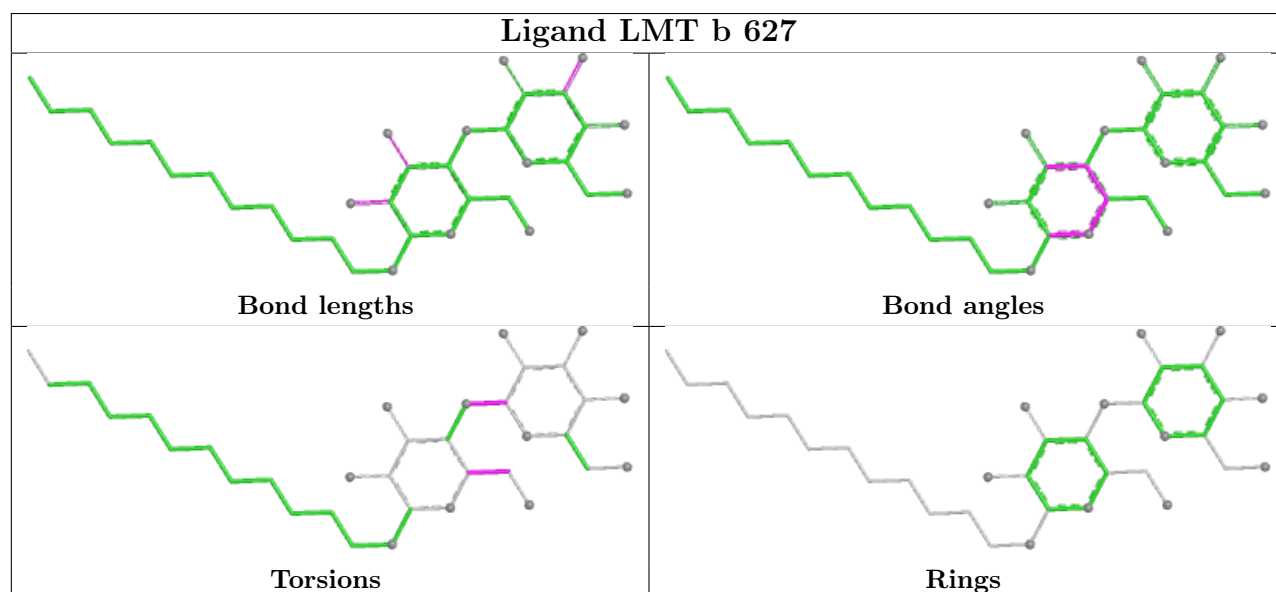
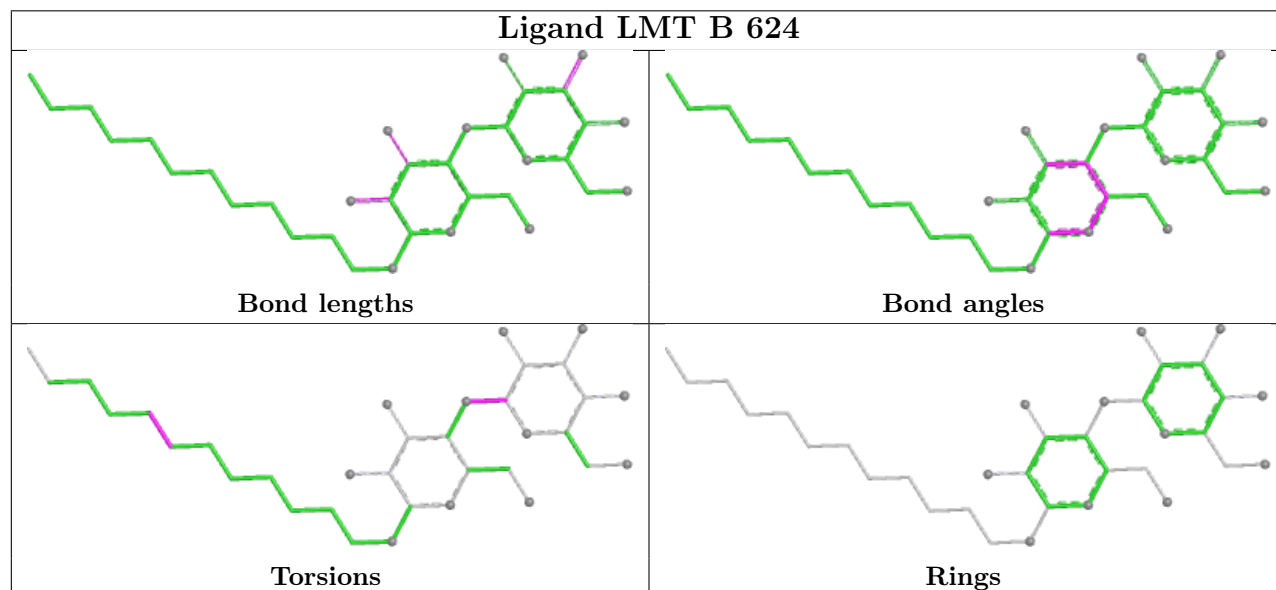
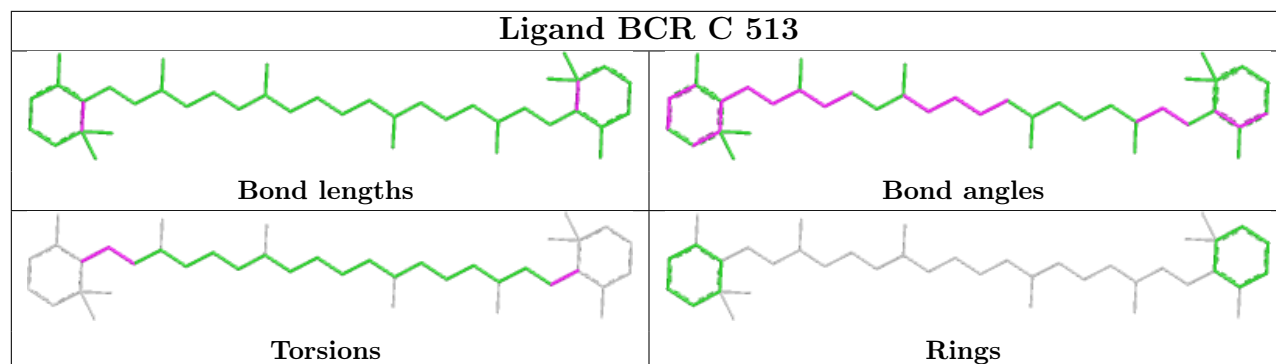


Ligand LHG a 412

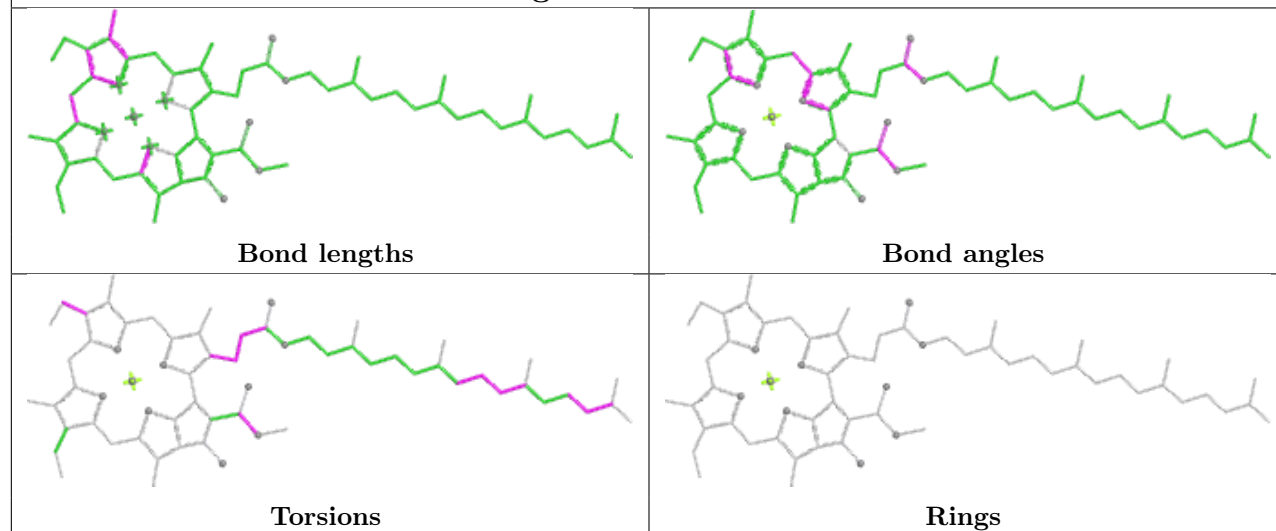


Ligand BCR c 514

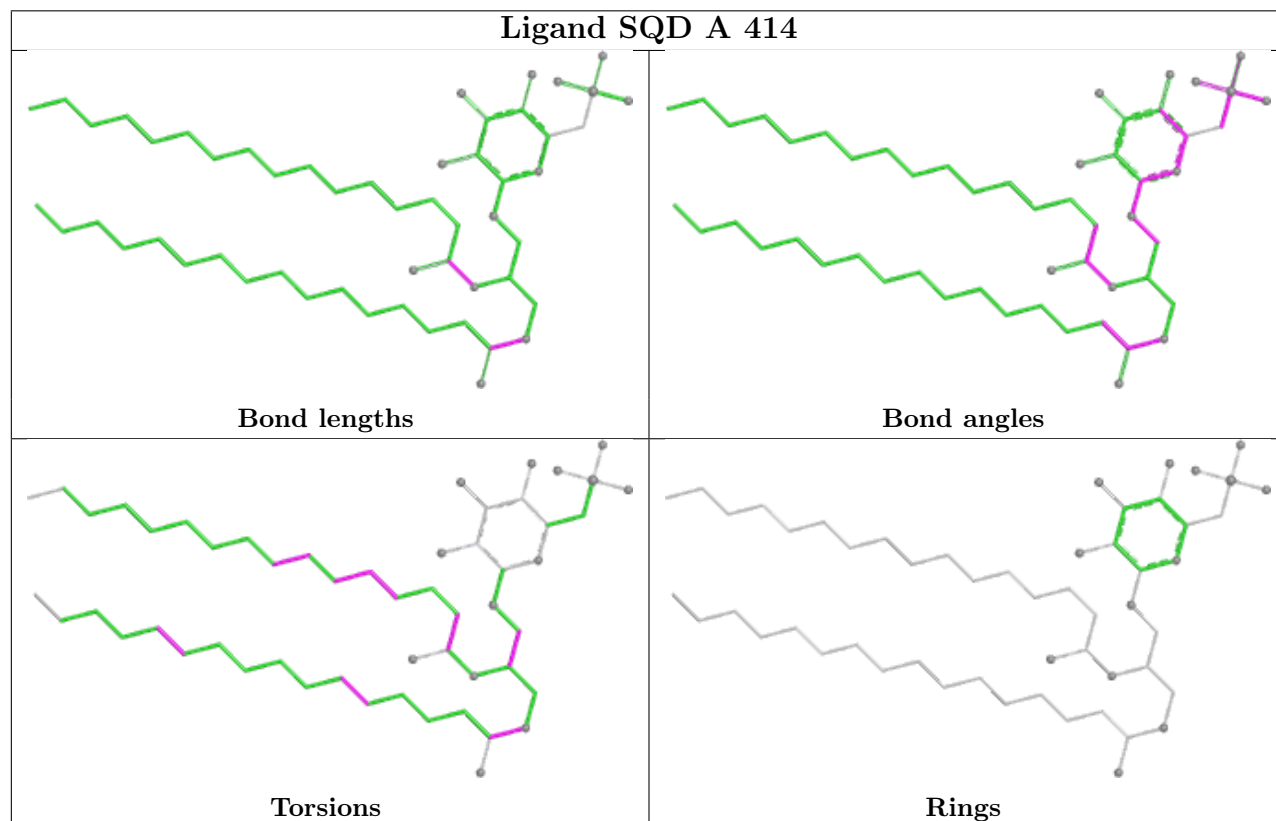




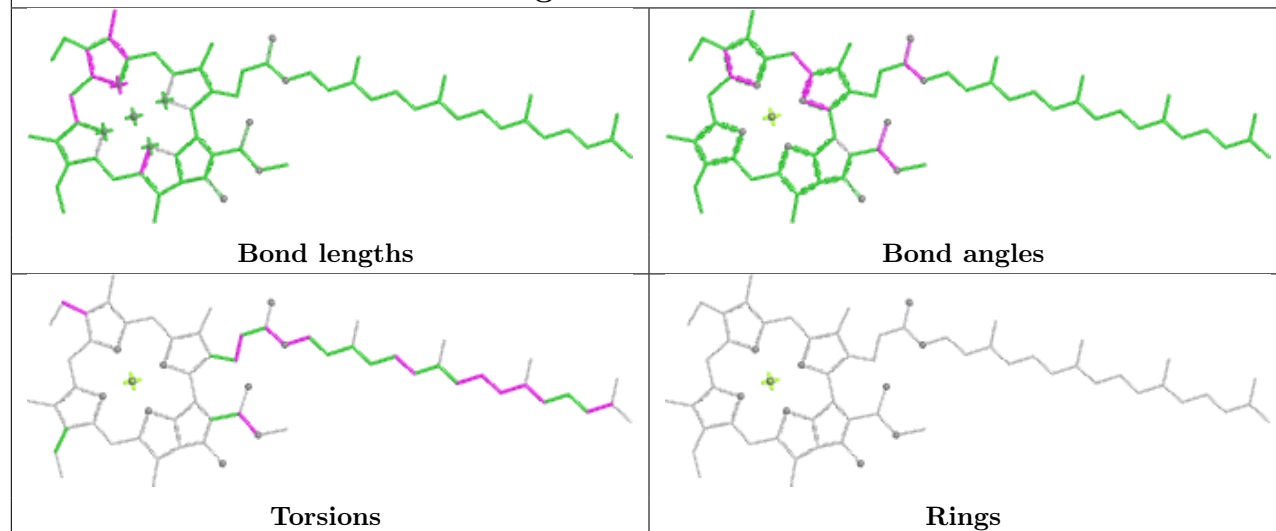
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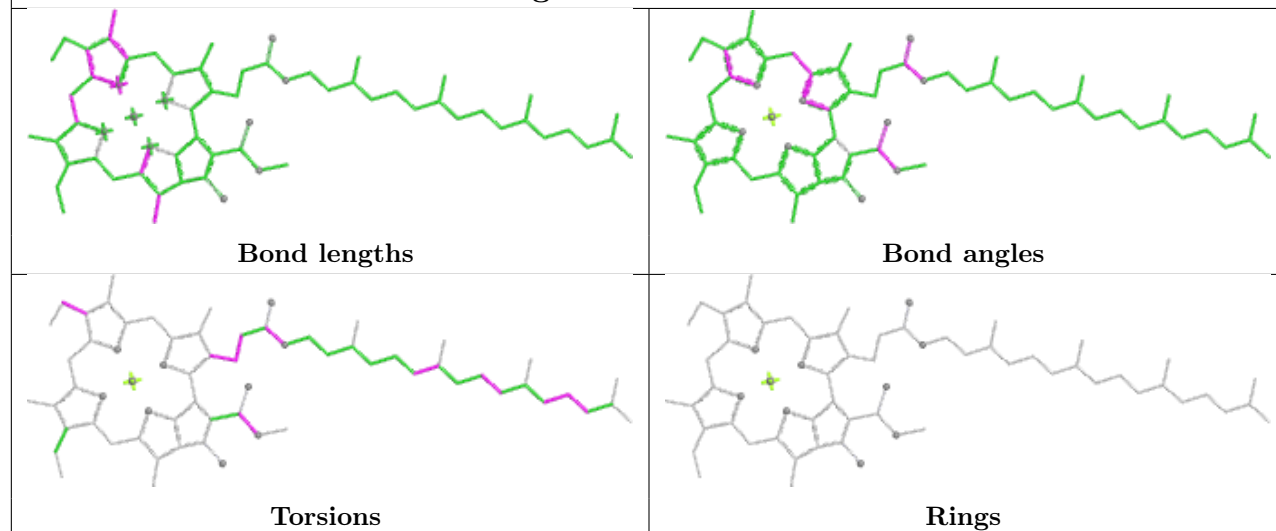
Ligand SQD A 414



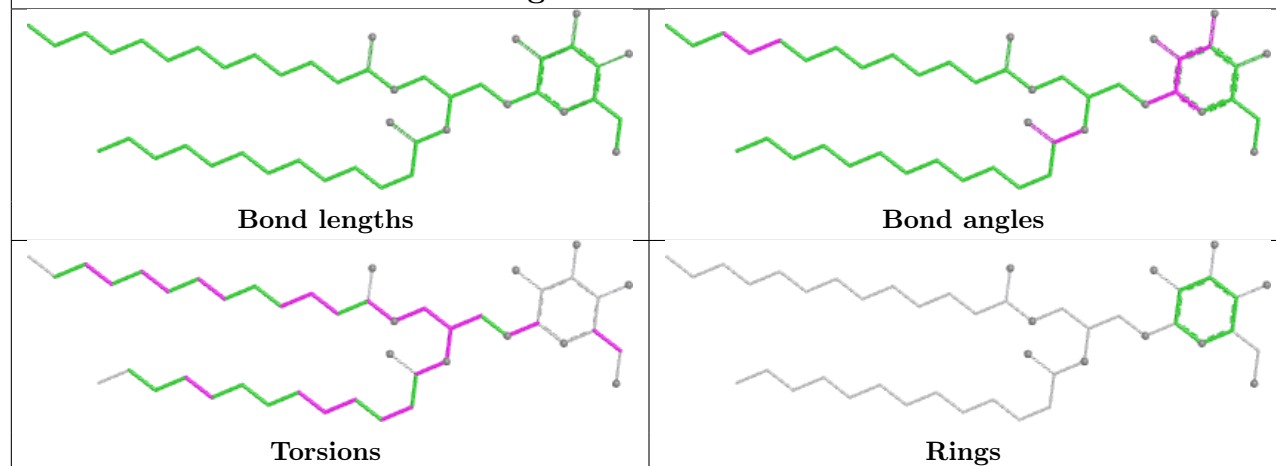
Ligand CLA b 613

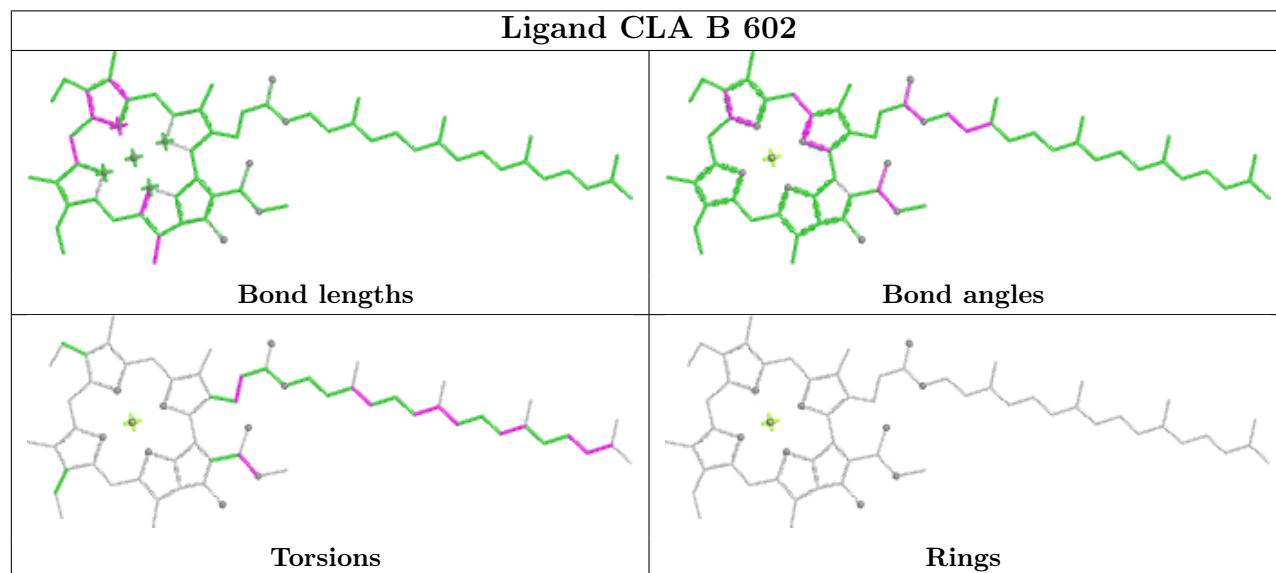
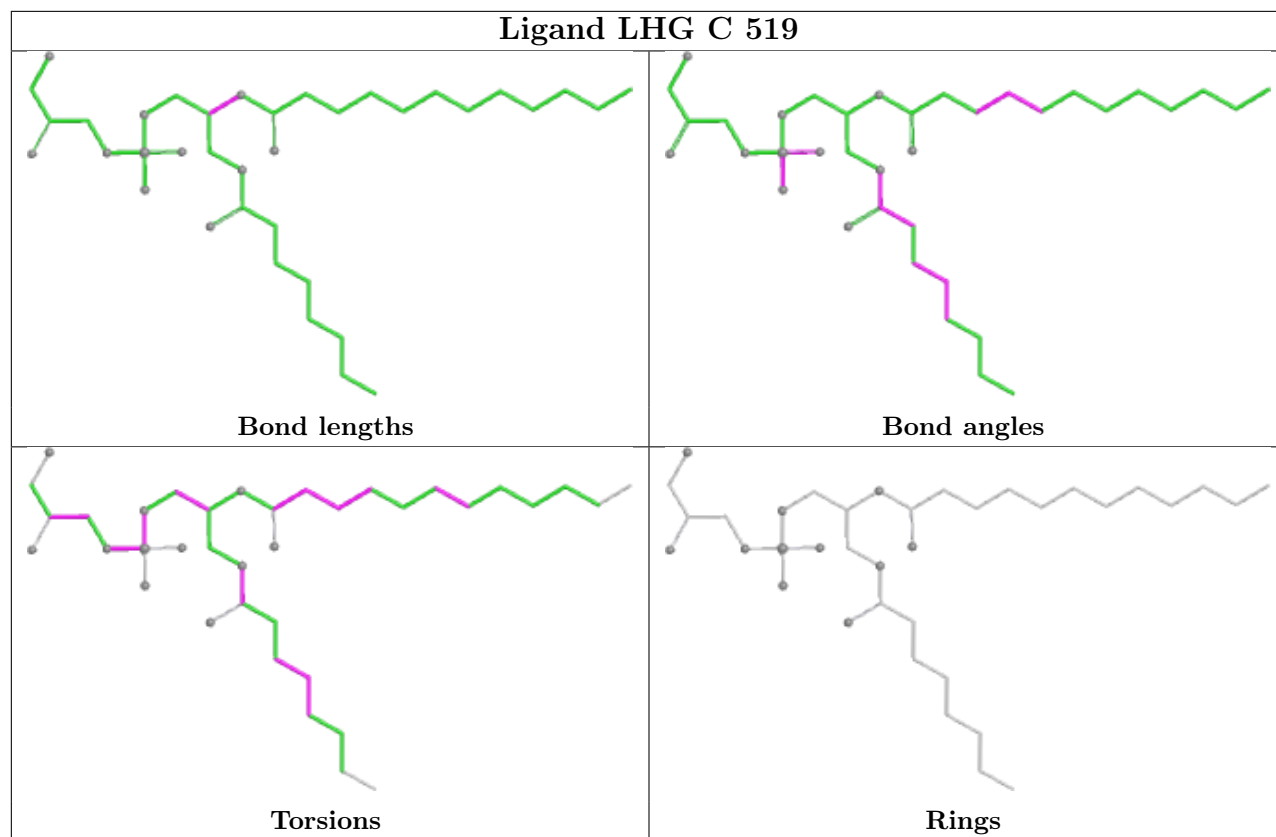


Ligand CLA C 520

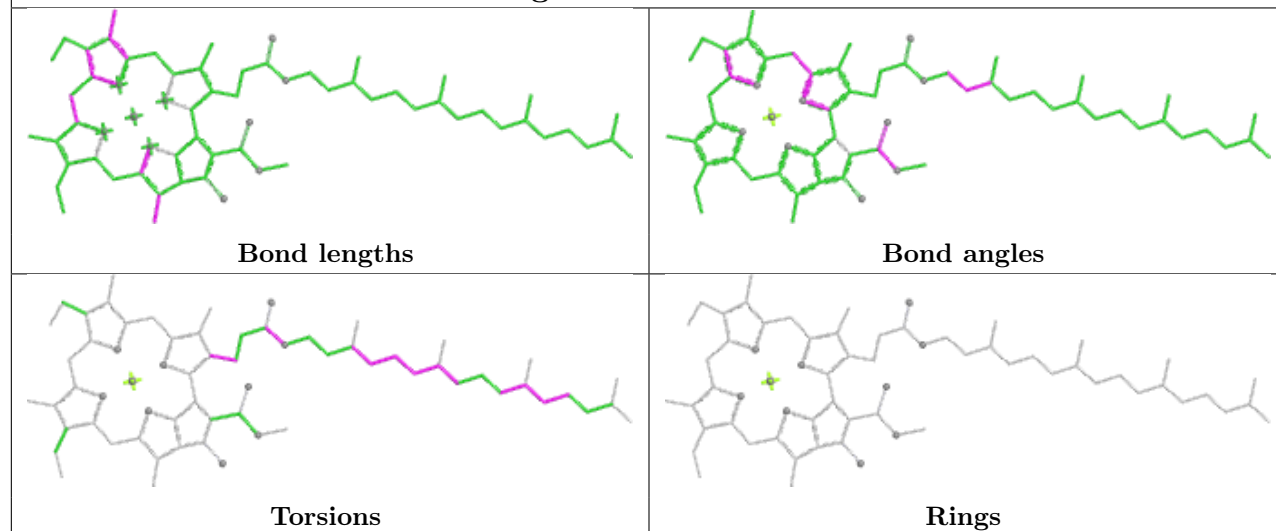


Ligand LMG C 518

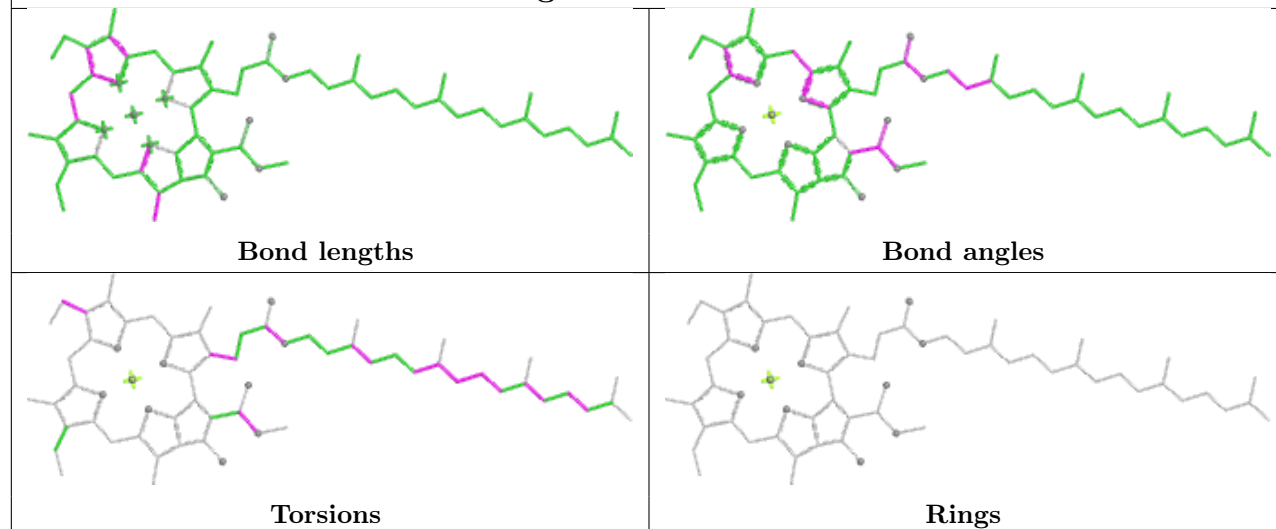




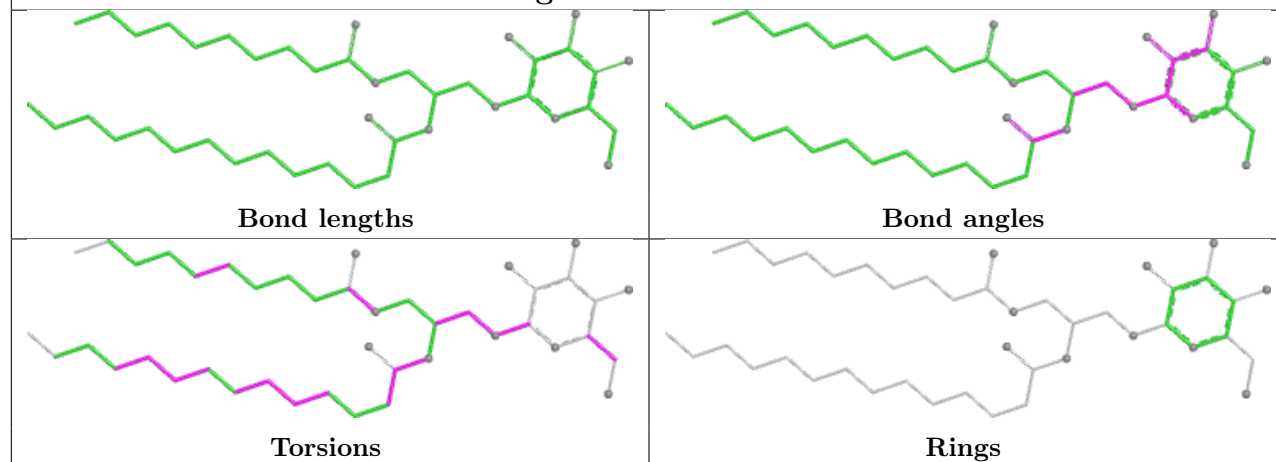
Ligand CLA H 101

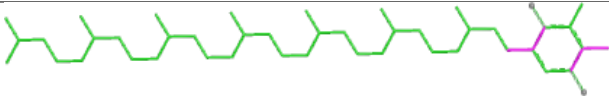
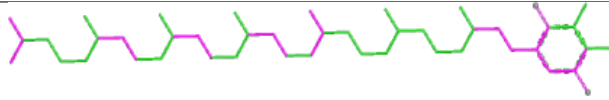
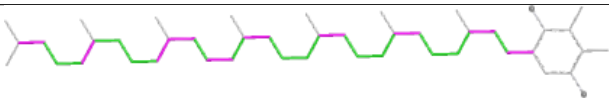
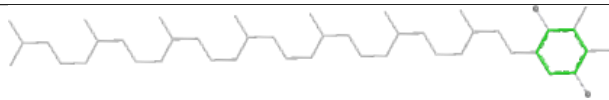


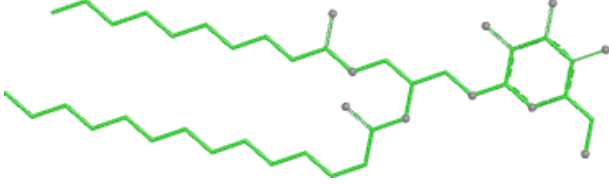
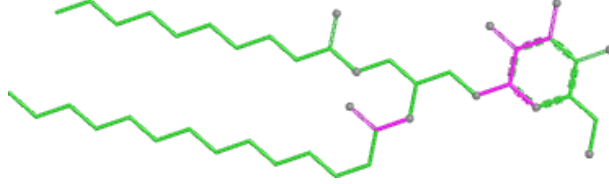
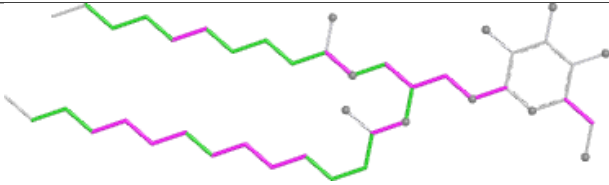
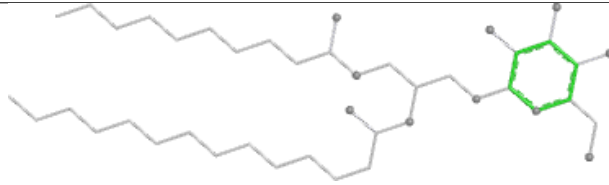
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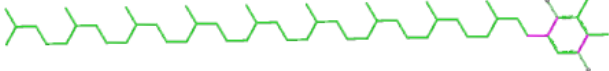
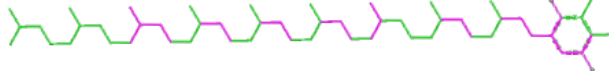
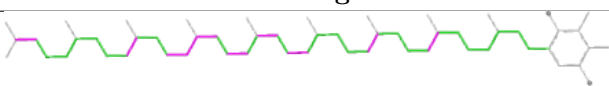
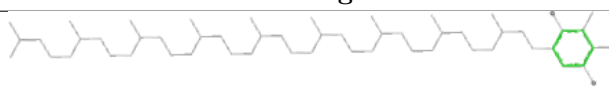


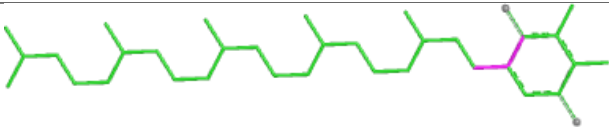
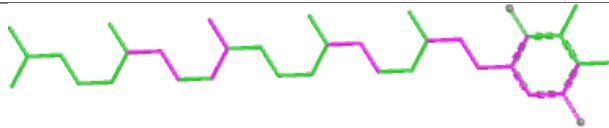
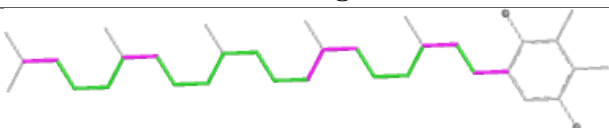
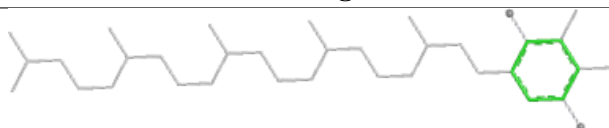
Ligand LMG i 101

