



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 01:10 AM EDT

PDB ID : 4TNJ / pdb_00004tnj
Title : RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 4.5 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 : 4.50 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

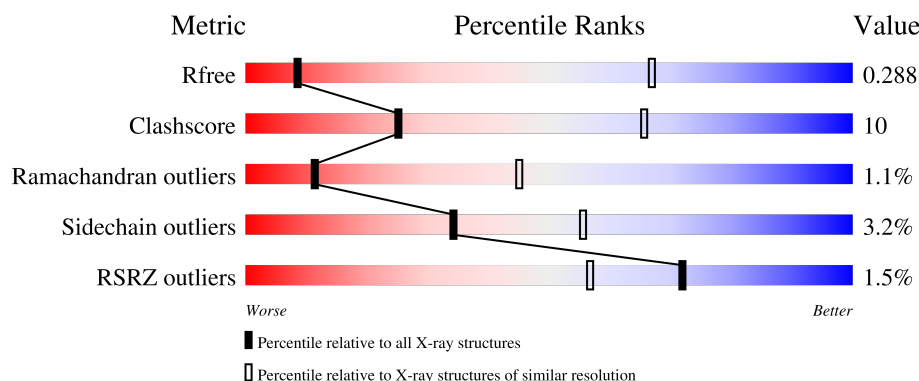
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

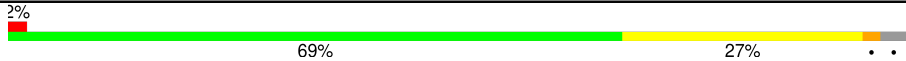
The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	

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Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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

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Mol	Chain	Length	Quality of chain
14	T	32	 81% 16% •
14	t	32	 81% 16% •
15	U	134	 3% 59% 13% • 28%
15	u	134	 % 59% 13% • 28%
16	V	163	 2% 77% 6% • 16%
16	v	163	 % 78% 5% • 16%
17	g	46	 41% 17% • 39%
17	y	46	 41% 15% • 39%
18	X	41	 59% 27% • • 10%
18	x	41	 66% 20% • • 10%
19	G	28	 100%
19	Y	28	 100%
20	Z	62	 2% 84% 13% •
20	z	62	 79% 18% •

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				

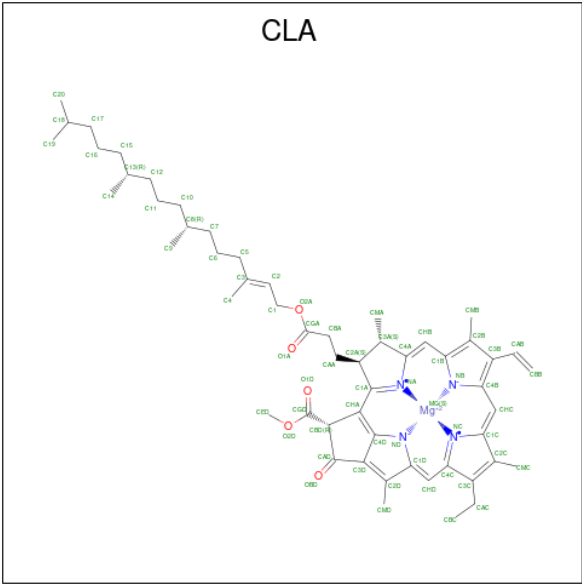
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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 1 1	0	0
21	a	1	Total Fe 1 1	0	0

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



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

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

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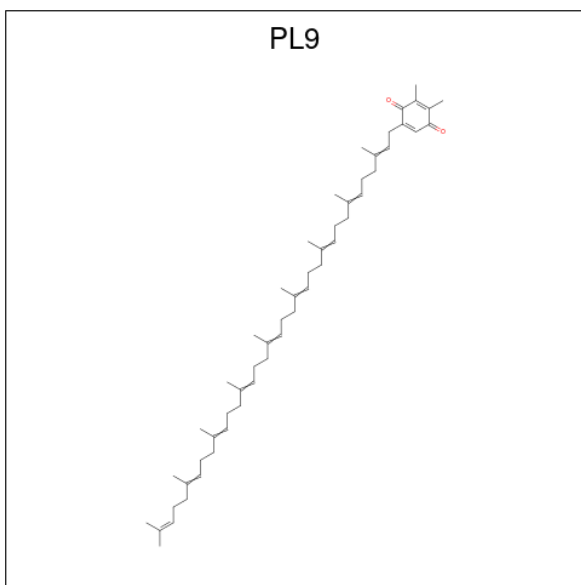
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 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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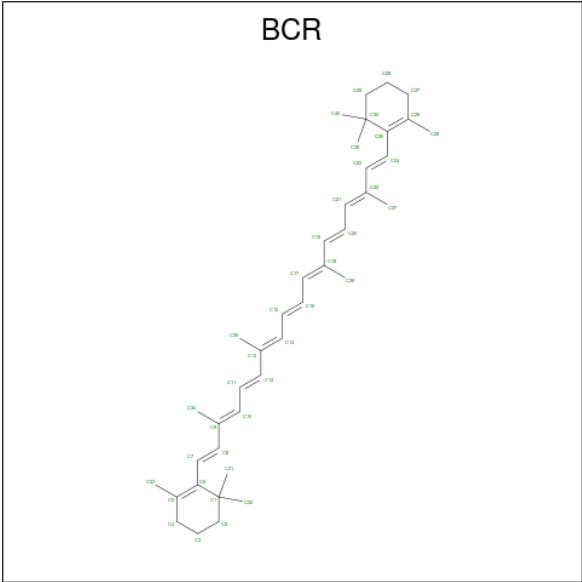
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: $C_{40}H_{56}$).



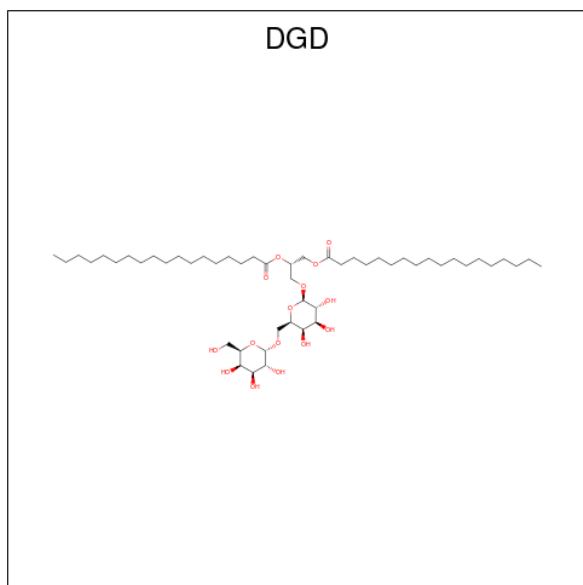
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	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: $C_{51}H_{96}O_{15}$).



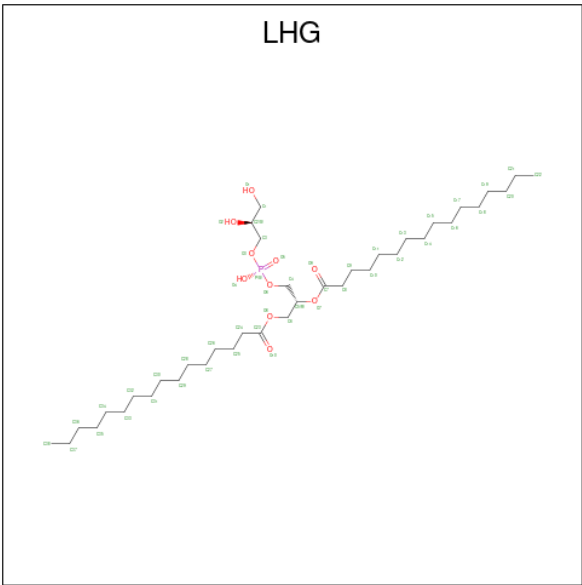
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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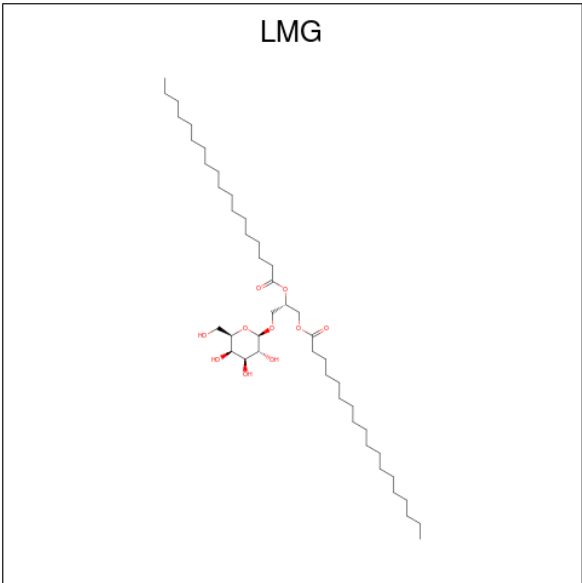
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

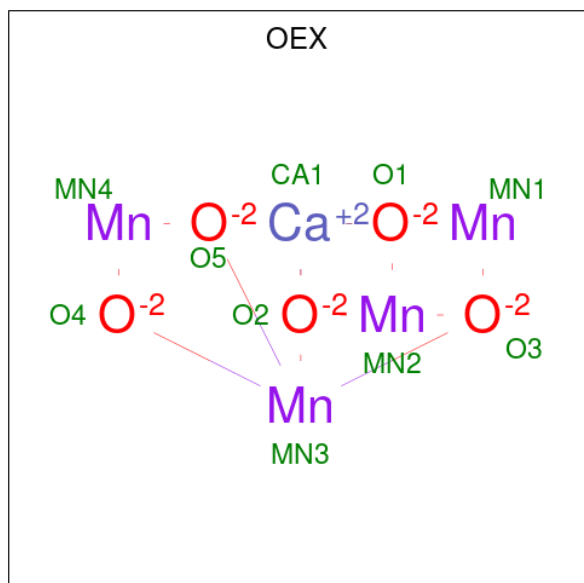


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	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	a	1	Total	C	O	0	0
			51	41	10		
27	b	1	Total	C	O	0	0
			49	39	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
			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		

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

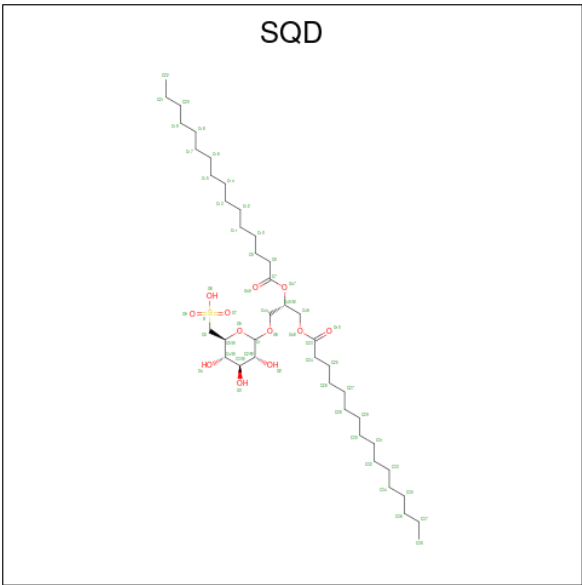
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

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



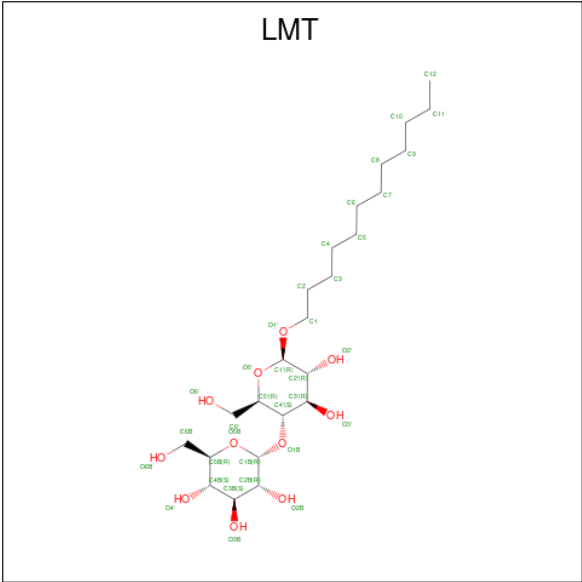
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



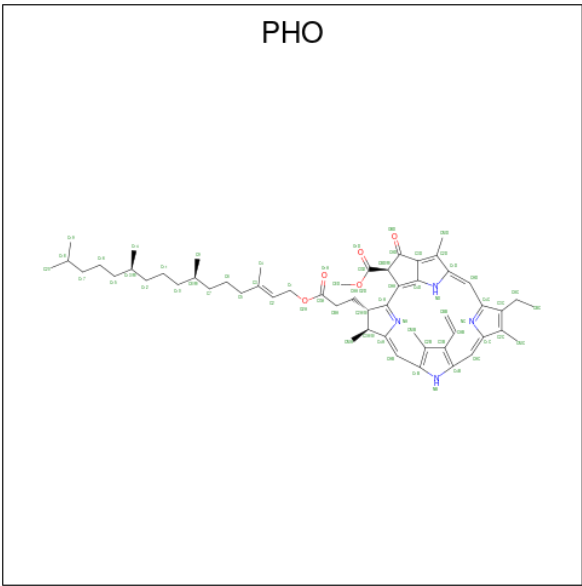
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0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



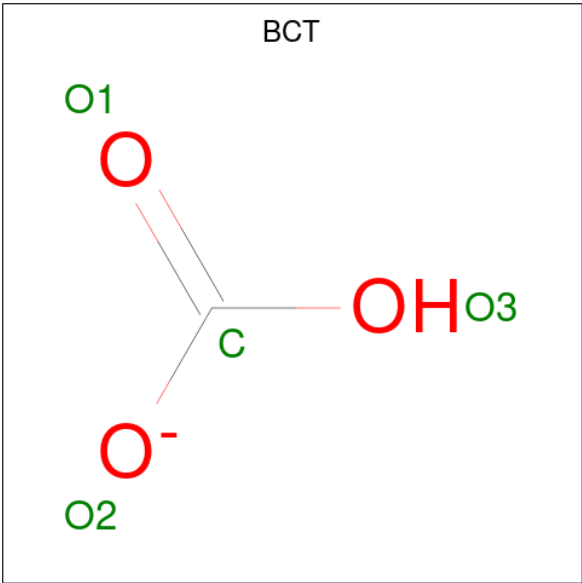
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	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: C₅₅H₇₄N₄O₅).



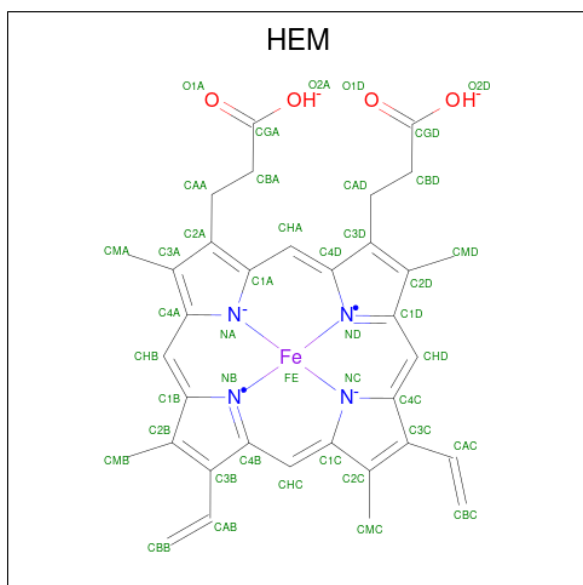
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

Continued on next page...

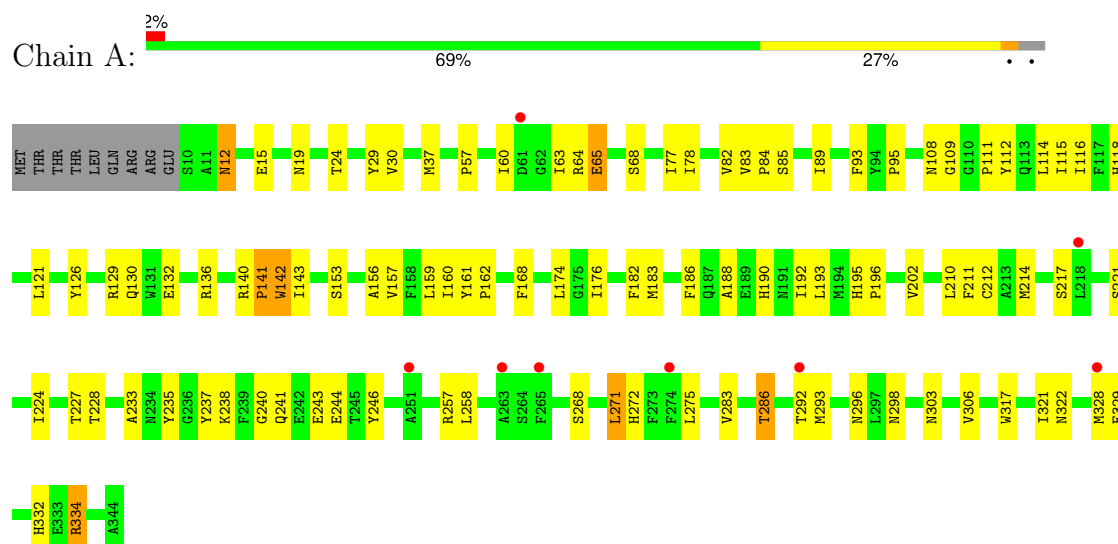
Continued from previous page...

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

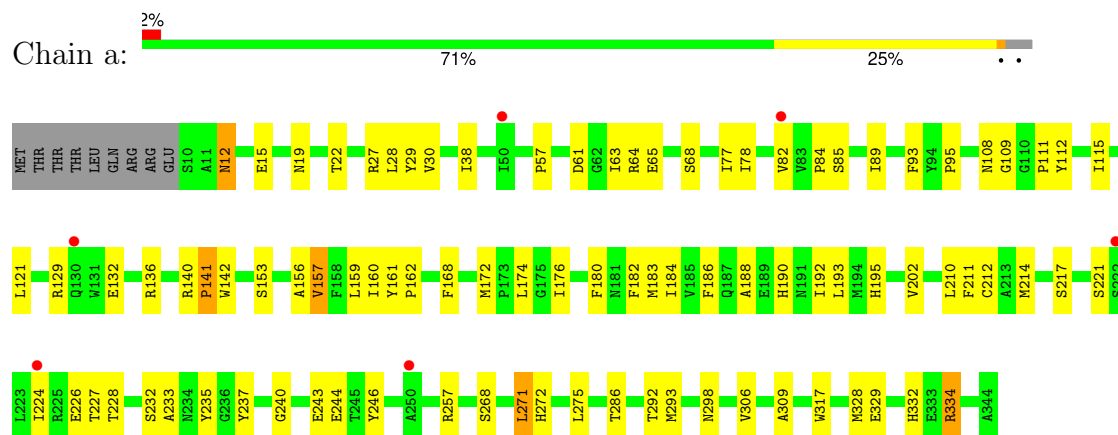
3 Residue-property plots

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

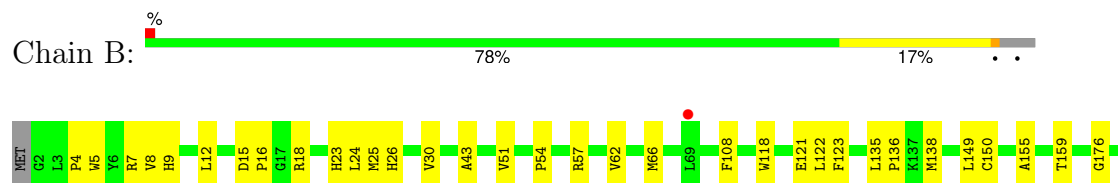
• Molecule 1: Photosystem Q(B) protein 1

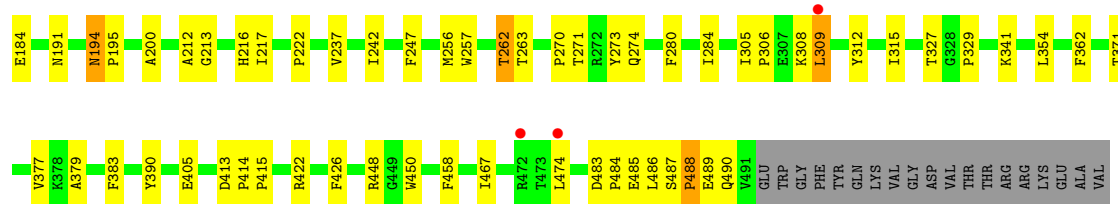


• Molecule 1: Photosystem Q(B) protein 1

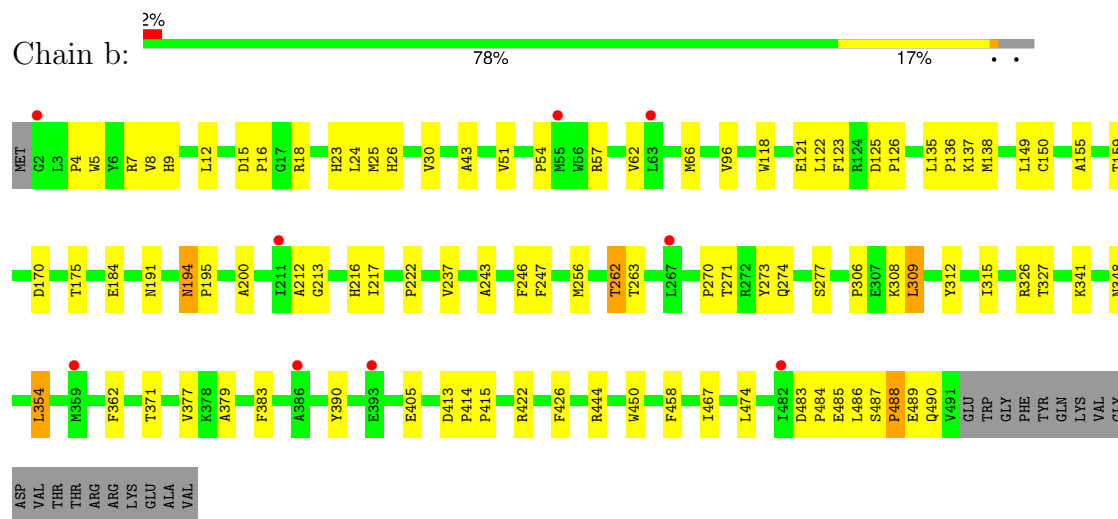


• Molecule 2: Photosystem II core light harvesting protein

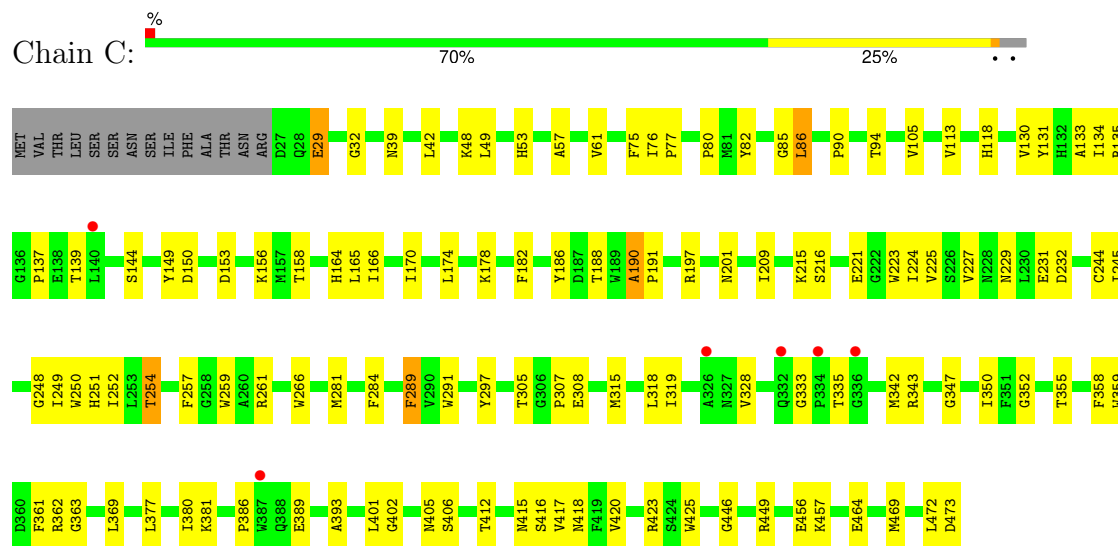




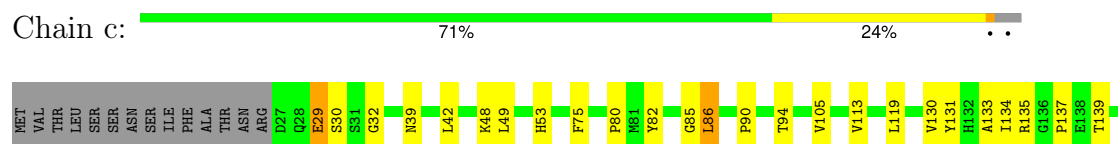
• Molecule 2: Photosystem II core light harvesting protein

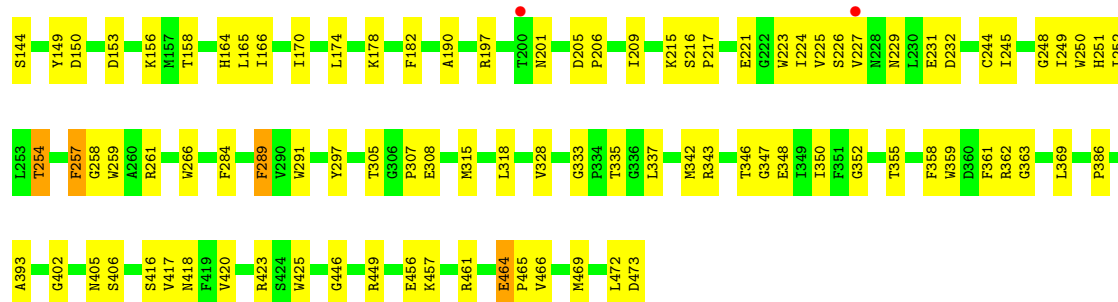


• Molecule 3: Photosystem II CP43 protein

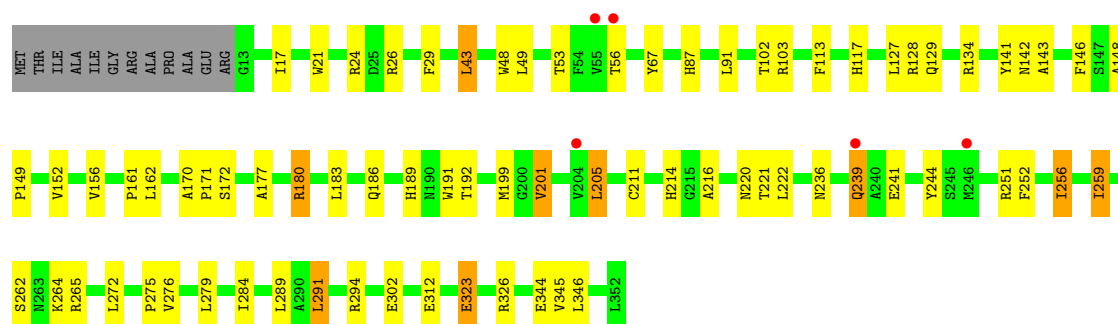
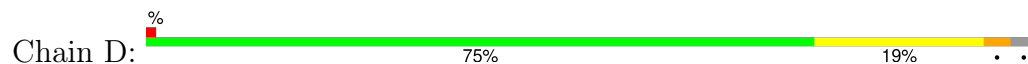


• Molecule 3: Photosystem II CP43 protein

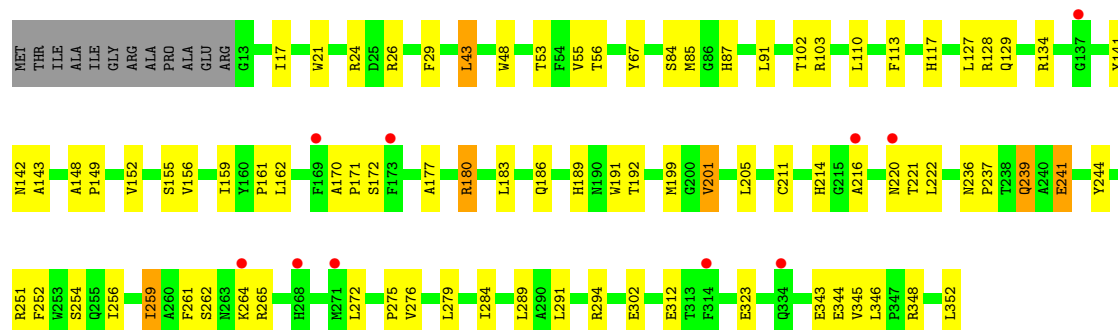




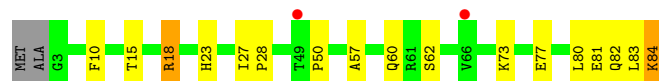
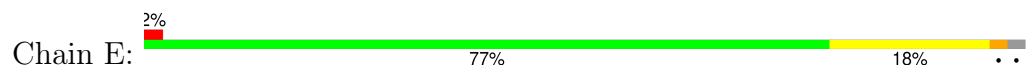
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein

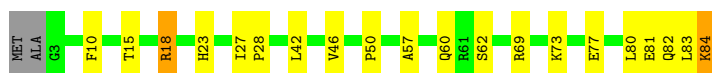


- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

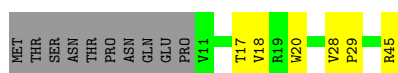




- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



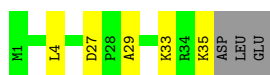
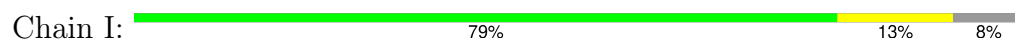
- Molecule 7: Photosystem II reaction center protein H



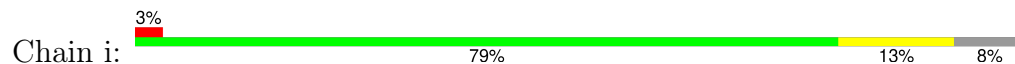
- Molecule 7: Photosystem II reaction center protein H



- 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



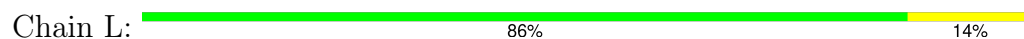
- Molecule 10: Photosystem II reaction center protein K



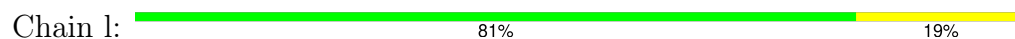
- Molecule 10: Photosystem II reaction center protein K



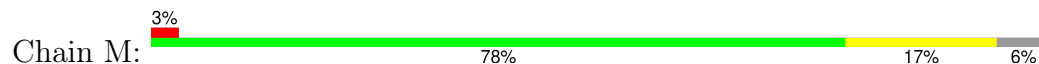
- Molecule 11: Photosystem II reaction center protein L



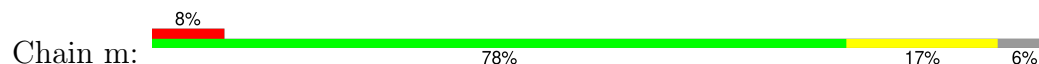
- Molecule 11: Photosystem II reaction center protein L

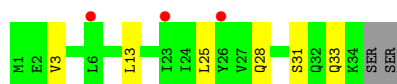


- Molecule 12: Photosystem II reaction center protein M

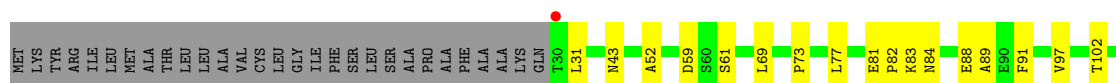


- Molecule 12: Photosystem II reaction center protein M

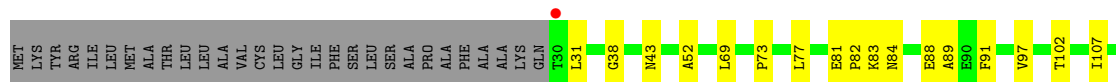




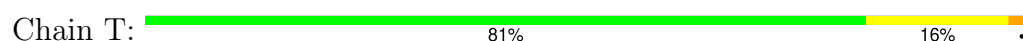
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



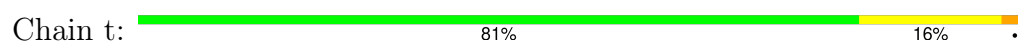
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



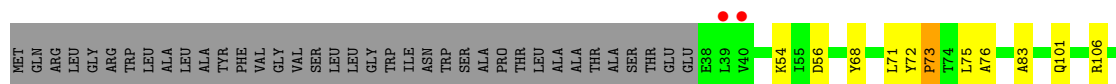
- Molecule 14: Photosystem II reaction center protein T



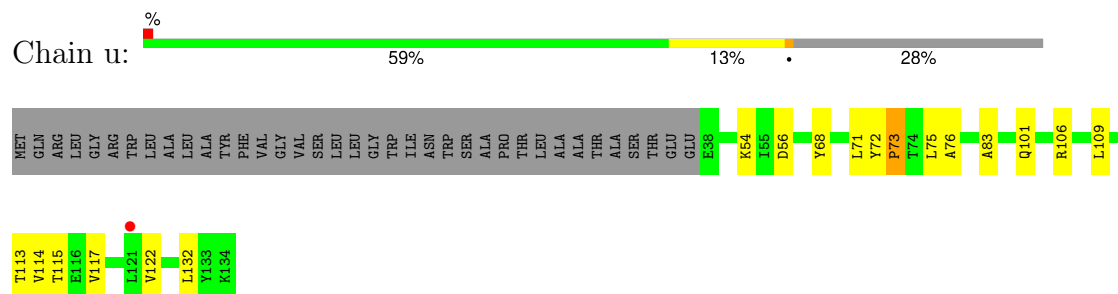
- Molecule 14: Photosystem II reaction center protein T



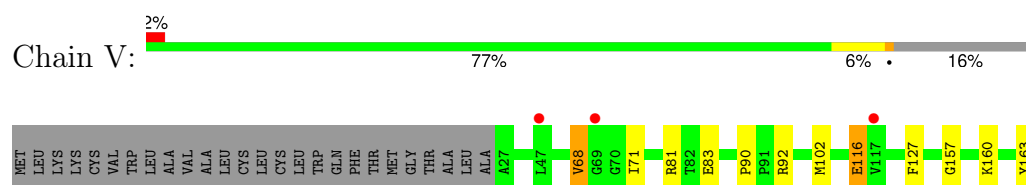
- Molecule 15: Photosystem II 12 kDa extrinsic protein



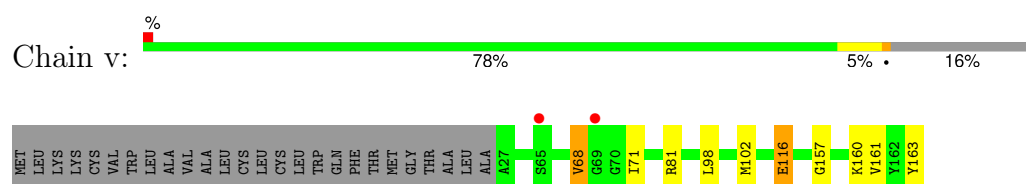
- Molecule 15: Photosystem II 12 kDa extrinsic protein



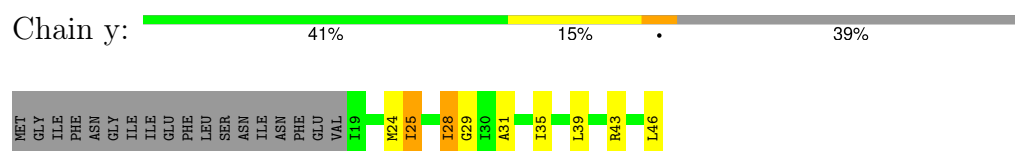
- Molecule 16: Cytochrome c-550



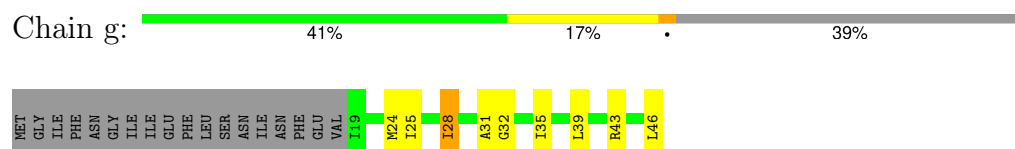
- Molecule 16: Cytochrome c-550



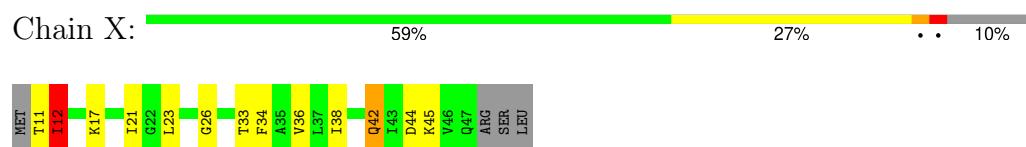
- Molecule 17: Photosystem II reaction center protein Ycf12



- 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

Chain Y: 100%

There are no outlier residues recorded for this chain.

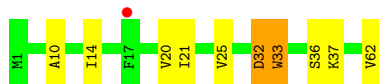
- Molecule 19: Photosystem II reaction center protein Y

Chain G: 100%

There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 2% 84% 13%



- Molecule 20: Photosystem II reaction center protein Z

Chain z: 79% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.30Å 228.71Å 307.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 4.50 72.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.97-4.50) 96.8 (72.97-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 4.46Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.276 , 0.284 0.280 , 0.288	Depositor DCC
R_{free} test set	2668 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	153.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 124.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.30	0/2713	0.79	2/3700 (0.1%)
2	B	0.30	0/3986	0.80	8/5433 (0.1%)
2	b	0.30	0/3986	0.81	8/5433 (0.1%)
3	C	0.30	0/3556	0.80	8/4842 (0.2%)
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	0.77	0/3818
5	E	0.31	0/685	0.83	0/933
5	e	0.31	0/685	0.84	0/933
6	F	0.34	0/291	0.75	0/397
6	f	0.34	0/291	0.76	0/397
7	H	0.34	0/520	0.73	0/709
7	h	0.33	0/520	0.73	0/709
8	I	0.29	0/293	0.78	0/395
8	i	0.30	0/293	0.78	0/395
9	J	0.29	0/255	0.85	0/346
9	j	0.30	0/255	0.84	0/346
10	K	0.44	0/303	0.86	0/416
10	k	0.45	0/303	0.87	0/416
11	L	0.29	0/311	0.72	0/422
11	l	0.28	0/311	0.72	0/422
12	M	0.30	0/270	0.79	0/367
12	m	0.30	0/270	0.79	0/367
13	O	0.27	0/1876	0.70	0/2548
13	o	0.28	0/1876	0.70	2/2548 (0.1%)
14	T	0.27	0/284	0.76	0/381
14	t	0.27	0/284	0.74	0/381
15	U	0.30	0/785	0.77	0/1064
15	u	0.30	0/785	0.79	0/1064
16	V	0.29	0/1081	0.76	2/1468 (0.1%)
16	v	0.30	0/1081	0.76	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.34	0/202	0.77	0/272
17	y	0.33	0/202	0.77	0/272
18	X	0.38	0/273	0.80	0/370
18	x	0.38	0/273	0.80	0/370
20	Z	0.31	0/490	0.83	0/669
20	z	0.31	0/490	0.85	0/669
All	All	0.30	0/41950	0.78	40/57100 (0.1%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	483	ASP	CA-C-N	10.70	133.21	119.84
2	b	483	ASP	C-N-CA	10.70	133.21	119.84
2	B	483	ASP	CA-C-N	10.56	133.04	119.84
2	B	483	ASP	C-N-CA	10.56	133.04	119.84
3	C	363	GLY	CA-C-N	6.37	125.86	119.24
3	C	363	GLY	C-N-CA	6.37	125.86	119.24
3	c	363	GLY	CA-C-N	6.29	125.78	119.24
3	c	363	GLY	C-N-CA	6.29	125.78	119.24
3	C	190	ALA	CA-C-N	6.19	125.67	119.24
3	C	190	ALA	C-N-CA	6.19	125.67	119.24
3	c	190	ALA	CA-C-N	6.18	125.67	119.24
3	c	190	ALA	C-N-CA	6.18	125.67	119.24
2	B	413	ASP	CA-C-N	5.72	126.27	120.38
2	B	413	ASP	C-N-CA	5.72	126.27	120.38
2	b	15	ASP	CA-C-N	5.69	125.81	119.32
2	b	15	ASP	C-N-CA	5.69	125.81	119.32
2	b	194	ASN	CA-C-N	5.65	125.32	119.05
2	b	194	ASN	C-N-CA	5.65	125.32	119.05
2	b	413	ASP	CA-C-N	5.65	126.20	120.38
2	b	413	ASP	C-N-CA	5.65	126.20	120.38
2	B	15	ASP	CA-C-N	5.52	125.61	119.32
2	B	15	ASP	C-N-CA	5.52	125.61	119.32
2	B	194	ASN	CA-C-N	5.47	125.12	119.05
2	B	194	ASN	C-N-CA	5.47	125.12	119.05
3	c	333	GLY	CA-C-N	5.33	126.51	119.84
3	c	333	GLY	C-N-CA	5.33	126.51	119.84
16	V	127	PHE	CA-C-N	5.24	126.39	119.84
16	V	127	PHE	C-N-CA	5.24	126.39	119.84
3	C	464	GLU	CA-C-N	5.20	126.34	119.84
3	C	464	GLU	C-N-CA	5.20	126.34	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	333	GLY	CA-C-N	5.19	126.33	119.84
3	C	333	GLY	C-N-CA	5.19	126.33	119.84
13	o	200	LEU	CA-C-N	5.15	125.19	119.32
13	o	200	LEU	C-N-CA	5.15	125.19	119.32
1	a	195	HIS	CA-C-N	5.05	125.08	119.32
1	a	195	HIS	C-N-CA	5.05	125.08	119.32
1	A	65	GLU	CA-C-N	5.03	125.31	119.93
1	A	65	GLU	C-N-CA	5.03	125.31	119.93
3	c	464	GLU	CA-C-N	5.01	126.11	119.84
3	c	464	GLU	C-N-CA	5.01	126.11	119.84

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	77	0
1	a	2628	0	2524	66	0
2	B	3850	0	3718	61	0
2	b	3850	0	3718	61	0
3	C	3444	0	3365	77	0
3	c	3444	0	3365	76	0
4	D	2706	0	2608	60	0
4	d	2706	0	2608	66	0
5	E	666	0	651	11	0
5	e	666	0	651	13	0
6	F	282	0	291	6	0
6	f	282	0	291	4	0
7	H	507	0	521	14	0
7	h	507	0	521	15	0
8	I	286	0	308	3	0
8	i	286	0	308	3	0
9	J	249	0	262	8	0
9	j	249	0	262	7	0
10	K	293	0	305	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	11	0
11	L	304	0	316	4	0
11	l	304	0	316	5	0
12	M	267	0	289	6	0
12	m	267	0	289	6	0
13	O	1845	0	1801	26	0
13	o	1845	0	1801	27	0
14	T	275	0	288	5	0
14	t	275	0	288	5	0
15	U	774	0	773	8	0
15	u	774	0	773	8	0
16	V	1060	0	1068	8	0
16	v	1060	0	1068	8	0
17	g	201	0	226	6	0
17	y	201	0	226	7	0
18	X	270	0	299	9	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	9	0
20	z	479	0	516	10	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	28	0
22	B	975	0	1080	55	0
22	C	845	0	936	33	0
22	D	130	0	144	12	0
22	H	65	0	72	8	0
22	a	260	0	288	27	0
22	b	975	0	1080	46	0
22	c	845	0	936	34	0
22	d	130	0	144	12	0
22	h	65	0	72	11	0
23	A	45	0	61	3	0
23	D	55	0	80	7	0
23	J	35	0	45	0	0
23	a	45	0	61	3	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	12	0
24	C	120	0	168	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	40	0	56	3	0
24	H	40	0	56	2	0
24	J	40	0	56	2	0
24	a	40	0	56	3	0
24	b	160	0	224	10	0
24	c	120	0	168	16	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	1	0
24	y	40	0	56	8	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	2	0
25	a	56	0	70	3	0
25	b	110	0	136	6	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	2	0
26	a	39	0	51	1	0
26	c	37	0	44	2	0
27	A	93	0	126	3	0
27	B	98	0	136	5	0
27	C	93	0	126	4	0
27	D	94	0	128	7	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	1	0
27	a	93	0	126	4	0
27	b	98	0	136	4	0
27	c	93	0	126	4	0
27	d	94	0	128	8	0
27	e	44	0	58	1	0
27	i	43	0	56	1	0
27	m	42	0	54	1	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	47	0	61	3	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	9	0
30	b	47	0	61	1	0
30	d	43	0	50	3	0
30	f	45	0	54	2	0
31	B	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	1	0
31	M	70	0	92	0	0
31	b	140	0	184	6	0
31	d	31	0	35	0	0
31	i	35	0	46	1	0
32	D	128	0	148	12	0
32	a	64	0	74	5	0
32	d	64	0	74	7	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	5	0
34	f	43	0	30	4	0
34	v	43	0	30	5	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51374	984	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 (984) 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	1.56	0.87
3:c:39:ASN:HB2	22:c:507:CLA:HBA1	1.58	0.86
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.60	0.82
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.61	0.81
3:c:362:ARG:H	25:c:515:DGD:HE4	1.46	0.80
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:82:PRO:HG3	13:o:89:ALA:HB2	1.66	0.78
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.66	0.77
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.67	0.77
3:C:362:ARG:H	25:C:515:DGD:HE4	1.50	0.75
34:v:201:HEM:HBC2	34:v:201:HEM:HHD	1.68	0.73
22:b:609:CLA:H72	24:b:623:BCR:H311	1.71	0.73
4:d:199:MET:HG2	23:d:406:PL9:H322	1.70	0.73
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.71	0.72
22:B:605:CLA:H72	24:B:619:BCR:H311	1.71	0.72
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.71	0.72
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.72	0.71
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.71	0.71
4:D:199:MET:HG2	23:D:407:PL9:H322	1.73	0.71
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.73	0.71
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.56	0.70
10:k:21:LEU:HD13	17:g:24:MET:HE2	1.73	0.70
25:c:517:DGD:HAF2	22:c:520:CLA:H202	1.74	0.70
10:K:21:LEU:HD13	17:y:24:MET:HE2	1.73	0.70
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.74	0.69
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.74	0.69
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.74	0.69
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.74	0.69
1:a:192:ILE:HA	1:a:293:MET:HE1	1.73	0.69
4:d:21:TRP:O	4:d:26:ARG:NH2	2.26	0.69
1:a:129:ARG:HH21	4:d:256:ILE:HD12	1.57	0.69
2:b:24:LEU:HD21	22:b:619:CLA:HAB	1.73	0.69
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.74	0.68
22:C:506:CLA:H112	24:C:514:BCR:H362	1.75	0.68
17:y:35:ILE:HG22	20:Z:21:ILE:HG23	1.76	0.68
24:b:621:BCR:H19C	24:b:622:BCR:H363	1.77	0.67
3:c:165:LEU:HD21	22:c:505:CLA:HAB	1.74	0.67
13:o:69:LEU:HB3	13:o:107:ILE:HB	1.75	0.67
1:A:15:GLU:O	1:A:19:ASN:ND2	2.26	0.67
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.75	0.67
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.76	0.67
4:d:29:PHE:O	4:d:128:ARG:NH2	2.28	0.67
5:e:60:GLN:OE1	5:e:84:LYS:NZ	2.28	0.67
4:d:236:ASN:ND2	4:d:239:GLN:O	2.28	0.67
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.67
3:c:250:TRP:O	3:c:254:THR:OG1	2.12	0.67
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:63:ILE:HB	3:c:335:THR:HG21	1.75	0.67
22:c:507:CLA:HBC3	22:c:509:CLA:H92	1.76	0.67
1:A:192:ILE:HA	1:A:293:MET:HE1	1.75	0.66
4:d:152:VAL:HG21	4:d:279:LEU:HD12	1.75	0.66
16:v:102:MET:HE3	34:v:201:HEM:HBB2	1.77	0.66
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.66
4:D:29:PHE:O	4:D:128:ARG:NH2	2.29	0.66
22:b:611:CLA:H42	4:d:127:LEU:HD11	1.75	0.66
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.66
4:D:236:ASN:ND2	4:D:239:GLN:O	2.29	0.66
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.77	0.65
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.77	0.65
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.77	0.65
4:D:259:ILE:HG12	27:D:408:LMG:H292	1.78	0.65
1:A:63:ILE:HB	3:C:335:THR:HG21	1.79	0.65
4:d:259:ILE:HG12	27:d:407:LMG:H292	1.77	0.65
22:B:607:CLA:HBA2	30:D:403:SQD:H101	1.79	0.65
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.78	0.65
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
1:a:190:HIS:HB3	1:a:293:MET:HE2	1.77	0.65
12:m:31:SER:HA	27:m:101:LMG:HC1	1.79	0.65
3:C:250:TRP:O	3:C:254:THR:OG1	2.11	0.65
16:V:102:MET:HE3	34:V:201:HEM:HBB2	1.79	0.64
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.30	0.64
2:b:271:THR:HG22	2:b:273:TYR:H	1.62	0.64
1:a:174:LEU:HD22	32:d:401:PHO:H151	1.79	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.79	0.64
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.80	0.64
4:d:189:HIS:HA	4:d:294:ARG:HD2	1.79	0.64
1:A:174:LEU:HD22	32:D:401:PHO:H151	1.80	0.63
30:D:403:SQD:H171	30:D:403:SQD:H301	1.81	0.63
22:A:404:CLA:H142	22:D:405:CLA:H151	1.80	0.63
1:a:183:MET:HB3	22:a:404:CLA:HBC2	1.80	0.63
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.80	0.63
2:B:271:THR:HG22	2:B:273:TYR:H	1.64	0.63
3:c:291:TRP:O	3:c:305:THR:OG1	2.17	0.63
32:a:407:PHO:H151	22:d:404:CLA:H172	1.80	0.63
3:c:48:LYS:NZ	3:c:133:ALA:O	2.31	0.63
30:d:402:SQD:H301	30:d:402:SQD:H171	1.80	0.63
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.80	0.63
1:a:15:GLU:O	1:a:19:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:329:GLU:O	1:a:332:HIS:ND1	2.32	0.62
3:C:406:SER:O	3:C:418:ASN:ND2	2.33	0.62
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
3:C:297:TYR:O	3:C:423:ARG:NH2	2.32	0.62
13:o:77:LEU:HB3	13:o:91:PHE:HB3	1.80	0.62
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.82	0.62
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.65	0.62
22:a:404:CLA:HHC	22:a:404:CLA:HBB1	1.81	0.62
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.82	0.62
2:B:121:GLU:O	7:H:12:ARG:NH2	2.33	0.61
30:a:401:SQD:H311	24:a:410:BCR:H342	1.83	0.61
1:a:214:MET:HE2	1:a:214:MET:HA	1.83	0.61
2:b:149:LEU:HG	22:b:606:CLA:HBC1	1.83	0.61
3:c:150:ASP:HB3	3:c:153:ASP:HB2	1.83	0.61
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.83	0.61
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.81	0.61
2:B:327:THR:HG21	27:B:621:LMG:H111	1.83	0.60
4:D:186:GLN:HB2	22:D:405:CLA:HBC1	1.82	0.60
22:b:611:CLA:HBA2	30:d:402:SQD:H101	1.83	0.60
3:c:216:SER:HB3	3:c:221:GLU:HB2	1.83	0.60
12:M:28:GLN:HA	12:m:28:GLN:HA	1.84	0.60
22:a:404:CLA:H71	22:a:405:CLA:HAB	1.83	0.60
3:C:49:LEU:O	3:C:53:HIS:ND1	2.34	0.60
3:c:297:TYR:O	3:c:423:ARG:NH2	2.35	0.60
17:g:35:ILE:HG22	20:z:21:ILE:HG23	1.83	0.60
22:a:406:CLA:H142	22:d:404:CLA:H151	1.83	0.60
3:c:342:MET:HE3	3:c:352:GLY:HA2	1.83	0.60
12:M:31:SER:HA	27:M:101:LMG:HC1	1.83	0.60
1:a:221:SER:HB3	4:d:141:TYR:HB2	1.83	0.60
3:c:49:LEU:O	3:c:53:HIS:ND1	2.33	0.60
4:D:216:ALA:O	4:D:220:ASN:ND2	2.34	0.59
9:j:15:THR:HG21	10:k:38:VAL:HG13	1.84	0.59
22:B:615:CLA:H2	30:a:401:SQD:H61	1.84	0.59
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.85	0.59
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.68	0.59
3:c:406:SER:O	3:c:418:ASN:ND2	2.35	0.59
22:c:506:CLA:H112	24:c:514:BCR:H362	1.85	0.59
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.85	0.59
22:A:403:CLA:H203	32:D:401:PHO:H71	1.84	0.59
30:A:413:SQD:H172	26:C:519:LHG:H172	1.85	0.59
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:262:THR:OG1	22:b:606:CLA:O1D	2.20	0.59
4:d:186:GLN:HB2	22:d:404:CLA:HBC1	1.84	0.59
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.84	0.58
13:O:83:LYS:HG2	13:O:84:ASN:H	1.68	0.58
22:b:611:CLA:H151	22:b:612:CLA:H203	1.85	0.58
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.68	0.58
30:A:414:SQD:H61	22:b:619:CLA:H2	1.84	0.58
30:a:415:SQD:H172	26:c:519:LHG:H172	1.85	0.58
22:h:101:CLA:H2	22:h:101:CLA:HBD	1.86	0.58
34:v:201:HEM:HBB2	34:v:201:HEM:HMB1	1.85	0.58
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.85	0.58
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.85	0.58
2:b:121:GLU:O	7:h:12:ARG:NH2	2.35	0.58
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.33	0.58
12:m:25:LEU:O	12:m:28:GLN:HG3	2.04	0.58
22:a:404:CLA:H122	32:d:401:PHO:H3A	1.85	0.58
2:b:12:LEU:HB2	22:b:615:CLA:HMC2	1.86	0.58
22:b:606:CLA:H193	7:h:42:LEU:HD12	1.85	0.58
3:c:449:ARG:HE	22:c:504:CLA:HED1	1.68	0.58
22:c:503:CLA:H172	22:c:509:CLA:HBB2	1.85	0.58
1:A:329:GLU:O	1:A:332:HIS:ND1	2.35	0.58
3:c:284:PHE:HB3	25:c:515:DGD:HA51	1.86	0.58
4:d:214:HIS:ND1	23:d:406:PL9:O2	2.25	0.58
6:f:17:THR:HG23	6:f:20:TRP:H	1.69	0.58
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.85	0.57
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.69	0.57
20:z:33:TRP:HA	20:z:36:SER:HB3	1.87	0.57
4:D:192:THR:HG23	22:D:405:CLA:HBC2	1.86	0.57
1:a:64:ARG:O	13:o:178:ARG:NH2	2.36	0.57
13:o:230:VAL:HG13	13:o:237:ILE:HG22	1.86	0.57
4:D:24:ARG:NH2	18:X:44:ASP:O	2.37	0.57
3:c:215:LYS:HB3	3:c:223:TRP:HA	1.86	0.57
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.87	0.57
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.86	0.57
3:c:164:HIS:ND1	22:c:506:CLA:OBD	2.33	0.57
2:b:62:VAL:HG12	2:b:66:MET:HE2	1.87	0.57
27:d:407:LMG:HO4	27:d:407:LMG:HO5	1.52	0.57
27:D:408:LMG:O6	11:L:15:THR:HG21	2.05	0.57
1:A:214:MET:HA	1:A:214:MET:HE2	1.86	0.57
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.87	0.57
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:42:LEU:HD21	22:c:510:CLA:H2A	1.87	0.56
27:d:410:LMG:H171	24:f:102:BCR:H383	1.87	0.56
2:B:256:MET:O	2:B:448:ARG:NH1	2.34	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.23	0.56
27:d:407:LMG:O6	11:l:15:THR:HG21	2.05	0.56
13:o:83:LYS:HG2	13:o:84:ASN:H	1.69	0.56
1:A:64:ARG:O	13:O:178:ARG:NH2	2.39	0.56
2:b:25:MET:HE3	24:b:620:BCR:H23C	1.88	0.56
4:d:192:THR:HG23	22:d:404:CLA:HBC2	1.88	0.56
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
22:B:607:CLA:H151	22:B:608:CLA:H203	1.88	0.56
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.87	0.56
12:M:25:LEU:O	12:M:28:GLN:HG3	2.06	0.56
1:a:328:MET:HE1	4:d:183:LEU:HD22	1.87	0.56
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.87	0.56
3:C:118:HIS:CE1	27:C:518:LMG:H192	2.41	0.56
1:a:217:SER:HA	4:d:272:LEU:HD12	1.87	0.56
15:u:56:ASP:OD2	15:u:115:THR:OG1	2.21	0.56
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.35	0.55
32:D:402:PHO:H151	22:D:405:CLA:H172	1.88	0.55
27:a:413:LMG:H231	23:d:406:PL9:H352	1.88	0.55
3:c:229:ASN:HD22	3:c:231:GLU:HB2	1.71	0.55
22:c:508:CLA:HBD	22:c:508:CLA:H121	1.87	0.55
4:d:216:ALA:O	4:d:220:ASN:ND2	2.37	0.55
2:b:184:GLU:H	2:b:200:ALA:HB2	1.72	0.55
17:g:39:LEU:HD21	20:z:25:VAL:HA	1.88	0.55
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.87	0.55
22:b:618:CLA:H111	22:b:618:CLA:H172	1.88	0.55
4:d:222:LEU:HD23	4:d:244:TYR:HB3	1.88	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.55
22:D:406:CLA:H43	18:X:23:LEU:HA	1.89	0.55
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.89	0.55
30:d:402:SQD:H241	30:d:402:SQD:H111	1.89	0.55
22:A:404:CLA:H93	22:D:405:CLA:H152	1.89	0.55
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.88	0.55
2:b:487:SER:N	2:b:488:PRO:HD2	2.21	0.55
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.89	0.55
27:D:408:LMG:HO4	27:D:408:LMG:HO5	1.52	0.55
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.89	0.55
4:d:24:ARG:NH2	18:x:44:ASP:O	2.40	0.55
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:405:CLA:HED1	23:d:406:PL9:H372	1.87	0.55
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.88	0.55
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.89	0.55
22:a:405:CLA:H203	32:d:401:PHO:H71	1.89	0.55
22:b:606:CLA:C2D	22:b:608:CLA:H2	2.37	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.54
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.54
22:H:101:CLA:H2	22:H:101:CLA:HBD	1.88	0.54
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.89	0.54
25:b:601:DGD:HD1	31:b:603:LMT:H32	1.88	0.54
1:A:268:SER:O	1:A:272:HIS:ND1	2.37	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.54
1:a:153:SER:HB3	22:a:404:CLA:HED1	1.88	0.54
2:B:262:THR:HG22	2:B:263:THR:HG23	1.89	0.54
24:A:407:BCR:H321	30:A:414:SQD:H321	1.90	0.54
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.40	0.54
25:b:601:DGD:O1B	25:b:601:DGD:O2D	2.25	0.54
1:A:217:SER:HA	4:D:272:LEU:HD12	1.90	0.54
27:A:410:LMG:H231	23:D:407:PL9:H352	1.90	0.54
22:d:405:CLA:H42	18:x:26:GLY:HA3	1.90	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
2:b:458:PHE:HB3	22:b:607:CLA:HBC2	1.90	0.54
2:B:25:MET:HE3	24:B:616:BCR:H23C	1.88	0.54
30:B:626:SQD:H1	30:B:626:SQD:H462	1.89	0.54
22:b:612:CLA:HMD1	7:h:27:THR:HB	1.90	0.54
25:c:517:DGD:HA22	9:j:29:PHE:HE1	1.71	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.90	0.54
22:A:403:CLA:HMA2	23:D:407:PL9:H411	1.90	0.54
3:c:229:ASN:ND2	3:c:232:ASP:OD1	2.34	0.54
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.43	0.54
34:f:101:HEM:HBC2	34:f:101:HEM:HMC2	1.90	0.54
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.33	0.54
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.43	0.54
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.90	0.54
25:B:625:DGD:O1B	25:B:625:DGD:O2D	2.26	0.53
1:a:244:GLU:HG3	1:a:246:TYR:H	1.73	0.53
22:b:607:CLA:HBD	22:b:608:CLA:H43	1.90	0.53
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.89	0.53
1:a:65:GLU:OE2	1:a:334:ARG:NH2	2.40	0.53
2:b:155:ALA:O	2:b:159:THR:OG1	2.20	0.53
30:b:602:SQD:H1	30:b:602:SQD:H462	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:LEU:O	7:H:15:ASN:ND2	2.38	0.53
22:c:507:CLA:H172	25:c:516:DGD:HBW2	1.89	0.53
20:z:33:TRP:O	20:z:37:LYS:HB2	2.08	0.53
7:h:55:LEU:HB2	7:h:58:VAL:HG12	1.90	0.53
22:A:402:CLA:H122	32:D:401:PHO:H3A	1.90	0.53
24:A:407:BCR:H342	30:A:414:SQD:H311	1.91	0.53
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.90	0.53
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.91	0.53
1:a:85:SER:HA	1:a:109:GLY:HA3	1.90	0.53
30:A:413:SQD:H311	22:C:507:CLA:H71	1.91	0.53
2:B:155:ALA:O	2:B:159:THR:OG1	2.22	0.53
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.39	0.53
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.90	0.53
1:a:29:TYR:O	1:a:129:ARG:NH1	2.42	0.53
4:d:302:GLU:OE1	13:o:186:LYS:NZ	2.41	0.53
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.53
30:f:103:SQD:H131	18:x:36:VAL:HG11	1.90	0.53
13:o:180:ALA:HB1	13:o:191:ALA:HB2	1.91	0.53
22:D:406:CLA:H42	18:X:26:GLY:HA3	1.91	0.53
4:D:214:HIS:ND1	23:D:407:PL9:O2	2.29	0.53
15:u:72:TYR:HB3	15:u:73:PRO:HD3	1.91	0.53
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.91	0.52
1:A:244:GLU:HG3	1:A:246:TYR:H	1.73	0.52
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.90	0.52
26:C:519:LHG:H271	26:C:519:LHG:H101	1.89	0.52
2:b:262:THR:HG22	2:b:263:THR:HG23	1.89	0.52
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.92	0.52
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.90	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.92	0.52
2:b:474:LEU:O	4:d:134:ARG:NH1	2.43	0.52
22:b:606:CLA:C3D	22:b:608:CLA:H2	2.39	0.52
3:c:305:THR:HG22	3:c:308:GLU:HB2	1.92	0.52
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.91	0.52
1:a:121:LEU:HD13	25:a:411:DGD:HB92	1.92	0.52
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.91	0.52
3:c:85:GLY:N	25:c:516:DGD:HE4	2.24	0.52
22:c:501:CLA:C2D	22:c:503:CLA:H2	2.39	0.52
30:a:415:SQD:H223	25:c:517:DGD:HAE1	1.92	0.52
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.92	0.52
1:a:183:MET:HE1	22:a:405:CLA:HMD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:327:THR:HG21	27:b:625:LMG:H111	1.92	0.52
22:b:608:CLA:H202	22:b:612:CLA:HBB2	1.92	0.52
3:c:29:GLU:HB3	10:k:46:ARG:HH11	1.74	0.52
22:B:605:CLA:OBD	31:B:622:LMT:O6'	2.21	0.51
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.34	0.51
22:b:614:CLA:H41	22:b:617:CLA:HBC3	1.91	0.51
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.75	0.51
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.92	0.51
2:b:270:PRO:HG3	2:b:312:TYR:HD2	1.75	0.51
5:e:10:PHE:N	27:e:101:LMG:O3	2.42	0.51
1:A:211:PHE:HA	1:A:214:MET:HB2	1.91	0.51
30:A:413:SQD:H223	25:C:517:DGD:HAE1	1.91	0.51
4:d:275:PRO:O	4:d:279:LEU:HD23	2.10	0.51
3:C:85:GLY:N	25:C:516:DGD:HE4	2.25	0.51
1:A:132:GLU:O	1:A:136:ARG:HG2	2.10	0.51
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.74	0.51
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.44	0.51
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.92	0.51
13:O:73:PRO:HG2	13:O:102:THR:HB	1.92	0.51
17:y:39:LEU:HD21	20:Z:25:VAL:HA	1.92	0.51
18:x:12:ILE:HG12	18:x:16:LEU:HD12	1.92	0.51
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.93	0.51
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.51
34:F:101:HEM:HBC2	34:F:101:HEM:HMC2	1.92	0.51
1:a:212:CYS:HB2	4:d:211:CYS:HB2	1.93	0.51
1:a:268:SER:O	1:a:272:HIS:ND1	2.39	0.51
2:b:341:LYS:HA	2:b:405:GLU:HB2	1.93	0.50
2:b:150:CYS:HA	22:b:606:CLA:HBC2	1.92	0.50
3:c:209:ILE:HG23	24:c:514:BCR:H382	1.92	0.50
30:f:103:SQD:H162	18:x:33:THR:HA	1.93	0.50
16:v:81:ARG:CZ	16:v:157:GLY:HA3	2.42	0.50
22:c:504:CLA:HBA1	22:c:504:CLA:HBD	1.94	0.50
22:C:504:CLA:HBA1	22:C:504:CLA:HBD	1.93	0.50
2:b:4:PRO:HD2	2:b:7:ARG:HD2	1.92	0.50
3:c:305:THR:HG23	3:c:307:PRO:HD2	1.92	0.50
22:A:403:CLA:HED1	23:D:407:PL9:H372	1.93	0.50
24:D:411:BCR:H383	27:D:412:LMG:H171	1.92	0.50
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.24	0.50
1:a:132:GLU:O	1:a:136:ARG:HG2	2.11	0.50
22:b:610:CLA:HBB1	27:b:625:LMG:H341	1.93	0.50
3:c:75:PHE:HD1	3:c:86:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:45:ILE:HD11	22:h:101:CLA:H42	1.94	0.50
9:j:14:ALA:O	9:j:18:GLY:N	2.42	0.50
17:g:24:MET:O	17:g:28:ILE:HG23	2.12	0.50
27:d:407:LMG:H111	11:l:19:LEU:HD21	1.93	0.50
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.47	0.50
8:I:4:LEU:HD22	31:b:603:LMT:H62	1.94	0.50
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.46	0.50
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.93	0.50
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.93	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.46	0.50
3:c:405:ASN:HB2	25:c:517:DGD:HG31	1.93	0.50
22:A:403:CLA:CHA	22:A:403:CLA:HBA1	2.42	0.50
2:b:383:PHE:CZ	13:o:193:GLY:HA2	2.47	0.50
22:b:617:CLA:H51	24:b:620:BCR:H372	1.93	0.50
25:c:517:DGD:HA22	9:j:29:PHE:CE1	2.47	0.50
26:c:519:LHG:H101	26:c:519:LHG:H271	1.94	0.50
5:e:57:ALA:HB3	5:e:60:GLN:HB3	1.94	0.50
13:o:168:PHE:HB2	13:o:225:LEU:HB2	1.92	0.50
2:B:271:THR:HB	2:B:274:GLN:HG3	1.94	0.49
30:a:415:SQD:H311	22:c:507:CLA:H71	1.94	0.49
22:C:510:CLA:HMB1	24:C:513:BCR:H382	1.94	0.49
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.94	0.49
22:a:405:CLA:H42	23:d:406:PL9:H162	1.95	0.49
4:d:102:THR:OG1	25:d:408:DGD:HD62	2.11	0.49
22:A:404:CLA:H161	23:A:406:PL9:H253	1.93	0.49
4:d:43:LEU:HD23	4:d:117:HIS:CE1	2.46	0.49
5:e:15:THR:HG23	9:j:8:ILE:O	2.12	0.49
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.28	0.49
2:b:135:LEU:HA	2:b:138:MET:HE3	1.94	0.49
27:A:415:LMG:H112	2:b:43:ALA:HA	1.95	0.49
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.47	0.49
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.94	0.49
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.93	0.49
22:a:406:CLA:HAB	22:d:404:CLA:H72	1.94	0.49
22:c:501:CLA:H193	22:c:506:CLA:H111	1.94	0.49
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.76	0.49
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.94	0.49
30:D:403:SQD:H241	30:D:403:SQD:H111	1.95	0.49
30:a:401:SQD:H321	24:a:410:BCR:H321	1.94	0.49
15:u:54:LYS:HD2	15:u:113:THR:HG23	1.94	0.49
1:A:183:MET:HE1	22:A:403:CLA:HMD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.94	0.49
17:y:24:MET:O	17:y:28:ILE:HG23	2.13	0.49
22:b:611:CLA:H51	22:b:612:CLA:H101	1.95	0.49
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.95	0.49
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.95	0.49
22:b:609:CLA:OBD	31:b:626:LMT:O6'	2.23	0.49
25:b:624:DGD:HAW2	22:h:101:CLA:H152	1.94	0.49
22:a:405:CLA:HMA2	23:d:406:PL9:H411	1.95	0.49
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.94	0.49
2:B:135:LEU:HA	2:B:138:MET:HE3	1.95	0.49
22:B:612:CLA:H51	27:B:624:LMG:H231	1.95	0.49
10:K:26:PRO:O	10:K:29:PRO:HD2	2.12	0.49
1:a:57:PRO:HG3	1:a:68:SER:HB3	1.95	0.49
1:A:85:SER:HA	1:A:109:GLY:HA3	1.95	0.48
32:a:407:PHO:HBC3	4:d:279:LEU:HG	1.95	0.48
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.94	0.48
13:O:154:SER:N	13:O:169:LYS:O	2.45	0.48
15:u:75:LEU:HD21	15:u:101:GLN:HB3	1.94	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
1:a:211:PHE:HA	1:a:214:MET:HB2	1.94	0.48
4:d:221:THR:HG23	4:d:244:TYR:HB2	1.95	0.48
13:o:118:SER:HB3	13:o:157:PRO:HA	1.95	0.48
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.95	0.48
1:a:227:THR:HG21	1:a:233:ALA:HA	1.95	0.48
22:a:405:CLA:CHA	22:a:405:CLA:HBA1	2.42	0.48
2:b:271:THR:HB	2:b:274:GLN:HG3	1.95	0.48
10:k:12:PRO:HB2	10:k:15:TYR:HD2	1.77	0.48
31:B:627:LMT:H62	8:i:4:LEU:HD22	1.94	0.48
3:c:197:ARG:NH2	3:c:231:GLU:OE2	2.47	0.48
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.96	0.48
15:u:68:TYR:HB2	15:u:71:LEU:HD12	1.94	0.48
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.46	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.95	0.48
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.43	0.48
3:c:131:TYR:HE1	3:c:135:ARG:HD2	1.78	0.48
10:k:26:PRO:O	10:k:29:PRO:HD2	2.14	0.48
1:A:210:LEU:HG	32:D:402:PHO:NC	2.29	0.48
1:a:12:ASN:HB3	1:a:15:GLU:HB3	1.94	0.48
2:b:306:PRO:HG2	2:b:309:LEU:HB2	1.94	0.48
22:A:405:CLA:H162	22:A:405:CLA:H141	1.69	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:PRO:HG3	7:H:27:THR:H	1.79	0.48
13:o:223:ILE:HG13	13:o:243:SER:HB3	1.96	0.48
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.95	0.48
1:A:258:LEU:O	4:D:128:ARG:NH1	2.47	0.48
2:B:383:PHE:N	4:D:344:GLU:O	2.34	0.48
1:a:190:HIS:O	1:a:298:ASN:HB3	2.14	0.48
3:c:130:VAL:O	3:c:134:ILE:HG12	2.14	0.48
24:c:513:BCR:H391	10:k:36:ALA:HB2	1.95	0.48
13:o:73:PRO:HG2	13:o:102:THR:HB	1.95	0.48
2:B:327:THR:HG22	22:B:606:CLA:H12	1.96	0.48
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.96	0.48
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.96	0.48
22:a:404:CLA:HBA1	22:a:404:CLA:H3A	1.52	0.48
4:D:275:PRO:O	4:D:279:LEU:HD23	2.13	0.47
1:a:232:SER:OG	27:a:413:LMG:O3	2.25	0.47
4:d:262:SER:N	27:d:407:LMG:O3	2.43	0.47
22:d:405:CLA:H43	18:x:23:LEU:HA	1.96	0.47
22:B:611:CLA:H171	22:B:612:CLA:HBB2	1.95	0.47
31:B:628:LMT:H122	14:t:7:VAL:HG12	1.95	0.47
4:D:279:LEU:HG	32:D:402:PHO:HBC3	1.96	0.47
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.47
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.44	0.47
2:b:122:LEU:O	7:h:15:ASN:ND2	2.45	0.47
2:b:247:PHE:HE1	22:h:101:CLA:H101	1.78	0.47
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.78	0.47
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.47
4:d:17:ILE:HG21	18:x:42:GLN:HG3	1.97	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.47
22:B:615:CLA:H12	22:B:615:CLA:H72	1.96	0.47
4:d:85:MET:HA	5:e:69:ARG:HB3	1.96	0.47
1:a:78:ILE:O	1:a:176:ILE:HB	2.14	0.47
2:b:25:MET:HG2	24:b:620:BCR:H23C	1.97	0.47
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.45	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.78	0.47
22:B:612:CLA:H171	27:B:624:LMG:H401	1.97	0.47
22:B:614:CLA:H172	22:B:614:CLA:H111	1.97	0.47
32:D:401:PHO:H62	32:D:401:PHO:H41	1.46	0.47
2:b:450:TRP:NE1	22:b:610:CLA:HBA1	2.29	0.47
22:b:606:CLA:H2	22:b:608:CLA:H93	1.97	0.47
24:c:513:BCR:H11C	24:g:101:BCR:H322	1.97	0.47
1:a:317:TRP:CZ3	4:d:180:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:611:CLA:H18	22:b:612:CLA:H192	1.96	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.41	0.47
1:A:298:ASN:ND2	3:C:402:GLY:O	2.48	0.47
24:B:619:BCR:H20C	24:B:619:BCR:H361	1.77	0.47
30:F:102:SQD:H162	18:X:33:THR:HA	1.96	0.47
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.97	0.47
1:a:156:ALA:HA	1:a:160:ILE:HB	1.97	0.47
27:i:101:LMG:H181	31:i:102:LMT:H42	1.96	0.47
18:x:11:THR:HG23	18:x:12:ILE:HG22	1.96	0.47
25:B:625:DGD:HD1	31:B:627:LMT:H32	1.97	0.47
3:C:223:TRP:CG	3:C:224:ILE:H	2.32	0.47
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.80	0.47
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.47
22:c:506:CLA:H92	22:c:506:CLA:H62	1.76	0.47
1:A:78:ILE:O	1:A:176:ILE:HB	2.15	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
1:a:224:ILE:O	4:d:265:ARG:NH2	2.47	0.46
2:b:170:ASP:OD1	2:b:175:THR:N	2.44	0.46
2:b:222:PRO:HG3	7:h:27:THR:H	1.80	0.46
13:o:230:VAL:HG12	13:o:231:ASP:H	1.80	0.46
1:A:121:LEU:HD13	25:A:408:DGD:HB92	1.97	0.46
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.81	0.46
3:c:166:ILE:O	3:c:170:ILE:HG13	2.15	0.46
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.97	0.46
3:c:343:ARG:NH1	3:c:347:GLY:O	2.48	0.46
3:c:361:PHE:HD1	25:c:515:DGD:HE61	1.80	0.46
2:B:474:LEU:O	4:D:134:ARG:NH1	2.48	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.98	0.46
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.98	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.96	0.46
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.96	0.46
3:c:315:MET:HE1	3:c:369:LEU:HD12	1.97	0.46
5:e:18:ARG:NH1	34:f:101:HEM:O1A	2.48	0.46
1:A:190:HIS:O	1:A:298:ASN:HB3	2.15	0.46
2:B:371:THR:HG22	2:B:377:VAL:HA	1.97	0.46
22:B:613:CLA:H51	24:B:616:BCR:H372	1.97	0.46
1:a:210:LEU:HG	32:a:407:PHO:NC	2.31	0.46
3:c:461:ARG:NH1	4:d:241:GLU:OE1	2.46	0.46
22:c:512:CLA:HAB	24:c:521:BCR:H24C	1.97	0.46
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.47	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.96	0.46
30:F:102:SQD:H131	18:X:36:VAL:HG11	1.98	0.46
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.98	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.49	0.46
27:D:408:LMG:H111	11:L:19:LEU:HD21	1.97	0.46
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.97	0.46
2:b:315:ILE:HG22	2:b:426:PHE:HB3	1.98	0.46
3:c:158:THR:O	3:c:251:HIS:HB3	2.16	0.46
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.96	0.46
13:o:144:LEU:HD13	13:o:259:VAL:HG11	1.97	0.46
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.97	0.46
2:b:327:THR:HG22	22:b:610:CLA:H12	1.98	0.46
25:b:624:DGD:HA71	22:h:101:CLA:H193	1.97	0.46
3:c:386:PRO:HB3	16:v:116:GLU:HG2	1.97	0.46
22:a:405:CLA:H41	22:a:405:CLA:H62	1.78	0.46
3:c:113:VAL:HG11	27:c:518:LMG:H132	1.97	0.46
13:o:240:THR:HG22	13:o:264:VAL:HG12	1.98	0.46
24:x:101:BCR:H20C	24:x:101:BCR:H361	1.78	0.46
20:z:29:SER:HA	20:z:30:PRO:HD3	1.82	0.46
1:A:114:LEU:O	1:A:118:HIS:ND1	2.45	0.45
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.98	0.45
1:a:159:LEU:C	1:a:162:PRO:HD2	2.41	0.45
2:B:43:ALA:HA	27:a:402:LMG:H112	1.97	0.45
25:B:620:DGD:HAW2	22:H:101:CLA:H152	1.99	0.45
3:C:158:THR:O	3:C:251:HIS:HB3	2.15	0.45
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.98	0.45
22:C:510:CLA:H93	22:C:510:CLA:H61	1.82	0.45
2:b:247:PHE:HB2	22:b:611:CLA:HBC1	1.97	0.45
4:d:348:ARG:NH2	4:d:352:LEU:O	2.37	0.45
5:e:23:HIS:NE2	34:f:101:HEM:ND	2.64	0.45
7:h:45:ILE:HD12	22:h:101:CLA:HAA2	1.98	0.45
22:h:101:CLA:H162	22:h:101:CLA:H122	1.53	0.45
20:z:32:ASP:CG	20:z:33:TRP:H	2.24	0.45
24:B:616:BCR:H20C	24:B:616:BCR:H361	1.76	0.45
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.45
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.74	0.45
22:b:619:CLA:H72	22:b:619:CLA:H12	1.98	0.45
22:c:508:CLA:H11	22:c:508:CLA:H51	1.81	0.45
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.99	0.45
1:a:193:LEU:HD11	22:a:404:CLA:HMC2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:223:TRP:CD2	3:c:224:ILE:HG13	2.51	0.45
22:c:504:CLA:H11	24:c:514:BCR:H312	1.99	0.45
4:D:48:TRP:CE2	32:D:402:PHO:H161	2.52	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.15	0.45
24:y:101:BCR:H20C	24:y:101:BCR:H361	1.82	0.45
22:A:402:CLA:H3A	22:A:402:CLA:HBA1	1.53	0.45
4:D:146:PHE:C	4:D:149:PRO:HD2	2.42	0.45
3:c:223:TRP:CG	3:c:224:ILE:H	2.32	0.45
10:k:40:GLN:HA	10:k:43:VAL:HG12	1.98	0.45
22:A:402:CLA:H51	32:D:401:PHO:C3B	2.47	0.45
27:B:621:LMG:H421	4:D:284:ILE:HD13	1.99	0.45
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.65	0.45
24:b:620:BCR:H333	12:m:13:LEU:HD12	1.97	0.45
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.98	0.45
27:d:407:LMG:O9	27:d:407:LMG:HC1	2.17	0.45
9:j:38:SER:OG	9:j:39:SER:N	2.48	0.45
16:v:102:MET:HE3	34:v:201:HEM:HMB1	1.99	0.45
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.99	0.45
22:C:509:CLA:H2	22:C:509:CLA:H61	1.72	0.45
1:a:140:ARG:NH2	26:a:412:LHG:O5	2.36	0.45
3:c:86:LEU:HB3	3:c:90:PRO:HD3	1.98	0.45
15:u:117:VAL:HG13	15:u:122:VAL:HG21	1.98	0.45
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.45
24:C:514:BCR:H20C	24:C:514:BCR:H361	1.84	0.45
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.80	0.45
16:V:102:MET:HE3	34:V:201:HEM:HMB1	1.98	0.45
27:a:413:LMG:O5	11:l:13:ASN:ND2	2.50	0.45
2:b:18:ARG:HD3	2:b:118:TRP:HB3	1.98	0.45
24:b:622:BCR:H24C	24:b:622:BCR:H371	1.81	0.45
4:d:43:LEU:HD23	4:d:117:HIS:HE1	1.82	0.45
7:h:46:LEU:HD13	22:h:101:CLA:H72	1.98	0.45
16:v:160:LYS:HA	16:v:163:TYR:CD2	2.52	0.45
24:B:618:BCR:H20C	24:B:618:BCR:H361	1.82	0.45
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.82	0.45
3:C:224:ILE:O	3:C:227:VAL:HG23	2.17	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.49	0.45
24:a:410:BCR:H24C	24:a:410:BCR:H371	1.82	0.45
2:b:277:SER:OG	25:b:624:DGD:O5E	2.33	0.45
2:b:326:ARG:HB3	2:b:444:ARG:HG2	1.99	0.45
3:c:137:PRO:HB2	3:c:139:THR:O	2.17	0.45
4:d:56:THR:HG21	5:e:50:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:29:ALA:HA	8:i:35:LYS:HB2	1.99	0.45
30:A:414:SQD:H332	22:b:609:CLA:H203	1.99	0.44
3:C:315:MET:HE1	3:C:369:LEU:HD12	1.98	0.44
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.52	0.44
4:D:102:THR:OG1	25:D:409:DGD:HD62	2.17	0.44
14:T:7:VAL:HG12	31:b:604:LMT:H122	1.98	0.44
13:o:184:ASP:OD2	13:o:188:ARG:HB2	2.17	0.44
17:g:32:GLY:O	17:g:35:ILE:HG12	2.17	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.17	0.44
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.99	0.44
22:B:605:CLA:H18	22:B:615:CLA:H121	1.99	0.44
22:B:611:CLA:H122	22:B:611:CLA:H162	1.76	0.44
10:K:37:PHE:HB3	24:y:101:BCR:C40	2.47	0.44
20:Z:33:TRP:O	20:Z:33:TRP:CD1	2.70	0.44
2:b:213:GLY:O	2:b:217:ILE:HG13	2.17	0.44
3:c:318:LEU:HG	3:c:328:VAL:HG11	1.99	0.44
3:c:337:LEU:HA	13:o:131:PRO:HG3	1.99	0.44
5:e:60:GLN:HG2	5:e:62:SER:H	1.82	0.44
22:h:101:CLA:H41	22:h:101:CLA:H62	1.56	0.44
22:B:604:CLA:H62	22:B:604:CLA:H41	1.80	0.44
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.44
24:y:101:BCR:H323	24:y:101:BCR:HC31	1.64	0.44
2:b:5:TRP:HZ3	22:b:614:CLA:H51	1.82	0.44
2:b:135:LEU:HD22	2:b:237:VAL:HG21	1.98	0.44
2:b:256:MET:HA	2:b:263:THR:HG21	1.99	0.44
4:d:244:TYR:OH	4:d:264:LYS:HE3	2.18	0.44
2:B:213:GLY:O	2:B:217:ILE:HG13	2.17	0.44
22:C:512:CLA:H3A	22:C:512:CLA:HBA2	1.72	0.44
32:a:407:PHO:H161	4:d:48:TRP:CE2	2.52	0.44
3:c:80:PRO:HB3	3:c:82:TYR:CE1	2.51	0.44
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.50	0.44
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.00	0.44
3:C:137:PRO:HB2	3:C:139:THR:O	2.17	0.44
2:b:96:VAL:HG22	22:b:609:CLA:HBA1	1.99	0.44
3:c:347:GLY:HA3	13:o:43:ASN:HB2	1.99	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	1.99	0.44
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.53	0.44
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.89	0.44
24:C:513:BCR:H11C	24:y:101:BCR:H322	2.00	0.44
13:O:118:SER:HB3	13:O:157:PRO:HA	2.00	0.44
22:b:608:CLA:H62	22:b:608:CLA:H41	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:512:CLA:HAB	24:c:521:BCR:H371	1.99	0.44
24:g:101:BCR:HC32	20:z:13:VAL:HG13	2.00	0.44
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.82	0.44
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.53	0.44
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.86	0.44
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.48	0.44
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.44
24:C:513:BCR:H353	24:y:101:BCR:H321	1.99	0.44
1:a:214:MET:HE1	4:d:142:ASN:HD21	1.81	0.44
1:a:317:TRP:HZ3	4:d:180:ARG:HD3	1.83	0.44
24:b:623:BCR:H15C	24:b:623:BCR:H351	1.88	0.44
3:C:130:VAL:O	3:C:134:ILE:HG12	2.18	0.44
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.99	0.44
1:a:271:LEU:HD11	23:a:409:PL9:C4	2.48	0.44
22:a:406:CLA:H93	22:d:404:CLA:H152	1.99	0.44
2:b:26:HIS:CE1	22:b:615:CLA:HMA2	2.52	0.44
2:b:30:VAL:HG12	22:b:608:CLA:HHD	2.00	0.44
24:c:513:BCR:H343	24:c:513:BCR:H311	2.00	0.44
24:j:102:BCR:H15C	24:j:102:BCR:H351	1.77	0.44
1:A:141:PRO:HB2	1:A:142:TRP:H	1.66	0.44
26:A:409:LHG:H382	22:C:509:CLA:H93	2.00	0.44
22:B:607:CLA:H51	22:B:608:CLA:H101	1.99	0.44
4:D:262:SER:N	27:D:408:LMG:O3	2.46	0.44
22:b:615:CLA:H171	22:b:616:CLA:HBB2	1.99	0.44
3:c:245:ILE:O	3:c:249:ILE:HG12	2.18	0.44
3:c:346:THR:HG21	13:o:38:GLY:HA2	1.98	0.44
5:e:27:ILE:HB	5:e:28:PRO:HD3	2.00	0.44
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.00	0.44
22:B:605:CLA:H3A	22:B:605:CLA:HBA2	1.27	0.43
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.43
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.43
1:a:157:VAL:HG13	1:a:172:MET:HB3	2.00	0.43
24:c:513:BCR:H371	24:c:513:BCR:H24C	1.81	0.43
24:B:616:BCR:H383	30:B:626:SQD:H111	1.99	0.43
3:C:456:GLU:OE1	3:C:456:GLU:N	2.51	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.53	0.43
7:H:46:LEU:HD13	22:H:101:CLA:H72	2.00	0.43
22:c:520:CLA:H142	22:c:520:CLA:H112	1.77	0.43
20:z:33:TRP:O	20:z:33:TRP:CD1	2.71	0.43
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.43
27:D:408:LMG:HC1	27:D:408:LMG:O9	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.43
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.43
22:a:406:CLA:HAB	22:d:404:CLA:H42	2.00	0.43
3:c:29:GLU:HB2	3:c:30:SER:H	1.65	0.43
3:c:90:PRO:O	3:c:94:THR:HG23	2.18	0.43
25:B:620:DGD:HA71	22:H:101:CLA:H193	2.01	0.43
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.27	0.43
4:d:84:SER:HB2	4:d:85:MET:HE2	2.01	0.43
13:o:143:PRO:HG2	13:o:248:ASP:HB3	1.99	0.43
1:A:193:LEU:HD11	22:A:402:CLA:HMC2	2.01	0.43
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.54	0.43
2:B:329:PRO:HB3	22:B:606:CLA:HED1	2.01	0.43
32:D:401:PHO:H13	32:D:401:PHO:H102	1.82	0.43
6:F:22:ALA:O	6:F:25:THR:OG1	2.34	0.43
7:H:12:ARG:O	7:H:12:ARG:HD3	2.18	0.43
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.01	0.43
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.43
22:b:613:CLA:H12	22:b:613:CLA:H51	1.89	0.43
3:c:456:GLU:HG2	3:c:457:LYS:HG3	2.01	0.43
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.84	0.43
22:A:403:CLA:H51	22:A:403:CLA:H11	1.81	0.43
2:B:108:PHE:HB2	30:B:626:SQD:H223	2.00	0.43
22:B:607:CLA:H18	22:B:608:CLA:H192	2.01	0.43
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.01	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.43
23:a:409:PL9:H371	23:a:409:PL9:H351	1.83	0.43
22:b:619:CLA:H111	22:b:619:CLA:H143	1.73	0.43
3:c:466:VAL:HG13	4:d:251:ARG:HD2	2.00	0.43
25:c:516:DGD:HA91	25:c:516:DGD:HAW2	1.74	0.43
1:A:240:GLY:HA3	14:T:29:ILE:HG22	2.00	0.43
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.83	0.43
24:H:102:BCR:H20C	24:H:102:BCR:H361	1.79	0.43
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.54	0.43
1:A:159:LEU:C	1:A:162:PRO:HD2	2.43	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.53	0.43
1:a:111:PRO:O	1:a:115:ILE:HG13	2.18	0.43
22:b:606:CLA:H61	22:b:606:CLA:H41	1.63	0.43
24:c:513:BCR:H361	24:c:513:BCR:H20C	1.79	0.43
4:d:252:PHE:O	4:d:256:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:O	1:A:129:ARG:NH1	2.52	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.93	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.43
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.00	0.43
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.19	0.43
22:H:101:CLA:H41	22:H:101:CLA:H62	1.56	0.43
1:a:28:LEU:HB2	30:a:401:SQD:H91	2.01	0.43
24:c:521:BCR:H20C	24:c:521:BCR:H361	1.81	0.43
4:d:53:THR:HG22	4:d:67:TYR:CD2	2.52	0.43
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.43
22:B:613:CLA:H91	22:B:613:CLA:H112	1.85	0.43
31:B:628:LMT:H1B	31:B:628:LMT:H3'	1.53	0.43
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.01	0.43
24:C:521:BCR:H24C	24:C:521:BCR:H371	1.82	0.43
32:D:402:PHO:CHB	22:D:405:CLA:H101	2.49	0.43
15:U:72:TYR:O	15:U:76:ALA:HB3	2.18	0.43
17:y:25:ILE:O	17:y:29:GLY:N	2.51	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.42
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.42
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.01	0.42
1:a:27:ARG:NH1	4:d:254:SER:O	2.48	0.42
22:a:405:CLA:H51	22:a:405:CLA:H11	1.82	0.42
22:a:406:CLA:H143	22:a:406:CLA:H161	1.88	0.42
2:b:371:THR:HG22	2:b:377:VAL:HA	2.00	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	1.80	0.42
13:o:81:GLU:HA	13:o:82:PRO:HD3	1.79	0.42
15:u:72:TYR:O	15:u:76:ALA:HB3	2.19	0.42
16:v:98:LEU:O	16:v:102:MET:HG3	2.20	0.42
24:g:101:BCR:H20C	24:g:101:BCR:H361	1.80	0.42
1:A:183:MET:HA	22:A:402:CLA:HMD2	2.01	0.42
22:A:403:CLA:H162	22:A:403:CLA:H202	1.76	0.42
22:B:605:CLA:H203	30:a:401:SQD:H332	2.01	0.42
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.78	0.42
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.01	0.42
5:E:81:GLU:C	5:E:83:LEU:H	2.27	0.42
32:a:407:PHO:CHB	22:d:404:CLA:H101	2.49	0.42
22:c:510:CLA:H121	24:c:513:BCR:H21C	2.00	0.42
22:c:510:CLA:H141	20:z:20:VAL:HG13	2.02	0.42
27:c:522:LMG:H322	10:k:27:VAL:HG23	2.01	0.42
4:d:201:VAL:HB	22:d:404:CLA:HMB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:12:ARG:O	7:h:12:ARG:HD3	2.19	0.42
9:j:9:PRO:HB2	9:j:12:ILE:HG13	2.00	0.42
22:D:405:CLA:H92	22:D:405:CLA:H62	1.80	0.42
24:y:101:BCR:H15C	24:y:101:BCR:H351	1.90	0.42
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.01	0.42
1:a:182:PHE:O	1:a:186:PHE:HB2	2.19	0.42
3:c:425:TRP:CE2	22:c:520:CLA:HBA1	2.54	0.42
3:c:473:ASP:HB2	14:t:26:PRO:HB3	2.00	0.42
22:c:512:CLA:H3A	22:c:512:CLA:HBA2	1.73	0.42
32:d:401:PHO:H13	32:d:401:PHO:H102	1.87	0.42
1:A:141:PRO:HG3	3:C:446:GLY:C	2.44	0.42
22:A:404:CLA:H161	22:A:404:CLA:H143	1.85	0.42
22:B:608:CLA:H11	7:H:35:MET:HE1	2.00	0.42
24:B:616:BCR:H15C	24:B:616:BCR:H351	1.85	0.42
22:C:512:CLA:HAB	24:C:521:BCR:H371	2.02	0.42
4:d:113:PHE:O	4:d:117:HIS:HB2	2.19	0.42
1:A:156:ALA:HA	1:A:160:ILE:HB	2.00	0.42
2:B:25:MET:HG2	24:B:616:BCR:H23C	2.00	0.42
22:B:605:CLA:C3D	31:B:622:LMT:H11	2.50	0.42
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.01	0.42
3:C:402:GLY:HA3	3:C:420:VAL:HG22	2.01	0.42
22:C:511:CLA:H13	22:C:511:CLA:H61	2.01	0.42
22:C:520:CLA:H112	22:C:520:CLA:H142	1.76	0.42
32:D:401:PHO:H202	32:D:401:PHO:H162	1.86	0.42
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.42
25:a:411:DGD:HA32	3:c:217:PRO:HD3	2.00	0.42
22:b:610:CLA:H193	11:l:27:LEU:HD11	2.02	0.42
22:b:616:CLA:H171	27:b:628:LMG:H401	2.00	0.42
24:b:620:BCR:H24C	24:b:620:BCR:H371	1.88	0.42
4:d:55:VAL:HG21	4:d:110:LEU:HD12	2.02	0.42
15:u:106:ARG:HA	15:u:109:LEU:HG	2.01	0.42
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.54	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.00	0.42
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.19	0.42
1:a:257:ARG:HH22	2:b:488:PRO:C	2.28	0.42
2:b:16:PRO:HB2	2:b:123:PHE:CG	2.54	0.42
22:b:609:CLA:H3A	22:b:609:CLA:HBA2	1.25	0.42
27:c:518:LMG:H292	27:c:518:LMG:H111	2.01	0.42
22:c:520:CLA:H141	22:c:520:CLA:H161	1.81	0.42
22:c:520:CLA:O2D	27:c:522:LMG:O2	2.37	0.42
2:B:26:HIS:CE1	22:B:611:CLA:HMA2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.92	0.42
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.02	0.42
22:C:501:CLA:H141	22:C:501:CLA:H162	1.78	0.42
25:D:409:DGD:O5E	25:D:409:DGD:O4E	2.25	0.42
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.77	0.42
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.20	0.42
22:a:405:CLA:H202	22:a:405:CLA:H162	1.75	0.42
3:c:205:ASP:HA	3:c:206:PRO:HD2	1.93	0.42
1:A:238:LYS:O	1:A:241:GLN:HG3	2.20	0.42
3:C:245:ILE:O	3:C:249:ILE:HG12	2.19	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.02	0.42
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.42
22:a:404:CLA:H151	32:d:401:PHO:H72	2.02	0.42
22:b:615:CLA:H162	22:b:615:CLA:H122	1.73	0.42
3:c:149:TYR:HA	3:c:156:LYS:HD3	2.02	0.42
3:c:393:ALA:HB1	34:v:201:HEM:HBC1	2.02	0.42
24:c:514:BCR:H15C	24:c:514:BCR:H351	1.83	0.42
4:d:129:GLN:OE1	4:d:143:ALA:HA	2.19	0.42
10:k:31:LEU:HB3	24:g:101:BCR:C15	2.50	0.42
13:o:178:ARG:HD2	13:o:182:PHE:CD1	2.54	0.42
22:A:403:CLA:HAA1	23:D:407:PL9:H362	2.01	0.42
22:B:601:CLA:HMB2	24:H:102:BCR:H393	2.02	0.42
27:C:522:LMG:H112	24:J:102:BCR:H373	2.01	0.42
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.42
16:V:90:PRO:O	16:V:92:ARG:HD3	2.19	0.42
2:b:212:ALA:O	2:b:216:HIS:ND1	2.46	0.42
31:b:604:LMT:H3'	31:b:604:LMT:H1B	1.53	0.42
22:b:611:CLA:CHA	22:b:611:CLA:HBA1	2.50	0.42
24:c:513:BCR:H15C	24:c:513:BCR:H351	1.89	0.42
4:d:155:SER:HA	4:d:159:ILE:HB	2.01	0.42
11:l:4:ASN:OD1	11:l:6:ASN:ND2	2.42	0.42
16:v:68:VAL:O	16:v:71:ILE:HG12	2.20	0.42
18:x:12:ILE:HA	18:x:16:LEU:HD12	2.01	0.42
1:A:182:PHE:O	1:A:186:PHE:HB2	2.20	0.42
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.02	0.42
2:B:212:ALA:O	2:B:216:HIS:ND1	2.51	0.42
3:C:113:VAL:HG11	27:C:518:LMG:H132	2.02	0.42
22:c:510:CLA:H122	10:k:32:PHE:HE1	1.85	0.42
5:e:42:LEU:O	5:e:46:VAL:HG23	2.20	0.42
10:k:12:PRO:HB2	10:k:15:TYR:CD2	2.55	0.42
1:A:235:TYR:C	1:A:237:TYR:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.02	0.41
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.02	0.41
24:D:411:BCR:H361	24:D:411:BCR:H20C	1.81	0.41
2:b:383:PHE:N	4:d:344:GLU:O	2.39	0.41
4:d:236:ASN:HA	4:d:237:PRO:HD2	1.95	0.41
13:o:135:GLN:HE21	13:o:135:GLN:HB3	1.72	0.41
13:o:135:GLN:HG2	13:o:141:ARG:HG3	2.02	0.41
1:A:224:ILE:O	4:D:265:ARG:NH2	2.52	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41
1:A:303:ASN:O	3:C:415:ASN:ND2	2.41	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.87	0.41
22:C:510:CLA:H171	20:Z:20:VAL:HA	2.02	0.41
22:C:520:CLA:H141	22:C:520:CLA:H161	1.85	0.41
22:H:101:CLA:H162	22:H:101:CLA:H122	1.51	0.41
13:O:59:ASP:C	13:O:61:SER:H	2.29	0.41
13:O:206:GLU:CD	13:O:206:GLU:H	2.27	0.41
18:X:17:LYS:O	18:X:21:ILE:HG13	2.20	0.41
3:c:402:GLY:HA3	3:c:420:VAL:HG22	2.01	0.41
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.02	0.41
32:d:401:PHO:H41	32:d:401:PHO:H62	1.45	0.41
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.03	0.41
24:C:514:BCR:H15C	24:C:514:BCR:H351	1.84	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	0.41
6:F:45:ARG:NH2	9:J:40:LEU:O	2.53	0.41
3:c:131:TYR:CE1	3:c:135:ARG:HD2	2.56	0.41
1:A:37:MET:HE1	1:A:129:ARG:CZ	2.50	0.41
22:C:504:CLA:H11	24:C:514:BCR:H312	2.02	0.41
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.41
24:D:411:BCR:H11C	24:D:411:BCR:H341	1.94	0.41
27:I:101:LMG:H181	31:I:102:LMT:H42	2.02	0.41
1:a:38:ILE:HD13	30:a:401:SQD:H121	2.03	0.41
22:a:406:CLA:H161	23:a:409:PL9:H253	2.02	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.56	0.41
3:c:248:GLY:O	3:c:252:ILE:HG12	2.20	0.41
3:c:350:ILE:HG21	3:c:359:TRP:HB2	2.02	0.41
24:c:521:BCR:H15C	24:c:521:BCR:H351	1.84	0.41
1:A:24:THR:O	4:D:251:ARG:NH2	2.44	0.41
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.56	0.41
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.41
1:a:61:ASP:HB2	1:a:63:ILE:HG12	2.03	0.41
3:c:456:GLU:OE1	3:c:456:GLU:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:z:10:ALA:O	20:z:14:ILE:HG13	2.21	0.41
22:A:403:CLA:H42	23:D:407:PL9:H162	2.02	0.41
22:B:602:CLA:H192	22:B:602:CLA:H162	1.77	0.41
3:C:166:ILE:O	3:C:170:ILE:HG13	2.20	0.41
3:C:259:TRP:H	3:C:259:TRP:CD1	2.38	0.41
10:K:31:LEU:HB3	24:y:101:BCR:C15	2.50	0.41
13:O:192:SER:OG	13:O:193:GLY:N	2.53	0.41
25:a:411:DGD:HD2	25:a:411:DGD:HG32	1.76	0.41
3:c:119:LEU:HG	24:c:513:BCR:H10C	2.01	0.41
3:c:223:TRP:O	3:c:226:SER:OG	2.33	0.41
3:c:259:TRP:CD1	3:c:259:TRP:H	2.39	0.41
22:c:509:CLA:H2	22:c:509:CLA:H61	1.73	0.41
13:o:192:SER:OG	13:o:193:GLY:N	2.53	0.41
22:A:403:CLA:H62	22:A:403:CLA:H41	1.78	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD2	1.95	0.41
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.56	0.41
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.35	0.41
1:a:334:ARG:NH2	4:d:312:GLU:OE2	2.53	0.41
27:b:625:LMG:H421	4:d:284:ILE:HD13	2.01	0.41
3:c:307:PRO:HB3	3:c:358:PHE:HB3	2.03	0.41
5:e:81:GLU:C	5:e:83:LEU:H	2.29	0.41
13:o:240:THR:HA	13:o:264:VAL:HA	2.02	0.41
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.41
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.50	0.41
5:E:60:GLN:HG2	5:E:62:SER:H	1.86	0.41
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.56	0.41
18:X:34:PHE:O	18:X:38:ILE:HG12	2.21	0.41
22:a:408:CLA:H141	22:a:408:CLA:H162	1.69	0.41
4:d:156:VAL:HG12	4:d:171:PRO:HG3	2.01	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.98	0.41
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.41
1:A:271:LEU:HD21	23:A:406:PL9:HC71	2.02	0.41
22:A:402:CLA:HHC	22:A:402:CLA:CBB	2.50	0.41
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.41
22:B:604:CLA:H141	22:B:604:CLA:H161	1.90	0.41
3:C:420:VAL:H	25:C:516:DGD:HE62	1.85	0.41
13:O:223:ILE:HG13	13:O:243:SER:HB3	2.02	0.41
1:a:22:THR:HG21	8:i:30:ARG:HD3	2.03	0.41
1:a:129:ARG:NH2	4:d:256:ILE:HD12	2.30	0.41
1:a:183:MET:HA	22:a:404:CLA:HMD2	2.02	0.41
2:b:125:ASP:HA	2:b:126:PRO:HD3	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:191:ASN:HB2	7:h:58:VAL:HG23	2.03	0.41
22:b:606:CLA:HBB2	22:b:606:CLA:H92	2.03	0.41
22:b:618:CLA:H52	22:b:618:CLA:H12	1.86	0.41
3:c:464:GLU:HA	3:c:465:PRO:HD2	1.79	0.41
4:d:343:GLU:HG2	16:v:161:VAL:HG11	2.02	0.41
22:d:404:CLA:H61	22:d:404:CLA:H41	1.66	0.41
24:g:101:BCR:H323	24:g:101:BCR:HC31	1.63	0.41
1:A:257:ARG:HH22	2:B:488:PRO:C	2.29	0.41
22:B:602:CLA:H161	22:B:602:CLA:H141	1.82	0.41
22:B:602:CLA:H41	22:B:602:CLA:H61	1.67	0.41
16:V:83:GLU:H	16:V:83:GLU:CD	2.29	0.41
1:a:240:GLY:HA3	14:t:29:ILE:HG22	2.02	0.41
3:c:257:PHE:HB3	3:c:258:GLY:H	1.62	0.41
3:c:346:THR:OG1	3:c:348:GLU:OE1	2.37	0.41
22:c:508:CLA:H92	22:c:508:CLA:H62	1.71	0.41
3:C:57:ALA:O	3:C:61:VAL:HG23	2.20	0.40
3:C:248:GLY:O	3:C:252:ILE:HG12	2.21	0.40
3:C:377:LEU:O	3:C:381:LYS:HB2	2.21	0.40
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.90	0.40
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.03	0.40
17:y:31:ALA:O	17:y:35:ILE:HG23	2.22	0.40
1:a:309:ALA:HA	6:f:45:ARG:HB2	2.03	0.40
2:b:135:LEU:HB2	2:b:136:PRO:HD3	2.02	0.40
2:b:194:ASN:HA	2:b:195:PRO:HD3	1.93	0.40
3:c:261:ARG:HA	3:c:266:TRP:HZ2	1.86	0.40
4:d:87:HIS:CD2	4:d:162:LEU:HD23	2.56	0.40
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.86	0.40
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.51	0.40
22:B:604:CLA:H202	22:B:608:CLA:HBB2	2.03	0.40
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.02	0.40
22:D:405:CLA:H3A	22:D:405:CLA:HBA1	1.86	0.40
17:y:28:ILE:O	24:y:101:BCR:H14C	2.21	0.40
1:a:235:TYR:C	1:a:237:TYR:H	2.29	0.40
2:b:54:PRO:HD2	2:b:57:ARG:HG3	2.02	0.40
2:b:414:PRO:HB2	2:b:415:PRO:HD3	2.02	0.40
24:b:622:BCR:H11C	24:b:622:BCR:H341	1.88	0.40
22:c:508:CLA:H141	22:c:511:CLA:HMD3	2.02	0.40
22:c:511:CLA:H13	22:c:511:CLA:H61	2.04	0.40
4:d:261:PHE:HA	27:d:407:LMG:O2	2.21	0.40
7:h:19:GLY:O	7:h:21:VAL:HG13	2.22	0.40
1:A:317:TRP:O	1:A:321:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.40
22:B:604:CLA:H202	22:B:604:CLA:H162	1.88	0.40
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.86	0.40
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.03	0.40
24:C:521:BCR:H351	24:C:521:BCR:H15C	1.84	0.40
4:D:49:LEU:O	4:D:53:THR:HG23	2.22	0.40
25:b:601:DGD:HB22	31:b:603:LMT:H72	2.02	0.40
7:h:12:ARG:N	7:h:13:PRO:HD2	2.36	0.40
22:h:101:CLA:H62	22:h:101:CLA:H93	1.84	0.40
17:g:31:ALA:O	17:g:35:ILE:HG23	2.20	0.40
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.03	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
1:A:140:ARG:HH22	26:A:409:LHG:P	2.44	0.40
1:A:141:PRO:O	1:A:143:ILE:N	2.53	0.40
1:A:322:ASN:OD1	3:C:412:THR:HA	2.21	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.89	0.40
22:B:607:CLA:H172	22:D:406:CLA:H3A	2.03	0.40
4:D:201:VAL:O	4:D:205:LEU:HB2	2.22	0.40
4:D:252:PHE:O	4:D:256:ILE:HG22	2.21	0.40
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.04	0.40
1:a:141:PRO:HG3	3:c:446:GLY:C	2.46	0.40
1:a:180:PHE:O	1:a:184:ILE:HG13	2.22	0.40
22:c:508:CLA:H142	22:c:508:CLA:H112	1.84	0.40
7:h:46:LEU:HB2	22:h:101:CLA:H61	2.02	0.40
22:A:404:CLA:HAB	22:D:405:CLA:H72	2.04	0.40
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.04	0.40
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.03	0.40
22:C:512:CLA:HAB	24:C:521:BCR:H24C	2.03	0.40
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.85	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.37	0.40
1:a:176:ILE:HD12	22:a:405:CLA:HED3	2.03	0.40
22:a:404:CLA:H51	32:d:401:PHO:C3B	2.52	0.40
2:b:137:LYS:HB2	2:b:137:LYS:HE3	1.96	0.40
2:b:348:ASN:HB3	2:b:354:LEU:HD21	2.03	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%)	310 (93%)	19 (6%)	4 (1%)	10	43
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	10	43
2	B	488/510 (96%)	450 (92%)	34 (7%)	4 (1%)	16	53
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	21	58
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	14	49
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	14	49
4	D	338/352 (96%)	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%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	22
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	22
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	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10	43
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	21
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	21
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	30
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	30
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	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%)	4673 (91%)	410 (8%)	55 (1%)	11	45

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
7	H	26	GLY
9	J	38	SER
13	O	52	ALA
14	T	30	THR
17	y	43	ARG
18	X	12	ILE
18	X	45	LYS

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Mol	Chain	Res	Type
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
7	h	26	GLY
9	j	38	SER
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
4	D	239	GLN
13	O	88	GLU
13	O	271	PRO
2	b	489	GLU
4	d	239	GLN
13	o	88	GLU
1	A	142	TRP
2	B	489	GLU
3	C	32	GLY
5	E	82	GLN
1	a	334	ARG
3	c	32	GLY
5	e	82	GLN
13	o	271	PRO
1	A	334	ARG
3	C	144	SER
7	H	16	SER
15	U	73	PRO
1	a	142	TRP
3	c	144	SER
7	h	16	SER
15	u	73	PRO
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY

5.3.2 Protein sidechains [i](#)

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%)	260 (96%)	11 (4%)	27	49
2	B	390/407 (96%)	380 (97%)	10 (3%)	40	60
2	b	390/407 (96%)	380 (97%)	10 (3%)	40	60
3	C	347/362 (96%)	336 (97%)	11 (3%)	34	55
3	c	347/362 (96%)	336 (97%)	11 (3%)	34	55
4	D	275/283 (97%)	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	41
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	41
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
15	u	84/112 (75%)	82 (98%)	2 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	116/138 (84%)	114 (98%)	2 (2%)	53	67
16	v	116/138 (84%)	114 (98%)	2 (2%)	53	67
17	g	20/37 (54%)	17 (85%)	3 (15%)	3	14
17	y	20/37 (54%)	17 (85%)	3 (15%)	3	14
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%)	4110 (97%)	134 (3%)	34	55

All (134) 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
3	C	254	THR

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

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Mol	Chain	Res	Type
1	a	157	VAL
1	a	202	VAL
1	a	226	GLU
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	275	LEU
1	a	286	THR
1	a	292	THR
1	a	306	VAL
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	354	LEU
2	b	362	PHE
2	b	422	ARG
2	b	467	ILE
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	174	LEU
3	c	201	ASN
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	417	VAL
3	c	469	MET
3	c	472	LEU
4	d	43	LEU
4	d	91	LEU
4	d	180	ARG
4	d	201	VAL
4	d	205	LEU
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	323	GLU
4	d	345	VAL
4	d	346	LEU

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Mol	Chain	Res	Type
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	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 (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	337	HIS
2	B	9	HIS
2	B	26	HIS
2	B	223	GLN
2	B	374	ASN
3	C	44	ASN
3	C	56	HIS
3	C	118	HIS
3	C	229	ASN
4	D	117	HIS
4	D	186	GLN
4	D	250	ASN
4	D	301	GLN

