



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 03:06 AM EDT

PDB ID : 4TNI / pdb_00004tni
Title : RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 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 : 4.60 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

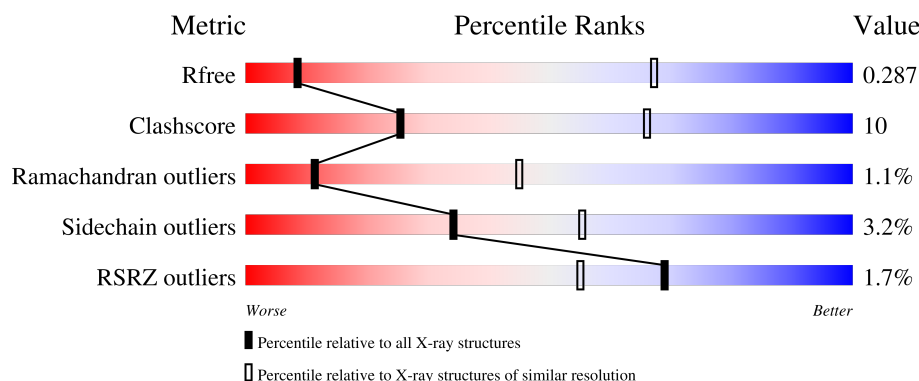
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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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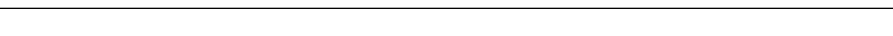
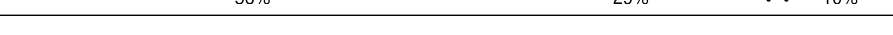
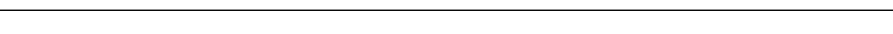
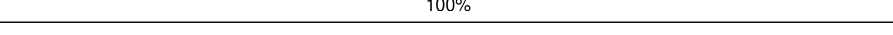
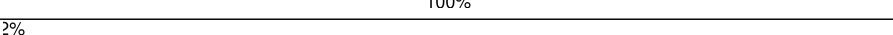
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 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	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

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				

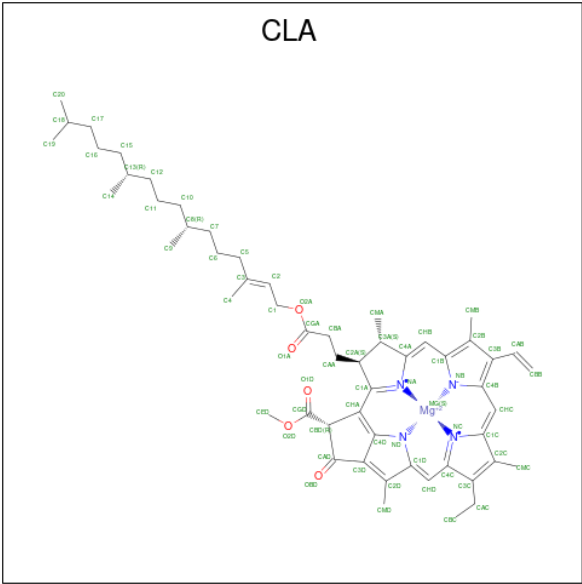
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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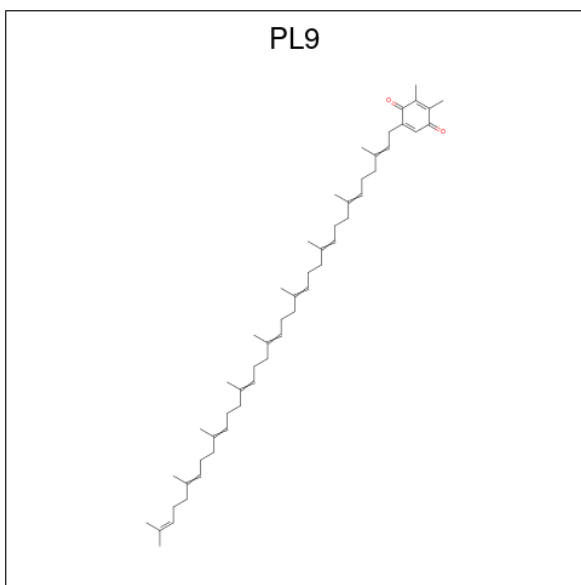
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22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55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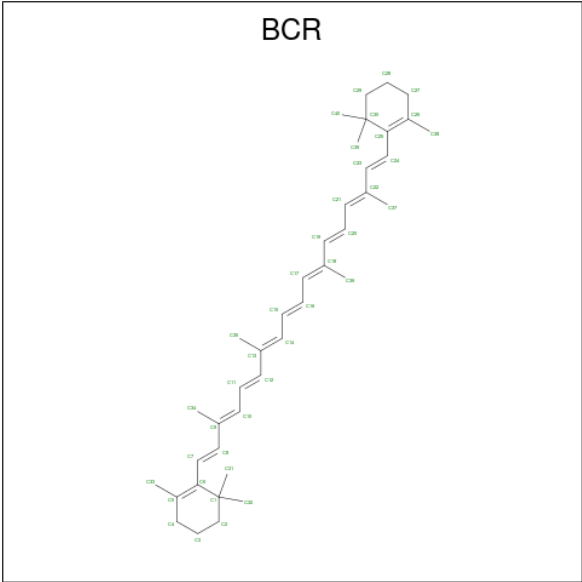
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



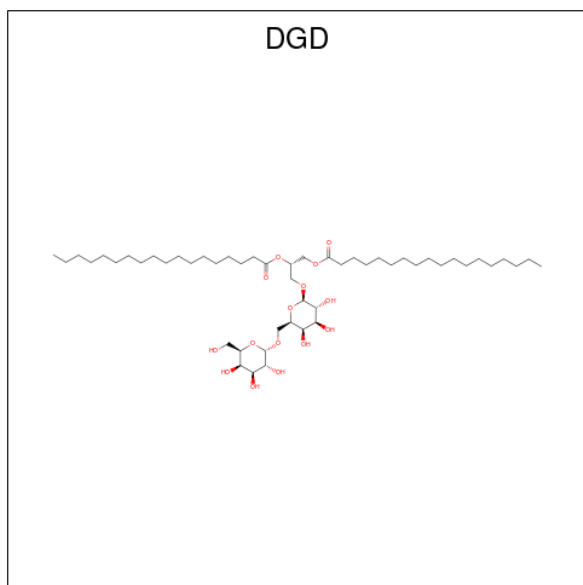
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total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

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

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



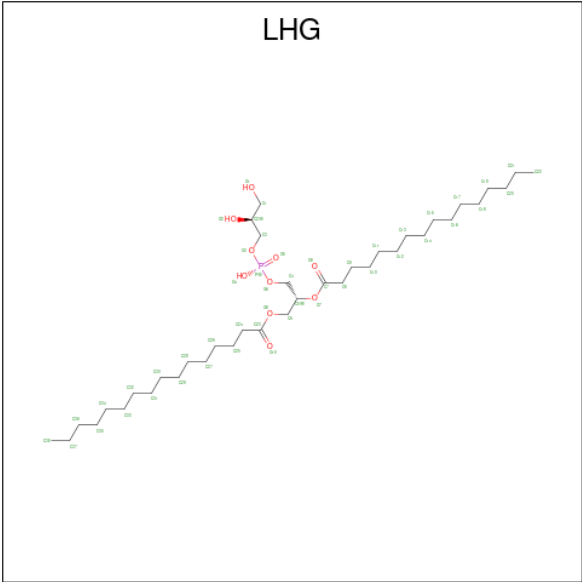
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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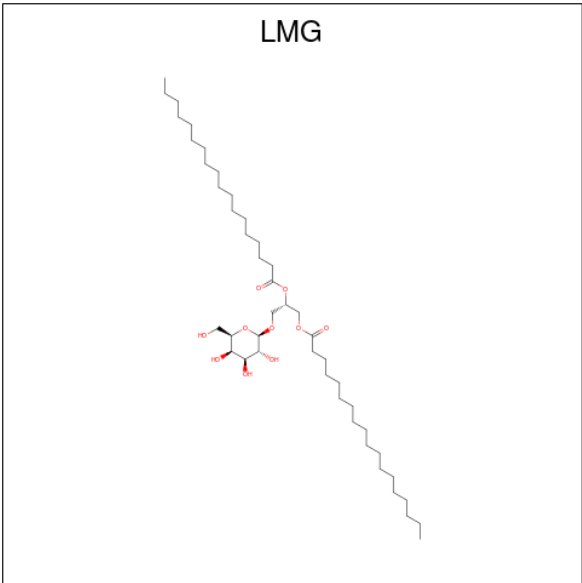
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

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



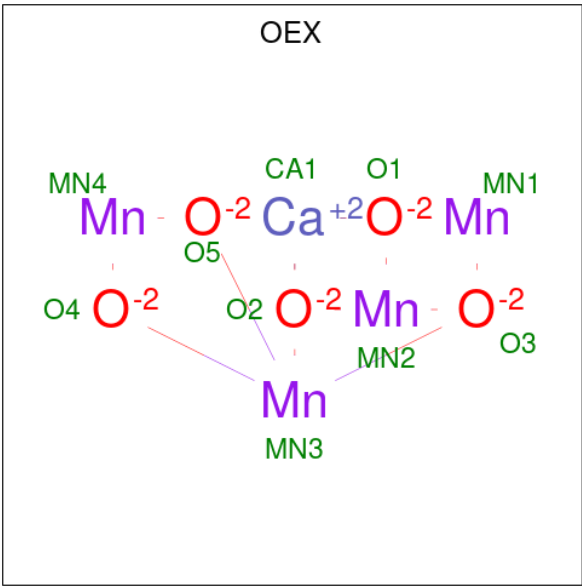
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

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



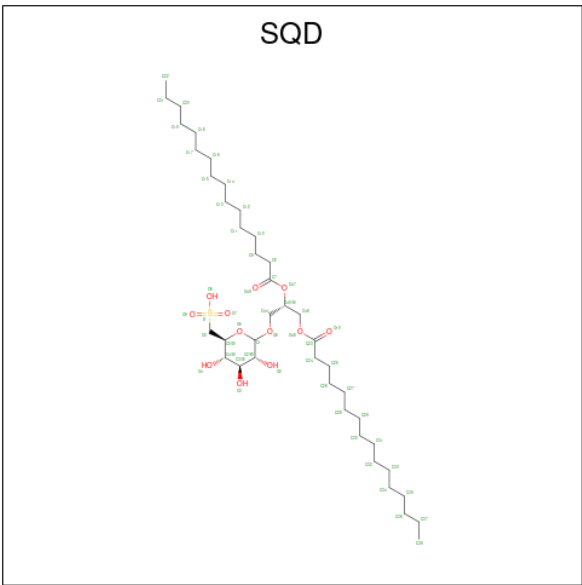
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total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

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



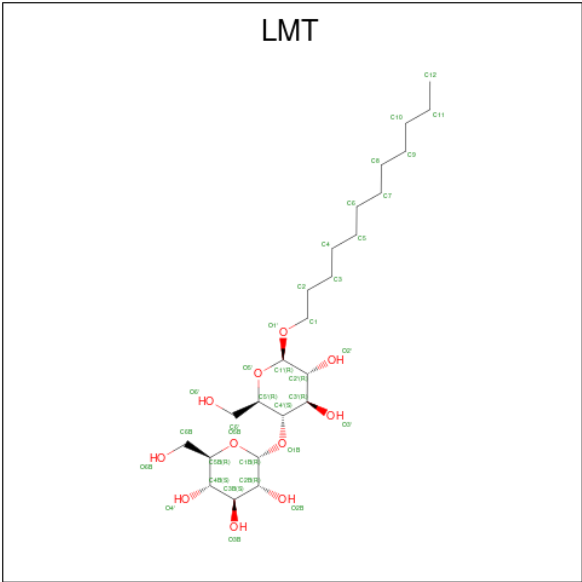
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
28	A	1	10	1	4	5	0	0
28	a	1	10	1	4	5	0	0

- Molecule 29 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
29	A	1	Total	C	O	S	0	0
			51	38	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			43	30	12	1		
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	F	1	Total	C	O	S	0	0
			45	32	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O	S	0	0
			51	38	12	1		
29	b	1	Total	C	O	S	0	0
			47	34	12	1		
29	d	1	Total	C	O	S	0	0
			43	30	12	1		
29	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 30 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



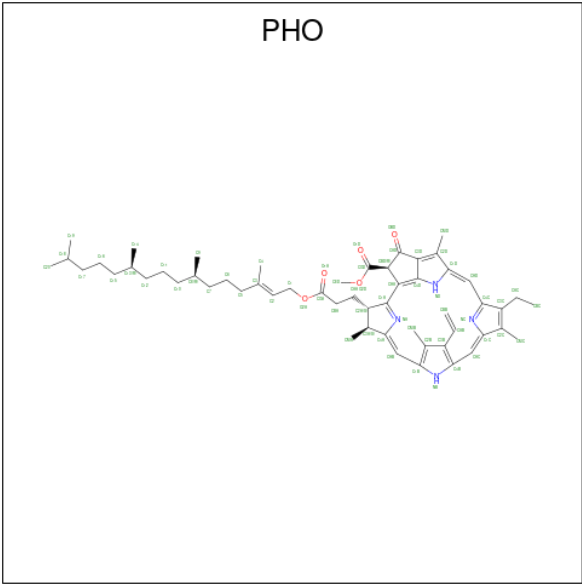
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		

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Continued from previous page...

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

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).

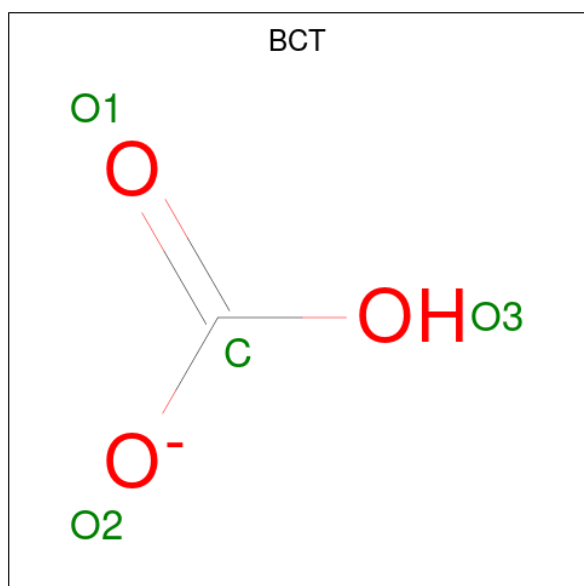


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	D	1	Total C N O 64 55 4 5	0	0
31	D	1	Total C N O 64 55 4 5	0	0
31	d	1	Total C N O 64 55 4 5	0	0
31	d	1	Total C N O 64 55 4 5	0	0

- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	D	1	Total Cl 1 1	0	0
32	a	1	Total Cl 1 1	0	0

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



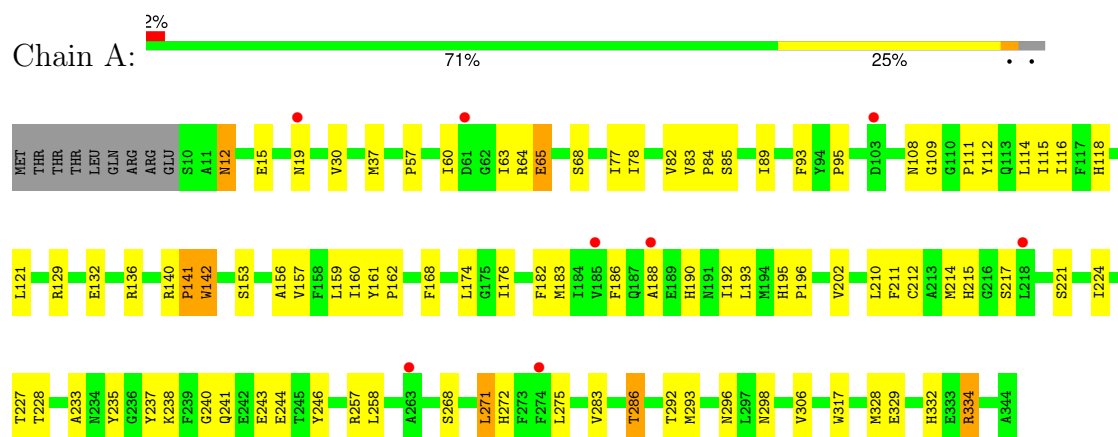
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 4 1 3	0	0
33	d	1	Total C O 4 1 3	0	0

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

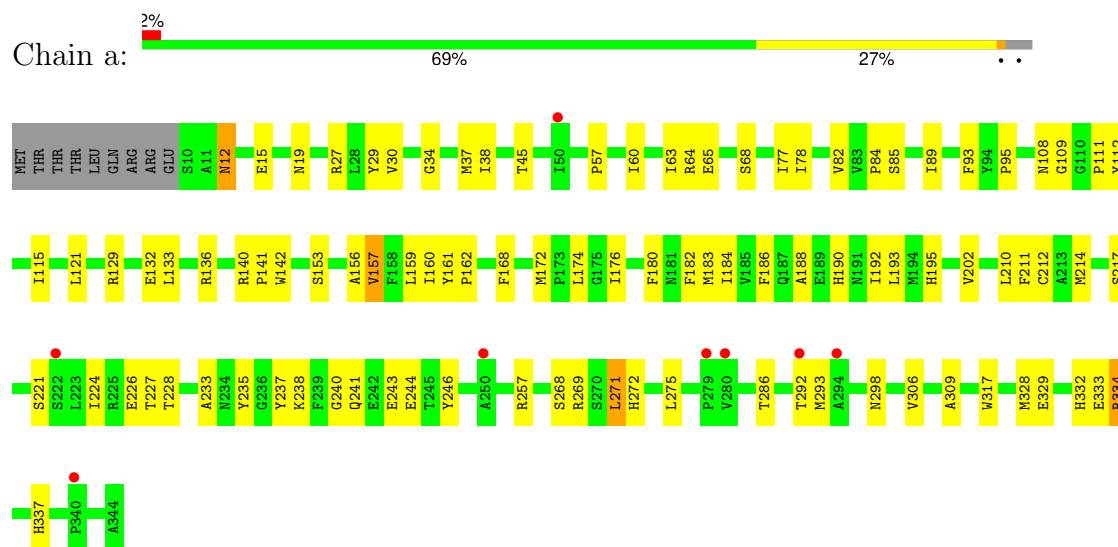
3 Residue-property plots [i](#)

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

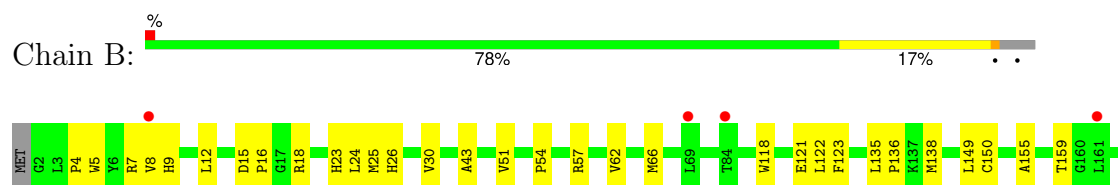
• Molecule 1: Photosystem Q(B) protein 1

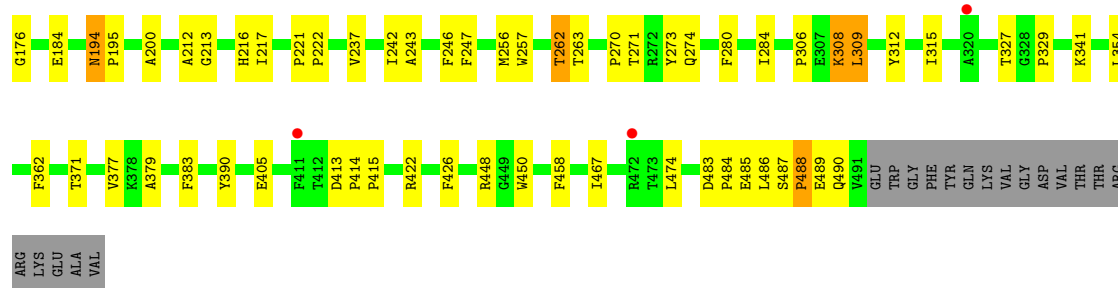


• Molecule 1: Photosystem Q(B) protein 1

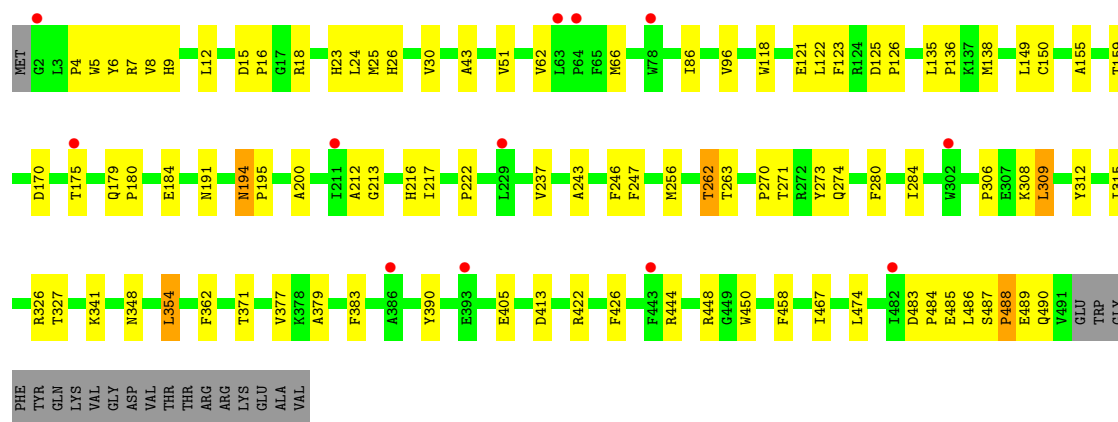
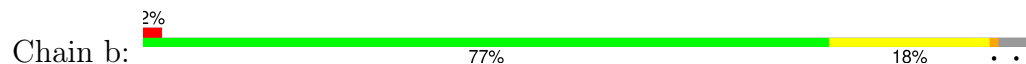


• Molecule 2: Photosystem II core light harvesting protein

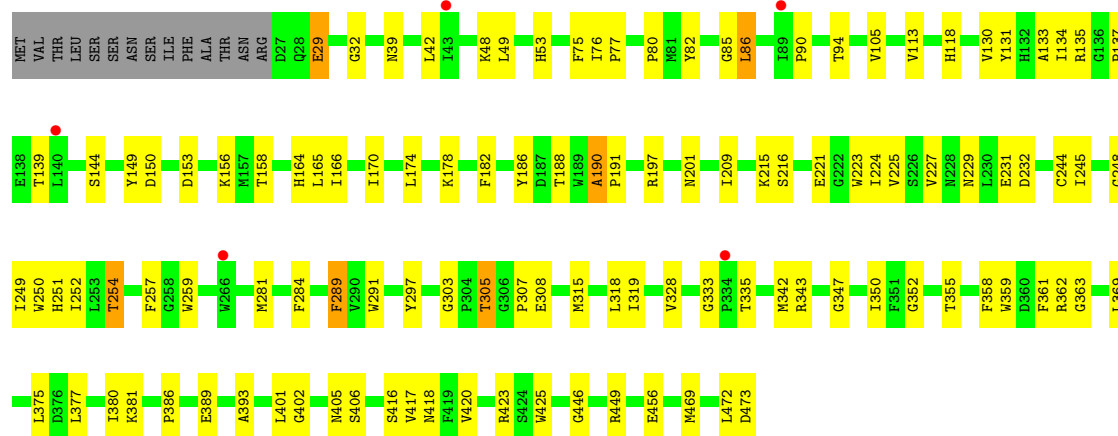




• Molecule 2: Photosystem II core light harvesting protein

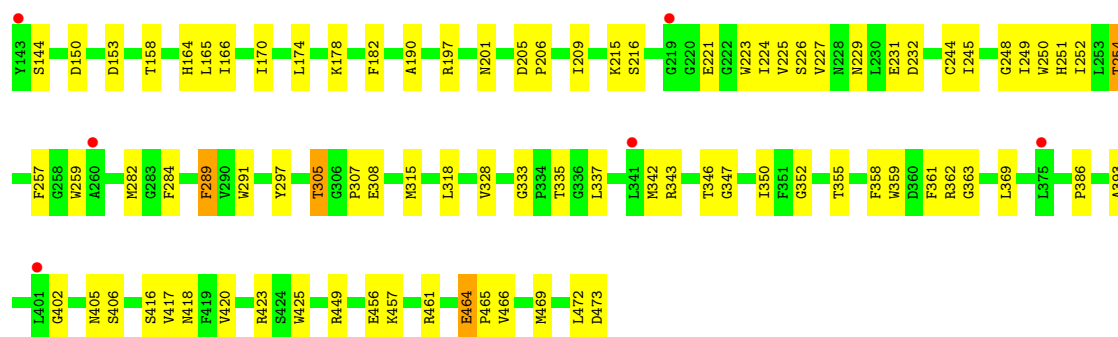


• Molecule 3: Photosystem II CP43 protein

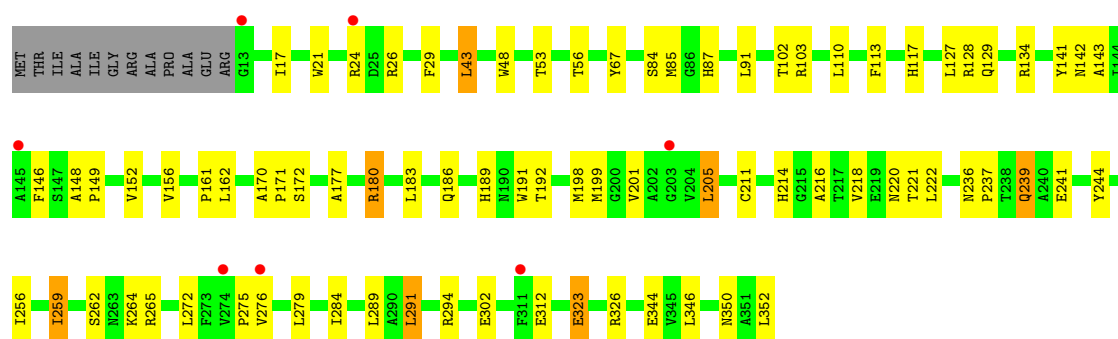
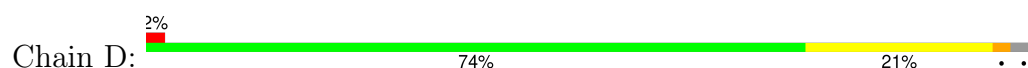


• Molecule 3: Photosystem II CP43 protein

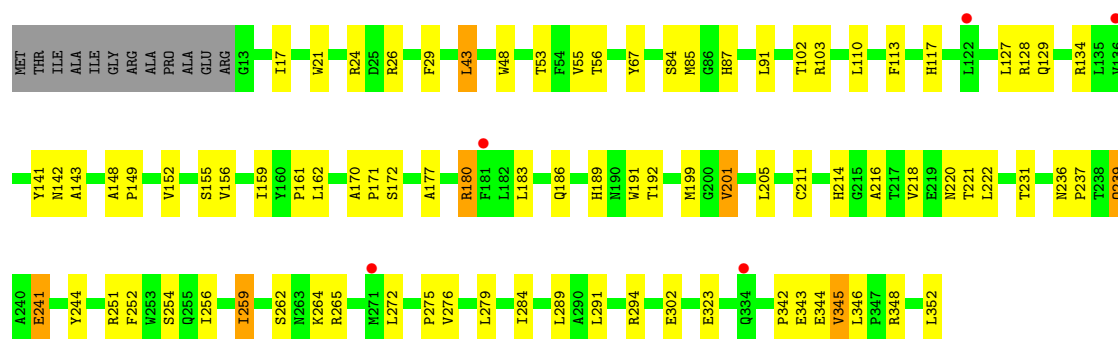




• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha





- Molecule 6: Cytochrome b559 subunit beta



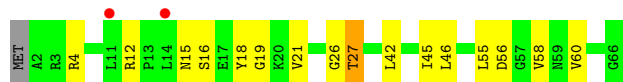
- Molecule 6: Cytochrome b559 subunit beta



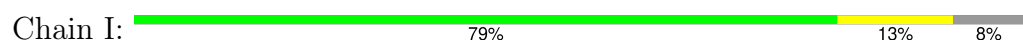
- Molecule 7: Photosystem II reaction center protein H



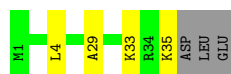
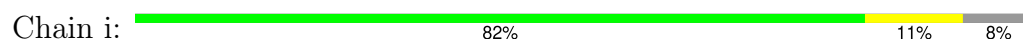
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





- Molecule 9: Photosystem II reaction center protein J



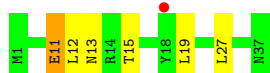
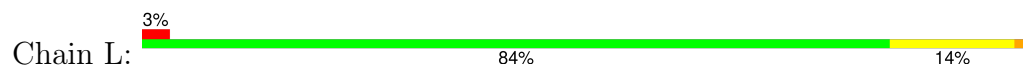
- Molecule 10: Photosystem II reaction center protein K



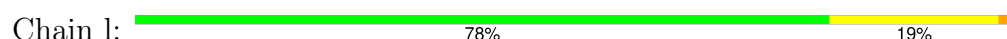
- Molecule 10: Photosystem II reaction center protein K



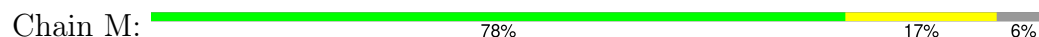
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

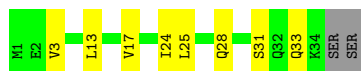


- Molecule 12: Photosystem II reaction center protein M

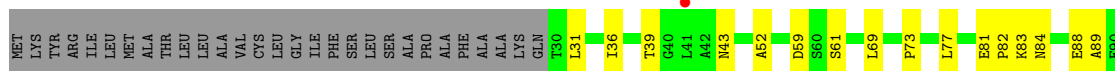


- Molecule 12: Photosystem II reaction center protein M

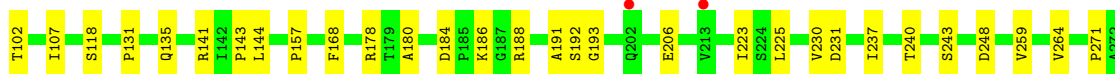




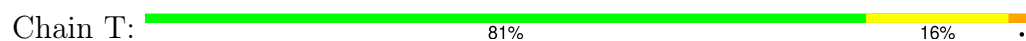
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



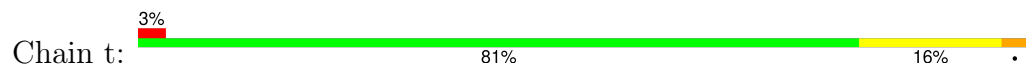
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



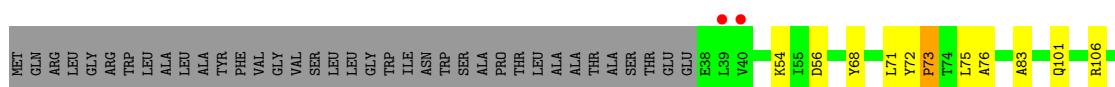
• Molecule 14: Photosystem II reaction center protein T



• Molecule 14: Photosystem II reaction center protein T

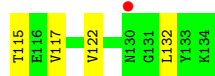
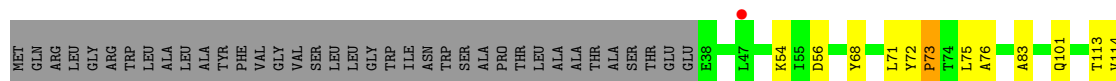


• Molecule 15: Photosystem II 12 kDa extrinsic protein

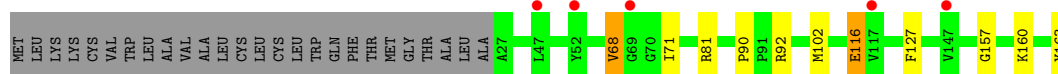
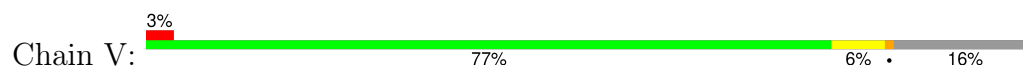




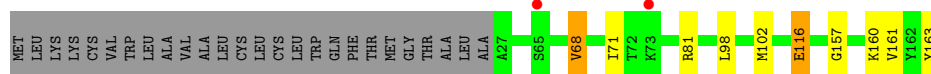
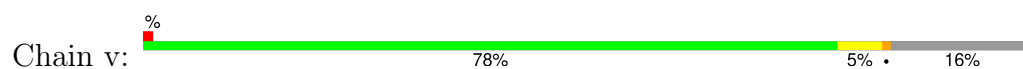
- Molecule 15: Photosystem II 12 kDa extrinsic protein



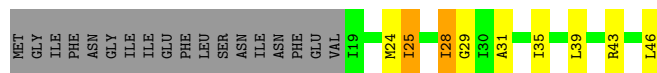
- Molecule 16: Cytochrome c-550



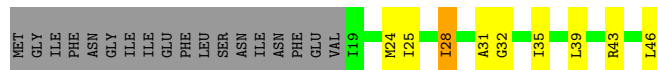
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

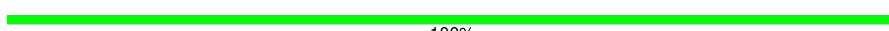


- Molecule 18: Photosystem II reaction center X protein

Chain x:  61% 24% • • 10%

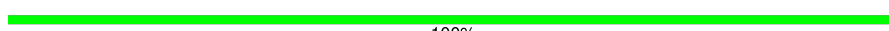


- Molecule 19: Photosystem II reaction center protein Y

Chain Y:  100%

There are no outlier residues recorded for this chain.

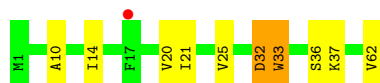
- Molecule 19: Photosystem II reaction center protein Y

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  2% 84% 13% •



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  2% 84% 13% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.43Å 228.81Å 307.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.96 – 4.60 72.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.96-4.60) 97.6 (72.96-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.278 , 0.284 0.283 , 0.287	Depositor DCC
R_{free} test set	2522 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	159.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 127.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: FE2, DGD, BCR, LMG, PL9, BCT, LMT, OEX, CL, HEM, CLA, CA, LHG, SQD, PHO

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	0.77	2/3700 (0.1%)
1	a	0.30	0/2713	0.78	3/3700 (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	0.79	6/4842 (0.1%)
3	c	0.30	0/3556	0.80	8/4842 (0.2%)
4	D	0.29	0/2801	0.76	0/3818
4	d	0.29	0/2801	0.77	0/3818
5	E	0.31	0/685	0.82	0/933
5	e	0.31	0/685	0.83	0/933
6	F	0.34	0/291	0.74	0/397
6	f	0.34	0/291	0.74	0/397
7	H	0.33	0/520	0.73	0/709
7	h	0.33	0/520	0.73	0/709
8	I	0.29	0/293	0.77	0/395
8	i	0.29	0/293	0.78	0/395
9	J	0.30	0/255	0.84	0/346
9	j	0.30	0/255	0.84	0/346
10	K	0.44	0/303	0.85	0/416
10	k	0.45	0/303	0.86	0/416
11	L	0.28	0/311	0.72	0/422
11	l	0.28	0/311	0.71	0/422
12	M	0.30	0/270	0.77	0/367
12	m	0.33	0/270	0.84	1/367 (0.3%)
13	O	0.27	0/1876	0.71	0/2548
13	o	0.27	0/1876	0.70	0/2548
14	T	0.27	0/284	0.74	0/381
14	t	0.27	0/284	0.73	0/381
15	U	0.30	0/785	0.77	0/1064
15	u	0.30	0/785	0.78	0/1064
16	V	0.29	0/1081	0.75	2/1468 (0.1%)
16	v	0.29	0/1081	0.75	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.32	0/202	0.78	0/272
17	y	0.32	0/202	0.76	0/272
18	X	0.38	0/273	0.79	0/370
18	x	0.37	0/273	0.79	0/370
20	Z	0.31	0/490	0.83	0/669
20	z	0.31	0/490	0.84	0/669
All	All	0.30	0/41950	0.78	38/57100 (0.1%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	483	ASP	CA-C-N	10.64	133.14	119.84
2	b	483	ASP	C-N-CA	10.64	133.14	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	6.26	125.75	119.24
3	c	363	GLY	C-N-CA	6.26	125.75	119.24
3	c	190	ALA	CA-C-N	6.18	125.66	119.24
3	c	190	ALA	C-N-CA	6.18	125.66	119.24
3	C	363	GLY	CA-C-N	6.09	125.58	119.24
3	C	363	GLY	C-N-CA	6.09	125.58	119.24
3	C	190	ALA	CA-C-N	6.06	125.54	119.24
3	C	190	ALA	C-N-CA	6.06	125.54	119.24
2	b	15	ASP	CA-C-N	5.92	126.07	119.32
2	b	15	ASP	C-N-CA	5.92	126.07	119.32
2	B	413	ASP	CA-C-N	5.73	126.29	120.38
2	B	413	ASP	C-N-CA	5.73	126.29	120.38
2	b	194	ASN	CA-C-N	5.58	125.25	119.05
2	b	194	ASN	C-N-CA	5.58	125.25	119.05
2	b	413	ASP	CA-C-N	5.52	126.07	120.38
2	b	413	ASP	C-N-CA	5.52	126.07	120.38
2	B	15	ASP	CA-C-N	5.45	125.54	119.32
2	B	15	ASP	C-N-CA	5.45	125.54	119.32
2	B	194	ASN	CA-C-N	5.41	125.05	119.05
2	B	194	ASN	C-N-CA	5.41	125.05	119.05
3	C	333	GLY	CA-C-N	5.25	126.40	119.84
3	C	333	GLY	C-N-CA	5.25	126.40	119.84
1	a	195	HIS	CA-C-N	5.22	125.28	119.32
1	a	195	HIS	C-N-CA	5.22	125.28	119.32
3	c	333	GLY	CA-C-N	5.22	126.37	119.84
3	c	333	GLY	C-N-CA	5.22	126.37	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	GLU	CA-C-N	5.13	125.42	119.93
1	A	65	GLU	C-N-CA	5.13	125.42	119.93
1	a	38	ILE	CB-CA-C	-5.11	108.85	113.70
3	c	464	GLU	CA-C-N	5.07	126.17	119.84
3	c	464	GLU	C-N-CA	5.07	126.17	119.84
16	V	127	PHE	CA-C-N	5.03	126.13	119.84
16	V	127	PHE	C-N-CA	5.03	126.13	119.84
12	m	17	VAL	CB-CA-C	-5.03	108.92	113.70

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	71	0
1	a	2628	0	2524	68	0
2	B	3850	0	3718	59	0
2	b	3850	0	3718	62	0
3	C	3444	0	3365	72	0
3	c	3444	0	3365	71	0
4	D	2706	0	2608	63	0
4	d	2706	0	2608	68	0
5	E	666	0	651	13	0
5	e	666	0	651	15	0
6	F	282	0	291	5	0
6	f	282	0	291	5	0
7	H	507	0	521	13	0
7	h	507	0	521	13	0
8	I	286	0	308	3	0
8	i	286	0	308	2	0
9	J	249	0	262	7	0
9	j	249	0	262	7	0
10	K	293	0	305	11	0
10	k	293	0	305	9	0
11	L	304	0	316	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	l	304	0	316	6	0
12	M	267	0	289	6	0
12	m	267	0	289	7	0
13	O	1845	0	1801	28	0
13	o	1845	0	1801	29	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	7	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	8	0
17	g	201	0	226	7	0
17	y	201	0	226	7	0
18	X	270	0	299	10	0
18	x	270	0	299	9	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	9	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	27	0
22	B	975	0	1080	52	0
22	C	845	0	936	28	0
22	D	130	0	144	10	0
22	H	65	0	72	8	0
22	a	260	0	288	25	0
22	b	975	0	1080	50	0
22	c	845	0	936	32	0
22	d	130	0	144	11	0
22	h	65	0	72	9	0
23	A	45	0	61	4	0
23	D	55	0	80	8	0
23	J	35	0	45	1	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	3	0
24	B	160	0	224	11	0
24	C	80	0	112	11	0
24	F	40	0	56	3	0
24	H	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	J	40	0	56	1	0
24	K	40	0	56	3	0
24	a	40	0	56	2	0
24	b	160	0	224	13	0
24	c	120	0	168	15	0
24	f	40	0	56	2	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	7	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	11	0
25	D	63	0	87	1	0
25	a	56	0	70	2	0
25	b	110	0	136	4	0
25	c	181	0	245	10	0
25	d	63	0	87	2	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	49	0	68	3	0
27	C	93	0	126	3	0
27	D	143	0	196	9	0
27	E	44	0	58	1	0
27	I	43	0	56	0	0
27	M	42	0	54	2	0
27	a	93	0	126	3	0
27	b	49	0	68	5	0
27	c	93	0	126	3	0
27	d	143	0	196	10	0
27	e	44	0	58	1	0
27	i	43	0	56	1	0
27	m	42	0	54	1	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	105	0	147	8	0
29	B	90	0	111	4	0
29	F	45	0	54	2	0
29	a	105	0	147	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	b	47	0	61	1	0
29	d	43	0	50	4	0
29	f	45	0	54	3	0
30	B	140	0	184	6	0
30	D	31	0	35	0	0
30	I	35	0	46	0	0
30	M	70	0	91	0	0
30	b	140	0	183	5	0
30	d	31	0	35	0	0
30	i	35	0	46	1	0
31	D	128	0	148	12	0
31	d	128	0	148	10	0
32	D	1	0	0	0	0
32	a	1	0	0	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	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	51372	970	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 (970) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.55	0.87
3:c:39:ASN:HB2	22:c:507:CLA:HBA1	1.58	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.81
3:c:362:ARG:H	25:c:515:DGD:HE4	1.44	0.81
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.62	0.81
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.61	0.80
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.63	0.79
34:V:201:HEM:HBC2	34:V:201:HEM:HHB	1.66	0.77
13:o:82:PRO:HG3	13:o:89:ALA:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:362:ARG:H	25:C:515:DGD:HE4	1.51	0.76
4:D:199:MET:HG2	23:D:407:PL9:H322	1.69	0.74
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.70	0.74
34:v:201:HEM:HBC2	34:v:201:HEM:HHD	1.69	0.73
22:B:605:CLA:H72	24:B:619:BCR:H311	1.70	0.73
4:d:199:MET:HG2	23:d:407:PL9:H322	1.71	0.72
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.70	0.72
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.72	0.72
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.72	0.71
22:b:609:CLA:H72	24:b:623:BCR:H311	1.71	0.71
1:a:192:ILE:HA	1:a:293:MET:HE1	1.71	0.71
25:c:517:DGD:HAF2	22:c:520:CLA:H202	1.73	0.70
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.73	0.70
1:a:129:ARG:HH21	4:d:256:ILE:HD12	1.55	0.70
2:b:24:LEU:HD21	22:b:619:CLA:HAB	1.72	0.70
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.74	0.70
4:D:29:PHE:O	4:D:128:ARG:NH2	2.25	0.70
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.56	0.70
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.74	0.69
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.73	0.69
3:C:250:TRP:O	3:C:254:THR:OG1	2.10	0.69
10:k:21:LEU:HD13	17:g:24:MET:HE2	1.75	0.68
10:K:21:LEU:HD13	17:y:24:MET:HE2	1.75	0.68
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.74	0.68
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.68
5:e:60:GLN:OE1	5:e:84:LYS:NZ	2.27	0.68
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.75	0.67
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.67
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.76	0.67
4:d:259:ILE:HG12	27:d:409:LMG:H292	1.76	0.67
13:o:69:LEU:HB3	13:o:107:ILE:HB	1.75	0.67
1:a:63:ILE:HB	3:c:335:THR:HG21	1.75	0.67
4:d:152:VAL:HG21	4:d:279:LEU:HD12	1.76	0.67
3:c:165:LEU:HD21	22:c:505:CLA:HAB	1.76	0.67
1:A:63:ILE:HB	3:C:335:THR:HG21	1.77	0.67
17:y:35:ILE:HG22	20:Z:21:ILE:HG23	1.77	0.67
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.76	0.67
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.76	0.67
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.76	0.66
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.77	0.66
12:m:31:SER:HA	27:m:101:LMG:HC1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:259:ILE:HG12	27:D:409:LMG:H292	1.78	0.66
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.28	0.66
22:b:611:CLA:H42	4:d:127:LEU:HD11	1.76	0.66
3:c:250:TRP:O	3:c:254:THR:OG1	2.13	0.66
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.66
22:C:506:CLA:H112	24:C:514:BCR:H362	1.77	0.66
4:d:236:ASN:ND2	4:d:239:GLN:O	2.29	0.66
1:A:15:GLU:O	1:A:19:ASN:ND2	2.27	0.66
1:A:192:ILE:HA	1:A:293:MET:HE1	1.76	0.65
4:d:21:TRP:O	4:d:26:ARG:NH2	2.26	0.65
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
29:d:403:SQD:H171	29:d:403:SQD:H301	1.78	0.65
4:d:189:HIS:HA	4:d:294:ARG:HD2	1.77	0.65
4:D:186:GLN:HB2	22:D:405:CLA:HBC1	1.79	0.65
4:D:236:ASN:ND2	4:D:239:GLN:O	2.30	0.65
1:a:174:LEU:HD22	31:d:401:PHO:H151	1.79	0.64
3:c:216:SER:HB3	3:c:221:GLU:HB2	1.79	0.64
22:c:507:CLA:HBC3	22:c:509:CLA:H92	1.78	0.64
22:A:404:CLA:H142	22:D:405:CLA:H151	1.79	0.64
24:b:621:BCR:H19C	24:b:622:BCR:H363	1.80	0.64
22:B:607:CLA:HBA2	29:B:622:SQD:H101	1.80	0.64
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.78	0.64
16:V:102:MET:HE3	34:V:201:HEM:HBB2	1.80	0.64
16:v:102:MET:HE3	34:v:201:HEM:HBB2	1.80	0.64
1:a:183:MET:HB3	22:a:404:CLA:HBC2	1.79	0.63
2:b:271:THR:HG22	2:b:273:TYR:H	1.63	0.63
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.63
1:a:190:HIS:HB3	1:a:293:MET:HE2	1.79	0.63
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.80	0.63
3:C:406:SER:O	3:C:418:ASN:ND2	2.32	0.63
3:c:48:LYS:NZ	3:c:133:ALA:O	2.31	0.63
31:d:402:PHO:H151	22:d:405:CLA:H172	1.80	0.63
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.80	0.63
3:c:291:TRP:O	3:c:305:THR:OG1	2.17	0.63
4:d:29:PHE:O	4:d:128:ARG:NH2	2.32	0.63
13:o:77:LEU:HB3	13:o:91:PHE:HB3	1.80	0.63
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
3:c:150:ASP:HB3	3:c:153:ASP:HB2	1.81	0.62
2:B:121:GLU:O	7:H:12:ARG:NH2	2.32	0.62
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.81	0.62
3:c:406:SER:O	3:c:418:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:149:LEU:HG	22:b:606:CLA:HBC1	1.82	0.62
3:C:49:LEU:O	3:C:53:HIS:ND1	2.32	0.62
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.81	0.62
1:A:174:LEU:HD22	31:D:401:PHO:H151	1.82	0.61
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.81	0.61
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.82	0.61
1:a:329:GLU:O	1:a:332:HIS:ND1	2.32	0.61
22:h:101:CLA:H2	22:h:101:CLA:HBD	1.83	0.61
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.61
3:c:297:TYR:O	3:c:423:ARG:NH2	2.34	0.61
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.82	0.61
3:c:49:LEU:O	3:c:53:HIS:ND1	2.32	0.61
22:a:404:CLA:H122	31:d:401:PHO:H3A	1.81	0.61
22:c:506:CLA:H112	24:c:514:BCR:H362	1.83	0.61
22:a:404:CLA:HHC	22:a:404:CLA:HBB1	1.82	0.61
3:c:342:MET:HE3	3:c:352:GLY:HA2	1.82	0.61
9:j:15:THR:HG21	10:k:38:VAL:HG13	1.83	0.61
1:a:214:MET:HE2	1:a:214:MET:HA	1.84	0.60
6:f:17:THR:HG23	6:f:20:TRP:H	1.66	0.60
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.84	0.60
29:A:412:SQD:H172	26:C:519:LHG:H172	1.84	0.60
1:a:15:GLU:O	1:a:19:ASN:ND2	2.35	0.60
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.84	0.60
22:b:611:CLA:HBA2	29:d:403:SQD:H101	1.84	0.60
4:d:186:GLN:HB2	22:d:405:CLA:HBC1	1.83	0.60
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.67	0.60
22:a:404:CLA:H71	22:a:405:CLA:HAB	1.83	0.60
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.84	0.60
1:a:221:SER:HB3	4:d:141:TYR:HB2	1.83	0.60
2:B:327:THR:HG21	27:B:621:LMG:H111	1.83	0.60
12:M:31:SER:HA	27:M:101:LMG:HC1	1.83	0.59
4:D:216:ALA:O	4:D:220:ASN:ND2	2.34	0.59
22:c:503:CLA:H172	22:c:509:CLA:HBB2	1.83	0.59
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.85	0.59
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.67	0.59
22:a:406:CLA:H142	22:d:405:CLA:H151	1.84	0.59
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.59
4:D:24:ARG:NH2	18:X:44:ASP:O	2.36	0.59
1:a:328:MET:HE1	4:d:183:LEU:HD22	1.84	0.59
2:b:262:THR:OG1	22:b:606:CLA:O1D	2.20	0.59
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:606:CLA:H193	7:h:42:LEU:HD12	1.84	0.59
17:g:35:ILE:HG22	20:z:21:ILE:HG23	1.84	0.59
29:A:413:SQD:H61	22:b:619:CLA:H2	1.85	0.59
29:a:401:SQD:H311	24:a:409:BCR:H342	1.85	0.59
12:M:28:GLN:HA	12:m:28:GLN:HA	1.85	0.59
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.84	0.58
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.58
22:B:615:CLA:H2	29:a:401:SQD:H61	1.85	0.58
3:c:215:LYS:HB3	3:c:223:TRP:HA	1.85	0.58
29:B:622:SQD:H171	29:B:622:SQD:H301	1.86	0.58
2:b:121:GLU:O	7:h:12:ARG:NH2	2.35	0.58
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.85	0.58
20:z:33:TRP:HA	20:z:36:SER:HB3	1.86	0.58
29:a:415:SQD:H172	26:c:519:LHG:H172	1.86	0.58
2:b:12:LEU:HB2	22:b:615:CLA:HMC2	1.86	0.58
3:c:449:ARG:HE	22:c:504:CLA:HED1	1.69	0.58
4:d:216:ALA:O	4:d:220:ASN:ND2	2.34	0.58
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.85	0.57
1:A:329:GLU:O	1:A:332:HIS:ND1	2.36	0.57
3:C:118:HIS:CE1	27:C:518:LMG:H192	2.39	0.57
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.86	0.57
2:b:62:VAL:HG12	2:b:66:MET:HE2	1.86	0.57
27:D:409:LMG:O6	11:L:15:THR:HG21	2.05	0.57
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.69	0.57
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.69	0.57
13:o:230:VAL:HG13	13:o:237:ILE:HG22	1.86	0.57
1:A:214:MET:HA	1:A:214:MET:HE2	1.85	0.57
25:c:517:DGD:HA22	9:j:29:PHE:HE1	1.68	0.57
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.85	0.57
34:v:201:HEM:HBB2	34:v:201:HEM:HMB1	1.86	0.57
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.86	0.57
13:O:83:LYS:HG2	13:O:84:ASN:H	1.69	0.57
3:c:164:HIS:ND1	22:c:506:CLA:OBD	2.33	0.57
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.87	0.57
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.86	0.57
1:A:268:SER:O	1:A:272:HIS:ND1	2.35	0.57
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.87	0.57
1:a:64:ARG:O	13:o:178:ARG:NH2	2.37	0.56
3:c:42:LEU:HD21	22:c:510:CLA:H2A	1.87	0.56
22:A:402:CLA:H122	31:D:401:PHO:H3A	1.87	0.56
12:m:25:LEU:O	12:m:28:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:404:CLA:H93	22:D:405:CLA:H152	1.87	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.23	0.56
22:H:101:CLA:H2	22:H:101:CLA:HBD	1.87	0.56
1:a:217:SER:HA	4:d:272:LEU:HD12	1.87	0.56
4:d:24:ARG:NH2	18:x:44:ASP:O	2.39	0.56
27:d:412:LMG:H171	24:f:102:BCR:H383	1.88	0.56
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.35	0.56
1:a:65:GLU:OE2	1:a:334:ARG:NH2	2.37	0.56
4:d:192:THR:HG23	22:d:405:CLA:HBC2	1.88	0.56
27:d:409:LMG:HO4	27:d:409:LMG:HO5	1.53	0.56
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
4:D:192:THR:HG23	22:D:405:CLA:HBC2	1.88	0.55
4:d:214:HIS:ND1	23:d:407:PL9:O2	2.28	0.55
29:d:403:SQD:H241	29:d:403:SQD:H111	1.88	0.55
13:o:83:LYS:HG2	13:o:84:ASN:H	1.70	0.55
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.87	0.55
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.88	0.55
22:b:607:CLA:HBD	22:b:608:CLA:H43	1.88	0.55
17:g:39:LEU:HD21	20:z:25:VAL:HA	1.88	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.88	0.55
22:A:403:CLA:H203	31:D:401:PHO:H71	1.87	0.55
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.40	0.55
4:D:214:HIS:ND1	23:D:407:PL9:O2	2.27	0.55
22:b:606:CLA:C2D	22:b:608:CLA:H2	2.37	0.55
27:A:410:LMG:H231	23:D:407:PL9:H352	1.89	0.55
22:D:406:CLA:H43	18:X:23:LEU:HA	1.89	0.55
22:d:406:CLA:H42	18:x:26:GLY:HA3	1.89	0.55
27:d:409:LMG:O6	11:l:15:THR:HG21	2.06	0.55
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.88	0.55
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.39	0.55
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.88	0.55
1:a:85:SER:HA	1:a:109:GLY:HA3	1.88	0.55
3:c:229:ASN:ND2	3:c:232:ASP:OD1	2.33	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.55
1:a:29:TYR:O	1:a:129:ARG:NH1	2.40	0.55
2:b:184:GLU:H	2:b:200:ALA:HB2	1.72	0.55
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.88	0.55
15:u:56:ASP:OD2	15:u:115:THR:OG1	2.21	0.55
22:A:403:CLA:HMA2	23:D:407:PL9:H411	1.89	0.55
27:a:412:LMG:H231	23:d:407:PL9:H352	1.89	0.55
2:B:256:MET:O	2:B:448:ARG:NH1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.55
22:b:611:CLA:H151	22:b:612:CLA:H203	1.89	0.55
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54
2:b:487:SER:N	2:b:488:PRO:HD2	2.22	0.54
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.35	0.54
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.37	0.54
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.54
2:b:458:PHE:HB3	22:b:607:CLA:HBC2	1.89	0.54
22:c:508:CLA:HBD	22:c:508:CLA:H121	1.88	0.54
34:f:101:HEM:HBC2	34:f:101:HEM:HMC2	1.90	0.54
1:A:64:ARG:O	13:O:178:ARG:NH2	2.41	0.54
2:B:25:MET:HE3	24:B:616:BCR:H23C	1.89	0.54
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.88	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.54
4:d:222:LEU:HD23	4:d:244:TYR:HB3	1.89	0.54
2:B:262:THR:HG22	2:B:263:THR:HG23	1.89	0.54
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.38	0.54
27:D:409:LMG:HO4	27:D:409:LMG:HO5	1.52	0.54
22:b:612:CLA:HMD1	7:h:27:THR:HB	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:603:CLA:HBC2	1.90	0.54
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.90	0.54
22:a:405:CLA:HED1	23:d:407:PL9:H372	1.87	0.54
31:D:402:PHO:H151	22:D:405:CLA:H172	1.89	0.54
3:c:229:ASN:HD22	3:c:231:GLU:HB2	1.73	0.54
24:A:407:BCR:H342	29:A:413:SQD:H311	1.90	0.54
2:b:270:PRO:HG3	2:b:312:TYR:HD2	1.73	0.54
25:B:625:DGD:O1B	25:B:625:DGD:O2D	2.25	0.54
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.54
13:O:73:PRO:HG2	13:O:102:THR:HB	1.90	0.54
26:c:519:LHG:H101	26:c:519:LHG:H271	1.90	0.54
22:b:614:CLA:H41	22:b:617:CLA:HBC3	1.89	0.54
22:c:501:CLA:C2D	22:c:503:CLA:H2	2.37	0.54
22:A:403:CLA:HED1	23:D:407:PL9:H372	1.90	0.53
2:b:327:THR:HG21	27:b:625:LMG:H111	1.90	0.53
22:a:405:CLA:H203	31:d:401:PHO:H71	1.90	0.53
20:z:33:TRP:O	20:z:37:LYS:HB2	2.08	0.53
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.89	0.53
2:b:155:ALA:O	2:b:159:THR:OG1	2.21	0.53
29:f:103:SQD:H131	18:x:36:VAL:HG11	1.89	0.53
22:c:507:CLA:H172	25:c:516:DGD:HBW2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.90	0.53
1:A:217:SER:HA	4:D:272:LEU:HD12	1.91	0.53
29:B:626:SQD:H1	29:B:626:SQD:H462	1.90	0.53
1:a:121:LEU:HD13	25:a:410:DGD:HB92	1.91	0.53
2:b:474:LEU:O	4:d:134:ARG:NH1	2.42	0.53
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.53
22:B:607:CLA:H151	22:B:608:CLA:H203	1.90	0.53
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.91	0.53
29:a:415:SQD:H311	22:c:507:CLA:H71	1.91	0.53
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.44	0.53
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.91	0.53
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.44	0.53
3:c:284:PHE:HB3	25:c:515:DGD:HA51	1.91	0.53
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.91	0.53
1:a:268:SER:O	1:a:272:HIS:ND1	2.37	0.53
22:B:605:CLA:OBD	30:B:623:LMT:O6'	2.20	0.52
34:F:101:HEM:HBC2	34:F:101:HEM:HMC2	1.91	0.52
13:o:180:ALA:HB1	13:o:191:ALA:HB2	1.92	0.52
24:A:407:BCR:H321	29:A:413:SQD:H321	1.91	0.52
2:B:271:THR:HB	2:B:274:GLN:HG3	1.91	0.52
25:b:601:DGD:O1B	25:b:601:DGD:O2D	2.26	0.52
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.91	0.52
5:e:10:PHE:N	27:e:101:LMG:O3	2.41	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
3:c:305:THR:HG22	3:c:308:GLU:HB2	1.91	0.52
1:a:244:GLU:HG3	1:a:246:TYR:H	1.74	0.52
22:b:606:CLA:C3D	22:b:608:CLA:H2	2.39	0.52
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.91	0.52
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.34	0.52
22:a:405:CLA:HMA2	23:d:407:PL9:H411	1.92	0.52
2:b:262:THR:HG22	2:b:263:THR:HG23	1.90	0.52
3:c:29:GLU:HB3	10:k:46:ARG:HH11	1.74	0.52
18:x:11:THR:HG23	18:x:12:ILE:HG22	1.92	0.52
1:A:211:PHE:HA	1:A:214:MET:HB2	1.91	0.52
22:b:618:CLA:H111	22:b:618:CLA:H172	1.92	0.52
3:c:305:THR:HG23	3:c:307:PRO:HD2	1.90	0.52
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.92	0.52
26:C:519:LHG:H271	26:C:519:LHG:H101	1.90	0.52
7:h:45:ILE:HD11	22:h:101:CLA:H42	1.92	0.52
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.91	0.51
1:a:153:SER:HB3	22:a:404:CLA:HED1	1.91	0.51
25:b:601:DGD:HD1	30:b:603:LMT:H32	1.91	0.51
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.91	0.51
22:D:406:CLA:H42	18:X:26:GLY:HA3	1.92	0.51
1:a:212:CYS:HB2	4:d:211:CYS:HB2	1.92	0.51
2:b:25:MET:HE3	24:b:620:BCR:H23C	1.91	0.51
4:d:275:PRO:O	4:d:279:LEU:HD23	2.10	0.51
15:u:72:TYR:HB3	15:u:73:PRO:HD3	1.92	0.51
22:a:405:CLA:H42	23:d:407:PL9:H162	1.93	0.51
3:c:197:ARG:NH2	3:c:231:GLU:OE2	2.44	0.51
29:A:412:SQD:H311	22:C:507:CLA:H71	1.93	0.51
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.92	0.51
29:b:602:SQD:H1	29:b:602:SQD:H462	1.91	0.51
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.93	0.51
7:h:55:LEU:HB2	7:h:58:VAL:HG12	1.92	0.51
13:o:240:THR:HG22	13:o:264:VAL:HG12	1.93	0.51
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.74	0.51
17:y:39:LEU:HD21	20:Z:25:VAL:HA	1.92	0.51
3:c:85:GLY:N	25:c:516:DGD:HE4	2.25	0.51
22:c:504:CLA:HBA1	22:c:504:CLA:HBD	1.93	0.51
25:c:517:DGD:HA22	9:j:29:PHE:CE1	2.46	0.51
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.93	0.51
1:a:57:PRO:HG3	1:a:68:SER:HB3	1.93	0.51
1:a:183:MET:HE1	22:a:405:CLA:HMD2	1.93	0.51
1:A:132:GLU:O	1:A:136:ARG:HG2	2.11	0.51
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.93	0.51
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.92	0.51
2:b:135:LEU:HA	2:b:138:MET:HE3	1.93	0.51
22:b:609:CLA:OBD	30:b:626:LMT:O6'	2.21	0.51
7:h:45:ILE:HD12	22:h:101:CLA:HAA2	1.93	0.50
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.94	0.50
3:c:131:TYR:HE1	3:c:135:ARG:HD2	1.75	0.50
3:C:85:GLY:N	25:C:516:DGD:HE4	2.26	0.50
22:b:608:CLA:H202	22:b:612:CLA:HBB2	1.93	0.50
2:B:135:LEU:HA	2:B:138:MET:HE3	1.94	0.50
8:I:4:LEU:HD22	30:b:603:LMT:H62	1.93	0.50
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.93	0.50
3:c:405:ASN:HB2	25:c:517:DGD:HG31	1.93	0.50
17:g:24:MET:O	17:g:28:ILE:HG23	2.12	0.50
10:k:26:PRO:O	10:k:29:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:403:CLA:CHA	22:A:403:CLA:HBA1	2.42	0.50
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.94	0.50
2:b:150:CYS:HA	22:b:606:CLA:HBC2	1.92	0.50
4:d:85:MET:HA	5:e:69:ARG:HB3	1.92	0.50
1:A:244:GLU:HG3	1:A:246:TYR:H	1.76	0.50
16:v:81:ARG:CZ	16:v:157:GLY:HA3	2.42	0.50
29:A:412:SQD:H223	25:C:517:DGD:HAE1	1.93	0.50
22:C:504:CLA:HBA1	22:C:504:CLA:HBD	1.94	0.50
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.94	0.50
2:b:4:PRO:HD2	2:b:7:ARG:HD2	1.93	0.50
2:b:341:LYS:HA	2:b:405:GLU:HB2	1.94	0.50
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.93	0.50
4:d:279:LEU:HG	31:d:402:PHO:HBC3	1.94	0.50
25:d:410:DGD:O5E	25:d:410:DGD:O4E	2.25	0.50
2:b:271:THR:HB	2:b:274:GLN:HG3	1.94	0.50
3:c:361:PHE:HD1	25:c:515:DGD:HE61	1.77	0.50
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.27	0.49
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.93	0.49
13:o:168:PHE:HB2	13:o:225:LEU:HB2	1.92	0.49
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.49
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.45	0.49
1:a:132:GLU:O	1:a:136:ARG:HG2	2.12	0.49
2:b:383:PHE:CZ	13:o:193:GLY:HA2	2.47	0.49
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.47	0.49
4:d:348:ARG:NH2	4:d:352:LEU:O	2.33	0.49
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.95	0.49
2:B:327:THR:HG22	22:B:606:CLA:H12	1.94	0.49
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.77	0.49
18:x:12:ILE:HG12	18:x:16:LEU:HD12	1.95	0.49
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.49
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.75	0.49
22:a:406:CLA:HAB	22:d:405:CLA:H72	1.94	0.49
13:o:73:PRO:HG2	13:o:102:THR:HB	1.94	0.49
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.42	0.49
1:a:190:HIS:O	1:a:298:ASN:HB3	2.13	0.49
2:b:122:LEU:O	7:h:15:ASN:ND2	2.43	0.49
27:d:409:LMG:H111	11:l:19:LEU:HD21	1.94	0.49
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.78	0.49
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.94	0.49
5:e:57:ALA:HB3	5:e:60:GLN:HB3	1.95	0.49
1:A:210:LEU:HG	31:D:402:PHO:NC	2.28	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
29:f:103:SQD:H162	18:x:33:THR:HA	1.95	0.49
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.49
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.47	0.49
22:b:610:CLA:HBB1	27:b:625:LMG:H341	1.95	0.49
22:b:611:CLA:H51	22:b:612:CLA:H101	1.95	0.49
5:e:15:THR:HG23	9:j:8:ILE:O	2.12	0.49
2:B:222:PRO:HG3	7:H:27:THR:H	1.78	0.48
22:B:612:CLA:H51	27:D:408:LMG:H231	1.95	0.48
29:B:622:SQD:H241	29:B:622:SQD:H111	1.96	0.48
30:B:627:LMT:H62	8:i:4:LEU:HD22	1.94	0.48
29:F:103:SQD:H162	18:X:33:THR:HA	1.94	0.48
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.95	0.48
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.25	0.48
1:A:78:ILE:O	1:A:176:ILE:HB	2.13	0.48
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.48	0.48
29:a:415:SQD:H223	25:c:517:DGD:HAE1	1.95	0.48
3:c:166:ILE:O	3:c:170:ILE:HG13	2.13	0.48
22:d:406:CLA:H43	18:x:23:LEU:HA	1.95	0.48
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.94	0.48
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.48
2:b:327:THR:HG22	22:b:610:CLA:H12	1.95	0.48
4:d:43:LEU:HD23	4:d:117:HIS:CE1	2.47	0.48
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.94	0.48
25:B:625:DGD:HD1	30:B:627:LMT:H32	1.95	0.48
27:A:414:LMG:H112	2:b:43:ALA:HA	1.95	0.48
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.48
1:a:211:PHE:HA	1:a:214:MET:HB2	1.95	0.48
4:d:102:THR:OG1	25:d:410:DGD:HD62	2.12	0.48
1:A:183:MET:HE1	22:A:403:CLA:HMD2	1.95	0.48
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.44	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.95	0.48
29:a:401:SQD:H321	24:a:409:BCR:H321	1.96	0.48
9:j:14:ALA:O	9:j:18:GLY:N	2.44	0.48
13:o:118:SER:HB3	13:o:157:PRO:HA	1.96	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.48
22:a:405:CLA:CHA	22:a:405:CLA:HBA1	2.42	0.48
22:b:617:CLA:H51	24:b:620:BCR:H372	1.94	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:140:ARG:NH2	26:a:411:LHG:O5	2.34	0.48
5:e:18:ARG:NH1	34:f:101:HEM:O1A	2.46	0.48
13:o:144:LEU:HD13	13:o:259:VAL:HG11	1.95	0.48
27:C:518:LMG:H292	27:C:518:LMG:H111	1.95	0.48
29:F:103:SQD:H131	18:X:36:VAL:HG11	1.96	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.79	0.47
25:b:624:DGD:HAW2	22:h:101:CLA:H152	1.95	0.47
3:c:209:ILE:HG23	24:c:514:BCR:H382	1.95	0.47
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.96	0.47
4:D:279:LEU:HG	31:D:402:PHO:HBC3	1.96	0.47
27:D:412:LMG:H171	24:F:102:BCR:H383	1.95	0.47
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.47
4:d:302:GLU:OE1	13:o:186:LYS:NZ	2.40	0.47
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.44	0.47
10:k:12:PRO:HB2	10:k:15:TYR:HD2	1.79	0.47
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.46	0.47
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.94	0.47
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.95	0.47
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.50	0.47
3:C:158:THR:O	3:C:251:HIS:HB3	2.14	0.47
1:a:156:ALA:HA	1:a:160:ILE:HB	1.97	0.47
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.97	0.47
3:c:461:ARG:NH1	4:d:241:GLU:OE1	2.45	0.47
2:b:247:PHE:HE1	22:h:101:CLA:H101	1.78	0.47
22:B:615:CLA:H12	22:B:615:CLA:H72	1.97	0.47
3:C:223:TRP:CG	3:C:224:ILE:H	2.32	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.97	0.47
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.97	0.47
22:b:616:CLA:H51	27:d:408:LMG:H231	1.97	0.47
3:c:158:THR:O	3:c:251:HIS:HB3	2.15	0.47
13:o:223:ILE:HG13	13:o:243:SER:HB3	1.97	0.47
1:a:210:LEU:HG	31:d:402:PHO:NC	2.30	0.47
3:c:130:VAL:O	3:c:134:ILE:HG12	2.15	0.47
15:u:75:LEU:HD21	15:u:101:GLN:HB3	1.96	0.47
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.97	0.47
2:b:450:TRP:NE1	22:b:610:CLA:HBA1	2.29	0.47
22:c:501:CLA:H193	22:c:506:CLA:H111	1.97	0.47
24:c:513:BCR:H391	10:k:36:ALA:HB2	1.96	0.47
4:d:262:SER:N	27:d:409:LMG:O3	2.44	0.47