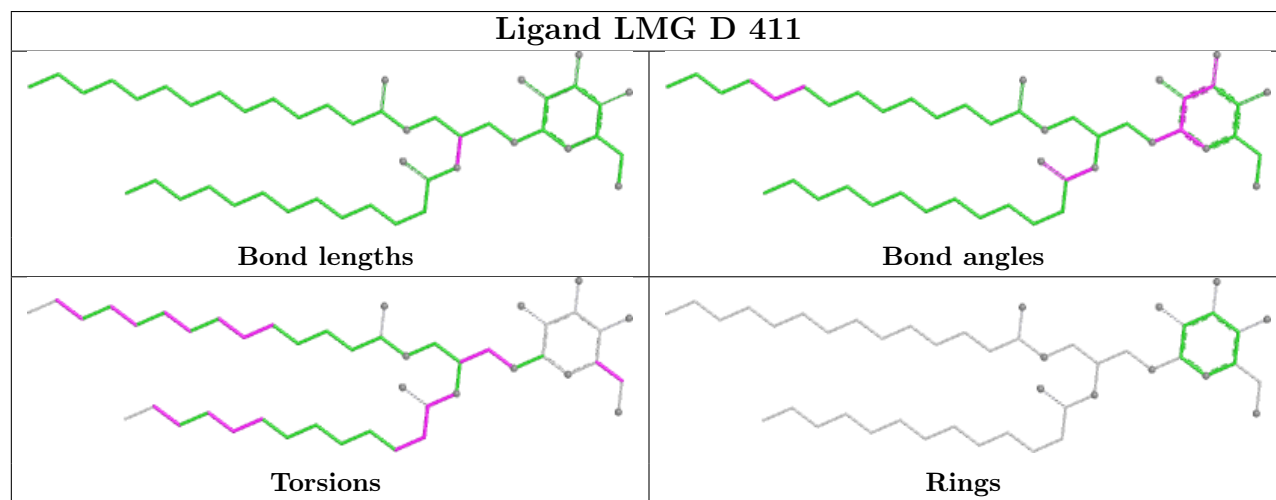
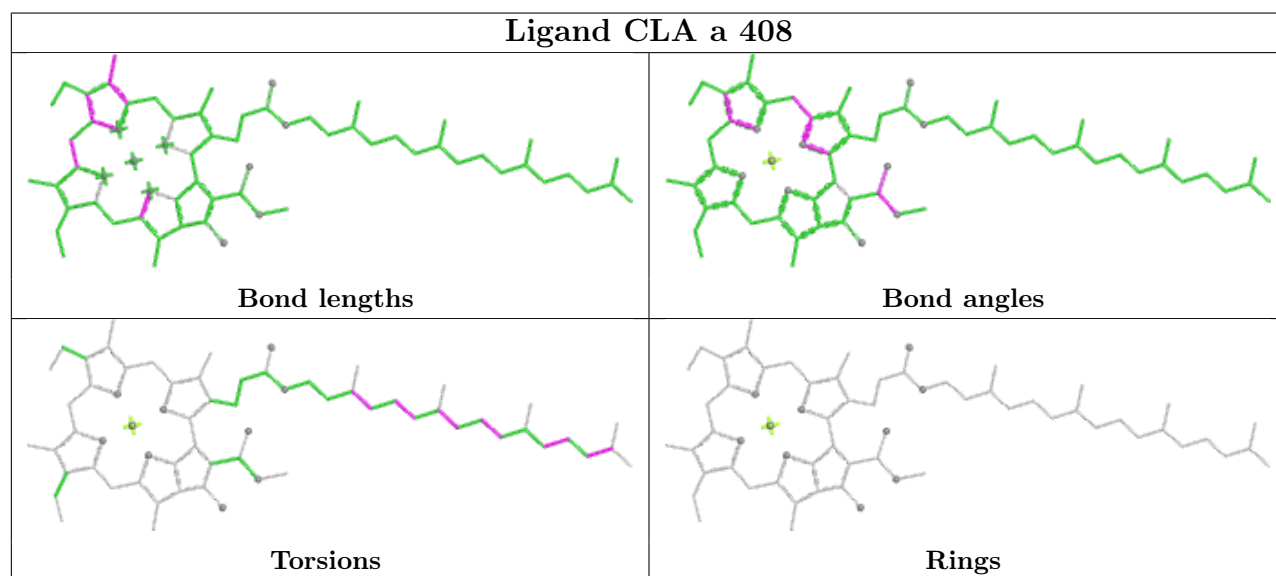
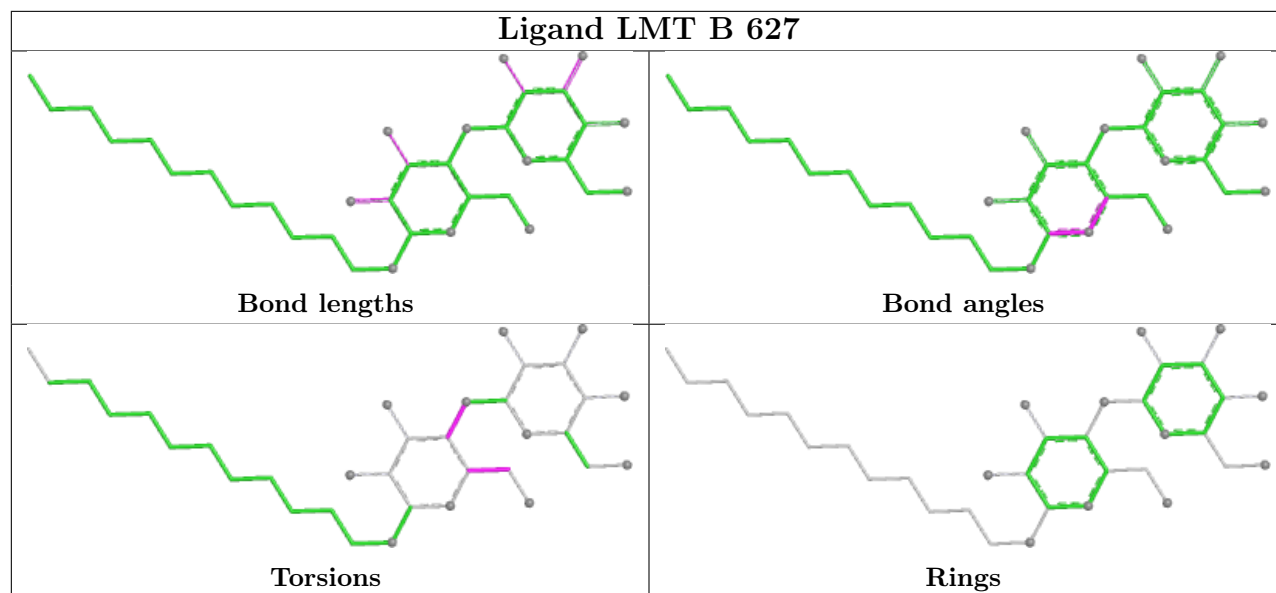


Ligand PL9 a 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

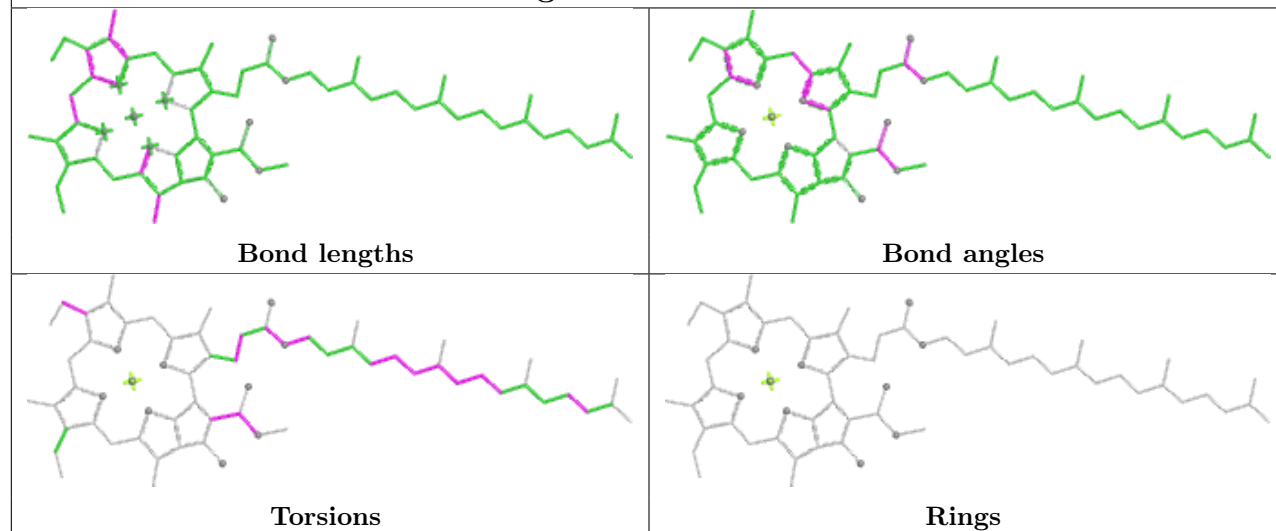
Ligand LMG I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

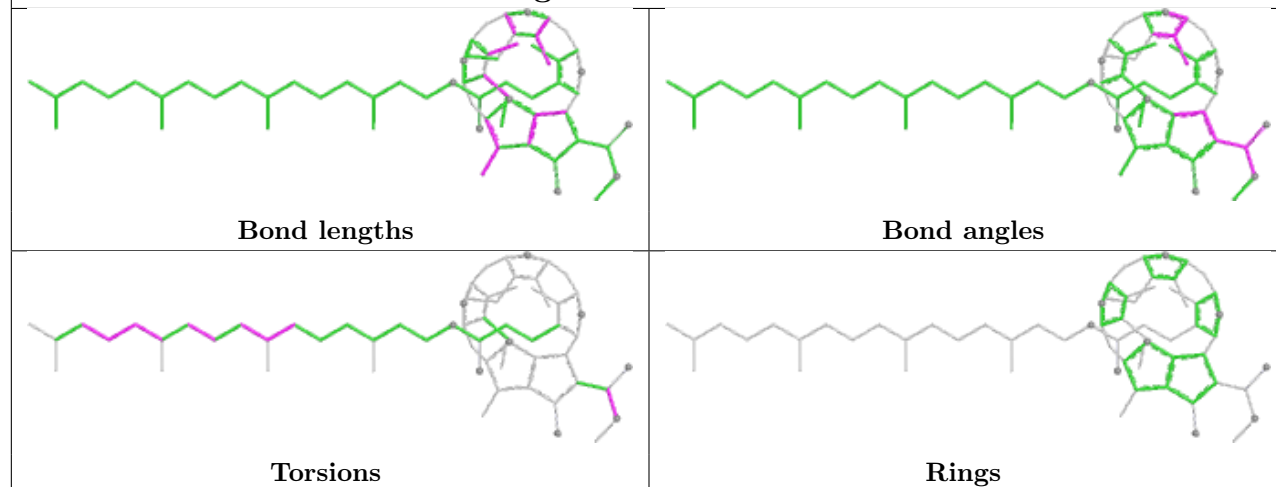
Ligand PL9 J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



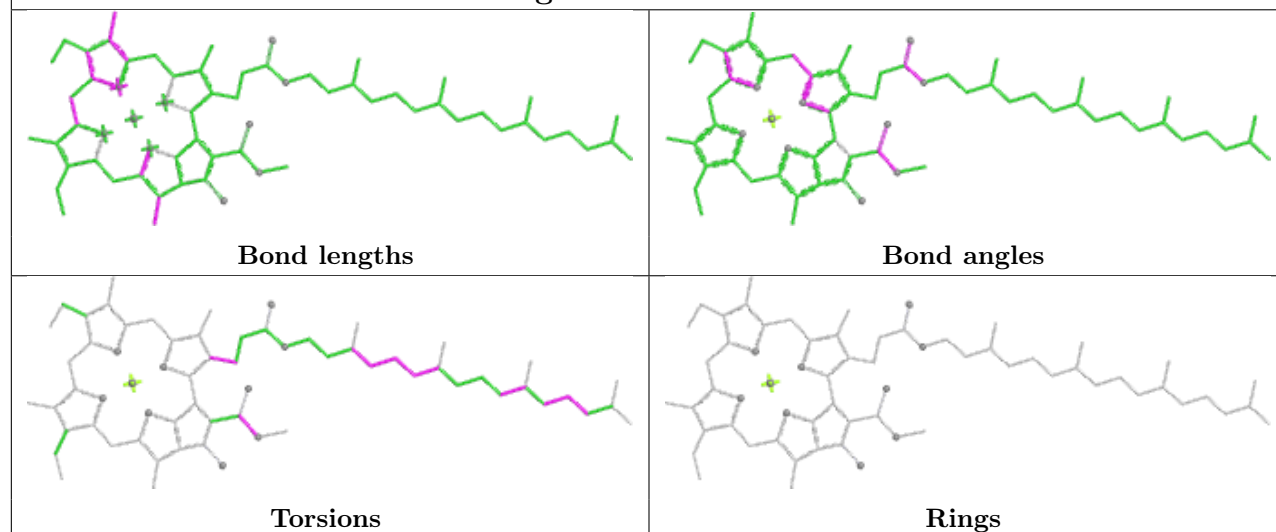
Ligand CLA c 508

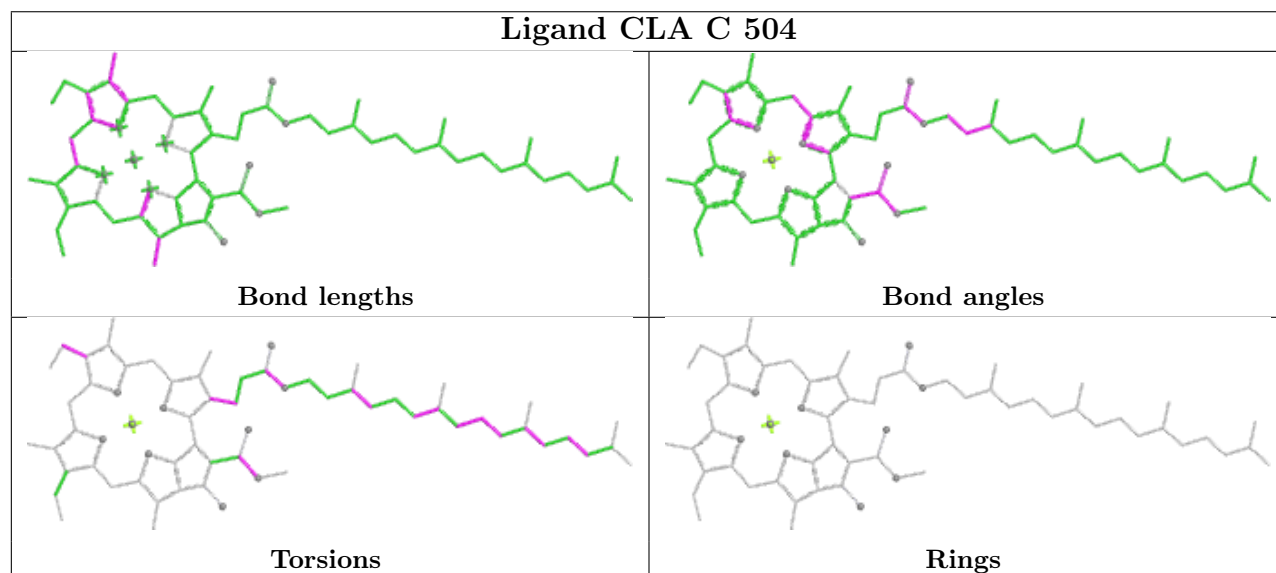
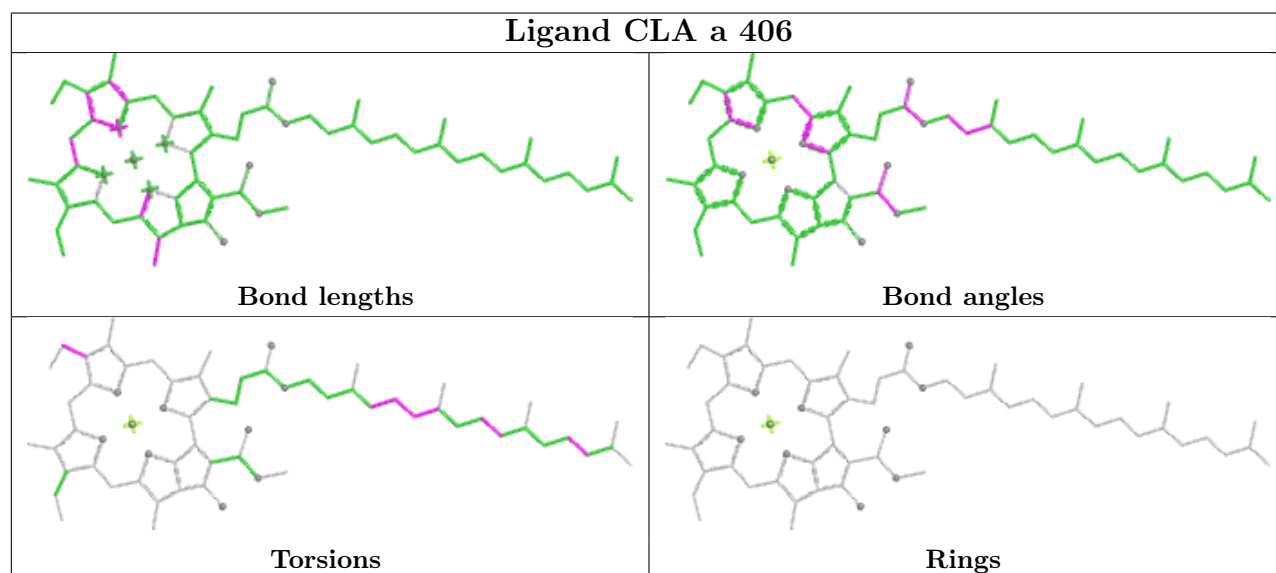
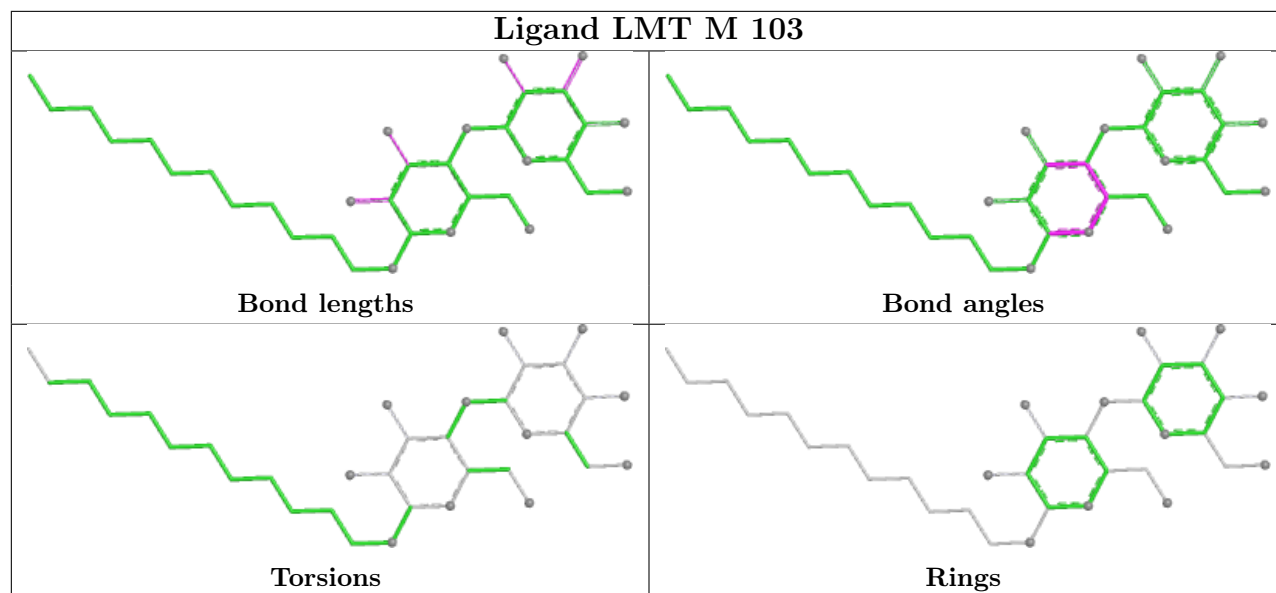


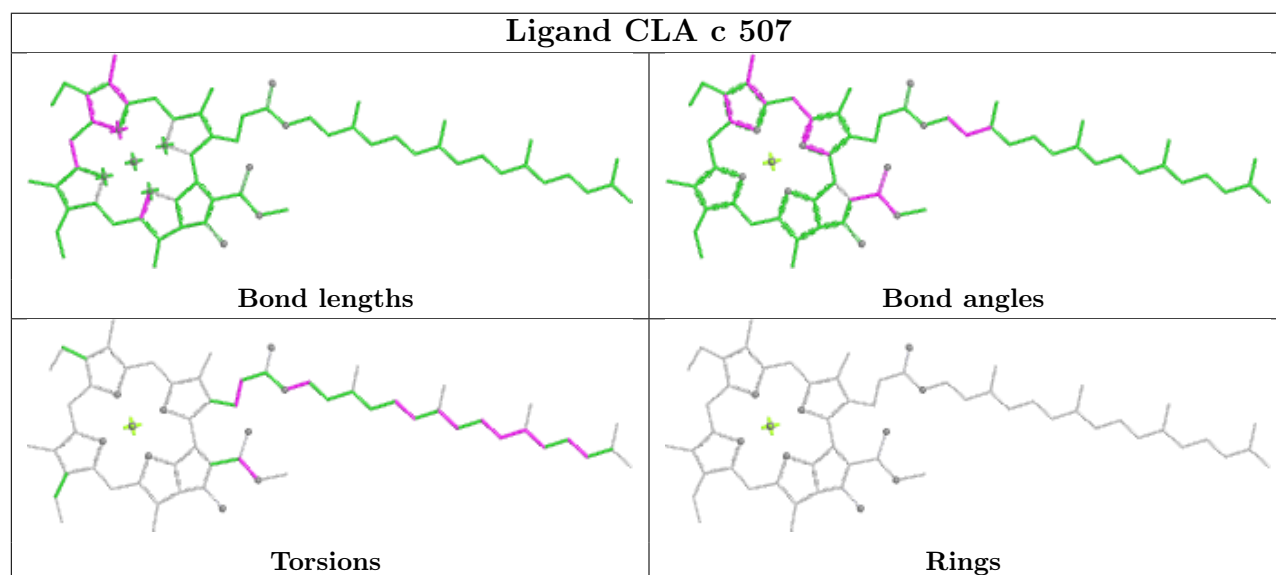
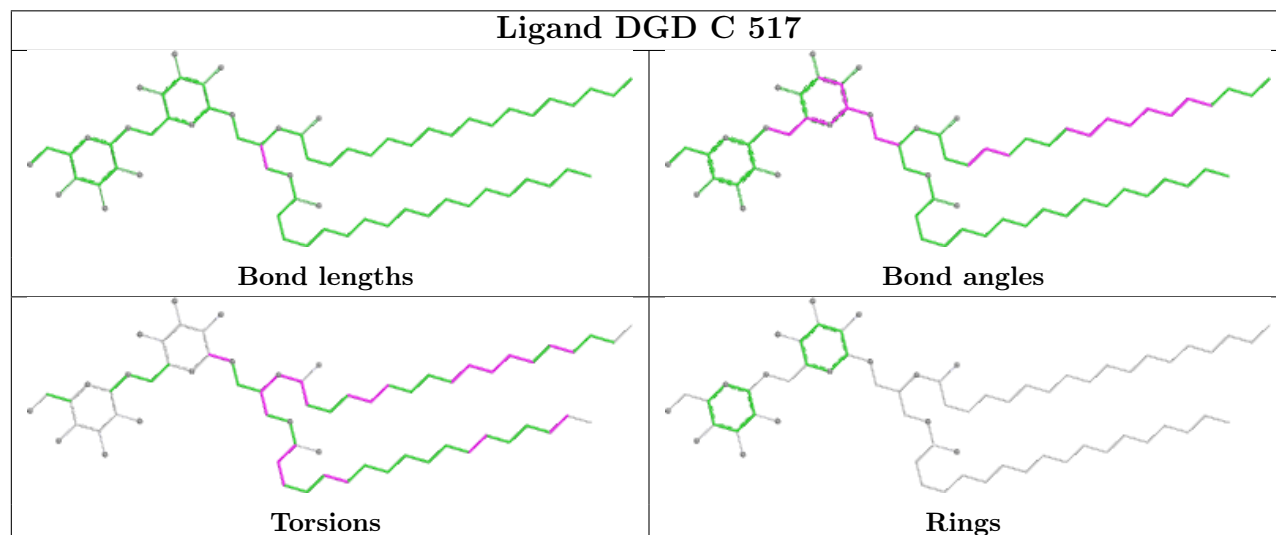
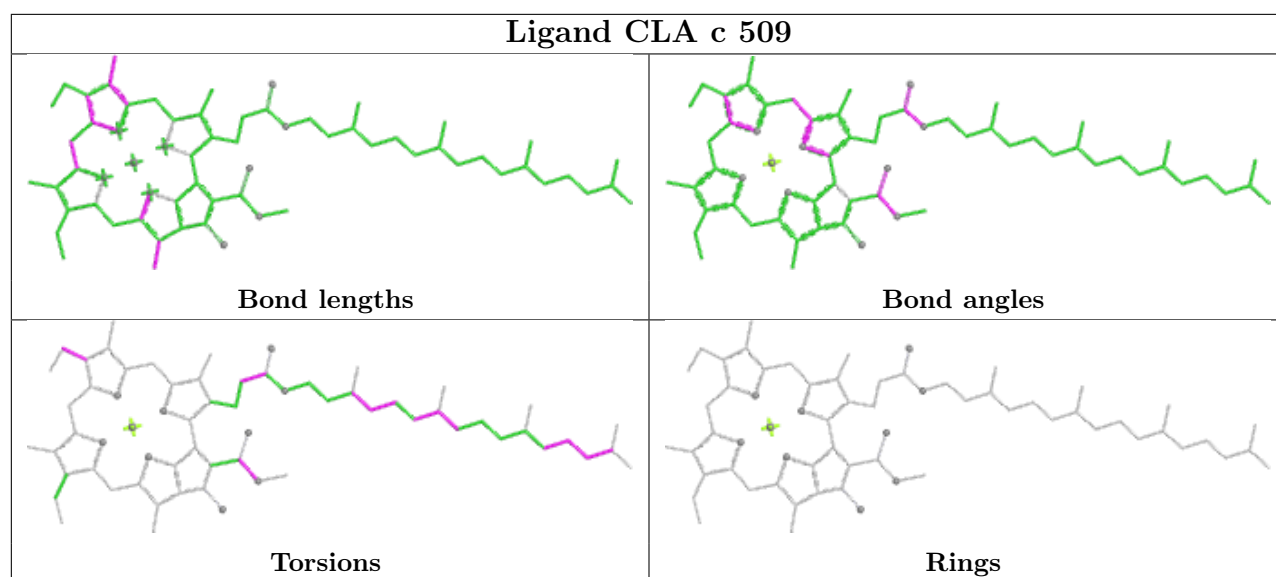
Ligand PHO a 407