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Mol	Chain	Res	Type
4	D	322	ASN
12	M	32	GLN
12	M	33	GLN
13	O	150	ASN
13	O	173	ASN
15	U	93	ASN
15	U	111	HIS
1	a	241	GLN
1	a	337	HIS
2	b	26	HIS
2	b	223	GLN
2	b	282	GLN
2	b	331	ASN
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	250	ASN
4	d	301	GLN
13	o	130	GLN
13	o	150	ASN
13	o	173	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	B	610	2	69,73,73	1.23	6 (8%)	82,113,113	1.29	7 (8%)
27	LMG	d	407	-	48,48,55	0.75	0	56,56,63	1.37	4 (7%)
22	CLA	D	405	-	69,73,73	1.20	7 (10%)	82,113,113	1.21	5 (6%)
22	CLA	B	603	2	69,73,73	1.18	8 (11%)	82,113,113	1.34	7 (8%)
22	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
22	CLA	b	607	2	69,73,73	1.19	8 (11%)	82,113,113	1.32	7 (8%)
24	BCR	A	407	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
25	DGD	B	620	-	59,59,67	0.89	1 (1%)	73,73,81	1.34	8 (10%)
32	PHO	D	401	-	58,69,69	2.16	9 (15%)	55,99,99	1.41	6 (10%)
22	CLA	h	101	-	69,73,73	1.20	6 (8%)	82,113,113	1.24	5 (6%)
30	SQD	a	401	-	52,54,54	0.96	3 (5%)	62,65,65	1.49	9 (14%)
22	CLA	C	504	3	69,73,73	1.18	7 (10%)	82,113,113	1.31	5 (6%)
27	LMG	b	628	-	49,49,55	0.76	1 (2%)	57,57,63	1.31	4 (7%)
30	SQD	A	413	-	49,51,54	0.97	2 (4%)	59,62,65	1.66	9 (15%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.29	5 (9%)
23	PL9	a	409	-	45,45,55	1.01	4 (8%)	56,57,69	1.53	10 (17%)
22	CLA	b	610	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
23	PL9	A	406	-	45,45,55	0.97	4 (8%)	56,57,69	1.54	11 (19%)
31	LMT	b	627	-	36,36,36	1.07	3 (8%)	47,47,47	1.00	2 (4%)
22	CLA	c	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
24	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	B	604	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
22	CLA	C	510	3	69,73,73	1.19	6 (8%)	82,113,113	1.31	6 (7%)
24	BCR	g	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	9 (16%)
32	PHO	D	402	-	58,69,69	2.20	9 (15%)	55,99,99	1.42	5 (9%)
22	CLA	A	402	1	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
27	LMG	I	101	-	43,43,55	0.79	0	51,51,63	1.27	4 (7%)
30	SQD	a	415	-	49,51,54	0.97	2 (4%)	59,62,65	1.68	9 (15%)
27	LMG	B	624	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCT	D	404	21	3,3,3	1.11	0	2,3,3	4.21	2 (100%)
24	BCR	b	622	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	9 (16%)
22	CLA	c	507	3	69,73,73	1.19	8 (11%)	82,113,113	1.30	7 (8%)
24	BCR	C	514	-	41,41,41	1.13	3 (7%)	56,56,56	1.30	9 (16%)
25	DGD	b	624	-	59,59,67	0.90	1 (1%)	73,73,81	1.33	6 (8%)
25	DGD	C	515	-	54,54,67	0.97	2 (3%)	68,68,81	1.27	6 (8%)
22	CLA	C	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	c	503	-	69,73,73	1.20	7 (10%)	82,113,113	1.28	5 (6%)
25	DGD	b	601	-	53,53,67	1.05	3 (5%)	67,67,81	1.33	7 (10%)
31	LMT	b	603	-	36,36,36	1.10	5 (13%)	47,47,47	0.95	1 (2%)
22	CLA	C	503	3	69,73,73	1.19	7 (10%)	82,113,113	1.28	4 (4%)
22	CLA	c	505	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	c	508	3	69,73,73	1.19	6 (8%)	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%)
31	LMT	B	628	-	36,36,36	1.11	5 (13%)	47,47,47	1.04	1 (2%)
25	DGD	d	408	-	64,64,67	0.91	2 (3%)	78,78,81	1.34	9 (11%)
24	BCR	b	623	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	8 (14%)
24	BCR	H	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	4 (7%)
26	LHG	C	519	-	36,36,48	0.72	2 (5%)	39,42,54	1.28	4 (10%)
25	DGD	c	517	-	67,67,67	0.87	0	81,81,81	1.39	9 (11%)
31	LMT	B	623	-	36,36,36	1.07	3 (8%)	47,47,47	1.01	2 (4%)
22	CLA	C	502	3	69,73,73	1.19	9 (13%)	82,113,113	1.27	5 (6%)
22	CLA	c	510	3	69,73,73	1.20	5 (7%)	82,113,113	1.29	6 (7%)
25	DGD	C	517	-	67,67,67	0.87	0	81,81,81	1.40	9 (11%)
22	CLA	b	605	-	69,73,73	1.21	7 (10%)	82,113,113	1.26	5 (6%)
31	LMT	B	627	-	36,36,36	1.10	4 (11%)	47,47,47	0.96	1 (2%)
27	LMG	d	410	-	46,46,55	0.79	1 (2%)	54,54,63	1.31	6 (11%)
24	BCR	C	513	-	41,41,41	1.15	2 (4%)	56,56,56	1.35	10 (17%)
24	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
22	CLA	c	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)
31	LMT	i	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.00	2 (4%)
25	DGD	a	411	-	57,57,67	0.93	1 (1%)	71,71,81	1.39	8 (11%)
23	PL9	d	406	-	55,55,55	1.00	3 (5%)	68,69,69	1.51	13 (19%)
22	CLA	d	405	-	69,73,73	1.19	5 (7%)	82,113,113	1.26	5 (6%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.28	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	611	2	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.33	7 (12%)
22	CLA	b	609	2	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
31	LMT	M	102	-	36,36,36	1.12	6 (16%)	47,47,47	1.00	2 (4%)
24	BCR	D	411	-	41,41,41	1.15	3 (7%)	56,56,56	1.23	7 (12%)
24	BCR	c	513	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	10 (17%)
25	DGD	C	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.43	13 (16%)
22	CLA	b	615	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
27	LMG	a	413	-	51,51,55	0.74	0	59,59,63	1.35	8 (13%)
34	HEM	v	201	16	50,50,50	1.99	10 (20%)	67,82,82	1.24	4 (5%)
22	CLA	d	404	-	69,73,73	1.20	6 (8%)	82,113,113	1.22	5 (6%)
22	CLA	a	404	1	69,73,73	1.19	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	C	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.28	5 (6%)
27	LMG	A	415	-	42,42,55	0.83	1 (2%)	50,50,63	1.26	4 (8%)
27	LMG	D	408	-	48,48,55	0.75	0	56,56,63	1.38	4 (7%)
29	OEX	A	412	3,1	0,14,14	-	-	-	-	-
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.29	5 (9%)
32	PHO	d	401	-	58,69,69	2.16	9 (15%)	55,99,99	1.41	7 (12%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	b	619	2	69,73,73	1.19	8 (11%)	82,113,113	1.24	5 (6%)
34	HEM	V	201	16	50,50,50	1.98	10 (20%)	67,82,82	1.21	2 (2%)
24	BCR	f	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	6 (10%)
22	CLA	c	502	-	69,73,73	1.19	9 (13%)	82,113,113	1.27	5 (6%)
22	CLA	a	406	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
22	CLA	b	612	2	69,73,73	1.20	7 (10%)	82,113,113	1.22	5 (6%)
23	PL9	J	101	-	35,35,55	0.98	2 (5%)	44,45,69	1.58	8 (18%)
24	BCR	x	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	3 (5%)
22	CLA	a	405	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
26	LHG	A	409	-	38,38,48	0.70	1 (2%)	41,44,54	1.21	3 (7%)
24	BCR	b	621	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	7 (12%)
24	BCR	c	514	-	41,41,41	1.13	3 (7%)	56,56,56	1.31	9 (16%)
22	CLA	b	606	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	7 (8%)
30	SQD	b	602	-	45,47,54	1.02	4 (8%)	55,58,65	1.74	9 (16%)
27	LMG	E	101	-	44,44,55	0.74	0	52,52,63	1.31	5 (9%)
22	CLA	A	405	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	y	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	a	408	1	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
31	LMT	D	410	-	32,32,36	1.15	4 (12%)	43,43,47	1.02	2 (4%)
22	CLA	B	601	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	6 (7%)
25	DGD	A	408	-	57,57,67	0.92	0	71,71,81	1.40	8 (11%)
22	CLA	b	614	2	69,73,73	1.23	6 (8%)	82,113,113	1.29	6 (7%)
23	PL9	D	407	-	55,55,55	1.02	4 (7%)	68,69,69	1.50	13 (19%)
23	PL9	j	101	-	35,35,55	0.96	2 (5%)	44,45,69	1.58	8 (18%)
24	BCR	C	521	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	9 (16%)
33	BCT	d	403	21	3,3,3	1.11	0	2,3,3	4.19	2 (100%)
22	CLA	B	613	2	69,73,73	1.18	6 (8%)	82,113,113	1.25	5 (6%)
31	LMT	b	626	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	1 (2%)
22	CLA	c	520	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
24	BCR	c	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	9 (16%)
22	CLA	c	509	3	69,73,73	1.19	8 (11%)	82,113,113	1.23	5 (6%)
22	CLA	C	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
27	LMG	M	101	-	42,42,55	0.85	0	50,50,63	1.24	4 (8%)
22	CLA	B	615	2	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
22	CLA	H	101	-	69,73,73	1.20	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	B	608	2	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	B	612	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	7 (8%)
22	CLA	b	613	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	B	614	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	D	406	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)
22	CLA	B	606	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
31	LMT	I	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.01	2 (4%)
24	BCR	J	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.58	11 (19%)
24	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.30	7 (12%)
27	LMG	C	522	-	48,48,55	0.76	0	56,56,63	1.32	5 (8%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.33	7 (10%)
22	CLA	A	404	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.30	5 (9%)
27	LMG	a	402	-	42,42,55	0.83	1 (2%)	50,50,63	1.26	4 (8%)
30	SQD	A	414	-	52,54,54	0.96	2 (3%)	62,65,65	1.50	8 (12%)
25	DGD	D	409	-	64,64,67	0.90	0	78,78,81	1.33	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	f	101	5,6	50,50,50	1.96	8 (16%)	67,82,82	1.32	4 (5%)
31	LMT	b	604	-	36,36,36	1.11	3 (8%)	47,47,47	1.03	1 (2%)
30	SQD	d	402	-	41,43,54	1.05	3 (7%)	51,54,65	1.73	10 (19%)
22	CLA	C	520	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
31	LMT	B	622	-	36,36,36	1.10	3 (8%)	47,47,47	0.97	1 (2%)
22	CLA	b	617	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
34	HEM	F	101	5,6	50,50,50	1.97	9 (18%)	67,82,82	1.31	4 (5%)
22	CLA	b	608	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
25	DGD	c	516	-	63,63,67	0.91	2 (3%)	77,77,81	1.43	12 (15%)
22	CLA	B	602	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	C	509	3	69,73,73	1.19	7 (10%)	82,113,113	1.22	5 (6%)
22	CLA	b	616	-	69,73,73	1.18	6 (8%)	82,113,113	1.27	7 (8%)
30	SQD	f	103	-	43,45,54	1.04	3 (6%)	53,56,65	1.56	11 (20%)
30	SQD	D	403	-	41,43,54	1.05	3 (7%)	51,54,65	1.72	10 (19%)
24	BCR	b	620	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	6 (10%)
27	LMG	i	101	-	43,43,55	0.82	0	51,51,63	1.27	6 (11%)
26	LHG	c	519	-	36,36,48	0.74	2 (5%)	39,42,54	1.29	4 (10%)
22	CLA	A	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
24	BCR	j	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.58	12 (21%)
27	LMG	D	412	-	46,46,55	0.78	1 (2%)	54,54,63	1.31	5 (9%)
22	CLA	b	618	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	c	504	3	69,73,73	1.19	6 (8%)	82,113,113	1.30	6 (7%)
24	BCR	B	616	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	8 (14%)
22	CLA	C	508	3	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
31	LMT	M	103	-	36,36,36	1.11	4 (11%)	47,47,47	0.99	2 (4%)
22	CLA	c	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
22	CLA	B	607	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
22	CLA	C	501	3	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	B	609	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	C	511	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
27	LMG	m	101	-	42,42,55	0.85	0	50,50,63	1.24	4 (8%)
27	LMG	A	410	-	51,51,55	0.73	0	59,59,63	1.36	7 (11%)
30	SQD	F	102	-	43,45,54	1.04	3 (6%)	53,56,65	1.57	10 (18%)
31	LMT	d	409	-	32,32,36	1.15	3 (9%)	43,43,47	0.99	2 (4%)
26	LHG	a	412	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	3 (7%)

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	1.32	5 (8%)
30	SQD	B	626	-	45,47,54	1.02	4 (8%)	55,58,65	1.71	10 (18%)
24	BCR	a	410	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
22	CLA	C	507	3	69,73,73	1.19	8 (11%)	82,113,113	1.29	7 (8%)
29	OEX	a	414	3,1	0,14,14	-	-	-	-	-
22	CLA	B	605	2	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	c	501	3	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	610	2	-	12/39/115/115	-
27	LMG	d	407	-	-	20/43/63/70	0/1/1/1
22	CLA	D	405	-	-	14/39/115/115	-
22	CLA	B	603	2	-	7/39/115/115	-
22	CLA	B	611	-	-	10/39/115/115	-
22	CLA	b	607	2	-	7/39/115/115	-
24	BCR	A	407	-	-	3/29/63/63	0/2/2/2
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2
32	PHO	D	401	-	-	11/37/103/103	0/5/6/6
22	CLA	h	101	-	-	15/39/115/115	-
30	SQD	a	401	-	-	12/49/69/69	0/1/1/1
22	CLA	C	504	3	-	17/39/115/115	-
27	LMG	b	628	-	-	24/44/64/70	0/1/1/1
30	SQD	A	413	-	-	19/46/66/69	0/1/1/1
27	LMG	c	518	-	-	21/40/60/70	0/1/1/1
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
22	CLA	b	610	-	-	9/39/115/115	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
31	LMT	b	627	-	-	2/21/61/61	0/2/2/2
22	CLA	c	512	3	-	19/39/115/115	-
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
22	CLA	B	604	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	510	3	-	13/39/115/115	-
24	BCR	g	101	-	-	4/29/63/63	0/2/2/2
32	PHO	D	402	-	-	10/37/103/103	0/5/6/6
22	CLA	A	402	1	-	8/39/115/115	-
27	LMG	I	101	-	-	18/38/58/70	0/1/1/1
30	SQD	a	415	-	-	17/46/66/69	0/1/1/1
27	LMG	B	624	-	-	25/44/64/70	0/1/1/1
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
22	CLA	c	507	3	-	13/39/115/115	-
24	BCR	C	514	-	-	4/29/63/63	0/2/2/2
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
22	CLA	C	512	3	-	15/39/115/115	-
22	CLA	c	503	-	-	11/39/115/115	-
25	DGD	b	601	-	-	18/41/81/95	0/2/2/2
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	C	503	3	-	12/39/115/115	-
22	CLA	c	505	3	-	16/39/115/115	-
22	CLA	c	508	3	-	18/39/115/115	-
32	PHO	a	407	-	-	11/37/103/103	0/5/6/6
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
25	DGD	d	408	-	-	35/52/92/95	0/2/2/2
24	BCR	b	623	-	-	4/29/63/63	0/2/2/2
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
26	LHG	C	519	-	-	16/41/41/53	-
25	DGD	c	517	-	-	20/55/95/95	0/2/2/2
31	LMT	B	623	-	-	4/21/61/61	0/2/2/2
22	CLA	C	502	3	-	9/39/115/115	-
22	CLA	c	510	3	-	15/39/115/115	-
25	DGD	C	517	-	-	21/55/95/95	0/2/2/2
22	CLA	b	605	-	-	15/39/115/115	-
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
27	LMG	d	410	-	-	15/41/61/70	0/1/1/1
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
22	CLA	c	511	-	-	17/39/115/115	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
25	DGD	a	411	-	-	14/45/85/95	0/2/2/2
23	PL9	d	406	-	-	11/53/73/73	0/1/1/1
22	CLA	d	405	-	-	8/39/115/115	-
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
22	CLA	b	611	2	-	13/39/115/115	-
27	LMG	B	621	-	-	15/44/64/70	0/1/1/1
22	CLA	b	609	2	-	17/39/115/115	-
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
24	BCR	D	411	-	-	5/29/63/63	0/2/2/2
24	BCR	c	513	-	-	6/29/63/63	0/2/2/2
25	DGD	C	516	-	-	19/51/91/95	0/2/2/2
22	CLA	b	615	-	-	10/39/115/115	-
27	LMG	a	413	-	-	26/46/66/70	0/1/1/1
34	HEM	v	201	16	-	5/14/54/54	-
22	CLA	d	404	-	-	11/39/115/115	-
22	CLA	a	404	1	-	8/39/115/115	-
22	CLA	C	505	3	-	16/39/115/115	-
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
27	LMG	D	408	-	-	21/43/63/70	0/1/1/1
32	PHO	d	401	-	-	10/37/103/103	0/5/6/6
27	LMG	C	518	-	-	22/40/60/70	0/1/1/1
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
22	CLA	b	619	2	-	19/39/115/115	-
34	HEM	V	201	16	-	5/14/54/54	-
24	BCR	f	102	-	-	6/29/63/63	0/2/2/2
22	CLA	c	502	-	-	10/39/115/115	-
22	CLA	a	406	-	-	8/39/115/115	-
22	CLA	b	612	2	-	8/39/115/115	-
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	a	405	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	A	409	-	-	13/43/43/53	-
24	BCR	b	621	-	-	7/29/63/63	0/2/2/2
24	BCR	c	514	-	-	4/29/63/63	0/2/2/2
22	CLA	b	606	2	-	13/39/115/115	-
30	SQD	b	602	-	-	14/42/62/69	0/1/1/1
27	LMG	E	101	-	-	18/39/59/70	0/1/1/1
22	CLA	A	405	1	-	8/39/115/115	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	a	408	1	-	7/39/115/115	-
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
22	CLA	B	601	-	-	16/39/115/115	-
25	DGD	A	408	-	-	15/45/85/95	0/2/2/2
22	CLA	b	614	2	-	11/39/115/115	-
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
24	BCR	C	521	-	-	5/29/63/63	0/2/2/2
22	CLA	B	613	2	-	13/39/115/115	-
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
22	CLA	c	520	-	-	12/39/115/115	-
24	BCR	c	521	-	-	4/29/63/63	0/2/2/2
22	CLA	c	509	3	-	17/39/115/115	-
22	CLA	C	506	-	-	13/39/115/115	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
22	CLA	B	615	2	-	19/39/115/115	-
22	CLA	H	101	-	-	15/39/115/115	-
22	CLA	B	608	2	-	8/39/115/115	-
22	CLA	B	612	-	-	16/39/115/115	-
22	CLA	b	613	-	-	18/39/115/115	-
22	CLA	B	614	-	-	9/39/115/115	-
22	CLA	D	406	-	-	8/39/115/115	-
22	CLA	B	606	-	-	10/39/115/115	-
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	C	522	-	-	19/43/63/70	0/1/1/1
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
22	CLA	A	404	-	-	10/39/115/115	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
30	SQD	A	414	-	-	10/49/69/69	0/1/1/1
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2
34	HEM	f	101	5,6	-	2/14/54/54	-
31	LMT	b	604	-	-	4/21/61/61	0/2/2/2
30	SQD	d	402	-	-	14/38/58/69	0/1/1/1
22	CLA	C	520	-	-	13/39/115/115	-
31	LMT	B	622	-	-	3/21/61/61	0/2/2/2
22	CLA	b	617	2	-	13/39/115/115	-
34	HEM	F	101	5,6	-	2/14/54/54	-
22	CLA	b	608	2	-	16/39/115/115	-
25	DGD	c	516	-	-	19/51/91/95	0/2/2/2
22	CLA	B	602	2	-	15/39/115/115	-
22	CLA	C	509	3	-	16/39/115/115	-
22	CLA	b	616	-	-	16/39/115/115	-
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
30	SQD	D	403	-	-	14/38/58/69	0/1/1/1
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
27	LMG	i	101	-	-	19/38/58/70	0/1/1/1
26	LHG	c	519	-	-	17/41/41/53	-
22	CLA	A	403	-	-	13/39/115/115	-
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
27	LMG	D	412	-	-	14/41/61/70	0/1/1/1
22	CLA	b	618	-	-	9/39/115/115	-
22	CLA	c	504	3	-	17/39/115/115	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
22	CLA	C	508	3	-	19/39/115/115	-
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	c	506	-	-	12/39/115/115	-
22	CLA	B	607	2	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	501	3	-	16/39/115/115	-
22	CLA	B	609	-	-	18/39/115/115	-
22	CLA	C	511	-	-	17/39/115/115	-
27	LMG	m	101	-	-	17/37/57/70	0/1/1/1
27	LMG	A	410	-	-	25/46/66/70	0/1/1/1
30	SQD	F	102	-	-	10/40/60/69	0/1/1/1
31	LMT	d	409	-	-	0/17/57/61	0/2/2/2
26	LHG	a	412	-	-	11/43/43/53	-
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
30	SQD	B	626	-	-	13/42/62/69	0/1/1/1
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
22	CLA	C	507	3	-	13/39/115/115	-
22	CLA	B	605	2	-	14/39/115/115	-
22	CLA	c	501	3	-	14/39/115/115	-

All (749) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	402	PHO	C1B-C2B	9.70	1.50	1.39
32	d	401	PHO	C1B-C2B	9.65	1.50	1.39
32	D	401	PHO	C1B-C2B	9.57	1.50	1.39
32	a	407	PHO	C1B-C2B	9.56	1.50	1.39
32	D	402	PHO	C3B-C4B	8.74	1.50	1.41
32	a	407	PHO	C3B-C4B	8.65	1.50	1.41
32	D	401	PHO	C3B-C4B	8.52	1.50	1.41
32	d	401	PHO	C3B-C4B	8.35	1.49	1.41
34	v	201	HEM	C3D-C2D	8.17	1.54	1.36
34	V	201	HEM	C3D-C2D	8.17	1.54	1.36
34	F	101	HEM	C3D-C2D	7.92	1.53	1.36
34	f	101	HEM	C3D-C2D	7.86	1.53	1.36
34	F	101	HEM	FE-ND	5.37	2.11	1.94
34	f	101	HEM	FE-ND	5.24	2.11	1.94
34	V	201	HEM	FE-ND	5.21	2.10	1.94
34	v	201	HEM	FE-ND	5.03	2.10	1.94
34	f	101	HEM	FE-NB	4.50	2.08	1.94
34	v	201	HEM	FE-NB	4.45	2.08	1.94
32	a	407	PHO	C1D-C2D	4.38	1.44	1.39
34	F	101	HEM	FE-NB	4.36	2.08	1.94
32	D	402	PHO	C1D-C2D	4.30	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	FE-NB	4.24	2.08	1.94
32	d	401	PHO	C1D-C2D	4.13	1.44	1.39
34	V	201	HEM	FE-NA	4.08	2.08	1.95
32	D	401	PHO	C1D-C2D	4.06	1.44	1.39
24	H	102	BCR	C1-C6	-3.89	1.48	1.53
24	y	101	BCR	C1-C6	-3.88	1.48	1.53
34	v	201	HEM	FE-NA	3.83	2.07	1.95
24	D	411	BCR	C1-C6	-3.83	1.48	1.53
32	D	401	PHO	C4D-CHA	3.83	1.45	1.39
32	D	402	PHO	C4D-CHA	3.82	1.45	1.39
32	a	407	PHO	C4D-CHA	3.79	1.45	1.39
24	g	101	BCR	C1-C6	-3.79	1.48	1.53
22	h	101	CLA	C1D-ND	3.78	1.42	1.37
24	f	102	BCR	C1-C6	-3.78	1.48	1.53
32	d	401	PHO	C4D-CHA	3.77	1.45	1.39
22	b	605	CLA	C1D-ND	3.77	1.42	1.37
24	x	101	BCR	C1-C6	-3.76	1.49	1.53
22	B	601	CLA	C1D-ND	3.76	1.42	1.37
22	c	503	CLA	C1D-ND	3.76	1.42	1.37
22	c	510	CLA	C1D-ND	3.76	1.42	1.37
22	C	501	CLA	C1D-ND	3.76	1.42	1.37
22	d	405	CLA	C1D-ND	3.74	1.42	1.37
22	d	404	CLA	C1D-ND	3.73	1.42	1.37
22	C	512	CLA	C1D-ND	3.73	1.42	1.37
22	B	608	CLA	C1D-ND	3.71	1.42	1.37
22	D	405	CLA	C1D-ND	3.71	1.42	1.37
22	c	505	CLA	C1D-ND	3.71	1.42	1.37
22	C	510	CLA	C1D-ND	3.71	1.42	1.37
22	c	501	CLA	C1D-ND	3.70	1.42	1.37
34	F	101	HEM	FE-NA	3.70	2.07	1.95
22	H	101	CLA	C1D-ND	3.70	1.42	1.37
22	b	608	CLA	C1D-ND	3.70	1.42	1.37
22	C	505	CLA	C1D-ND	3.70	1.42	1.37
22	b	612	CLA	C1D-ND	3.70	1.42	1.37
22	c	512	CLA	C1D-ND	3.69	1.42	1.37
22	D	406	CLA	C1D-ND	3.69	1.42	1.37
22	b	618	CLA	C1D-ND	3.69	1.42	1.37
22	C	503	CLA	C1D-ND	3.67	1.42	1.37
22	A	403	CLA	C1D-ND	3.67	1.42	1.37
22	B	604	CLA	C1D-ND	3.67	1.42	1.37
22	a	405	CLA	C1D-ND	3.67	1.42	1.37
22	A	405	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	C1D-ND	3.66	1.42	1.37
22	a	408	CLA	C1D-ND	3.66	1.42	1.37
22	b	613	CLA	C1D-ND	3.66	1.42	1.37
22	b	609	CLA	C1D-ND	3.65	1.42	1.37
22	b	616	CLA	C1D-ND	3.65	1.42	1.37
22	c	508	CLA	C1D-ND	3.65	1.42	1.37
22	c	506	CLA	C1D-ND	3.64	1.42	1.37
22	c	502	CLA	C1D-ND	3.63	1.42	1.37
22	b	606	CLA	C1D-ND	3.63	1.42	1.37
34	f	101	HEM	FE-NA	3.62	2.07	1.95
22	B	613	CLA	C1D-ND	3.62	1.42	1.37
22	C	502	CLA	C1D-ND	3.62	1.42	1.37
24	C	513	BCR	C1-C6	-3.62	1.49	1.53
22	C	511	CLA	C1D-ND	3.62	1.42	1.37
22	B	614	CLA	C1D-ND	3.62	1.42	1.37
22	a	406	CLA	C1D-ND	3.61	1.42	1.37
22	B	603	CLA	C1D-ND	3.61	1.42	1.37
22	B	606	CLA	C1D-ND	3.60	1.42	1.37
22	C	520	CLA	C1D-ND	3.60	1.42	1.37
22	c	504	CLA	C1D-ND	3.60	1.42	1.37
22	B	605	CLA	C1D-ND	3.60	1.42	1.37
22	b	607	CLA	C1D-ND	3.59	1.42	1.37
22	c	520	CLA	C1D-ND	3.59	1.42	1.37
22	C	504	CLA	C1D-ND	3.59	1.42	1.37
22	B	612	CLA	C1D-ND	3.59	1.42	1.37
24	B	616	BCR	C1-C6	-3.58	1.49	1.53
24	b	620	BCR	C1-C6	-3.58	1.49	1.53
22	b	611	CLA	C1D-ND	3.58	1.42	1.37
22	B	602	CLA	C1D-ND	3.57	1.42	1.37
22	c	511	CLA	C1D-ND	3.57	1.42	1.37
22	b	610	CLA	C1D-ND	3.56	1.42	1.37
22	c	507	CLA	C1D-ND	3.55	1.42	1.37
22	B	607	CLA	C1D-ND	3.55	1.42	1.37
22	A	404	CLA	C1D-ND	3.55	1.42	1.37
24	C	514	BCR	C1-C6	-3.54	1.49	1.53
22	b	617	CLA	C1D-ND	3.54	1.42	1.37
22	B	609	CLA	C1D-ND	3.54	1.42	1.37
24	c	513	BCR	C1-C6	-3.54	1.49	1.53
22	B	615	CLA	C1D-ND	3.53	1.42	1.37
24	c	514	BCR	C1-C6	-3.53	1.49	1.53
22	a	404	CLA	C1D-ND	3.52	1.42	1.37
22	C	507	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	619	CLA	C1D-ND	3.51	1.42	1.37
22	C	508	CLA	C1D-ND	3.48	1.42	1.37
22	A	402	CLA	C1D-ND	3.48	1.42	1.37
24	b	622	BCR	C30-C25	-3.47	1.49	1.53
22	B	610	CLA	C1D-ND	3.46	1.42	1.37
22	c	509	CLA	C1D-ND	3.46	1.42	1.37
22	C	509	CLA	C1D-ND	3.46	1.42	1.37
24	y	101	BCR	C30-C25	-3.42	1.49	1.53
22	b	614	CLA	C1D-ND	3.42	1.42	1.37
24	b	621	BCR	C1-C6	-3.39	1.49	1.53
24	g	101	BCR	C30-C25	-3.39	1.49	1.53
24	B	618	BCR	C30-C25	-3.37	1.49	1.53
24	B	619	BCR	C30-C25	-3.36	1.49	1.53
34	v	201	HEM	FE-NC	3.35	2.06	1.95
24	C	521	BCR	C30-C25	-3.34	1.49	1.53
24	b	623	BCR	C30-C25	-3.34	1.49	1.53
24	a	410	BCR	C1-C6	-3.34	1.49	1.53
24	b	620	BCR	C30-C25	-3.34	1.49	1.53
24	B	617	BCR	C1-C6	-3.33	1.49	1.53
24	c	521	BCR	C30-C25	-3.32	1.49	1.53
24	a	410	BCR	C30-C25	-3.31	1.49	1.53
24	A	407	BCR	C30-C25	-3.31	1.49	1.53
24	B	616	BCR	C30-C25	-3.30	1.49	1.53
24	D	411	BCR	C30-C25	-3.30	1.49	1.53
24	b	623	BCR	C1-C6	-3.30	1.49	1.53
24	B	618	BCR	C1-C6	-3.28	1.49	1.53
24	f	102	BCR	C30-C25	-3.28	1.49	1.53
22	A	402	CLA	C4B-NB	3.27	1.42	1.37
24	B	619	BCR	C1-C6	-3.26	1.49	1.53
24	b	622	BCR	C1-C6	-3.26	1.49	1.53
24	A	407	BCR	C1-C6	-3.26	1.49	1.53
22	B	601	CLA	C4B-NB	3.24	1.42	1.37
24	J	102	BCR	C30-C25	-3.24	1.49	1.53
22	a	404	CLA	C4B-NB	3.23	1.42	1.37
22	b	605	CLA	C4B-NB	3.23	1.42	1.37
22	b	615	CLA	C1D-ND	3.23	1.42	1.37
24	j	102	BCR	C30-C25	-3.23	1.49	1.53
22	c	508	CLA	C4B-NB	3.22	1.42	1.37
24	x	101	BCR	C30-C25	-3.21	1.49	1.53
22	c	509	CLA	C4B-NB	3.21	1.42	1.37
22	B	611	CLA	C1D-ND	3.21	1.42	1.37
22	C	509	CLA	C4B-NB	3.21	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	BCR	C30-C25	-3.20	1.49	1.53
22	b	619	CLA	C4B-NB	3.20	1.42	1.37
22	b	614	CLA	C4B-NB	3.20	1.42	1.37
22	C	508	CLA	C4B-NB	3.19	1.42	1.37
24	j	102	BCR	C1-C6	-3.18	1.49	1.53
24	J	102	BCR	C1-C6	-3.18	1.49	1.53
22	C	505	CLA	C4B-NB	3.18	1.42	1.37
22	c	511	CLA	C4B-NB	3.18	1.42	1.37
30	A	414	SQD	O48-C23	3.17	1.42	1.33
30	a	401	SQD	O48-C23	3.17	1.42	1.33
34	f	101	HEM	FE-NC	3.17	2.05	1.95
30	d	402	SQD	O48-C23	3.17	1.42	1.33
22	B	610	CLA	C4B-NB	3.16	1.42	1.37
22	B	615	CLA	C4B-NB	3.16	1.42	1.37
24	c	514	BCR	C30-C25	-3.16	1.49	1.53
22	a	405	CLA	C4B-NB	3.16	1.42	1.37
24	C	514	BCR	C30-C25	-3.15	1.49	1.53
24	C	521	BCR	C1-C6	-3.15	1.49	1.53
22	c	505	CLA	C4B-NB	3.15	1.42	1.37
30	b	602	SQD	O48-C23	3.15	1.42	1.33
22	c	520	CLA	C4B-NB	3.15	1.42	1.37
22	c	504	CLA	C4B-NB	3.14	1.42	1.37
22	d	405	CLA	C4B-NB	3.14	1.42	1.37
22	c	512	CLA	C4B-NB	3.14	1.42	1.37
22	b	612	CLA	C4B-NB	3.14	1.42	1.37
22	C	507	CLA	C4B-NB	3.14	1.42	1.37
22	b	610	CLA	C4B-NB	3.14	1.42	1.37
22	d	404	CLA	C4B-NB	3.14	1.42	1.37
30	f	103	SQD	O48-C23	3.13	1.42	1.33
30	B	626	SQD	O48-C23	3.13	1.42	1.33
24	H	102	BCR	C30-C25	-3.13	1.49	1.53
30	a	415	SQD	O48-C23	3.12	1.42	1.33
22	B	606	CLA	C4B-NB	3.12	1.42	1.37
22	b	618	CLA	C4B-NB	3.12	1.42	1.37
22	B	608	CLA	C4B-NB	3.12	1.42	1.37
22	D	406	CLA	C4B-NB	3.12	1.42	1.37
30	D	403	SQD	O48-C23	3.11	1.42	1.33
22	C	512	CLA	C4B-NB	3.11	1.42	1.37
22	c	503	CLA	C4B-NB	3.11	1.42	1.37
34	f	101	HEM	CAC-C3C	3.11	1.55	1.47
22	H	101	CLA	C4B-NB	3.11	1.41	1.37
30	F	102	SQD	O48-C23	3.11	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	CAB-C3B	3.11	1.55	1.47
22	b	614	CLA	CMB-C2B	-3.11	1.44	1.50
22	c	507	CLA	C4B-NB	3.10	1.41	1.37
30	A	413	SQD	O48-C23	3.10	1.42	1.33
22	B	604	CLA	C4B-NB	3.10	1.41	1.37
24	c	521	BCR	C1-C6	-3.10	1.49	1.53
22	C	511	CLA	C4B-NB	3.10	1.41	1.37
22	B	614	CLA	C4B-NB	3.09	1.41	1.37
22	C	510	CLA	C4B-NB	3.09	1.41	1.37
34	v	201	HEM	CAB-C3B	3.09	1.55	1.47
22	c	510	CLA	C4B-NB	3.09	1.41	1.37
22	A	403	CLA	C4B-NB	3.09	1.41	1.37
22	a	408	CLA	C4B-NB	3.09	1.41	1.37
22	B	607	CLA	C4B-NB	3.08	1.41	1.37
34	F	101	HEM	CAC-C3C	3.07	1.55	1.47
22	C	503	CLA	C4B-NB	3.07	1.41	1.37
22	a	406	CLA	C4B-NB	3.07	1.41	1.37
22	b	608	CLA	C4B-NB	3.06	1.41	1.37
22	h	101	CLA	C4B-NB	3.06	1.41	1.37
22	B	609	CLA	C4B-NB	3.06	1.41	1.37
34	F	101	HEM	FE-NC	3.06	2.05	1.95
22	b	615	CLA	C4B-NB	3.06	1.41	1.37
22	A	405	CLA	C4B-NB	3.05	1.41	1.37
22	D	405	CLA	C4B-NB	3.05	1.41	1.37
22	b	611	CLA	C4B-NB	3.04	1.41	1.37
22	b	613	CLA	C4B-NB	3.04	1.41	1.37
22	C	520	CLA	C4B-NB	3.04	1.41	1.37
34	V	201	HEM	CAC-C3C	3.04	1.55	1.47
22	b	617	CLA	C4B-NB	3.03	1.41	1.37
22	C	501	CLA	C4B-NB	3.03	1.41	1.37
22	b	609	CLA	C4B-NB	3.02	1.41	1.37
22	B	610	CLA	CMB-C2B	-3.02	1.44	1.50
22	C	502	CLA	C4B-NB	3.02	1.41	1.37
22	b	616	CLA	C4B-NB	3.02	1.41	1.37
34	v	201	HEM	CAC-C3C	3.02	1.55	1.47
22	B	611	CLA	C4B-NB	3.01	1.41	1.37
22	B	605	CLA	C4B-NB	3.01	1.41	1.37
22	c	501	CLA	C4B-NB	3.01	1.41	1.37
22	C	504	CLA	C4B-NB	3.00	1.41	1.37
22	B	612	CLA	C4B-NB	3.00	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	C4B-NB	2.99	1.41	1.37
22	c	506	CLA	C4B-NB	2.99	1.41	1.37
22	A	404	CLA	C4B-NB	2.98	1.41	1.37
24	c	513	BCR	C30-C25	-2.97	1.50	1.53
22	B	613	CLA	C4B-NB	2.97	1.41	1.37
24	B	617	BCR	C30-C25	-2.96	1.50	1.53
22	B	602	CLA	C4B-NB	2.96	1.41	1.37
22	B	603	CLA	C4B-NB	2.96	1.41	1.37
24	b	621	BCR	C30-C25	-2.94	1.50	1.53
30	A	414	SQD	O47-C7	2.94	1.42	1.34
22	b	606	CLA	C4B-NB	2.94	1.41	1.37
30	D	403	SQD	O47-C7	2.93	1.42	1.34
34	F	101	HEM	CAB-C3B	2.92	1.55	1.47
30	d	402	SQD	O47-C7	2.92	1.42	1.34
22	c	504	CLA	C1B-C2B	2.92	1.50	1.43
30	F	102	SQD	O47-C7	2.91	1.42	1.34
30	a	401	SQD	O47-C7	2.90	1.42	1.34
30	a	415	SQD	O47-C7	2.89	1.42	1.34
30	A	413	SQD	O47-C7	2.89	1.42	1.34
34	f	101	HEM	CAB-C3B	2.89	1.55	1.47
22	C	501	CLA	C1B-C2B	2.89	1.49	1.43
22	c	501	CLA	C1B-C2B	2.88	1.49	1.43
22	d	404	CLA	C1B-C2B	2.87	1.49	1.43
22	b	619	CLA	C1B-C2B	2.87	1.49	1.43
22	D	405	CLA	C1B-C2B	2.87	1.49	1.43
23	a	409	PL9	C3-C4	-2.86	1.45	1.49
25	b	601	DGD	C1E-C2E	2.86	1.60	1.52
30	b	602	SQD	O47-C7	2.85	1.42	1.34
22	B	615	CLA	C1B-C2B	2.84	1.49	1.43
22	b	607	CLA	C1B-C2B	2.84	1.49	1.43
30	B	626	SQD	O47-C7	2.84	1.42	1.34
30	f	103	SQD	O47-C7	2.84	1.42	1.34
22	c	511	CLA	C1B-C2B	2.83	1.49	1.43
22	H	101	CLA	C1B-C2B	2.83	1.49	1.43
22	h	101	CLA	C1B-C2B	2.83	1.49	1.43
22	C	504	CLA	C1B-C2B	2.83	1.49	1.43
22	c	503	CLA	C1B-C2B	2.81	1.49	1.43
22	C	503	CLA	C1B-C2B	2.81	1.49	1.43
22	B	603	CLA	C1B-C2B	2.81	1.49	1.43
22	b	609	CLA	C1B-C2B	2.81	1.49	1.43
22	b	618	CLA	C1B-C2B	2.80	1.49	1.43
22	c	510	CLA	C1B-C2B	2.79	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	406	PL9	C7-C3	-2.79	1.47	1.51
22	b	617	CLA	C1B-C2B	2.79	1.49	1.43
22	B	604	CLA	C1B-C2B	2.79	1.49	1.43
22	b	616	CLA	C1B-C2B	2.79	1.49	1.43
22	B	614	CLA	C1B-C2B	2.79	1.49	1.43
22	C	510	CLA	C1B-C2B	2.79	1.49	1.43
22	C	511	CLA	C1B-C2B	2.78	1.49	1.43
25	B	625	DGD	C1E-C2E	2.78	1.60	1.52
22	C	502	CLA	C1B-C2B	2.78	1.49	1.43
22	B	608	CLA	C1B-C2B	2.78	1.49	1.43
22	D	406	CLA	C1B-C2B	2.78	1.49	1.43
22	B	601	CLA	C1B-C2B	2.78	1.49	1.43
22	a	406	CLA	C1B-C2B	2.78	1.49	1.43
22	B	613	CLA	C1B-C2B	2.77	1.49	1.43
22	B	611	CLA	C1B-C2B	2.77	1.49	1.43
22	b	605	CLA	C1B-C2B	2.77	1.49	1.43
22	B	605	CLA	C1B-C2B	2.77	1.49	1.43
22	b	610	CLA	C1B-C2B	2.76	1.49	1.43
22	d	405	CLA	C1B-C2B	2.76	1.49	1.43
22	B	606	CLA	C1B-C2B	2.76	1.49	1.43
22	B	602	CLA	C1B-C2B	2.76	1.49	1.43
22	b	615	CLA	C1B-C2B	2.76	1.49	1.43
22	c	512	CLA	C1B-C2B	2.76	1.49	1.43
22	b	612	CLA	C1B-C2B	2.76	1.49	1.43
22	b	608	CLA	C1B-C2B	2.76	1.49	1.43
22	c	520	CLA	C1B-C2B	2.76	1.49	1.43
22	c	502	CLA	C1B-C2B	2.75	1.49	1.43
22	C	505	CLA	C1B-C2B	2.75	1.49	1.43
22	B	612	CLA	C1B-C2B	2.75	1.49	1.43
22	C	512	CLA	C1B-C2B	2.75	1.49	1.43
34	V	201	HEM	FE-NC	2.74	2.04	1.95
22	b	606	CLA	C1B-C2B	2.74	1.49	1.43
22	C	509	CLA	C1B-C2B	2.73	1.49	1.43
22	A	405	CLA	C1B-C2B	2.73	1.49	1.43
22	c	508	CLA	C1B-C2B	2.73	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	613	CLA	C1B-C2B	2.72	1.49	1.43
22	c	505	CLA	C1B-C2B	2.71	1.49	1.43
22	C	508	CLA	C1B-C2B	2.71	1.49	1.43
22	A	404	CLA	C1B-C2B	2.71	1.49	1.43
22	a	408	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	C1B-C2B	2.70	1.49	1.43
22	B	607	CLA	C1B-C2B	2.70	1.49	1.43
22	C	520	CLA	C1B-C2B	2.70	1.49	1.43
22	a	405	CLA	C1B-C2B	2.69	1.49	1.43
25	C	515	DGD	O2G-C2G	-2.69	1.40	1.46
23	D	407	PL9	C3-C4	-2.68	1.45	1.49
22	a	404	CLA	C3B-C4B	2.67	1.50	1.42
22	A	402	CLA	C3B-C4B	2.67	1.50	1.42
22	C	507	CLA	C1B-C2B	2.66	1.49	1.43
23	d	406	PL9	C3-C4	-2.66	1.45	1.49
22	B	609	CLA	C1B-C2B	2.65	1.49	1.43
22	b	611	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	2.64	1.49	1.43
32	D	402	PHO	CMC-C2C	-2.62	1.46	1.50
23	D	407	PL9	C7-C3	-2.60	1.47	1.51
22	c	507	CLA	C1B-C2B	2.59	1.49	1.43
22	A	402	CLA	C1B-C2B	2.59	1.49	1.43
32	a	407	PHO	C3D-C4D	2.58	1.44	1.41
22	a	404	CLA	C1B-C2B	2.57	1.49	1.43
32	D	402	PHO	C3D-C4D	2.56	1.44	1.41
32	D	401	PHO	C3D-C4D	2.56	1.44	1.41
32	a	407	PHO	CMC-C2C	-2.55	1.46	1.50
32	D	401	PHO	CMC-C2C	-2.54	1.46	1.50
23	J	101	PL9	C7-C3	-2.54	1.47	1.51
32	d	401	PHO	CMC-C2C	-2.53	1.46	1.50
32	d	401	PHO	C3D-C4D	2.51	1.44	1.41
32	d	401	PHO	CMD-C2D	-2.48	1.46	1.51
23	a	409	PL9	C7-C3	-2.48	1.48	1.51
22	c	508	CLA	C3B-C4B	2.48	1.49	1.42
22	a	405	CLA	C3B-C4B	2.46	1.49	1.42
32	D	402	PHO	CMD-C2D	-2.46	1.46	1.51
22	b	614	CLA	MG-NB	-2.45	2.00	2.05
22	C	508	CLA	C3B-C4B	2.45	1.49	1.42
31	b	627	LMT	O3'-C3'	-2.45	1.36	1.43
23	j	101	PL9	C7-C3	-2.45	1.48	1.51
32	a	407	PHO	CMD-C2D	-2.45	1.46	1.51
31	M	102	LMT	O3'-C3'	-2.44	1.36	1.43
32	D	401	PHO	CMB-C2B	-2.44	1.46	1.51
32	d	401	PHO	CMB-C2B	-2.44	1.46	1.51
32	D	401	PHO	CMD-C2D	-2.44	1.46	1.51
31	B	623	LMT	O3'-C3'	-2.44	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	610	CLA	MG-NB	-2.43	2.01	2.05
22	A	403	CLA	C3B-C4B	2.43	1.49	1.42
31	D	410	LMT	O3'-C3'	-2.43	1.36	1.43
25	c	515	DGD	O2G-C2G	-2.43	1.40	1.46
22	B	613	CLA	CHC-C1C	2.43	1.43	1.38
31	d	409	LMT	O3'-C3'	-2.42	1.37	1.43
32	D	402	PHO	CAC-C3C	-2.41	1.47	1.51
32	D	402	PHO	CMB-C2B	-2.41	1.46	1.51
32	a	407	PHO	CMB-C2B	-2.41	1.46	1.51
31	M	103	LMT	O3'-C3'	-2.40	1.37	1.43
22	h	101	CLA	CHC-C1C	2.40	1.43	1.38
22	d	405	CLA	C3B-C4B	2.39	1.49	1.42
32	d	401	PHO	CAC-C3C	-2.39	1.47	1.51
22	c	520	CLA	C3B-C4B	2.39	1.49	1.42
22	B	608	CLA	CHC-C1C	2.39	1.43	1.38
31	b	603	LMT	O3'-C3'	-2.39	1.37	1.43
22	C	505	CLA	C3B-C4B	2.39	1.49	1.42
22	C	520	CLA	C3B-C4B	2.38	1.49	1.42
22	c	509	CLA	C3B-C4B	2.38	1.49	1.42
22	c	505	CLA	C3B-C4B	2.38	1.49	1.42
31	I	102	LMT	O3'-C3'	-2.38	1.37	1.43
22	b	612	CLA	C3B-C4B	2.37	1.49	1.42
22	b	605	CLA	C3B-C4B	2.37	1.49	1.42
31	b	626	LMT	O3'-C3'	-2.37	1.37	1.43
22	B	601	CLA	C3B-C4B	2.37	1.49	1.42
22	B	613	CLA	C3B-C4B	2.37	1.49	1.42
22	b	612	CLA	CHC-C1C	2.37	1.43	1.38
22	H	101	CLA	CHC-C1C	2.37	1.43	1.38
31	B	622	LMT	O3'-C3'	-2.36	1.37	1.43
22	B	607	CLA	C3B-C4B	2.36	1.49	1.42
22	H	101	CLA	C3B-C4B	2.36	1.49	1.42
22	h	101	CLA	C3B-C4B	2.36	1.49	1.42
22	b	611	CLA	C3B-C4B	2.36	1.49	1.42
22	C	507	CLA	C3B-C4B	2.35	1.49	1.42
23	D	407	PL9	C6-C1	-2.35	1.44	1.48
22	c	510	CLA	C3B-C4B	2.35	1.49	1.42
31	B	627	LMT	O3'-C3'	-2.35	1.37	1.43
31	b	604	LMT	O3'-C3'	-2.35	1.37	1.43
22	b	606	CLA	C3B-C4B	2.35	1.49	1.42
22	c	512	CLA	C3B-C4B	2.35	1.49	1.42
31	i	102	LMT	O3'-C3'	-2.34	1.37	1.43
22	B	608	CLA	C3B-C4B	2.34	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	406	CLA	C3B-C4B	2.34	1.49	1.42
22	c	511	CLA	C3B-C4B	2.34	1.49	1.42
22	B	607	CLA	CHC-C1C	2.34	1.43	1.38
22	B	615	CLA	C3B-C4B	2.34	1.49	1.42
25	B	625	DGD	C4D-C5D	2.34	1.58	1.53
22	C	512	CLA	C3B-C4B	2.34	1.49	1.42
25	C	516	DGD	O2G-C2G	-2.34	1.41	1.46
22	b	611	CLA	CHC-C1C	2.34	1.43	1.38
22	a	404	CLA	CHC-C1C	2.34	1.43	1.38
32	D	401	PHO	CAC-C3C	-2.34	1.47	1.51
22	C	509	CLA	C3B-C4B	2.34	1.49	1.42
32	a	407	PHO	CAC-C3C	-2.34	1.47	1.51
22	C	511	CLA	C3B-C4B	2.34	1.49	1.42
22	a	408	CLA	C3B-C4B	2.34	1.49	1.42
22	C	510	CLA	C3B-C4B	2.34	1.49	1.42
22	c	502	CLA	CHC-C1C	2.34	1.43	1.38
22	d	404	CLA	C3B-C4B	2.33	1.49	1.42
22	B	611	CLA	CMD-C2D	-2.33	1.46	1.50
22	c	507	CLA	C3B-C4B	2.33	1.49	1.42
22	B	612	CLA	C3B-C4B	2.33	1.49	1.42
22	d	405	CLA	CHC-C1C	2.33	1.43	1.38
22	a	406	CLA	C3B-C4B	2.33	1.49	1.42
22	C	512	CLA	CHC-C1C	2.33	1.43	1.38
22	D	405	CLA	CHC-C1C	2.33	1.43	1.38
22	b	619	CLA	C3B-C4B	2.33	1.49	1.42
22	B	614	CLA	C3B-C4B	2.33	1.49	1.42
22	b	606	CLA	CHC-C1C	2.33	1.43	1.38
22	b	618	CLA	C3B-C4B	2.33	1.49	1.42
22	c	512	CLA	CHC-C1C	2.33	1.43	1.38
22	b	614	CLA	C1B-C2B	2.32	1.48	1.43
22	b	616	CLA	C3B-C4B	2.32	1.49	1.42
22	c	507	CLA	CHC-C1C	2.31	1.43	1.38
22	b	617	CLA	C3B-C4B	2.31	1.49	1.42
22	b	615	CLA	C3B-C4B	2.31	1.49	1.42
22	D	405	CLA	C3B-C4B	2.31	1.49	1.42
22	A	404	CLA	C3B-C4B	2.31	1.49	1.42
22	C	506	CLA	C3B-C4B	2.31	1.49	1.42
22	b	617	CLA	CHC-C1C	2.31	1.43	1.38
22	B	611	CLA	C3B-C4B	2.31	1.49	1.42
22	B	605	CLA	C3B-C4B	2.31	1.49	1.42
22	d	404	CLA	CHC-C1C	2.31	1.43	1.38
22	C	509	CLA	CHC-C1C	2.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	503	CLA	C3B-C4B	2.30	1.49	1.42
22	B	609	CLA	C3B-C4B	2.30	1.49	1.42
22	c	511	CLA	CHC-C1C	2.30	1.43	1.38
22	B	602	CLA	C3B-C4B	2.30	1.49	1.42
22	b	615	CLA	CMD-C2D	-2.30	1.46	1.50
22	C	505	CLA	CHC-C1C	2.29	1.43	1.38
22	c	509	CLA	CHC-C1C	2.29	1.43	1.38
22	b	616	CLA	CHC-C1C	2.29	1.43	1.38
22	c	502	CLA	C3B-C4B	2.29	1.49	1.42
27	D	412	LMG	O7-C8	-2.29	1.41	1.46
22	B	604	CLA	C3B-C4B	2.29	1.49	1.42
22	C	504	CLA	CHC-C1C	2.29	1.43	1.38
22	b	613	CLA	C3B-C4B	2.29	1.49	1.42
22	b	608	CLA	C3B-C4B	2.29	1.49	1.42
22	C	511	CLA	CHC-C1C	2.29	1.43	1.38
22	B	606	CLA	C3B-C4B	2.29	1.49	1.42
22	C	503	CLA	C3B-C4B	2.29	1.49	1.42
22	C	502	CLA	C3B-C4B	2.28	1.49	1.42
31	B	628	LMT	O3'-C3'	-2.28	1.37	1.43
31	I	102	LMT	O2'-C2'	-2.28	1.37	1.43
22	B	610	CLA	C1B-C2B	2.28	1.48	1.43
22	B	609	CLA	CHC-C1C	2.28	1.43	1.38
22	b	609	CLA	C3B-C4B	2.28	1.49	1.42
22	C	501	CLA	C3B-C4B	2.27	1.49	1.42
22	c	505	CLA	CHC-C1C	2.27	1.43	1.38
22	A	405	CLA	C3B-C4B	2.27	1.49	1.42
22	B	602	CLA	CHC-C1C	2.27	1.43	1.38
22	a	406	CLA	CHC-C1C	2.27	1.43	1.38
22	C	510	CLA	CHC-C1C	2.27	1.43	1.38
22	B	614	CLA	CHC-C1C	2.27	1.43	1.38
22	A	402	CLA	CHC-C1C	2.27	1.43	1.38
22	c	504	CLA	C3B-C4B	2.26	1.49	1.42
22	C	506	CLA	CHC-C1C	2.26	1.43	1.38
22	b	610	CLA	C3B-C4B	2.26	1.49	1.42
22	b	618	CLA	CHC-C1C	2.26	1.43	1.38
23	a	409	PL9	C53-C6	-2.26	1.46	1.50
22	C	508	CLA	CHC-C1C	2.26	1.43	1.38
23	A	406	PL9	C7-C3	-2.26	1.48	1.51
22	c	510	CLA	CHC-C1C	2.26	1.43	1.38
22	B	605	CLA	CHC-C1C	2.26	1.43	1.38
26	a	412	LHG	O7-C5	-2.26	1.41	1.46
22	c	504	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	CHC-C1C	2.26	1.43	1.38
22	a	408	CLA	CHC-C1C	2.26	1.43	1.38
22	b	613	CLA	CHC-C1C	2.26	1.43	1.38
22	B	604	CLA	CHC-C1C	2.26	1.43	1.38
22	C	504	CLA	C3B-C4B	2.25	1.49	1.42
22	b	607	CLA	CHC-C1C	2.25	1.43	1.38
25	c	516	DGD	O2G-C2G	-2.25	1.41	1.46
22	b	608	CLA	CHC-C1C	2.25	1.43	1.38
22	b	607	CLA	C3B-C4B	2.25	1.49	1.42
22	c	506	CLA	C3B-C4B	2.25	1.49	1.42
22	A	404	CLA	CHC-C1C	2.25	1.43	1.38
22	B	603	CLA	CHC-C1C	2.24	1.43	1.38
22	B	612	CLA	CHC-C1C	2.24	1.43	1.38
22	c	503	CLA	CHC-C1C	2.24	1.43	1.38
22	c	508	CLA	CHC-C1C	2.24	1.43	1.38
31	i	102	LMT	O2'-C2'	-2.24	1.37	1.43
27	d	410	LMG	O7-C8	-2.23	1.41	1.46
23	A	406	PL9	C53-C6	-2.23	1.46	1.50
22	B	603	CLA	C3B-C4B	2.23	1.49	1.42
25	b	624	DGD	O2G-C2G	-2.23	1.41	1.46
31	M	102	LMT	O3B-C3B	-2.23	1.37	1.43
22	c	504	CLA	CMD-C2D	-2.23	1.46	1.50
22	B	606	CLA	CHC-C1C	2.23	1.42	1.38
22	D	406	CLA	CHC-C1C	2.23	1.42	1.38
22	c	520	CLA	CHC-C1C	2.22	1.42	1.38
22	A	403	CLA	CHC-C1C	2.22	1.42	1.38
22	B	601	CLA	CHC-C1C	2.22	1.42	1.38
27	b	625	LMG	C4-C5	2.21	1.57	1.53
22	C	507	CLA	CHC-C1C	2.21	1.42	1.38
22	C	520	CLA	CHC-C1C	2.21	1.42	1.38
22	b	609	CLA	CHC-C1C	2.21	1.42	1.38
25	b	601	DGD	C4D-C5D	2.21	1.57	1.53
25	B	620	DGD	O2G-C2G	-2.21	1.41	1.46
31	B	628	LMT	O3B-C3B	-2.21	1.37	1.43
22	C	501	CLA	CHC-C1C	2.21	1.42	1.38
22	c	501	CLA	C3B-C4B	2.21	1.49	1.42
22	c	506	CLA	CHC-C1C	2.21	1.42	1.38
22	b	619	CLA	CHC-C1C	2.20	1.42	1.38
22	C	503	CLA	CHC-C1C	2.20	1.42	1.38
23	A	406	PL9	C6-C1	-2.20	1.44	1.48
22	c	507	CLA	CMB-C2B	-2.20	1.46	1.50
22	C	507	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	CHC-C1C	2.20	1.42	1.38
31	b	604	LMT	O3B-C3B	-2.19	1.37	1.43
22	c	509	CLA	CMD-C2D	-2.19	1.46	1.50
31	b	627	LMT	O3B-C3B	-2.19	1.37	1.43
22	B	615	CLA	CHC-C1C	2.18	1.42	1.38
22	C	504	CLA	CMD-C2D	-2.18	1.46	1.50
22	b	615	CLA	CHC-C1C	2.18	1.42	1.38
30	b	602	SQD	O2-C2	-2.18	1.37	1.43
31	M	103	LMT	O3B-C3B	-2.18	1.37	1.43
31	I	102	LMT	O2B-C2B	-2.17	1.37	1.43
22	b	605	CLA	CHC-C1C	2.17	1.42	1.38
31	B	627	LMT	O2'-C2'	-2.17	1.37	1.43
31	b	603	LMT	O3B-C3B	-2.17	1.37	1.43
31	B	622	LMT	O3B-C3B	-2.17	1.37	1.43
22	C	509	CLA	CMD-C2D	-2.16	1.46	1.50
30	B	626	SQD	O2-C2	-2.16	1.37	1.43
31	B	623	LMT	O3B-C3B	-2.16	1.37	1.43
26	c	519	LHG	P-O6	2.16	1.67	1.59
22	B	607	CLA	CMD-C2D	-2.15	1.46	1.50
22	c	501	CLA	CHC-C1C	2.15	1.42	1.38
22	a	405	CLA	CHC-C1C	2.15	1.42	1.38
31	I	102	LMT	O3B-C3B	-2.15	1.37	1.43
22	B	611	CLA	CHC-C1C	2.15	1.42	1.38
22	A	405	CLA	CHC-C1C	2.14	1.42	1.38
31	i	102	LMT	O2B-C2B	-2.14	1.37	1.43
31	D	410	LMT	O3B-C3B	-2.14	1.37	1.43
31	d	409	LMT	O3B-C3B	-2.14	1.37	1.43
26	c	519	LHG	O7-C5	-2.14	1.41	1.46
22	b	606	CLA	MG-NB	-2.14	2.01	2.05
22	b	611	CLA	CMD-C2D	-2.14	1.46	1.50
31	b	603	LMT	O2'-C2'	-2.13	1.37	1.43
31	M	102	LMT	O2'-C2'	-2.13	1.37	1.43
22	B	603	CLA	CMD-C2D	-2.13	1.46	1.50
22	A	404	CLA	MG-NB	-2.13	2.01	2.05
26	C	519	LHG	O7-C5	-2.12	1.41	1.46
31	b	626	LMT	O3B-C3B	-2.12	1.37	1.43
22	A	402	CLA	CMD-C2D	-2.12	1.46	1.50
31	M	103	LMT	O2'-C2'	-2.11	1.37	1.43
23	J	101	PL9	C3-C4	-2.11	1.46	1.49
34	V	201	HEM	CMB-C2B	2.11	1.55	1.50
27	B	621	LMG	C4-C5	2.11	1.57	1.53
31	i	102	LMT	O3B-C3B	-2.11	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	CMC-C2C	2.11	1.55	1.50
31	B	627	LMT	O3B-C3B	-2.11	1.37	1.43
25	B	625	DGD	C3G-C2G	2.11	1.57	1.50
23	a	409	PL9	C6-C1	-2.11	1.45	1.48
23	d	406	PL9	C6-C1	-2.11	1.45	1.48
22	a	404	CLA	CMD-C2D	-2.11	1.46	1.50
25	C	515	DGD	O1G-C1G	-2.11	1.40	1.45
22	b	607	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	602	CLA	MG-NB	-2.10	2.01	2.05
22	B	610	CLA	C3B-C4B	2.10	1.48	1.42
31	b	626	LMT	O2'-C2'	-2.10	1.37	1.43
31	b	604	LMT	O2'-C2'	-2.10	1.37	1.43
34	F	101	HEM	CMC-C2C	2.10	1.55	1.50
31	B	622	LMT	O2'-C2'	-2.10	1.37	1.43
34	v	201	HEM	CMD-C2D	2.09	1.55	1.50
22	a	404	CLA	CMB-C2B	-2.09	1.46	1.50
22	b	613	CLA	MG-NB	-2.09	2.01	2.05
34	v	201	HEM	CMB-C2B	2.09	1.55	1.50
22	C	520	CLA	MG-NB	-2.09	2.01	2.05
31	b	627	LMT	O2'-C2'	-2.08	1.37	1.43
22	A	403	CLA	CMB-C2B	-2.08	1.46	1.50
31	B	628	LMT	O2'-C2'	-2.08	1.37	1.43
25	c	516	DGD	O5D-C6D	-2.08	1.40	1.43
31	b	603	LMT	O2B-C2B	-2.08	1.37	1.43
22	b	611	CLA	MG-NB	-2.08	2.01	2.05
24	C	514	BCR	C38-C26	-2.08	1.47	1.50
31	B	627	LMT	O2B-C2B	-2.08	1.37	1.43
22	B	604	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	601	DGD	C3G-C2G	2.08	1.57	1.50
22	B	609	CLA	CMB-C2B	-2.08	1.46	1.50
22	c	506	CLA	MG-NB	-2.08	2.01	2.05
22	b	611	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	607	CLA	CMB-C2B	-2.07	1.46	1.50
22	b	608	CLA	CMD-C2D	-2.07	1.46	1.50
27	a	402	LMG	O7-C8	-2.07	1.41	1.46
22	A	404	CLA	CMD-C2D	-2.07	1.46	1.50
22	C	505	CLA	CMB-C2B	-2.07	1.46	1.50
22	C	508	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	603	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	612	CLA	MG-NB	-2.07	2.01	2.05
22	C	502	CLA	MG-NB	-2.07	2.01	2.05
22	b	607	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	BCR	C38-C26	-2.07	1.47	1.50
34	V	201	HEM	CMD-C2D	2.07	1.55	1.50
22	a	406	CLA	CMD-C2D	-2.07	1.46	1.50
23	j	101	PL9	C3-C4	-2.06	1.46	1.49
22	c	503	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	405	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	405	CLA	MG-NB	-2.06	2.01	2.05
22	B	605	CLA	MG-NB	-2.06	2.01	2.05
22	A	402	CLA	CMB-C2B	-2.06	1.46	1.50
31	M	102	LMT	O2B-C2B	-2.06	1.37	1.43
27	B	624	LMG	O7-C8	-2.06	1.41	1.46
22	B	611	CLA	MG-NB	-2.06	2.01	2.05
25	d	408	DGD	C1D-C2D	2.06	1.58	1.52
25	d	408	DGD	O1G-C1G	-2.06	1.40	1.45
31	M	103	LMT	O2B-C2B	-2.06	1.37	1.43
22	B	602	CLA	CMD-C2D	-2.06	1.46	1.50
22	b	619	CLA	CMC-C2C	-2.06	1.46	1.50
22	A	404	CLA	CMB-C2B	-2.05	1.46	1.50
22	c	505	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	502	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	609	CLA	MG-NB	-2.05	2.01	2.05
22	A	403	CLA	CMD-C2D	-2.05	1.46	1.50
31	M	102	LMT	O1'-C1'	-2.05	1.36	1.40
22	C	503	CLA	CMD-C2D	-2.05	1.46	1.50
25	a	411	DGD	O1G-C1G	-2.05	1.40	1.45
22	C	509	CLA	CMB-C2B	-2.05	1.46	1.50
27	b	628	LMG	O7-C8	-2.05	1.41	1.46
22	B	603	CLA	MG-NB	-2.05	2.01	2.05
22	c	507	CLA	MG-NB	-2.05	2.01	2.05
22	C	506	CLA	MG-NB	-2.05	2.01	2.05
22	c	502	CLA	MG-NB	-2.05	2.01	2.05
22	B	601	CLA	CMB-C2B	-2.05	1.46	1.50
24	g	101	BCR	C33-C5	-2.05	1.47	1.50
26	A	409	LHG	O7-C5	-2.05	1.41	1.46
22	b	619	CLA	CMD-C2D	-2.04	1.46	1.50
22	c	508	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	614	CLA	C3B-C4B	2.04	1.48	1.42
22	C	511	CLA	MG-NB	-2.04	2.01	2.05
22	a	405	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	605	CLA	CMB-C2B	-2.04	1.46	1.50
31	B	623	LMT	O2'-C2'	-2.04	1.37	1.43
22	B	607	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	406	CLA	CMB-C2B	-2.04	1.46	1.50
22	D	406	CLA	MG-NB	-2.04	2.01	2.05
22	C	501	CLA	CMB-C2B	-2.04	1.46	1.50
22	a	405	CLA	CMB-C2B	-2.04	1.46	1.50
22	a	408	CLA	CMD-C2D	-2.04	1.46	1.50
22	C	507	CLA	CMD-C2D	-2.04	1.46	1.50
22	c	509	CLA	CMB-C2B	-2.03	1.46	1.50
27	A	415	LMG	O7-C8	-2.03	1.41	1.46
22	b	617	CLA	MG-NB	-2.03	2.01	2.05
22	B	605	CLA	CMB-C2B	-2.03	1.46	1.50
22	c	507	CLA	CMD-C2D	-2.03	1.46	1.50
23	D	407	PL9	C53-C6	-2.03	1.46	1.50
22	C	504	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	613	CLA	CMB-C2B	-2.03	1.46	1.50
22	c	502	CLA	CMC-C2C	-2.03	1.46	1.50
22	c	502	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	615	CLA	CMD-C2D	-2.03	1.46	1.50
22	C	502	CLA	CMD-C2D	-2.03	1.46	1.50
22	H	101	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	610	CLA	CMD-C2D	-2.03	1.46	1.50
22	C	502	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	615	CLA	CMC-C2C	-2.03	1.46	1.50
22	b	615	CLA	MG-NB	-2.03	2.01	2.05
31	M	102	LMT	O4'-C4B	-2.03	1.37	1.43
22	C	507	CLA	MG-NB	-2.03	2.01	2.05
31	b	626	LMT	O2B-C2B	-2.03	1.37	1.43
22	B	613	CLA	MG-NB	-2.03	2.01	2.05
22	b	610	CLA	MG-NB	-2.03	2.01	2.05
22	B	606	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	615	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	608	CLA	CMB-C2B	-2.03	1.46	1.50
30	d	402	SQD	O2-C2	-2.02	1.37	1.43
22	b	612	CLA	CMD-C2D	-2.02	1.46	1.50
30	b	602	SQD	O3-C3	-2.02	1.37	1.43
31	d	409	LMT	O2'-C2'	-2.02	1.37	1.43
22	C	503	CLA	MG-NB	-2.02	2.01	2.05
22	C	511	CLA	CMD-C2D	-2.02	1.46	1.50
22	H	101	CLA	CMD-C2D	-2.02	1.46	1.50
22	D	405	CLA	CMB-C2B	-2.02	1.46	1.50
22	h	101	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	501	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	626	SQD	O3-C3	-2.02	1.38	1.43
31	D	410	LMT	O2B-C2B	-2.02	1.38	1.43
22	b	609	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	520	CLA	CMB-C2B	-2.02	1.46	1.50
22	c	520	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	605	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	509	CLA	MG-NB	-2.02	2.01	2.05
22	C	505	CLA	CMD-C2D	-2.02	1.46	1.50
22	b	610	CLA	CMB-C2B	-2.02	1.46	1.50
22	d	404	CLA	CMB-C2B	-2.02	1.46	1.50
31	B	628	LMT	O4'-C4B	-2.02	1.38	1.43
22	b	617	CLA	CMD-C2D	-2.02	1.46	1.50
30	f	103	SQD	O2-C2	-2.02	1.38	1.43
22	b	607	CLA	MG-NB	-2.02	2.01	2.05
22	B	609	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	511	CLA	CMD-C2D	-2.02	1.46	1.50
22	b	609	CLA	CMB-C2B	-2.02	1.46	1.50
31	B	628	LMT	O2B-C2B	-2.01	1.38	1.43
22	A	405	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	606	CLA	CMD-C2D	-2.01	1.46	1.50
22	C	520	CLA	CMB-C2B	-2.01	1.46	1.50
22	a	408	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	502	CLA	CMB-C2B	-2.01	1.46	1.50
22	b	606	CLA	CMD-C2D	-2.01	1.46	1.50
34	v	201	HEM	CMA-C3A	2.01	1.54	1.50
34	F	101	HEM	CMA-C3A	2.01	1.54	1.50
22	B	601	CLA	CMD-C2D	-2.01	1.46	1.50
22	C	510	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	501	CLA	CMD-C2D	-2.01	1.46	1.50
31	D	410	LMT	O2'-C2'	-2.01	1.38	1.43
22	D	405	CLA	CMD-C2D	-2.01	1.46	1.50
26	C	519	LHG	P-O6	2.01	1.67	1.59
22	B	604	CLA	CMB-C2B	-2.01	1.46	1.50
22	b	609	CLA	MG-NB	-2.01	2.01	2.05
22	B	614	CLA	CMD-C2D	-2.01	1.46	1.50
22	C	520	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	608	CLA	CMD-C2D	-2.01	1.46	1.50
31	b	603	LMT	O4'-C4B	-2.01	1.38	1.43
24	D	411	BCR	C33-C5	-2.00	1.47	1.50
34	V	201	HEM	CMA-C3A	2.00	1.54	1.50
22	b	608	CLA	CMB-C2B	-2.00	1.46	1.50
22	B	614	CLA	CMB-C2B	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	CMB-C2B	-2.00	1.46	1.50
22	c	503	CLA	MG-NB	-2.00	2.01	2.05
30	D	403	SQD	O2-C2	-2.00	1.38	1.43
22	B	614	CLA	CMC-C2C	-2.00	1.46	1.50
22	B	615	CLA	CMB-C2B	-2.00	1.46	1.50
22	b	619	CLA	CMB-C2B	-2.00	1.46	1.50
22	c	512	CLA	CMB-C2B	-2.00	1.46	1.50
22	b	616	CLA	CMD-C2D	-2.00	1.46	1.50
30	F	102	SQD	O2-C2	-2.00	1.38	1.43
30	a	401	SQD	O47-C45	-2.00	1.41	1.46
22	C	512	CLA	CMB-C2B	-2.00	1.46	1.50
22	b	612	CLA	CMB-C2B	-2.00	1.46	1.50
22	b	618	CLA	CMD-C2D	-2.00	1.46	1.50
22	B	615	CLA	MG-NB	-2.00	2.01	2.05

All (1029) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.16	109.94	106.68
22	c	504	CLA	C4A-NA-C1A	7.08	109.91	106.68
22	C	510	CLA	C4A-NA-C1A	7.06	109.90	106.68
22	B	603	CLA	C4A-NA-C1A	7.02	109.88	106.68
22	B	611	CLA	C4A-NA-C1A	7.02	109.88	106.68
22	b	609	CLA	C4A-NA-C1A	6.98	109.86	106.68
22	b	615	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	b	607	CLA	C4A-NA-C1A	6.94	109.84	106.68
22	a	405	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	520	CLA	C4A-NA-C1A	6.82	109.79	106.68
22	C	501	CLA	C4A-NA-C1A	6.75	109.76	106.68
22	c	503	CLA	C4A-NA-C1A	6.75	109.76	106.68
22	C	503	CLA	C4A-NA-C1A	6.72	109.75	106.68
22	b	616	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	c	510	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	b	618	CLA	C4A-NA-C1A	6.70	109.74	106.68
22	C	520	CLA	C4A-NA-C1A	6.70	109.73	106.68
22	c	501	CLA	C4A-NA-C1A	6.68	109.73	106.68
22	B	605	CLA	C4A-NA-C1A	6.67	109.72	106.68
22	c	511	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	B	615	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	C	512	CLA	C4A-NA-C1A	6.63	109.70	106.68
22	c	512	CLA	C4A-NA-C1A	6.59	109.68	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	C4A-NA-C1A	6.57	109.68	106.68
22	C	511	CLA	C4A-NA-C1A	6.56	109.67	106.68
22	B	604	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	B	614	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	b	619	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	b	608	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	B	606	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	c	506	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	B	612	CLA	C4A-NA-C1A	6.52	109.66	106.68
22	C	505	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	a	406	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	d	404	CLA	C4A-NA-C1A	6.50	109.65	106.68
22	A	405	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	B	609	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	b	617	CLA	C4A-NA-C1A	6.44	109.61	106.68
22	B	607	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	c	505	CLA	C4A-NA-C1A	6.41	109.60	106.68
22	D	405	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	a	408	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	c	508	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	h	101	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	B	602	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	C	507	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	B	613	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	c	507	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	b	610	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	d	405	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	b	611	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	C	502	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	C	508	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	c	502	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	B	601	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	B	608	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	H	101	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	D	406	CLA	C4A-NA-C1A	6.21	109.51	106.68
22	A	404	CLA	C4A-NA-C1A	6.15	109.48	106.68
22	b	605	CLA	C4A-NA-C1A	6.13	109.47	106.68
22	b	606	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	b	613	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	C	509	CLA	C4A-NA-C1A	6.08	109.45	106.68
22	A	402	CLA	C4A-NA-C1A	6.05	109.44	106.68
22	a	404	CLA	C4A-NA-C1A	6.05	109.44	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C4A-NA-C1A	6.01	109.42	106.68
22	b	612	CLA	C4A-NA-C1A	5.99	109.41	106.68
32	D	402	PHO	C4D-CHA-CBD	-5.90	105.62	108.45
32	D	401	PHO	C4D-CHA-CBD	-5.82	105.66	108.45
32	a	407	PHO	C4D-CHA-CBD	-5.76	105.69	108.45
30	b	602	SQD	O6-C1-C2	5.74	116.99	108.27
32	d	401	PHO	C4D-CHA-CBD	-5.73	105.71	108.45
33	D	404	BCT	O2-C-O1	5.58	133.96	119.68
33	d	403	BCT	O2-C-O1	5.56	133.90	119.68
23	j	101	PL9	C7-C3-C4	5.54	121.48	116.91
30	B	626	SQD	O6-C1-C2	5.54	116.68	108.27
23	J	101	PL9	C7-C3-C4	5.46	121.41	116.91
34	v	201	HEM	C4D-ND-C1D	5.40	111.60	105.21
30	a	415	SQD	O6-C1-C2	5.38	116.45	108.27
22	b	614	CLA	C4A-NA-C1A	5.34	109.11	106.68
22	B	610	CLA	C4A-NA-C1A	5.33	109.11	106.68
23	A	406	PL9	C7-C3-C4	5.27	121.25	116.91
34	V	201	HEM	C4D-ND-C1D	5.23	111.41	105.21
23	d	406	PL9	C7-C3-C4	5.20	121.19	116.91
34	f	101	HEM	C4D-ND-C1D	5.16	111.31	105.21
23	D	407	PL9	C7-C3-C4	5.13	121.14	116.91
34	F	101	HEM	C4D-ND-C1D	5.12	111.27	105.21
30	A	413	SQD	O6-C1-C2	5.07	115.97	108.27
23	a	409	PL9	C7-C3-C4	5.03	121.05	116.91
30	D	403	SQD	O6-C1-C2	4.62	115.28	108.27
30	d	402	SQD	O6-C1-C2	4.58	115.22	108.27
25	A	408	DGD	O3G-C3G-C2G	-4.57	99.69	110.82
25	a	411	DGD	O3G-C3G-C2G	-4.57	99.70	110.82
30	A	413	SQD	O9-S-C6	4.42	113.36	106.76
26	a	412	LHG	O4-P-O5	4.40	132.92	112.44
26	C	519	LHG	O4-P-O5	4.38	132.83	112.44
26	c	519	LHG	O4-P-O5	4.38	132.82	112.44
26	A	409	LHG	O4-P-O5	4.38	132.80	112.44
30	d	402	SQD	O5-C5-C4	4.36	117.56	109.70
25	C	517	DGD	O3G-C3G-C2G	-4.30	100.36	110.82
30	D	403	SQD	O5-C5-C4	4.28	117.40	109.70
23	j	101	PL9	C7-C3-C2	-4.23	118.40	123.39
30	a	415	SQD	O9-S-C6	4.23	113.08	106.76
23	J	101	PL9	C7-C3-C2	-4.20	118.44	123.39
23	d	406	PL9	C7-C3-C2	-4.06	118.61	123.39
30	b	602	SQD	O5-C5-C4	4.05	116.99	109.70
30	B	626	SQD	O5-C5-C4	4.04	116.99	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	517	DGD	O3G-C3G-C2G	-4.03	101.01	110.82
24	C	513	BCR	C2-C1-C6	4.02	116.28	110.44
30	A	414	SQD	O5-C5-C4	4.00	116.91	109.70
30	D	403	SQD	O9-S-O7	-4.00	100.83	113.82
30	d	402	SQD	O9-S-O7	-3.99	100.84	113.82
24	c	513	BCR	C2-C1-C6	3.99	116.23	110.44
30	f	103	SQD	O9-S-O7	-3.98	100.86	113.82
30	F	102	SQD	O9-S-O7	-3.98	100.89	113.82
23	D	407	PL9	C7-C3-C2	-3.97	118.71	123.39
23	A	406	PL9	C7-C3-C2	-3.96	118.72	123.39
30	A	413	SQD	O9-S-O7	-3.95	100.98	113.82
30	A	413	SQD	O47-C7-C8	3.94	120.00	111.48
30	a	415	SQD	O9-S-O7	-3.93	101.04	113.82
30	b	602	SQD	O9-S-O7	-3.92	101.07	113.82
30	B	626	SQD	O9-S-O7	-3.92	101.09	113.82
30	a	415	SQD	O47-C7-C8	3.91	119.94	111.48
30	a	401	SQD	O9-S-O7	-3.89	101.16	113.82
30	A	414	SQD	O9-S-O7	-3.86	101.27	113.82
27	d	407	LMG	C1-C2-C3	-3.85	101.92	110.01
23	a	409	PL9	C7-C3-C2	-3.82	118.88	123.39
27	D	408	LMG	C1-C2-C3	-3.80	102.02	110.01
30	a	401	SQD	O5-C5-C4	3.78	116.50	109.70
30	a	415	SQD	O5-C5-C4	3.73	116.42	109.70
32	d	401	PHO	C2B-C1B-NB	-3.72	106.74	109.43
25	d	408	DGD	O6D-C1D-O3G	-3.70	101.29	110.04
25	D	409	DGD	O6D-C1D-O3G	-3.67	101.37	110.04
30	B	626	SQD	O47-C7-C8	3.66	119.40	111.48
30	A	414	SQD	O7-S-C6	3.65	112.21	106.76
30	b	602	SQD	O47-C7-C8	3.65	119.37	111.48
30	b	602	SQD	O7-S-C6	3.64	112.20	106.76
24	J	102	BCR	C11-C10-C9	-3.64	122.18	127.28
30	f	103	SQD	O5-C5-C4	3.63	116.25	109.70
32	D	401	PHO	C2B-C1B-NB	-3.63	106.81	109.43
30	F	102	SQD	O5-C5-C4	3.61	116.20	109.70
32	D	402	PHO	C2B-C1B-NB	-3.58	106.84	109.43
30	a	401	SQD	O7-S-C6	3.58	112.09	106.76
30	A	413	SQD	O5-C5-C4	3.58	116.14	109.70
30	f	103	SQD	O7-S-C6	3.56	112.06	106.76
25	c	516	DGD	O3G-C3G-C2G	-3.54	102.22	110.82
25	C	516	DGD	O3G-C3G-C2G	-3.53	102.23	110.82
24	J	102	BCR	C3-C4-C5	-3.50	107.82	114.06
24	A	407	BCR	C2-C1-C6	3.49	115.51	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	F	102	SQD	O6-C1-C2	3.49	113.57	108.27
30	B	626	SQD	O7-S-C6	3.49	111.96	106.76
24	J	102	BCR	C2-C1-C6	3.49	115.50	110.44
24	j	102	BCR	C2-C1-C6	3.48	115.50	110.44
24	j	102	BCR	C24-C23-C22	-3.48	121.09	126.23
30	A	414	SQD	O47-C7-C8	3.47	118.98	111.48
32	a	407	PHO	C2B-C1B-NB	-3.45	106.94	109.43
24	j	102	BCR	C3-C4-C5	-3.43	107.94	114.06
24	j	102	BCR	C11-C10-C9	-3.43	122.47	127.28
30	b	602	SQD	O9-S-C6	3.42	111.86	106.76
30	D	403	SQD	O47-C7-C8	3.40	118.84	111.48
30	B	626	SQD	O9-S-C6	3.39	111.82	106.76
30	F	102	SQD	O7-S-C6	3.39	111.82	106.76
30	F	102	SQD	O47-C7-C8	3.37	118.77	111.48
25	c	515	DGD	O3G-C3G-C2G	-3.37	102.63	110.82
25	C	515	DGD	O3G-C3G-C2G	-3.36	102.65	110.82
30	d	402	SQD	O9-S-C6	3.36	111.77	106.76
24	a	410	BCR	C2-C1-C6	3.34	115.29	110.44
30	f	103	SQD	O47-C7-C8	3.33	118.69	111.48
30	D	403	SQD	O9-S-C6	3.33	111.72	106.76
30	d	402	SQD	O47-C7-C8	3.31	118.63	111.48
24	B	618	BCR	C2-C1-C6	3.31	115.24	110.44
25	c	516	DGD	O5D-C6D-C5D	-3.30	101.98	109.42
30	d	402	SQD	C3-C4-C5	3.30	116.22	110.23
25	B	620	DGD	O3G-C3G-C2G	-3.29	102.82	110.82
24	J	102	BCR	C24-C23-C22	-3.27	121.39	126.23
30	a	401	SQD	O47-C7-C8	3.27	118.56	111.48
22	B	603	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
24	b	622	BCR	C2-C1-C6	3.26	115.18	110.44
22	c	503	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
22	b	606	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
30	f	103	SQD	O6-C1-C2	3.21	113.15	108.27
22	b	609	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
25	b	624	DGD	O6D-C1D-O3G	-3.21	102.46	110.04
22	B	613	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
22	c	507	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
22	B	605	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
25	b	624	DGD	O3G-C3G-C2G	-3.19	103.07	110.82
25	c	516	DGD	O6D-C1D-O3G	-3.18	102.53	110.04
22	b	617	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
30	D	403	SQD	O7-S-C6	3.16	111.47	106.76
24	B	619	BCR	C2-C1-C6	3.16	115.03	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	402	CLA	C3B-C4B-NB	-3.16	107.71	110.53
24	f	102	BCR	C29-C30-C25	3.15	115.02	110.44
25	d	408	DGD	O3G-C3G-C2G	-3.15	103.17	110.82
22	a	404	CLA	C3B-C4B-NB	-3.14	107.72	110.53
22	C	502	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
31	B	628	LMT	C1'-O5'-C5'	-3.14	107.59	113.72
24	b	623	BCR	C2-C1-C6	3.14	114.99	110.44
25	B	620	DGD	O6D-C1D-O3G	-3.13	102.64	110.04
32	D	402	PHO	O1D-CGD-CBD	3.13	129.47	124.72
30	a	415	SQD	C3-C4-C5	3.12	115.89	110.23
22	C	504	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
22	C	503	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
25	A	408	DGD	O6D-C1D-O3G	-3.11	102.70	110.04
24	J	102	BCR	C7-C8-C9	-3.11	121.64	126.23
22	B	604	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
32	a	407	PHO	O1D-CGD-CBD	3.09	129.41	124.72
32	d	401	PHO	O1D-CGD-CBD	3.09	129.41	124.72
30	D	403	SQD	C3-C4-C5	3.09	115.84	110.23
24	c	521	BCR	C2-C1-C6	3.09	114.92	110.44
30	a	401	SQD	O9-S-C6	3.08	111.36	106.76
24	g	101	BCR	C33-C5-C6	-3.08	121.12	124.48
25	C	516	DGD	O5D-C6D-C5D	-3.08	102.47	109.42
22	C	505	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
24	b	621	BCR	C15-C14-C13	-3.08	122.96	127.28
22	b	607	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
22	b	610	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
22	c	504	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
30	a	401	SQD	C44-O6-C1	3.07	120.37	113.80
25	B	625	DGD	O5D-C1E-C2E	3.07	112.93	108.27
30	a	415	SQD	O7-S-C6	3.06	111.33	106.76
24	b	622	BCR	C24-C23-C22	-3.06	121.71	126.23
22	c	502	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
25	D	409	DGD	O3G-C3G-C2G	-3.05	103.40	110.82
24	j	102	BCR	C7-C8-C9	-3.05	121.72	126.23
25	C	516	DGD	O6D-C1D-O3G	-3.05	102.84	110.04
22	B	606	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
30	A	413	SQD	C3-C4-C5	3.04	115.75	110.23
24	D	411	BCR	C29-C30-C25	3.04	114.86	110.44
22	B	608	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
30	A	413	SQD	O7-S-C6	3.04	111.29	106.76
22	C	507	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
22	b	612	CLA	O2D-CGD-O1D	-3.03	117.96	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
22	b	605	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
22	c	505	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
25	c	517	DGD	C1D-C2D-C3D	-3.01	103.68	110.01
24	y	101	BCR	C33-C5-C6	-3.01	121.20	124.48
22	C	508	CLA	C3B-C4B-NB	-3.01	107.84	110.53
24	B	617	BCR	C15-C16-C17	-3.01	117.37	123.52
25	c	515	DGD	O6D-C1D-O3G	-3.01	102.94	110.04
31	b	604	LMT	C1'-O5'-C5'	-3.00	107.85	113.72
24	J	102	BCR	C27-C26-C25	3.00	126.76	122.70
22	b	611	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
30	d	402	SQD	O7-S-C6	3.00	111.23	106.76
22	b	613	CLA	C3B-C4B-NB	-3.00	107.86	110.53
32	D	401	PHO	O1D-CGD-CBD	2.99	129.26	124.72
24	j	102	BCR	C15-C14-C13	-2.99	123.09	127.28
24	H	102	BCR	C33-C5-C6	-2.98	121.23	124.48
22	b	608	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	c	508	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	C	510	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
25	b	601	DGD	O5D-C1E-C2E	2.97	112.78	108.27
22	H	101	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
22	a	406	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	C	521	BCR	C2-C1-C6	2.96	114.74	110.44
24	y	101	BCR	C27-C26-C25	2.96	126.70	122.70
22	a	404	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	c	511	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
25	C	515	DGD	O6D-C1D-O3G	-2.95	103.08	110.04
24	B	618	BCR	C29-C30-C25	2.95	114.72	110.44
25	a	411	DGD	O6D-C1D-O3G	-2.95	103.08	110.04
22	c	509	CLA	C3B-C4B-NB	-2.95	107.90	110.53
22	C	506	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
31	B	623	LMT	C3'-C4'-C5'	-2.94	104.42	110.93
22	B	613	CLA	C3B-C4B-NB	-2.94	107.91	110.53
25	C	517	DGD	C1D-C2D-C3D	-2.94	103.83	110.01
31	i	102	LMT	O1'-C1'-C2'	2.93	112.73	108.27
22	B	601	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	B	607	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	b	613	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
24	b	622	BCR	C29-C30-C25	2.92	114.69	110.44
22	c	506	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	A	403	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	B	612	CLA	O2D-CGD-O1D	-2.92	118.16	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	628	LMG	O6-C1-O1	-2.92	103.14	110.04
22	B	609	CLA	C3B-C4B-NB	-2.92	107.92	110.53
24	b	621	BCR	C15-C16-C17	-2.92	117.54	123.52
24	x	101	BCR	C33-C5-C6	-2.92	121.30	124.48
22	b	611	CLA	C3B-C4B-NB	-2.92	107.93	110.53
22	D	406	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	c	512	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	g	101	BCR	C27-C26-C25	2.91	126.64	122.70
22	c	520	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
25	B	625	DGD	C1D-C2D-C3D	-2.91	103.88	110.01
22	A	402	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	b	616	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	C	501	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
25	b	601	DGD	C1D-C2D-C3D	-2.90	103.91	110.01
22	C	512	CLA	C3B-C4B-NB	-2.90	107.94	110.53
30	F	102	SQD	O8-S-C6	2.90	111.57	105.97
22	c	502	CLA	C3B-C4B-NB	-2.90	107.94	110.53
24	D	411	BCR	C33-C5-C6	-2.90	121.33	124.48
34	F	101	HEM	C3B-C4B-NB	-2.89	107.39	109.47
30	A	414	SQD	C44-O6-C1	2.89	120.00	113.80
30	f	103	SQD	O8-S-C6	2.89	111.55	105.97
22	B	614	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
34	f	101	HEM	C3B-C4B-NB	-2.89	107.39	109.47
24	j	102	BCR	C27-C26-C25	2.89	126.61	122.70
22	c	510	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
22	C	509	CLA	C3B-C4B-NB	-2.88	107.95	110.53
24	B	617	BCR	C15-C14-C13	-2.88	123.24	127.28
22	C	520	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	A	404	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
30	A	414	SQD	O9-S-C6	2.88	111.06	106.76
23	D	407	PL9	C22-C23-C24	-2.88	121.03	127.62
26	a	412	LHG	O8-C23-C24	2.87	120.60	111.83
31	I	102	LMT	O1'-C1'-C2'	2.87	112.63	108.27
27	B	624	LMG	O6-C1-O1	-2.87	103.26	110.04
22	d	405	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
30	B	626	SQD	C3-C4-C5	2.87	115.43	110.23
25	C	517	DGD	CDB-CCB-CBB	-2.86	99.90	114.37
24	f	102	BCR	C33-C5-C6	-2.86	121.36	124.48
22	C	511	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	C	520	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	c	512	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	c	517	DGD	CDB-CCB-CBB	-2.86	99.92	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	501	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
31	b	627	LMT	C3'-C4'-C5'	-2.86	104.59	110.93
22	b	617	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	A	404	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	B	607	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	b	612	CLA	C3B-C4B-NB	-2.86	107.98	110.53
24	B	617	BCR	C33-C5-C6	-2.86	121.37	124.48
22	d	404	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	J	102	BCR	C15-C14-C13	-2.85	123.29	127.28
26	A	409	LHG	O8-C23-C24	2.85	120.51	111.83
22	B	603	CLA	C1-C2-C3	-2.84	121.54	126.20
34	F	101	HEM	C3B-C2B-C1B	2.84	108.55	106.41
30	b	602	SQD	C3-C4-C5	2.83	115.37	110.23
22	b	607	CLA	C1-C2-C3	-2.83	121.55	126.20
25	c	516	DGD	CDB-CCB-CBB	-2.83	100.04	114.37
24	y	101	BCR	C7-C8-C9	-2.83	122.04	126.23
22	b	618	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
22	B	609	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
22	D	405	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
32	D	402	PHO	O2D-CGD-O1D	-2.83	118.34	123.85
24	b	620	BCR	C33-C5-C6	-2.83	121.40	124.48
22	a	408	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
22	h	101	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
23	A	406	PL9	C22-C23-C24	-2.82	121.17	127.62
22	B	605	CLA	C3B-C4B-NB	-2.82	108.02	110.53
24	B	616	BCR	C33-C5-C6	-2.82	121.41	124.48
22	c	503	CLA	C3B-C4B-NB	-2.81	108.02	110.53
34	f	101	HEM	C3B-C2B-C1B	2.81	108.52	106.41
25	C	516	DGD	CDB-CCB-CBB	-2.81	100.18	114.37
22	B	611	CLA	C3B-C4B-NB	-2.81	108.03	110.53
22	C	512	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
22	C	511	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	b	615	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	a	409	PL9	C22-C23-C24	-2.79	121.23	127.62
22	b	614	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	d	406	PL9	C22-C23-C24	-2.78	121.25	127.62
24	b	621	BCR	C33-C5-C6	-2.78	121.45	124.48
22	c	509	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
22	C	502	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	c	520	CLA	C3B-C4B-NB	-2.77	108.05	110.53
22	c	507	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	a	405	CLA	O2D-CGD-O1D	-2.77	118.45	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	506	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	b	601	DGD	C3G-C2G-C1G	-2.77	105.33	111.78
25	b	601	DGD	O3G-C3G-C2G	-2.76	104.09	110.82
22	A	405	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
24	C	514	BCR	C15-C16-C17	-2.76	117.88	123.52
22	C	506	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	c	511	CLA	C3B-C4B-NB	-2.76	108.07	110.53
24	y	101	BCR	C38-C26-C25	-2.75	121.48	124.48
22	b	608	CLA	C3B-C4B-NB	-2.75	108.07	110.53
25	c	517	DGD	C1D-O6D-C5D	-2.75	108.36	113.72
23	J	101	PL9	C7-C8-C9	-2.75	122.10	126.83
23	d	406	PL9	C40-C39-C41	2.74	119.98	115.23
24	c	521	BCR	C15-C16-C17	-2.74	117.91	123.52
32	D	401	PHO	O2D-CGD-O1D	-2.74	118.52	123.85
23	J	101	PL9	C22-C23-C24	-2.74	121.35	127.62
25	C	517	DGD	C1D-O6D-C5D	-2.74	108.37	113.72
22	C	509	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
24	B	618	BCR	C24-C23-C22	-2.73	122.19	126.23
22	B	603	CLA	C3B-C4B-NB	-2.73	108.09	110.53
27	C	518	LMG	O6-C1-O1	-2.73	103.60	110.04
25	B	625	DGD	C3G-C2G-C1G	-2.73	105.43	111.78
22	b	619	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
32	d	401	PHO	O2D-CGD-O1D	-2.72	118.55	123.85
24	g	101	BCR	C38-C26-C25	-2.72	121.51	124.48
25	D	409	DGD	CDB-CCB-CBB	-2.72	100.63	114.37
24	b	621	BCR	C28-C27-C26	-2.72	109.21	114.06
22	b	618	CLA	C3B-C4B-NB	-2.72	108.11	110.53
23	j	101	PL9	C22-C23-C24	-2.72	121.41	127.62
24	g	101	BCR	C7-C8-C9	-2.71	122.22	126.23
22	B	610	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
32	a	407	PHO	O2D-CGD-O1D	-2.71	118.58	123.85
22	b	619	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	b	606	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	C	514	BCR	C29-C30-C25	2.70	114.37	110.44
27	c	518	LMG	O6-C1-O1	-2.70	103.66	110.04
24	c	514	BCR	C29-C30-C25	2.70	114.36	110.44
25	d	408	DGD	CDB-CCB-CBB	-2.70	100.71	114.37
23	d	406	PL9	C7-C8-C9	-2.70	122.18	126.83
24	b	623	BCR	C7-C8-C9	-2.70	122.25	126.23
24	c	514	BCR	C11-C10-C9	-2.70	123.50	127.28
32	a	407	PHO	CMB-C2B-C3B	2.70	130.07	124.68
26	c	519	LHG	O8-C23-C24	2.70	120.05	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	C	519	LHG	O8-C23-C24	2.69	120.04	111.83
25	B	625	DGD	O3G-C3G-C2G	-2.69	104.28	110.82
22	b	609	CLA	CHB-C4A-NA	2.69	128.28	124.40
22	A	403	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	B	608	CLA	C3B-C4B-NB	-2.69	108.13	110.53
32	D	402	PHO	CMB-C2B-C3B	2.69	130.06	124.68
22	A	403	CLA	CHB-C4A-NA	2.69	128.28	124.40
24	B	617	BCR	C28-C27-C26	-2.69	109.27	114.06
22	a	406	CLA	C3B-C4B-NB	-2.68	108.14	110.53
27	I	101	LMG	O6-C1-O1	-2.68	103.71	110.04
22	B	614	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	c	514	BCR	C28-C27-C26	-2.68	109.28	114.06
24	C	521	BCR	C15-C16-C17	-2.68	118.04	123.52
23	D	407	PL9	C7-C8-C9	-2.68	122.22	126.83
23	j	101	PL9	C7-C8-C9	-2.67	122.23	126.83
22	B	602	CLA	C3B-C4B-NB	-2.67	108.14	110.53
22	c	510	CLA	C3B-C4B-NB	-2.67	108.15	110.53
22	d	405	CLA	C3B-C4B-NB	-2.67	108.15	110.53
22	a	405	CLA	CHB-C4A-NA	2.67	128.25	124.40
24	C	514	BCR	C28-C27-C26	-2.66	109.31	114.06
27	i	101	LMG	O6-C1-O1	-2.66	103.76	110.04
22	b	607	CLA	C3B-C4B-NB	-2.66	108.16	110.53
24	j	102	BCR	C33-C5-C6	-2.66	121.59	124.48
22	C	503	CLA	C3B-C4B-NB	-2.65	108.16	110.53
22	B	615	CLA	C3B-C4B-NB	-2.65	108.16	110.53
24	b	622	BCR	C11-C10-C9	-2.65	123.56	127.28
24	B	618	BCR	C11-C10-C9	-2.65	123.56	127.28
23	D	407	PL9	C40-C39-C41	2.65	119.82	115.23
24	J	102	BCR	C33-C5-C6	-2.64	121.61	124.48
22	C	504	CLA	C3B-C4B-NB	-2.64	108.18	110.53
24	B	619	BCR	C27-C26-C25	2.64	126.27	122.70
27	E	101	LMG	C1-C2-C3	-2.63	104.47	110.01
24	C	513	BCR	C24-C23-C22	-2.63	122.34	126.23
22	C	510	CLA	CHB-C4A-NA	2.63	128.20	124.40
24	c	521	BCR	C27-C26-C25	2.63	126.26	122.70
24	c	513	BCR	C7-C8-C9	-2.63	122.35	126.23
22	B	610	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
22	D	406	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	c	514	BCR	C15-C16-C17	-2.62	118.17	123.52
22	C	506	CLA	CHB-C4A-NA	2.61	128.17	124.40
24	j	102	BCR	C15-C16-C17	-2.61	118.17	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	C	521	BCR	C27-C26-C25	2.61	126.23	122.70
31	M	102	LMT	C1'-O5'-C5'	-2.60	108.64	113.72
30	F	102	SQD	O9-S-C6	2.60	110.64	106.76
24	b	623	BCR	C27-C26-C25	2.60	126.22	122.70
22	B	603	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	B	619	BCR	C7-C8-C9	-2.60	122.39	126.23
22	c	506	CLA	CHB-C4A-NA	2.60	128.15	124.40
22	C	510	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	B	605	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	b	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
30	d	402	SQD	O8-S-C6	2.59	110.97	105.97
30	B	626	SQD	C4-C3-C2	2.59	115.38	110.83
22	B	615	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
24	C	513	BCR	C15-C16-C17	-2.59	118.22	123.52
31	b	626	LMT	C1'-O5'-C5'	-2.59	108.67	113.72
22	c	501	CLA	C3B-C4B-NB	-2.58	108.23	110.53
22	b	608	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	c	514	BCR	C15-C14-C13	-2.58	123.66	127.28
24	A	407	BCR	C27-C26-C25	2.58	126.19	122.70
24	B	617	BCR	C29-C30-C25	2.58	114.18	110.44
24	b	621	BCR	C29-C30-C25	2.58	114.18	110.44
22	C	501	CLA	C3B-C4B-NB	-2.58	108.23	110.53
30	b	602	SQD	C4-C3-C2	2.57	115.35	110.83
22	c	508	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
22	C	512	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	c	520	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	B	610	CLA	C3B-C4B-NB	-2.57	108.24	110.53
32	D	401	PHO	CMB-C2B-C3B	2.57	129.81	124.68
22	b	607	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	B	618	BCR	C15-C14-C13	-2.57	123.68	127.28
22	a	406	CLA	CHB-C4A-NA	2.56	128.10	124.40
30	f	103	SQD	C44-O6-C1	2.56	119.29	113.80
31	B	622	LMT	C1'-O5'-C5'	-2.56	108.72	113.72
25	c	516	DGD	O6E-C1E-O5D	-2.56	104.00	110.04
22	C	505	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	C	520	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	a	405	CLA	C3B-C4B-NB	-2.56	108.25	110.53
22	b	615	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
25	d	408	DGD	C3G-C2G-C1G	-2.55	105.83	111.78
22	c	512	CLA	CHB-C4A-NA	2.55	128.09	124.40
24	a	410	BCR	C27-C26-C25	2.55	126.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	504	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	C	514	BCR	C33-C5-C6	-2.54	121.72	124.48
22	C	504	CLA	CHB-C4A-NA	2.54	128.06	124.40
30	D	403	SQD	O48-C23-C24	2.53	119.56	111.83
22	b	614	CLA	C1-C2-C3	-2.53	122.04	126.20
24	y	101	BCR	C1-C6-C5	-2.53	119.17	122.64
24	j	102	BCR	C29-C30-C25	2.53	114.12	110.44
22	a	408	CLA	C3B-C4B-NB	-2.53	108.27	110.53
24	J	102	BCR	C29-C30-C25	2.53	114.12	110.44
31	M	102	LMT	C3'-C4'-C5'	-2.53	105.32	110.93
22	B	604	CLA	C3B-C4B-NB	-2.53	108.27	110.53
22	C	501	CLA	CHB-C4A-NA	2.53	128.05	124.40
22	B	608	CLA	C1-C2-C3	-2.53	122.06	126.20
24	C	513	BCR	C15-C14-C13	-2.53	123.74	127.28
24	c	513	BCR	C11-C10-C9	-2.53	123.74	127.28
27	D	408	LMG	O6-C1-C2	-2.53	105.18	110.37
22	d	405	CLA	C1-C2-C3	-2.53	122.06	126.20
23	a	409	PL9	C7-C8-C9	-2.52	122.49	126.83
22	B	606	CLA	C3B-C4B-NB	-2.52	108.28	110.53
22	c	510	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	a	410	BCR	C33-C5-C6	-2.52	121.73	124.48
24	b	620	BCR	C2-C1-C6	2.52	114.10	110.44
24	c	521	BCR	C15-C14-C13	-2.52	123.75	127.28
22	H	101	CLA	C3B-C4B-NB	-2.52	108.28	110.53
22	b	618	CLA	CHB-C4A-NA	2.52	128.03	124.40
24	C	514	BCR	C15-C14-C13	-2.52	123.75	127.28
27	b	625	LMG	C1-C2-C3	-2.51	104.72	110.01
25	D	409	DGD	CFB-CEB-CDB	-2.51	101.67	114.37
22	B	609	CLA	CHB-C4A-NA	2.51	128.02	124.40
22	C	503	CLA	CHB-C4A-NA	2.51	128.02	124.40
22	c	511	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	C	521	BCR	C15-C14-C13	-2.51	123.76	127.28
30	d	402	SQD	C44-O6-C1	2.51	119.17	113.80
24	C	513	BCR	C8-C7-C6	-2.50	120.31	127.00
24	c	514	BCR	C33-C5-C6	-2.50	121.75	124.48
22	c	505	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	b	622	BCR	C15-C14-C13	-2.50	123.77	127.28
22	c	508	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	h	101	CLA	C3B-C4B-NB	-2.50	108.30	110.53
30	D	403	SQD	O8-S-C6	2.49	110.79	105.97
24	b	623	BCR	C3-C4-C5	-2.49	109.61	114.06
22	c	505	CLA	C3B-C4B-NB	-2.49	108.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	408	DGD	C3D-C4D-C5D	-2.49	105.71	110.23
27	M	101	LMG	C1-C2-C3	-2.49	104.77	110.01
22	c	503	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	D	405	CLA	C3B-C4B-NB	-2.49	108.31	110.53
22	B	610	CLA	C1-C2-C3	-2.49	122.12	126.20
23	a	409	PL9	C27-C28-C29	-2.49	121.93	127.62
22	b	614	CLA	CMB-C2B-C1B	-2.49	121.64	125.42
24	B	616	BCR	C2-C1-C6	2.48	114.05	110.44
22	b	615	CLA	CHB-C4A-NA	2.48	127.98	124.40
34	f	101	HEM	C1B-NB-C4B	2.48	108.15	105.21
27	B	621	LMG	C1-C2-C3	-2.48	104.79	110.01
27	a	402	LMG	O6-C1-O1	-2.48	104.18	110.04
27	d	410	LMG	C38-C37-C36	-2.48	101.83	114.37
22	b	605	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	B	616	BCR	C27-C26-C25	2.48	126.05	122.70
24	c	513	BCR	C8-C7-C6	-2.48	120.38	127.00
27	D	412	LMG	C38-C37-C36	-2.48	101.85	114.37
24	c	513	BCR	C15-C14-C13	-2.48	123.81	127.28
22	B	611	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
22	C	508	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
31	M	103	LMT	C3'-C4'-C5'	-2.47	105.44	110.93
31	D	410	LMT	C1'-O5'-C5'	-2.47	108.89	113.72
22	B	614	CLA	CHB-C4A-NA	2.47	127.97	124.40
27	d	407	LMG	C38-C37-C36	-2.47	101.88	114.37
25	d	408	DGD	CFB-CEB-CDB	-2.47	101.88	114.37
22	a	404	CLA	CHB-C4A-NA	2.47	127.97	124.40
30	d	402	SQD	O48-C23-C24	2.47	119.37	111.83
24	B	618	BCR	C15-C16-C17	-2.47	118.47	123.52
22	c	501	CLA	CHB-C4A-NA	2.47	127.96	124.40
22	b	614	CLA	C3B-C4B-NB	-2.47	108.33	110.53
22	d	405	CLA	CHB-C4A-NA	2.47	127.96	124.40
34	F	101	HEM	C1B-NB-C4B	2.47	108.13	105.21
30	a	401	SQD	O48-C23-C24	2.47	119.35	111.83
25	C	517	DGD	O5D-C6D-C5D	-2.46	103.87	109.42
23	D	407	PL9	C27-C28-C29	-2.46	121.99	127.62
22	C	507	CLA	C1-C2-C3	-2.46	122.16	126.20
22	C	511	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	c	504	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	B	619	BCR	C3-C4-C5	-2.46	109.67	114.06
25	A	408	DGD	CBB-CAB-C9B	-2.46	101.94	114.37
22	B	604	CLA	CHB-C4A-NA	2.46	127.94	124.40
27	A	410	LMG	C40-C39-C38	-2.46	101.96	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	404	CLA	CHB-C4A-NA	2.45	127.94	124.40
22	B	601	CLA	C3B-C4B-NB	-2.45	108.34	110.53
24	A	407	BCR	C33-C5-C6	-2.45	121.81	124.48
24	B	616	BCR	C11-C10-C9	-2.45	123.84	127.28
22	D	406	CLA	CHB-C4A-NA	2.45	127.93	124.40
22	B	607	CLA	CHB-C4A-NA	2.45	127.93	124.40
22	b	616	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	g	101	BCR	C1-C6-C5	-2.45	119.29	122.64
25	a	411	DGD	CBB-CAB-C9B	-2.44	102.02	114.37
24	c	513	BCR	C15-C16-C17	-2.44	118.52	123.52
25	c	516	DGD	C3G-C2G-C1G	-2.44	106.09	111.78
30	D	403	SQD	C44-O6-C1	2.44	119.03	113.80
31	b	603	LMT	C1'-O5'-C5'	-2.44	108.95	113.72
22	b	611	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	h	101	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	C	516	DGD	O6E-C1E-O5D	-2.44	104.28	110.04
32	d	401	PHO	CMB-C2B-C3B	2.44	129.55	124.68
24	C	514	BCR	C11-C10-C9	-2.44	123.86	127.28
22	B	608	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	b	620	BCR	C27-C26-C25	2.43	125.99	122.70
31	d	409	LMT	C3'-C4'-C5'	-2.43	105.53	110.93
22	C	505	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	M	103	LMT	C1'-O5'-C5'	-2.43	108.97	113.72
27	e	101	LMG	O6-C1-O1	-2.43	104.30	110.04
22	B	612	CLA	CHB-C4A-NA	2.43	127.91	124.40
30	a	401	SQD	C1-O5-C5	2.43	118.46	113.72
22	B	602	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	a	408	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	C	508	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	C	511	CLA	O2A-CGA-O1A	-2.42	117.56	123.63
27	D	408	LMG	C38-C37-C36	-2.42	102.12	114.37
27	A	415	LMG	O6-C1-O1	-2.42	104.33	110.04
30	F	102	SQD	C3-C4-C5	2.42	114.62	110.23
22	B	606	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	A	402	CLA	CHB-C4A-NA	2.42	127.89	124.40
27	C	522	LMG	C40-C39-C38	-2.42	102.15	114.37
22	B	612	CLA	C3B-C4B-NB	-2.42	108.37	110.53
27	c	522	LMG	O6-C1-O1	-2.41	104.34	110.04
24	C	521	BCR	C24-C23-C22	-2.41	122.66	126.23
27	c	522	LMG	C40-C39-C38	-2.41	102.17	114.37
26	c	519	LHG	C11-C10-C9	-2.41	102.17	114.37
30	A	414	SQD	O48-C23-C24	2.41	119.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	415	SQD	O48-C23-C24	2.41	119.19	111.83
22	B	611	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	c	511	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
23	A	406	PL9	C7-C8-C9	-2.41	122.68	126.83
22	b	610	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	c	507	CLA	CHB-C4A-NA	2.41	127.87	124.40
23	j	101	PL9	O2-C1-C6	2.41	124.31	120.48
22	b	606	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	c	502	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	b	622	BCR	C15-C16-C17	-2.40	118.60	123.52
27	a	413	LMG	C40-C39-C38	-2.40	102.22	114.37
25	B	620	DGD	CBB-CAB-C9B	-2.40	102.22	114.37
22	A	405	CLA	C3B-C4B-NB	-2.40	108.39	110.53
27	B	624	LMG	C38-C37-C36	-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
22	B	603	CLA	O1D-CGD-CBD	2.40	129.25	124.52
27	A	410	LMG	C1-C2-C3	-2.40	104.97	110.01
25	b	624	DGD	CBB-CAB-C9B	-2.40	102.25	114.37
23	D	407	PL9	C37-C38-C39	-2.40	122.14	127.62
22	C	502	CLA	CHB-C4A-NA	2.39	127.86	124.40
22	d	404	CLA	C3B-C4B-NB	-2.39	108.39	110.53
23	D	407	PL9	C32-C33-C34	-2.39	122.15	127.62
23	d	406	PL9	C37-C38-C39	-2.39	122.15	127.62
24	C	513	BCR	C27-C26-C25	2.39	125.93	122.70
22	B	615	CLA	CHB-C4A-NA	2.39	127.85	124.40
23	J	101	PL9	O2-C1-C6	2.39	124.28	120.48
23	d	406	PL9	C27-C28-C29	-2.39	122.16	127.62
25	C	517	DGD	CFB-CEB-CDB	-2.39	102.30	114.37
31	B	627	LMT	C1'-O5'-C5'	-2.39	109.06	113.72
27	C	522	LMG	O6-C1-O1	-2.39	104.40	110.04
22	b	617	CLA	CHB-C4A-NA	2.39	127.84	124.40
24	c	513	BCR	C3-C4-C5	-2.39	109.80	114.06
24	b	620	BCR	C11-C10-C9	-2.39	123.93	127.28
31	i	102	LMT	C1'-O5'-C5'	-2.39	109.06	113.72
22	B	613	CLA	CHB-C4A-NA	2.39	127.84	124.40
25	c	516	DGD	CFB-CEB-CDB	-2.39	102.31	114.37
24	C	513	BCR	C3-C4-C5	-2.38	109.81	114.06
27	b	628	LMG	C38-C37-C36	-2.38	102.33	114.37
24	c	513	BCR	C27-C26-C25	2.38	125.92	122.70
25	c	517	DGD	CFB-CEB-CDB	-2.38	102.33	114.37
23	a	409	PL9	C41-C39-C40	2.38	120.07	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	413	SQD	O48-C23-C24	2.38	119.09	111.83
22	A	405	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	c	517	DGD	O5D-C6D-C5D	-2.37	104.07	109.42
25	D	409	DGD	C3G-C2G-C1G	-2.37	106.26	111.78
22	c	502	CLA	C1-C2-C3	-2.37	122.32	126.20
25	C	515	DGD	C3G-C2G-C1G	-2.37	106.27	111.78
22	b	619	CLA	CHB-C4A-NA	2.37	127.82	124.40
22	c	507	CLA	C1-C2-C3	-2.37	122.32	126.20
30	f	103	SQD	O9-S-C6	2.36	110.29	106.76
27	e	101	LMG	C1-C2-C3	-2.36	105.04	110.01
24	c	513	BCR	C24-C23-C22	-2.36	122.74	126.23
22	b	612	CLA	CHB-C4A-NA	2.36	127.81	124.40
30	A	414	SQD	C1-O5-C5	2.36	118.33	113.72
23	d	406	PL9	C32-C33-C34	-2.36	122.23	127.62
23	a	409	PL9	C20-C19-C21	2.36	119.32	115.23
24	b	623	BCR	C11-C10-C9	-2.36	123.97	127.28
25	C	516	DGD	C3G-C2G-C1G	-2.36	106.29	111.78
25	B	620	DGD	C1D-C2D-C3D	-2.35	105.06	110.01
24	C	521	BCR	C33-C5-C6	-2.35	121.92	124.48
26	C	519	LHG	C11-C10-C9	-2.35	102.47	114.37
27	m	101	LMG	O2-C2-C1	-2.35	104.47	110.08
22	D	406	CLA	C1-C2-C3	-2.35	122.35	126.20
25	b	601	DGD	O6D-C1D-O3G	-2.35	104.50	110.04
23	d	406	PL9	O1-C4-C3	-2.35	118.26	120.73
31	D	410	LMT	C3'-C4'-C5'	-2.34	105.73	110.93
27	A	410	LMG	C38-C37-C36	-2.34	102.52	114.37
22	C	509	CLA	CHB-C4A-NA	2.34	127.78	124.40
23	a	409	PL9	O2-C1-C6	2.34	124.21	120.48
22	C	507	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	a	413	LMG	C1-C2-C3	-2.34	105.09	110.01
27	d	407	LMG	O6-C1-C2	-2.34	105.56	110.37
23	d	406	PL9	O2-C1-C6	2.34	124.20	120.48
27	E	101	LMG	O6-C1-O1	-2.34	104.53	110.04
22	c	507	CLA	O2D-CGD-CBD	2.33	115.31	111.23
27	B	621	LMG	O6-C1-O1	-2.33	104.53	110.04
22	c	509	CLA	CHB-C4A-NA	2.33	127.77	124.40
22	b	616	CLA	C3B-C4B-NB	-2.33	108.45	110.53
23	d	406	PL9	C20-C19-C21	2.33	119.27	115.23
27	d	410	LMG	O6-C1-O1	-2.33	104.54	110.04
22	b	613	CLA	CHB-C4A-NA	2.33	127.76	124.40
31	d	409	LMT	C1'-O5'-C5'	-2.33	109.17	113.72
24	B	616	BCR	C15-C14-C13	-2.33	124.01	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	516	DGD	CFB-CEB-CDB	-2.33	102.61	114.37
24	J	102	BCR	C15-C16-C17	-2.32	118.76	123.52
22	C	502	CLA	C1-C2-C3	-2.32	122.39	126.20
24	B	619	BCR	C38-C26-C25	-2.32	121.95	124.48
27	B	624	LMG	O2-C2-C1	-2.32	104.55	110.08
24	x	101	BCR	C29-C30-C25	2.32	113.81	110.44
22	H	101	CLA	CHB-C4A-NA	2.32	127.74	124.40
27	A	410	LMG	O3-C3-C2	-2.32	104.92	110.38
24	C	521	BCR	C11-C10-C9	-2.32	124.03	127.28
24	b	623	BCR	C38-C26-C25	-2.31	121.96	124.48
27	C	518	LMG	C38-C37-C36	-2.31	102.69	114.37
23	A	406	PL9	C41-C39-C40	2.31	119.90	114.59
27	b	625	LMG	C40-C39-C38	-2.31	102.70	114.37
24	b	623	BCR	C24-C23-C22	-2.31	122.82	126.23
27	i	101	LMG	O2-C2-C1	-2.31	104.58	110.08
27	a	413	LMG	C38-C37-C36	-2.30	102.72	114.37
27	B	621	LMG	C40-C39-C38	-2.30	102.72	114.37
25	C	516	DGD	C3D-C4D-C5D	-2.30	106.06	110.23
23	A	406	PL9	O2-C1-C6	2.30	124.14	120.48
22	B	601	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	D	412	LMG	C1-C2-C3	-2.30	105.17	110.01
30	B	626	SQD	O48-C23-C24	2.30	118.84	111.83
23	J	101	PL9	C20-C19-C21	2.30	119.21	115.23
27	m	101	LMG	C1-C2-C3	-2.30	105.18	110.01
27	c	518	LMG	C38-C37-C36	-2.29	102.77	114.37
24	b	622	BCR	C7-C8-C9	-2.29	122.84	126.23
24	c	521	BCR	C33-C5-C6	-2.29	121.98	124.48
23	D	407	PL9	C20-C19-C21	2.28	119.19	115.23
23	D	407	PL9	O1-C4-C3	-2.28	118.32	120.73
27	C	522	LMG	O2-C2-C1	-2.28	104.63	110.08
27	b	625	LMG	C38-C37-C36	-2.28	102.83	114.37
22	B	606	CLA	C1-C2-C3	-2.28	122.46	126.20
22	c	503	CLA	O2D-CGD-CBD	2.28	115.22	111.23
25	C	515	DGD	C1D-C2D-C3D	-2.28	105.21	110.01
24	f	102	BCR	C27-C26-C25	2.28	125.78	122.70
27	D	412	LMG	O6-C1-O1	-2.28	104.66	110.04
25	A	408	DGD	C3G-C2G-C1G	-2.27	106.48	111.78
23	D	407	PL9	O2-C1-C6	2.27	124.10	120.48
25	B	620	DGD	C3G-C2G-C1G	-2.27	106.49	111.78
25	D	409	DGD	C3D-C4D-C5D	-2.27	106.12	110.23
24	B	618	BCR	C7-C8-C9	-2.27	122.88	126.23
31	I	102	LMT	C1'-O5'-C5'	-2.27	109.30	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	PL9	C20-C19-C21	2.27	119.16	115.23
27	c	522	LMG	C38-C37-C36	-2.26	102.95	114.37
27	c	522	LMG	O2-C2-C1	-2.26	104.69	110.08
25	b	624	DGD	C1D-C2D-C3D	-2.26	105.26	110.01
24	H	102	BCR	C29-C30-C25	2.26	113.72	110.44
22	b	607	CLA	O1D-CGD-CBD	2.26	128.97	124.52
25	A	408	DGD	O5D-C6D-C5D	-2.26	104.33	109.42
27	b	628	LMG	O2-C2-C1	-2.25	104.71	110.08
27	b	625	LMG	O6-C1-O1	-2.25	104.72	110.04
24	b	620	BCR	C15-C14-C13	-2.25	124.12	127.28
25	c	516	DGD	C3D-C4D-C5D	-2.25	106.15	110.23
22	d	404	CLA	O1D-CGD-CBD	2.25	128.96	124.52
25	B	625	DGD	O6D-C1D-O3G	-2.25	104.73	110.04
25	a	411	DGD	C1D-C2D-C3D	-2.25	105.28	110.01
27	I	101	LMG	O2-C2-C1	-2.25	104.72	110.08
22	H	101	CLA	C1-C2-C3	-2.25	122.52	126.20
27	C	522	LMG	C38-C37-C36	-2.25	103.02	114.37
24	a	410	BCR	C38-C26-C25	-2.24	122.03	124.48
23	a	409	PL9	O1-C4-C3	-2.24	118.37	120.73
22	b	605	CLA	CHB-C4A-NA	2.24	127.63	124.40
27	c	518	LMG	O7-C10-O9	-2.24	118.47	123.70
27	M	101	LMG	O2-C2-C1	-2.24	104.74	110.08
23	d	406	PL9	O2-C1-C2	-2.24	116.74	121.83
24	A	407	BCR	C15-C14-C13	-2.23	124.14	127.28
23	j	101	PL9	O2-C1-C2	-2.23	116.75	121.83
24	a	410	BCR	C15-C16-C17	-2.23	118.95	123.52
22	a	404	CLA	C1-C2-C3	-2.23	122.54	126.20
22	B	605	CLA	O1D-CGD-CBD	2.23	128.92	124.52
22	D	405	CLA	O1D-CGD-CBD	2.23	128.92	124.52
27	B	621	LMG	C38-C37-C36	-2.23	103.09	114.37
24	D	411	BCR	C27-C26-C25	2.23	125.72	122.70
30	b	602	SQD	O48-C23-C24	2.23	118.64	111.83
31	B	623	LMT	C1'-O5'-C5'	-2.23	109.37	113.72
27	m	101	LMG	C1-O6-C5	-2.23	109.37	113.72
24	c	521	BCR	C24-C23-C22	-2.23	122.94	126.23
25	a	411	DGD	C3G-C2G-C1G	-2.23	106.59	111.78
24	f	102	BCR	C15-C16-C17	-2.23	118.96	123.52
24	D	411	BCR	C11-C10-C9	-2.23	124.16	127.28
24	C	514	BCR	C38-C26-C25	-2.22	122.06	124.48
24	b	622	BCR	C27-C26-C25	2.22	125.71	122.70
24	A	407	BCR	C38-C26-C25	-2.22	122.06	124.48
30	a	415	SQD	C4-C3-C2	2.22	114.73	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	412	LMG	O3-C3-C2	-2.22	105.15	110.38
22	b	612	CLA	C1-C2-C3	-2.22	122.56	126.20
24	A	407	BCR	C15-C16-C17	-2.22	118.98	123.52
27	D	408	LMG	O6-C1-O1	-2.21	104.82	110.04
24	C	514	BCR	C24-C23-C22	-2.21	122.97	126.23
30	f	103	SQD	C3-C4-C5	2.21	114.23	110.23
23	J	101	PL9	O2-C1-C2	-2.21	116.81	121.83
22	C	507	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
22	c	507	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
24	c	514	BCR	C38-C26-C25	-2.20	122.08	124.48
27	b	628	LMG	O3-C3-C2	-2.20	105.18	110.38
22	B	603	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
27	C	518	LMG	O7-C10-O9	-2.20	118.56	123.70
24	c	521	BCR	C11-C10-C9	-2.20	124.19	127.28
24	D	411	BCR	C7-C8-C9	-2.20	122.98	126.23
25	c	516	DGD	CBB-CAB-C9B	-2.20	103.26	114.37
22	b	618	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
27	d	410	LMG	C1-C2-C3	-2.20	105.39	110.01
24	g	101	BCR	C3-C2-C1	-2.19	106.66	114.43
24	B	619	BCR	C24-C23-C22	-2.19	122.99	126.23
25	C	516	DGD	CBB-CAB-C9B	-2.19	103.28	114.37
22	b	605	CLA	C1-C2-C3	-2.19	122.61	126.20
27	B	624	LMG	O3-C3-C2	-2.19	105.21	110.38
23	j	101	PL9	C20-C19-C21	2.19	119.03	115.23
22	d	404	CLA	CHB-C4A-NA	2.19	127.56	124.40
22	B	611	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
27	a	402	LMG	O1-C7-C8	-2.18	105.51	110.82
22	B	602	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
27	d	410	LMG	O3-C3-C2	-2.18	105.23	110.38
22	D	405	CLA	CHB-C4A-NA	2.18	127.55	124.40
24	f	102	BCR	C11-C10-C9	-2.18	124.22	127.28
22	c	506	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
30	F	102	SQD	O48-C23-C24	2.18	118.47	111.83
27	a	413	LMG	O3-C3-C2	-2.17	105.25	110.38
24	C	513	BCR	C7-C8-C9	-2.17	123.02	126.23
27	C	518	LMG	O2-C2-C1	-2.17	104.90	110.08
22	B	610	CLA	CHB-C1B-NB	2.17	127.31	124.05
24	g	101	BCR	C15-C16-C17	-2.17	119.08	123.52
24	a	410	BCR	C24-C23-C22	-2.17	123.03	126.23
22	c	509	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
30	F	102	SQD	C44-O6-C1	2.17	118.44	113.80
27	I	101	LMG	O7-C10-O9	-2.17	118.64	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	C1-C2-C3	-2.17	122.65	126.20
22	B	612	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
25	C	517	DGD	CBB-CAB-C9B	-2.16	103.43	114.37
25	b	624	DGD	C3G-C2G-C1G	-2.16	106.75	111.78
24	y	101	BCR	C3-C2-C1	-2.16	106.79	114.43
24	H	102	BCR	C16-C15-C14	-2.16	119.10	123.52
25	a	411	DGD	CAB-C9B-C8B	-2.16	103.46	114.37
27	A	415	LMG	O7-C10-O9	-2.16	118.66	123.70
22	b	615	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
27	e	101	LMG	O1-C7-C8	-2.16	105.58	110.82
24	J	102	BCR	C35-C13-C14	-2.15	119.33	122.82
22	b	616	CLA	C1-C2-C3	-2.15	122.67	126.20
25	b	601	DGD	CBB-CAB-C9B	-2.15	103.48	114.37
24	c	514	BCR	C24-C23-C22	-2.15	123.05	126.23
27	c	518	LMG	O2-C2-C1	-2.15	104.95	110.08
24	b	622	BCR	C33-C5-C6	-2.15	122.14	124.48
25	A	408	DGD	CAB-C9B-C8B	-2.15	103.49	114.37
24	D	411	BCR	C15-C16-C17	-2.15	119.12	123.52
32	d	401	PHO	C1-C2-C3	-2.15	122.68	126.20
22	B	614	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
31	b	627	LMT	C1'-O5'-C5'	-2.14	109.53	113.72
26	a	412	LHG	C27-C26-C25	-2.14	103.53	114.37
27	d	407	LMG	O6-C1-O1	-2.14	104.98	110.04
25	B	625	DGD	CBB-CAB-C9B	-2.14	103.54	114.37
24	B	616	BCR	C15-C16-C17	-2.14	119.14	123.52
25	c	517	DGD	CBB-CAB-C9B	-2.14	103.54	114.37
25	c	515	DGD	C1D-C2D-C3D	-2.14	105.50	110.01
25	a	411	DGD	O5D-C6D-C5D	-2.14	104.59	109.42
25	C	516	DGD	CAB-C9B-C8B	-2.14	103.55	114.37
23	D	407	PL9	O2-C1-C2	-2.14	116.96	121.83
27	B	621	LMG	O2-C2-C1	-2.14	104.98	110.08
24	y	101	BCR	C15-C16-C17	-2.14	119.15	123.52
23	A	406	PL9	O1-C4-C3	-2.14	118.48	120.73
27	b	625	LMG	O2-C2-C1	-2.14	104.99	110.08
22	C	504	CLA	O1D-CGD-CBD	2.14	128.73	124.52
30	f	103	SQD	C1-O5-C5	2.13	117.89	113.72
22	B	612	CLA	C1-C2-C3	-2.13	122.70	126.20
27	A	415	LMG	O1-C7-C8	-2.13	105.63	110.82
22	b	606	CLA	C1-C2-C3	-2.13	122.70	126.20
25	c	516	DGD	O3D-C3D-C4D	-2.13	105.35	110.38
24	a	410	BCR	C15-C14-C13	-2.13	124.29	127.28
22	b	610	CLA	O2A-CGA-O1A	-2.13	118.30	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	522	LMG	O3-C3-C2	-2.13	105.36	110.38
22	C	506	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
24	C	514	BCR	C7-C8-C9	-2.13	123.09	126.23
22	B	611	CLA	C1-C2-C3	-2.13	122.71	126.20
22	b	614	CLA	CHB-C1B-NB	2.13	127.24	124.05
24	b	623	BCR	C15-C14-C13	-2.13	124.30	127.28
24	H	102	BCR	C27-C26-C25	2.12	125.57	122.70
25	C	516	DGD	O3D-C3D-C4D	-2.12	105.37	110.38
23	D	407	PL9	C12-C13-C14	-2.12	122.76	127.62
24	B	619	BCR	C11-C10-C9	-2.12	124.30	127.28
22	B	601	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
27	a	402	LMG	O3-C3-C2	-2.12	105.37	110.38
27	B	621	LMG	O3-C3-C2	-2.12	105.38	110.38
27	i	101	LMG	O1-C1-C2	-2.12	105.05	108.27
30	f	103	SQD	O48-C23-C24	2.12	118.29	111.83
22	b	616	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	c	504	CLA	O1D-CGD-CBD	2.12	128.69	124.52
22	b	616	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
27	I	101	LMG	O3-C3-C2	-2.12	105.39	110.38
22	C	501	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
32	D	401	PHO	O2A-CGA-O1A	-2.11	118.34	123.63
25	b	601	DGD	CAB-C9B-C8B	-2.11	103.69	114.37
22	C	510	CLA	C1-C2-C3	-2.11	122.74	126.20
25	C	517	DGD	CAB-C9B-C8B	-2.11	103.70	114.37
22	b	607	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
27	i	101	LMG	O3-C3-C2	-2.11	105.40	110.38
22	b	610	CLA	C1-C2-C3	-2.11	122.74	126.20
27	C	518	LMG	O3-C3-C2	-2.11	105.41	110.38
27	c	522	LMG	O3-C3-C2	-2.11	105.41	110.38
24	B	618	BCR	C27-C26-C25	2.10	125.55	122.70
22	b	606	CLA	O2D-CGD-CBD	2.10	114.91	111.23
34	v	201	HEM	C2A-C1A-NA	-2.10	107.82	110.15
22	B	606	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
27	a	413	LMG	O7-C10-O9	-2.10	118.79	123.70
27	b	625	LMG	O3-C3-C2	-2.10	105.42	110.38
24	j	102	BCR	C20-C21-C22	-2.10	124.33	127.28
27	B	624	LMG	O1-C1-C2	-2.10	105.08	108.27
23	A	406	PL9	O2-C1-C2	-2.10	117.06	121.83
23	a	409	PL9	O2-C1-C2	-2.10	117.06	121.83
22	C	520	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
27	A	410	LMG	O7-C10-O9	-2.10	118.80	123.70
22	B	612	CLA	O2A-CGA-O1A	-2.10	118.39	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
27	i	101	LMG	O1-C7-C8	-2.09	105.72	110.82
27	e	101	LMG	O7-C10-O9	-2.09	118.81	123.70
27	M	101	LMG	C1-O6-C5	-2.09	109.63	113.72
22	b	609	CLA	O1D-CGD-CBD	2.09	128.64	124.52
22	b	606	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
27	i	101	LMG	O7-C10-O9	-2.09	118.82	123.70
24	B	616	BCR	C38-C26-C25	-2.09	122.20	124.48
22	c	508	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
24	B	618	BCR	C33-C5-C6	-2.09	122.20	124.48
25	B	625	DGD	CAB-C9B-C8B	-2.09	103.81	114.37
30	A	413	SQD	C4-C3-C2	2.09	114.49	110.83
27	a	413	LMG	O2-C2-C1	-2.09	105.10	110.08
27	e	101	LMG	O3-C3-C2	-2.09	105.46	110.38
27	c	518	LMG	O3-C3-C2	-2.08	105.47	110.38
25	c	517	DGD	CAB-C9B-C8B	-2.08	103.84	114.37
24	b	621	BCR	C24-C23-C22	-2.08	123.16	126.23
24	B	616	BCR	C7-C8-C9	-2.08	123.16	126.23
25	b	624	DGD	CAB-C9B-C8B	-2.08	103.85	114.37
22	B	607	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
26	A	409	LHG	C27-C26-C25	-2.08	103.86	114.37
22	c	501	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	d	408	DGD	C5B-C4B-C3B	-2.08	103.86	114.37
27	M	101	LMG	O3-C3-C2	-2.08	105.48	110.38
25	c	516	DGD	C1D-O6D-C5D	-2.07	109.67	113.72
22	a	405	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
24	C	513	BCR	C11-C10-C9	-2.07	124.37	127.28
24	g	101	BCR	C15-C14-C13	-2.07	124.37	127.28
24	C	521	BCR	C38-C26-C25	-2.07	122.22	124.48
22	C	512	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	b	613	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	A	408	DGD	C1D-C2D-C3D	-2.07	105.65	110.01
27	A	415	LMG	O3-C3-C2	-2.07	105.50	110.38
25	c	516	DGD	CAB-C9B-C8B	-2.07	103.91	114.37
24	b	620	BCR	C15-C16-C17	-2.07	119.29	123.52
27	B	621	LMG	O7-C10-O9	-2.07	118.87	123.70
24	C	513	BCR	C38-C26-C25	-2.07	122.23	124.48
22	B	601	CLA	C1-C2-C3	-2.07	122.81	126.20
27	D	412	LMG	O7-C10-O9	-2.06	118.88	123.70
25	B	620	DGD	C4E-C3E-C2E	-2.06	107.21	110.83
25	c	515	DGD	O5D-C6D-C5D	-2.06	104.77	109.42
22	a	406	CLA	O2A-CGA-O1A	-2.06	118.47	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	403	BCT	O3-C-O1	-2.06	114.40	119.68
25	C	516	DGD	C1D-C2D-C3D	-2.06	105.67	110.01
22	A	403	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
22	c	520	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	d	410	LMG	O7-C10-O9	-2.06	118.89	123.70
25	D	409	DGD	CAB-C9B-C8B	-2.06	103.96	114.37
32	d	401	PHO	O2A-CGA-O1A	-2.06	118.48	123.63
27	a	413	LMG	O1-C1-C2	-2.06	105.15	108.27
25	D	409	DGD	C5B-C4B-C3B	-2.06	103.97	114.37
24	C	521	BCR	C7-C8-C9	-2.06	123.19	126.23
33	D	404	BCT	O3-C-O1	-2.06	114.42	119.68
22	h	101	CLA	C1-C2-C3	-2.06	122.83	126.20
22	A	402	CLA	C1-C2-C3	-2.05	122.83	126.20
24	D	411	BCR	C24-C23-C22	-2.05	123.20	126.23
24	x	101	BCR	C27-C26-C25	2.05	125.48	122.70
24	B	617	BCR	C24-C23-C22	-2.05	123.20	126.23
34	v	201	HEM	C1B-NB-C4B	2.05	107.64	105.21
24	j	102	BCR	C35-C13-C14	-2.05	119.50	122.82
23	d	406	PL9	C12-C13-C14	-2.05	122.94	127.62
27	d	410	LMG	O2-C2-C1	-2.04	105.20	110.08
22	c	504	CLA	C1-C2-C3	-2.04	122.85	126.20
34	V	201	HEM	C3B-C2B-C1B	2.04	107.94	106.41
27	A	410	LMG	O2-C2-C1	-2.04	105.22	110.08
24	f	102	BCR	C7-C8-C9	-2.04	123.22	126.23
27	E	101	LMG	O3-C3-C2	-2.04	105.57	110.38
27	b	625	LMG	O7-C10-O9	-2.04	118.94	123.70
22	A	404	CLA	C1-C2-C3	-2.04	122.86	126.20
25	d	408	DGD	CAB-C9B-C8B	-2.04	104.08	114.37
25	A	408	DGD	CDB-CCB-CBB	-2.04	99.62	113.36
27	m	101	LMG	O3-C3-C2	-2.04	105.58	110.38
24	B	617	BCR	C38-C26-C25	-2.03	122.26	124.48
23	A	406	PL9	C12-C13-C14	-2.03	122.97	127.62
25	C	517	DGD	C5B-C4B-C3B	-2.03	104.09	114.37
22	C	508	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	J	101	PL9	C12-C13-C14	-2.03	122.98	127.62
23	j	101	PL9	C12-C13-C14	-2.03	122.98	127.62
22	B	615	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	B	610	CLA	CHB-C4A-NA	2.03	127.33	124.40
22	B	613	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
24	g	101	BCR	C24-C23-C22	-2.03	123.24	126.23
24	c	513	BCR	C38-C26-C25	-2.03	122.27	124.48
25	C	515	DGD	O5D-C6D-C5D	-2.03	104.85	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	402	LMG	O7-C10-O9	-2.02	118.97	123.70
22	C	510	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	d	408	DGD	CBB-CAB-C9B	-2.02	104.14	114.37
30	B	626	SQD	O8-S-C6	2.02	109.88	105.97
22	C	505	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
24	A	407	BCR	C24-C23-C22	-2.02	123.24	126.23
24	c	514	BCR	C7-C8-C9	-2.02	123.24	126.23
24	c	521	BCR	C7-C8-C9	-2.02	123.24	126.23
25	c	517	DGD	C5B-C4B-C3B	-2.02	104.15	114.37
25	a	411	DGD	CDB-CCB-CBB	-2.02	99.72	113.36
22	B	609	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	C	519	LHG	C27-C26-C25	-2.02	104.16	114.37
22	a	406	CLA	C1-C2-C3	-2.02	122.89	126.20
22	C	509	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	C	515	DGD	C5B-C4B-C3B	-2.02	104.16	114.37
27	E	101	LMG	O1-C7-C8	-2.02	105.91	110.82
30	a	401	SQD	O8-S-C6	2.02	109.87	105.97
22	b	615	CLA	C1-C2-C3	-2.02	122.89	126.20
27	E	101	LMG	O7-C10-O9	-2.02	118.99	123.70
22	C	507	CLA	O2D-CGD-CBD	2.02	114.75	111.23
25	D	409	DGD	CBB-CAB-C9B	-2.01	104.18	114.37
22	a	404	CLA	O1D-CGD-CBD	2.01	128.49	124.52
25	c	515	DGD	C5B-C4B-C3B	-2.01	104.19	114.37
25	C	516	DGD	C1D-O6D-C5D	-2.01	109.79	113.72
27	a	413	LMG	C1-O6-C5	-2.01	109.79	113.72
22	c	505	CLA	C1-C2-C3	-2.01	122.90	126.20
22	a	408	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
25	B	620	DGD	CAB-C9B-C8B	-2.01	104.21	114.37
26	c	519	LHG	C27-C26-C25	-2.01	104.21	114.37
22	B	607	CLA	C1-C2-C3	-2.01	122.91	126.20
22	A	404	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
22	b	619	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
34	v	201	HEM	C3B-C2B-C1B	2.01	107.92	106.41
24	b	621	BCR	C38-C26-C25	-2.01	122.29	124.48
25	c	515	DGD	O2D-C2D-C1D	-2.01	105.30	110.08
24	c	521	BCR	C38-C26-C25	-2.01	122.30	124.48
22	c	510	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
25	B	620	DGD	C5B-C4B-C3B	-2.00	104.24	114.37
27	A	410	LMG	O1-C1-C2	-2.00	105.23	108.27