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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	0.47
22:C:510:CLA:HMB1	24:C:513:BCR:H382	1.97	0.47
1:a:227:THR:HG21	1:a:233:ALA:HA	1.97	0.47
1:a:317:TRP:CZ3	4:d:180:ARG:HD3	2.49	0.47
22:A:405:CLA:H141	22:A:405:CLA:H162	1.71	0.46
22:B:607:CLA:H18	22:B:608:CLA:H192	1.97	0.46
27:i:101:LMG:H181	30:i:102:LMT:H42	1.96	0.46
10:k:40:GLN:HA	10:k:43:VAL:HG12	1.97	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.98	0.46
4:D:275:PRO:O	4:D:279:LEU:HD23	2.14	0.46
1:a:78:ILE:O	1:a:176:ILE:HB	2.15	0.46
1:a:193:LEU:HD11	22:a:404:CLA:HMC2	1.97	0.46
22:b:619:CLA:H72	22:b:619:CLA:H12	1.97	0.46
8:i:29:ALA:HA	8:i:35:LYS:HB2	1.97	0.46
17:g:32:GLY:O	17:g:35:ILE:HG12	2.16	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46
4:D:48:TRP:CE2	31:D:402:PHO:H161	2.50	0.46
4:d:17:ILE:HG21	18:x:42:GLN:HG3	1.98	0.46
22:B:605:CLA:H18	22:B:615:CLA:H121	1.98	0.46
22:H:101:CLA:H41	22:H:101:CLA:H62	1.56	0.46
2:b:315:ILE:HG22	2:b:426:PHE:HB3	1.98	0.46
2:b:326:ARG:HB3	2:b:444:ARG:HG2	1.97	0.46
22:h:101:CLA:H41	22:h:101:CLA:H62	1.55	0.46
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.46
24:y:101:BCR:H20C	24:y:101:BCR:H361	1.80	0.46
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.97	0.46
3:c:75:PHE:HD1	3:c:86:LEU:HD21	1.79	0.46
3:c:343:ARG:NH1	3:c:347:GLY:O	2.49	0.46
22:h:101:CLA:H162	22:h:101:CLA:H122	1.53	0.46
24:x:101:BCR:H20C	24:x:101:BCR:H361	1.78	0.46
22:A:404:CLA:H161	23:A:406:PL9:H253	1.96	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.96	0.46
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.46
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.46
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.51	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
31:D:401:PHO:H41	31:D:401:PHO:H62	1.47	0.46
2:b:170:ASP:OD1	2:b:175:THR:N	2.45	0.46
3:c:223:TRP:CG	3:c:224:ILE:H	2.31	0.46
3:c:386:PRO:HB3	16:v:116:GLU:HG2	1.97	0.46
4:d:244:TYR:OH	4:d:264:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:54:LYS:HD2	15:u:113:THR:HG23	1.98	0.46
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.51	0.46
2:B:371:THR:HG22	2:B:377:VAL:HA	1.98	0.46
24:B:616:BCR:H20C	24:B:616:BCR:H361	1.76	0.46
22:C:510:CLA:H93	22:C:510:CLA:H61	1.81	0.46
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.79	0.46
2:b:306:PRO:HG2	2:b:309:LEU:HB2	1.97	0.46
3:c:223:TRP:CD2	3:c:224:ILE:HG13	2.50	0.46
13:o:230:VAL:HG12	13:o:231:ASP:H	1.80	0.46
2:B:383:PHE:N	4:D:344:GLU:O	2.36	0.46
24:C:513:BCR:H11C	24:y:101:BCR:H322	1.98	0.46
4:d:84:SER:HB2	4:d:85:MET:HE2	1.98	0.46
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.97	0.46
15:u:68:TYR:HB2	15:u:71:LEU:HD12	1.97	0.46
2:b:222:PRO:HG3	7:h:27:THR:H	1.81	0.45
3:c:318:LEU:HG	3:c:328:VAL:HG11	1.98	0.45
27:d:409:LMG:HC1	27:d:409:LMG:O9	2.16	0.45
20:z:32:ASP:CG	20:z:33:TRP:H	2.24	0.45
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.52	0.45
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.98	0.45
24:g:101:BCR:HC31	24:g:101:BCR:H323	1.69	0.45
1:A:121:LEU:HD13	25:A:408:DGD:HB92	1.99	0.45
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.45
22:C:509:CLA:H2	22:C:509:CLA:H61	1.72	0.45
4:D:102:THR:OG1	25:D:410:DGD:HD62	2.16	0.45
4:D:146:PHE:C	4:D:149:PRO:HD2	2.41	0.45
5:e:60:GLN:HG2	5:e:62:SER:H	1.81	0.45
27:M:101:LMG:H322	12:m:24:ILE:HG21	1.97	0.45
1:a:159:LEU:C	1:a:162:PRO:HD2	2.41	0.45
22:c:506:CLA:H92	22:c:506:CLA:H62	1.76	0.45
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.98	0.45
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.52	0.45
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.51	0.45
22:B:607:CLA:H51	22:B:608:CLA:H101	1.98	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.48	0.45
1:a:12:ASN:HB3	1:a:15:GLU:HB3	1.97	0.45
3:c:86:LEU:HB3	3:c:90:PRO:HD3	1.98	0.45
31:d:401:PHO:H41	31:d:401:PHO:H62	1.47	0.45
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.99	0.45
24:B:618:BCR:H20C	24:B:618:BCR:H361	1.82	0.45
27:D:409:LMG:H111	11:L:19:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:610:CLA:H193	11:l:27:LEU:HD11	1.99	0.45
3:c:337:LEU:HA	13:o:131:PRO:HG3	1.99	0.45
4:d:43:LEU:HD23	4:d:117:HIS:HE1	1.82	0.45
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.99	0.45
7:h:46:LEU:HD13	22:h:101:CLA:H72	1.97	0.45
16:v:160:LYS:HA	16:v:163:TYR:CD2	2.52	0.45
1:A:114:LEU:O	1:A:118:HIS:ND1	2.46	0.45
22:A:402:CLA:H3A	22:A:402:CLA:HBA1	1.53	0.45
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.99	0.45
2:b:212:ALA:O	2:b:216:HIS:ND1	2.44	0.45
13:o:184:ASP:OD2	13:o:188:ARG:HB2	2.16	0.45
22:B:604:CLA:H62	22:B:604:CLA:H41	1.79	0.45
22:B:614:CLA:H172	22:B:614:CLA:H111	1.99	0.45
24:C:514:BCR:H20C	24:C:514:BCR:H361	1.83	0.45
13:O:118:SER:HB3	13:O:157:PRO:HA	1.99	0.45
13:O:143:PRO:HG2	13:O:248:ASP:HB3	1.98	0.45
3:c:80:PRO:HB3	3:c:82:TYR:CE1	2.51	0.45
22:A:402:CLA:H51	31:D:401:PHO:C3B	2.47	0.45
22:B:611:CLA:H122	22:B:611:CLA:H162	1.76	0.45
30:B:628:LMT:H122	14:t:7:VAL:HG12	1.97	0.45
3:C:113:VAL:HG11	27:C:518:LMG:H132	1.99	0.45
3:c:137:PRO:HB2	3:c:139:THR:O	2.17	0.45
3:c:402:GLY:HA3	3:c:420:VAL:HG22	1.98	0.45
22:c:512:CLA:HAB	24:c:521:BCR:H24C	1.99	0.45
16:v:98:LEU:O	16:v:102:MET:HG3	2.17	0.45
1:A:224:ILE:O	4:D:265:ARG:NH2	2.49	0.45
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.80	0.45
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.45
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.31	0.45
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.45
14:T:7:VAL:HG12	30:b:604:LMT:H122	1.99	0.45
22:a:405:CLA:H202	22:a:405:CLA:H162	1.76	0.45
2:b:18:ARG:HD3	2:b:118:TRP:HB3	1.98	0.45
2:b:30:VAL:HG12	22:b:608:CLA:HHD	1.99	0.45
3:c:347:GLY:HA3	13:o:43:ASN:HB2	1.99	0.45
22:c:510:CLA:H121	24:c:513:BCR:H21C	1.98	0.45
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.79	0.44
3:c:131:TYR:CE1	3:c:135:ARG:HD2	2.53	0.44
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.42	0.44
22:B:605:CLA:H3A	22:B:605:CLA:HBA2	1.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:620:DGD:HA71	22:H:101:CLA:H193	2.00	0.44
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.99	0.44
1:a:214:MET:HE1	4:d:142:ASN:HD21	1.82	0.44
22:a:404:CLA:H3A	22:a:404:CLA:HBA1	1.52	0.44
22:c:508:CLA:H11	22:c:508:CLA:H51	1.82	0.44
24:c:521:BCR:H20C	24:c:521:BCR:H361	1.80	0.44
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.99	0.44
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.44
7:H:46:LEU:HD13	22:H:101:CLA:H72	2.00	0.44
22:c:504:CLA:H11	24:c:514:BCR:H312	2.00	0.44
22:B:613:CLA:H51	24:B:616:BCR:H372	1.98	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.44
24:H:102:BCR:H20C	24:H:102:BCR:H361	1.78	0.44
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.52	0.44
1:a:317:TRP:HZ3	4:d:180:ARG:HD3	1.82	0.44
23:a:408:PL9:H371	23:a:408:PL9:H351	1.81	0.44
4:d:221:THR:HG23	4:d:244:TYR:HB2	1.99	0.44
9:j:38:SER:OG	9:j:39:SER:N	2.49	0.44
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.99	0.44
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.86	0.44
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.41	0.44
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.44
5:E:60:GLN:HG2	5:E:62:SER:H	1.82	0.44
10:K:37:PHE:HB3	24:y:101:BCR:C40	2.47	0.44
2:b:213:GLY:O	2:b:217:ILE:HG13	2.17	0.44
20:z:29:SER:HA	20:z:30:PRO:HD3	1.83	0.44
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.99	0.44
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.83	0.44
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.98	0.44
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.26	0.44
20:Z:33:TRP:O	20:Z:33:TRP:CD1	2.71	0.44
22:a:406:CLA:H93	22:d:405:CLA:H152	1.98	0.44
3:c:113:VAL:HG11	27:c:518:LMG:H132	1.98	0.44
22:c:501:CLA:H162	22:c:501:CLA:H141	1.78	0.44
4:d:56:THR:HG21	5:e:50:PRO:HD3	2.00	0.44
2:B:474:LEU:O	4:D:134:ARG:NH1	2.50	0.44
1:a:45:THR:HG21	29:a:401:SQD:H201	1.99	0.44
2:B:26:HIS:CE1	22:B:611:CLA:HMA2	2.52	0.44
3:C:137:PRO:HB2	3:C:139:THR:O	2.18	0.44
3:C:224:ILE:O	3:C:227:VAL:HG23	2.18	0.44
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.00	0.44

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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	0.44
1:a:271:LEU:HD11	23:a:408:PL9:C4	2.48	0.44
2:b:26:HIS:CE1	22:b:615:CLA:HMA2	2.53	0.44
2:b:135:LEU:HD22	2:b:237:VAL:HG21	1.99	0.44
2:b:371:THR:HG22	2:b:377:VAL:HA	1.99	0.44
13:o:240:THR:HA	13:o:264:VAL:HA	1.99	0.44
15:u:117:VAL:HG13	15:u:122:VAL:HG21	1.99	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.18	0.44
2:B:213:GLY:O	2:B:217:ILE:HG13	2.18	0.44
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.44
4:D:262:SER:N	27:D:409:LMG:O3	2.46	0.44
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.00	0.44
16:V:102:MET:HE3	34:V:201:HEM:HMB1	1.99	0.44
22:a:406:CLA:H161	23:a:408:PL9:H253	2.00	0.44
22:b:610:CLA:H102	27:b:625:LMG:H392	2.00	0.44
3:c:223:TRP:O	3:c:226:SER:OG	2.31	0.44
5:e:49:THR:HA	5:e:50:PRO:HD3	1.90	0.44
13:o:143:PRO:HG2	13:o:248:ASP:HB3	1.98	0.44
1:A:156:ALA:HA	1:A:160:ILE:HB	1.99	0.43
22:C:512:CLA:H3A	22:C:512:CLA:HBA2	1.72	0.43
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.77	0.43
24:K:102:BCR:H24C	24:K:102:BCR:H371	1.81	0.43
24:b:623:BCR:H24C	24:b:623:BCR:H371	1.88	0.43
3:c:346:THR:HG21	13:o:38:GLY:HA2	1.99	0.43
13:o:81:GLU:HA	13:o:82:PRO:HD3	1.78	0.43
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.43
3:C:245:ILE:O	3:C:249:ILE:HG12	2.17	0.43
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.43
2:b:256:MET:HA	2:b:263:THR:HG21	2.00	0.43
25:b:624:DGD:HA71	22:h:101:CLA:H193	1.99	0.43
4:d:201:VAL:HB	22:d:405:CLA:HMB2	1.99	0.43
1:A:141:PRO:HB2	1:A:142:TRP:H	1.66	0.43
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.83	0.43
22:A:403:CLA:H51	22:A:403:CLA:H11	1.81	0.43
22:B:605:CLA:C3D	30:B:623:LMT:H11	2.49	0.43
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.18	0.43
5:E:81:GLU:C	5:E:83:LEU:H	2.26	0.43
6:F:22:ALA:O	6:F:25:THR:OG1	2.33	0.43
4:d:53:THR:HG22	4:d:67:TYR:CD2	2.52	0.43
1:A:271:LEU:HD21	23:A:406:PL9:HC71	1.99	0.43
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:401:PHO:H13	31:D:401:PHO:H102	1.82	0.43
22:D:405:CLA:H92	22:D:405:CLA:H62	1.79	0.43
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.43
22:b:619:CLA:H111	22:b:619:CLA:H143	1.74	0.43
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.00	0.43
24:j:102:BCR:H15C	24:j:102:BCR:H351	1.77	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.93	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
22:B:608:CLA:H11	7:H:35:MET:HE1	1.99	0.43
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.18	0.43
2:b:247:PHE:HB2	22:b:611:CLA:HBC1	1.99	0.43
3:c:315:MET:HE1	3:c:369:LEU:HD12	1.99	0.43
20:z:33:TRP:O	20:z:33:TRP:CD1	2.71	0.43
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.54	0.43
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.01	0.43
27:D:409:LMG:HC1	27:D:409:LMG:O9	2.18	0.43
22:b:606:CLA:H2	22:b:608:CLA:H93	2.01	0.43
22:b:616:CLA:H171	27:d:408:LMG:H401	1.99	0.43
24:b:623:BCR:H15C	24:b:623:BCR:H351	1.88	0.43
24:c:513:BCR:H371	24:c:513:BCR:H24C	1.81	0.43
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.01	0.43
16:v:68:VAL:O	16:v:71:ILE:HG12	2.19	0.43
1:A:141:PRO:HG3	3:C:446:GLY:C	2.43	0.43
22:A:404:CLA:H161	22:A:404:CLA:H143	1.86	0.43
30:B:628:LMT:H1B	30:B:628:LMT:H3'	1.53	0.43
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.43
2:b:5:TRP:HZ3	22:b:614:CLA:H51	1.84	0.43
4:d:87:HIS:CD2	4:d:162:LEU:HD23	2.54	0.43
11:l:4:ASN:OD1	11:l:6:ASN:ND2	2.41	0.43
1:A:235:TYR:C	1:A:237:TYR:H	2.26	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.43
1:a:309:ALA:HA	6:f:45:ARG:HB2	2.01	0.43
22:b:615:CLA:H162	22:b:615:CLA:H122	1.73	0.43
3:c:29:GLU:HB2	3:c:30:SER:H	1.64	0.43
3:c:224:ILE:O	3:c:227:VAL:HG23	2.19	0.43
3:c:245:ILE:O	3:c:249:ILE:HG12	2.19	0.43
3:c:473:ASP:HB2	14:t:26:PRO:HB3	2.00	0.43
4:d:48:TRP:CE2	31:d:402:PHO:H161	2.54	0.43
6:f:16:PHE:HB3	29:f:103:SQD:H241	2.01	0.43
16:v:102:MET:HE3	34:v:201:HEM:HMB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:g:101:BCR:H20C	24:g:101:BCR:H361	1.80	0.43
2:B:43:ALA:HA	27:a:402:LMG:H112	2.00	0.43
22:B:611:CLA:H171	22:B:612:CLA:HBB2	2.00	0.43
22:B:613:CLA:H91	22:B:613:CLA:H112	1.84	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.78	0.43
4:D:84:SER:HB2	4:D:85:MET:HE2	2.01	0.43
1:a:157:VAL:HG13	1:a:172:MET:HB3	2.01	0.43
3:c:90:PRO:O	3:c:94:THR:HG23	2.18	0.43
4:d:156:VAL:HG12	4:d:171:PRO:HG3	2.00	0.43
26:A:409:LHG:H382	22:C:509:CLA:H93	2.01	0.43
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.01	0.43
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.01	0.43
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.76	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
22:D:405:CLA:H3A	22:D:405:CLA:HBA1	1.82	0.43
1:a:224:ILE:O	4:d:265:ARG:NH2	2.44	0.43
5:e:23:HIS:NE2	34:f:101:HEM:ND	2.67	0.43
13:o:135:GLN:HG2	13:o:141:ARG:HG3	2.01	0.43
1:A:193:LEU:HD11	22:A:402:CLA:HMC2	2.01	0.42
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.42
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.42
24:C:513:BCR:H353	24:y:101:BCR:H321	2.01	0.42
7:H:12:ARG:O	7:H:12:ARG:HD3	2.19	0.42
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.42
25:a:410:DGD:HD2	25:a:410:DGD:HG32	1.75	0.42
2:b:383:PHE:N	4:d:344:GLU:O	2.37	0.42
22:b:606:CLA:H61	22:b:606:CLA:H41	1.64	0.42
22:b:611:CLA:CHA	22:b:611:CLA:HBA1	2.49	0.42
3:c:248:GLY:O	3:c:252:ILE:HG12	2.18	0.42
4:d:129:GLN:OE1	4:d:143:ALA:HA	2.19	0.42
1:A:37:MET:HE1	1:A:129:ARG:CZ	2.49	0.42
27:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
3:C:343:ARG:NH1	3:C:347:GLY:O	2.52	0.42
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.42
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.01	0.42
23:D:407:PL9:H401	23:D:407:PL9:H421	1.86	0.42
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.01	0.42
3:c:456:GLU:HG2	3:c:457:LYS:HG3	2.02	0.42
24:f:102:BCR:H15C	24:f:102:BCR:H351	1.91	0.42
15:u:72:TYR:O	15:u:76:ALA:HB3	2.19	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:620:DGD:HAW2	22:H:101:CLA:H152	2.02	0.42
22:C:504:CLA:H11	24:C:514:BCR:H312	2.01	0.42
2:b:86:ILE:H	2:b:86:ILE:HG13	1.73	0.42
24:c:513:BCR:H15C	24:c:513:BCR:H351	1.89	0.42
1:A:183:MET:HA	22:A:402:CLA:HMD2	2.01	0.42
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.01	0.42
1:a:27:ARG:NH1	4:d:254:SER:O	2.48	0.42
1:a:111:PRO:O	1:a:115:ILE:HG13	2.18	0.42
1:a:129:ARG:NH2	4:d:256:ILE:HD12	2.30	0.42
22:c:511:CLA:H13	22:c:511:CLA:H61	2.02	0.42
1:A:140:ARG:HH22	26:A:409:LHG:P	2.41	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.91	0.42
22:B:605:CLA:H203	29:a:401:SQD:H332	2.02	0.42
24:B:616:BCR:H15C	24:B:616:BCR:H351	1.86	0.42
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.02	0.42
3:C:377:LEU:O	3:C:381:LYS:HB2	2.20	0.42
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.01	0.42
22:a:404:CLA:H51	31:d:401:PHO:C3B	2.50	0.42
22:a:406:CLA:H161	22:a:406:CLA:H143	1.87	0.42
22:c:512:CLA:HBA2	22:c:512:CLA:H3A	1.72	0.42
7:h:12:ARG:O	7:h:12:ARG:HD3	2.19	0.42
13:o:41:LEU:HD12	13:o:41:LEU:HA	1.92	0.42
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.85	0.42
22:B:612:CLA:H171	27:D:408:LMG:H401	2.01	0.42
22:C:511:CLA:H143	22:C:512:CLA:H162	2.02	0.42
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.67	0.42
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.00	0.42
27:a:412:LMG:O5	11:l:13:ASN:ND2	2.52	0.42
22:A:403:CLA:H42	23:D:407:PL9:H162	2.01	0.42
24:C:514:BCR:H15C	24:C:514:BCR:H351	1.84	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
1:a:60:ILE:HD12	1:a:84:PRO:HD2	2.01	0.42
22:b:613:CLA:H12	22:b:613:CLA:H51	1.89	0.42
24:b:623:BCR:H20C	24:b:623:BCR:H361	1.76	0.42
4:d:113:PHE:O	4:d:117:HIS:HB2	2.19	0.42
13:o:135:GLN:HE21	13:o:135:GLN:HB3	1.72	0.42
29:A:412:SQD:H171	23:J:101:PL9:H522	2.01	0.42
3:C:456:GLU:OE1	3:C:456:GLU:N	2.52	0.42
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.02	0.42
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.02	0.42
2:b:25:MET:HG2	24:b:620:BCR:H23C	2.02	0.42
24:b:620:BCR:H333	12:m:13:LEU:HD12	2.01	0.42
3:c:425:TRP:CE2	22:c:520:CLA:HBA1	2.54	0.42
22:c:520:CLA:H142	22:c:520:CLA:H112	1.78	0.42
3:C:315:MET:HE1	3:C:369:LEU:HD12	2.01	0.42
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.01	0.42
31:D:401:PHO:H202	31:D:401:PHO:H162	1.87	0.42
13:O:192:SER:OG	13:O:193:GLY:N	2.52	0.42
15:U:72:TYR:O	15:U:76:ALA:HB3	2.19	0.42
22:a:405:CLA:H51	22:a:405:CLA:H11	1.83	0.42
22:c:509:CLA:H2	22:c:509:CLA:H61	1.72	0.42
22:c:520:CLA:H141	22:c:520:CLA:H161	1.83	0.42
5:e:81:GLU:C	5:e:83:LEU:H	2.28	0.42
10:k:31:LEU:HB3	24:g:101:BCR:C15	2.50	0.42
18:x:17:LYS:O	18:x:21:ILE:HG13	2.19	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.42
2:B:329:PRO:HB3	22:B:606:CLA:HED1	2.02	0.42
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.89	0.42
1:a:182:PHE:O	1:a:186:PHE:HB2	2.20	0.42
1:a:257:ARG:HH22	2:b:488:PRO:C	2.28	0.42
22:c:510:CLA:H141	20:z:20:VAL:HG13	2.02	0.42
4:d:155:SER:HA	4:d:159:ILE:HB	2.01	0.42
4:d:236:ASN:HA	4:d:237:PRO:HD2	1.94	0.42
5:e:42:LEU:O	5:e:46:VAL:HG23	2.20	0.42
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.19	0.41
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.41
22:b:609:CLA:H3A	22:b:609:CLA:HBA2	1.25	0.41
3:c:456:GLU:OE1	3:c:456:GLU:N	2.50	0.41
22:c:508:CLA:H141	22:c:511:CLA:HMD3	2.01	0.41
22:d:406:CLA:H61	22:d:406:CLA:H41	1.85	0.41
9:j:9:PRO:HB2	9:j:12:ILE:HG13	2.01	0.41
17:g:28:ILE:O	24:g:101:BCR:H14C	2.20	0.41
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.85	0.41
24:B:618:BCR:H24C	24:B:618:BCR:H371	1.83	0.41
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.50	0.41
22:C:512:CLA:HAB	24:K:102:BCR:H371	2.02	0.41
4:D:350:ASN:O	4:D:352:LEU:N	2.48	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.41
16:V:90:PRO:O	16:V:92:ARG:HD3	2.19	0.41
22:a:406:CLA:HAB	22:d:405:CLA:H42	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:16:PRO:HB2	2:b:123:PHE:CG	2.55	0.41
4:d:252:PHE:O	4:d:256:ILE:HG22	2.20	0.41
13:o:206:GLU:H	13:o:206:GLU:CD	2.28	0.41
17:g:31:ALA:O	17:g:35:ILE:HG23	2.19	0.41
22:A:403:CLA:H162	22:A:403:CLA:H202	1.76	0.41
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.85	0.41
4:D:85:MET:HA	5:E:69:ARG:HB3	2.03	0.41
22:a:407:CLA:H141	22:a:407:CLA:H162	1.69	0.41
2:b:135:LEU:HB2	2:b:136:PRO:HD3	2.02	0.41
2:b:348:ASN:HB3	2:b:354:LEU:HD21	2.01	0.41
22:b:608:CLA:H41	22:b:608:CLA:H62	1.78	0.41
22:b:611:CLA:H18	22:b:612:CLA:H192	2.01	0.41
3:c:205:ASP:HA	3:c:206:PRO:HD2	1.93	0.41
1:A:238:LYS:O	1:A:241:GLN:HG3	2.21	0.41
22:A:403:CLA:H62	22:A:403:CLA:H41	1.76	0.41
22:A:403:CLA:HED2	4:D:198:MET:SD	2.60	0.41
22:B:602:CLA:HBB2	22:B:602:CLA:H92	2.03	0.41
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.84	0.41
24:F:102:BCR:H11C	24:F:102:BCR:H341	1.94	0.41
13:O:206:GLU:CD	13:O:206:GLU:H	2.27	0.41
27:b:625:LMG:H421	4:d:284:ILE:HD13	2.01	0.41
3:c:350:ILE:HG21	3:c:359:TRP:HB2	2.02	0.41
3:c:464:GLU:HA	3:c:465:PRO:HD2	1.78	0.41
27:c:522:LMG:H322	10:k:27:VAL:HG23	2.02	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.01	0.41
22:B:601:CLA:HMB2	24:H:102:BCR:H393	2.02	0.41
3:C:248:GLY:O	3:C:252:ILE:HG12	2.21	0.41
3:C:259:TRP:H	3:C:259:TRP:CD1	2.38	0.41
24:F:102:BCR:H361	24:F:102:BCR:H20C	1.81	0.41
22:H:101:CLA:H162	22:H:101:CLA:H122	1.50	0.41
10:K:31:LEU:HB3	24:y:101:BCR:C15	2.50	0.41
17:y:25:ILE:O	17:y:29:GLY:N	2.53	0.41
18:X:34:PHE:O	18:X:38:ILE:HG12	2.20	0.41
22:b:618:CLA:H12	22:b:618:CLA:H52	1.84	0.41
3:c:282:MET:HG2	22:c:501:CLA:H61	2.01	0.41
24:c:521:BCR:H15C	24:c:521:BCR:H351	1.84	0.41
1:A:257:ARG:HH22	2:B:488:PRO:C	2.29	0.41
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.56	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:31:ALA:O	17:y:35:ILE:HG23	2.21	0.41
1:a:235:TYR:C	1:a:237:TYR:H	2.29	0.41
1:a:240:GLY:HA3	14:t:29:ILE:HG22	2.02	0.41
3:c:466:VAL:HG13	4:d:251:ARG:HD2	2.01	0.41
1:A:215:HIS:ND1	23:A:406:PL9:O1	2.54	0.41
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.03	0.41
13:O:36:ILE:O	13:O:39:THR:OG1	2.34	0.41
1:a:89:ILE:HG12	13:o:99:ARG:NH2	2.36	0.41
1:a:269:ARG:NH1	4:d:231:THR:HB	2.36	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.56	0.41
2:b:280:PHE:O	2:b:284:ILE:HG13	2.20	0.41
4:d:55:VAL:HG21	4:d:110:LEU:HD12	2.03	0.41
5:e:7:GLU:H	5:e:7:GLU:CD	2.28	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.97	0.41
1:A:182:PHE:O	1:A:186:PHE:HB2	2.21	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.88	0.41
31:D:402:PHO:CHB	22:D:405:CLA:H101	2.51	0.41
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.56	0.41
1:a:153:SER:HB2	22:a:404:CLA:H43	2.03	0.41
22:b:610:CLA:H122	27:b:625:LMG:H412	2.03	0.41
24:c:513:BCR:H11C	24:g:101:BCR:H322	2.03	0.41
24:c:513:BCR:H361	24:c:513:BCR:H20C	1.80	0.41
13:o:192:SER:OG	13:o:193:GLY:N	2.53	0.41
1:A:258:LEU:O	4:D:128:ARG:NH1	2.54	0.41
22:A:403:CLA:HAA1	23:D:407:PL9:H362	2.02	0.41
24:A:407:BCR:H11C	24:A:407:BCR:H341	1.94	0.41
22:B:602:CLA:H192	22:B:602:CLA:H162	1.77	0.41
3:C:303:GLY:O	3:C:423:ARG:NE	2.41	0.41
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.54	0.41
7:H:19:GLY:O	7:H:21:VAL:HG13	2.21	0.41
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.21	0.41
1:a:34:GLY:HA2	1:a:37:MET:HB3	2.03	0.41
1:a:333:GLU:HB2	1:a:337:HIS:HE1	1.85	0.41
22:b:611:CLA:H143	22:b:611:CLA:H161	1.91	0.41
3:c:119:LEU:HG	24:c:513:BCR:H10C	2.02	0.41
3:c:259:TRP:CD1	3:c:259:TRP:H	2.39	0.41
3:c:393:ALA:HB1	34:v:201:HEM:HBC1	2.03	0.41
4:d:342:PRO:O	4:d:345:VAL:HG12	2.20	0.41
4:d:343:GLU:HG2	16:v:161:VAL:HG11	2.02	0.41
31:d:401:PHO:H13	31:d:401:PHO:H102	1.89	0.41
7:h:19:GLY:O	7:h:21:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.94	0.41
24:H:102:BCR:HC31	24:H:102:BCR:H323	1.89	0.41
24:y:101:BCR:H15C	24:y:101:BCR:H351	1.91	0.41
22:a:404:CLA:H102	22:a:404:CLA:H62	1.85	0.41
2:b:96:VAL:HG22	22:b:609:CLA:HBA1	2.03	0.41
2:b:191:ASN:HB2	7:h:58:VAL:HG23	2.03	0.41
30:b:604:LMT:H3'	30:b:604:LMT:H1B	1.55	0.41
22:c:512:CLA:HAB	24:c:521:BCR:H371	2.02	0.41
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.40
22:B:605:CLA:H62	22:B:605:CLA:H41	1.86	0.40
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.03	0.40
13:O:59:ASP:C	13:O:61:SER:H	2.30	0.40
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.57	0.40
17:y:28:ILE:O	24:y:101:BCR:H14C	2.21	0.40
1:a:238:LYS:O	1:a:241:GLN:HG3	2.21	0.40
2:b:125:ASP:HA	2:b:126:PRO:HD3	1.98	0.40
2:B:212:ALA:O	2:B:216:HIS:ND1	2.52	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.04	0.40
3:C:375:LEU:HB3	3:C:380:ILE:HD11	2.04	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.37	0.40
24:K:102:BCR:H361	24:K:102:BCR:H20C	1.81	0.40
2:b:179:GLN:HA	2:b:180:PRO:HD3	1.96	0.40
2:b:256:MET:O	2:b:448:ARG:NH1	2.39	0.40
24:b:622:BCR:H11C	24:b:622:BCR:H341	1.89	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.04	0.40
22:B:602:CLA:H61	22:B:602:CLA:H41	1.67	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.90	0.40
1:a:317:TRP:CD1	4:d:177:ALA:HB2	2.55	0.40
24:b:620:BCR:H361	24:b:620:BCR:H20C	1.76	0.40
3:c:307:PRO:HB3	3:c:358:PHE:HB3	2.03	0.40
22:c:510:CLA:H171	20:z:20:VAL:HA	2.02	0.40
27:c:518:LMG:H292	27:c:518:LMG:H111	2.03	0.40
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
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.40
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.52	0.40
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.51	0.40
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.86	0.40
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:11:GLU:HG2	11:L:12:LEU:N	2.35	0.40
1:a:180:PHE:O	1:a:184:ILE:HG13	2.22	0.40
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.57	0.40
22:b:606:CLA:H161	22:b:606:CLA:H141	1.85	0.40
24:b:620:BCR:H24C	24:b:620:BCR:H371	1.90	0.40
24:b:622:BCR:H15C	24:b:622:BCR:H351	1.85	0.40
24:c:514:BCR:H15C	24:c:514:BCR:H351	1.84	0.40
29:d:403:SQD:H45	29:d:403:SQD:H81	1.87	0.40
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.04	0.40
29:A:413:SQD:H332	22:b:609:CLA:H203	2.04	0.40
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.89	0.40
5:E:7:GLU:CD	5:E:7:GLU:H	2.30	0.40
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.40
1:a:29:TYR:CG	1:a:133:LEU:HD13	2.55	0.40
2:b:6:TYR:OH	27:d:408:LMG:HC5	2.22	0.40
2:b:194:ASN:HA	2:b:195:PRO:HD3	1.92	0.40
22:b:615:CLA:H171	22:b:616:CLA:HBB2	2.04	0.40
11:l:11:GLU:HG2	11:l:12:LEU:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	10	42
1	a	333/344 (97%)	309 (93%)	20 (6%)	4 (1%)	10	42
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	16	53
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	21	58
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	14	49
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	42
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10	42
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	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%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2	19
17	y	26/46 (56%)	19 (73%)	6 (23%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	35
All	All	5138/5618 (92%)	4675 (91%)	408 (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
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	45	LYS
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
13	o	52	ALA
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
2	B	489	GLU
4	D	239	GLN
13	O	88	GLU
13	O	271	PRO
18	X	12	ILE
2	b	489	GLU
3	c	32	GLY
4	d	239	GLN
7	h	26	GLY

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	261 (96%)	10 (4%)	30	51
1	a	271/280 (97%)	260 (96%)	11 (4%)	27	49
2	B	390/407 (96%)	379 (97%)	11 (3%)	38	59
2	b	390/407 (96%)	380 (97%)	10 (3%)	40	60
3	C	347/362 (96%)	335 (96%)	12 (4%)	32	53
3	c	347/362 (96%)	335 (96%)	12 (4%)	32	53
4	D	275/283 (97%)	265 (96%)	10 (4%)	31	52
4	d	275/283 (97%)	264 (96%)	11 (4%)	28	49
5	E	72/73 (99%)	68 (94%)	4 (6%)	19	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	72/73 (99%)	68 (94%)	4 (6%)	19	41
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	50 (94%)	3 (6%)	18	40
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	40
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	57
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	57
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
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	13
17	y	20/37 (54%)	17 (85%)	3 (15%)	3	13
18	X	30/34 (88%)	28 (93%)	2 (7%)	15	36
18	x	30/34 (88%)	28 (93%)	2 (7%)	15	36
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%)	4109 (97%)	135 (3%)	34	55

All (135) 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	308	LYS
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	305	THR
3	C	355	THR
3	C	417	VAL
3	C	469	MET
3	C	472	LEU
4	D	43	LEU
4	D	91	LEU
4	D	180	ARG
4	D	201	VAL
4	D	205	LEU
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	323	GLU
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	y	25	ILE
17	y	28	ILE
17	y	46	LEU
18	X	12	ILE
18	X	42	GLN
20	Z	33	TRP
20	Z	62	VAL
1	a	30	VAL
1	a	157	VAL
1	a	202	VAL
1	a	226	GLU
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	275	LEU
1	a	286	THR
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

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Mol	Chain	Res	Type
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	305	THR
3	c	355	THR
3	c	417	VAL
3	c	469	MET
3	c	472	LEU
4	d	43	LEU
4	d	91	LEU
4	d	180	ARG
4	d	201	VAL
4	d	205	LEU
4	d	241	GLU
4	d	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

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

Mol	Chain	Res	Type
1	A	165	GLN
1	A	241	GLN
1	A	303	ASN
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
3	C	441	HIS
4	D	117	HIS
4	D	186	GLN
4	D	250	ASN
4	D	301	GLN
4	D	322	ASN
12	M	33	GLN
13	O	150	ASN
13	O	173	ASN
15	U	93	ASN
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