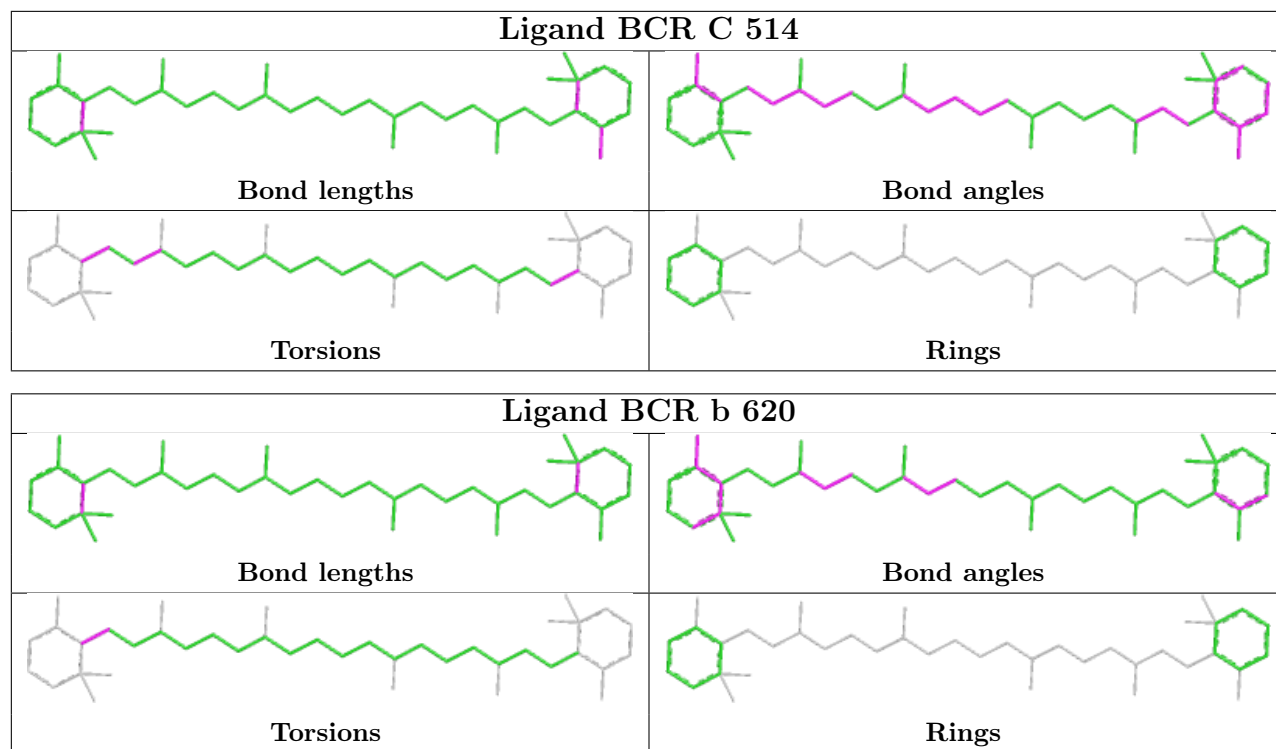


Ligand CLA b 611









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%)	0.04	5 (1%) 72 57	205, 207, 208, 208	0
1	a	335/344 (97%)	-0.15	1 (0%) 90 80	204, 207, 208, 209	0
2	B	490/510 (96%)	-0.14	6 (1%) 76 62	205, 207, 208, 208	0
2	b	490/510 (96%)	-0.09	9 (1%) 67 54	205, 207, 208, 209	0
3	C	447/461 (96%)	-0.05	10 (2%) 62 50	205, 207, 208, 209	0
3	c	447/461 (96%)	-0.13	2 (0%) 88 77	206, 207, 208, 209	0
4	D	340/352 (96%)	-0.01	5 (1%) 72 57	204, 207, 208, 209	0
4	d	340/352 (96%)	-0.15	4 (1%) 76 62	204, 207, 208, 208	0
5	E	82/84 (97%)	-0.13	2 (2%) 59 49	205, 207, 208, 208	0
5	e	82/84 (97%)	-0.06	1 (1%) 76 62	206, 207, 208, 208	0
6	F	35/45 (77%)	-0.08	0 100 100	206, 207, 208, 208	0
6	f	35/45 (77%)	-0.20	0 100 100	206, 207, 208, 208	0
7	H	65/66 (98%)	0.31	4 (6%) 26 28	206, 207, 208, 209	0
7	h	65/66 (98%)	0.15	3 (4%) 37 34	206, 207, 208, 208	0
8	I	35/38 (92%)	-0.15	0 100 100	206, 207, 208, 208	0
8	i	35/38 (92%)	-0.15	1 (2%) 53 43	206, 207, 208, 208	0
9	J	34/40 (85%)	-0.25	0 100 100	205, 207, 207, 208	0
9	j	34/40 (85%)	-0.16	0 100 100	206, 207, 208, 209	0
10	K	37/46 (80%)	-0.22	0 100 100	206, 207, 208, 208	0
10	k	37/46 (80%)	-0.13	0 100 100	206, 207, 208, 209	0
11	L	37/37 (100%)	-0.19	0 100 100	205, 207, 208, 208	0
11	l	37/37 (100%)	-0.13	0 100 100	206, 207, 208, 209	0
12	M	34/36 (94%)	-0.00	0 100 100	205, 206, 207, 208	0
12	m	34/36 (94%)	0.06	1 (2%) 53 43	205, 207, 207, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	-0.03	5 (2%) 63 51	205, 207, 208, 209	0
13	o	243/272 (89%)	-0.12	2 (0%) 82 69	205, 207, 208, 209	0
14	T	32/32 (100%)	-0.11	0 100 100	206, 207, 208, 209	0
14	t	32/32 (100%)	0.03	0 100 100	205, 206, 208, 208	0
15	U	97/134 (72%)	0.00	3 (3%) 51 42	205, 207, 208, 208	0
15	u	97/134 (72%)	0.14	0 100 100	205, 207, 208, 208	0
16	V	137/163 (84%)	0.04	4 (2%) 53 43	205, 207, 208, 208	0
16	v	137/163 (84%)	-0.09	1 (0%) 84 71	206, 207, 208, 208	0
17	g	28/46 (60%)	-0.04	1 (3%) 46 39	206, 207, 208, 209	0
17	y	28/46 (60%)	-0.20	0 100 100	206, 207, 208, 208	0
18	X	37/41 (90%)	0.06	0 100 100	205, 207, 208, 209	0
18	x	37/41 (90%)	0.06	0 100 100	206, 207, 208, 208	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	-0.15	1 (1%) 70 56	205, 207, 208, 209	0
20	z	62/62 (100%)	-0.21	0 100 100	206, 207, 208, 209	0
All	All	5214/5674 (91%)	-0.07	71 (1%) 73 59	204, 207, 208, 209	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	63	LEU	4.4
2	B	309	LEU	4.3
7	H	27	THR	4.3
16	V	47	LEU	3.9
4	D	145	ALA	3.8
2	b	211	ILE	3.8
2	b	386	ALA	3.7
13	O	209	ALA	3.7
1	A	61	ASP	3.6
4	D	144	ILE	3.4
2	B	214	LEU	3.4
4	d	334	GLN	3.3
7	h	27	THR	3.3
7	h	14	LEU	3.2
16	V	74	THR	3.2
4	D	314	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
15	U	39	LEU	3.2
3	C	105	VAL	3.2
7	h	11	LEU	3.1
1	A	263	ALA	3.1
7	H	30	LEU	3.0
3	C	151	TRP	3.0
12	m	26	TYR	2.9
13	O	201	PRO	2.9
2	b	482	ILE	2.8
3	C	368	PRO	2.8
13	o	200	LEU	2.8
4	D	56	THR	2.8
2	b	55	MET	2.8
3	C	149	TYR	2.8
2	b	443	PHE	2.7
3	C	140	LEU	2.6
7	H	64	ALA	2.6
4	d	136	VAL	2.5
2	b	229	LEU	2.5
1	A	67	VAL	2.5
2	B	475	PHE	2.5
2	B	5	TRP	2.5
13	O	195	ASP	2.4
2	b	302	TRP	2.4
20	Z	17	PHE	2.4
1	A	251	ALA	2.3
3	C	44	ASN	2.3
2	b	393	GLU	2.3
15	U	74	THR	2.3
2	B	443	PHE	2.3
16	v	69	GLY	2.3
2	B	471	ALA	2.3
13	O	200	LEU	2.3
1	a	50	ILE	2.2
15	U	40	VAL	2.2
3	c	463	SER	2.2
3	c	260	ALA	2.2
3	C	334	PRO	2.2
7	H	63	LYS	2.2
13	O	234	THR	2.2
3	C	267	SER	2.2
1	A	102	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	303	ILE	2.1
5	E	66	VAL	2.1
3	C	462	GLU	2.1
4	d	137	GLY	2.1
17	g	20	ALA	2.1
16	V	139	VAL	2.1
5	e	84	LYS	2.1
13	o	204	LYS	2.1
5	E	84	LYS	2.1
4	D	307	GLU	2.1
8	i	6	ILE	2.0
16	V	143	GLY	2.0
3	C	87	ILE	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($\text{\AA}^2$)	Q<0.9
31	LMT	d	410	31/35	0.48	0.17	206,208,209,210	0
31	LMT	i	102	35/35	0.50	0.17	206,208,209,210	0
31	LMT	I	102	35/35	0.54	0.18	205,207,209,210	0
22	CLA	b	605	65/65	0.61	0.22	205,208,209,209	0
31	LMT	B	623	35/35	0.65	0.14	205,208,209,210	0
35	CA	K	101	1/1	0.65	0.17	210,210,210,210	0
31	LMT	b	626	35/35	0.67	0.14	205,208,210,210	0
31	LMT	b	627	35/35	0.68	0.13	205,208,210,210	0
22	CLA	B	601	65/65	0.69	0.17	206,207,208,209	0
31	LMT	D	410	31/35	0.70	0.13	206,208,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	J	102	40/40	0.71	0.26	205,207,208,209	0
27	LMG	E	101	44/55	0.71	0.24	204,207,209,210	0
26	LHG	c	519	37/49	0.72	0.19	205,207,211,214	0
33	BCT	d	403	4/4	0.74	0.24	207,207,207,208	0
35	CA	O	301	1/1	0.75	0.08	207,207,207,207	0
25	DGD	B	625	52/66	0.76	0.18	205,208,210,210	0
27	LMG	c	518	45/55	0.76	0.17	206,207,208,208	0
23	PL9	A	406	45/55	0.76	0.29	205,206,207,208	0
22	CLA	b	619	65/65	0.77	0.15	205,207,208,209	0
35	CA	o	301	1/1	0.77	0.12	209,209,209,209	0
31	LMT	b	603	35/35	0.78	0.12	205,207,208,209	0
27	LMG	C	518	45/55	0.78	0.16	205,206,208,208	0
22	CLA	c	512	65/65	0.78	0.15	205,207,208,208	0
25	DGD	D	409	63/66	0.78	0.18	205,208,209,211	0
25	DGD	d	409	63/66	0.78	0.19	205,208,210,211	0
31	LMT	B	628	35/35	0.78	0.17	204,207,209,209	0
24	BCR	j	102	40/40	0.78	0.24	206,207,209,209	0
27	LMG	A	415	42/55	0.78	0.22	204,207,208,209	0
31	LMT	M	102	35/35	0.78	0.20	205,207,208,209	0
30	SQD	B	626	47/54	0.79	0.15	204,207,209,211	0
30	SQD	d	402	43/54	0.80	0.17	205,207,209,211	0
27	LMG	a	402	42/55	0.80	0.19	204,207,209,209	0
31	LMT	B	627	35/35	0.80	0.11	205,207,209,209	0
30	SQD	F	103	45/54	0.80	0.21	205,207,209,210	0
31	LMT	B	624	35/35	0.81	0.13	205,207,210,210	0
25	DGD	C	517	66/66	0.81	0.18	205,206,207,208	0
23	PL9	J	101	35/55	0.81	0.27	204,207,208,209	0
22	CLA	C	506	65/65	0.81	0.18	204,207,207,208	0
30	SQD	A	413	51/54	0.81	0.18	205,207,208,208	0
26	LHG	C	519	37/49	0.82	0.14	204,207,210,212	0
25	DGD	C	516	62/66	0.82	0.13	204,206,208,208	0
25	DGD	A	408	56/66	0.82	0.18	206,207,209,210	0
25	DGD	c	517	66/66	0.83	0.17	204,206,207,208	0
24	BCR	c	521	40/40	0.83	0.16	205,207,208,209	0
27	LMG	b	625	49/55	0.83	0.20	205,206,207,208	0
25	DGD	b	601	52/66	0.83	0.15	204,207,208,209	0
30	SQD	b	602	47/54	0.84	0.16	205,207,209,212	0
24	BCR	H	102	40/40	0.84	0.20	206,207,208,208	0
27	LMG	I	101	43/55	0.84	0.16	204,207,209,210	0
22	CLA	a	406	65/65	0.84	0.21	205,207,208,209	0
24	BCR	a	410	40/40	0.84	0.22	205,206,207,207	0
24	BCR	b	621	40/40	0.84	0.19	204,206,207,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	c	513	40/40	0.84	0.18	204,206,207,208	0
22	CLA	C	512	65/65	0.84	0.15	205,207,208,209	0
25	DGD	a	411	56/66	0.84	0.16	205,207,209,209	0
27	LMG	l	101	51/55	0.85	0.19	205,206,208,208	0
25	DGD	c	516	62/66	0.85	0.16	205,207,208,209	0
23	PL9	d	406	55/55	0.85	0.16	204,206,207,208	0
32	PHO	D	402	64/64	0.85	0.16	205,206,207,208	0
30	SQD	a	401	54/54	0.86	0.16	205,207,209,211	0
22	CLA	c	506	65/65	0.86	0.15	206,207,208,208	0
24	BCR	x	101	40/40	0.86	0.21	205,207,208,208	0
27	LMG	m	101	42/55	0.86	0.18	203,207,208,209	0
22	CLA	c	505	65/65	0.87	0.14	204,206,208,208	0
22	CLA	b	613	65/65	0.87	0.13	205,207,208,209	0
24	BCR	g	101	40/40	0.87	0.17	204,206,207,207	0
27	LMG	e	101	44/55	0.87	0.17	204,207,208,209	0
22	CLA	c	510	65/65	0.87	0.13	206,207,208,209	0
22	CLA	A	405	65/65	0.87	0.15	204,206,208,208	0
31	LMT	b	604	35/35	0.87	0.16	205,207,209,209	0
27	LMG	M	101	42/55	0.87	0.17	205,207,209,210	0
25	DGD	C	515	53/66	0.88	0.15	204,206,207,208	0
22	CLA	B	605	65/65	0.88	0.12	205,206,207,208	0
24	BCR	K	102	40/40	0.88	0.20	204,207,208,209	0
23	PL9	j	101	35/55	0.88	0.23	205,208,209,209	0
24	BCR	C	514	40/40	0.88	0.17	205,206,207,207	0
27	LMG	B	621	49/55	0.88	0.16	204,206,207,208	0
24	BCR	b	623	40/40	0.88	0.13	204,206,207,207	0
22	CLA	c	502	65/65	0.88	0.15	205,207,208,208	0
27	LMG	i	101	43/55	0.89	0.12	205,207,209,209	0
22	CLA	C	520	65/65	0.89	0.15	205,207,208,209	0
24	BCR	b	622	40/40	0.89	0.22	204,206,207,207	0
22	CLA	c	503	65/65	0.89	0.13	205,207,208,208	0
30	SQD	B	622	43/54	0.89	0.15	205,207,209,212	0
32	PHO	D	401	64/64	0.89	0.14	203,206,207,208	0
22	CLA	b	606	65/65	0.89	0.14	205,206,207,207	0
27	LMG	C	521	48/55	0.89	0.18	204,206,207,208	0
27	LMG	c	522	48/55	0.89	0.19	205,206,207,208	0
31	LMT	M	103	35/35	0.89	0.14	205,206,208,210	0
24	BCR	b	620	40/40	0.89	0.21	205,206,207,208	0
30	SQD	A	414	54/54	0.90	0.14	204,207,208,210	0
22	CLA	C	508	65/65	0.90	0.13	205,206,207,208	0
25	DGD	b	624	58/66	0.90	0.19	205,206,207,208	0
22	CLA	C	510	65/65	0.90	0.12	205,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	BCR	y	101	40/40	0.90	0.18	205,206,207,207	0
30	SQD	a	415	51/54	0.90	0.15	205,206,208,208	0
22	CLA	C	511	65/65	0.90	0.13	205,207,208,208	0
23	PL9	D	406	55/55	0.90	0.17	204,206,207,207	0
22	CLA	c	501	65/65	0.90	0.13	205,207,208,209	0
22	CLA	B	613	65/65	0.90	0.13	205,206,207,208	0
22	CLA	B	615	65/65	0.90	0.13	205,206,208,208	0
22	CLA	C	505	65/65	0.90	0.14	205,206,207,208	0
21	FE2	a	403	1/1	0.90	0.17	211,211,211,211	0
35	CA	k	101	1/1	0.90	0.07	204,204,204,204	0
27	LMG	D	408	48/55	0.90	0.13	202,206,208,208	0
27	LMG	d	408	48/55	0.91	0.16	204,206,207,208	0
26	LHG	A	409	39/49	0.91	0.19	205,206,208,209	0
22	CLA	B	607	65/65	0.91	0.15	205,206,207,209	0
25	DGD	B	620	58/66	0.91	0.16	203,206,208,209	0
23	PL9	a	409	45/55	0.91	0.18	204,206,207,208	0
22	CLA	c	508	65/65	0.91	0.10	205,207,208,208	0
22	CLA	b	607	65/65	0.91	0.11	205,206,207,209	0
24	BCR	A	407	40/40	0.91	0.15	205,206,207,208	0
24	BCR	B	616	40/40	0.91	0.11	205,206,207,207	0
27	LMG	D	411	46/55	0.91	0.15	205,206,207,208	0
24	BCR	B	619	40/40	0.91	0.12	205,206,207,207	0
24	BCR	c	514	40/40	0.91	0.17	205,206,207,208	0
22	CLA	b	609	65/65	0.91	0.11	205,207,208,209	0
25	DGD	c	515	53/66	0.91	0.16	205,207,208,209	0
30	SQD	f	103	45/54	0.91	0.14	205,207,208,210	0
22	CLA	h	101	65/65	0.91	0.15	204,207,208,209	0
22	CLA	b	610	65/65	0.91	0.13	205,206,207,208	0
22	CLA	A	404	65/65	0.91	0.16	204,206,207,208	0
22	CLA	a	405	65/65	0.92	0.14	202,206,207,208	0
22	CLA	c	511	65/65	0.92	0.12	205,207,208,209	0
24	BCR	F	102	40/40	0.92	0.17	205,206,207,208	0
22	CLA	b	617	65/65	0.92	0.13	205,206,208,209	0
22	CLA	B	604	65/65	0.92	0.12	205,207,208,208	0
22	CLA	B	602	65/65	0.92	0.13	204,206,208,209	0
22	CLA	C	504	65/65	0.92	0.13	205,206,207,207	0
22	CLA	B	603	65/65	0.92	0.12	204,206,207,208	0
22	CLA	c	504	65/65	0.92	0.15	205,207,208,208	0
32	PHO	d	401	64/64	0.92	0.13	204,206,207,207	0
22	CLA	b	608	65/65	0.92	0.12	205,206,207,208	0
22	CLA	B	609	65/65	0.92	0.11	205,206,208,208	0
22	CLA	D	404	65/65	0.92	0.12	203,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	c	509	65/65	0.92	0.12	204,206,208,209	0
24	BCR	B	617	40/40	0.92	0.15	204,206,207,208	0
27	LMG	d	407	49/55	0.93	0.17	205,206,207,207	0
22	CLA	c	520	65/65	0.93	0.13	205,207,207,208	0
27	LMG	D	407	49/55	0.93	0.15	205,206,207,208	0
22	CLA	d	404	65/65	0.93	0.15	204,206,207,207	0
22	CLA	C	509	65/65	0.93	0.12	205,206,207,208	0
22	CLA	B	611	65/65	0.93	0.10	204,206,207,208	0
28	CL	A	411	1/1	0.93	0.15	207,207,207,207	0
32	PHO	a	407	64/64	0.93	0.11	205,207,207,208	0
22	CLA	b	618	65/65	0.93	0.12	205,207,208,208	0
26	LHG	a	412	39/49	0.93	0.14	205,207,208,210	0
24	BCR	B	618	40/40	0.93	0.18	204,205,207,207	0
22	CLA	C	503	65/65	0.93	0.12	205,207,207,208	0
24	BCR	C	513	40/40	0.93	0.12	205,206,207,208	0
22	CLA	H	101	65/65	0.93	0.14	205,206,207,208	0
22	CLA	b	615	65/65	0.94	0.09	205,206,207,208	0
22	CLA	C	502	65/65	0.94	0.13	205,206,207,208	0
24	BCR	f	102	40/40	0.94	0.15	206,206,207,208	0
27	LMG	d	411	46/55	0.94	0.14	204,206,207,208	0
22	CLA	A	402	65/65	0.94	0.14	205,206,207,208	0
22	CLA	D	405	65/65	0.94	0.14	205,206,207,207	0
22	CLA	B	614	65/65	0.94	0.11	205,206,207,208	0
22	CLA	B	608	65/65	0.94	0.12	205,207,208,209	0
22	CLA	C	501	65/65	0.94	0.10	205,206,207,208	0
22	CLA	d	405	65/65	0.94	0.14	204,206,207,208	0
22	CLA	b	611	65/65	0.94	0.12	205,206,207,208	0
22	CLA	b	612	65/65	0.94	0.12	205,206,207,209	0
22	CLA	a	408	65/65	0.94	0.12	205,206,207,209	0
27	LMG	A	410	51/55	0.94	0.14	204,206,207,208	0
22	CLA	A	403	65/65	0.95	0.12	204,206,207,207	0
28	CL	a	413	1/1	0.95	0.14	204,204,204,204	0
22	CLA	a	404	65/65	0.95	0.10	205,206,207,208	0
34	HEM	f	101	43/43	0.95	0.12	206,207,207,208	0
34	HEM	v	201	43/43	0.95	0.12	205,207,207,208	0
22	CLA	B	610	65/65	0.95	0.09	205,206,207,207	0
22	CLA	B	606	65/65	0.95	0.12	205,206,207,208	0
22	CLA	c	507	65/65	0.95	0.10	205,207,208,208	0
22	CLA	C	507	65/65	0.95	0.14	205,206,208,210	0
33	BCT	D	403	4/4	0.96	0.06	206,206,206,206	0
21	FE2	A	401	1/1	0.96	0.07	206,206,206,206	0
34	HEM	F	101	43/43	0.96	0.10	205,207,208,209	0

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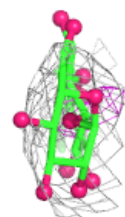
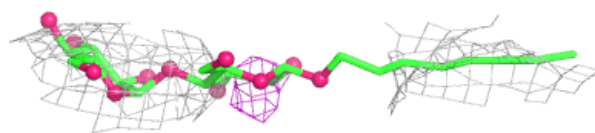
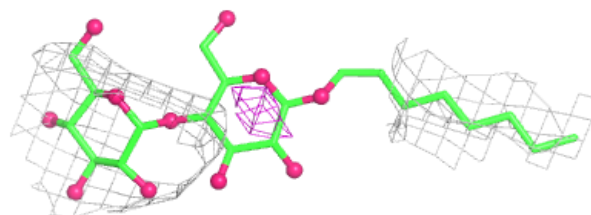
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HEM	V	201	43/43	0.96	0.16	203,206,207,208	0
22	CLA	B	612	65/65	0.96	0.10	204,206,207,207	0
22	CLA	b	616	65/65	0.97	0.17	204,206,208,209	0
22	CLA	b	614	65/65	0.97	0.12	205,206,207,208	0
29	OEX	A	412	10/10	0.98	0.07	198,204,206,206	0
29	OEX	a	414	10/10	0.98	0.08	198,203,205,207	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.

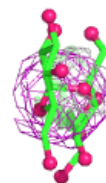
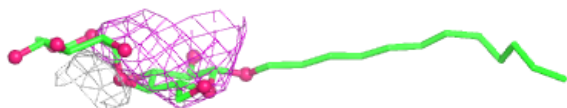
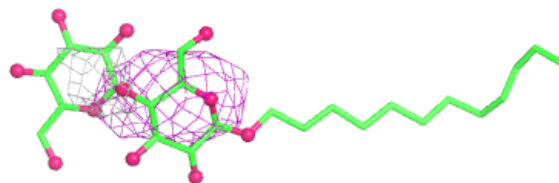
Electron density around LMT d 410:

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

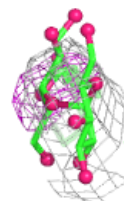
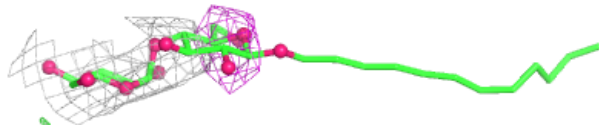
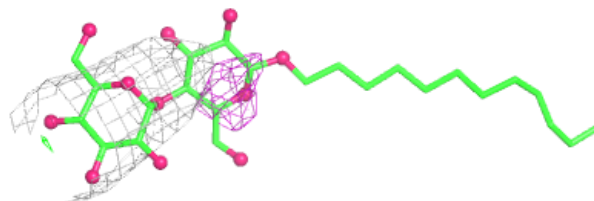


Electron density around LMT i 102:

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

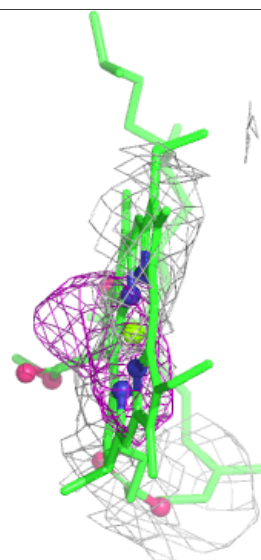
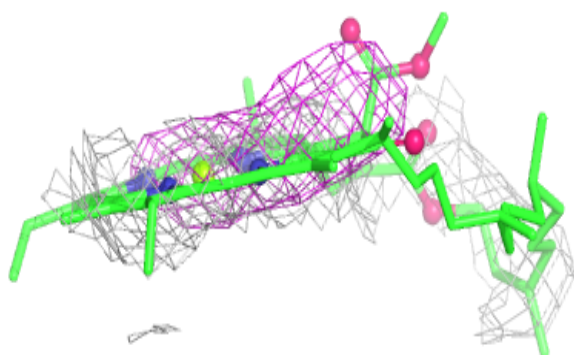
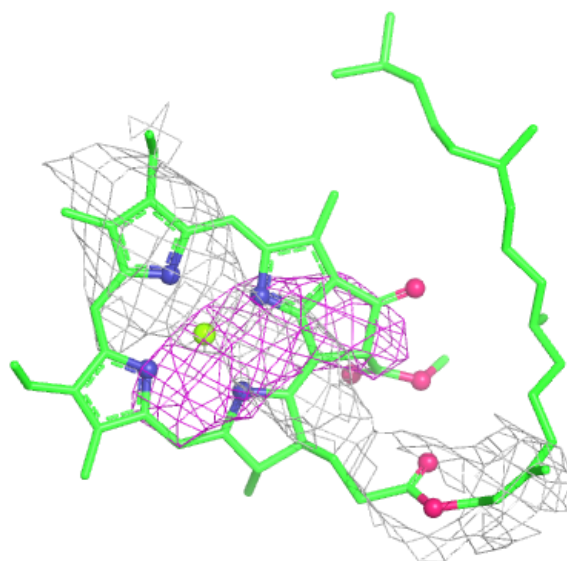
**Electron density around LMT I 102:**

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



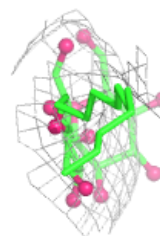
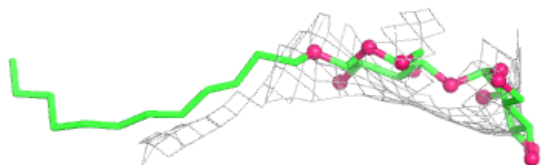
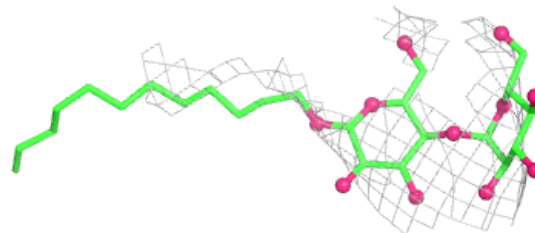
Electron density around CLA b 605:

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

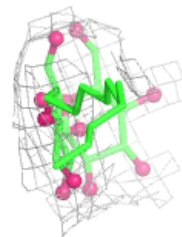
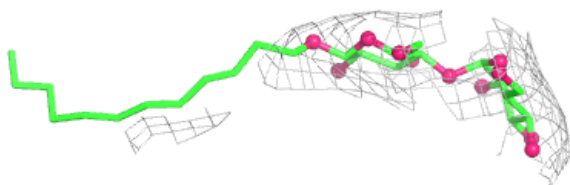
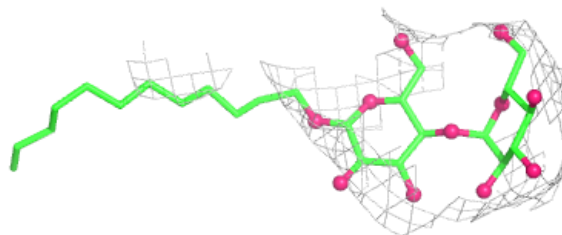


Electron density around LMT B 623:

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

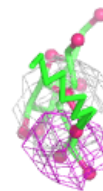
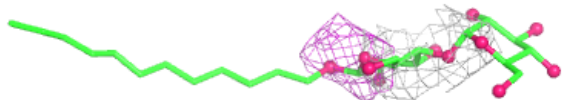
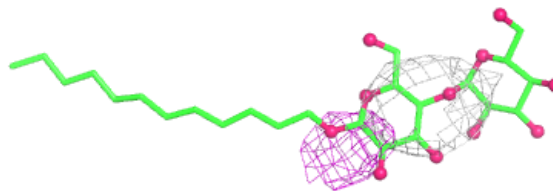
**Electron density around LMT b 626:**

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



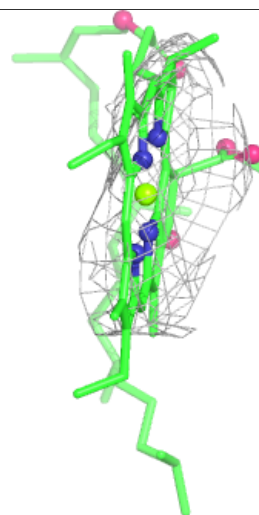
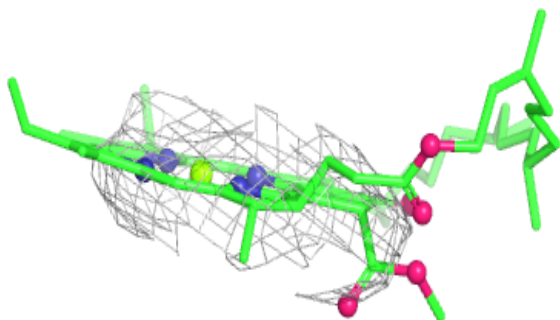
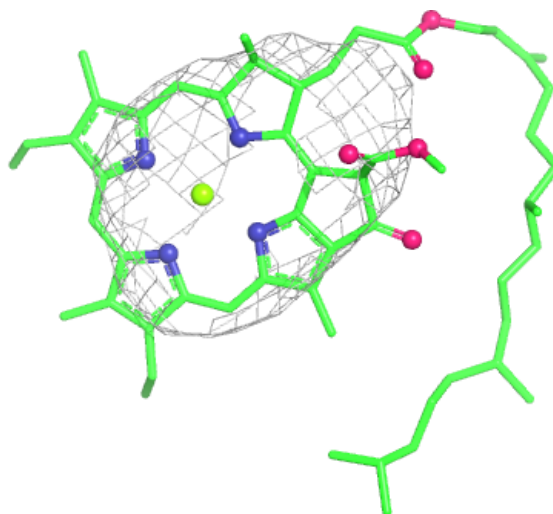
Electron density around LMT b 627:

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



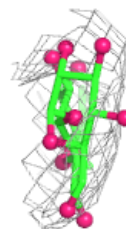
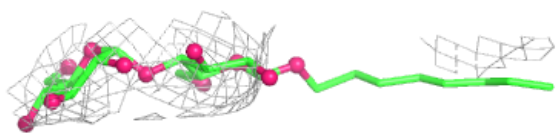
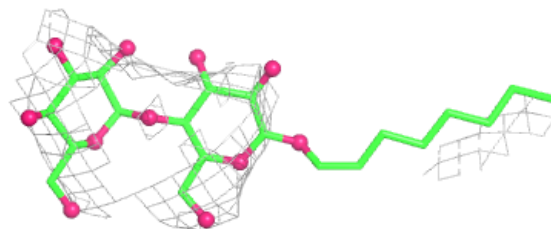
Electron density around CLA B 601:

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and green (positive)

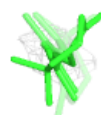
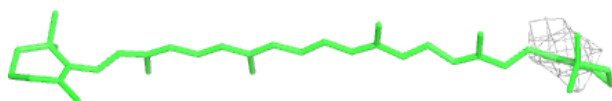
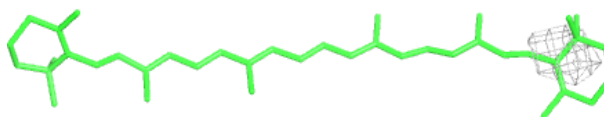


Electron density around LMT D 410:

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

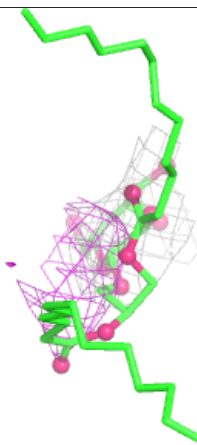
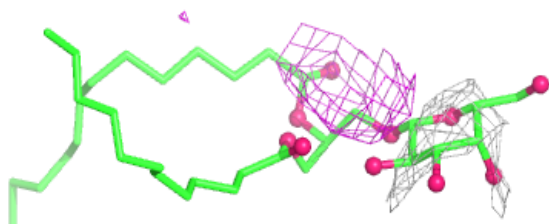
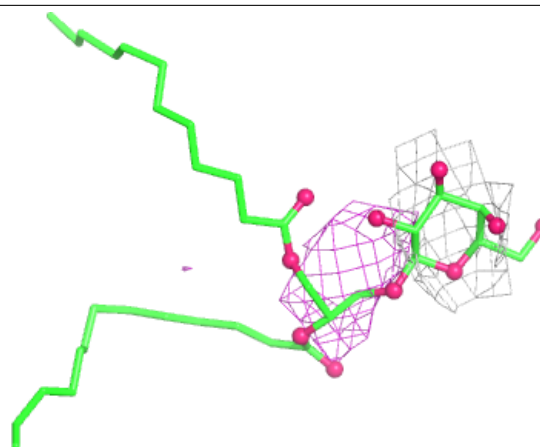
**Electron density around BCR J 102:**

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



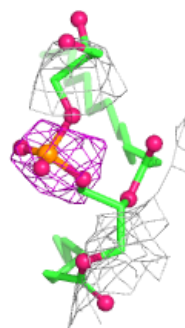
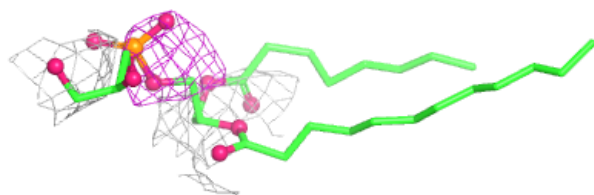
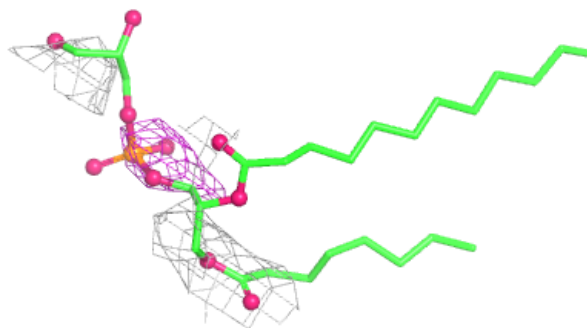
Electron density around LMG E 101:

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

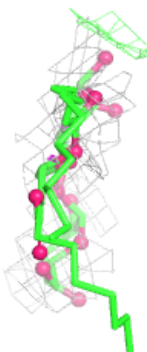
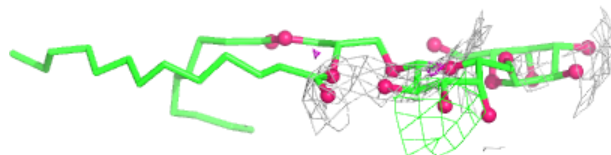
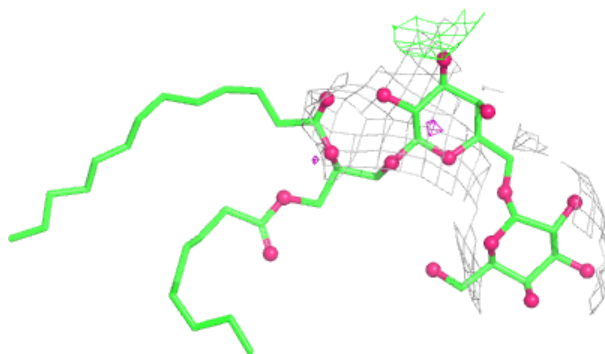


Electron density around LHG c 519:

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

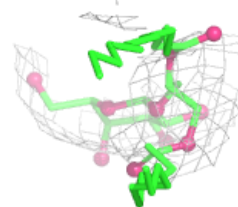
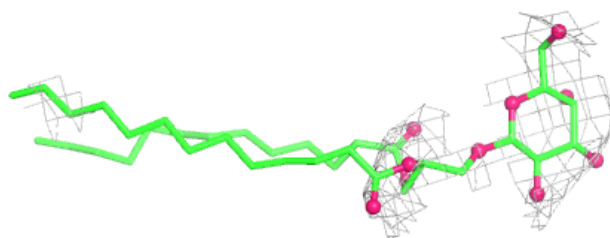
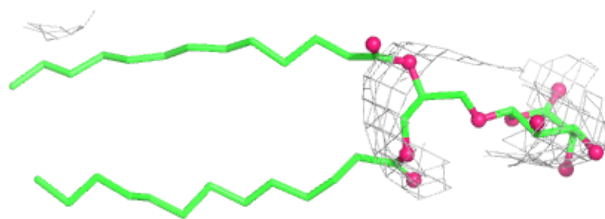
**Electron density around DGD B 625:**

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

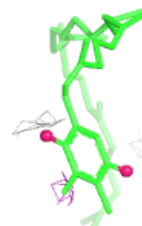
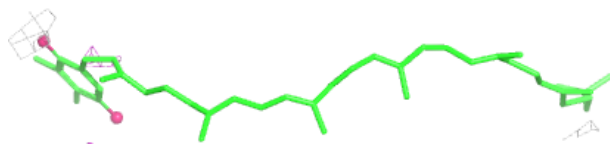
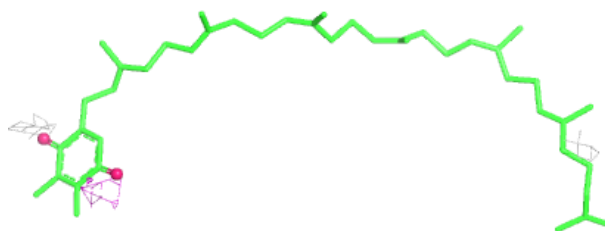


Electron density around LMG c 518:

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

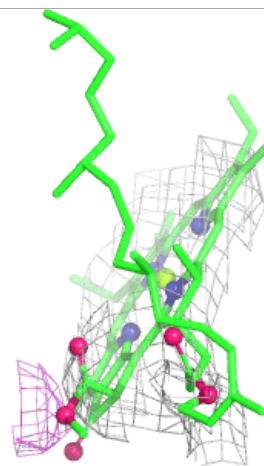
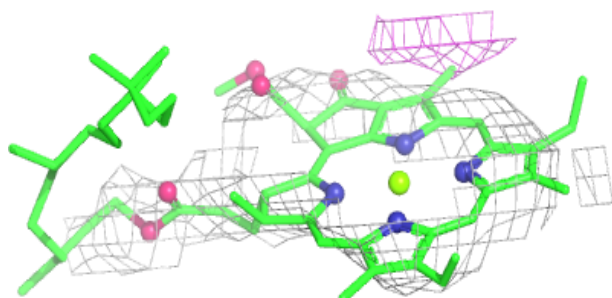
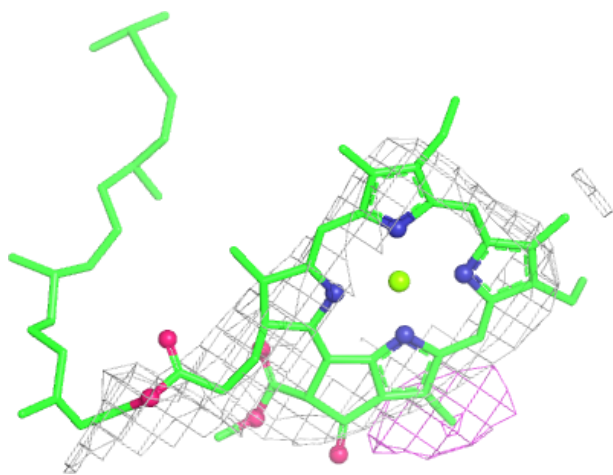
**Electron density around PL9 A 406:**

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



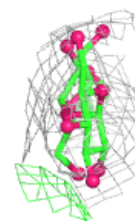
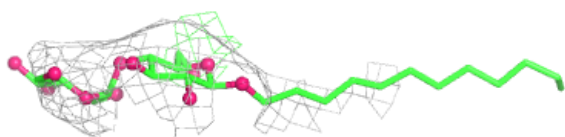
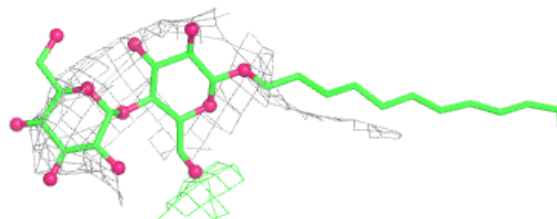
Electron density around CLA b 619:

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

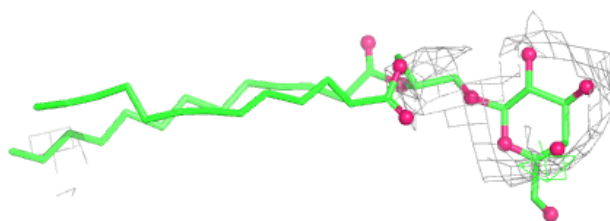
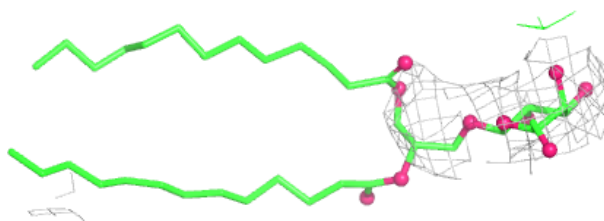


Electron density around LMT b 603:

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

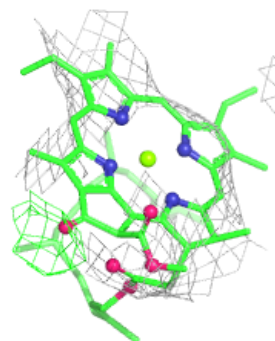
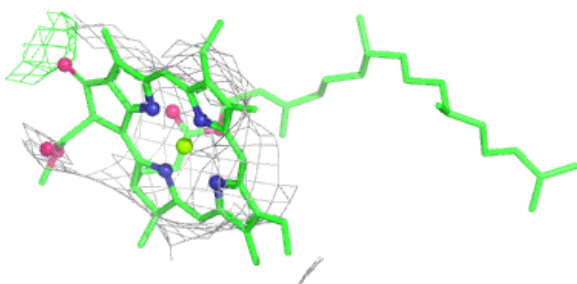
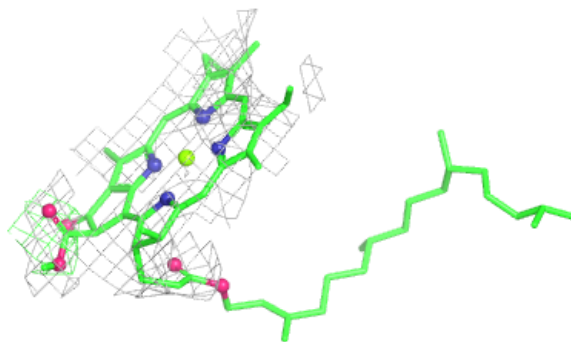
**Electron density around LMG C 518:**