There are no chirality outliers.

All (2081) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	404	CLA	C4B-C3B-CAB-CBB
22	B	601	CLA	CBD-CGD-O2D-CED
22	B	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	C4B-C3B-CAB-CBB
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C2B-C3B-CAB-CBB
22	B	608	CLA	C4B-C3B-CAB-CBB
22	B	609	CLA	C2B-C3B-CAB-CBB
22	B	609	CLA	C4B-C3B-CAB-CBB
22	B	609	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	C2B-C3B-CAB-CBB
22	B	610	CLA	C4B-C3B-CAB-CBB
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	C2B-C3B-CAB-CBB
22	B	615	CLA	C4B-C3B-CAB-CBB
22	B	615	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	C2B-C3B-CAB-CBB
22	C	509	CLA	C4B-C3B-CAB-CBB
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	C6-C7-C8-C9
22	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	C6-C7-C8-C9
22	a	404	CLA	CBD-CGD-O2D-CED
22	a	405	CLA	C1A-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

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Mol	Chain	Res	Type	Atoms
22	b	608	CLA	CBD-CGD-O2D-CED
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	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	613	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	C2B-C3B-CAB-CBB
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	c	511	CLA	C1A-C2A-CAA-CBA
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

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Mol	Chain	Res	Type	Atoms
23	A	406	PL9	C27-C28-C29-C31
23	A	406	PL9	C37-C38-C39-C41
23	D	407	PL9	C27-C28-C29-C31
23	D	407	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-C11
23	a	409	PL9	C12-C13-C14-C15
23	a	409	PL9	C12-C13-C14-C16
23	a	409	PL9	C17-C18-C19-C21
23	a	409	PL9	C22-C23-C24-C25
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	C	521	BCR	C7-C8-C9-C34
24	D	411	BCR	C7-C8-C9-C10
24	H	102	BCR	C21-C22-C23-C24
24	J	102	BCR	C21-C22-C23-C24
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-C10
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

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Mol	Chain	Res	Type	Atoms
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	O1B-C1B-O2G-C2G
25	D	409	DGD	O6D-C1D-O3G-C3G
25	a	411	DGD	C2D-C1D-O3G-C3G
25	b	601	DGD	O1B-C1B-O2G-C2G
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	b	624	DGD	C2E-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	O6D-C1D-O3G-C3G
25	d	408	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	B	624	LMG	O1-C7-C8-O7
27	B	624	LMG	C11-C10-O7-C8
27	B	624	LMG	O10-C28-O8-C9
27	C	518	LMG	O9-C10-O7-C8
27	C	518	LMG	C11-C10-O7-C8
27	D	408	LMG	O6-C1-O1-C7
27	D	412	LMG	O9-C10-O7-C8
27	D	412	LMG	C11-C10-O7-C8
27	M	101	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
27	b	625	LMG	C11-C10-O7-C8
27	b	628	LMG	O1-C7-C8-O7
27	b	628	LMG	C11-C10-O7-C8
27	c	518	LMG	O9-C10-O7-C8
27	c	518	LMG	C11-C10-O7-C8
27	d	407	LMG	O6-C1-O1-C7
27	d	410	LMG	O9-C10-O7-C8
27	d	410	LMG	C11-C10-O7-C8
27	m	101	LMG	O9-C10-O7-C8
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	C5-C6-S-O7
30	A	413	SQD	C5-C6-S-O8
30	A	413	SQD	C5-C6-S-O9
30	A	414	SQD	C24-C23-O48-C46
30	B	626	SQD	O5-C5-C6-S
30	D	403	SQD	C2-C1-O6-C44
30	D	403	SQD	O5-C1-O6-C44
30	D	403	SQD	O49-C7-O47-C45
30	D	403	SQD	C8-C7-O47-C45
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	O5-C1-O6-C44
30	d	402	SQD	O49-C7-O47-C45
30	d	402	SQD	C8-C7-O47-C45
22	B	603	CLA	O1D-CGD-O2D-CED
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	b	619	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	615	CLA	O1D-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	C	520	CLA	CBD-CGD-O2D-CED
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	614	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	520	CLA	CBD-CGD-O2D-CED
27	E	101	LMG	O10-C28-O8-C9
27	e	101	LMG	O10-C28-O8-C9
30	A	414	SQD	O10-C23-O48-C46
30	a	401	SQD	O10-C23-O48-C46
23	A	406	PL9	C37-C38-C39-C40
23	a	409	PL9	C37-C38-C39-C40
27	C	518	LMG	C8-C9-O8-C28
27	a	413	LMG	C29-C28-O8-C9
27	d	407	LMG	C29-C28-O8-C9
30	F	102	SQD	C24-C23-O48-C46
30	f	103	SQD	C24-C23-O48-C46
22	B	606	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	O10-C28-O8-C9
27	C	518	LMG	O10-C28-O8-C9
27	D	408	LMG	O10-C28-O8-C9
27	a	413	LMG	O10-C28-O8-C9
27	b	628	LMG	O10-C28-O8-C9
27	c	518	LMG	O10-C28-O8-C9
27	d	407	LMG	O10-C28-O8-C9
30	F	102	SQD	O10-C23-O48-C46
30	f	103	SQD	O10-C23-O48-C46
22	B	609	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	b	608	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
31	B	627	LMT	C3'-C4'-O1B-C1B
31	b	603	LMT	C3'-C4'-O1B-C1B
25	d	408	DGD	O1B-C1B-O2G-C2G
27	A	415	LMG	O9-C10-O7-C8
27	B	621	LMG	O9-C10-O7-C8
27	B	624	LMG	O9-C10-O7-C8
27	I	101	LMG	O9-C10-O7-C8
27	a	402	LMG	O9-C10-O7-C8
27	b	625	LMG	O9-C10-O7-C8
27	b	628	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
32	d	401	PHO	C3-C5-C6-C7
27	c	518	LMG	C8-C9-O8-C28
22	b	613	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	c	522	LMG	C29-C28-O8-C9
22	B	605	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	a	402	LMG	C11-C10-O7-C8
27	m	101	LMG	C11-C10-O7-C8
30	F	102	SQD	C8-C7-O47-C45
22	B	601	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	O1D-CGD-O2D-CED
25	b	624	DGD	C4D-C5D-C6D-O5D
27	I	101	LMG	O6-C5-C6-O5
22	B	602	CLA	C4-C3-C5-C6
22	D	405	CLA	C4-C3-C5-C6
22	H	101	CLA	C4-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
22	b	608	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	405	CLA	C2-C3-C5-C6
22	H	101	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
22	h	101	CLA	C2-C3-C5-C6
31	i	102	LMT	C3'-C4'-O1B-C1B
22	C	520	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
22	c	505	CLA	O1D-CGD-O2D-CED
22	c	520	CLA	O1D-CGD-O2D-CED
25	A	408	DGD	O6E-C5E-C6E-O5E
27	i	101	LMG	O6-C5-C6-O5
22	B	609	CLA	C2A-CAA-CBA-CGA
31	I	102	LMT	C3'-C4'-O1B-C1B
25	D	409	DGD	C2A-C1A-O1G-C1G
25	d	408	DGD	C2A-C1A-O1G-C1G
27	B	624	LMG	C29-C28-O8-C9
27	C	522	LMG	C29-C28-O8-C9
27	b	628	LMG	C29-C28-O8-C9
25	B	620	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	O6E-C5E-C6E-O5E
23	J	101	PL9	C7-C8-C9-C10
23	a	409	PL9	C17-C18-C19-C20
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	C	516	DGD	C4E-C5E-C6E-O5E
25	D	409	DGD	O1A-C1A-O1G-C1G
25	d	408	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
27	C	522	LMG	O10-C28-O8-C9
27	e	101	LMG	O9-C10-O7-C8
22	C	507	CLA	O1D-CGD-O2D-CED
25	c	516	DGD	C4E-C5E-C6E-O5E
22	C	508	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	c	508	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
22	H	101	CLA	C3-C5-C6-C7
32	D	401	PHO	C3-C5-C6-C7
22	B	607	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
32	D	402	PHO	CBD-CGD-O2D-CED
26	A	409	LHG	O2-C2-C3-O3
26	a	412	LHG	O2-C2-C3-O3
22	B	613	CLA	O1D-CGD-O2D-CED
22	C	501	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
27	E	101	LMG	C29-C28-O8-C9
27	e	101	LMG	C29-C28-O8-C9
25	a	411	DGD	O6E-C5E-C6E-O5E
27	b	628	LMG	O6-C5-C6-O5
25	C	515	DGD	O6E-C5E-C6E-O5E
25	c	515	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	C4E-C5E-C6E-O5E
27	I	101	LMG	C4-C5-C6-O5
22	C	511	CLA	CBD-CGD-O2D-CED
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	d	407	LMG	C11-C10-O7-C8
30	f	103	SQD	C8-C7-O47-C45
22	b	614	CLA	O1D-CGD-O2D-CED
27	i	101	LMG	C4-C5-C6-O5
22	B	608	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	b	611	CLA	CBD-CGD-O2D-CED
27	B	624	LMG	O6-C5-C6-O5
22	B	610	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	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	c	522	LMG	O10-C28-O8-C9
23	A	406	PL9	C24-C26-C27-C28
23	a	409	PL9	C24-C26-C27-C28
22	c	512	CLA	CBD-CGD-O2D-CED
25	A	408	DGD	C4E-C5E-C6E-O5E
22	b	610	CLA	C2A-CAA-CBA-CGA
25	B	620	DGD	O6E-C1E-O5D-C6D
25	C	515	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	522	LMG	O6-C1-O1-C7
27	E	101	LMG	O6-C1-O1-C7
27	a	402	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
25	C	516	DGD	O6E-C5E-C6E-O5E
25	c	516	DGD	O6E-C5E-C6E-O5E
25	B	620	DGD	C4E-C5E-C6E-O5E
32	d	401	PHO	CBA-CGA-O2A-C1
22	B	611	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
27	C	518	LMG	O6-C5-C6-O5
23	a	409	PL9	C7-C8-C9-C10
22	B	615	CLA	O1A-CGA-O2A-C1
27	c	518	LMG	O6-C5-C6-O5
22	B	606	CLA	O1D-CGD-O2D-CED
25	d	408	DGD	C2B-C1B-O2G-C2G
27	i	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
32	d	401	PHO	O1A-CGA-O2A-C1
27	E	101	LMG	O9-C10-O7-C8
27	d	407	LMG	O9-C10-O7-C8
22	C	512	CLA	CBA-CGA-O2A-C1
22	b	619	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
32	D	401	PHO	CBA-CGA-O2A-C1
25	C	515	DGD	C4E-C5E-C6E-O5E
27	C	518	LMG	C4-C5-C6-O5
27	c	518	LMG	C4-C5-C6-O5
25	c	515	DGD	C4E-C5E-C6E-O5E
22	b	608	CLA	C2-C3-C5-C6
22	B	607	CLA	C6-C7-C8-C9
22	B	609	CLA	C14-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C9
22	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	a	411	DGD	C4E-C5E-C6E-O5E
25	c	517	DGD	C2D-C1D-O3G-C3G
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
27	c	518	LMG	C2-C1-O1-C7
27	c	522	LMG	C2-C1-O1-C7
27	d	407	LMG	C2-C1-O1-C7
27	e	101	LMG	C2-C1-O1-C7
30	a	415	SQD	C2-C1-O6-C44
30	b	602	SQD	O10-C23-O48-C46
32	D	401	PHO	O1A-CGA-O2A-C1
24	B	617	BCR	C37-C22-C23-C24
24	H	102	BCR	C7-C8-C9-C34
24	H	102	BCR	C37-C22-C23-C24
24	J	102	BCR	C37-C22-C23-C24
24	y	101	BCR	C7-C8-C9-C34
24	f	102	BCR	C37-C22-C23-C24
24	g	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C37-C22-C23-C24
24	B	617	BCR	C7-C8-C9-C10
24	b	621	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	V	201	HEM	C2D-C3D-CAD-CBD
22	B	606	CLA	C2A-CAA-CBA-CGA
27	C	518	LMG	C10-C11-C12-C13
22	B	605	CLA	O1D-CGD-O2D-CED
22	b	619	CLA	O1A-CGA-O2A-C1
27	I	101	LMG	C11-C10-O7-C8
27	c	522	LMG	O6-C5-C6-O5
25	C	516	DGD	O2G-C2G-C3G-O3G
25	c	516	DGD	O2G-C2G-C3G-O3G
27	m	101	LMG	O1-C7-C8-O7
22	B	606	CLA	C15-C16-C17-C18
22	B	611	CLA	C5-C6-C7-C8
22	b	610	CLA	C15-C16-C17-C18
22	c	509	CLA	CBD-CGD-O2D-CED
23	D	407	PL9	C27-C28-C29-C30
22	B	615	CLA	C5-C6-C7-C8
22	h	101	CLA	C3-C5-C6-C7
22	b	609	CLA	O1D-CGD-O2D-CED
32	a	407	PHO	O1D-CGD-O2D-CED
22	A	404	CLA	C10-C11-C12-C13
22	b	615	CLA	C13-C15-C16-C17
22	b	619	CLA	C5-C6-C7-C8
27	c	522	LMG	C4-C5-C6-O5
22	b	615	CLA	C5-C6-C7-C8
32	a	407	PHO	C15-C16-C17-C18
27	b	628	LMG	C4-C5-C6-O5
27	A	415	LMG	C28-C29-C30-C31
27	B	621	LMG	C10-C11-C12-C13
23	D	407	PL9	C29-C31-C32-C33
23	d	406	PL9	C29-C31-C32-C33
22	A	402	CLA	C3-C5-C6-C7
22	B	611	CLA	C13-C15-C16-C17
25	C	515	DGD	C1B-C2B-C3B-C4B
25	d	408	DGD	C1B-C2B-C3B-C4B
27	D	412	LMG	C10-C11-C12-C13
27	b	625	LMG	C10-C11-C12-C13
27	d	410	LMG	C10-C11-C12-C13
22	C	512	CLA	O1A-CGA-O2A-C1
27	c	522	LMG	C11-C10-O7-C8
22	B	609	CLA	C8-C10-C11-C12
22	C	520	CLA	C15-C16-C17-C18
22	a	406	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	C10-C11-C12-C13
22	c	520	CLA	C13-C15-C16-C17
22	c	520	CLA	C15-C16-C17-C18
32	D	402	PHO	C15-C16-C17-C18
22	C	507	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2A-CAA-CBA-CGA
22	b	613	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
22	B	603	CLA	C13-C15-C16-C17
22	B	608	CLA	C13-C15-C16-C17
22	C	501	CLA	C8-C10-C11-C12
22	C	501	CLA	C15-C16-C17-C18
22	C	505	CLA	C13-C15-C16-C17
22	C	507	CLA	C10-C11-C12-C13
22	b	610	CLA	C13-C15-C16-C17
22	b	612	CLA	C13-C15-C16-C17
22	b	614	CLA	C15-C16-C17-C18
22	b	619	CLA	C10-C11-C12-C13
22	c	505	CLA	C5-C6-C7-C8
22	c	507	CLA	C10-C11-C12-C13
22	c	508	CLA	C5-C6-C7-C8
22	d	404	CLA	C13-C15-C16-C17
25	D	409	DGD	C1B-C2B-C3B-C4B
25	c	515	DGD	C1B-C2B-C3B-C4B
27	C	518	LMG	C28-C29-C30-C31
27	C	522	LMG	C10-C11-C12-C13
27	c	518	LMG	C10-C11-C12-C13
27	c	518	LMG	C28-C29-C30-C31
27	c	522	LMG	C10-C11-C12-C13
22	a	404	CLA	C3-C5-C6-C7
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	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	615	CLA	C10-C11-C12-C13
22	C	503	CLA	C10-C11-C12-C13
22	C	504	CLA	C10-C11-C12-C13
22	C	505	CLA	C15-C16-C17-C18
22	C	508	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C15-C16-C17-C18
22	C	520	CLA	C13-C15-C16-C17
22	D	405	CLA	C13-C15-C16-C17
22	D	405	CLA	C15-C16-C17-C18
22	b	605	CLA	C13-C15-C16-C17
22	b	607	CLA	C13-C15-C16-C17
22	b	613	CLA	C8-C10-C11-C12
22	c	504	CLA	C10-C11-C12-C13
22	c	505	CLA	C13-C15-C16-C17
22	c	505	CLA	C15-C16-C17-C18
22	c	509	CLA	C15-C16-C17-C18
22	d	404	CLA	C15-C16-C17-C18
22	B	604	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
30	B	626	SQD	O10-C23-O48-C46
22	B	601	CLA	C13-C15-C16-C17
22	B	606	CLA	C13-C15-C16-C17
22	c	501	CLA	C15-C16-C17-C18
27	D	408	LMG	O9-C10-O7-C8
22	C	512	CLA	O1D-CGD-O2D-CED
22	c	511	CLA	O1D-CGD-O2D-CED
22	A	403	CLA	C15-C16-C17-C18
22	B	612	CLA	C5-C6-C7-C8
22	C	507	CLA	C15-C16-C17-C18
22	c	506	CLA	C5-C6-C7-C8
22	c	510	CLA	C5-C6-C7-C8
22	B	604	CLA	C2-C3-C5-C6
25	b	624	DGD	C1B-C2B-C3B-C4B
22	B	607	CLA	O1D-CGD-O2D-CED
32	D	402	PHO	O1D-CGD-O2D-CED
22	A	404	CLA	C15-C16-C17-C18
22	a	405	CLA	C15-C16-C17-C18
22	b	611	CLA	C15-C16-C17-C18
22	c	501	CLA	C10-C11-C12-C13
22	c	507	CLA	C15-C16-C17-C18
27	I	101	LMG	C29-C28-O8-C9
27	C	522	LMG	C11-C10-O7-C8
22	C	512	CLA	C15-C16-C17-C18
25	C	517	DGD	O1B-C1B-O2G-C2G
25	c	517	DGD	O1B-C1B-O2G-C2G
27	c	522	LMG	O9-C10-O7-C8
22	B	601	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	CBA-CGA-O2A-C1
22	b	608	CLA	CBA-CGA-O2A-C1
22	c	511	CLA	CBA-CGA-O2A-C1
22	c	520	CLA	CBA-CGA-O2A-C1
30	b	602	SQD	C24-C23-O48-C46
22	B	607	CLA	C5-C6-C7-C8
22	B	607	CLA	C15-C16-C17-C18
22	B	610	CLA	C15-C16-C17-C18
22	C	506	CLA	C5-C6-C7-C8
22	a	406	CLA	C15-C16-C17-C18
22	c	501	CLA	C8-C10-C11-C12
22	c	512	CLA	C15-C16-C17-C18
22	b	619	CLA	C3-C5-C6-C7
22	C	511	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	C5-C6-C7-C8
22	C	510	CLA	C5-C6-C7-C8
22	B	614	CLA	C13-C15-C16-C17
22	b	619	CLA	C13-C15-C16-C17
22	a	405	CLA	C6-C7-C8-C9
27	C	522	LMG	O9-C10-O7-C8
30	F	102	SQD	O49-C7-O47-C45
25	D	409	DGD	C2D-C1D-O3G-C3G
25	D	409	DGD	C2E-C1E-O5D-C6D
25	d	408	DGD	C2D-C1D-O3G-C3G
25	d	408	DGD	C2E-C1E-O5D-C6D
27	I	101	LMG	C2-C1-O1-C7
27	i	101	LMG	C2-C1-O1-C7
22	b	618	CLA	C13-C15-C16-C17
27	a	402	LMG	C28-C29-C30-C31
25	C	515	DGD	C1A-C2A-C3A-C4A
22	C	501	CLA	C10-C11-C12-C13
22	b	611	CLA	C5-C6-C7-C8
22	c	520	CLA	C10-C11-C12-C13
24	B	617	BCR	C7-C8-C9-C34
24	b	621	BCR	C7-C8-C9-C34
24	C	521	BCR	C7-C8-C9-C10
22	b	608	CLA	O1A-CGA-O2A-C1
31	b	604	LMT	O1'-C1-C2-C3
22	A	402	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
22	c	520	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C13-C15-C16-C17
30	a	415	SQD	C7-C8-C9-C10
27	C	522	LMG	C4-C5-C6-O5
27	C	518	LMG	C9-C8-O7-C10
27	e	101	LMG	C7-C8-O7-C10
22	b	611	CLA	O1D-CGD-O2D-CED
27	d	410	LMG	O6-C5-C6-O5
24	H	102	BCR	C11-C10-C9-C8
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	B	624	LMG	O6-C1-O1-C7
27	b	628	LMG	O6-C1-O1-C7
30	b	602	SQD	C8-C7-O47-C45
23	A	406	PL9	C33-C34-C36-C37
23	a	409	PL9	C33-C34-C36-C37
27	C	522	LMG	O6-C5-C6-O5
31	B	628	LMT	O1'-C1-C2-C3
27	i	101	LMG	C29-C28-O8-C9
27	m	101	LMG	C29-C28-O8-C9
30	B	626	SQD	C24-C23-O48-C46
31	B	622	LMT	C1-C2-C3-C4
22	C	520	CLA	C10-C11-C12-C13
27	D	412	LMG	O6-C5-C6-O5
22	c	508	CLA	C2-C1-O2A-CGA
22	B	604	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	O1A-CGA-O2A-C1
25	C	516	DGD	C2A-C3A-C4A-C5A
27	A	410	LMG	C34-C35-C36-C37
27	b	625	LMG	C31-C32-C33-C34
31	I	102	LMT	C6-C7-C8-C9
31	i	102	LMT	C6-C7-C8-C9
25	b	601	DGD	C5B-C6B-C7B-C8B
30	F	102	SQD	C12-C13-C14-C15
30	b	602	SQD	C11-C10-C9-C8
22	c	512	CLA	O1D-CGD-O2D-CED
27	M	101	LMG	O6-C5-C6-O5
22	b	616	CLA	C5-C6-C7-C8
25	B	620	DGD	C3B-C4B-C5B-C6B
25	D	409	DGD	C4B-C5B-C6B-C7B
25	c	516	DGD	C4A-C5A-C6A-C7A
25	d	408	DGD	CEB-CFB-CGB-CHB

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Mol	Chain	Res	Type	Atoms
27	C	518	LMG	C29-C30-C31-C32
27	I	101	LMG	C14-C15-C16-C17
27	i	101	LMG	C12-C13-C14-C15
22	C	511	CLA	O1A-CGA-O2A-C1
22	C	520	CLA	CBA-CGA-O2A-C1
25	B	625	DGD	C5B-C6B-C7B-C8B
25	B	625	DGD	C9B-CAB-CBB-CCB
25	D	409	DGD	C5B-C6B-C7B-C8B
25	D	409	DGD	CCB-CDB-CEB-CFB
25	b	601	DGD	C9B-CAB-CBB-CCB
25	b	624	DGD	C3B-C4B-C5B-C6B
25	b	624	DGD	C6B-C7B-C8B-C9B
25	c	515	DGD	C3B-C4B-C5B-C6B
25	c	516	DGD	C2A-C3A-C4A-C5A
25	d	408	DGD	CCB-CDB-CEB-CFB
27	A	415	LMG	C30-C31-C32-C33
27	B	621	LMG	C31-C32-C33-C34
27	c	518	LMG	C29-C30-C31-C32
30	f	103	SQD	C12-C13-C14-C15
25	C	515	DGD	C3B-C4B-C5B-C6B
25	D	409	DGD	CEB-CFB-CGB-CHB
25	a	411	DGD	C8B-C9B-CAB-CBB
25	d	408	DGD	C5B-C6B-C7B-C8B
27	I	101	LMG	C12-C13-C14-C15
27	a	402	LMG	C30-C31-C32-C33
27	a	413	LMG	C34-C35-C36-C37
22	B	611	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	C5-C6-C7-C8
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	620	DGD	C1B-C2B-C3B-C4B
27	a	402	LMG	O6-C5-C6-O5
27	A	410	LMG	C33-C34-C35-C36
27	c	522	LMG	C12-C13-C14-C15
27	i	101	LMG	C16-C17-C18-C19
25	c	515	DGD	C3A-C4A-C5A-C6A
22	C	503	CLA	C11-C12-C13-C15
25	C	515	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
25	d	408	DGD	C4B-C5B-C6B-C7B
22	C	503	CLA	C5-C6-C7-C8
31	b	626	LMT	C1-C2-C3-C4
25	A	408	DGD	C8B-C9B-CAB-CBB
27	B	624	LMG	C18-C19-C20-C21
27	C	522	LMG	C12-C13-C14-C15
27	a	413	LMG	C33-C34-C35-C36
30	B	626	SQD	C9-C10-C11-C12
22	B	615	CLA	C3-C5-C6-C7
22	B	606	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	C	506	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	C3A-C2A-CAA-CBA
22	a	405	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	615	CLA	O1D-CGD-O2D-CED
27	A	415	LMG	C15-C16-C17-C18
27	a	402	LMG	C32-C33-C34-C35
25	B	620	DGD	C7A-C8A-C9A-CAA
30	A	413	SQD	C14-C15-C16-C17
22	H	101	CLA	C5-C6-C7-C8
27	B	624	LMG	C4-C5-C6-O5
25	b	624	DGD	O6D-C5D-C6D-O5D
22	c	520	CLA	O1A-CGA-O2A-C1
25	C	515	DGD	C2B-C3B-C4B-C5B
25	C	517	DGD	CBA-CCA-CDA-CEA
27	d	407	LMG	C14-C15-C16-C17
34	V	201	HEM	C4D-C3D-CAD-CBD
25	B	620	DGD	C6B-C7B-C8B-C9B
30	a	415	SQD	C14-C15-C16-C17
25	D	409	DGD	C7B-C8B-C9B-CAB
25	b	624	DGD	C7A-C8A-C9A-CAA
25	d	408	DGD	C7B-C8B-C9B-CAB
27	D	408	LMG	C14-C15-C16-C17
27	b	628	LMG	C18-C19-C20-C21
30	B	626	SQD	C11-C10-C9-C8
25	c	517	DGD	C1A-C2A-C3A-C4A
27	B	624	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
27	E	101	LMG	C28-C29-C30-C31
25	c	515	DGD	C2B-C3B-C4B-C5B
27	A	415	LMG	C18-C19-C20-C21
30	b	602	SQD	C9-C10-C11-C12
25	C	516	DGD	C4A-C5A-C6A-C7A
25	c	517	DGD	CBA-CCA-CDA-CEA
27	B	624	LMG	C31-C32-C33-C34
27	D	408	LMG	C19-C20-C21-C22
27	I	101	LMG	C16-C17-C18-C19
27	i	101	LMG	C14-C15-C16-C17
25	B	620	DGD	O6D-C5D-C6D-O5D
30	a	415	SQD	C27-C28-C29-C30
27	a	413	LMG	C31-C32-C33-C34
22	A	404	CLA	C2B-C3B-CAB-CBB
22	B	606	CLA	C2B-C3B-CAB-CBB
22	a	406	CLA	C2B-C3B-CAB-CBB
22	b	610	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
30	B	626	SQD	C8-C7-O47-C45
26	C	519	LHG	C24-C23-O8-C6
30	F	102	SQD	C11-C12-C13-C14
27	A	410	LMG	C31-C32-C33-C34
22	B	605	CLA	C2A-CAA-CBA-CGA
22	a	404	CLA	C2A-CAA-CBA-CGA
25	B	625	DGD	C1A-C2A-C3A-C4A
27	b	628	LMG	C28-C29-C30-C31
25	C	517	DGD	C9B-CAB-CBB-CCB
25	c	517	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C30-C31-C32-C33
27	d	407	LMG	C19-C20-C21-C22
25	C	515	DGD	C4A-C5A-C6A-C7A
27	a	402	LMG	C15-C16-C17-C18
27	b	628	LMG	C31-C32-C33-C34
26	A	409	LHG	O9-C7-O7-C5
30	f	103	SQD	O49-C7-O47-C45
23	j	101	PL9	C15-C14-C16-C17
22	C	509	CLA	O1D-CGD-O2D-CED
25	a	411	DGD	C5B-C6B-C7B-C8B
25	b	624	DGD	C4B-C5B-C6B-C7B
25	c	517	DGD	CAB-CBB-CCB-CDB
27	a	402	LMG	C18-C19-C20-C21
27	a	413	LMG	C30-C31-C32-C33
30	A	413	SQD	C27-C28-C29-C30
30	f	103	SQD	C11-C12-C13-C14
22	H	101	CLA	C13-C15-C16-C17
25	B	625	DGD	C2B-C3B-C4B-C5B
27	A	415	LMG	C32-C33-C34-C35
22	D	406	CLA	CBA-CGA-O2A-C1
22	b	614	CLA	CBA-CGA-O2A-C1
22	d	405	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C29-C28-O8-C9
22	C	520	CLA	O1A-CGA-O2A-C1
22	A	403	CLA	C6-C7-C8-C9
22	a	404	CLA	C11-C12-C13-C14
22	b	612	CLA	C6-C7-C8-C9
27	C	518	LMG	C34-C35-C36-C37
25	d	408	DGD	O6E-C1E-O5D-C6D
25	B	625	DGD	C4A-C5A-C6A-C7A
27	m	101	LMG	C29-C30-C31-C32
22	h	101	CLA	C5-C6-C7-C8
25	A	408	DGD	C5B-C6B-C7B-C8B
25	c	515	DGD	C4A-C5A-C6A-C7A
25	c	515	DGD	C1A-C2A-C3A-C4A
25	C	517	DGD	CAB-CBB-CCB-CDB
25	D	409	DGD	C5A-C6A-C7A-C8A
25	b	601	DGD	C4A-C5A-C6A-C7A
27	c	518	LMG	C34-C35-C36-C37
22	c	509	CLA	C3-C5-C6-C7
22	b	605	CLA	C16-C17-C18-C20
22	c	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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
26	a	412	LHG	C23-C24-C25-C26
27	e	101	LMG	C28-C29-C30-C31
30	A	413	SQD	C7-C8-C9-C10
26	a	412	LHG	O9-C7-O7-C5
25	B	620	DGD	C4B-C5B-C6B-C7B
25	b	601	DGD	C2B-C3B-C4B-C5B
30	b	602	SQD	C11-C12-C13-C14
22	C	506	CLA	CBD-CGD-O2D-CED
24	D	411	BCR	C37-C22-C23-C24
24	b	621	BCR	C37-C22-C23-C24
24	j	102	BCR	C37-C22-C23-C24
25	C	516	DGD	C1A-C2A-C3A-C4A
25	d	408	DGD	C5A-C6A-C7A-C8A
27	a	413	LMG	C14-C15-C16-C17
22	c	502	CLA	C3-C5-C6-C7
27	A	410	LMG	C8-C7-O1-C1
27	D	408	LMG	C8-C7-O1-C1
27	d	407	LMG	C8-C7-O1-C1
31	B	628	LMT	C7-C8-C9-C10
22	C	520	CLA	C2A-CAA-CBA-CGA
22	B	612	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C20
27	I	101	LMG	C13-C14-C15-C16
27	i	101	LMG	C13-C14-C15-C16
30	F	102	SQD	C10-C11-C12-C13
22	c	509	CLA	C4-C3-C5-C6
23	d	406	PL9	C35-C34-C36-C37
27	A	410	LMG	C14-C15-C16-C17
22	B	603	CLA	C8-C10-C11-C12
22	a	408	CLA	C10-C11-C12-C13
22	b	607	CLA	C8-C10-C11-C12
30	f	103	SQD	C10-C11-C12-C13
27	D	412	LMG	C17-C18-C19-C20
22	C	509	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	a	405	CLA	C3-C5-C6-C7
27	e	101	LMG	O6-C5-C6-O5
22	C	505	CLA	C10-C11-C12-C13
22	C	512	CLA	C13-C15-C16-C17
22	h	101	CLA	C13-C15-C16-C17
27	d	407	LMG	C32-C33-C34-C35
25	C	517	DGD	C1A-C2A-C3A-C4A
25	b	601	DGD	C1A-C2A-C3A-C4A
31	B	622	LMT	O1'-C1-C2-C3
25	D	409	DGD	C6B-C7B-C8B-C9B
22	B	601	CLA	C10-C11-C12-C13
22	C	511	CLA	C13-C15-C16-C17
25	b	624	DGD	C5B-C6B-C7B-C8B
26	a	412	LHG	C25-C26-C27-C28
27	D	408	LMG	C32-C33-C34-C35
31	b	604	LMT	C7-C8-C9-C10
25	c	516	DGD	C1A-C2A-C3A-C4A
27	a	413	LMG	C4-C5-C6-O5
22	A	405	CLA	C10-C11-C12-C13
22	D	406	CLA	C15-C16-C17-C18
22	c	505	CLA	C10-C11-C12-C13
27	E	101	LMG	C15-C16-C17-C18
27	c	518	LMG	C12-C13-C14-C15
27	c	518	LMG	C36-C37-C38-C39
27	A	410	LMG	O1-C7-C8-O7
27	I	101	LMG	O1-C7-C8-O7
27	M	101	LMG	O1-C7-C8-O7
27	i	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
27	C	518	LMG	C12-C13-C14-C15
27	d	407	LMG	C15-C16-C17-C18
30	B	626	SQD	C11-C12-C13-C14
27	D	408	LMG	C15-C16-C17-C18
27	M	101	LMG	C29-C30-C31-C32
27	e	101	LMG	C15-C16-C17-C18
30	d	402	SQD	C9-C10-C11-C12
22	b	605	CLA	C10-C11-C12-C13
27	m	101	LMG	O6-C5-C6-O5
27	C	518	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
27	D	408	LMG	C13-C14-C15-C16
30	D	403	SQD	C9-C10-C11-C12
25	B	620	DGD	C5B-C6B-C7B-C8B
27	A	415	LMG	C31-C32-C33-C34
27	B	624	LMG	C30-C31-C32-C33
22	C	508	CLA	C2-C1-O2A-CGA
27	E	101	LMG	O6-C5-C6-O5
23	d	406	PL9	C47-C48-C49-C51
25	c	516	DGD	CAB-CBB-CCB-CDB
26	a	412	LHG	C30-C31-C32-C33
27	b	628	LMG	C30-C31-C32-C33
27	b	628	LMG	C36-C37-C38-C39
34	v	201	HEM	C2D-C3D-CAD-CBD
34	v	201	HEM	C4D-C3D-CAD-CBD
22	c	512	CLA	C4-C3-C5-C6
27	D	412	LMG	C34-C35-C36-C37
27	d	410	LMG	C17-C18-C19-C20
22	c	501	CLA	C2A-CAA-CBA-CGA
22	C	504	CLA	CBA-CGA-O2A-C1
25	C	515	DGD	C2A-C3A-C4A-C5A
26	A	409	LHG	C30-C31-C32-C33
22	c	511	CLA	C13-C15-C16-C17
31	I	102	LMT	C5'-C4'-O1B-C1B
27	A	410	LMG	C15-C16-C17-C18
26	C	519	LHG	C24-C25-C26-C27
22	b	614	CLA	O1A-CGA-O2A-C1
22	C	502	CLA	C3-C5-C6-C7
27	d	410	LMG	C34-C35-C36-C37
22	B	615	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	D	405	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	508	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	C13-C15-C16-C17
26	c	519	LHG	C24-C25-C26-C27
27	B	624	LMG	C17-C18-C19-C20
25	A	408	DGD	C3B-C4B-C5B-C6B
25	C	516	DGD	CAB-CBB-CCB-CDB
31	i	102	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
23	D	407	PL9	C47-C48-C49-C51
27	a	402	LMG	C31-C32-C33-C34
25	D	409	DGD	CAB-CBB-CCB-CDB
26	A	409	LHG	C25-C26-C27-C28
22	A	403	CLA	C3-C5-C6-C7
22	B	605	CLA	C12-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C7
22	C	502	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C10-C8-C7
22	D	405	CLA	C12-C13-C15-C16
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	503	CLA	C11-C12-C13-C15
22	c	504	CLA	C6-C7-C8-C10
22	c	504	CLA	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
22	c	510	CLA	C12-C13-C15-C16
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	613	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20
22	d	405	CLA	C15-C16-C17-C18
27	A	415	LMG	C17-C18-C19-C20
22	a	408	CLA	C13-C15-C16-C17
25	C	515	DGD	C4B-C5B-C6B-C7B
31	b	627	LMT	C2B-C1B-O1B-C4'
22	C	509	CLA	C4-C3-C5-C6
22	C	509	CLA	C2-C3-C5-C6
22	C	512	CLA	C2-C3-C5-C6
25	D	409	DGD	C2A-C3A-C4A-C5A
25	d	408	DGD	C2A-C3A-C4A-C5A
22	D	406	CLA	O1A-CGA-O2A-C1
25	d	408	DGD	C6B-C7B-C8B-C9B
31	b	626	LMT	O1'-C1-C2-C3
27	A	410	LMG	C11-C10-O7-C8
22	C	501	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
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	505	CLA	C14-C13-C15-C16
22	C	510	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	b	606	CLA	C6-C7-C8-C9
22	b	618	CLA	C11-C10-C8-C9
22	c	502	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	c	505	CLA	C14-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C9
22	d	404	CLA	C14-C13-C15-C16
25	D	409	DGD	C3A-C4A-C5A-C6A
25	d	408	DGD	CAB-CBB-CCB-CDB
30	B	626	SQD	C12-C13-C14-C15
22	c	504	CLA	CBA-CGA-O2A-C1
26	c	519	LHG	C24-C23-O8-C6
22	C	503	CLA	C8-C10-C11-C12
22	c	502	CLA	C13-C15-C16-C17
27	B	621	LMG	C34-C35-C36-C37
25	c	515	DGD	C2A-C3A-C4A-C5A
27	b	625	LMG	C34-C35-C36-C37
31	B	623	LMT	C2B-C1B-O1B-C4'
25	d	408	DGD	C3A-C4A-C5A-C6A
25	A	408	DGD	C1B-C2B-C3B-C4B
25	a	411	DGD	C1B-C2B-C3B-C4B
25	A	408	DGD	C1G-C2G-C3G-O3G
25	c	517	DGD	O1G-C1G-C2G-C3G
27	B	621	LMG	C7-C8-C9-O8
27	B	624	LMG	O1-C7-C8-C9
27	C	522	LMG	C7-C8-C9-O8
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	a	413	LMG	O1-C7-C8-C9
27	b	625	LMG	C7-C8-C9-O8
27	b	628	LMG	O1-C7-C8-C9
27	c	522	LMG	C7-C8-C9-O8
27	d	407	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	i	101	LMG	O1-C7-C8-C9
27	m	101	LMG	C7-C8-C9-O8
30	A	414	SQD	O6-C44-C45-C46
30	B	626	SQD	C44-C45-C46-O48
30	b	602	SQD	C44-C45-C46-O48
27	B	624	LMG	C36-C37-C38-C39
27	d	407	LMG	C13-C14-C15-C16
22	d	405	CLA	O1A-CGA-O2A-C1
25	D	409	DGD	C8B-C9B-CAB-CBB
27	b	625	LMG	C13-C14-C15-C16
27	D	412	LMG	C31-C32-C33-C34
27	b	628	LMG	C17-C18-C19-C20
26	c	519	LHG	C25-C26-C27-C28
22	A	405	CLA	C5-C6-C7-C8
25	d	408	DGD	C8B-C9B-CAB-CBB
24	b	621	BCR	C20-C21-C22-C37
22	b	607	CLA	C15-C16-C17-C18
27	C	522	LMG	C16-C17-C18-C19
30	b	602	SQD	C12-C13-C14-C15
27	a	413	LMG	C15-C16-C17-C18
22	C	512	CLA	C4-C3-C5-C6
22	c	509	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
22	c	503	CLA	C8-C10-C11-C12
27	d	410	LMG	C31-C32-C33-C34
22	c	508	CLA	O1A-CGA-O2A-C1
27	A	415	LMG	O6-C5-C6-O5
25	a	411	DGD	C3B-C4B-C5B-C6B
22	a	408	CLA	C5-C6-C7-C8
25	A	408	DGD	C4B-C5B-C6B-C7B
25	c	515	DGD	C4B-C5B-C6B-C7B
26	A	409	LHG	C23-C24-C25-C26
27	B	624	LMG	C15-C16-C17-C18
22	c	509	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	CBA-CGA-O2A-C1
22	C	508	CLA	CBA-CGA-O2A-C1
27	A	410	LMG	C4-C5-C6-O5
25	D	409	DGD	C1G-C2G-O2G-C1B
25	d	408	DGD	C1G-C2G-O2G-C1B
27	E	101	LMG	C7-C8-O7-C10
27	c	518	LMG	C9-C8-O7-C10
25	B	625	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
25	c	516	DGD	O6D-C5D-C6D-O5D
24	j	102	BCR	C18-C19-C20-C21
25	C	517	DGD	C3B-C4B-C5B-C6B
25	c	517	DGD	C3B-C4B-C5B-C6B
27	d	407	LMG	C28-C29-C30-C31
22	C	504	CLA	O1A-CGA-O2A-C1
24	J	102	BCR	C20-C21-C22-C23
22	B	603	CLA	C15-C16-C17-C18
22	C	504	CLA	C15-C16-C17-C18
22	C	510	CLA	CBA-CGA-O2A-C1
32	d	401	PHO	CBD-CGD-O2D-CED
23	A	406	PL9	C35-C34-C36-C37
23	D	407	PL9	C35-C34-C36-C37
22	C	504	CLA	C2-C3-C5-C6
27	B	621	LMG	C13-C14-C15-C16
27	c	522	LMG	C16-C17-C18-C19
22	B	601	CLA	C16-C17-C18-C20
22	B	613	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C19
27	B	624	LMG	C32-C33-C34-C35
30	a	401	SQD	C10-C11-C12-C13
25	C	516	DGD	O6D-C5D-C6D-O5D
27	b	628	LMG	C32-C33-C34-C35
25	C	515	DGD	O2G-C2G-C3G-O3G
25	c	517	DGD	O1G-C1G-C2G-O2G
27	a	413	LMG	O1-C7-C8-O7
27	m	101	LMG	O7-C8-C9-O8
25	a	411	DGD	C4B-C5B-C6B-C7B
27	i	101	LMG	C31-C32-C33-C34
30	A	413	SQD	C17-C18-C19-C20
30	a	415	SQD	C17-C18-C19-C20
27	A	410	LMG	C8-C9-O8-C28
27	I	101	LMG	C18-C19-C20-C21
27	e	101	LMG	C18-C19-C20-C21
27	E	101	LMG	O7-C10-C11-C12
27	E	101	LMG	C17-C18-C19-C20
27	i	101	LMG	C18-C19-C20-C21
27	c	522	LMG	C17-C18-C19-C20
22	B	609	CLA	C16-C17-C18-C20
22	C	511	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
25	c	516	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
25	D	409	DGD	CDB-CEB-CFB-CGB
25	d	408	DGD	CDB-CEB-CFB-CGB
22	b	613	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	CBA-CGA-O2A-C1
27	A	415	LMG	C11-C12-C13-C14
27	a	413	LMG	C11-C10-O7-C8
23	d	406	PL9	C27-C28-C29-C30
25	b	601	DGD	O6D-C5D-C6D-O5D
22	C	502	CLA	C13-C15-C16-C17
22	b	617	CLA	C5-C6-C7-C8
25	C	516	DGD	C4D-C5D-C6D-O5D
22	b	617	CLA	C16-C17-C18-C20
22	c	504	CLA	C4-C3-C5-C6
23	D	407	PL9	C15-C14-C16-C17
27	C	522	LMG	C34-C35-C36-C37
25	D	409	DGD	CAA-CBA-CCA-CDA
26	C	519	LHG	C11-C10-C9-C8
26	c	519	LHG	C11-C10-C9-C8
30	A	414	SQD	C10-C11-C12-C13
22	B	602	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	507	CLA	C11-C10-C8-C9
22	D	405	CLA	C14-C13-C15-C16
22	b	609	CLA	C14-C13-C15-C16
22	b	618	CLA	C14-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C14
22	c	504	CLA	C6-C7-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
32	D	402	PHO	C14-C13-C15-C16
32	a	407	PHO	C14-C13-C15-C16
30	A	413	SQD	C10-C11-C12-C13
27	I	101	LMG	O10-C28-O8-C9
25	D	409	DGD	CBA-CCA-CDA-CEA
27	a	402	LMG	C17-C18-C19-C20
22	c	504	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	B	624	LMG	C2-C1-O1-C7
27	b	628	LMG	C2-C1-O1-C7
25	d	408	DGD	CBA-CCA-CDA-CEA
25	c	517	DGD	CFA-CGA-CHA-CIA
22	B	602	CLA	C6-C7-C8-C10
22	B	607	CLA	C6-C7-C8-C10
22	B	608	CLA	C12-C13-C15-C16
22	B	610	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
22	B	615	CLA	C11-C10-C8-C7
22	C	501	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	C11-C10-C8-C7
22	C	508	CLA	C11-C10-C8-C7
22	C	509	CLA	C6-C7-C8-C10
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	H	101	CLA	C6-C7-C8-C10
22	b	606	CLA	C6-C7-C8-C10
22	b	609	CLA	C12-C13-C15-C16
22	b	619	CLA	C12-C13-C15-C16
22	c	502	CLA	C12-C13-C15-C16
22	c	505	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	511	CLA	C11-C12-C13-C15
22	B	615	CLA	C15-C16-C17-C18
22	b	619	CLA	C8-C10-C11-C12
22	c	501	CLA	C13-C15-C16-C17
22	B	601	CLA	C16-C17-C18-C19
27	i	101	LMG	C17-C18-C19-C20
22	c	504	CLA	O1A-CGA-O2A-C1
26	c	519	LHG	O10-C23-O8-C6
27	E	101	LMG	C19-C20-C21-C22
22	A	402	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	C4-C3-C5-C6
22	a	404	CLA	C3A-C2A-CAA-CBA
23	d	406	PL9	C15-C14-C16-C17
22	B	613	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	b	628	LMG	C15-C16-C17-C18
22	A	405	CLA	C13-C15-C16-C17
27	D	412	LMG	C38-C39-C40-C41
27	d	410	LMG	C38-C39-C40-C41
22	C	508	CLA	O1A-CGA-O2A-C1
26	C	519	LHG	O10-C23-O8-C6
27	e	101	LMG	C19-C20-C21-C22
27	a	413	LMG	O6-C5-C6-O5
22	B	604	CLA	C5-C6-C7-C8
27	a	402	LMG	C11-C12-C13-C14
22	b	608	CLA	C10-C11-C12-C13
25	B	625	DGD	C1G-C2G-C3G-O3G
25	C	516	DGD	C1G-C2G-C3G-O3G
25	C	517	DGD	O1G-C1G-C2G-C3G
25	D	409	DGD	C1G-C2G-C3G-O3G
25	c	516	DGD	C1G-C2G-C3G-O3G
25	d	408	DGD	C1G-C2G-C3G-O3G
27	A	410	LMG	O1-C7-C8-C9
27	C	518	LMG	O1-C7-C8-C9
27	M	101	LMG	O1-C7-C8-C9
27	c	518	LMG	O1-C7-C8-C9
27	m	101	LMG	O1-C7-C8-C9
30	a	401	SQD	O6-C44-C45-C46
25	C	517	DGD	CFA-CGA-CHA-CIA
22	c	511	CLA	C3-C5-C6-C7
22	B	609	CLA	C16-C17-C18-C19
22	b	613	CLA	C16-C17-C18-C19
22	B	613	CLA	C5-C6-C7-C8
27	B	624	LMG	C19-C20-C21-C22
27	C	522	LMG	C17-C18-C19-C20
27	b	625	LMG	C17-C18-C19-C20
27	B	621	LMG	C17-C18-C19-C20
27	E	101	LMG	C18-C19-C20-C21
27	b	628	LMG	C19-C20-C21-C22
22	c	504	CLA	C2-C3-C5-C6
22	B	610	CLA	O1A-CGA-O2A-C1
27	D	412	LMG	C19-C20-C21-C22
22	b	617	CLA	C15-C16-C17-C18
25	d	408	DGD	CAA-CBA-CCA-CDA
22	B	604	CLA	C15-C16-C17-C18
25	B	625	DGD	C5A-C6A-C7A-C8A
27	I	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	J	101	PL9	C27-C28-C29-C30
31	B	627	LMT	C5'-C4'-O1B-C1B
24	B	616	BCR	C1-C6-C7-C8
24	C	513	BCR	C1-C6-C7-C8
24	D	411	BCR	C1-C6-C7-C8
24	J	102	BCR	C1-C6-C7-C8
24	b	620	BCR	C1-C6-C7-C8
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
25	D	409	DGD	C1A-C2A-C3A-C4A
25	D	409	DGD	C3B-C4B-C5B-C6B
25	c	516	DGD	C3A-C4A-C5A-C6A
27	b	628	LMG	C13-C14-C15-C16
31	B	623	LMT	O5B-C1B-O1B-C4'
22	C	508	CLA	C15-C16-C17-C18
26	C	519	LHG	C25-C26-C27-C28
27	D	408	LMG	C29-C30-C31-C32
22	C	511	CLA	C16-C17-C18-C19
22	c	512	CLA	C2A-CAA-CBA-CGA
22	B	615	CLA	C8-C10-C11-C12
25	C	517	DGD	O1G-C1G-C2G-O2G
25	c	515	DGD	O2G-C2G-C3G-O3G
27	C	518	LMG	O1-C7-C8-O7
27	C	522	LMG	O7-C8-C9-O8
27	M	101	LMG	O7-C8-C9-O8
27	c	518	LMG	O1-C7-C8-O7
27	c	522	LMG	O7-C8-C9-O8
30	D	403	SQD	O6-C44-C45-O47
30	b	602	SQD	O47-C45-C46-O48
30	d	402	SQD	O6-C44-C45-O47
31	b	603	LMT	C5'-C4'-O1B-C1B
23	A	406	PL9	C4-C3-C7-C8
23	a	409	PL9	C4-C3-C7-C8
30	a	415	SQD	C31-C32-C33-C34
27	m	101	LMG	C30-C31-C32-C33
30	A	414	SQD	C9-C10-C11-C12
22	a	405	CLA	C5-C6-C7-C8
22	b	613	CLA	C5-C6-C7-C8
23	j	101	PL9	C27-C28-C29-C30
27	A	410	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
30	a	415	SQD	C10-C11-C12-C13
27	I	101	LMG	C17-C18-C19-C20
27	e	101	LMG	C17-C18-C19-C20
30	A	413	SQD	C31-C32-C33-C34
27	D	408	LMG	C28-C29-C30-C31
22	C	511	CLA	C3-C5-C6-C7
22	B	608	CLA	C14-C13-C15-C16
22	C	501	CLA	C11-C12-C13-C14
22	D	405	CLA	C6-C7-C8-C9
22	b	612	CLA	C14-C13-C15-C16
27	d	410	LMG	C19-C20-C21-C22
31	b	627	LMT	O5B-C1B-O1B-C4'
22	C	510	CLA	O1A-CGA-O2A-C1
25	d	408	DGD	C3B-C4B-C5B-C6B
27	c	522	LMG	C34-C35-C36-C37
22	b	617	CLA	C16-C17-C18-C19
25	c	516	DGD	C4B-C5B-C6B-C7B
25	d	408	DGD	C4E-C5E-C6E-O5E
22	b	608	CLA	C15-C16-C17-C18
25	b	601	DGD	C5A-C6A-C7A-C8A
22	b	608	CLA	C5-C6-C7-C8
22	b	619	CLA	C15-C16-C17-C18
22	c	506	CLA	O1D-CGD-O2D-CED
25	D	409	DGD	C2B-C3B-C4B-C5B
31	B	628	LMT	C2-C3-C4-C5
24	B	617	BCR	C20-C21-C22-C37
25	C	517	DGD	CDB-CEB-CFB-CGB
22	B	609	CLA	C10-C11-C12-C13
22	c	511	CLA	C5-C6-C7-C8
22	A	403	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	609	CLA	C11-C12-C13-C15
22	B	612	CLA	C11-C10-C8-C7
22	B	612	CLA	C11-C12-C13-C15
22	B	615	CLA	C12-C13-C15-C16
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C10
22	C	511	CLA	C12-C13-C15-C16
22	a	405	CLA	C12-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C10-C8-C7
22	b	611	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
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
27	c	518	LMG	C13-C14-C15-C16
30	f	103	SQD	C29-C30-C31-C32
25	C	516	DGD	C3A-C4A-C5A-C6A
24	J	102	BCR	C7-C8-C9-C10
24	c	514	BCR	C7-C8-C9-C10
34	F	101	HEM	C3D-CAD-CBD-CGD
27	i	101	LMG	O10-C28-O8-C9
27	a	413	LMG	C8-C7-O1-C1
30	D	403	SQD	C45-C44-O6-C1
30	D	403	SQD	C5-C6-S-O8
30	d	402	SQD	C45-C44-O6-C1
30	d	402	SQD	C5-C6-S-O8
31	b	603	LMT	C4'-C5'-C6'-O6'
22	C	506	CLA	O1D-CGD-O2D-CED
30	b	602	SQD	O49-C7-O47-C45
22	c	510	CLA	O1A-CGA-O2A-C1
32	D	401	PHO	C5-C6-C7-C8
27	B	624	LMG	C20-C21-C22-C23
27	d	407	LMG	C29-C30-C31-C32
22	C	511	CLA	C5-C6-C7-C8
32	D	402	PHO	C10-C11-C12-C13
25	b	624	DGD	C5A-C6A-C7A-C8A
22	b	613	CLA	O1A-CGA-O2A-C1
22	B	603	CLA	CBA-CGA-O2A-C1
22	b	615	CLA	C10-C11-C12-C13
30	B	626	SQD	C17-C18-C19-C20
23	D	407	PL9	C24-C26-C27-C28
25	a	411	DGD	C1G-C2G-C3G-O3G
25	b	601	DGD	C1G-C2G-C3G-O3G
30	A	413	SQD	C44-C45-C46-O48
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

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Mol	Chain	Res	Type	Atoms
30	b	602	SQD	C10-C11-C12-C13
27	d	407	LMG	C36-C37-C38-C39
22	B	613	CLA	C2A-CAA-CBA-CGA
25	d	408	DGD	C1A-C2A-C3A-C4A
25	a	411	DGD	O2G-C2G-C3G-O3G
27	B	621	LMG	O7-C8-C9-O8
27	b	625	LMG	O7-C8-C9-O8
30	B	626	SQD	O47-C45-C46-O48
22	B	611	CLA	C10-C11-C12-C13
22	A	403	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C12-C13-C14
22	B	612	CLA	C11-C12-C13-C14
22	C	507	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	a	405	CLA	C14-C13-C15-C16
22	b	616	CLA	C11-C12-C13-C14
22	c	501	CLA	C11-C12-C13-C14
22	c	507	CLA	C14-C13-C15-C16
32	d	401	PHO	C6-C7-C8-C9
27	b	625	LMG	C28-C29-C30-C31
30	B	626	SQD	C10-C11-C12-C13
22	B	605	CLA	CBA-CGA-O2A-C1
25	C	516	DGD	C4B-C5B-C6B-C7B
27	A	410	LMG	C20-C21-C22-C23
27	C	518	LMG	C13-C14-C15-C16
22	A	404	CLA	C5-C6-C7-C8
30	A	413	SQD	C15-C16-C17-C18
30	a	415	SQD	C15-C16-C17-C18
27	b	628	LMG	C20-C21-C22-C23
32	d	401	PHO	C5-C6-C7-C8
25	c	517	DGD	CDB-CEB-CFB-CGB
26	A	409	LHG	C2-C3-O3-P
25	d	408	DGD	C2B-C3B-C4B-C5B
22	C	507	CLA	C5-C6-C7-C8
22	b	613	CLA	C10-C11-C12-C13
22	b	607	CLA	CBA-CGA-O2A-C1
22	B	604	CLA	C10-C11-C12-C13
27	c	522	LMG	C35-C36-C37-C38
30	A	414	SQD	C32-C33-C34-C35
22	A	403	CLA	C5-C6-C7-C8
27	A	410	LMG	C29-C30-C31-C32
30	F	102	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
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	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
25	d	408	DGD	C4A-C5A-C6A-C7A
22	b	615	CLA	C4-C3-C5-C6
23	a	409	PL9	C35-C34-C36-C37
24	C	514	BCR	C7-C8-C9-C10
24	j	102	BCR	C7-C8-C9-C10
25	D	409	DGD	C4A-C5A-C6A-C7A
22	c	506	CLA	C3-C5-C6-C7
25	D	409	DGD	C4E-C5E-C6E-O5E
22	c	508	CLA	C15-C16-C17-C18
27	e	101	LMG	O7-C10-C11-C12
32	D	401	PHO	CBD-CGD-O2D-CED
30	B	626	SQD	O49-C7-O47-C45
22	A	405	CLA	C11-C10-C8-C7
22	B	602	CLA	C11-C12-C13-C15
22	B	607	CLA	C11-C12-C13-C15
22	B	609	CLA	C12-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C15
22	D	406	CLA	C11-C10-C8-C7
22	H	101	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
26	c	519	LHG	O2-C2-C3-O3
22	B	614	CLA	CBA-CGA-O2A-C1
30	D	403	SQD	C10-C11-C12-C13
27	C	522	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	d	401	PHO	O1D-CGD-O2D-CED
27	B	621	LMG	C28-C29-C30-C31
22	B	611	CLA	C4-C3-C5-C6
22	C	512	CLA	C3A-C2A-CAA-CBA
22	A	405	CLA	C16-C17-C18-C19
27	B	624	LMG	C16-C17-C18-C19
26	C	519	LHG	O6-C4-C5-O7
26	c	519	LHG	O6-C4-C5-O7
22	C	508	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	C11-C10-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	C	511	CLA	C14-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	b	618	CLA	C6-C7-C8-C9
22	b	619	CLA	C11-C10-C8-C9
22	c	511	CLA	C14-C13-C15-C16
22	B	603	CLA	O1A-CGA-O2A-C1
22	B	605	CLA	O1A-CGA-O2A-C1
27	c	518	LMG	C32-C33-C34-C35
23	D	407	PL9	C32-C33-C34-C36
22	a	408	CLA	C16-C17-C18-C19
22	B	609	CLA	C5-C6-C7-C8
32	D	402	PHO	C13-C15-C16-C17
32	a	407	PHO	C13-C15-C16-C17
27	D	408	LMG	C31-C32-C33-C34
25	c	515	DGD	C5A-C6A-C7A-C8A
22	C	506	CLA	C3-C5-C6-C7
27	a	413	LMG	C20-C21-C22-C23
22	b	607	CLA	O1A-CGA-O2A-C1
25	B	620	DGD	O1A-C1A-O1G-C1G
27	m	101	LMG	O10-C28-O8-C9
25	A	408	DGD	O2G-C2G-C3G-O3G
25	D	409	DGD	O2G-C2G-C3G-O3G
25	d	408	DGD	O2G-C2G-C3G-O3G
27	d	407	LMG	C31-C32-C33-C34
27	e	101	LMG	O1-C7-C8-C9
30	D	403	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
30	d	402	SQD	O6-C44-C45-C46
22	b	609	CLA	C13-C15-C16-C17
23	d	406	PL9	C13-C14-C16-C17
27	a	413	LMG	C16-C17-C18-C19
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
32	a	407	PHO	C10-C11-C12-C13
22	C	504	CLA	C8-C10-C11-C12
25	b	624	DGD	CCA-CDA-CEA-CFA
31	b	604	LMT	C2-C3-C4-C5
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	616	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
26	A	409	LHG	C3-O3-P-O5
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
23	D	407	PL9	C20-C19-C21-C22
23	d	406	PL9	C20-C19-C21-C22
22	B	601	CLA	C2B-C3B-CAB-CBB
22	B	605	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
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
24	f	102	BCR	C7-C8-C9-C34
27	a	413	LMG	C10-C11-C12-C13
24	H	102	BCR	C7-C8-C9-C10
27	b	625	LMG	C12-C13-C14-C15
30	a	401	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	h	101	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	C3-C5-C6-C7
25	B	620	DGD	CAB-CBB-CCB-CDB
22	B	614	CLA	O1A-CGA-O2A-C1
25	C	517	DGD	C3G-C2G-O2G-C1B
25	c	517	DGD	C3G-C2G-O2G-C1B
26	A	409	LHG	C6-C5-O7-C7
26	a	412	LHG	C6-C5-O7-C7
27	m	101	LMG	C9-C8-O7-C10
27	B	621	LMG	C12-C13-C14-C15
30	f	103	SQD	C24-C25-C26-C27
22	b	616	CLA	C10-C11-C12-C13
26	C	519	LHG	O6-C4-C5-C6
26	c	519	LHG	O6-C4-C5-C6
27	M	101	LMG	O10-C28-O8-C9
22	A	404	CLA	C6-C7-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	609	CLA	C11-C12-C13-C14
22	B	610	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	b	606	CLA	C11-C12-C13-C14
22	b	616	CLA	C11-C10-C8-C9
22	b	619	CLA	C11-C12-C13-C14
22	b	619	CLA	C14-C13-C15-C16
22	c	510	CLA	C11-C10-C8-C9
22	d	404	CLA	C6-C7-C8-C9
32	D	401	PHO	C6-C7-C8-C9
32	D	402	PHO	C11-C10-C8-C9
22	A	404	CLA	C6-C7-C8-C10
22	B	601	CLA	C6-C7-C8-C10
22	b	606	CLA	C11-C12-C13-C15
22	c	508	CLA	C6-C7-C8-C10
26	c	519	LHG	C7-C8-C9-C10
30	a	401	SQD	C32-C33-C34-C35
27	A	410	LMG	O6-C1-O1-C7
22	A	405	CLA	C16-C17-C18-C20
30	d	402	SQD	C10-C11-C12-C13
22	h	101	CLA	O1A-CGA-O2A-C1
30	a	415	SQD	C11-C10-C9-C8
22	B	612	CLA	C10-C11-C12-C13
27	a	402	LMG	C16-C17-C18-C19
27	b	628	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	c	516	DGD	C6A-C7A-C8A-C9A
27	C	518	LMG	C32-C33-C34-C35
26	a	412	LHG	C2-C3-O3-P
25	c	517	DGD	C8B-C9B-CAB-CBB
30	b	602	SQD	C17-C18-C19-C20
27	D	408	LMG	O1-C7-C8-O7
27	d	407	LMG	O1-C7-C8-O7
27	E	101	LMG	C31-C32-C33-C34
25	b	624	DGD	CAB-CBB-CCB-CDB
27	a	413	LMG	C29-C30-C31-C32
22	C	511	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	C2A-CAA-CBA-CGA
23	J	101	PL9	C15-C14-C16-C17
22	a	408	CLA	C16-C17-C18-C20
22	c	511	CLA	CAA-CBA-CGA-O2A
23	D	407	PL9	C13-C14-C16-C17
23	d	406	PL9	C24-C26-C27-C28
27	A	410	LMG	C10-C11-C12-C13
22	a	406	CLA	C5-C6-C7-C8
30	A	413	SQD	C11-C10-C9-C8
32	D	401	PHO	O1D-CGD-O2D-CED
24	c	513	BCR	C11-C12-C13-C35
27	A	410	LMG	C38-C39-C40-C41
23	d	406	PL9	C32-C33-C34-C36
25	C	515	DGD	C5A-C6A-C7A-C8A
22	b	616	CLA	C8-C10-C11-C12
25	B	625	DGD	C2G-C3G-O3G-C1D
25	b	601	DGD	C2G-C3G-O3G-C1D
27	d	410	LMG	C8-C7-O1-C1
27	B	624	LMG	C13-C14-C15-C16
22	d	405	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C16-C17-C18-C20
22	A	403	CLA	C4-C3-C5-C6
22	B	610	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
23	D	407	PL9	C40-C39-C41-C42
27	D	412	LMG	C16-C17-C18-C19
27	B	624	LMG	C10-C11-C12-C13
22	b	617	CLA	C2C-C3C-CAC-CBC
22	b	606	CLA	C16-C17-C18-C19
22	B	607	CLA	C11-C12-C13-C14
22	B	615	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
22	b	611	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
32	a	407	PHO	C6-C7-C8-C9
32	a	407	PHO	C11-C10-C8-C9
22	B	609	CLA	CBA-CGA-O2A-C1
22	b	608	CLA	C4B-C3B-CAB-CBB
34	f	101	HEM	C3D-CAD-CBD-CGD
22	a	405	CLA	C4-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
27	m	101	LMG	C31-C32-C33-C34
22	c	504	CLA	C8-C10-C11-C12
25	C	517	DGD	C8B-C9B-CAB-CBB
27	M	101	LMG	C31-C32-C33-C34
22	C	505	CLA	C6-C7-C8-C10
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	510	CLA	C11-C10-C8-C7
22	b	608	CLA	C8-C10-C11-C12
25	b	624	DGD	O1A-C1A-O1G-C1G
25	c	515	DGD	C5B-C6B-C7B-C8B
30	a	401	SQD	C12-C13-C14-C15
25	B	620	DGD	C5A-C6A-C7A-C8A
27	c	522	LMG	C32-C33-C34-C35
26	C	519	LHG	O2-C2-C3-O3
27	A	410	LMG	C16-C17-C18-C19
27	A	415	LMG	C12-C13-C14-C15
27	C	522	LMG	C32-C33-C34-C35
27	A	415	LMG	C16-C17-C18-C19
22	B	605	CLA	C13-C15-C16-C17
22	c	512	CLA	C3A-C2A-CAA-CBA
22	B	611	CLA	C2-C3-C5-C6
27	b	625	LMG	C15-C16-C17-C18
27	a	413	LMG	C35-C36-C37-C38
27	c	522	LMG	C30-C31-C32-C33
27	d	410	LMG	C16-C17-C18-C19
22	b	616	CLA	C13-C15-C16-C17
22	a	405	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	C	515	DGD	C5B-C6B-C7B-C8B
27	a	413	LMG	C11-C12-C13-C14
22	b	615	CLA	C2-C3-C5-C6
26	c	519	LHG	C1-C2-C3-O3
25	C	516	DGD	C7B-C8B-C9B-CAB
22	B	614	CLA	C6-C7-C8-C9
22	B	615	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	C14-C13-C15-C16
22	D	406	CLA	C11-C10-C8-C9
22	b	605	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
22	c	520	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C10-C8-C9
27	M	101	LMG	C30-C31-C32-C33
22	B	602	CLA	C16-C17-C18-C19
22	c	509	CLA	C16-C17-C18-C19
27	M	101	LMG	C16-C17-C18-C19
27	B	624	LMG	C29-C30-C31-C32
27	M	101	LMG	C9-C8-O7-C10
22	b	606	CLA	C15-C16-C17-C18
22	b	614	CLA	C2-C3-C5-C6
22	B	609	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	C8-C10-C11-C12
27	B	621	LMG	C15-C16-C17-C18
25	d	408	DGD	CBB-CCB-CDB-CEB
27	e	101	LMG	C31-C32-C33-C34
22	C	512	CLA	C1A-C2A-CAA-CBA
22	d	404	CLA	C1A-C2A-CAA-CBA
22	B	604	CLA	C2B-C3B-CAB-CBB
22	C	508	CLA	C2B-C3B-CAB-CBB
22	b	608	CLA	C2B-C3B-CAB-CBB
22	c	508	CLA	C2B-C3B-CAB-CBB
22	c	520	CLA	C2B-C3B-CAB-CBB
24	A	407	BCR	C1-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C30
24	B	616	BCR	C5-C6-C7-C8
24	B	619	BCR	C1-C6-C7-C8
24	B	619	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
24	C	513	BCR	C5-C6-C7-C8
24	C	513	BCR	C23-C24-C25-C30
24	C	521	BCR	C23-C24-C25-C30
24	D	411	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
27	D	408	LMG	C18-C19-C20-C21
22	B	602	CLA	C15-C16-C17-C18
22	c	510	CLA	C4-C3-C5-C6
25	c	516	DGD	C7B-C8B-C9B-CAB
30	A	414	SQD	C12-C13-C14-C15
22	C	507	CLA	C11-C12-C13-C15
22	C	520	CLA	C6-C7-C8-C10
22	D	405	CLA	C11-C10-C8-C7
22	b	605	CLA	C6-C7-C8-C10
22	b	605	CLA	C12-C13-C15-C16
22	b	609	CLA	C6-C7-C8-C10
22	c	505	CLA	C6-C7-C8-C10
22	c	505	CLA	C11-C10-C8-C7
32	D	402	PHO	C11-C10-C8-C7
32	a	407	PHO	C11-C10-C8-C7
27	D	408	LMG	C36-C37-C38-C39
30	F	102	SQD	C24-C25-C26-C27
25	D	409	DGD	CBB-CCB-CDB-CEB
30	F	102	SQD	C9-C10-C11-C12
30	a	415	SQD	C12-C13-C14-C15
27	A	410	LMG	C35-C36-C37-C38
22	b	609	CLA	C16-C17-C18-C19
27	C	522	LMG	C30-C31-C32-C33
22	C	510	CLA	C4-C3-C5-C6
22	B	604	CLA	C8-C10-C11-C12
22	B	612	CLA	C13-C15-C16-C17
22	c	510	CLA	C2-C3-C5-C6
27	a	413	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
22	b	613	CLA	C2-C1-O2A-CGA
27	a	413	LMG	C8-C9-O8-C28
22	B	605	CLA	C16-C17-C18-C20
30	a	401	SQD	C26-C27-C28-C29
25	d	408	DGD	O6E-C5E-C6E-O5E
27	b	625	LMG	C29-C28-O8-C9
22	C	512	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
25	b	601	DGD	C2A-C3A-C4A-C5A
25	B	620	DGD	CCA-CDA-CEA-CFA
27	A	410	LMG	C17-C18-C19-C20
25	b	624	DGD	C4A-C5A-C6A-C7A
25	c	515	DGD	O6D-C1D-O3G-C3G
27	e	101	LMG	C14-C15-C16-C17
22	b	606	CLA	C16-C17-C18-C20
31	B	623	LMT	C6-C7-C8-C9
27	b	628	LMG	C29-C30-C31-C32
30	A	413	SQD	C12-C13-C14-C15
30	f	103	SQD	C9-C10-C11-C12
27	d	410	LMG	O1-C7-C8-C9
25	B	620	DGD	C7B-C8B-C9B-CAB
27	e	101	LMG	C30-C31-C32-C33
27	a	402	LMG	C12-C13-C14-C15
22	b	617	CLA	C4C-C3C-CAC-CBC
22	C	501	CLA	C13-C15-C16-C17
22	C	503	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
22	C	509	CLA	C16-C17-C18-C19
22	B	604	CLA	C4B-C3B-CAB-CBB
22	D	406	CLA	C4B-C3B-CAB-CBB
22	d	405	CLA	C4B-C3B-CAB-CBB
22	c	509	CLA	C16-C17-C18-C20
27	A	410	LMG	C11-C12-C13-C14
22	c	502	CLA	C16-C17-C18-C20
27	b	625	LMG	O1-C7-C8-O7
27	e	101	LMG	O1-C7-C8-O7
25	c	517	DGD	CBB-CCB-CDB-CEB
26	A	409	LHG	C27-C28-C29-C30
22	B	607	CLA	C13-C15-C16-C17
30	f	103	SQD	C14-C15-C16-C17
22	C	512	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
32	D	402	PHO	C6-C7-C8-C10
25	a	411	DGD	C2A-C3A-C4A-C5A
27	m	101	LMG	C17-C18-C19-C20
22	A	403	CLA	C11-C10-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	c	509	CLA	C11-C10-C8-C9
25	A	408	DGD	C2A-C3A-C4A-C5A
27	D	412	LMG	C8-C7-O1-C1
22	A	403	CLA	C2-C1-O2A-CGA
22	B	609	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
22	b	616	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
32	D	401	PHO	C2-C1-O2A-CGA
22	B	613	CLA	C2C-C3C-CAC-CBC
22	c	509	CLA	C13-C15-C16-C17
22	b	609	CLA	CBA-CGA-O2A-C1
22	b	618	CLA	CBA-CGA-O2A-C1
25	b	601	DGD	C4E-C5E-C6E-O5E
22	C	520	CLA	C3A-C2A-CAA-CBA
22	D	405	CLA	C3A-C2A-CAA-CBA
27	D	408	LMG	C34-C35-C36-C37
31	B	622	LMT	C4-C5-C6-C7
26	A	409	LHG	C4-C5-O7-C7
26	a	412	LHG	C4-C5-O7-C7
22	b	618	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	C16-C17-C18-C20
22	c	507	CLA	C5-C6-C7-C8
22	b	609	CLA	O1A-CGA-O2A-C1
22	C	501	CLA	C16-C17-C18-C20
25	B	625	DGD	C2A-C3A-C4A-C5A
25	C	516	DGD	O6E-C1E-O5D-C6D
25	D	409	DGD	C8A-C9A-CAA-CBA
30	a	415	SQD	C16-C17-C18-C19
27	B	621	LMG	C29-C28-O8-C9
25	C	515	DGD	C1G-C2G-C3G-O3G
25	c	515	DGD	C1G-C2G-C3G-O3G
27	E	101	LMG	O1-C7-C8-C9
27	c	518	LMG	C7-C8-C9-O8
22	D	406	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	C2A-CAA-CBA-CGA
27	E	101	LMG	C33-C34-C35-C36
30	A	413	SQD	C16-C17-C18-C19
26	C	519	LHG	O7-C7-C8-C9
27	a	413	LMG	O7-C10-C11-C12
27	m	101	LMG	C16-C17-C18-C19
22	A	405	CLA	C11-C10-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	H	101	CLA	C11-C12-C13-C14
22	a	405	CLA	C11-C10-C8-C9
22	h	101	CLA	C11-C10-C8-C9
22	B	602	CLA	C16-C17-C18-C20
22	B	605	CLA	C16-C17-C18-C19
22	C	509	CLA	C16-C17-C18-C20
22	B	612	CLA	CAA-CBA-CGA-O2A
22	b	616	CLA	CAA-CBA-CGA-O2A
26	c	519	LHG	O7-C7-C8-C9
24	f	102	BCR	C21-C22-C23-C24
24	x	101	BCR	C7-C8-C9-C10
27	D	412	LMG	C36-C37-C38-C39
27	d	410	LMG	C11-C12-C13-C14
22	B	601	CLA	C11-C12-C13-C15
22	B	601	CLA	C12-C13-C15-C16
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	C12-C13-C15-C16
22	a	408	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C12-C13-C15
22	c	507	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	C11-C12-C13-C15
22	c	512	CLA	C12-C13-C15-C16
22	h	101	CLA	C12-C13-C15-C16
22	D	406	CLA	C2B-C3B-CAB-CBB
22	d	405	CLA	C2B-C3B-CAB-CBB
24	A	407	BCR	C23-C24-C25-C26
24	B	617	BCR	C1-C6-C7-C8
24	B	619	BCR	C5-C6-C7-C8
24	B	619	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
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-C26
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
27	B	621	LMG	C35-C36-C37-C38
27	E	101	LMG	C30-C31-C32-C33
30	A	413	SQD	C8-C7-O47-C45
22	d	404	CLA	CAA-CBA-CGA-O2A
22	A	402	CLA	C2-C1-O2A-CGA
25	B	625	DGD	CAB-CBB-CCB-CDB
22	B	611	CLA	CAA-CBA-CGA-O2A
27	A	410	LMG	O7-C10-C11-C12
25	A	408	DGD	O6E-C1E-O5D-C6D
25	b	601	DGD	O6D-C1D-O3G-C3G
25	C	517	DGD	C4A-C5A-C6A-C7A
27	M	101	LMG	C17-C18-C19-C20
22	C	509	CLA	C13-C15-C16-C17
22	A	405	CLA	C4-C3-C5-C6
22	D	405	CLA	C3-C5-C6-C7
26	C	519	LHG	C11-C12-C13-C14
27	a	402	LMG	O7-C10-C11-C12
25	C	517	DGD	CBB-CCB-CDB-CEB
26	c	519	LHG	C11-C12-C13-C14
34	V	201	HEM	CAA-CBA-CGA-O2A
32	D	401	PHO	C13-C15-C16-C17
30	f	103	SQD	C15-C16-C17-C18
22	b	615	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	C3-C5-C6-C7
22	C	501	CLA	C16-C17-C18-C19
22	a	408	CLA	C4-C3-C5-C6
22	B	613	CLA	C4C-C3C-CAC-CBC
25	C	517	DGD	O1G-C1A-C2A-C3A
25	c	517	DGD	O1G-C1A-C2A-C3A
27	C	522	LMG	O8-C28-C29-C30
22	b	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	A	403	CLA	C2-C3-C5-C6
22	a	405	CLA	C2-C3-C5-C6
25	c	517	DGD	C4A-C5A-C6A-C7A
27	A	415	LMG	O7-C10-C11-C12
22	H	101	CLA	O1A-CGA-O2A-C1
25	A	408	DGD	O6D-C5D-C6D-O5D
22	C	505	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C12-C13-C14
22	C	509	CLA	C11-C10-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	609	CLA	C6-C7-C8-C9
22	c	505	CLA	C6-C7-C8-C9
25	C	517	DGD	C4B-C5B-C6B-C7B
30	a	401	SQD	O47-C7-C8-C9
25	D	409	DGD	O6E-C5E-C6E-O5E
27	C	518	LMG	C7-C8-C9-O8
27	i	101	LMG	C7-C8-C9-O8
22	A	403	CLA	C4B-C3B-CAB-CBB
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	614	CLA	C4B-C3B-CAB-CBB
22	b	618	CLA	C4B-C3B-CAB-CBB
22	c	512	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	CBA-CGA-O2A-C1
25	B	625	DGD	O6D-C1D-O3G-C3G
25	C	515	DGD	O6D-C1D-O3G-C3G
25	a	411	DGD	O6E-C1E-O5D-C6D
25	c	516	DGD	O6E-C1E-O5D-C6D
27	M	101	LMG	O6-C1-O1-C7
27	m	101	LMG	O6-C1-O1-C7
22	D	405	CLA	CAA-CBA-CGA-O2A
22	c	501	CLA	CAA-CBA-CGA-O2A
22	c	509	CLA	CAA-CBA-CGA-O2A
30	A	414	SQD	O47-C7-C8-C9
27	B	621	LMG	O1-C7-C8-O7
27	d	410	LMG	O1-C7-C8-O7
34	v	201	HEM	CAA-CBA-CGA-O2A
31	B	623	LMT	O5'-C5'-C6'-O6'
24	D	411	BCR	C21-C22-C23-C24
25	c	517	DGD	C4B-C5B-C6B-C7B
22	C	501	CLA	CAA-CBA-CGA-O2A
27	c	522	LMG	O8-C28-C29-C30
22	b	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	B	620	DGD	C4A-C5A-C6A-C7A
26	C	519	LHG	C7-C8-C9-C10
22	C	509	CLA	CAA-CBA-CGA-O2A
30	d	402	SQD	O47-C7-C8-C9
25	a	411	DGD	C4A-C5A-C6A-C7A
30	D	403	SQD	C5-C6-S-O9
30	a	401	SQD	C5-C6-S-O9
30	d	402	SQD	C5-C6-S-O9
25	A	408	DGD	C4D-C5D-C6D-O5D
22	B	612	CLA	C2-C1-O2A-CGA
32	d	401	PHO	C2-C1-O2A-CGA
22	c	506	CLA	CAA-CBA-CGA-O2A
22	B	602	CLA	C11-C10-C8-C7
22	b	606	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
22	d	404	CLA	C11-C10-C8-C7
22	C	502	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	C8-C10-C11-C12
27	b	628	LMG	C10-C11-C12-C13
25	d	408	DGD	C8A-C9A-CAA-CBA
25	d	408	DGD	C9B-CAB-CBB-CCB
27	a	413	LMG	C17-C18-C19-C20
27	M	101	LMG	C7-C8-O7-C10
22	C	506	CLA	CAA-CBA-CGA-O2A
27	D	412	LMG	C32-C33-C34-C35
22	c	508	CLA	C8-C10-C11-C12
22	c	502	CLA	CBA-CGA-O2A-C1
30	D	403	SQD	O49-C7-C8-C9
22	B	602	CLA	C2A-CAA-CBA-CGA
22	B	610	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C19
25	C	517	DGD	O2G-C1B-C2B-C3B
22	A	404	CLA	O1A-CGA-O2A-C1
22	C	502	CLA	O1A-CGA-O2A-C1
34	V	201	HEM	CAA-CBA-CGA-O1A
27	d	407	LMG	C34-C35-C36-C37
22	C	509	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	O1A-CGA-O2A-C1
26	A	409	LHG	C24-C25-C26-C27
22	A	404	CLA	CBA-CGA-O2A-C1
22	B	601	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C11-C12-C13-C14
22	C	520	CLA	C6-C7-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C12-C13-C14
27	D	408	LMG	O7-C10-C11-C12
22	c	509	CLA	CAA-CBA-CGA-O1A
27	c	522	LMG	O10-C28-C29-C30
31	B	627	LMT	C4'-C5'-C6'-O6'
22	B	606	CLA	C4-C3-C5-C6
22	b	611	CLA	C4-C3-C5-C6
22	b	615	CLA	CAA-CBA-CGA-O1A
30	A	414	SQD	O49-C7-C8-C9
30	d	402	SQD	O49-C7-C8-C9
30	D	403	SQD	O5-C5-C6-S
30	d	402	SQD	O5-C5-C6-S
22	b	616	CLA	CAA-CBA-CGA-O1A
22	d	404	CLA	CAA-CBA-CGA-O1A
25	C	517	DGD	CEA-CFA-CGA-CHA
22	c	502	CLA	C16-C17-C18-C19
34	v	201	HEM	CAA-CBA-CGA-O1A
22	B	611	CLA	CAA-CBA-CGA-O1A
22	C	501	CLA	CAA-CBA-CGA-O1A
22	c	501	CLA	CAA-CBA-CGA-O1A
22	C	508	CLA	C8-C10-C11-C12
25	C	516	DGD	C6A-C7A-C8A-C9A
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	C	518	LMG	O7-C8-C9-O8
22	D	405	CLA	CAA-CBA-CGA-O1A
27	d	410	LMG	O9-C10-C11-C12
30	A	413	SQD	C9-C10-C11-C12
22	C	502	CLA	C16-C17-C18-C20
27	B	624	LMG	C7-C8-C9-O8
27	I	101	LMG	C7-C8-C9-O8
22	B	612	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
27	D	412	LMG	O9-C10-C11-C12
22	B	609	CLA	C13-C15-C16-C17
27	m	101	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	b	601	DGD	CAB-CBB-CCB-CDB
22	C	510	CLA	C2-C3-C5-C6
22	B	611	CLA	C3-C5-C6-C7
22	C	506	CLA	CAA-CBA-CGA-O1A
22	C	506	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
25	c	517	DGD	O2G-C1B-C2B-C3B
30	D	403	SQD	O47-C7-C8-C9
30	a	401	SQD	O49-C7-C8-C9
22	C	508	CLA	C10-C11-C12-C13
30	b	602	SQD	C15-C16-C17-C18
22	h	101	CLA	CAA-CBA-CGA-O2A
27	M	101	LMG	O8-C28-C29-C30
27	a	413	LMG	C39-C40-C41-C42
22	b	613	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
25	B	620	DGD	O2G-C1B-C2B-C3B
25	b	624	DGD	O2G-C1B-C2B-C3B
27	d	407	LMG	O7-C10-C11-C12
27	a	402	LMG	O9-C10-C11-C12
27	a	413	LMG	O9-C10-C11-C12
22	B	613	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

160 monomers are involved in 454 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	610	CLA	3	0
27	d	407	LMG	7	0
22	D	405	CLA	9	0
22	B	603	CLA	2	0
22	B	611	CLA	4	0
22	b	607	CLA	2	0
24	A	407	BCR	2	0
25	B	620	DGD	2	0
32	D	401	PHO	7	0
22	h	101	CLA	11	0
30	a	401	SQD	6	0
22	C	504	CLA	4	0
27	b	628	LMG	1	0
30	A	413	SQD	3	0
27	c	518	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	409	PL9	3	0
22	b	610	CLA	4	0
23	A	406	PL9	3	0
22	c	512	CLA	3	0
24	B	618	BCR	3	0
22	B	604	CLA	9	0
22	C	510	CLA	6	0
24	g	101	BCR	5	0
32	D	402	PHO	5	0
22	A	402	CLA	11	0
27	I	101	LMG	1	0
30	a	415	SQD	3	0
27	B	624	LMG	2	0
24	b	622	BCR	3	0
22	c	507	CLA	4	0
24	C	514	BCR	6	0
25	b	624	DGD	3	0
25	C	515	DGD	3	0
22	C	512	CLA	3	0
22	c	503	CLA	2	0
25	b	601	DGD	3	0
31	b	603	LMT	3	0
22	C	503	CLA	3	0
22	c	505	CLA	1	0
22	c	508	CLA	5	0
32	a	407	PHO	5	0
31	B	628	LMT	2	0
25	d	408	DGD	1	0
24	b	623	BCR	2	0
24	H	102	BCR	2	0
26	C	519	LHG	2	0
25	c	517	DGD	5	0
22	c	510	CLA	4	0
25	C	517	DGD	5	0
31	B	627	LMT	2	0
27	d	410	LMG	1	0
24	C	513	BCR	6	0
24	B	619	BCR	2	0
22	c	511	CLA	2	0
31	i	102	LMT	1	0
25	a	411	DGD	3	0
23	d	406	PL9	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	d	405	CLA	2	0
25	c	515	DGD	3	0
22	b	611	CLA	7	0
27	B	621	LMG	3	0
22	b	609	CLA	5	0
24	D	411	BCR	3	0
24	c	513	BCR	8	0
25	C	516	DGD	4	0
22	b	615	CLA	4	0
27	a	413	LMG	3	0
34	v	201	HEM	5	0
22	d	404	CLA	10	0
22	a	404	CLA	10	0
22	C	505	CLA	1	0
27	A	415	LMG	1	0
27	D	408	LMG	6	0
27	C	518	LMG	3	0
32	d	401	PHO	7	0
27	b	625	LMG	3	0
22	b	619	CLA	4	0
34	V	201	HEM	5	0
24	f	102	BCR	1	0
22	a	406	CLA	6	0
22	b	612	CLA	5	0
24	x	101	BCR	1	0
22	a	405	CLA	11	0
26	A	409	LHG	3	0
24	b	621	BCR	1	0
24	c	514	BCR	4	0
22	b	606	CLA	9	0
30	b	602	SQD	1	0
27	E	101	LMG	1	0
22	A	405	CLA	1	0
24	y	101	BCR	8	0
22	a	408	CLA	1	0
22	B	601	CLA	1	0
25	A	408	DGD	1	0
22	b	614	CLA	2	0
23	D	407	PL9	7	0
24	C	521	BCR	4	0
22	B	613	CLA	3	0
31	b	626	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	520	CLA	5	0
24	c	521	BCR	4	0
22	c	509	CLA	3	0
22	C	506	CLA	3	0
27	M	101	LMG	1	0
22	B	615	CLA	4	0
22	H	101	CLA	8	0
22	B	608	CLA	6	0
22	B	612	CLA	3	0
22	b	613	CLA	1	0
22	B	614	CLA	1	0
22	D	406	CLA	3	0
22	B	606	CLA	6	0
31	I	102	LMT	1	0
24	J	102	BCR	2	0
24	B	617	BCR	1	0
27	C	522	LMG	1	0
25	B	625	DGD	2	0
22	A	404	CLA	5	0
27	e	101	LMG	1	0
27	a	402	LMG	1	0
30	A	414	SQD	4	0
25	D	409	DGD	2	0
34	f	101	HEM	4	0
31	b	604	LMT	2	0
30	d	402	SQD	3	0
22	C	520	CLA	4	0
31	B	622	LMT	2	0
22	b	617	CLA	2	0
34	F	101	HEM	4	0
22	b	608	CLA	7	0
25	c	516	DGD	3	0
22	B	602	CLA	10	0
22	C	509	CLA	4	0
22	b	616	CLA	2	0
30	f	103	SQD	2	0
30	D	403	SQD	3	0
24	b	620	BCR	5	0
27	i	101	LMG	1	0
26	c	519	LHG	2	0
22	A	403	CLA	13	0
24	j	102	BCR	1	0