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Mol	Chain	Res	Type
3	c	56	HIS
3	c	229	ASN
3	c	441	HIS
4	d	117	HIS
4	d	250	ASN
4	d	301	GLN
12	m	33	GLN
13	o	130	GLN
13	o	150	ASN
13	o	173	ASN
15	u	93	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	b	605	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	6 (7%)
30	LMT	i	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	C	519	-	36,36,48	0.72	1 (2%)	39,42,54	1.30	4 (10%)
22	CLA	C	501	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
30	LMT	M	103	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
33	BCT	d	404	21	3,3,3	1.11	0	2,3,3	4.26	2 (100%)
22	CLA	c	510	3	69,73,73	1.20	5 (7%)	82,113,113	1.28	5 (6%)
22	CLA	d	405	-	69,73,73	1.19	7 (10%)	82,113,113	1.19	6 (7%)
27	LMG	d	412	-	46,46,55	0.77	1 (2%)	54,54,63	1.30	6 (11%)
22	CLA	A	405	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)
30	LMT	b	604	-	36,36,36	1.11	4 (11%)	47,47,47	1.05	1 (2%)
29	SQD	B	622	-	41,43,54	1.05	2 (4%)	51,54,65	1.68	11 (21%)
25	DGD	C	517	-	67,67,67	0.86	0	81,81,81	1.40	9 (11%)
27	LMG	a	412	-	51,51,55	0.75	0	59,59,63	1.34	6 (10%)
24	BCR	c	514	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	9 (16%)
22	CLA	B	613	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	1.24	5 (6%)
22	CLA	C	520	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
22	CLA	B	611	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	6 (7%)
22	CLA	b	608	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
24	BCR	y	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.27	8 (14%)
27	LMG	I	101	-	43,43,55	0.79	0	51,51,63	1.27	4 (7%)
22	CLA	B	612	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	7 (8%)
22	CLA	b	619	2	69,73,73	1.18	7 (10%)	82,113,113	1.23	4 (4%)
24	BCR	A	407	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	7 (12%)
25	DGD	b	624	-	59,59,67	0.90	1 (1%)	73,73,81	1.33	7 (9%)
22	CLA	c	504	3	69,73,73	1.19	6 (8%)	82,113,113	1.30	5 (6%)
26	LHG	A	409	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	3 (7%)
22	CLA	c	508	3	69,73,73	1.20	7 (10%)	82,113,113	1.24	5 (6%)
27	LMG	i	101	-	43,43,55	0.80	0	51,51,63	1.27	6 (11%)
22	CLA	a	406	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
24	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	7 (12%)
24	BCR	g	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.29	8 (14%)
27	LMG	D	408	-	49,49,55	0.76	1 (2%)	57,57,63	1.31	5 (8%)
22	CLA	B	606	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
27	LMG	d	409	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
22	CLA	C	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.28	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PL9	j	101	-	35,35,55	0.98	2 (5%)	44,45,69	1.58	9 (20%)
22	CLA	c	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
30	LMT	B	624	-	36,36,36	1.08	3 (8%)	47,47,47	1.02	2 (4%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.29	5 (9%)
22	CLA	a	405	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	5 (6%)
30	LMT	B	627	-	36,36,36	1.10	4 (11%)	47,47,47	0.96	1 (2%)
22	CLA	B	604	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
22	CLA	a	404	1	69,73,73	1.19	7 (10%)	82,113,113	1.25	7 (8%)
22	CLA	C	504	3	69,73,73	1.18	7 (10%)	82,113,113	1.31	5 (6%)
27	LMG	d	408	-	49,49,55	0.76	1 (2%)	57,57,63	1.31	5 (8%)
31	PHO	D	402	-	58,69,69	2.20	9 (15%)	55,99,99	1.42	5 (9%)
26	LHG	a	411	-	38,38,48	0.69	1 (2%)	41,44,54	1.23	3 (7%)
28	OEX	A	411	1,3	0,14,14	-	-	-	-	-
22	CLA	C	508	3	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	c	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.28	5 (6%)
25	DGD	C	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.42	12 (15%)
28	OEX	a	414	1,3	0,14,14	-	-	-	-	-
22	CLA	b	612	2	69,73,73	1.20	6 (8%)	82,113,113	1.22	5 (6%)
22	CLA	b	617	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
22	CLA	C	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	H	101	-	69,73,73	1.19	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	b	610	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
34	HEM	v	201	16	50,50,50	2.00	10 (20%)	67,82,82	1.25	4 (5%)
22	CLA	C	507	3	69,73,73	1.19	8 (11%)	82,113,113	1.29	6 (7%)
31	PHO	D	401	-	58,69,69	2.15	9 (15%)	55,99,99	1.42	6 (10%)
22	CLA	c	509	3	69,73,73	1.19	8 (11%)	82,113,113	1.24	5 (6%)
22	CLA	A	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
25	DGD	c	517	-	67,67,67	0.87	0	81,81,81	1.39	9 (11%)
30	LMT	d	411	-	32,32,36	1.16	4 (12%)	43,43,47	1.00	2 (4%)
27	LMG	A	410	-	51,51,55	0.74	0	59,59,63	1.36	7 (11%)
22	CLA	B	603	2	69,73,73	1.18	8 (11%)	82,113,113	1.35	7 (8%)
27	LMG	D	412	-	46,46,55	0.76	1 (2%)	54,54,63	1.31	6 (11%)
22	CLA	B	605	2	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
25	DGD	D	410	-	64,64,67	0.91	0	78,78,81	1.32	9 (11%)
23	PL9	J	101	-	35,35,55	1.00	2 (5%)	44,45,69	1.58	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
24	BCR	b	621	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	9 (16%)
31	PHO	d	402	-	58,69,69	2.18	9 (15%)	55,99,99	1.39	5 (9%)
29	SQD	f	103	-	43,45,54	1.03	2 (4%)	53,56,65	1.57	10 (18%)
22	CLA	C	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
24	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	8 (14%)
29	SQD	a	401	-	52,54,54	0.95	2 (3%)	62,65,65	1.48	9 (14%)
22	CLA	a	407	1	69,73,73	1.18	6 (8%)	82,113,113	1.24	5 (6%)
22	CLA	B	614	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
34	HEM	F	101	5,6	50,50,50	1.97	9 (18%)	67,82,82	1.32	4 (5%)
27	LMG	a	402	-	42,42,55	0.82	2 (4%)	50,50,63	1.26	5 (10%)
29	SQD	A	412	-	49,51,54	0.96	2 (4%)	59,62,65	1.67	10 (16%)
22	CLA	D	405	-	69,73,73	1.18	7 (10%)	82,113,113	1.20	5 (6%)
22	CLA	b	609	2	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
24	BCR	B	616	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)
25	DGD	b	601	-	53,53,67	1.04	4 (7%)	67,67,81	1.32	7 (10%)
22	CLA	A	402	1	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
23	PL9	D	407	-	55,55,55	1.06	4 (7%)	68,69,69	1.50	13 (19%)
22	CLA	c	507	3	69,73,73	1.18	8 (11%)	82,113,113	1.29	7 (8%)
24	BCR	j	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.60	12 (21%)
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.28	5 (9%)
34	HEM	f	101	5,6	50,50,50	1.97	8 (16%)	67,82,82	1.33	4 (5%)
30	LMT	b	603	-	36,36,36	1.10	4 (11%)	47,47,47	0.96	1 (2%)
22	CLA	c	501	3	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	b	614	2	69,73,73	1.24	7 (10%)	82,113,113	1.34	6 (7%)
22	CLA	b	618	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	b	613	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
29	SQD	A	413	-	52,54,54	0.95	3 (5%)	62,65,65	1.48	9 (14%)
22	CLA	b	607	2	69,73,73	1.19	8 (11%)	82,113,113	1.33	7 (8%)
22	CLA	B	610	2	69,73,73	1.24	6 (8%)	82,113,113	1.34	6 (7%)
30	LMT	D	411	-	32,32,36	1.16	4 (12%)	43,43,47	1.03	2 (4%)
22	CLA	C	511	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	b	616	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	7 (8%)
24	BCR	c	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	607	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	B	608	2	69,73,73	1.20	7 (10%)	82,113,113	1.25	5 (6%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	c	520	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
25	DGD	A	408	-	57,57,67	0.92	0	71,71,81	1.41	9 (12%)
29	SQD	a	415	-	49,51,54	0.97	2 (4%)	59,62,65	1.69	10 (16%)
24	BCR	b	622	-	41,41,41	1.13	2 (4%)	56,56,56	1.39	11 (19%)
25	DGD	d	410	-	64,64,67	0.92	2 (3%)	78,78,81	1.34	9 (11%)
22	CLA	B	609	-	69,73,73	1.19	8 (11%)	82,113,113	1.27	5 (6%)
24	BCR	f	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
24	BCR	H	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
24	BCR	F	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	6 (10%)
22	CLA	b	615	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
27	LMG	M	101	-	42,42,55	0.84	1 (2%)	50,50,63	1.23	4 (8%)
24	BCR	C	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	9 (16%)
22	CLA	b	606	2	69,73,73	1.18	7 (10%)	82,113,113	1.22	5 (6%)
22	CLA	c	502	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	5 (6%)
24	BCR	b	623	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	9 (16%)
30	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	1 (2%)
24	BCR	b	620	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
34	HEM	V	201	16	50,50,50	1.98	9 (18%)	67,82,82	1.22	4 (5%)
22	CLA	C	503	3	69,73,73	1.19	8 (11%)	82,113,113	1.26	4 (4%)
30	LMT	b	627	-	36,36,36	1.08	4 (11%)	47,47,47	1.00	2 (4%)
22	CLA	c	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
25	DGD	c	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.42	11 (14%)
22	CLA	d	406	-	69,73,73	1.19	5 (7%)	82,113,113	1.27	5 (6%)
22	CLA	A	404	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
29	SQD	B	626	-	45,47,54	1.01	3 (6%)	55,58,65	1.70	10 (18%)
22	CLA	C	502	3	69,73,73	1.19	9 (13%)	82,113,113	1.26	5 (6%)
24	BCR	B	618	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	9 (16%)
31	PHO	d	401	-	58,69,69	2.15	9 (15%)	55,99,99	1.42	7 (12%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
25	DGD	a	410	-	57,57,67	0.92	1 (1%)	71,71,81	1.40	9 (12%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.28	5 (9%)
22	CLA	B	601	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	615	2	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
30	LMT	B	628	-	36,36,36	1.12	4 (11%)	47,47,47	1.05	1 (2%)
24	BCR	a	409	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	7 (12%)
33	BCT	D	404	21	3,3,3	1.11	0	2,3,3	4.29	2 (100%)
22	CLA	B	602	2	69,73,73	1.17	7 (10%)	82,113,113	1.24	5 (6%)
30	LMT	I	102	-	36,36,36	1.09	4 (11%)	47,47,47	1.02	2 (4%)
24	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	D	406	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
23	PL9	A	406	-	45,45,55	1.01	4 (8%)	56,57,69	1.55	10 (17%)
24	BCR	J	102	-	41,41,41	1.11	3 (7%)	56,56,56	1.62	12 (21%)
27	LMG	m	101	-	42,42,55	0.84	0	50,50,63	1.23	4 (8%)
22	CLA	C	510	3	69,73,73	1.18	6 (8%)	82,113,113	1.30	6 (7%)
22	CLA	b	611	2	69,73,73	1.19	8 (11%)	82,113,113	1.24	4 (4%)
24	BCR	x	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	4 (7%)
27	LMG	D	409	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
22	CLA	c	503	-	69,73,73	1.20	8 (11%)	82,113,113	1.27	5 (6%)
23	PL9	a	408	-	45,45,55	1.05	4 (8%)	56,57,69	1.54	10 (17%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.26	6 (8%)
30	LMT	b	626	-	36,36,36	1.11	4 (11%)	47,47,47	0.96	1 (2%)
29	SQD	d	403	-	41,43,54	1.05	2 (4%)	51,54,65	1.70	11 (21%)
29	SQD	b	602	-	45,47,54	1.02	3 (6%)	55,58,65	1.72	10 (18%)
25	DGD	B	620	-	59,59,67	0.90	1 (1%)	73,73,81	1.34	9 (12%)
22	CLA	c	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)
22	CLA	h	101	-	69,73,73	1.20	8 (11%)	82,113,113	1.24	5 (6%)
23	PL9	d	407	-	55,55,55	1.05	3 (5%)	68,69,69	1.51	12 (17%)
27	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.29	4 (7%)
30	LMT	M	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.01	2 (4%)
25	DGD	C	515	-	54,54,67	0.97	2 (3%)	68,68,81	1.25	5 (7%)
27	LMG	C	521	-	48,48,55	0.77	1 (2%)	56,56,63	1.30	5 (8%)
24	BCR	C	514	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	9 (16%)
27	LMG	A	414	-	42,42,55	0.83	2 (4%)	50,50,63	1.25	4 (8%)
26	LHG	c	519	-	36,36,48	0.73	2 (5%)	39,42,54	1.30	4 (10%)
24	BCR	K	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	8 (14%)
29	SQD	F	103	-	43,45,54	1.03	2 (4%)	53,56,65	1.57	10 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	605	-	-	15/39/115/115	-
30	LMT	i	102	-	-	3/21/61/61	0/2/2/2
26	LHG	C	519	-	-	17/41/41/53	-
22	CLA	C	501	3	-	16/39/115/115	-
30	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	c	510	3	-	15/39/115/115	-
22	CLA	d	405	-	-	12/39/115/115	-
27	LMG	d	412	-	-	16/41/61/70	0/1/1/1
22	CLA	A	405	1	-	8/39/115/115	-
30	LMT	b	604	-	-	5/21/61/61	0/2/2/2
29	SQD	B	622	-	-	14/38/58/69	0/1/1/1
25	DGD	C	517	-	-	21/55/95/95	0/2/2/2
27	LMG	a	412	-	-	26/46/66/70	0/1/1/1
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
22	CLA	B	613	2	-	12/39/115/115	-
22	CLA	C	509	3	-	15/39/115/115	-
22	CLA	C	520	-	-	13/39/115/115	-
22	CLA	B	611	-	-	9/39/115/115	-
22	CLA	b	608	2	-	15/39/115/115	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
27	LMG	I	101	-	-	18/38/58/70	0/1/1/1
22	CLA	B	612	-	-	15/39/115/115	-
22	CLA	b	619	2	-	19/39/115/115	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
22	CLA	c	504	3	-	18/39/115/115	-
26	LHG	A	409	-	-	12/43/43/53	-
22	CLA	c	508	3	-	16/39/115/115	-
27	LMG	i	101	-	-	18/38/58/70	0/1/1/1
22	CLA	a	406	-	-	8/39/115/115	-
24	BCR	B	617	-	-	6/29/63/63	0/2/2/2
24	BCR	g	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	D	408	-	-	25/44/64/70	0/1/1/1
22	CLA	B	606	-	-	9/39/115/115	-
27	LMG	d	409	-	-	20/43/63/70	0/1/1/1
22	CLA	C	505	3	-	16/39/115/115	-
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
22	CLA	c	512	3	-	17/39/115/115	-
30	LMT	B	624	-	-	4/21/61/61	0/2/2/2
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
22	CLA	a	405	-	-	13/39/115/115	-
30	LMT	B	627	-	-	3/21/61/61	0/2/2/2
22	CLA	B	604	2	-	15/39/115/115	-
22	CLA	a	404	1	-	8/39/115/115	-
22	CLA	C	504	3	-	19/39/115/115	-
27	LMG	d	408	-	-	23/44/64/70	0/1/1/1
31	PHO	D	402	-	-	11/37/103/103	0/5/6/6
26	LHG	a	411	-	-	11/43/43/53	-
22	CLA	C	508	3	-	17/39/115/115	-
22	CLA	c	505	3	-	16/39/115/115	-
25	DGD	C	516	-	-	19/51/91/95	0/2/2/2
22	CLA	b	612	2	-	9/39/115/115	-
22	CLA	b	617	2	-	13/39/115/115	-
22	CLA	C	512	3	-	15/39/115/115	-
22	CLA	H	101	-	-	15/39/115/115	-
22	CLA	b	610	-	-	9/39/115/115	-
34	HEM	v	201	16	-	5/14/54/54	-
22	CLA	C	507	3	-	13/39/115/115	-
31	PHO	D	401	-	-	10/37/103/103	0/5/6/6
22	CLA	c	509	3	-	17/39/115/115	-
22	CLA	A	403	-	-	13/39/115/115	-
25	DGD	c	517	-	-	20/55/95/95	0/2/2/2
30	LMT	d	411	-	-	0/17/57/61	0/2/2/2
27	LMG	A	410	-	-	26/46/66/70	0/1/1/1
22	CLA	B	603	2	-	9/39/115/115	-
27	LMG	D	412	-	-	14/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	605	2	-	14/39/115/115	-
25	DGD	D	410	-	-	34/52/92/95	0/2/2/2
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
24	BCR	b	621	-	-	7/29/63/63	0/2/2/2
31	PHO	d	402	-	-	11/37/103/103	0/5/6/6
29	SQD	f	103	-	-	12/40/60/69	0/1/1/1
22	CLA	C	506	-	-	12/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
29	SQD	a	401	-	-	14/49/69/69	0/1/1/1
22	CLA	a	407	1	-	8/39/115/115	-
22	CLA	B	614	-	-	9/39/115/115	-
34	HEM	F	101	5,6	-	2/14/54/54	-
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
29	SQD	A	412	-	-	18/46/66/69	0/1/1/1
22	CLA	D	405	-	-	14/39/115/115	-
22	CLA	b	609	2	-	16/39/115/115	-
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
25	DGD	b	601	-	-	19/41/81/95	0/2/2/2
22	CLA	A	402	1	-	8/39/115/115	-
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
22	CLA	c	507	3	-	13/39/115/115	-
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
27	LMG	C	518	-	-	22/40/60/70	0/1/1/1
34	HEM	f	101	5,6	-	2/14/54/54	-
30	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	c	501	3	-	14/39/115/115	-
22	CLA	b	614	2	-	11/39/115/115	-
22	CLA	b	618	-	-	9/39/115/115	-
22	CLA	b	613	-	-	18/39/115/115	-
29	SQD	A	413	-	-	12/49/69/69	0/1/1/1
22	CLA	b	607	2	-	7/39/115/115	-
22	CLA	B	610	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	D	411	-	-	0/17/57/61	0/2/2/2
22	CLA	C	511	-	-	17/39/115/115	-
22	CLA	b	616	-	-	15/39/115/115	-
24	BCR	c	521	-	-	3/29/63/63	0/2/2/2
22	CLA	B	607	2	-	12/39/115/115	-
22	CLA	B	608	2	-	8/39/115/115	-
27	LMG	B	621	-	-	15/44/64/70	0/1/1/1
22	CLA	c	520	-	-	13/39/115/115	-
25	DGD	A	408	-	-	13/45/85/95	0/2/2/2
29	SQD	a	415	-	-	18/46/66/69	0/1/1/1
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
25	DGD	d	410	-	-	35/52/92/95	0/2/2/2
22	CLA	B	609	-	-	18/39/115/115	-
24	BCR	f	102	-	-	6/29/63/63	0/2/2/2
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
24	BCR	F	102	-	-	5/29/63/63	0/2/2/2
22	CLA	b	615	-	-	10/39/115/115	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
24	BCR	C	513	-	-	4/29/63/63	0/2/2/2
22	CLA	b	606	2	-	14/39/115/115	-
22	CLA	c	502	-	-	9/39/115/115	-
24	BCR	b	623	-	-	5/29/63/63	0/2/2/2
30	LMT	B	623	-	-	3/21/61/61	0/2/2/2
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
34	HEM	V	201	16	-	5/14/54/54	-
22	CLA	C	503	3	-	12/39/115/115	-
30	LMT	b	627	-	-	3/21/61/61	0/2/2/2
22	CLA	c	506	-	-	12/39/115/115	-
25	DGD	c	516	-	-	19/51/91/95	0/2/2/2
22	CLA	d	406	-	-	8/39/115/115	-
22	CLA	A	404	-	-	10/39/115/115	-
29	SQD	B	626	-	-	14/42/62/69	0/1/1/1
22	CLA	C	502	3	-	9/39/115/115	-
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
31	PHO	d	401	-	-	10/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
25	DGD	a	410	-	-	15/45/85/95	0/2/2/2
27	LMG	c	518	-	-	22/40/60/70	0/1/1/1
22	CLA	B	601	-	-	18/39/115/115	-
22	CLA	B	615	2	-	19/39/115/115	-
30	LMT	B	628	-	-	5/21/61/61	0/2/2/2
24	BCR	a	409	-	-	4/29/63/63	0/2/2/2
22	CLA	B	602	2	-	15/39/115/115	-
30	LMT	I	102	-	-	3/21/61/61	0/2/2/2
24	BCR	c	513	-	-	4/29/63/63	0/2/2/2
22	CLA	D	406	-	-	8/39/115/115	-
23	PL9	A	406	-	-	19/41/61/73	0/1/1/1
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
27	LMG	m	101	-	-	17/37/57/70	0/1/1/1
22	CLA	C	510	3	-	14/39/115/115	-
22	CLA	b	611	2	-	12/39/115/115	-
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
27	LMG	D	409	-	-	21/43/63/70	0/1/1/1
22	CLA	c	503	-	-	11/39/115/115	-
23	PL9	a	408	-	-	18/41/61/73	0/1/1/1
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
30	LMT	b	626	-	-	2/21/61/61	0/2/2/2
29	SQD	d	403	-	-	14/38/58/69	0/1/1/1
29	SQD	b	602	-	-	13/42/62/69	0/1/1/1
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2
22	CLA	c	511	-	-	17/39/115/115	-
22	CLA	h	101	-	-	15/39/115/115	-
23	PL9	d	407	-	-	12/53/73/73	0/1/1/1
27	LMG	E	101	-	-	19/39/59/70	0/1/1/1
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
27	LMG	C	521	-	-	20/43/63/70	0/1/1/1
24	BCR	C	514	-	-	4/29/63/63	0/2/2/2
27	LMG	A	414	-	-	15/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	c	519	-	-	17/41/41/53	-
24	BCR	K	102	-	-	5/29/63/63	0/2/2/2
29	SQD	F	103	-	-	11/40/60/69	0/1/1/1

All (752) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	402	PHO	C1B-C2B	9.76	1.50	1.39
31	d	401	PHO	C1B-C2B	9.67	1.50	1.39
31	d	402	PHO	C1B-C2B	9.57	1.50	1.39
31	D	401	PHO	C1B-C2B	9.55	1.50	1.39
31	D	402	PHO	C3B-C4B	8.71	1.50	1.41
31	d	402	PHO	C3B-C4B	8.68	1.50	1.41
31	D	401	PHO	C3B-C4B	8.47	1.50	1.41
31	d	401	PHO	C3B-C4B	8.29	1.49	1.41
34	V	201	HEM	C3D-C2D	8.18	1.54	1.36
34	v	201	HEM	C3D-C2D	8.17	1.54	1.36
34	F	101	HEM	C3D-C2D	7.91	1.53	1.36
34	f	101	HEM	C3D-C2D	7.88	1.53	1.36
34	F	101	HEM	FE-ND	5.66	2.12	1.94
34	f	101	HEM	FE-ND	5.30	2.11	1.94
34	v	201	HEM	FE-ND	5.08	2.10	1.94
34	V	201	HEM	FE-ND	5.05	2.10	1.94
34	v	201	HEM	FE-NB	4.64	2.09	1.94
34	f	101	HEM	FE-NB	4.57	2.09	1.94
31	d	402	PHO	C1D-C2D	4.41	1.44	1.39
31	D	402	PHO	C1D-C2D	4.34	1.44	1.39
34	V	201	HEM	FE-NB	4.32	2.08	1.94
31	d	401	PHO	C1D-C2D	4.12	1.44	1.39
31	D	401	PHO	C1D-C2D	4.07	1.44	1.39
24	y	101	BCR	C1-C6	-4.02	1.48	1.53
34	F	101	HEM	FE-NB	4.01	2.07	1.94
24	H	102	BCR	C1-C6	-3.95	1.48	1.53
24	g	101	BCR	C1-C6	-3.92	1.48	1.53
24	F	102	BCR	C1-C6	-3.90	1.48	1.53
34	V	201	HEM	FE-NA	3.88	2.08	1.95
34	f	101	HEM	FE-NA	3.87	2.07	1.95
24	x	101	BCR	C1-C6	-3.85	1.48	1.53
24	f	102	BCR	C1-C6	-3.84	1.48	1.53
31	D	402	PHO	C4D-CHA	3.84	1.45	1.39
31	D	401	PHO	C4D-CHA	3.81	1.45	1.39
22	C	501	CLA	C1D-ND	3.78	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	401	PHO	C4D-CHA	3.78	1.45	1.39
22	B	601	CLA	C1D-ND	3.77	1.42	1.37
22	c	503	CLA	C1D-ND	3.77	1.42	1.37
22	b	605	CLA	C1D-ND	3.77	1.42	1.37
34	F	101	HEM	FE-NA	3.76	2.07	1.95
34	v	201	HEM	FE-NA	3.75	2.07	1.95
31	d	402	PHO	C4D-CHA	3.75	1.45	1.39
22	C	512	CLA	C1D-ND	3.74	1.42	1.37
22	B	608	CLA	C1D-ND	3.74	1.42	1.37
22	c	510	CLA	C1D-ND	3.73	1.42	1.37
22	c	512	CLA	C1D-ND	3.72	1.42	1.37
22	h	101	CLA	C1D-ND	3.72	1.42	1.37
22	d	406	CLA	C1D-ND	3.72	1.42	1.37
22	b	618	CLA	C1D-ND	3.71	1.42	1.37
22	c	501	CLA	C1D-ND	3.70	1.42	1.37
22	a	407	CLA	C1D-ND	3.68	1.42	1.37
22	A	403	CLA	C1D-ND	3.68	1.42	1.37
22	C	505	CLA	C1D-ND	3.68	1.42	1.37
22	c	505	CLA	C1D-ND	3.68	1.42	1.37
22	C	510	CLA	C1D-ND	3.68	1.42	1.37
22	H	101	CLA	C1D-ND	3.68	1.42	1.37
22	c	506	CLA	C1D-ND	3.67	1.42	1.37
22	b	608	CLA	C1D-ND	3.67	1.42	1.37
22	A	405	CLA	C1D-ND	3.67	1.42	1.37
22	b	612	CLA	C1D-ND	3.67	1.42	1.37
22	b	616	CLA	C1D-ND	3.66	1.42	1.37
22	B	604	CLA	C1D-ND	3.65	1.42	1.37
22	C	506	CLA	C1D-ND	3.65	1.42	1.37
22	D	406	CLA	C1D-ND	3.65	1.42	1.37
22	b	613	CLA	C1D-ND	3.65	1.42	1.37
22	B	614	CLA	C1D-ND	3.64	1.42	1.37
22	C	503	CLA	C1D-ND	3.64	1.42	1.37
22	b	607	CLA	C1D-ND	3.64	1.42	1.37
22	C	511	CLA	C1D-ND	3.64	1.42	1.37
22	c	508	CLA	C1D-ND	3.63	1.42	1.37
22	d	405	CLA	C1D-ND	3.63	1.42	1.37
22	b	609	CLA	C1D-ND	3.63	1.42	1.37
22	C	502	CLA	C1D-ND	3.62	1.42	1.37
22	b	606	CLA	C1D-ND	3.62	1.42	1.37
22	B	603	CLA	C1D-ND	3.62	1.42	1.37
22	c	502	CLA	C1D-ND	3.62	1.42	1.37
22	B	612	CLA	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	C1D-ND	3.62	1.42	1.37
22	C	520	CLA	C1D-ND	3.61	1.42	1.37
24	B	616	BCR	C1-C6	-3.61	1.49	1.53
24	C	514	BCR	C1-C6	-3.61	1.49	1.53
22	C	504	CLA	C1D-ND	3.61	1.42	1.37
22	B	605	CLA	C1D-ND	3.60	1.42	1.37
22	a	405	CLA	C1D-ND	3.60	1.42	1.37
22	B	607	CLA	C1D-ND	3.60	1.42	1.37
22	B	606	CLA	C1D-ND	3.60	1.42	1.37
22	b	611	CLA	C1D-ND	3.59	1.42	1.37
24	c	514	BCR	C1-C6	-3.59	1.49	1.53
22	B	613	CLA	C1D-ND	3.58	1.42	1.37
22	a	406	CLA	C1D-ND	3.58	1.42	1.37
22	b	610	CLA	C1D-ND	3.58	1.42	1.37
22	c	520	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
24	b	620	BCR	C1-C6	-3.56	1.49	1.53
34	v	201	HEM	FE-NC	3.54	2.06	1.95
22	B	609	CLA	C1D-ND	3.53	1.42	1.37
22	A	404	CLA	C1D-ND	3.53	1.42	1.37
22	a	404	CLA	C1D-ND	3.53	1.42	1.37
24	b	621	BCR	C1-C6	-3.53	1.49	1.53
22	c	507	CLA	C1D-ND	3.52	1.42	1.37
22	b	617	CLA	C1D-ND	3.52	1.42	1.37
24	y	101	BCR	C30-C25	-3.51	1.49	1.53
22	B	615	CLA	C1D-ND	3.51	1.42	1.37
24	b	622	BCR	C30-C25	-3.50	1.49	1.53
22	C	509	CLA	C1D-ND	3.50	1.42	1.37
22	C	507	CLA	C1D-ND	3.50	1.42	1.37
22	b	619	CLA	C1D-ND	3.50	1.42	1.37
22	C	508	CLA	C1D-ND	3.49	1.42	1.37
22	c	509	CLA	C1D-ND	3.48	1.42	1.37
22	A	402	CLA	C1D-ND	3.47	1.42	1.37
22	B	610	CLA	C1D-ND	3.47	1.42	1.37
22	D	405	CLA	C1D-ND	3.46	1.42	1.37
24	B	617	BCR	C1-C6	-3.45	1.49	1.53
24	J	102	BCR	C30-C25	-3.45	1.49	1.53
24	C	513	BCR	C1-C6	-3.45	1.49	1.53
24	g	101	BCR	C30-C25	-3.45	1.49	1.53
22	b	614	CLA	C1D-ND	3.44	1.42	1.37
24	j	102	BCR	C30-C25	-3.43	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	BCR	C1-C6	-3.40	1.49	1.53
24	B	618	BCR	C30-C25	-3.39	1.49	1.53
24	K	102	BCR	C30-C25	-3.38	1.49	1.53
24	F	102	BCR	C30-C25	-3.36	1.49	1.53
24	c	521	BCR	C30-C25	-3.33	1.49	1.53
24	A	407	BCR	C30-C25	-3.32	1.49	1.53
22	A	402	CLA	C4B-NB	3.31	1.42	1.37
24	B	618	BCR	C1-C6	-3.31	1.49	1.53
22	c	508	CLA	C4B-NB	3.31	1.42	1.37
24	a	409	BCR	C30-C25	-3.30	1.49	1.53
24	f	102	BCR	C30-C25	-3.30	1.49	1.53
24	b	623	BCR	C1-C6	-3.29	1.49	1.53
22	b	614	CLA	CMB-C2B	-3.29	1.44	1.50
24	B	619	BCR	C30-C25	-3.29	1.49	1.53
24	B	616	BCR	C30-C25	-3.29	1.49	1.53
24	b	620	BCR	C30-C25	-3.28	1.49	1.53
22	C	509	CLA	C4B-NB	3.27	1.42	1.37
24	b	623	BCR	C30-C25	-3.26	1.49	1.53
22	b	615	CLA	C1D-ND	3.26	1.42	1.37
22	B	601	CLA	C4B-NB	3.26	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
22	a	404	CLA	C4B-NB	3.26	1.42	1.37
22	b	605	CLA	C4B-NB	3.26	1.42	1.37
24	A	407	BCR	C1-C6	-3.26	1.49	1.53
24	a	409	BCR	C1-C6	-3.25	1.49	1.53
22	C	508	CLA	C4B-NB	3.25	1.42	1.37
22	B	611	CLA	C1D-ND	3.22	1.42	1.37
22	b	619	CLA	C4B-NB	3.22	1.42	1.37
22	C	505	CLA	C4B-NB	3.22	1.42	1.37
22	c	509	CLA	C4B-NB	3.22	1.42	1.37
22	b	614	CLA	C4B-NB	3.21	1.42	1.37
24	C	514	BCR	C30-C25	-3.21	1.49	1.53
24	K	102	BCR	C1-C6	-3.20	1.49	1.53
22	B	610	CLA	CMB-C2B	-3.20	1.44	1.50
29	a	401	SQD	O48-C23	3.19	1.42	1.33
22	B	610	CLA	C4B-NB	3.18	1.42	1.37
22	c	505	CLA	C4B-NB	3.18	1.42	1.37
22	B	615	CLA	C4B-NB	3.18	1.42	1.37
22	c	511	CLA	C4B-NB	3.18	1.42	1.37
24	C	513	BCR	C30-C25	-3.17	1.49	1.53
24	c	514	BCR	C30-C25	-3.17	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	C4B-NB	3.17	1.42	1.37
29	b	602	SQD	O48-C23	3.17	1.42	1.33
22	c	504	CLA	C4B-NB	3.16	1.42	1.37
29	d	403	SQD	O48-C23	3.16	1.42	1.33
29	f	103	SQD	O48-C23	3.15	1.42	1.33
22	b	612	CLA	C4B-NB	3.15	1.42	1.37
22	b	615	CLA	C4B-NB	3.15	1.42	1.37
22	c	520	CLA	C4B-NB	3.15	1.42	1.37
22	B	614	CLA	C4B-NB	3.14	1.42	1.37
29	F	103	SQD	O48-C23	3.14	1.42	1.33
22	c	503	CLA	C4B-NB	3.14	1.42	1.37
22	D	405	CLA	C4B-NB	3.14	1.42	1.37
22	b	610	CLA	C4B-NB	3.13	1.42	1.37
22	d	406	CLA	C4B-NB	3.13	1.42	1.37
34	V	201	HEM	CAB-C3B	3.13	1.55	1.47
22	a	405	CLA	C4B-NB	3.12	1.42	1.37
29	A	413	SQD	O48-C23	3.12	1.42	1.33
22	b	618	CLA	C4B-NB	3.12	1.42	1.37
22	B	611	CLA	C4B-NB	3.12	1.42	1.37
22	B	606	CLA	C4B-NB	3.12	1.42	1.37
29	B	622	SQD	O48-C23	3.12	1.42	1.33
24	x	101	BCR	C30-C25	-3.12	1.49	1.53
29	B	626	SQD	O48-C23	3.11	1.42	1.33
34	v	201	HEM	CAB-C3B	3.11	1.55	1.47
22	B	608	CLA	C4B-NB	3.11	1.41	1.37
34	f	101	HEM	CAC-C3C	3.11	1.55	1.47
22	c	510	CLA	C4B-NB	3.11	1.41	1.37
22	B	609	CLA	C4B-NB	3.11	1.41	1.37
24	c	521	BCR	C1-C6	-3.10	1.49	1.53
22	a	406	CLA	C4B-NB	3.10	1.41	1.37
29	a	415	SQD	O48-C23	3.09	1.42	1.33
22	d	405	CLA	C4B-NB	3.09	1.41	1.37
22	c	512	CLA	C4B-NB	3.09	1.41	1.37
22	C	511	CLA	C4B-NB	3.09	1.41	1.37
22	A	403	CLA	C4B-NB	3.09	1.41	1.37
22	H	101	CLA	C4B-NB	3.08	1.41	1.37
22	c	507	CLA	C4B-NB	3.08	1.41	1.37
22	B	604	CLA	C4B-NB	3.08	1.41	1.37
22	b	608	CLA	C4B-NB	3.07	1.41	1.37
34	F	101	HEM	CAC-C3C	3.07	1.55	1.47
22	A	405	CLA	C4B-NB	3.07	1.41	1.37
24	H	102	BCR	C30-C25	-3.07	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	C4B-NB	3.06	1.41	1.37
22	D	406	CLA	C4B-NB	3.06	1.41	1.37
29	A	412	SQD	O48-C23	3.05	1.42	1.33
22	h	101	CLA	C4B-NB	3.05	1.41	1.37
22	C	510	CLA	C4B-NB	3.05	1.41	1.37
34	F	101	HEM	FE-NC	3.05	2.05	1.95
34	V	201	HEM	FE-NC	3.05	2.05	1.95
22	a	407	CLA	C4B-NB	3.05	1.41	1.37
22	b	611	CLA	C4B-NB	3.05	1.41	1.37
22	b	609	CLA	C4B-NB	3.04	1.41	1.37
22	C	502	CLA	C4B-NB	3.03	1.41	1.37
34	v	201	HEM	CAC-C3C	3.03	1.55	1.47
34	f	101	HEM	FE-NC	3.02	2.05	1.95
22	B	607	CLA	C4B-NB	3.02	1.41	1.37
34	V	201	HEM	CAC-C3C	3.02	1.55	1.47
22	A	404	CLA	C4B-NB	3.02	1.41	1.37
22	C	503	CLA	C4B-NB	3.01	1.41	1.37
22	b	616	CLA	C4B-NB	3.01	1.41	1.37
22	B	605	CLA	C4B-NB	3.01	1.41	1.37
22	B	613	CLA	C4B-NB	3.01	1.41	1.37
22	C	504	CLA	C4B-NB	3.01	1.41	1.37
22	C	520	CLA	C4B-NB	3.00	1.41	1.37
22	c	501	CLA	C4B-NB	2.99	1.41	1.37
22	b	617	CLA	C4B-NB	2.99	1.41	1.37
24	J	102	BCR	C1-C6	-2.99	1.50	1.53
22	C	501	CLA	C4B-NB	2.99	1.41	1.37
22	b	613	CLA	C4B-NB	2.99	1.41	1.37
24	j	102	BCR	C1-C6	-2.98	1.50	1.53
22	b	607	CLA	C4B-NB	2.98	1.41	1.37
24	c	513	BCR	C30-C25	-2.98	1.50	1.53
22	c	506	CLA	C4B-NB	2.98	1.41	1.37
22	c	502	CLA	C4B-NB	2.97	1.41	1.37
22	B	612	CLA	C4B-NB	2.97	1.41	1.37
22	b	606	CLA	C4B-NB	2.96	1.41	1.37
22	C	506	CLA	C4B-NB	2.95	1.41	1.37
29	d	403	SQD	O47-C7	2.94	1.42	1.34
22	B	603	CLA	C4B-NB	2.94	1.41	1.37
34	F	101	HEM	CAB-C3B	2.93	1.55	1.47
22	B	602	CLA	C4B-NB	2.93	1.41	1.37
23	d	407	PL9	C7-C3	-2.92	1.47	1.51
24	b	621	BCR	C30-C25	-2.92	1.50	1.53
29	B	622	SQD	O47-C7	2.92	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	C1B-C2B	2.91	1.50	1.43
24	B	617	BCR	C30-C25	-2.91	1.50	1.53
29	a	415	SQD	O47-C7	2.90	1.42	1.34
34	f	101	HEM	CAB-C3B	2.90	1.55	1.47
29	a	401	SQD	O47-C7	2.90	1.42	1.34
29	A	413	SQD	O47-C7	2.89	1.42	1.34
29	A	412	SQD	O47-C7	2.89	1.42	1.34
22	D	405	CLA	C1B-C2B	2.89	1.49	1.43
25	b	601	DGD	C1E-C2E	2.89	1.61	1.52
23	a	408	PL9	C3-C4	-2.88	1.45	1.49
22	C	501	CLA	C1B-C2B	2.88	1.49	1.43
29	F	103	SQD	O47-C7	2.87	1.42	1.34
22	b	619	CLA	C1B-C2B	2.86	1.49	1.43
22	d	405	CLA	C1B-C2B	2.85	1.49	1.43
22	B	611	CLA	C1B-C2B	2.85	1.49	1.43
22	c	501	CLA	C1B-C2B	2.85	1.49	1.43
22	C	504	CLA	C1B-C2B	2.84	1.49	1.43
29	b	602	SQD	O47-C7	2.83	1.42	1.34
23	D	407	PL9	C3-C4	-2.83	1.45	1.49
29	B	626	SQD	O47-C7	2.82	1.42	1.34
22	B	615	CLA	C1B-C2B	2.82	1.49	1.43
22	h	101	CLA	C1B-C2B	2.82	1.49	1.43
29	f	103	SQD	O47-C7	2.82	1.42	1.34
22	B	603	CLA	C1B-C2B	2.82	1.49	1.43
22	B	613	CLA	C1B-C2B	2.82	1.49	1.43
22	H	101	CLA	C1B-C2B	2.82	1.49	1.43
22	c	503	CLA	C1B-C2B	2.82	1.49	1.43
22	b	615	CLA	C1B-C2B	2.82	1.49	1.43
22	B	601	CLA	C1B-C2B	2.81	1.49	1.43
25	B	625	DGD	C1E-C2E	2.81	1.60	1.52
22	c	511	CLA	C1B-C2B	2.81	1.49	1.43
22	b	607	CLA	C1B-C2B	2.81	1.49	1.43
22	b	618	CLA	C1B-C2B	2.81	1.49	1.43
22	B	614	CLA	C1B-C2B	2.80	1.49	1.43
22	b	609	CLA	C1B-C2B	2.80	1.49	1.43
22	b	617	CLA	C1B-C2B	2.80	1.49	1.43
22	C	511	CLA	C1B-C2B	2.79	1.49	1.43
22	c	510	CLA	C1B-C2B	2.79	1.49	1.43
22	b	616	CLA	C1B-C2B	2.79	1.49	1.43
23	d	407	PL9	C3-C4	-2.79	1.45	1.49
22	b	612	CLA	C1B-C2B	2.78	1.49	1.43
22	a	406	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	C1B-C2B	2.78	1.49	1.43
22	c	502	CLA	C1B-C2B	2.78	1.49	1.43
22	b	605	CLA	C1B-C2B	2.78	1.49	1.43
22	C	503	CLA	C1B-C2B	2.77	1.49	1.43
22	B	608	CLA	C1B-C2B	2.77	1.49	1.43
22	B	606	CLA	C1B-C2B	2.77	1.49	1.43
22	C	510	CLA	C1B-C2B	2.77	1.49	1.43
22	b	608	CLA	C1B-C2B	2.76	1.49	1.43
22	B	612	CLA	C1B-C2B	2.76	1.49	1.43
22	B	604	CLA	C1B-C2B	2.76	1.49	1.43
22	B	605	CLA	C1B-C2B	2.75	1.49	1.43
22	d	406	CLA	C1B-C2B	2.75	1.49	1.43
22	c	520	CLA	C1B-C2B	2.75	1.49	1.43
22	C	512	CLA	C1B-C2B	2.75	1.49	1.43
22	A	404	CLA	C1B-C2B	2.75	1.49	1.43
22	b	606	CLA	C1B-C2B	2.75	1.49	1.43
22	b	610	CLA	C1B-C2B	2.75	1.49	1.43
22	c	512	CLA	C1B-C2B	2.74	1.49	1.43
22	c	506	CLA	C1B-C2B	2.74	1.49	1.43
22	c	508	CLA	C1B-C2B	2.73	1.49	1.43
22	B	602	CLA	C1B-C2B	2.73	1.49	1.43
22	D	406	CLA	C1B-C2B	2.73	1.49	1.43
22	C	509	CLA	C1B-C2B	2.71	1.49	1.43
22	C	505	CLA	C1B-C2B	2.71	1.49	1.43
22	A	405	CLA	C1B-C2B	2.71	1.49	1.43
22	c	505	CLA	C1B-C2B	2.71	1.49	1.43
22	C	506	CLA	C1B-C2B	2.71	1.49	1.43
22	C	508	CLA	C1B-C2B	2.71	1.49	1.43
22	c	509	CLA	C1B-C2B	2.70	1.49	1.43
22	B	607	CLA	C1B-C2B	2.70	1.49	1.43
22	b	613	CLA	C1B-C2B	2.69	1.49	1.43
23	A	406	PL9	C3-C4	-2.69	1.45	1.49
23	D	407	PL9	C7-C3	-2.69	1.47	1.51
22	B	609	CLA	C1B-C2B	2.69	1.49	1.43
22	a	405	CLA	C1B-C2B	2.68	1.49	1.43
22	C	520	CLA	C1B-C2B	2.68	1.49	1.43
22	C	507	CLA	C1B-C2B	2.68	1.49	1.43
22	a	407	CLA	C1B-C2B	2.67	1.49	1.43
25	C	515	DGD	O2G-C2G	-2.67	1.40	1.46
22	b	611	CLA	C1B-C2B	2.66	1.49	1.43
22	A	402	CLA	C3B-C4B	2.65	1.50	1.42
22	A	403	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	PL9	C7-C3	-2.64	1.47	1.51
22	a	404	CLA	C3B-C4B	2.64	1.50	1.42
31	D	402	PHO	CMC-C2C	-2.62	1.46	1.50
22	A	402	CLA	C1B-C2B	2.60	1.49	1.43
22	c	507	CLA	C1B-C2B	2.58	1.49	1.43
31	d	402	PHO	C3D-C4D	2.57	1.44	1.41
31	d	402	PHO	CMC-C2C	-2.57	1.46	1.50
22	B	610	CLA	MG-NB	-2.56	2.00	2.05
22	a	404	CLA	C1B-C2B	2.55	1.49	1.43
31	d	401	PHO	CMC-C2C	-2.54	1.46	1.50
31	d	401	PHO	C3D-C4D	2.54	1.44	1.41
22	b	614	CLA	MG-NB	-2.53	2.00	2.05
31	D	401	PHO	CMC-C2C	-2.53	1.46	1.50
31	D	402	PHO	C3D-C4D	2.53	1.44	1.41
31	D	401	PHO	C3D-C4D	2.52	1.44	1.41
30	d	411	LMT	O3'-C3'	-2.49	1.36	1.43
30	b	627	LMT	O3'-C3'	-2.49	1.36	1.43
31	d	401	PHO	CMD-C2D	-2.47	1.46	1.51
30	D	411	LMT	O3'-C3'	-2.47	1.36	1.43
30	M	102	LMT	O3'-C3'	-2.47	1.36	1.43
30	I	102	LMT	O3'-C3'	-2.47	1.36	1.43
31	D	402	PHO	CMD-C2D	-2.46	1.46	1.51
30	M	103	LMT	O3'-C3'	-2.46	1.36	1.43
22	c	508	CLA	C3B-C4B	2.46	1.49	1.42
31	D	401	PHO	CMD-C2D	-2.46	1.46	1.51
22	a	405	CLA	C3B-C4B	2.45	1.49	1.42
31	d	401	PHO	CMB-C2B	-2.45	1.46	1.51
31	d	402	PHO	CMD-C2D	-2.45	1.46	1.51
30	b	626	LMT	O3'-C3'	-2.45	1.36	1.43
22	B	608	CLA	CHC-C1C	2.45	1.43	1.38
31	D	401	PHO	CMB-C2B	-2.45	1.46	1.51
22	B	613	CLA	CHC-C1C	2.44	1.43	1.38
31	D	402	PHO	CAC-C3C	-2.44	1.47	1.51
22	C	508	CLA	C3B-C4B	2.43	1.49	1.42
30	b	603	LMT	O3'-C3'	-2.43	1.36	1.43
30	b	604	LMT	O3'-C3'	-2.43	1.36	1.43
22	A	403	CLA	C3B-C4B	2.43	1.49	1.42
30	B	627	LMT	O3'-C3'	-2.42	1.37	1.43
30	B	624	LMT	O3'-C3'	-2.42	1.37	1.43
25	B	625	DGD	C4D-C5D	2.41	1.58	1.53
31	d	401	PHO	CAC-C3C	-2.41	1.47	1.51
30	i	102	LMT	O3'-C3'	-2.40	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	h	101	CLA	CHC-C1C	2.40	1.43	1.38
31	d	402	PHO	CMB-C2B	-2.40	1.46	1.51
22	b	605	CLA	C3B-C4B	2.40	1.49	1.42
30	B	623	LMT	O3'-C3'	-2.40	1.37	1.43
22	C	505	CLA	C3B-C4B	2.39	1.49	1.42
31	D	402	PHO	CMB-C2B	-2.39	1.46	1.51
22	c	520	CLA	C3B-C4B	2.39	1.49	1.42
22	b	612	CLA	CHC-C1C	2.38	1.43	1.38
22	H	101	CLA	CHC-C1C	2.38	1.43	1.38
22	C	520	CLA	C3B-C4B	2.38	1.49	1.42
22	B	613	CLA	C3B-C4B	2.38	1.49	1.42
22	c	505	CLA	C3B-C4B	2.38	1.49	1.42
22	b	611	CLA	CHC-C1C	2.37	1.43	1.38
22	B	601	CLA	C3B-C4B	2.37	1.49	1.42
22	c	511	CLA	C3B-C4B	2.36	1.49	1.42
23	J	101	PL9	C7-C3	-2.36	1.48	1.51
22	b	606	CLA	C3B-C4B	2.36	1.49	1.42
22	b	611	CLA	C3B-C4B	2.36	1.49	1.42
22	b	612	CLA	C3B-C4B	2.36	1.49	1.42
22	c	510	CLA	C3B-C4B	2.36	1.49	1.42
22	c	509	CLA	C3B-C4B	2.36	1.49	1.42
22	d	406	CLA	C3B-C4B	2.36	1.49	1.42
25	c	515	DGD	O2G-C2G	-2.35	1.41	1.46
23	A	406	PL9	C7-C3	-2.35	1.48	1.51
22	h	101	CLA	C3B-C4B	2.35	1.49	1.42
22	b	606	CLA	CHC-C1C	2.35	1.43	1.38
30	B	628	LMT	O3'-C3'	-2.35	1.37	1.43
22	C	511	CLA	C3B-C4B	2.35	1.49	1.42
31	d	402	PHO	CAC-C3C	-2.35	1.47	1.51
22	B	608	CLA	C3B-C4B	2.35	1.49	1.42
22	b	615	CLA	C3B-C4B	2.34	1.49	1.42
22	b	617	CLA	CHC-C1C	2.34	1.43	1.38
22	B	611	CLA	CMD-C2D	-2.34	1.46	1.50
22	H	101	CLA	C3B-C4B	2.34	1.49	1.42
22	C	507	CLA	C3B-C4B	2.34	1.49	1.42
22	b	618	CLA	C3B-C4B	2.33	1.49	1.42
22	a	406	CLA	C3B-C4B	2.33	1.49	1.42
22	D	405	CLA	C3B-C4B	2.33	1.49	1.42
22	B	614	CLA	C3B-C4B	2.33	1.49	1.42
31	D	401	PHO	CAC-C3C	-2.33	1.47	1.51
22	C	509	CLA	C3B-C4B	2.33	1.49	1.42
22	c	507	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CHC-C1C	2.33	1.43	1.38
22	a	404	CLA	CHC-C1C	2.33	1.43	1.38
22	B	612	CLA	C3B-C4B	2.32	1.49	1.42
22	d	406	CLA	CHC-C1C	2.32	1.43	1.38
22	c	512	CLA	C3B-C4B	2.32	1.49	1.42
22	c	502	CLA	CHC-C1C	2.32	1.43	1.38
22	b	619	CLA	C3B-C4B	2.32	1.49	1.42
22	B	607	CLA	C3B-C4B	2.32	1.49	1.42
22	C	510	CLA	C3B-C4B	2.32	1.49	1.42
22	B	615	CLA	C3B-C4B	2.32	1.49	1.42
22	B	611	CLA	C3B-C4B	2.32	1.49	1.42
23	D	407	PL9	C6-C1	-2.31	1.44	1.48
22	C	505	CLA	CHC-C1C	2.31	1.43	1.38
22	D	406	CLA	C3B-C4B	2.31	1.49	1.42
23	a	408	PL9	C53-C6	-2.31	1.46	1.50
22	A	404	CLA	C3B-C4B	2.31	1.49	1.42
22	C	512	CLA	CHC-C1C	2.30	1.43	1.38
22	c	511	CLA	CHC-C1C	2.30	1.43	1.38
22	b	617	CLA	C3B-C4B	2.30	1.49	1.42
22	c	512	CLA	CHC-C1C	2.30	1.43	1.38
22	c	507	CLA	CHC-C1C	2.30	1.43	1.38
22	a	407	CLA	C3B-C4B	2.30	1.49	1.42
22	b	616	CLA	C3B-C4B	2.30	1.49	1.42
22	B	609	CLA	C3B-C4B	2.30	1.49	1.42
25	c	516	DGD	O2G-C2G	-2.30	1.41	1.46
22	C	511	CLA	CHC-C1C	2.30	1.43	1.38
22	d	405	CLA	CHC-C1C	2.30	1.43	1.38
22	c	509	CLA	CHC-C1C	2.29	1.43	1.38
22	C	512	CLA	C3B-C4B	2.29	1.49	1.42
22	B	602	CLA	C3B-C4B	2.29	1.49	1.42
22	B	604	CLA	C3B-C4B	2.29	1.49	1.42
22	a	406	CLA	CHC-C1C	2.29	1.43	1.38
22	c	505	CLA	CHC-C1C	2.29	1.43	1.38
22	C	502	CLA	CHC-C1C	2.29	1.43	1.38
22	C	502	CLA	C3B-C4B	2.29	1.49	1.42
22	c	504	CLA	CHC-C1C	2.29	1.43	1.38
22	c	503	CLA	C3B-C4B	2.29	1.49	1.42
22	B	606	CLA	C3B-C4B	2.28	1.49	1.42
22	C	509	CLA	CHC-C1C	2.28	1.43	1.38
22	D	405	CLA	CHC-C1C	2.28	1.43	1.38
22	b	613	CLA	C3B-C4B	2.28	1.49	1.42
26	a	411	LHG	O7-C5	-2.28	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	CMD-C2D	-2.28	1.46	1.50
22	b	608	CLA	C3B-C4B	2.28	1.49	1.42
22	a	407	CLA	CHC-C1C	2.28	1.43	1.38
22	B	609	CLA	CHC-C1C	2.28	1.43	1.38
22	B	603	CLA	CHC-C1C	2.28	1.43	1.38
22	b	616	CLA	CHC-C1C	2.28	1.43	1.38
23	j	101	PL9	C7-C3	-2.28	1.48	1.51
22	C	504	CLA	CHC-C1C	2.27	1.43	1.38
22	B	604	CLA	CHC-C1C	2.27	1.43	1.38
22	b	607	CLA	CHC-C1C	2.27	1.43	1.38
22	c	502	CLA	C3B-C4B	2.27	1.49	1.42
22	B	605	CLA	C3B-C4B	2.27	1.49	1.42
25	C	516	DGD	O2G-C2G	-2.27	1.41	1.46
22	B	614	CLA	CHC-C1C	2.27	1.43	1.38
22	b	618	CLA	CHC-C1C	2.27	1.43	1.38
22	C	506	CLA	C3B-C4B	2.26	1.49	1.42
22	b	610	CLA	C3B-C4B	2.26	1.49	1.42
22	d	405	CLA	C3B-C4B	2.26	1.49	1.42
22	B	602	CLA	CHC-C1C	2.26	1.43	1.38
22	c	508	CLA	CHC-C1C	2.26	1.43	1.38
22	C	508	CLA	CHC-C1C	2.26	1.43	1.38
22	c	506	CLA	C3B-C4B	2.26	1.49	1.42
23	A	406	PL9	C53-C6	-2.26	1.46	1.50
22	c	510	CLA	CHC-C1C	2.26	1.43	1.38
22	A	405	CLA	C3B-C4B	2.26	1.49	1.42
22	A	404	CLA	CHC-C1C	2.25	1.43	1.38
22	c	504	CLA	C3B-C4B	2.25	1.49	1.42
22	C	503	CLA	C3B-C4B	2.25	1.49	1.42
22	b	609	CLA	C3B-C4B	2.24	1.49	1.42
27	D	412	LMG	O7-C8	-2.24	1.41	1.46
22	C	520	CLA	CHC-C1C	2.24	1.43	1.38
24	g	101	BCR	C33-C5	-2.24	1.47	1.50
25	B	620	DGD	O2G-C2G	-2.24	1.41	1.46
22	b	613	CLA	CHC-C1C	2.24	1.43	1.38
22	B	603	CLA	C3B-C4B	2.24	1.49	1.42
22	A	403	CLA	CHC-C1C	2.24	1.43	1.38
23	J	101	PL9	C3-C4	-2.23	1.46	1.49
30	I	102	LMT	O2'-C2'	-2.23	1.37	1.43
22	B	605	CLA	CHC-C1C	2.23	1.43	1.38
22	B	606	CLA	CHC-C1C	2.23	1.42	1.38
22	b	608	CLA	CHC-C1C	2.23	1.42	1.38
25	C	515	DGD	O1G-C1G	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	CHC-C1C	2.22	1.42	1.38
22	c	503	CLA	CHC-C1C	2.22	1.42	1.38
22	C	504	CLA	C3B-C4B	2.22	1.49	1.42
22	A	402	CLA	CHC-C1C	2.22	1.42	1.38
22	B	612	CLA	CHC-C1C	2.22	1.42	1.38
22	b	610	CLA	CHC-C1C	2.22	1.42	1.38
27	B	621	LMG	C4-C5	2.22	1.57	1.53
22	b	607	CLA	C3B-C4B	2.22	1.49	1.42
27	d	412	LMG	O7-C8	-2.22	1.41	1.46
22	c	504	CLA	CMD-C2D	-2.22	1.46	1.50
30	I	102	LMT	O2B-C2B	-2.22	1.37	1.43
22	C	501	CLA	C3B-C4B	2.22	1.49	1.42
22	c	520	CLA	CHC-C1C	2.22	1.42	1.38
22	C	506	CLA	CHC-C1C	2.21	1.42	1.38
22	C	507	CLA	CMB-C2B	-2.21	1.46	1.50
22	B	610	CLA	C1B-NB	-2.20	1.35	1.37
30	i	102	LMT	O2'-C2'	-2.20	1.37	1.43
22	B	601	CLA	CHC-C1C	2.20	1.42	1.38
30	b	626	LMT	O2'-C2'	-2.20	1.37	1.43
30	i	102	LMT	O2B-C2B	-2.20	1.37	1.43
22	b	605	CLA	CHC-C1C	2.20	1.42	1.38
22	c	507	CLA	CMB-C2B	-2.20	1.46	1.50
22	b	609	CLA	CHC-C1C	2.20	1.42	1.38
22	C	504	CLA	CMD-C2D	-2.20	1.46	1.50
23	j	101	PL9	C3-C4	-2.20	1.46	1.49
22	C	507	CLA	CHC-C1C	2.19	1.42	1.38
23	A	406	PL9	C6-C1	-2.19	1.44	1.48
27	D	408	LMG	O7-C8	-2.19	1.41	1.46
22	c	506	CLA	CHC-C1C	2.19	1.42	1.38
22	b	615	CLA	CHC-C1C	2.19	1.42	1.38
22	c	509	CLA	CMD-C2D	-2.19	1.46	1.50
22	C	501	CLA	CHC-C1C	2.18	1.42	1.38
22	C	503	CLA	CHC-C1C	2.18	1.42	1.38
22	c	501	CLA	C3B-C4B	2.17	1.49	1.42
22	D	406	CLA	CHC-C1C	2.17	1.42	1.38
22	D	405	CLA	CMD-C2D	-2.17	1.46	1.50
25	b	624	DGD	O2G-C2G	-2.17	1.41	1.46
22	b	619	CLA	CHC-C1C	2.17	1.42	1.38
22	A	405	CLA	CHC-C1C	2.17	1.42	1.38
22	B	611	CLA	CHC-C1C	2.16	1.42	1.38
24	y	101	BCR	C33-C5	-2.16	1.47	1.50
30	M	103	LMT	O2'-C2'	-2.16	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	102	LMT	O1'-C1'	-2.15	1.36	1.40
22	B	615	CLA	CHC-C1C	2.15	1.42	1.38
30	B	623	LMT	O2'-C2'	-2.15	1.37	1.43
22	b	614	CLA	C1B-C2B	2.15	1.48	1.43
26	C	519	LHG	O7-C5	-2.15	1.41	1.46
30	M	103	LMT	O3B-C3B	-2.15	1.37	1.43
22	b	613	CLA	MG-NB	-2.15	2.01	2.05
30	b	627	LMT	O2'-C2'	-2.15	1.37	1.43
27	b	625	LMG	C4-C5	2.15	1.57	1.53
30	B	628	LMT	O3B-C3B	-2.14	1.37	1.43
30	B	627	LMT	O2'-C2'	-2.14	1.37	1.43
34	f	101	HEM	CMC-C2C	2.14	1.55	1.50
22	B	610	CLA	C1B-C2B	2.14	1.48	1.43
22	c	501	CLA	CHC-C1C	2.14	1.42	1.38
22	C	509	CLA	CMD-C2D	-2.14	1.46	1.50
30	M	102	LMT	O3B-C3B	-2.14	1.37	1.43
22	B	602	CLA	MG-NB	-2.13	2.01	2.05
30	b	627	LMT	O3B-C3B	-2.13	1.37	1.43
26	A	409	LHG	O7-C5	-2.13	1.41	1.46
22	b	611	CLA	CMD-C2D	-2.13	1.46	1.50
30	M	103	LMT	O2B-C2B	-2.13	1.37	1.43
22	a	405	CLA	CHC-C1C	2.13	1.42	1.38
23	a	408	PL9	C6-C1	-2.13	1.45	1.48
30	M	102	LMT	O2'-C2'	-2.13	1.37	1.43
22	b	614	CLA	C1B-NB	-2.13	1.35	1.37
30	D	411	LMT	O3B-C3B	-2.13	1.37	1.43
30	b	603	LMT	O2B-C2B	-2.13	1.37	1.43
22	B	603	CLA	CMD-C2D	-2.13	1.46	1.50
22	C	503	CLA	MG-NB	-2.12	2.01	2.05
26	c	519	LHG	O7-C5	-2.12	1.41	1.46
30	b	603	LMT	O3B-C3B	-2.12	1.37	1.43
30	B	623	LMT	O3B-C3B	-2.12	1.37	1.43
30	M	102	LMT	O2B-C2B	-2.12	1.37	1.43
30	b	626	LMT	O2B-C2B	-2.12	1.37	1.43
22	c	507	CLA	MG-NB	-2.12	2.01	2.05
30	b	604	LMT	O3B-C3B	-2.11	1.37	1.43
34	F	101	HEM	CMC-C2C	2.11	1.55	1.50
30	I	102	LMT	O3B-C3B	-2.11	1.37	1.43
30	B	624	LMT	O3B-C3B	-2.11	1.37	1.43
25	a	410	DGD	O1G-C1G	-2.11	1.40	1.45
22	A	402	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	607	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	CMB-C2B	-2.11	1.46	1.50
22	b	606	CLA	MG-NB	-2.10	2.01	2.05
34	V	201	HEM	CMB-C2B	2.10	1.55	1.50
30	B	627	LMT	O2B-C2B	-2.10	1.37	1.43
30	D	411	LMT	O2'-C2'	-2.10	1.37	1.43
30	d	411	LMT	O3B-C3B	-2.10	1.37	1.43
29	b	602	SQD	O2-C2	-2.10	1.37	1.43
25	b	601	DGD	C4D-C5D	2.10	1.57	1.53
22	B	605	CLA	MG-NB	-2.09	2.01	2.05
30	b	603	LMT	O2'-C2'	-2.09	1.37	1.43
22	A	404	CLA	CMD-C2D	-2.09	1.46	1.50
22	C	509	CLA	CMB-C2B	-2.09	1.46	1.50
22	a	404	CLA	CMD-C2D	-2.09	1.46	1.50
22	a	406	CLA	CMD-C2D	-2.09	1.46	1.50
22	c	509	CLA	CMB-C2B	-2.09	1.46	1.50
30	b	604	LMT	O2B-C2B	-2.09	1.37	1.43
30	d	411	LMT	O2'-C2'	-2.09	1.37	1.43
24	C	514	BCR	C38-C26	-2.08	1.47	1.50
30	D	411	LMT	O2B-C2B	-2.08	1.37	1.43
30	b	626	LMT	O3B-C3B	-2.08	1.37	1.43
30	i	102	LMT	O3B-C3B	-2.08	1.37	1.43
34	v	201	HEM	CMD-C2D	2.08	1.55	1.50
30	B	624	LMT	O2'-C2'	-2.08	1.37	1.43
22	b	619	CLA	CMC-C2C	-2.08	1.46	1.50
22	C	506	CLA	MG-NB	-2.08	2.01	2.05
22	C	520	CLA	MG-NB	-2.08	2.01	2.05
22	B	607	CLA	CMB-C2B	-2.08	1.46	1.50
22	b	611	CLA	CMB-C2B	-2.08	1.46	1.50
25	B	625	DGD	C3G-C2G	2.08	1.57	1.50
26	c	519	LHG	P-O6	2.08	1.67	1.59
30	B	627	LMT	O3B-C3B	-2.08	1.37	1.43
30	B	628	LMT	O2'-C2'	-2.08	1.37	1.43
22	A	403	CLA	CMB-C2B	-2.08	1.46	1.50
30	B	628	LMT	O2B-C2B	-2.08	1.37	1.43
22	b	607	CLA	CMD-C2D	-2.07	1.46	1.50
34	v	201	HEM	CMB-C2B	2.07	1.55	1.50
22	b	611	CLA	MG-NB	-2.07	2.01	2.05
25	d	410	DGD	C1D-C2D	2.07	1.58	1.52
22	B	607	CLA	MG-NB	-2.07	2.01	2.05
22	c	506	CLA	MG-NB	-2.07	2.01	2.05
29	B	626	SQD	O2-C2	-2.07	1.37	1.43
22	B	609	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	CMB-C2B	-2.07	1.46	1.50
22	b	619	CLA	CMD-C2D	-2.07	1.46	1.50
22	b	607	CLA	CMB-C2B	-2.07	1.46	1.50
34	V	201	HEM	CMD-C2D	2.07	1.55	1.50
22	B	615	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	615	CLA	CMD-C2D	-2.07	1.46	1.50
30	B	623	LMT	O2B-C2B	-2.06	1.37	1.43
22	B	603	CLA	MG-NB	-2.06	2.01	2.05
22	A	404	CLA	MG-NB	-2.06	2.01	2.05
22	D	406	CLA	MG-NB	-2.06	2.01	2.05
30	d	411	LMT	O2B-C2B	-2.06	1.37	1.43
23	d	407	PL9	C6-C1	-2.06	1.45	1.48
22	D	405	CLA	MG-NB	-2.06	2.01	2.05
22	C	501	CLA	CMB-C2B	-2.06	1.46	1.50
22	d	405	CLA	CMD-C2D	-2.06	1.46	1.50
22	c	502	CLA	MG-NB	-2.06	2.01	2.05
22	a	405	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	404	CLA	CMB-C2B	-2.06	1.46	1.50
22	C	502	CLA	MG-NB	-2.06	2.01	2.05
22	A	405	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	402	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	403	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	612	CLA	MG-NB	-2.05	2.01	2.05
22	B	602	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	609	CLA	MG-NB	-2.05	2.01	2.05
22	b	617	CLA	MG-NB	-2.05	2.01	2.05
22	c	501	CLA	CMB-C2B	-2.05	1.46	1.50
22	a	407	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	505	CLA	CMB-C2B	-2.05	1.46	1.50
24	J	102	BCR	C38-C26	-2.05	1.47	1.50
27	A	414	LMG	O7-C8	-2.05	1.41	1.46
24	c	514	BCR	C38-C26	-2.05	1.47	1.50
22	a	405	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	508	CLA	CMD-C2D	-2.05	1.46	1.50
22	a	406	CLA	CMB-C2B	-2.05	1.46	1.50
25	b	601	DGD	C3G-C2G	2.04	1.57	1.50
23	D	407	PL9	C53-C6	-2.04	1.46	1.50
30	b	604	LMT	O2'-C2'	-2.04	1.37	1.43
22	d	405	CLA	CMB-C2B	-2.04	1.46	1.50
27	a	402	LMG	O7-C8	-2.04	1.41	1.46
22	b	607	CLA	MG-NB	-2.04	2.01	2.05
27	C	521	LMG	O7-C8	-2.04	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	608	CLA	CMD-C2D	-2.04	1.46	1.50
22	C	508	CLA	CMB-C2B	-2.04	1.46	1.50
22	H	101	CLA	CMD-C2D	-2.04	1.46	1.50
22	C	502	CLA	CMC-C2C	-2.04	1.46	1.50
22	c	505	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	606	CLA	CMB-C2B	-2.04	1.46	1.50
22	A	405	CLA	MG-NB	-2.04	2.01	2.05
22	B	605	CLA	CMB-C2B	-2.03	1.46	1.50
34	v	201	HEM	CMA-C3A	2.03	1.54	1.50
22	B	601	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	610	CLA	CMB-C2B	-2.03	1.46	1.50
22	C	505	CLA	CMD-C2D	-2.03	1.46	1.50
24	j	102	BCR	C38-C26	-2.03	1.47	1.50
22	C	502	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	605	CLA	CMB-C2B	-2.03	1.46	1.50
22	C	512	CLA	CMB-C2B	-2.03	1.46	1.50
22	C	520	CLA	CMB-C2B	-2.03	1.46	1.50
22	c	508	CLA	CMD-C2D	-2.03	1.46	1.50
22	C	502	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	CMB-C2B	-2.02	1.46	1.50
22	h	101	CLA	CMD-C2D	-2.02	1.46	1.50
30	M	103	LMT	O1'-C1'	-2.02	1.36	1.40
22	B	608	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	615	CLA	MG-NB	-2.02	2.01	2.05
25	d	410	DGD	O1G-C1G	-2.02	1.40	1.45
22	c	508	CLA	CMB-C2B	-2.02	1.46	1.50
22	H	101	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	609	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	612	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	405	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	604	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	611	CLA	MG-NB	-2.02	2.01	2.05
22	C	504	CLA	CMB-C2B	-2.02	1.46	1.50
22	C	507	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	503	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	615	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	615	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	614	CLA	CMD-C2D	-2.02	1.46	1.50
22	b	610	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	CMB-C2B	-2.02	1.46	1.50
22	c	520	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	502	CLA	CMD-C2D	-2.02	1.46	1.50
22	b	608	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	520	CLA	CMB-C2B	-2.01	1.46	1.50
22	b	614	CLA	MG-ND	-2.01	2.01	2.05
22	C	510	CLA	CMB-C2B	-2.01	1.46	1.50
22	b	606	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	609	CLA	CMD-C2D	-2.01	1.46	1.50
22	h	101	CLA	CMB-C2B	-2.01	1.46	1.50
22	b	617	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	610	CLA	MG-NB	-2.01	2.01	2.05
22	C	511	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	609	CLA	CMD-C2D	-2.01	1.46	1.50
22	C	503	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	503	CLA	MG-NB	-2.01	2.01	2.05
22	h	101	CLA	MG-NB	-2.01	2.01	2.05
22	c	507	CLA	CMD-C2D	-2.01	1.46	1.50
22	C	507	CLA	MG-NB	-2.01	2.01	2.05
22	c	509	CLA	MG-NB	-2.01	2.01	2.05
22	B	606	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	616	CLA	CMD-C2D	-2.01	1.46	1.50
29	A	413	SQD	O3-C3	-2.01	1.38	1.43
27	M	101	LMG	C4-C5	2.01	1.57	1.53
22	b	609	CLA	MG-NB	-2.01	2.01	2.05
27	A	414	LMG	C4-C5	2.01	1.57	1.53
22	D	406	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	503	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	601	DGD	C1G-C2G	2.01	1.57	1.50
27	d	408	LMG	O7-C8	-2.01	1.41	1.46
22	B	615	CLA	MG-NB	-2.01	2.01	2.05
22	B	608	CLA	CMD-C2D	-2.00	1.46	1.50
22	B	613	CLA	CMD-C2D	-2.00	1.46	1.50
22	C	503	CLA	CMD-C2D	-2.00	1.46	1.50
34	F	101	HEM	CMA-C3A	2.00	1.54	1.50
22	c	502	CLA	CMC-C2C	-2.00	1.46	1.50
22	b	618	CLA	CMD-C2D	-2.00	1.46	1.50
22	c	511	CLA	CMD-C2D	-2.00	1.46	1.50
22	B	601	CLA	CMD-C2D	-2.00	1.46	1.50
22	c	505	CLA	CMD-C2D	-2.00	1.46	1.50
24	F	102	BCR	C33-C5	-2.00	1.47	1.50
22	C	511	CLA	MG-NB	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	402	LMG	C4-C5	2.00	1.57	1.53
30	b	627	LMT	O2B-C2B	-2.00	1.38	1.43
22	B	613	CLA	MG-NB	-2.00	2.01	2.05