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

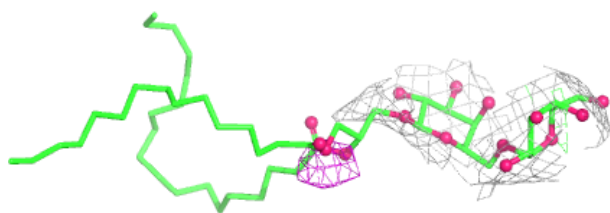
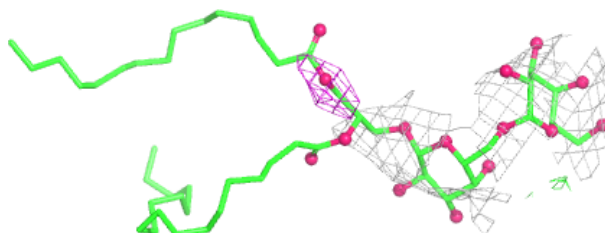


Electron density around CLA c 512:

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

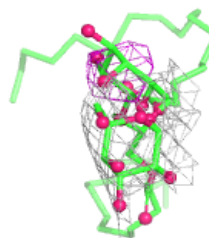
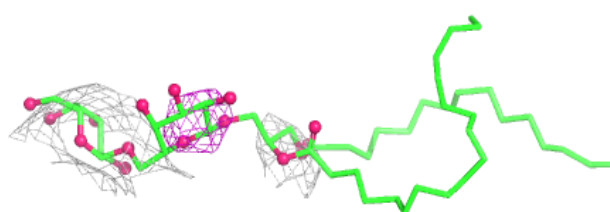
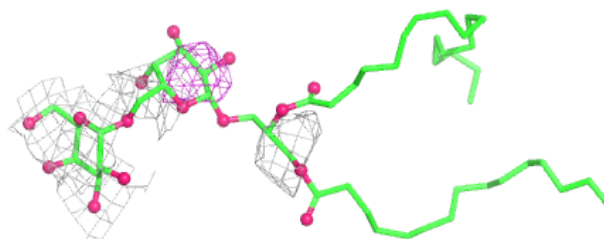
**Electron density around DGD D 409:**

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

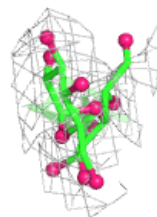
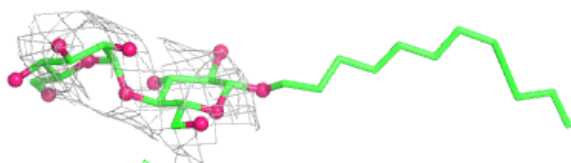
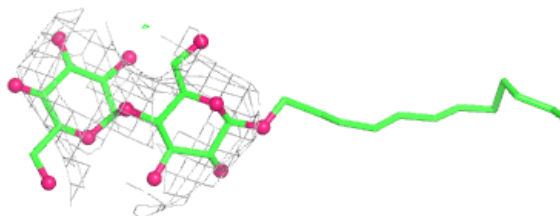


Electron density around DGD d 409:

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

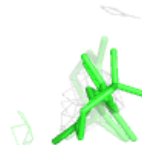
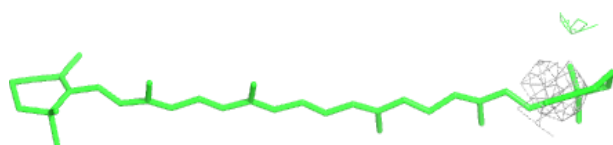
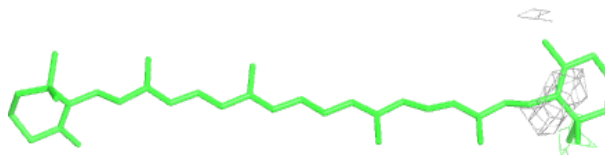
**Electron density around LMT B 628:**

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

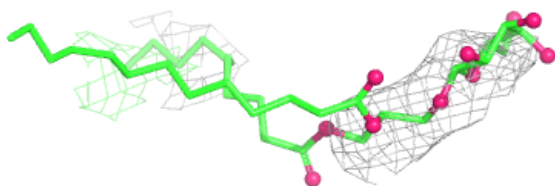
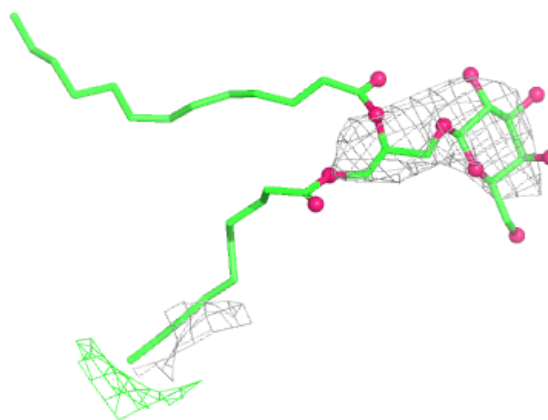


Electron density around BCR j 102:

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

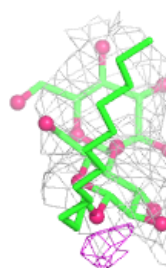
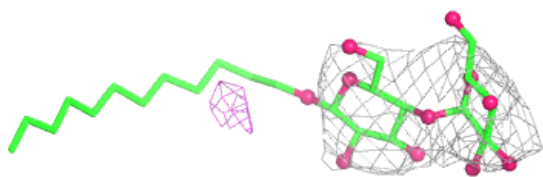
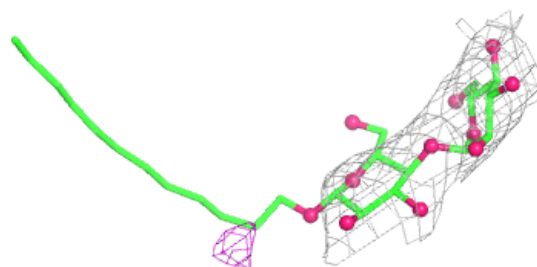
**Electron density around LMG A 415:**

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

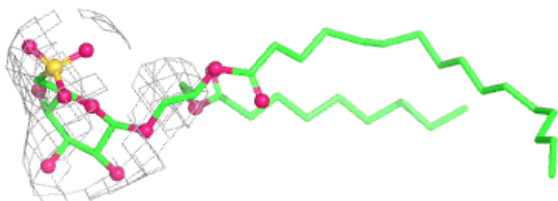
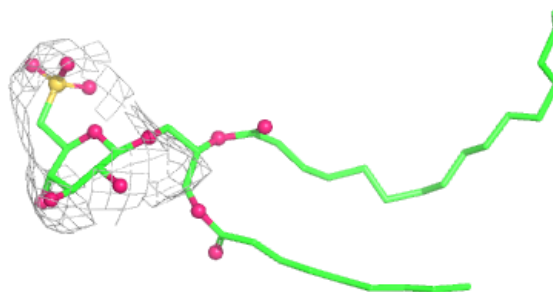


Electron density around LMT M 102:

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

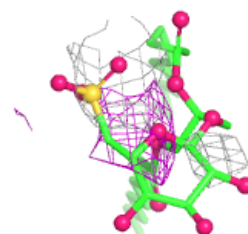
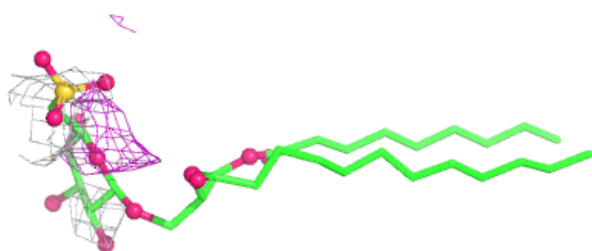
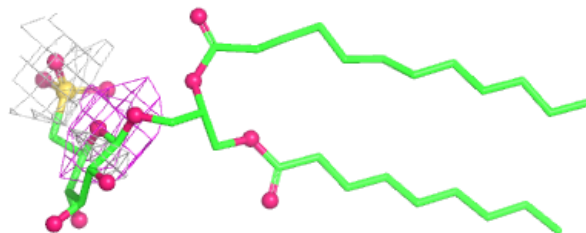
**Electron density around SQD B 626:**

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

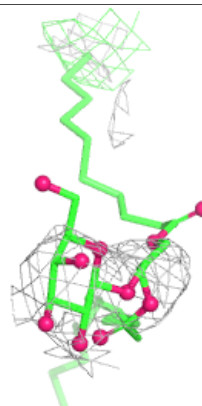
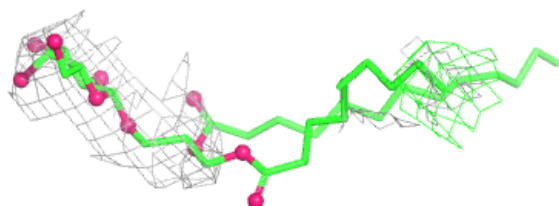
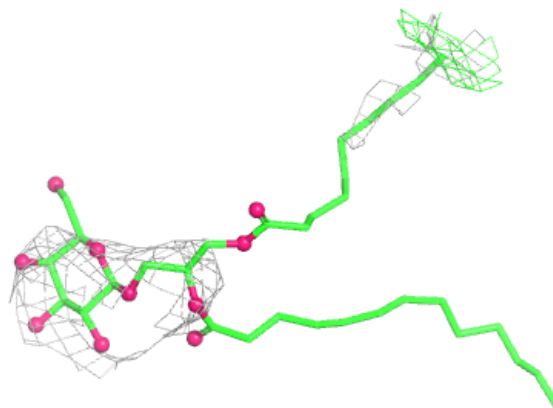


Electron density around SQD d 402:

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

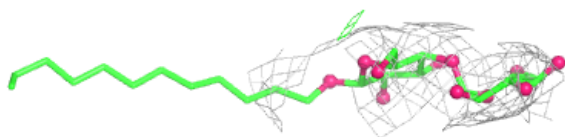
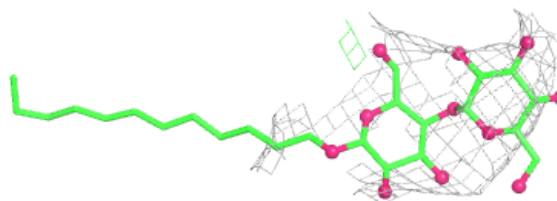
**Electron density around LMG a 402:**

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

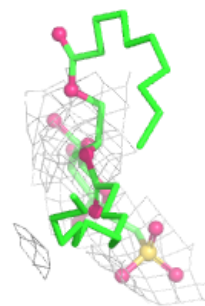


Electron density around LMT B 627:

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

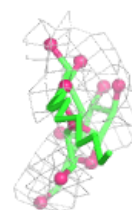
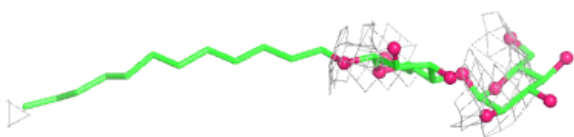
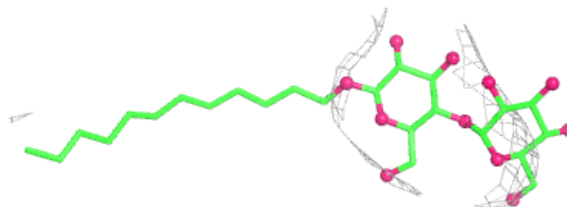
**Electron density around SQD F 103:**

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

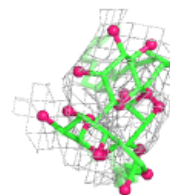
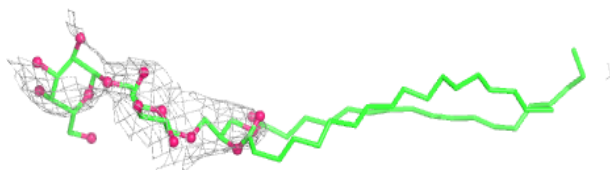
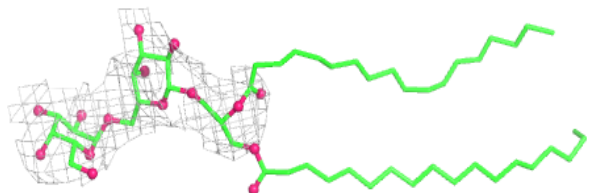


Electron density around LMT B 624:

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

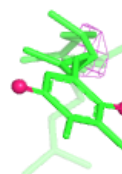
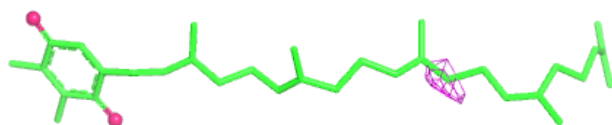
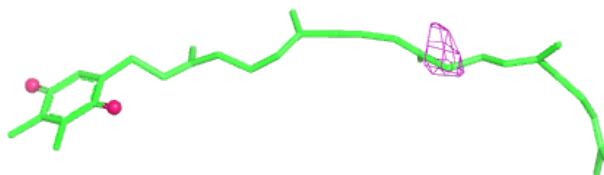
**Electron density around DGD C 517:**

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

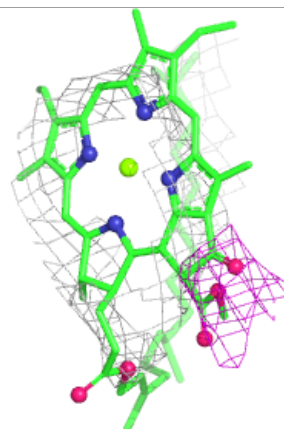
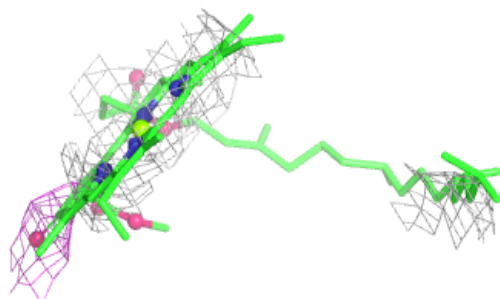
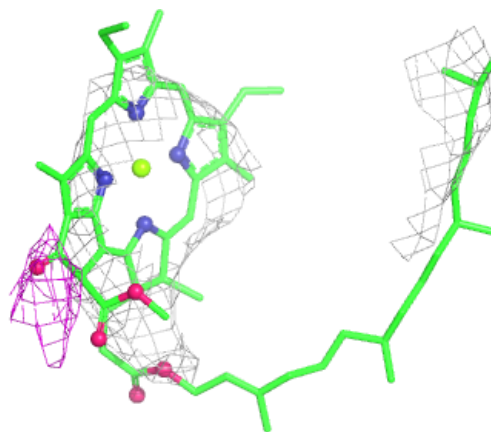


Electron density around PL9 J 101:

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

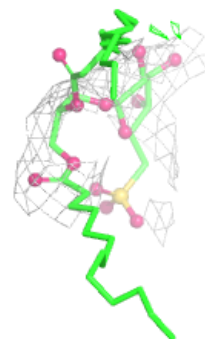
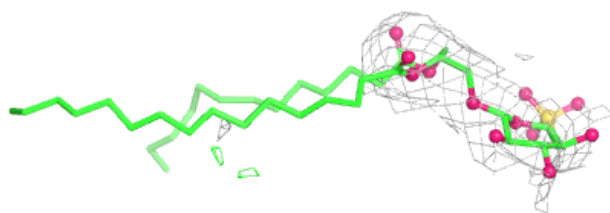
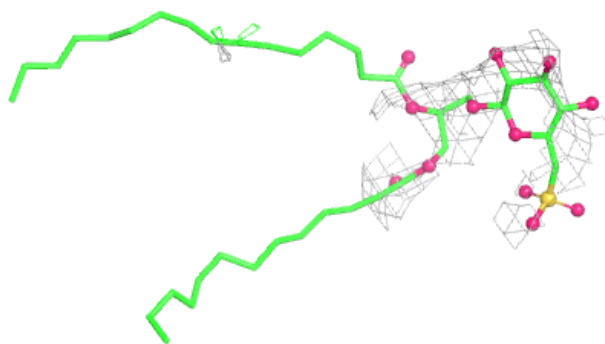
**Electron density around CLA C 506:**

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

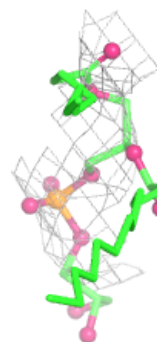
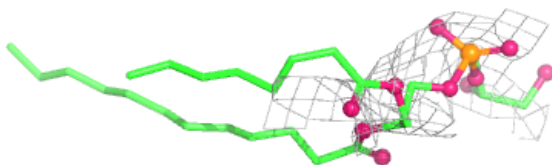
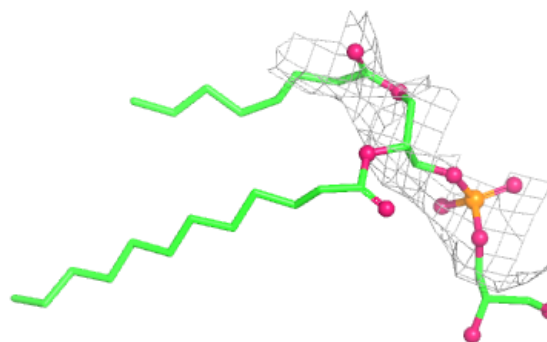


Electron density around SQD A 413:

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

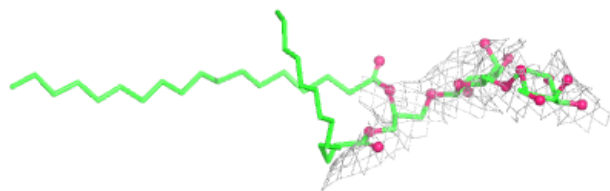
**Electron density around LHG C 519:**

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

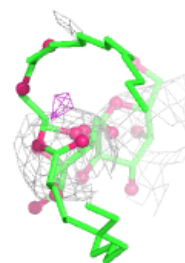
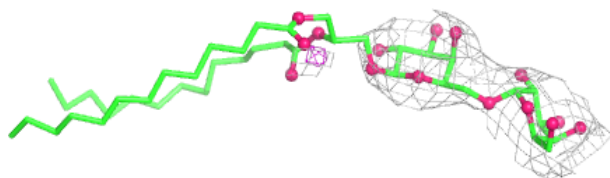
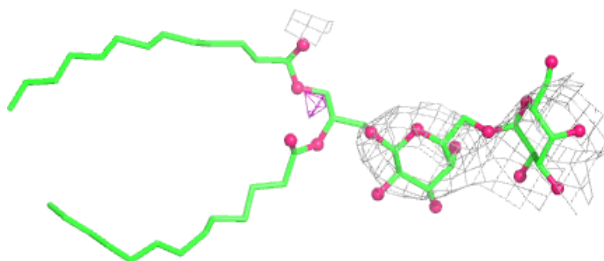


Electron density around DGD C 516:

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

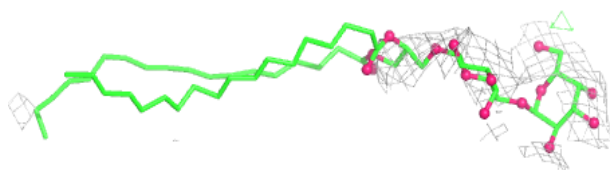
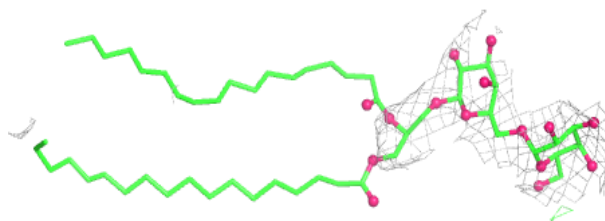
**Electron density around DGD A 408:**

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

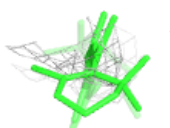
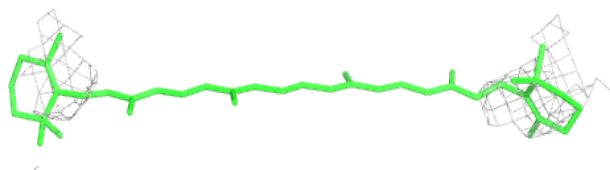
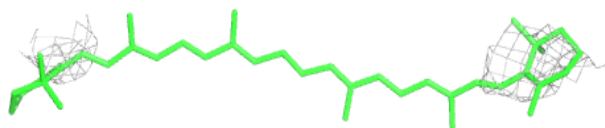


Electron density around DGD c 517:

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

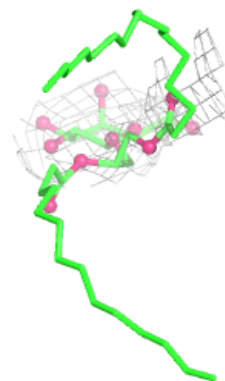
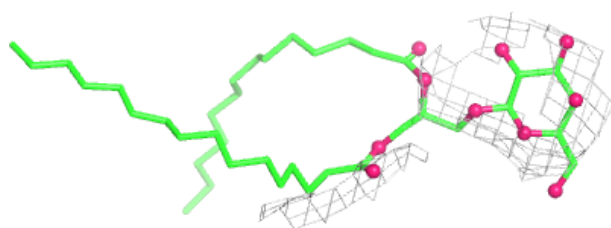
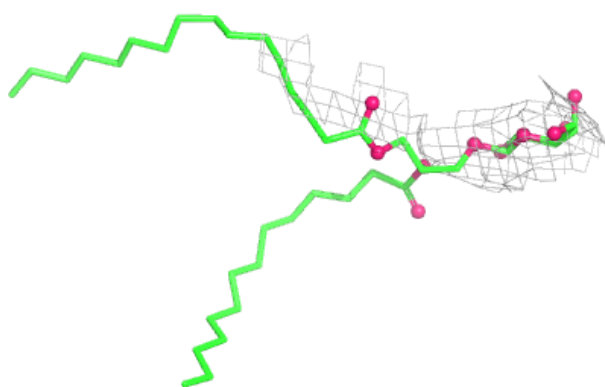
**Electron density around BCR c 521:**

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

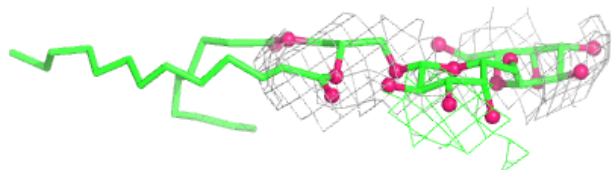
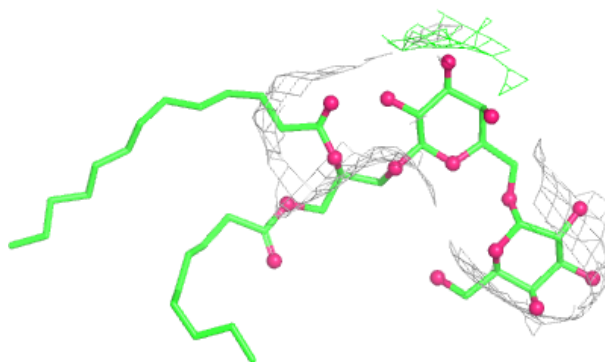


Electron density around LMG b 625:

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

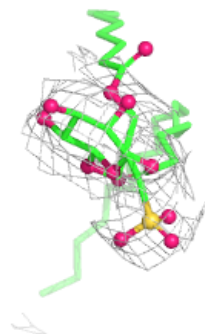
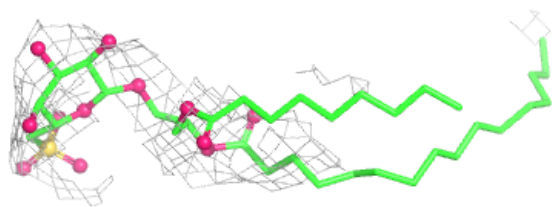
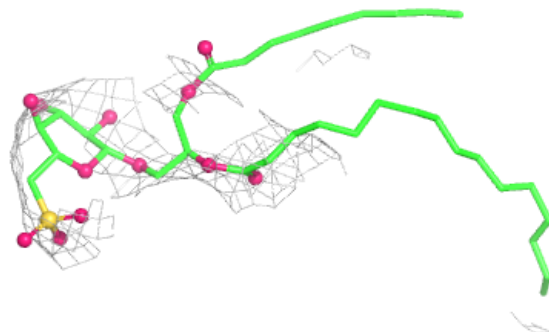
**Electron density around DGD b 601:**

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

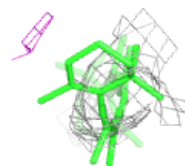
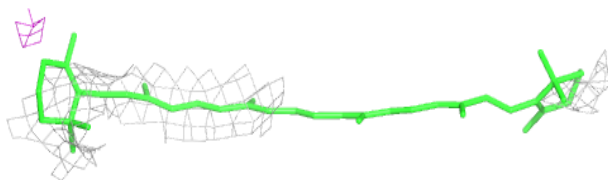
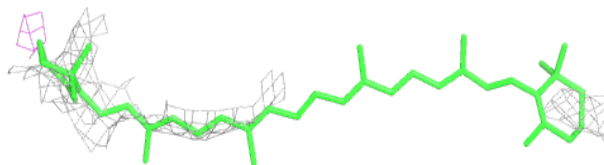


Electron density around SQD b 602:

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

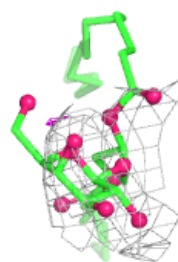
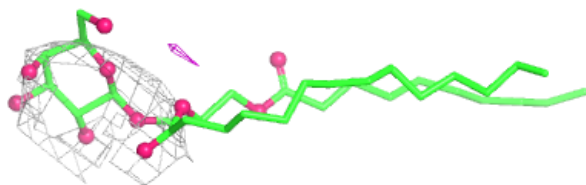
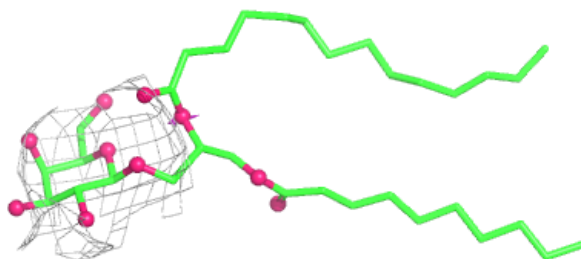
**Electron density around BCR H 102:**

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

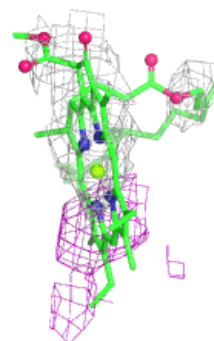
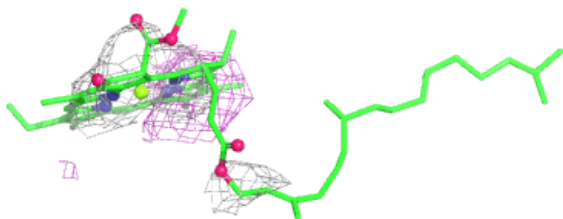
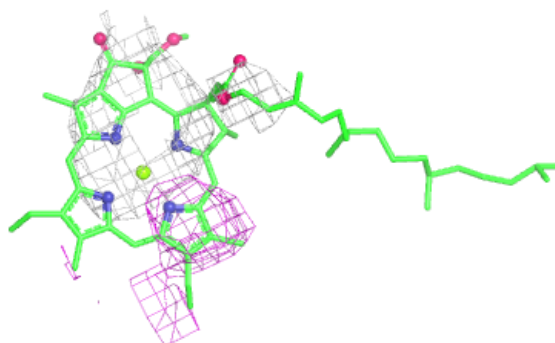


Electron density around LMG I 101:

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

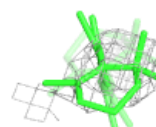
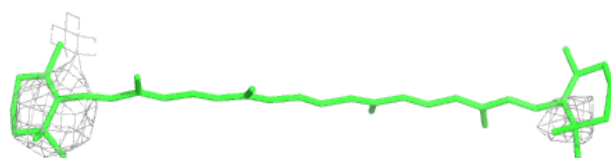
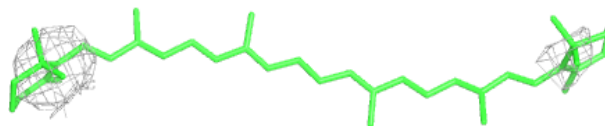
**Electron density around CLA a 406:**

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

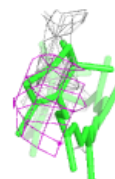
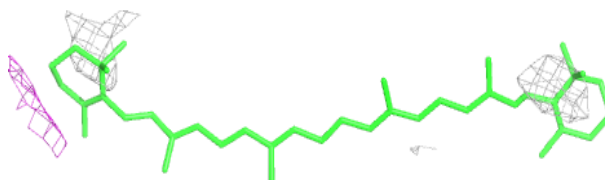


Electron density around BCR a 410:

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

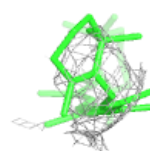
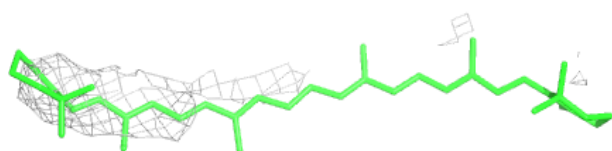
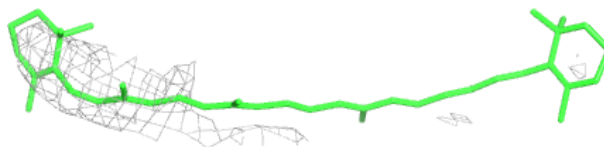
**Electron density around BCR b 621:**

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

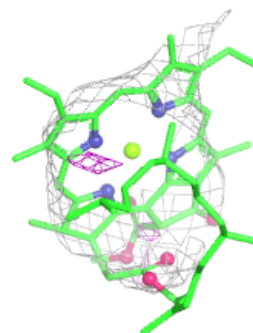
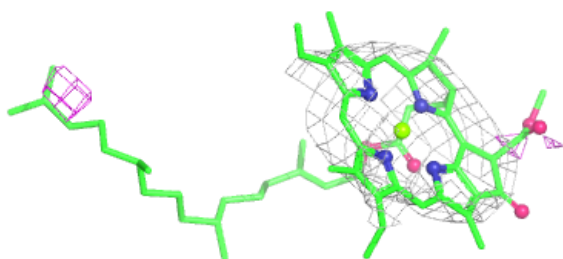
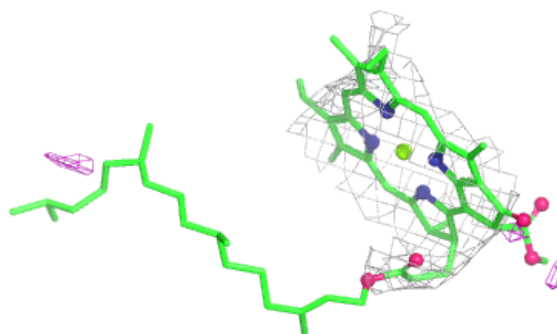


Electron density around BCR c 513:

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

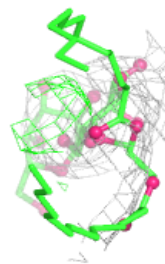
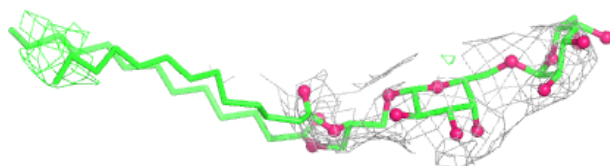
**Electron density around CLA C 512:**

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



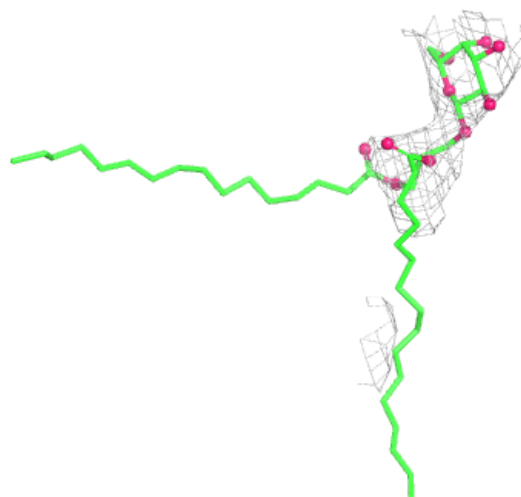
Electron density around DGD a 411:

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



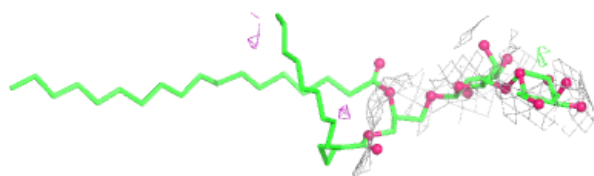
Electron density around LMG 1 101:

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

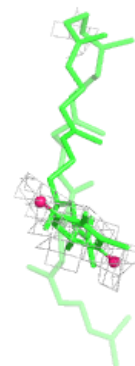
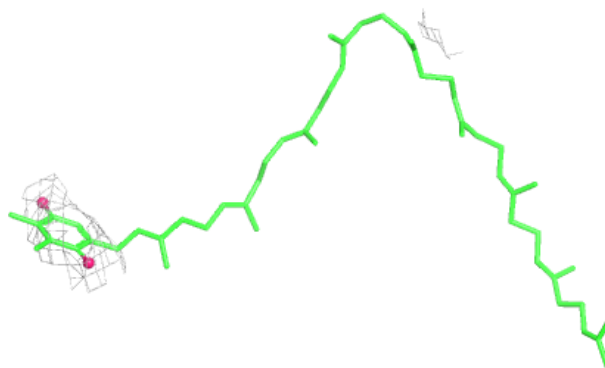


Electron density around DGD c 516:

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

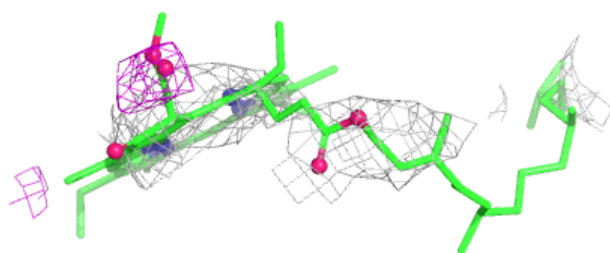
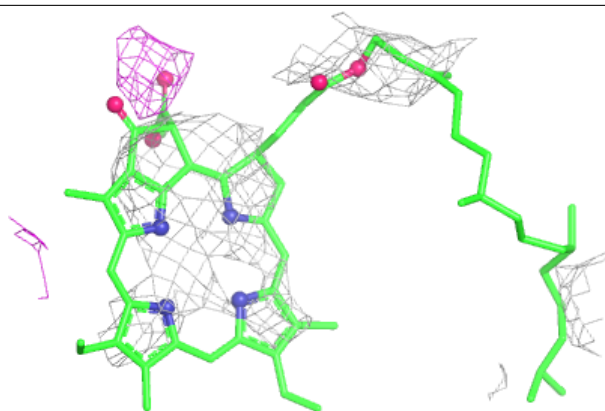
**Electron density around PL9 d 406:**