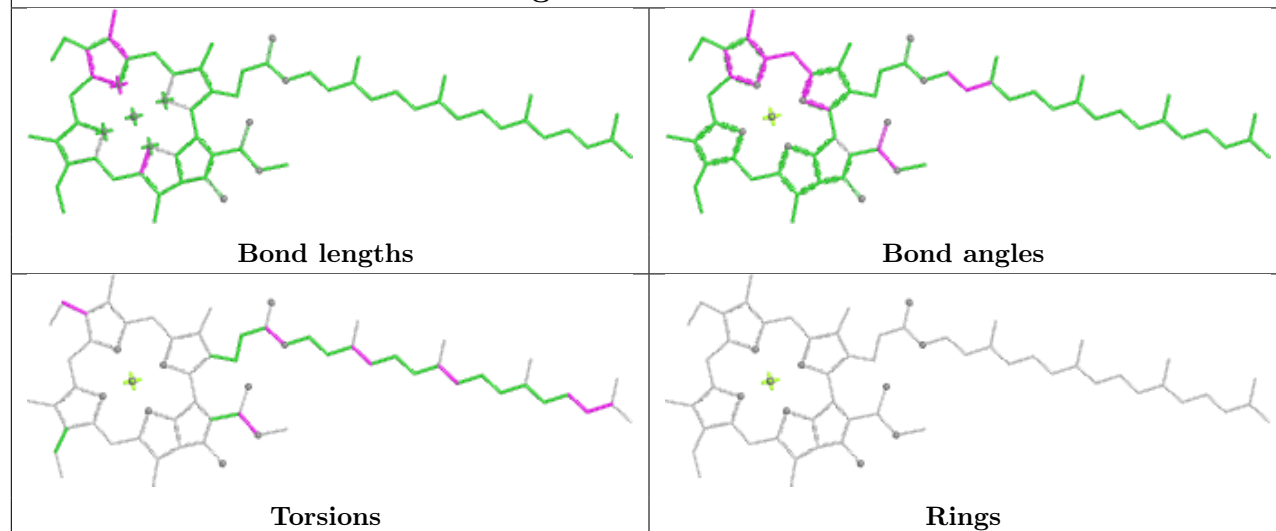
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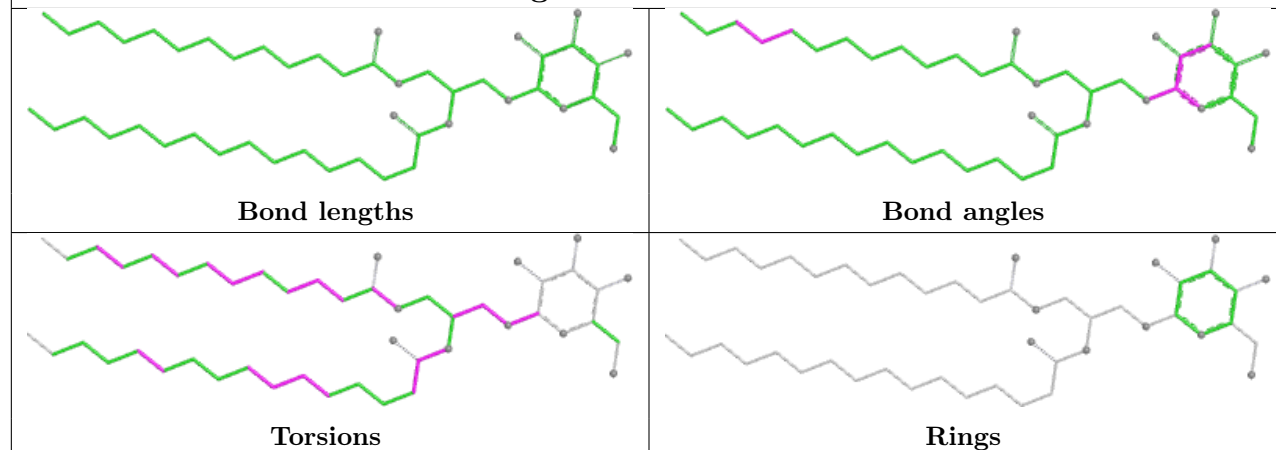
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	412	LMG	1	0
22	b	618	CLA	2	0
22	c	504	CLA	3	0
24	B	616	BCR	7	0
22	C	508	CLA	1	0
22	c	506	CLA	4	0
22	B	607	CLA	8	0
22	C	501	CLA	3	0
22	C	511	CLA	1	0
27	m	101	LMG	1	0
27	A	410	LMG	2	0
30	F	102	SQD	2	0
26	a	412	LHG	1	0
27	c	522	LMG	2	0
30	B	626	SQD	3	0
24	a	410	BCR	3	0
22	C	507	CLA	4	0
22	B	605	CLA	6	0
22	c	501	CLA	3	0

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

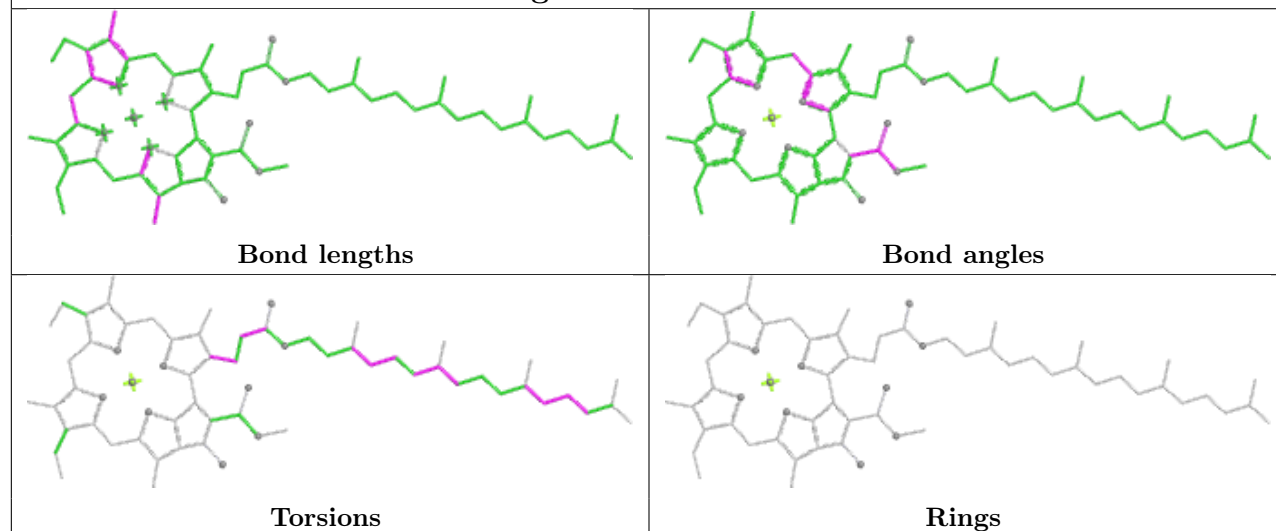
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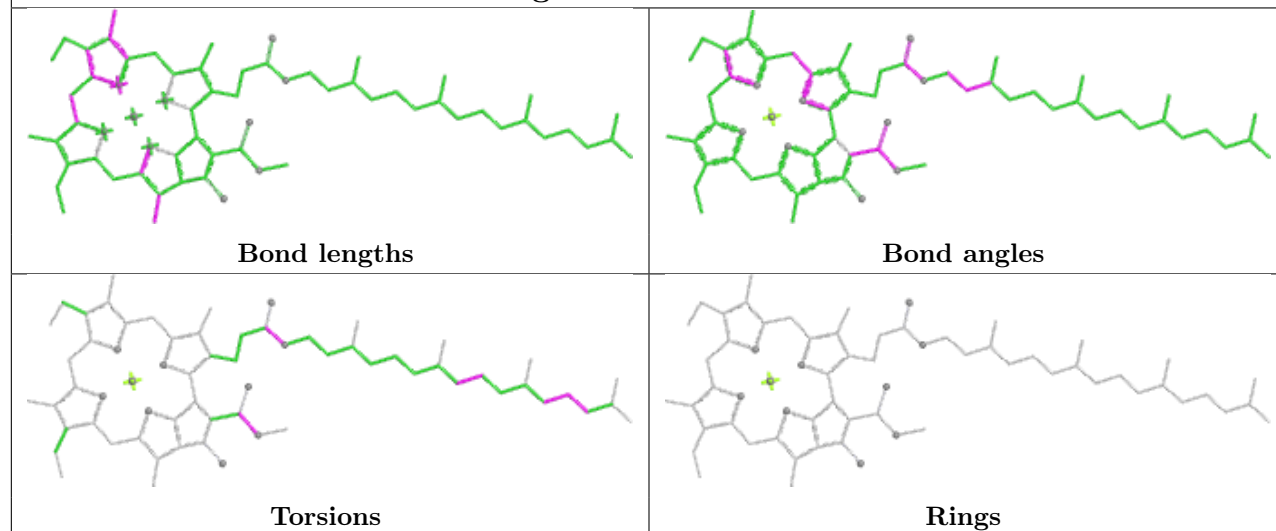
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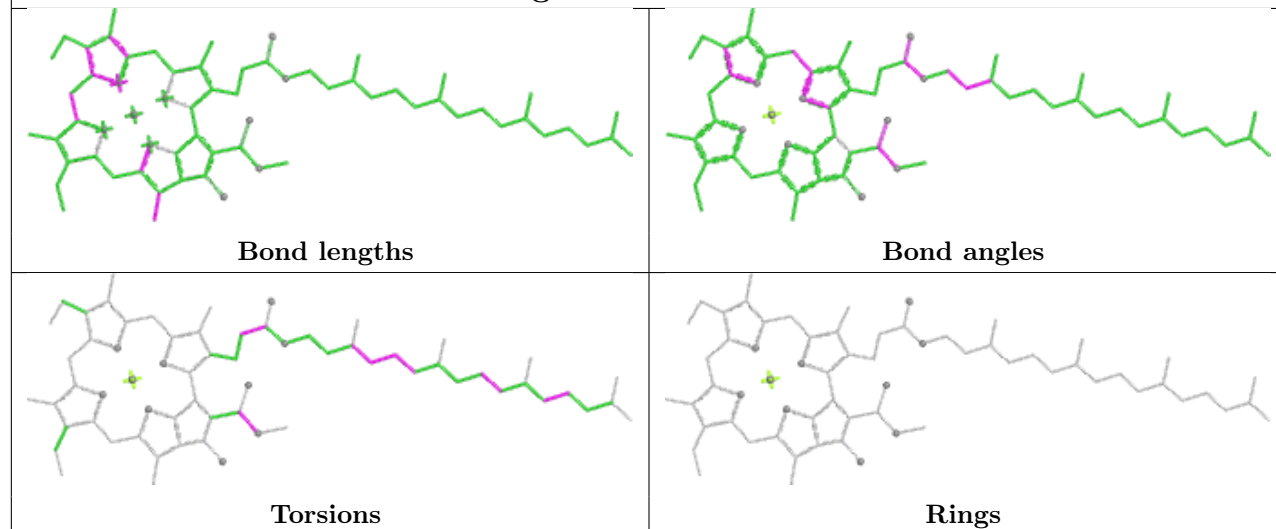
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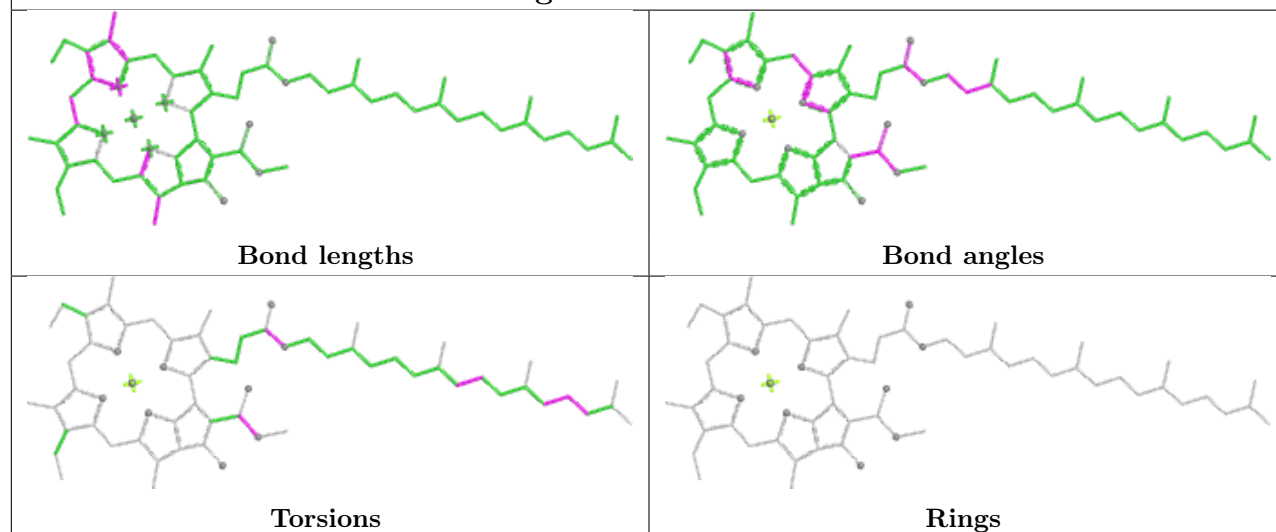
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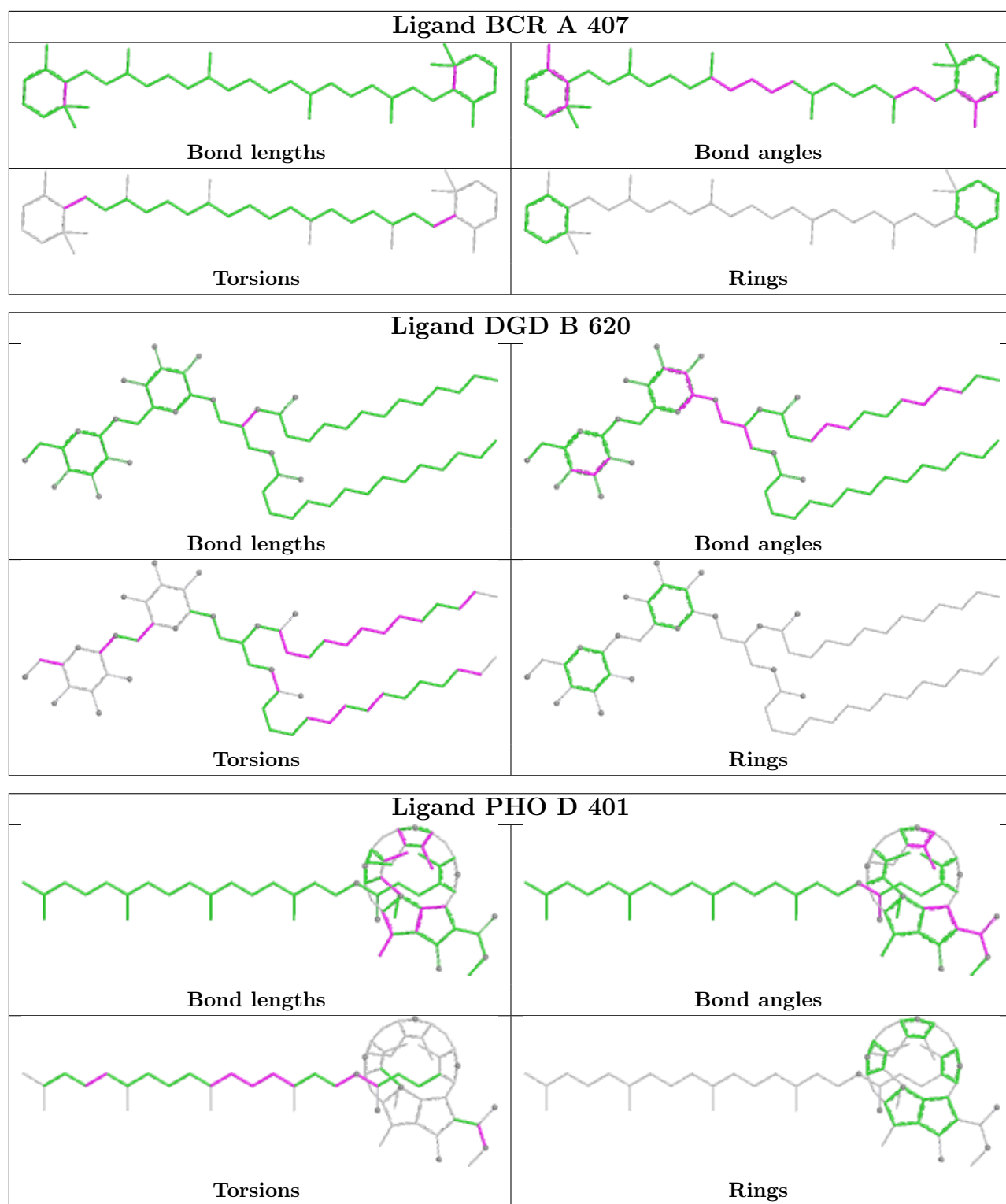


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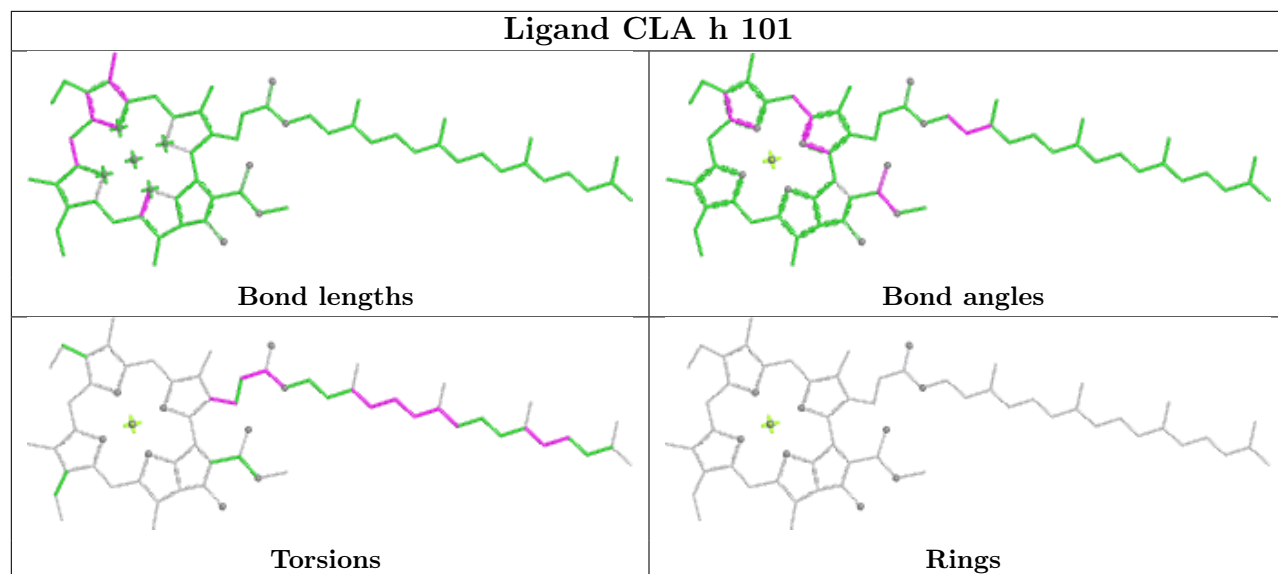


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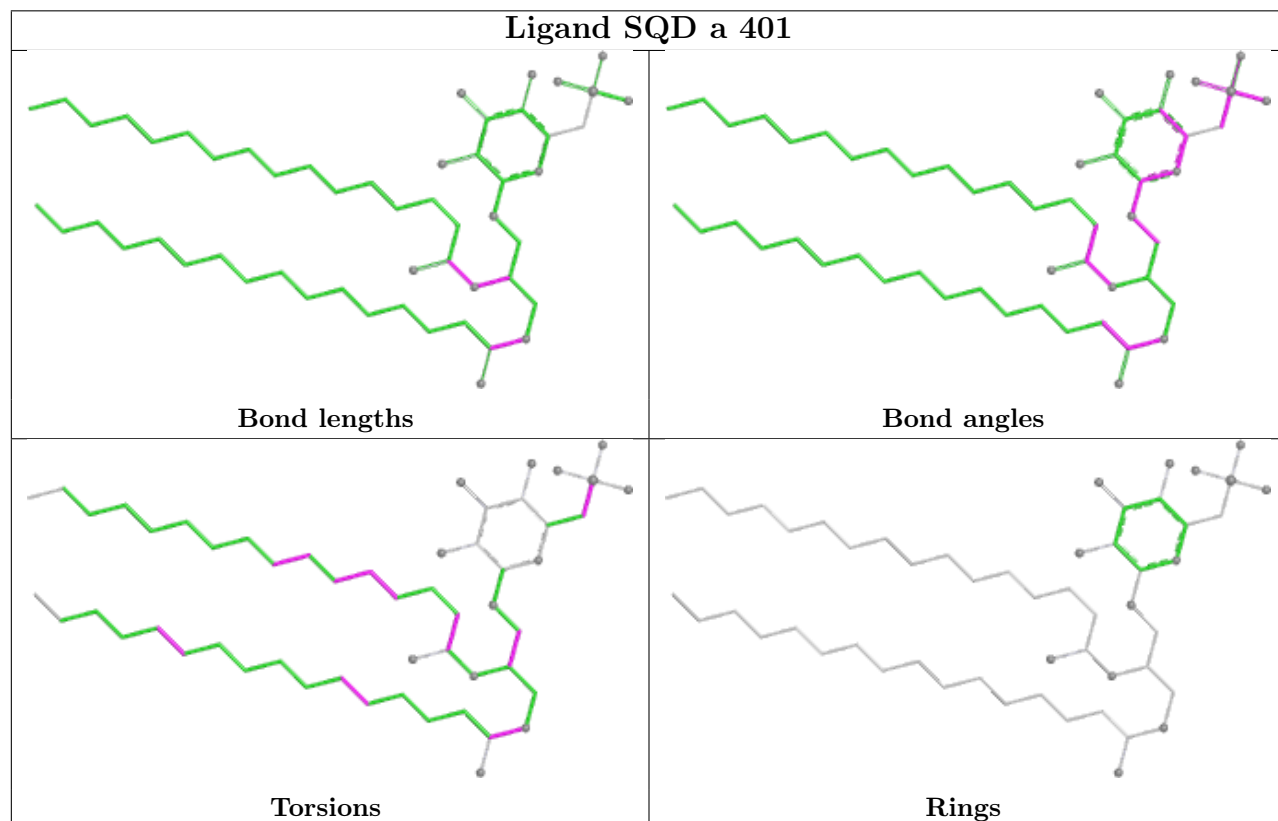


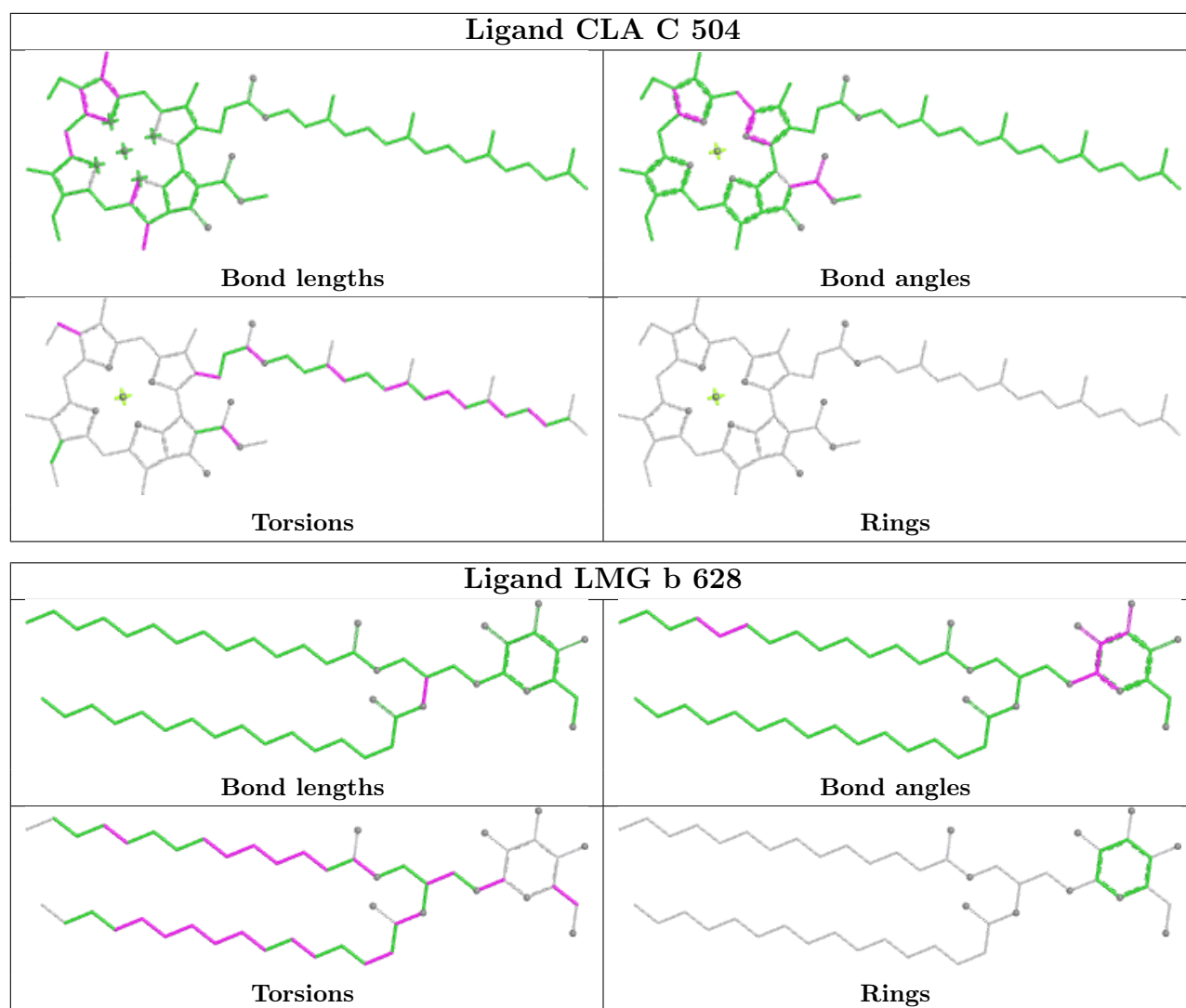


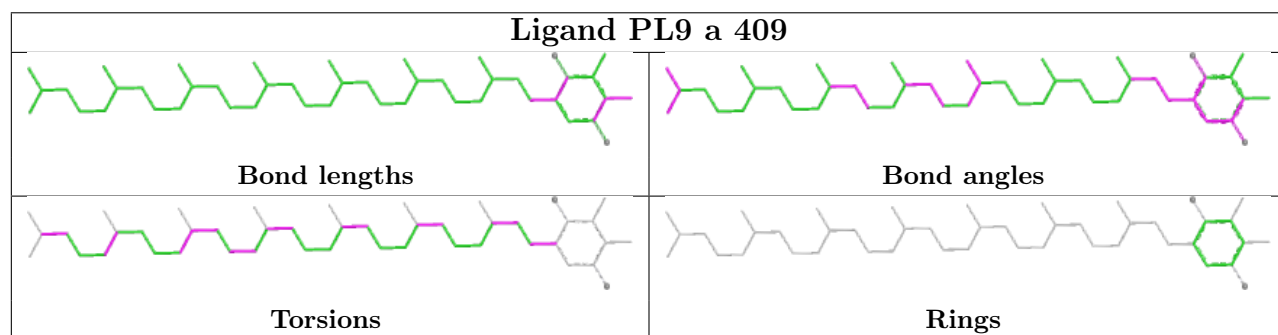
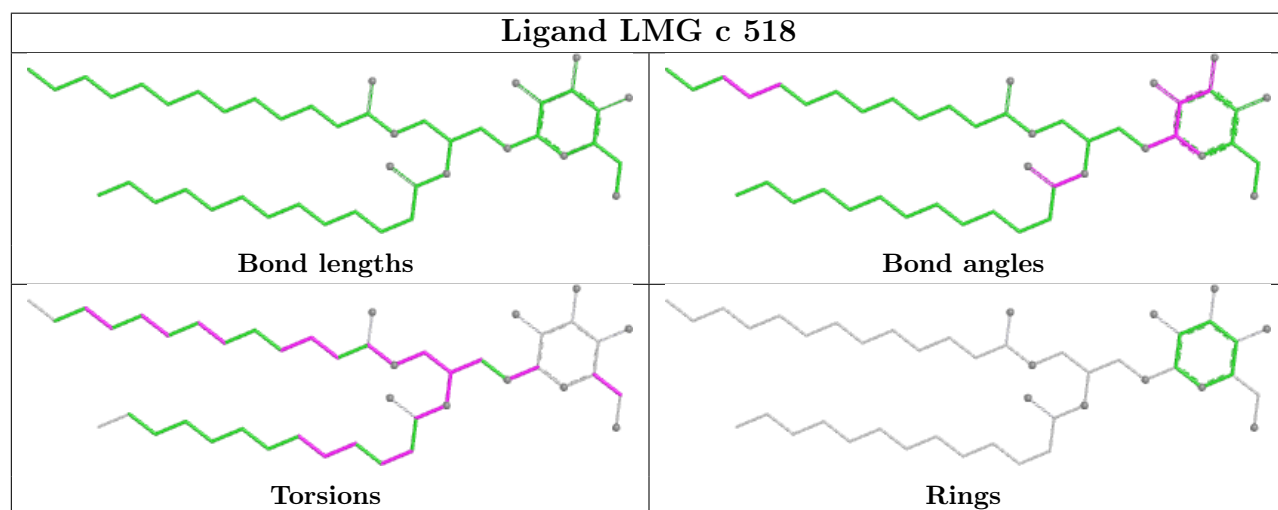
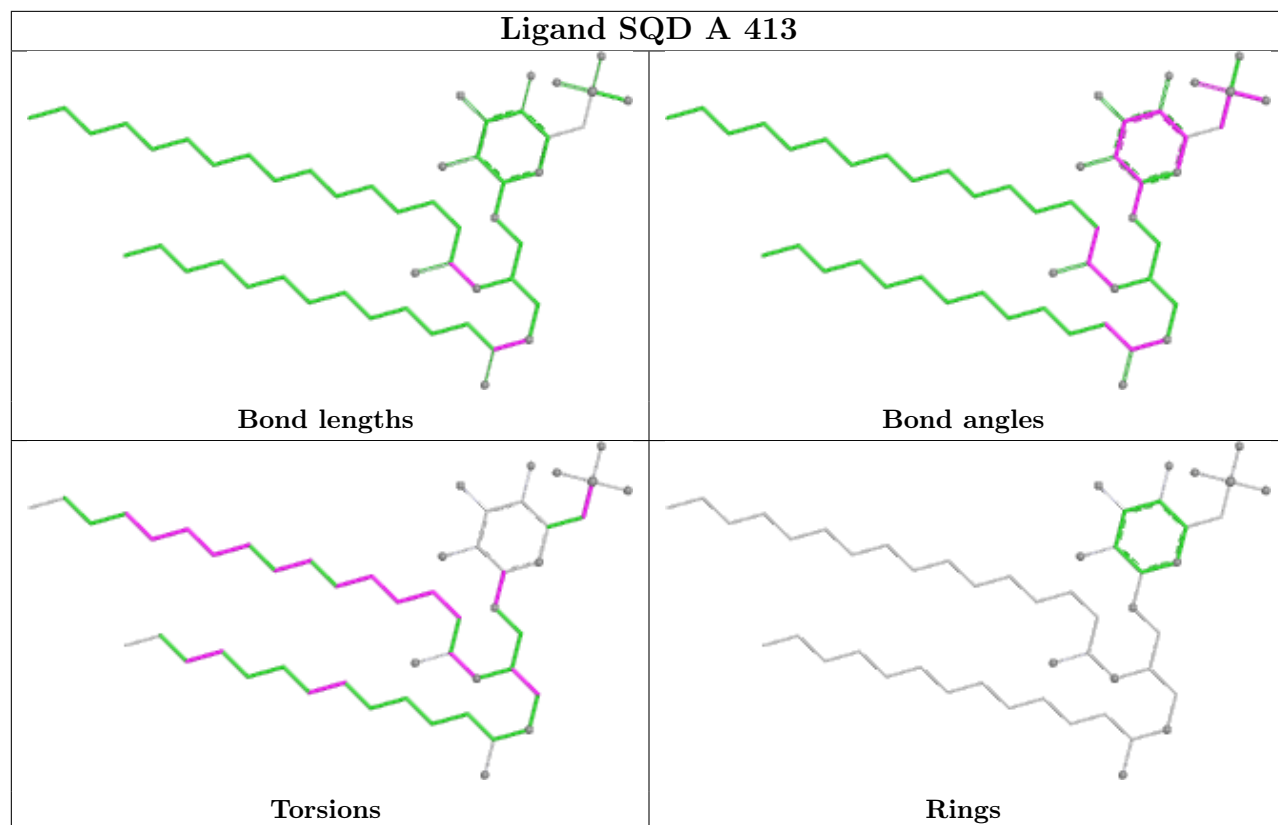
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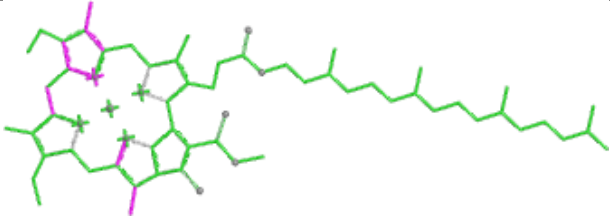
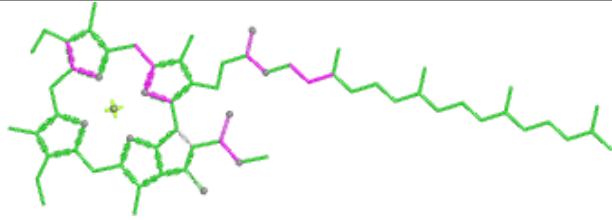
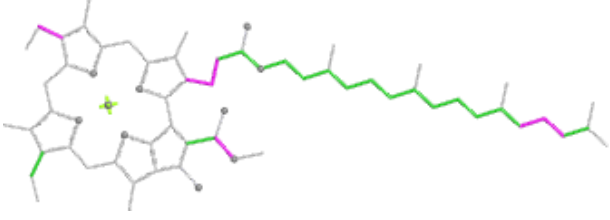
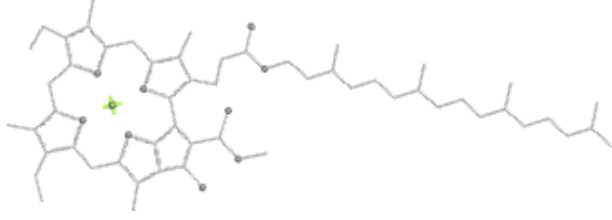
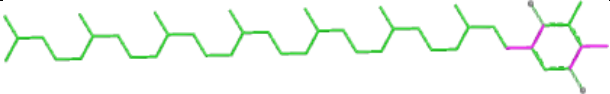
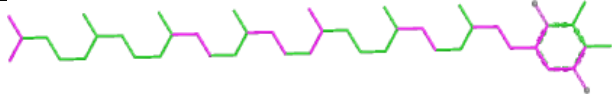
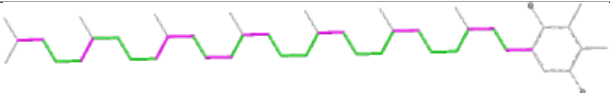
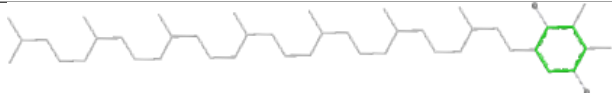
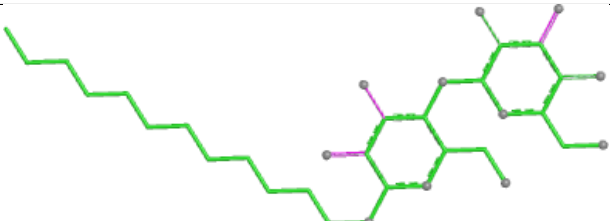
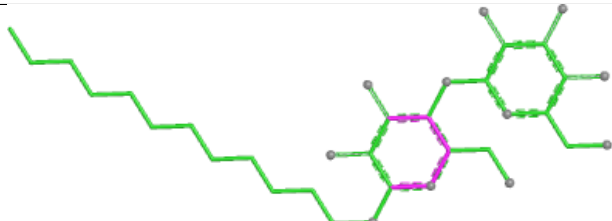
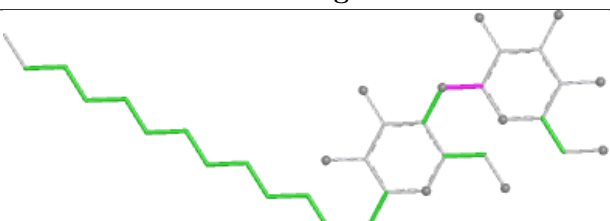
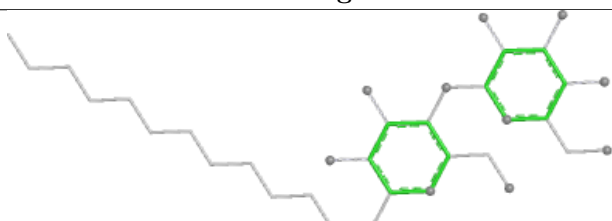


Ligand SQD a 401

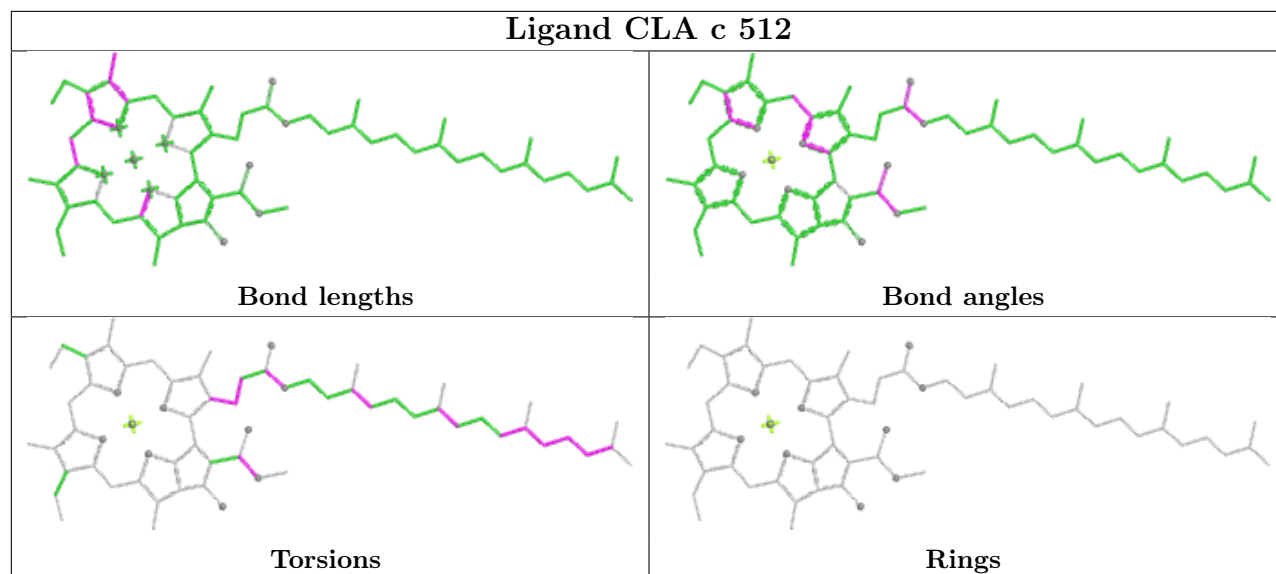




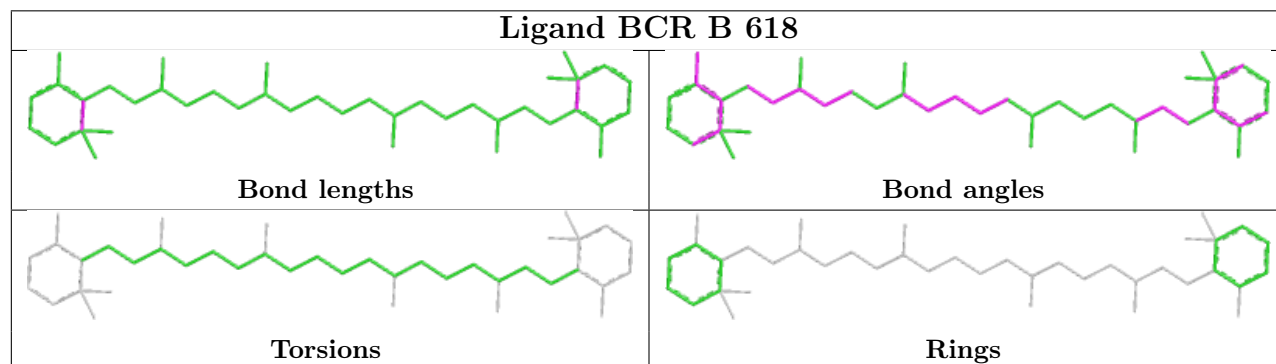


Ligand CLA b 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT b 627	
 Bond lengths	 Bond angles
 Torsions	 Rings

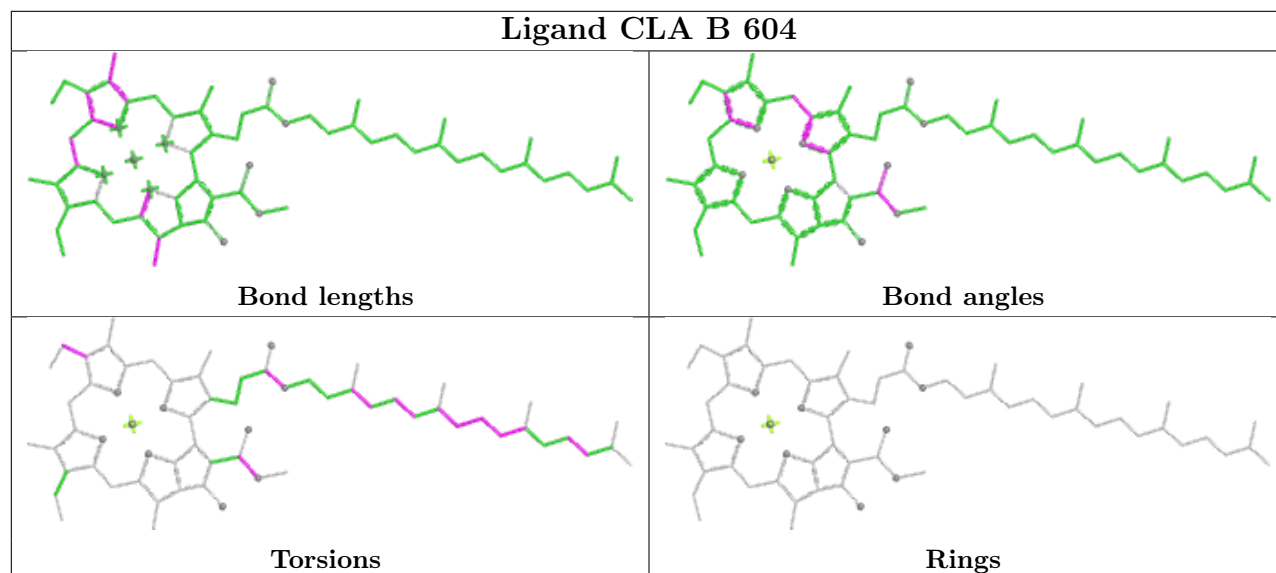
Ligand CLA c 512



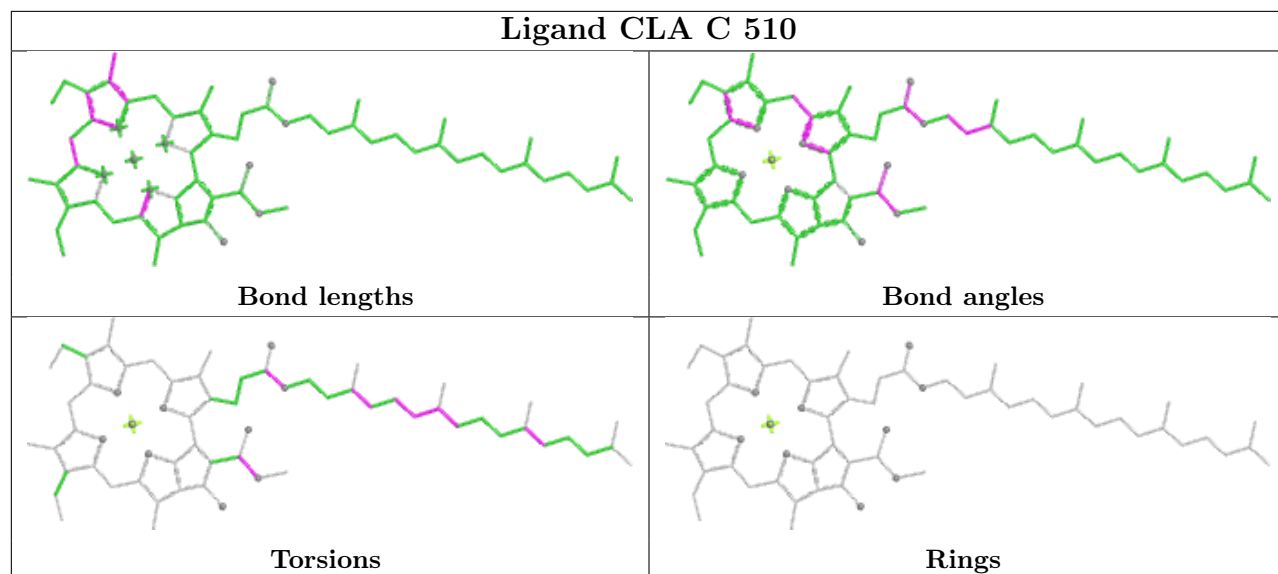
Ligand BCR B 618



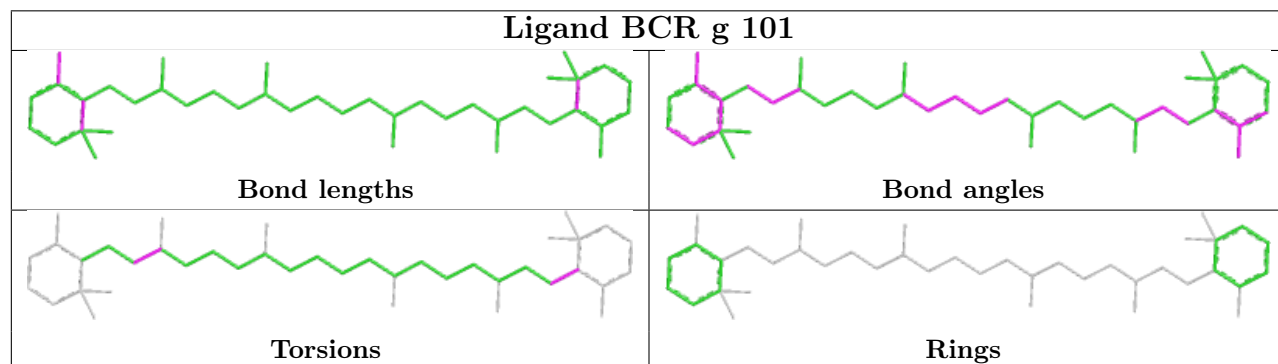
Ligand CLA B 604



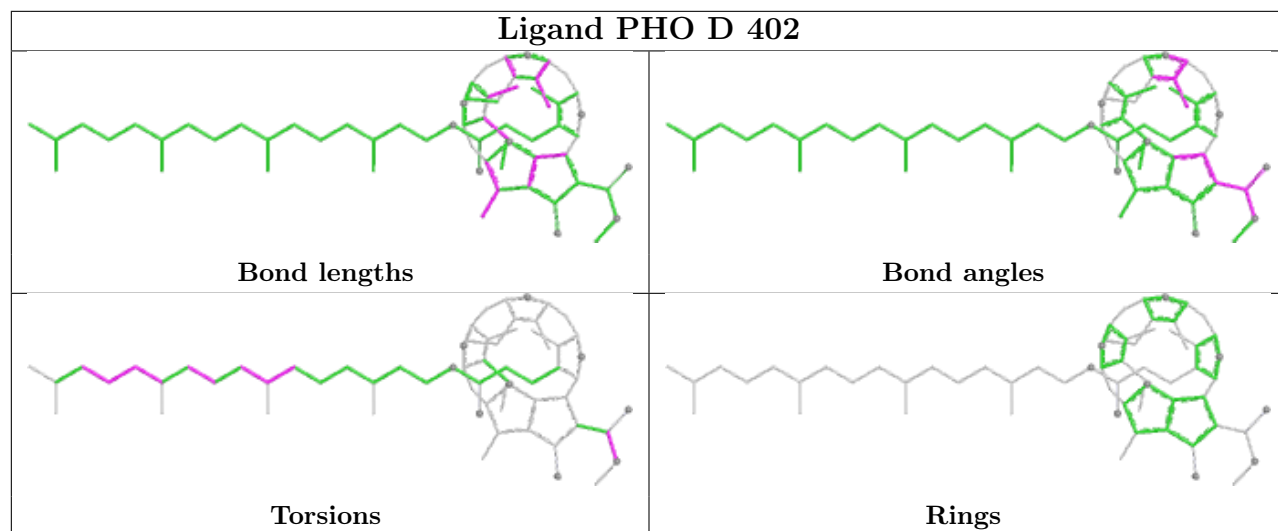
Ligand CLA C 510

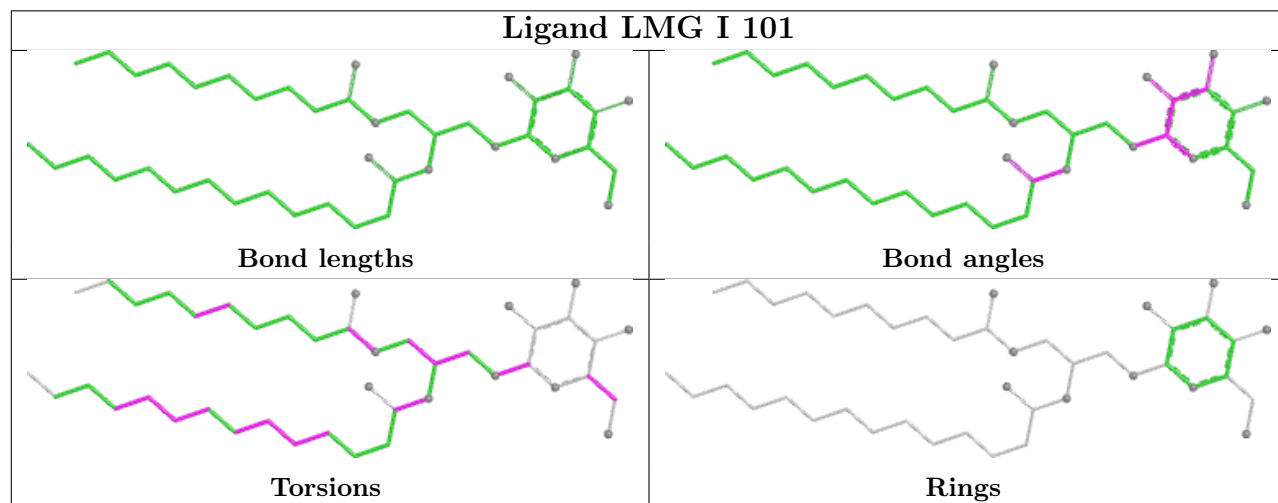
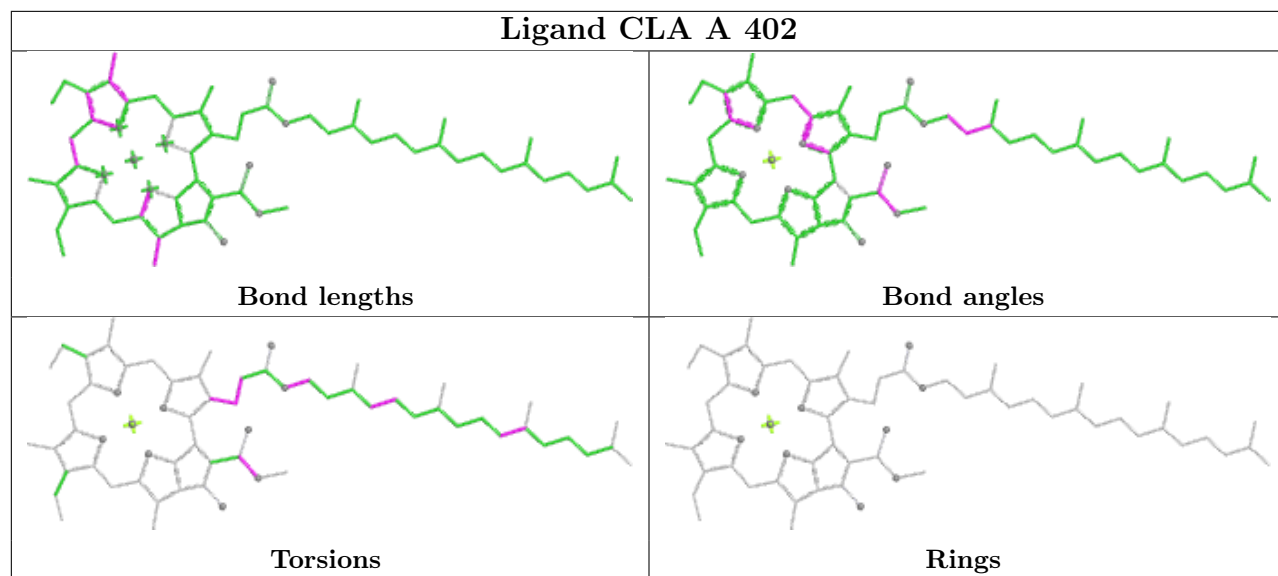


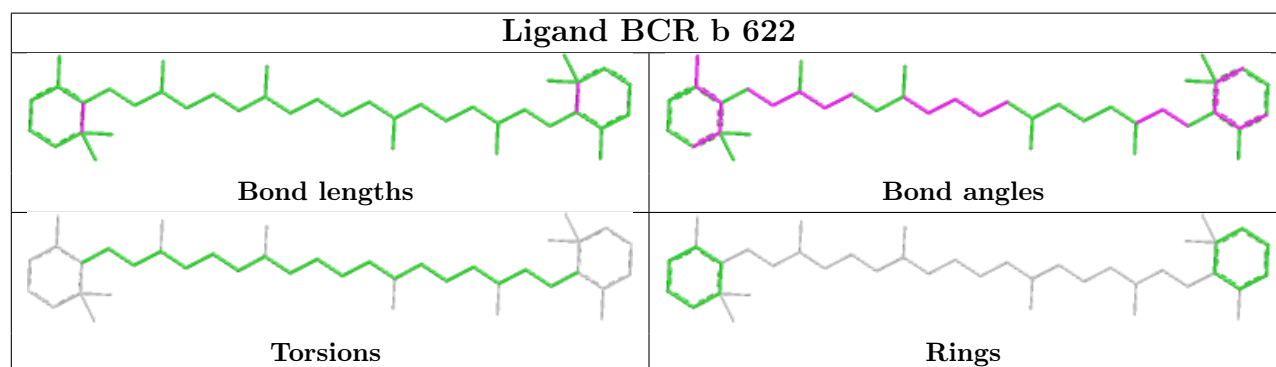
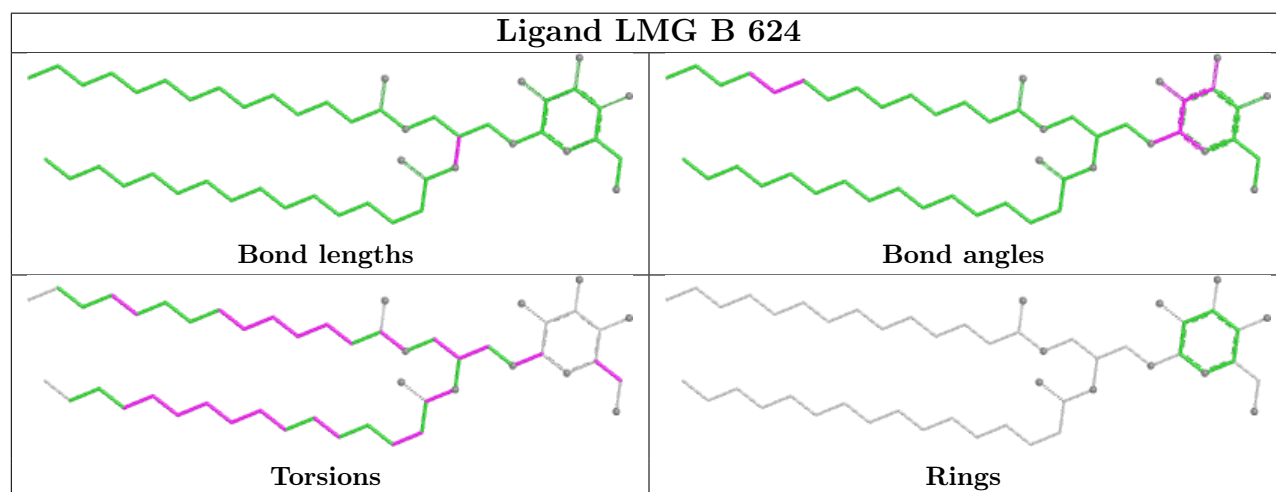
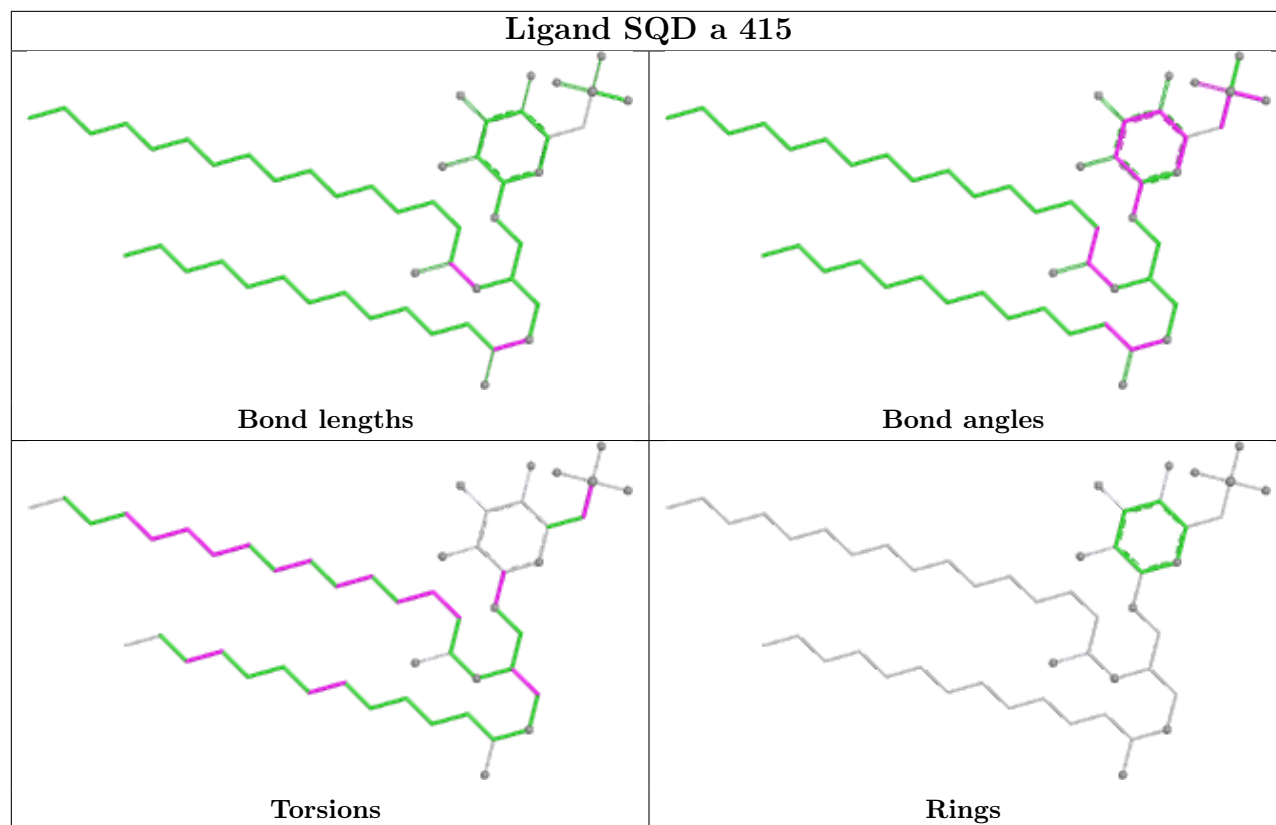
Ligand BCR g 101

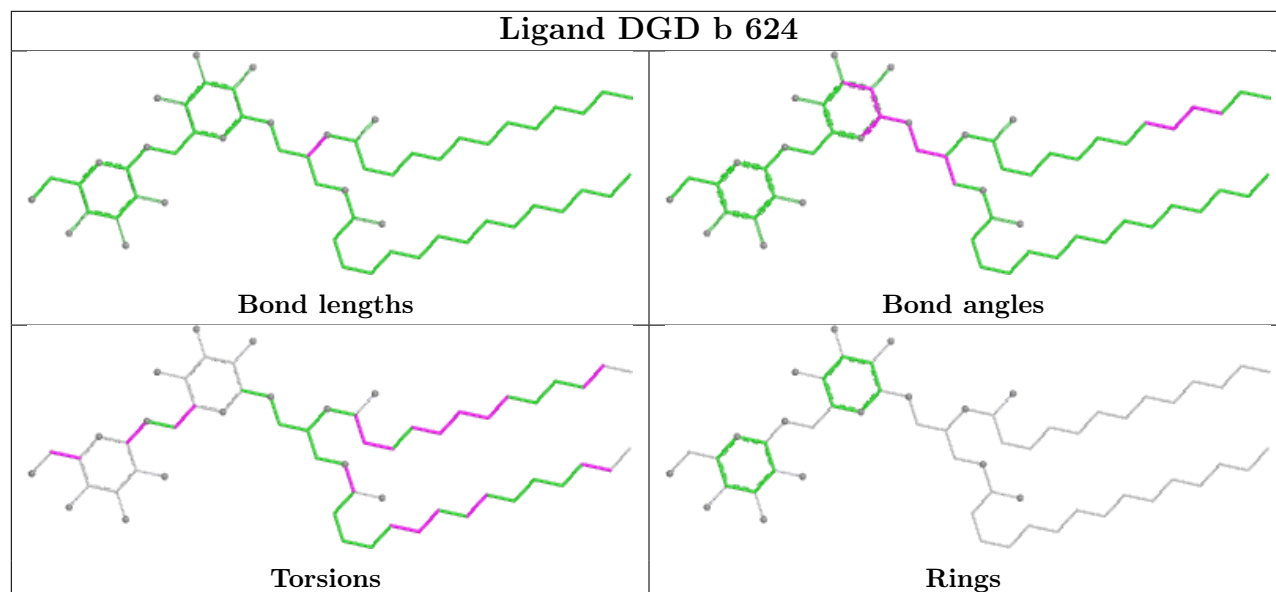
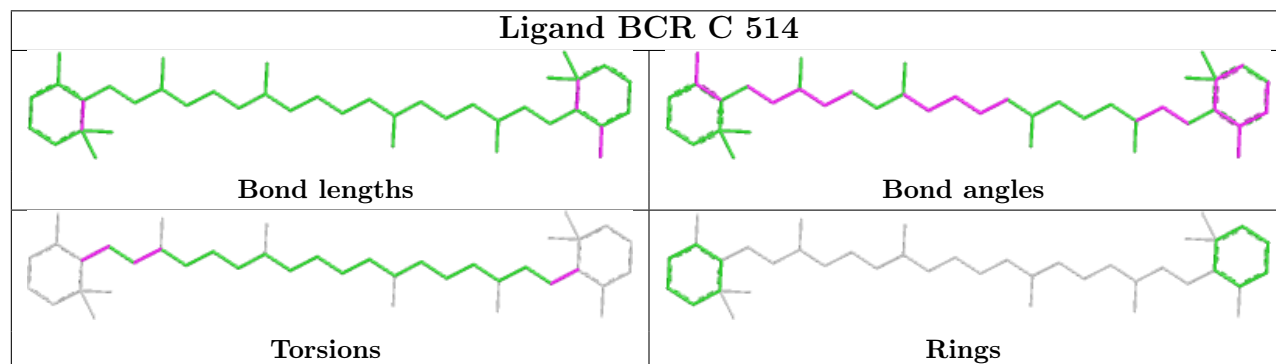
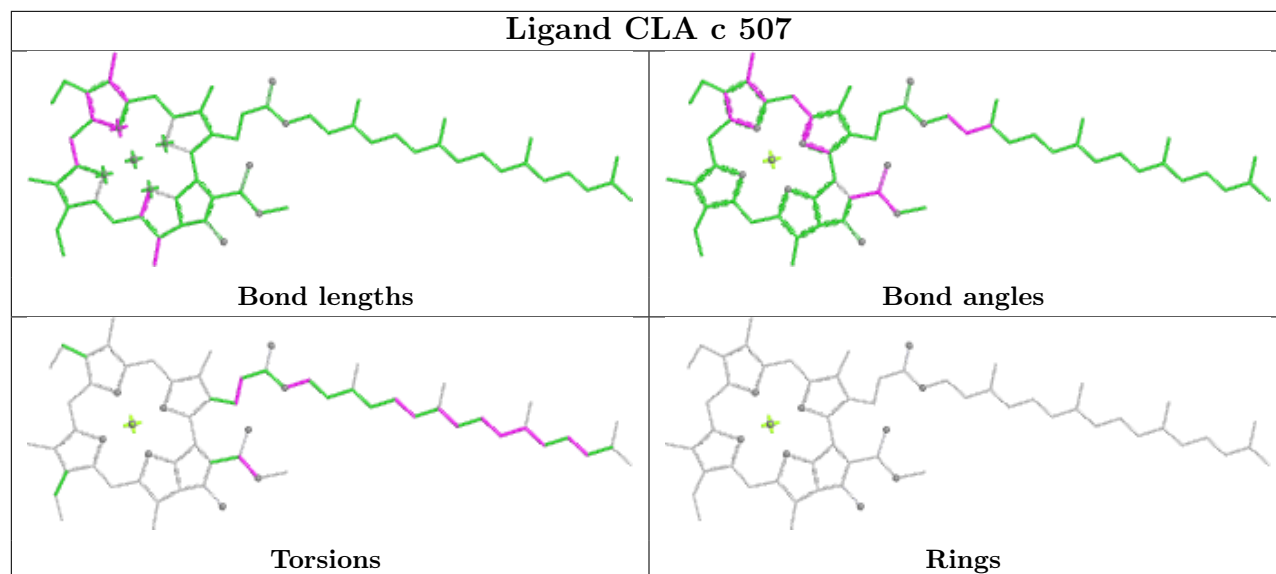


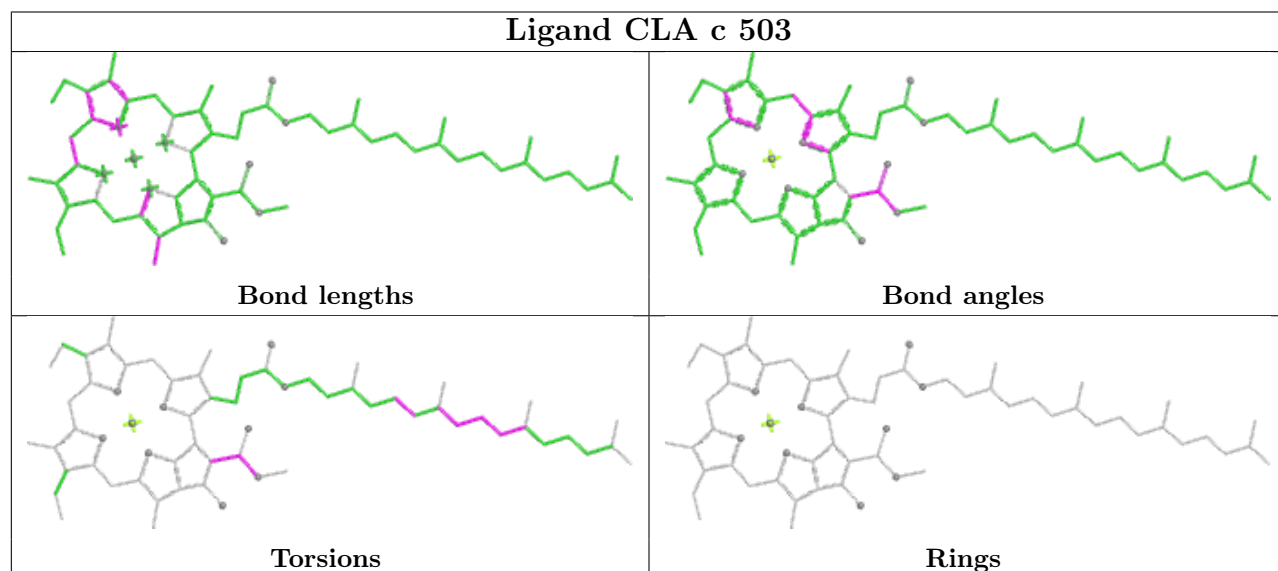
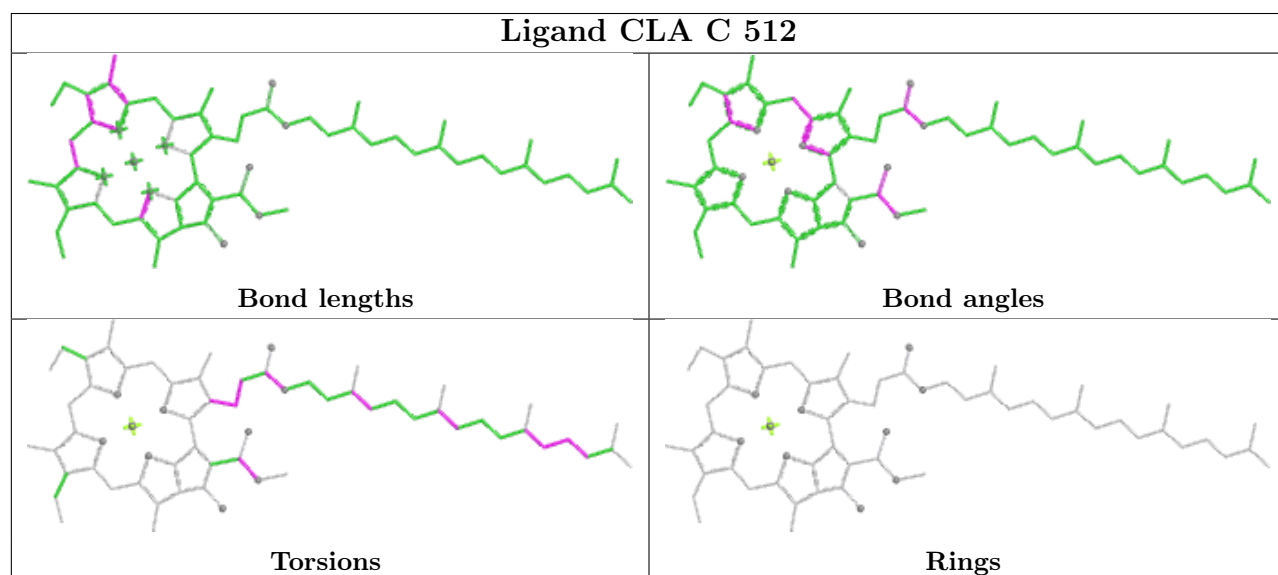
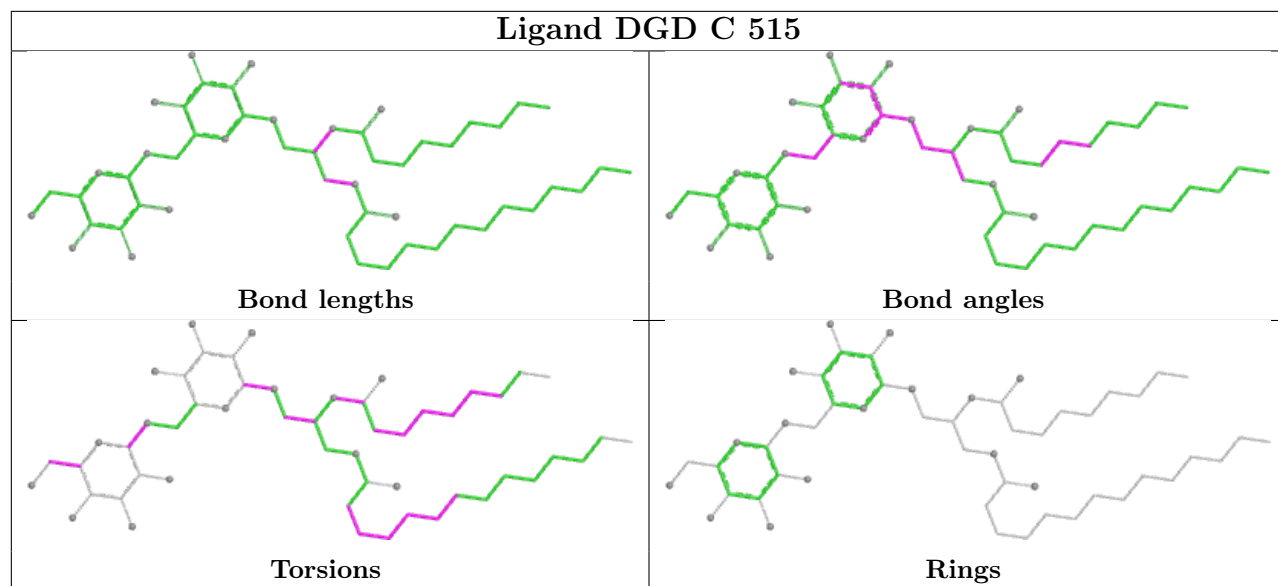
Ligand PHO D 402

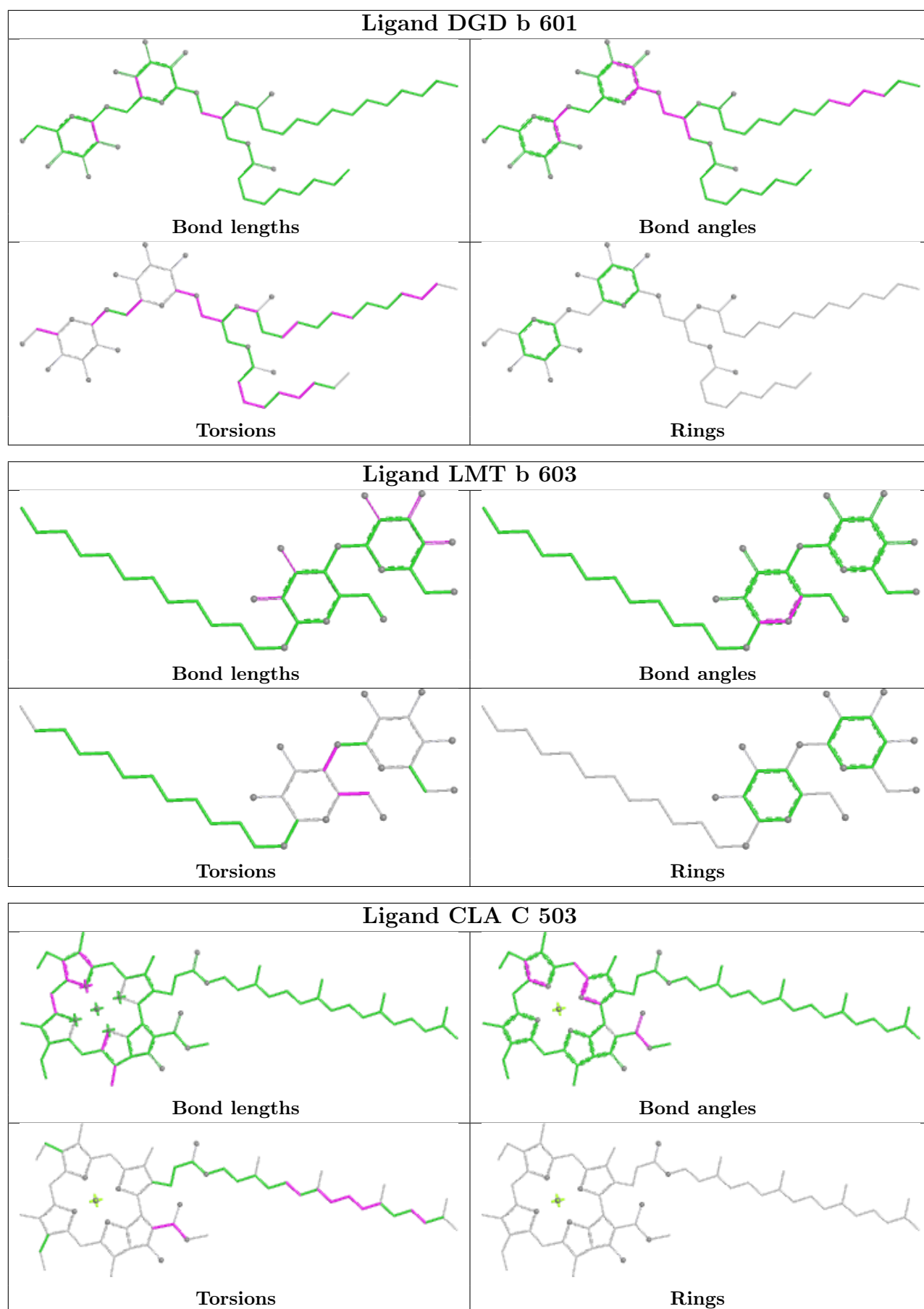




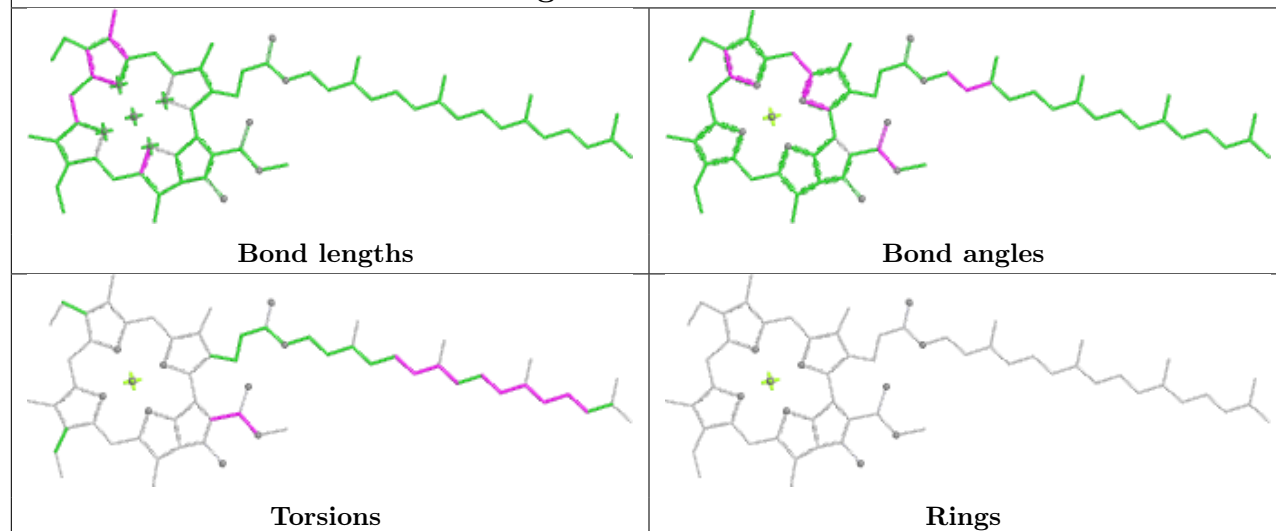




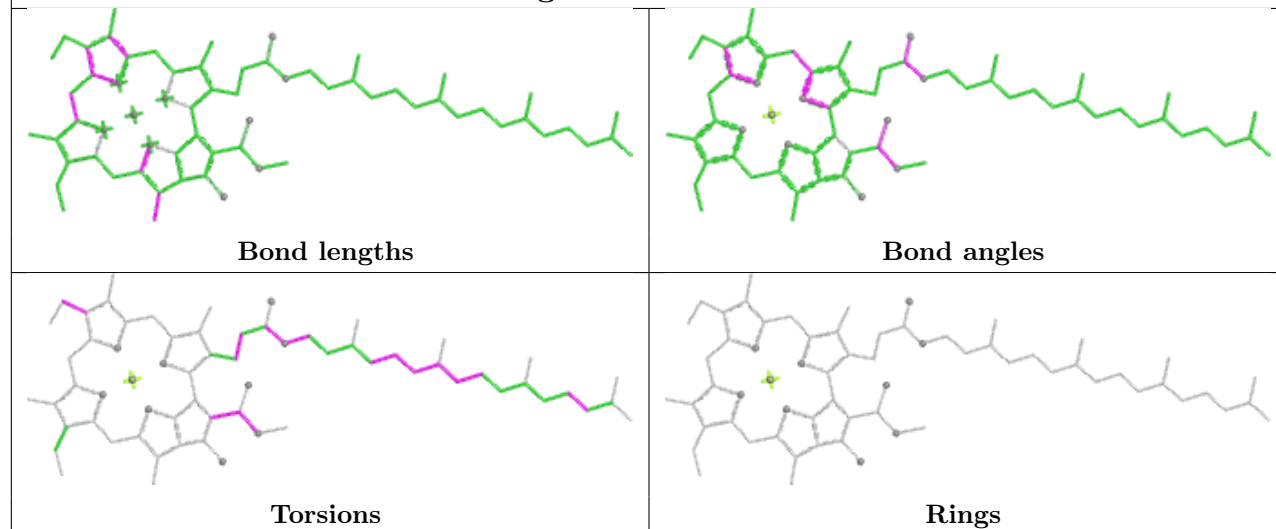




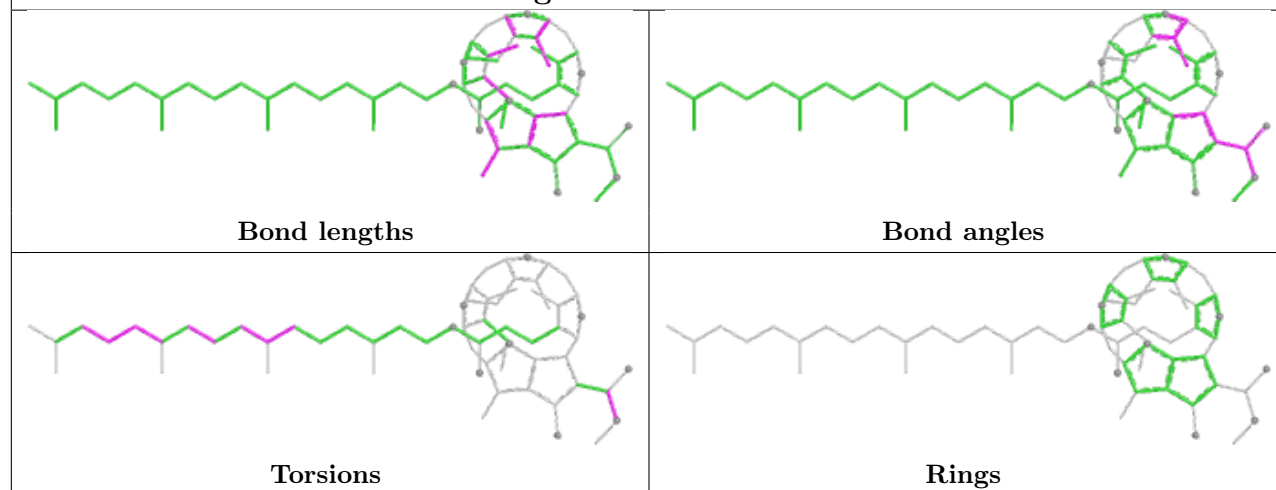
Ligand CLA c 505

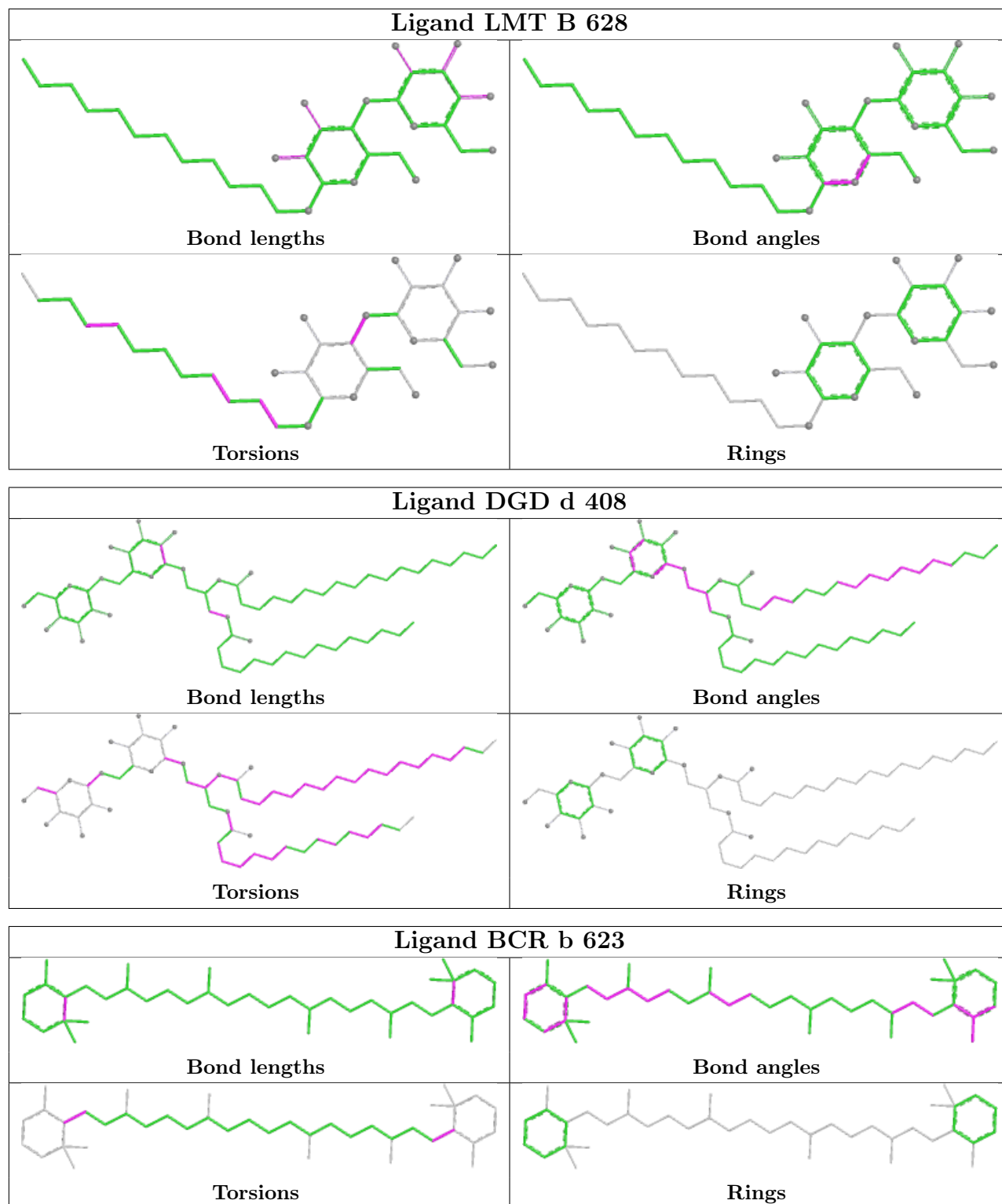


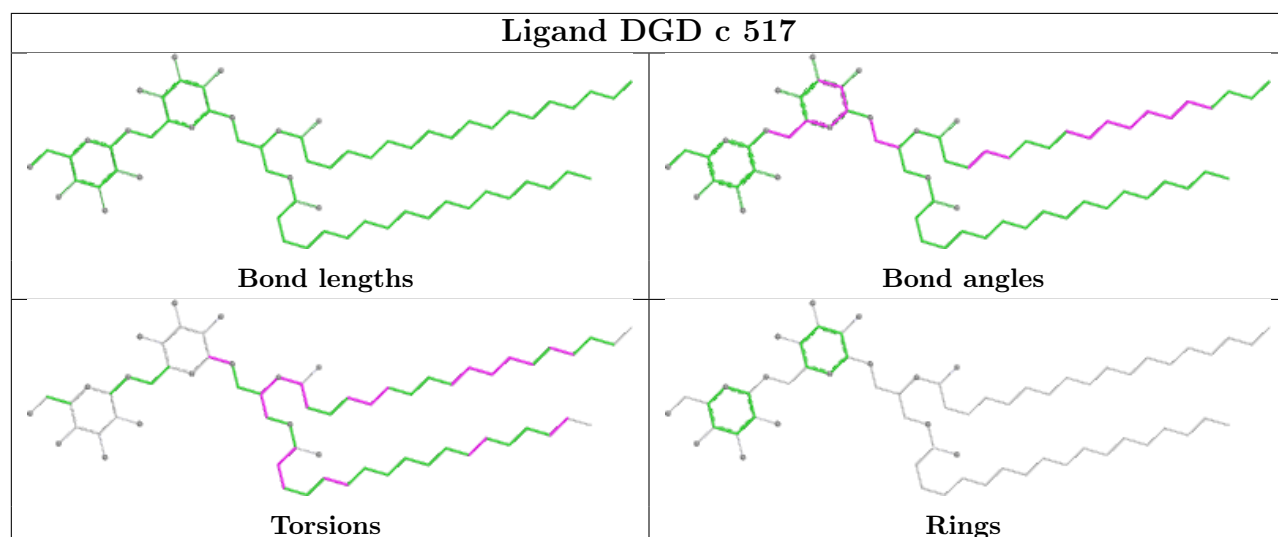
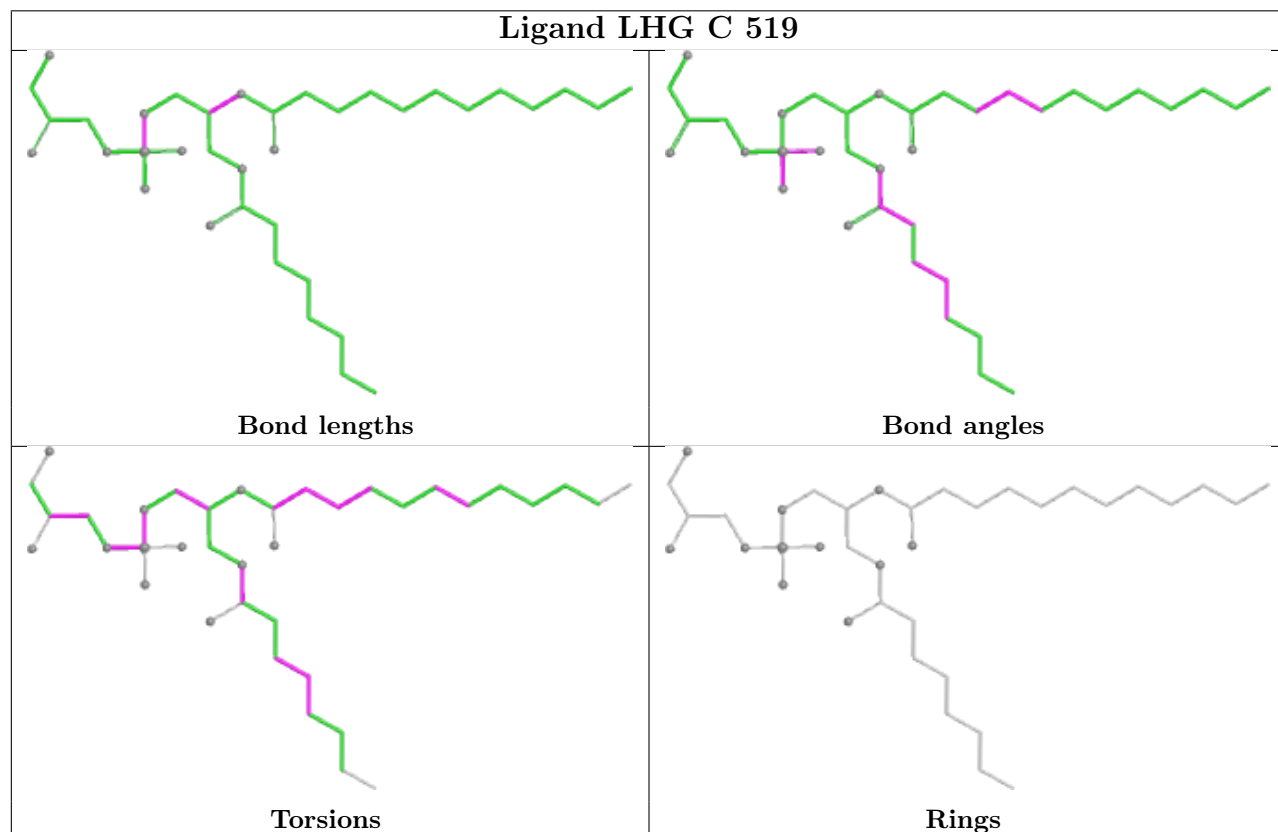
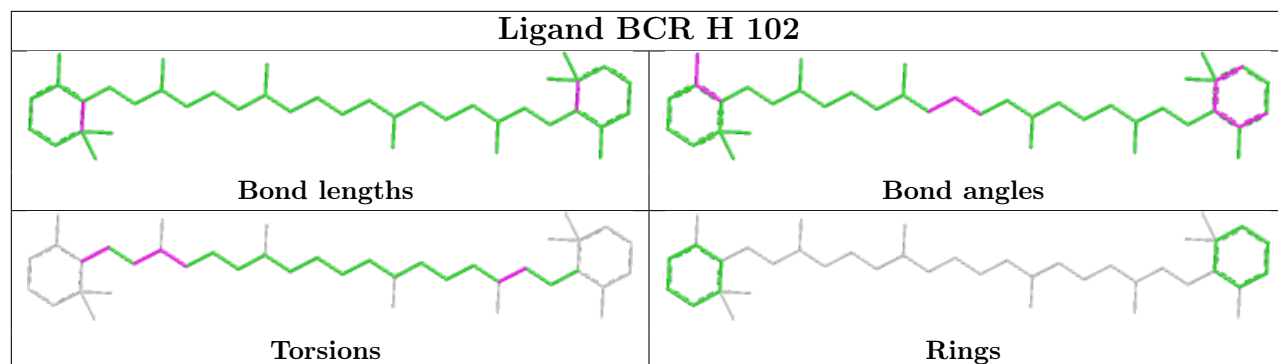
Ligand CLA c 508

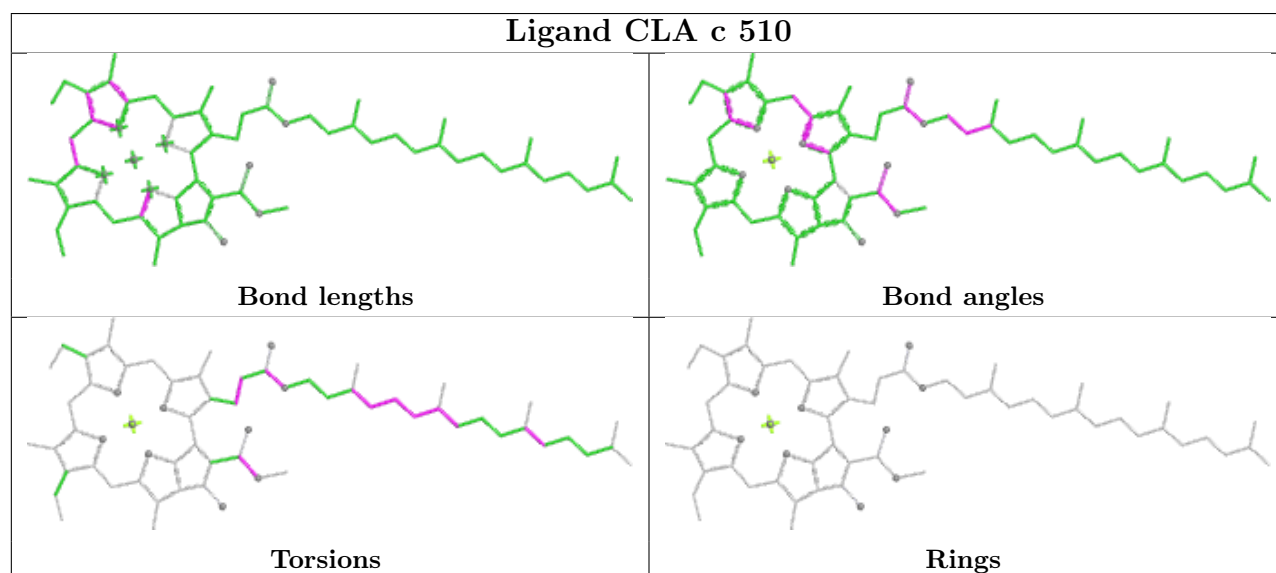
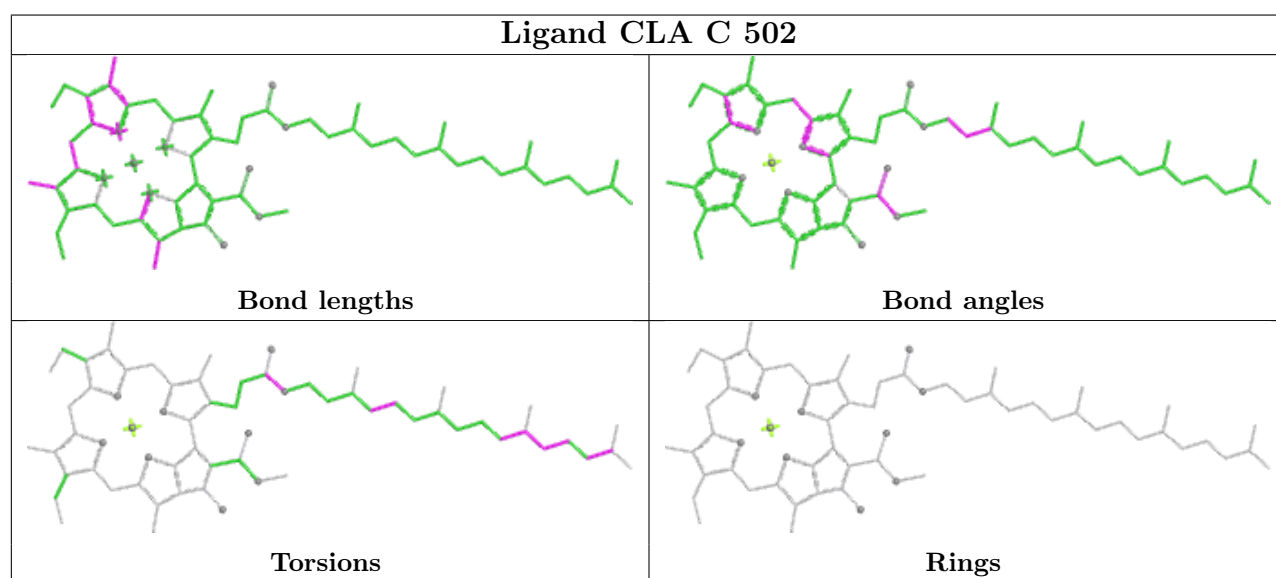
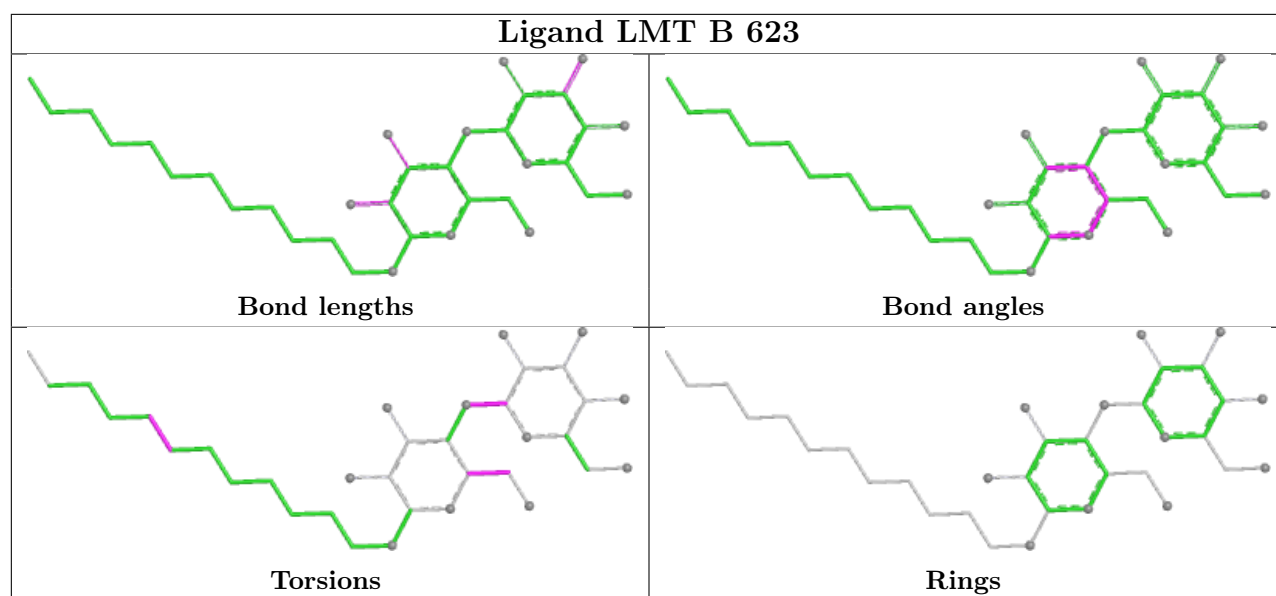


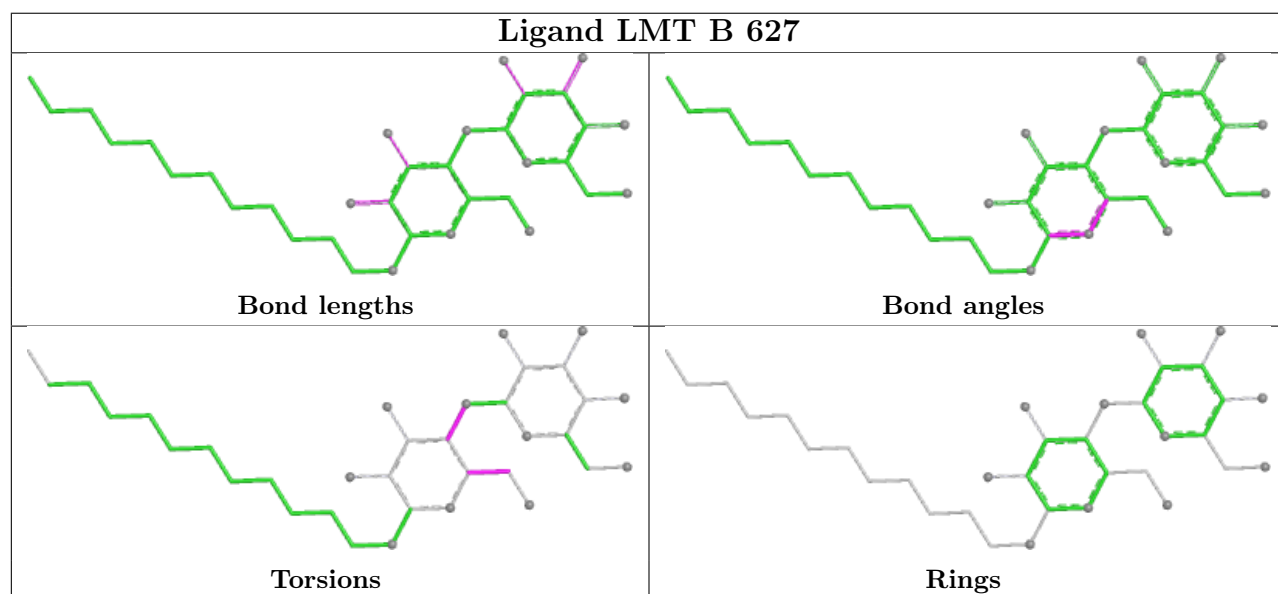
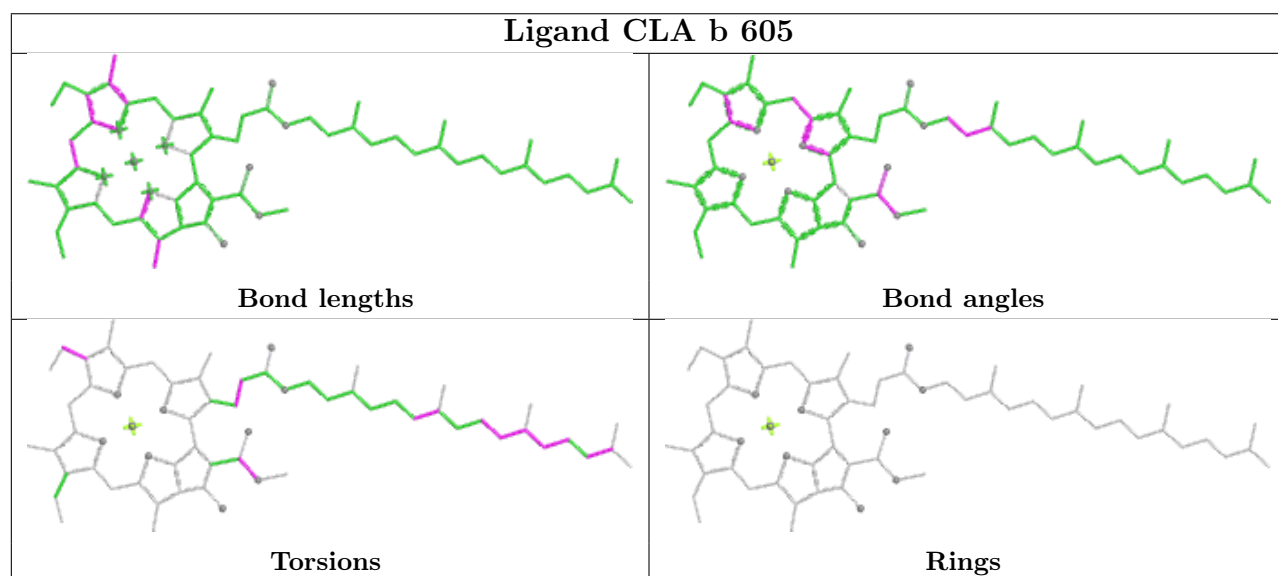
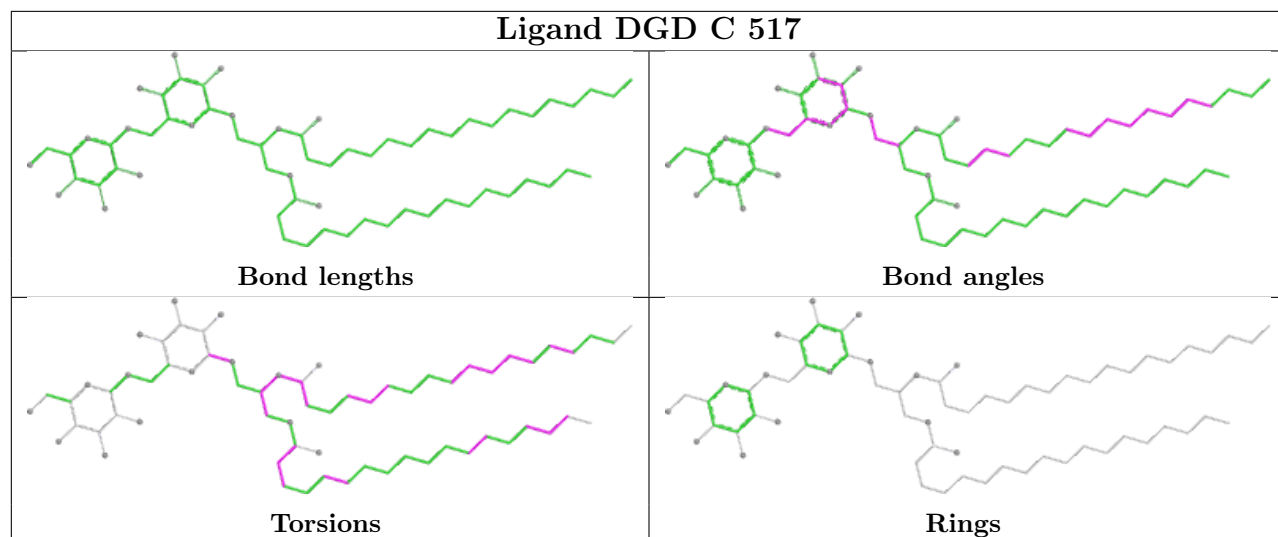
Ligand PHO a 407

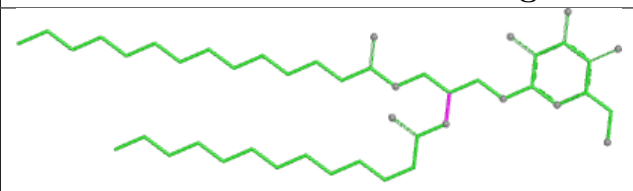
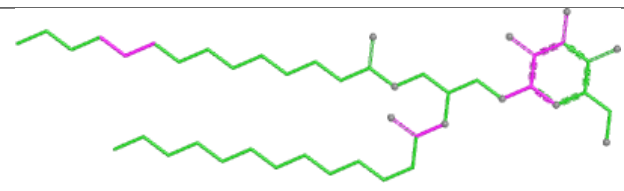
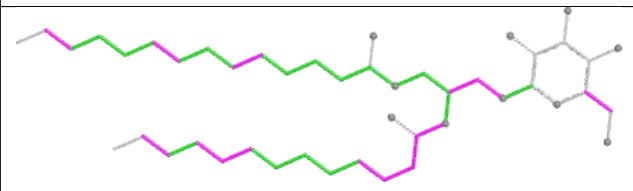
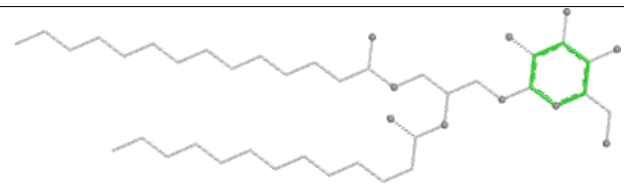


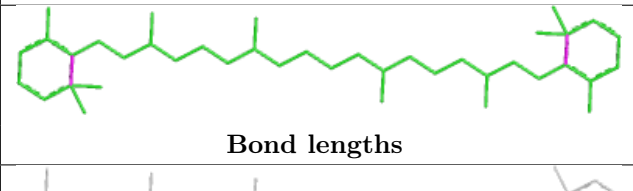
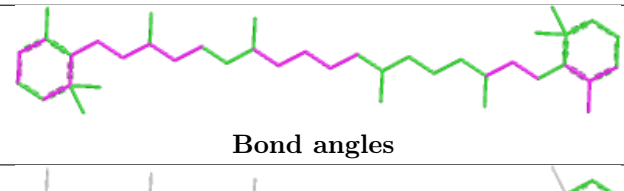
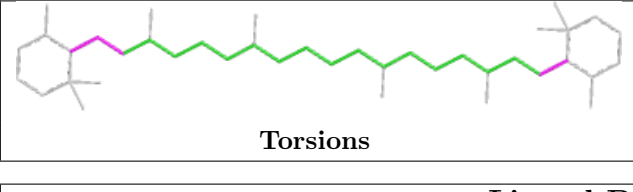
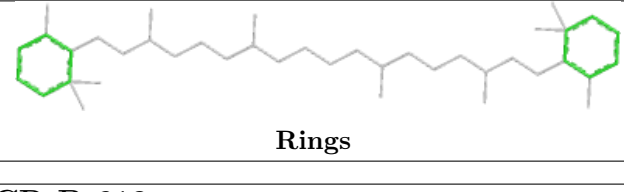