All (1031) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.27	110.00	106.68
22	B	611	CLA	C4A-NA-C1A	7.25	109.99	106.68
22	c	504	CLA	C4A-NA-C1A	7.17	109.95	106.68
22	B	603	CLA	C4A-NA-C1A	7.15	109.94	106.68
22	b	615	CLA	C4A-NA-C1A	7.01	109.88	106.68
22	b	609	CLA	C4A-NA-C1A	6.99	109.87	106.68
22	C	510	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	b	607	CLA	C4A-NA-C1A	6.95	109.85	106.68
22	C	501	CLA	C4A-NA-C1A	6.89	109.82	106.68
22	A	403	CLA	C4A-NA-C1A	6.85	109.80	106.68
22	c	503	CLA	C4A-NA-C1A	6.84	109.80	106.68
22	a	405	CLA	C4A-NA-C1A	6.79	109.78	106.68
22	b	616	CLA	C4A-NA-C1A	6.79	109.78	106.68
22	C	520	CLA	C4A-NA-C1A	6.78	109.77	106.68
22	c	501	CLA	C4A-NA-C1A	6.78	109.77	106.68
22	B	605	CLA	C4A-NA-C1A	6.76	109.76	106.68
22	b	618	CLA	C4A-NA-C1A	6.73	109.75	106.68
22	C	511	CLA	C4A-NA-C1A	6.72	109.75	106.68
22	b	608	CLA	C4A-NA-C1A	6.69	109.73	106.68
22	B	606	CLA	C4A-NA-C1A	6.69	109.73	106.68
22	c	520	CLA	C4A-NA-C1A	6.67	109.72	106.68
22	A	405	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	c	511	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	C	512	CLA	C4A-NA-C1A	6.63	109.70	106.68
22	B	614	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	B	615	CLA	C4A-NA-C1A	6.61	109.70	106.68
22	C	506	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	B	612	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	c	506	CLA	C4A-NA-C1A	6.57	109.67	106.68
22	b	617	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	C	505	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	a	406	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	c	510	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	C	507	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	B	604	CLA	C4A-NA-C1A	6.52	109.65	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	a	407	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	c	505	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	b	619	CLA	C4A-NA-C1A	6.46	109.62	106.68
22	h	101	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	B	607	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	B	613	CLA	C4A-NA-C1A	6.44	109.61	106.68
22	H	101	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	B	608	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	B	609	CLA	C4A-NA-C1A	6.41	109.60	106.68
22	b	610	CLA	C4A-NA-C1A	6.41	109.60	106.68
22	A	404	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	c	508	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	c	502	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	c	512	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	c	507	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	B	602	CLA	C4A-NA-C1A	6.33	109.57	106.68
22	D	405	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	d	406	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	b	611	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	C	508	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	C	502	CLA	C4A-NA-C1A	6.21	109.51	106.68
22	A	402	CLA	C4A-NA-C1A	6.18	109.50	106.68
22	C	509	CLA	C4A-NA-C1A	6.17	109.49	106.68
22	c	509	CLA	C4A-NA-C1A	6.16	109.49	106.68
22	D	406	CLA	C4A-NA-C1A	6.14	109.48	106.68
22	b	613	CLA	C4A-NA-C1A	6.13	109.47	106.68
22	d	405	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	B	601	CLA	C4A-NA-C1A	6.11	109.47	106.68
22	b	605	CLA	C4A-NA-C1A	6.09	109.46	106.68
22	b	612	CLA	C4A-NA-C1A	6.07	109.45	106.68
22	a	404	CLA	C4A-NA-C1A	6.01	109.42	106.68
22	b	606	CLA	C4A-NA-C1A	6.01	109.42	106.68
31	D	402	PHO	C4D-CHA-CBD	-5.87	105.64	108.45
31	D	401	PHO	C4D-CHA-CBD	-5.86	105.64	108.45
31	d	401	PHO	C4D-CHA-CBD	-5.85	105.65	108.45
29	a	415	SQD	O6-C1-C2	5.83	117.13	108.27
31	d	402	PHO	C4D-CHA-CBD	-5.80	105.67	108.45
29	A	412	SQD	O6-C1-C2	5.68	116.91	108.27
33	D	404	BCT	O2-C-O1	5.67	134.18	119.68
33	d	404	BCT	O2-C-O1	5.63	134.08	119.68
29	b	602	SQD	O6-C1-C2	5.57	116.74	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	101	PL9	C7-C3-C4	5.57	121.50	116.91
22	b	614	CLA	C4A-NA-C1A	5.50	109.19	106.68
23	J	101	PL9	C7-C3-C4	5.48	121.42	116.91
34	v	201	HEM	C4D-ND-C1D	5.45	111.66	105.21
29	B	626	SQD	O6-C1-C2	5.44	116.53	108.27
22	B	610	CLA	C4A-NA-C1A	5.40	109.14	106.68
23	A	406	PL9	C7-C3-C4	5.33	121.30	116.91
34	V	201	HEM	C4D-ND-C1D	5.28	111.46	105.21
34	f	101	HEM	C4D-ND-C1D	5.19	111.36	105.21
23	d	407	PL9	C7-C3-C4	5.16	121.16	116.91
23	D	407	PL9	C7-C3-C4	5.11	121.12	116.91
34	F	101	HEM	C4D-ND-C1D	5.10	111.24	105.21
23	a	408	PL9	C7-C3-C4	5.07	121.08	116.91
25	A	408	DGD	O3G-C3G-C2G	-4.77	99.22	110.82
25	a	410	DGD	O3G-C3G-C2G	-4.67	99.45	110.82
29	d	403	SQD	O5-C5-C4	4.57	117.94	109.70
29	B	622	SQD	O5-C5-C4	4.49	117.79	109.70
26	c	519	LHG	O4-P-O5	4.43	133.05	112.44
26	C	519	LHG	O4-P-O5	4.43	133.04	112.44
26	a	411	LHG	O4-P-O5	4.42	133.03	112.44
26	A	409	LHG	O4-P-O5	4.39	132.89	112.44
25	C	517	DGD	O3G-C3G-C2G	-4.39	100.13	110.82
29	d	403	SQD	O6-C1-C2	4.30	114.81	108.27
29	B	622	SQD	O6-C1-C2	4.29	114.79	108.27
23	j	101	PL9	C7-C3-C2	-4.27	118.36	123.39
23	J	101	PL9	C7-C3-C2	-4.22	118.41	123.39
25	c	517	DGD	O3G-C3G-C2G	-4.19	100.62	110.82
29	A	412	SQD	O9-S-C6	4.13	112.92	106.76
23	d	407	PL9	C7-C3-C2	-4.11	118.55	123.39
29	a	415	SQD	O9-S-C6	4.05	112.80	106.76
24	C	513	BCR	C2-C1-C6	4.03	116.29	110.44
29	F	103	SQD	O9-S-O7	-4.02	100.74	113.82
23	D	407	PL9	C7-C3-C2	-4.01	118.66	123.39
29	f	103	SQD	O9-S-O7	-4.01	100.78	113.82
23	A	406	PL9	C7-C3-C2	-4.01	118.66	123.39
24	c	513	BCR	C2-C1-C6	4.00	116.25	110.44
29	A	412	SQD	O9-S-O7	-3.97	100.90	113.82
24	J	102	BCR	C11-C10-C9	-3.97	121.71	127.28
29	a	415	SQD	O9-S-O7	-3.96	100.93	113.82
29	d	403	SQD	O9-S-O7	-3.95	100.97	113.82
29	A	413	SQD	O5-C5-C4	3.95	116.81	109.70
29	B	622	SQD	O9-S-O7	-3.92	101.06	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	401	SQD	O9-S-O7	-3.92	101.07	113.82
29	B	626	SQD	O9-S-O7	-3.92	101.08	113.82
24	J	102	BCR	C2-C1-C6	3.92	116.13	110.44
24	j	102	BCR	C2-C1-C6	3.91	116.12	110.44
23	a	408	PL9	C7-C3-C2	-3.91	118.78	123.39
29	b	602	SQD	O9-S-O7	-3.90	101.12	113.82
29	A	413	SQD	O9-S-O7	-3.90	101.13	113.82
29	B	626	SQD	O5-C5-C4	3.90	116.72	109.70
29	a	401	SQD	O5-C5-C4	3.88	116.70	109.70
29	b	602	SQD	O5-C5-C4	3.84	116.61	109.70
27	D	409	LMG	C1-C2-C3	-3.83	101.95	110.01
27	d	409	LMG	C1-C2-C3	-3.80	102.01	110.01
24	j	102	BCR	C11-C10-C9	-3.79	121.97	127.28
31	d	401	PHO	C2B-C1B-NB	-3.78	106.70	109.43
29	a	415	SQD	O5-C5-C4	3.72	116.41	109.70
29	a	415	SQD	O47-C7-C8	3.72	119.53	111.48
29	f	103	SQD	O5-C5-C4	3.68	116.33	109.70
31	D	402	PHO	C2B-C1B-NB	-3.68	106.77	109.43
31	D	401	PHO	C2B-C1B-NB	-3.66	106.79	109.43
29	F	103	SQD	O5-C5-C4	3.64	116.27	109.70
25	d	410	DGD	O6D-C1D-O3G	-3.63	101.46	110.04
29	A	412	SQD	O47-C7-C8	3.63	119.33	111.48
29	A	412	SQD	O5-C5-C4	3.62	116.23	109.70
25	D	410	DGD	O6D-C1D-O3G	-3.61	101.51	110.04
29	b	602	SQD	O47-C7-C8	3.59	119.24	111.48
29	B	626	SQD	O47-C7-C8	3.59	119.24	111.48
29	f	103	SQD	O7-S-C6	3.51	111.99	106.76
24	A	407	BCR	C2-C1-C6	3.50	115.53	110.44
29	F	103	SQD	O7-S-C6	3.48	111.95	106.76
25	C	516	DGD	O3G-C3G-C2G	-3.47	102.37	110.82
25	c	516	DGD	O3G-C3G-C2G	-3.47	102.39	110.82
31	d	402	PHO	C2B-C1B-NB	-3.46	106.93	109.43
29	d	403	SQD	O47-C7-C8	3.46	118.97	111.48
29	B	622	SQD	O47-C7-C8	3.46	118.96	111.48
29	F	103	SQD	O6-C1-C2	3.43	113.49	108.27
29	F	103	SQD	O47-C7-C8	3.42	118.88	111.48
29	a	401	SQD	O7-S-C6	3.38	111.81	106.76
24	a	409	BCR	C2-C1-C6	3.38	115.34	110.44
29	A	413	SQD	O7-S-C6	3.36	111.78	106.76
29	b	602	SQD	O9-S-C6	3.35	111.76	106.76
29	B	626	SQD	O9-S-C6	3.34	111.75	106.76
29	f	103	SQD	O47-C7-C8	3.34	118.71	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413	SQD	O47-C7-C8	3.34	118.70	111.48
24	B	618	BCR	C2-C1-C6	3.33	115.28	110.44
25	B	620	DGD	O3G-C3G-C2G	-3.30	102.78	110.82
24	b	622	BCR	C24-C23-C22	-3.29	121.37	126.23
24	j	102	BCR	C24-C23-C22	-3.28	121.38	126.23
24	b	622	BCR	C2-C1-C6	3.27	115.20	110.44
25	C	515	DGD	O3G-C3G-C2G	-3.26	102.89	110.82
25	c	516	DGD	O5D-C6D-C5D	-3.24	102.11	109.42
25	c	515	DGD	O3G-C3G-C2G	-3.24	102.93	110.82
22	B	605	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
24	J	102	BCR	C24-C23-C22	-3.24	121.44	126.23
29	f	103	SQD	O6-C1-C2	3.23	113.17	108.27
25	b	624	DGD	O3G-C3G-C2G	-3.22	102.98	110.82
29	b	602	SQD	O7-S-C6	3.22	111.56	106.76
22	a	404	CLA	C3B-C4B-NB	-3.22	107.66	110.53
22	B	603	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
22	b	609	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
22	B	610	CLA	CMB-C2B-C1B	-3.21	120.54	125.42
29	a	401	SQD	O47-C7-C8	3.21	118.42	111.48
22	B	613	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
25	b	624	DGD	O6D-C1D-O3G	-3.17	102.54	110.04
24	J	102	BCR	C27-C26-C25	3.17	126.98	122.70
29	a	401	SQD	C44-O6-C1	3.16	120.57	113.80
25	B	620	DGD	O6D-C1D-O3G	-3.16	102.58	110.04
22	c	503	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
31	d	402	PHO	O1D-CGD-CBD	3.15	129.50	124.72
24	B	617	BCR	C15-C16-C17	-3.15	117.08	123.52
31	D	402	PHO	O1D-CGD-CBD	3.14	129.49	124.72
30	B	628	LMT	C1'-O5'-C5'	-3.14	107.59	113.72
25	c	516	DGD	O6D-C1D-O3G	-3.14	102.62	110.04
22	b	617	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
22	b	606	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
29	A	412	SQD	O7-S-C6	3.14	111.44	106.76
24	c	521	BCR	C2-C1-C6	3.13	114.99	110.44
29	B	622	SQD	O7-S-C6	3.13	111.42	106.76
22	b	614	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
25	C	516	DGD	O5D-C6D-C5D	-3.11	102.40	109.42
24	j	102	BCR	C7-C8-C9	-3.11	121.63	126.23
29	B	626	SQD	O7-S-C6	3.11	111.39	106.76
22	A	402	CLA	C3B-C4B-NB	-3.10	107.76	110.53
25	d	410	DGD	O3G-C3G-C2G	-3.10	103.28	110.82
22	c	507	CLA	O2D-CGD-O1D	-3.10	117.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	102	BCR	C3-C4-C5	-3.10	108.53	114.06
29	B	626	SQD	C3-C4-C5	3.10	115.84	110.23
24	J	102	BCR	C7-C8-C9	-3.09	121.66	126.23
22	b	607	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
25	A	408	DGD	O6D-C1D-O3G	-3.09	102.75	110.04
24	j	102	BCR	C27-C26-C25	3.09	126.88	122.70
31	d	401	PHO	O1D-CGD-CBD	3.09	129.41	124.72
22	C	505	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	b	621	BCR	C15-C16-C17	-3.08	117.21	123.52
29	d	403	SQD	O9-S-C6	3.08	111.36	106.76
22	C	503	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
29	a	415	SQD	O7-S-C6	3.08	111.35	106.76
22	B	608	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
25	C	516	DGD	O6D-C1D-O3G	-3.07	102.79	110.04
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
22	C	502	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
24	B	617	BCR	C33-C5-C6	-3.07	121.14	124.48
30	b	604	LMT	C1'-O5'-C5'	-3.07	107.73	113.72
29	b	602	SQD	C3-C4-C5	3.06	115.78	110.23
24	b	621	BCR	C33-C5-C6	-3.06	121.15	124.48
31	D	401	PHO	O1D-CGD-CBD	3.06	129.36	124.72
22	B	606	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
22	C	504	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
22	b	605	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
25	B	625	DGD	O5D-C1E-C2E	3.05	112.90	108.27
24	b	623	BCR	C2-C1-C6	3.04	114.86	110.44
24	B	619	BCR	C2-C1-C6	3.04	114.86	110.44
24	j	102	BCR	C3-C4-C5	-3.04	108.63	114.06
25	D	410	DGD	O3G-C3G-C2G	-3.03	103.44	110.82
24	f	102	BCR	C29-C30-C25	3.00	114.80	110.44
22	b	611	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
22	b	608	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
24	y	101	BCR	C27-C26-C25	2.99	126.75	122.70
24	F	102	BCR	C33-C5-C6	-2.99	121.22	124.48
30	B	624	LMT	C3'-C4'-C5'	-2.99	104.31	110.93
24	H	102	BCR	C33-C5-C6	-2.98	121.23	124.48
27	d	408	LMG	O6-C1-O1	-2.98	103.00	110.04
22	B	602	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	B	604	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
29	B	622	SQD	O9-S-C6	2.97	111.19	106.76
22	b	612	CLA	O2D-CGD-O1D	-2.97	118.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	DGD	O6D-C1D-O3G	-2.97	103.04	110.04
22	a	406	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
24	K	102	BCR	C2-C1-C6	2.96	114.74	110.44
22	C	507	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
22	c	505	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
22	b	613	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	C	506	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
29	d	403	SQD	O7-S-C6	2.96	111.17	106.76
25	a	410	DGD	O6D-C1D-O3G	-2.95	103.06	110.04
30	I	102	LMT	O1'-C1'-C2'	2.95	112.76	108.27
22	a	404	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
24	g	101	BCR	C27-C26-C25	2.95	126.69	122.70
24	f	102	BCR	C33-C5-C6	-2.95	121.27	124.48
24	x	101	BCR	C33-C5-C6	-2.95	121.27	124.48
34	F	101	HEM	C3B-C4B-NB	-2.94	107.35	109.47
22	C	508	CLA	C3B-C4B-NB	-2.94	107.91	110.53
22	B	609	CLA	C3B-C4B-NB	-2.94	107.91	110.53
22	B	607	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	c	520	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
22	c	511	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	C	501	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	C	510	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
22	b	616	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
22	c	501	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	c	506	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	d	406	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	A	402	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	b	611	CLA	C3B-C4B-NB	-2.92	107.92	110.53
22	c	512	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	A	403	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	c	510	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	b	613	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	c	512	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	B	605	CLA	C3B-C4B-NB	-2.91	107.93	110.53
25	C	515	DGD	O6D-C1D-O3G	-2.91	103.17	110.04
29	d	403	SQD	C3-C4-C5	2.91	115.51	110.23
34	f	101	HEM	C3B-C4B-NB	-2.90	107.38	109.47
30	i	102	LMT	O1'-C1'-C2'	2.90	112.68	108.27
22	B	601	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
25	c	517	DGD	CDB-CCB-CBB	-2.90	99.70	114.37
22	H	101	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
25	C	517	DGD	CDB-CCB-CBB	-2.90	99.70	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	627	LMT	C3'-C4'-C5'	-2.90	104.50	110.93
22	b	612	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	b	601	DGD	O5D-C1E-C2E	2.90	112.67	108.27
24	B	618	BCR	C29-C30-C25	2.89	114.64	110.44
24	F	102	BCR	C29-C30-C25	2.89	114.64	110.44
22	C	520	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	B	609	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
22	B	613	CLA	C3B-C4B-NB	-2.88	107.95	110.53
22	B	612	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	b	618	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
34	F	101	HEM	C3B-C2B-C1B	2.87	108.57	106.41
22	c	502	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	c	508	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	C	502	CLA	C3B-C4B-NB	-2.87	107.97	110.53
26	A	409	LHG	O8-C23-C24	2.87	120.58	111.83
22	B	614	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
22	C	512	CLA	C3B-C4B-NB	-2.87	107.97	110.53
29	A	413	SQD	C44-O6-C1	2.87	119.94	113.80
22	c	509	CLA	C3B-C4B-NB	-2.86	107.97	110.53
23	A	406	PL9	C22-C23-C24	-2.86	121.08	127.62
22	C	520	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	B	607	CLA	C3B-C4B-NB	-2.86	107.98	110.53
29	f	103	SQD	O9-S-C6	2.86	111.02	106.76
22	C	509	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	c	517	DGD	C1D-C2D-C3D	-2.85	104.01	110.01
22	D	406	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	c	516	DGD	CDB-CCB-CBB	-2.85	99.97	114.37
27	D	408	LMG	O6-C1-O1	-2.84	103.32	110.04
22	d	405	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
23	a	408	PL9	C22-C23-C24	-2.84	121.13	127.62
29	A	412	SQD	C3-C4-C5	2.84	115.38	110.23
22	C	509	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
22	c	502	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	A	404	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	a	411	LHG	O8-C23-C24	2.83	120.46	111.83
31	D	402	PHO	O2D-CGD-O1D	-2.83	118.34	123.85
22	b	607	CLA	C1-C2-C3	-2.83	121.56	126.20
22	B	603	CLA	C1-C2-C3	-2.83	121.56	126.20
29	a	401	SQD	O9-S-C6	2.83	110.98	106.76
25	C	516	DGD	CDB-CCB-CBB	-2.82	100.10	114.37
24	c	521	BCR	C15-C16-C17	-2.82	117.76	123.52
24	K	102	BCR	C15-C16-C17	-2.81	117.76	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	617	CLA	C3B-C4B-NB	-2.81	108.02	110.53
29	A	413	SQD	O9-S-C6	2.81	110.96	106.76
22	b	609	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	C	511	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	b	614	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
22	h	101	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
22	b	606	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	B	625	DGD	C1D-C2D-C3D	-2.80	104.12	110.01
34	f	101	HEM	C3B-C2B-C1B	2.80	108.51	106.41
24	b	621	BCR	C15-C14-C13	-2.80	123.36	127.28
23	d	407	PL9	C40-C39-C41	2.80	120.08	115.23
22	c	511	CLA	C3B-C4B-NB	-2.80	108.03	110.53
29	a	415	SQD	C3-C4-C5	2.79	115.30	110.23
25	b	601	DGD	C3G-C2G-C1G	-2.79	105.27	111.78
24	C	514	BCR	C15-C16-C17	-2.79	117.81	123.52
24	b	622	BCR	C29-C30-C25	2.79	114.49	110.44
29	B	622	SQD	C3-C4-C5	2.79	115.29	110.23
25	C	517	DGD	C1D-C2D-C3D	-2.79	104.14	110.01
22	C	512	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	B	608	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	D	410	DGD	CDB-CCB-CBB	-2.78	100.31	114.37
22	c	507	CLA	C3B-C4B-NB	-2.78	108.05	110.53
23	D	407	PL9	C22-C23-C24	-2.78	121.27	127.62
22	B	610	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
22	c	520	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	C	511	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
22	B	602	CLA	C3B-C4B-NB	-2.77	108.06	110.53
29	F	103	SQD	O9-S-C6	2.77	110.89	106.76
22	c	509	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	B	618	BCR	C24-C23-C22	-2.77	122.14	126.23
24	j	102	BCR	C15-C14-C13	-2.77	123.40	127.28
25	d	410	DGD	CDB-CCB-CBB	-2.77	100.39	114.37
22	a	405	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
22	c	503	CLA	C3B-C4B-NB	-2.75	108.07	110.53
31	D	401	PHO	O2D-CGD-O1D	-2.75	118.49	123.85
22	A	404	CLA	C3B-C4B-NB	-2.75	108.07	110.53
22	D	406	CLA	C3B-C4B-NB	-2.75	108.08	110.53
22	C	503	CLA	C3B-C4B-NB	-2.75	108.08	110.53
22	C	506	CLA	C3B-C4B-NB	-2.74	108.08	110.53
25	B	625	DGD	C3G-C2G-C1G	-2.74	105.39	111.78
29	F	103	SQD	O8-S-C6	2.74	111.27	105.97
22	c	506	CLA	C3B-C4B-NB	-2.74	108.08	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	101	BCR	C7-C8-C9	-2.74	122.18	126.23
24	c	513	BCR	C11-C10-C9	-2.74	123.44	127.28
31	d	401	PHO	O2D-CGD-O1D	-2.73	118.53	123.85
24	B	619	BCR	C3-C4-C5	-2.73	109.18	114.06
25	b	601	DGD	C1D-C2D-C3D	-2.73	104.26	110.01
23	D	407	PL9	C40-C39-C41	2.73	119.97	115.23
22	a	407	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
27	C	518	LMG	O6-C1-O1	-2.72	103.61	110.04
25	b	601	DGD	O3G-C3G-C2G	-2.72	104.20	110.82
24	y	101	BCR	C38-C26-C25	-2.72	121.52	124.48
22	A	403	CLA	C3B-C4B-NB	-2.72	108.10	110.53
24	b	623	BCR	C3-C4-C5	-2.72	109.21	114.06
24	J	102	BCR	C15-C14-C13	-2.72	123.47	127.28
22	b	607	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	b	619	CLA	C3B-C4B-NB	-2.71	108.11	110.53
27	i	101	LMG	O6-C1-O1	-2.71	103.65	110.04
24	B	617	BCR	C28-C27-C26	-2.71	109.23	114.06
22	B	603	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	b	619	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	g	101	BCR	C38-C26-C25	-2.70	121.54	124.48
22	b	608	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	A	405	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
23	J	101	PL9	C22-C23-C24	-2.70	121.45	127.62
26	C	519	LHG	O8-C23-C24	2.69	120.04	111.83
22	b	615	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	c	519	LHG	O8-C23-C24	2.69	120.03	111.83
22	c	510	CLA	C3B-C4B-NB	-2.68	108.13	110.53
24	c	514	BCR	C11-C10-C9	-2.68	123.51	127.28
24	b	621	BCR	C28-C27-C26	-2.68	109.27	114.06
24	C	514	BCR	C29-C30-C25	2.68	114.34	110.44
27	I	101	LMG	O6-C1-O1	-2.68	103.71	110.04
23	d	407	PL9	C22-C23-C24	-2.68	121.49	127.62
31	d	402	PHO	CMB-C2B-C3B	2.68	130.03	124.68
23	d	407	PL9	C7-C8-C9	-2.67	122.22	126.83
22	d	406	CLA	C3B-C4B-NB	-2.67	108.14	110.53
22	c	508	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
24	g	101	BCR	C7-C8-C9	-2.67	122.29	126.23
22	D	405	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
31	D	402	PHO	CMB-C2B-C3B	2.66	130.01	124.68
23	J	101	PL9	C7-C8-C9	-2.66	122.24	126.83
22	a	406	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	A	403	CLA	CHB-C4A-NA	2.66	128.24	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C29-C30-C25	2.66	114.30	110.44
24	c	521	BCR	C27-C26-C25	2.66	126.30	122.70
24	C	513	BCR	C15-C16-C17	-2.66	118.08	123.52
24	B	618	BCR	C11-C10-C9	-2.66	123.55	127.28
22	b	618	CLA	C3B-C4B-NB	-2.66	108.16	110.53
24	b	620	BCR	C33-C5-C6	-2.66	121.58	124.48
31	d	402	PHO	O2D-CGD-O1D	-2.66	118.68	123.85
22	B	614	CLA	C3B-C4B-NB	-2.65	108.16	110.53
23	j	101	PL9	C22-C23-C24	-2.65	121.55	127.62
24	B	616	BCR	C33-C5-C6	-2.65	121.59	124.48
22	B	603	CLA	CHB-C4A-NA	2.65	128.23	124.40
25	B	625	DGD	O3G-C3G-C2G	-2.65	104.37	110.82
22	B	615	CLA	C3B-C4B-NB	-2.65	108.17	110.53
27	c	518	LMG	O6-C1-O1	-2.65	103.79	110.04
22	a	405	CLA	C3B-C4B-NB	-2.65	108.17	110.53
29	b	602	SQD	C4-C3-C2	2.65	115.47	110.83
24	K	102	BCR	C27-C26-C25	2.64	126.28	122.70
29	f	103	SQD	O8-S-C6	2.64	111.08	105.97
23	j	101	PL9	C7-C8-C9	-2.64	122.28	126.83
24	C	513	BCR	C24-C23-C22	-2.63	122.34	126.23
22	d	406	CLA	C1-C2-C3	-2.63	121.89	126.20
22	a	405	CLA	CHB-C4A-NA	2.63	128.19	124.40
22	B	611	CLA	C3B-C4B-NB	-2.62	108.19	110.53
30	M	102	LMT	C1'-O5'-C5'	-2.62	108.60	113.72
22	b	607	CLA	CHB-C4A-NA	2.62	128.18	124.40
22	B	615	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	b	610	CLA	C3B-C4B-NB	-2.62	108.19	110.53
25	C	517	DGD	C1D-O6D-C5D	-2.62	108.61	113.72
24	c	514	BCR	C15-C16-C17	-2.61	118.17	123.52
25	c	517	DGD	C1D-O6D-C5D	-2.61	108.62	113.72
24	B	618	BCR	C15-C16-C17	-2.61	118.17	123.52
27	a	402	LMG	O6-C1-O1	-2.61	103.88	110.04
24	B	618	BCR	C15-C14-C13	-2.61	123.62	127.28
23	D	407	PL9	C7-C8-C9	-2.61	122.34	126.83
24	c	514	BCR	C28-C27-C26	-2.61	109.41	114.06
24	g	101	BCR	C33-C5-C6	-2.61	121.64	124.48
22	B	604	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	b	608	CLA	CHB-C4A-NA	2.60	128.15	124.40
30	B	623	LMT	C1'-O5'-C5'	-2.59	108.65	113.72
24	A	407	BCR	C27-C26-C25	2.59	126.21	122.70
22	C	510	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	C	506	CLA	CHB-C4A-NA	2.59	128.14	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	407	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	C	505	CLA	CHB-C4A-NA	2.59	128.13	124.40
24	J	102	BCR	C38-C26-C25	-2.59	121.66	124.48
22	b	615	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
24	b	620	BCR	C2-C1-C6	2.58	114.19	110.44
29	d	403	SQD	O8-S-C6	2.58	110.96	105.97
22	C	510	CLA	C3B-C4B-NB	-2.58	108.22	110.53
22	C	520	CLA	CHB-C4A-NA	2.58	128.13	124.40
22	b	614	CLA	C1-C2-C3	-2.58	121.97	126.20
22	c	506	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	C	514	BCR	C11-C10-C9	-2.58	123.66	127.28
24	C	514	BCR	C28-C27-C26	-2.58	109.46	114.06
31	D	401	PHO	CMB-C2B-C3B	2.58	129.83	124.68
24	B	619	BCR	C7-C8-C9	-2.58	122.42	126.23
22	C	504	CLA	CHB-C4A-NA	2.57	128.12	124.40
22	b	609	CLA	CHB-C4A-NA	2.57	128.12	124.40
22	H	101	CLA	C3B-C4B-NB	-2.57	108.23	110.53
24	a	409	BCR	C27-C26-C25	2.57	126.18	122.70
24	b	623	BCR	C27-C26-C25	2.57	126.18	122.70
22	c	501	CLA	C3B-C4B-NB	-2.57	108.24	110.53
22	C	501	CLA	C3B-C4B-NB	-2.57	108.24	110.53
23	a	408	PL9	C7-C8-C9	-2.57	122.41	126.83
24	B	619	BCR	C27-C26-C25	2.57	126.17	122.70
22	c	505	CLA	C3B-C4B-NB	-2.57	108.24	110.53
24	b	621	BCR	C29-C30-C25	2.56	114.16	110.44
24	B	617	BCR	C29-C30-C25	2.56	114.15	110.44
24	c	521	BCR	C15-C14-C13	-2.56	123.69	127.28
22	C	504	CLA	C3B-C4B-NB	-2.56	108.25	110.53
24	B	617	BCR	C15-C14-C13	-2.55	123.70	127.28
24	b	622	BCR	C11-C10-C9	-2.55	123.70	127.28
22	B	610	CLA	C1-C2-C3	-2.55	122.01	126.20
22	h	101	CLA	C3B-C4B-NB	-2.55	108.25	110.53
24	C	514	BCR	C15-C14-C13	-2.55	123.70	127.28
22	c	504	CLA	C3B-C4B-NB	-2.55	108.25	110.53
24	b	622	BCR	C15-C16-C17	-2.55	118.31	123.52
29	B	626	SQD	C4-C3-C2	2.55	115.30	110.83
30	M	102	LMT	C3'-C4'-C5'	-2.55	105.28	110.93
24	C	513	BCR	C15-C14-C13	-2.55	123.71	127.28
22	c	511	CLA	CHB-C4A-NA	2.55	128.07	124.40
25	D	410	DGD	CFB-CEB-CDB	-2.55	101.50	114.37
24	j	102	BCR	C15-C16-C17	-2.54	118.31	123.52
24	y	101	BCR	C1-C6-C5	-2.54	119.16	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	406	CLA	CHB-C4A-NA	2.54	128.07	124.40
24	b	623	BCR	C7-C8-C9	-2.54	122.47	126.23
22	c	520	CLA	CHB-C4A-NA	2.54	128.07	124.40
27	M	101	LMG	C1-C2-C3	-2.54	104.67	110.01
24	j	102	BCR	C38-C26-C25	-2.54	121.72	124.48
24	y	101	BCR	C33-C5-C6	-2.54	121.72	124.48
27	A	414	LMG	O6-C1-O1	-2.54	104.05	110.04
34	F	101	HEM	C1B-NB-C4B	2.54	108.21	105.21
22	B	608	CLA	C1-C2-C3	-2.53	122.05	126.20
22	C	507	CLA	C3B-C4B-NB	-2.53	108.27	110.53
22	B	605	CLA	CHB-C4A-NA	2.53	128.06	124.40
22	C	508	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
22	b	605	CLA	C3B-C4B-NB	-2.53	108.27	110.53
24	c	513	BCR	C15-C16-C17	-2.53	118.34	123.52
22	C	512	CLA	CHB-C4A-NA	2.53	128.04	124.40
22	c	508	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	c	505	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	C	501	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	B	608	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	C	511	CLA	CHB-C4A-NA	2.52	128.03	124.40
30	M	103	LMT	C3'-C4'-C5'	-2.52	105.35	110.93
22	C	505	CLA	C3B-C4B-NB	-2.51	108.28	110.53
30	b	626	LMT	C1'-O5'-C5'	-2.51	108.82	113.72
24	C	514	BCR	C33-C5-C6	-2.51	121.74	124.48
24	K	102	BCR	C24-C23-C22	-2.51	122.52	126.23
22	B	610	CLA	C3B-C4B-NB	-2.51	108.29	110.53
22	B	611	CLA	CHB-C4A-NA	2.51	128.02	124.40
22	b	615	CLA	CHB-C4A-NA	2.51	128.02	124.40
22	B	611	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
22	b	618	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	d	410	DGD	CFB-CEB-CDB	-2.50	101.72	114.37
22	c	504	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	M	103	LMT	C1'-O5'-C5'	-2.50	108.84	113.72
29	d	403	SQD	C44-O6-C1	2.50	119.15	113.80
22	a	407	CLA	CHB-C4A-NA	2.50	128.00	124.40
34	f	101	HEM	C1B-NB-C4B	2.50	108.16	105.21
29	A	412	SQD	O48-C23-C24	2.50	119.44	111.83
23	a	408	PL9	C41-C39-C40	2.49	120.33	114.59
27	d	412	LMG	C38-C37-C36	-2.49	101.77	114.37
22	B	604	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	c	514	BCR	C33-C5-C6	-2.49	121.77	124.48
22	c	510	CLA	CHB-C4A-NA	2.49	127.99	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	405	CLA	C3B-C4B-NB	-2.49	108.31	110.53
25	d	410	DGD	C3G-C2G-C1G	-2.49	105.99	111.78
24	B	616	BCR	C2-C1-C6	2.49	114.05	110.44
27	d	409	LMG	C38-C37-C36	-2.49	101.81	114.37
25	C	517	DGD	O5D-C6D-C5D	-2.48	103.82	109.42
27	D	412	LMG	C38-C37-C36	-2.48	101.83	114.37
25	a	410	DGD	CBB-CAB-C9B	-2.48	101.83	114.37
22	c	501	CLA	CHB-C4A-NA	2.48	127.98	124.40
27	B	621	LMG	C1-C2-C3	-2.48	104.79	110.01
23	D	407	PL9	C27-C28-C29	-2.48	121.95	127.62
25	c	517	DGD	O5D-C6D-C5D	-2.48	103.83	109.42
22	A	404	CLA	CHB-C4A-NA	2.48	127.97	124.40
27	A	410	LMG	C40-C39-C38	-2.47	101.86	114.37
24	j	102	BCR	C29-C30-C25	2.47	114.03	110.44
22	c	512	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	B	606	CLA	C3B-C4B-NB	-2.47	108.32	110.53
22	B	614	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	B	609	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	B	612	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	c	503	CLA	CHB-C4A-NA	2.47	127.97	124.40
29	B	622	SQD	O8-S-C6	2.47	110.74	105.97
24	c	513	BCR	C15-C14-C13	-2.47	123.82	127.28
25	A	408	DGD	CBB-CAB-C9B	-2.47	101.89	114.37
23	A	406	PL9	C7-C8-C9	-2.47	122.58	126.83
22	B	606	CLA	CHB-C4A-NA	2.46	127.96	124.40
22	C	508	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	b	614	CLA	C3B-C4B-NB	-2.46	108.33	110.53
22	b	610	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	g	101	BCR	C1-C6-C5	-2.46	119.27	122.64
29	f	103	SQD	C44-O6-C1	2.46	119.07	113.80
30	D	411	LMT	C1'-O5'-C5'	-2.46	108.92	113.72
22	B	607	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	B	622	SQD	O48-C23-C24	2.46	119.33	111.83
22	b	616	CLA	CHB-C4A-NA	2.46	127.95	124.40
31	d	401	PHO	CMB-C2B-C3B	2.46	129.59	124.68
24	b	623	BCR	C11-C10-C9	-2.45	123.84	127.28
24	b	622	BCR	C15-C14-C13	-2.45	123.84	127.28
26	c	519	LHG	C11-C10-C9	-2.45	101.99	114.37
22	d	406	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	K	102	BCR	C15-C14-C13	-2.45	123.84	127.28
29	a	401	SQD	O48-C23-C24	2.45	119.30	111.83
22	a	404	CLA	CHB-C4A-NA	2.45	127.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	DGD	O6E-C1E-O5D	-2.45	104.27	110.04
24	c	513	BCR	C7-C8-C9	-2.44	122.62	126.23
22	B	610	CLA	CHB-C1B-NB	2.44	127.71	124.05
22	B	601	CLA	C3B-C4B-NB	-2.44	108.35	110.53
23	a	408	PL9	C27-C28-C29	-2.44	122.05	127.62
25	C	516	DGD	O6E-C1E-O5D	-2.44	104.29	110.04
24	J	102	BCR	C35-C13-C14	-2.44	118.87	122.82
22	C	507	CLA	C1-C2-C3	-2.43	122.21	126.20
24	b	620	BCR	C11-C10-C9	-2.43	123.86	127.28
24	B	616	BCR	C27-C26-C25	2.43	125.99	122.70
23	A	406	PL9	C27-C28-C29	-2.43	122.06	127.62
22	C	511	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
30	d	411	LMT	C3'-C4'-C5'	-2.43	105.54	110.93
24	J	102	BCR	C29-C30-C25	2.43	113.97	110.44
27	D	409	LMG	C38-C37-C36	-2.43	102.10	114.37
27	d	408	LMG	C38-C37-C36	-2.43	102.10	114.37
25	B	620	DGD	CBB-CAB-C9B	-2.43	102.10	114.37
27	E	101	LMG	O6-C1-O1	-2.43	104.31	110.04
22	c	502	CLA	CHB-C4A-NA	2.43	127.90	124.40
23	d	407	PL9	C27-C28-C29	-2.43	122.07	127.62
22	A	402	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	D	406	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	b	614	CLA	CHB-C1B-NB	2.42	127.68	124.05
22	d	405	CLA	C3B-C4B-NB	-2.42	108.37	110.53
22	b	617	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	C	503	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	b	624	DGD	CBB-CAB-C9B	-2.42	102.13	114.37
22	B	613	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	A	405	CLA	CHB-C4A-NA	2.42	127.89	124.40
26	C	519	LHG	C11-C10-C9	-2.42	102.14	114.37
23	a	408	PL9	C20-C19-C21	2.42	119.42	115.23
27	c	522	LMG	O6-C1-O1	-2.42	104.33	110.04
27	a	412	LMG	C40-C39-C38	-2.42	102.15	114.37
29	B	622	SQD	C44-O6-C1	2.42	118.98	113.80
22	B	603	CLA	O1D-CGD-CBD	2.41	129.28	124.52
23	j	101	PL9	O2-C1-C6	2.41	124.32	120.48
23	A	406	PL9	C41-C39-C40	2.41	120.14	114.59
24	b	620	BCR	C27-C26-C25	2.41	125.96	122.70
24	B	616	BCR	C11-C10-C9	-2.41	123.90	127.28
27	C	521	LMG	C40-C39-C38	-2.41	102.19	114.37
25	C	517	DGD	CFB-CEB-CDB	-2.41	102.19	114.37
22	h	101	CLA	CHB-C4A-NA	2.41	127.88	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	PL9	O2-C1-C6	2.41	124.31	120.48
29	a	415	SQD	O48-C23-C24	2.41	119.17	111.83
25	c	517	DGD	CFB-CEB-CDB	-2.40	102.21	114.37
22	b	611	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	B	612	CLA	C3B-C4B-NB	-2.40	108.39	110.53
22	B	602	CLA	CHB-C4A-NA	2.40	127.87	124.40
27	B	621	LMG	O6-C1-O1	-2.40	104.37	110.04
24	c	513	BCR	C27-C26-C25	2.40	125.95	122.70
24	C	513	BCR	C27-C26-C25	2.40	125.94	122.70
30	b	603	LMT	C1'-O5'-C5'	-2.40	109.04	113.72
24	c	514	BCR	C15-C14-C13	-2.40	123.92	127.28
22	c	507	CLA	CHB-C4A-NA	2.40	127.86	124.40
27	c	522	LMG	C40-C39-C38	-2.39	102.28	114.37
23	J	101	PL9	O2-C1-C6	2.39	124.28	120.48
22	H	101	CLA	CHB-C4A-NA	2.39	127.84	124.40
25	c	515	DGD	C3G-C2G-C1G	-2.39	106.22	111.78
23	D	407	PL9	C37-C38-C39	-2.38	122.17	127.62
25	c	516	DGD	CFB-CEB-CDB	-2.38	102.31	114.37
25	c	516	DGD	C3G-C2G-C1G	-2.38	106.23	111.78
27	D	408	LMG	C38-C37-C36	-2.38	102.34	114.37
22	C	502	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	b	612	CLA	CHB-C4A-NA	2.38	127.83	124.40
23	D	407	PL9	C20-C19-C21	2.38	119.36	115.23
22	c	509	CLA	CHB-C4A-NA	2.38	127.83	124.40
23	d	407	PL9	O2-C1-C6	2.37	124.26	120.48
25	C	515	DGD	C3G-C2G-C1G	-2.37	106.25	111.78
27	E	101	LMG	C1-C2-C3	-2.37	105.02	110.01
23	A	406	PL9	O2-C1-C6	2.37	124.25	120.48
24	a	409	BCR	C15-C16-C17	-2.37	118.66	123.52
23	J	101	PL9	C20-C19-C21	2.37	119.35	115.23
27	C	521	LMG	O6-C1-O1	-2.37	104.44	110.04
30	B	627	LMT	C1'-O5'-C5'	-2.37	109.09	113.72
22	b	606	CLA	CHB-C4A-NA	2.37	127.82	124.40
27	e	101	LMG	O6-C1-O1	-2.37	104.45	110.04
27	D	409	LMG	O6-C1-C2	-2.37	105.50	110.37
29	d	403	SQD	O48-C23-C24	2.37	119.05	111.83
27	b	625	LMG	C1-C2-C3	-2.37	105.03	110.01
25	C	516	DGD	C3G-C2G-C1G	-2.36	106.27	111.78
27	A	410	LMG	C38-C37-C36	-2.36	102.42	114.37
30	D	411	LMT	C3'-C4'-C5'	-2.36	105.69	110.93
24	f	102	BCR	C27-C26-C25	2.36	125.90	122.70
22	C	509	CLA	CHB-C4A-NA	2.36	127.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	407	PL9	C37-C38-C39	-2.36	122.22	127.62
24	c	513	BCR	C24-C23-C22	-2.36	122.74	126.23
22	C	507	CLA	CHB-C4A-NA	2.36	127.81	124.40
29	a	415	SQD	C4-C3-C2	2.36	114.97	110.83
23	d	407	PL9	C20-C19-C21	2.36	119.32	115.23
22	b	613	CLA	CHB-C4A-NA	2.36	127.80	124.40
24	B	619	BCR	C11-C10-C9	-2.35	123.98	127.28
24	F	102	BCR	C27-C26-C25	2.35	125.88	122.70
27	C	518	LMG	C38-C37-C36	-2.35	102.49	114.37
25	A	408	DGD	O5D-C6D-C5D	-2.35	104.12	109.42
29	B	626	SQD	O48-C23-C24	2.35	119.00	111.83
25	D	410	DGD	C3G-C2G-C1G	-2.35	106.31	111.78
22	A	405	CLA	C3B-C4B-NB	-2.35	108.44	110.53
24	j	102	BCR	C35-C13-C14	-2.34	119.02	122.82
30	i	102	LMT	C1'-O5'-C5'	-2.34	109.14	113.72
24	F	102	BCR	C11-C10-C9	-2.34	123.99	127.28
22	c	511	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
29	A	413	SQD	O48-C23-C24	2.34	118.96	111.83
22	B	615	CLA	CHB-C4A-NA	2.34	127.77	124.40
22	B	606	CLA	C1-C2-C3	-2.34	122.37	126.20
24	J	102	BCR	C15-C16-C17	-2.33	118.74	123.52
22	c	507	CLA	C1-C2-C3	-2.33	122.37	126.20
27	B	621	LMG	C40-C39-C38	-2.33	102.58	114.37
27	c	518	LMG	C38-C37-C36	-2.33	102.58	114.37
25	C	516	DGD	CFB-CEB-CDB	-2.33	102.58	114.37
24	x	101	BCR	C29-C30-C25	2.33	113.83	110.44
24	C	513	BCR	C11-C10-C9	-2.33	124.01	127.28
27	d	412	LMG	O6-C1-O1	-2.33	104.55	110.04
24	K	102	BCR	C11-C10-C9	-2.33	124.02	127.28
23	D	407	PL9	C32-C33-C34	-2.33	122.30	127.62
24	J	102	BCR	C20-C21-C22	-2.32	124.02	127.28
22	C	502	CLA	C1-C2-C3	-2.32	122.39	126.20
27	b	625	LMG	O6-C1-O1	-2.32	104.56	110.04
29	a	401	SQD	C1-O5-C5	2.32	118.25	113.72
27	A	410	LMG	O3-C3-C2	-2.32	104.91	110.38
22	D	406	CLA	C1-C2-C3	-2.32	122.40	126.20
24	j	102	BCR	C20-C21-C22	-2.32	124.03	127.28
25	b	601	DGD	O6D-C1D-O3G	-2.31	104.58	110.04
27	a	412	LMG	C38-C37-C36	-2.31	102.68	114.37
24	A	407	BCR	C15-C16-C17	-2.31	118.79	123.52
27	b	625	LMG	C40-C39-C38	-2.31	102.70	114.37
29	a	401	SQD	O8-S-C6	2.31	110.43	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	BCR	C15-C16-C17	-2.31	118.80	123.52
23	D	407	PL9	O2-C1-C6	2.31	124.15	120.48
29	B	626	SQD	O8-S-C6	2.30	110.42	105.97
30	d	411	LMT	C1'-O5'-C5'	-2.30	109.22	113.72
24	f	102	BCR	C11-C10-C9	-2.30	124.05	127.28
22	b	607	CLA	O1D-CGD-CBD	2.30	129.06	124.52
22	b	619	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	e	101	LMG	C1-C2-C3	-2.29	105.19	110.01
24	C	513	BCR	C3-C4-C5	-2.29	109.97	114.06
24	B	616	BCR	C15-C14-C13	-2.29	124.07	127.28
22	b	616	CLA	C3B-C4B-NB	-2.29	108.49	110.53
29	b	602	SQD	O48-C23-C24	2.28	118.80	111.83
24	b	620	BCR	C15-C14-C13	-2.28	124.07	127.28
27	C	521	LMG	C38-C37-C36	-2.28	102.82	114.37
24	F	102	BCR	C15-C16-C17	-2.28	118.85	123.52
24	c	521	BCR	C11-C10-C9	-2.28	124.08	127.28
22	b	605	CLA	CHB-C4A-NA	2.28	127.69	124.40
23	d	407	PL9	O1-C4-C3	-2.28	118.33	120.73
25	d	410	DGD	C3D-C4D-C5D	-2.28	106.10	110.23
27	D	412	LMG	O6-C1-O1	-2.28	104.66	110.04
23	j	101	PL9	C20-C19-C21	2.27	119.17	115.23
24	a	409	BCR	C33-C5-C6	-2.27	122.01	124.48
22	c	507	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
27	b	625	LMG	C38-C37-C36	-2.27	102.91	114.37
22	B	601	CLA	CHB-C4A-NA	2.26	127.67	124.40
27	a	412	LMG	O3-C3-C2	-2.26	105.05	110.38
29	F	103	SQD	C44-O6-C1	2.26	118.64	113.80
27	m	101	LMG	O2-C2-C1	-2.26	104.70	110.08
29	F	103	SQD	O48-C23-C24	2.26	118.71	111.83
24	B	617	BCR	C11-C10-C9	-2.25	124.12	127.28
24	H	102	BCR	C29-C30-C25	2.25	113.71	110.44
29	A	412	SQD	C4-C3-C2	2.25	114.78	110.83
24	b	622	BCR	C27-C26-C25	2.25	125.75	122.70
24	c	513	BCR	C3-C4-C5	-2.25	110.04	114.06
24	K	102	BCR	C33-C5-C6	-2.25	122.03	124.48
27	A	410	LMG	C1-C2-C3	-2.25	105.28	110.01
24	A	407	BCR	C15-C14-C13	-2.25	124.12	127.28
30	I	102	LMT	C1'-O5'-C5'	-2.25	109.33	113.72
29	A	413	SQD	O8-S-C6	2.25	110.31	105.97
23	D	407	PL9	O1-C4-C3	-2.25	118.36	120.73
27	c	518	LMG	O7-C10-O9	-2.25	118.45	123.70
25	A	408	DGD	C3G-C2G-C1G	-2.25	106.55	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	407	PL9	C32-C33-C34	-2.25	122.48	127.62
24	f	102	BCR	C15-C16-C17	-2.24	118.93	123.52
27	c	522	LMG	C38-C37-C36	-2.24	103.04	114.37
25	B	620	DGD	C1D-C2D-C3D	-2.24	105.30	110.01
22	b	610	CLA	C1-C2-C3	-2.24	122.53	126.20
27	D	412	LMG	O3-C3-C2	-2.24	105.11	110.38
22	b	612	CLA	C1-C2-C3	-2.23	122.54	126.20
24	a	409	BCR	C15-C14-C13	-2.23	124.14	127.28
27	I	101	LMG	O7-C10-O9	-2.23	118.48	123.70
27	B	621	LMG	C38-C37-C36	-2.23	103.08	114.37
29	b	602	SQD	O8-S-C6	2.23	110.28	105.97
24	A	407	BCR	C33-C5-C6	-2.23	122.05	124.48
24	c	521	BCR	C24-C23-C22	-2.23	122.94	126.23
22	c	506	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
25	a	410	DGD	C3G-C2G-C1G	-2.23	106.59	111.78
24	b	622	BCR	C7-C8-C9	-2.23	122.94	126.23
27	m	101	LMG	C1-C2-C3	-2.22	105.33	110.01
22	b	605	CLA	C1-C2-C3	-2.22	122.56	126.20
25	a	410	DGD	O5D-C6D-C5D	-2.22	104.41	109.42
27	D	408	LMG	O2-C2-C1	-2.22	104.79	110.08
24	H	102	BCR	C16-C15-C14	-2.22	118.98	123.52
22	b	618	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
25	B	625	DGD	O6D-C1D-O3G	-2.21	104.81	110.04
24	g	101	BCR	C15-C16-C17	-2.21	118.99	123.52
27	D	412	LMG	C1-C2-C3	-2.21	105.36	110.01
27	d	409	LMG	O6-C1-O1	-2.21	104.82	110.04
25	b	624	DGD	C1D-C2D-C3D	-2.21	105.36	110.01
27	C	521	LMG	O2-C2-C1	-2.21	104.81	110.08
25	B	620	DGD	C3G-C2G-C1G	-2.21	106.64	111.78
27	C	518	LMG	O7-C10-O9	-2.21	118.55	123.70
27	D	409	LMG	O6-C1-O1	-2.21	104.83	110.04
24	b	623	BCR	C24-C23-C22	-2.21	122.97	126.23
25	a	410	DGD	CAB-C9B-C8B	-2.20	103.22	114.37
24	b	621	BCR	C7-C8-C9	-2.20	122.97	126.23
23	A	406	PL9	C20-C19-C21	2.20	119.05	115.23
22	B	605	CLA	O1D-CGD-CBD	2.20	128.86	124.52
22	H	101	CLA	C1-C2-C3	-2.20	122.59	126.20
22	c	502	CLA	C1-C2-C3	-2.20	122.59	126.20
27	i	101	LMG	O2-C2-C1	-2.20	104.83	110.08
24	C	513	BCR	C7-C8-C9	-2.20	122.99	126.23
27	A	410	LMG	O7-C10-O9	-2.19	118.57	123.70
27	a	412	LMG	O7-C10-O9	-2.19	118.58	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	DGD	CBB-CAB-C9B	-2.19	103.28	114.37
26	a	411	LHG	C27-C26-C25	-2.19	103.29	114.37
30	B	624	LMT	C1'-O5'-C5'	-2.19	109.44	113.72
25	C	516	DGD	O3D-C3D-C4D	-2.19	105.21	110.38
22	d	405	CLA	O1D-CGD-CBD	2.19	128.84	124.52
27	m	101	LMG	C1-O6-C5	-2.19	109.44	113.72
25	c	516	DGD	O3D-C3D-C4D	-2.19	105.21	110.38
24	F	102	BCR	C7-C8-C9	-2.19	123.00	126.23
34	v	201	HEM	C2A-C1A-NA	-2.19	107.72	110.15
22	c	507	CLA	O2D-CGD-CBD	2.19	115.05	111.23
27	I	101	LMG	O2-C2-C1	-2.19	104.87	110.08
22	B	601	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
25	A	408	DGD	CAB-C9B-C8B	-2.18	103.33	114.37
22	B	603	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
25	C	516	DGD	CBB-CAB-C9B	-2.18	103.33	114.37
24	b	621	BCR	C11-C10-C9	-2.18	124.22	127.28
22	B	611	CLA	C1-C2-C3	-2.18	122.62	126.20
24	c	521	BCR	C33-C5-C6	-2.18	122.11	124.48
27	d	412	LMG	C1-C2-C3	-2.18	105.42	110.01
25	C	517	DGD	CBB-CAB-C9B	-2.18	103.35	114.37
23	d	407	PL9	O2-C1-C2	-2.18	116.87	121.83
27	d	408	LMG	O3-C3-C2	-2.18	105.25	110.38
27	d	408	LMG	O2-C2-C1	-2.17	104.89	110.08
27	A	414	LMG	O7-C10-O9	-2.17	118.62	123.70
24	B	617	BCR	C7-C8-C9	-2.17	123.02	126.23
23	j	101	PL9	O2-C1-C2	-2.17	116.89	121.83
24	b	623	BCR	C38-C26-C25	-2.17	122.11	124.48
25	b	601	DGD	CBB-CAB-C9B	-2.17	103.39	114.37
22	C	507	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
24	y	101	BCR	C15-C16-C17	-2.17	119.08	123.52
27	a	412	LMG	C1-C2-C3	-2.17	105.44	110.01
24	C	514	BCR	C38-C26-C25	-2.17	122.11	124.48
24	B	618	BCR	C7-C8-C9	-2.17	123.02	126.23
25	b	624	DGD	C3G-C2G-C1G	-2.17	106.73	111.78
27	i	101	LMG	O1-C7-C8	-2.17	105.55	110.82
25	C	515	DGD	C1D-C2D-C3D	-2.17	105.45	110.01
25	a	410	DGD	C1D-C2D-C3D	-2.17	105.45	110.01
24	C	514	BCR	C24-C23-C22	-2.17	123.03	126.23
29	F	103	SQD	C3-C4-C5	2.16	114.15	110.23
29	f	103	SQD	C3-C4-C5	2.16	114.15	110.23
25	C	516	DGD	CAB-C9B-C8B	-2.16	103.45	114.37
29	B	622	SQD	C4-C3-C2	2.16	114.62	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C38-C26-C25	-2.16	122.13	124.48
25	C	516	DGD	C3D-C4D-C5D	-2.16	106.32	110.23
33	D	404	BCT	O3-C-O1	-2.16	114.16	119.68
27	d	409	LMG	O6-C1-C2	-2.16	105.94	110.37
24	b	623	BCR	C33-C5-C6	-2.16	122.13	124.48
24	B	619	BCR	C24-C23-C22	-2.16	123.05	126.23
22	c	509	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
22	b	616	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
27	D	408	LMG	O3-C3-C2	-2.15	105.31	110.38
23	J	101	PL9	O2-C1-C2	-2.15	116.94	121.83
25	D	410	DGD	C3D-C4D-C5D	-2.15	106.33	110.23
24	g	101	BCR	C3-C2-C1	-2.15	106.82	114.43
22	D	405	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	B	602	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
29	a	415	SQD	O8-S-C6	2.15	110.12	105.97
24	c	514	BCR	C24-C23-C22	-2.15	123.06	126.23
25	B	625	DGD	CBB-CAB-C9B	-2.15	103.51	114.37
27	a	402	LMG	O3-C3-C2	-2.15	105.31	110.38
27	b	625	LMG	O3-C3-C2	-2.15	105.31	110.38
22	b	607	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
27	B	621	LMG	O3-C3-C2	-2.15	105.32	110.38
27	i	101	LMG	O7-C10-O9	-2.15	118.69	123.70
25	c	517	DGD	CBB-CAB-C9B	-2.15	103.52	114.37
27	I	101	LMG	O3-C3-C2	-2.14	105.32	110.38
30	b	627	LMT	C1'-O5'-C5'	-2.14	109.53	113.72
33	d	404	BCT	O3-C-O1	-2.14	114.19	119.68
24	B	618	BCR	C27-C26-C25	2.14	125.60	122.70
29	f	103	SQD	O48-C23-C24	2.14	118.37	111.83
26	A	409	LHG	C27-C26-C25	-2.14	103.54	114.37
22	c	504	CLA	O1D-CGD-CBD	2.14	128.74	124.52
29	d	403	SQD	C4-C3-C2	2.14	114.59	110.83
22	b	615	CLA	C1-C2-C3	-2.14	122.69	126.20
27	c	522	LMG	O2-C2-C1	-2.14	104.98	110.08
22	b	615	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
23	a	408	PL9	O1-C4-C3	-2.14	118.48	120.73
27	d	412	LMG	O3-C3-C2	-2.14	105.34	110.38
31	d	401	PHO	C1-C2-C3	-2.14	122.70	126.20
25	b	601	DGD	CAB-C9B-C8B	-2.13	103.58	114.37
25	B	620	DGD	C4E-C3E-C2E	-2.13	107.08	110.83
22	B	612	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
22	C	506	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
23	D	407	PL9	O2-C1-C2	-2.13	116.99	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	611	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
24	H	102	BCR	C27-C26-C25	2.13	125.58	122.70
23	A	406	PL9	O2-C1-C2	-2.12	117.00	121.83
22	c	510	CLA	C1-C2-C3	-2.12	122.72	126.20
23	a	408	PL9	O2-C1-C2	-2.12	117.00	121.83
25	d	410	DGD	C5B-C4B-C3B	-2.12	103.64	114.37
22	B	612	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
22	C	501	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
27	b	625	LMG	O2-C2-C1	-2.12	105.03	110.08
25	c	517	DGD	CAB-C9B-C8B	-2.12	103.66	114.37
34	V	201	HEM	C3B-C2B-C1B	2.12	108.00	106.41
22	b	609	CLA	O1D-CGD-CBD	2.12	128.69	124.52
22	c	503	CLA	O2D-CGD-CBD	2.12	114.93	111.23
24	b	622	BCR	C33-C5-C6	-2.12	122.17	124.48
27	D	412	LMG	O7-C10-O9	-2.12	118.76	123.70
25	B	625	DGD	CAB-C9B-C8B	-2.11	103.68	114.37
29	A	412	SQD	O8-S-C6	2.11	110.06	105.97
24	a	409	BCR	C24-C23-C22	-2.11	123.11	126.23
22	b	616	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
25	c	515	DGD	C1D-C2D-C3D	-2.11	105.57	110.01
22	d	405	CLA	CHB-C4A-NA	2.11	127.44	124.40
24	B	619	BCR	C33-C5-C6	-2.11	122.18	124.48
27	M	101	LMG	O2-C2-C1	-2.11	105.05	110.08
24	c	514	BCR	C38-C26-C25	-2.11	122.19	124.48
27	a	402	LMG	O1-C7-C8	-2.11	105.69	110.82
27	c	522	LMG	O3-C3-C2	-2.11	105.41	110.38
22	B	606	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
22	B	614	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
22	b	610	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
26	C	519	LHG	C27-C26-C25	-2.10	103.73	114.37
34	v	201	HEM	C1B-NB-C4B	2.10	107.70	105.21
22	c	508	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
22	b	616	CLA	C1-C2-C3	-2.10	122.75	126.20
23	D	407	PL9	C12-C13-C14	-2.10	122.81	127.62
27	C	521	LMG	O3-C3-C2	-2.10	105.42	110.38
27	i	101	LMG	O3-C3-C2	-2.10	105.42	110.38
25	D	410	DGD	C5B-C4B-C3B	-2.10	103.75	114.37
27	d	412	LMG	O7-C10-O9	-2.10	118.80	123.70
22	C	520	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
22	c	520	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
24	y	101	BCR	C3-C2-C1	-2.10	107.01	114.43
27	i	101	LMG	O1-C1-C2	-2.10	105.09	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	h	101	CLA	C1-C2-C3	-2.09	122.77	126.20
22	C	508	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	C	517	DGD	CAB-C9B-C8B	-2.09	103.80	114.37
27	B	621	LMG	O7-C10-O9	-2.09	118.81	123.70
24	C	514	BCR	C7-C8-C9	-2.09	123.14	126.23
27	e	101	LMG	O3-C3-C2	-2.09	105.45	110.38
22	C	512	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	B	601	CLA	C1-C2-C3	-2.09	122.77	126.20
25	c	516	DGD	CAB-C9B-C8B	-2.09	103.81	114.37
22	D	405	CLA	CHB-C4A-NA	2.09	127.41	124.40
27	A	414	LMG	O3-C3-C2	-2.09	105.45	110.38
22	a	405	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
24	K	102	BCR	C7-C8-C9	-2.09	123.15	126.23
22	C	504	CLA	O1D-CGD-CBD	2.09	128.63	124.52
22	c	501	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
27	c	518	LMG	O3-C3-C2	-2.08	105.46	110.38
25	A	408	DGD	CDB-CCB-CBB	-2.08	99.30	113.36
26	c	519	LHG	C27-C26-C25	-2.08	103.84	114.37
25	C	515	DGD	C5B-C4B-C3B	-2.08	103.85	114.37
25	a	410	DGD	CDB-CCB-CBB	-2.08	99.32	113.36
22	b	606	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	c	515	DGD	C5B-C4B-C3B	-2.08	103.87	114.37
24	A	407	BCR	C38-C26-C25	-2.08	122.22	124.48
27	b	625	LMG	O7-C10-O9	-2.08	118.85	123.70
22	B	612	CLA	C1-C2-C3	-2.08	122.80	126.20
27	C	518	LMG	O2-C2-C1	-2.08	105.13	110.08
27	e	101	LMG	O1-C7-C8	-2.08	105.77	110.82
27	c	518	LMG	O2-C2-C1	-2.07	105.13	110.08
24	b	621	BCR	C24-C23-C22	-2.07	123.17	126.23
22	a	404	CLA	C1-C2-C3	-2.07	122.81	126.20
24	x	101	BCR	C27-C26-C25	2.07	125.50	122.70
22	c	512	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
25	A	408	DGD	C1D-C2D-C3D	-2.06	105.67	110.01
22	C	510	CLA	C1-C2-C3	-2.06	122.82	126.20
24	b	620	BCR	C15-C16-C17	-2.06	119.30	123.52
22	B	609	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
24	H	102	BCR	C7-C8-C9	-2.06	123.19	126.23
27	M	101	LMG	C1-O6-C5	-2.06	109.70	113.72
24	a	409	BCR	C38-C26-C25	-2.06	122.24	124.48
22	d	405	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
25	D	410	DGD	CAB-C9B-C8B	-2.06	103.96	114.37
23	A	406	PL9	O1-C4-C3	-2.06	118.56	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	518	LMG	O3-C3-C2	-2.06	105.53	110.38
22	a	406	CLA	C1-C2-C3	-2.06	122.83	126.20
24	x	101	BCR	C16-C15-C14	-2.06	119.31	123.52
25	c	516	DGD	C3D-C4D-C5D	-2.05	106.51	110.23
25	D	410	DGD	CBB-CAB-C9B	-2.05	103.98	114.37
27	a	412	LMG	O2-C2-C1	-2.05	105.18	110.08
24	c	513	BCR	C8-C7-C6	-2.05	121.52	127.00
22	B	607	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
27	E	101	LMG	O1-C7-C8	-2.05	105.83	110.82
27	A	410	LMG	O2-C2-C1	-2.05	105.19	110.08
25	d	410	DGD	CAB-C9B-C8B	-2.05	104.00	114.37
27	d	412	LMG	O2-C2-C1	-2.05	105.19	110.08
24	B	618	BCR	C33-C5-C6	-2.05	122.25	124.48
29	A	413	SQD	C1-O5-C5	2.05	117.72	113.72
34	V	201	HEM	C2A-C1A-NA	-2.05	107.88	110.15
24	B	616	BCR	C7-C8-C9	-2.05	123.21	126.23
24	b	622	BCR	C20-C21-C22	-2.05	124.41	127.28
25	b	624	DGD	CAB-C9B-C8B	-2.05	104.02	114.37
25	d	410	DGD	CBB-CAB-C9B	-2.05	104.03	114.37
27	E	101	LMG	O3-C3-C2	-2.05	105.56	110.38
27	B	621	LMG	O2-C2-C1	-2.04	105.20	110.08
27	a	402	LMG	O2-C2-C1	-2.04	105.21	110.08
31	d	401	PHO	O2A-CGA-O1A	-2.04	118.52	123.63
24	b	623	BCR	C15-C16-C17	-2.04	119.34	123.52
31	D	401	PHO	O2A-CGA-O1A	-2.04	118.52	123.63
24	C	513	BCR	C8-C7-C6	-2.04	121.55	127.00
22	A	403	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
27	M	101	LMG	O3-C3-C2	-2.04	105.57	110.38
27	A	414	LMG	O1-C7-C8	-2.04	105.86	110.82
25	c	517	DGD	C5B-C4B-C3B	-2.04	104.08	114.37
25	C	517	DGD	C5B-C4B-C3B	-2.03	104.08	114.37
25	B	620	DGD	C5B-C4B-C3B	-2.03	104.09	114.37
22	b	613	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	j	101	PL9	C12-C13-C14	-2.03	122.97	127.62
24	f	102	BCR	C7-C8-C9	-2.03	123.23	126.23
27	e	101	LMG	O7-C10-O9	-2.03	118.96	123.70
25	C	516	DGD	C5B-C4B-C3B	-2.03	104.12	114.37
25	c	515	DGD	O5D-C6D-C5D	-2.03	104.85	109.42
24	A	407	BCR	C11-C10-C9	-2.03	124.44	127.28
24	b	622	BCR	C29-C28-C27	2.02	115.73	111.28
25	A	408	DGD	C5B-C4B-C3B	-2.02	104.14	114.37
27	D	408	LMG	O7-C10-O9	-2.02	118.98	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	BCR	C35-C13-C14	-2.02	119.54	122.82
22	C	510	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
22	b	605	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
22	c	505	CLA	C1-C2-C3	-2.02	122.89	126.20
25	a	410	DGD	C5B-C4B-C3B	-2.02	104.15	114.37
22	A	402	CLA	C1-C2-C3	-2.02	122.89	126.20
25	B	620	DGD	CAB-C9B-C8B	-2.02	104.16	114.37
22	B	615	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	g	101	BCR	C24-C23-C22	-2.02	123.25	126.23
22	C	509	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
27	m	101	LMG	O3-C3-C2	-2.02	105.62	110.38
24	c	521	BCR	C7-C8-C9	-2.02	123.25	126.23
23	J	101	PL9	C12-C13-C14	-2.02	123.01	127.62
27	D	412	LMG	O2-C2-C1	-2.01	105.28	110.08
22	a	407	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
24	H	102	BCR	C15-C16-C17	-2.01	119.40	123.52
24	y	101	BCR	C24-C23-C22	-2.01	123.26	126.23
22	A	404	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
34	v	201	HEM	C3B-C2B-C1B	2.01	107.92	106.41
22	a	404	CLA	O1D-CGD-CBD	2.01	128.48	124.52
22	a	404	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
23	j	101	PL9	O1-C4-C3	-2.01	118.61	120.73
27	a	402	LMG	O7-C10-O9	-2.01	119.01	123.70
25	b	624	DGD	C5B-C4B-C3B	-2.01	104.22	114.37
34	V	201	HEM	C1B-NB-C4B	2.01	107.58	105.21
27	A	410	LMG	O1-C1-C2	-2.01	105.23	108.27
27	d	408	LMG	O7-C10-O9	-2.00	119.02	123.70
25	B	620	DGD	CDB-CCB-CBB	-2.00	99.84	113.36
24	c	514	BCR	C7-C8-C9	-2.00	123.27	126.23
22	B	613	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