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

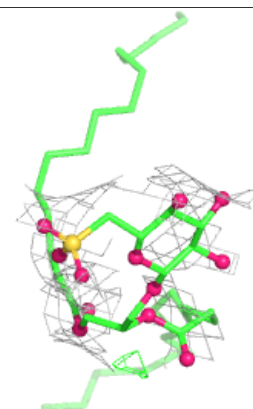
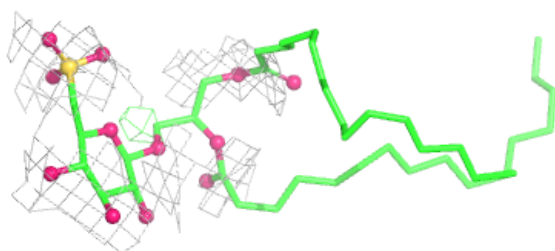
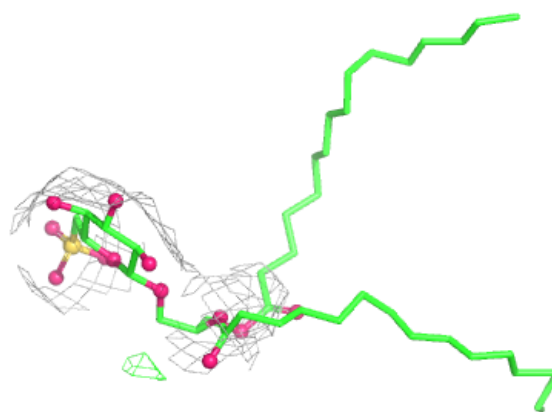


Electron density around PHO D 402:

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

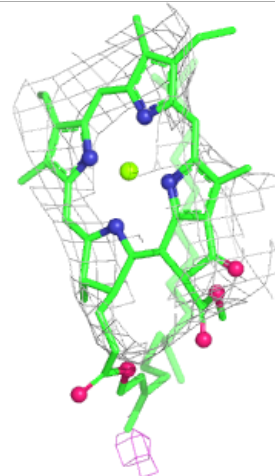
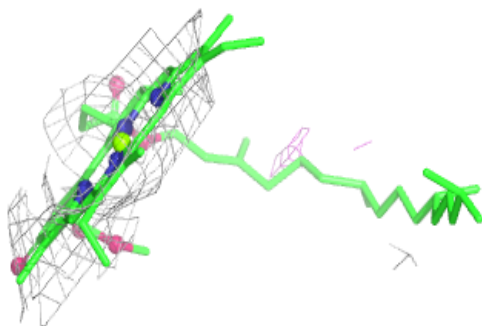
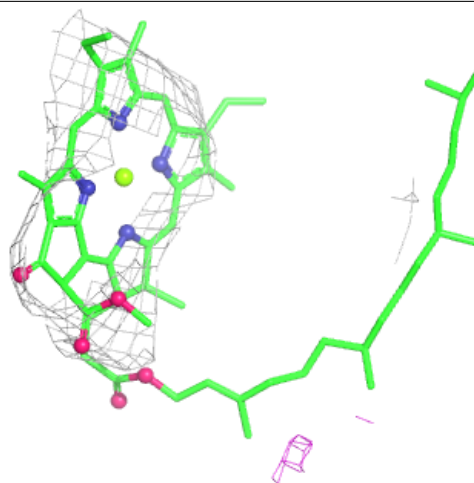
**Electron density around SQD a 401:**

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



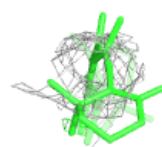
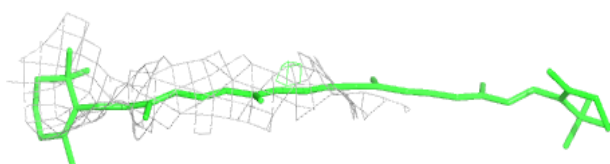
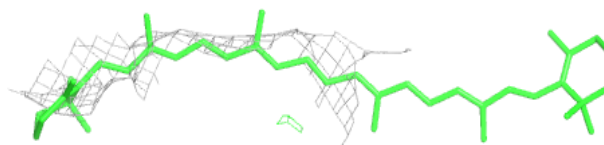
Electron density around CLA c 506:

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

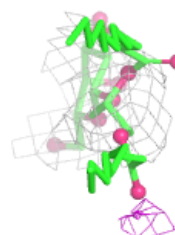
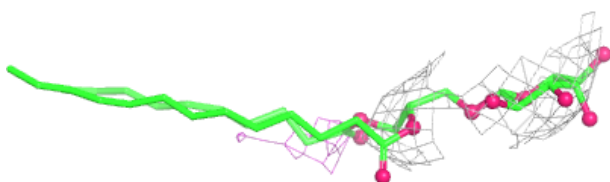
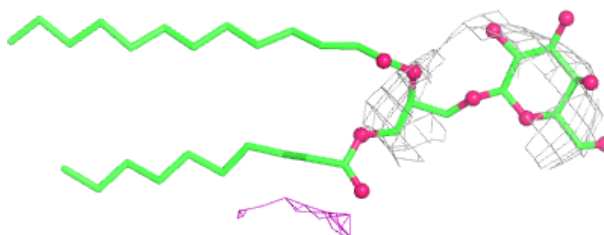


Electron density around BCR x 101:

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

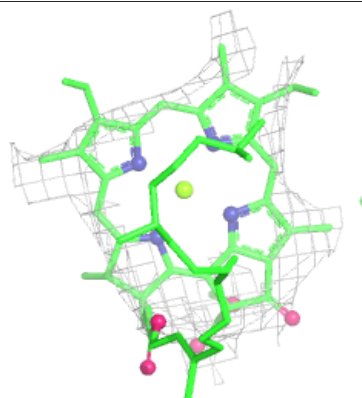
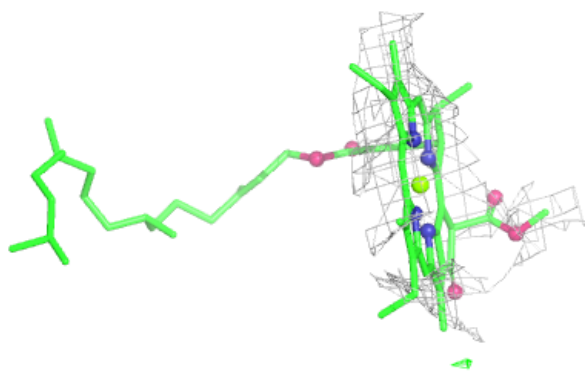
**Electron density around LMG m 101:**

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

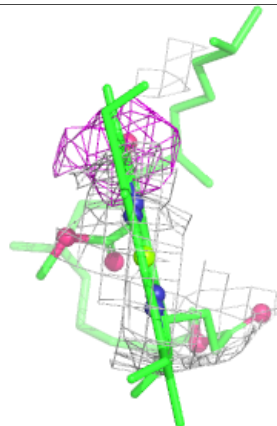
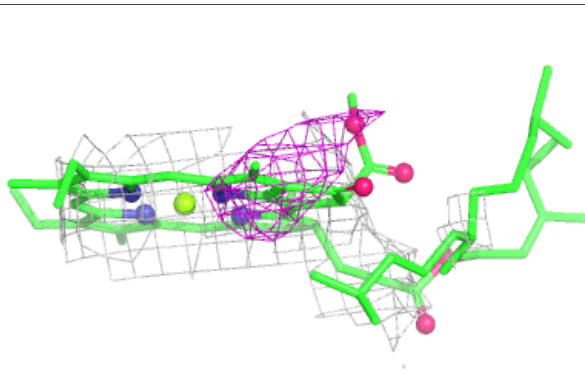
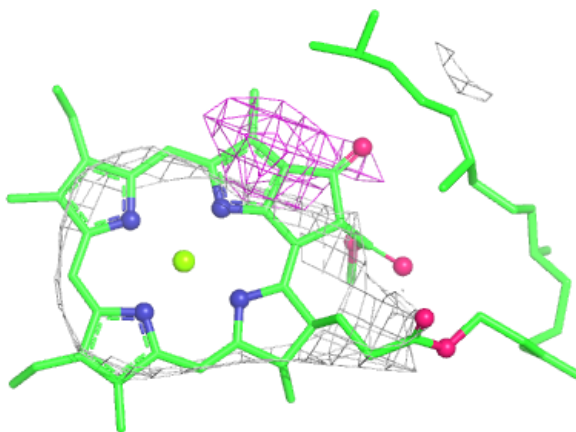


Electron density around CLA c 505:

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

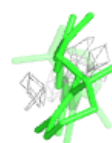
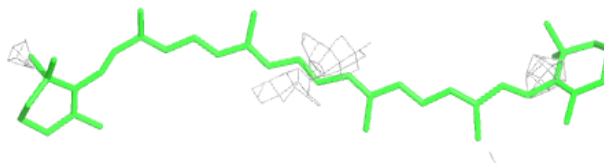
**Electron density around CLA b 613:**

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

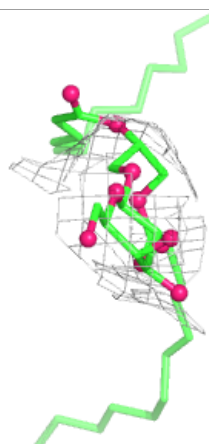
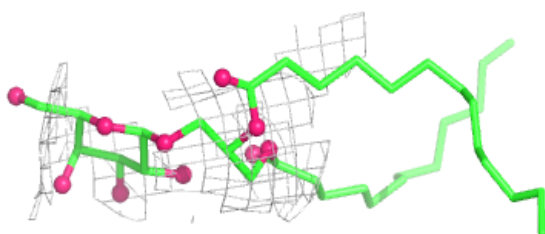
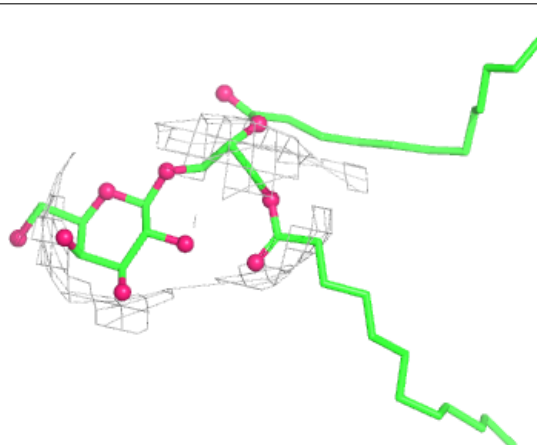


Electron density around BCR g 101:

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

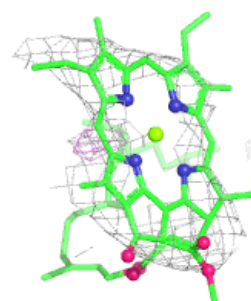
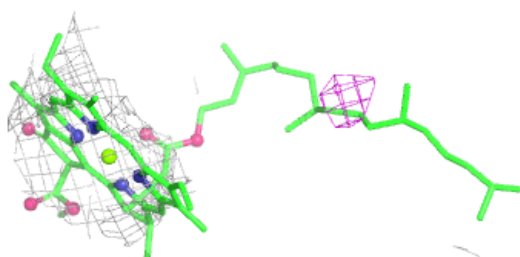
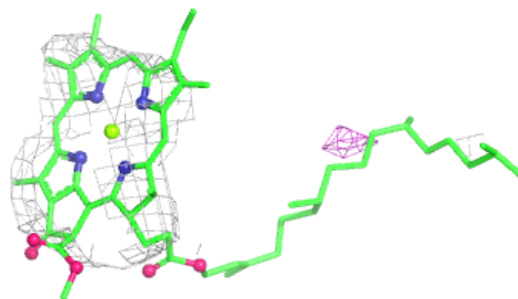
**Electron density around LMG e 101:**

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

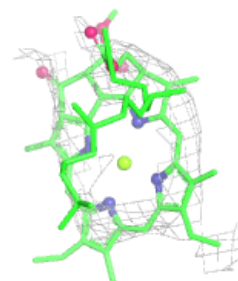
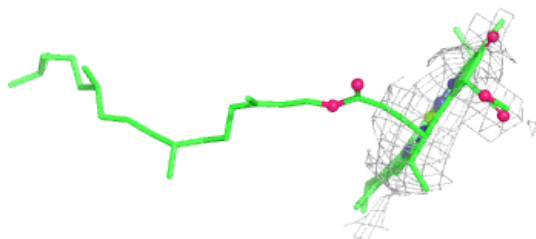
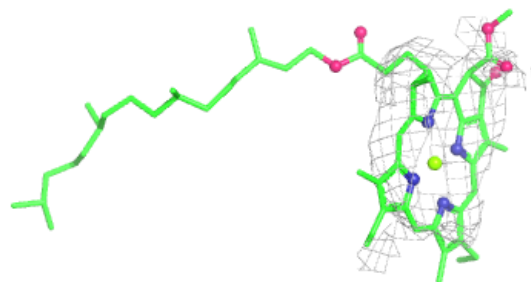


Electron density around CLA c 510:

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

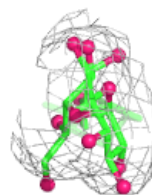
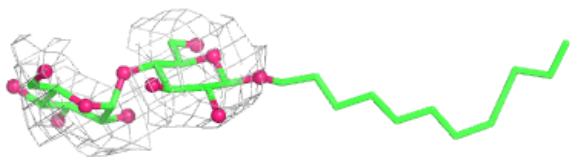
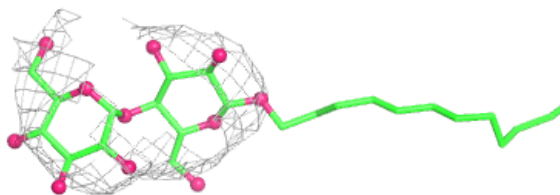
**Electron density around CLA A 405:**

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

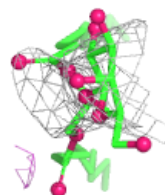
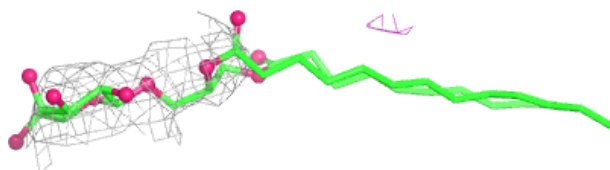
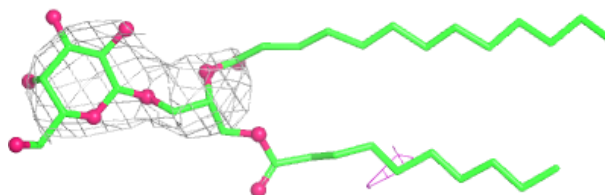


Electron density around LMT b 604:

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

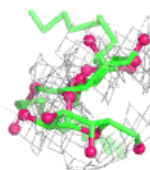
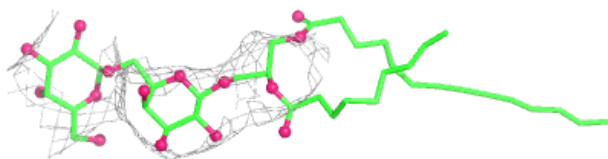
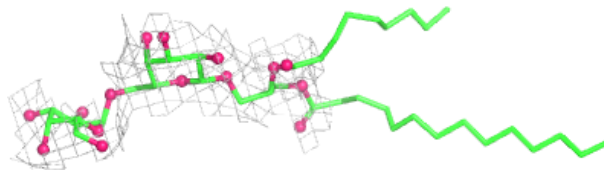
**Electron density around LMG M 101:**

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

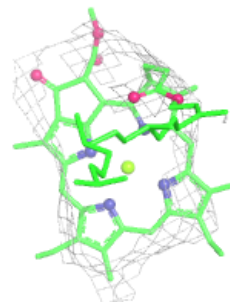
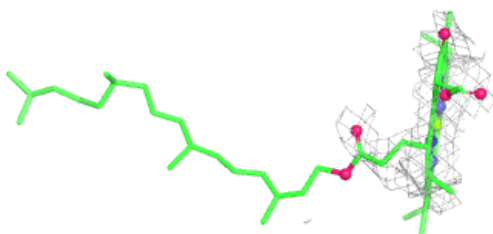
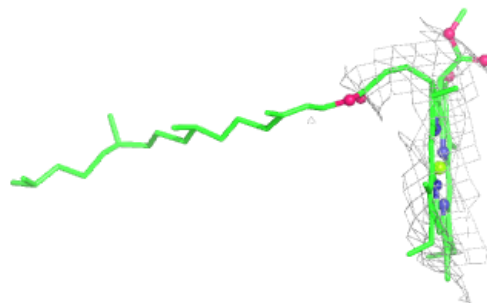


Electron density around DGD C 515:

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

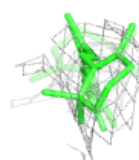
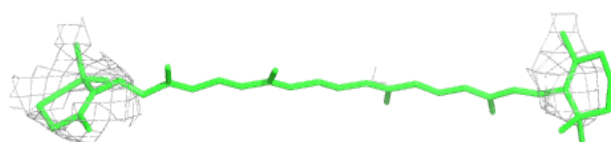
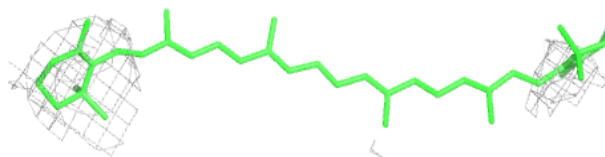
**Electron density around CLA B 605:**

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

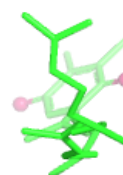
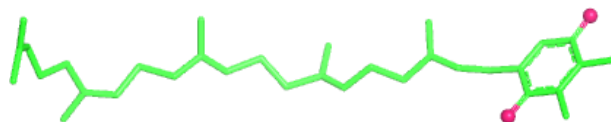
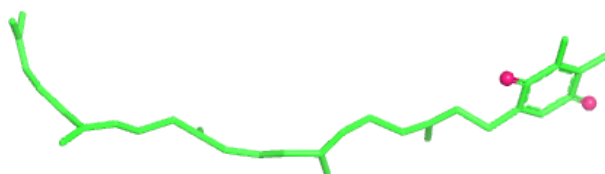


Electron density around BCR K 102:

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

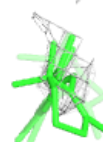
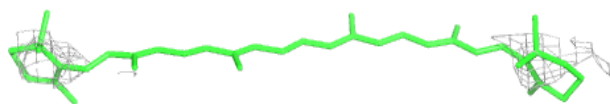
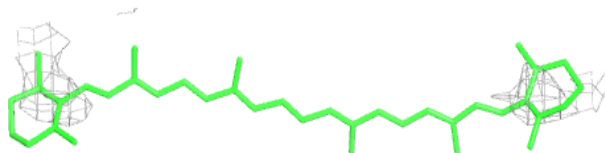
**Electron density around PL9 j 101:**

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

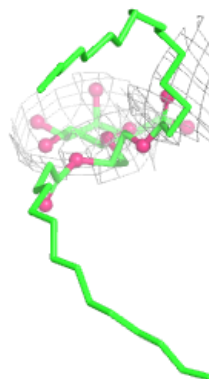
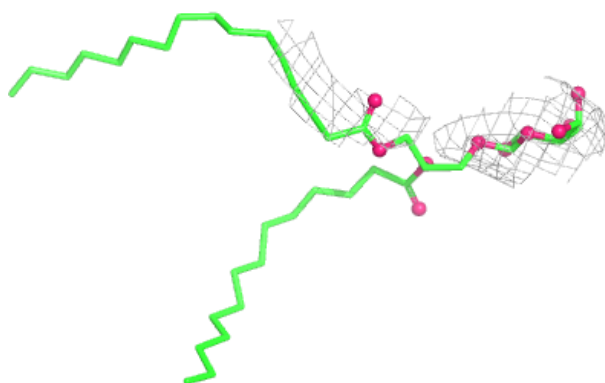


Electron density around BCR C 514:

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

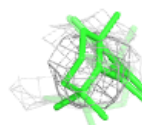
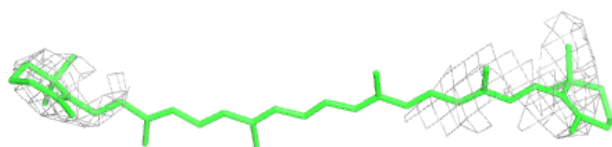
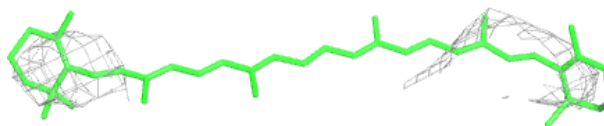
**Electron density around LMG B 621:**

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

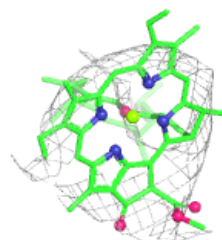
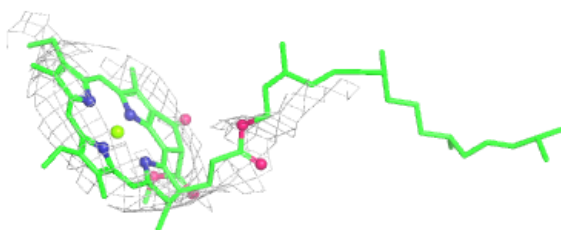


Electron density around BCR b 623:

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

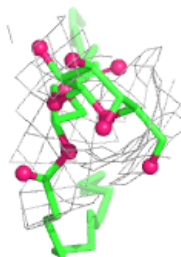
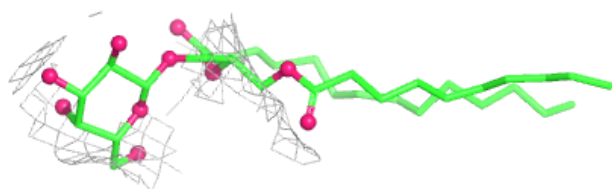
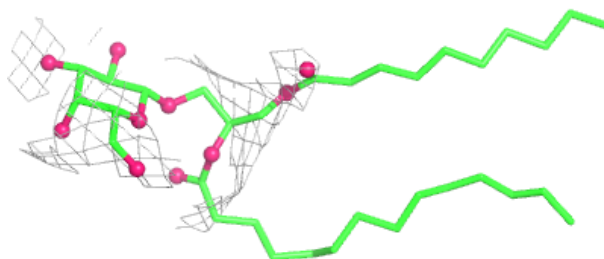
**Electron density around CLA c 502:**

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

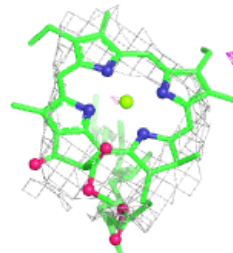
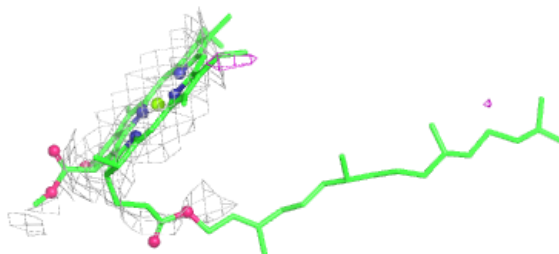


Electron density around LMG i 101:

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

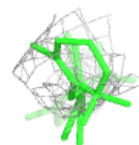
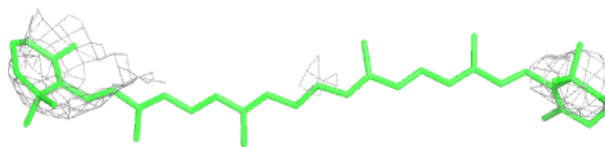
**Electron density around CLA C 520:**

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

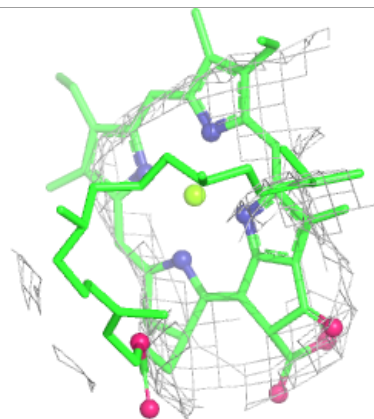
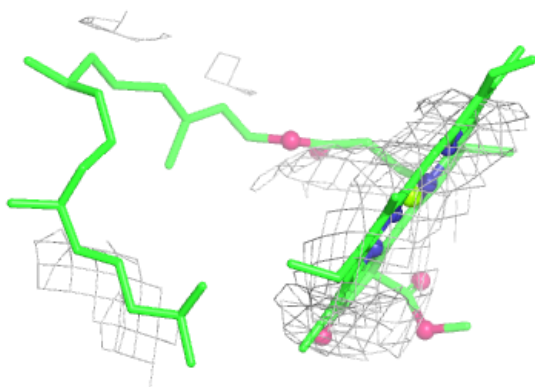
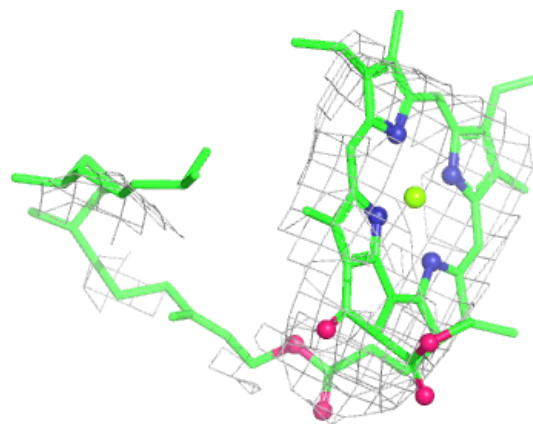


Electron density around BCR b 622:

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

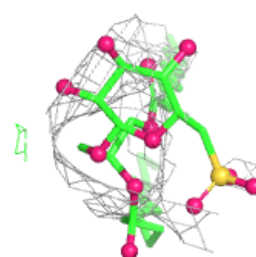
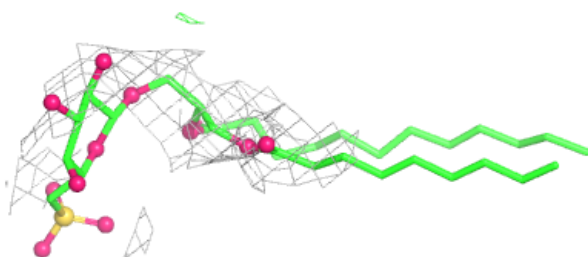
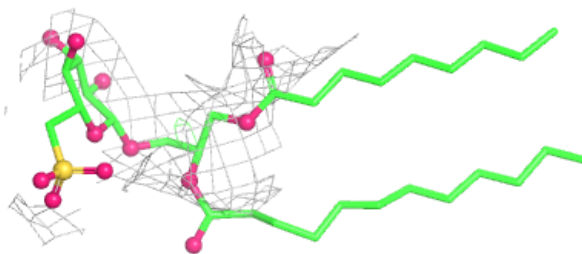
**Electron density around CLA c 503:**

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

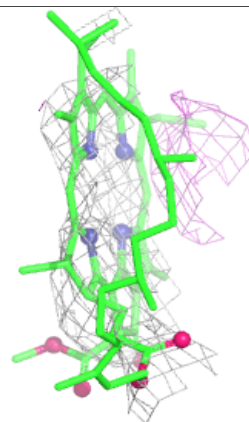
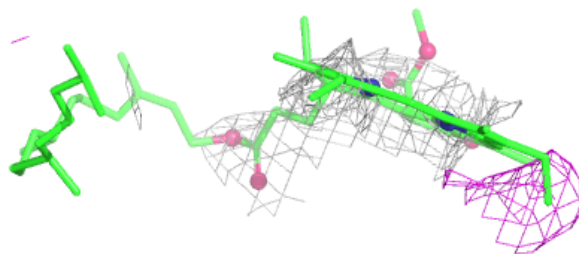
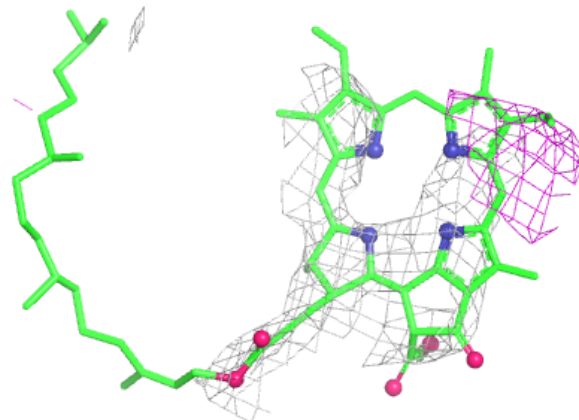


Electron density around SQD B 622:

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

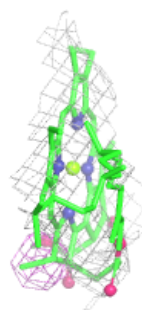
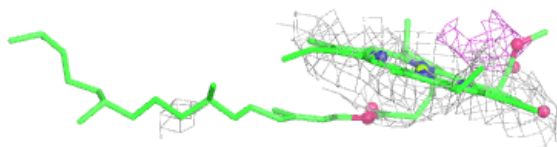
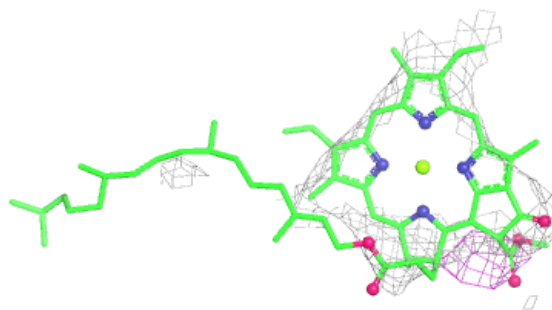
**Electron density around PHO D 401:**

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

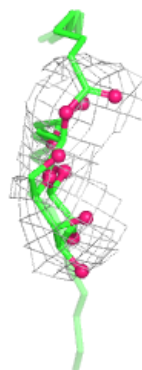
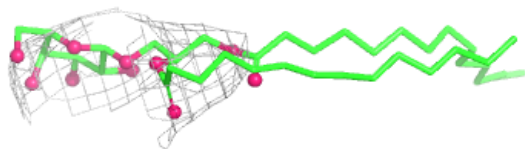
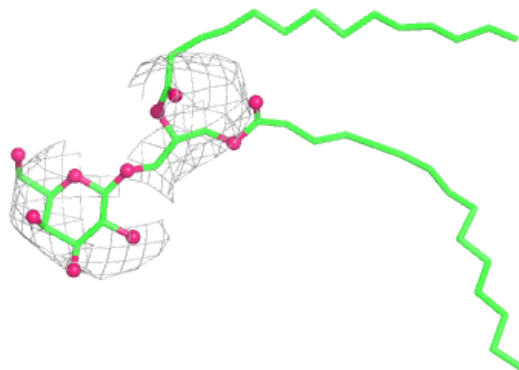


Electron density around CLA b 606:

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

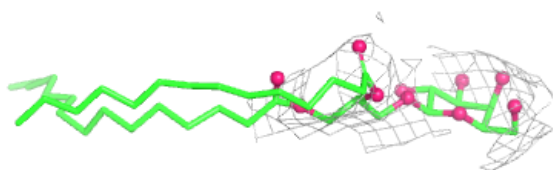
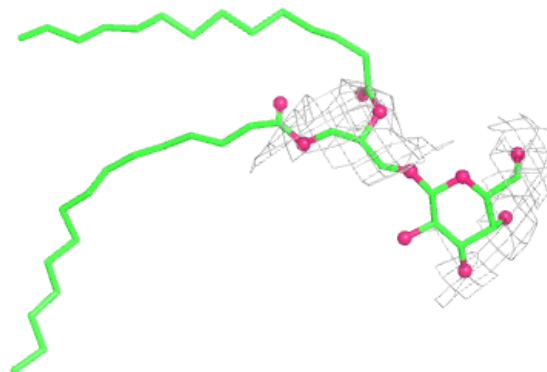
**Electron density around LMG C 521:**

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

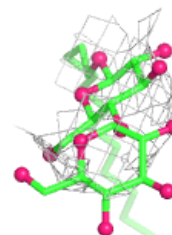
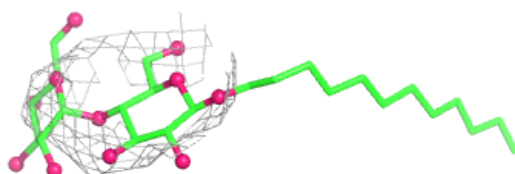
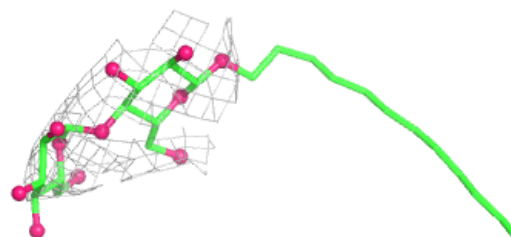


Electron density around LMG c 522:

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

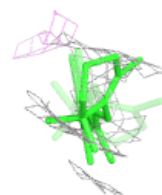
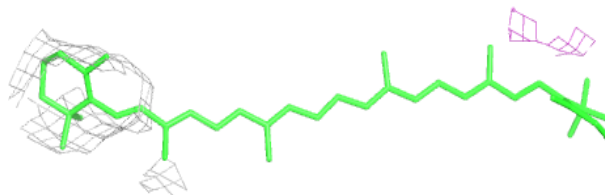
**Electron density around LMT M 103:**

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

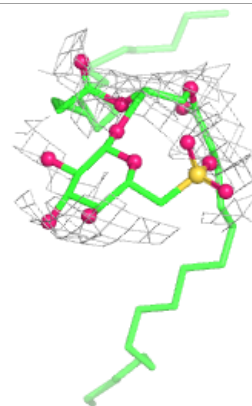
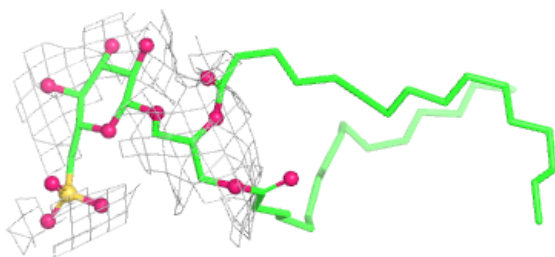
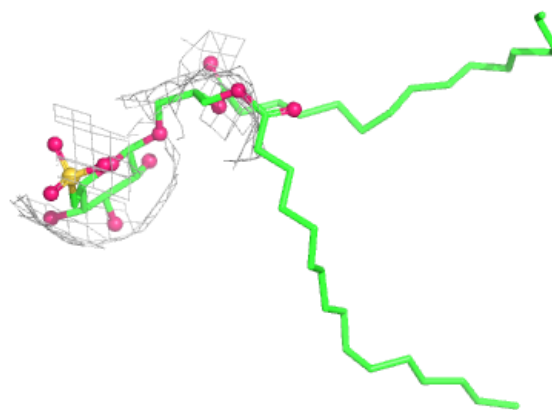