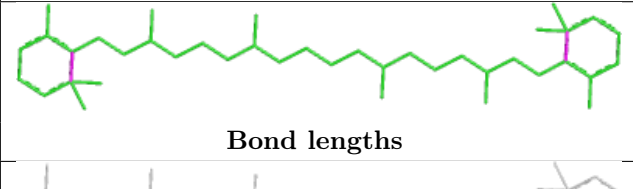
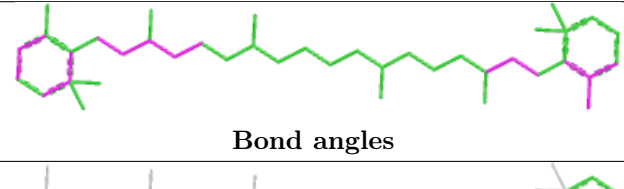
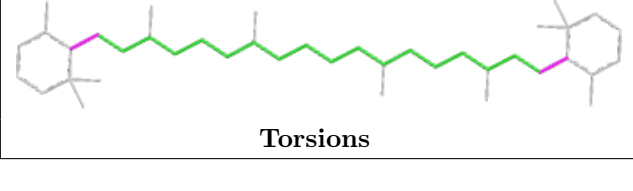
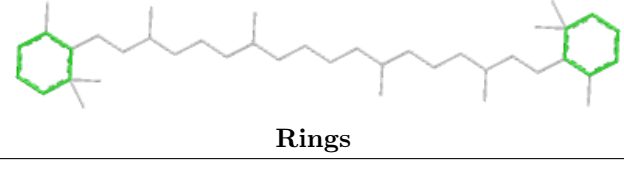




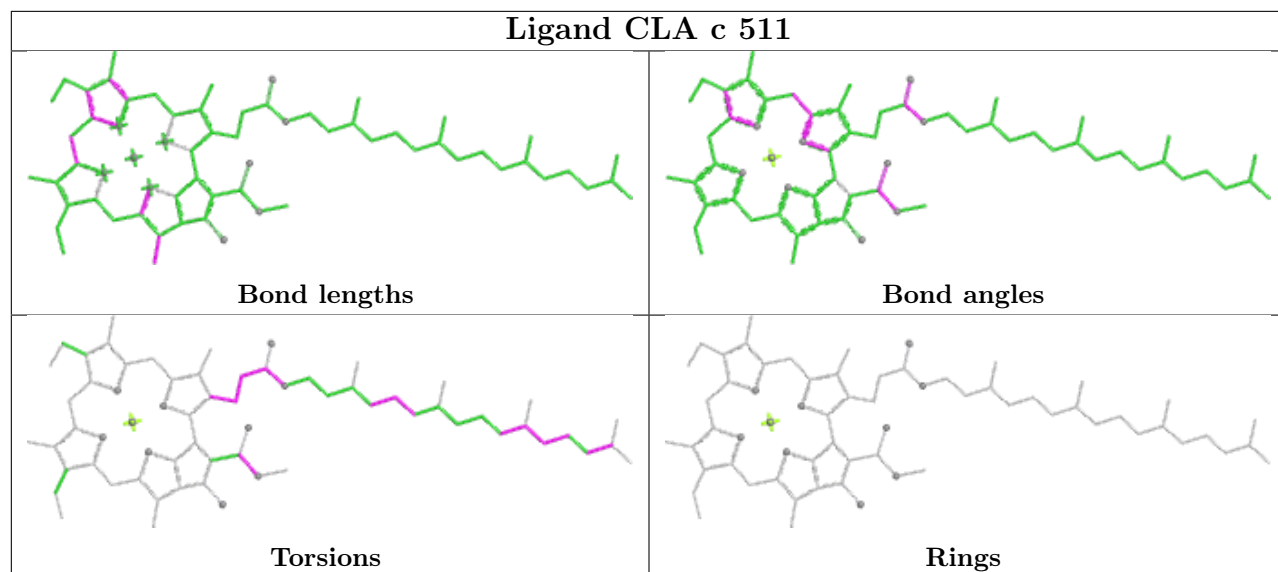


Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

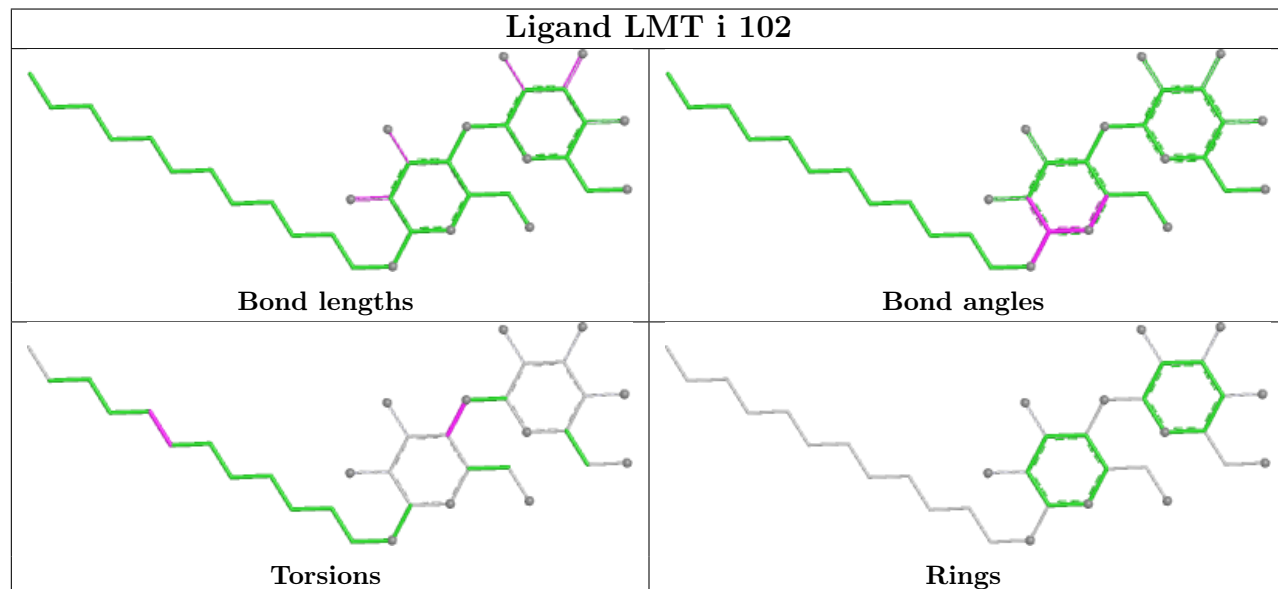
Ligand BCR C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

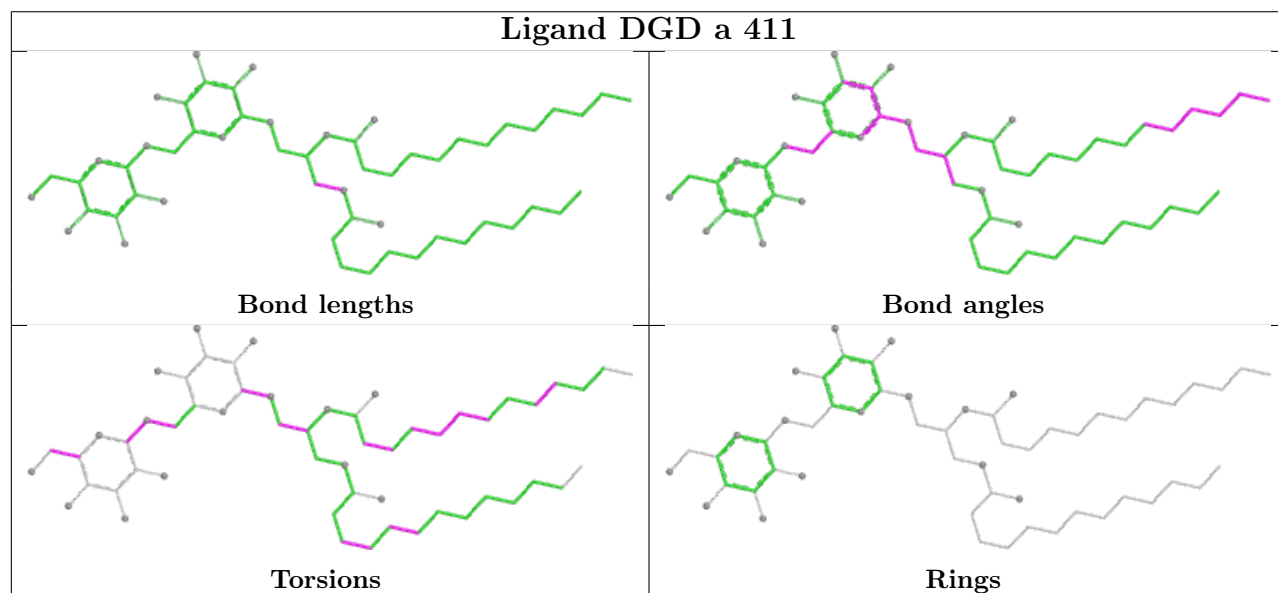
Ligand CLA c 511

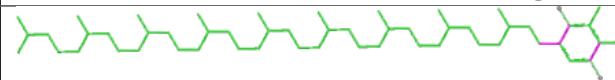
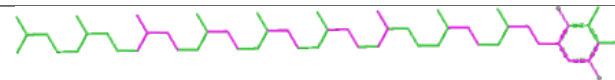
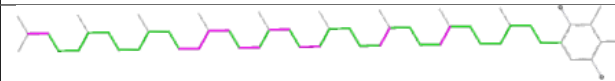
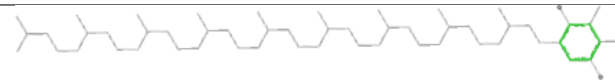


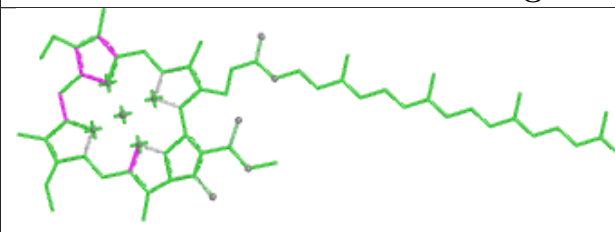
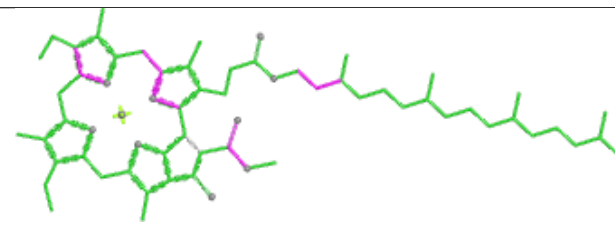
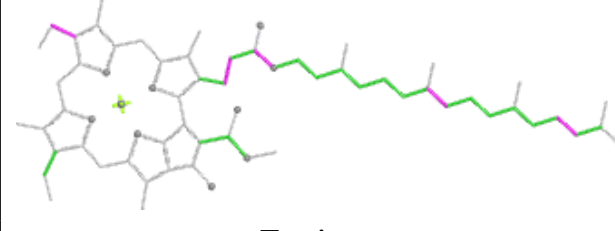
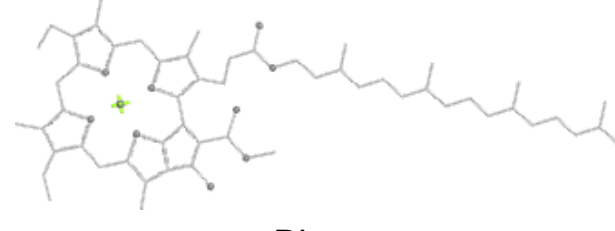
Ligand LMT i 102

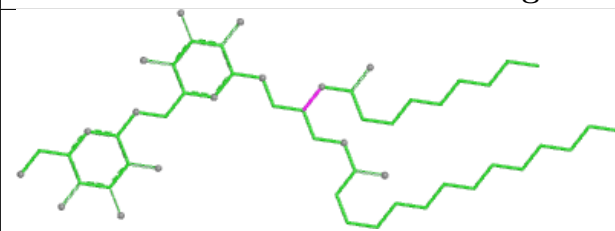
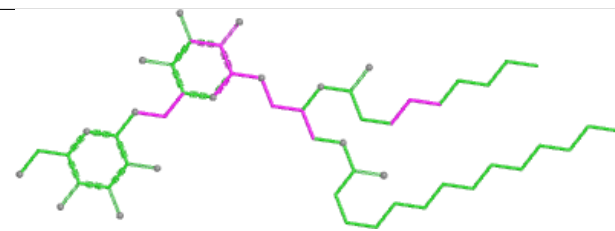
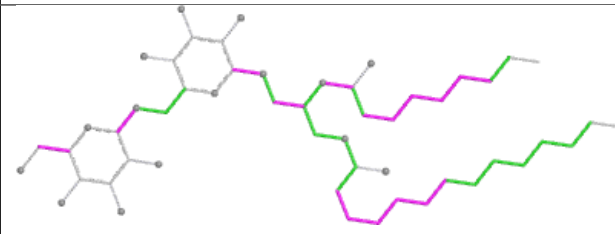
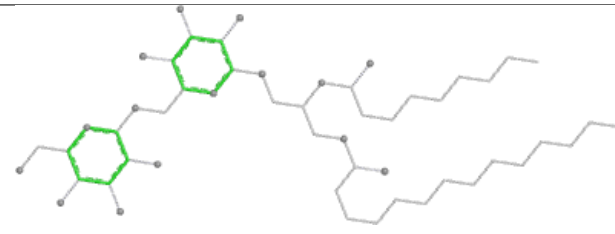


Ligand DGD a 411

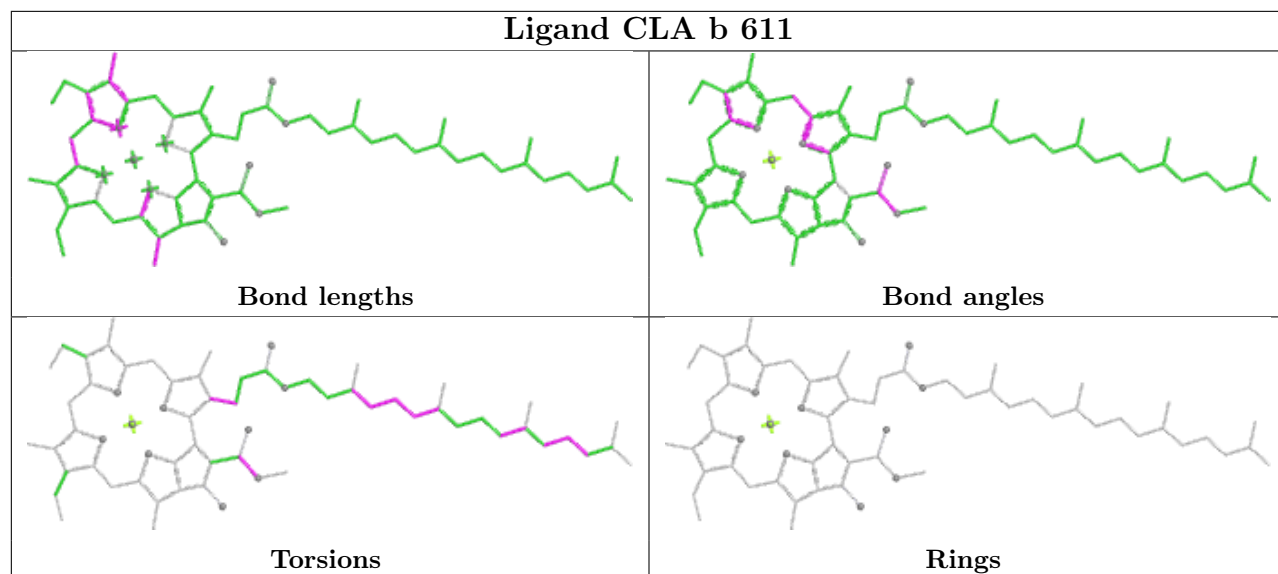


Ligand PL9 d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

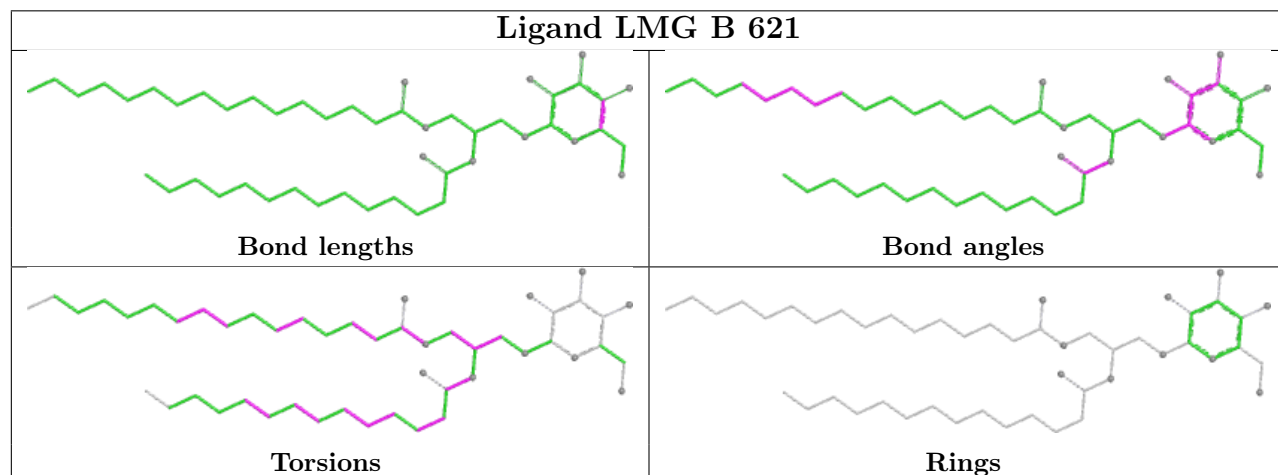
Ligand CLA d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

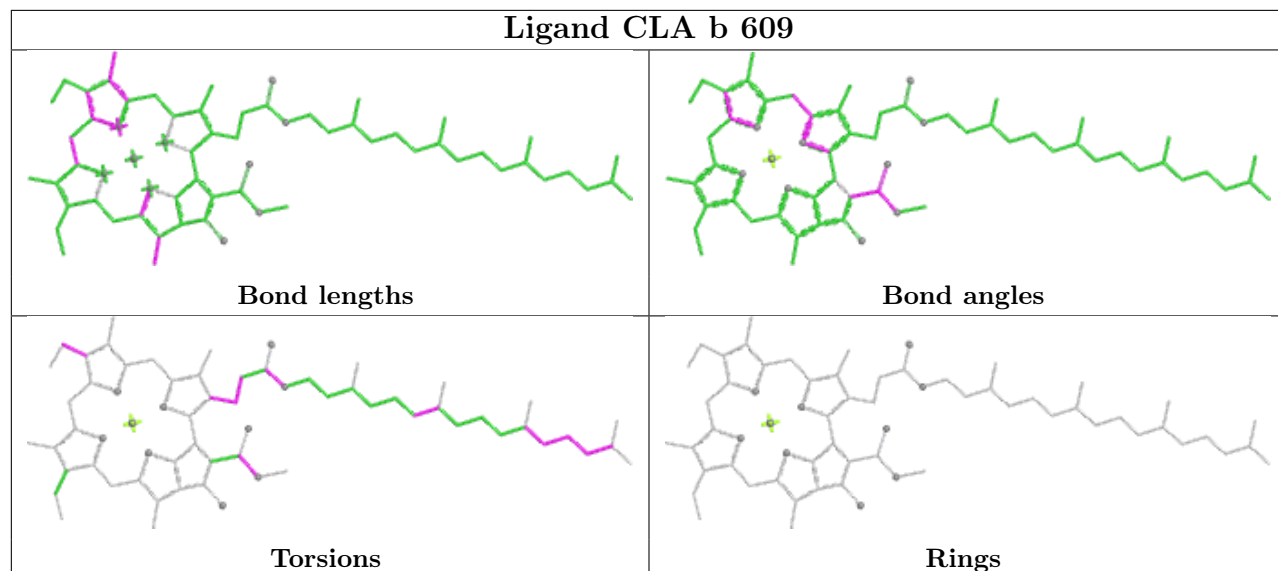
Ligand CLA b 611

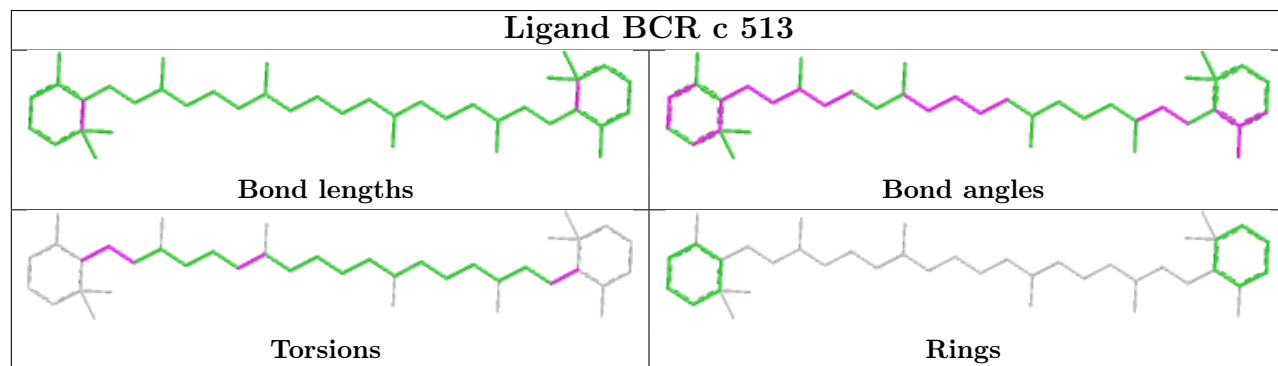
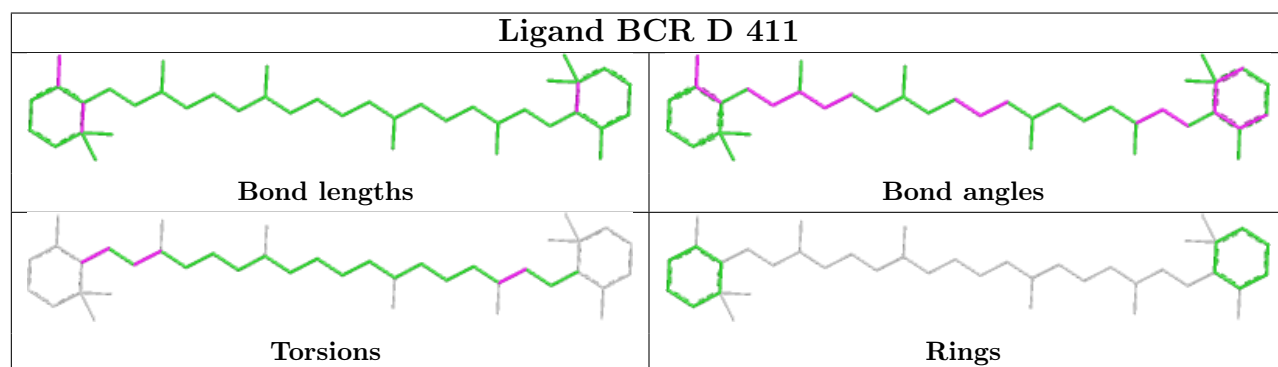
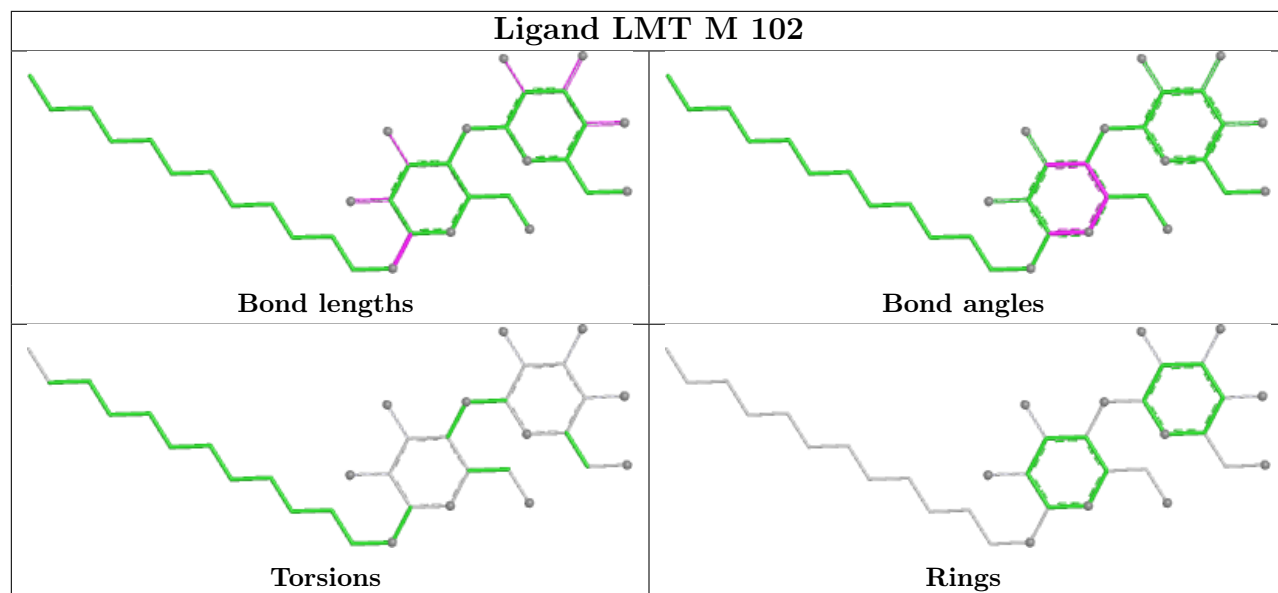


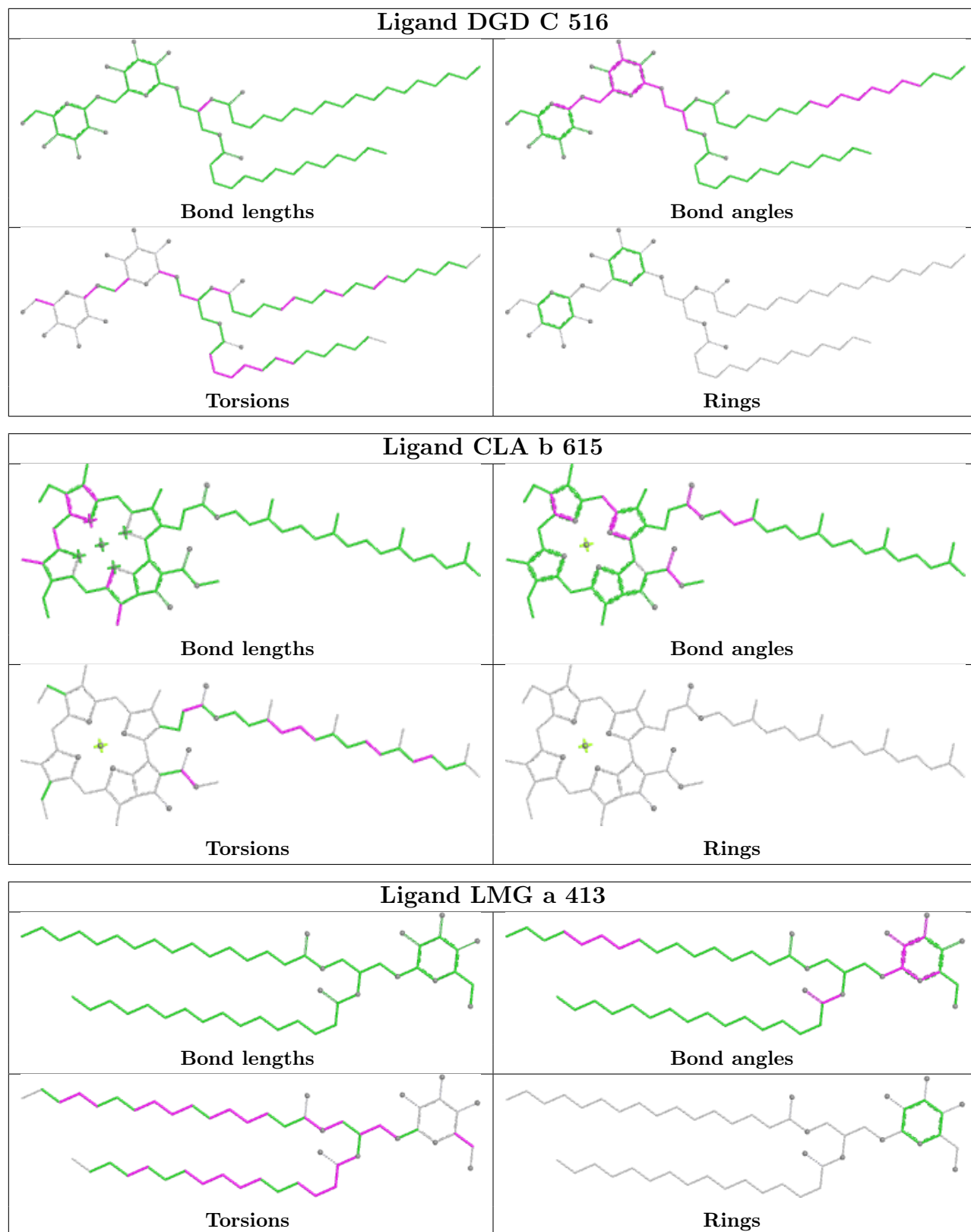
Ligand LMG B 621

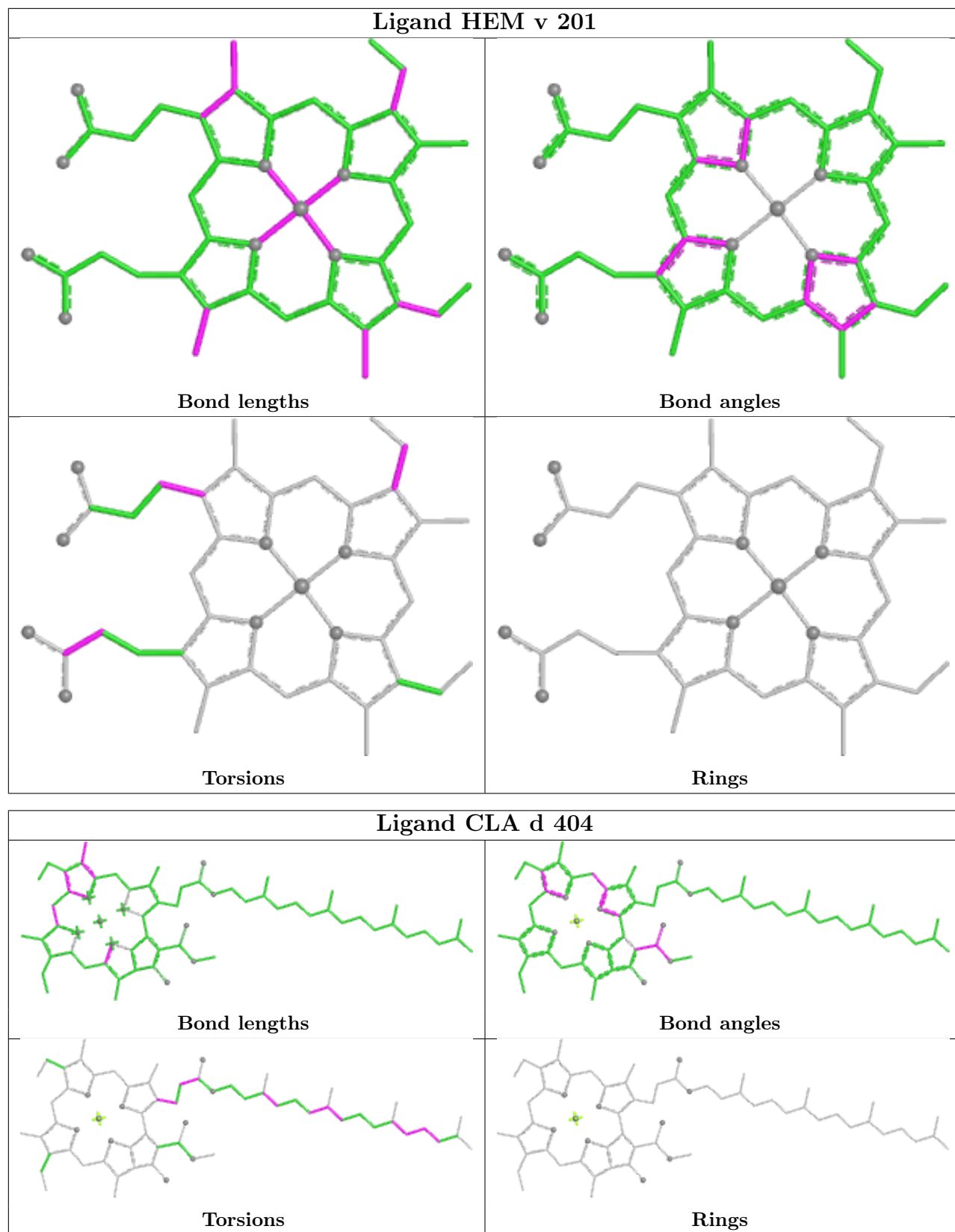


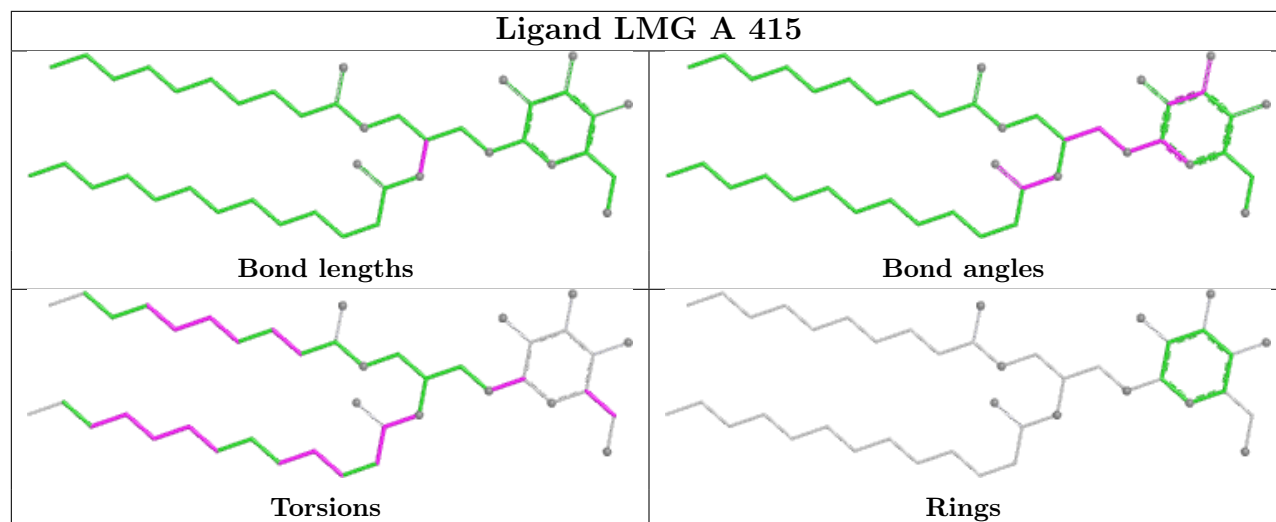
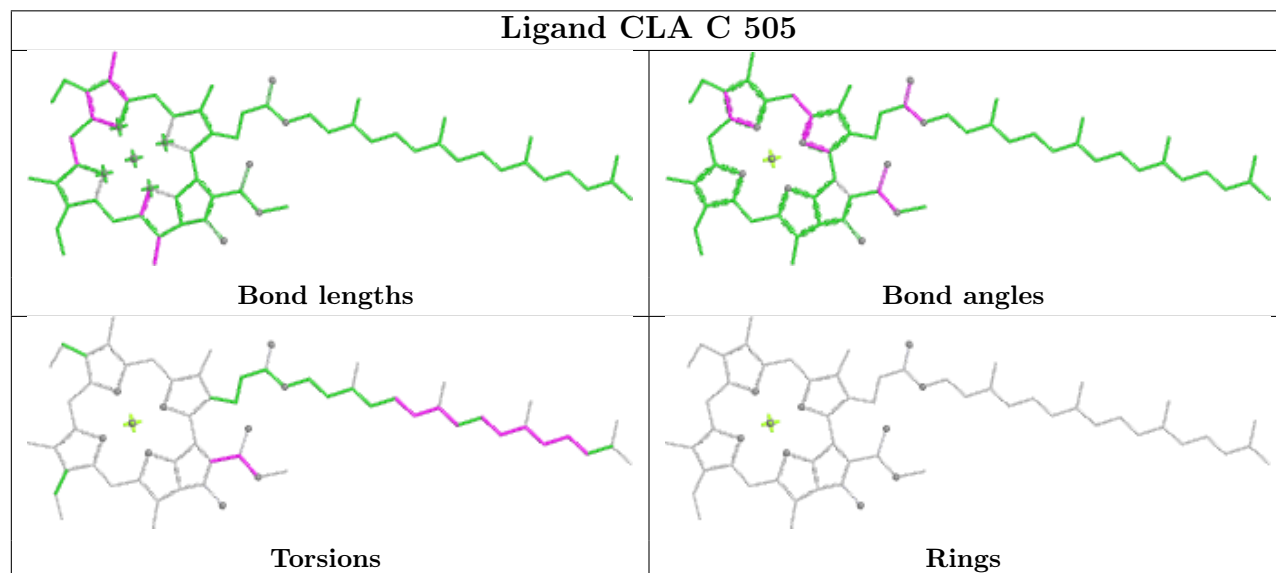
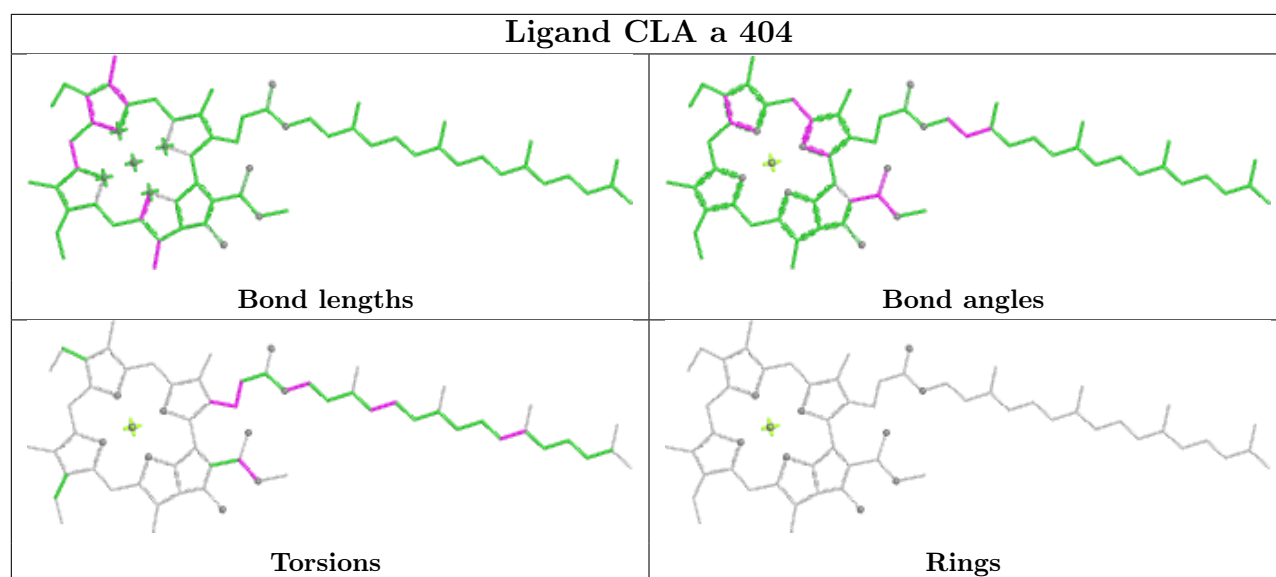
Ligand CLA b 609

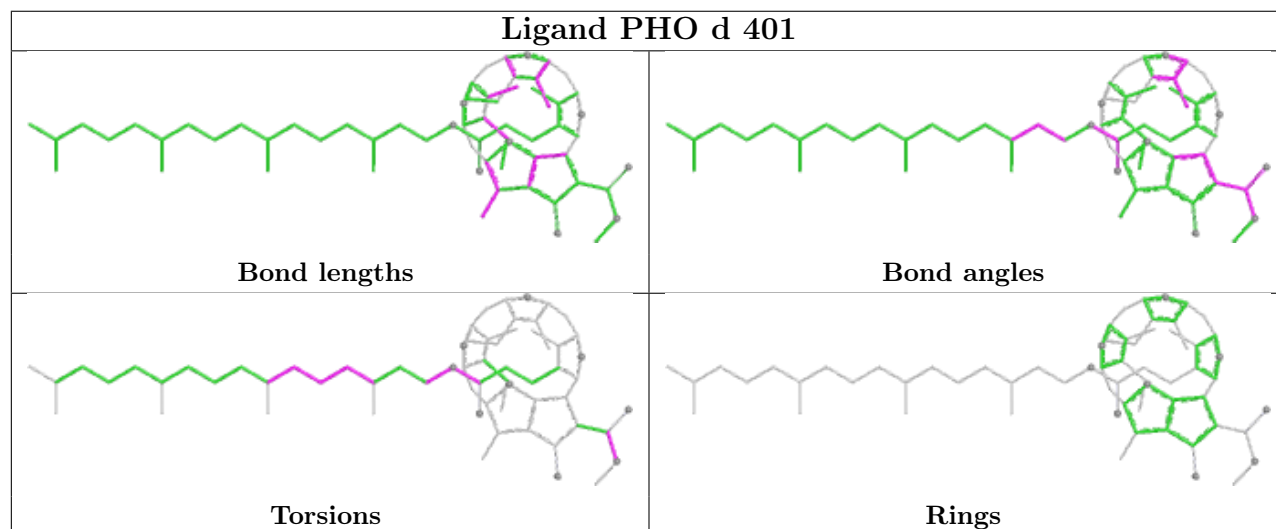
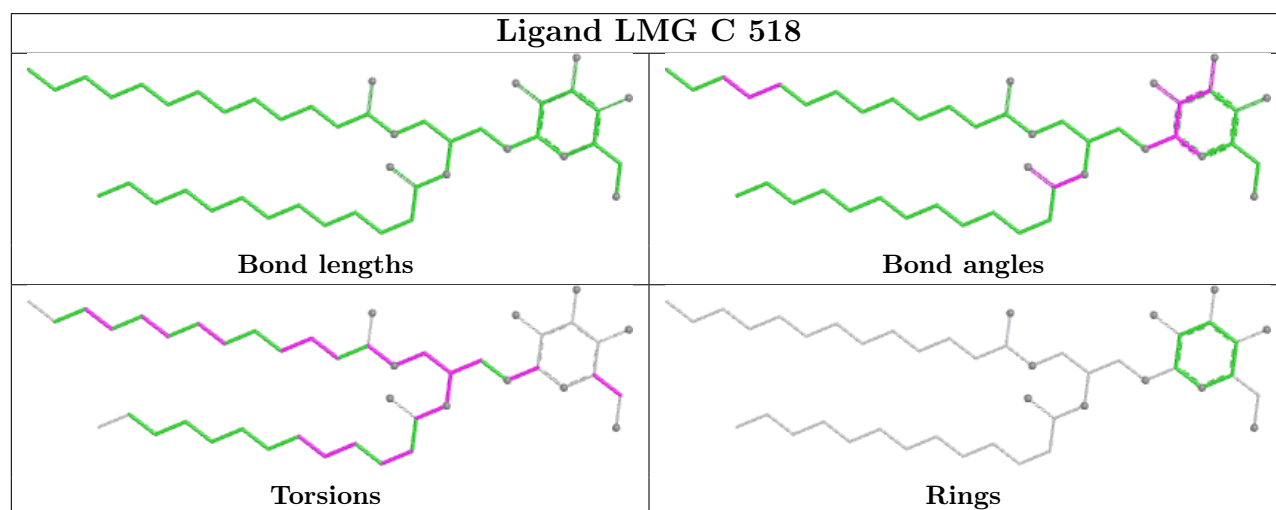
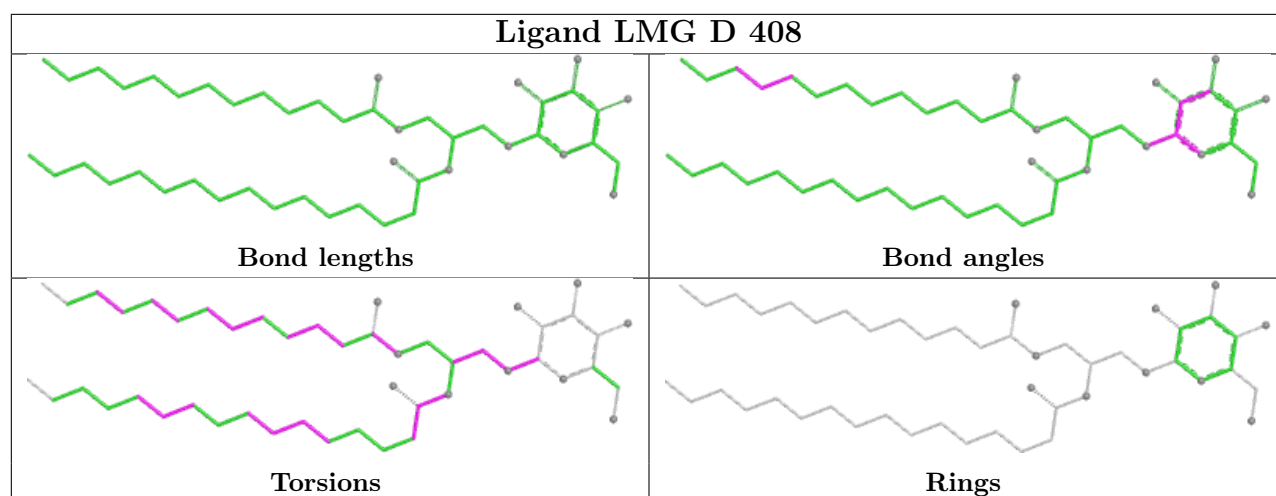


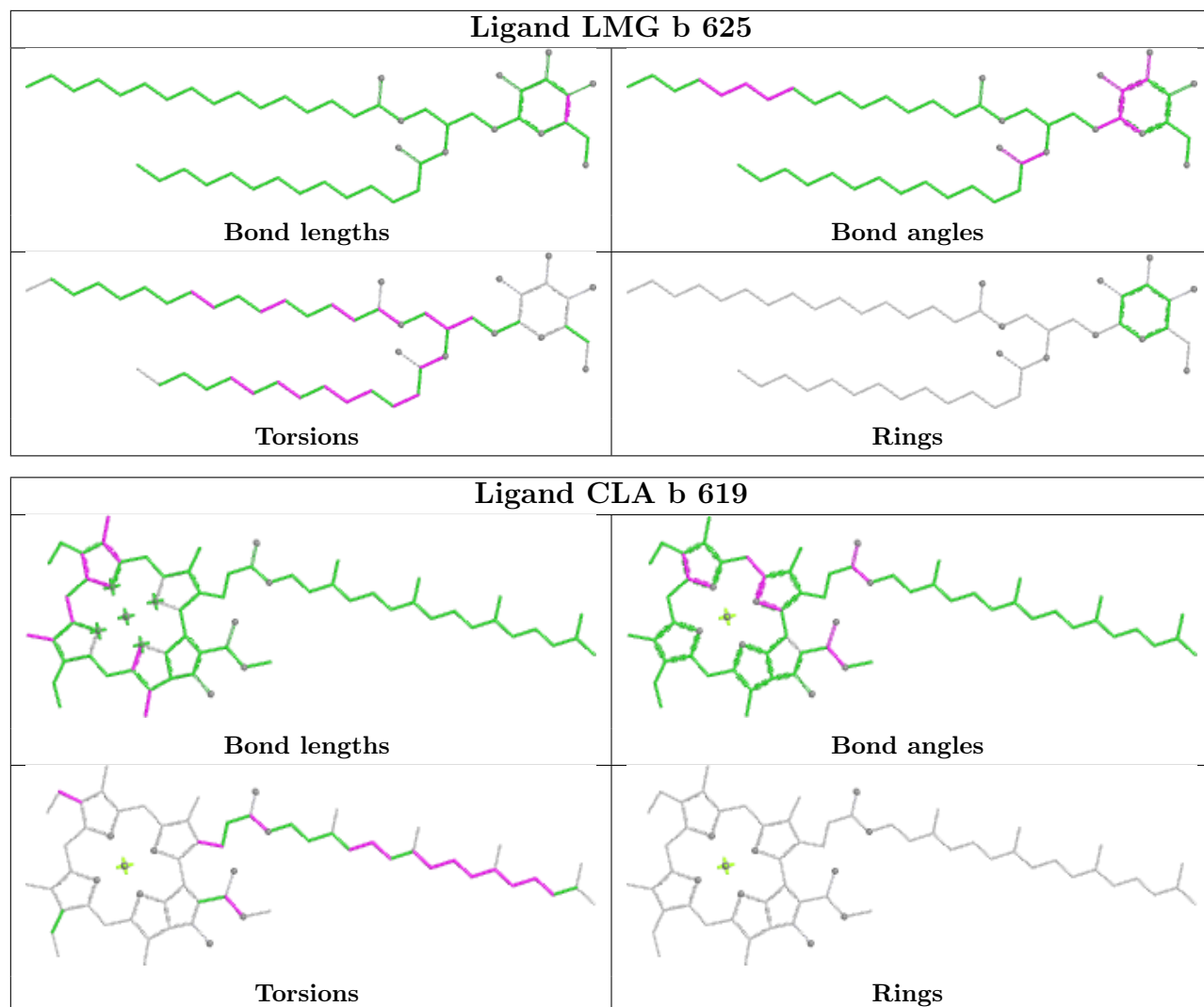


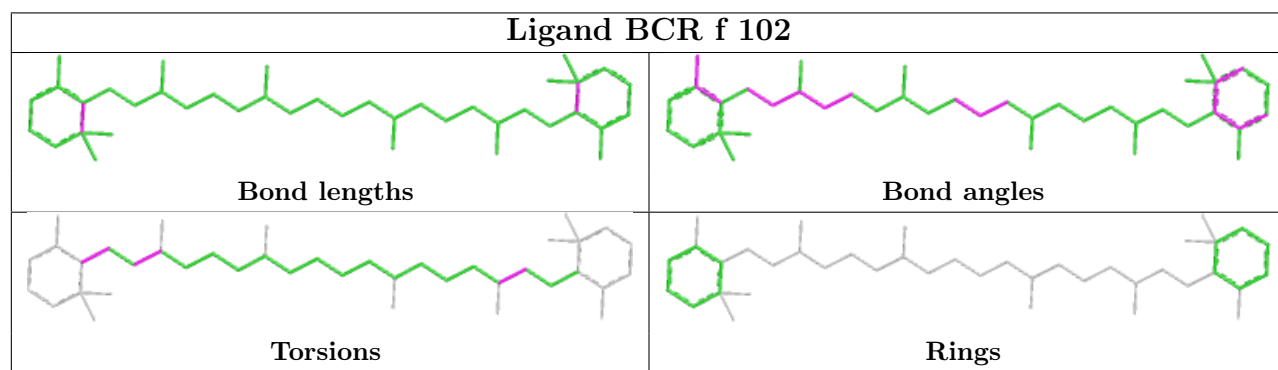
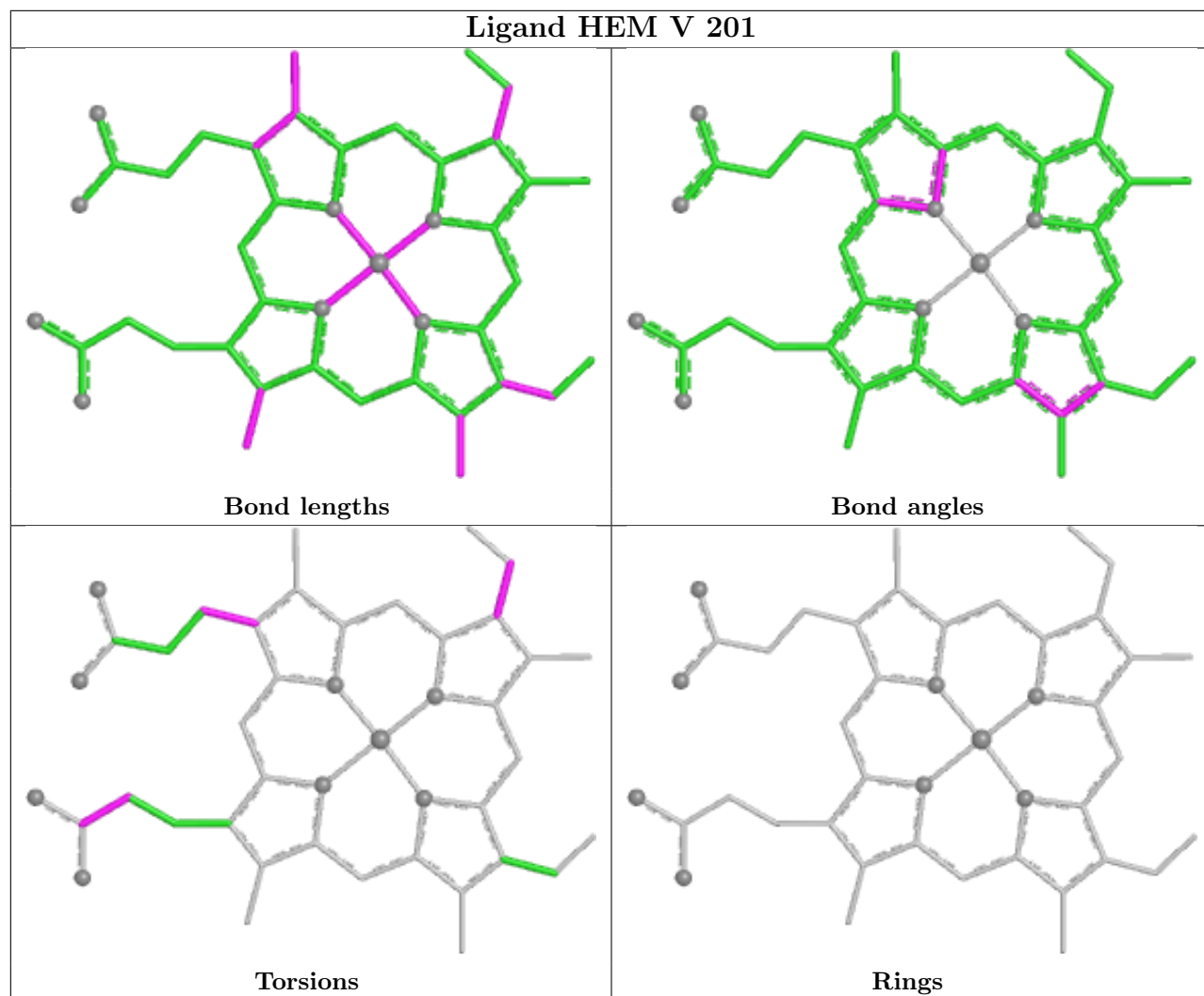




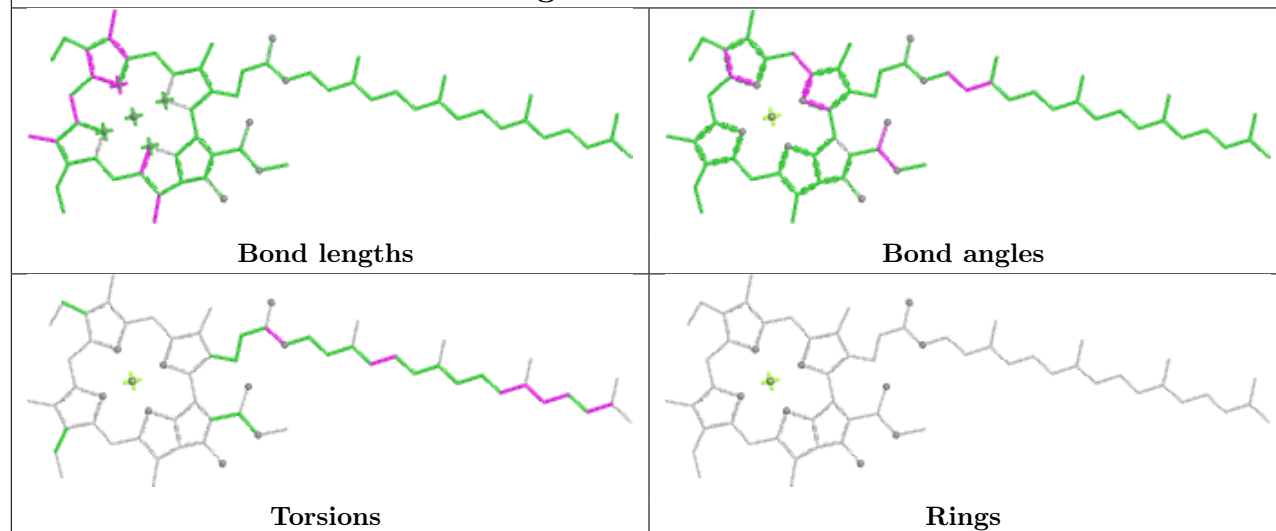




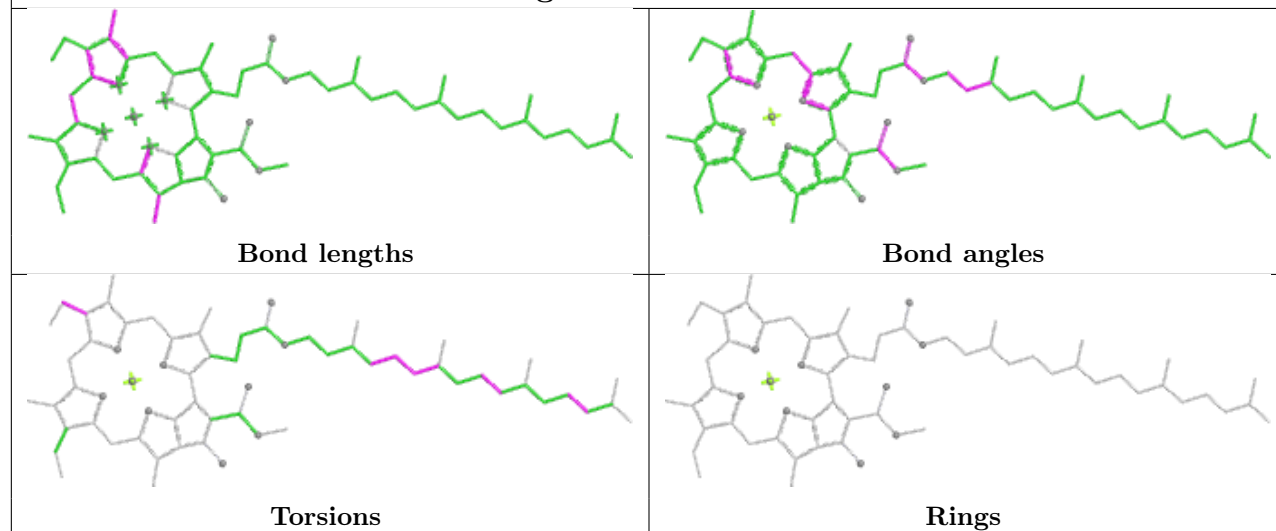




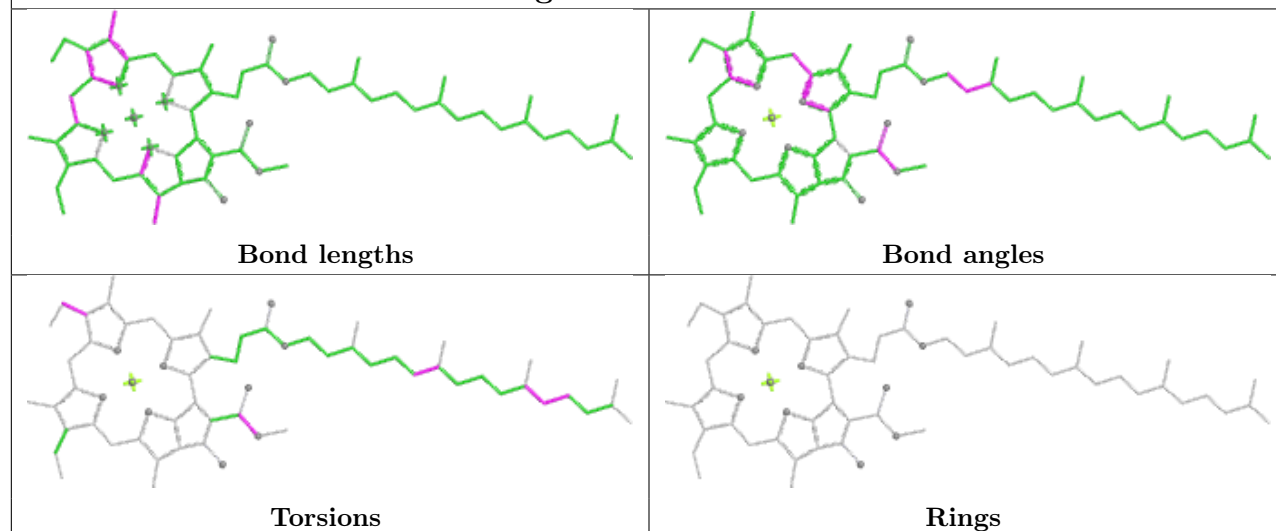
Ligand CLA c 502

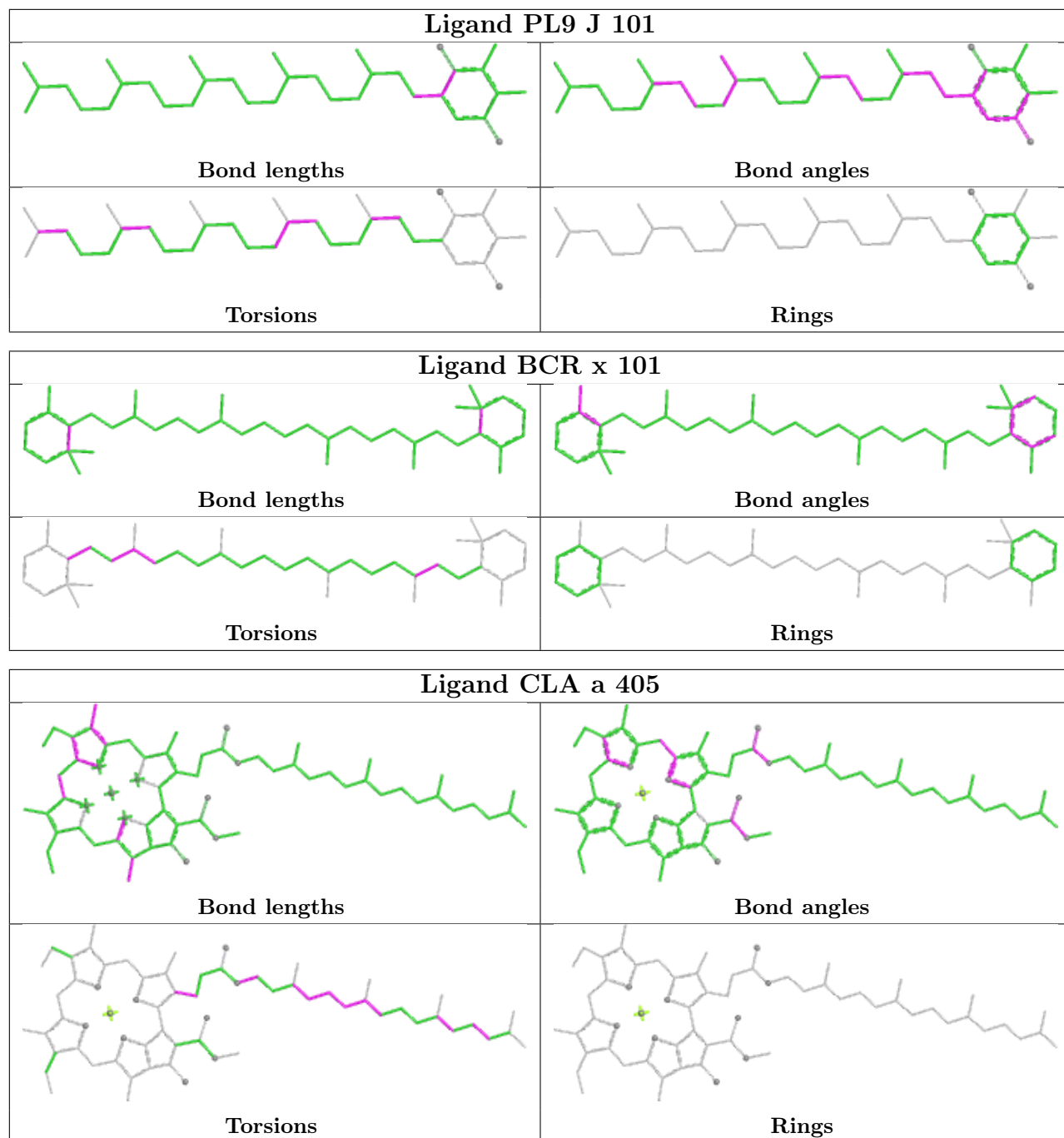


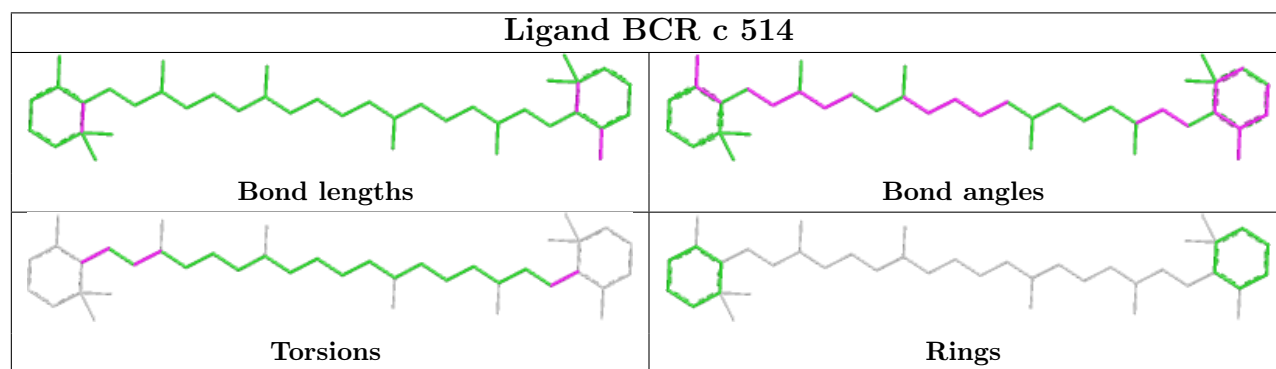
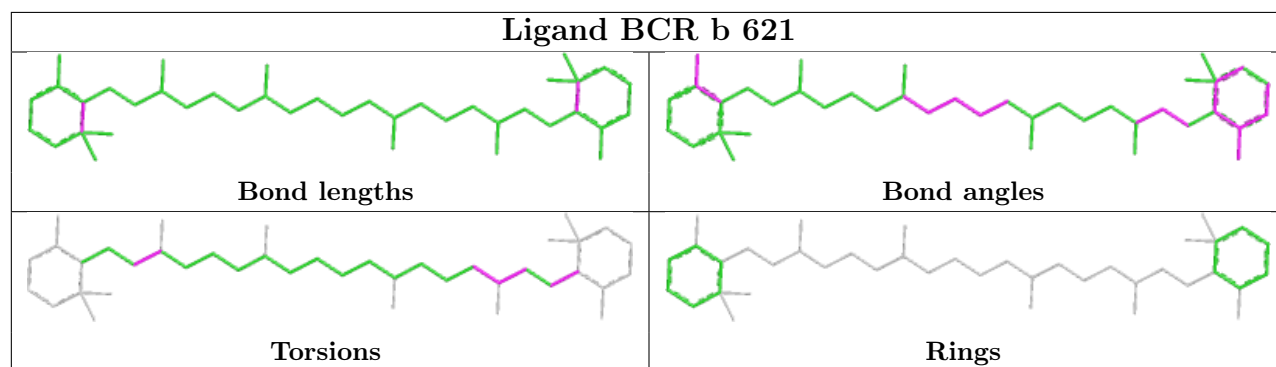
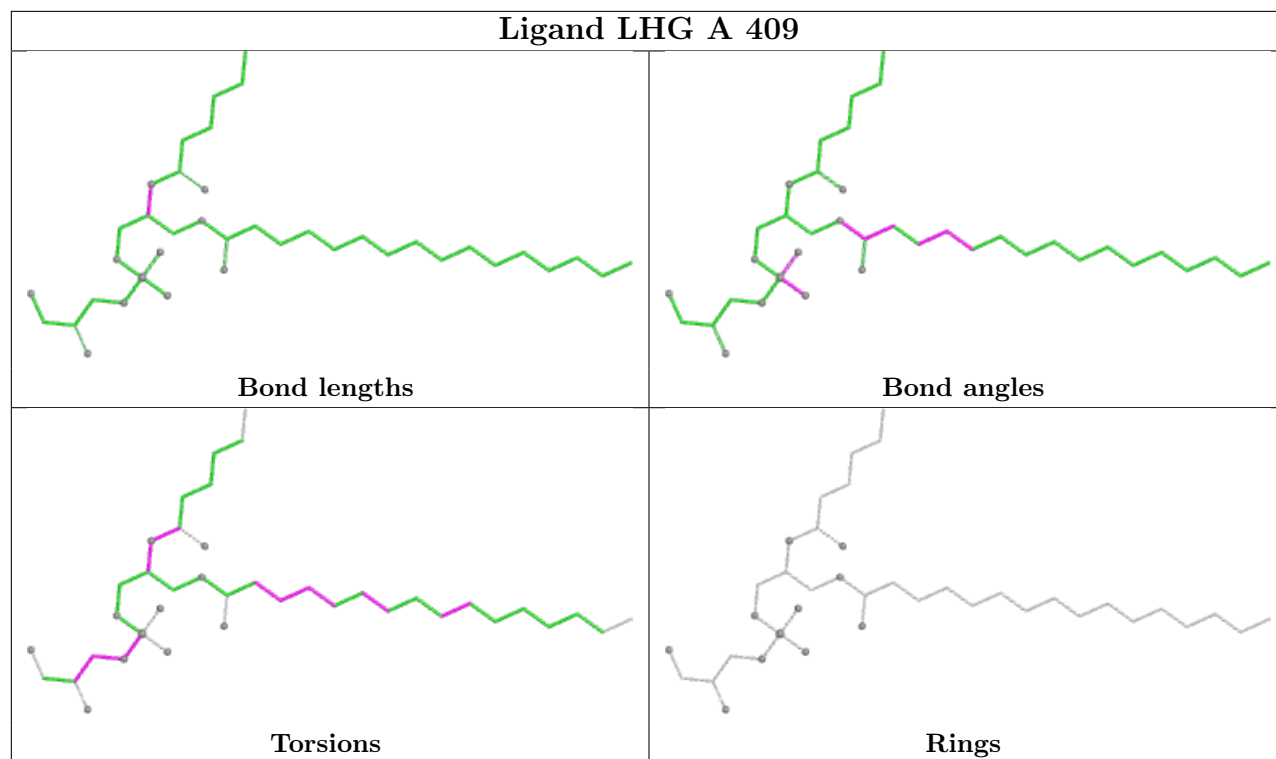
Ligand CLA a 406



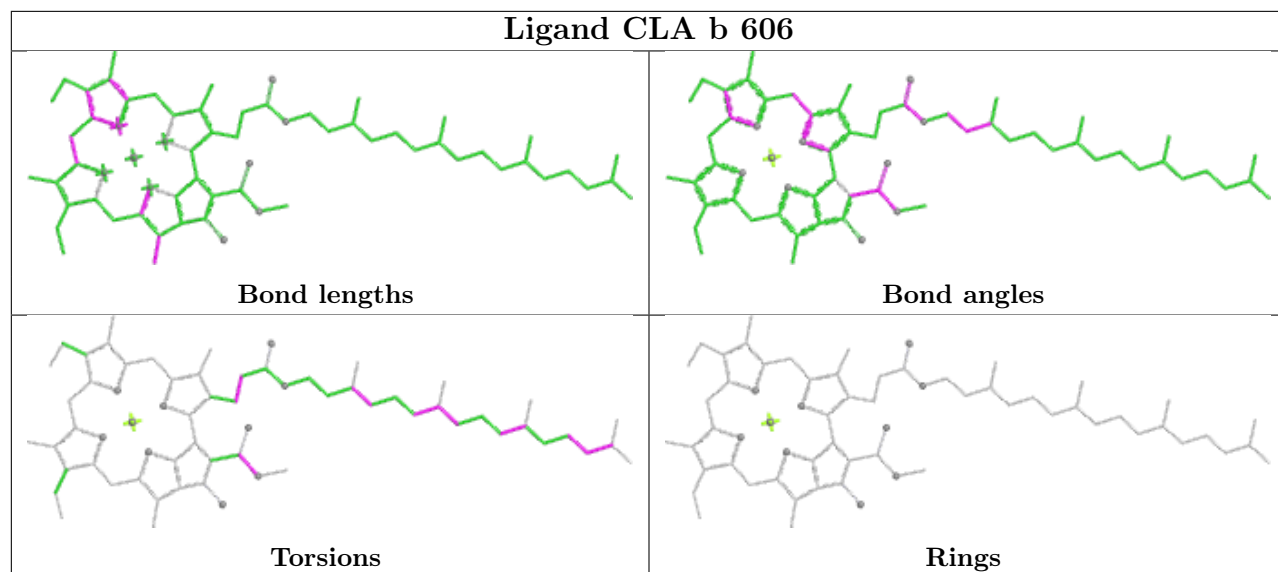
Ligand CLA b 612



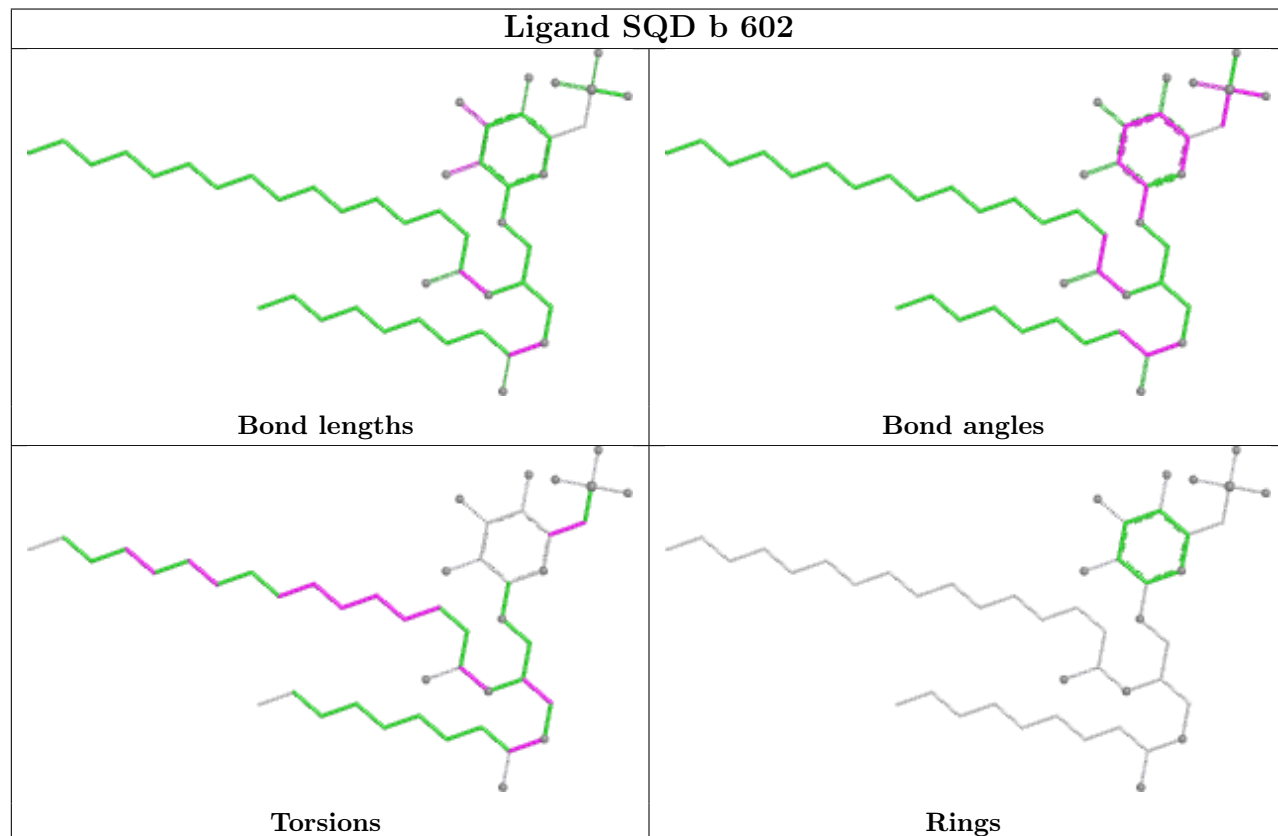


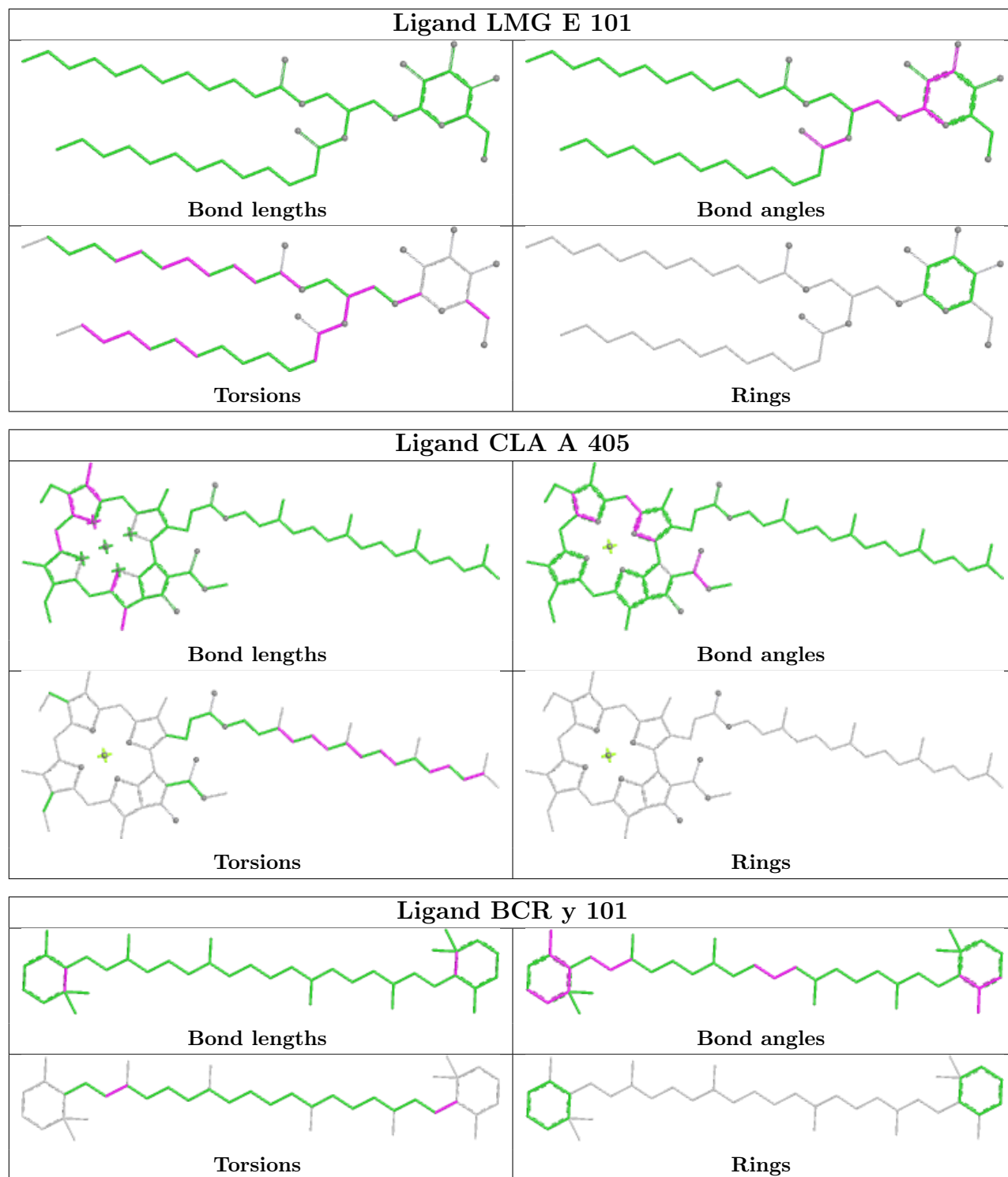


Ligand CLA b 606

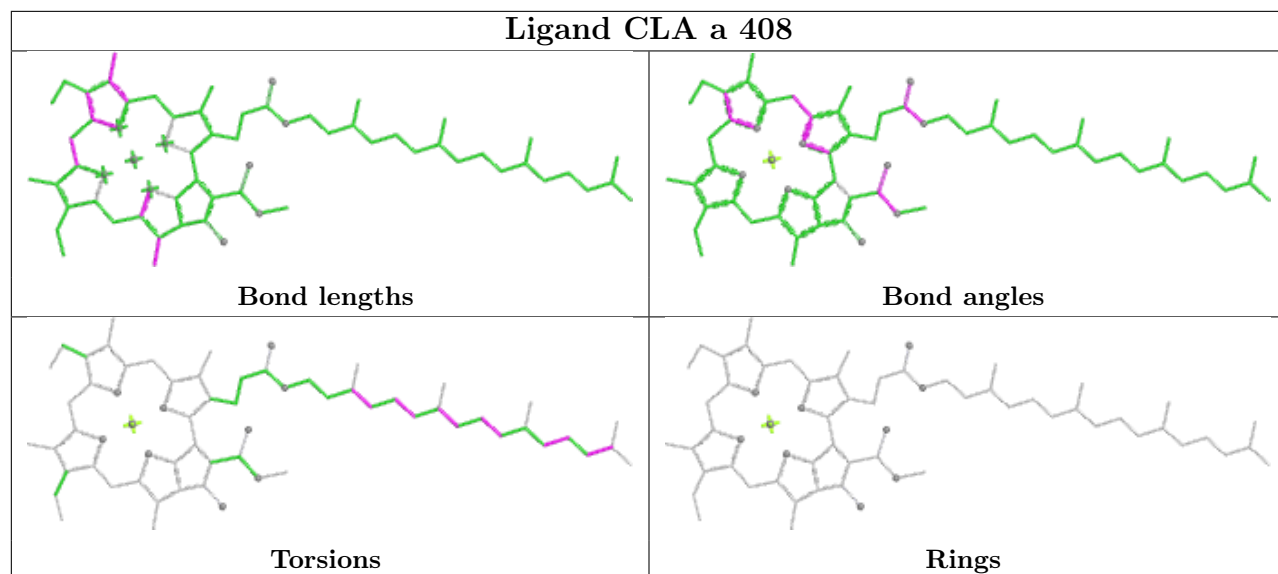


Ligand SQD b 602

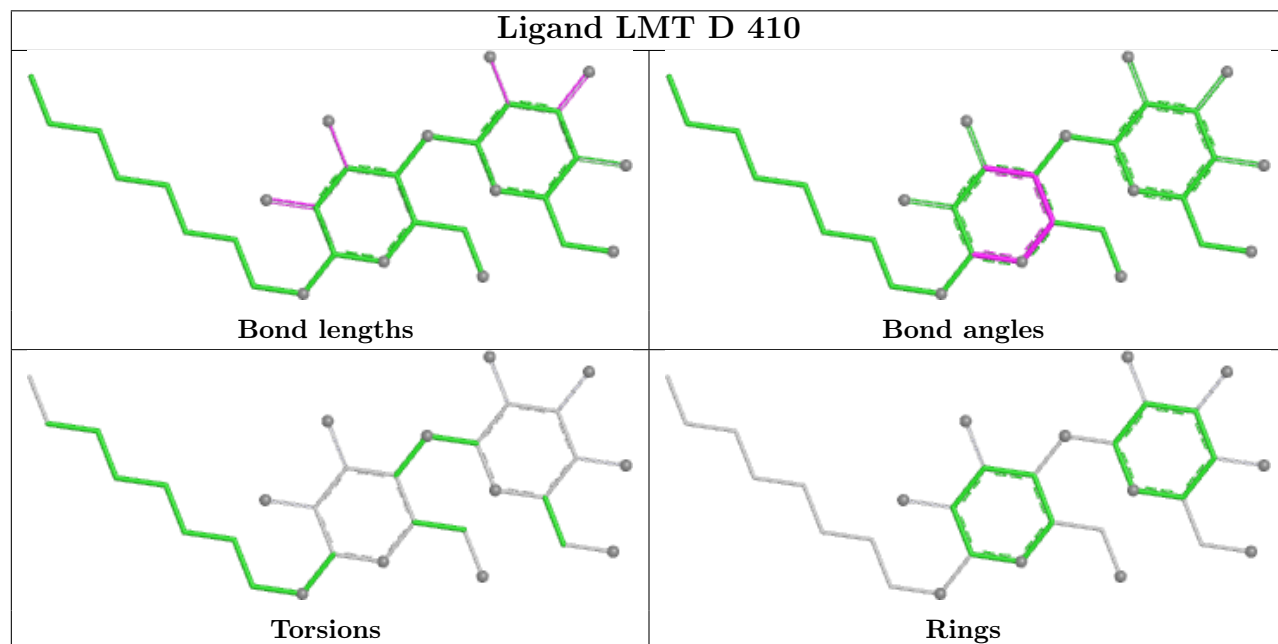




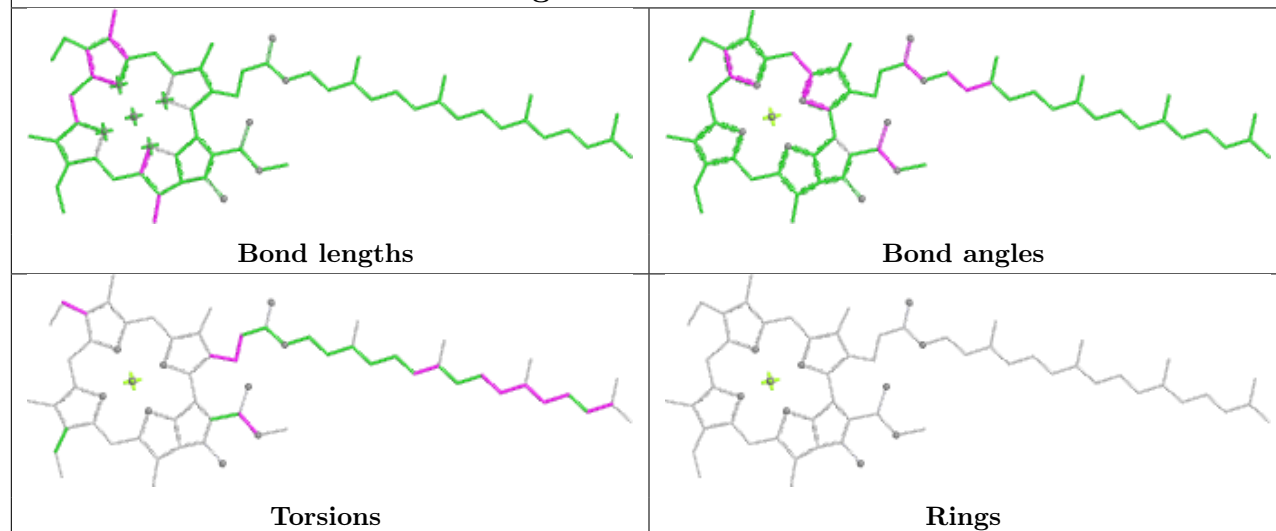
Ligand CLA a 408



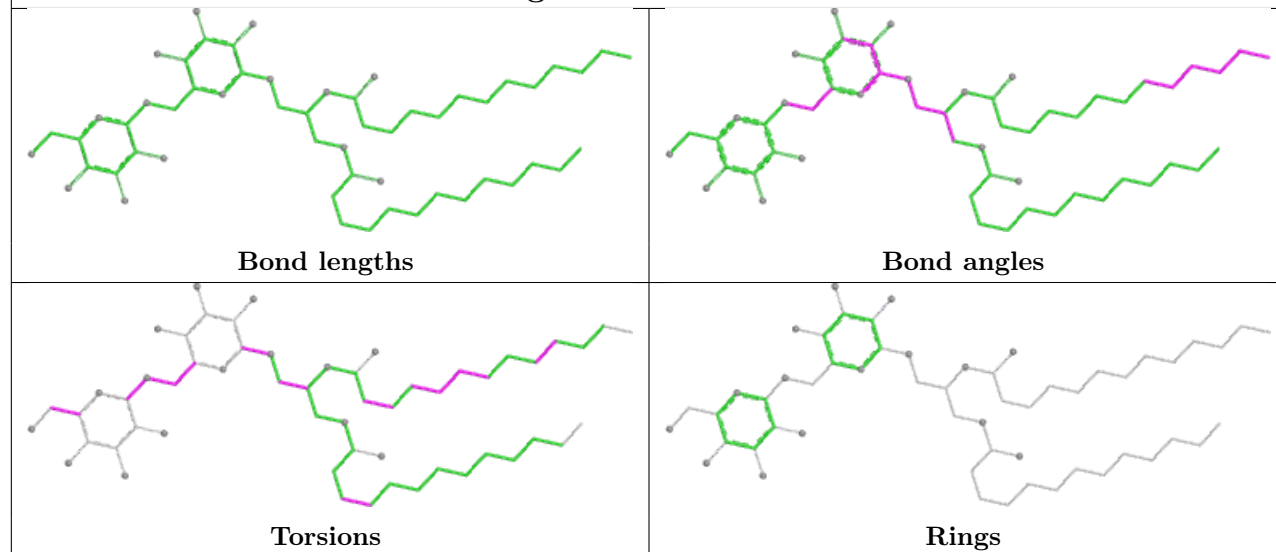
Ligand LMT D 410



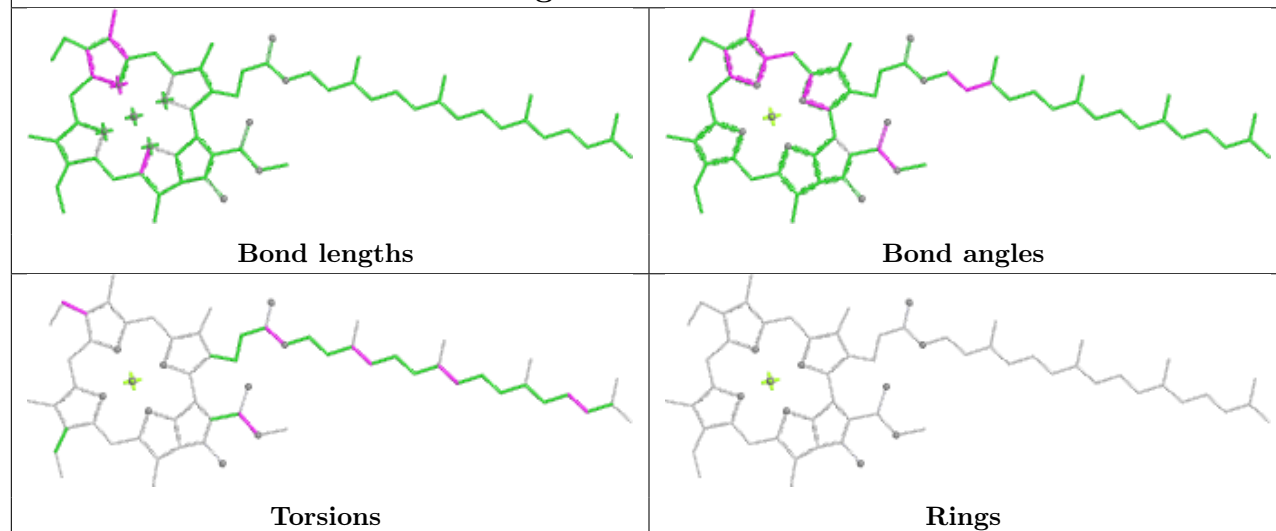
Ligand CLA B 601

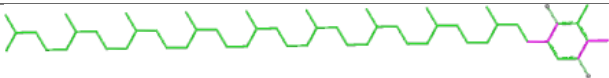
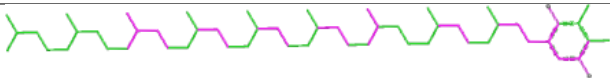
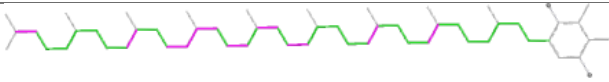
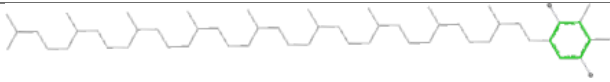


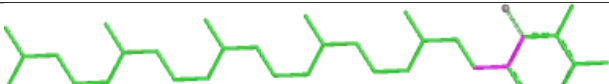
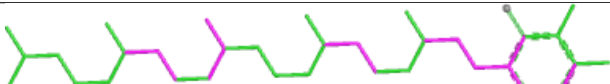
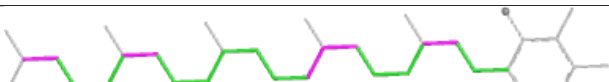
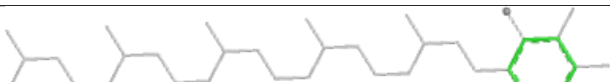
Ligand DGD A 408

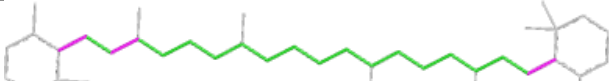


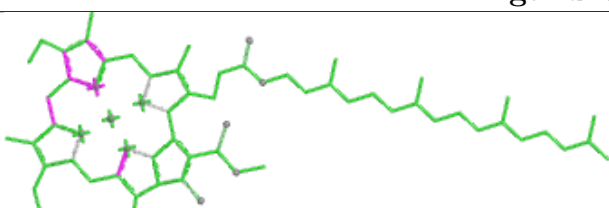
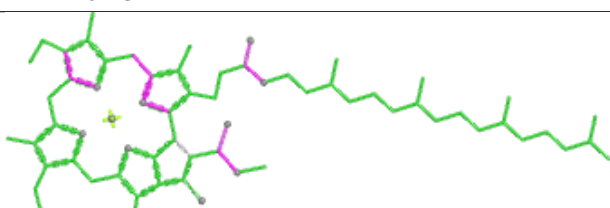
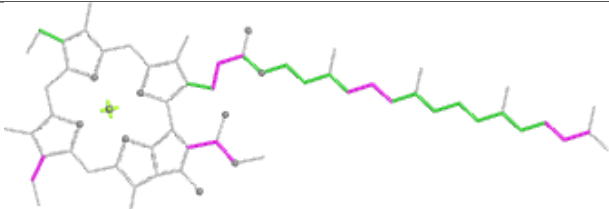
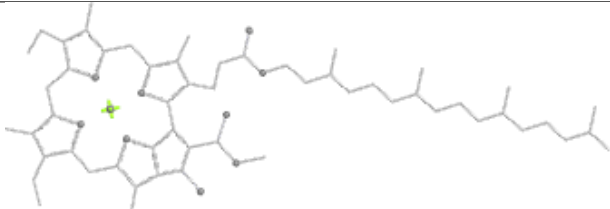
Ligand CLA b 614

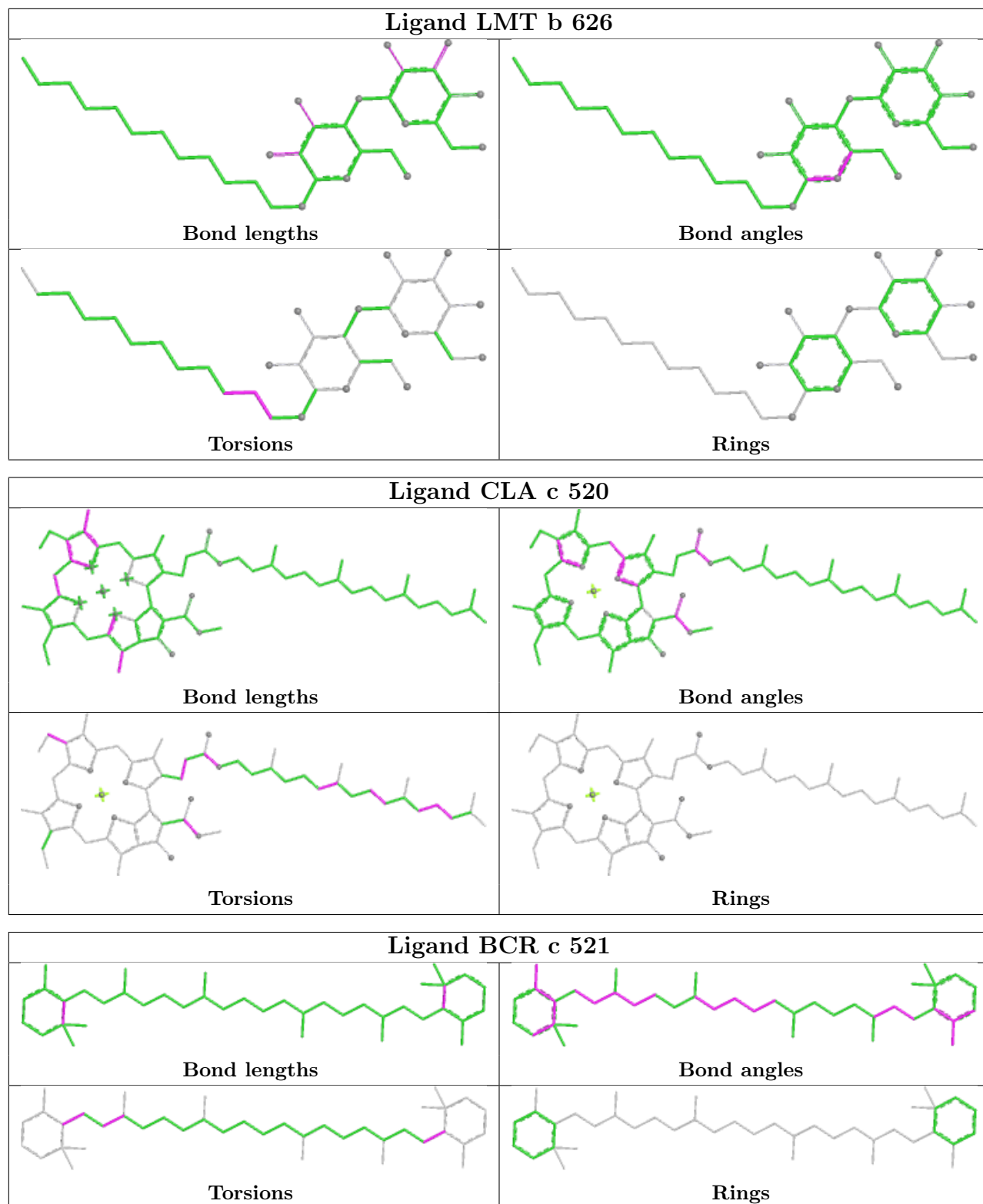


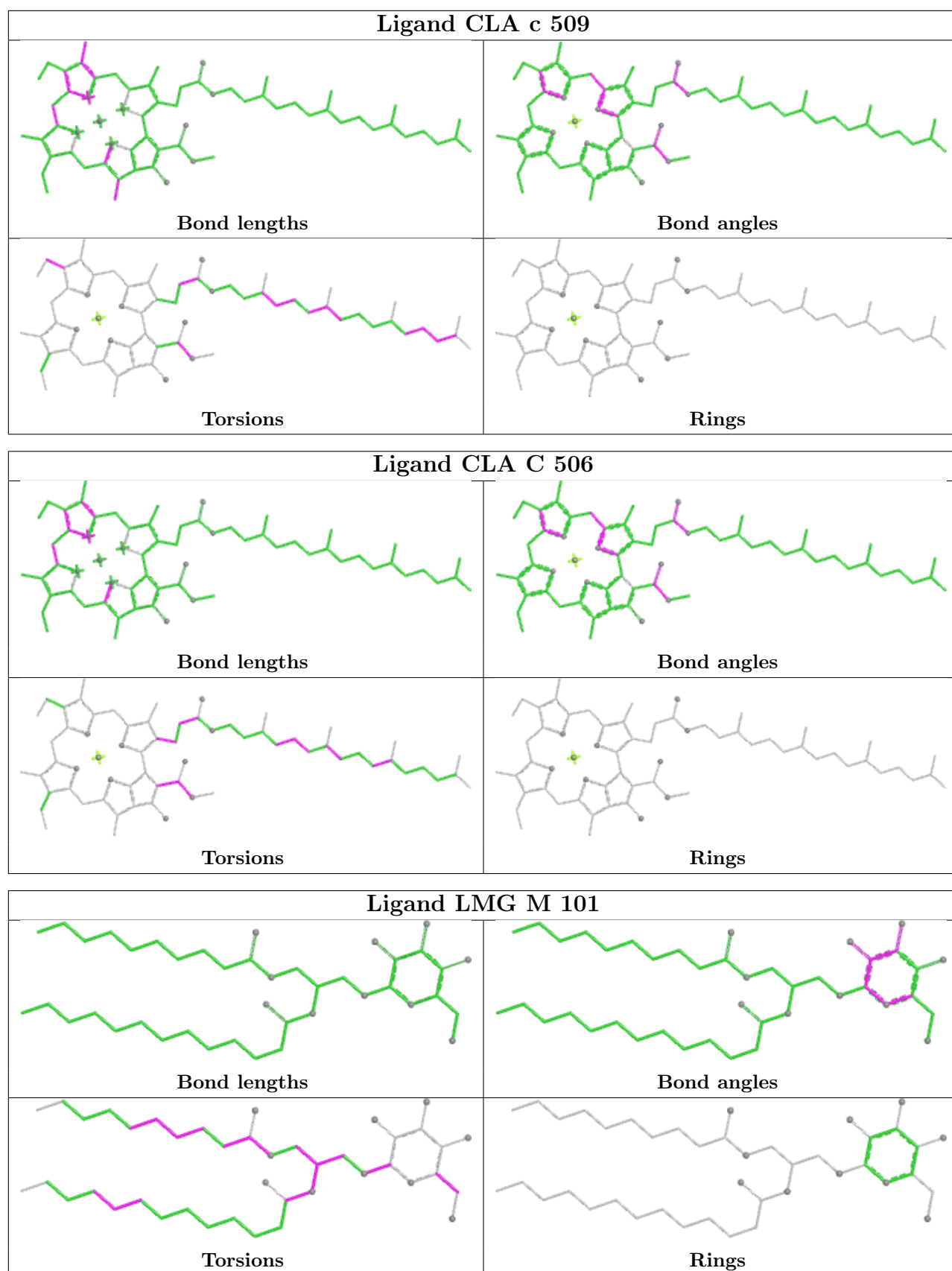
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

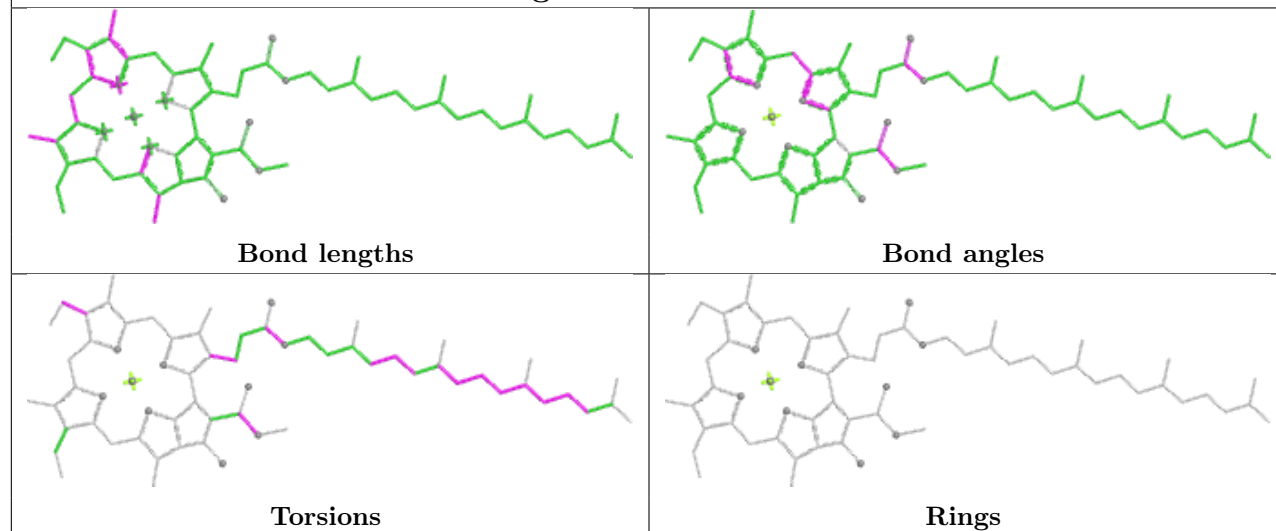
Ligand BCR C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

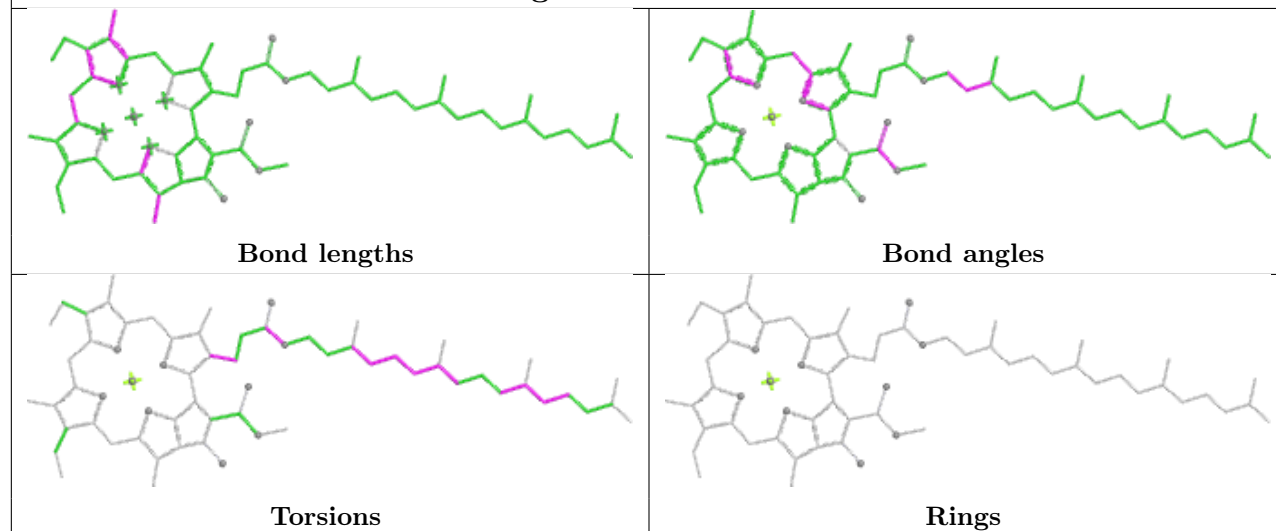




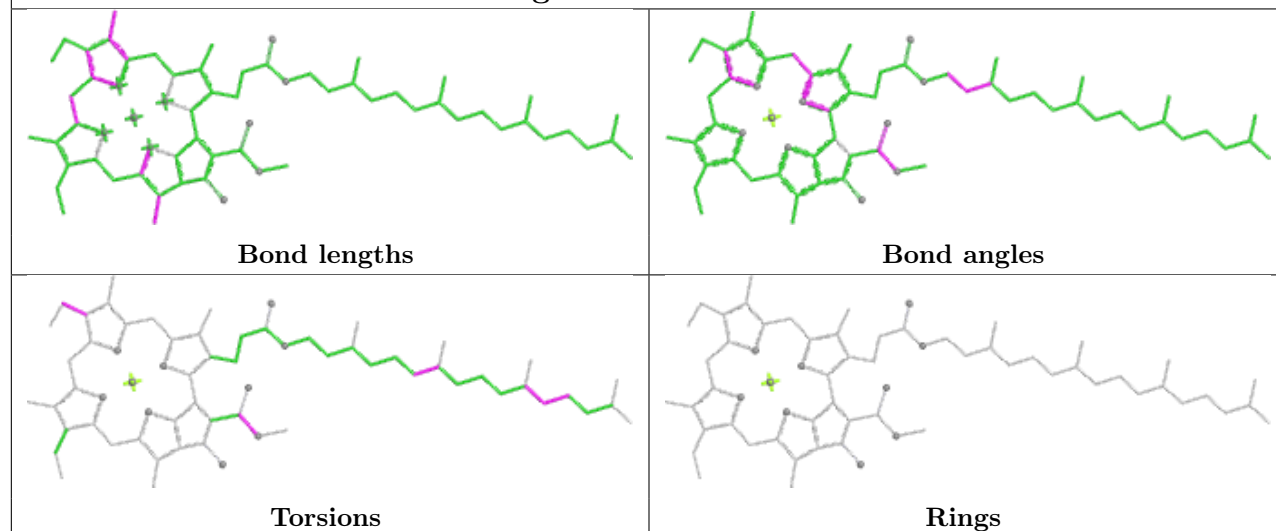
Ligand CLA B 615

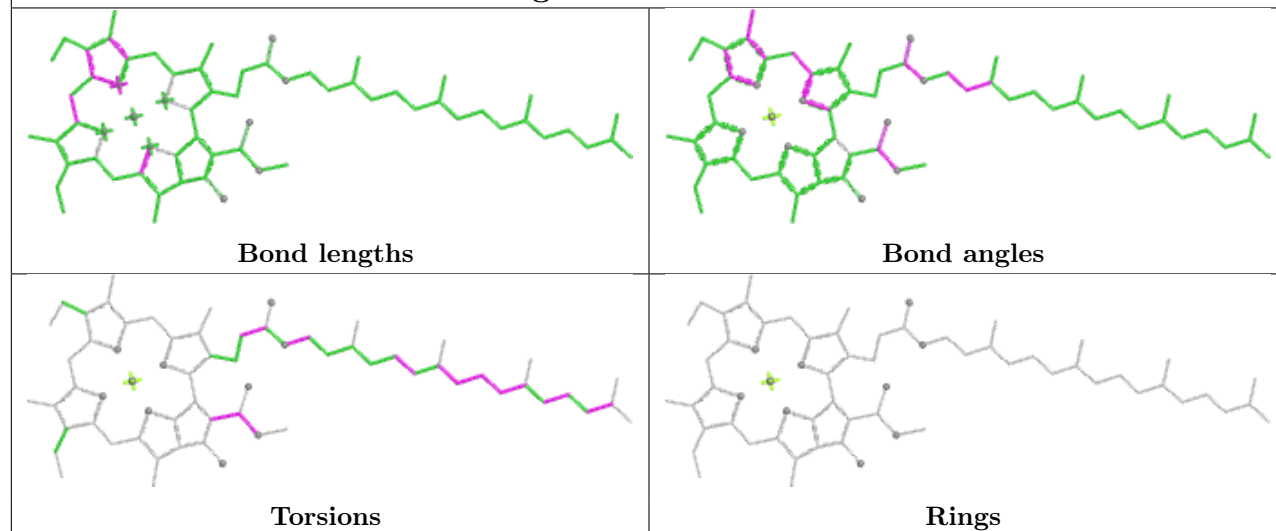
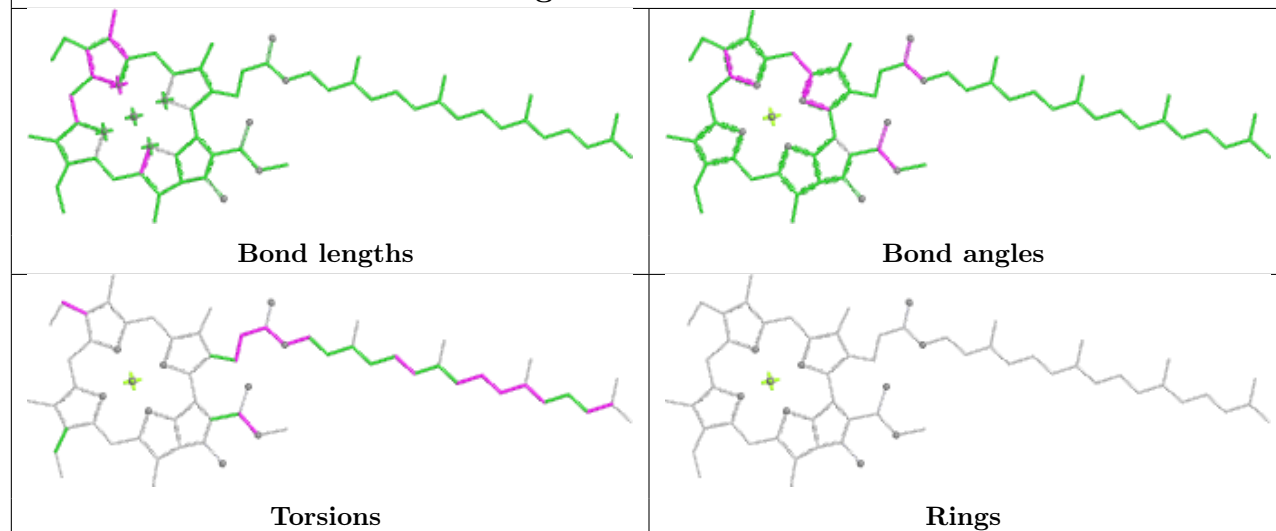
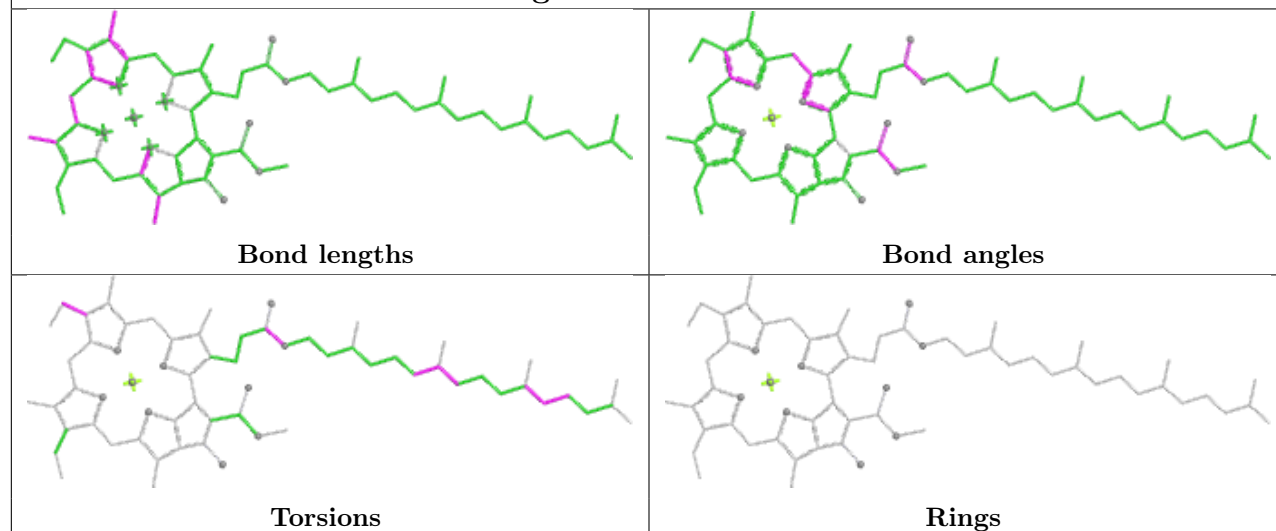