There are no chirality outliers.

All (2091) 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

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Mol	Chain	Res	Type	Atoms
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	511	CLA	C1A-C2A-CAA-CBA
22	D	405	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	606	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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	617	CLA	CAD-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O2D
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-O1D
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	405	CLA	C2-C3-C5-C6
22	d	405	CLA	C4-C3-C5-C6
22	h	101	CLA	C1A-C2A-CAA-CBA
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-C21
23	A	406	PL9	C22-C23-C24-C25
23	A	406	PL9	C27-C28-C29-C30
23	A	406	PL9	C27-C28-C29-C31
23	A	406	PL9	C37-C38-C39-C40
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	408	PL9	C7-C8-C9-C11

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Mol	Chain	Res	Type	Atoms
23	a	408	PL9	C12-C13-C14-C15
23	a	408	PL9	C12-C13-C14-C16
23	a	408	PL9	C17-C18-C19-C21
23	a	408	PL9	C22-C23-C24-C25
23	a	408	PL9	C27-C28-C29-C30
23	a	408	PL9	C27-C28-C29-C31
23	a	408	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
24	B	617	BCR	C21-C22-C23-C24
24	B	617	BCR	C23-C24-C25-C26
24	C	513	BCR	C6-C7-C8-C9
24	F	102	BCR	C7-C8-C9-C10
24	H	102	BCR	C21-C22-C23-C24
24	J	102	BCR	C21-C22-C23-C24
24	K	102	BCR	C7-C8-C9-C10
24	K	102	BCR	C7-C8-C9-C34
24	y	101	BCR	C7-C8-C9-C10
24	b	621	BCR	C21-C22-C23-C24
24	b	621	BCR	C23-C24-C25-C26
24	c	513	BCR	C6-C7-C8-C9
24	c	521	BCR	C7-C8-C9-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	C21-C22-C23-C24
25	A	408	DGD	C2D-C1D-O3G-C3G
25	B	620	DGD	C2E-C1E-O5D-C6D
25	B	625	DGD	O1B-C1B-O2G-C2G
25	B	625	DGD	O2G-C2G-C3G-O3G
25	B	625	DGD	C2E-C1E-O5D-C6D
25	B	625	DGD	O6E-C1E-O5D-C6D
25	C	515	DGD	C2B-C1B-O2G-C2G
25	C	515	DGD	O1B-C1B-O2G-C2G
25	C	515	DGD	C2E-C1E-O5D-C6D
25	C	516	DGD	C2B-C1B-O2G-C2G
25	C	516	DGD	O1B-C1B-O2G-C2G
25	C	516	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
25	C	517	DGD	C2D-C1D-O3G-C3G
25	C	517	DGD	O6D-C1D-O3G-C3G
25	D	410	DGD	O6D-C1D-O3G-C3G
25	a	410	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	C2D-C1D-O3G-C3G
25	c	517	DGD	O6D-C1D-O3G-C3G
25	d	410	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	411	LHG	C1-C2-C3-O3
26	c	519	LHG	C3-O3-P-O6
26	c	519	LHG	C4-O6-P-O3
26	c	519	LHG	C4-O6-P-O4
27	B	621	LMG	C11-C10-O7-C8
27	C	518	LMG	O9-C10-O7-C8
27	C	518	LMG	C11-C10-O7-C8
27	C	521	LMG	C2-C1-O1-C7
27	D	408	LMG	O1-C7-C8-O7
27	D	408	LMG	C11-C10-O7-C8
27	D	408	LMG	O10-C28-O8-C9
27	D	409	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
27	b	625	LMG	C11-C10-O7-C8
27	c	518	LMG	O9-C10-O7-C8
27	c	518	LMG	C11-C10-O7-C8
27	d	408	LMG	O1-C7-C8-O7
27	d	408	LMG	C11-C10-O7-C8
27	d	409	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
27	d	412	LMG	O9-C10-O7-C8
27	d	412	LMG	C11-C10-O7-C8
27	e	101	LMG	C7-C8-O7-C10
27	m	101	LMG	O9-C10-O7-C8
29	A	412	SQD	C5-C6-S-O7
29	A	412	SQD	C5-C6-S-O8
29	A	412	SQD	C5-C6-S-O9
29	A	413	SQD	C24-C23-O48-C46
29	B	622	SQD	C2-C1-O6-C44
29	B	622	SQD	O5-C1-O6-C44
29	B	622	SQD	O49-C7-O47-C45
29	B	622	SQD	C8-C7-O47-C45
29	B	626	SQD	O5-C5-C6-S
29	a	401	SQD	C24-C23-O48-C46
29	a	415	SQD	C5-C6-S-O7
29	a	415	SQD	C5-C6-S-O8
29	a	415	SQD	C5-C6-S-O9
29	b	602	SQD	O5-C5-C6-S
29	d	403	SQD	C2-C1-O6-C44
29	d	403	SQD	O5-C1-O6-C44
29	d	403	SQD	O49-C7-O47-C45
29	d	403	SQD	C8-C7-O47-C45
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	504	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
30	B	628	LMT	C3'-C4'-O1B-C1B
30	b	604	LMT	C3'-C4'-O1B-C1B
22	A	402	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	a	404	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	520	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	616	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
29	A	413	SQD	O10-C23-O48-C46
29	a	401	SQD	O10-C23-O48-C46
23	a	408	PL9	C37-C38-C39-C40
27	C	518	LMG	C8-C9-O8-C28
22	C	510	CLA	O1D-CGD-O2D-CED
27	a	412	LMG	C29-C28-O8-C9
27	d	409	LMG	C29-C28-O8-C9
29	F	103	SQD	C24-C23-O48-C46
29	f	103	SQD	C24-C23-O48-C46
27	A	410	LMG	O10-C28-O8-C9
27	C	518	LMG	O10-C28-O8-C9
27	D	409	LMG	O10-C28-O8-C9
27	a	412	LMG	O10-C28-O8-C9
27	c	518	LMG	O10-C28-O8-C9
27	d	408	LMG	O10-C28-O8-C9
27	d	409	LMG	O10-C28-O8-C9
27	e	101	LMG	O10-C28-O8-C9
29	F	103	SQD	O10-C23-O48-C46
29	f	103	SQD	O10-C23-O48-C46
22	B	601	CLA	O1D-CGD-O2D-CED
30	B	627	LMT	C3'-C4'-O1B-C1B
30	b	603	LMT	C3'-C4'-O1B-C1B
22	B	604	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
25	D	410	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
25	d	410	DGD	O1B-C1B-O2G-C2G
27	A	414	LMG	O9-C10-O7-C8
27	B	621	LMG	O9-C10-O7-C8
27	D	408	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	d	408	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
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	409	LMG	C29-C28-O8-C9
27	c	518	LMG	C29-C28-O8-C9
27	I	101	LMG	O6-C5-C6-O5
27	i	101	LMG	O6-C5-C6-O5
22	B	605	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
31	D	402	PHO	CBD-CGD-O2D-CED
31	d	402	PHO	CBD-CGD-O2D-CED
25	B	625	DGD	C2B-C1B-O2G-C2G
25	b	601	DGD	C2B-C1B-O2G-C2G
25	c	516	DGD	C2B-C1B-O2G-C2G
27	M	101	LMG	C11-C10-O7-C8
27	m	101	LMG	C11-C10-O7-C8
22	B	612	CLA	O1D-CGD-O2D-CED
22	C	520	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
22	b	616	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	C4-C3-C5-C6
22	B	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
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
22	h	101	CLA	C4-C3-C5-C6
23	A	406	PL9	C30-C29-C31-C32
23	a	408	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
30	I	102	LMT	C3'-C4'-O1B-C1B
30	i	102	LMT	C3'-C4'-O1B-C1B
22	c	505	CLA	O1D-CGD-O2D-CED
25	A	408	DGD	O6E-C5E-C6E-O5E
22	b	610	CLA	C2A-CAA-CBA-CGA
31	d	401	PHO	C3-C5-C6-C7
25	D	410	DGD	C2A-C1A-O1G-C1G
25	d	410	DGD	C2A-C1A-O1G-C1G
27	C	521	LMG	C29-C28-O8-C9
27	D	408	LMG	C29-C28-O8-C9
27	c	522	LMG	C29-C28-O8-C9
27	d	408	LMG	C29-C28-O8-C9
23	A	406	PL9	C17-C18-C19-C20
23	J	101	PL9	C7-C8-C9-C10
23	a	408	PL9	C7-C8-C9-C10
23	a	408	PL9	C17-C18-C19-C20
23	j	101	PL9	C7-C8-C9-C10
25	B	620	DGD	C4D-C5D-C6D-O5D
25	b	624	DGD	C4D-C5D-C6D-O5D
23	A	406	PL9	C22-C23-C24-C26
23	J	101	PL9	C7-C8-C9-C11
23	a	408	PL9	C22-C23-C24-C26
23	j	101	PL9	C7-C8-C9-C11
25	B	620	DGD	O6E-C5E-C6E-O5E
25	a	410	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	O6E-C5E-C6E-O5E
25	D	410	DGD	O1A-C1A-O1G-C1G
25	d	410	DGD	O1A-C1A-O1G-C1G
25	C	516	DGD	C4E-C5E-C6E-O5E
25	c	516	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
23	J	101	PL9	C27-C28-C29-C31
22	C	508	CLA	C3-C5-C6-C7
31	D	401	PHO	C3-C5-C6-C7
22	B	607	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
26	A	409	LHG	O2-C2-C3-O3
26	a	411	LHG	O2-C2-C3-O3
22	C	505	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	CBA-CGA-O2A-C1
27	E	101	LMG	C29-C28-O8-C9
27	e	101	LMG	C29-C28-O8-C9
27	D	408	LMG	O6-C5-C6-O5
27	d	408	LMG	O6-C5-C6-O5
27	C	521	LMG	O10-C28-O8-C9
27	c	522	LMG	O10-C28-O8-C9
22	b	610	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	c	520	CLA	O1D-CGD-O2D-CED
25	b	624	DGD	C4E-C5E-C6E-O5E
27	i	101	LMG	C4-C5-C6-O5
25	D	410	DGD	C2B-C1B-O2G-C2G
27	A	414	LMG	C11-C10-O7-C8
27	D	409	LMG	C11-C10-O7-C8
27	a	402	LMG	C11-C10-O7-C8
27	d	409	LMG	C11-C10-O7-C8
29	F	103	SQD	C8-C7-O47-C45
29	f	103	SQD	C8-C7-O47-C45
22	b	614	CLA	O1D-CGD-O2D-CED
25	C	515	DGD	O6E-C5E-C6E-O5E
27	I	101	LMG	C4-C5-C6-O5
23	j	101	PL9	C27-C28-C29-C31
22	B	613	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	C3-C5-C6-C7
22	b	611	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
25	c	515	DGD	O6E-C5E-C6E-O5E
22	B	608	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	610	CLA	O1D-CGD-O2D-CED
22	C	501	CLA	O1D-CGD-O2D-CED
31	D	401	PHO	C4-C3-C5-C6
31	d	401	PHO	C4-C3-C5-C6
31	D	401	PHO	C2-C3-C5-C6
31	d	401	PHO	C2-C3-C5-C6
27	e	101	LMG	O9-C10-O7-C8
23	A	406	PL9	C24-C26-C27-C28
23	a	408	PL9	C24-C26-C27-C28
25	A	408	DGD	C4E-C5E-C6E-O5E
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	C2A-CAA-CBA-CGA
22	b	617	CLA	O1D-CGD-O2D-CED
25	B	620	DGD	O6E-C1E-O5D-C6D
25	C	516	DGD	O6D-C1D-O3G-C3G
25	b	624	DGD	O6E-C1E-O5D-C6D
25	c	515	DGD	O6E-C1E-O5D-C6D
25	c	516	DGD	O6D-C1D-O3G-C3G
27	C	518	LMG	O6-C1-O1-C7
27	C	521	LMG	O6-C1-O1-C7
27	E	101	LMG	O6-C1-O1-C7
27	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	B	620	DGD	C4E-C5E-C6E-O5E
22	c	512	CLA	CBA-CGA-O2A-C1
31	d	401	PHO	CBA-CGA-O2A-C1
22	B	611	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
25	C	516	DGD	O6E-C5E-C6E-O5E
27	C	518	LMG	O6-C5-C6-O5
22	B	615	CLA	O1A-CGA-O2A-C1
25	c	516	DGD	O6E-C5E-C6E-O5E
27	c	518	LMG	O6-C5-C6-O5
25	d	410	DGD	C2B-C1B-O2G-C2G
27	i	101	LMG	C11-C10-O7-C8
25	a	410	DGD	C4E-C5E-C6E-O5E
27	C	518	LMG	C4-C5-C6-O5
31	d	401	PHO	O1A-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
22	b	619	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	D	401	PHO	CBA-CGA-O2A-C1
22	C	509	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	O1D-CGD-O2D-CED
27	c	522	LMG	O6-C5-C6-O5
25	C	515	DGD	C4E-C5E-C6E-O5E
22	B	604	CLA	C2-C3-C5-C6
22	b	608	CLA	C2-C3-C5-C6
22	h	101	CLA	C3-C5-C6-C7
22	B	607	CLA	C6-C7-C8-C9
22	B	609	CLA	C14-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C9
22	C	510	CLA	C6-C7-C8-C9
22	b	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
27	c	518	LMG	C4-C5-C6-O5
27	c	522	LMG	C4-C5-C6-O5
27	C	518	LMG	C2-C1-O1-C7
27	D	409	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	409	LMG	C2-C1-O1-C7
27	e	101	LMG	C2-C1-O1-C7
29	A	412	SQD	C2-C1-O6-C44
29	a	415	SQD	C2-C1-O6-C44
27	C	518	LMG	C10-C11-C12-C13
31	D	401	PHO	O1A-CGA-O2A-C1
31	d	402	PHO	O1D-CGD-O2D-CED
24	H	102	BCR	C7-C8-C9-C34
24	H	102	BCR	C37-C22-C23-C24
24	y	101	BCR	C7-C8-C9-C34
24	g	101	BCR	C7-C8-C9-C34
24	x	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
34	V	201	HEM	C2D-C3D-CAD-CBD
25	c	515	DGD	C4E-C5E-C6E-O5E
22	b	619	CLA	O1A-CGA-O2A-C1
29	b	602	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
22	H	101	CLA	C3-C5-C6-C7
27	E	101	LMG	O9-C10-O7-C8
27	I	101	LMG	C11-C10-O7-C8
27	c	522	LMG	C11-C10-O7-C8
25	C	516	DGD	O2G-C2G-C3G-O3G
25	c	516	DGD	O2G-C2G-C3G-O3G
27	m	101	LMG	O1-C7-C8-O7
27	d	408	LMG	C4-C5-C6-O5
22	c	511	CLA	CBA-CGA-O2A-C1
22	B	605	CLA	O1D-CGD-O2D-CED
23	D	407	PL9	C27-C28-C29-C30
22	A	404	CLA	C10-C11-C12-C13
22	B	608	CLA	C13-C15-C16-C17
22	B	611	CLA	C5-C6-C7-C8
22	B	615	CLA	C5-C6-C7-C8
22	C	508	CLA	C5-C6-C7-C8
22	b	612	CLA	C13-C15-C16-C17
22	b	615	CLA	C5-C6-C7-C8
22	b	609	CLA	O1D-CGD-O2D-CED
22	c	511	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	C13-C15-C16-C17
22	b	619	CLA	C5-C6-C7-C8
25	d	410	DGD	C1B-C2B-C3B-C4B
27	C	521	LMG	C10-C11-C12-C13
27	c	522	LMG	C10-C11-C12-C13
25	C	517	DGD	O1B-C1B-O2G-C2G
23	D	407	PL9	C29-C31-C32-C33
23	d	407	PL9	C29-C31-C32-C33
22	A	402	CLA	C3-C5-C6-C7
22	B	611	CLA	C13-C15-C16-C17
22	b	610	CLA	C15-C16-C17-C18
22	c	508	CLA	C5-C6-C7-C8
31	d	402	PHO	C15-C16-C17-C18
25	D	410	DGD	C1B-C2B-C3B-C4B
25	c	515	DGD	C1B-C2B-C3B-C4B
27	A	414	LMG	C28-C29-C30-C31
27	D	412	LMG	C10-C11-C12-C13
27	c	518	LMG	C10-C11-C12-C13
27	d	412	LMG	C10-C11-C12-C13
29	B	626	SQD	O10-C23-O48-C46
22	c	509	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	C	520	CLA	C13-C15-C16-C17
22	C	520	CLA	C15-C16-C17-C18
22	D	405	CLA	C15-C16-C17-C18
22	a	406	CLA	C10-C11-C12-C13
22	b	613	CLA	C8-C10-C11-C12
22	b	619	CLA	C10-C11-C12-C13
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	C	501	CLA	C8-C10-C11-C12
22	D	405	CLA	C13-C15-C16-C17
22	c	505	CLA	C13-C15-C16-C17
22	c	507	CLA	C15-C16-C17-C18
25	C	515	DGD	C1B-C2B-C3B-C4B
27	C	518	LMG	C28-C29-C30-C31
27	c	518	LMG	C28-C29-C30-C31
22	C	511	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	O1A-CGA-O2A-C1
22	a	404	CLA	C3-C5-C6-C7
25	C	515	DGD	O6E-C1E-O5D-C6D
27	A	414	LMG	O6-C1-O1-C7
27	I	101	LMG	O6-C1-O1-C7
27	i	101	LMG	O6-C1-O1-C7
29	A	412	SQD	O5-C1-O6-C44
29	a	415	SQD	O5-C1-O6-C44
31	D	402	PHO	O1D-CGD-O2D-CED
22	B	603	CLA	C13-C15-C16-C17
22	B	606	CLA	C13-C15-C16-C17
22	B	609	CLA	C8-C10-C11-C12
22	B	615	CLA	C10-C11-C12-C13
22	C	503	CLA	C10-C11-C12-C13
22	C	505	CLA	C15-C16-C17-C18
22	C	507	CLA	C10-C11-C12-C13
22	C	509	CLA	C15-C16-C17-C18
22	b	607	CLA	C13-C15-C16-C17
22	c	501	CLA	C15-C16-C17-C18
22	c	503	CLA	C10-C11-C12-C13
22	c	505	CLA	C5-C6-C7-C8
22	c	509	CLA	C15-C16-C17-C18
22	c	520	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	c	520	CLA	C15-C16-C17-C18
22	d	405	CLA	C13-C15-C16-C17
22	d	405	CLA	C15-C16-C17-C18
31	D	402	PHO	C15-C16-C17-C18
22	b	608	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
27	B	621	LMG	C10-C11-C12-C13
22	B	601	CLA	C13-C15-C16-C17
22	C	501	CLA	C15-C16-C17-C18
22	b	605	CLA	C13-C15-C16-C17
22	b	610	CLA	C13-C15-C16-C17
22	c	506	CLA	C5-C6-C7-C8
25	c	517	DGD	O1B-C1B-O2G-C2G
27	d	409	LMG	O9-C10-O7-C8
27	D	408	LMG	C4-C5-C6-O5
22	A	403	CLA	C15-C16-C17-C18
22	A	404	CLA	C15-C16-C17-C18
22	C	505	CLA	C13-C15-C16-C17
22	c	507	CLA	C10-C11-C12-C13
27	b	625	LMG	C10-C11-C12-C13
22	C	512	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	C15-C16-C17-C18
22	b	614	CLA	C15-C16-C17-C18
22	c	501	CLA	C10-C11-C12-C13
22	c	504	CLA	C10-C11-C12-C13
22	C	511	CLA	CBA-CGA-O2A-C1
27	i	101	LMG	C29-C28-O8-C9
27	C	521	LMG	C11-C10-O7-C8
22	c	511	CLA	O1A-CGA-O2A-C1
25	b	624	DGD	C1B-C2B-C3B-C4B
22	B	607	CLA	C15-C16-C17-C18
22	c	505	CLA	C15-C16-C17-C18
22	B	607	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	C15-C16-C17-C18
27	D	409	LMG	O9-C10-O7-C8
27	c	522	LMG	O9-C10-O7-C8
22	B	601	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	CBA-CGA-O2A-C1
29	b	602	SQD	C24-C23-O48-C46
22	B	615	CLA	C13-C15-C16-C17
22	C	506	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	C15-C16-C17-C18
22	C	510	CLA	C5-C6-C7-C8
22	a	405	CLA	C15-C16-C17-C18
22	b	611	CLA	C15-C16-C17-C18
22	b	618	CLA	C13-C15-C16-C17
22	b	619	CLA	C13-C15-C16-C17
22	c	501	CLA	C8-C10-C11-C12
22	c	510	CLA	C5-C6-C7-C8
27	a	402	LMG	C28-C29-C30-C31
22	C	504	CLA	C10-C11-C12-C13
22	b	611	CLA	C5-C6-C7-C8
22	c	512	CLA	C15-C16-C17-C18
22	B	607	CLA	C5-C6-C7-C8
22	B	612	CLA	C5-C6-C7-C8
22	B	614	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
22	a	406	CLA	C15-C16-C17-C18
27	I	101	LMG	C29-C28-O8-C9
23	A	406	PL9	C33-C34-C36-C37
22	b	619	CLA	C3-C5-C6-C7
27	d	412	LMG	O6-C5-C6-O5
27	C	521	LMG	O9-C10-O7-C8
29	F	103	SQD	O49-C7-O47-C45
25	D	410	DGD	C2D-C1D-O3G-C3G
25	D	410	DGD	C2E-C1E-O5D-C6D
25	d	410	DGD	C2D-C1D-O3G-C3G
25	d	410	DGD	C2E-C1E-O5D-C6D
27	I	101	LMG	C2-C1-O1-C7
27	i	101	LMG	C2-C1-O1-C7
30	b	604	LMT	O1'-C1-C2-C3
29	a	415	SQD	C7-C8-C9-C10
24	B	617	BCR	C7-C8-C9-C34
24	B	617	BCR	C37-C22-C23-C24
24	J	102	BCR	C37-C22-C23-C24
24	b	621	BCR	C7-C8-C9-C34
24	b	621	BCR	C37-C22-C23-C24
24	j	102	BCR	C37-C22-C23-C24
22	B	604	CLA	O1A-CGA-O2A-C1
22	c	520	CLA	C2A-CAA-CBA-CGA
22	C	520	CLA	C10-C11-C12-C13
22	c	520	CLA	C10-C11-C12-C13
27	C	518	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
22	b	608	CLA	O1A-CGA-O2A-C1
22	B	615	CLA	C3-C5-C6-C7
22	c	509	CLA	C3-C5-C6-C7
34	V	201	HEM	C4D-C3D-CAD-CBD
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	410	DGD	O6E-C1E-O5D-C6D
27	D	408	LMG	O6-C1-O1-C7
27	d	408	LMG	O6-C1-O1-C7
22	b	611	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	O1D-CGD-O2D-CED
27	a	402	LMG	O6-C5-C6-O5
22	c	520	CLA	CBA-CGA-O2A-C1
29	B	626	SQD	C24-C23-O48-C46
22	c	508	CLA	C2-C1-O2A-CGA
22	C	511	CLA	O1A-CGA-O2A-C1
22	C	501	CLA	C10-C11-C12-C13
22	b	616	CLA	C5-C6-C7-C8
29	F	103	SQD	C12-C13-C14-C15
30	I	102	LMT	C6-C7-C8-C9
30	B	623	LMT	C1-C2-C3-C4
25	C	516	DGD	C2A-C3A-C4A-C5A
25	a	410	DGD	C8B-C9B-CAB-CBB
25	b	601	DGD	C9B-CAB-CBB-CCB
25	c	515	DGD	C3B-C4B-C5B-C6B
27	C	518	LMG	C29-C30-C31-C32
27	b	625	LMG	C31-C32-C33-C34
25	B	620	DGD	C1B-C2B-C3B-C4B
25	C	515	DGD	C3B-C4B-C5B-C6B
25	b	601	DGD	C5B-C6B-C7B-C8B
25	b	624	DGD	C3B-C4B-C5B-C6B
27	c	522	LMG	C12-C13-C14-C15
30	i	102	LMT	C6-C7-C8-C9
30	b	626	LMT	C1-C2-C3-C4
25	B	620	DGD	C6B-C7B-C8B-C9B
25	B	625	DGD	C5B-C6B-C7B-C8B
25	B	625	DGD	C9B-CAB-CBB-CCB
25	D	410	DGD	C4B-C5B-C6B-C7B
25	D	410	DGD	CCB-CDB-CEB-CFB
25	c	516	DGD	C2A-C3A-C4A-C5A
25	c	516	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C33-C34-C35-C36
27	A	410	LMG	C34-C35-C36-C37
27	A	414	LMG	C30-C31-C32-C33
27	B	621	LMG	C31-C32-C33-C34
27	I	101	LMG	C12-C13-C14-C15
27	I	101	LMG	C14-C15-C16-C17
27	a	402	LMG	C30-C31-C32-C33
27	c	518	LMG	C29-C30-C31-C32
29	b	602	SQD	C11-C10-C9-C8
29	f	103	SQD	C12-C13-C14-C15
29	f	103	SQD	O49-C7-O47-C45
25	D	410	DGD	C5B-C6B-C7B-C8B
25	d	410	DGD	C5B-C6B-C7B-C8B
25	d	410	DGD	CCB-CDB-CEB-CFB
27	i	101	LMG	C12-C13-C14-C15
22	B	605	CLA	C4B-C3B-CAB-CBB
22	C	501	CLA	C4B-C3B-CAB-CBB
22	C	504	CLA	C4B-C3B-CAB-CBB
22	b	609	CLA	C4B-C3B-CAB-CBB
22	c	501	CLA	C4B-C3B-CAB-CBB
22	c	504	CLA	C4B-C3B-CAB-CBB
25	D	410	DGD	CEB-CFB-CGB-CHB
25	d	410	DGD	CEB-CFB-CGB-CHB
27	a	412	LMG	C34-C35-C36-C37
22	b	615	CLA	O1D-CGD-O2D-CED
22	B	605	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
25	A	408	DGD	C8B-C9B-CAB-CBB
25	C	515	DGD	C3A-C4A-C5A-C6A
27	D	408	LMG	C18-C19-C20-C21
29	B	626	SQD	C9-C10-C11-C12
29	B	626	SQD	C8-C7-O47-C45
29	b	602	SQD	C8-C7-O47-C45
25	c	515	DGD	C3A-C4A-C5A-C6A
22	C	503	CLA	C11-C12-C13-C15
22	D	405	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
25	C	515	DGD	C2B-C3B-C4B-C5B
25	b	624	DGD	C6B-C7B-C8B-C9B
25	d	410	DGD	C4B-C5B-C6B-C7B
27	a	412	LMG	C33-C34-C35-C36
25	C	515	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
27	m	101	LMG	C29-C28-O8-C9
22	C	503	CLA	C5-C6-C7-C8
22	c	503	CLA	C5-C6-C7-C8
25	B	620	DGD	C3B-C4B-C5B-C6B
27	C	521	LMG	C12-C13-C14-C15
27	i	101	LMG	C16-C17-C18-C19
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	b	619	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
25	C	517	DGD	CBA-CCA-CDA-CEA
29	B	626	SQD	C11-C10-C9-C8
23	a	408	PL9	C33-C34-C36-C37
25	b	624	DGD	C7A-C8A-C9A-CAA
22	H	101	CLA	C5-C6-C7-C8
22	B	611	CLA	O1D-CGD-O2D-CED
25	c	517	DGD	C1A-C2A-C3A-C4A
27	d	408	LMG	C18-C19-C20-C21
27	M	101	LMG	O6-C5-C6-O5
27	a	402	LMG	C32-C33-C34-C35
25	c	515	DGD	C2B-C3B-C4B-C5B
27	A	414	LMG	C15-C16-C17-C18
27	D	409	LMG	C14-C15-C16-C17
22	C	520	CLA	CBA-CGA-O2A-C1
26	C	519	LHG	C24-C23-O8-C6
25	d	410	DGD	C7B-C8B-C9B-CAB
29	b	602	SQD	C9-C10-C11-C12
27	D	408	LMG	C28-C29-C30-C31
25	B	620	DGD	C7A-C8A-C9A-CAA
25	D	410	DGD	C7B-C8B-C9B-CAB
27	A	414	LMG	C18-C19-C20-C21
27	D	409	LMG	C19-C20-C21-C22
27	d	409	LMG	C14-C15-C16-C17
27	i	101	LMG	C14-C15-C16-C17
29	A	412	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	a	415	SQD	C14-C15-C16-C17
30	B	628	LMT	O1'-C1-C2-C3
27	C	521	LMG	C4-C5-C6-O5
27	A	410	LMG	C30-C31-C32-C33
27	D	408	LMG	C31-C32-C33-C34
29	a	415	SQD	C27-C28-C29-C30
25	B	620	DGD	O6D-C5D-C6D-O5D
25	b	624	DGD	O6D-C5D-C6D-O5D
27	a	402	LMG	C18-C19-C20-C21
25	C	516	DGD	C4A-C5A-C6A-C7A
25	c	517	DGD	CBA-CCA-CDA-CEA
27	a	402	LMG	C15-C16-C17-C18
25	B	625	DGD	C1A-C2A-C3A-C4A
27	d	408	LMG	C28-C29-C30-C31
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	513	BCR	C1-C6-C7-C8
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
27	a	412	LMG	C30-C31-C32-C33
25	c	517	DGD	C2B-C1B-O2G-C2G
22	a	407	CLA	C10-C11-C12-C13
25	C	517	DGD	C9B-CAB-CBB-CCB
27	I	101	LMG	C16-C17-C18-C19
27	a	412	LMG	C31-C32-C33-C34
29	F	103	SQD	C11-C12-C13-C14
29	A	412	SQD	C27-C28-C29-C30
22	A	402	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	a	404	CLA	C2A-CAA-CBA-CGA
27	E	101	LMG	C28-C29-C30-C31
27	A	410	LMG	C31-C32-C33-C34
27	A	414	LMG	C32-C33-C34-C35
22	c	520	CLA	O1A-CGA-O2A-C1
27	d	408	LMG	C31-C32-C33-C34
29	f	103	SQD	C11-C12-C13-C14
26	A	409	LHG	O9-C7-O7-C5
25	a	410	DGD	C5B-C6B-C7B-C8B
25	b	624	DGD	C4B-C5B-C6B-C7B
25	c	517	DGD	CAB-CBB-CCB-CDB
22	B	612	CLA	C16-C17-C18-C19
25	B	625	DGD	C2B-C3B-C4B-C5B
25	c	517	DGD	C9B-CAB-CBB-CCB
27	d	409	LMG	C19-C20-C21-C22
25	c	515	DGD	C1A-C2A-C3A-C4A
29	A	412	SQD	C7-C8-C9-C10
22	b	614	CLA	CBA-CGA-O2A-C1
22	c	508	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C29-C28-O8-C9
22	a	405	CLA	C3-C5-C6-C7
27	D	412	LMG	C17-C18-C19-C20
25	A	408	DGD	C5B-C6B-C7B-C8B
25	C	515	DGD	C4A-C5A-C6A-C7A
25	d	410	DGD	O6E-C1E-O5D-C6D
22	B	603	CLA	C8-C10-C11-C12
22	C	511	CLA	C13-C15-C16-C17
22	h	101	CLA	C5-C6-C7-C8
27	D	412	LMG	O6-C5-C6-O5
25	b	601	DGD	C4A-C5A-C6A-C7A
25	c	515	DGD	C4A-C5A-C6A-C7A
27	c	518	LMG	C12-C13-C14-C15
25	C	517	DGD	CAB-CBB-CCB-CDB
27	I	101	LMG	C13-C14-C15-C16
27	d	409	LMG	C15-C16-C17-C18
26	c	519	LHG	C24-C23-O8-C6
22	b	605	CLA	C16-C17-C18-C20
25	C	517	DGD	C2B-C1B-O2G-C2G
26	A	409	LHG	C8-C7-O7-C5
26	a	411	LHG	C8-C7-O7-C5
27	E	101	LMG	C11-C10-O7-C8
27	e	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
25	C	517	DGD	C1A-C2A-C3A-C4A
25	a	410	DGD	C1B-C2B-C3B-C4B
27	C	518	LMG	C34-C35-C36-C37
22	H	101	CLA	C13-C15-C16-C17
22	b	607	CLA	C8-C10-C11-C12
27	C	521	LMG	O6-C5-C6-O5
26	a	411	LHG	O9-C7-O7-C5
25	b	601	DGD	C2B-C3B-C4B-C5B
27	c	518	LMG	C34-C35-C36-C37
24	f	102	BCR	C37-C22-C23-C24
25	B	625	DGD	C4A-C5A-C6A-C7A
22	c	502	CLA	C3-C5-C6-C7
27	m	101	LMG	O6-C5-C6-O5
27	D	409	LMG	C8-C7-O1-C1
27	d	409	LMG	C8-C7-O1-C1
30	B	628	LMT	C7-C8-C9-C10
22	C	520	CLA	C2A-CAA-CBA-CGA
22	B	612	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C19
26	a	411	LHG	C25-C26-C27-C28
27	a	412	LMG	C14-C15-C16-C17
27	m	101	LMG	C29-C30-C31-C32
23	j	101	PL9	C15-C14-C16-C17
27	i	101	LMG	C13-C14-C15-C16
29	F	103	SQD	C10-C11-C12-C13
22	A	405	CLA	C10-C11-C12-C13
22	h	101	CLA	C13-C15-C16-C17
25	D	410	DGD	C6B-C7B-C8B-C9B
29	b	602	SQD	C11-C12-C13-C14
25	A	408	DGD	C1B-C2B-C3B-C4B
27	e	101	LMG	C28-C29-C30-C31
25	B	620	DGD	C4B-C5B-C6B-C7B
25	d	410	DGD	C5A-C6A-C7A-C8A
22	c	512	CLA	C13-C15-C16-C17
22	b	616	CLA	C16-C17-C18-C20
25	b	624	DGD	C5B-C6B-C7B-C8B
26	a	411	LHG	C30-C31-C32-C33
27	D	409	LMG	C32-C33-C34-C35
27	d	409	LMG	C32-C33-C34-C35
22	C	520	CLA	O1A-CGA-O2A-C1
25	D	410	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
30	b	604	LMT	C7-C8-C9-C10
25	c	516	DGD	C1A-C2A-C3A-C4A
22	C	505	CLA	C10-C11-C12-C13
26	A	409	LHG	C30-C31-C32-C33
27	d	412	LMG	C34-C35-C36-C37
27	e	101	LMG	O6-C5-C6-O5
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
29	A	412	SQD	O47-C45-C46-O48
29	A	413	SQD	O6-C44-C45-O47
29	a	401	SQD	O6-C44-C45-O47
29	a	415	SQD	O47-C45-C46-O48
27	A	410	LMG	C14-C15-C16-C17
27	D	408	LMG	C30-C31-C32-C33
27	D	409	LMG	C15-C16-C17-C18
29	f	103	SQD	C10-C11-C12-C13
30	B	623	LMT	O1'-C1-C2-C3
27	C	518	LMG	C12-C13-C14-C15
22	C	512	CLA	C13-C15-C16-C17
22	c	505	CLA	C10-C11-C12-C13
22	d	406	CLA	C15-C16-C17-C18
27	A	414	LMG	O6-C5-C6-O5
25	B	620	DGD	C5B-C6B-C7B-C8B
25	c	516	DGD	CAB-CBB-CCB-CDB
26	A	409	LHG	C25-C26-C27-C28
27	c	518	LMG	C36-C37-C38-C39
27	d	408	LMG	C36-C37-C38-C39
27	E	101	LMG	C15-C16-C17-C18
27	d	408	LMG	C30-C31-C32-C33
27	e	101	LMG	C15-C16-C17-C18
29	B	622	SQD	C9-C10-C11-C12
29	B	626	SQD	C11-C12-C13-C14
22	c	509	CLA	C4-C3-C5-C6
22	C	509	CLA	C3-C5-C6-C7
25	C	516	DGD	CAB-CBB-CCB-CDB
27	D	412	LMG	C34-C35-C36-C37
29	d	403	SQD	C9-C10-C11-C12
22	c	501	CLA	C2A-CAA-CBA-CGA
27	M	101	LMG	C29-C30-C31-C32
22	D	406	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	D	407	PL9	C47-C48-C49-C51
23	d	407	PL9	C47-C48-C49-C51
22	c	506	CLA	CBD-CGD-O2D-CED
25	D	410	DGD	C3A-C4A-C5A-C6A
25	d	410	DGD	C6B-C7B-C8B-C9B
27	A	414	LMG	C31-C32-C33-C34
27	B	621	LMG	C34-C35-C36-C37
27	C	518	LMG	C36-C37-C38-C39
22	c	508	CLA	O1A-CGA-O2A-C1
22	C	502	CLA	C3-C5-C6-C7
26	c	519	LHG	C24-C25-C26-C27
27	d	412	LMG	C17-C18-C19-C20
27	D	409	LMG	C13-C14-C15-C16
22	B	615	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	b	619	CLA	C1A-C2A-CAA-CBA
22	c	501	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C10-C11-C12-C13
25	C	515	DGD	C2A-C3A-C4A-C5A
30	I	102	LMT	C5'-C4'-O1B-C1B
30	i	102	LMT	C5'-C4'-O1B-C1B
22	B	603	CLA	C15-C16-C17-C18
27	E	101	LMG	O6-C5-C6-O5
25	D	410	DGD	C2A-C3A-C4A-C5A
25	d	410	DGD	CAB-CBB-CCB-CDB
25	b	601	DGD	C1A-C2A-C3A-C4A
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	C	504	CLA	C6-C7-C8-C10
22	H	101	CLA	C6-C7-C8-C10
22	b	618	CLA	C11-C10-C8-C7
22	b	618	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C10-C8-C7
22	c	504	CLA	C6-C7-C8-C10
22	c	510	CLA	C6-C7-C8-C10
22	c	510	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	C12-C13-C15-C16
22	h	101	CLA	C6-C7-C8-C10
31	D	402	PHO	C12-C13-C15-C16
31	d	402	PHO	C12-C13-C15-C16
25	d	410	DGD	C2A-C3A-C4A-C5A
26	C	519	LHG	C24-C25-C26-C27
22	B	609	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20
22	C	509	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	CBA-CGA-O2A-C1
25	B	625	DGD	O6D-C5D-C6D-O5D
25	C	516	DGD	C1A-C2A-C3A-C4A
26	a	411	LHG	C23-C24-C25-C26
25	D	410	DGD	CAB-CBB-CCB-CDB
25	d	410	DGD	C3A-C4A-C5A-C6A
27	D	412	LMG	C31-C32-C33-C34
22	C	509	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
22	C	512	CLA	C2-C3-C5-C6
27	A	410	LMG	C15-C16-C17-C18
22	b	614	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	C13-C15-C16-C17
30	b	626	LMT	O1'-C1-C2-C3
22	C	501	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C11-C12-C13-C14
22	B	602	CLA	C6-C7-C8-C9
22	B	614	CLA	C11-C10-C8-C9
22	C	502	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C12-C13-C14
22	C	504	CLA	C14-C13-C15-C16
22	C	510	CLA	C14-C13-C15-C16
22	a	405	CLA	C6-C7-C8-C9
22	b	606	CLA	C6-C7-C8-C9
22	b	612	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