Electron density around BCR b 620:

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

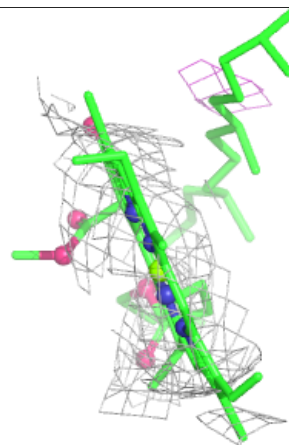
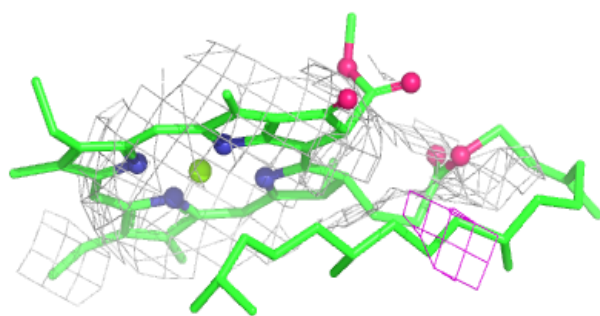
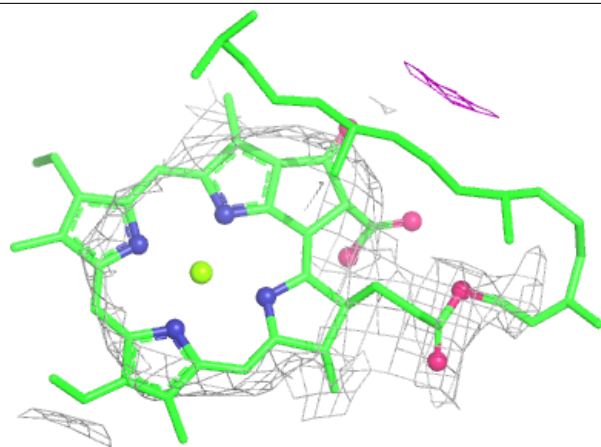
**Electron density around SQD A 414:**

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

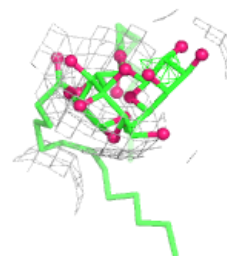
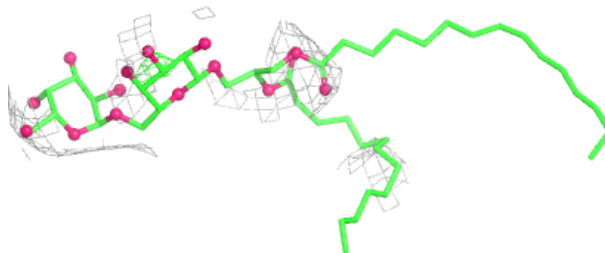


Electron density around CLA C 508:

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

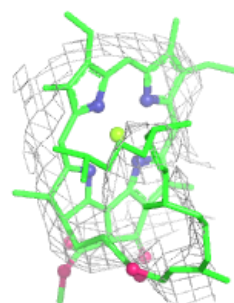
**Electron density around DGD b 624:**

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

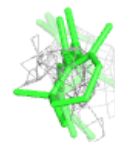
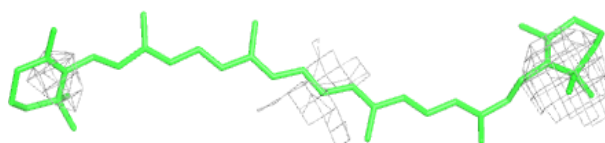


Electron density around CLA C 510:

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

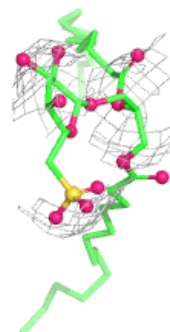
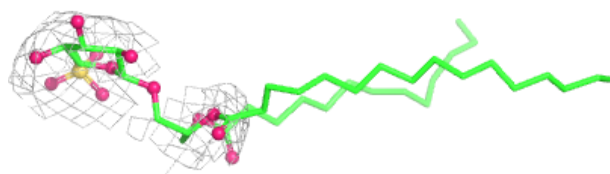
**Electron density around BCR y 101:**

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

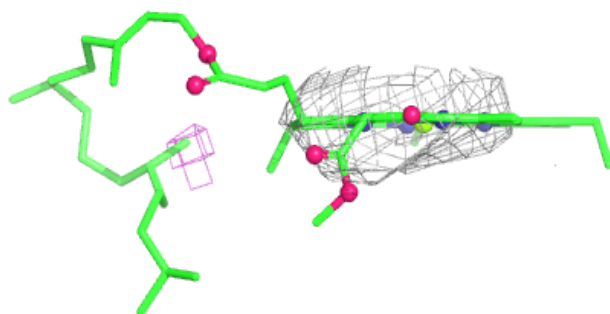
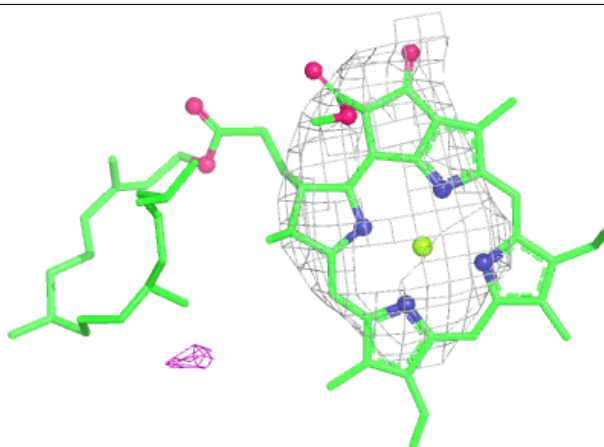


Electron density around SQD a 415:

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

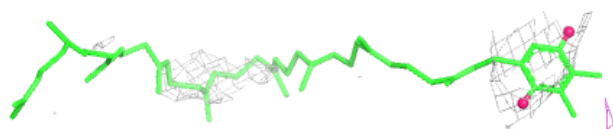
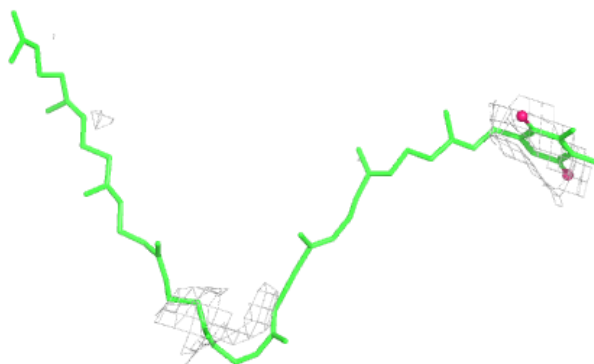
**Electron density around CLA C 511:**

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

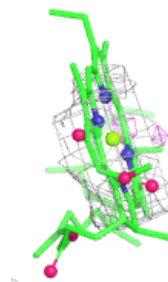
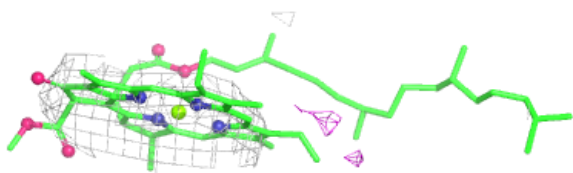
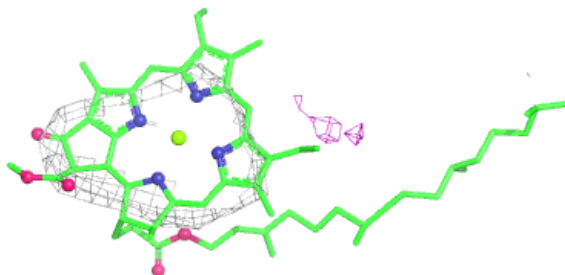


Electron density around PL9 D 406:

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

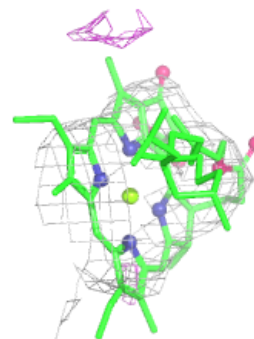
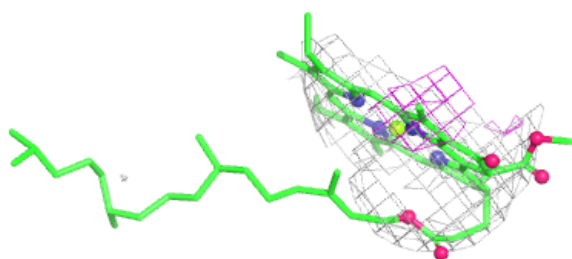
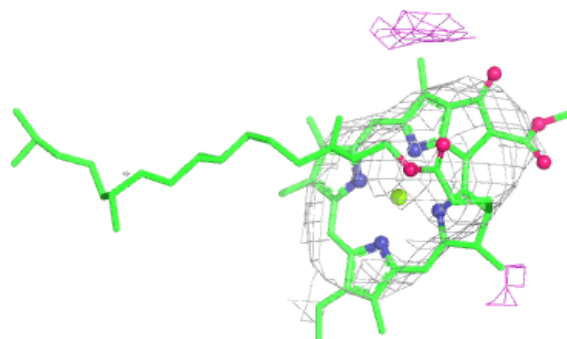
**Electron density around CLA c 501:**

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



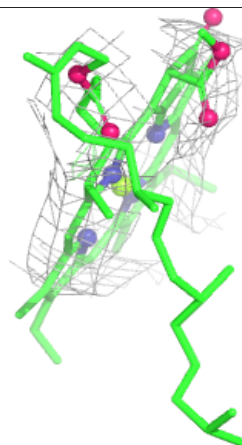
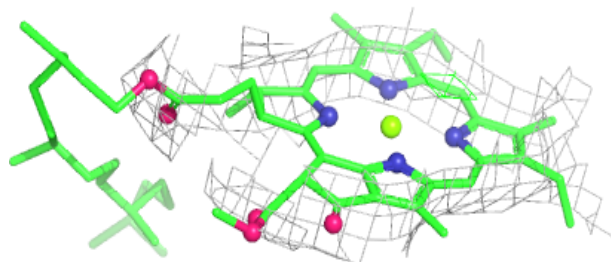
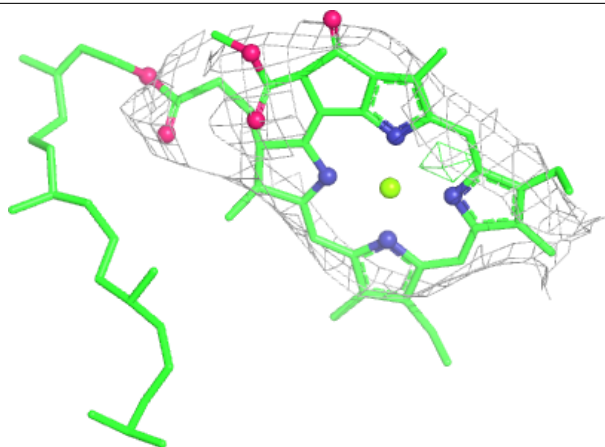
Electron density around CLA B 613:

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



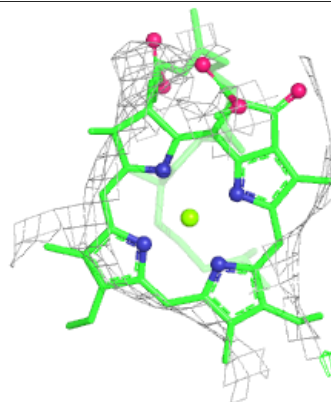
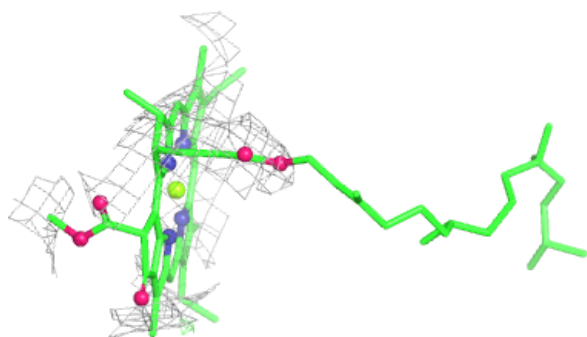
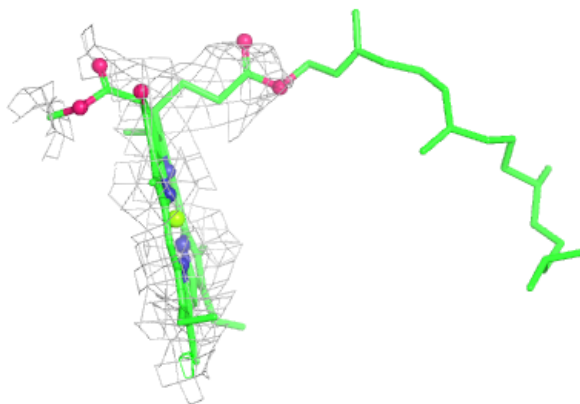
Electron density around CLA B 615:

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

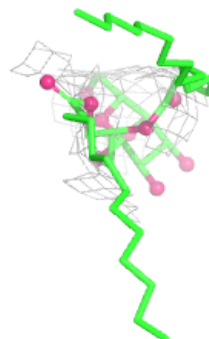
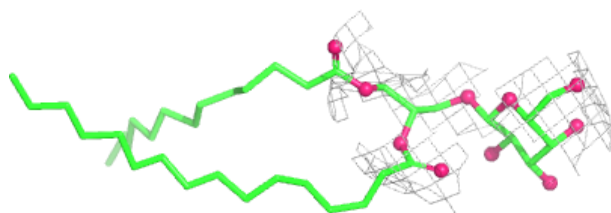
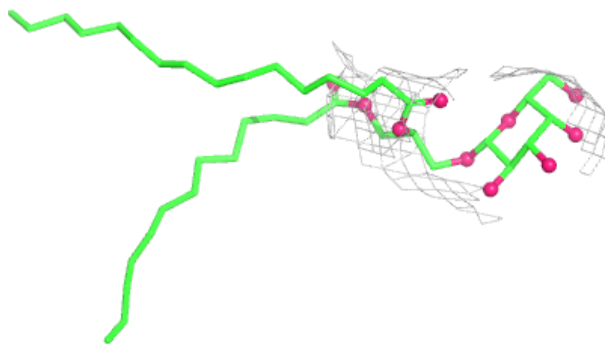


Electron density around CLA C 505:

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

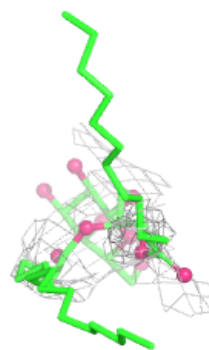
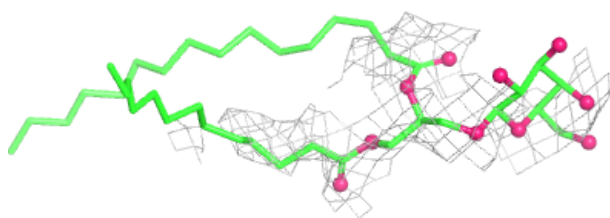
**Electron density around LMG D 408:**

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

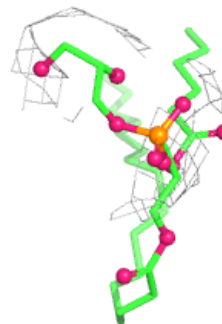
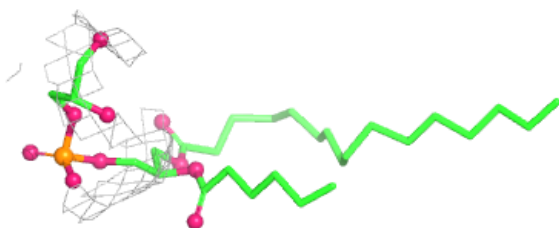


Electron density around LMG d 408:

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

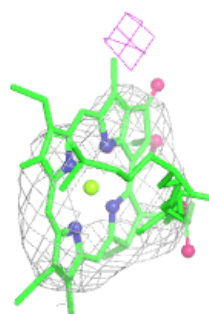
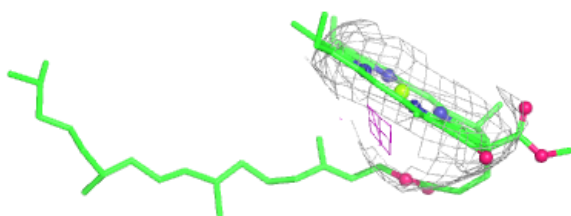
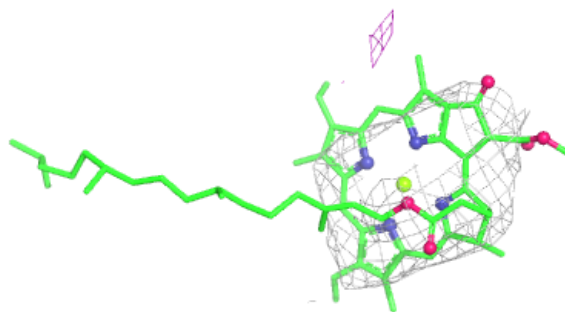
**Electron density around LHG A 409:**

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

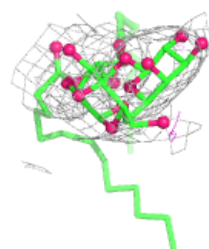
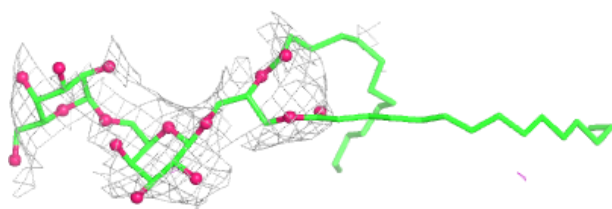
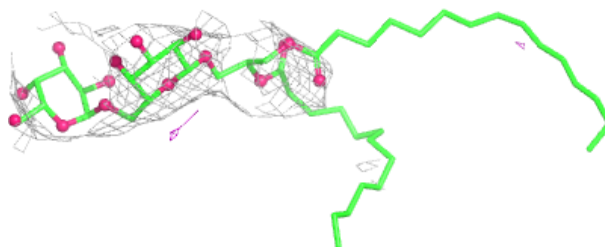


Electron density around CLA B 607:

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

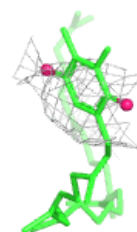
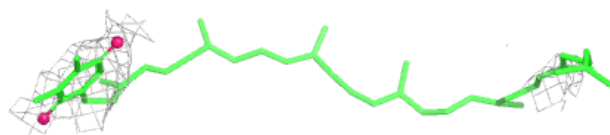
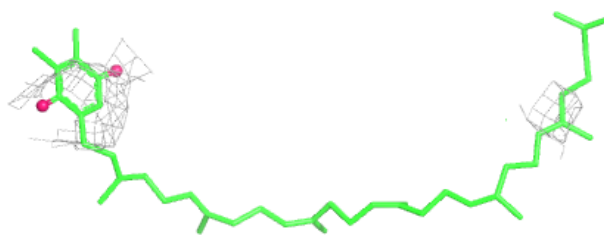
**Electron density around DGD B 620:**

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

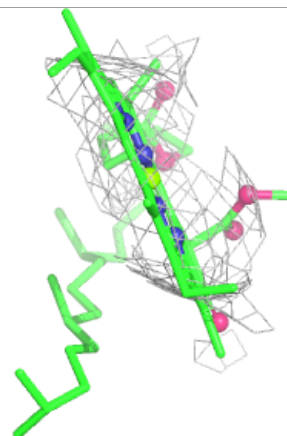
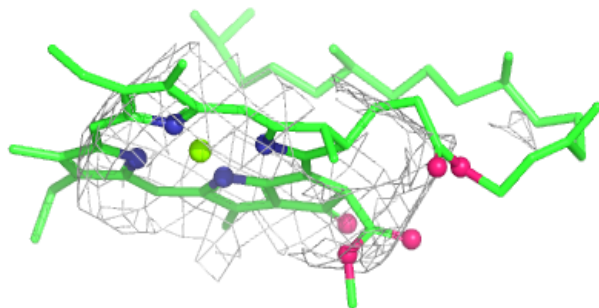
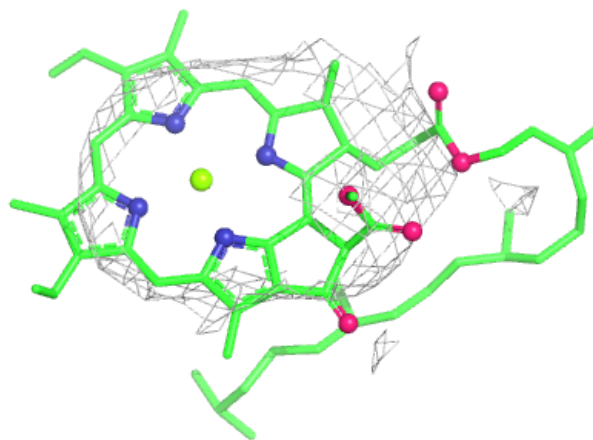


Electron density around PL9 a 409:

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

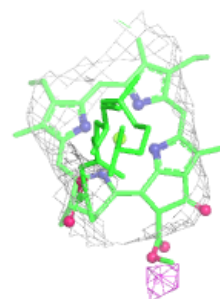
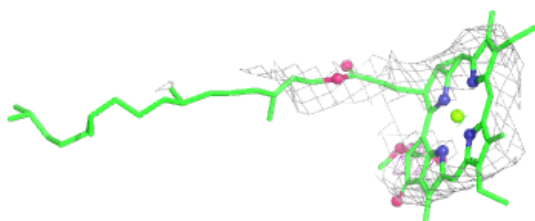
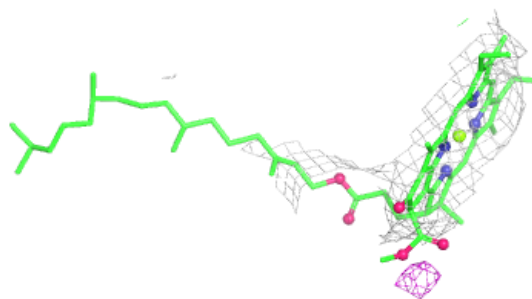
**Electron density around CLA c 508:**

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

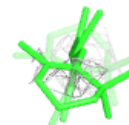
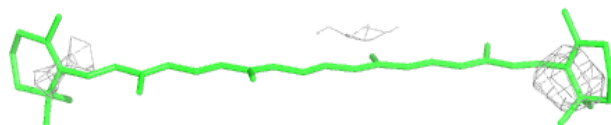
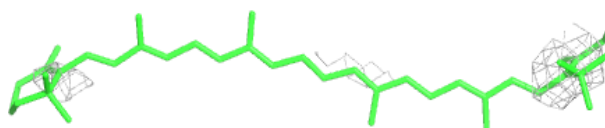


Electron density around CLA b 607:

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

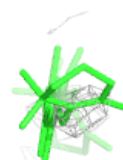
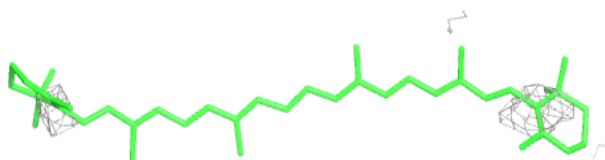
**Electron density around BCR A 407:**

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

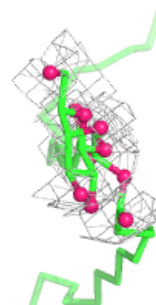
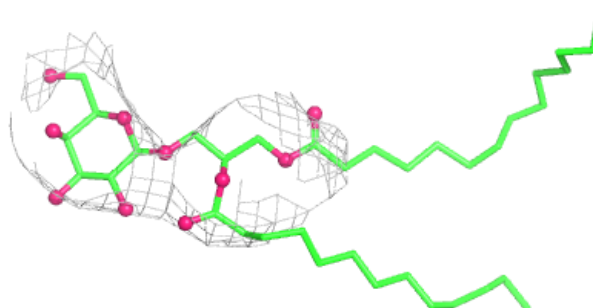


Electron density around BCR B 616:

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

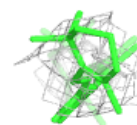
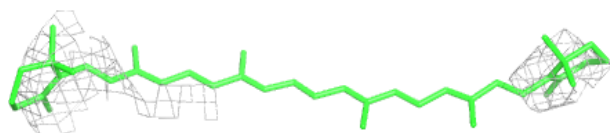
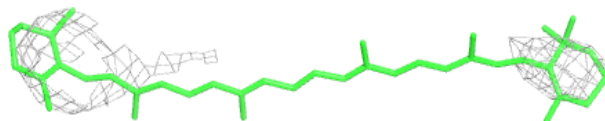
**Electron density around LMG D 411:**

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

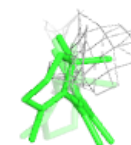
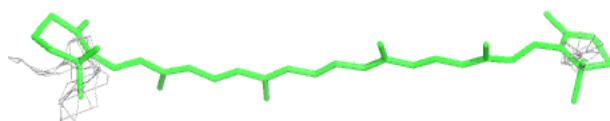
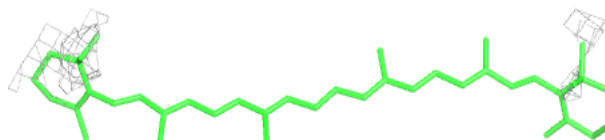


Electron density around BCR B 619:

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

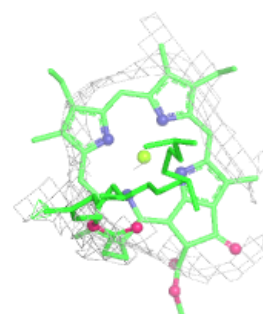
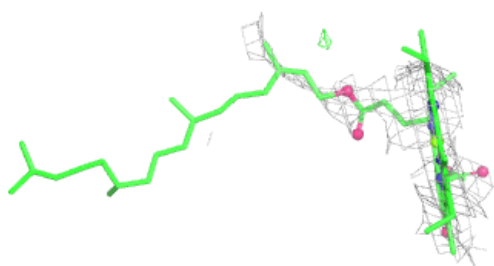
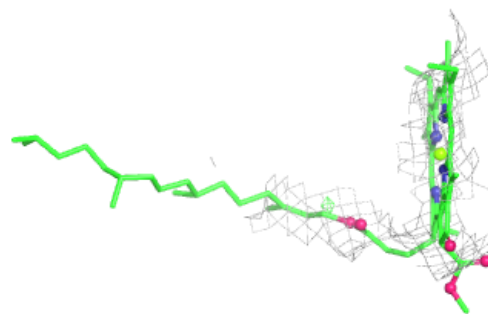
**Electron density around BCR c 514:**

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

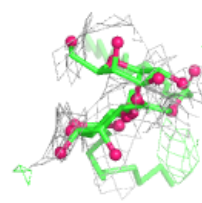
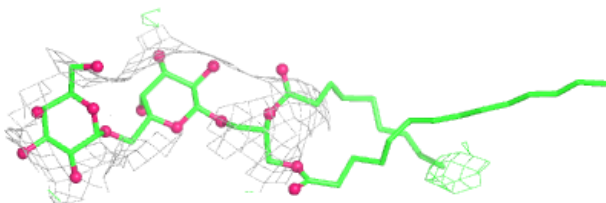
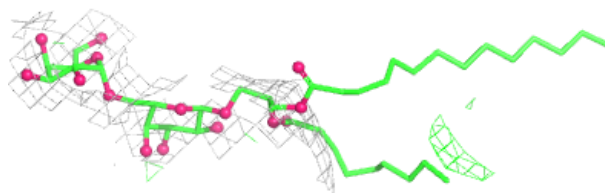


Electron density around CLA b 609:

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

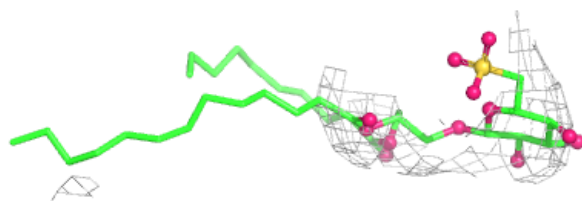
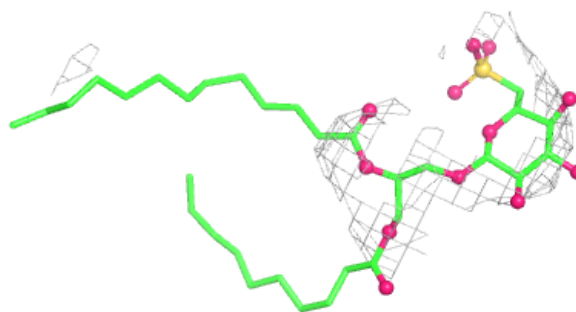
**Electron density around DGD c 515:**

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

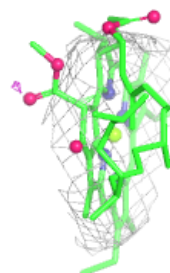
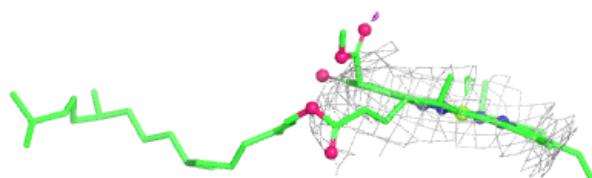
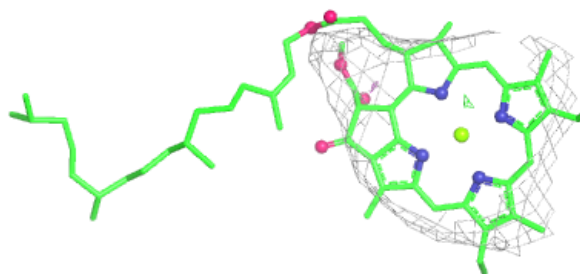


Electron density around SQD f 103:

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

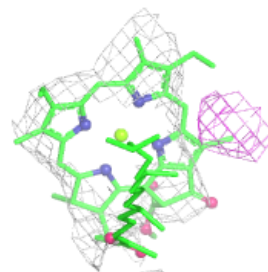
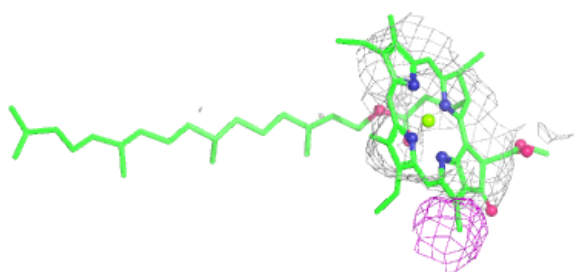
**Electron density around CLA h 101:**

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

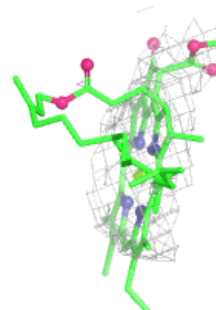
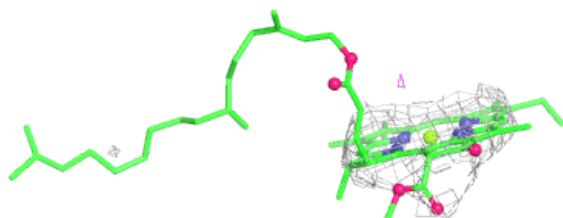
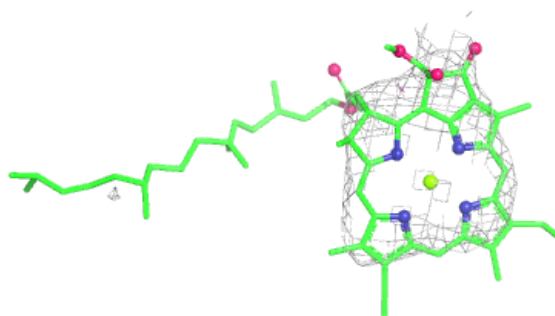


Electron density around CLA b 610:

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

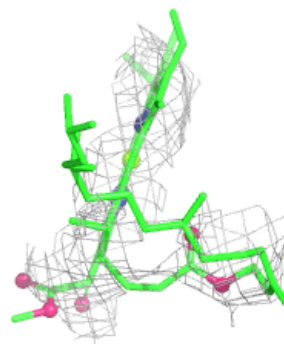
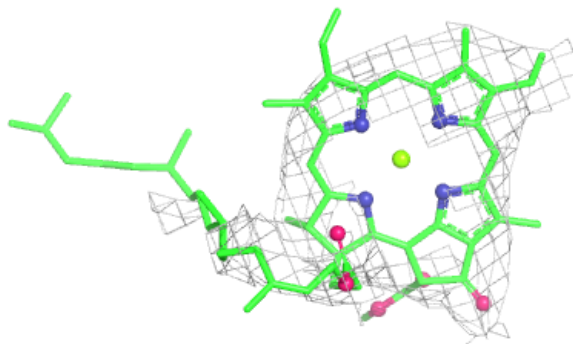
**Electron density around CLA A 404:**

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



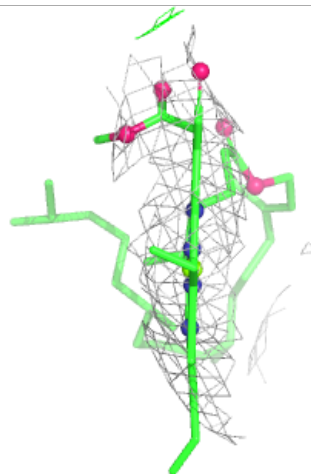
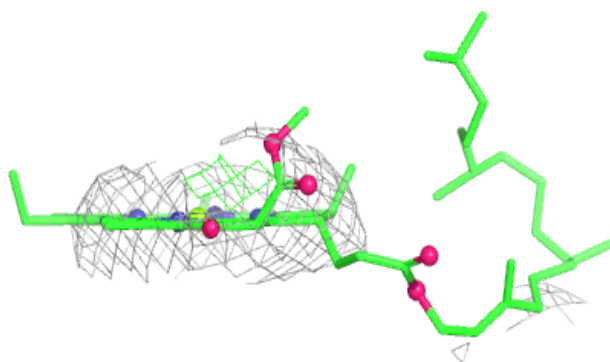
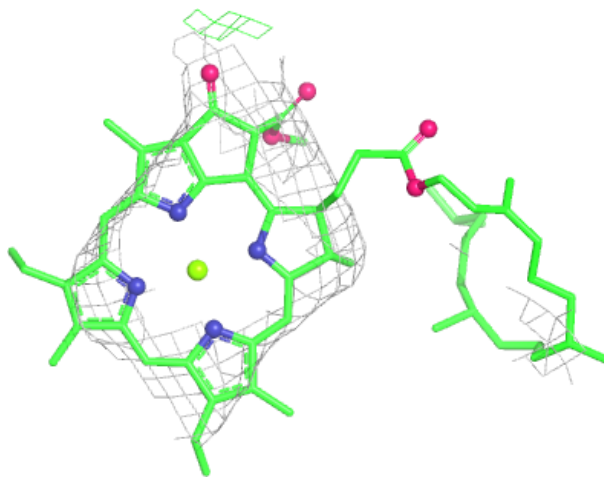
Electron density around CLA a 405:

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



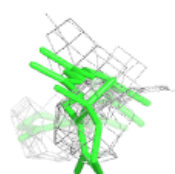
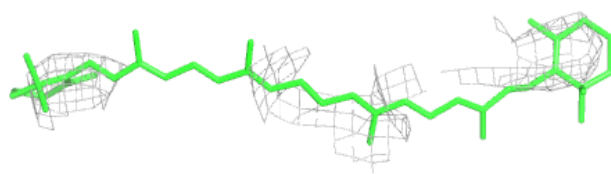
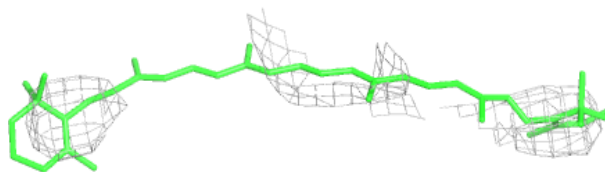
Electron density around CLA c 511:

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

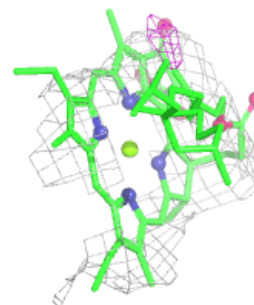
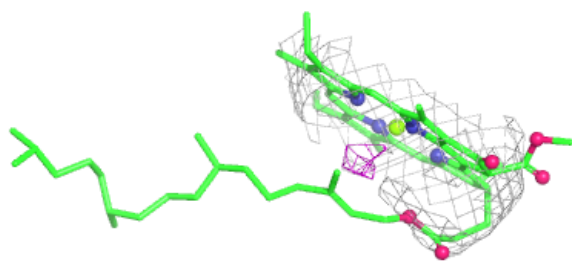
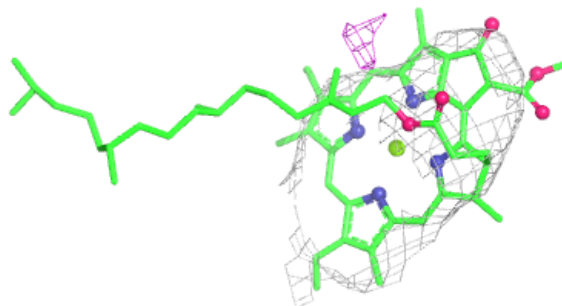


Electron density around BCR F 102:

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

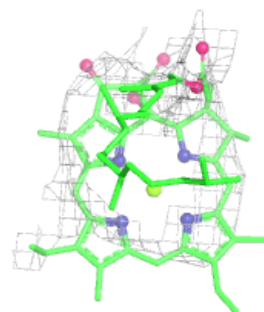
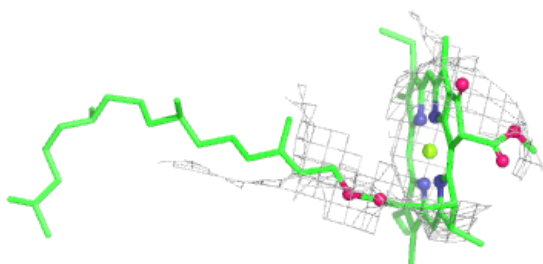
**Electron density around CLA b 617:**

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

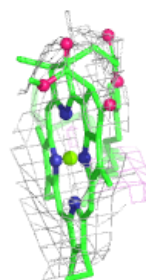
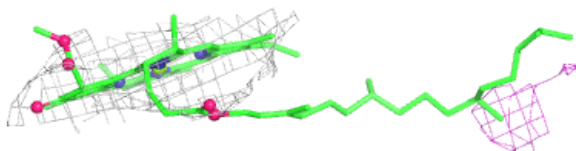
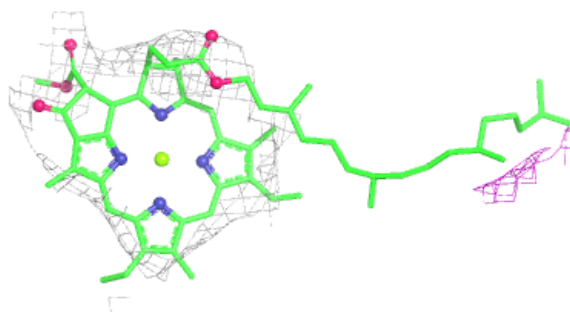


Electron density around CLA B 604:

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

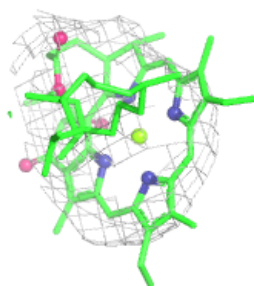
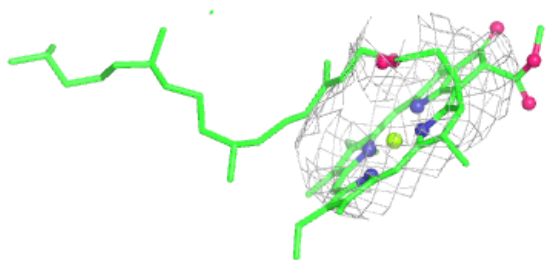
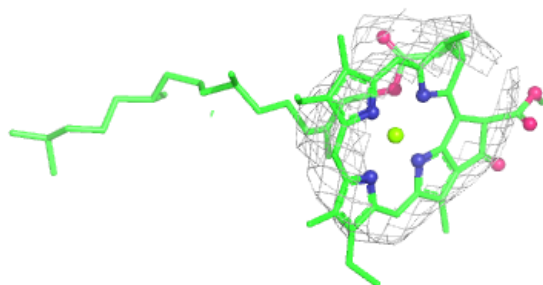
**Electron density around CLA B 602:**

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

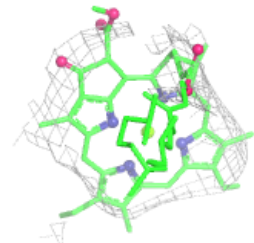
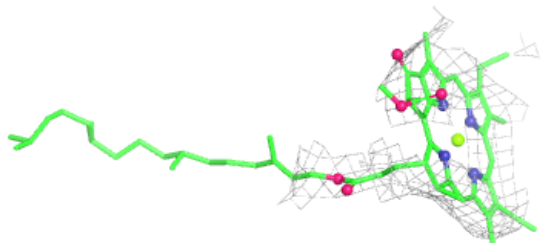
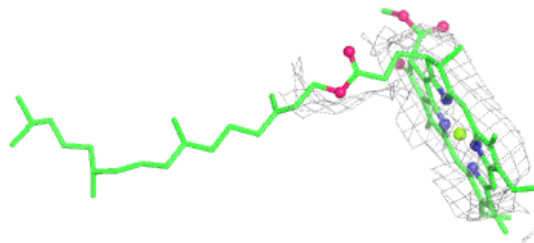


Electron density around CLA C 504:

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

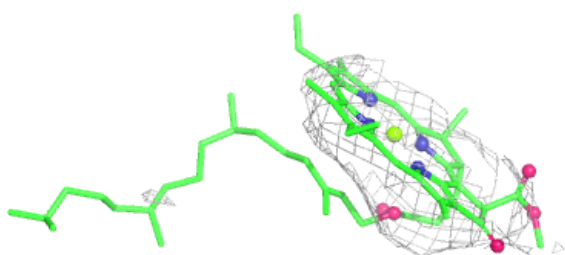
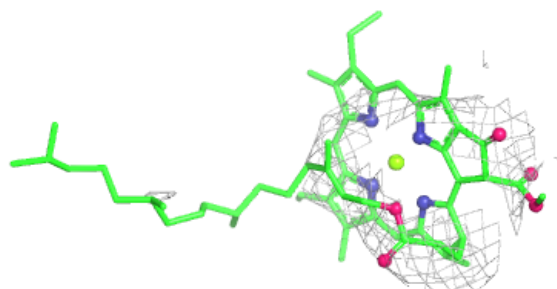
**Electron density around CLA B 603:**

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

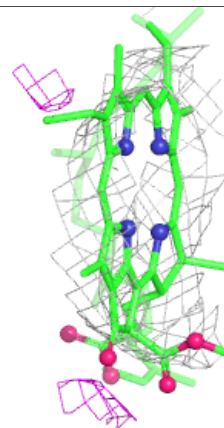
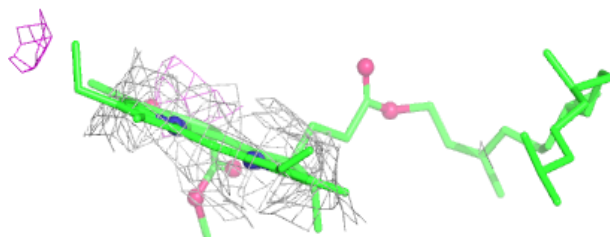
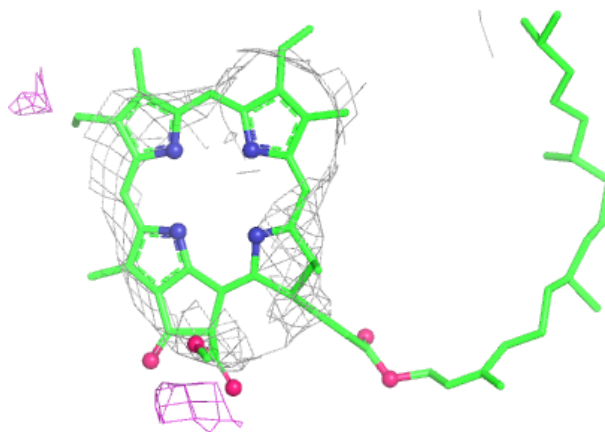


Electron density around CLA c 504:

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

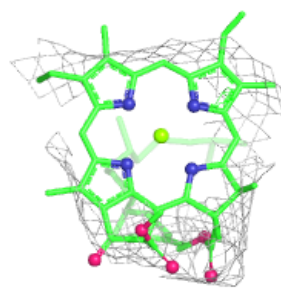
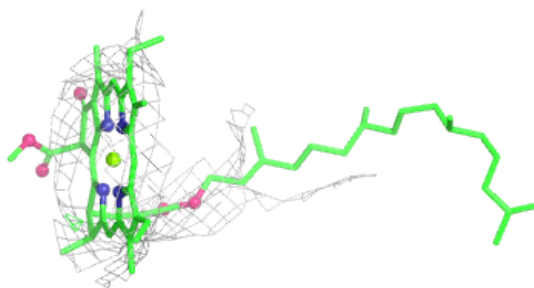
**Electron density around PHO d 401:**

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



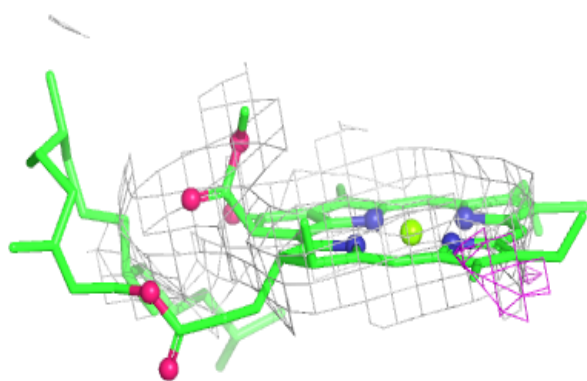
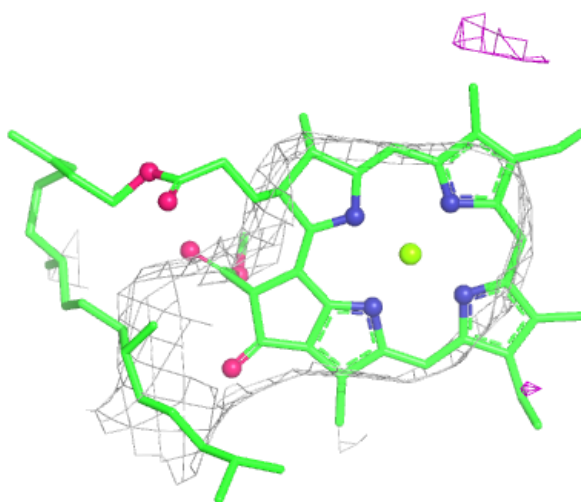
Electron density around CLA b 608:

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



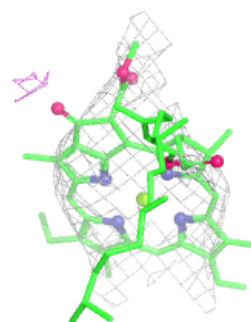
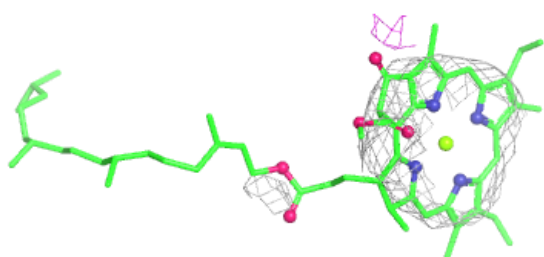
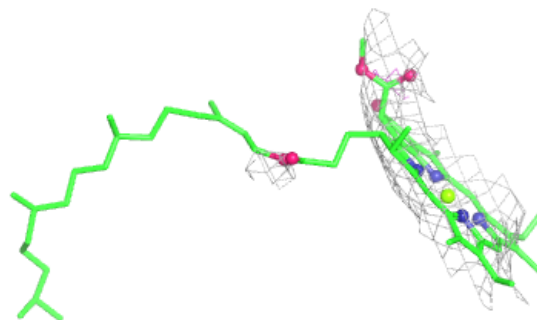
Electron density around CLA B 609:

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



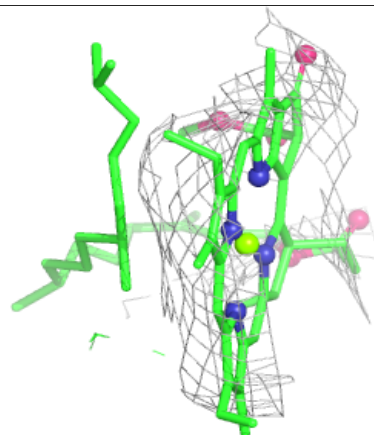
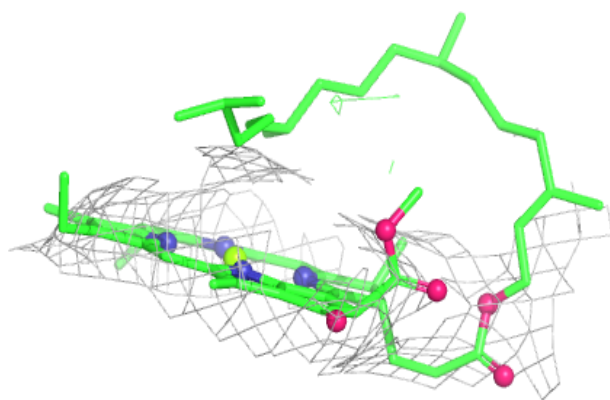
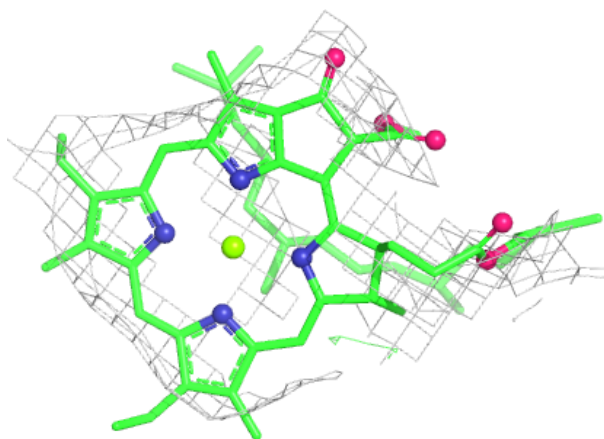
Electron density around CLA D 404:

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

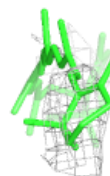
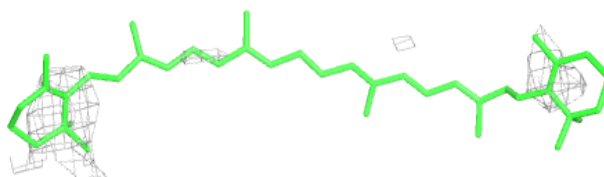


Electron density around CLA c 509:

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

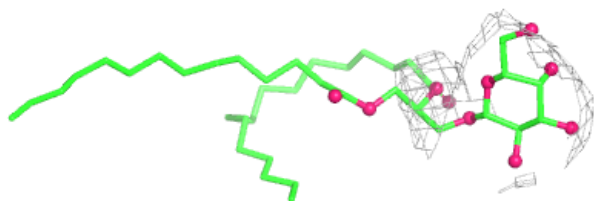
**Electron density around BCR B 617:**

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

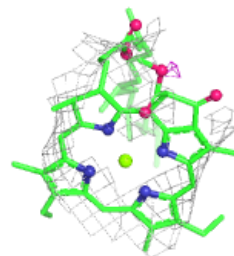
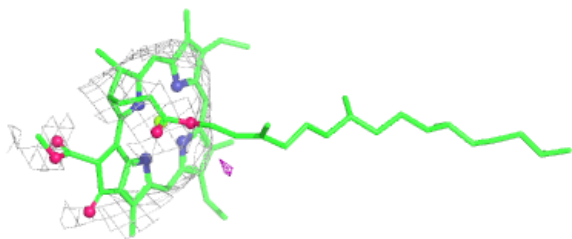
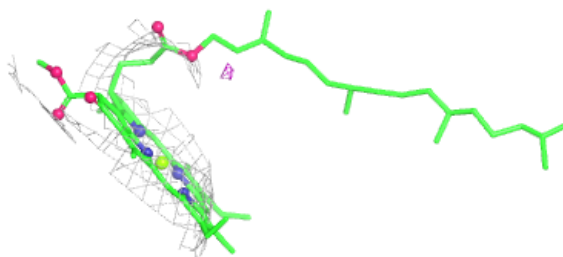


Electron density around LMG d 407:

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

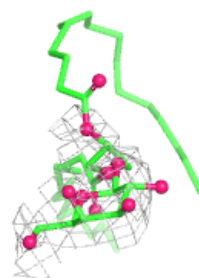
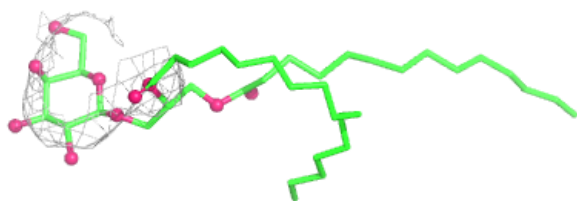
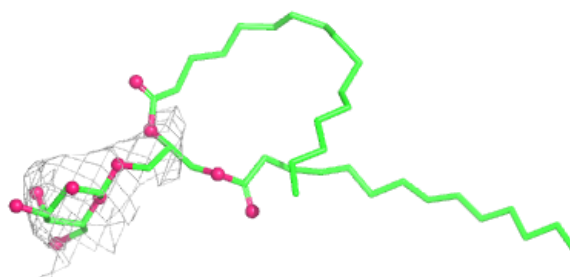
**Electron density around CLA c 520:**

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

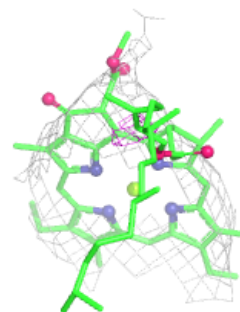
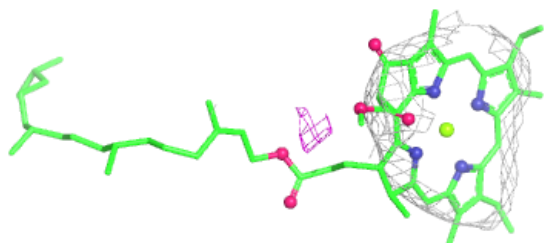
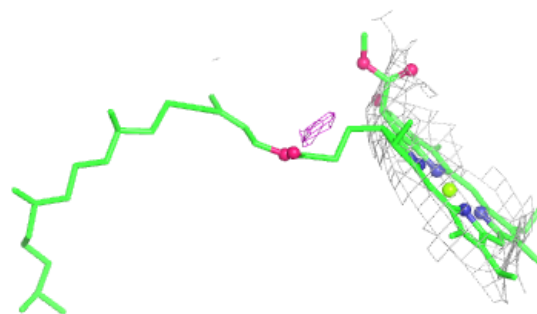


Electron density around LMG D 407:

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

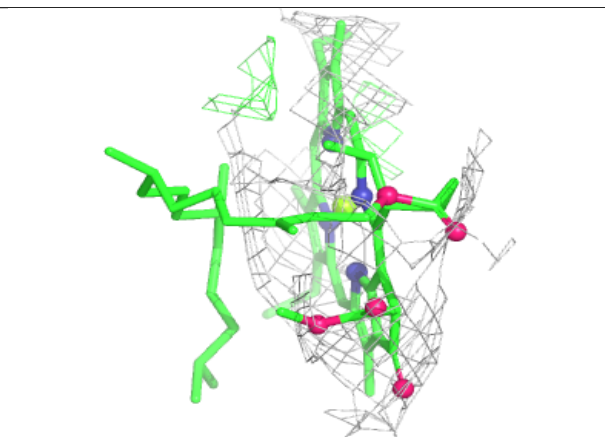
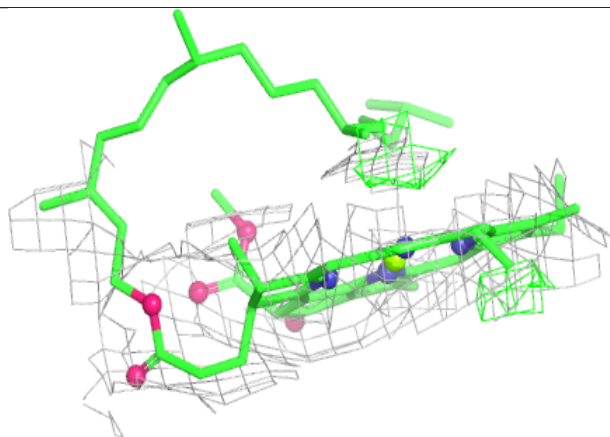
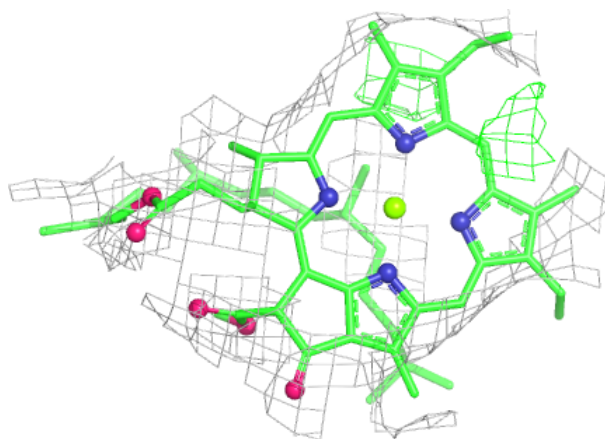
**Electron density around CLA d 404:**

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

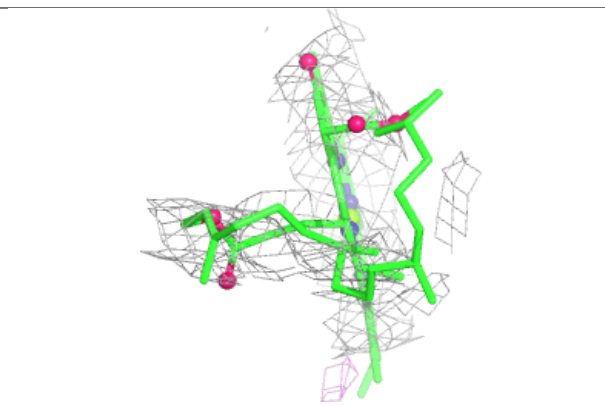
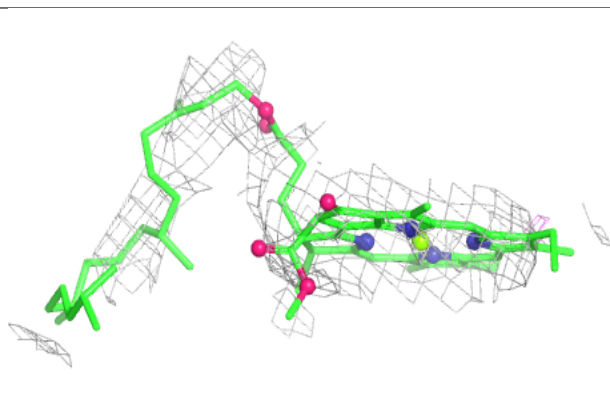
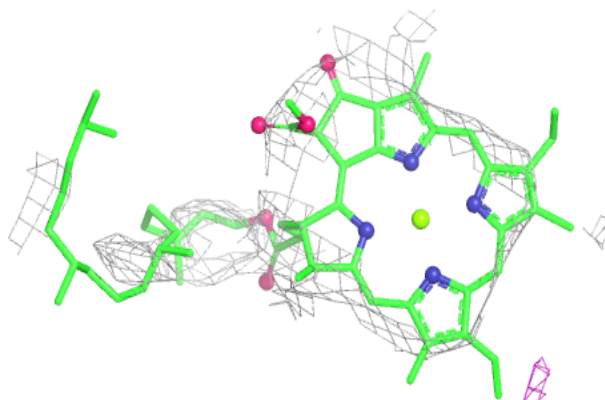


Electron density around CLA C 509:

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

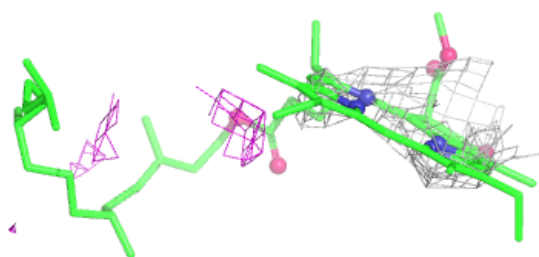
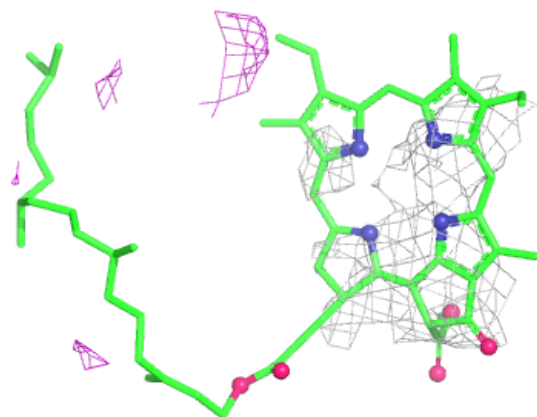
**Electron density around CLA B 611:**

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



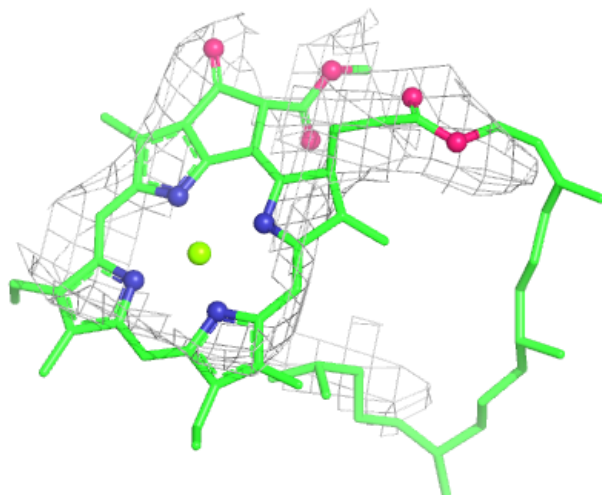
Electron density around PHO a 407:

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



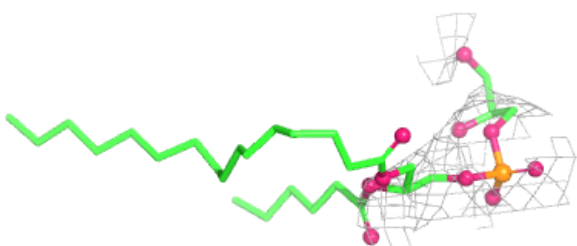
Electron density around CLA b 618:

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

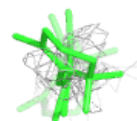
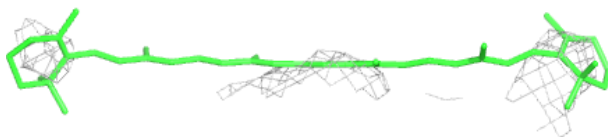
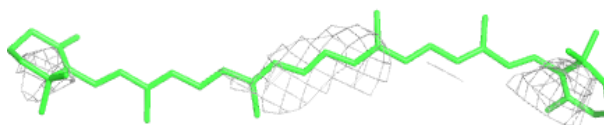


Electron density around LHG a 412:

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

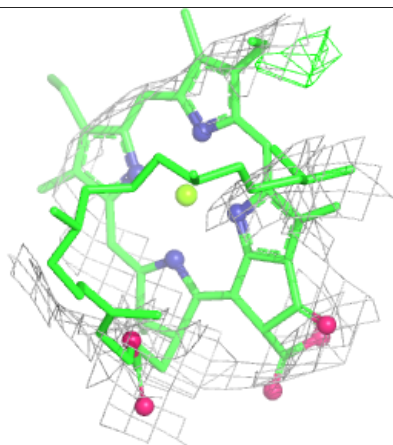
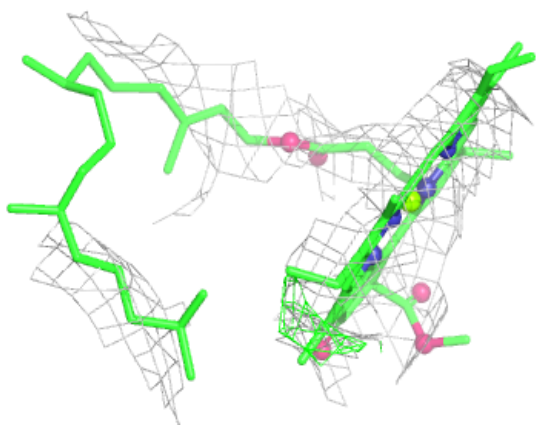
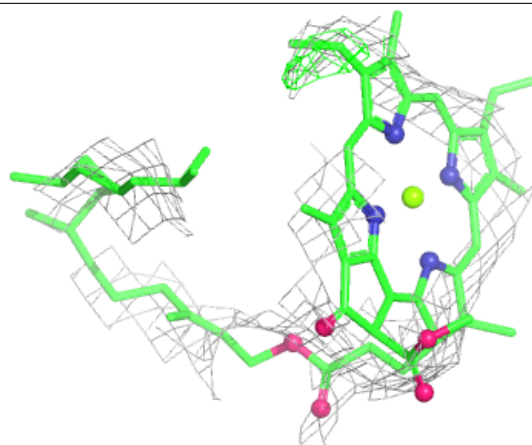
**Electron density around BCR B 618:**

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

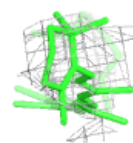
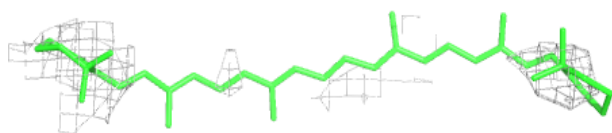
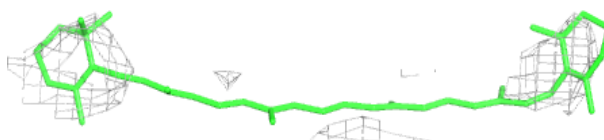


Electron density around CLA C 503:

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

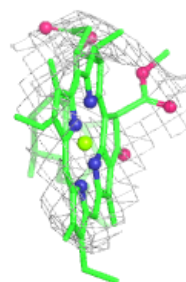
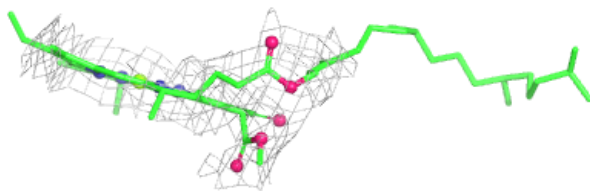
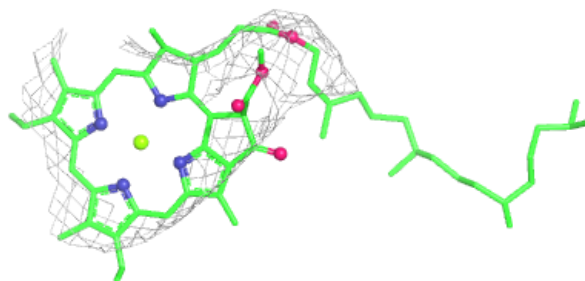
**Electron density around BCR C 513:**

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

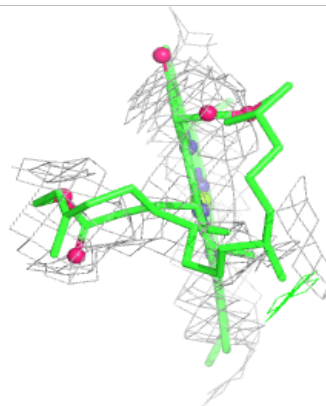
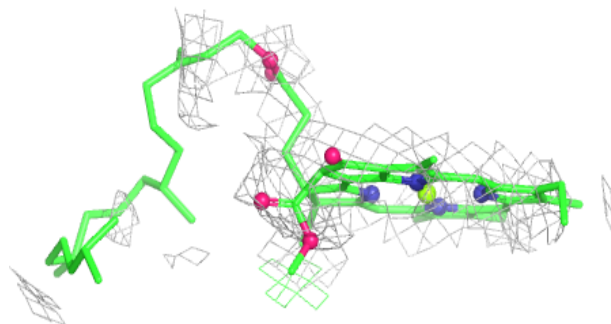
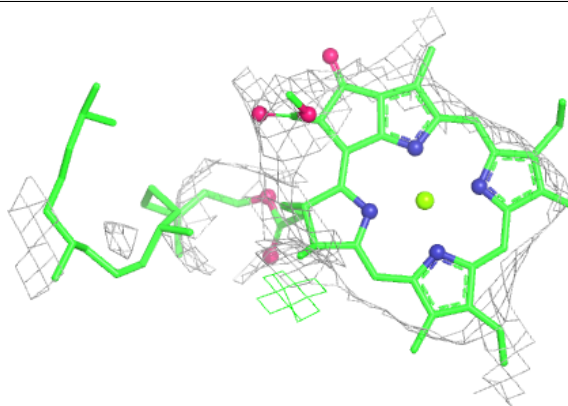


Electron density around CLA H 101:

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

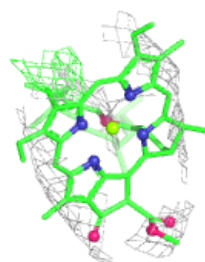
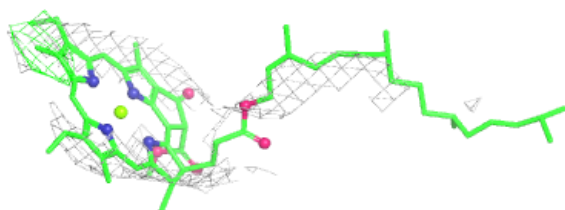
**Electron density around CLA b 615:**