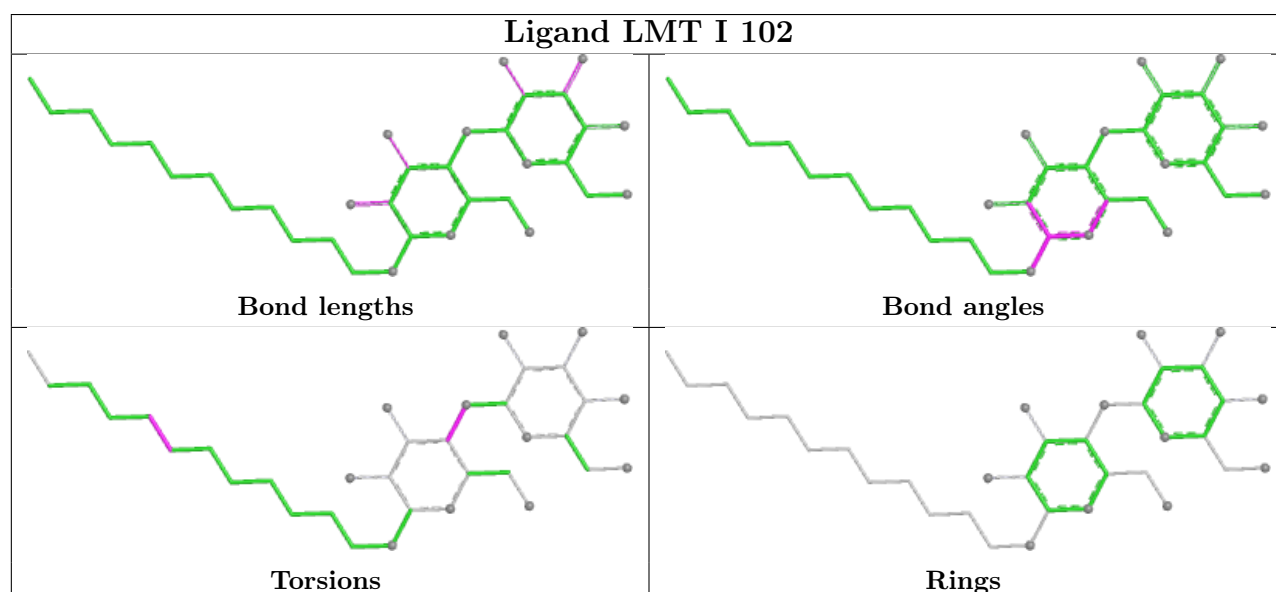
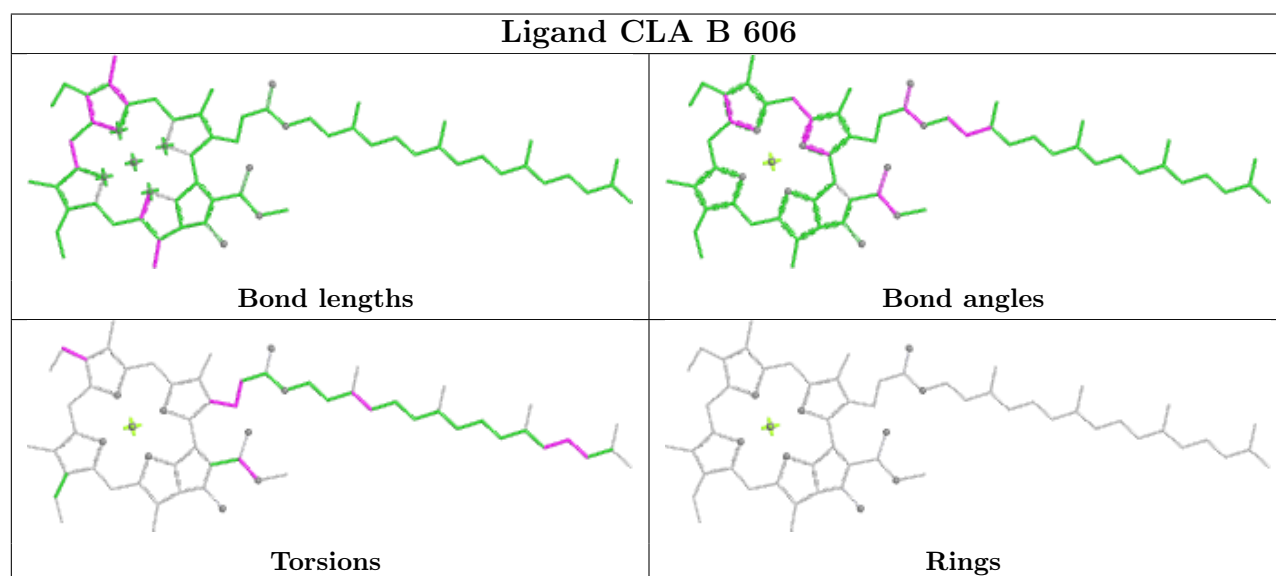
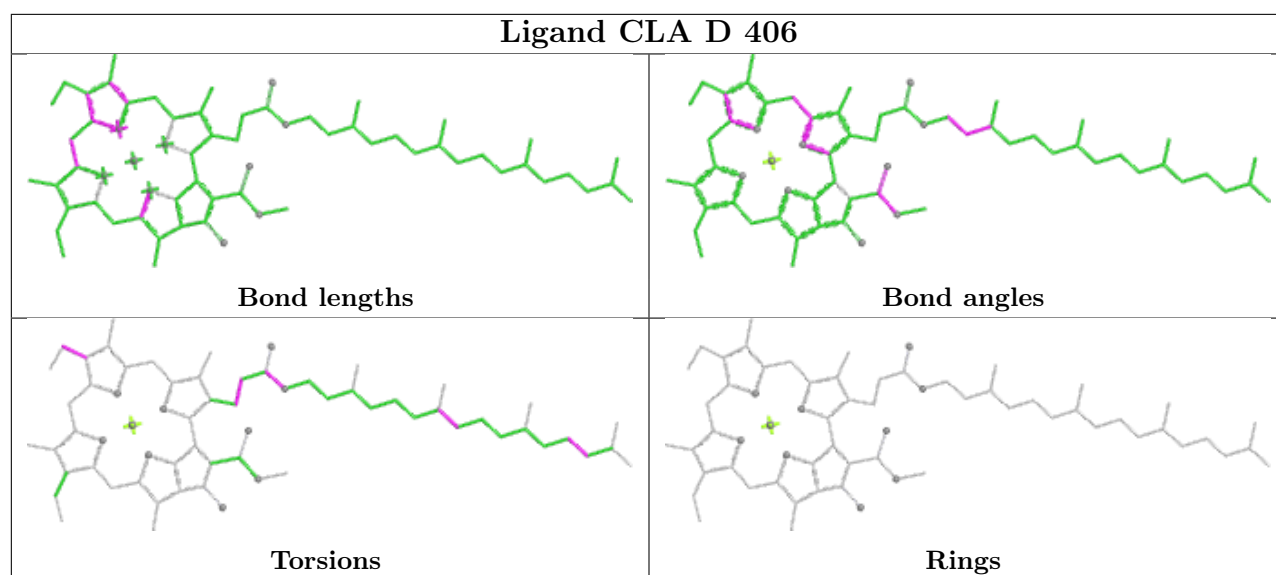
Ligand CLA H 101

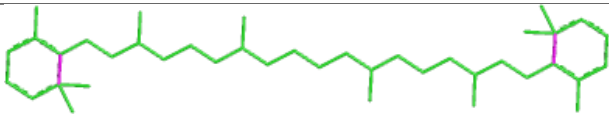
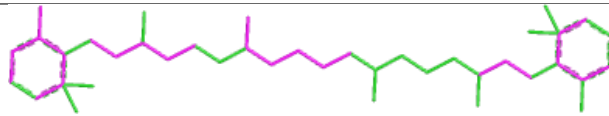
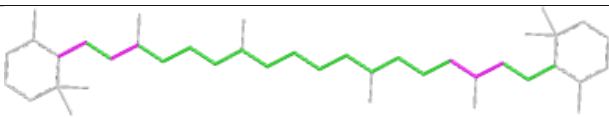
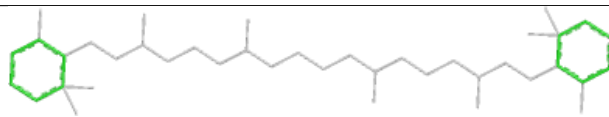


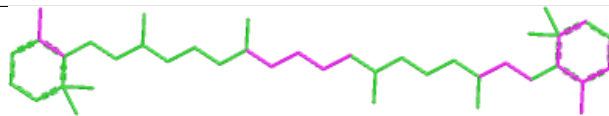
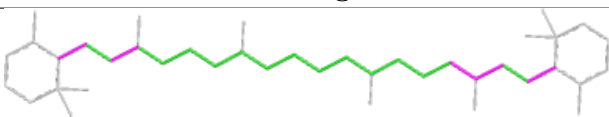
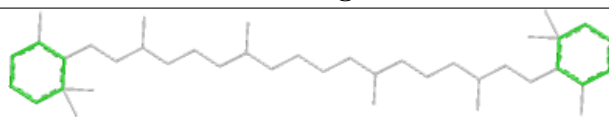
Ligand CLA B 608

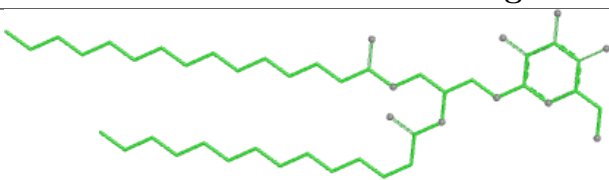
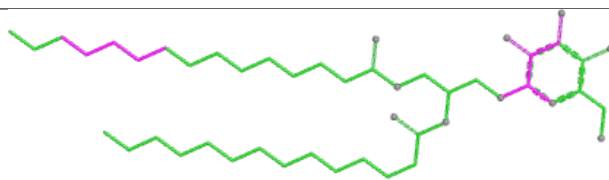
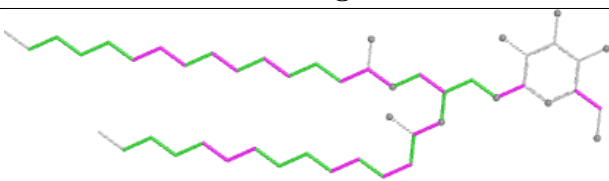
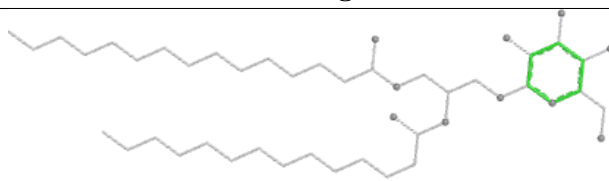


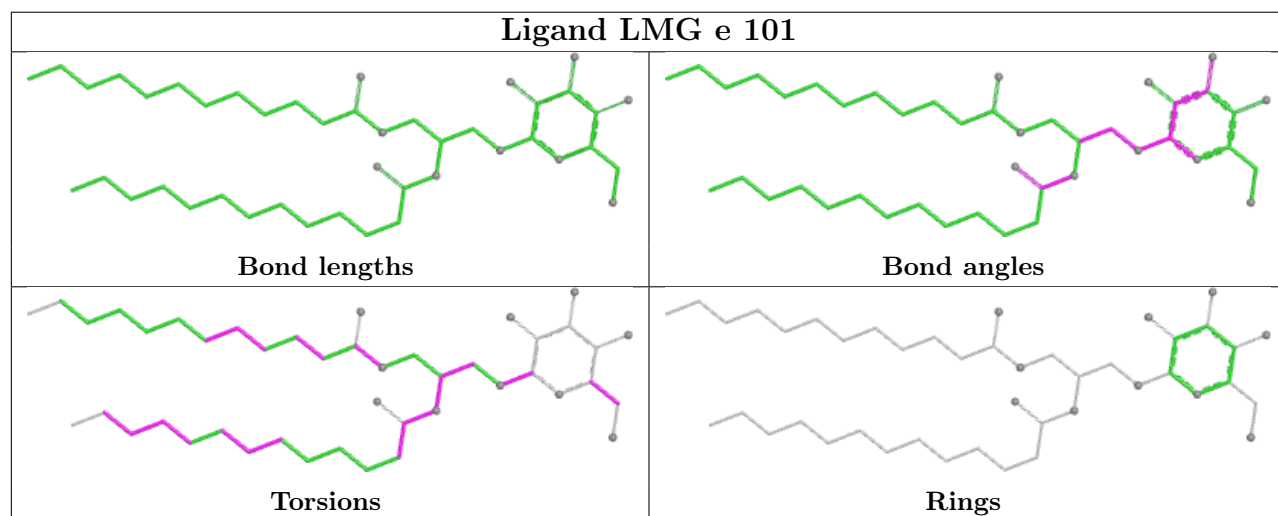
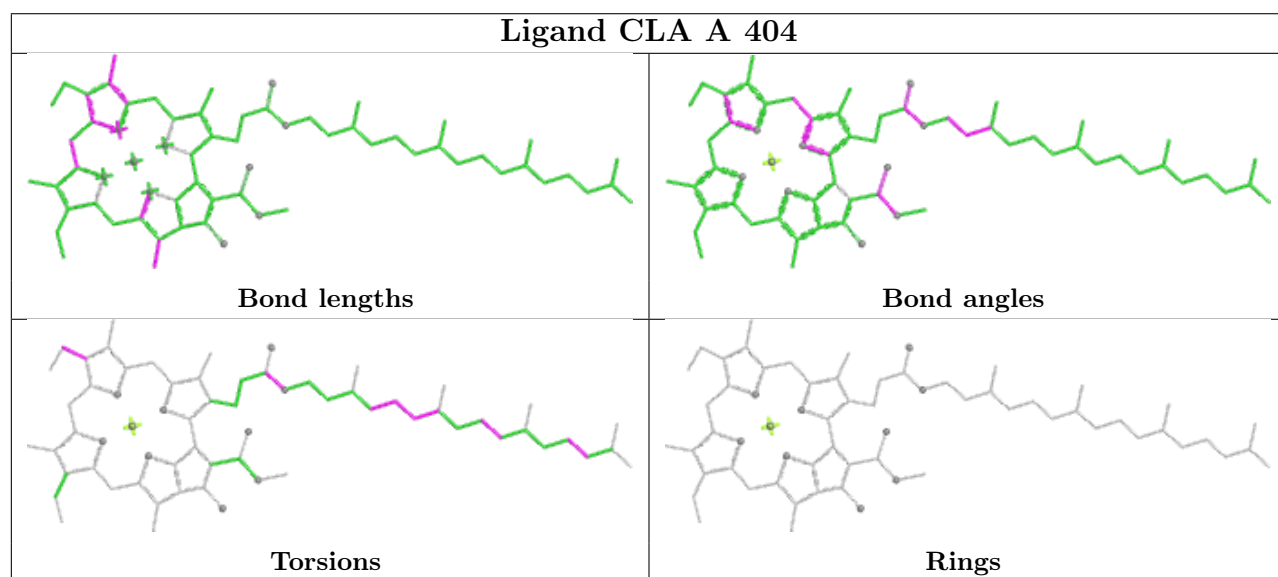
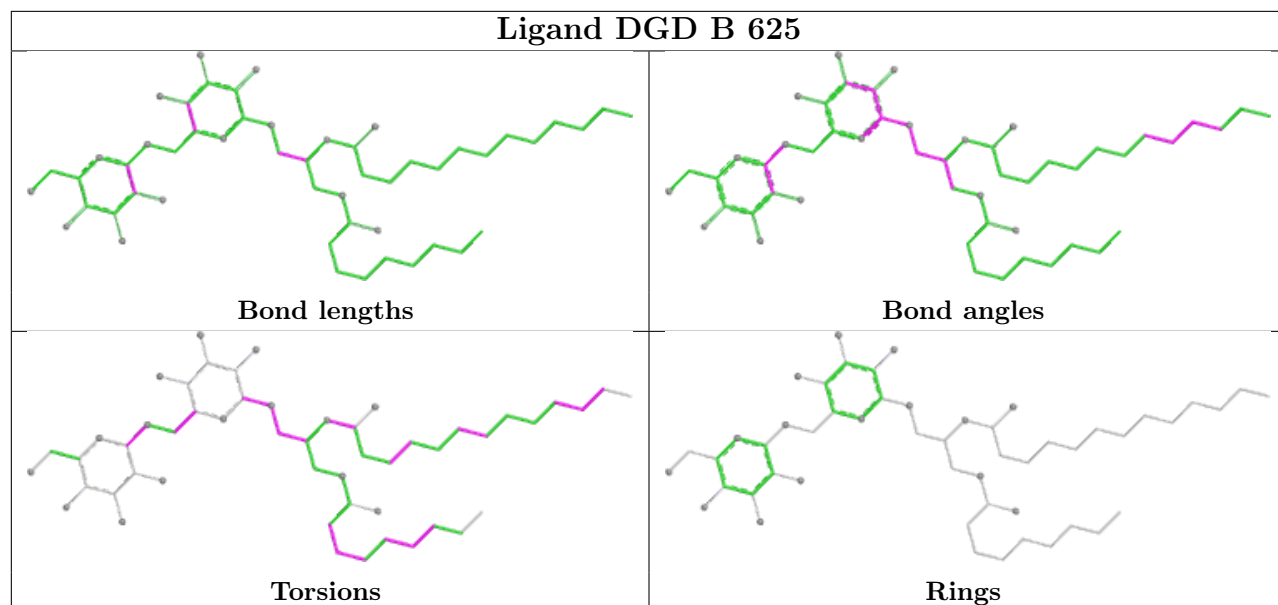
Ligand CLA B 612**Ligand CLA b 613****Ligand CLA B 614**

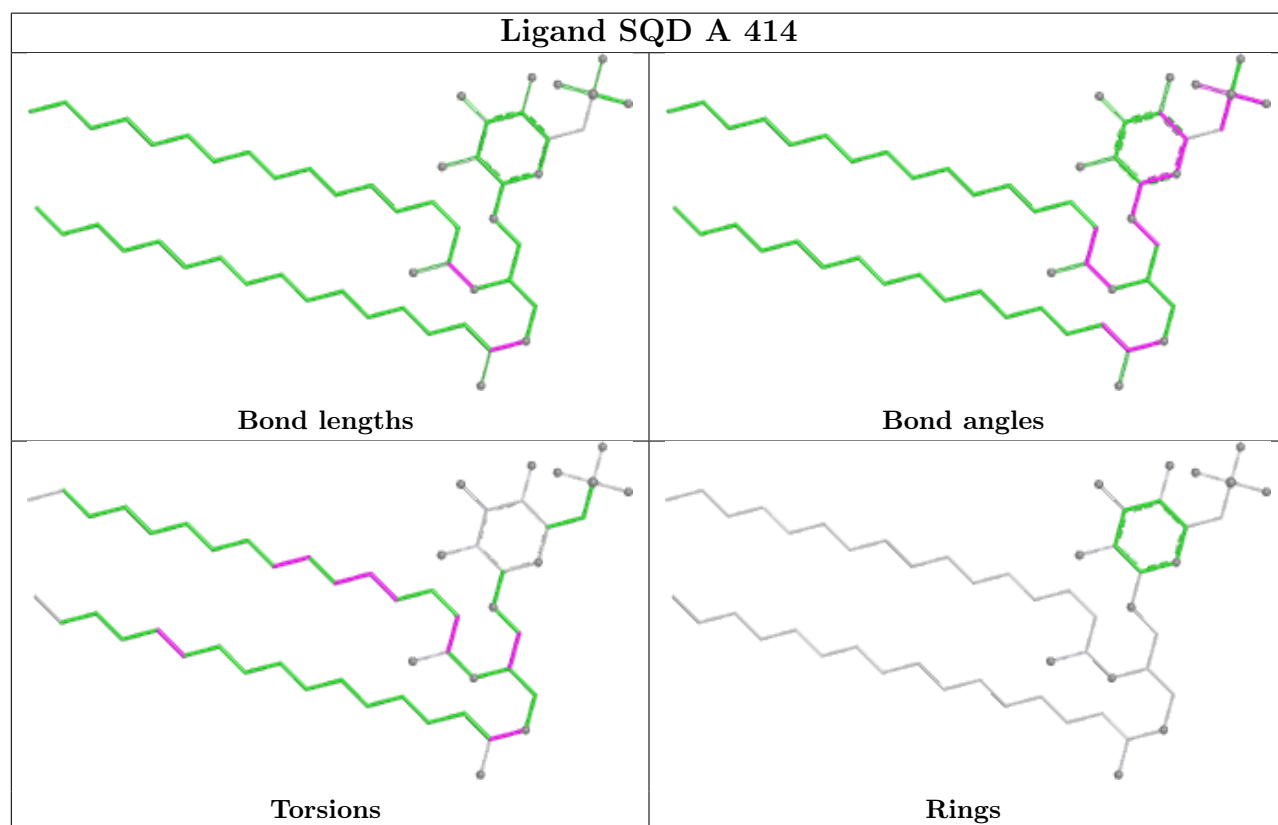
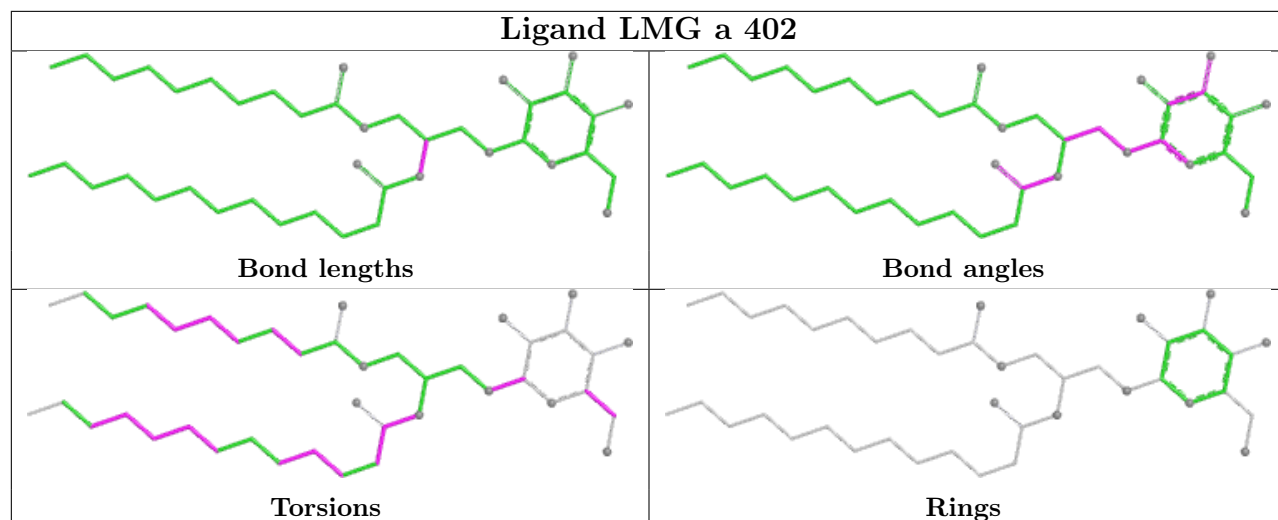


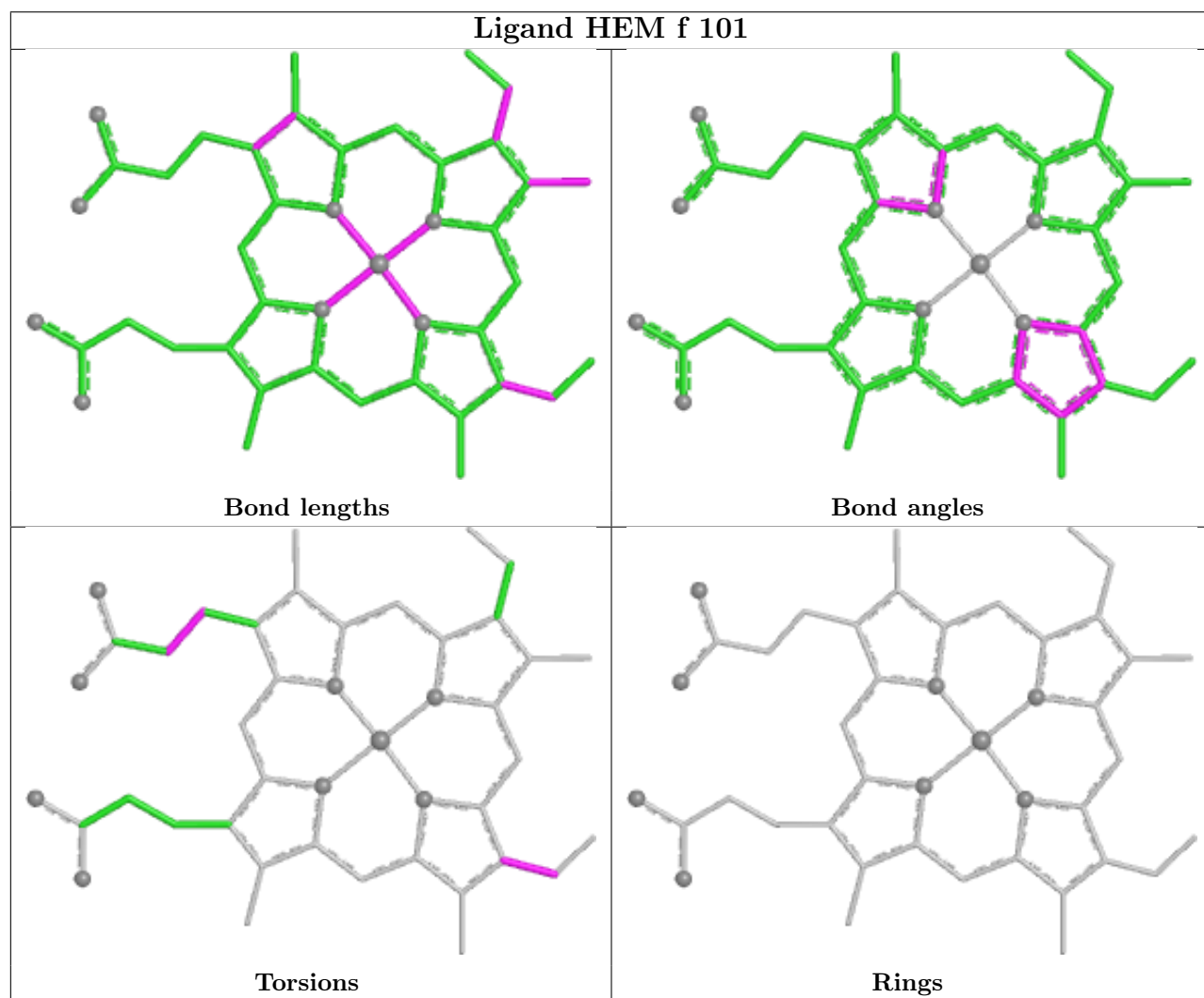
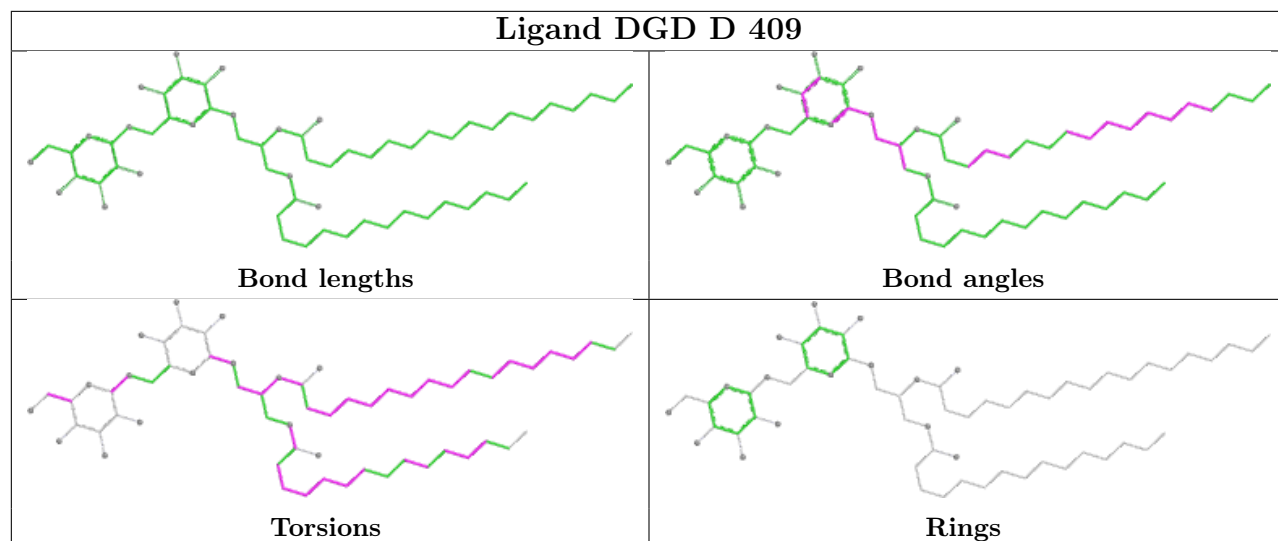
Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

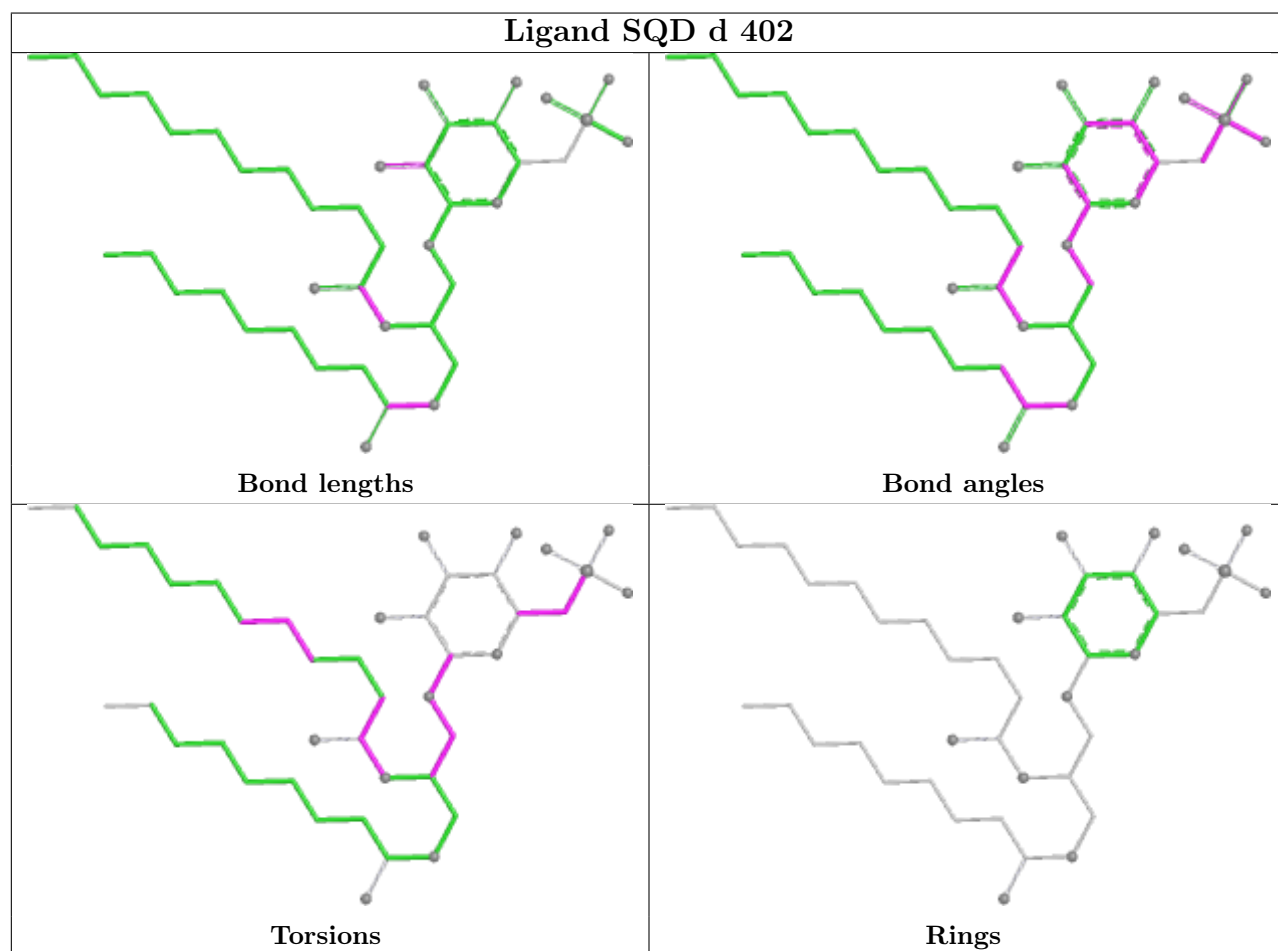
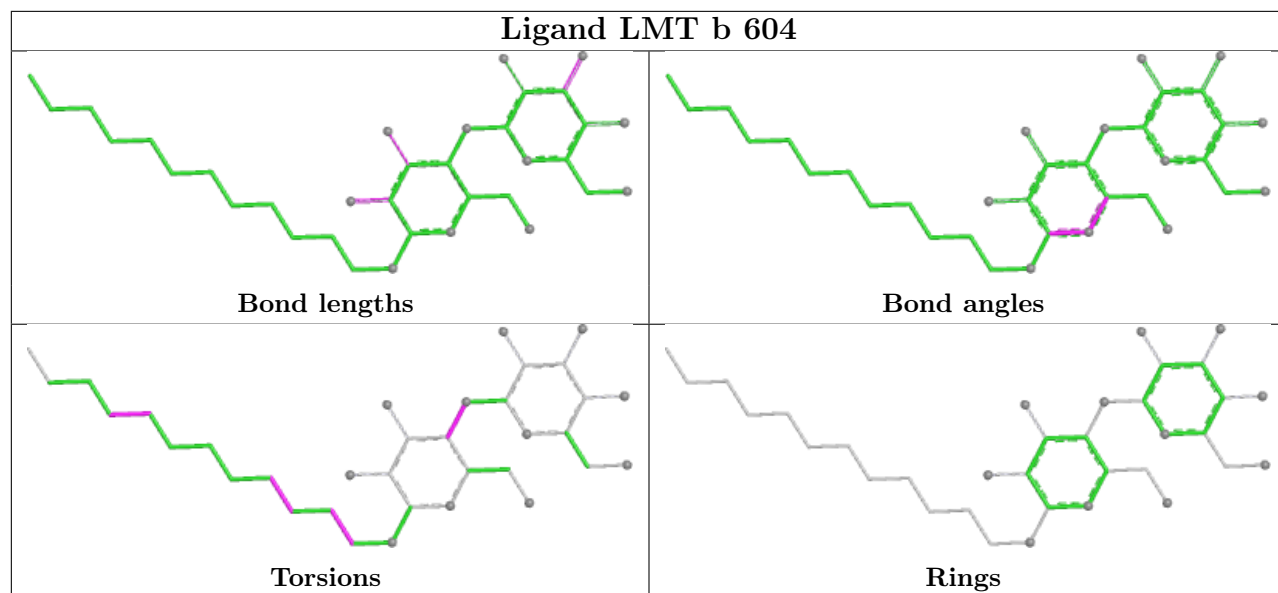
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

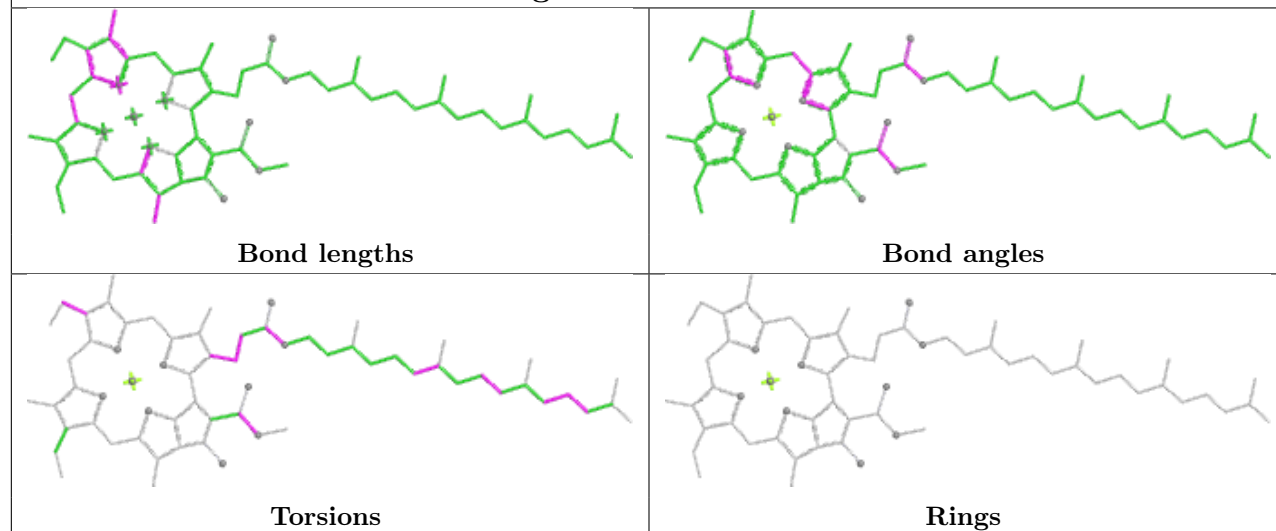




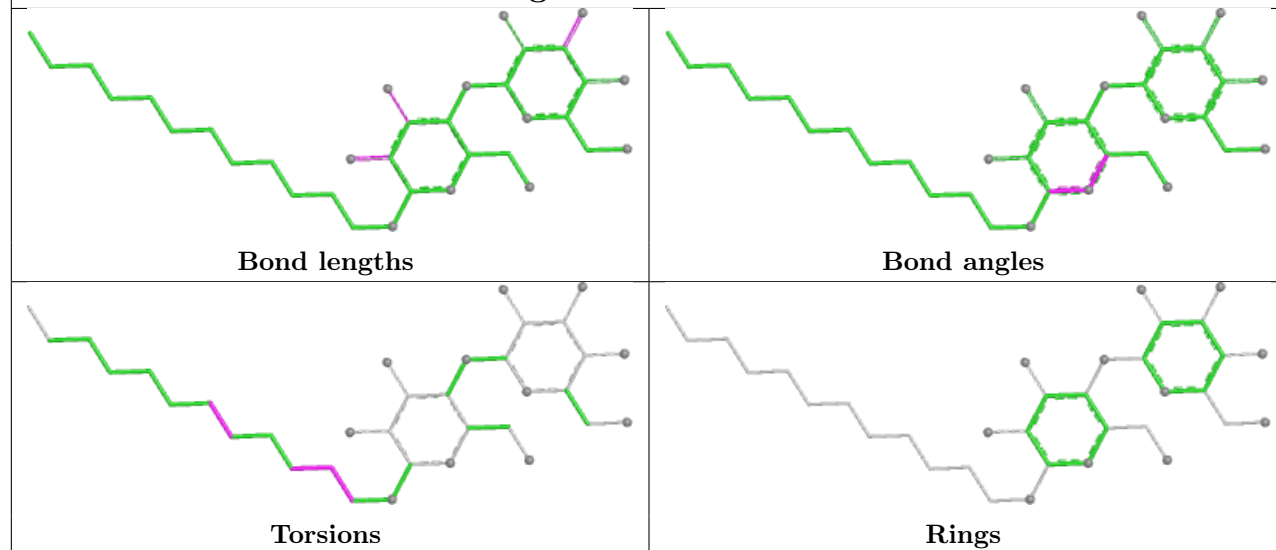




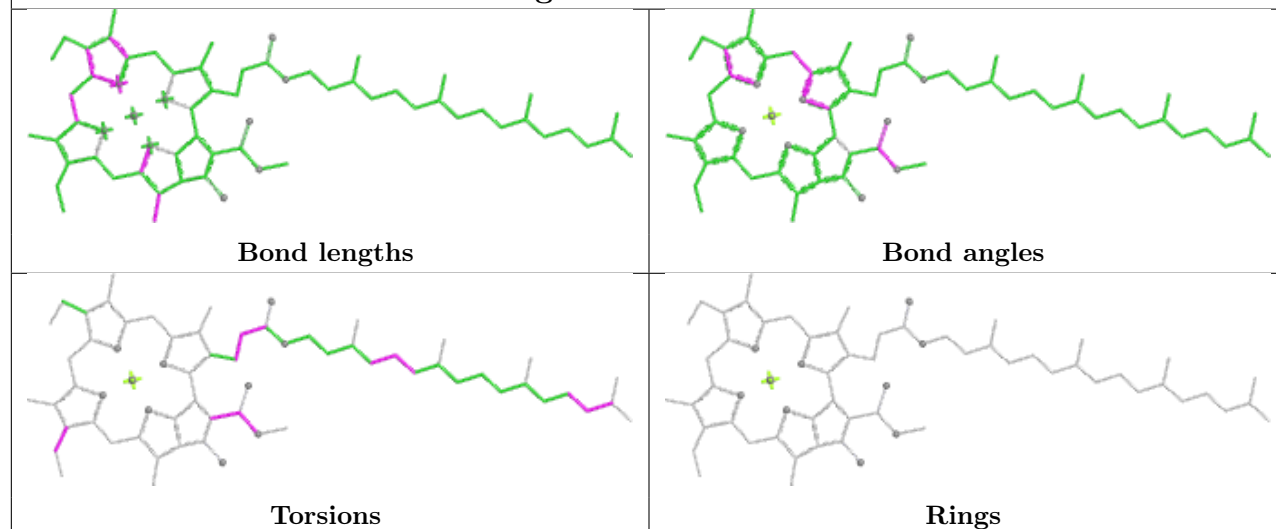
Ligand CLA C 520

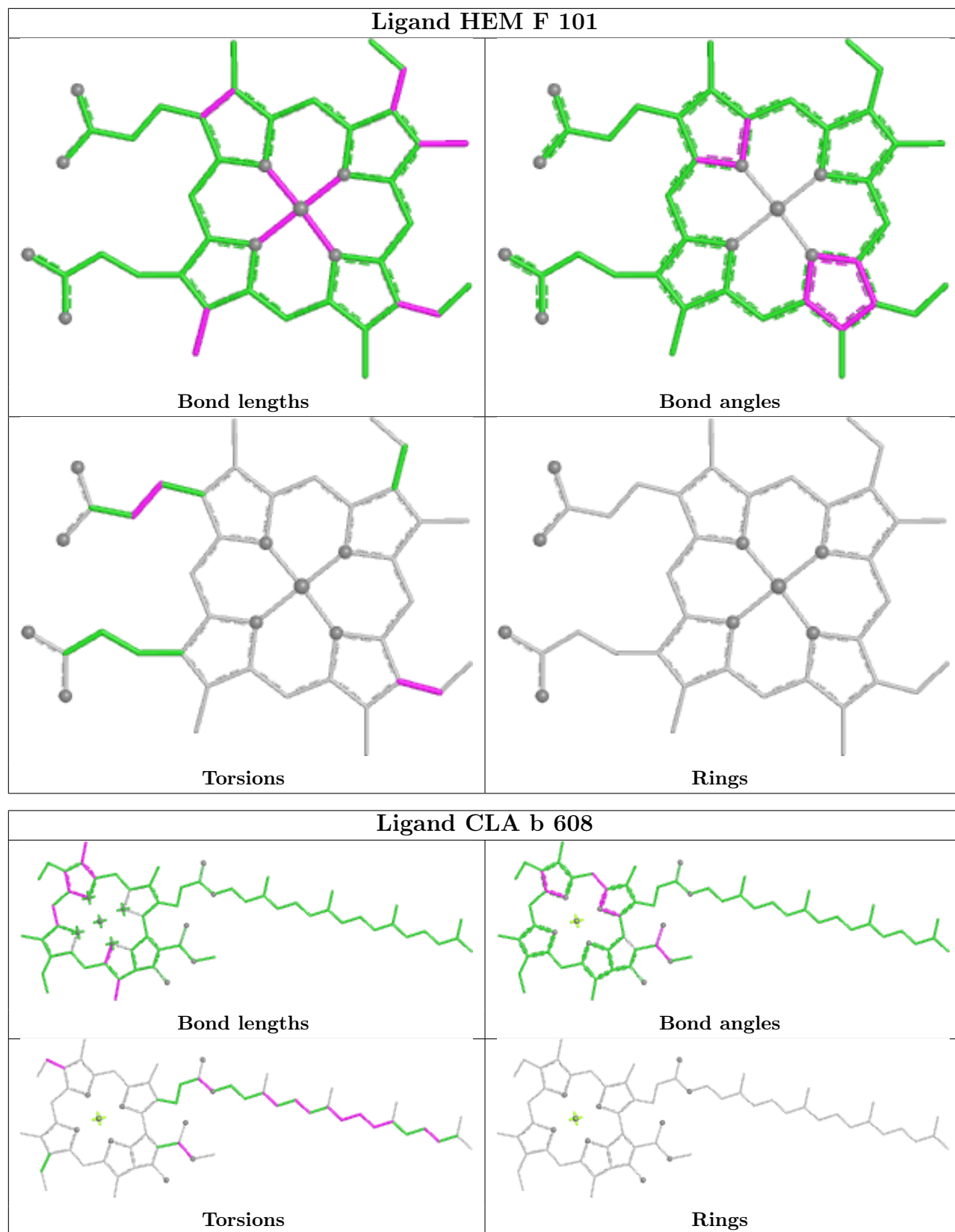


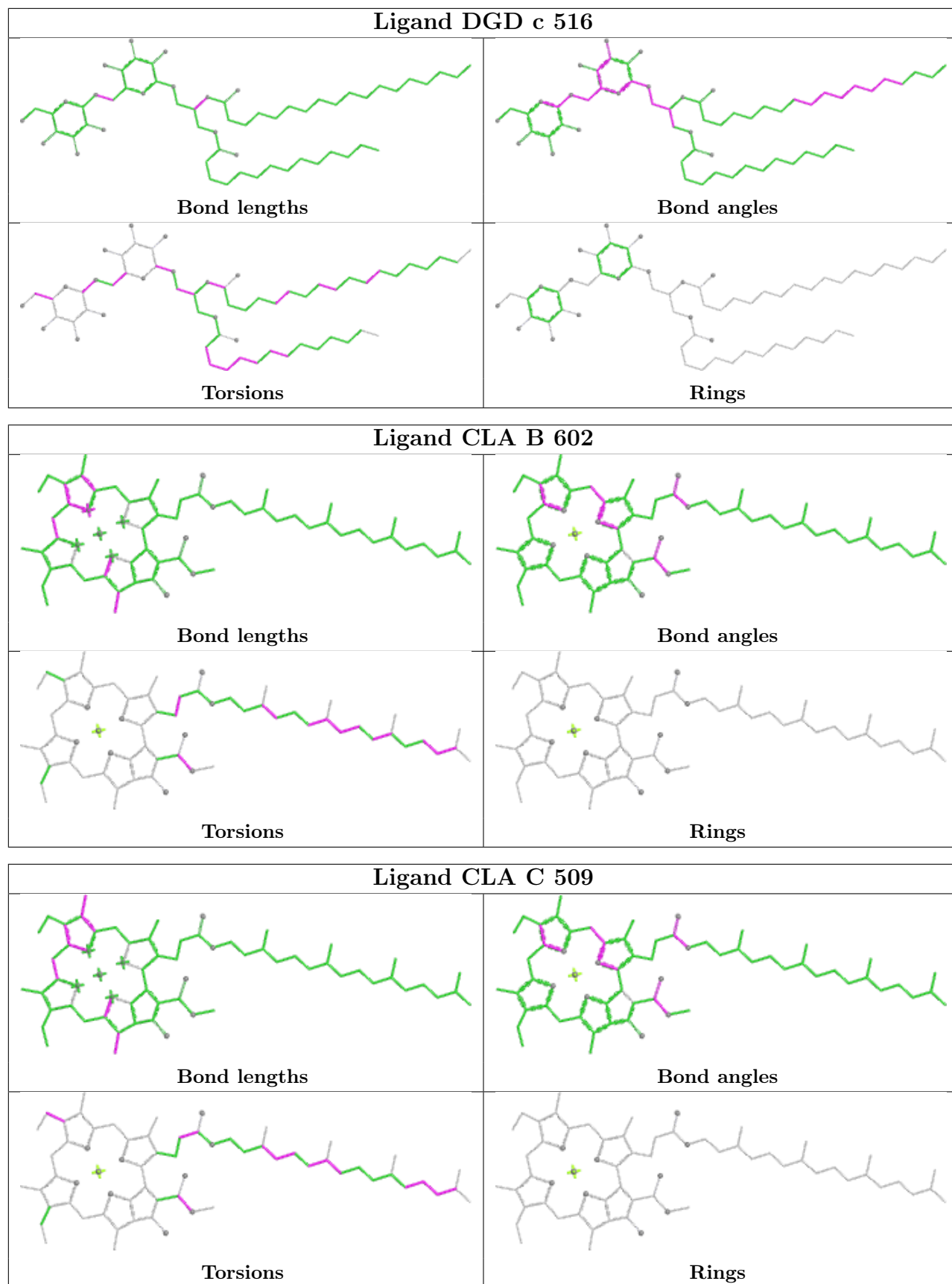
Ligand LMT B 622



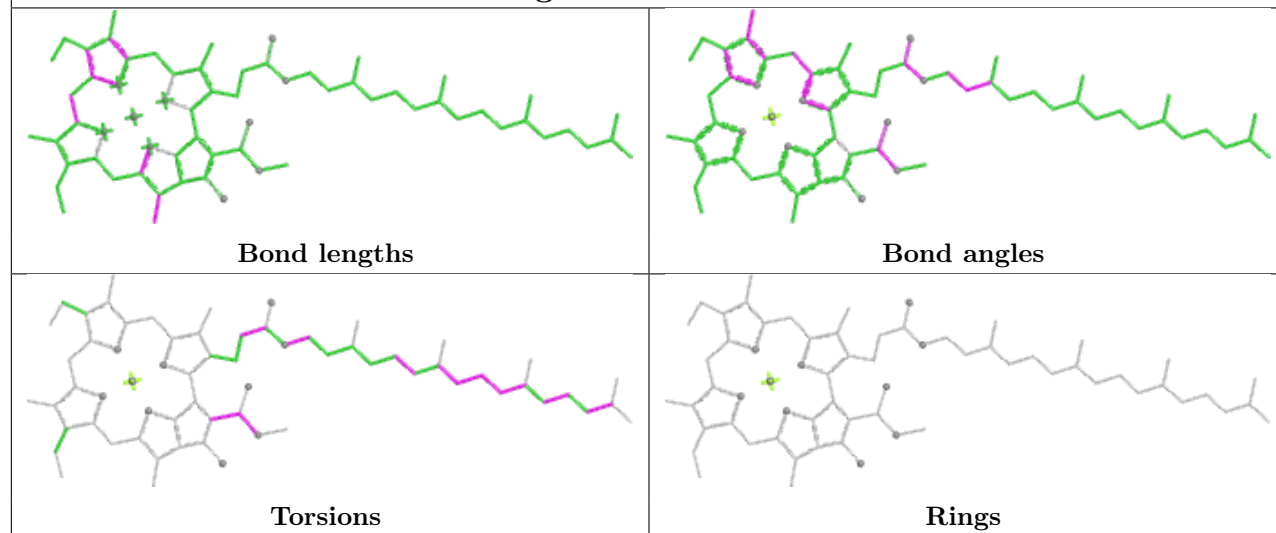
Ligand CLA b 617



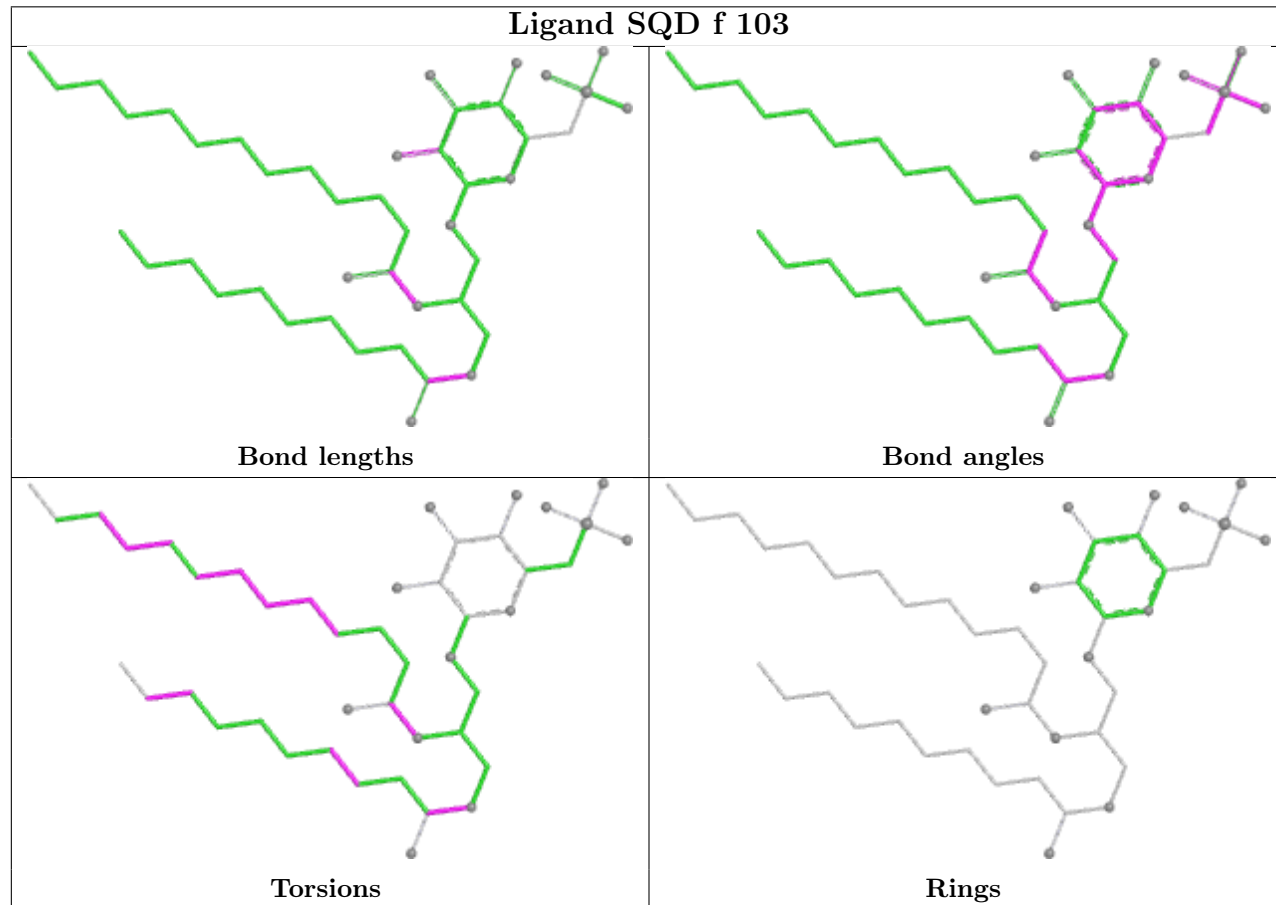


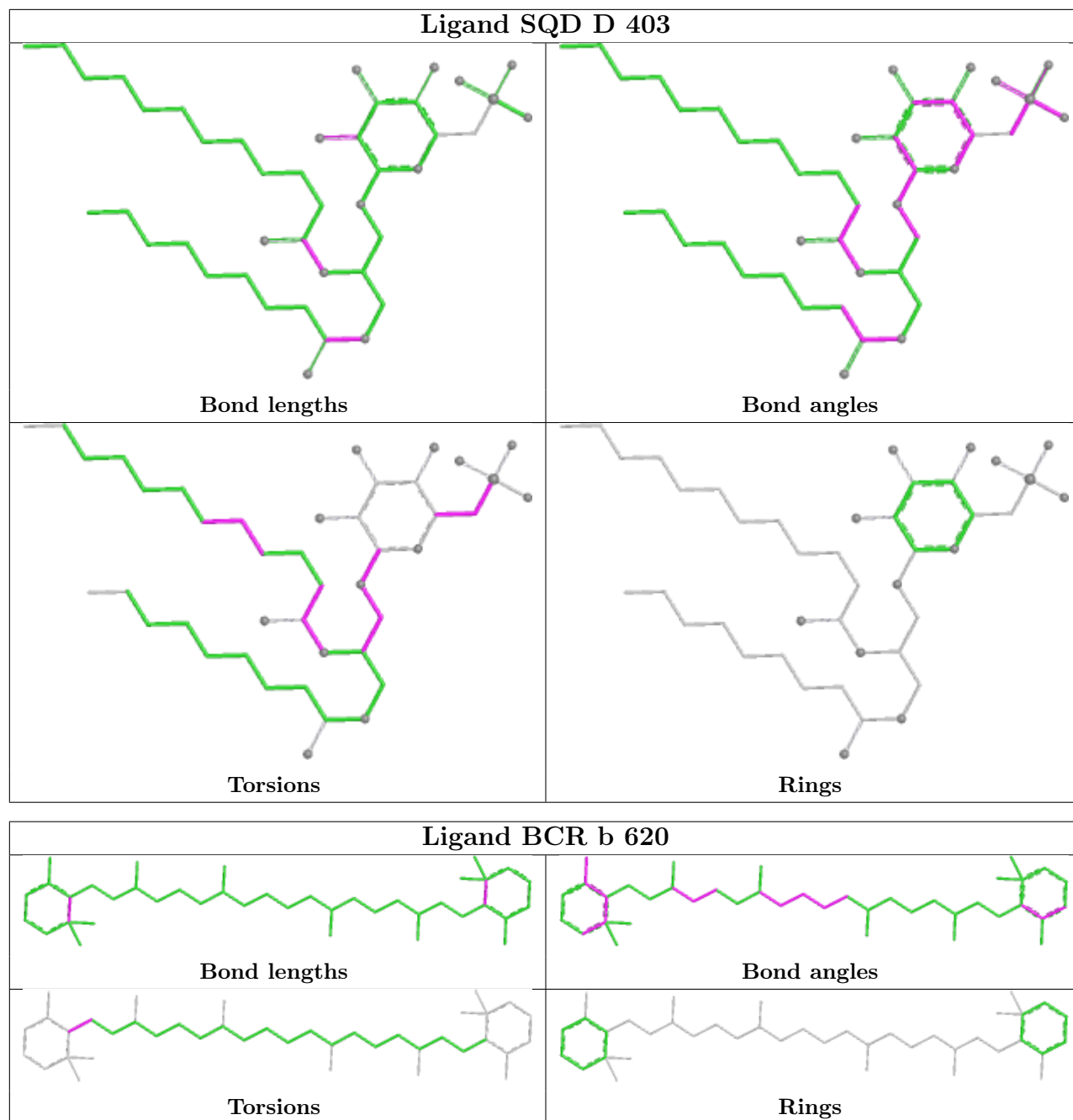


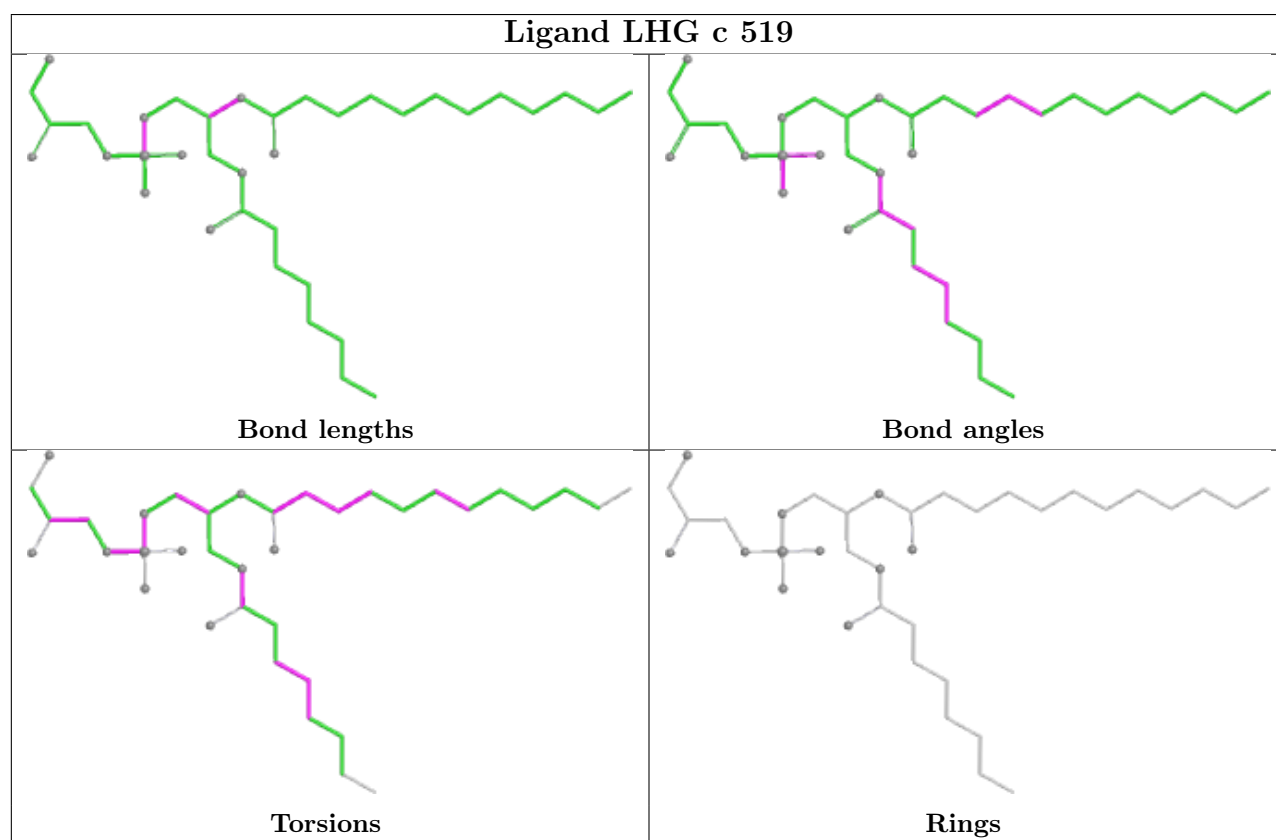
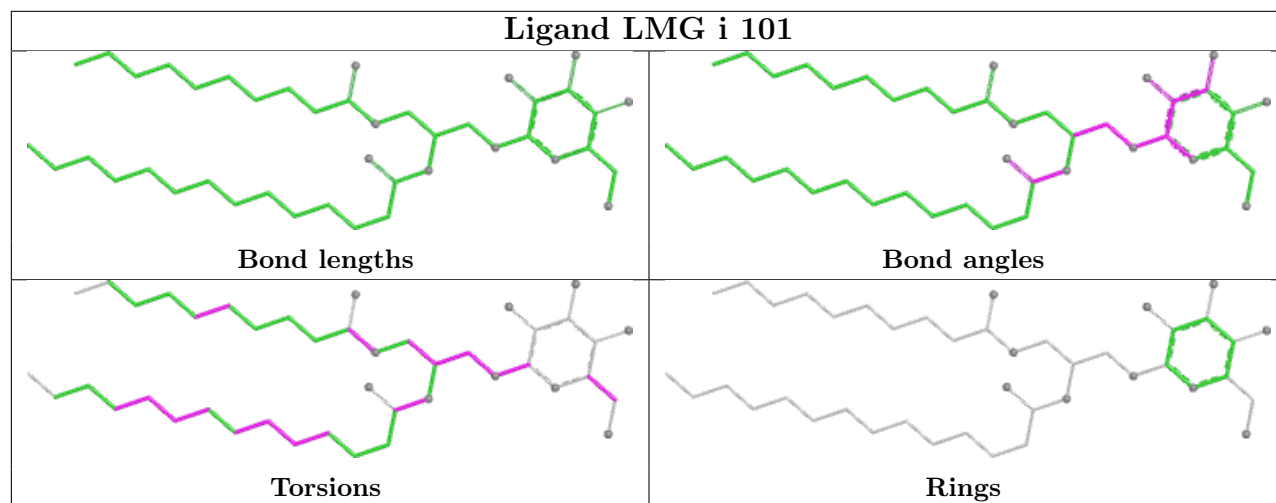
Ligand CLA b 616

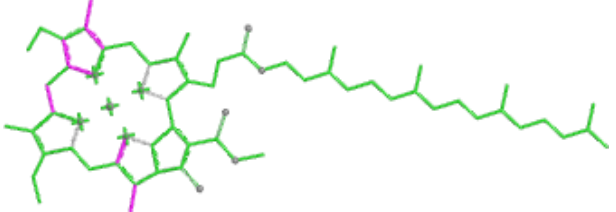
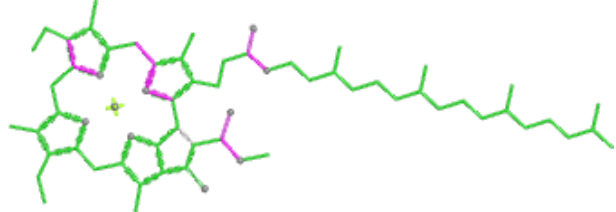
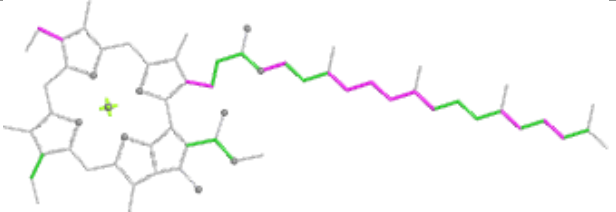
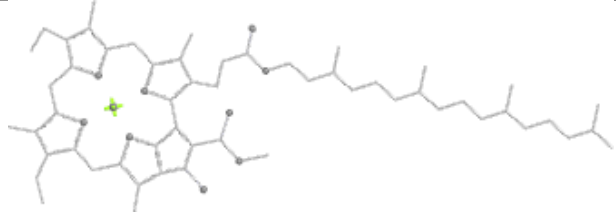
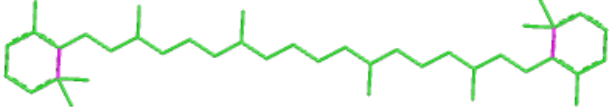
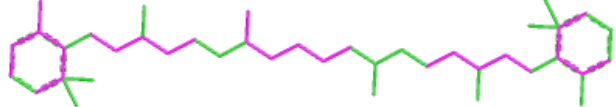
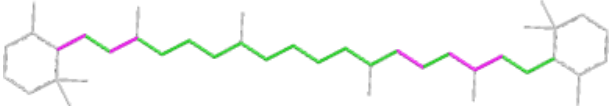
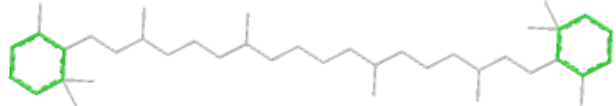
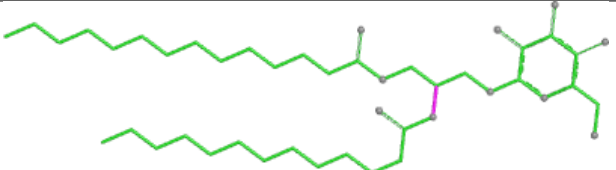
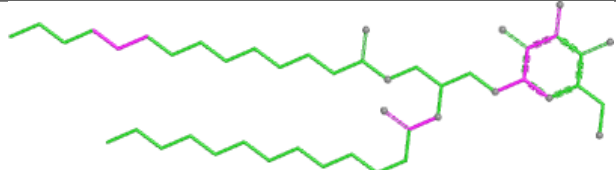
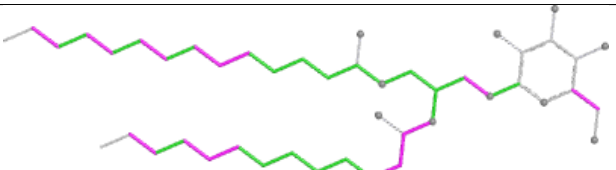
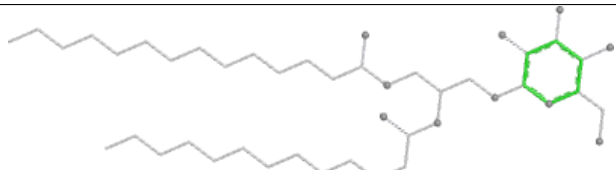


Ligand SQD f 103

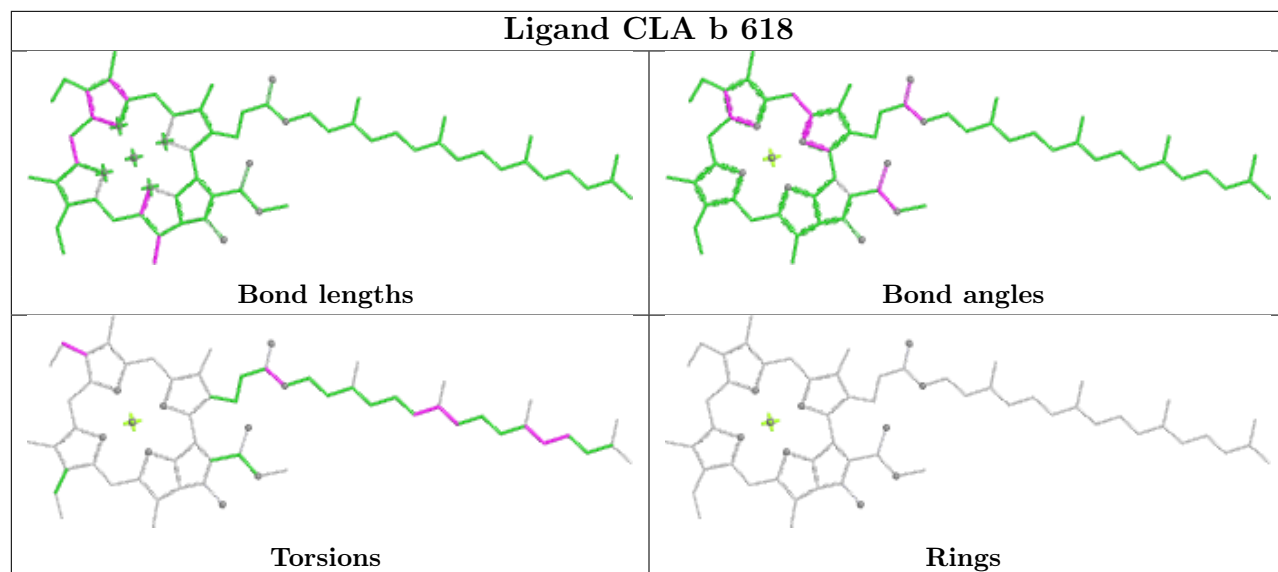




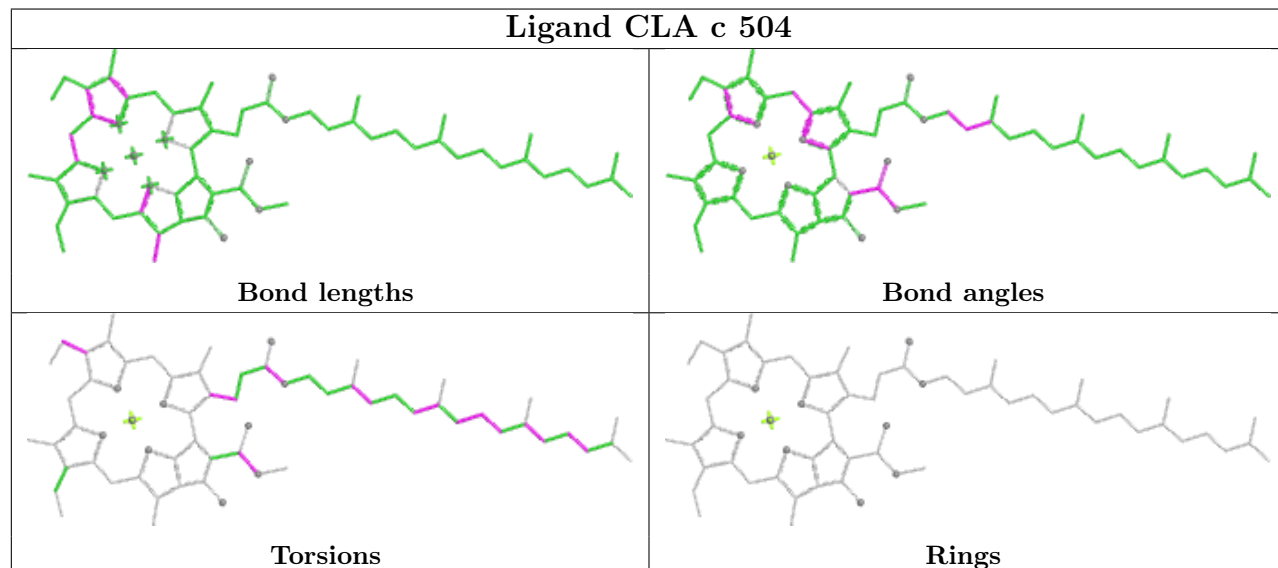


Ligand CLA A 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR j 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG D 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

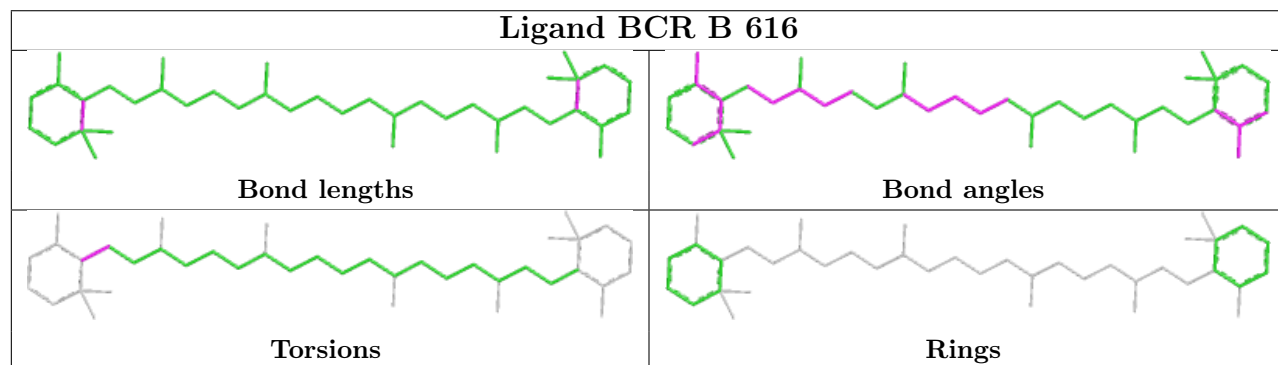
Ligand CLA b 618



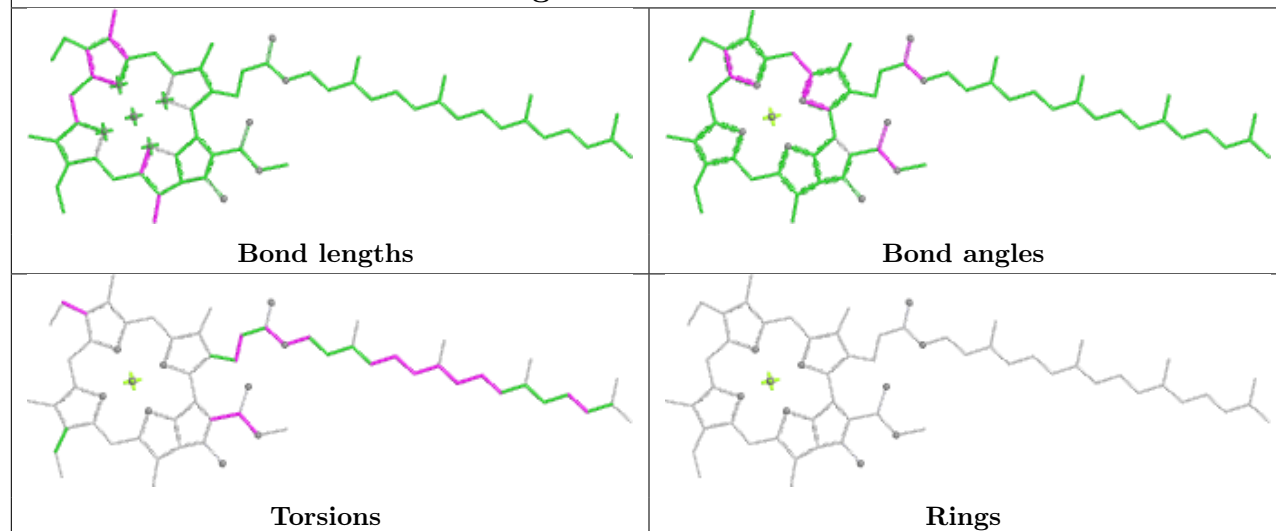
Ligand CLA c 504



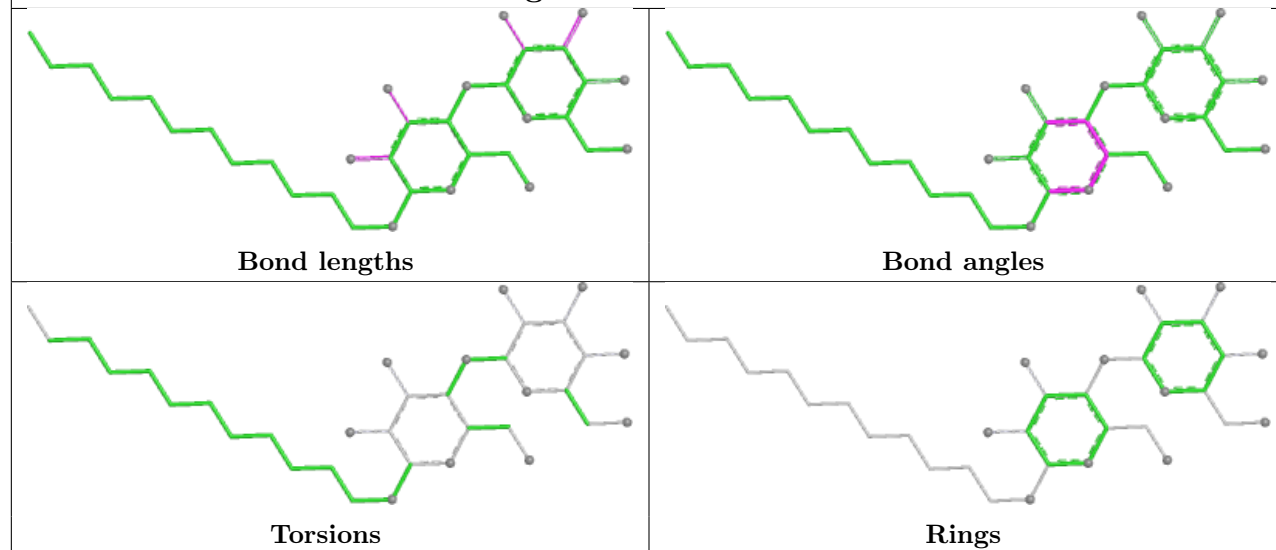
Ligand BCR B 616



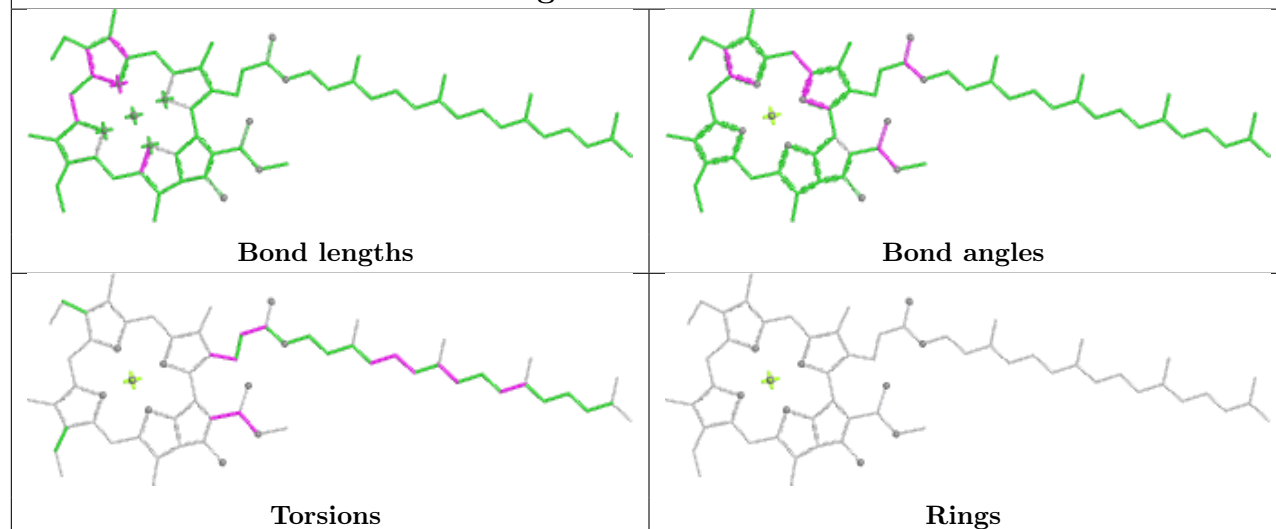
Ligand CLA C 508



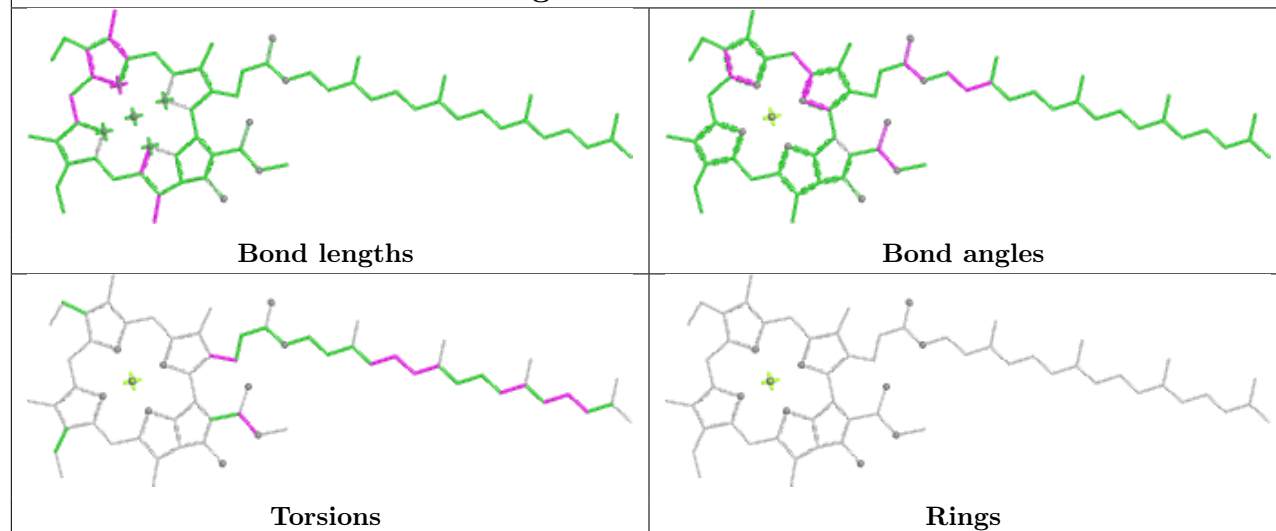
Ligand LMT M 103



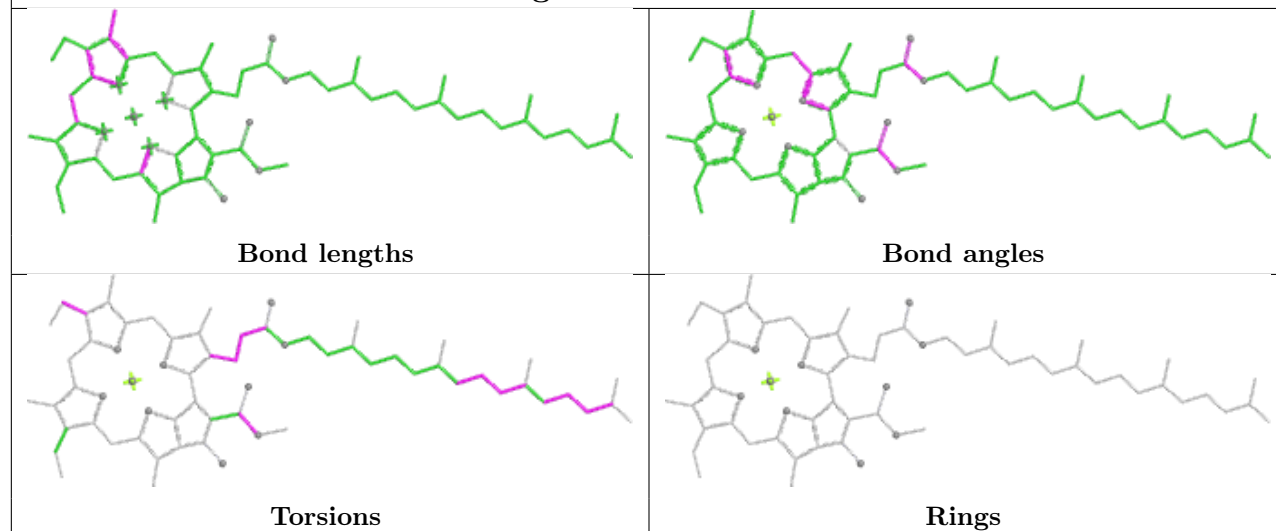
Ligand CLA c 506



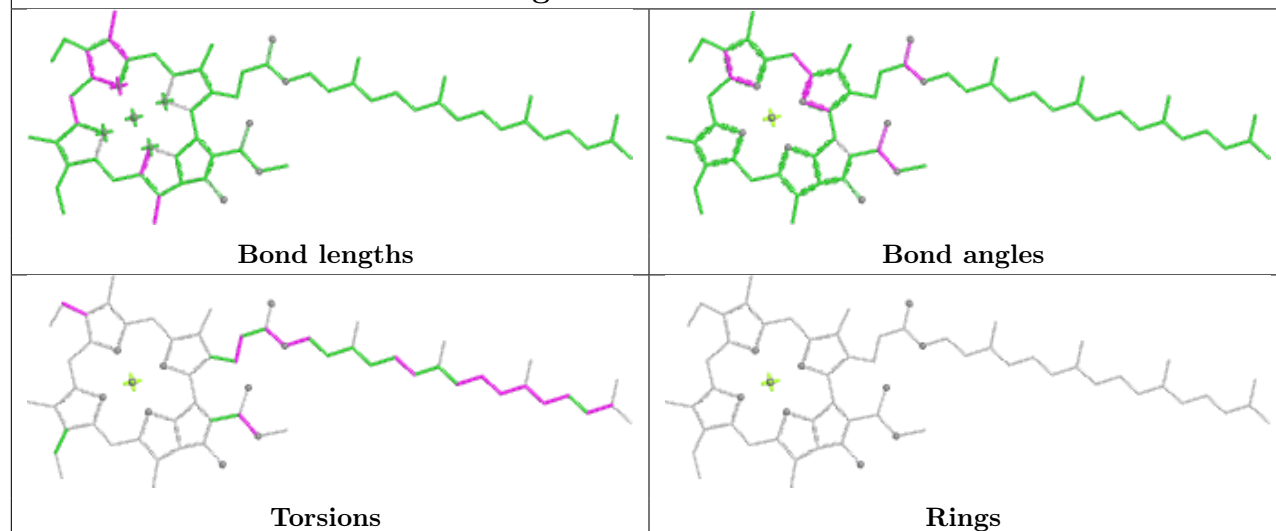
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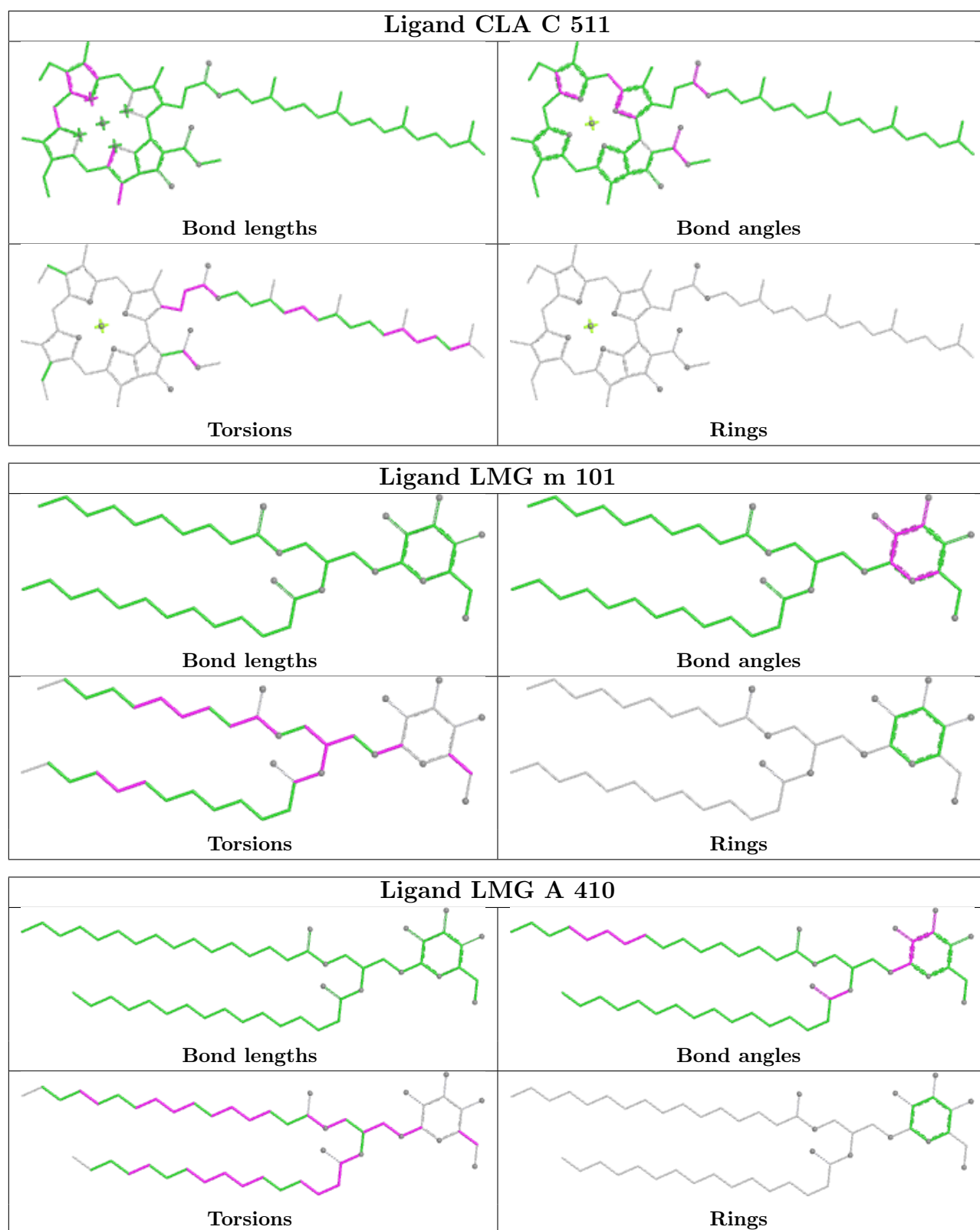


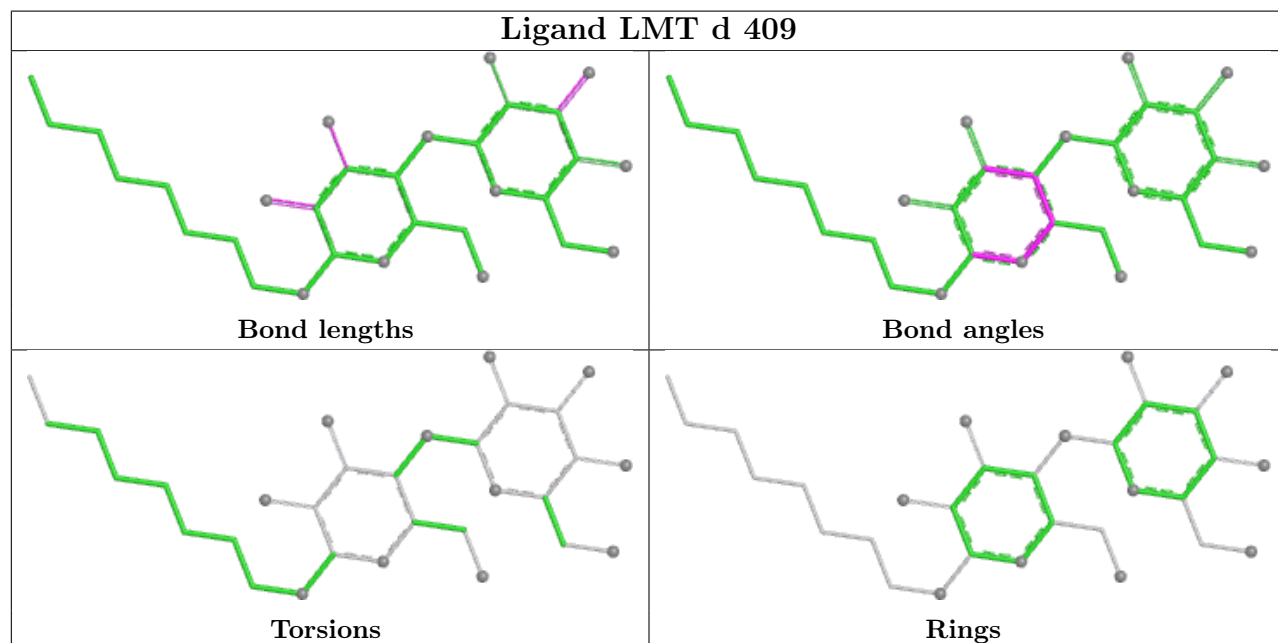
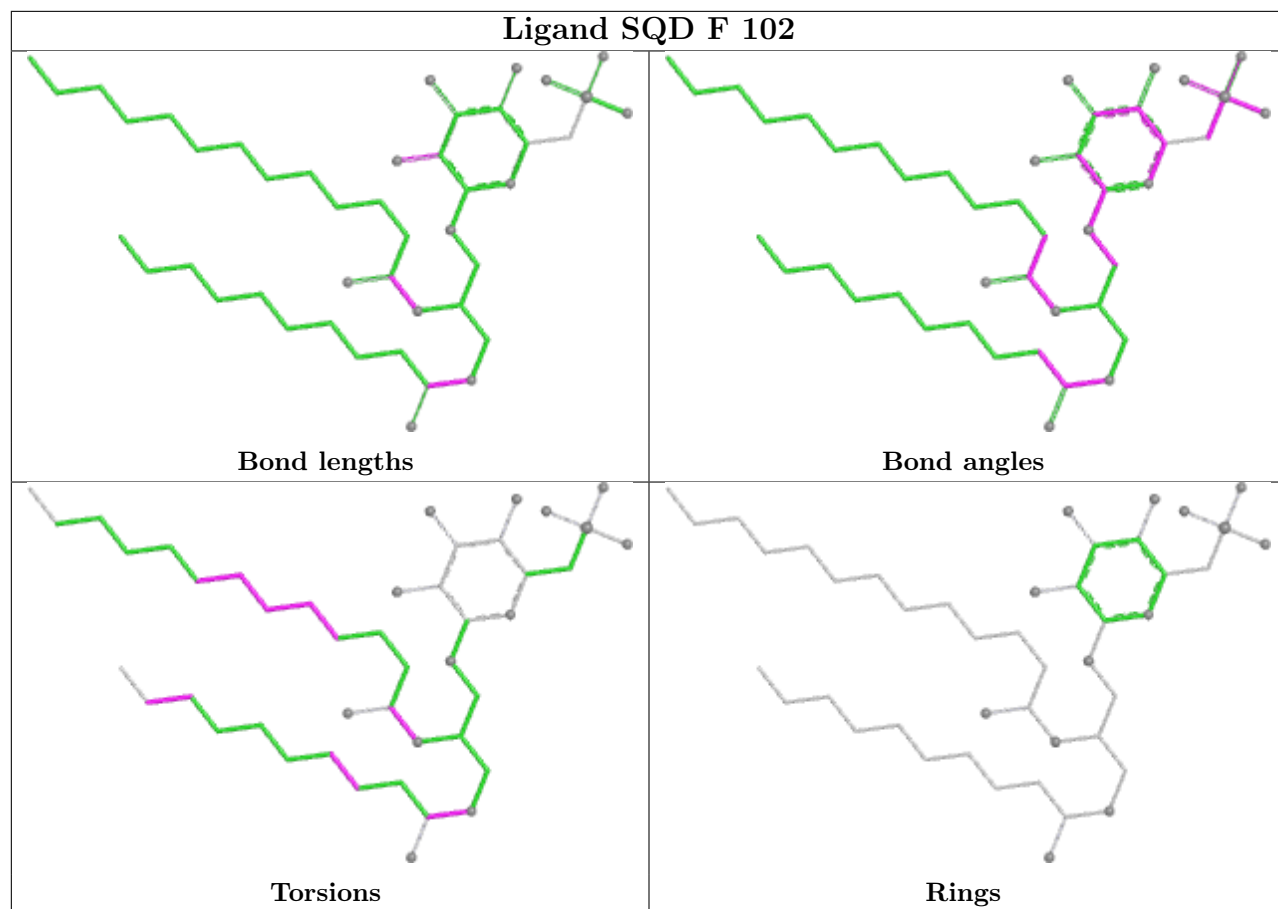
Ligand CLA C 501

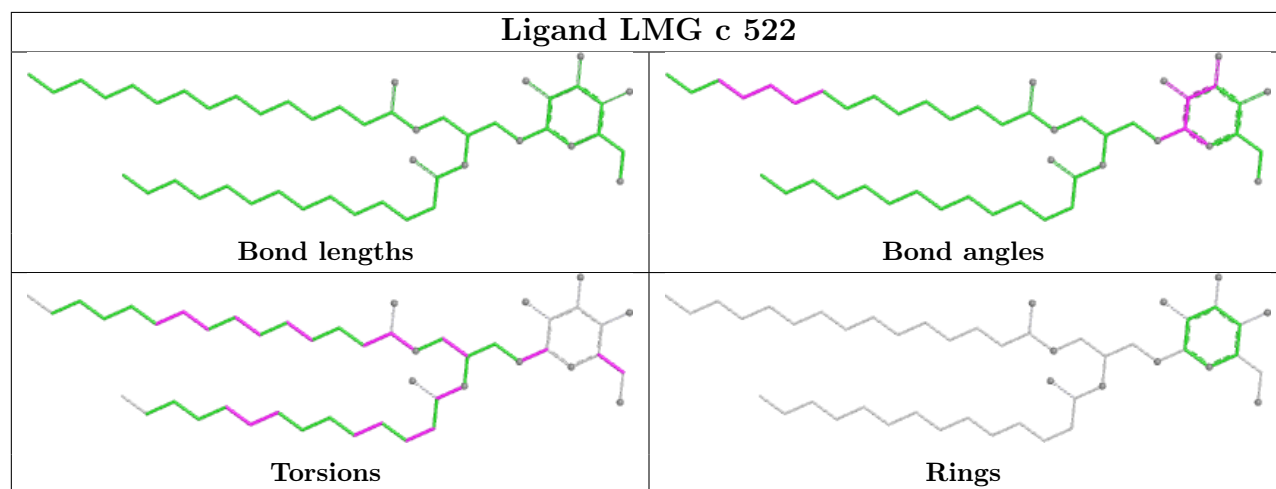
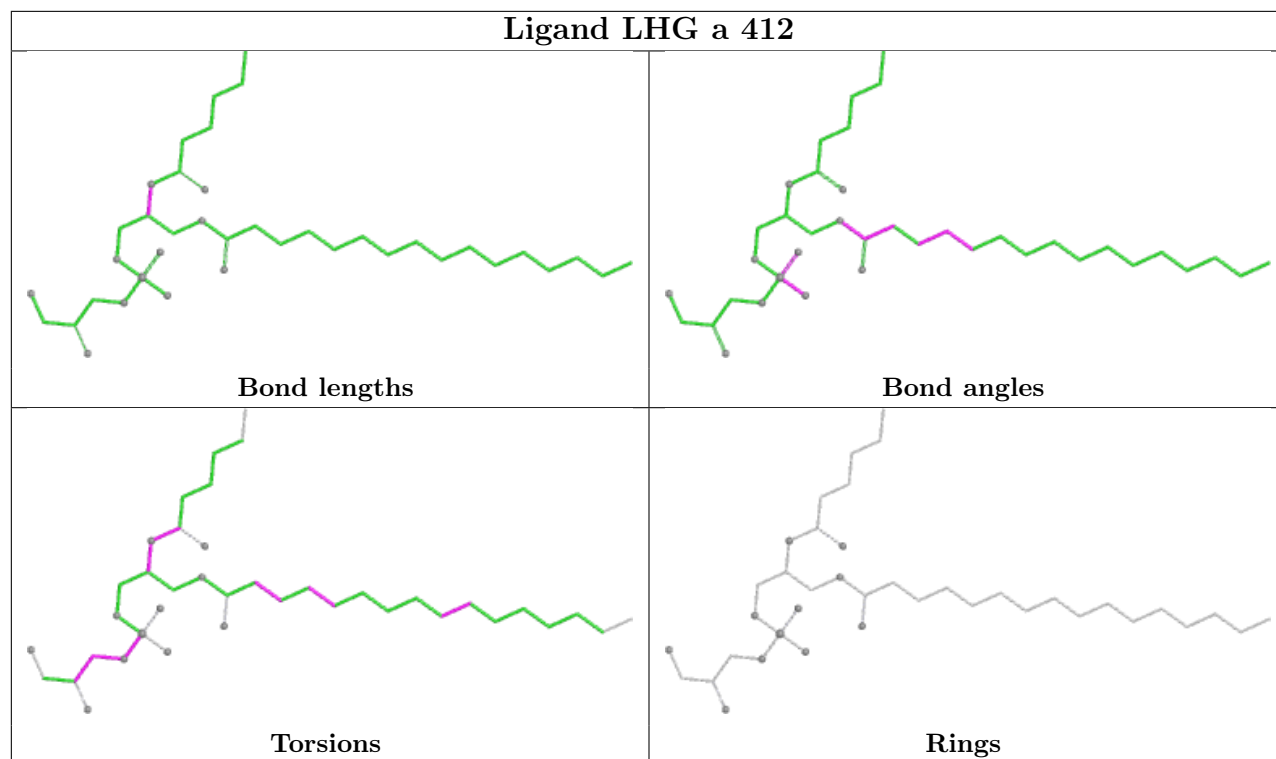


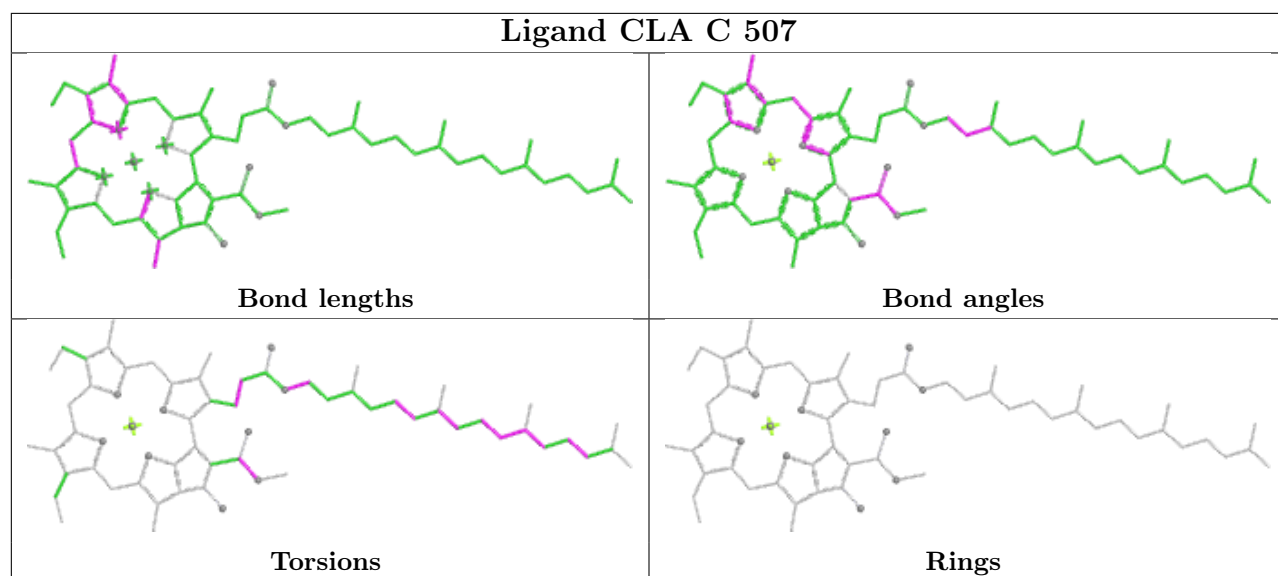
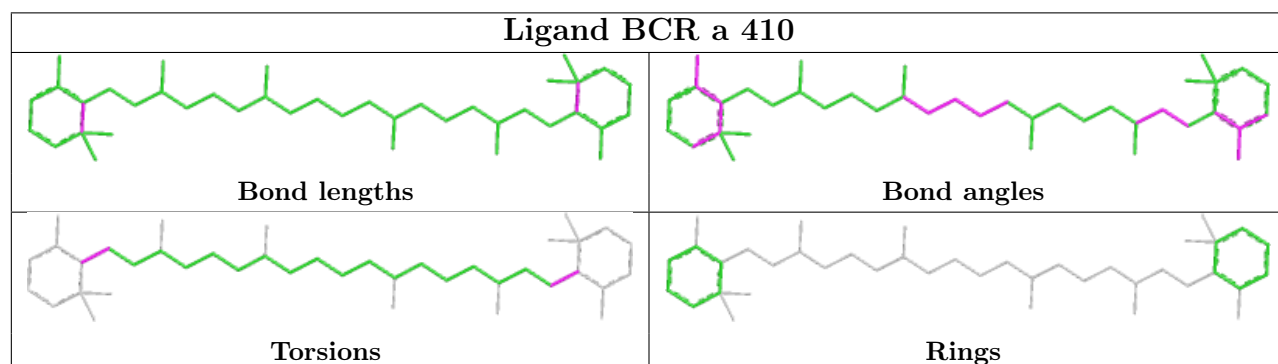
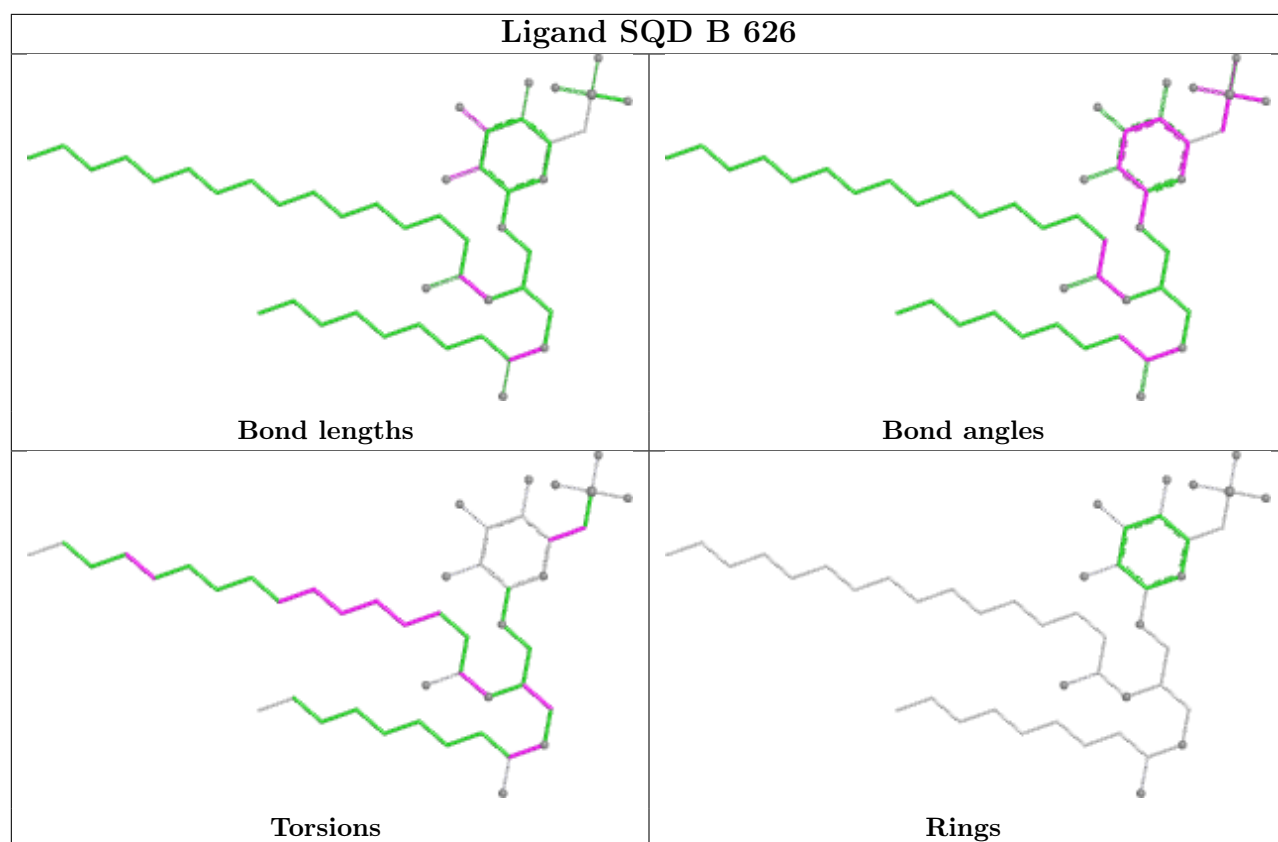
Ligand CLA B 609