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	C14-C13-C15-C16
27	D	408	LMG	C17-C18-C19-C20
29	B	626	SQD	C12-C13-C14-C15
27	d	409	LMG	C13-C14-C15-C16
22	B	610	CLA	CBA-CGA-O2A-C1
22	c	504	CLA	CBA-CGA-O2A-C1
22	d	406	CLA	CBA-CGA-O2A-C1
25	D	410	DGD	CAA-CBA-CCA-CDA
27	d	408	LMG	C17-C18-C19-C20
30	b	627	LMT	C2B-C1B-O1B-C4'
34	v	201	HEM	C4D-C3D-CAD-CBD
27	D	408	LMG	C2-C1-O1-C7
30	B	624	LMT	C2B-C1B-O1B-C4'
25	C	515	DGD	C4B-C5B-C6B-C7B
25	c	515	DGD	C2A-C3A-C4A-C5A
27	D	408	LMG	C36-C37-C38-C39
27	d	412	LMG	C31-C32-C33-C34
25	A	408	DGD	C1G-C2G-C3G-O3G
25	C	517	DGD	O1G-C1G-C2G-C3G
25	c	516	DGD	C1G-C2G-C3G-O3G
25	c	517	DGD	O1G-C1G-C2G-C3G
27	B	621	LMG	C7-C8-C9-O8
27	C	521	LMG	C7-C8-C9-O8
27	D	408	LMG	O1-C7-C8-C9
27	D	409	LMG	O1-C7-C8-C9
27	I	101	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
27	b	625	LMG	C7-C8-C9-O8
27	c	522	LMG	C7-C8-C9-O8
27	d	408	LMG	O1-C7-C8-C9
27	d	409	LMG	O1-C7-C8-C9
27	i	101	LMG	O1-C7-C8-C9
27	m	101	LMG	C7-C8-C9-O8
29	b	602	SQD	C44-C45-C46-O48
25	d	410	DGD	C8B-C9B-CAB-CBB
27	A	414	LMG	C17-C18-C19-C20
22	B	601	CLA	C10-C11-C12-C13
26	c	519	LHG	C25-C26-C27-C28
22	C	510	CLA	CBA-CGA-O2A-C1
22	D	406	CLA	CBA-CGA-O2A-C1
22	B	601	CLA	C16-C17-C18-C20
22	B	613	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	b	625	LMG	C34-C35-C36-C37
29	b	602	SQD	C12-C13-C14-C15
25	A	408	DGD	C3B-C4B-C5B-C6B
27	i	101	LMG	O10-C28-O8-C9
27	a	402	LMG	C31-C32-C33-C34
27	a	412	LMG	C15-C16-C17-C18
22	C	509	CLA	C2-C3-C5-C6
22	c	509	CLA	C2-C3-C5-C6
27	D	408	LMG	C15-C16-C17-C18
34	v	201	HEM	C2D-C3D-CAD-CBD
22	A	405	CLA	C5-C6-C7-C8
22	C	502	CLA	C13-C15-C16-C17
22	C	503	CLA	C8-C10-C11-C12
22	b	607	CLA	C15-C16-C17-C18
22	b	608	CLA	C15-C16-C17-C18
22	c	503	CLA	C8-C10-C11-C12
27	C	521	LMG	C16-C17-C18-C19
27	c	522	LMG	C16-C17-C18-C19
25	D	410	DGD	C8B-C9B-CAB-CBB
25	C	517	DGD	C3B-C4B-C5B-C6B
22	C	508	CLA	CBA-CGA-O2A-C1
25	D	410	DGD	C1G-C2G-O2G-C1B
25	d	410	DGD	C1G-C2G-O2G-C1B
27	E	101	LMG	C7-C8-O7-C10
27	c	518	LMG	C9-C8-O7-C10
22	a	407	CLA	C5-C6-C7-C8
22	c	502	CLA	C13-C15-C16-C17
25	A	408	DGD	C4B-C5B-C6B-C7B
25	a	410	DGD	C3B-C4B-C5B-C6B
22	B	609	CLA	C16-C17-C18-C19
25	c	515	DGD	C4B-C5B-C6B-C7B
27	B	621	LMG	C13-C14-C15-C16
22	C	506	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	C11-C10-O7-C8
27	b	625	LMG	C13-C14-C15-C16
25	B	625	DGD	C5A-C6A-C7A-C8A
25	a	410	DGD	C4B-C5B-C6B-C7B
22	C	512	CLA	C4-C3-C5-C6
23	d	407	PL9	C35-C34-C36-C37
22	c	512	CLA	C2-C3-C5-C6
25	c	517	DGD	C3B-C4B-C5B-C6B
27	i	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C19
27	I	101	LMG	C18-C19-C20-C21
27	e	101	LMG	C18-C19-C20-C21
25	C	516	DGD	O6D-C5D-C6D-O5D
25	c	516	DGD	O6D-C5D-C6D-O5D
27	d	408	LMG	C32-C33-C34-C35
29	A	412	SQD	C17-C18-C19-C20
25	C	515	DGD	O2G-C2G-C3G-O3G
25	C	517	DGD	O1G-C1G-C2G-O2G
25	c	517	DGD	O1G-C1G-C2G-O2G
27	a	412	LMG	O1-C7-C8-O7
29	a	401	SQD	C10-C11-C12-C13
29	a	415	SQD	C17-C18-C19-C20
22	C	504	CLA	O1A-CGA-O2A-C1
27	a	402	LMG	C17-C18-C19-C20
22	C	511	CLA	C3-C5-C6-C7
25	d	410	DGD	CDB-CEB-CFB-CGB
26	c	519	LHG	C11-C10-C9-C8
27	D	408	LMG	C32-C33-C34-C35
22	c	509	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	CBA-CGA-O2A-C1
29	A	412	SQD	C10-C11-C12-C13
23	d	407	PL9	C27-C28-C29-C30
25	b	601	DGD	O6D-C5D-C6D-O5D
22	d	406	CLA	O1A-CGA-O2A-C1
26	A	409	LHG	C23-C24-C25-C26
22	C	504	CLA	C15-C16-C17-C18
22	a	407	CLA	C13-C15-C16-C17
22	b	617	CLA	C5-C6-C7-C8
25	C	516	DGD	C4D-C5D-C6D-O5D
25	c	516	DGD	C4D-C5D-C6D-O5D
22	B	613	CLA	C16-C17-C18-C19
22	b	617	CLA	C16-C17-C18-C20
23	D	407	PL9	C35-C34-C36-C37
25	d	410	DGD	C4E-C5E-C6E-O5E
25	D	410	DGD	CDB-CEB-CFB-CGB
22	A	403	CLA	C6-C7-C8-C9
22	B	605	CLA	C14-C13-C15-C16
22	B	608	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	C14-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C14
22	C	504	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	C	511	CLA	C11-C12-C13-C14
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
31	D	402	PHO	C14-C13-C15-C16
31	d	402	PHO	C14-C13-C15-C16
22	B	615	CLA	C15-C16-C17-C18
22	B	610	CLA	O1A-CGA-O2A-C1
29	A	413	SQD	C10-C11-C12-C13
27	A	410	LMG	C8-C9-O8-C28
22	B	601	CLA	C16-C17-C18-C19
23	D	407	PL9	C32-C33-C34-C36
25	D	410	DGD	CBA-CCA-CDA-CEA
27	d	408	LMG	C2-C1-O1-C7
26	C	519	LHG	C11-C10-C9-C8
26	C	519	LHG	C25-C26-C27-C28
27	d	408	LMG	C19-C20-C21-C22
27	i	101	LMG	C17-C18-C19-C20
27	d	409	LMG	C28-C29-C30-C31
27	a	412	LMG	C11-C10-O7-C8
22	B	602	CLA	C6-C7-C8-C10
22	B	607	CLA	C6-C7-C8-C10
22	B	609	CLA	C11-C12-C13-C15
22	B	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	C12-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	508	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C15
22	b	606	CLA	C6-C7-C8-C10
22	b	609	CLA	C12-C13-C15-C16
22	b	612	CLA	C12-C13-C15-C16
22	b	619	CLA	C12-C13-C15-C16
22	c	502	CLA	C12-C13-C15-C16
22	c	504	CLA	C12-C13-C15-C16
22	c	505	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	511	CLA	C11-C12-C13-C15
22	B	613	CLA	C5-C6-C7-C8
22	B	615	CLA	C8-C10-C11-C12
22	C	508	CLA	C15-C16-C17-C18
22	c	504	CLA	C15-C16-C17-C18
25	c	517	DGD	CFA-CGA-CHA-CIA
25	d	410	DGD	CBA-CCA-CDA-CEA
22	b	608	CLA	C10-C11-C12-C13
27	c	522	LMG	C17-C18-C19-C20
27	d	408	LMG	C15-C16-C17-C18
22	D	406	CLA	O1A-CGA-O2A-C1
27	C	521	LMG	C17-C18-C19-C20
22	A	402	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	C4-C3-C5-C6
22	a	404	CLA	C3A-C2A-CAA-CBA
22	c	504	CLA	C4-C3-C5-C6
23	D	407	PL9	C15-C14-C16-C17
23	d	407	PL9	C15-C14-C16-C17
27	d	409	LMG	C29-C30-C31-C32
27	E	101	LMG	O7-C10-C11-C12
23	J	101	PL9	C27-C28-C29-C30
22	c	504	CLA	O1A-CGA-O2A-C1
27	a	412	LMG	C4-C5-C6-O5
27	E	101	LMG	C17-C18-C19-C20
27	C	521	LMG	C34-C35-C36-C37
22	C	511	CLA	C16-C17-C18-C19
27	D	412	LMG	C38-C39-C40-C41
27	E	101	LMG	C19-C20-C21-C22
22	C	508	CLA	O1A-CGA-O2A-C1
22	C	510	CLA	O1A-CGA-O2A-C1
27	d	412	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
27	A	414	LMG	C11-C12-C13-C14
27	e	101	LMG	C19-C20-C21-C22
27	I	101	LMG	C31-C32-C33-C34
22	b	619	CLA	C8-C10-C11-C12
25	B	625	DGD	C1G-C2G-C3G-O3G
25	C	516	DGD	C1G-C2G-C3G-O3G
25	a	410	DGD	C1G-C2G-C3G-O3G
25	d	410	DGD	C1G-C2G-C3G-O3G
27	A	410	LMG	O1-C7-C8-C9
27	C	518	LMG	O1-C7-C8-C9
27	a	412	LMG	O1-C7-C8-C9
27	c	518	LMG	O1-C7-C8-C9
27	m	101	LMG	O1-C7-C8-C9
29	A	412	SQD	C44-C45-C46-O48
29	A	413	SQD	O6-C44-C45-C46
29	B	626	SQD	C44-C45-C46-O48
29	a	401	SQD	O6-C44-C45-C46
27	D	412	LMG	C19-C20-C21-C22
27	d	408	LMG	C13-C14-C15-C16
22	b	613	CLA	C16-C17-C18-C19
27	I	101	LMG	C17-C18-C19-C20
29	a	415	SQD	C31-C32-C33-C34
27	E	101	LMG	C18-C19-C20-C21
26	C	519	LHG	O10-C23-O8-C6
27	c	522	LMG	C34-C35-C36-C37
27	D	408	LMG	C19-C20-C21-C22
27	D	409	LMG	C29-C30-C31-C32
25	C	517	DGD	CDB-CEB-CFB-CGB
27	b	625	LMG	C17-C18-C19-C20
27	i	101	LMG	C31-C32-C33-C34
24	B	616	BCR	C1-C6-C7-C8
24	C	513	BCR	C1-C6-C7-C8
24	F	102	BCR	C1-C6-C7-C8
24	J	102	BCR	C1-C6-C7-C8
24	b	620	BCR	C1-C6-C7-C8
24	f	102	BCR	C1-C6-C7-C8
24	j	102	BCR	C1-C6-C7-C8
27	a	402	LMG	C11-C12-C13-C14
22	c	511	CLA	C3-C5-C6-C7
27	B	621	LMG	C17-C18-C19-C20
30	B	628	LMT	C2-C3-C4-C5
22	b	617	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	619	CLA	C15-C16-C17-C18
29	a	415	SQD	C10-C11-C12-C13
30	B	624	LMT	O5B-C1B-O1B-C4'
27	A	410	LMG	C4-C5-C6-O5
23	j	101	PL9	C27-C28-C29-C30
27	e	101	LMG	C17-C18-C19-C20
22	c	512	CLA	C2A-CAA-CBA-CGA
25	c	515	DGD	O2G-C2G-C3G-O3G
27	B	621	LMG	O7-C8-C9-O8
27	C	518	LMG	O1-C7-C8-O7
27	C	521	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
27	m	101	LMG	O7-C8-C9-O8
29	b	602	SQD	O47-C45-C46-O48
29	d	403	SQD	O6-C44-C45-O47
27	d	412	LMG	C19-C20-C21-C22
25	D	410	DGD	C3B-C4B-C5B-C6B
23	A	406	PL9	C4-C3-C7-C8
23	a	408	PL9	C4-C3-C7-C8
25	C	516	DGD	C3A-C4A-C5A-C6A
22	c	504	CLA	C2-C3-C5-C6
22	b	617	CLA	C16-C17-C18-C19
25	d	410	DGD	C3B-C4B-C5B-C6B
25	C	517	DGD	CFA-CGA-CHA-CIA
27	D	409	LMG	C28-C29-C30-C31
31	D	401	PHO	CBD-CGD-O2D-CED
22	B	608	CLA	C14-C13-C15-C16
22	C	507	CLA	C14-C13-C15-C16
22	a	404	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
31	d	401	PHO	C6-C7-C8-C9
22	B	604	CLA	C5-C6-C7-C8
29	A	412	SQD	C31-C32-C33-C34
30	B	627	LMT	C5'-C4'-O1B-C1B
30	b	603	LMT	C5'-C4'-O1B-C1B
22	B	613	CLA	C15-C16-C17-C18
22	a	405	CLA	C5-C6-C7-C8
22	c	501	CLA	C13-C15-C16-C17
25	D	410	DGD	C1A-C2A-C3A-C4A
30	b	627	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	CBA-CGA-O2A-C1
22	C	504	CLA	C2-C3-C5-C6
22	B	604	CLA	C10-C11-C12-C13
25	c	516	DGD	C3A-C4A-C5A-C6A
29	b	602	SQD	C10-C11-C12-C13
24	b	621	BCR	C20-C21-C22-C37
27	I	101	LMG	O10-C28-O8-C9
22	A	405	CLA	C13-C15-C16-C17
24	F	102	BCR	C37-C22-C23-C24
29	f	103	SQD	C29-C30-C31-C32
22	A	403	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	608	CLA	C12-C13-C15-C16
22	B	610	CLA	C11-C10-C8-C7
22	B	612	CLA	C11-C12-C13-C15
22	B	615	CLA	C12-C13-C15-C16
22	C	507	CLA	C12-C13-C15-C16
22	C	511	CLA	C12-C13-C15-C16
22	a	405	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
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	m	101	LMG	C30-C31-C32-C33
24	H	102	BCR	C7-C8-C9-C10
24	J	102	BCR	C7-C8-C9-C10
24	c	514	BCR	C7-C8-C9-C10
26	c	519	LHG	O10-C23-O8-C6
27	A	410	LMG	C8-C7-O1-C1
27	a	412	LMG	C8-C7-O1-C1
29	B	622	SQD	C45-C44-O6-C1
29	B	622	SQD	C5-C6-S-O8
29	d	403	SQD	C45-C44-O6-C1
29	d	403	SQD	C5-C6-S-O8
22	c	508	CLA	C15-C16-C17-C18
31	D	401	PHO	C5-C6-C7-C8
29	b	602	SQD	C17-C18-C19-C20
23	A	406	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
27	e	101	LMG	O7-C10-C11-C12
22	b	613	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	O1A-CGA-O2A-C1
25	b	601	DGD	C5A-C6A-C7A-C8A
25	c	516	DGD	C4B-C5B-C6B-C7B
22	B	609	CLA	C10-C11-C12-C13
29	a	415	SQD	C15-C16-C17-C18
31	D	402	PHO	C10-C11-C12-C13
29	A	412	SQD	C15-C16-C17-C18
26	C	519	LHG	O2-C2-C3-O3
22	C	511	CLA	C5-C6-C7-C8
24	J	102	BCR	C20-C21-C22-C23
26	c	519	LHG	O6-C4-C5-O7
23	D	407	PL9	C24-C26-C27-C28
25	D	410	DGD	C1G-C2G-C3G-O3G
25	b	601	DGD	C1G-C2G-C3G-O3G
27	M	101	LMG	O1-C7-C8-C9
29	a	415	SQD	C44-C45-C46-O48
22	b	613	CLA	C5-C6-C7-C8
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
22	c	506	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	C2A-CAA-CBA-CGA
29	B	626	SQD	C10-C11-C12-C13
25	a	410	DGD	O2G-C2G-C3G-O3G
29	B	622	SQD	O6-C44-C45-O47
31	d	401	PHO	C5-C6-C7-C8
22	A	403	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
22	B	612	CLA	C11-C12-C13-C14
22	C	501	CLA	C11-C12-C13-C14
22	D	405	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
25	C	516	DGD	C4B-C5B-C6B-C7B
27	C	518	LMG	C13-C14-C15-C16
22	b	607	CLA	CBA-CGA-O2A-C1
25	D	410	DGD	C2B-C3B-C4B-C5B
27	c	518	LMG	C13-C14-C15-C16
25	c	517	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C20-C21-C22-C23
27	d	408	LMG	C20-C21-C22-C23
22	B	604	CLA	C15-C16-C17-C18
22	B	611	CLA	C10-C11-C12-C13
22	b	608	CLA	C5-C6-C7-C8
22	c	511	CLA	C5-C6-C7-C8
27	d	409	LMG	C31-C32-C33-C34
25	d	410	DGD	CAA-CBA-CCA-CDA
27	D	408	LMG	C16-C17-C18-C19
22	C	508	CLA	C2-C1-O2A-CGA
22	A	405	CLA	C16-C17-C18-C19
25	d	410	DGD	C2B-C3B-C4B-C5B
23	a	408	PL9	C35-C34-C36-C37
23	d	407	PL9	C20-C19-C21-C22
22	b	615	CLA	C10-C11-C12-C13
22	a	407	CLA	C16-C17-C18-C19
22	b	613	CLA	C10-C11-C12-C13
27	d	409	LMG	C36-C37-C38-C39
22	B	603	CLA	O1A-CGA-O2A-C1
25	D	410	DGD	C4A-C5A-C6A-C7A
27	b	625	LMG	C28-C29-C30-C31
22	C	506	CLA	C3-C5-C6-C7
22	A	402	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C4B-C3B-CAB-CBB
22	C	508	CLA	C4B-C3B-CAB-CBB
22	C	520	CLA	C4B-C3B-CAB-CBB
22	a	404	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C4B-C3B-CAB-CBB
22	c	520	CLA	C4B-C3B-CAB-CBB
22	B	614	CLA	CBA-CGA-O2A-C1
29	B	626	SQD	C17-C18-C19-C20
22	A	403	CLA	C4-C3-C5-C6
22	B	611	CLA	C4-C3-C5-C6
24	j	102	BCR	C7-C8-C9-C10
29	A	413	SQD	C9-C10-C11-C12
26	C	519	LHG	O6-C4-C5-C6
26	c	519	LHG	O6-C4-C5-C6
31	d	401	PHO	CBD-CGD-O2D-CED
29	B	626	SQD	O49-C7-O47-C45
29	b	602	SQD	O49-C7-O47-C45
25	d	410	DGD	C1A-C2A-C3A-C4A
22	B	609	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	O1D-CGD-O2D-CED
22	A	405	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	B	609	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	C	508	CLA	C6-C7-C8-C10
22	C	509	CLA	C6-C7-C8-C10
22	D	406	CLA	C11-C10-C8-C7
22	b	611	CLA	C6-C7-C8-C10
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	406	CLA	C11-C10-C8-C7
22	h	101	CLA	C11-C10-C8-C7
31	d	402	PHO	C6-C7-C8-C10
25	b	624	DGD	C5A-C6A-C7A-C8A
29	F	103	SQD	C29-C30-C31-C32
27	C	521	LMG	C35-C36-C37-C38
27	D	409	LMG	C31-C32-C33-C34
27	a	412	LMG	C20-C21-C22-C23
29	A	413	SQD	C32-C33-C34-C35
26	A	409	LHG	C2-C3-O3-P
22	b	615	CLA	C4-C3-C5-C6
26	C	519	LHG	O6-C4-C5-O7
29	a	401	SQD	C9-C10-C11-C12
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	610	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	405	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	b	619	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	C11-C12-C13-C14
22	c	507	CLA	C14-C13-C15-C16
27	c	522	LMG	C35-C36-C37-C38
31	d	402	PHO	C10-C11-C12-C13
25	c	515	DGD	C5A-C6A-C7A-C8A
22	A	403	CLA	C5-C6-C7-C8
22	b	616	CLA	C13-C15-C16-C17
29	B	622	SQD	O5-C5-C6-S
22	c	506	CLA	C3-C5-C6-C7
29	f	103	SQD	C24-C25-C26-C27
22	b	607	CLA	O1A-CGA-O2A-C1
25	A	408	DGD	O2G-C2G-C3G-O3G
25	D	410	DGD	O2G-C2G-C3G-O3G
25	d	410	DGD	O2G-C2G-C3G-O3G
27	D	409	LMG	O1-C7-C8-O7
27	b	625	LMG	O7-C8-C9-O8
29	B	626	SQD	O47-C45-C46-O48
25	B	620	DGD	C5A-C6A-C7A-C8A
22	A	404	CLA	C5-C6-C7-C8
27	D	408	LMG	C20-C21-C22-C23
29	d	403	SQD	O6-C44-C45-C46
27	A	410	LMG	C29-C30-C31-C32
29	B	622	SQD	C10-C11-C12-C13
31	d	402	PHO	C13-C15-C16-C17
27	A	410	LMG	O6-C5-C6-O5
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
27	a	412	LMG	C16-C17-C18-C19
25	d	410	DGD	C4A-C5A-C6A-C7A
31	D	401	PHO	O1D-CGD-O2D-CED
29	d	403	SQD	C10-C11-C12-C13
22	B	614	CLA	O1A-CGA-O2A-C1
25	B	620	DGD	O1A-C1A-O1G-C1G
27	a	412	LMG	O6-C5-C6-O5
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	c	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
26	A	409	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
26	C	519	LHG	C3-O3-P-O5
26	C	519	LHG	C4-O6-P-O5
26	a	411	LHG	C3-O3-P-O5
26	c	519	LHG	C3-O3-P-O5
26	c	519	LHG	C4-O6-P-O5
29	a	401	SQD	C32-C33-C34-C35
22	B	612	CLA	C10-C11-C12-C13
23	J	101	PL9	C15-C14-C16-C17
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
22	c	520	CLA	C2B-C3B-CAB-CBB
24	b	623	BCR	C23-C24-C25-C30
23	D	407	PL9	C13-C14-C16-C17
23	d	407	PL9	C13-C14-C16-C17
26	a	411	LHG	C2-C3-O3-P
30	b	604	LMT	C2-C3-C4-C5
27	E	101	LMG	C31-C32-C33-C34
30	b	603	LMT	C4'-C5'-C6'-O6'
22	A	405	CLA	C16-C17-C18-C20
22	a	407	CLA	C16-C17-C18-C20
27	a	412	LMG	C10-C11-C12-C13
22	C	507	CLA	C5-C6-C7-C8
22	b	609	CLA	C13-C15-C16-C17
25	C	515	DGD	C5A-C6A-C7A-C8A
27	B	621	LMG	C12-C13-C14-C15
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	411	LHG	C6-C5-O7-C7
25	b	624	DGD	CCA-CDA-CEA-CFA
22	c	507	CLA	C5-C6-C7-C8
27	A	410	LMG	C10-C11-C12-C13
29	a	415	SQD	C11-C10-C9-C8
27	A	410	LMG	C16-C17-C18-C19
25	d	410	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
22	A	404	CLA	C6-C7-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	B	609	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C12-C13-C14
22	C	508	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	a	406	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	b	618	CLA	C6-C7-C8-C9
22	b	619	CLA	C11-C12-C13-C14
22	b	619	CLA	C14-C13-C15-C16
22	d	405	CLA	C6-C7-C8-C9
31	D	401	PHO	C6-C7-C8-C9
22	A	404	CLA	C6-C7-C8-C10
22	B	601	CLA	C6-C7-C8-C10
22	B	602	CLA	C11-C12-C13-C15
22	H	101	CLA	C11-C10-C8-C7
22	H	101	CLA	C12-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C10
31	D	402	PHO	C6-C7-C8-C10
22	b	617	CLA	C2C-C3C-CAC-CBC
26	c	519	LHG	C7-C8-C9-C10
27	c	518	LMG	C32-C33-C34-C35
29	A	412	SQD	C11-C10-C9-C8
27	A	410	LMG	O6-C1-O1-C7
22	b	616	CLA	C8-C10-C11-C12
27	A	414	LMG	C16-C17-C18-C19
25	c	516	DGD	C6A-C7A-C8A-C9A
22	B	610	CLA	C4-C3-C5-C6
27	c	522	LMG	C30-C31-C32-C33
22	c	510	CLA	C3-C5-C6-C7
27	A	410	LMG	C38-C39-C40-C41
25	c	516	DGD	C7B-C8B-C9B-CAB
27	B	621	LMG	C28-C29-C30-C31
22	C	504	CLA	C8-C10-C11-C12
27	d	409	LMG	O1-C7-C8-O7
25	B	620	DGD	CAB-CBB-CCB-CDB
27	C	518	LMG	C32-C33-C34-C35
27	D	408	LMG	C13-C14-C15-C16
34	F	101	HEM	C3D-CAD-CBD-CGD
27	a	402	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	a	406	CLA	C5-C6-C7-C8
22	a	405	CLA	C4-C3-C5-C6
23	d	407	PL9	C24-C26-C27-C28
27	e	101	LMG	O1-C7-C8-C9
29	B	622	SQD	O6-C44-C45-C46
25	d	410	DGD	CBB-CCB-CDB-CEB
22	C	511	CLA	CAA-CBA-CGA-O2A
24	f	102	BCR	C7-C8-C9-C34
25	D	410	DGD	CBB-CCB-CDB-CEB
23	d	407	PL9	C32-C33-C34-C36
24	C	514	BCR	C7-C8-C9-C10
22	b	609	CLA	CBA-CGA-O2A-C1
25	B	625	DGD	C2G-C3G-O3G-C1D
25	b	601	DGD	C2G-C3G-O3G-C1D
27	d	412	LMG	C8-C7-O1-C1
22	b	616	CLA	C10-C11-C12-C13
31	D	402	PHO	C13-C15-C16-C17
22	b	617	CLA	C2A-CAA-CBA-CGA
31	d	401	PHO	O1D-CGD-O2D-CED
27	a	412	LMG	C11-C12-C13-C14
26	c	519	LHG	O2-C2-C3-O3
23	D	407	PL9	C20-C19-C21-C22
27	b	625	LMG	C15-C16-C17-C18
25	C	516	DGD	C7B-C8B-C9B-CAB
27	A	414	LMG	C12-C13-C14-C15
22	B	607	CLA	C11-C12-C13-C14
22	B	615	CLA	C14-C13-C15-C16
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	508	CLA	C11-C10-C8-C9
22	c	510	CLA	C11-C10-C8-C9
31	D	402	PHO	C11-C10-C8-C9
31	d	402	PHO	C11-C10-C8-C9
22	B	609	CLA	CBA-CGA-O2A-C1
22	b	608	CLA	C4B-C3B-CAB-CBB
27	b	625	LMG	C12-C13-C14-C15
29	a	401	SQD	C12-C13-C14-C15
34	f	101	HEM	C3D-CAD-CBD-CGD
22	B	605	CLA	CBA-CGA-O2A-C1
22	h	101	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	C	515	DGD	C5B-C6B-C7B-C8B
25	b	624	DGD	O1A-C1A-O1G-C1G
22	b	614	CLA	C4-C3-C5-C6
22	c	511	CLA	CAA-CBA-CGA-O2A
29	A	413	SQD	C12-C13-C14-C15
27	C	521	LMG	C32-C33-C34-C35
27	d	412	LMG	C16-C17-C18-C19
22	C	506	CLA	C11-C10-C8-C7
22	C	520	CLA	C6-C7-C8-C10
22	D	405	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C10-C8-C7
22	b	609	CLA	O1A-CGA-O2A-C1
27	m	101	LMG	O10-C28-O8-C9
25	b	624	DGD	C4A-C5A-C6A-C7A
27	a	412	LMG	C35-C36-C37-C38
27	e	101	LMG	C31-C32-C33-C34
25	c	517	DGD	C8B-C9B-CAB-CBB
22	B	605	CLA	C13-C15-C16-C17
29	a	401	SQD	C26-C27-C28-C29
22	C	512	CLA	C3A-C2A-CAA-CBA
22	D	405	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
22	c	504	CLA	C8-C10-C11-C12
27	D	409	LMG	C36-C37-C38-C39
22	B	610	CLA	C2-C3-C5-C6
27	a	412	LMG	C8-C9-O8-C28
25	c	515	DGD	C5B-C6B-C7B-C8B
27	c	522	LMG	C32-C33-C34-C35
22	a	405	CLA	C2-C1-O2A-CGA
31	D	401	PHO	C2-C1-O2A-CGA
22	B	612	CLA	C8-C10-C11-C12
27	a	412	LMG	C29-C30-C31-C32
24	x	101	BCR	C7-C8-C9-C10
22	B	611	CLA	C2-C3-C5-C6
22	b	615	CLA	C2-C3-C5-C6
26	C	519	LHG	C1-C2-C3-O3
22	h	101	CLA	O1A-CGA-O2A-C1
22	b	618	CLA	CBA-CGA-O2A-C1
22	B	605	CLA	O1A-CGA-O2A-C1
22	B	609	CLA	O1A-CGA-O2A-C1
22	B	614	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	d	406	CLA	C11-C10-C8-C9
31	d	402	PHO	C6-C7-C8-C9
22	B	602	CLA	C16-C17-C18-C19
25	C	517	DGD	C8B-C9B-CAB-CBB
27	M	101	LMG	C16-C17-C18-C19
30	B	624	LMT	C6-C7-C8-C9
25	B	620	DGD	CCA-CDA-CEA-CFA
26	A	409	LHG	C4-C5-O7-C7
27	M	101	LMG	C9-C8-O7-C10
27	m	101	LMG	C9-C8-O7-C10
27	a	402	LMG	C12-C13-C14-C15
22	B	602	CLA	C15-C16-C17-C18
29	F	103	SQD	C24-C25-C26-C27
23	D	407	PL9	C40-C39-C41-C42
26	C	519	LHG	C7-C8-C9-C10
22	b	606	CLA	C16-C17-C18-C19
22	b	617	CLA	C4C-C3C-CAC-CBC
27	M	101	LMG	C31-C32-C33-C34
22	d	406	CLA	C2A-CAA-CBA-CGA
27	D	408	LMG	C29-C30-C31-C32
22	C	512	CLA	C1A-C2A-CAA-CBA
22	d	405	CLA	C1A-C2A-CAA-CBA
25	d	410	DGD	C8A-C9A-CAA-CBA
25	b	624	DGD	CAB-CBB-CCB-CDB
27	A	410	LMG	C17-C18-C19-C20
29	f	103	SQD	C14-C15-C16-C17
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	d	406	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
24	C	513	BCR	C5-C6-C7-C8
24	C	513	BCR	C23-C24-C25-C30
24	F	102	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	J	102	BCR	C5-C6-C7-C8
24	K	102	BCR	C23-C24-C25-C30
24	a	409	BCR	C1-C6-C7-C8
24	a	409	BCR	C23-C24-C25-C30
24	b	620	BCR	C5-C6-C7-C8
24	b	623	BCR	C1-C6-C7-C8
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	B	621	LMG	C15-C16-C17-C18
27	e	101	LMG	C30-C31-C32-C33
25	B	625	DGD	C2A-C3A-C4A-C5A
22	b	614	CLA	C2-C3-C5-C6
27	A	410	LMG	C35-C36-C37-C38
27	D	409	LMG	C18-C19-C20-C21
27	a	412	LMG	C38-C39-C40-C41
22	B	601	CLA	C12-C13-C15-C16
22	C	505	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C12-C13-C15
22	C	510	CLA	C11-C10-C8-C7
22	a	407	CLA	C11-C10-C8-C7
22	b	605	CLA	C6-C7-C8-C10
22	b	605	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10
22	c	508	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C10-C8-C7
31	D	402	PHO	C11-C10-C8-C7
31	d	402	PHO	C11-C10-C8-C7
22	c	509	CLA	C16-C17-C18-C19
27	d	408	LMG	C16-C17-C18-C19
29	F	103	SQD	C9-C10-C11-C12
25	b	601	DGD	C2A-C3A-C4A-C5A
27	m	101	LMG	C31-C32-C33-C34
26	c	519	LHG	C1-C2-C3-O3
22	C	510	CLA	C4-C3-C5-C6
22	B	612	CLA	C13-C15-C16-C17
27	C	521	LMG	C30-C31-C32-C33
22	C	507	CLA	C2-C1-O2A-CGA
22	b	608	CLA	C8-C10-C11-C12
24	F	102	BCR	C21-C22-C23-C24
22	b	609	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C11-C12-C13-C14
25	a	410	DGD	C2A-C3A-C4A-C5A
29	f	103	SQD	C9-C10-C11-C12
22	B	601	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
27	D	412	LMG	C16-C17-C18-C19
22	B	604	CLA	C8-C10-C11-C12
22	B	607	CLA	C13-C15-C16-C17
22	b	606	CLA	C15-C16-C17-C18
29	a	415	SQD	C12-C13-C14-C15
22	c	510	CLA	C4-C3-C5-C6
22	A	403	CLA	C2-C3-C5-C6
30	B	624	LMT	O5'-C5'-C6'-O6'
22	c	509	CLA	C13-C15-C16-C17
22	b	618	CLA	O1A-CGA-O2A-C1
27	d	408	LMG	C29-C30-C31-C32
25	B	620	DGD	C7B-C8B-C9B-CAB
25	C	517	DGD	C4A-C5A-C6A-C7A
25	C	515	DGD	C1G-C2G-C3G-O3G
27	d	412	LMG	O1-C7-C8-C9
30	b	604	LMT	C6-C7-C8-C9
22	c	510	CLA	C2A-CAA-CBA-CGA
25	c	517	DGD	CBB-CCB-CDB-CEB
22	B	605	CLA	C16-C17-C18-C20
23	d	407	PL9	C40-C39-C41-C42
22	B	604	CLA	C4B-C3B-CAB-CBB
22	d	406	CLA	C4B-C3B-CAB-CBB
27	D	412	LMG	C32-C33-C34-C35
27	D	408	LMG	C10-C11-C12-C13
25	A	408	DGD	C2A-C3A-C4A-C5A
27	D	412	LMG	C36-C37-C38-C39
22	c	510	CLA	C2-C3-C5-C6
25	c	515	DGD	O6D-C1D-O3G-C3G
22	C	512	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C10-C8-C7
25	C	516	DGD	C6A-C7A-C8A-C9A
22	A	403	CLA	C11-C10-C8-C9
22	C	512	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C11-C12-C13-C14
22	c	509	CLA	C11-C10-C8-C9
22	c	520	CLA	C6-C7-C8-C9
27	D	412	LMG	C8-C7-O1-C1
22	B	612	CLA	C2-C1-O2A-CGA
22	b	613	CLA	C2-C1-O2A-CGA
22	b	616	CLA	C2-C1-O2A-CGA
31	d	401	PHO	C2-C1-O2A-CGA
22	b	606	CLA	C16-C17-C18-C20
22	c	509	CLA	C16-C17-C18-C20
22	C	502	CLA	CBA-CGA-O2A-C1
22	A	405	CLA	C4-C3-C5-C6
22	C	520	CLA	C3A-C2A-CAA-CBA
22	a	407	CLA	C4-C3-C5-C6
22	c	520	CLA	C3A-C2A-CAA-CBA
22	C	502	CLA	O1A-CGA-O2A-C1
25	b	601	DGD	C4E-C5E-C6E-O5E
26	a	411	LHG	C4-C5-O7-C7
24	j	102	BCR	C18-C19-C20-C21
27	B	621	LMG	C35-C36-C37-C38
27	M	101	LMG	C30-C31-C32-C33
25	B	625	DGD	CAB-CBB-CCB-CDB
22	C	509	CLA	C13-C15-C16-C17
25	D	410	DGD	C4E-C5E-C6E-O5E
27	M	101	LMG	O10-C28-O8-C9
22	C	502	CLA	C16-C17-C18-C20
22	b	611	CLA	C13-C15-C16-C17
27	M	101	LMG	O6-C1-O1-C7
27	a	412	LMG	O6-C1-O1-C7
29	A	412	SQD	C16-C17-C18-C19
22	H	101	CLA	CBA-CGA-O2A-C1
25	c	515	DGD	C1G-C2G-C3G-O3G
27	C	518	LMG	C7-C8-C9-O8
27	I	101	LMG	C7-C8-C9-O8
27	c	518	LMG	C7-C8-C9-O8
22	H	101	CLA	O1A-CGA-O2A-C1
27	E	101	LMG	C30-C31-C32-C33
27	m	101	LMG	C16-C17-C18-C19
29	a	415	SQD	C16-C17-C18-C19
22	D	406	CLA	C2A-CAA-CBA-CGA
22	a	405	CLA	C2-C3-C5-C6
22	B	602	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	b	609	CLA	C16-C17-C18-C19
25	d	410	DGD	C9B-CAB-CBB-CCB
27	b	625	LMG	O1-C7-C8-O7
27	e	101	LMG	O1-C7-C8-O7
22	A	405	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C12-C13-C14
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	C	501	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C19
29	F	103	SQD	C14-C15-C16-C17
22	B	612	CLA	CAA-CBA-CGA-O2A
27	A	410	LMG	O7-C10-C11-C12
27	a	412	LMG	O7-C10-C11-C12
30	B	627	LMT	C4'-C5'-C6'-O6'
22	C	501	CLA	C13-C15-C16-C17
27	E	101	LMG	C33-C34-C35-C36
27	d	412	LMG	C11-C12-C13-C14
22	B	601	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C10-C8-C7
22	C	512	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C15
22	b	609	CLA	C6-C7-C8-C10
22	c	506	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	C12-C13-C15-C16
22	h	101	CLA	C12-C13-C15-C16
24	A	407	BCR	C5-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C26
24	B	619	BCR	C5-C6-C7-C8
24	B	619	BCR	C23-C24-C25-C26
24	C	514	BCR	C1-C6-C7-C8
24	K	102	BCR	C1-C6-C7-C8
24	K	102	BCR	C23-C24-C25-C26
24	a	409	BCR	C5-C6-C7-C8
24	a	409	BCR	C23-C24-C25-C26
24	b	623	BCR	C5-C6-C7-C8
24	b	623	BCR	C23-C24-C25-C26
24	c	514	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	c	514	BCR	C5-C6-C7-C8
24	c	521	BCR	C23-C24-C25-C30
22	b	616	CLA	CAA-CBA-CGA-O2A
26	C	519	LHG	O7-C7-C8-C9
26	c	519	LHG	O7-C7-C8-C9
22	A	402	CLA	C2-C1-O2A-CGA
22	A	403	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
29	A	412	SQD	C12-C13-C14-C15
22	B	611	CLA	CAA-CBA-CGA-O2A
22	d	405	CLA	CAA-CBA-CGA-O2A
25	B	625	DGD	O6D-C1D-O3G-C3G
25	a	410	DGD	O6E-C1E-O5D-C6D
30	B	623	LMT	C4-C5-C6-C7
22	C	506	CLA	CAA-CBA-CGA-O2A
25	b	601	DGD	CAB-CBB-CCB-CDB
22	b	606	CLA	C2A-CAA-CBA-CGA
27	b	625	LMG	C29-C28-O8-C9
22	B	605	CLA	C16-C17-C18-C19
27	c	518	LMG	C17-C18-C19-C20
22	b	609	CLA	C15-C16-C17-C18
27	A	414	LMG	O7-C10-C11-C12
27	d	412	LMG	C36-C37-C38-C39
34	V	201	HEM	CAA-CBA-CGA-O2A
22	C	501	CLA	CAA-CBA-CGA-O2A
25	C	517	DGD	O1G-C1A-C2A-C3A
23	A	406	PL9	C28-C29-C31-C32
25	a	410	DGD	O1A-C1A-O1G-C1G
22	C	510	CLA	C2A-CAA-CBA-CGA
29	a	401	SQD	C17-C18-C19-C20
22	c	506	CLA	CAA-CBA-CGA-O2A
27	c	522	LMG	O8-C28-C29-C30
29	a	401	SQD	O47-C7-C8-C9
22	A	404	CLA	O1A-CGA-O2A-C1
34	v	201	HEM	CAA-CBA-CGA-O2A
22	C	505	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C12-C13-C14
22	C	520	CLA	C6-C7-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	D	406	CLA	C11-C10-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	a	407	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C14-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C10-C8-C9
24	b	623	BCR	C7-C8-C9-C34
22	C	509	CLA	CAA-CBA-CGA-O2A
25	c	517	DGD	O1G-C1A-C2A-C3A
29	A	413	SQD	O47-C7-C8-C9
26	A	409	LHG	C24-C25-C26-C27
26	c	519	LHG	C11-C12-C13-C14
27	E	101	LMG	O1-C7-C8-C9
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	D	406	CLA	C4B-C3B-CAB-CBB
22	a	405	CLA	C4B-C3B-CAB-CBB
22	b	618	CLA	C4B-C3B-CAB-CBB
22	c	508	CLA	C4B-C3B-CAB-CBB
22	c	512	CLA	C1A-C2A-CAA-CBA
25	C	515	DGD	O6D-C1D-O3G-C3G
25	C	516	DGD	O6E-C1E-O5D-C6D
25	b	601	DGD	O6D-C1D-O3G-C3G
25	c	516	DGD	O6E-C1E-O5D-C6D
27	m	101	LMG	O6-C1-O1-C7
22	b	615	CLA	CAA-CBA-CGA-O2A
27	a	402	LMG	O7-C10-C11-C12
27	B	621	LMG	O1-C7-C8-O7
24	f	102	BCR	C21-C22-C23-C24
22	c	501	CLA	CAA-CBA-CGA-O2A
27	C	521	LMG	O8-C28-C29-C30
29	B	622	SQD	O47-C7-C8-C9
27	e	101	LMG	C14-C15-C16-C17
29	A	413	SQD	C26-C27-C28-C29
22	B	610	CLA	C16-C17-C18-C19
22	c	509	CLA	CAA-CBA-CGA-O2A
29	B	622	SQD	C5-C6-S-O9
29	a	401	SQD	C5-C6-S-O9
29	d	403	SQD	C5-C6-S-O9
22	B	613	CLA	C2C-C3C-CAC-CBC
29	d	403	SQD	O47-C7-C8-C9
22	B	602	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C12-C13-C15
22	C	506	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	C11-C10-C8-C7
22	c	512	CLA	C11-C12-C13-C15
25	a	410	DGD	C4A-C5A-C6A-C7A
22	C	501	CLA	C16-C17-C18-C19
22	C	509	CLA	C16-C17-C18-C20
22	c	502	CLA	C16-C17-C18-C20
27	M	101	LMG	C7-C8-O7-C10
22	D	405	CLA	CAA-CBA-CGA-O2A
22	b	606	CLA	C8-C10-C11-C12
22	A	404	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	C2A-CAA-CBA-CGA
25	c	517	DGD	C5B-C6B-C7B-C8B
34	V	201	HEM	CAA-CBA-CGA-O1A
22	B	603	CLA	C4C-C3C-CAC-CBC
25	B	620	DGD	C4A-C5A-C6A-C7A
29	A	413	SQD	C17-C18-C19-C20
25	c	517	DGD	C4A-C5A-C6A-C7A
25	C	517	DGD	O2G-C1B-C2B-C3B
22	B	601	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C10-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C12-C13-C14
31	D	402	PHO	C6-C7-C8-C9
22	b	616	CLA	CAA-CBA-CGA-O1A
29	B	622	SQD	O49-C7-C8-C9
22	B	601	CLA	C5-C6-C7-C8
25	C	517	DGD	C4B-C5B-C6B-C7B
27	C	521	LMG	O10-C28-C29-C30
29	d	403	SQD	O49-C7-C8-C9
27	D	409	LMG	C34-C35-C36-C37
27	D	409	LMG	O7-C10-C11-C12
29	d	403	SQD	O5-C5-C6-S
22	B	613	CLA	C4C-C3C-CAC-CBC
30	B	628	LMT	C6-C7-C8-C9
27	d	412	LMG	O9-C10-C11-C12
22	D	405	CLA	C3-C5-C6-C7
22	b	615	CLA	C3-C5-C6-C7
34	v	201	HEM	CAA-CBA-CGA-O1A
27	B	621	LMG	C29-C28-O8-C9
22	c	509	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	D	412	LMG	O9-C10-C11-C12
25	A	408	DGD	C5D-C6D-O5D-C1E
25	a	410	DGD	C5D-C6D-O5D-C1E
27	i	101	LMG	C8-C7-O1-C1
27	C	518	LMG	O7-C8-C9-O8
22	B	611	CLA	CAA-CBA-CGA-O1A
22	B	612	CLA	CAA-CBA-CGA-O1A
22	C	506	CLA	CAA-CBA-CGA-O1A
22	C	509	CLA	CAA-CBA-CGA-O1A
22	b	615	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
27	D	408	LMG	C7-C8-C9-O8
25	A	408	DGD	O6D-C5D-C6D-O5D
25	D	410	DGD	C8A-C9A-CAA-CBA
29	A	412	SQD	C9-C10-C11-C12
22	c	501	CLA	CAA-CBA-CGA-O1A
22	d	405	CLA	CAA-CBA-CGA-O1A
30	b	627	LMT	O5'-C5'-C6'-O6'
25	C	517	DGD	CBB-CCB-CDB-CEB
25	b	601	DGD	C8B-C9B-CAB-CBB
22	D	406	CLA	C8-C10-C11-C12
25	B	620	DGD	O2G-C1B-C2B-C3B
25	c	517	DGD	O2G-C1B-C2B-C3B
27	M	101	LMG	O8-C28-C29-C30
22	C	510	CLA	C2-C3-C5-C6
23	a	408	PL9	C28-C29-C31-C32
29	A	413	SQD	O49-C7-C8-C9
22	c	512	CLA	C16-C17-C18-C20
22	C	506	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
22	B	602	CLA	C8-C10-C11-C12
29	a	401	SQD	O49-C7-C8-C9
27	m	101	LMG	C17-C18-C19-C20
22	B	609	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
26	C	519	LHG	C11-C12-C13-C14
27	M	101	LMG	C17-C18-C19-C20
29	a	415	SQD	C32-C33-C34-C35
27	a	402	LMG	O9-C10-C11-C12
27	c	522	LMG	O10-C28-C29-C30
25	b	624	DGD	O2G-C1B-C2B-C3B
27	d	409	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	610	CLA	C16-C17-C18-C20
27	E	101	LMG	C14-C15-C16-C17
22	C	503	CLA	C15-C16-C17-C18
22	c	502	CLA	O1A-CGA-O2A-C1
29	a	401	SQD	C23-C24-C25-C26
27	d	412	LMG	C32-C33-C34-C35
22	B	601	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	CAA-CBA-CGA-O2A
22	b	613	CLA	CAA-CBA-CGA-O2A
22	h	101	CLA	CAA-CBA-CGA-O2A
27	m	101	LMG	O8-C28-C29-C30
22	c	502	CLA	C5-C6-C7-C8
22	C	501	CLA	CAA-CBA-CGA-O1A
22	D	405	CLA	CAA-CBA-CGA-O1A
27	a	412	LMG	O9-C10-C11-C12
23	A	406	PL9	C2-C3-C7-C8
25	D	410	DGD	C9B-CAB-CBB-CCB
22	b	617	CLA	CAA-CBA-CGA-O2A
27	a	412	LMG	C13-C14-C15-C16
29	f	103	SQD	C27-C28-C29-C30
25	C	517	DGD	O1A-C1A-C2A-C3A
27	A	410	LMG	O9-C10-C11-C12
22	B	603	CLA	C2C-C3C-CAC-CBC
27	d	409	LMG	C34-C35-C36-C37
29	B	626	SQD	C15-C16-C17-C18

There are no ring outliers.