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

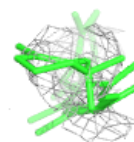
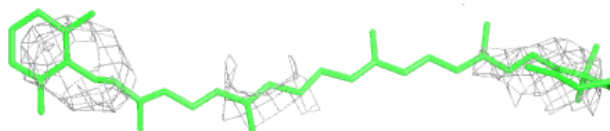


Electron density around CLA C 502:

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

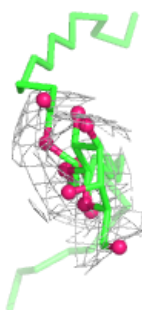
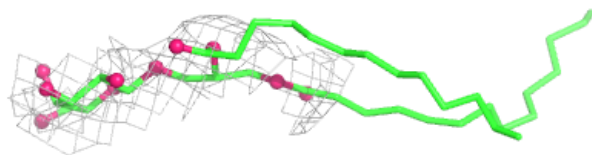
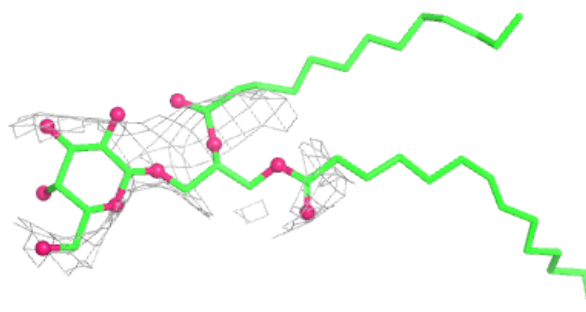
**Electron density around BCR f 102:**

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

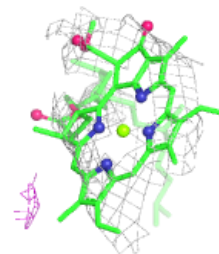
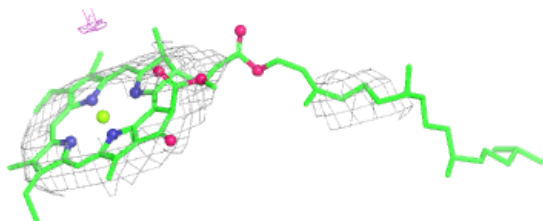
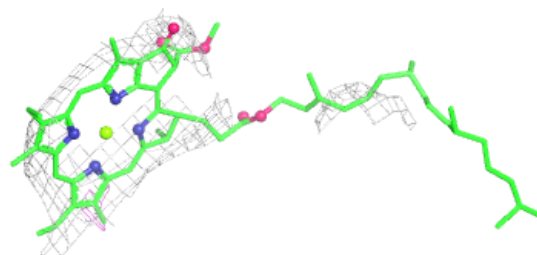


Electron density around LMG d 411:

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

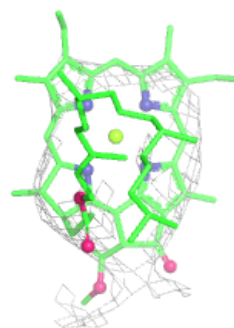
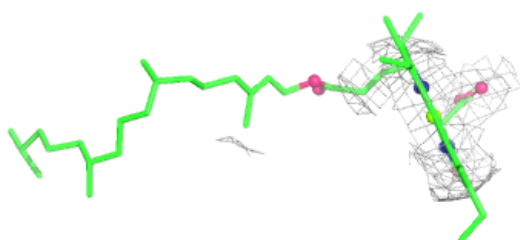
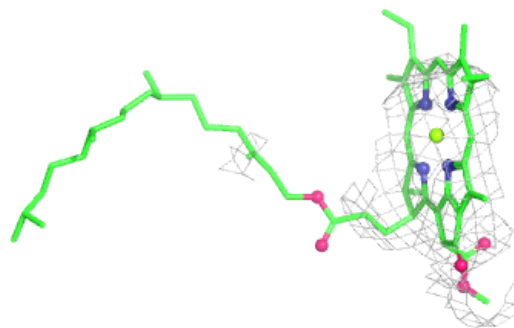
**Electron density around CLA A 402:**

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



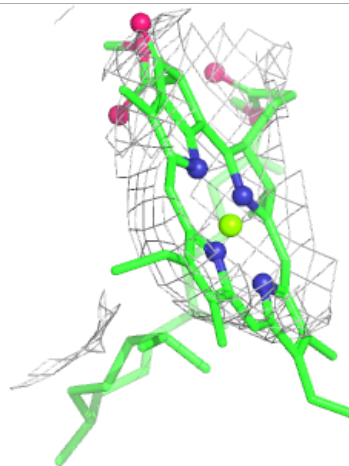
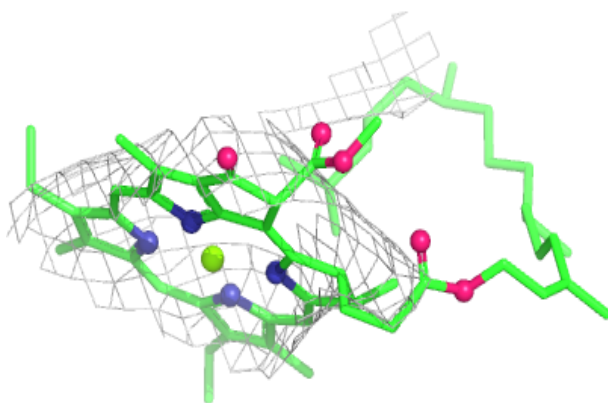
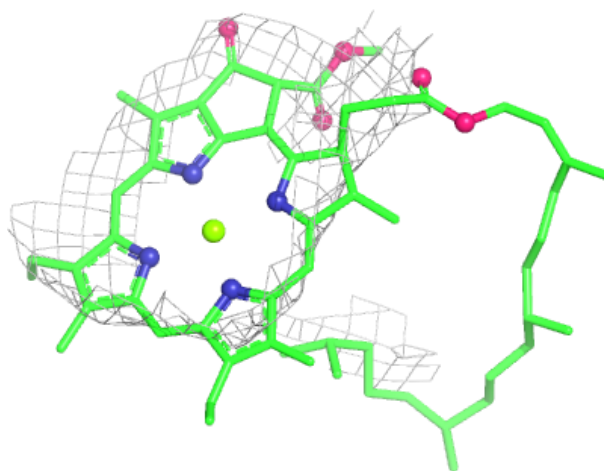
Electron density around CLA D 405:

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



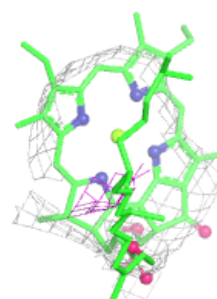
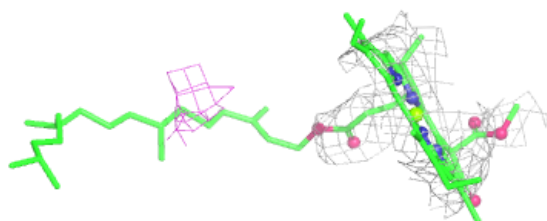
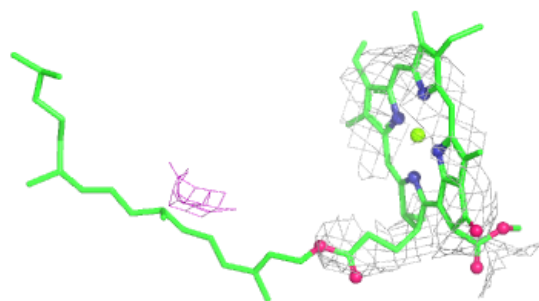
Electron density around CLA B 614:

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

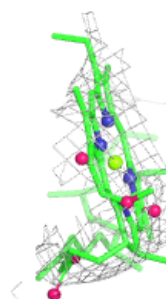
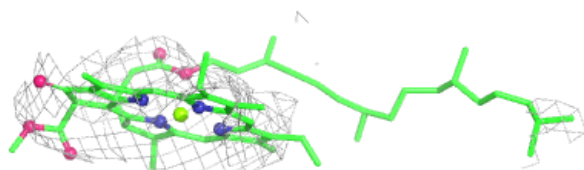
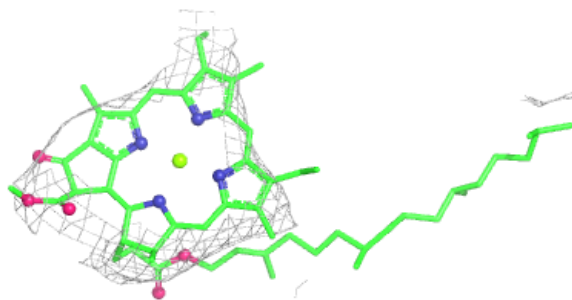


Electron density around CLA B 608:

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

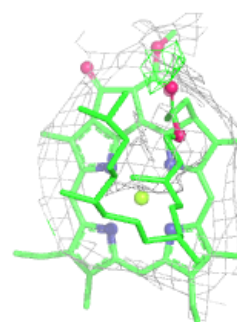
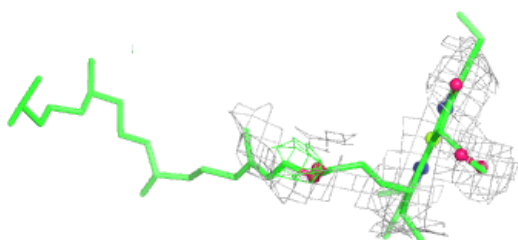
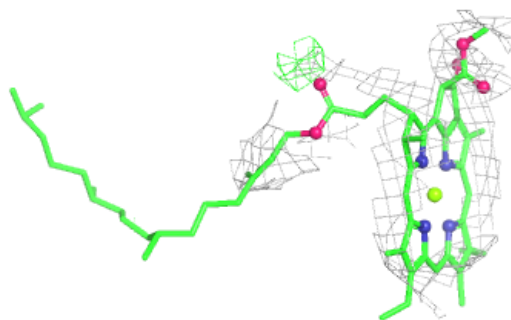
**Electron density around CLA C 501:**

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

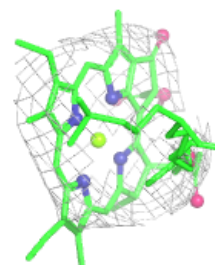
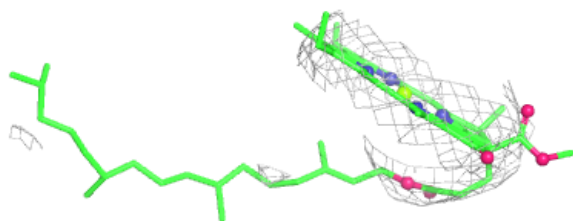
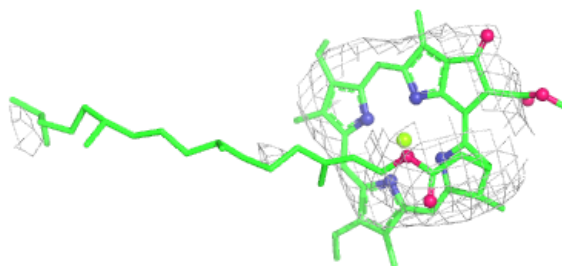


Electron density around CLA d 405:

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

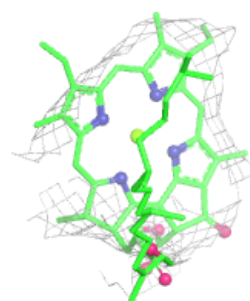
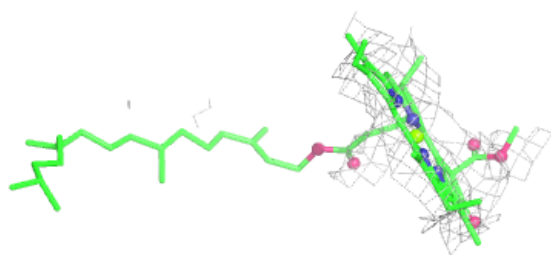
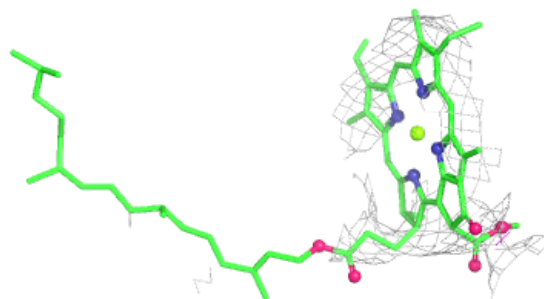
**Electron density around CLA b 611:**

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

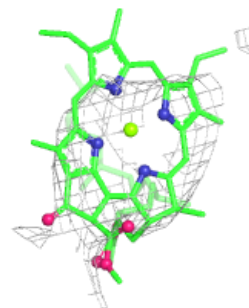
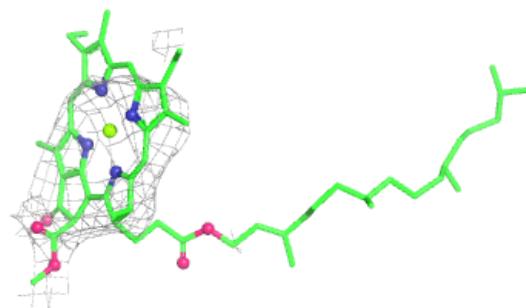


Electron density around CLA b 612:

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

**Electron density around CLA 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)



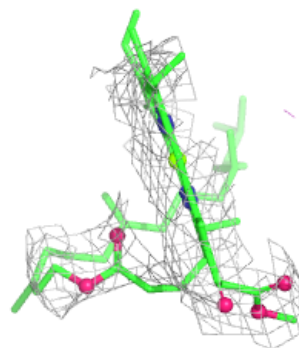
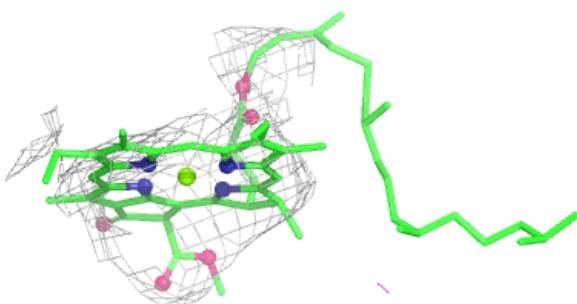
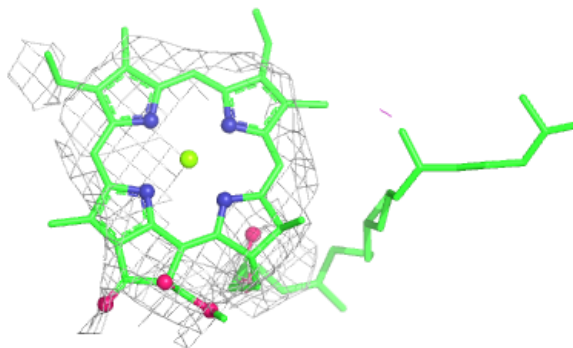
Electron density around LMG A 410:

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

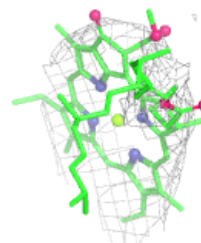
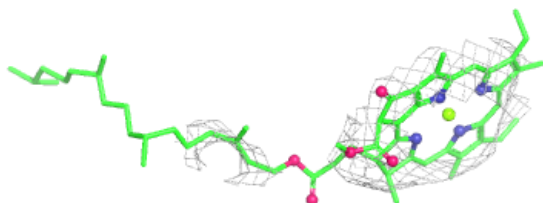
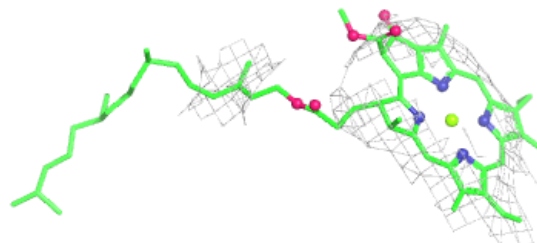


Electron density around CLA A 403:

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

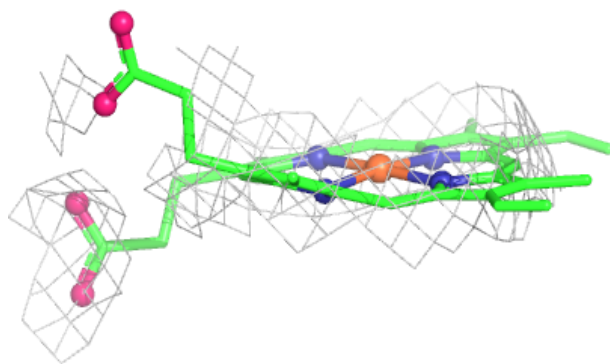
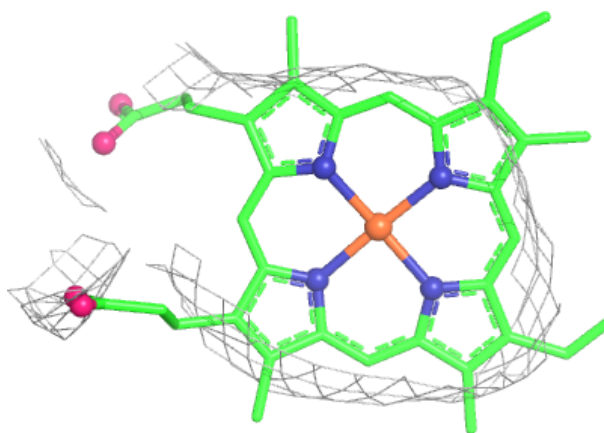
**Electron density around CLA a 404:**

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



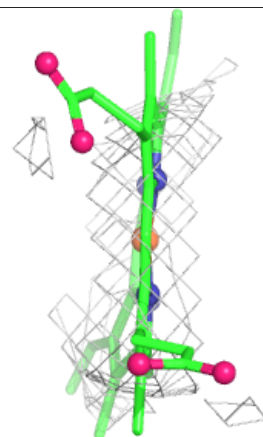
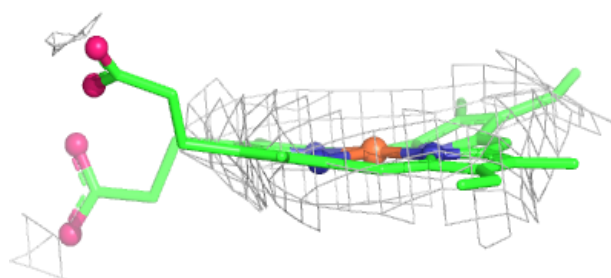
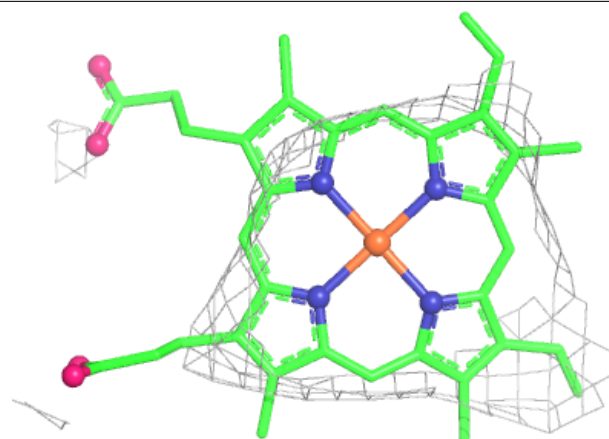
Electron density around HEM f 101:

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



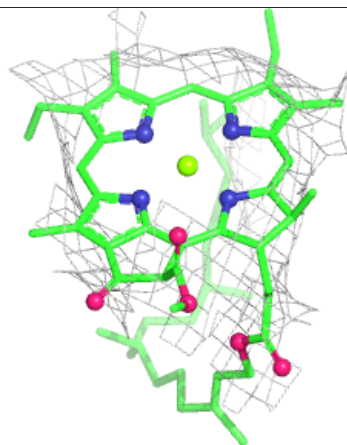
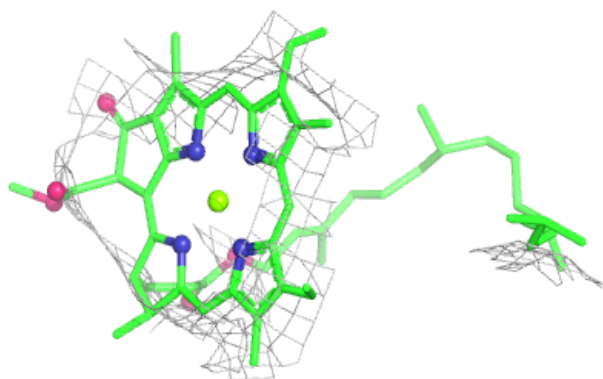
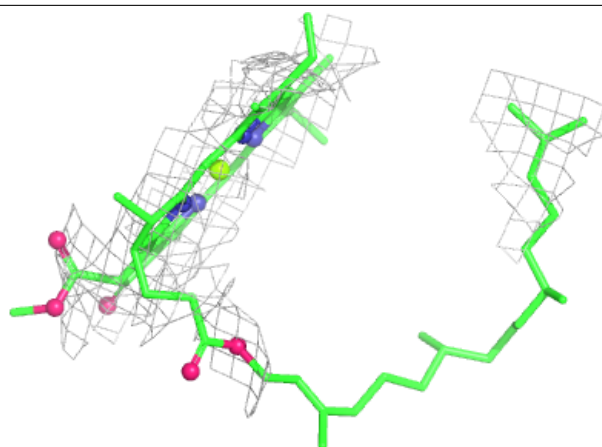
Electron density around HEM v 201:

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



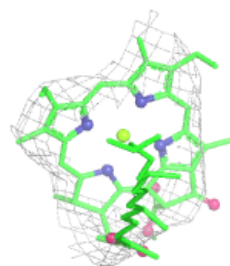
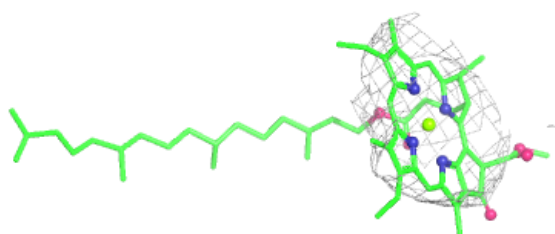
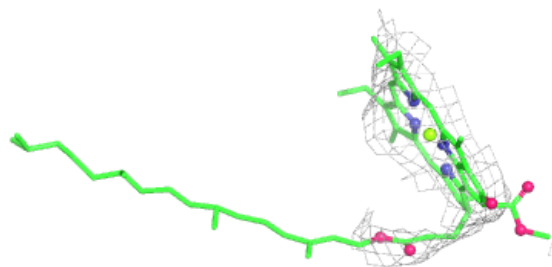
Electron density around CLA B 610:

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

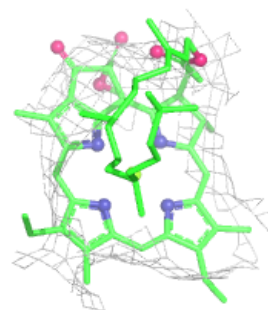
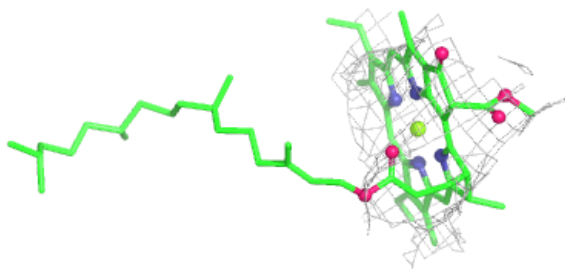
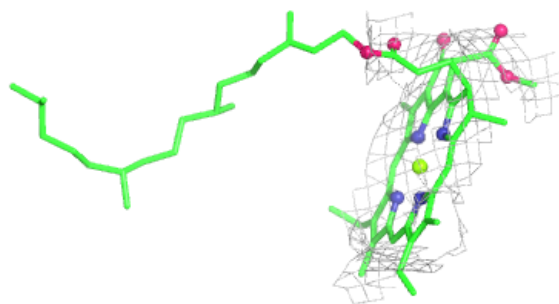


Electron density around CLA B 606:

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

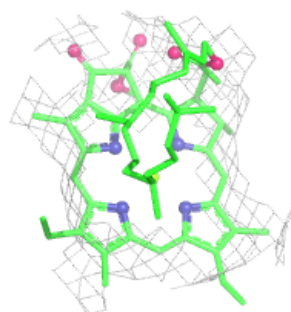
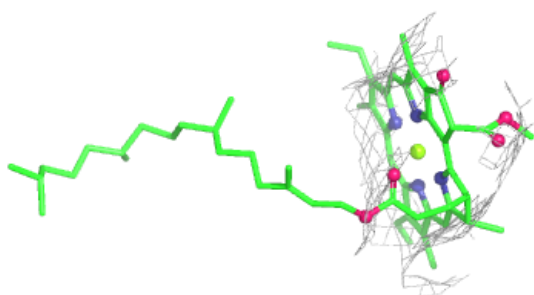
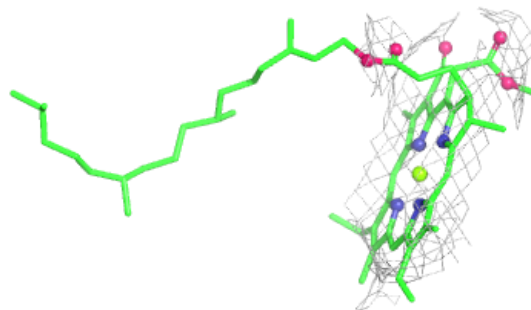
**Electron density around CLA c 507:**

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

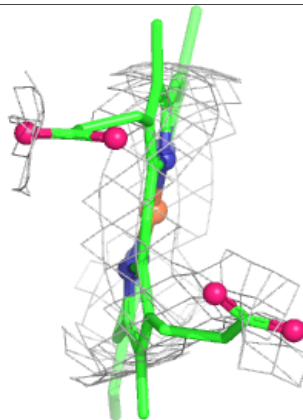
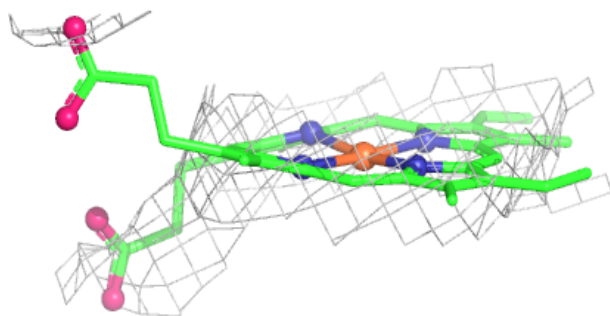
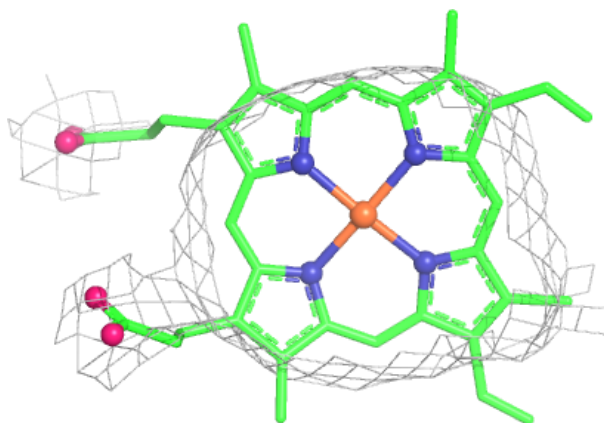


Electron density around CLA C 507:

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

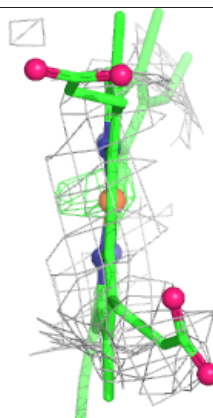
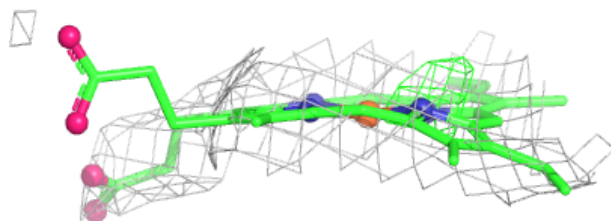
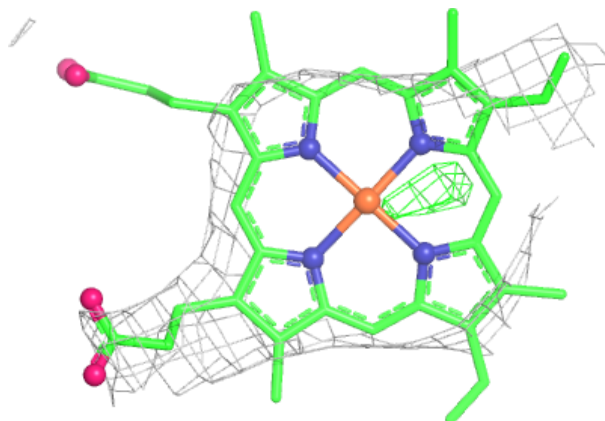
**Electron density around HEM F 101:**

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



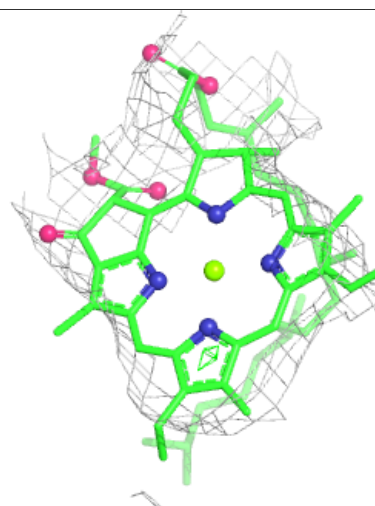
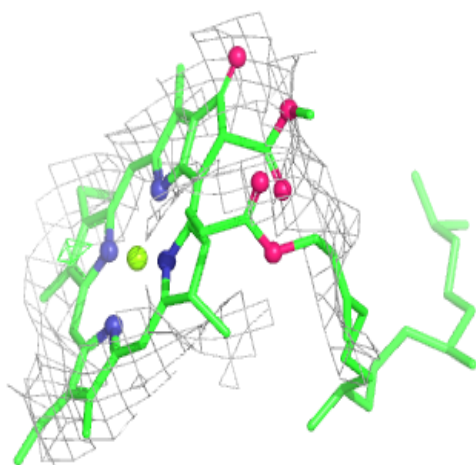
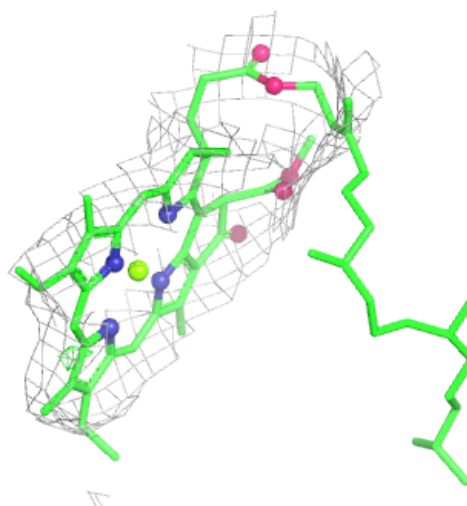
Electron density around HEM V 201:

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



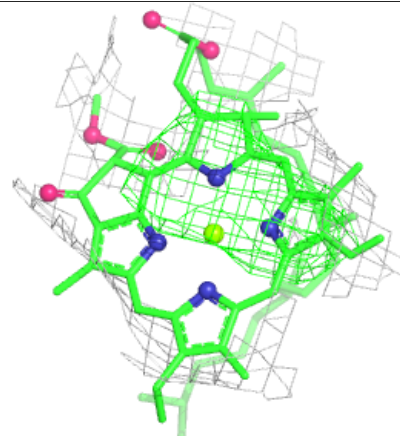
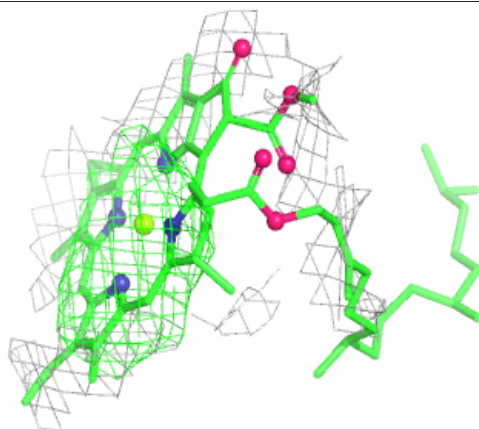
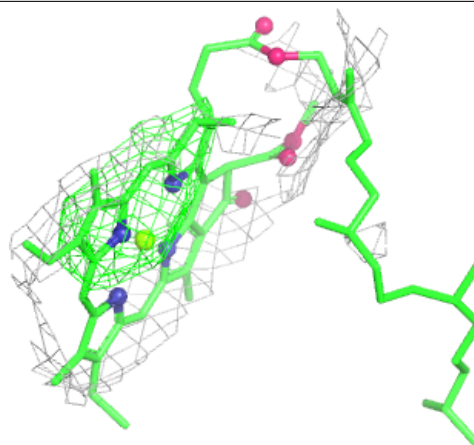
Electron density around CLA B 612:

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



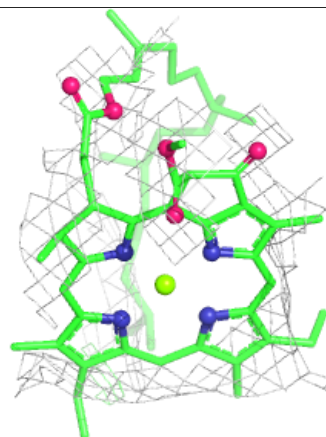
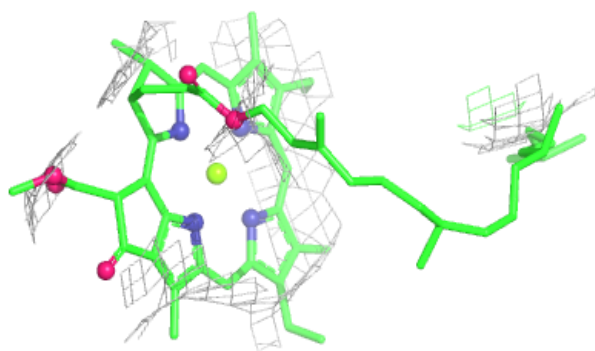
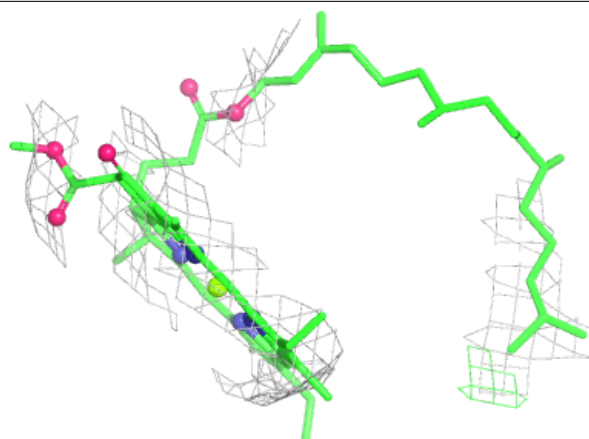
Electron density around CLA b 616:

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



Electron density around CLA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.