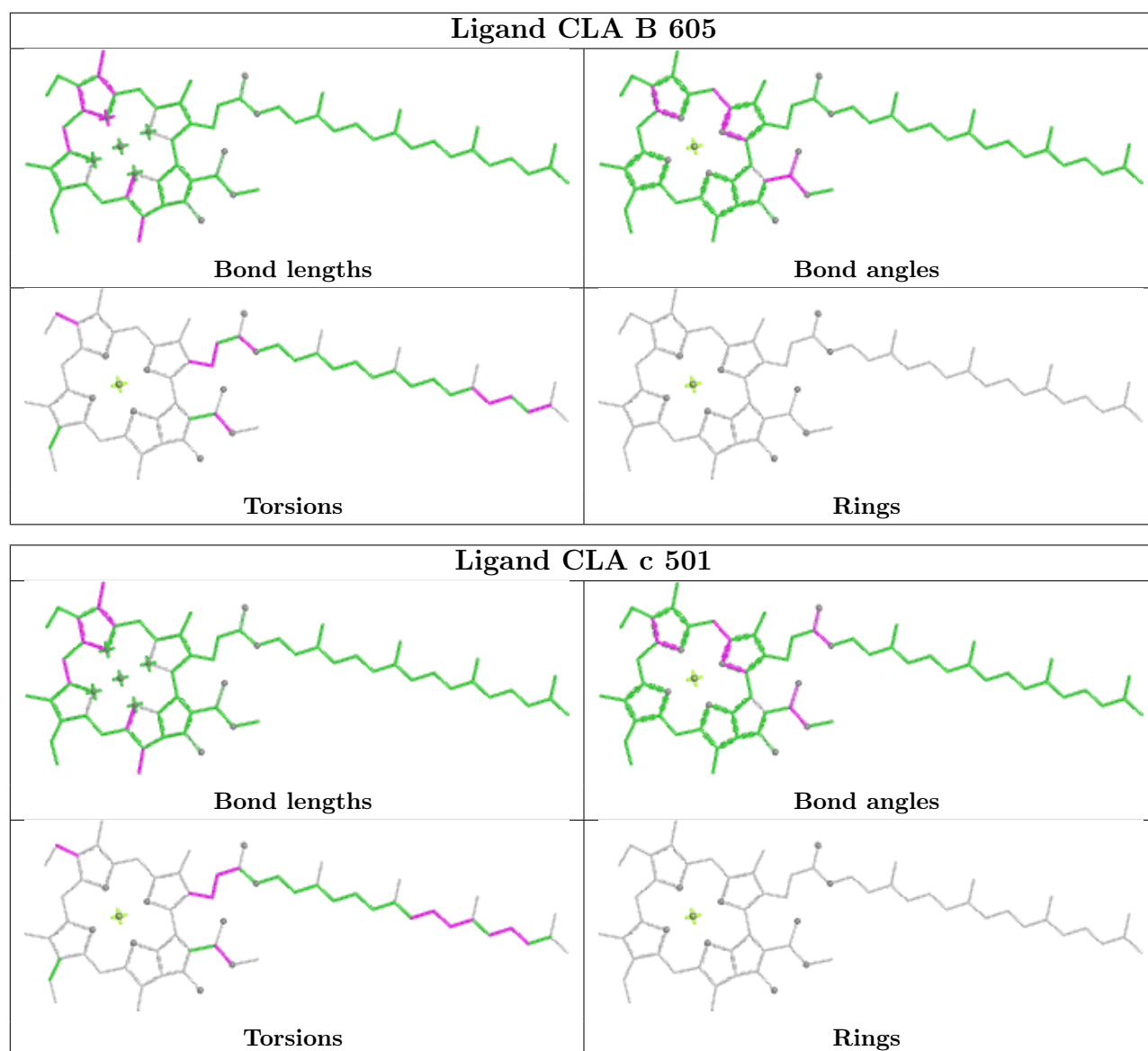












5.7 Other polymers [i](#)

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%)	0.12	8 (2%) 59 47	172, 174, 175, 176	0
1	a	335/344 (97%)	0.03	6 (1%) 67 53	172, 174, 175, 176	0
2	B	490/510 (96%)	-0.02	4 (0%) 82 69	172, 174, 175, 176	0
2	b	490/510 (96%)	0.00	9 (1%) 67 53	172, 174, 175, 176	0
3	C	447/461 (96%)	0.04	6 (1%) 75 60	172, 174, 175, 176	0
3	c	447/461 (96%)	-0.10	2 (0%) 88 77	173, 174, 175, 176	0
4	D	340/352 (96%)	0.08	5 (1%) 72 57	171, 174, 175, 176	0
4	d	340/352 (96%)	-0.01	10 (2%) 53 42	172, 174, 175, 175	0
5	E	82/84 (97%)	-0.03	2 (2%) 59 47	172, 174, 175, 175	0
5	e	82/84 (97%)	-0.21	0 100 100	173, 174, 175, 177	0
6	F	35/45 (77%)	0.12	2 (5%) 29 29	173, 174, 175, 175	0
6	f	35/45 (77%)	-0.21	0 100 100	174, 174, 175, 176	0
7	H	65/66 (98%)	0.13	0 100 100	173, 174, 175, 176	0
7	h	65/66 (98%)	0.15	1 (1%) 72 57	173, 174, 175, 176	0
8	I	35/38 (92%)	-0.17	0 100 100	173, 174, 175, 176	0
8	i	35/38 (92%)	0.05	1 (2%) 53 42	173, 174, 175, 176	0
9	J	34/40 (85%)	-0.14	0 100 100	173, 174, 175, 175	0
9	j	34/40 (85%)	0.06	0 100 100	173, 174, 175, 175	0
10	K	37/46 (80%)	-0.05	0 100 100	173, 174, 175, 175	0
10	k	37/46 (80%)	-0.08	0 100 100	174, 174, 175, 176	0
11	L	37/37 (100%)	0.09	0 100 100	172, 174, 175, 175	0
11	l	37/37 (100%)	0.11	0 100 100	173, 174, 175, 176	0
12	M	34/36 (94%)	0.13	1 (2%) 53 42	172, 174, 174, 176	0
12	m	34/36 (94%)	0.27	3 (8%) 15 19	173, 173, 174, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.09	5 (2%) 63 50	172, 174, 175, 176	0
13	o	243/272 (89%)	0.06	4 (1%) 70 55	172, 174, 175, 176	0
14	T	32/32 (100%)	0.01	0 100 100	173, 174, 176, 176	0
14	t	32/32 (100%)	0.15	0 100 100	173, 174, 175, 176	0
15	U	97/134 (72%)	0.26	4 (4%) 41 36	172, 174, 174, 175	0
15	u	97/134 (72%)	0.19	1 (1%) 79 64	173, 174, 175, 175	0
16	V	137/163 (84%)	0.18	3 (2%) 62 49	172, 174, 175, 175	0
16	v	137/163 (84%)	0.06	2 (1%) 72 57	173, 174, 175, 176	0
17	g	28/46 (60%)	0.21	0 100 100	174, 175, 176, 176	0
17	y	28/46 (60%)	-0.11	0 100 100	173, 174, 176, 176	0
18	X	37/41 (90%)	-0.02	0 100 100	173, 174, 175, 176	0
18	x	37/41 (90%)	0.13	0 100 100	173, 174, 175, 175	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	-0.17	1 (1%) 70 55	173, 174, 175, 176	0
20	z	62/62 (100%)	-0.12	0 100 100	173, 175, 176, 176	0
All	All	5214/5674 (91%)	0.03	80 (1%) 72 57	171, 174, 175, 177	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	309	LEU	4.9
15	U	39	LEU	4.8
13	O	195	ASP	4.6
15	U	40	VAL	4.5
1	A	265	PHE	4.4
2	B	474	LEU	4.1
1	A	263	ALA	4.1
2	B	69	LEU	3.7
1	A	61	ASP	3.6
4	d	169	PHE	3.6
16	V	47	LEU	3.5
1	a	50	ILE	3.4
4	D	56	THR	3.3
2	B	472	ARG	3.2
1	a	224	ILE	3.2
3	C	336	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
4	d	173	PHE	3.1
2	b	386	ALA	3.1
15	U	121	LEU	3.0
2	b	267	LEU	3.0
6	F	38	ALA	3.0
4	d	264	LYS	2.9
3	C	334	PRO	2.9
2	b	63	LEU	2.9
2	b	2	GLY	2.8
3	C	140	LEU	2.8
13	o	202	GLN	2.7
2	b	482	ILE	2.6
13	O	177	TYR	2.6
2	b	393	GLU	2.6
1	a	250	ALA	2.6
1	A	292	THR	2.6
15	u	121	LEU	2.5
1	a	222	SER	2.5
3	C	332	GLN	2.5
1	A	218	LEU	2.5
7	h	26	GLY	2.5
16	v	69	GLY	2.5
13	O	218	LEU	2.4
4	d	314	PHE	2.4
4	D	246	MET	2.3
4	d	271	MET	2.3
4	d	268	HIS	2.3
4	d	137	GLY	2.3
16	V	117	VAL	2.3
20	Z	17	PHE	2.3
12	m	6	LEU	2.3
13	o	200	LEU	2.3
13	o	203	ALA	2.3
5	E	66	VAL	2.3
1	A	328	MET	2.3
4	d	334	GLN	2.3
16	v	65	SER	2.2
1	A	274	PHE	2.2
4	D	239	GLN	2.2
1	A	251	ALA	2.2
1	a	130	GLN	2.2
4	D	204	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
12	m	23	ILE	2.2
12	M	21	PHE	2.2
1	a	82	VAL	2.2
2	b	55	MET	2.2
2	b	359	MET	2.2
3	C	326	ALA	2.1
3	c	227	VAL	2.1
4	D	55	VAL	2.1
12	m	26	TYR	2.1
4	d	216	ALA	2.1
16	V	69	GLY	2.1
15	U	122	VAL	2.1
2	b	211	ILE	2.1
8	i	8	VAL	2.1
13	O	186	LYS	2.1
13	O	30	THR	2.1
3	C	387	TRP	2.1
4	d	220	ASN	2.0
5	E	49	THR	2.0
13	o	30	THR	2.0
6	F	11	VAL	2.0
3	c	200	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	LMT	b	627	35/35	0.44	0.19	173,175,177,177	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMT	I	102	35/35	0.51	0.18	173,175,176,178	0
31	LMT	d	409	31/35	0.52	0.18	172,175,177,177	0
22	CLA	b	605	65/65	0.55	0.22	172,175,176,176	0
22	CLA	B	601	65/65	0.57	0.20	172,175,176,177	0
31	LMT	b	626	35/35	0.58	0.17	172,175,176,177	0
31	LMT	D	410	31/35	0.59	0.15	174,175,176,176	0
31	LMT	i	102	35/35	0.63	0.17	173,175,176,177	0
31	LMT	B	622	35/35	0.64	0.16	171,175,177,177	0
22	CLA	b	619	65/65	0.69	0.18	172,174,175,175	0
27	LMG	C	518	45/55	0.70	0.19	171,174,175,175	0
24	BCR	j	102	40/40	0.72	0.29	173,175,177,178	0
25	DGD	D	409	63/66	0.72	0.21	172,174,176,178	0
33	BCT	d	403	4/4	0.72	0.29	174,174,175,176	0
35	CA	o	301	1/1	0.72	0.14	180,180,180,180	0
24	BCR	J	102	40/40	0.73	0.28	172,174,176,177	0
31	LMT	B	627	35/35	0.73	0.14	172,175,177,177	0
31	LMT	B	628	35/35	0.75	0.18	172,174,177,178	0
35	CA	O	301	1/1	0.76	0.12	177,177,177,177	0
22	CLA	C	506	65/65	0.76	0.20	172,174,175,175	0
25	DGD	d	408	63/66	0.77	0.20	172,175,177,178	0
25	DGD	B	625	52/66	0.77	0.18	172,175,177,177	0
30	SQD	B	626	47/54	0.77	0.16	170,174,176,178	0
31	LMT	b	604	35/35	0.78	0.22	172,174,176,176	0
27	LMG	I	101	43/55	0.78	0.18	172,174,177,177	0
31	LMT	B	623	35/35	0.78	0.14	173,174,177,177	0
22	CLA	c	512	65/65	0.78	0.15	172,174,176,176	0
25	DGD	C	516	62/66	0.80	0.16	171,174,175,176	0
26	LHG	C	519	37/49	0.80	0.17	172,174,179,183	0
27	LMG	a	402	42/55	0.80	0.23	171,174,176,176	0
27	LMG	c	518	45/55	0.80	0.15	172,174,176,176	0
30	SQD	A	413	51/54	0.80	0.19	172,174,175,176	0
27	LMG	b	625	49/55	0.81	0.21	172,174,175,175	0
23	PL9	A	406	45/55	0.81	0.26	172,174,175,175	0
31	LMT	M	102	35/35	0.81	0.19	172,174,175,175	0
31	LMT	b	603	35/35	0.81	0.12	172,174,175,176	0
30	SQD	a	401	54/54	0.82	0.19	172,174,176,178	0
30	SQD	d	402	43/54	0.82	0.17	172,174,176,178	0
27	LMG	M	101	42/55	0.82	0.19	173,174,176,176	0
25	DGD	b	601	52/66	0.83	0.18	172,174,176,177	0
25	DGD	c	516	62/66	0.83	0.21	172,174,175,175	0
24	BCR	H	102	40/40	0.83	0.21	173,174,175,176	0
27	LMG	i	101	43/55	0.84	0.16	172,174,177,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	DGD	C	517	66/66	0.84	0.17	172,173,174,175	0
23	PL9	J	101	35/55	0.84	0.25	172,175,176,176	0
27	LMG	A	415	42/55	0.85	0.21	171,174,176,177	0
30	SQD	F	102	45/54	0.85	0.19	172,175,177,178	0
27	LMG	a	413	51/55	0.85	0.21	172,173,175,176	0
25	DGD	c	517	66/66	0.85	0.21	172,173,175,176	0
27	LMG	E	101	44/55	0.86	0.19	170,174,176,177	0
27	LMG	c	522	48/55	0.86	0.23	172,174,175,176	0
27	LMG	e	101	44/55	0.86	0.17	171,174,175,176	0
22	CLA	c	506	65/65	0.86	0.16	173,174,175,175	0
26	LHG	c	519	37/49	0.86	0.16	172,174,178,181	0
24	BCR	c	521	40/40	0.87	0.16	172,174,175,175	0
30	SQD	b	602	47/54	0.87	0.15	171,174,176,178	0
27	LMG	m	101	42/55	0.87	0.19	170,174,175,175	0
24	BCR	a	410	40/40	0.87	0.20	172,173,174,175	0
31	LMT	M	103	35/35	0.87	0.17	172,173,175,176	0
25	DGD	A	408	56/66	0.87	0.17	172,174,175,176	0
24	BCR	c	514	40/40	0.87	0.22	172,173,175,175	0
27	LMG	D	408	48/55	0.88	0.17	170,173,175,175	0
22	CLA	C	504	65/65	0.88	0.18	171,173,175,175	0
22	CLA	c	501	65/65	0.88	0.15	172,174,175,175	0
25	DGD	b	624	58/66	0.88	0.20	171,173,174,175	0
30	SQD	a	415	51/54	0.88	0.17	173,174,175,176	0
23	PL9	j	101	35/55	0.88	0.25	173,175,175,176	0
24	BCR	x	101	40/40	0.88	0.18	173,174,175,175	0
28	CL	A	411	1/1	0.88	0.13	172,172,172,172	0
22	CLA	C	512	65/65	0.89	0.12	172,174,176,177	0
24	BCR	B	619	40/40	0.89	0.16	172,173,174,175	0
24	BCR	C	521	40/40	0.89	0.18	172,174,175,176	0
22	CLA	c	505	65/65	0.89	0.15	172,174,175,175	0
22	CLA	C	505	65/65	0.89	0.16	172,174,175,176	0
22	CLA	b	606	65/65	0.89	0.15	172,173,174,174	0
27	LMG	C	522	48/55	0.89	0.18	172,174,174,175	0
25	DGD	a	411	56/66	0.89	0.16	173,174,175,176	0
22	CLA	h	101	65/65	0.89	0.19	171,174,175,175	0
22	CLA	b	609	65/65	0.89	0.14	172,174,175,175	0
35	CA	k	101	1/1	0.89	0.08	172,172,172,172	0
22	CLA	B	605	65/65	0.89	0.13	172,173,175,176	0
22	CLA	A	405	65/65	0.90	0.14	172,174,175,176	0
27	LMG	B	621	49/55	0.90	0.16	172,173,174,174	0
24	BCR	g	101	40/40	0.90	0.15	173,174,175,175	0
22	CLA	b	618	65/65	0.90	0.13	172,174,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	520	65/65	0.90	0.16	172,174,175,176	0
22	CLA	D	405	65/65	0.90	0.15	172,173,174,175	0
25	DGD	C	515	53/66	0.90	0.17	172,173,174,174	0
24	BCR	A	407	40/40	0.90	0.19	171,173,174,174	0
24	BCR	B	616	40/40	0.90	0.15	172,173,174,175	0
22	CLA	c	502	65/65	0.90	0.14	173,174,175,175	0
22	CLA	c	503	65/65	0.90	0.13	172,174,175,175	0
22	CLA	a	408	65/65	0.90	0.15	173,174,175,175	0
22	CLA	C	507	65/65	0.90	0.16	173,174,175,177	0
25	DGD	c	515	53/66	0.90	0.18	171,174,175,177	0
22	CLA	c	510	65/65	0.90	0.12	173,174,175,176	0
24	BCR	b	621	40/40	0.90	0.18	171,173,174,174	0
24	BCR	b	622	40/40	0.90	0.24	171,172,173,173	0
26	LHG	A	409	39/49	0.90	0.17	172,173,175,176	0
32	PHO	D	401	64/64	0.90	0.17	171,173,174,175	0
32	PHO	D	402	64/64	0.90	0.15	171,173,175,175	0
30	SQD	A	414	54/54	0.90	0.15	171,174,176,179	0
22	CLA	c	511	65/65	0.90	0.14	172,174,175,176	0
30	SQD	D	403	43/54	0.90	0.14	172,174,177,180	0
22	CLA	C	510	65/65	0.90	0.14	172,173,175,175	0
22	CLA	B	607	65/65	0.91	0.15	172,174,174,175	0
27	LMG	d	407	48/55	0.91	0.16	171,173,175,175	0
24	BCR	b	620	40/40	0.91	0.21	172,173,174,175	0
22	CLA	C	508	65/65	0.91	0.13	172,174,175,175	0
35	CA	K	101	1/1	0.91	0.13	177,177,177,177	0
22	CLA	a	406	65/65	0.91	0.16	172,174,175,176	0
24	BCR	y	101	40/40	0.91	0.15	173,173,174,175	0
27	LMG	A	410	51/55	0.91	0.17	171,173,174,175	0
23	PL9	d	406	55/55	0.92	0.16	172,173,175,175	0
22	CLA	c	508	65/65	0.92	0.11	172,174,175,175	0
24	BCR	b	623	40/40	0.92	0.13	171,173,174,174	0
24	BCR	c	513	40/40	0.92	0.16	172,173,175,175	0
22	CLA	B	615	65/65	0.92	0.13	172,174,175,175	0
22	CLA	B	604	65/65	0.92	0.11	172,173,175,175	0
24	BCR	B	617	40/40	0.92	0.18	172,173,174,174	0
22	CLA	A	404	65/65	0.92	0.17	170,173,174,175	0
26	LHG	a	412	39/49	0.92	0.17	171,174,176,177	0
24	BCR	C	513	40/40	0.92	0.15	172,173,174,174	0
24	BCR	C	514	40/40	0.92	0.15	172,173,175,175	0
25	DGD	B	620	58/66	0.92	0.17	171,173,175,176	0
22	CLA	c	520	65/65	0.92	0.15	173,174,174,175	0
27	LMG	B	624	49/55	0.92	0.18	171,173,174,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	B	602	65/65	0.92	0.14	171,173,174,175	0
22	CLA	B	613	65/65	0.92	0.14	172,174,174,175	0
23	PL9	D	407	55/55	0.92	0.18	171,173,174,175	0
27	LMG	D	412	46/55	0.92	0.15	172,174,175,175	0
22	CLA	a	405	65/65	0.92	0.17	170,172,174,175	0
23	PL9	a	409	45/55	0.92	0.17	171,173,174,175	0
30	SQD	f	103	45/54	0.92	0.14	172,174,176,178	0
27	LMG	d	410	46/55	0.93	0.15	172,173,175,175	0
22	CLA	C	509	65/65	0.93	0.13	173,173,174,174	0
22	CLA	c	504	65/65	0.93	0.14	172,174,175,175	0
22	CLA	H	101	65/65	0.93	0.14	172,174,175,175	0
22	CLA	b	612	65/65	0.93	0.12	171,174,175,176	0
22	CLA	b	613	65/65	0.93	0.12	172,174,175,175	0
24	BCR	f	102	40/40	0.93	0.17	171,173,175,175	0
32	PHO	a	407	64/64	0.93	0.12	173,174,175,175	0
32	PHO	d	401	64/64	0.93	0.14	172,173,174,174	0
22	CLA	C	503	65/65	0.93	0.13	172,174,175,176	0
22	CLA	C	511	65/65	0.93	0.13	172,174,175,175	0
22	CLA	B	609	65/65	0.93	0.13	172,174,175,175	0
22	CLA	B	610	65/65	0.93	0.12	172,174,174,175	0
22	CLA	d	405	65/65	0.93	0.13	172,174,175,175	0
22	CLA	b	617	65/65	0.94	0.17	173,173,175,176	0
22	CLA	b	607	65/65	0.94	0.12	172,173,175,176	0
22	CLA	c	507	65/65	0.94	0.12	172,174,175,176	0
22	CLA	b	608	65/65	0.94	0.13	172,173,175,176	0
22	CLA	B	603	65/65	0.94	0.11	171,173,175,175	0
22	CLA	b	610	65/65	0.94	0.14	172,173,175,175	0
22	CLA	A	402	65/65	0.94	0.14	172,173,174,175	0
22	CLA	D	406	65/65	0.94	0.13	172,174,175,176	0
27	LMG	b	628	49/55	0.94	0.17	172,174,175,175	0
22	CLA	d	404	65/65	0.94	0.13	172,173,174,174	0
22	CLA	A	403	65/65	0.95	0.13	171,173,174,175	0
22	CLA	B	611	65/65	0.95	0.10	171,173,174,174	0
22	CLA	b	611	65/65	0.95	0.11	172,174,175,175	0
22	CLA	B	608	65/65	0.95	0.13	172,174,175,175	0
22	CLA	B	614	65/65	0.95	0.10	172,174,175,175	0
24	BCR	B	618	40/40	0.95	0.16	171,172,174,174	0
22	CLA	b	615	65/65	0.95	0.10	172,173,174,175	0
29	OEX	A	412	10/10	0.95	0.10	165,169,172,173	0
29	OEX	a	414	10/10	0.95	0.11	168,171,173,177	0
22	CLA	B	606	65/65	0.95	0.13	172,173,174,175	0
34	HEM	F	101	43/43	0.95	0.11	173,174,175,176	0

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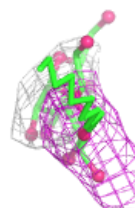
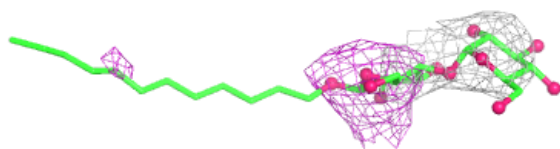
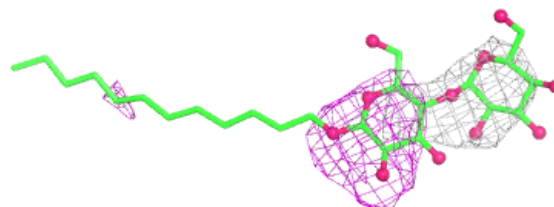
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HEM	V	201	43/43	0.95	0.17	172,173,175,175	0
34	HEM	f	101	43/43	0.95	0.12	173,174,175,175	0
22	CLA	C	501	65/65	0.95	0.11	172,174,174,175	0
22	CLA	c	509	65/65	0.95	0.09	172,173,175,175	0
24	BCR	D	411	40/40	0.95	0.14	171,173,174,175	0
22	CLA	C	502	65/65	0.95	0.15	173,174,174,175	0
22	CLA	b	614	65/65	0.96	0.12	172,173,174,175	0
34	HEM	v	201	43/43	0.96	0.12	171,174,175,175	0
33	BCT	D	404	4/4	0.96	0.05	173,174,174,174	0
22	CLA	B	612	65/65	0.96	0.13	171,173,175,175	0
28	CL	a	416	1/1	0.96	0.16	173,173,173,173	0
22	CLA	a	404	65/65	0.96	0.12	172,173,174,176	0
22	CLA	b	616	65/65	0.97	0.13	171,173,174,175	0
21	FE2	A	401	1/1	0.97	0.10	170,170,170,170	0
21	FE2	a	403	1/1	0.97	0.12	175,175,175,175	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.

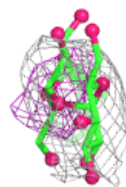
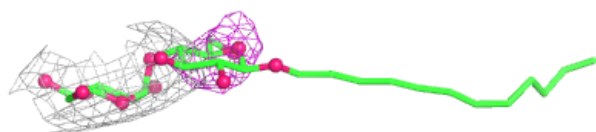
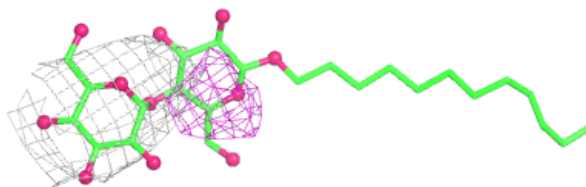
Electron density around LMT b 627:

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

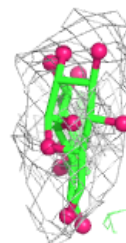
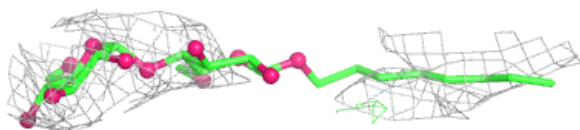
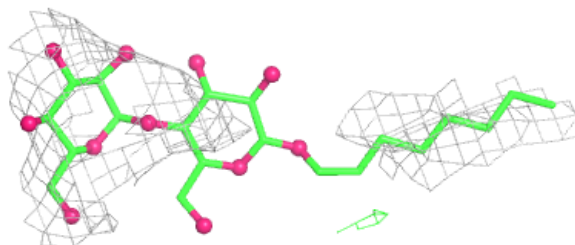


Electron density around LMT I 102:

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

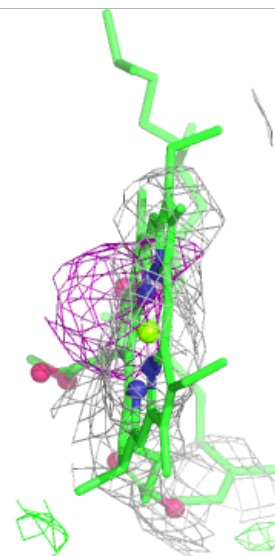
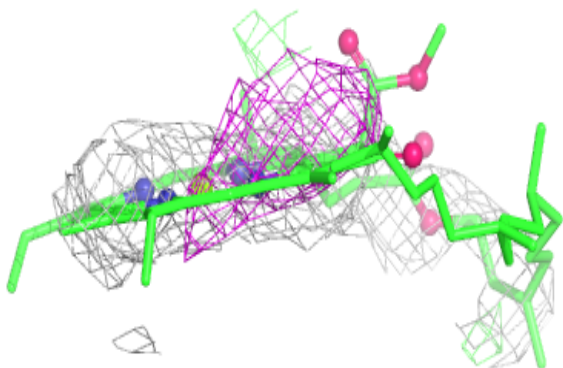
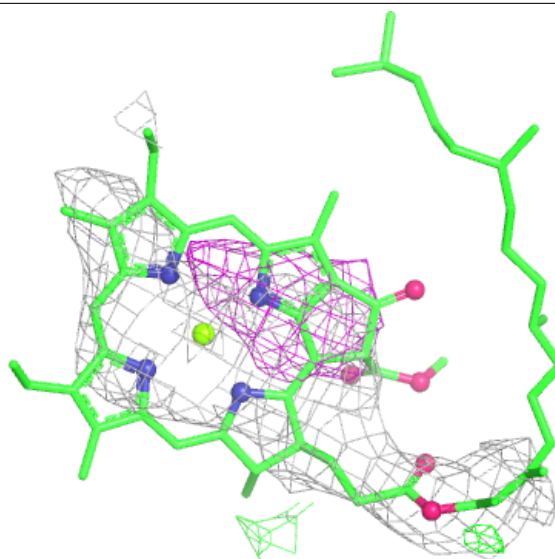
**Electron density around LMT d 409:**

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



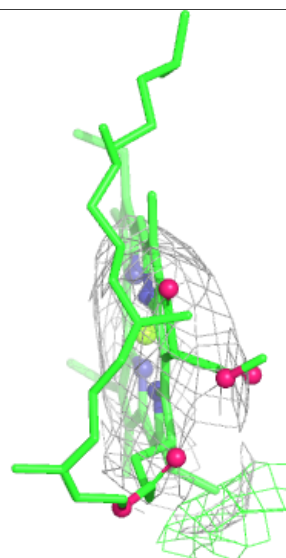
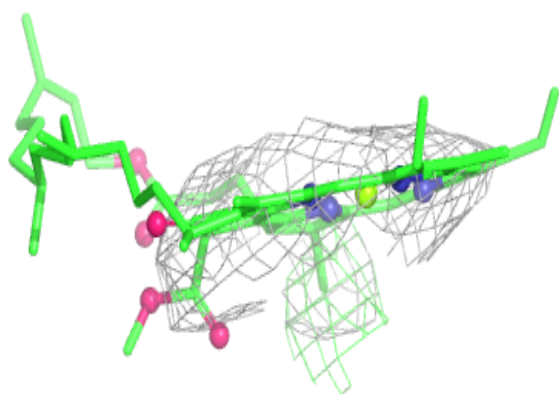
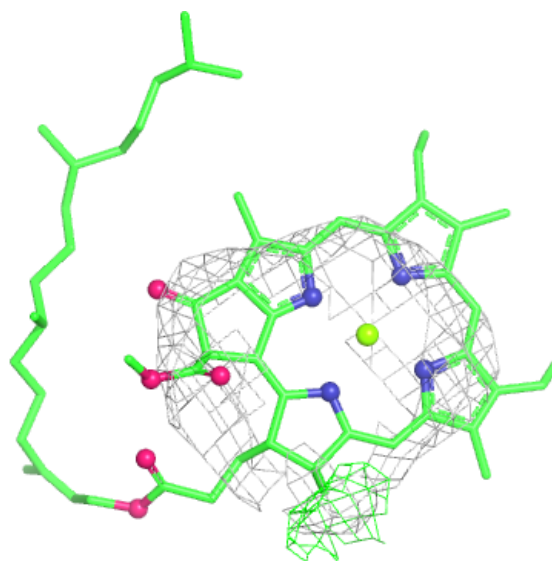
Electron density around CLA b 605:

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



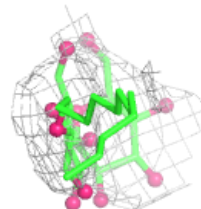
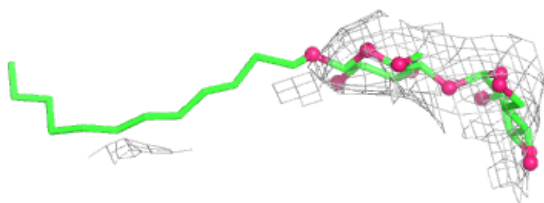
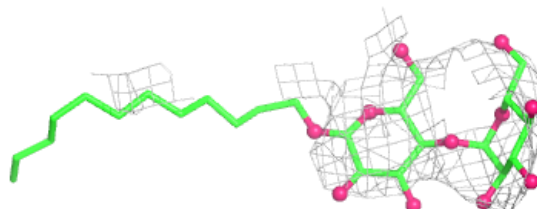
Electron density around CLA B 601:

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

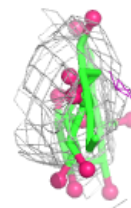
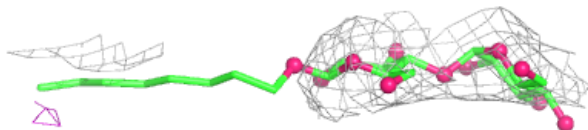
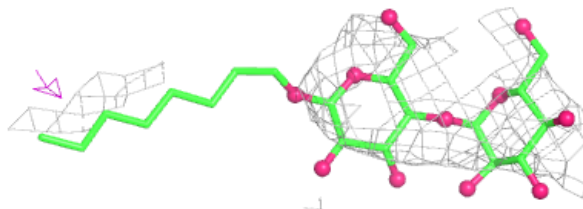


Electron density around LMT b 626:

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

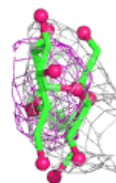
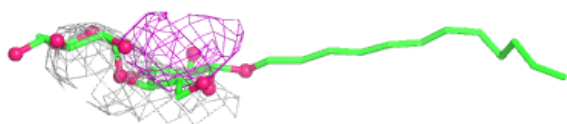
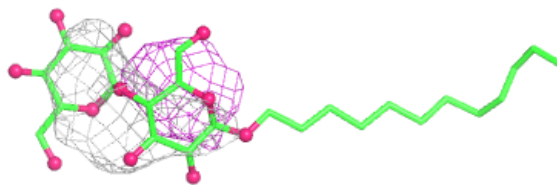
**Electron density around LMT D 410:**

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

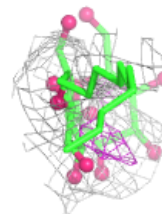
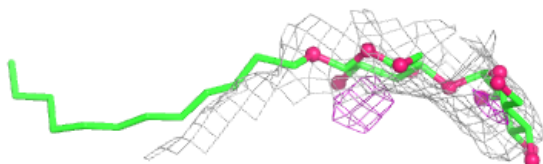
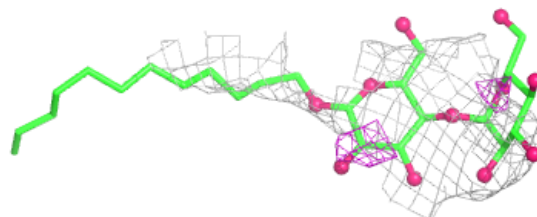


Electron density around LMT i 102:

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

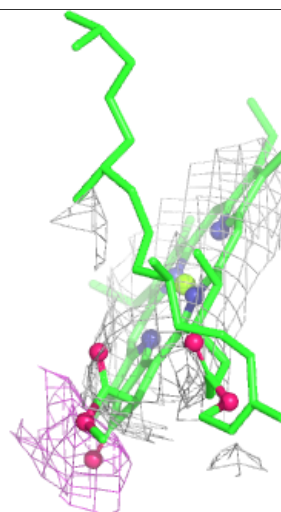
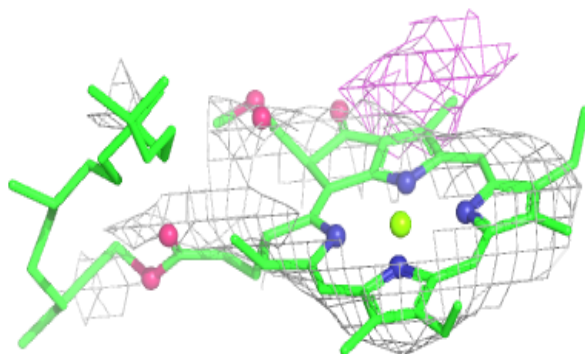
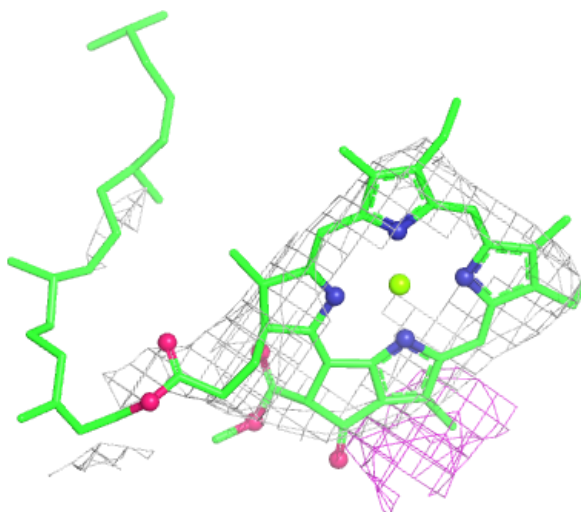
**Electron density around LMT B 622:**

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



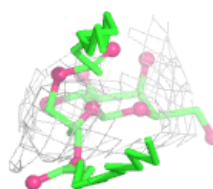
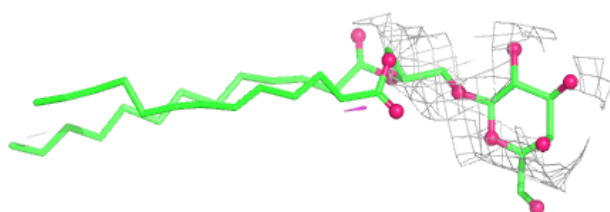
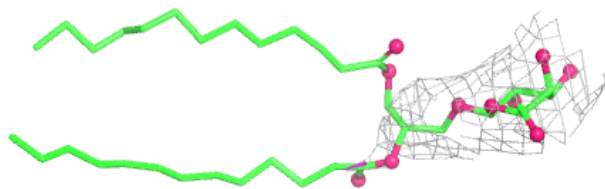
Electron density around CLA b 619:

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

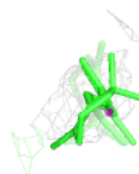
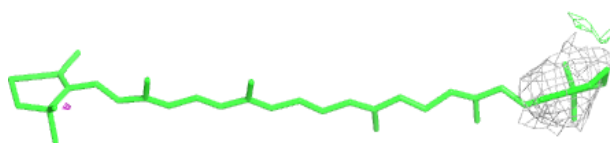
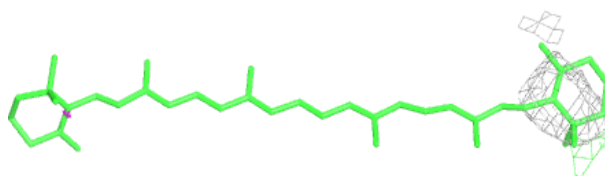


Electron density around LMG C 518:

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

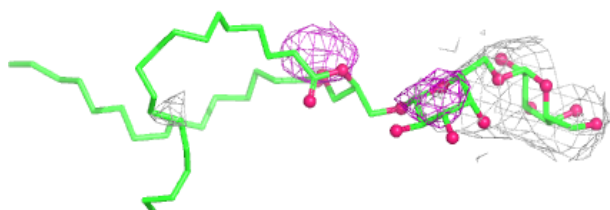
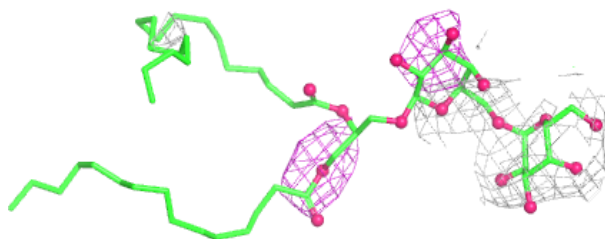
**Electron density around BCR j 102:**

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

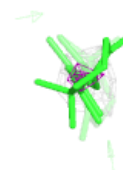
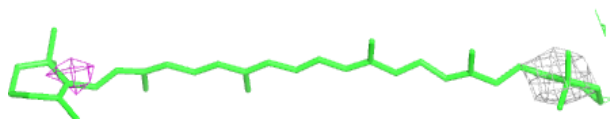
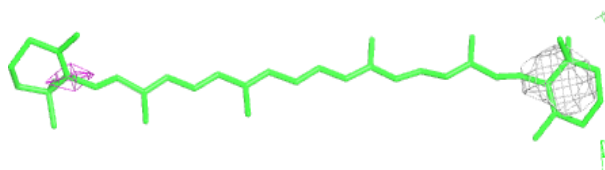


Electron density around DGD D 409:

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

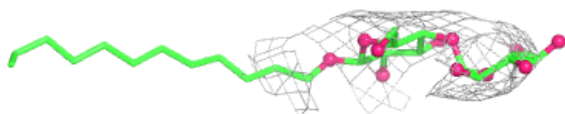
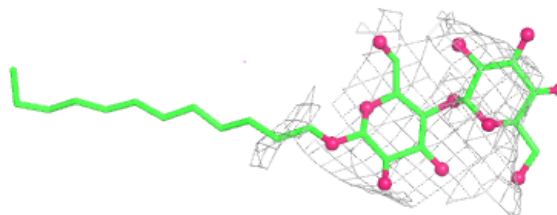
**Electron density around BCR J 102:**

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

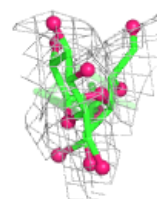
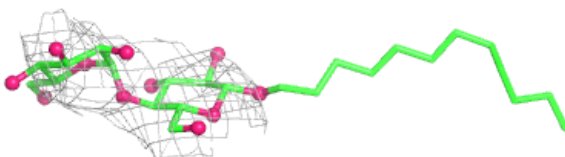
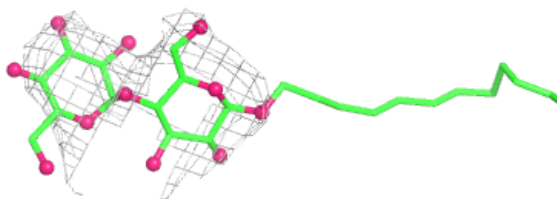


Electron density around LMT B 627:

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

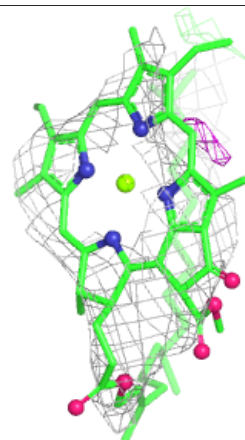
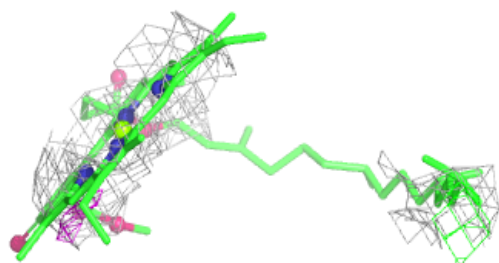
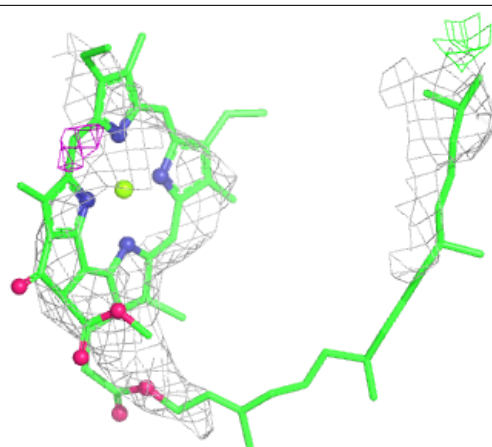
**Electron density around LMT B 628:**

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

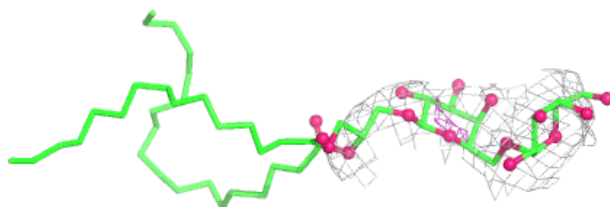
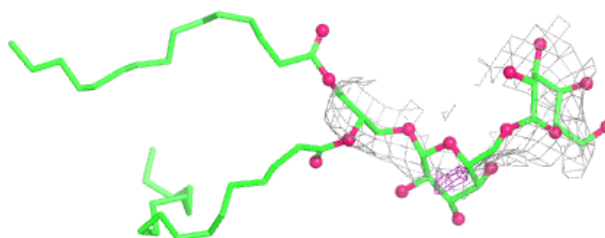


Electron density around CLA C 506:

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

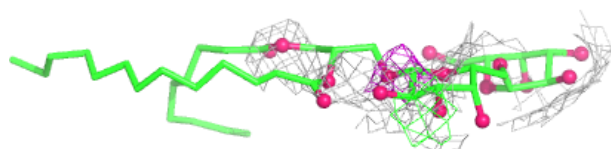
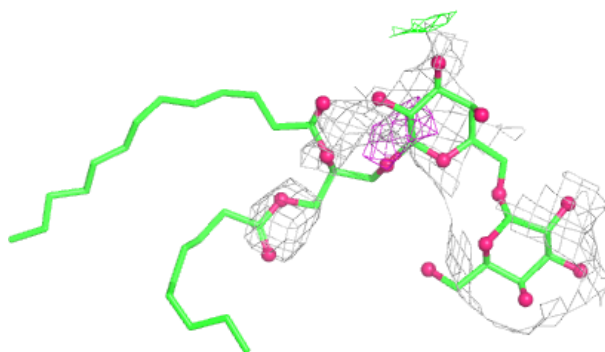
**Electron density around DGD d 408:**

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

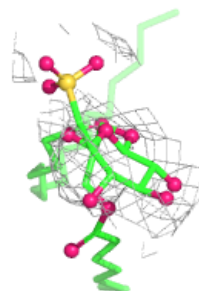
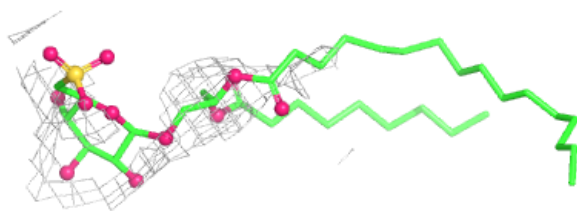


Electron density around DGD B 625:

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

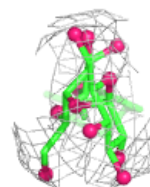
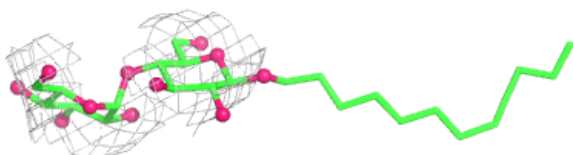
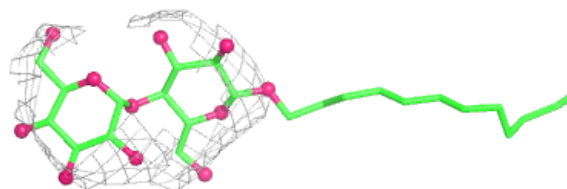
**Electron density around SQD B 626:**

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and green (positive)

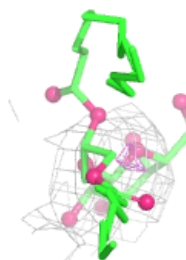
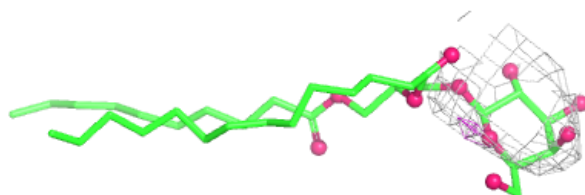
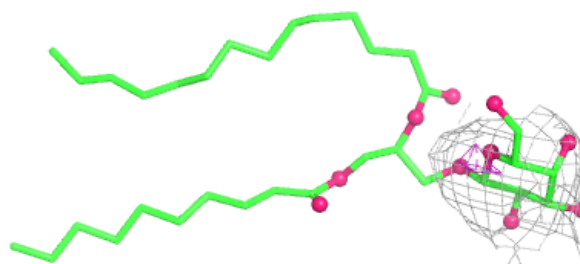


Electron density around LMT b 604:

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

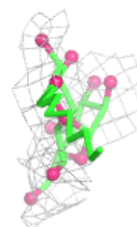
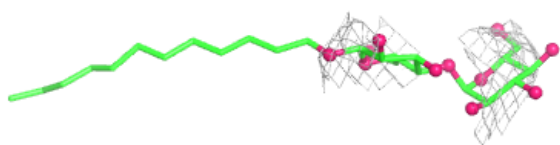
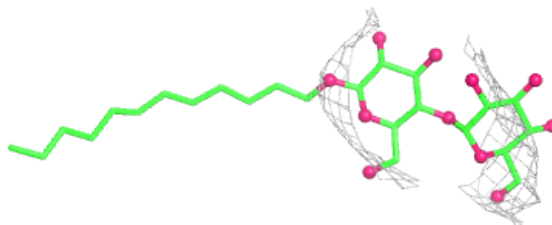
**Electron density around LMG I 101:**

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

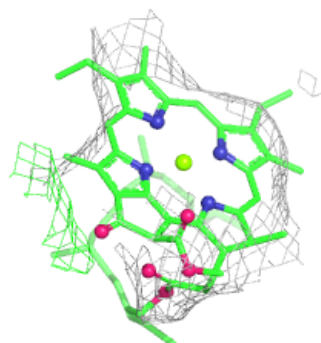
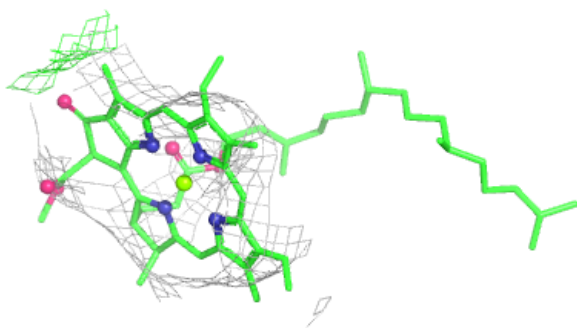
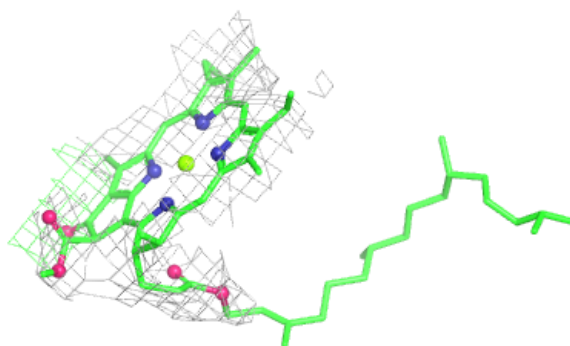


Electron density around LMT B 623:

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

**Electron density around CLA c 512:**

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

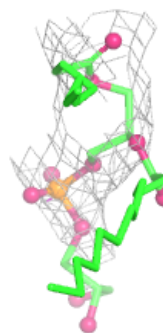
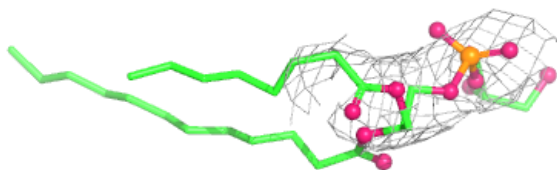
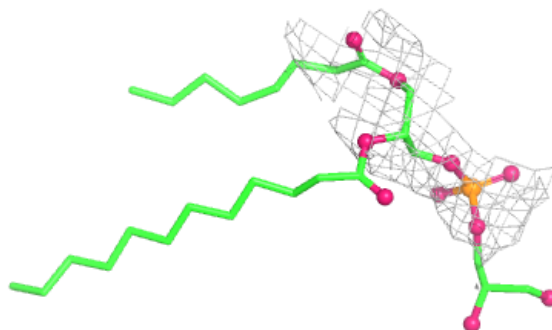


Electron density around DGD C 516:

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

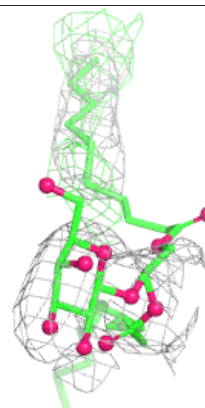
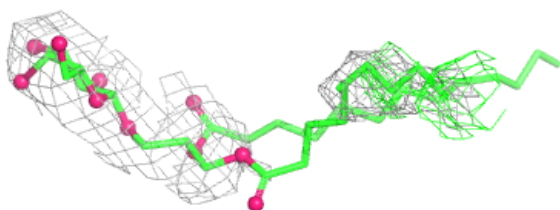
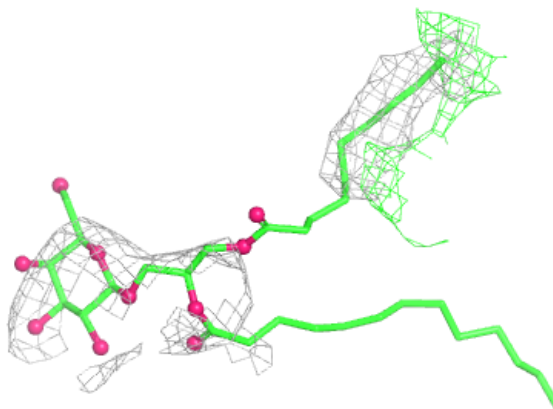
**Electron density around LHG C 519:**

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

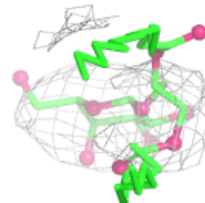
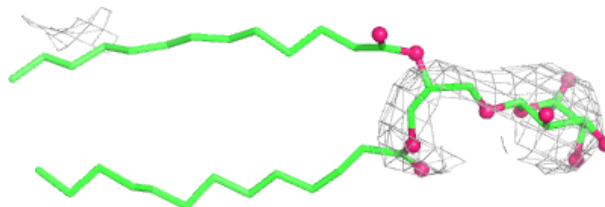


Electron density around LMG a 402:

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

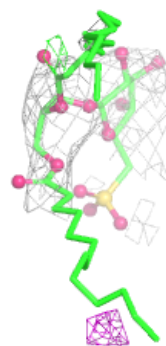
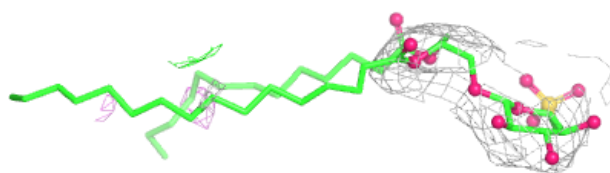
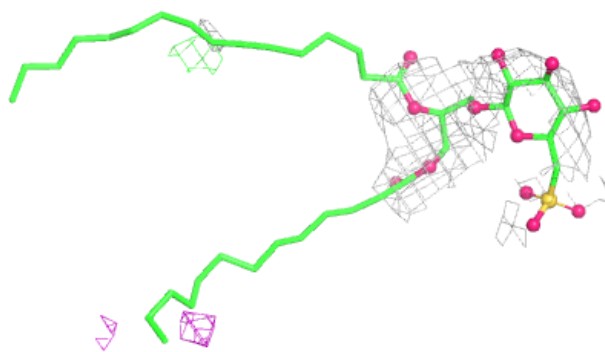
**Electron density around LMG c 518:**

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

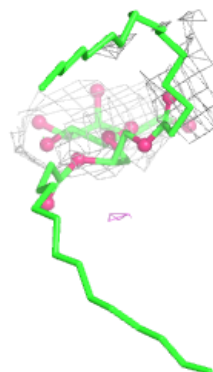
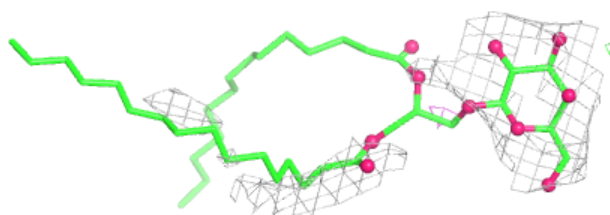


Electron density around SQD A 413:

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

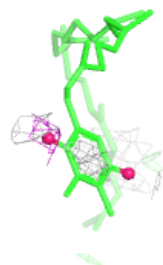
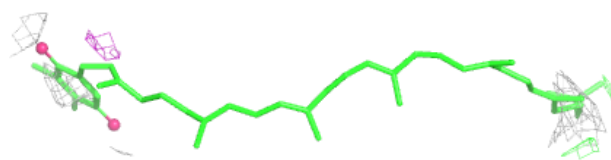
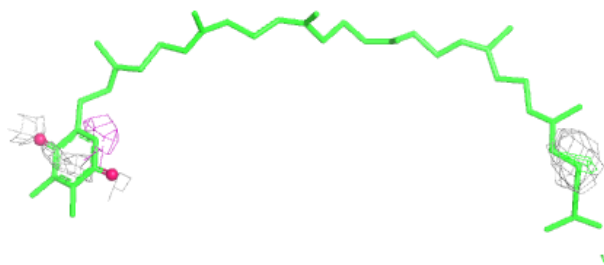
**Electron density around LMG b 625:**

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

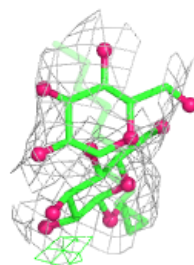
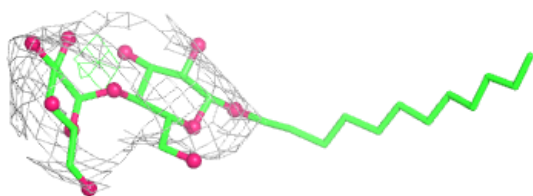


Electron density around PL9 A 406:

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

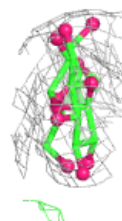
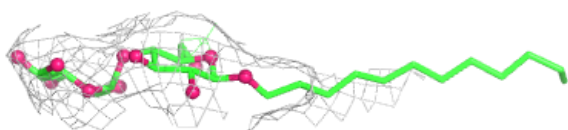
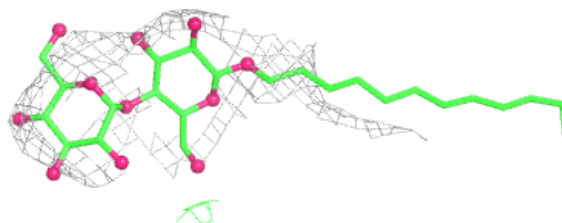
**Electron density around LMT M 102:**

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

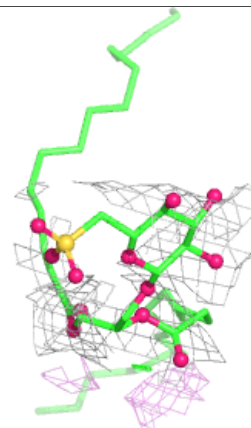
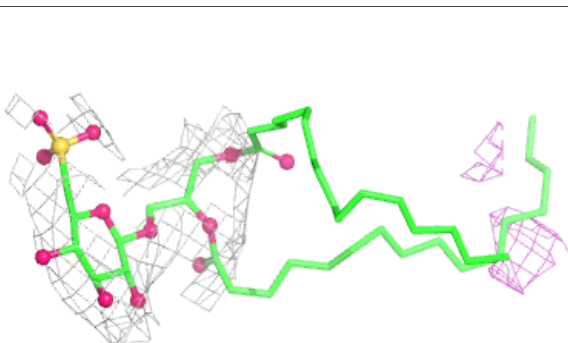
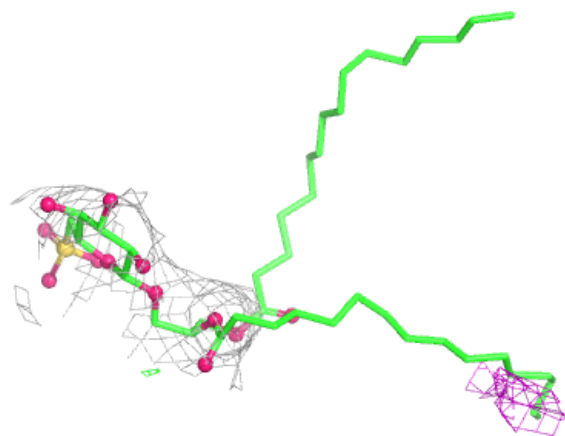


Electron density around LMT b 603:

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

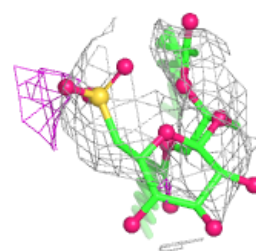
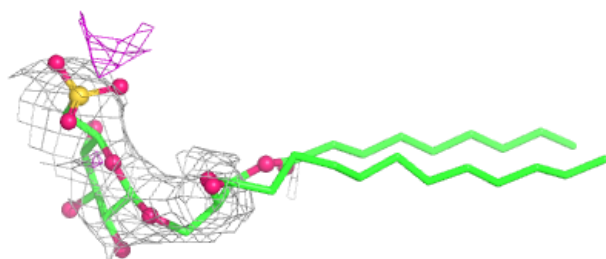
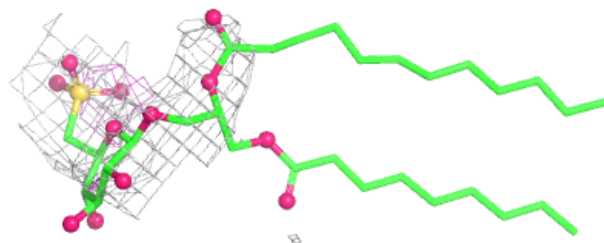
**Electron density around SQD a 401:**

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

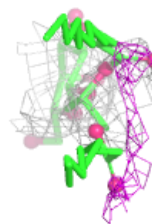
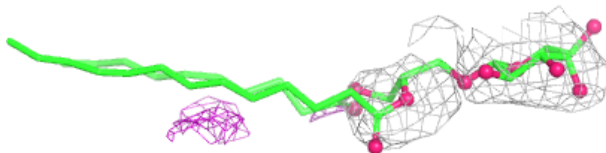
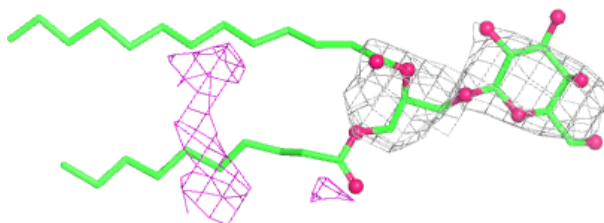


Electron density around SQD d 402:

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

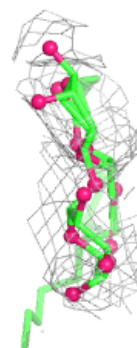
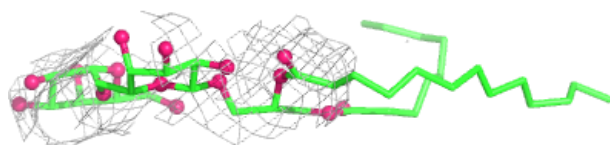
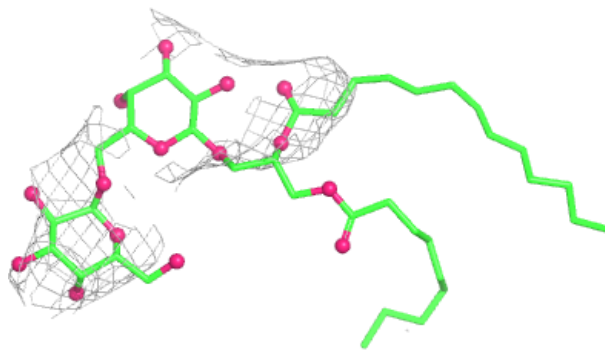
**Electron density around LMG M 101:**

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

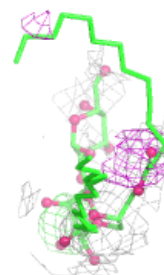
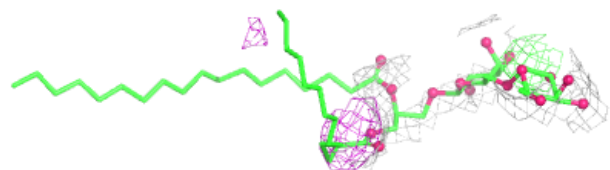


Electron density around DGD b 601:

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

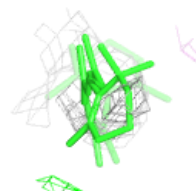
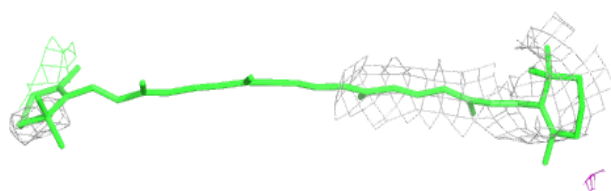
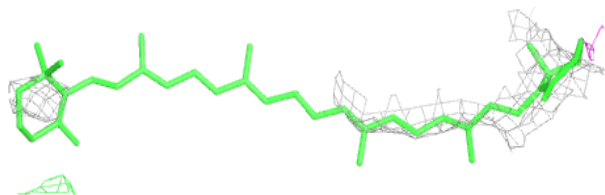
**Electron density around DGD c 516:**

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

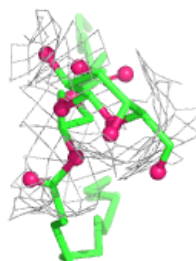
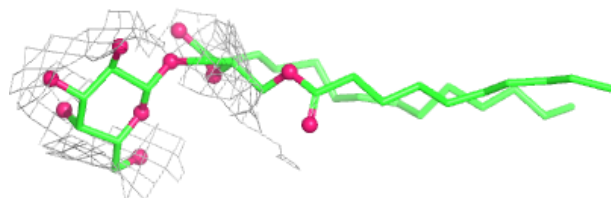
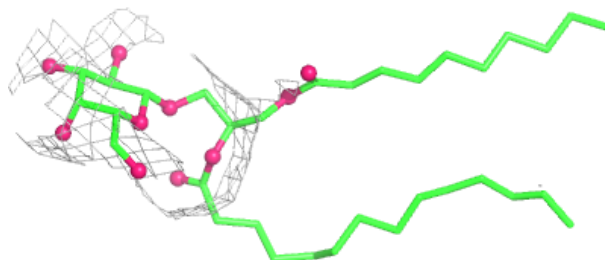


Electron density around BCR H 102:

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

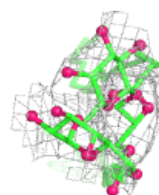
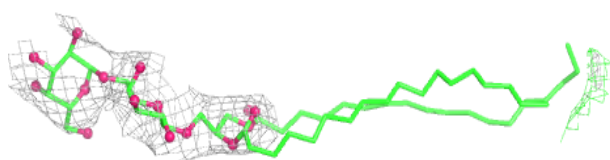
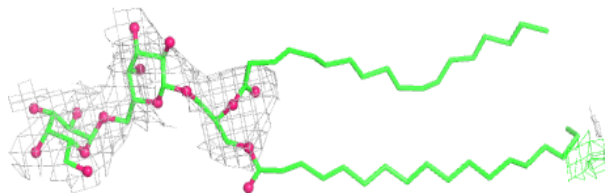
**Electron density around LMG i 101:**

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

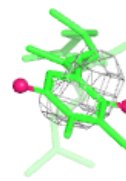
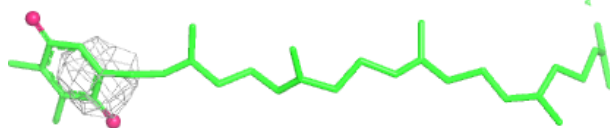
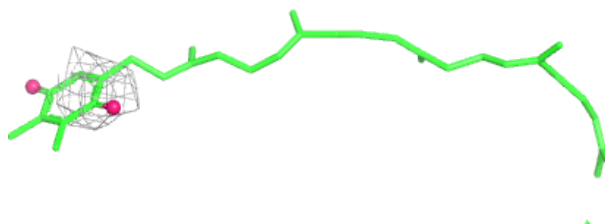


Electron density around DGD C 517:

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

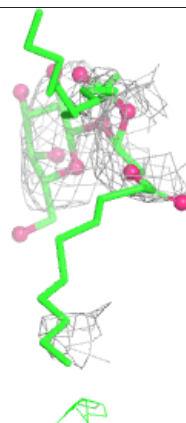
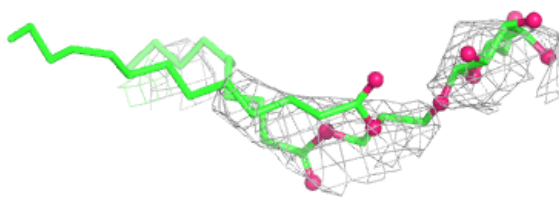
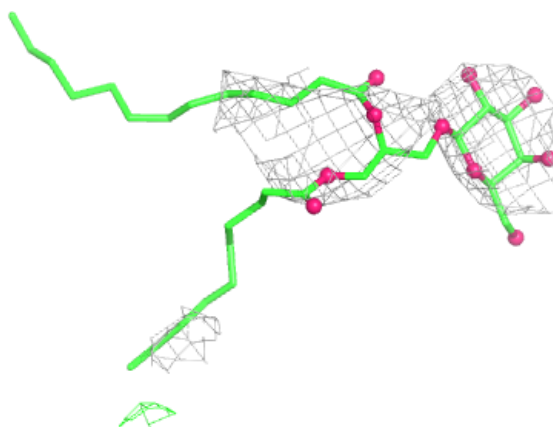
**Electron density around PL9 J 101:**

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

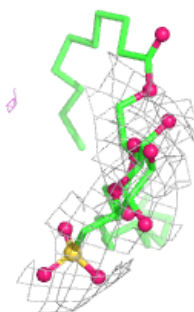
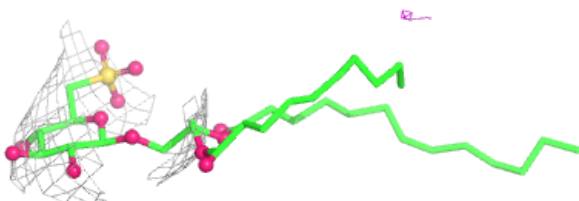
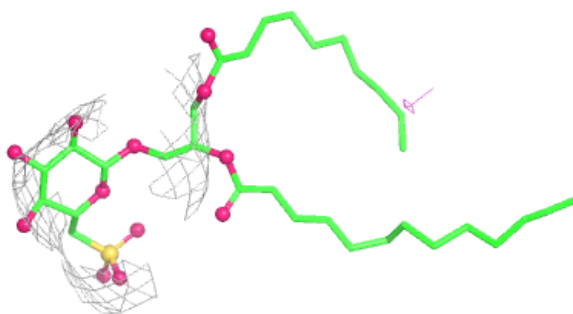


Electron density around LMG A 415:

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

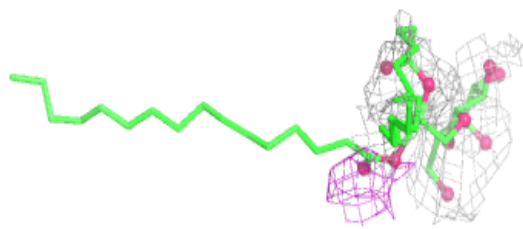
**Electron density around SQD F 102:**

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



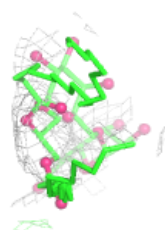
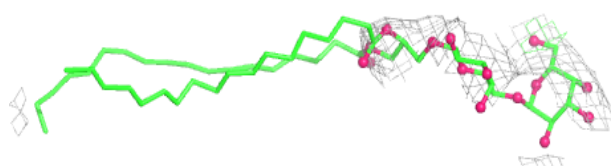
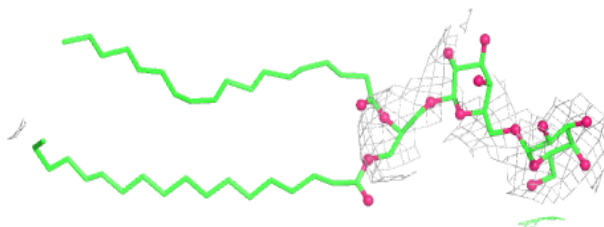
Electron density around LMG a 413:

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

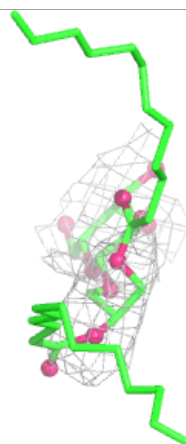
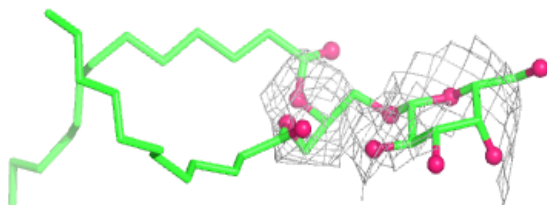
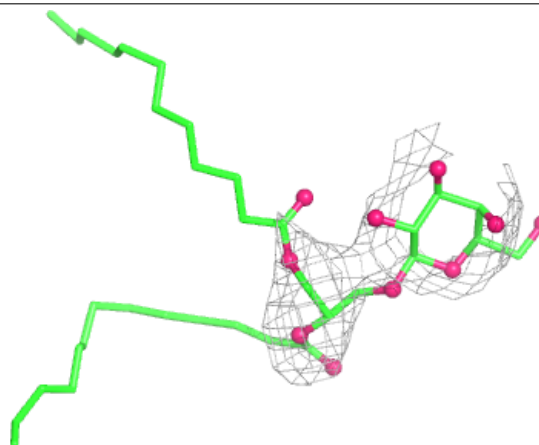


Electron density around DGD c 517:

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

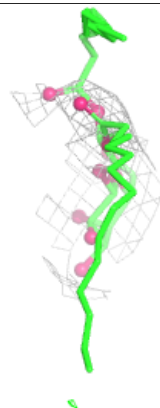
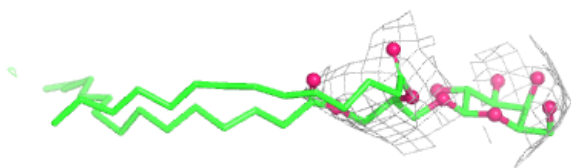
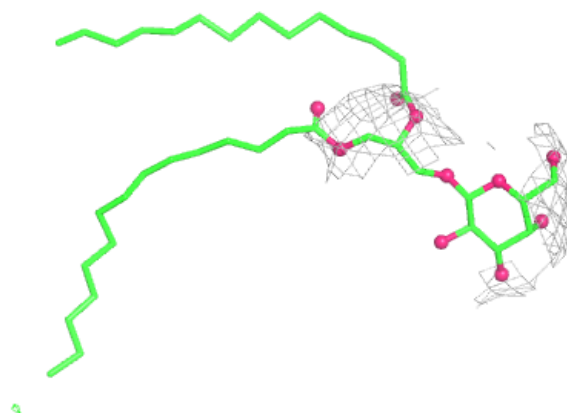
**Electron density around LMG E 101:**

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



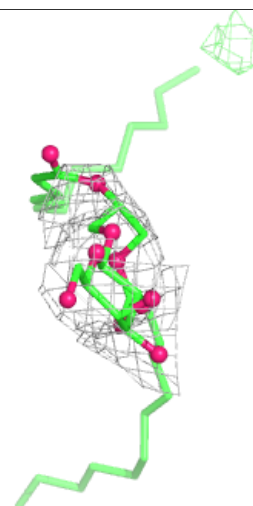
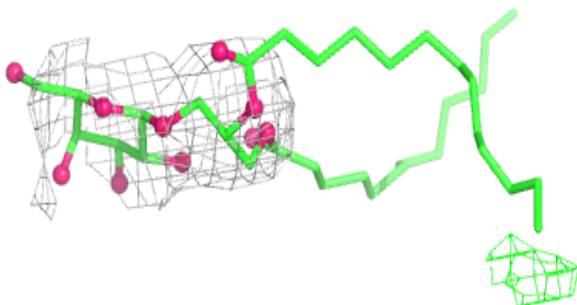
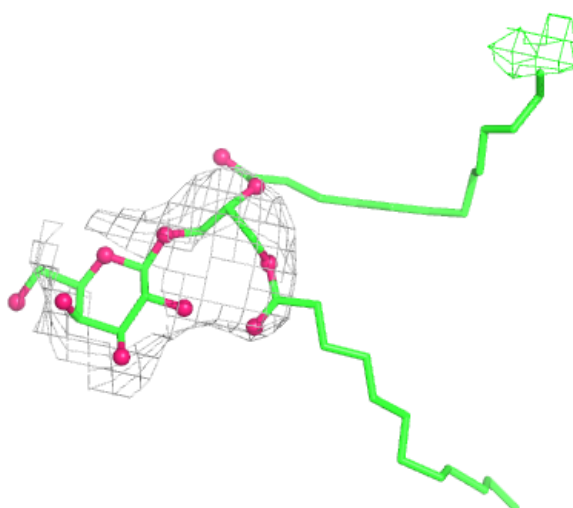
Electron density around LMG c 522:

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



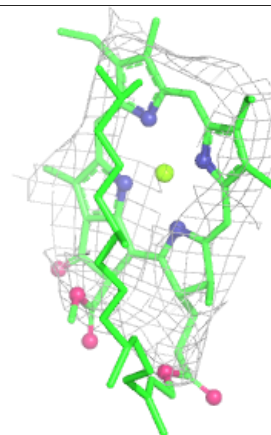
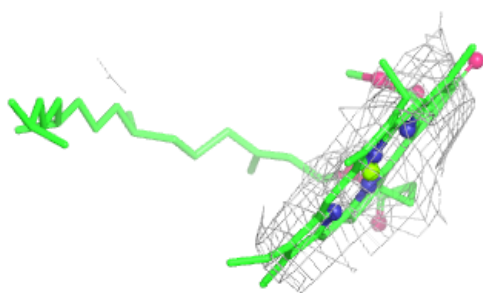
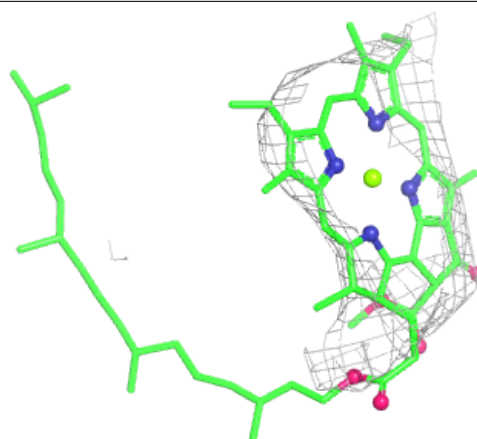
Electron density around LMG e 101:

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



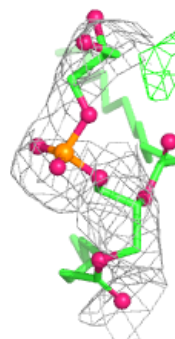
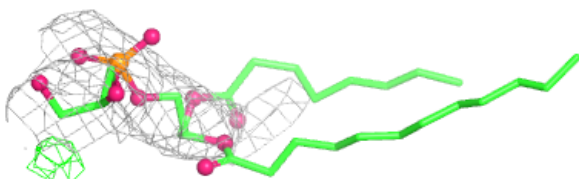
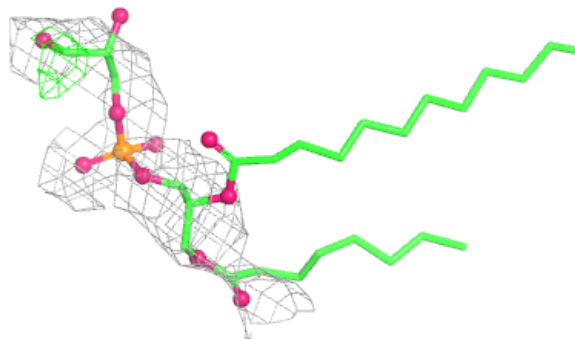
Electron density around CLA c 506:

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

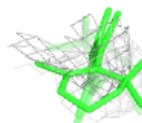
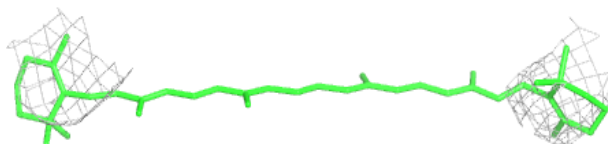
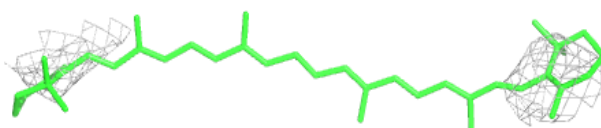


Electron density around LHG c 519:

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

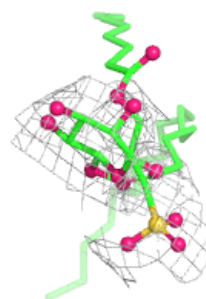
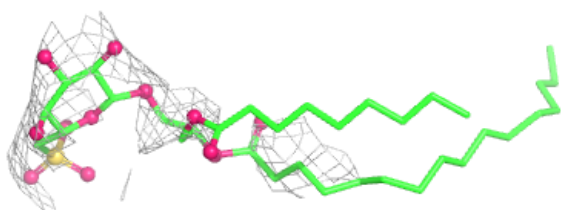
**Electron density around BCR c 521:**

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

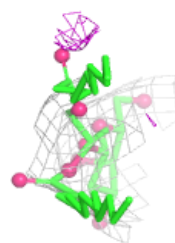
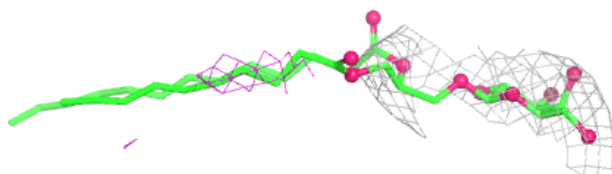
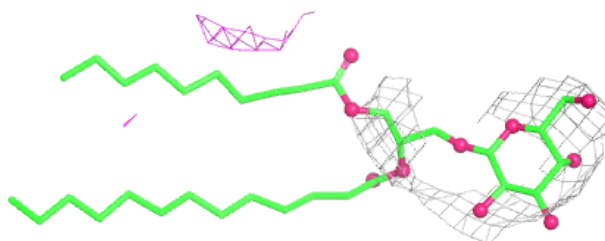


Electron density around SQD b 602:

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

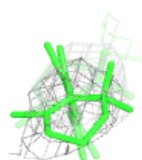
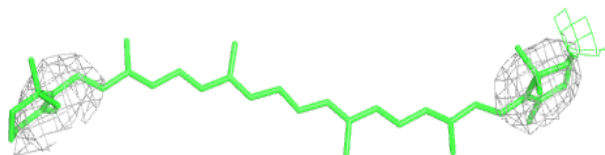
**Electron density around LMG m 101:**

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

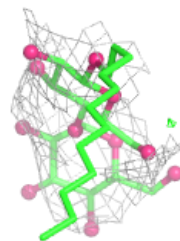
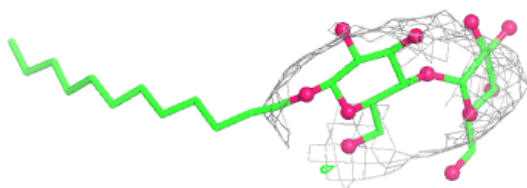


Electron density around BCR a 410:

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

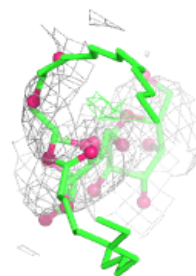
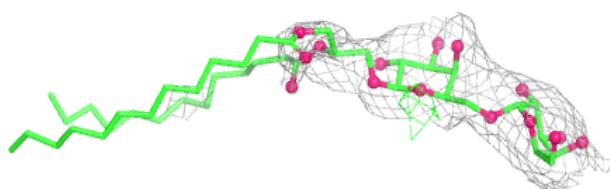
**Electron density around LMT M 103:**

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

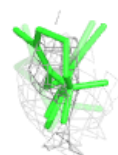
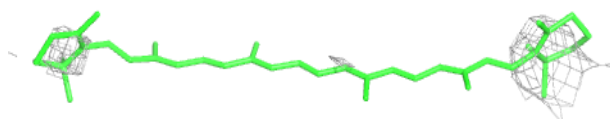
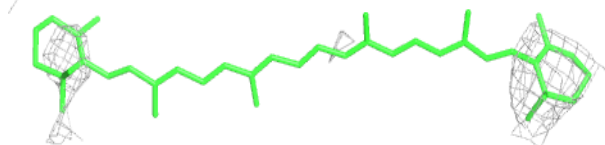


Electron density around DGD A 408:

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

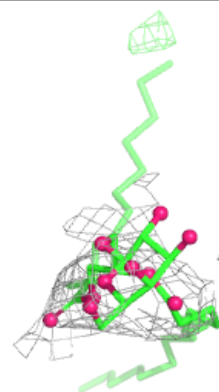
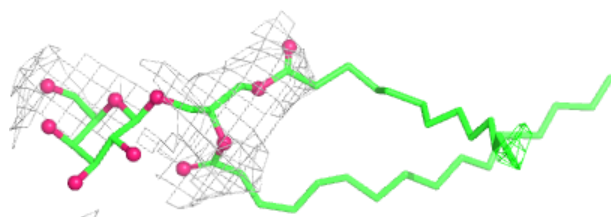
**Electron density around BCR c 514:**

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

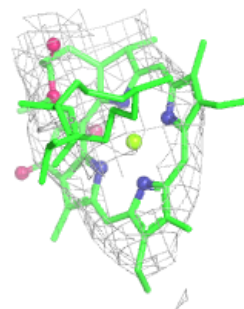
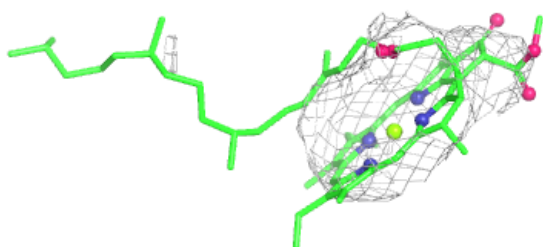
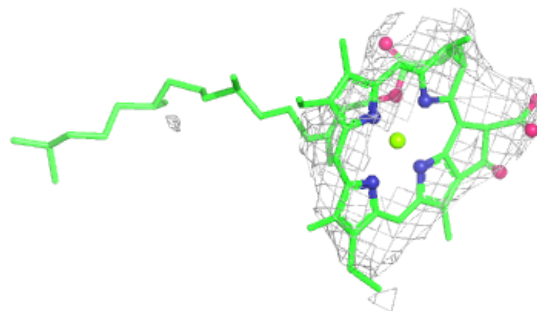


Electron density around LMG D 408:

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

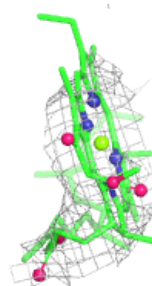
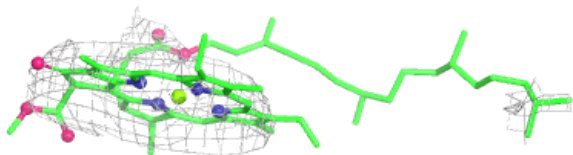
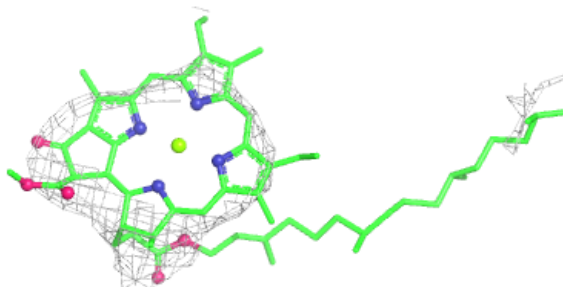
**Electron density around CLA C 504:**

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

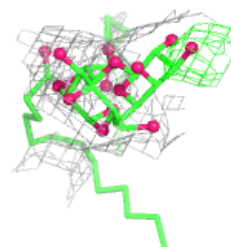
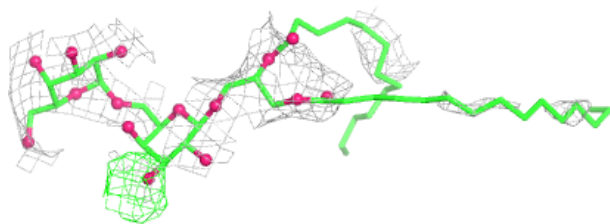


Electron density around CLA c 501:

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

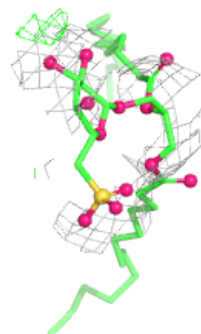
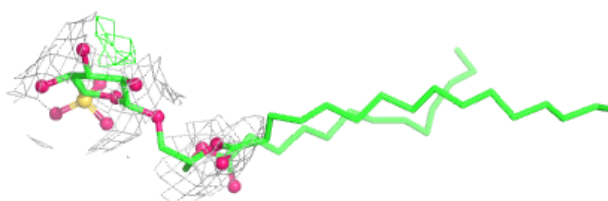
**Electron density around DGD b 624:**

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

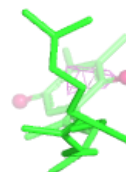
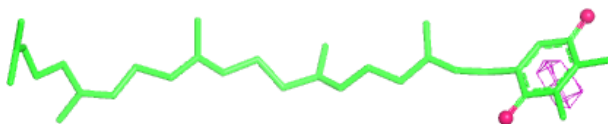
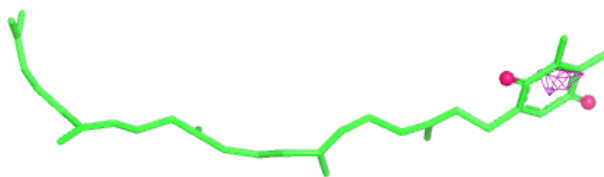


Electron density around SQD a 415:

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

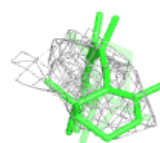
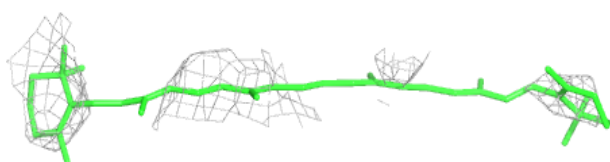
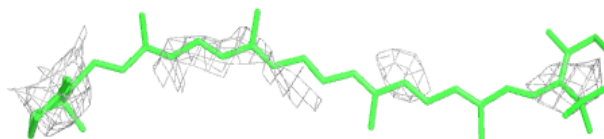
**Electron density around PL9 j 101:**

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

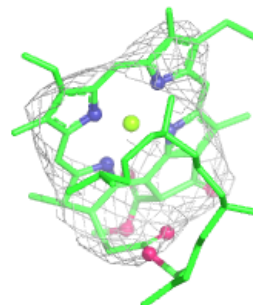
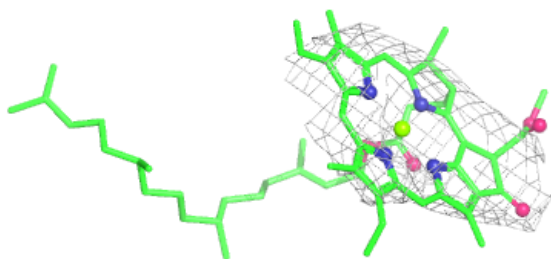
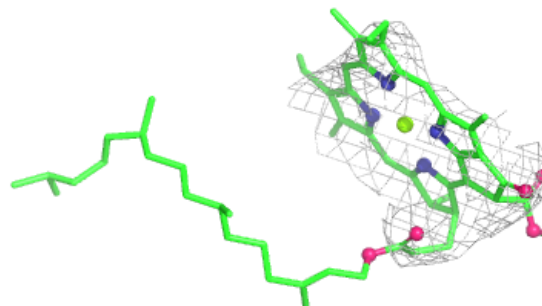


Electron density around BCR x 101:

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

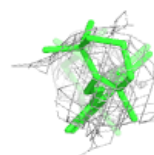
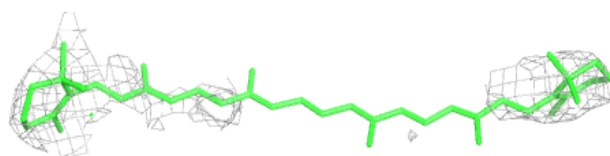
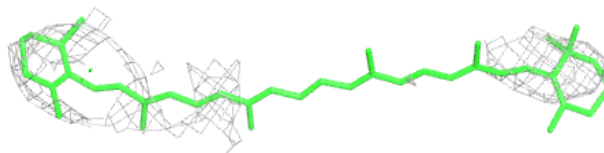
**Electron density around CLA C 512:**

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

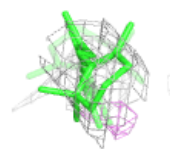
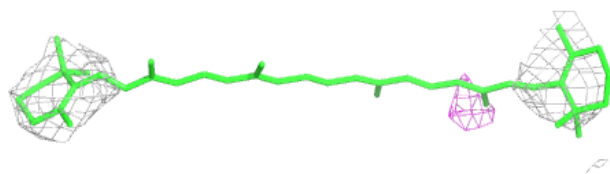
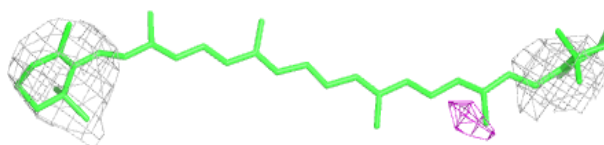


Electron density around BCR B 619:

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

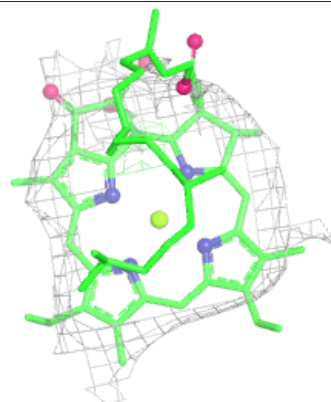
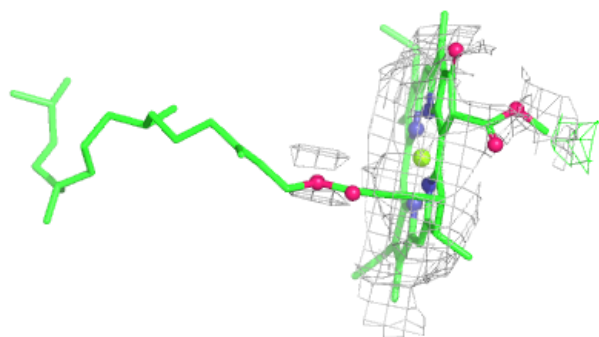
**Electron density around BCR C 521:**

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

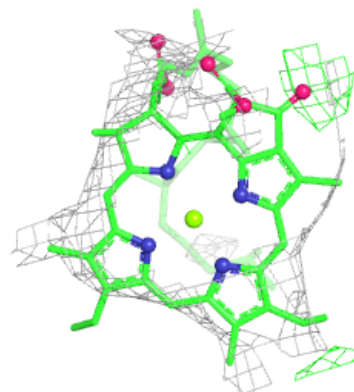
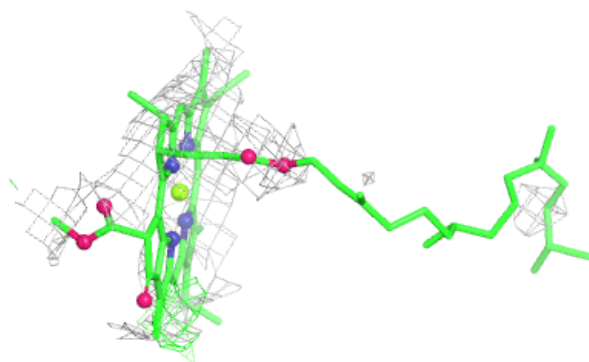
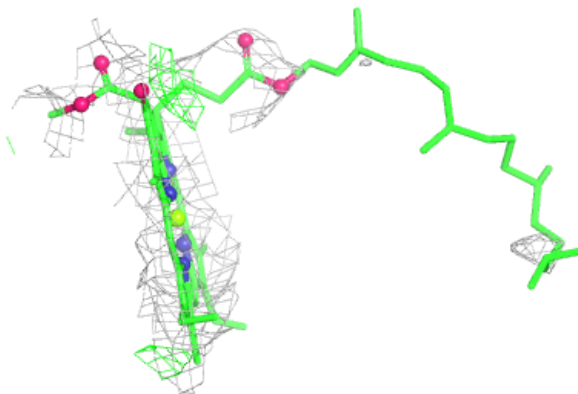


Electron density around CLA c 505:

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

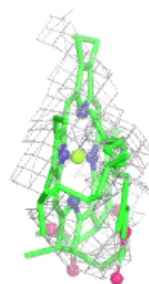
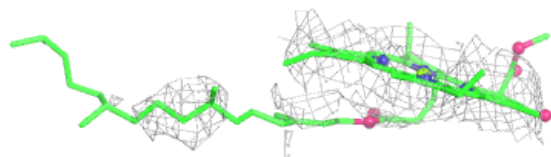
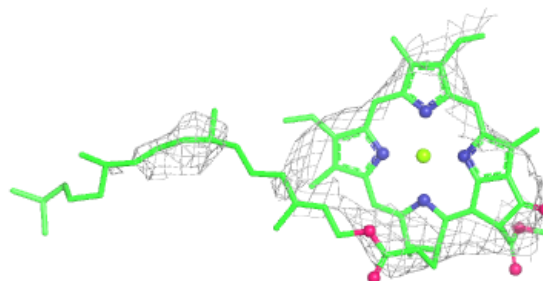
**Electron density around CLA C 505:**

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

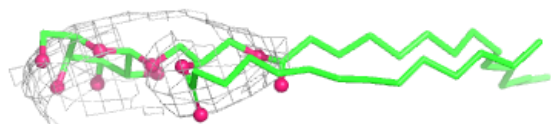
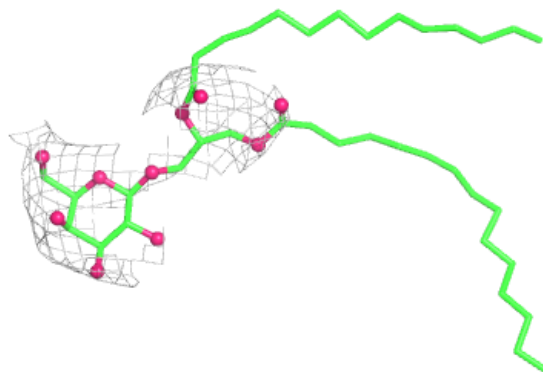


Electron density around CLA b 606:

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

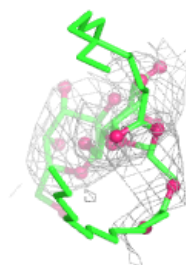
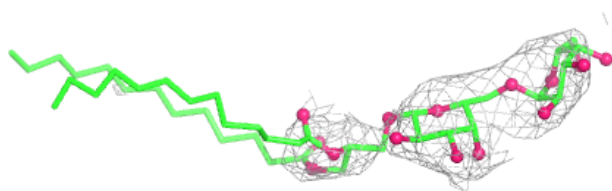
**Electron density around LMG C 522:**

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

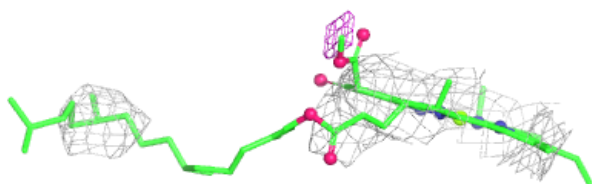
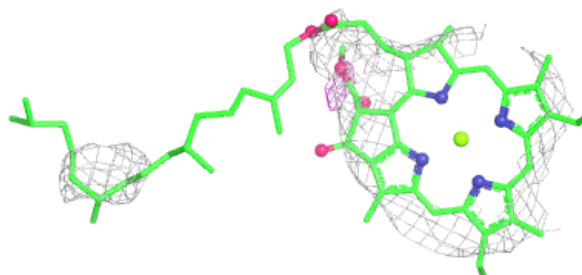


Electron density around DGD a 411:

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

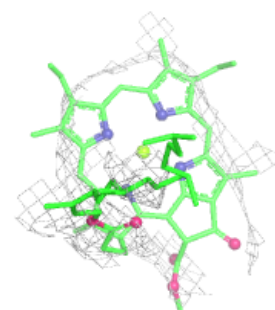
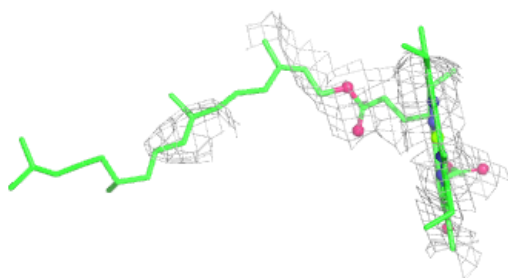
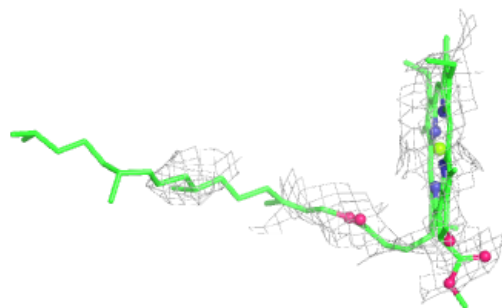
**Electron density around CLA h 101:**

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

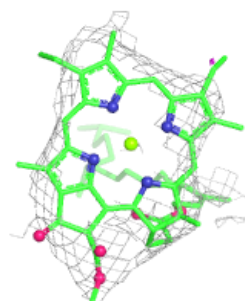
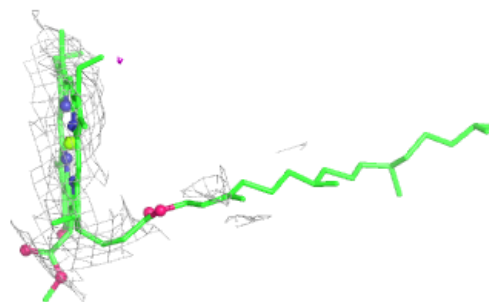


Electron density around CLA b 609:

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

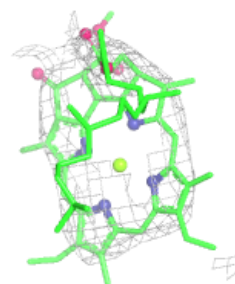
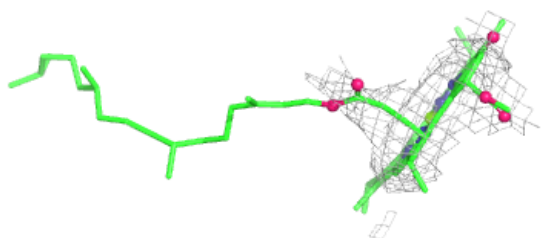
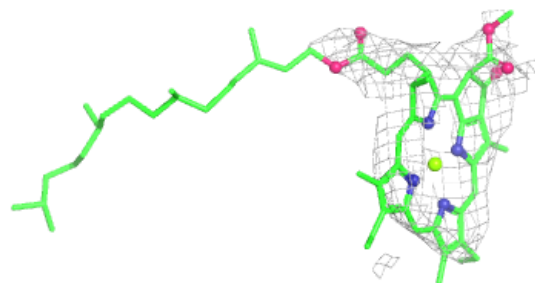
**Electron density around CLA B 605:**

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

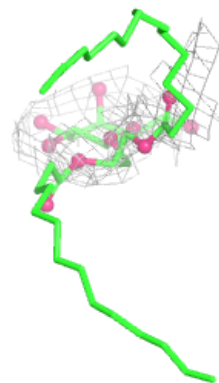
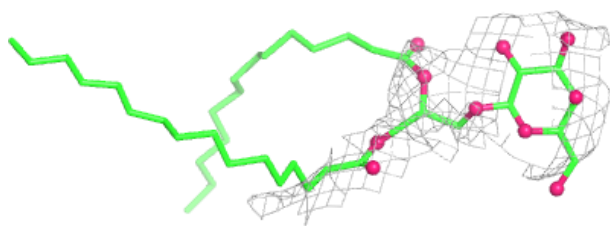
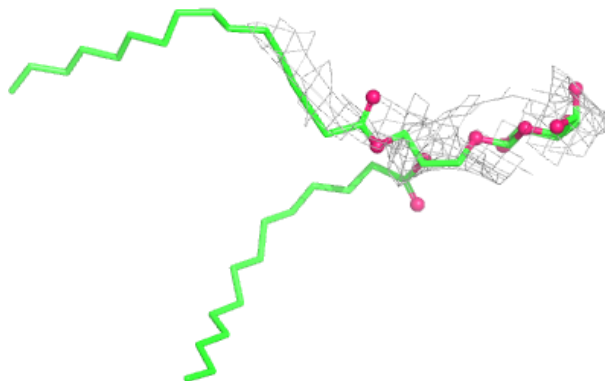


Electron density around CLA A 405:

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

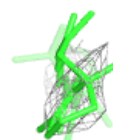
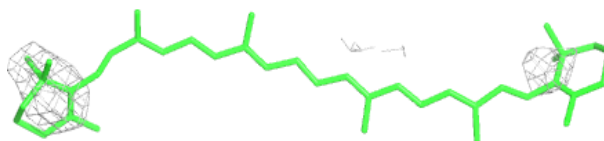
**Electron density around LMG B 621:**

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



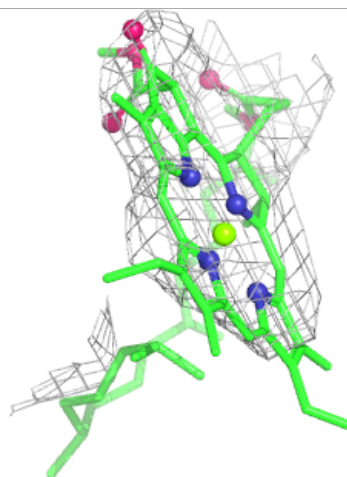
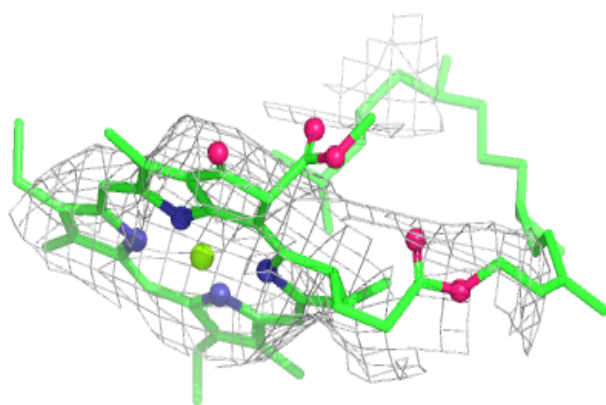
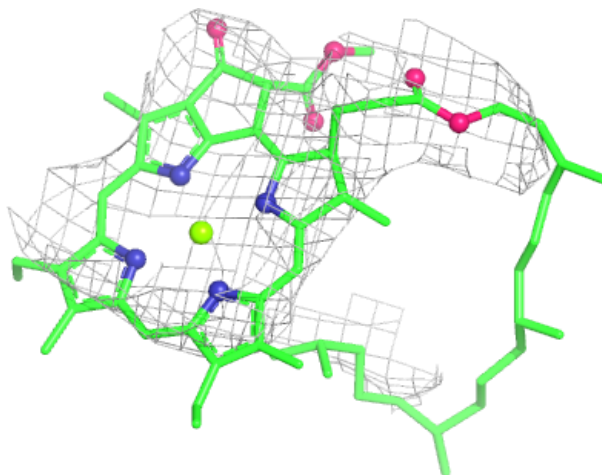
Electron density around BCR g 101:

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



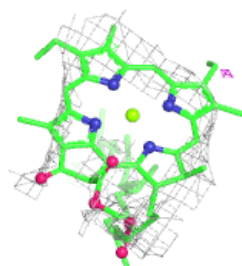
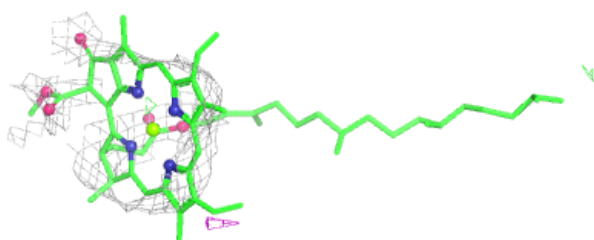
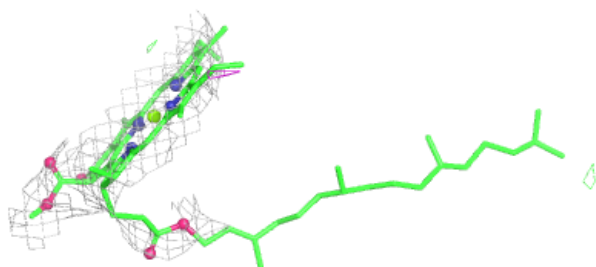
Electron density around CLA b 618:

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

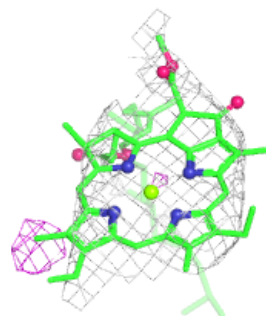
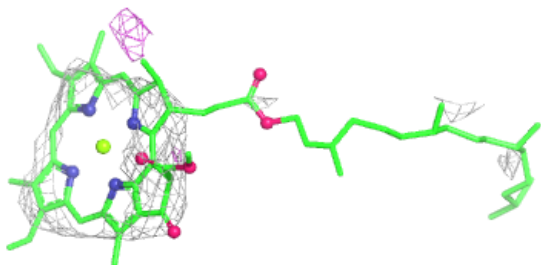
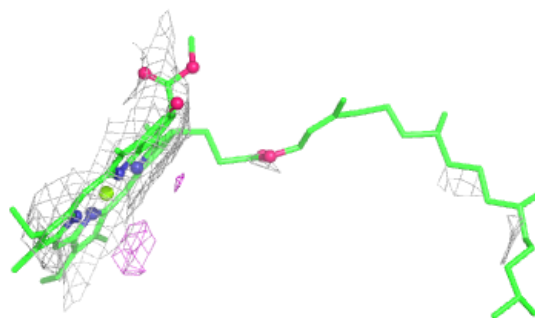


Electron density around CLA C 520:

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

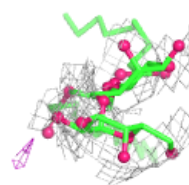
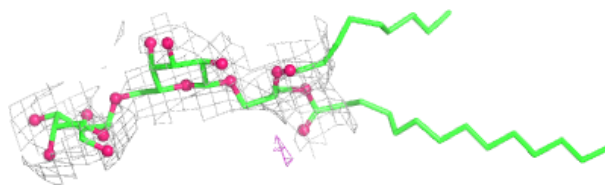
**Electron density around CLA D 405:**

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

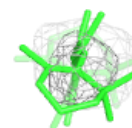
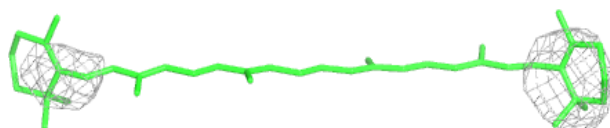
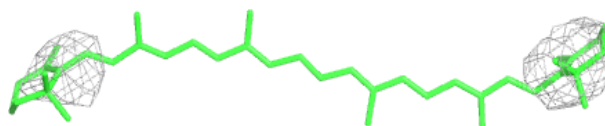


Electron density around DGD C 515:

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

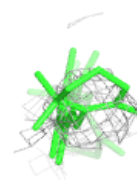
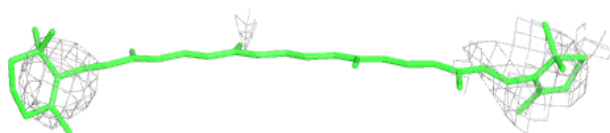
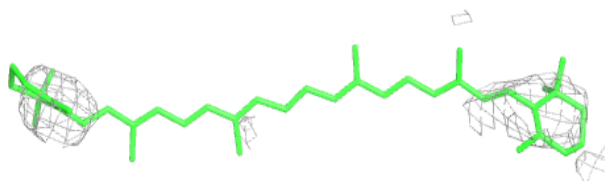
**Electron density around BCR A 407:**