158 monomers are involved in 440 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	i	102	LMT	1	0
26	C	519	LHG	2	0
22	C	501	CLA	2	0
22	c	510	CLA	4	0
22	d	405	CLA	8	0
27	d	412	LMG	1	0
22	A	405	CLA	1	0
30	b	604	LMT	2	0
29	B	622	SQD	3	0
25	C	517	DGD	5	0
27	a	412	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	514	BCR	4	0
22	B	613	CLA	3	0
22	C	509	CLA	4	0
22	C	520	CLA	2	0
22	B	611	CLA	4	0
22	b	608	CLA	7	0
24	y	101	BCR	7	0
22	B	612	CLA	3	0
22	b	619	CLA	4	0
24	A	407	BCR	3	0
25	b	624	DGD	2	0
22	c	504	CLA	3	0
26	A	409	LHG	3	0
22	c	508	CLA	3	0
27	i	101	LMG	1	0
22	a	406	CLA	6	0
24	B	617	BCR	2	0
24	g	101	BCR	5	0
27	D	408	LMG	2	0
22	B	606	CLA	6	0
27	d	409	LMG	6	0
22	C	505	CLA	1	0
22	c	512	CLA	3	0
27	e	101	LMG	1	0
22	a	405	CLA	9	0
30	B	627	LMT	2	0
22	B	604	CLA	6	0
22	a	404	CLA	10	0
22	C	504	CLA	4	0
27	d	408	LMG	3	0
31	D	402	PHO	5	0
26	a	411	LHG	1	0
22	C	508	CLA	1	0
22	c	505	CLA	1	0
25	C	516	DGD	3	0
22	b	612	CLA	5	0
22	b	617	CLA	2	0
22	C	512	CLA	3	0
22	H	101	CLA	8	0
22	b	610	CLA	6	0
34	v	201	HEM	5	0
22	C	507	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	401	PHO	7	0
22	c	509	CLA	3	0
22	A	403	CLA	14	0
25	c	517	DGD	5	0
27	A	410	LMG	2	0
22	B	603	CLA	2	0
27	D	412	LMG	1	0
22	B	605	CLA	7	0
25	D	410	DGD	1	0
23	J	101	PL9	1	0
27	b	625	LMG	5	0
24	b	621	BCR	1	0
31	d	402	PHO	4	0
29	f	103	SQD	3	0
22	C	506	CLA	3	0
24	B	619	BCR	1	0
29	a	401	SQD	5	0
22	a	407	CLA	1	0
22	B	614	CLA	1	0
34	F	101	HEM	4	0
27	a	402	LMG	1	0
29	A	412	SQD	4	0
22	D	405	CLA	8	0
22	b	609	CLA	5	0
25	B	625	DGD	2	0
24	B	616	BCR	5	0
25	b	601	DGD	2	0
22	A	402	CLA	10	0
23	D	407	PL9	8	0
22	c	507	CLA	4	0
24	j	102	BCR	1	0
27	C	518	LMG	3	0
34	f	101	HEM	4	0
30	b	603	LMT	2	0
22	c	501	CLA	4	0
22	b	614	CLA	2	0
22	b	618	CLA	2	0
22	b	613	CLA	1	0
29	A	413	SQD	4	0
22	b	607	CLA	2	0
22	B	610	CLA	3	0
22	C	511	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	616	CLA	3	0
24	c	521	BCR	4	0
22	B	607	CLA	7	0
22	B	608	CLA	5	0
27	B	621	LMG	3	0
22	c	520	CLA	4	0
25	A	408	DGD	1	0
29	a	415	SQD	3	0
24	b	622	BCR	3	0
25	d	410	DGD	2	0
24	f	102	BCR	2	0
24	H	102	BCR	3	0
24	F	102	BCR	3	0
22	b	615	CLA	4	0
27	M	101	LMG	2	0
24	C	513	BCR	5	0
22	b	606	CLA	9	0
24	b	623	BCR	4	0
30	B	623	LMT	2	0
24	b	620	BCR	6	0
34	V	201	HEM	5	0
22	C	503	CLA	3	0
22	c	506	CLA	4	0
25	c	516	DGD	2	0
22	d	406	CLA	3	0
22	A	404	CLA	4	0
29	B	626	SQD	1	0
24	B	618	BCR	4	0
31	d	401	PHO	6	0
27	c	522	LMG	1	0
25	a	410	DGD	2	0
27	c	518	LMG	2	0
22	B	601	CLA	1	0
22	B	615	CLA	4	0
30	B	628	LMT	2	0
24	a	409	BCR	2	0
22	B	602	CLA	10	0
24	c	513	BCR	7	0
22	D	406	CLA	2	0
23	A	406	PL9	4	0
24	J	102	BCR	1	0
27	m	101	LMG	1	0

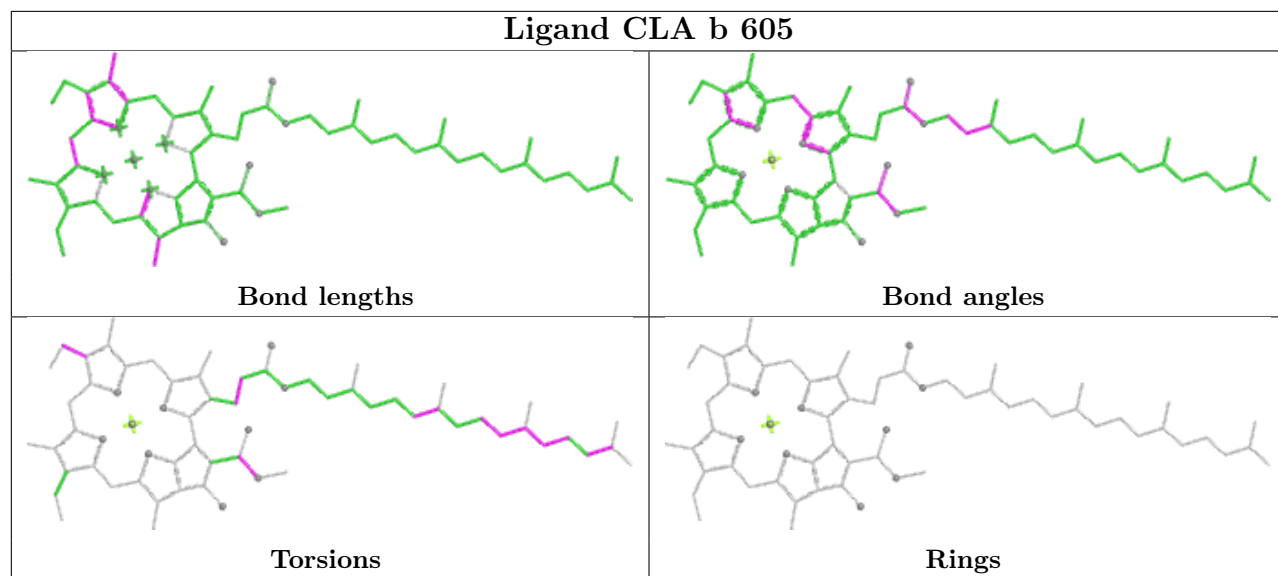
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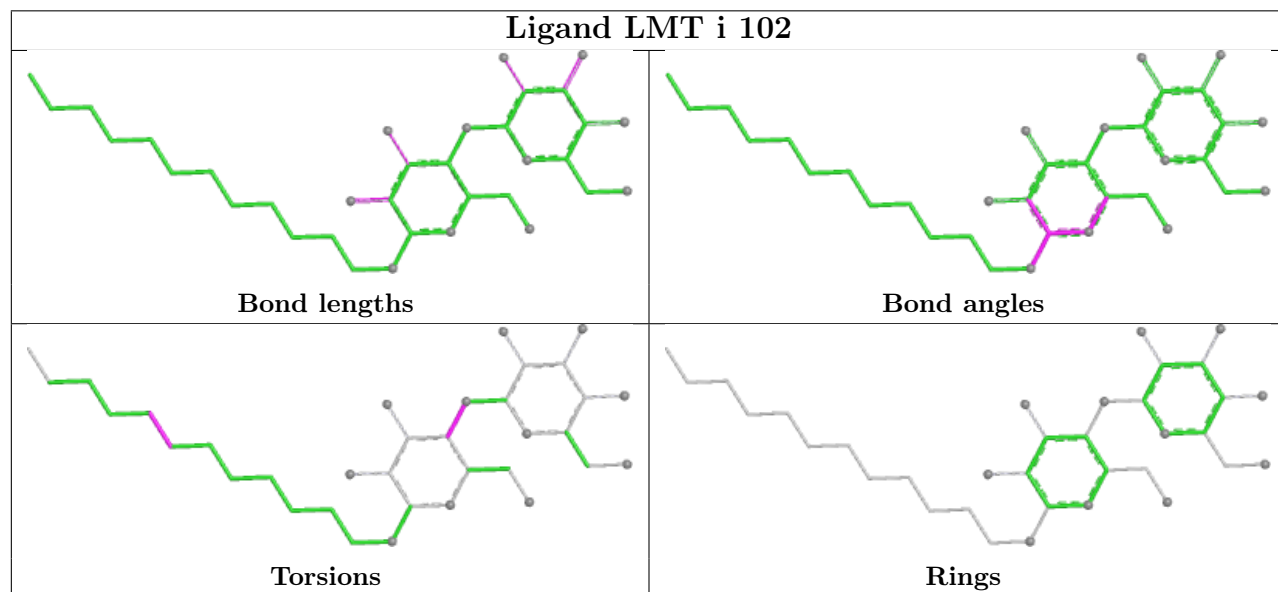
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	510	CLA	5	0
22	b	611	CLA	8	0
24	x	101	BCR	1	0
27	D	409	LMG	6	0
22	c	503	CLA	2	0
23	a	408	PL9	3	0
25	c	515	DGD	3	0
30	b	626	LMT	1	0
29	d	403	SQD	4	0
29	b	602	SQD	1	0
25	B	620	DGD	2	0
22	c	511	CLA	2	0
22	h	101	CLA	9	0
23	d	407	PL9	6	0
27	E	101	LMG	1	0
25	C	515	DGD	3	0
24	C	514	BCR	6	0
27	A	414	LMG	1	0
26	c	519	LHG	2	0
24	K	102	BCR	3	0
29	F	103	SQD	2	0

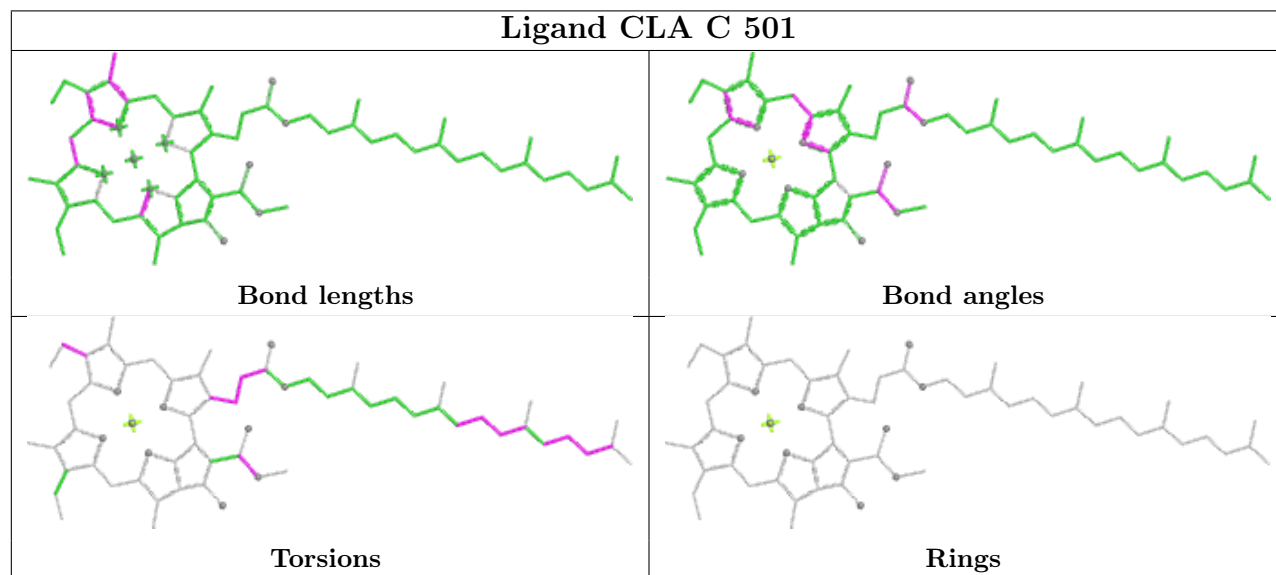
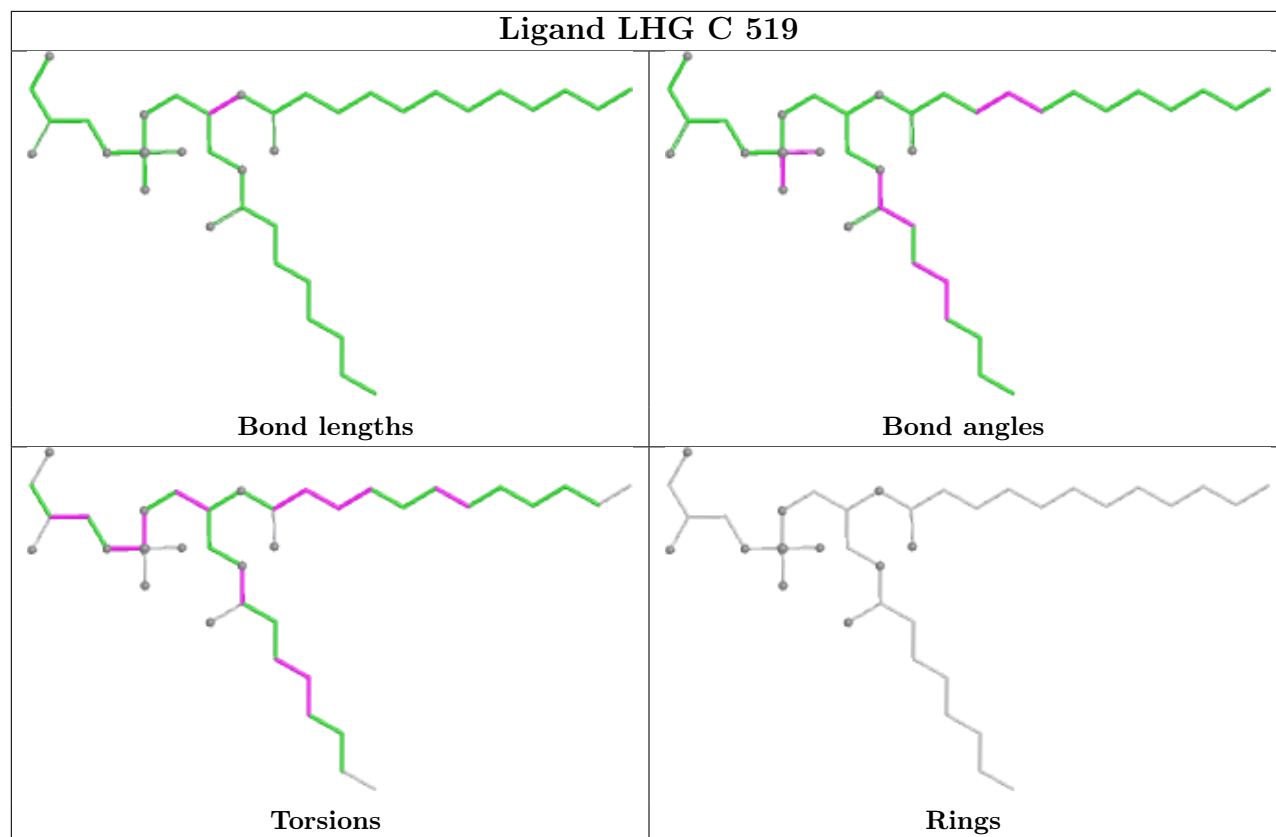
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

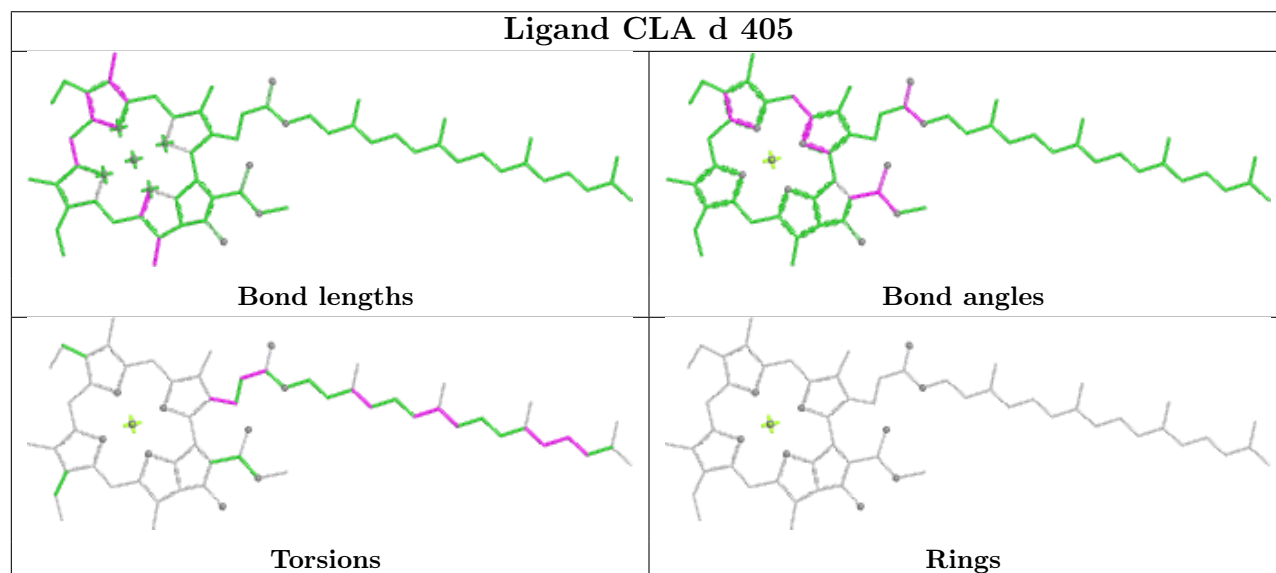
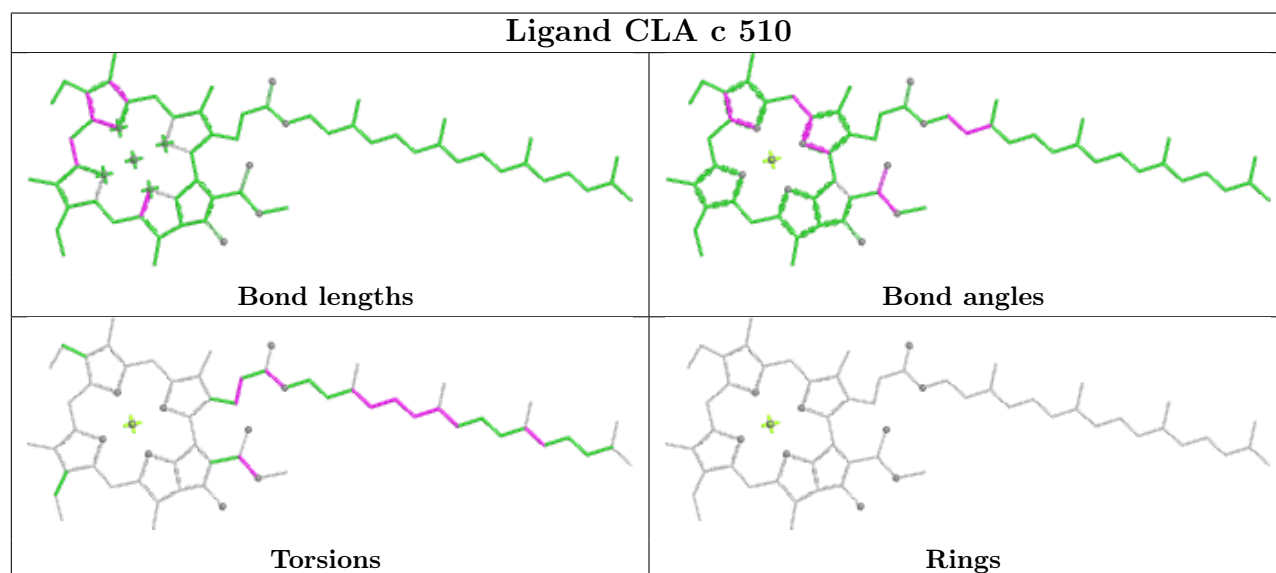
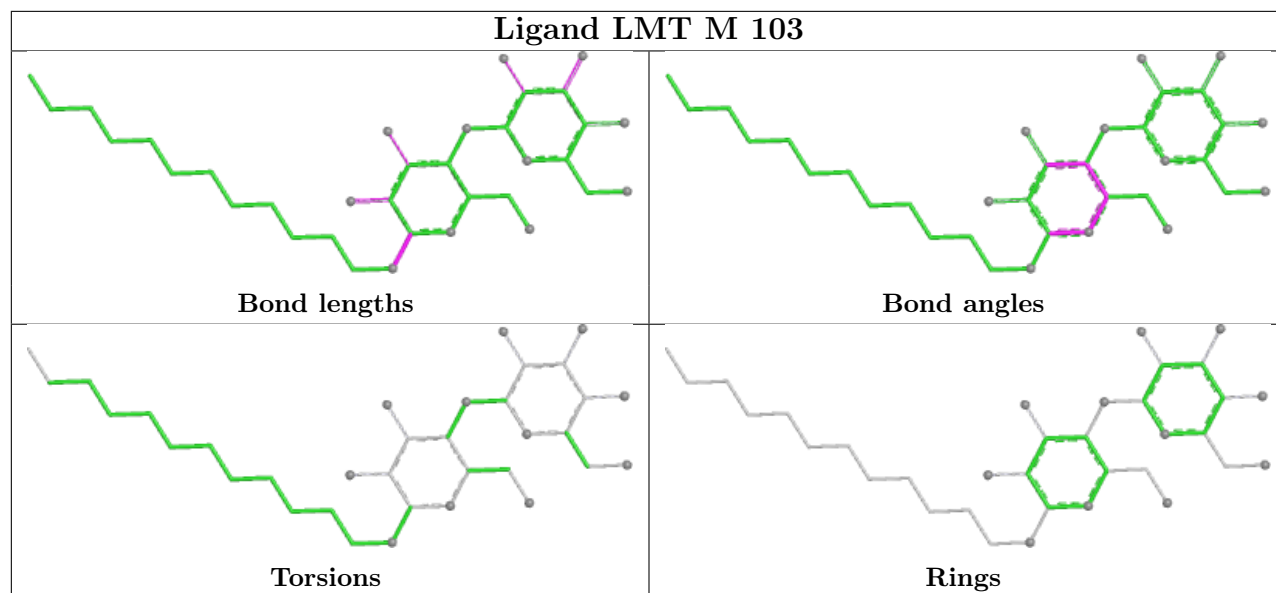
Ligand CLA b 605

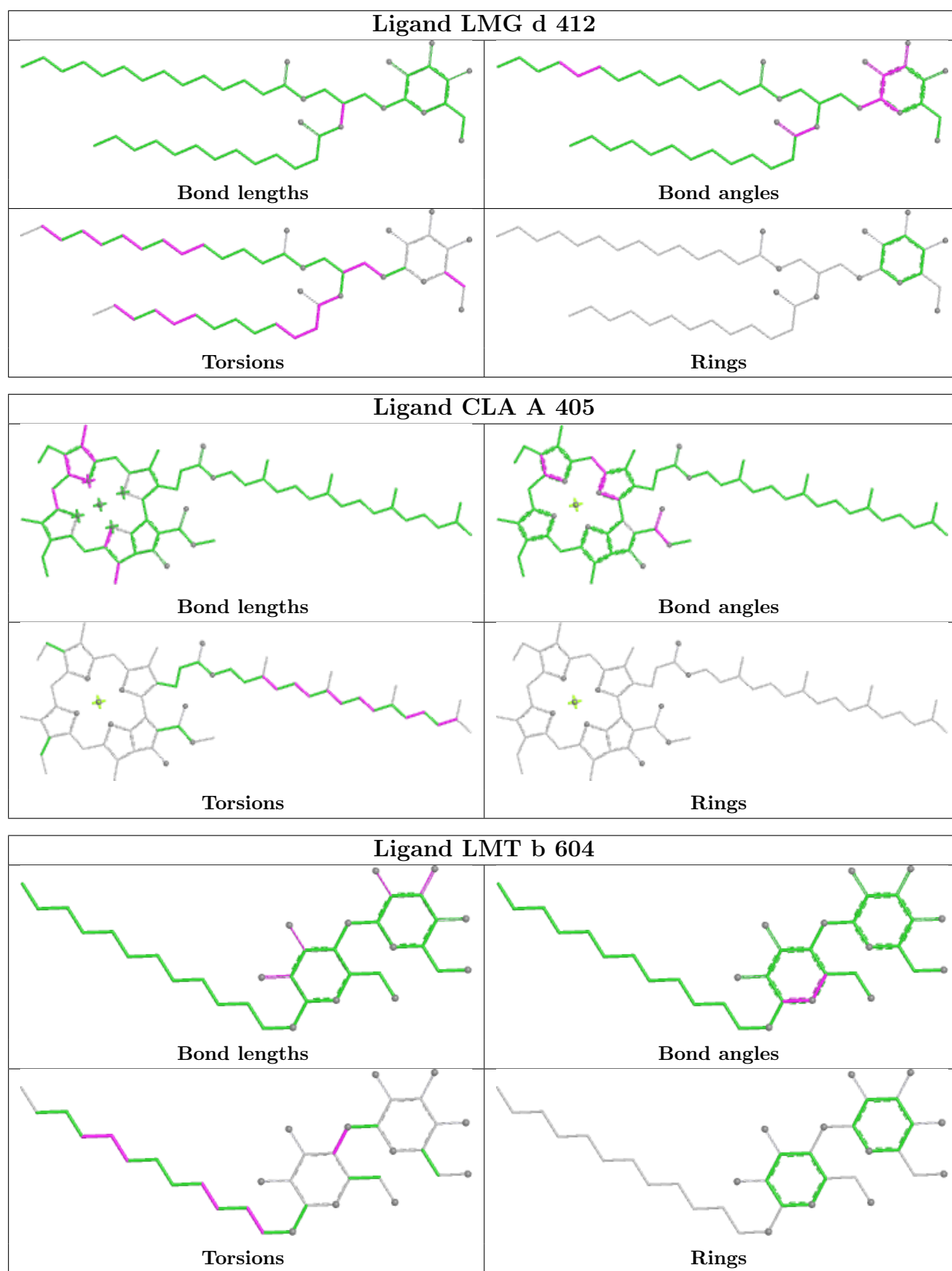


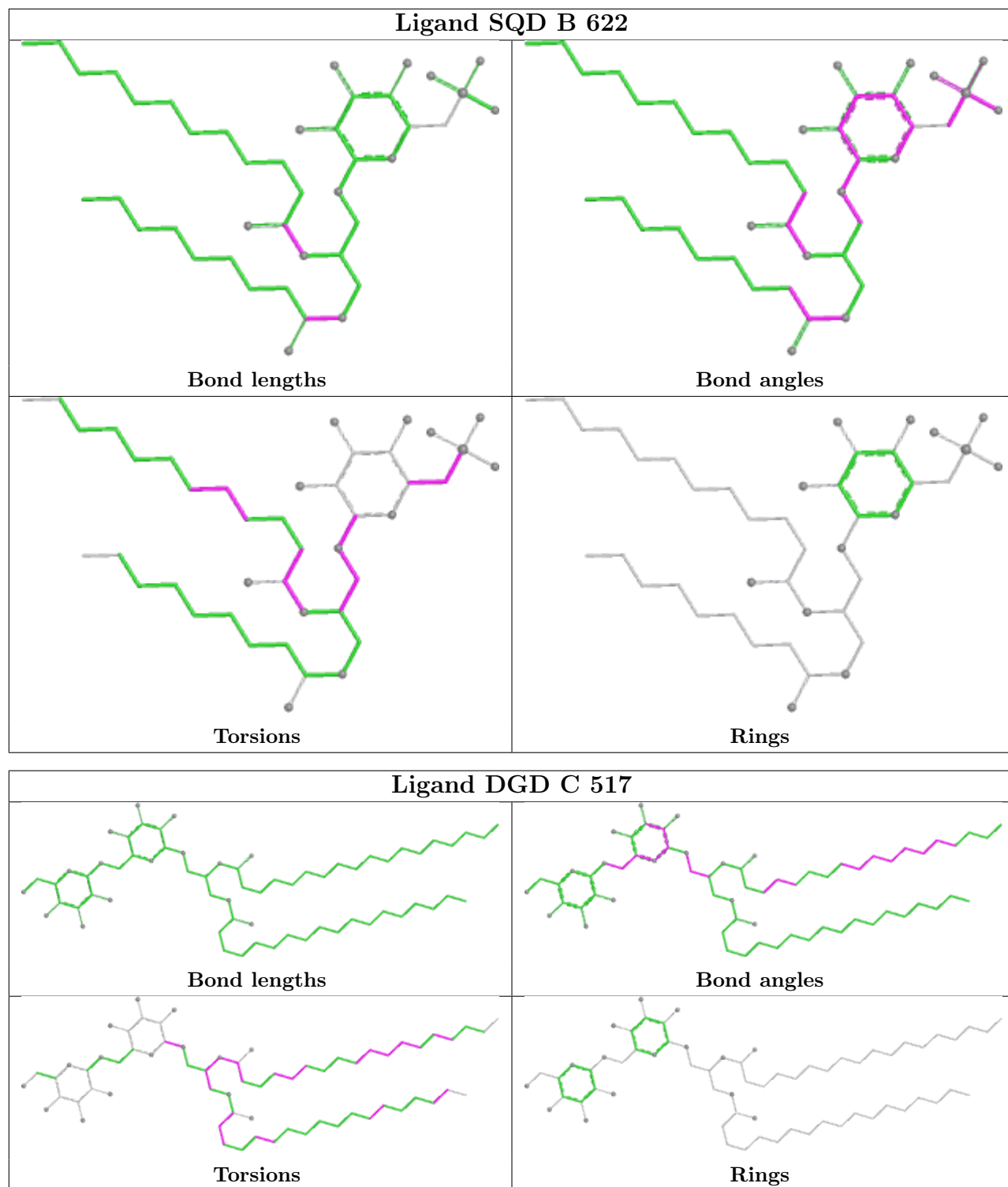
Ligand LMT i 102

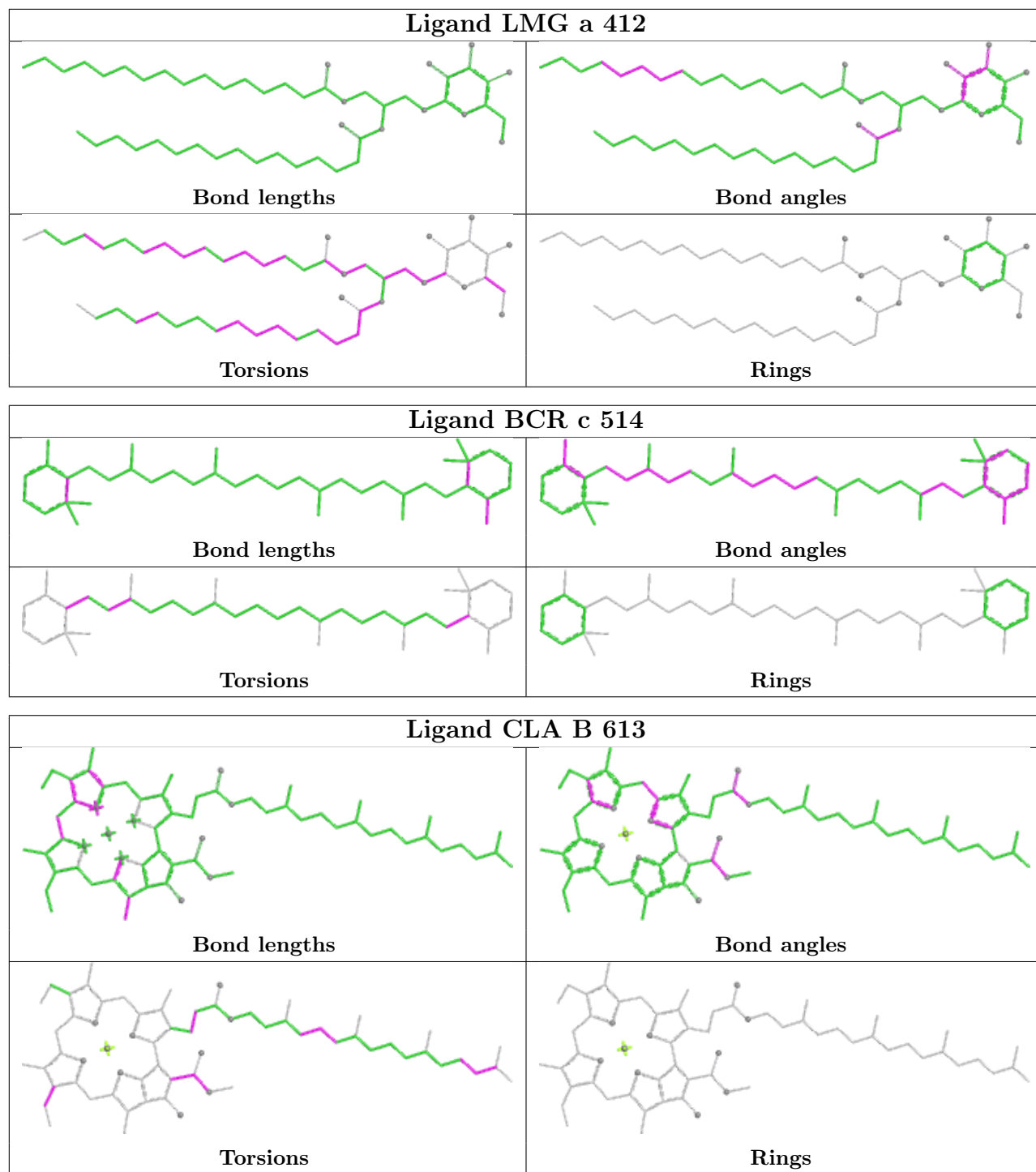




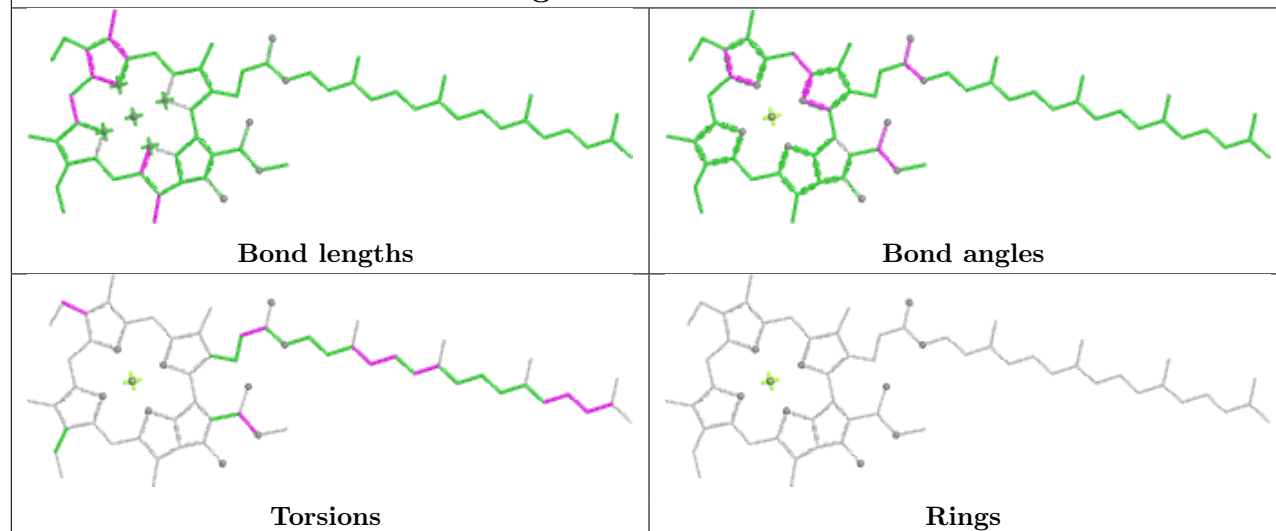




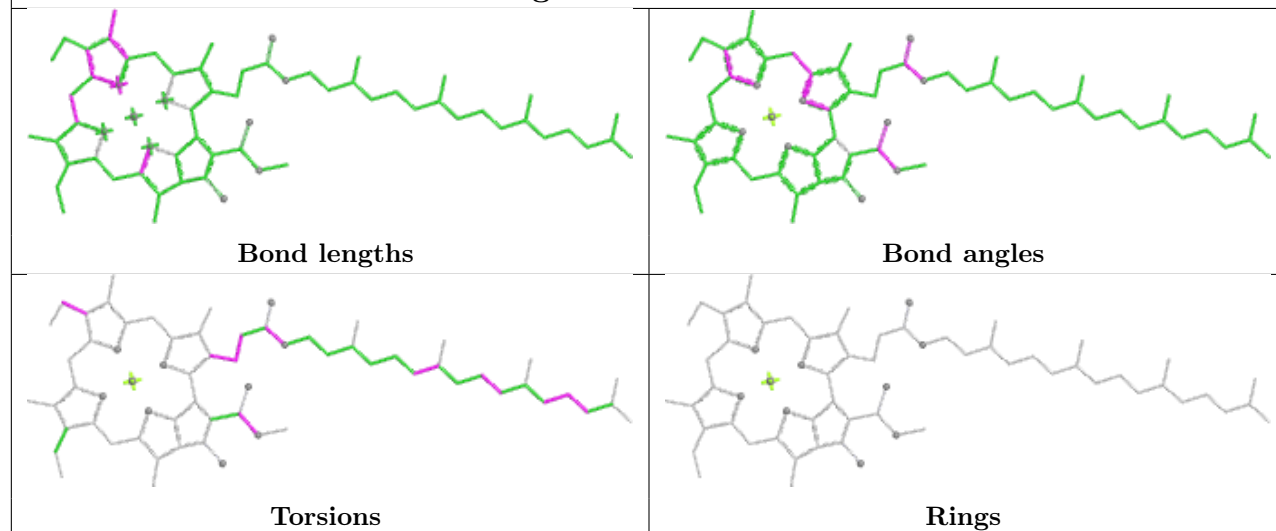




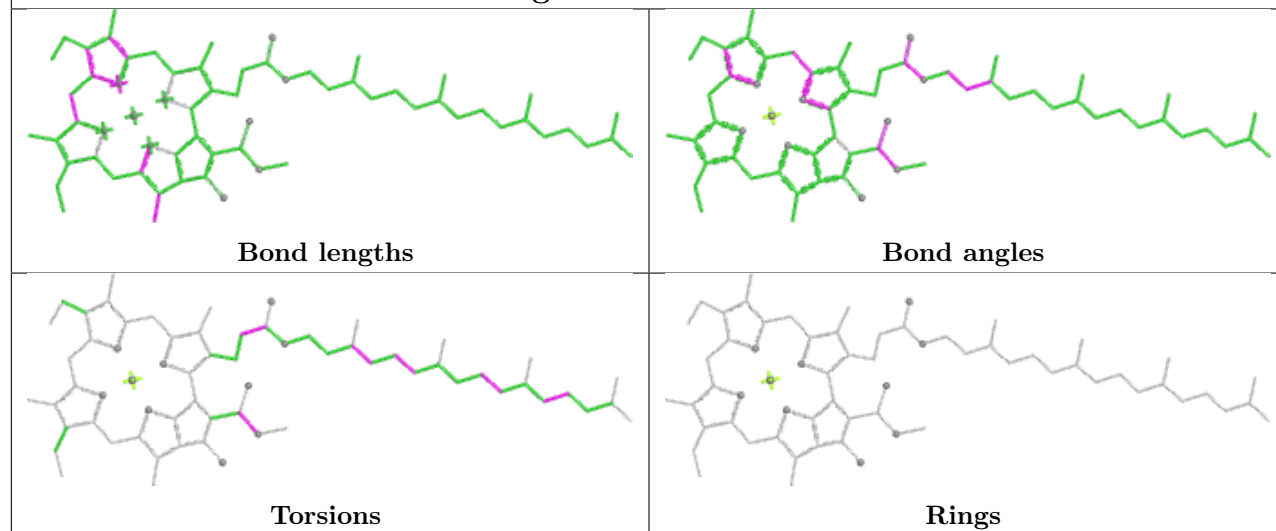
Ligand CLA C 509

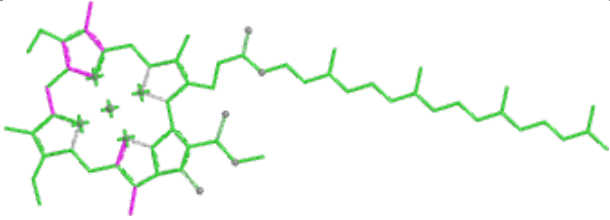
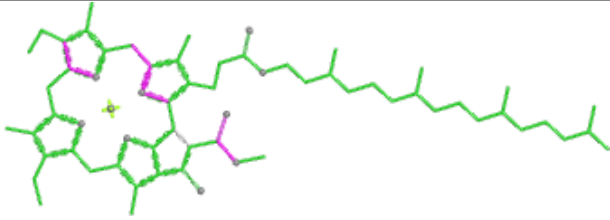
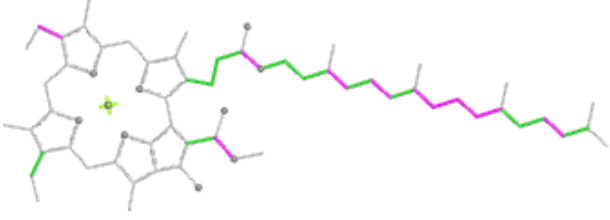
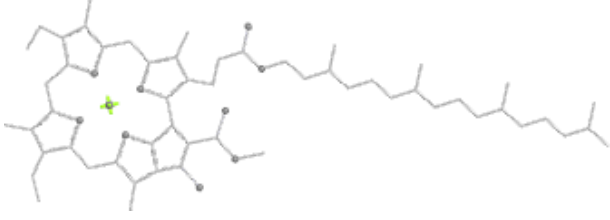
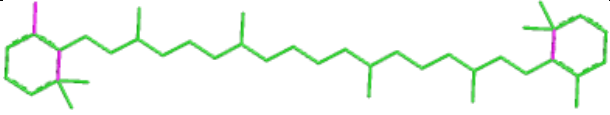
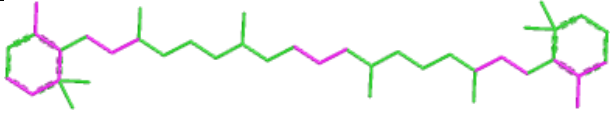
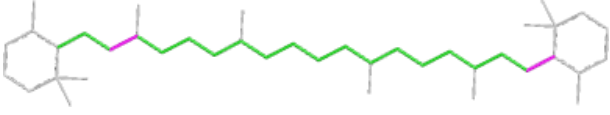
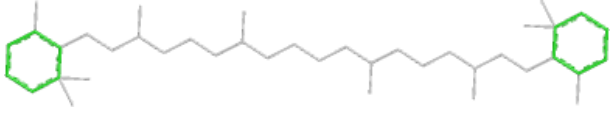
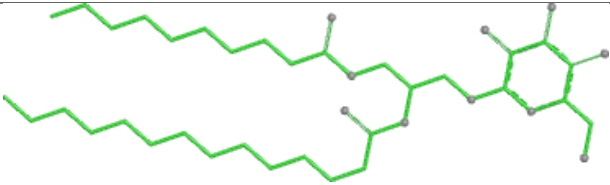
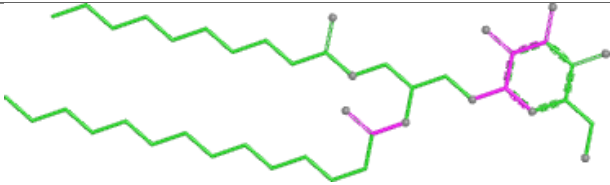
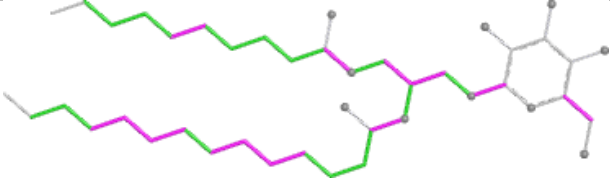
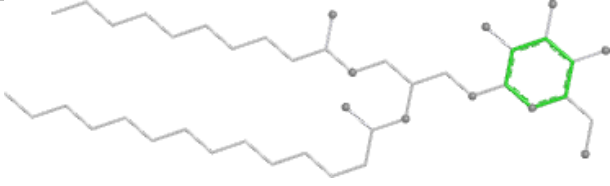


Ligand CLA C 520

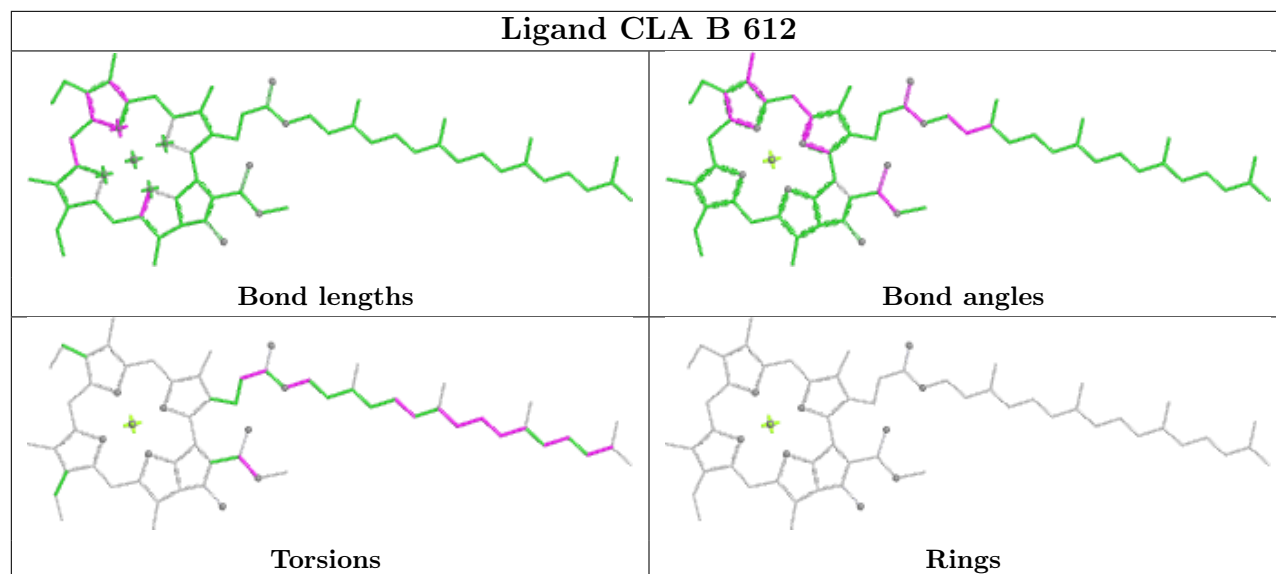


Ligand CLA B 611

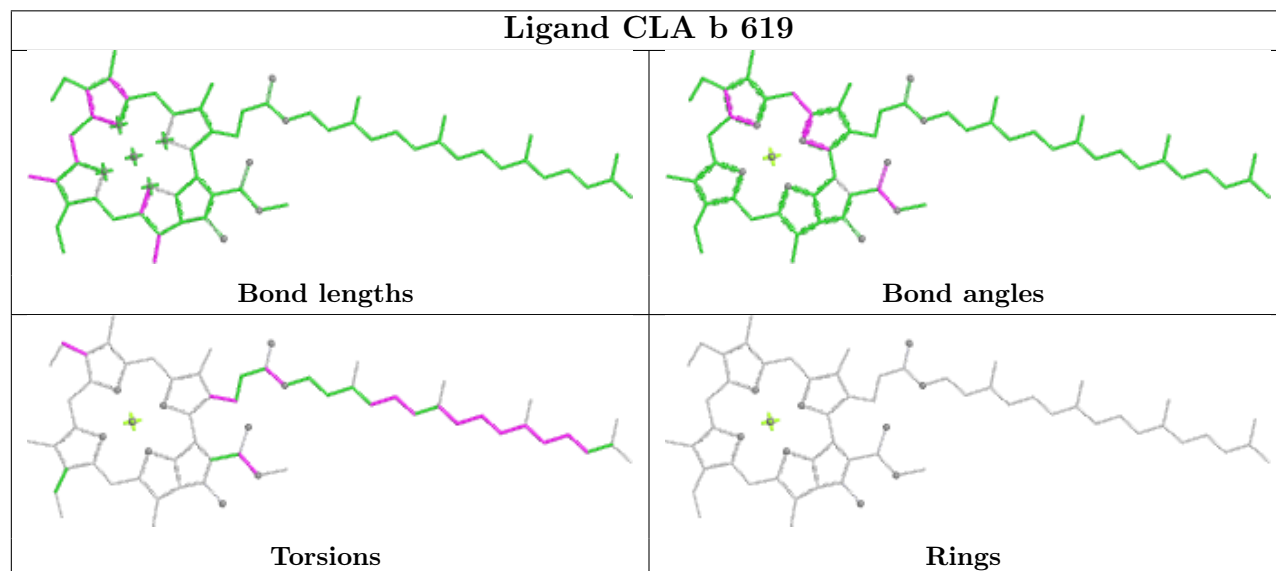


Ligand CLA b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

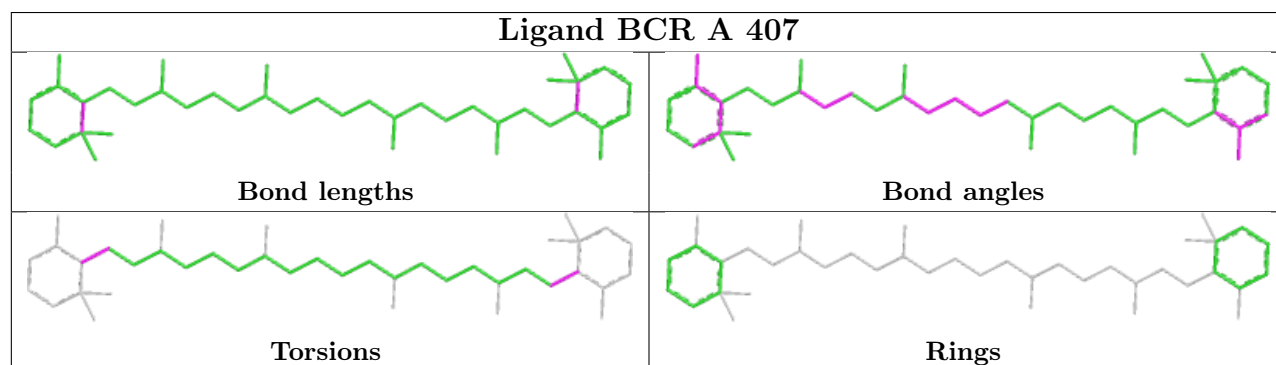
Ligand CLA B 612

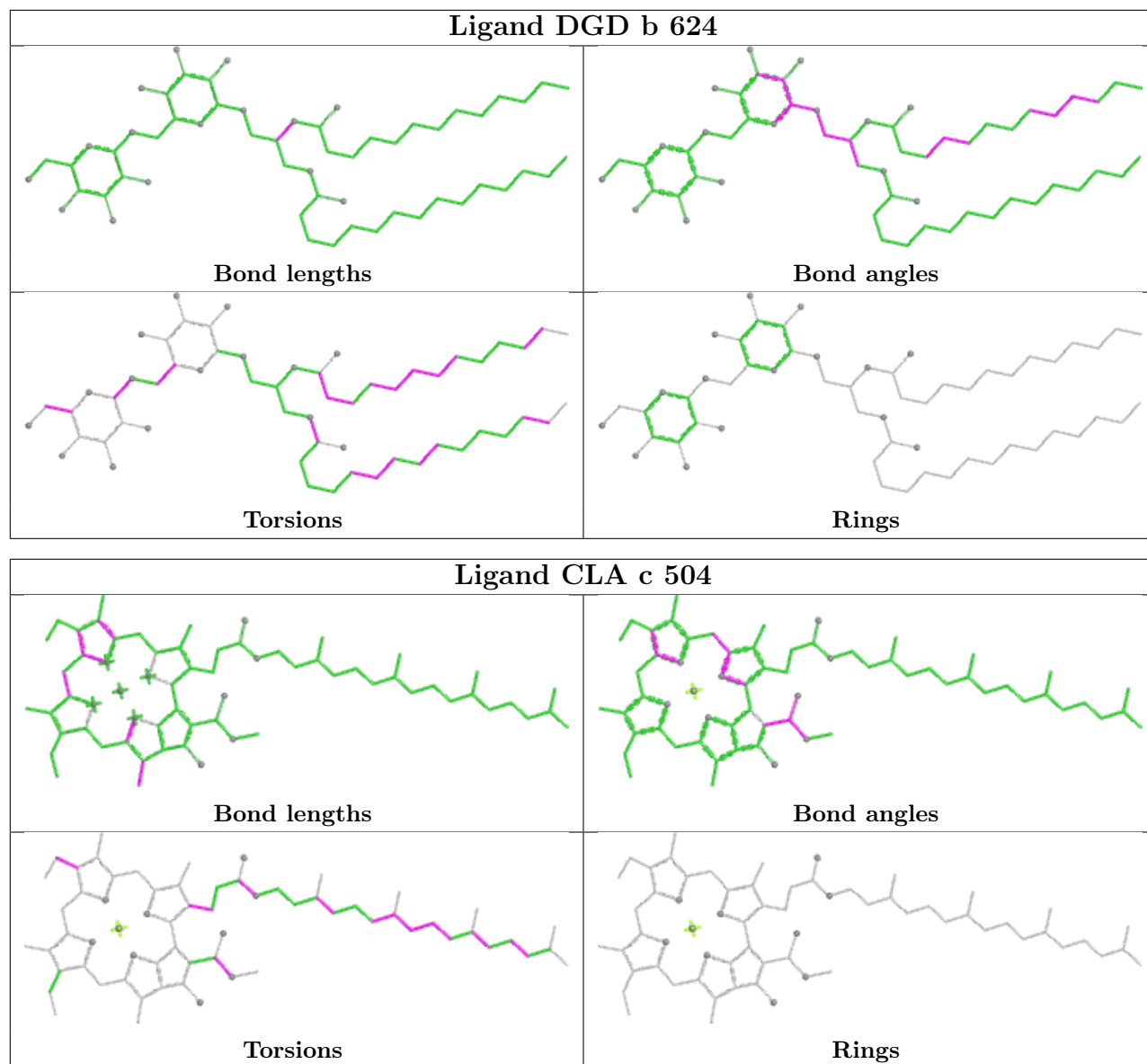


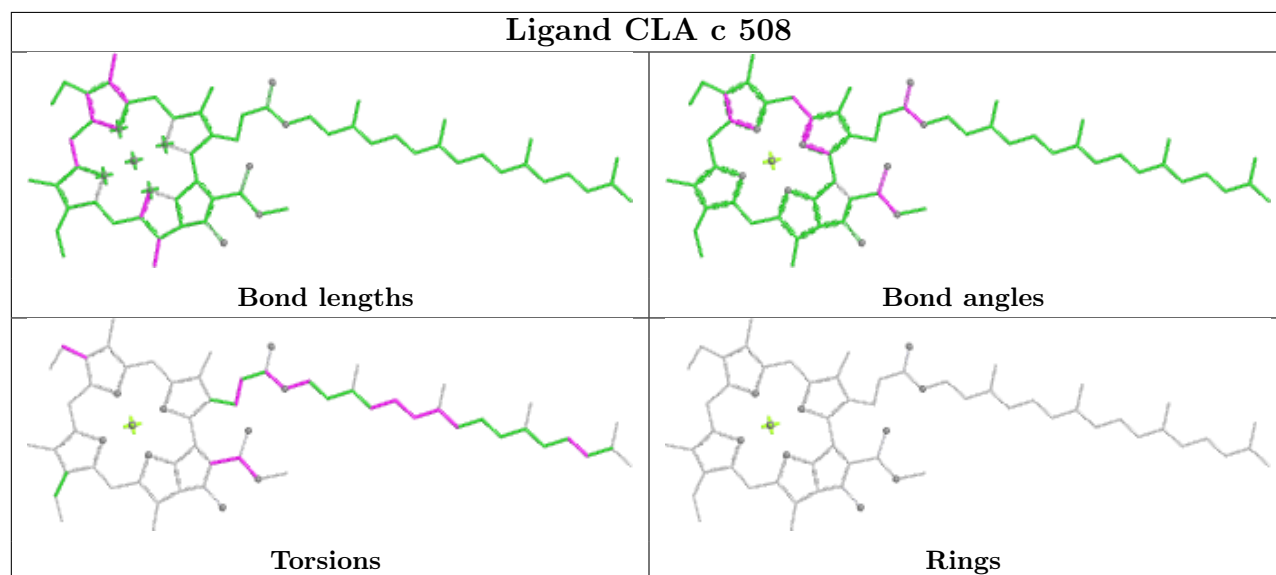
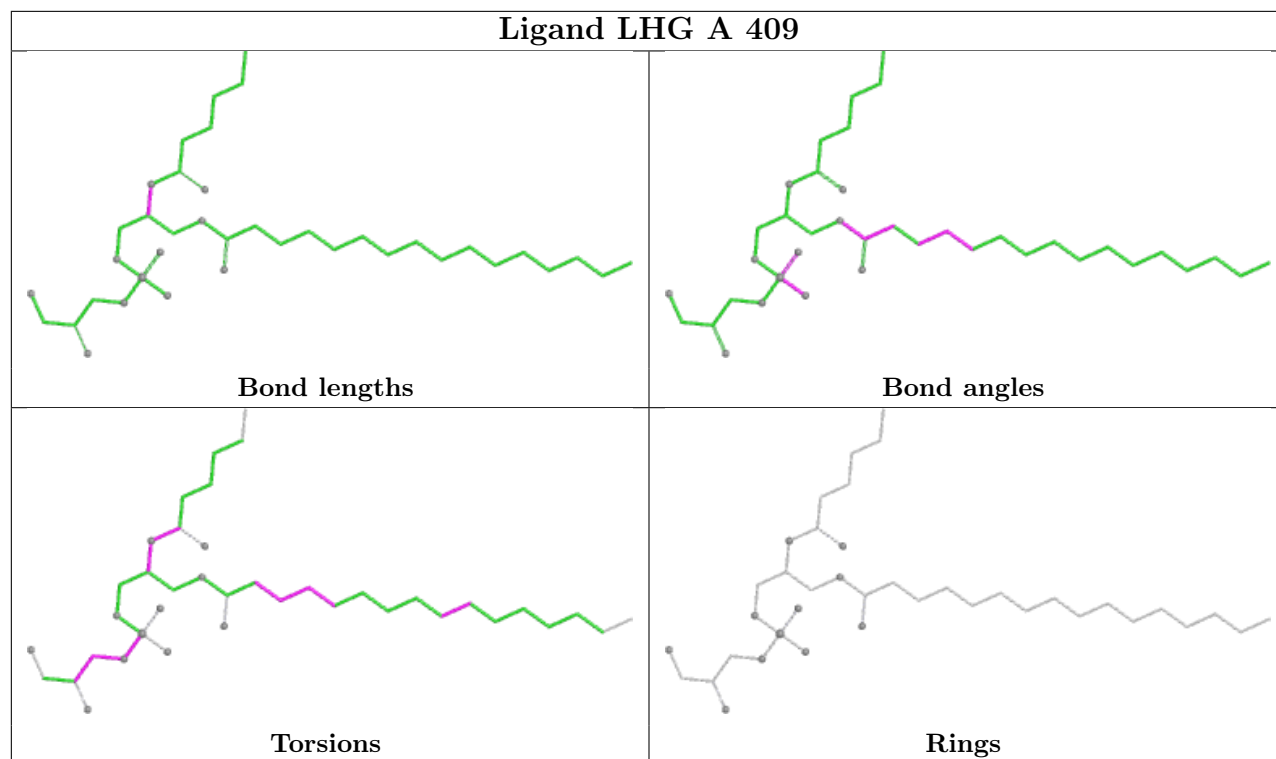
Ligand CLA b 619