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

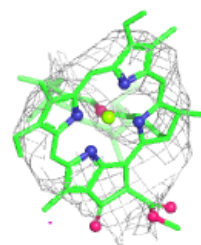
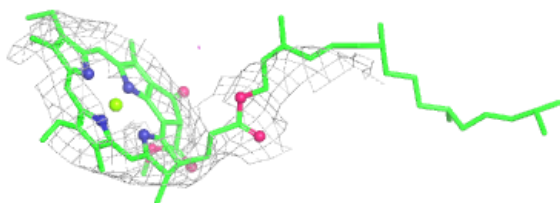


Electron density around BCR B 616:

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

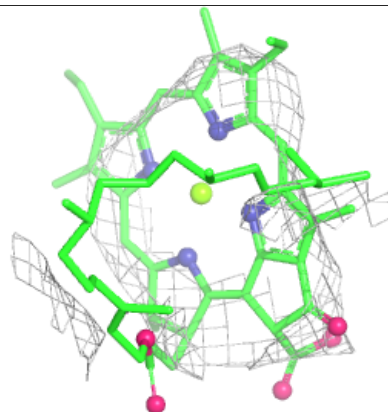
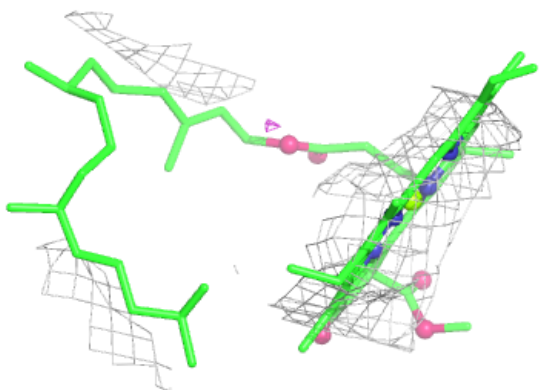
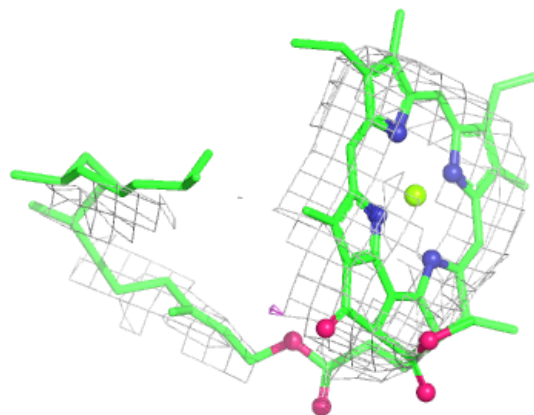
**Electron density around CLA c 502:**

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

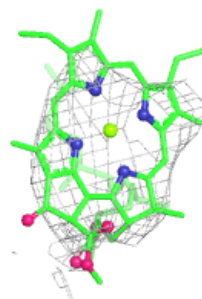
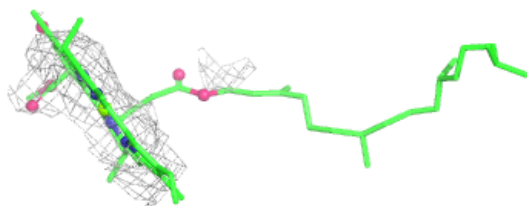
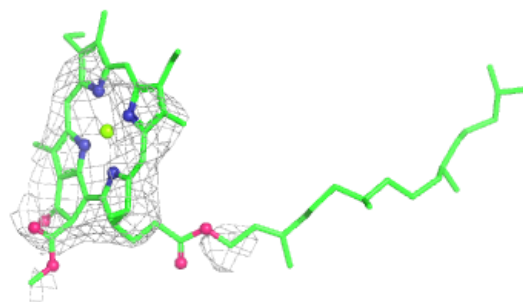


Electron density around CLA c 503:

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

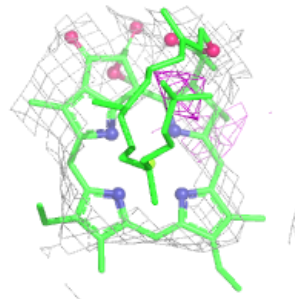
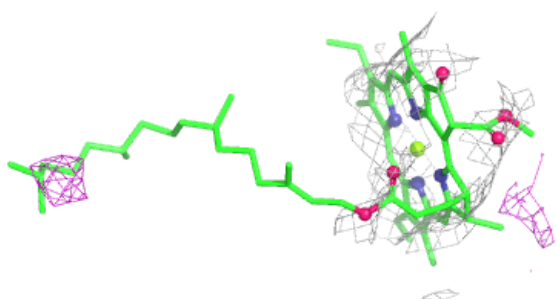
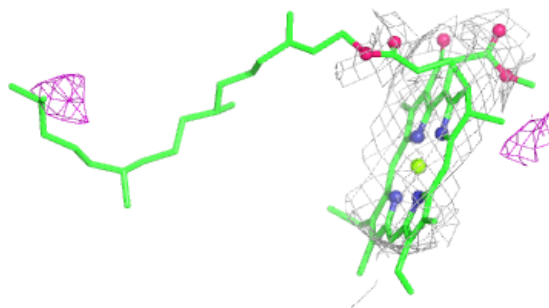
**Electron density around CLA a 408:**

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

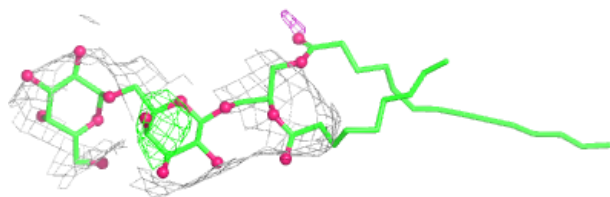
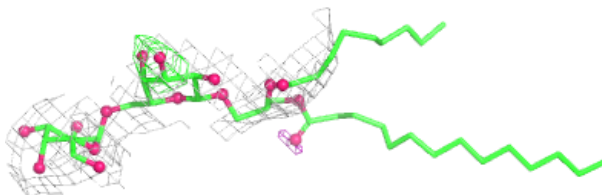


Electron density around CLA C 507:

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

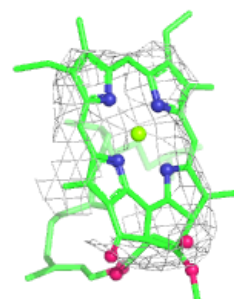
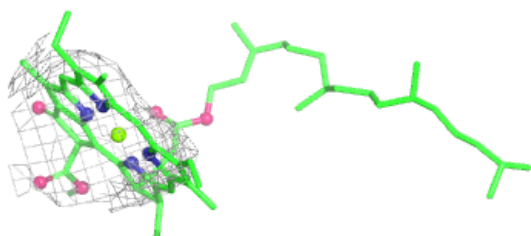
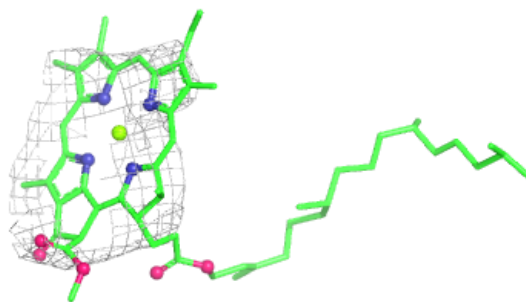
**Electron density around DGD c 515:**

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

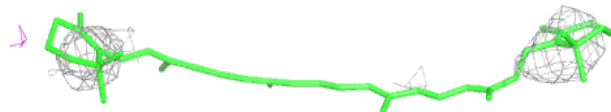
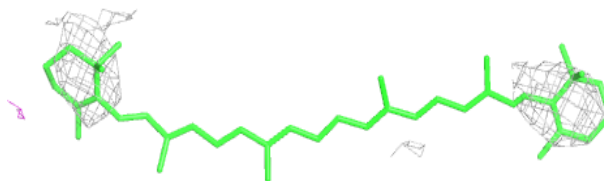


Electron density around CLA c 510:

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

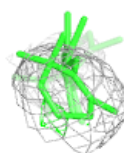
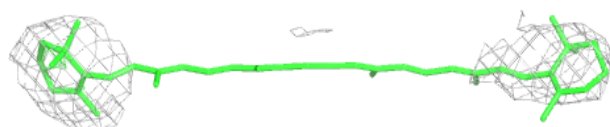
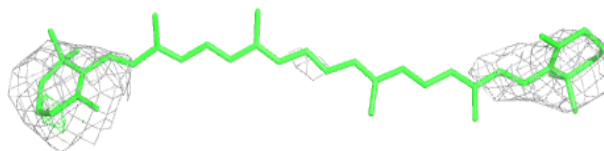
**Electron density around BCR b 621:**

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

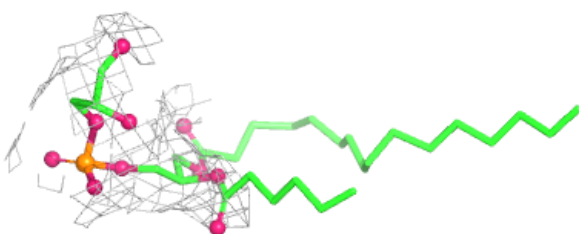
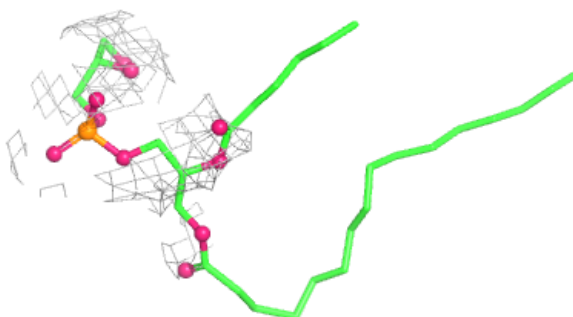


Electron density around BCR b 622:

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

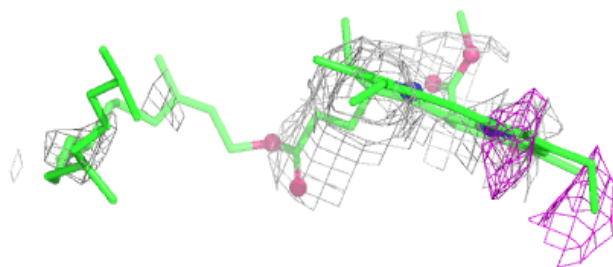
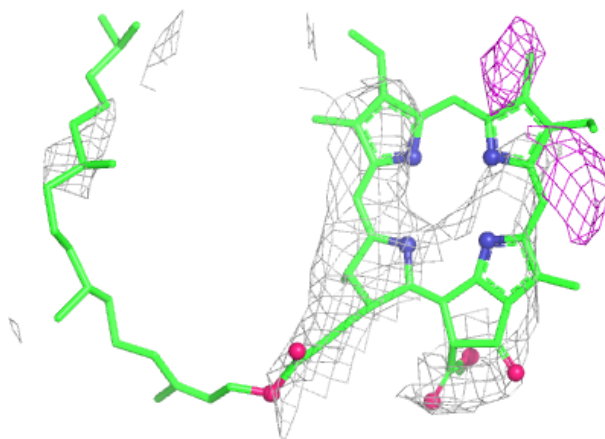
**Electron density around LHG A 409:**

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



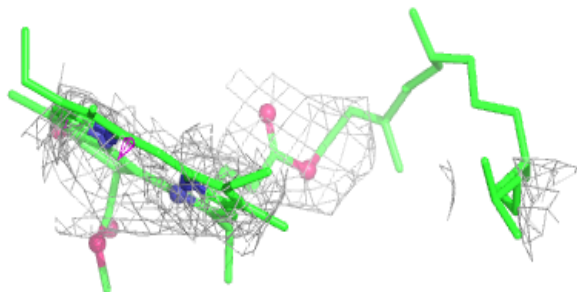
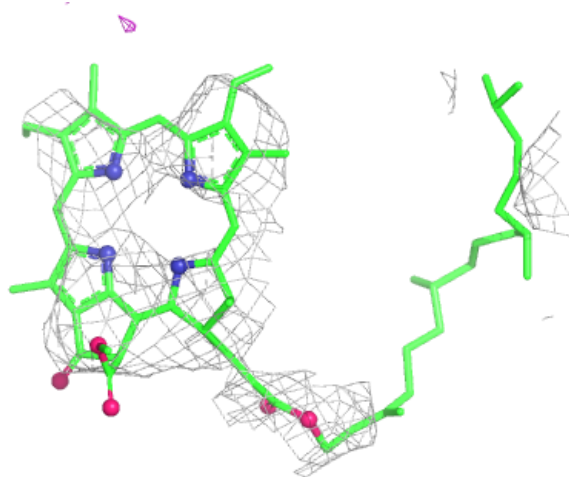
Electron density around PHO D 401:

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



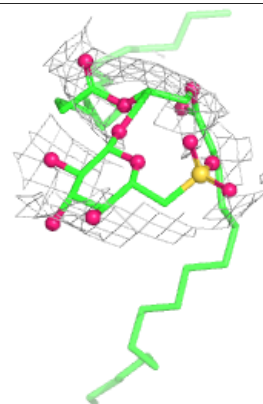
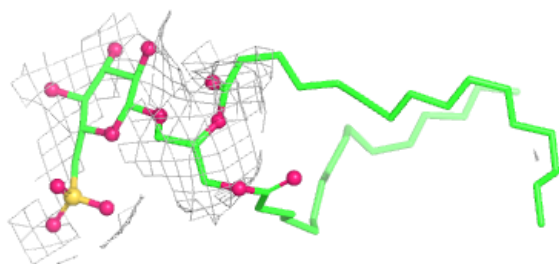
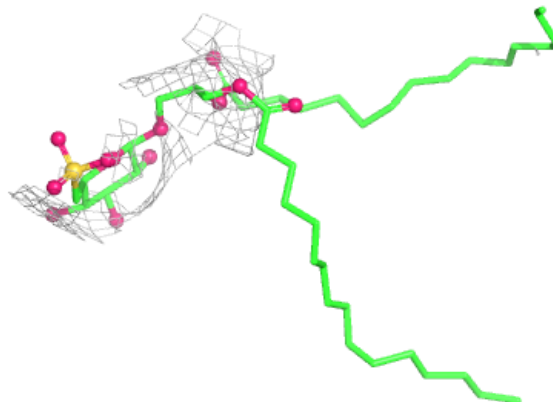
Electron density around PHO D 402:

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



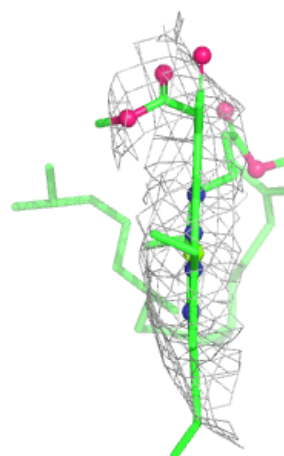
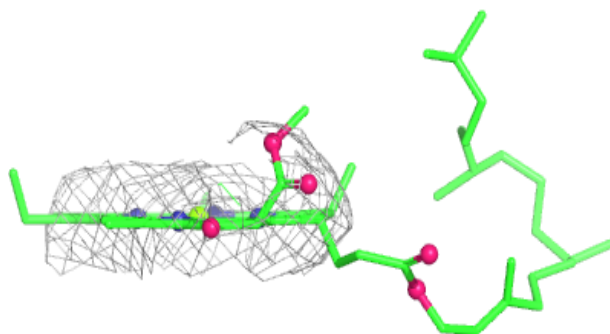
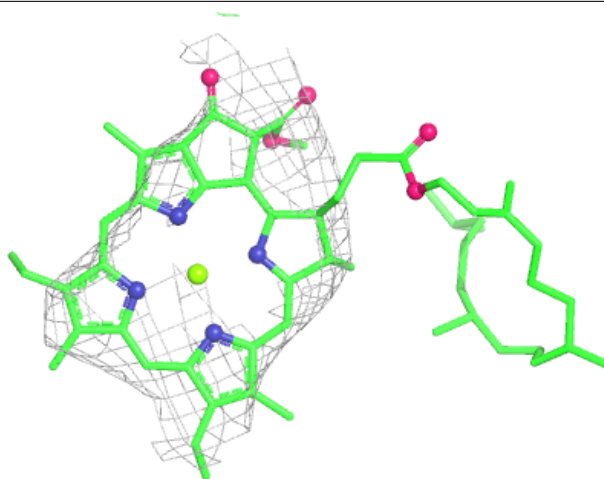
Electron density around SQD A 414:

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



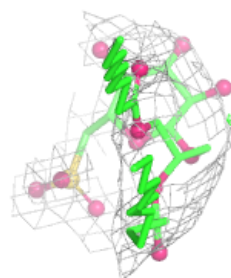
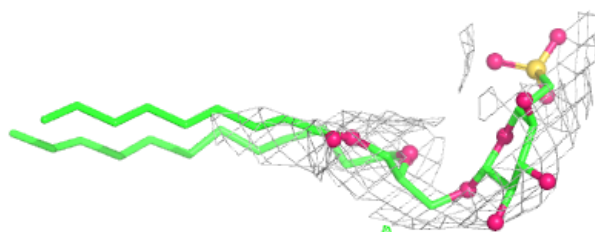
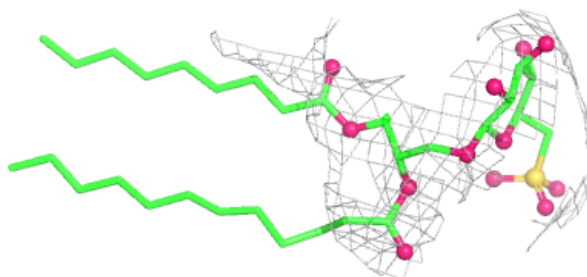
Electron density around CLA c 511:

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

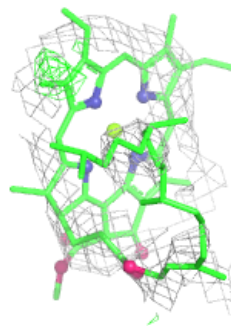
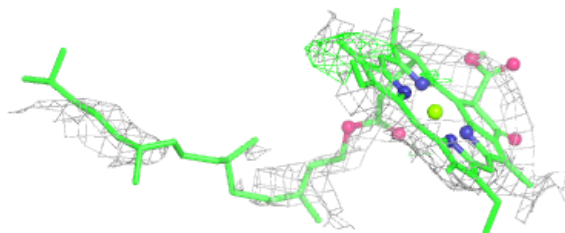


Electron density around SQD D 403:

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

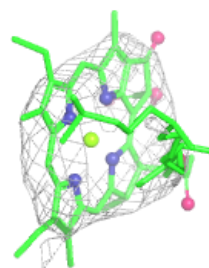
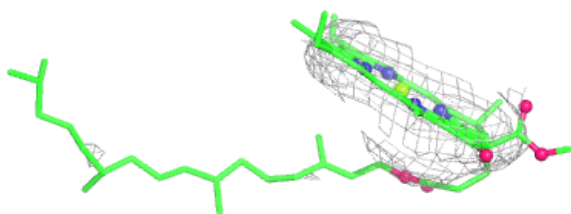
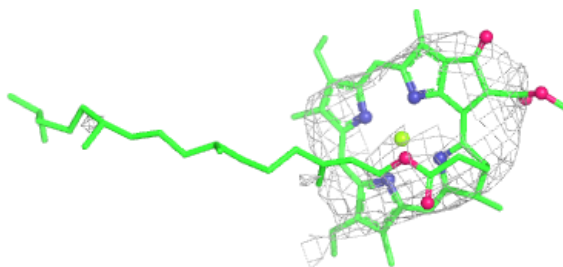
**Electron density around CLA C 510:**

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

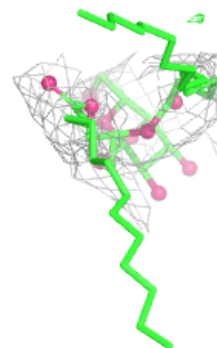
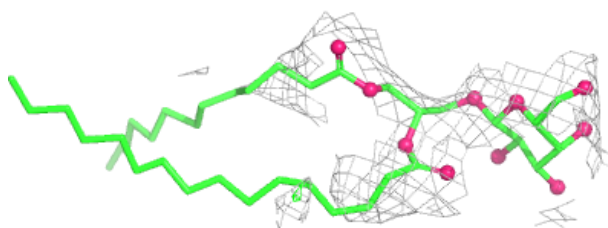
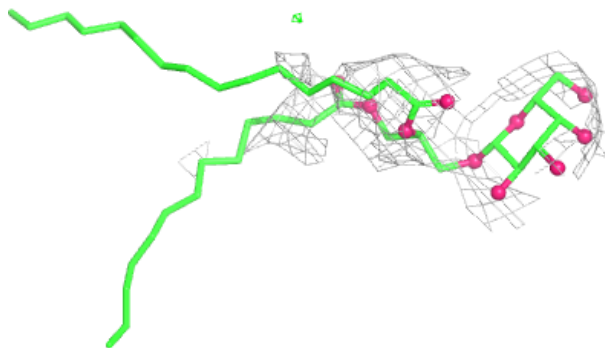


Electron density around CLA B 607:

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

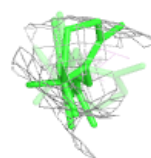
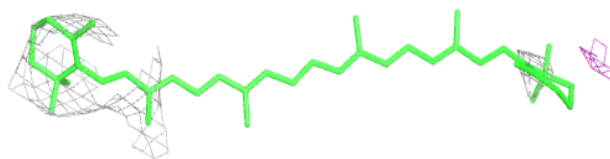
**Electron density around LMG d 407:**

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



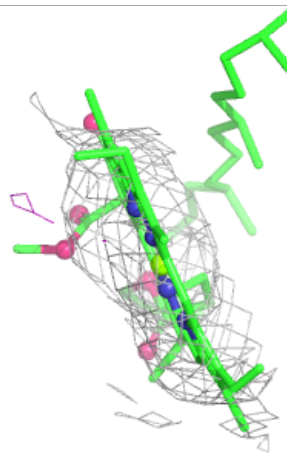
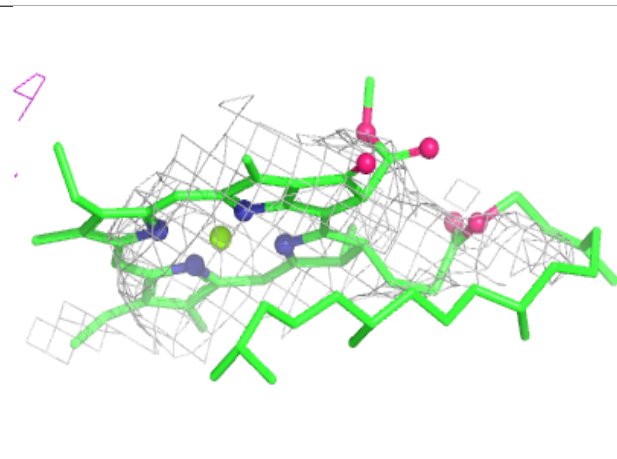
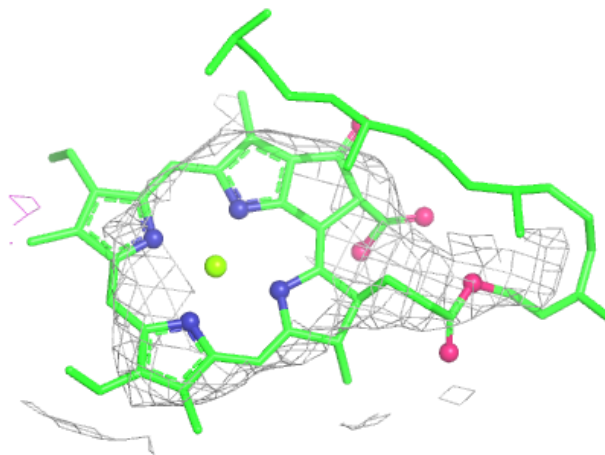
Electron density around BCR b 620:

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



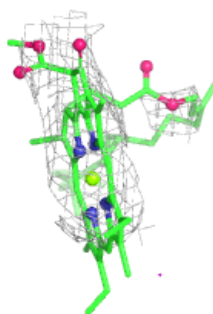
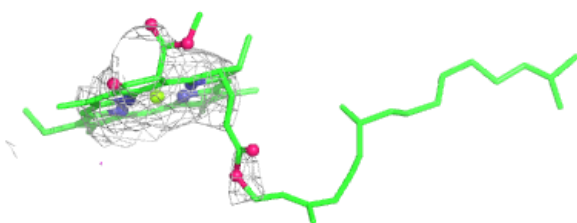
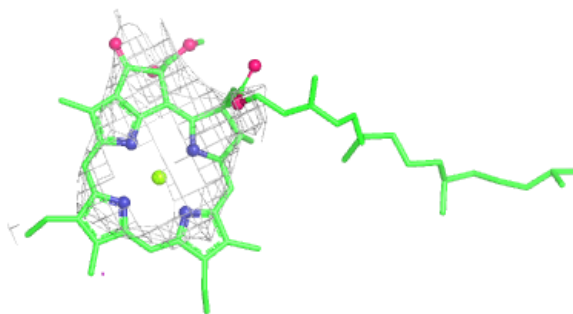
Electron density around CLA C 508:

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

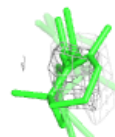
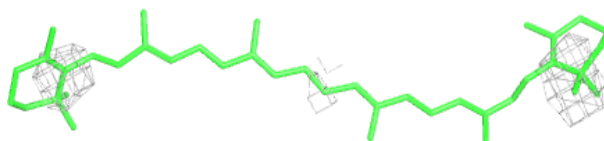


Electron density around CLA a 406:

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

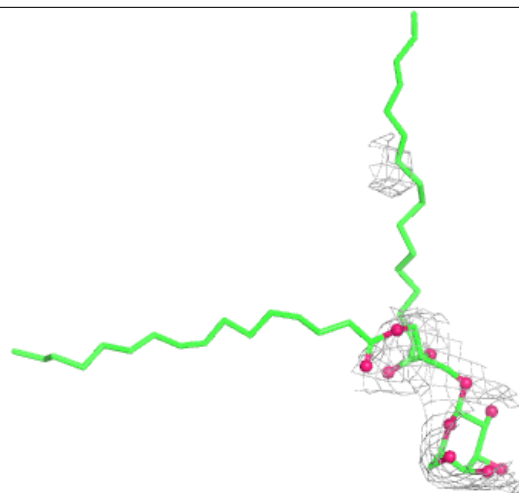
**Electron density around BCR y 101:**

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



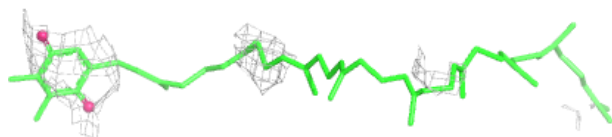
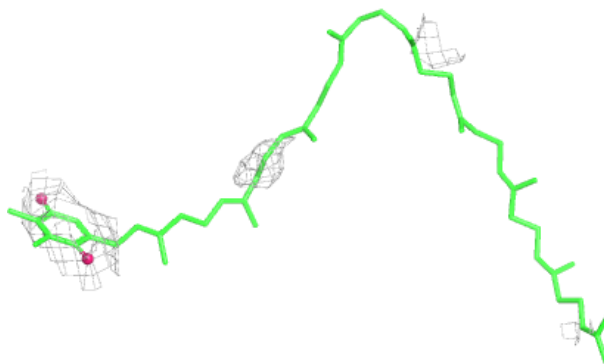
Electron density around LMG A 410:

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

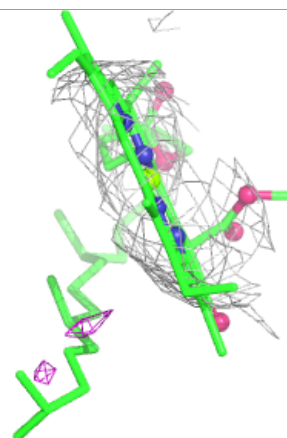
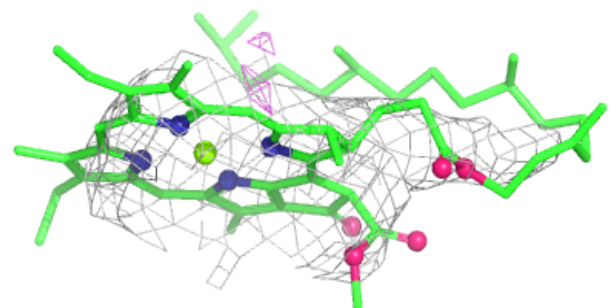
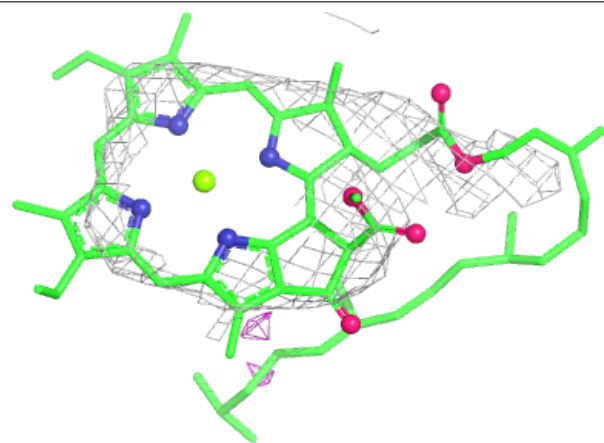


Electron density around PL9 d 406:

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

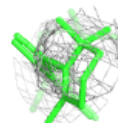
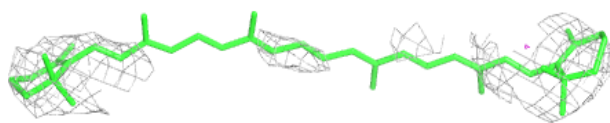
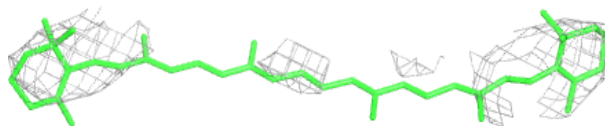
**Electron density around CLA c 508:**

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

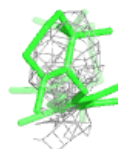
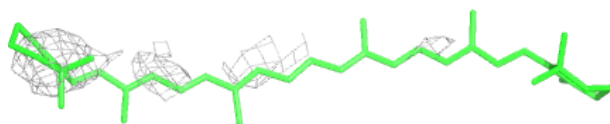
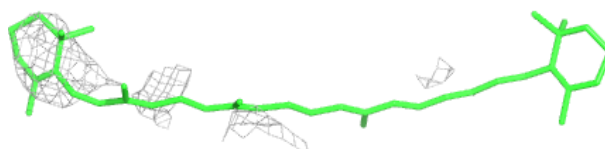


Electron density around BCR b 623:

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

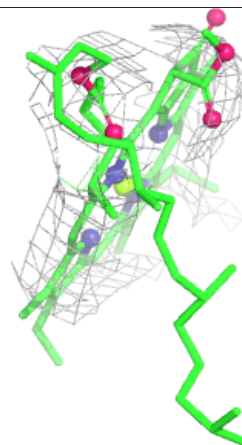
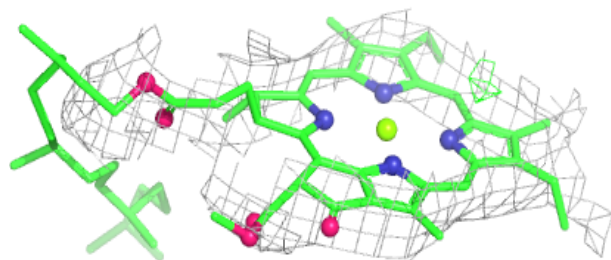
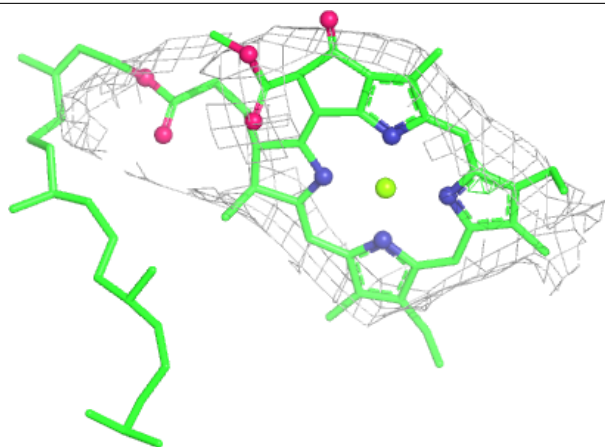
**Electron density around BCR c 513:**

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



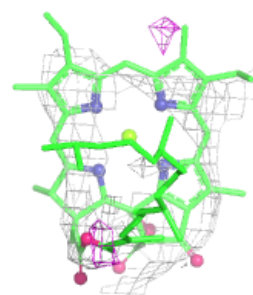
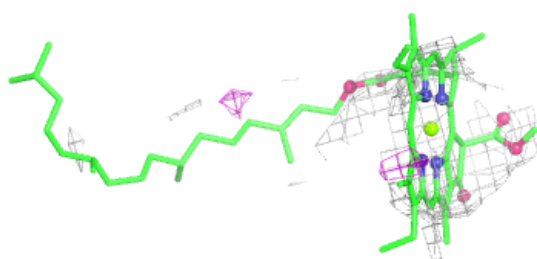
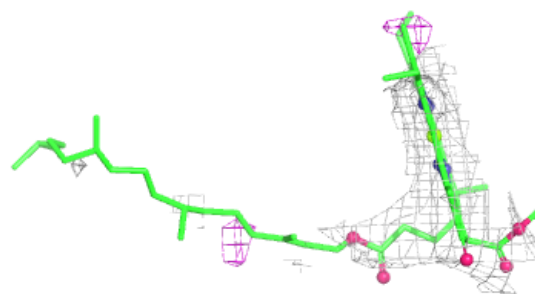
Electron density around CLA B 615:

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

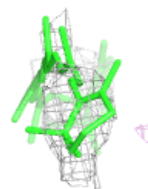
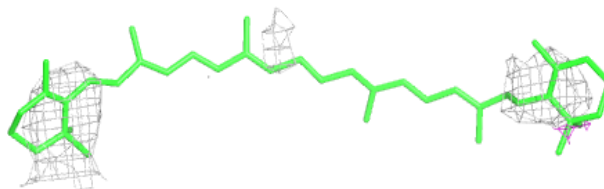


Electron density around CLA B 604:

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

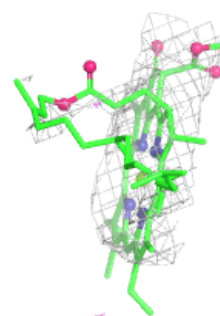
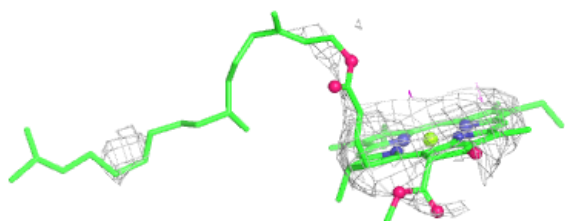
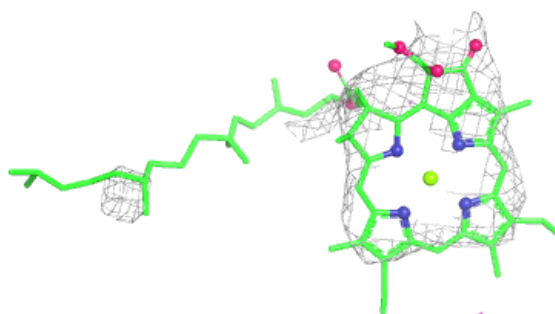
**Electron density around BCR B 617:**

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

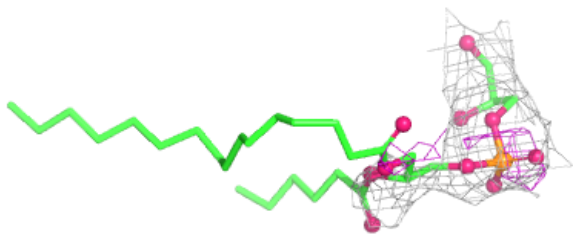
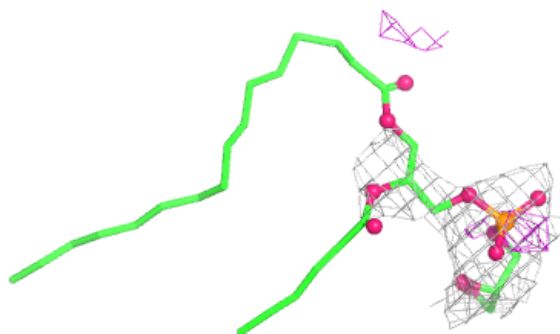


Electron density around CLA A 404:

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

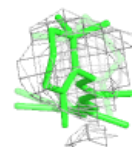
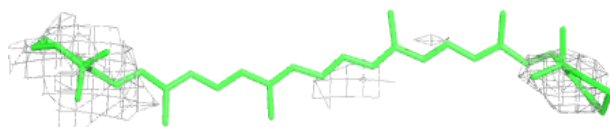
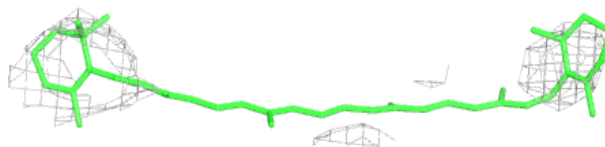
**Electron density around LHG a 412:**

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

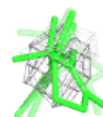
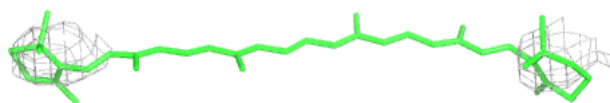
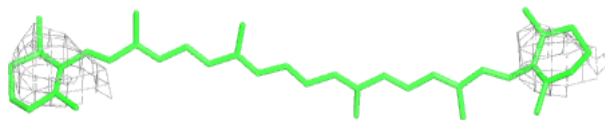


Electron density around BCR C 513:

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

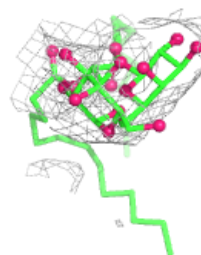
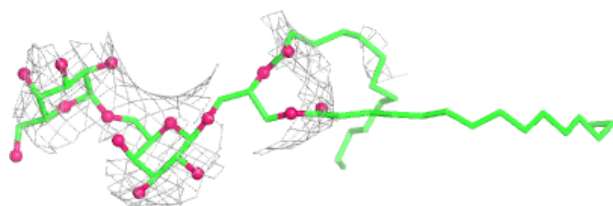
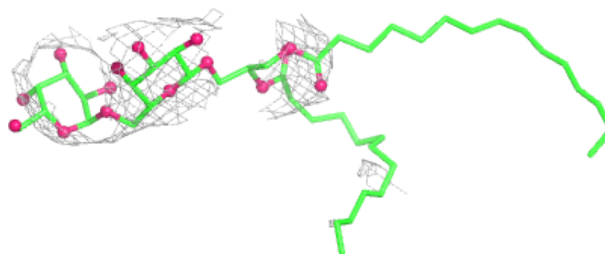
**Electron density around BCR C 514:**

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

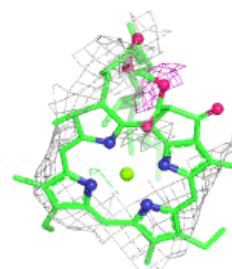
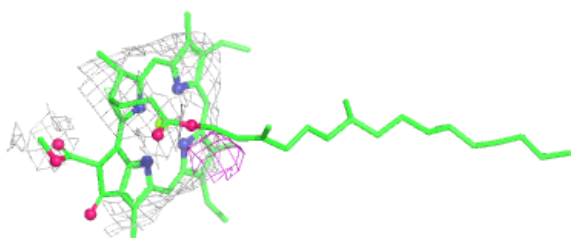
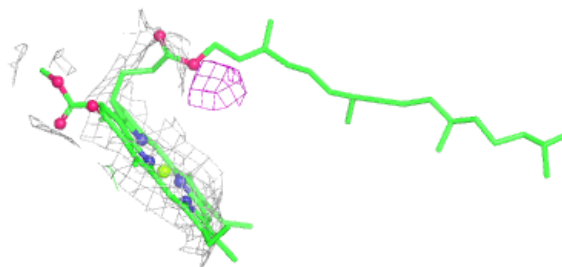


Electron density around DGD B 620:

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

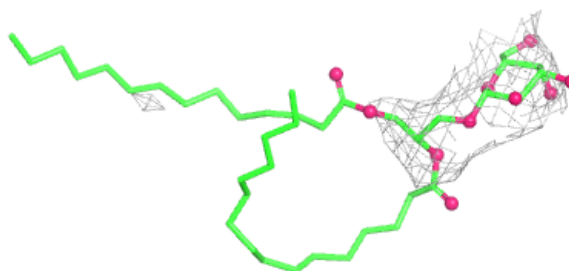
**Electron density around CLA c 520:**

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

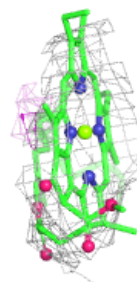
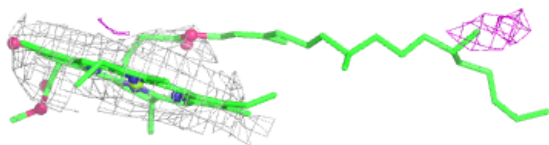
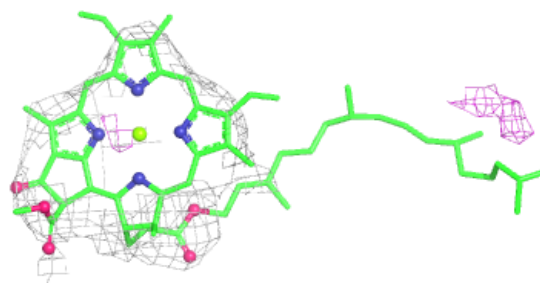


Electron density around LMG B 624:

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

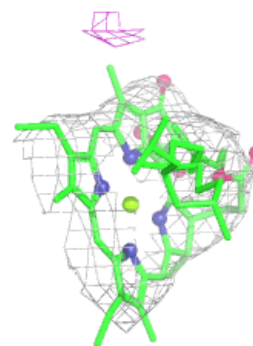
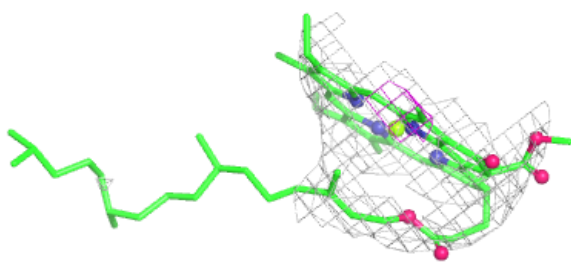
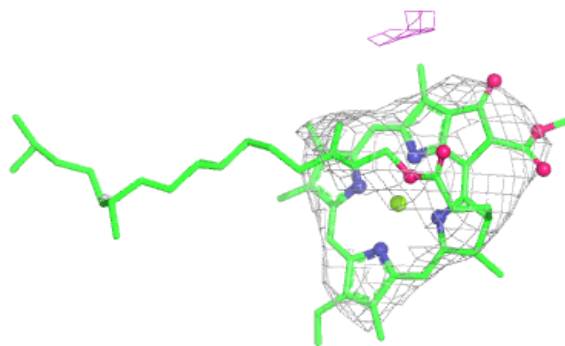
**Electron density around CLA B 602:**

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

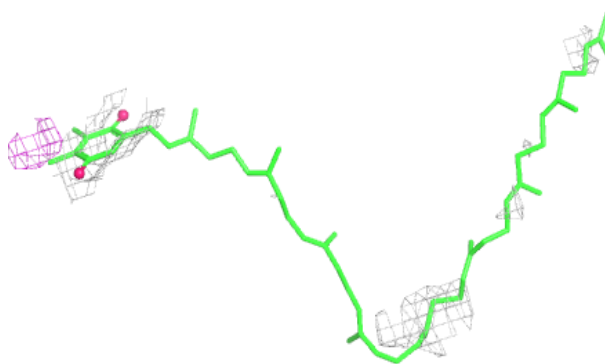


Electron density around CLA B 613:

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

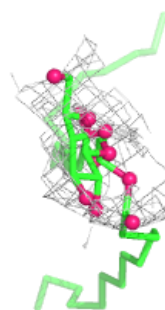
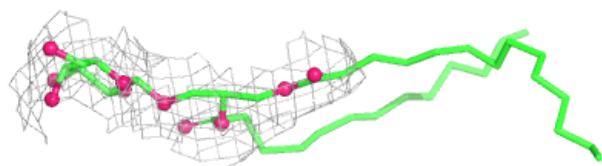
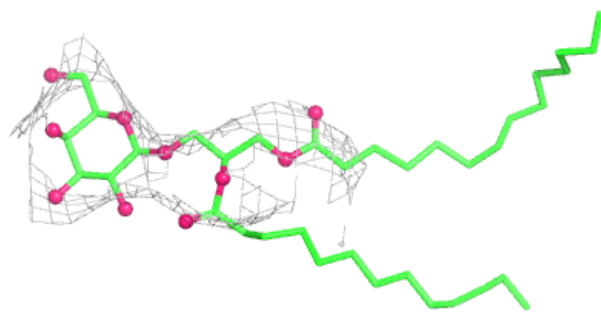
**Electron density around PL9 D 407:**

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

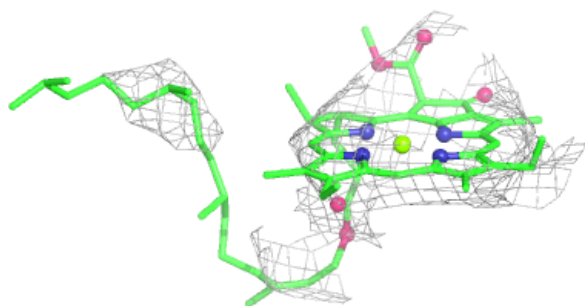
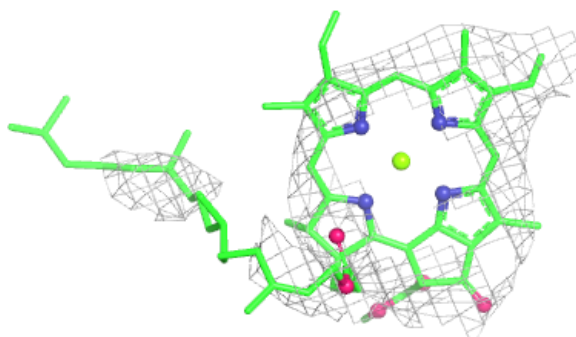


Electron density around LMG D 412:

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

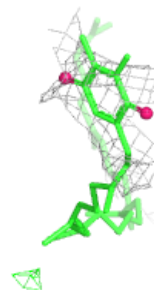
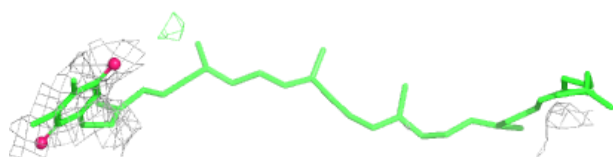
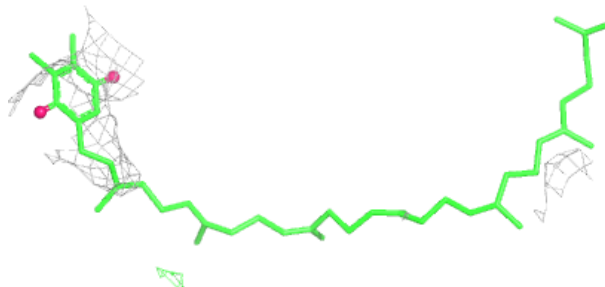
**Electron density around CLA a 405:**

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

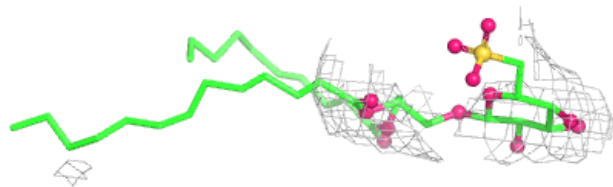
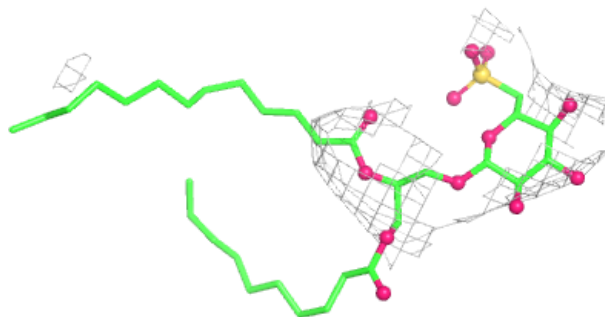


Electron density around PL9 a 409:

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

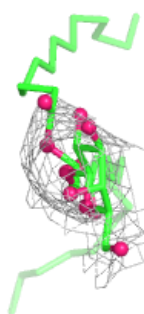
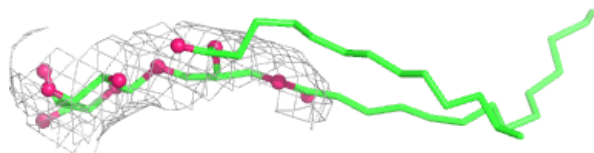
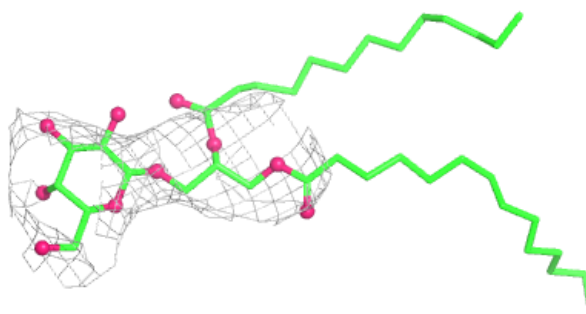
**Electron density around SQD f 103:**

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



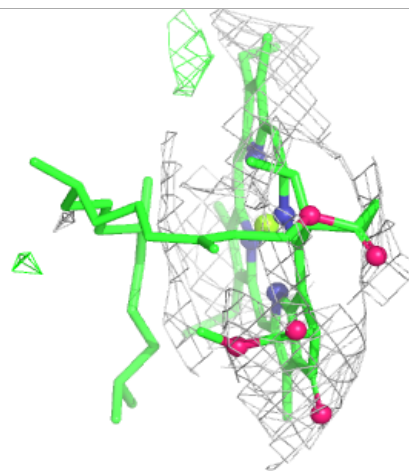
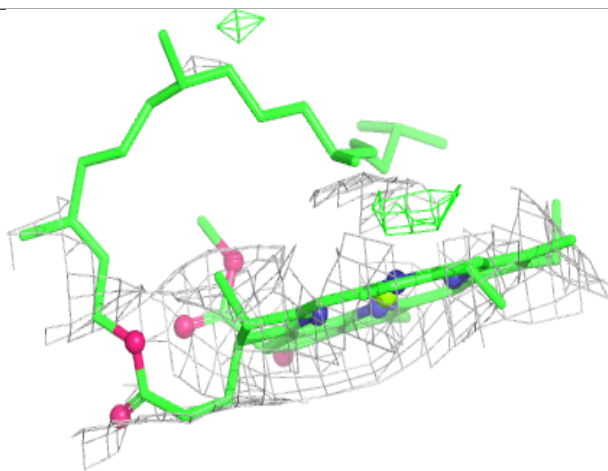
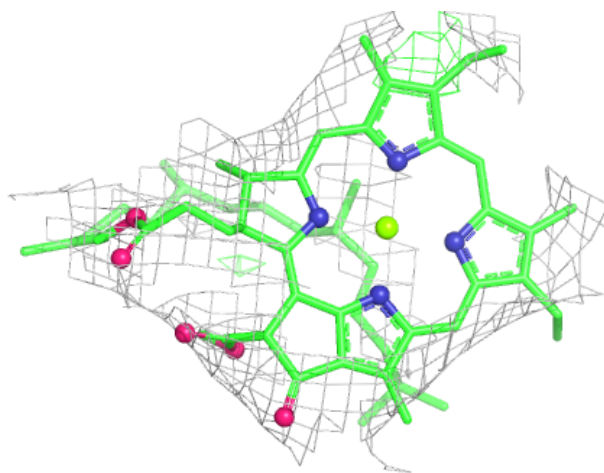
Electron density around LMG d 410:

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



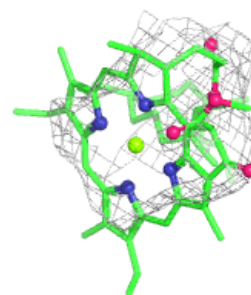
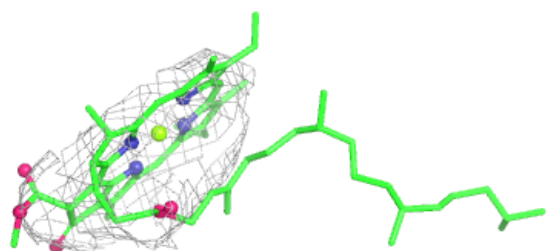
Electron density around CLA C 509:

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

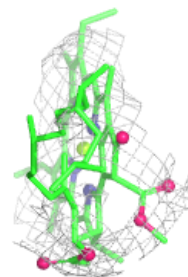
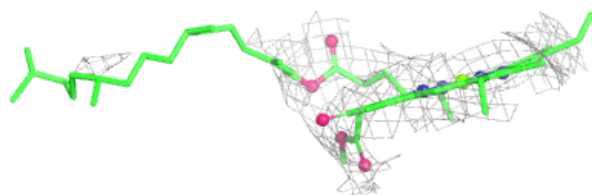
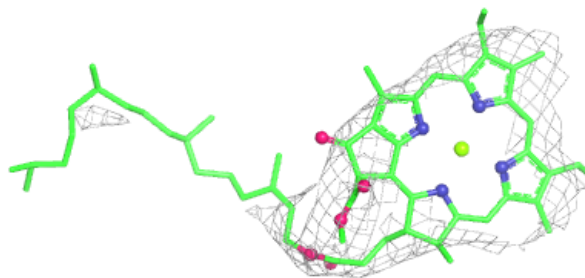


Electron density around CLA c 504:

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

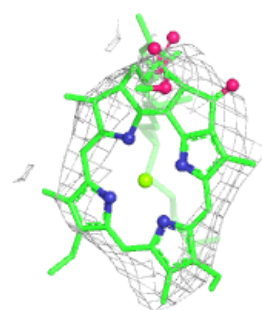
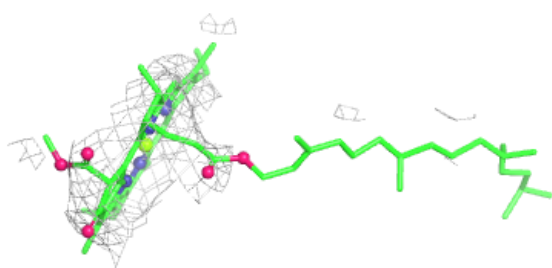
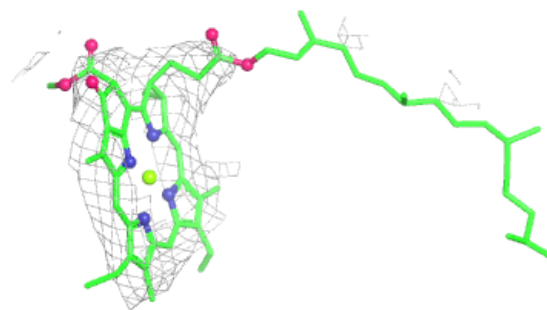
**Electron density around CLA H 101:**

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

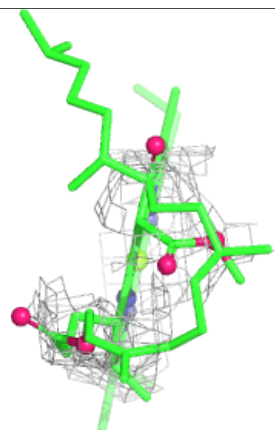
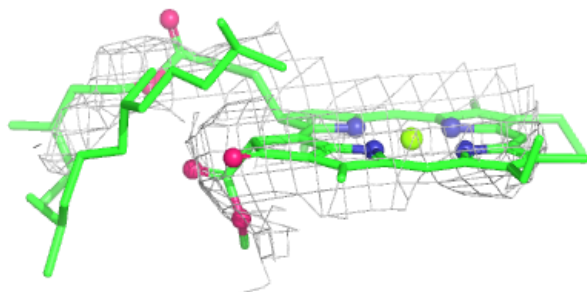
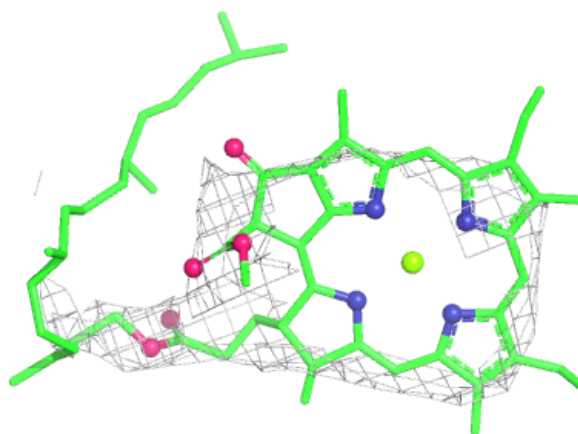


Electron density around CLA b 612:

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

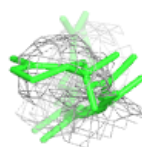
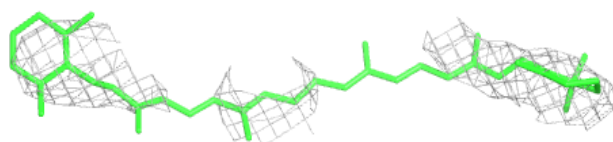
**Electron density around CLA b 613:**

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

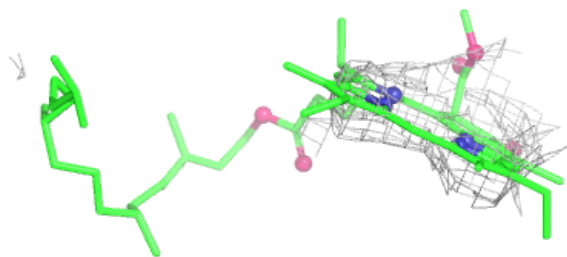
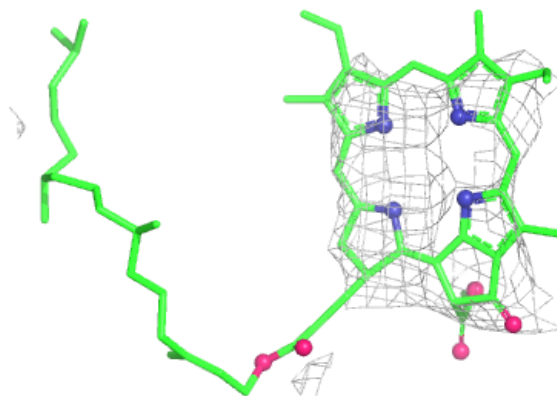


Electron density around BCR f 102:

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

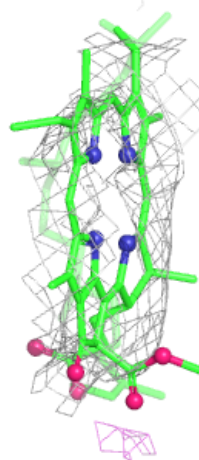
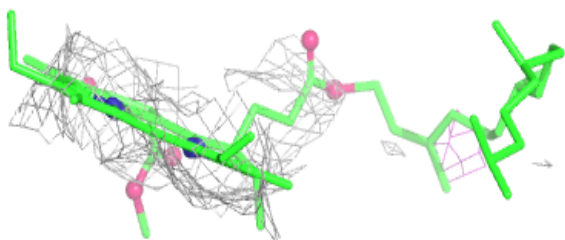
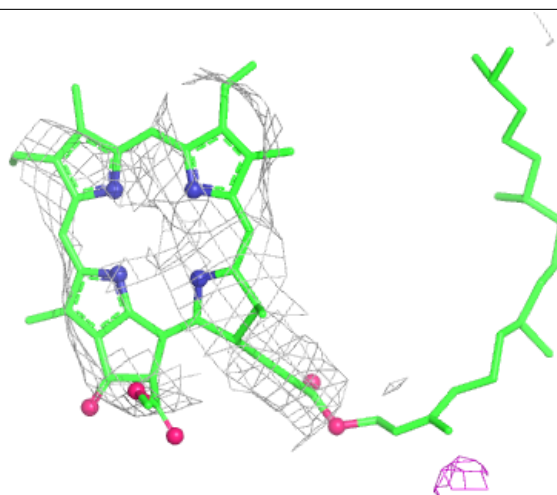
**Electron density around PHO a 407:**

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



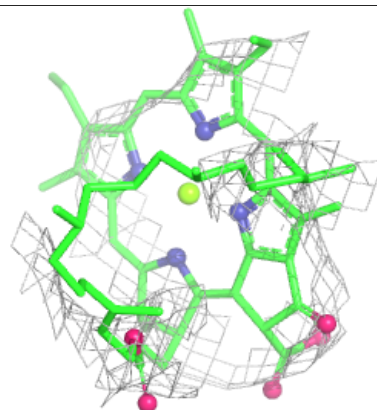
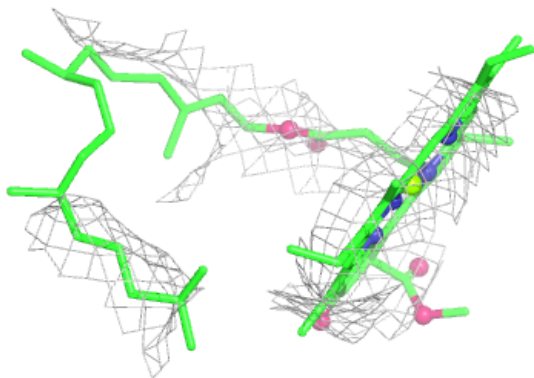
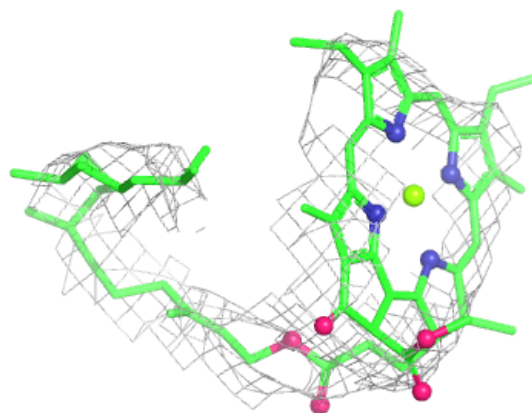
Electron density around PHO d 401:

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



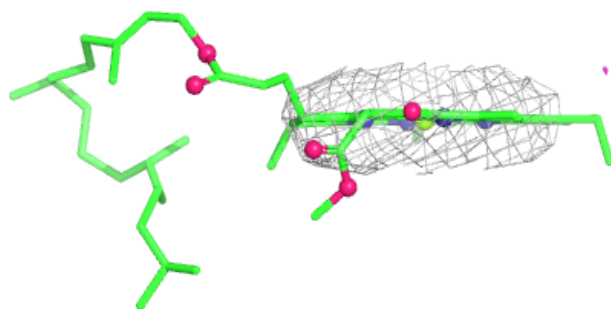
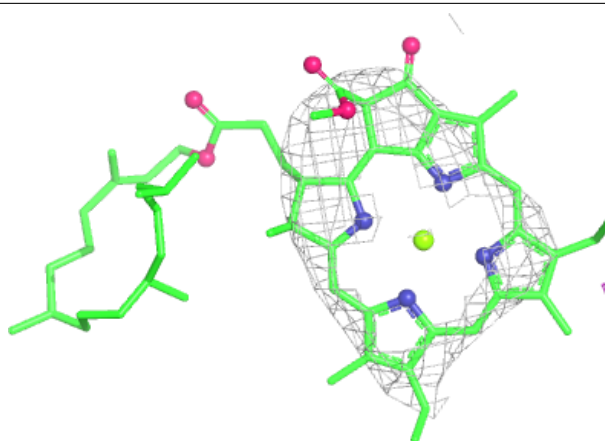
Electron density around CLA C 503:

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



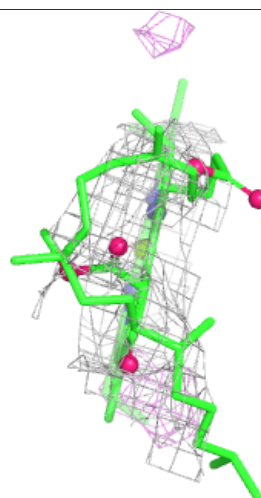
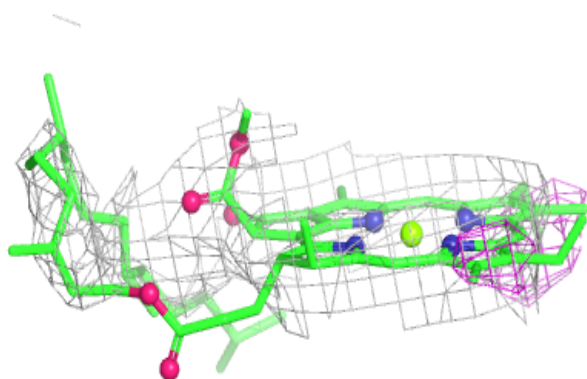
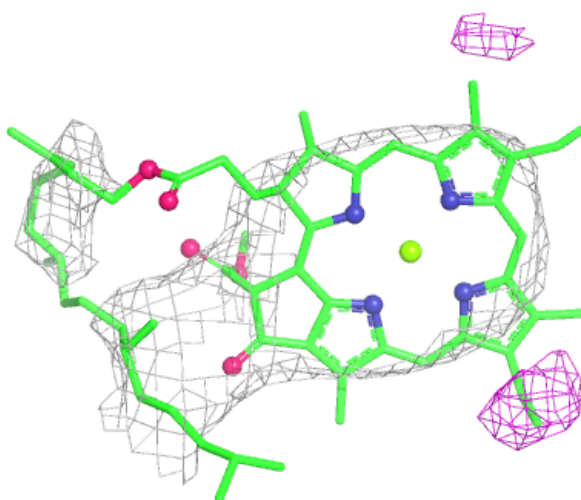
Electron density around CLA C 511:

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



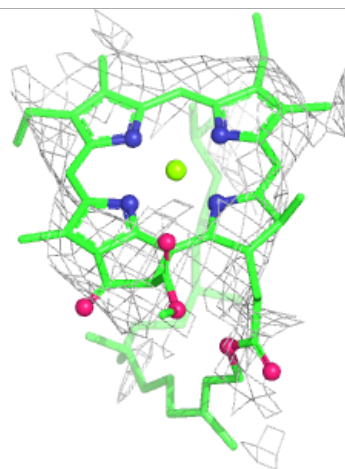
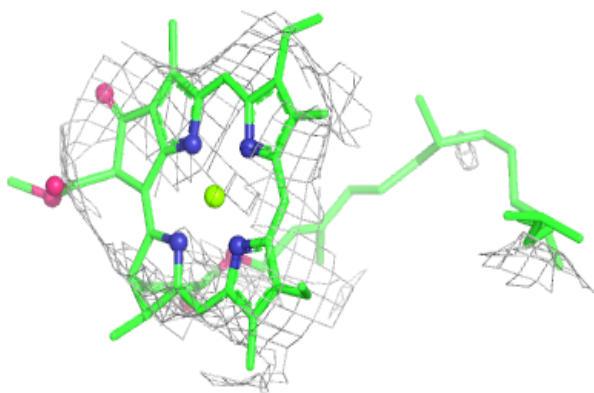
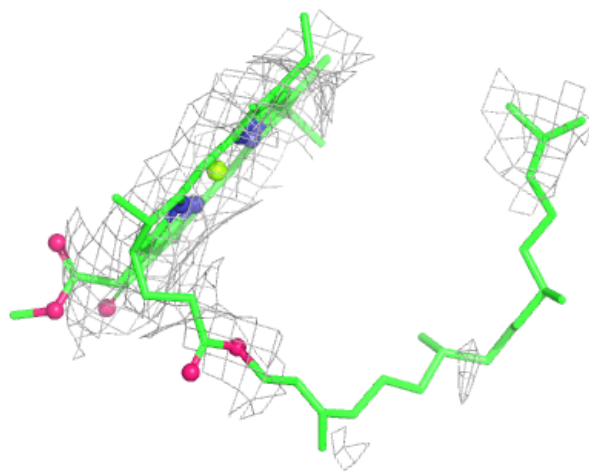
Electron density around CLA B 609:

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



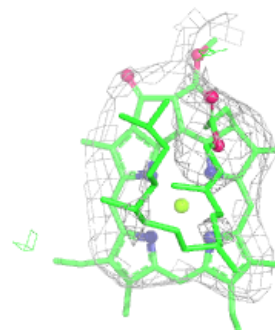
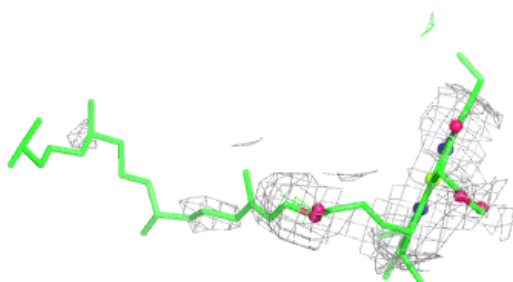
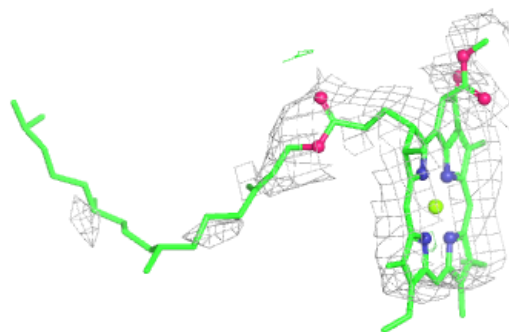
Electron density around CLA B 610:

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

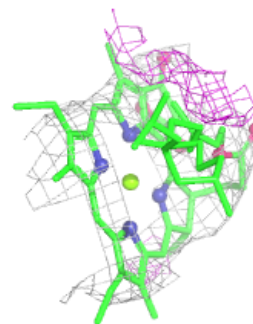
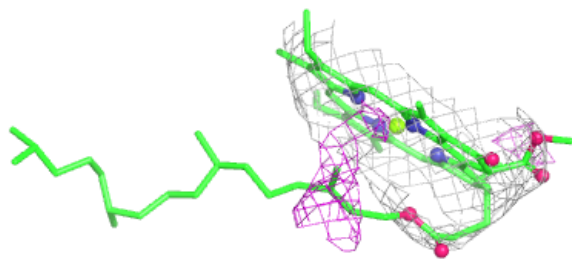
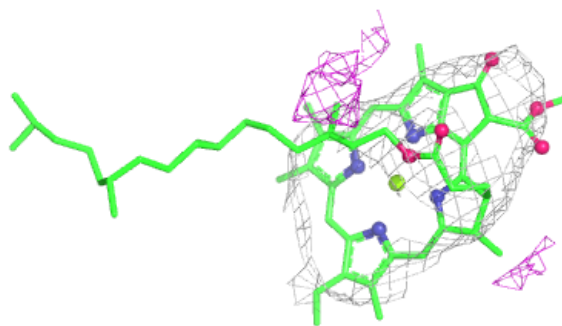


Electron density around CLA d 405:

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

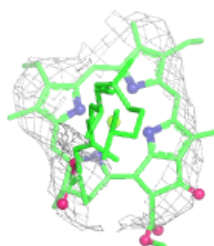
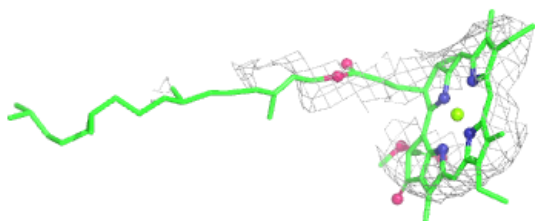
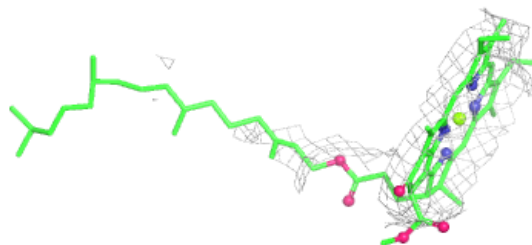
**Electron density around CLA b 617:**

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

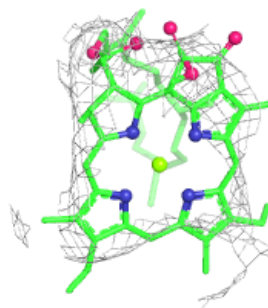
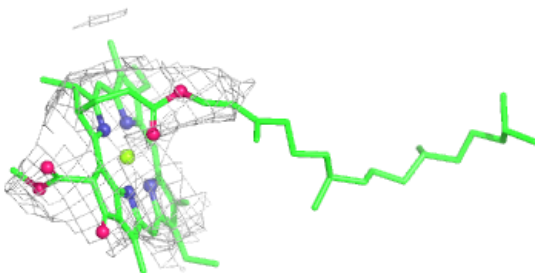
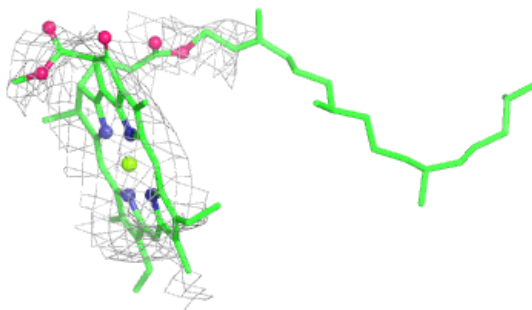


Electron density around CLA b 607:

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

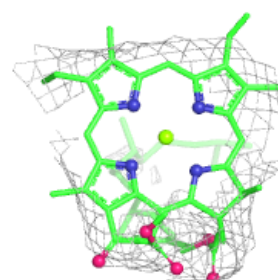
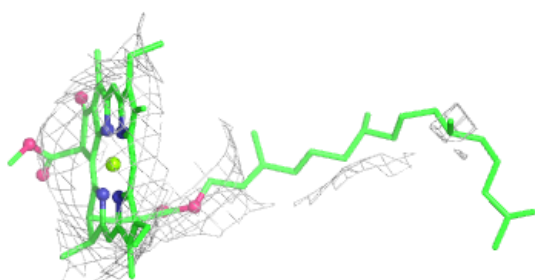
**Electron density around CLA c 507:**

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

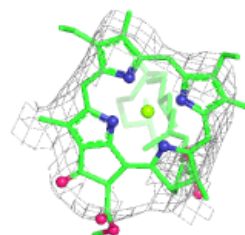
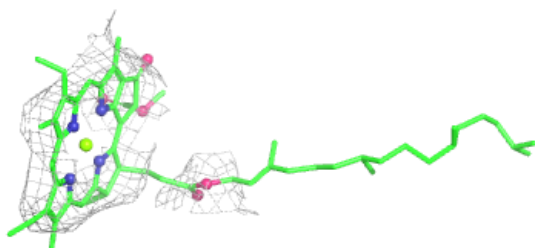
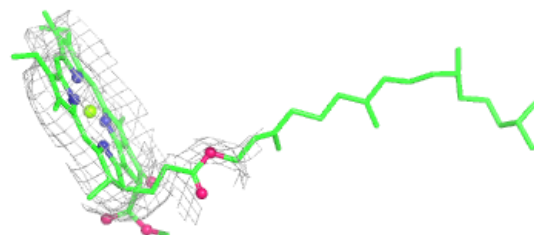


Electron density around CLA b 608:

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

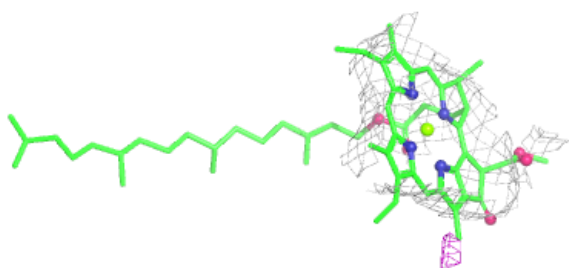
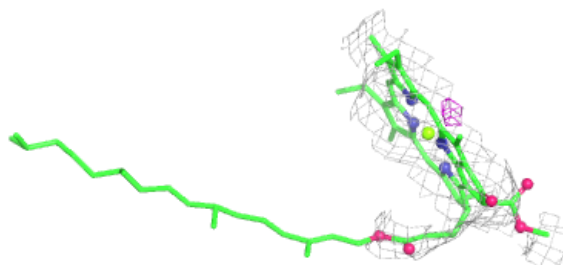
**Electron density around CLA B 603:**

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

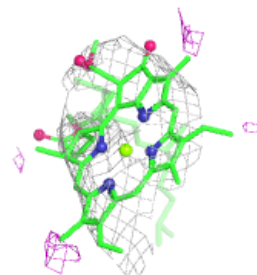
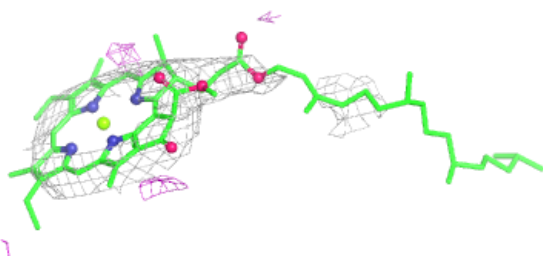
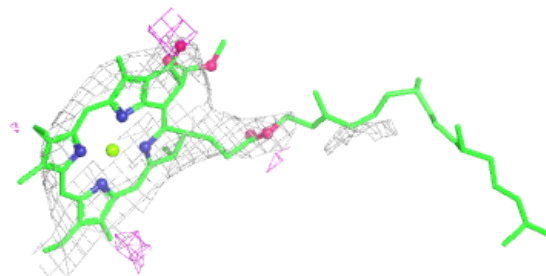


Electron density around CLA b 610:

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

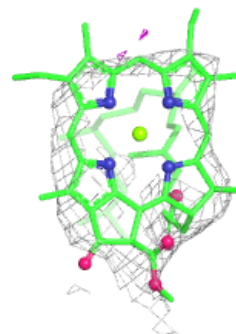
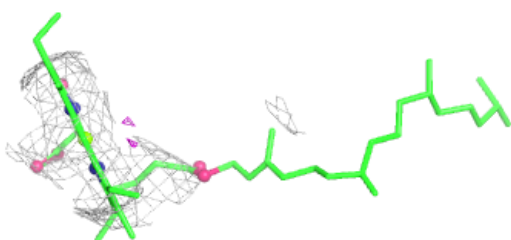
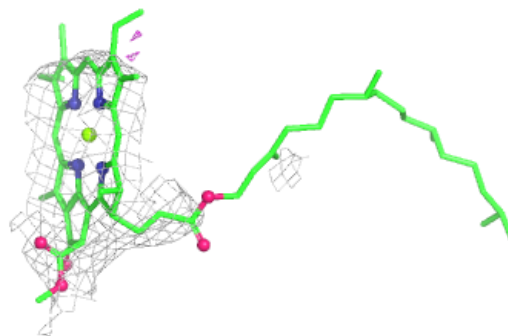
**Electron density around CLA A 402:**

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

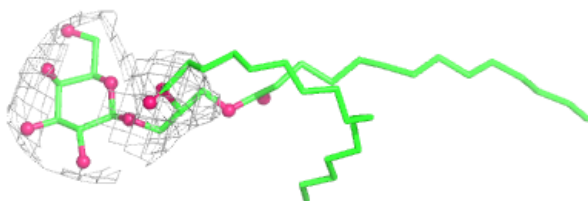
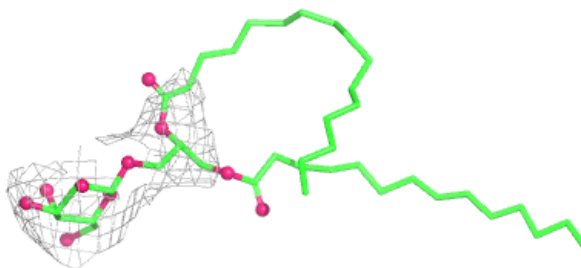


Electron density around CLA D 406:

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

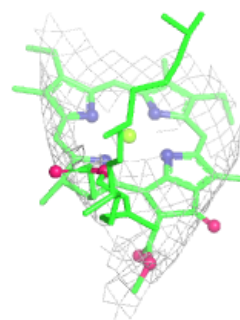
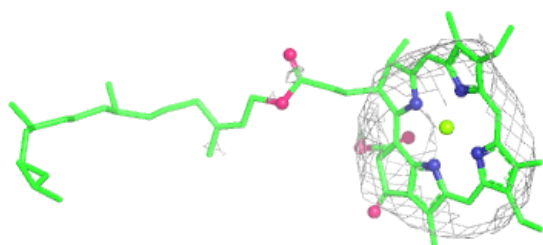
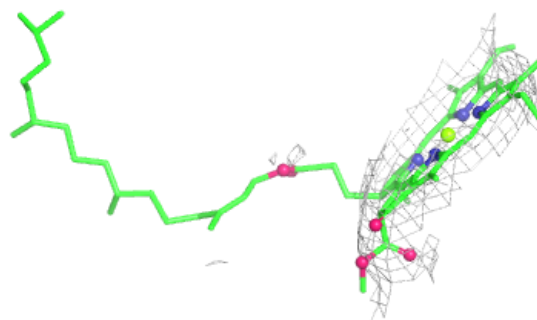
**Electron density around LMG b 628:**

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

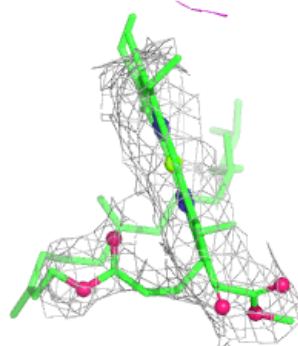
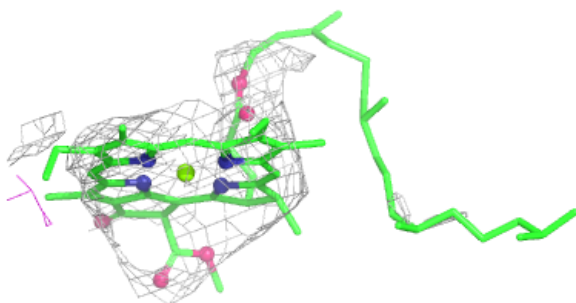
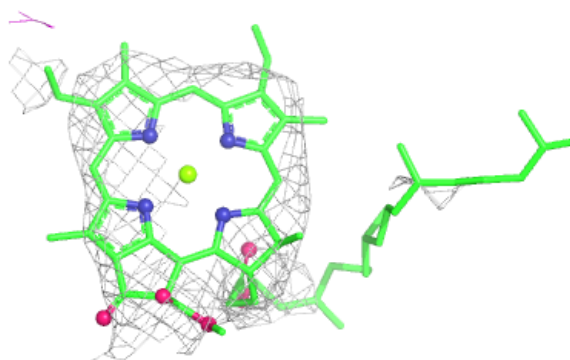


Electron density around CLA d 404:

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

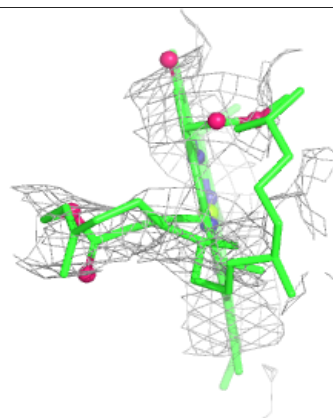
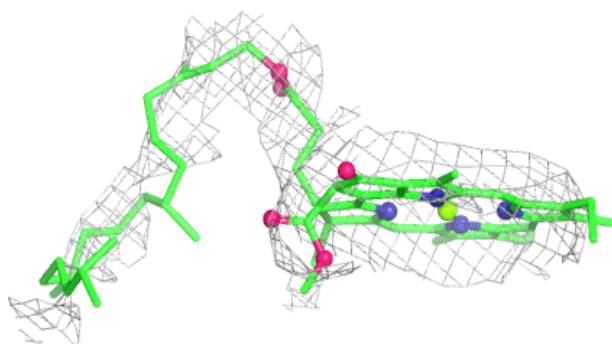
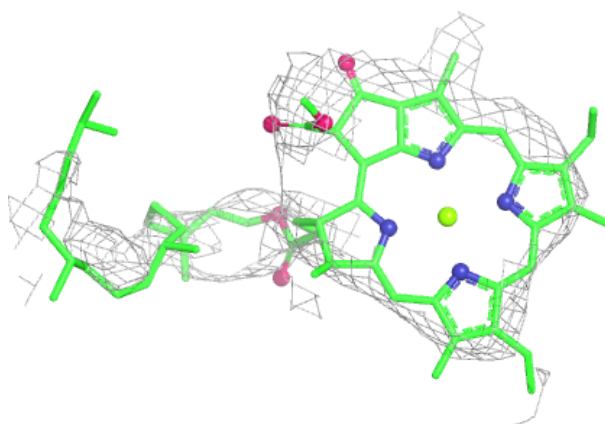
**Electron density around CLA A 403:**

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

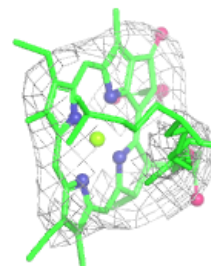
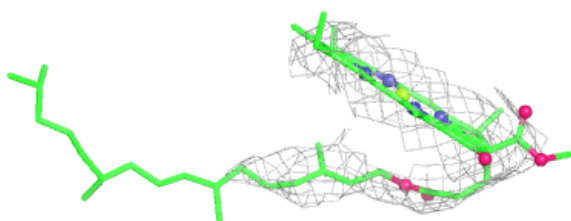


Electron density around CLA B 611:

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

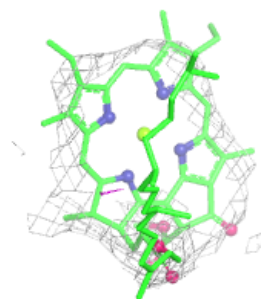
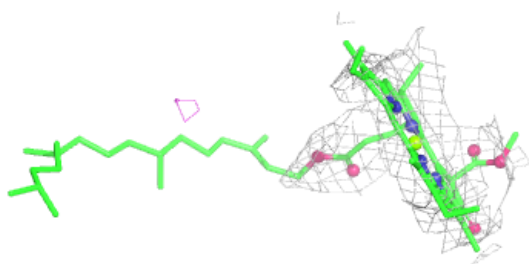
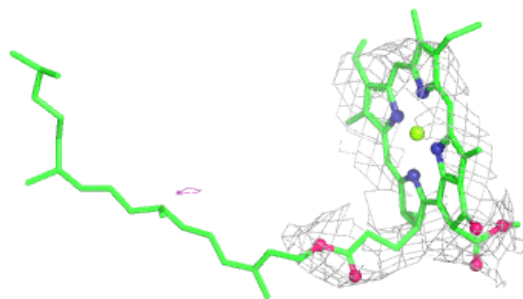
**Electron density around CLA b 611:**

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



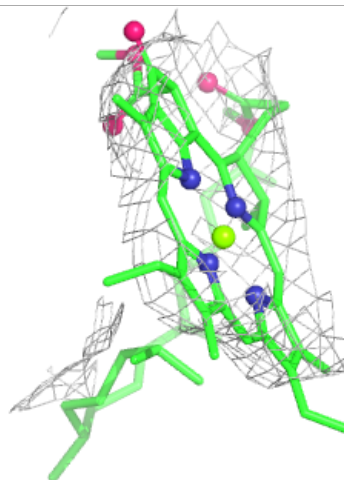
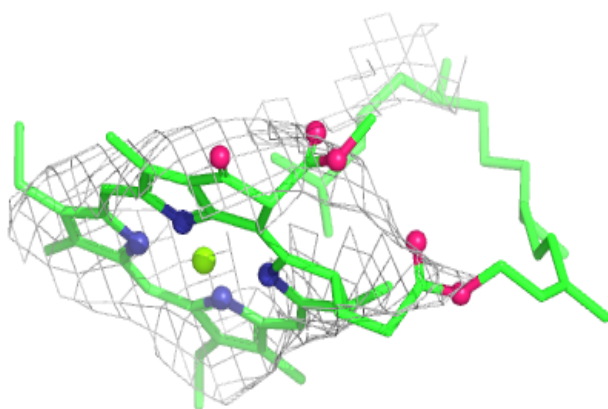
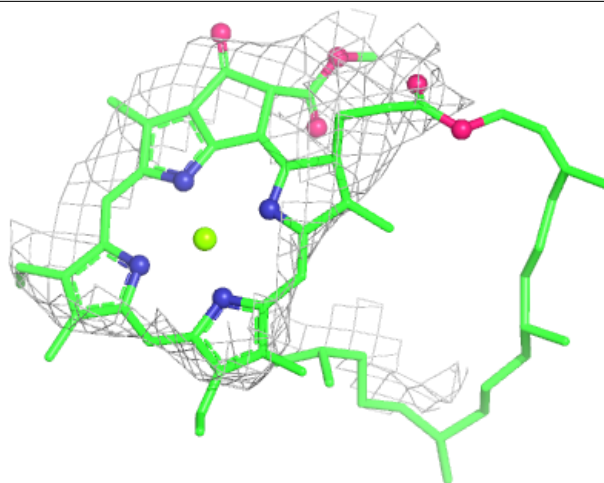
Electron density around CLA B 608:

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



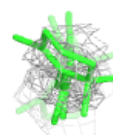
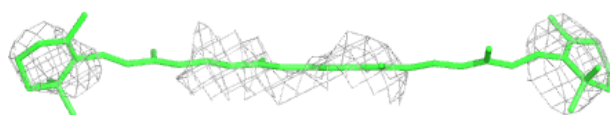
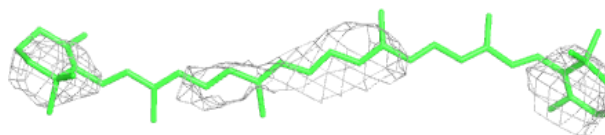
Electron density around CLA B 614:

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

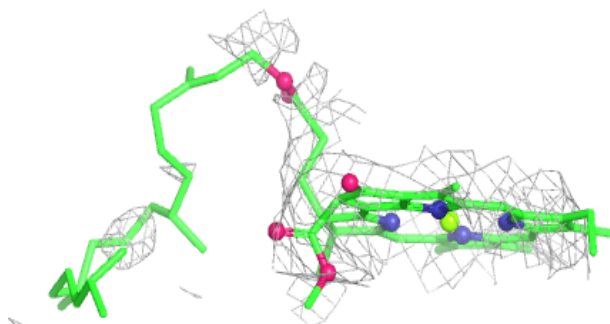
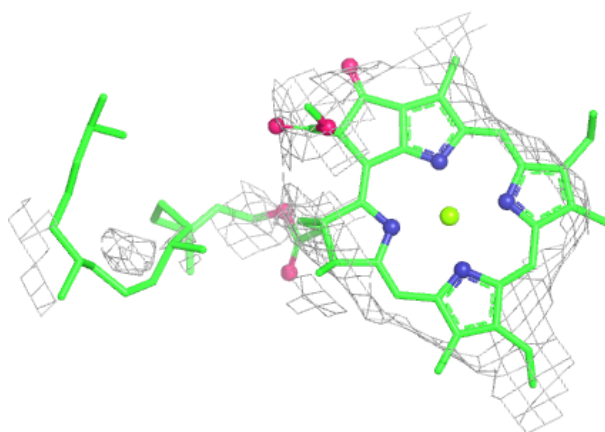


Electron density around BCR B 618:

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

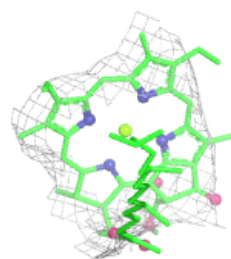
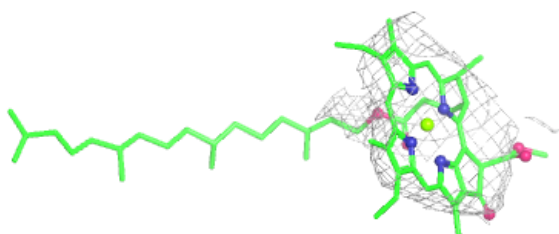
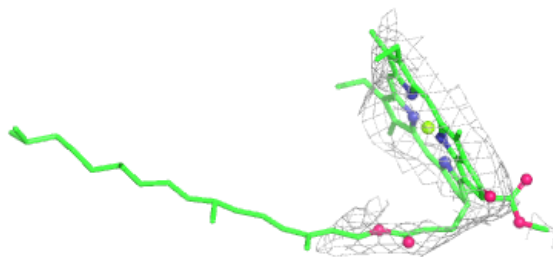
**Electron density around CLA b 615:**

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



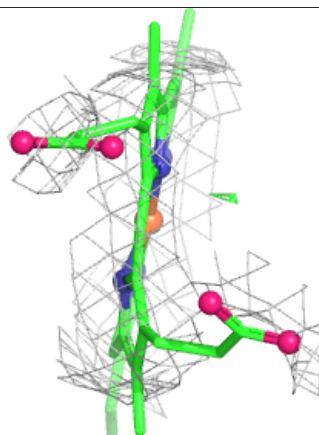
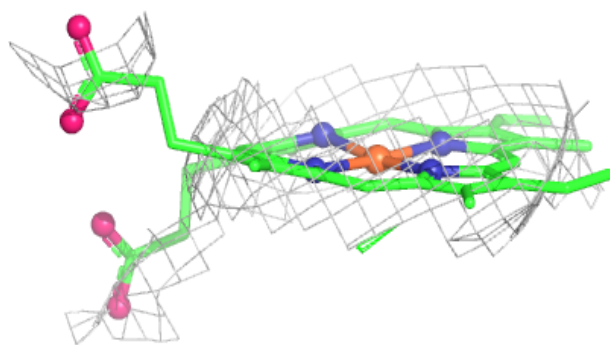
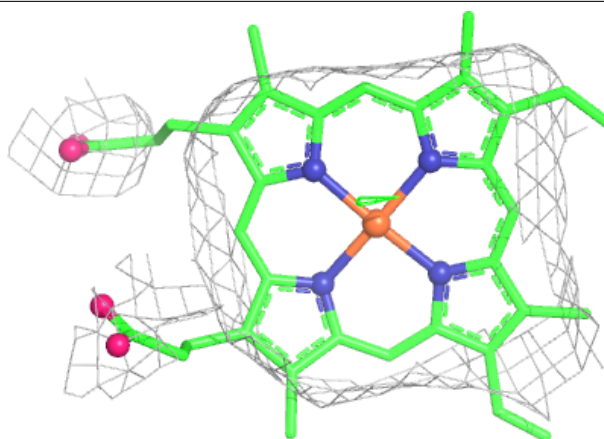
Electron density around CLA B 606:

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



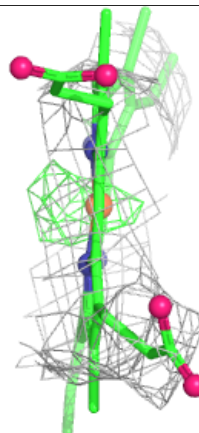
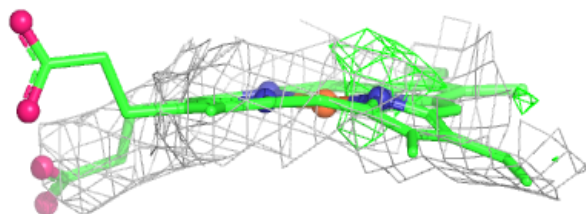
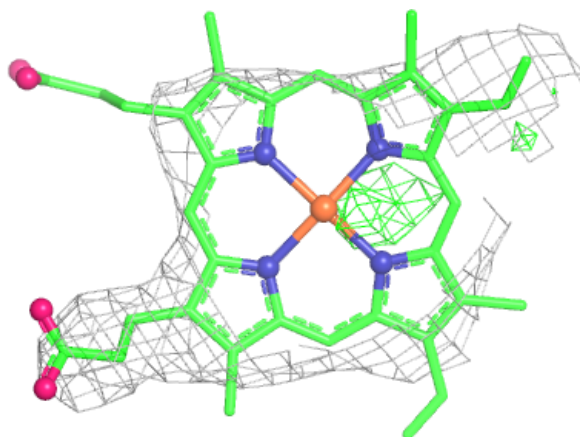
Electron density around HEM F 101:

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

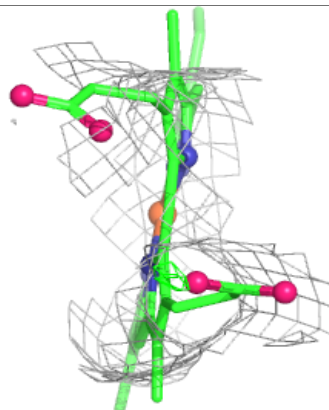
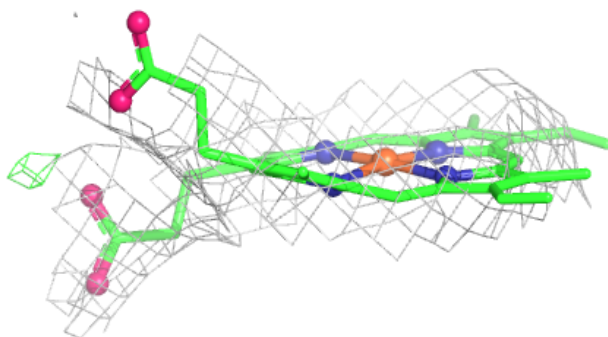
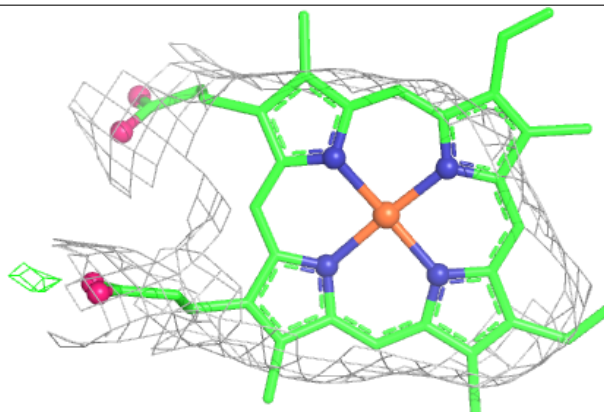


Electron density around HEM V 201:

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

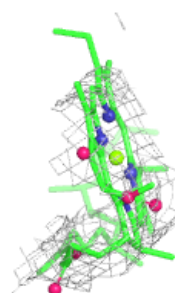
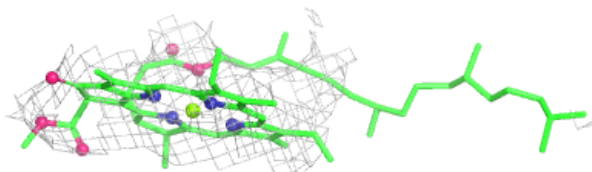
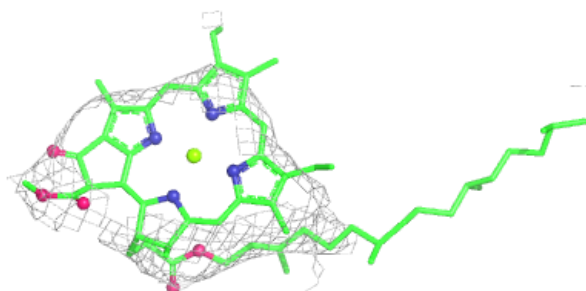
**Electron density around HEM f 101:**

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

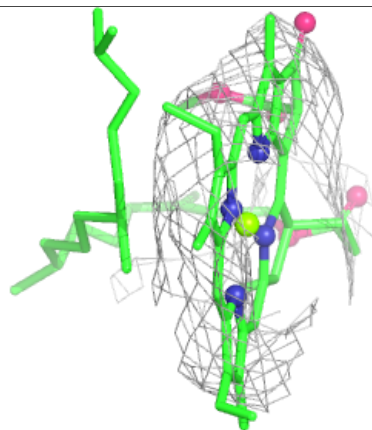
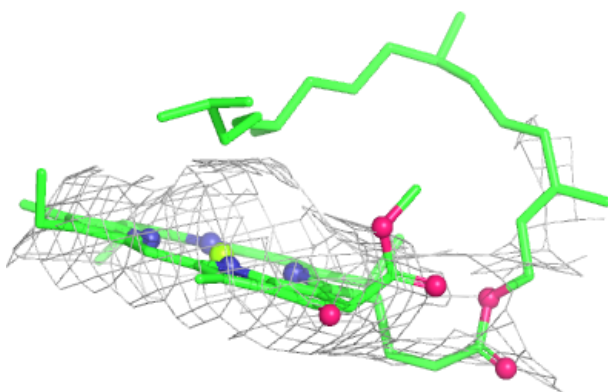
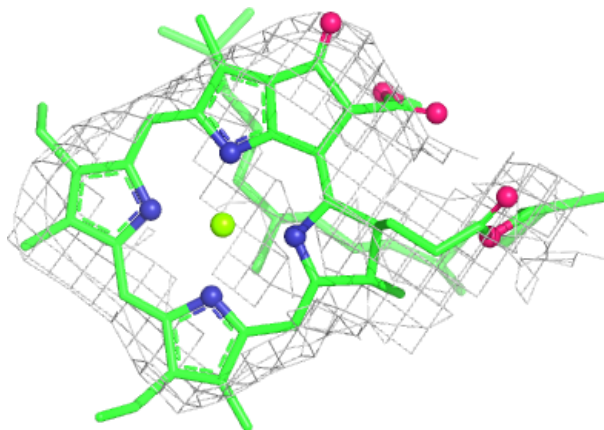


Electron density around CLA C 501:

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

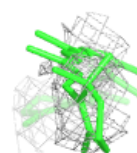
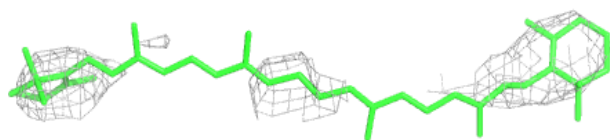
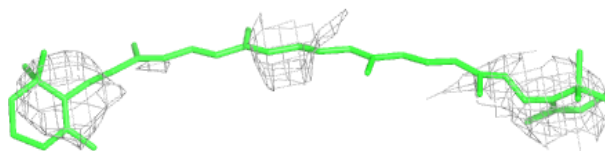
**Electron density around CLA c 509:**

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

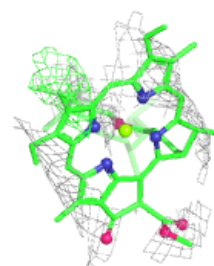
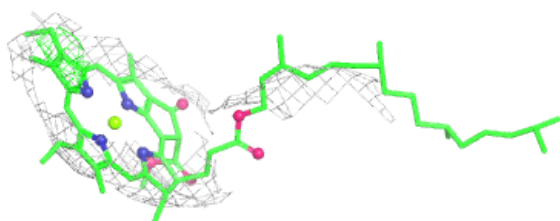


Electron density around BCR D 411:

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

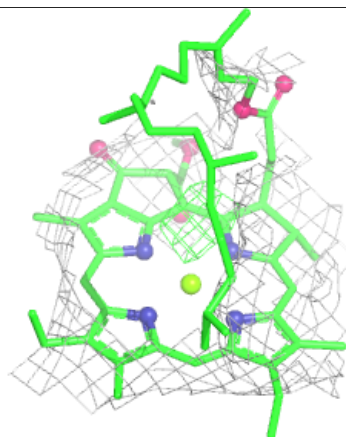
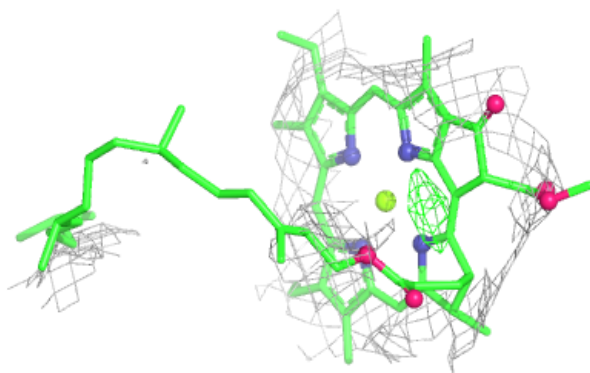
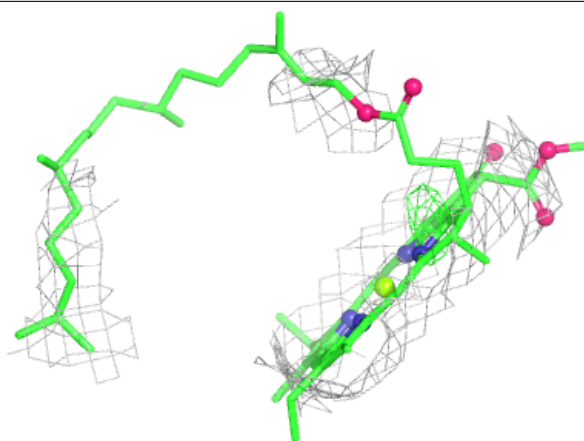
**Electron density around CLA C 502:**

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



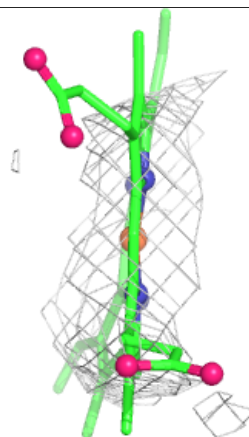
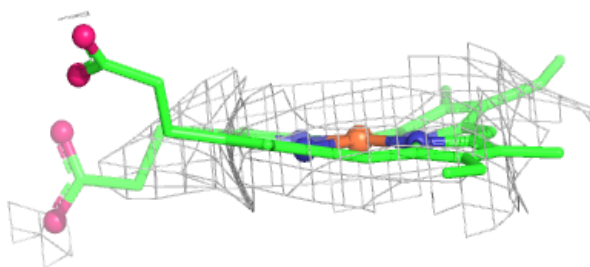
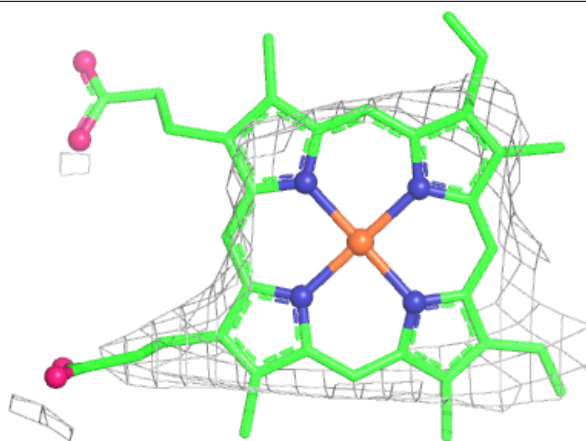
Electron density around CLA b 614:

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



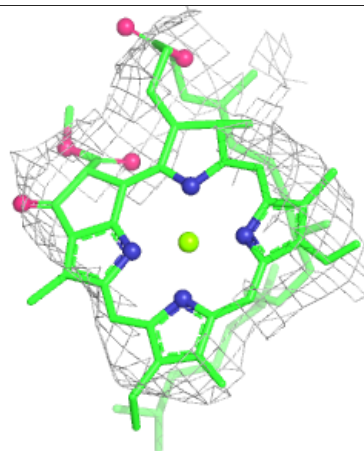
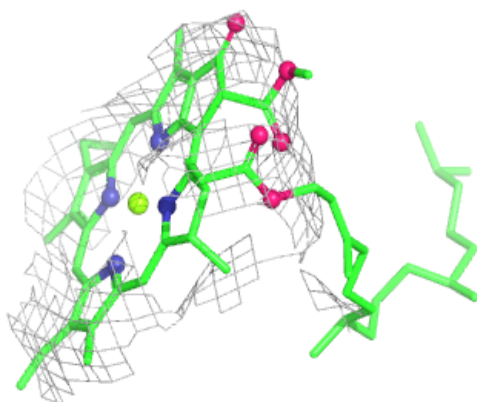
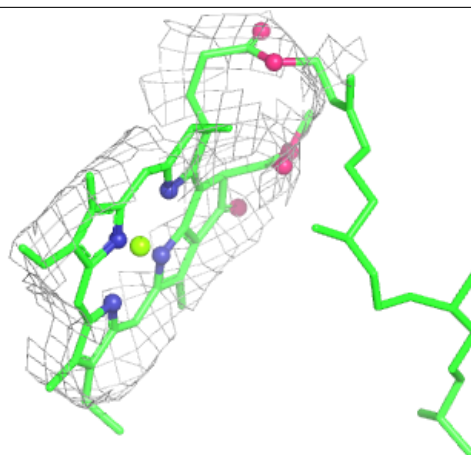
Electron density around HEM v 201:

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



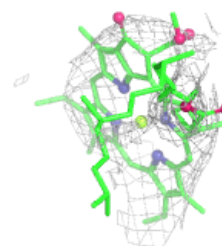
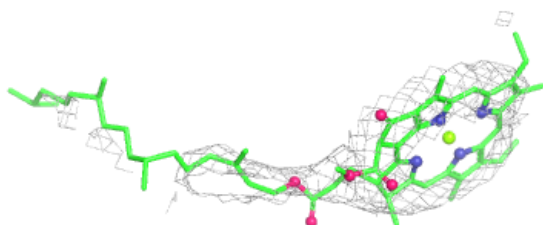
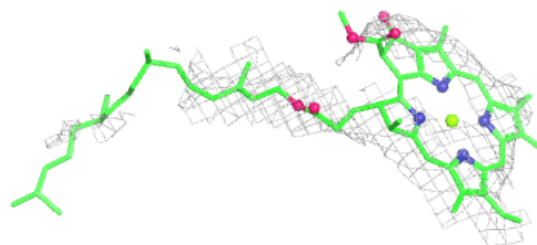
Electron density around CLA B 612:

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



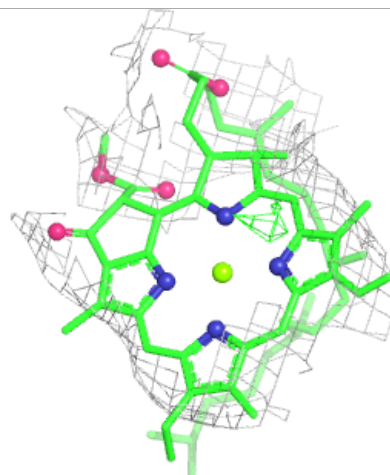
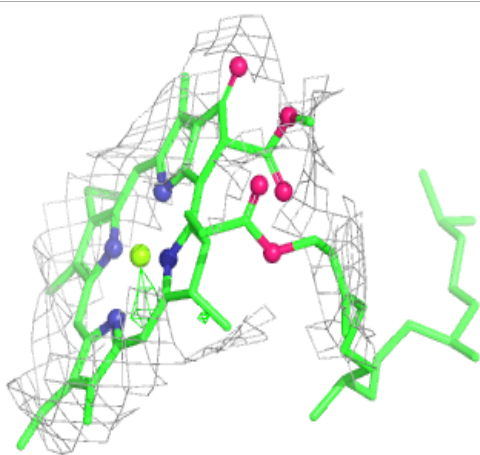
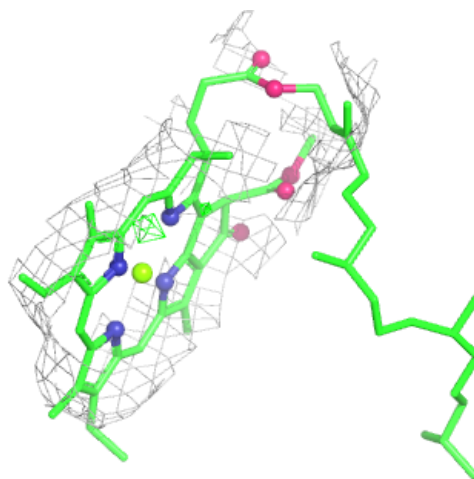
Electron density around CLA a 404:

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



Electron density around CLA b 616:

$2mF_o-DF_c$ (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.