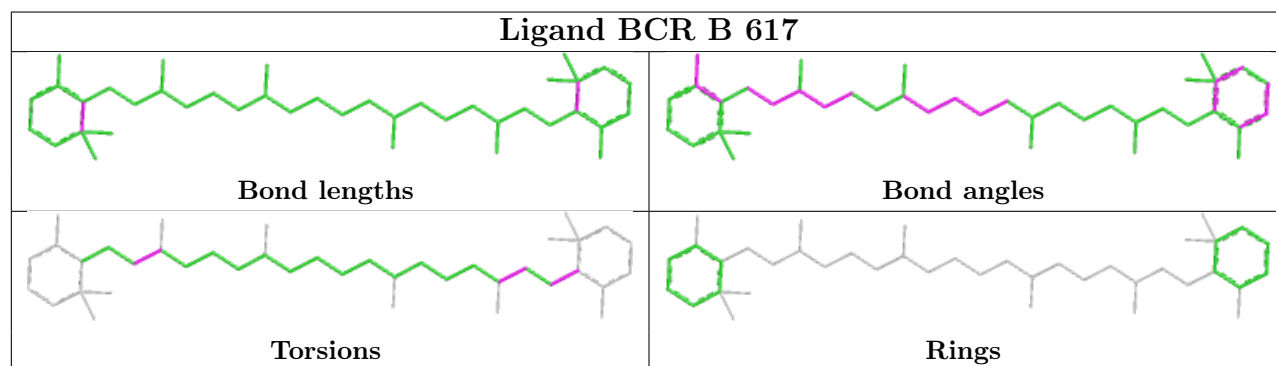
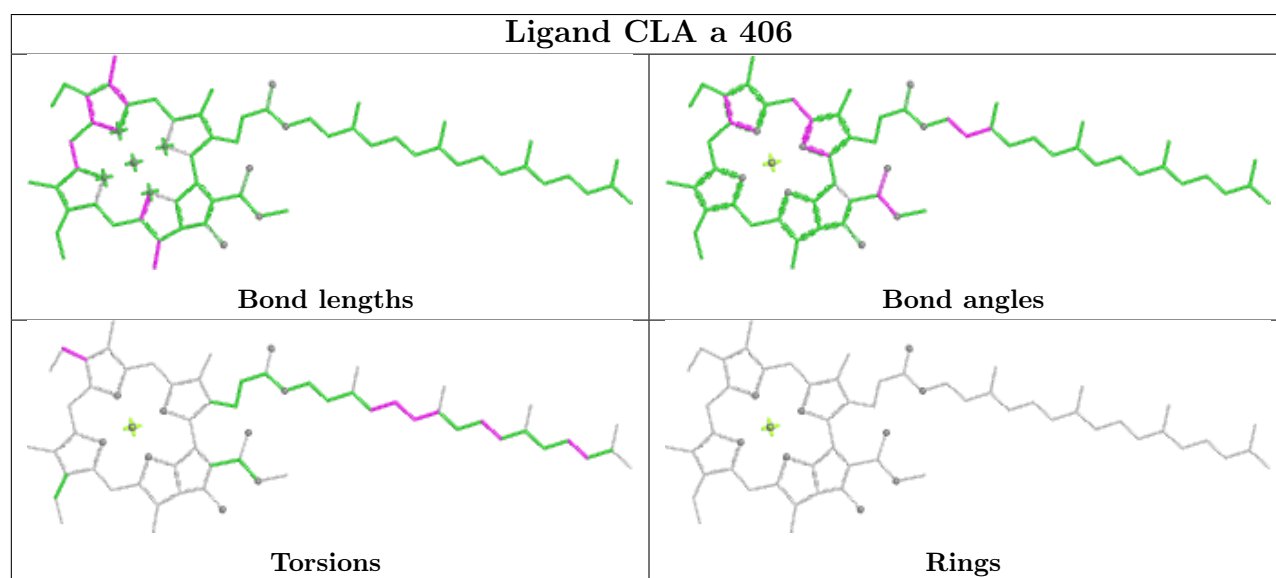
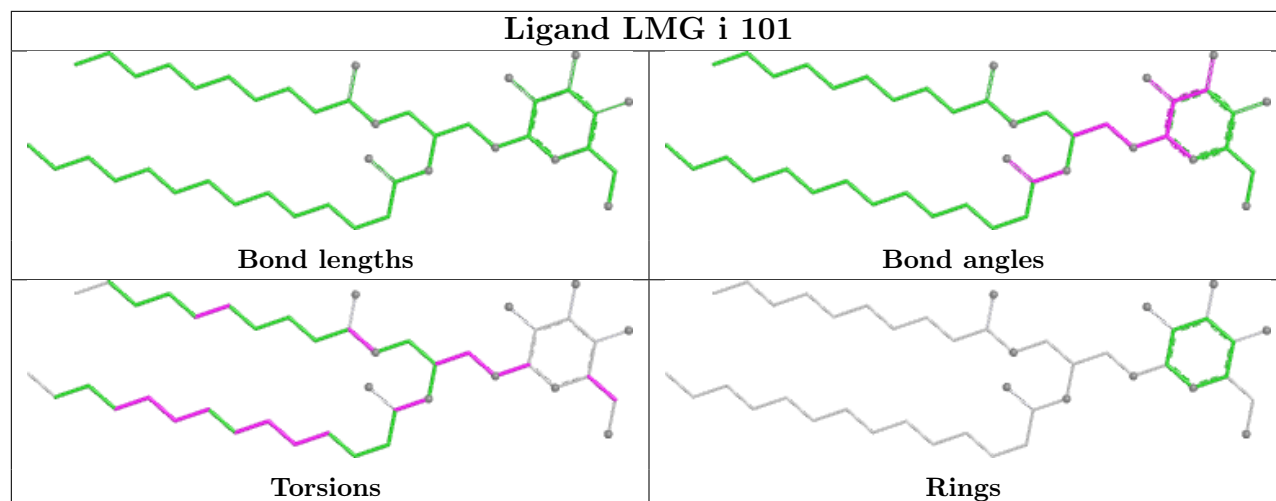


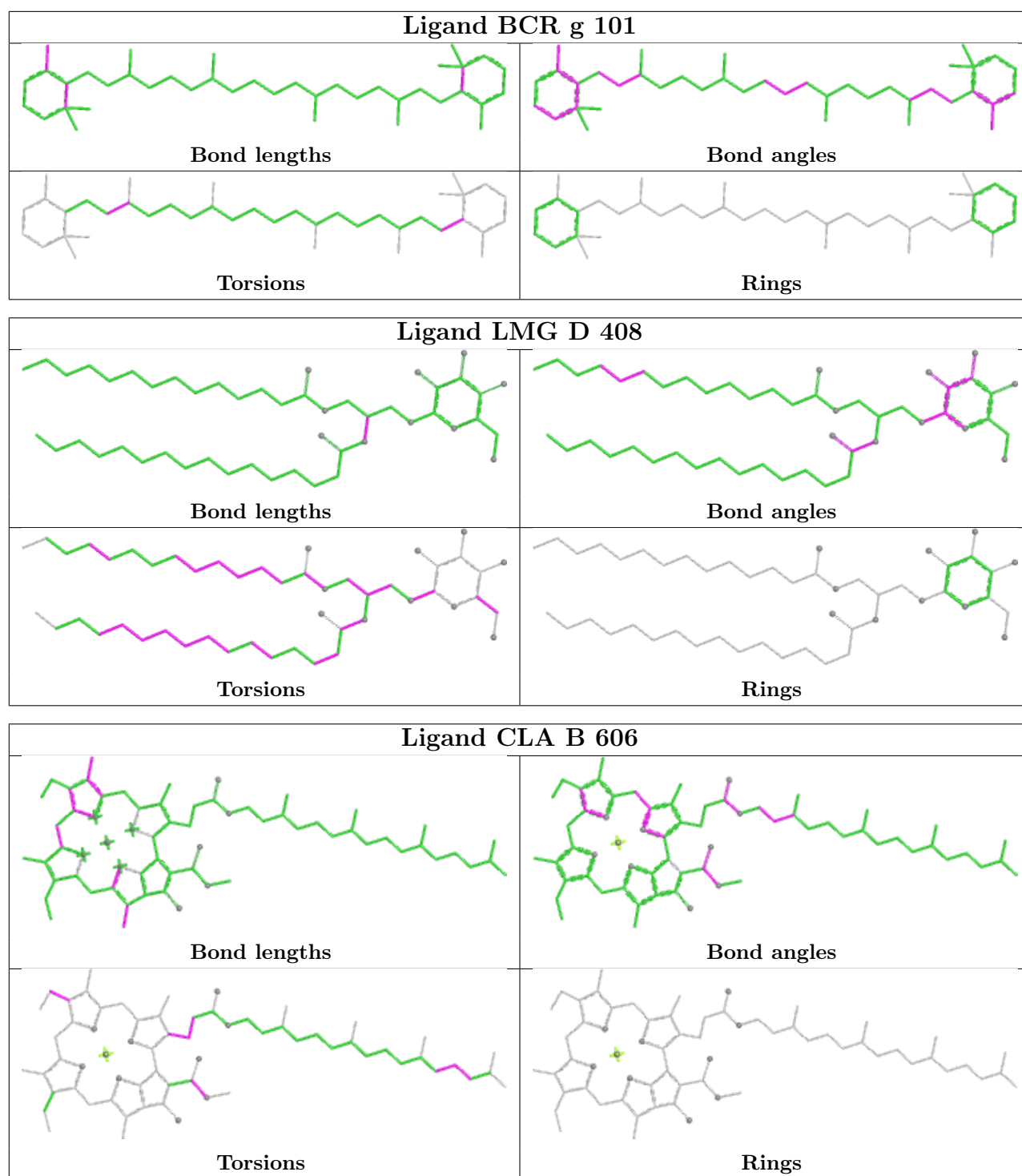
Ligand BCR A 407

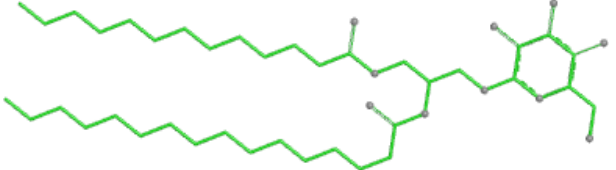
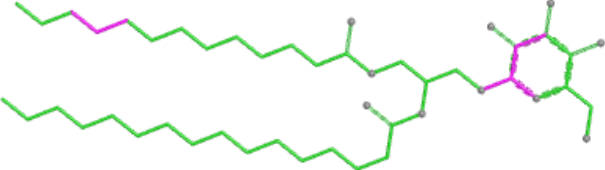
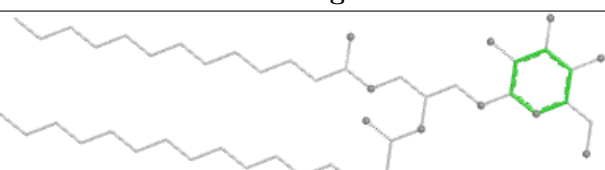
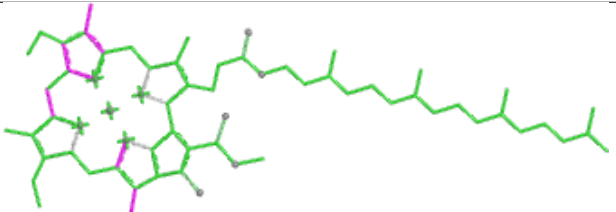
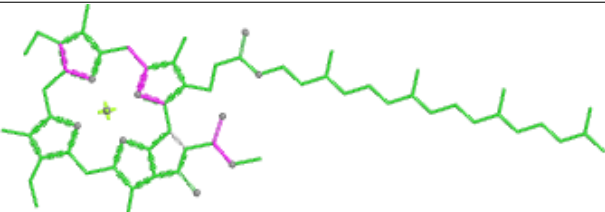
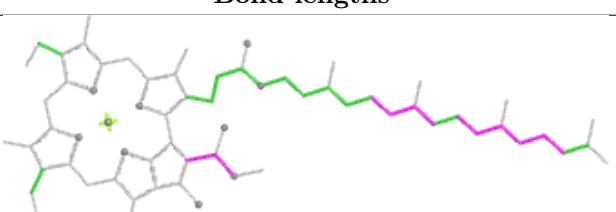
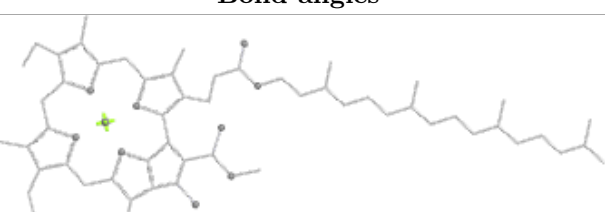
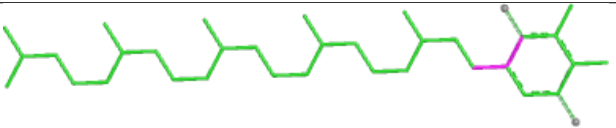
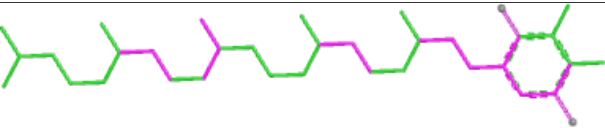
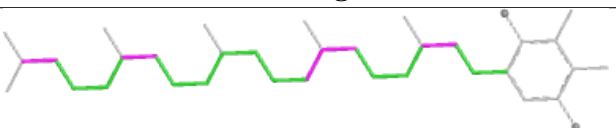
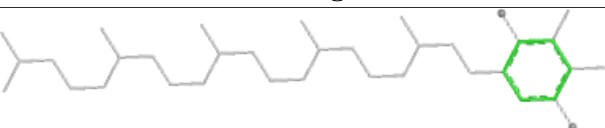




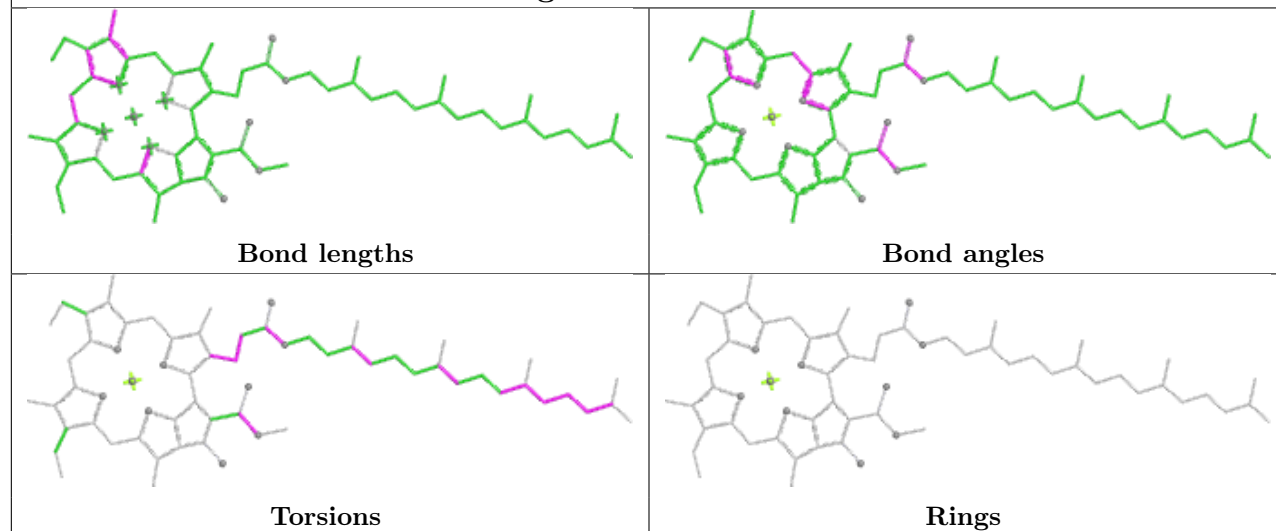




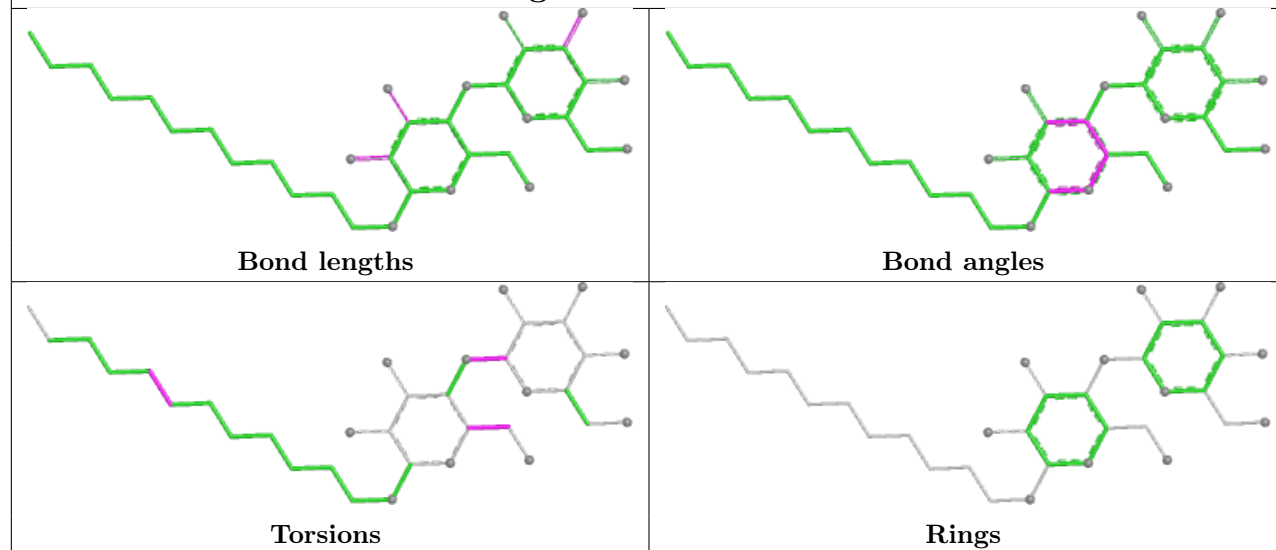


Ligand LMG d 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

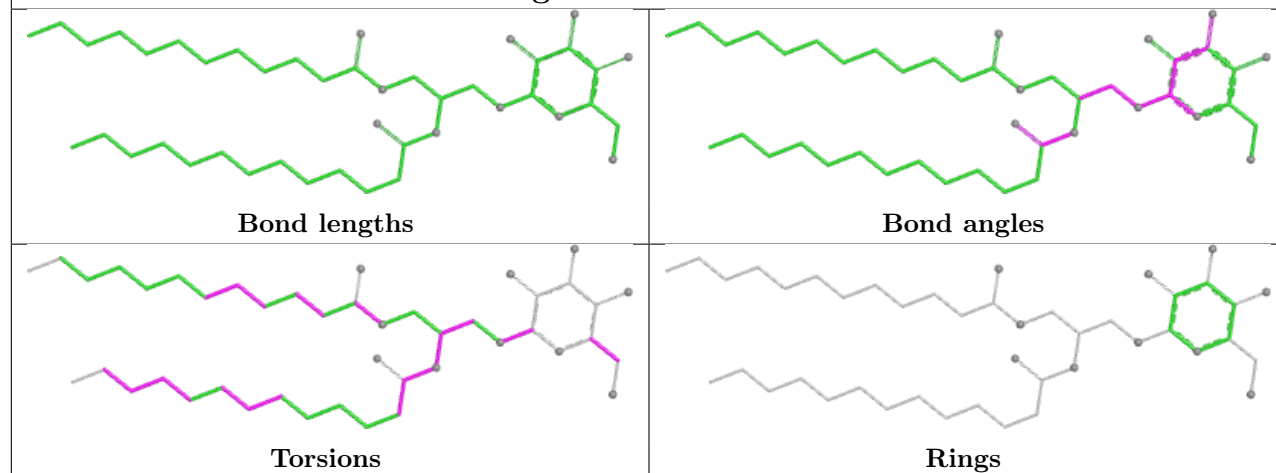
Ligand CLA c 512



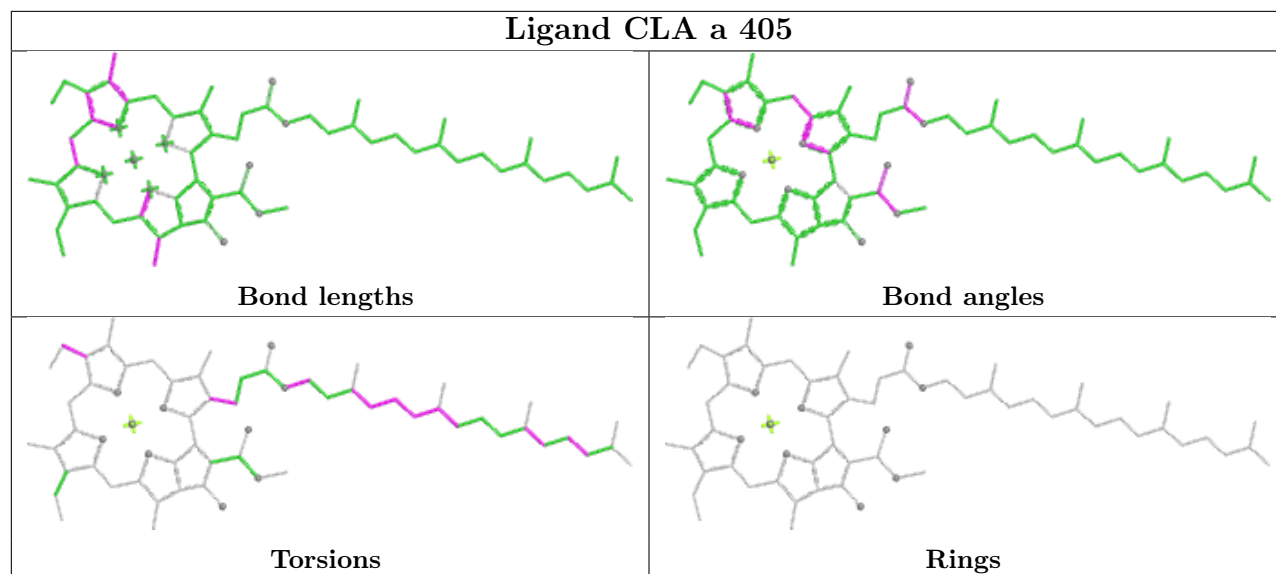
Ligand LMT B 624



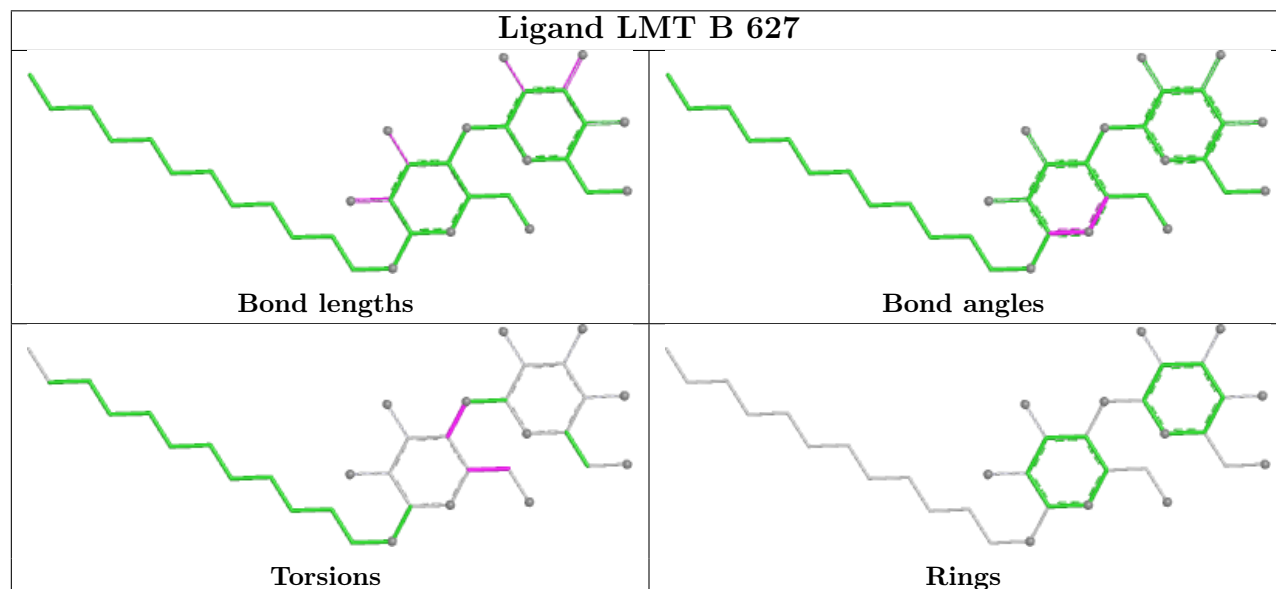
Ligand LMG e 101



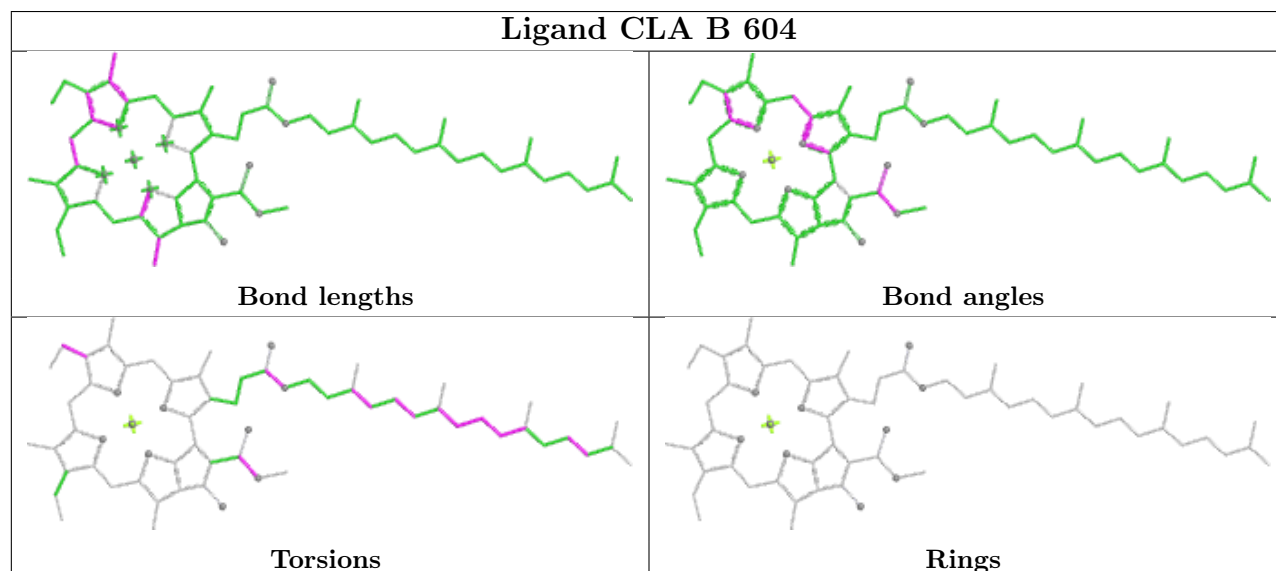
Ligand CLA a 405



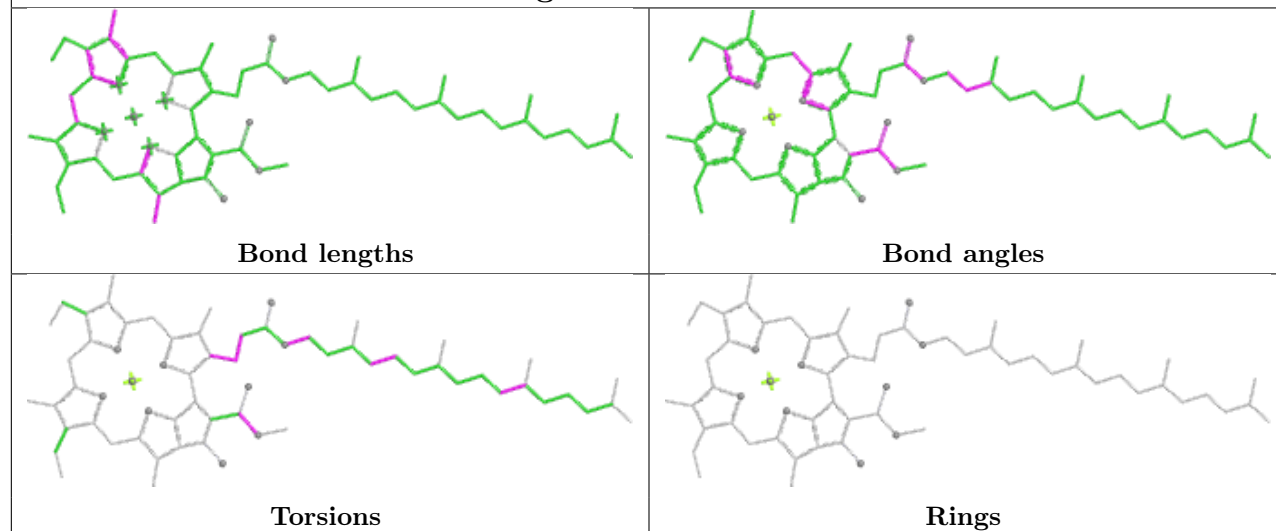
Ligand LMT B 627



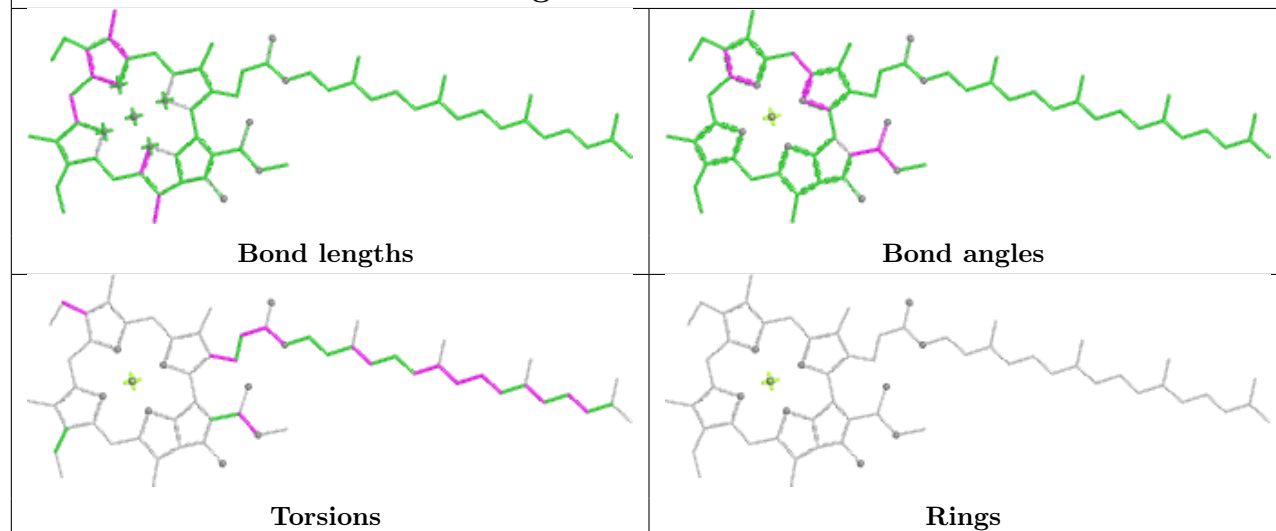
Ligand CLA B 604



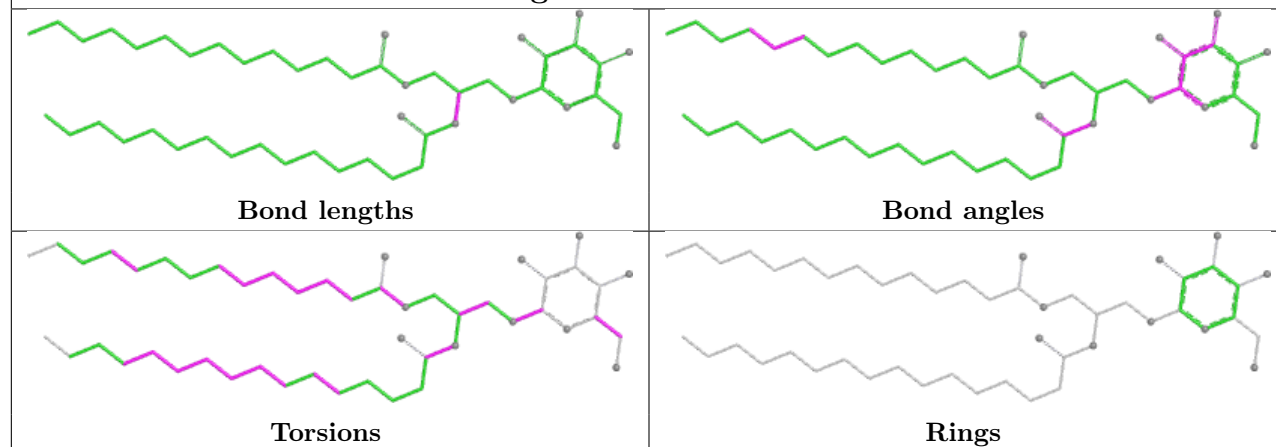
Ligand CLA a 404

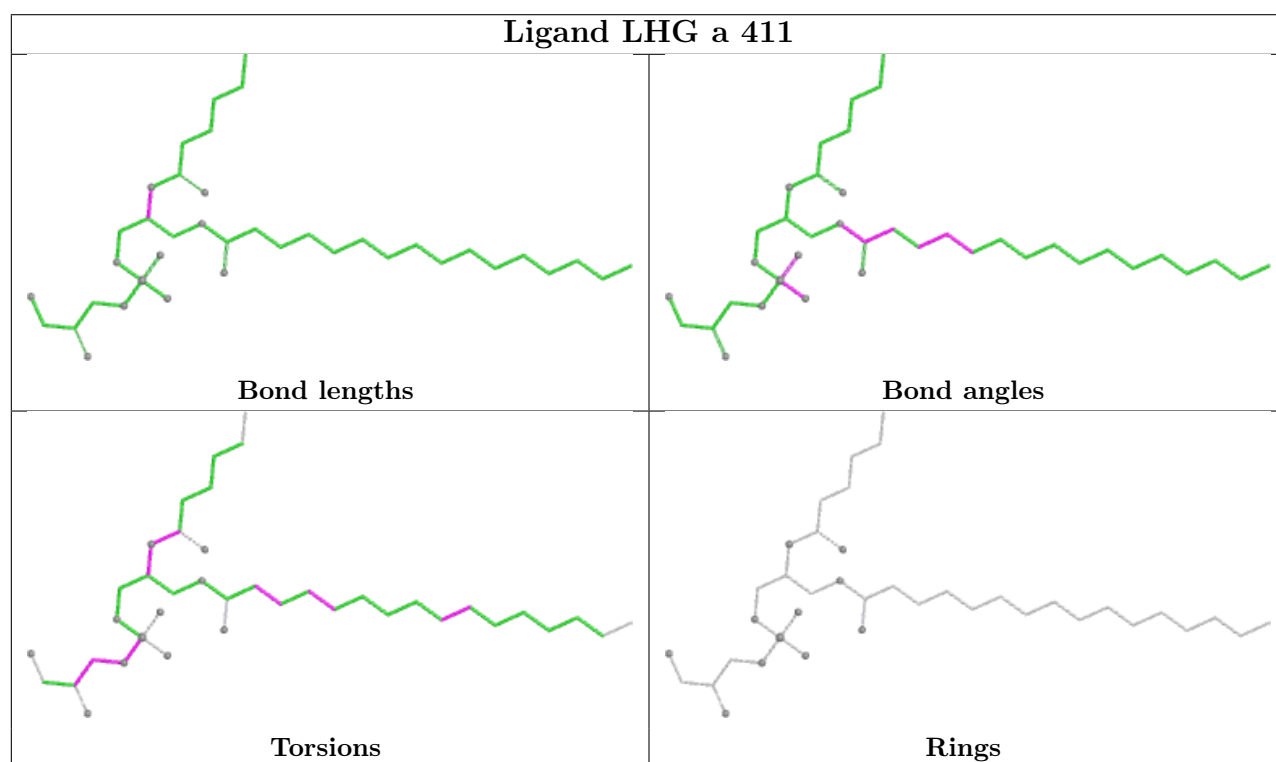
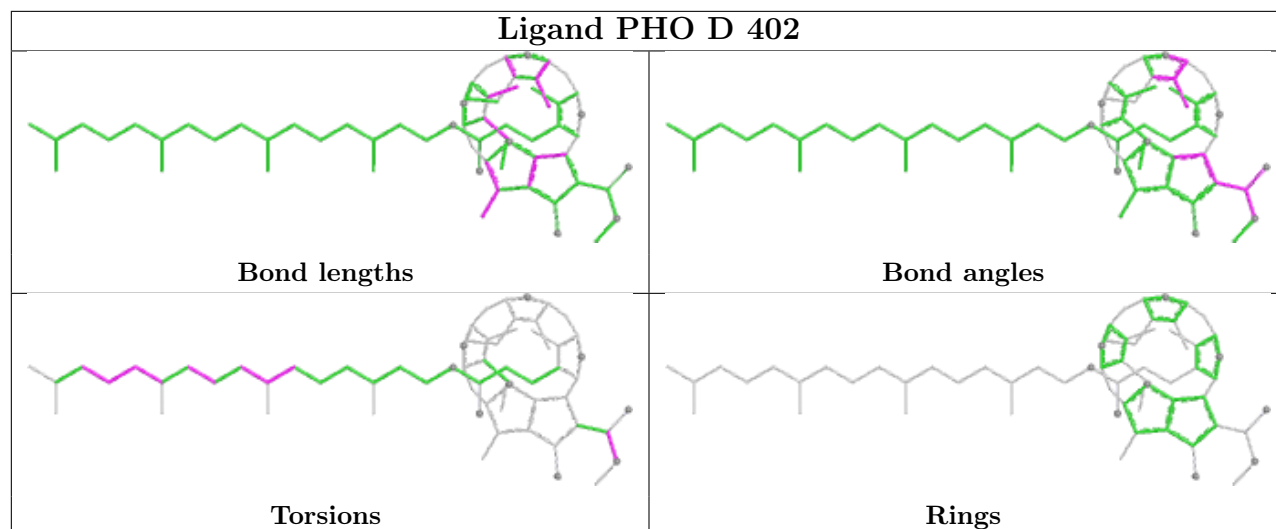


Ligand CLA C 504

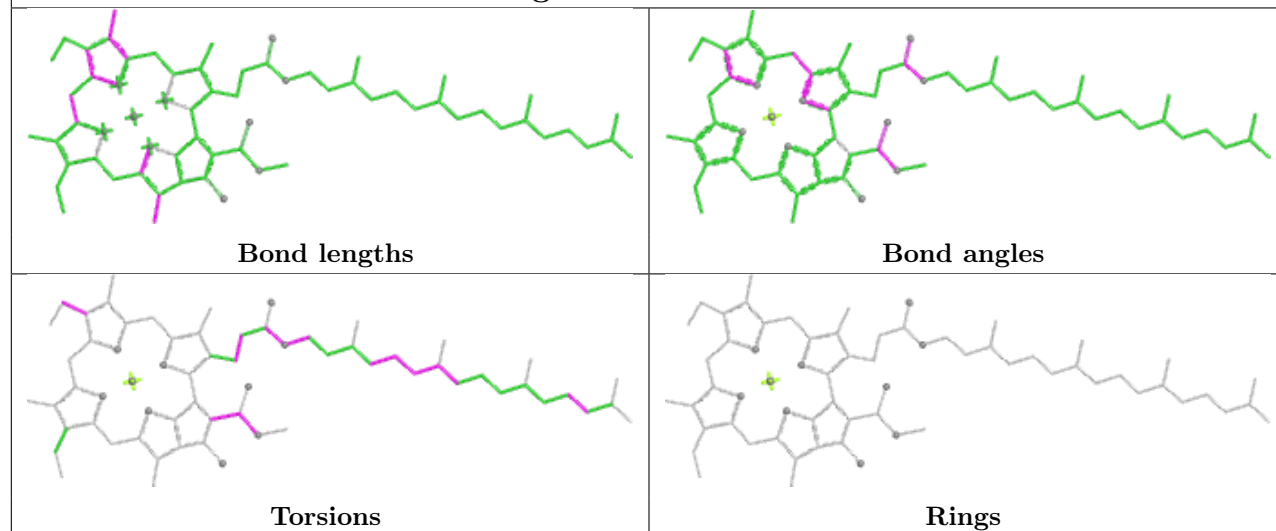


Ligand LMG d 408

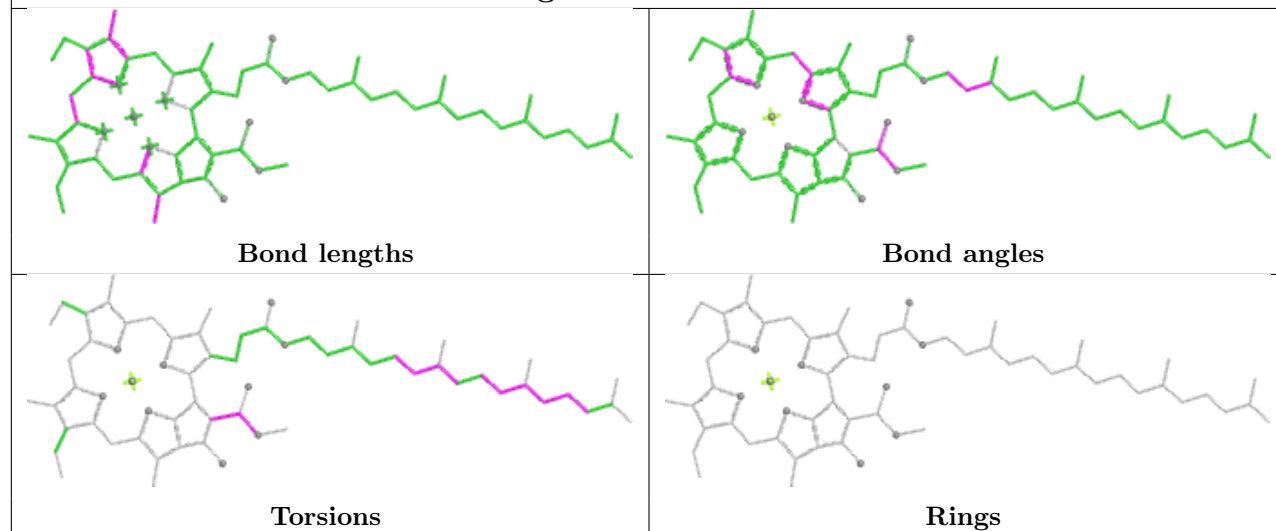




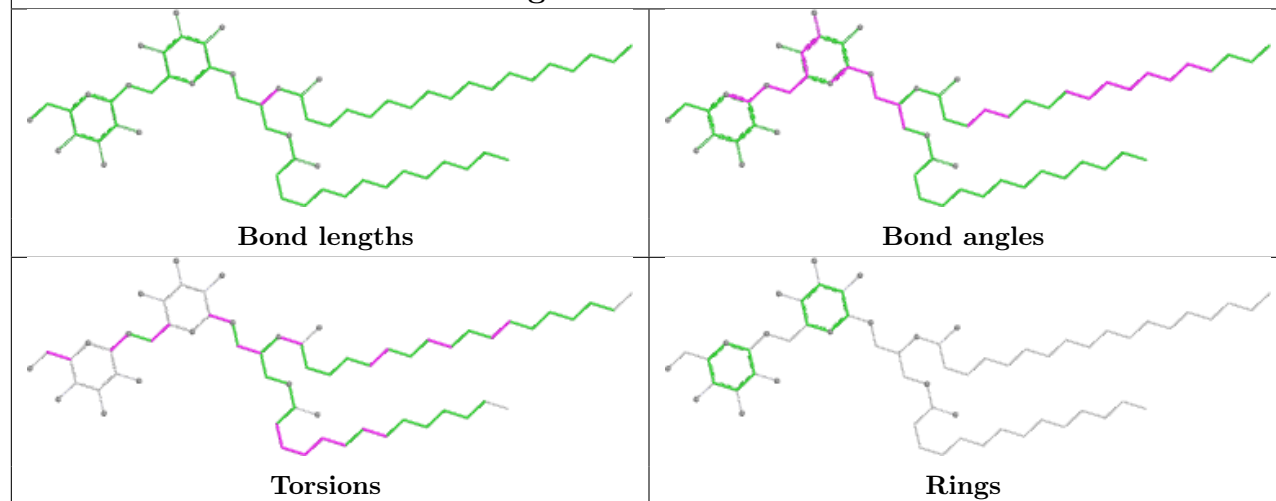
Ligand CLA C 508



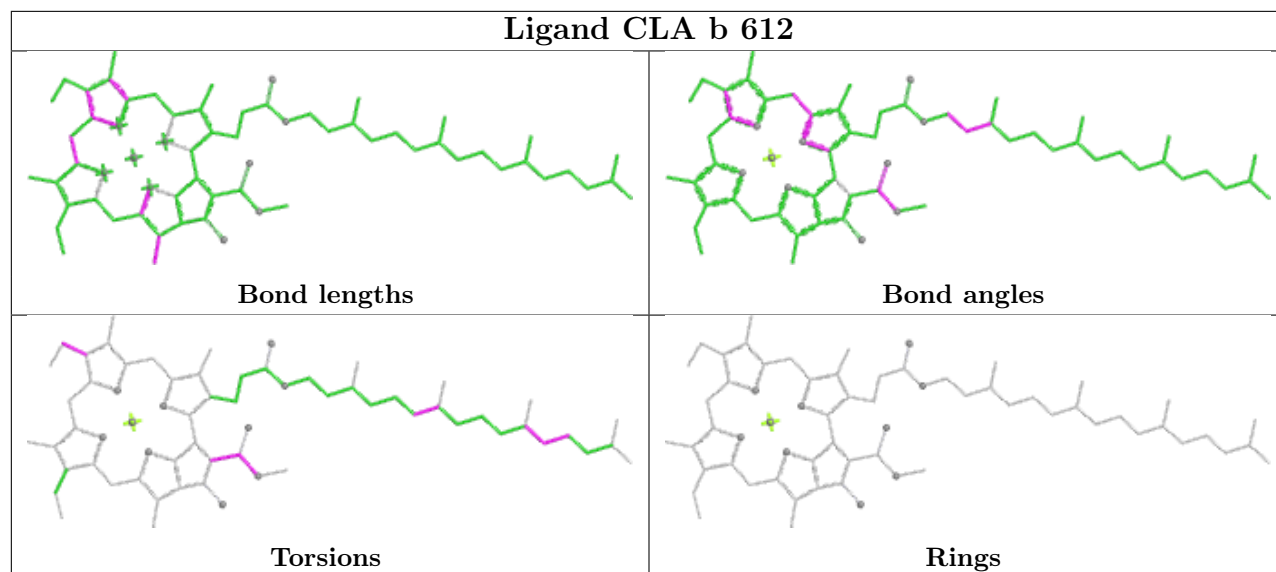
Ligand CLA c 505



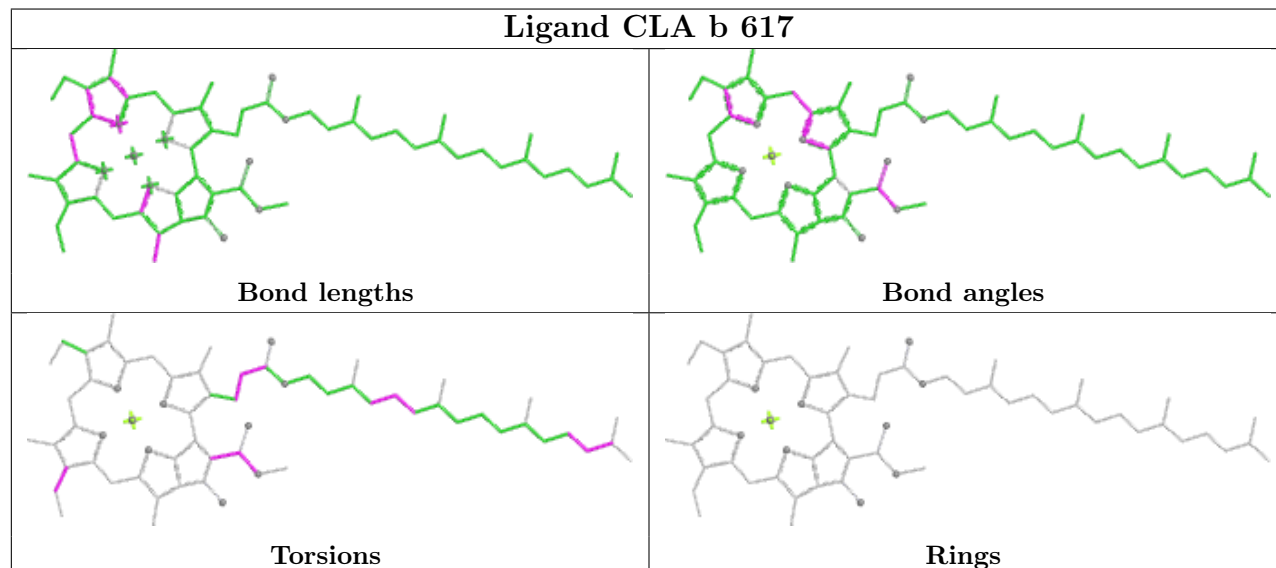
Ligand DGD C 516



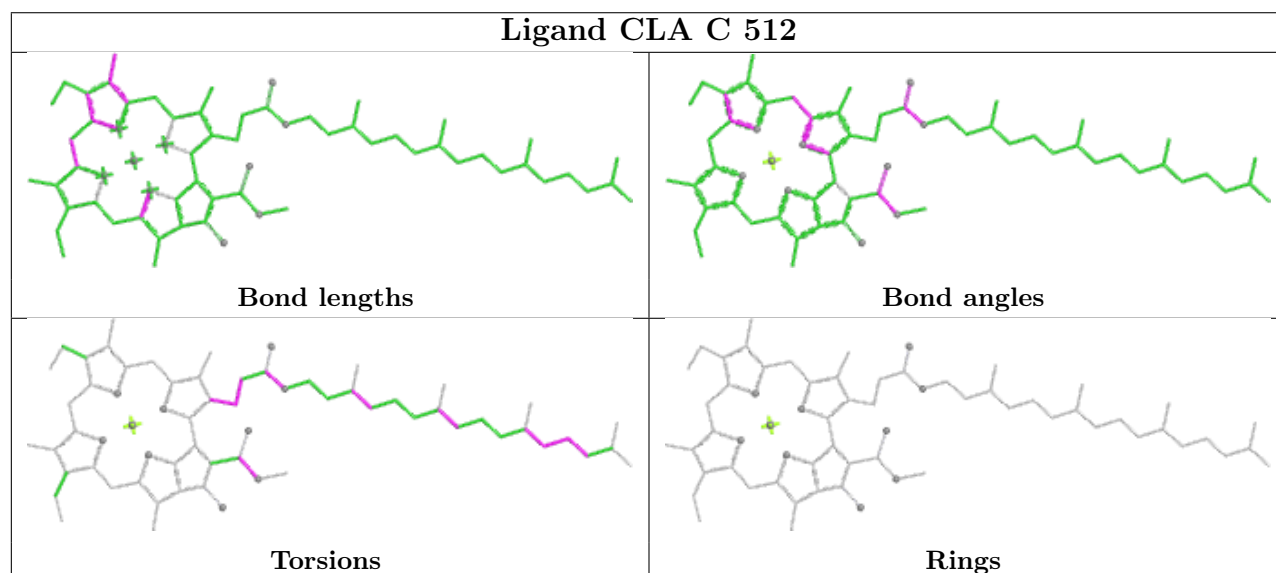
Ligand CLA b 612



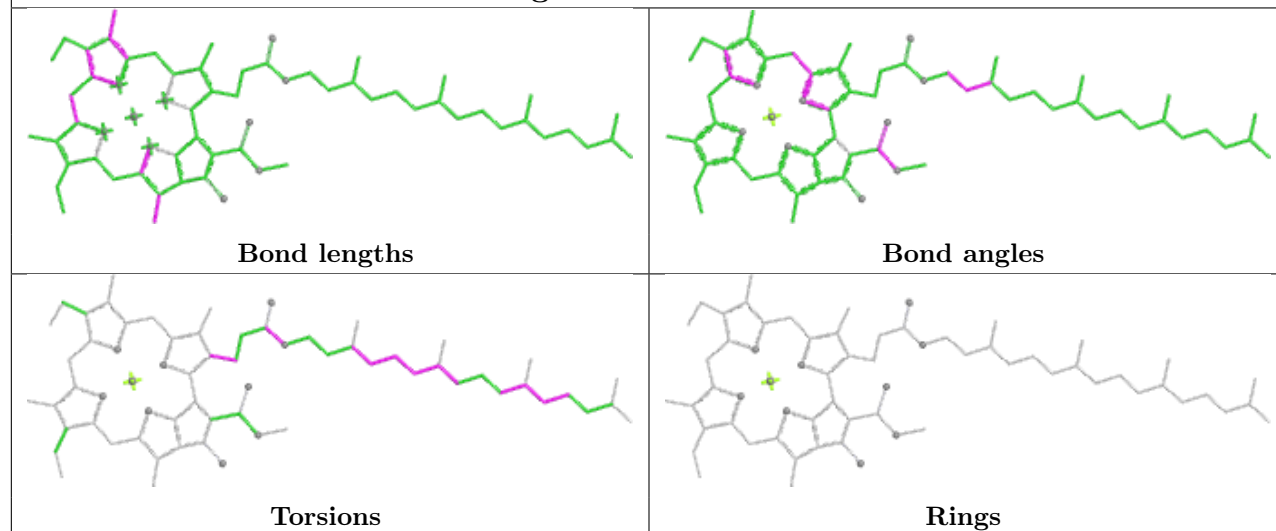
Ligand CLA b 617



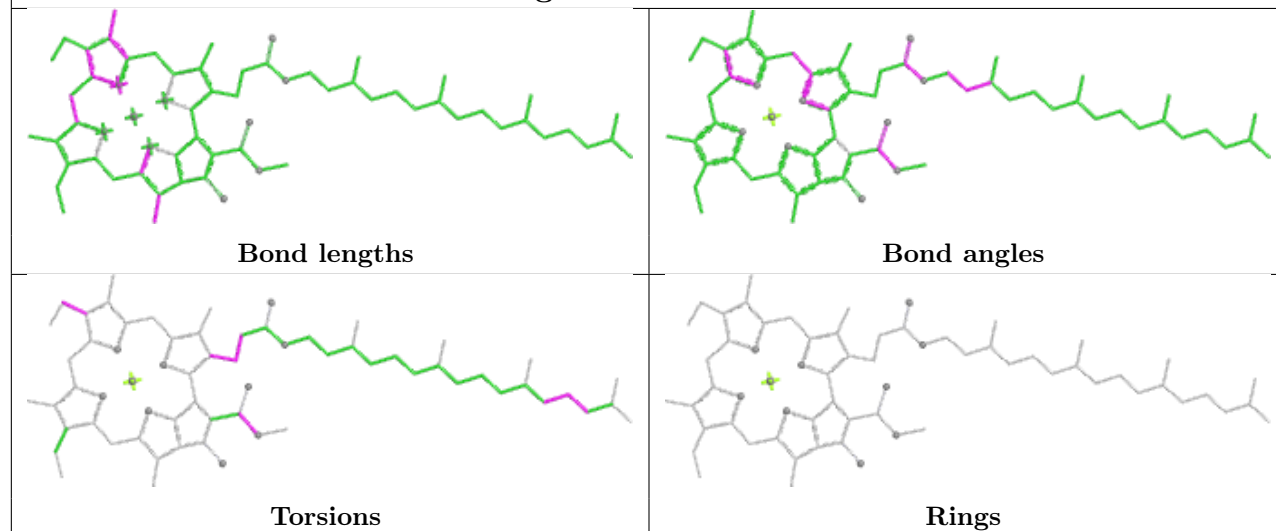
Ligand CLA C 512



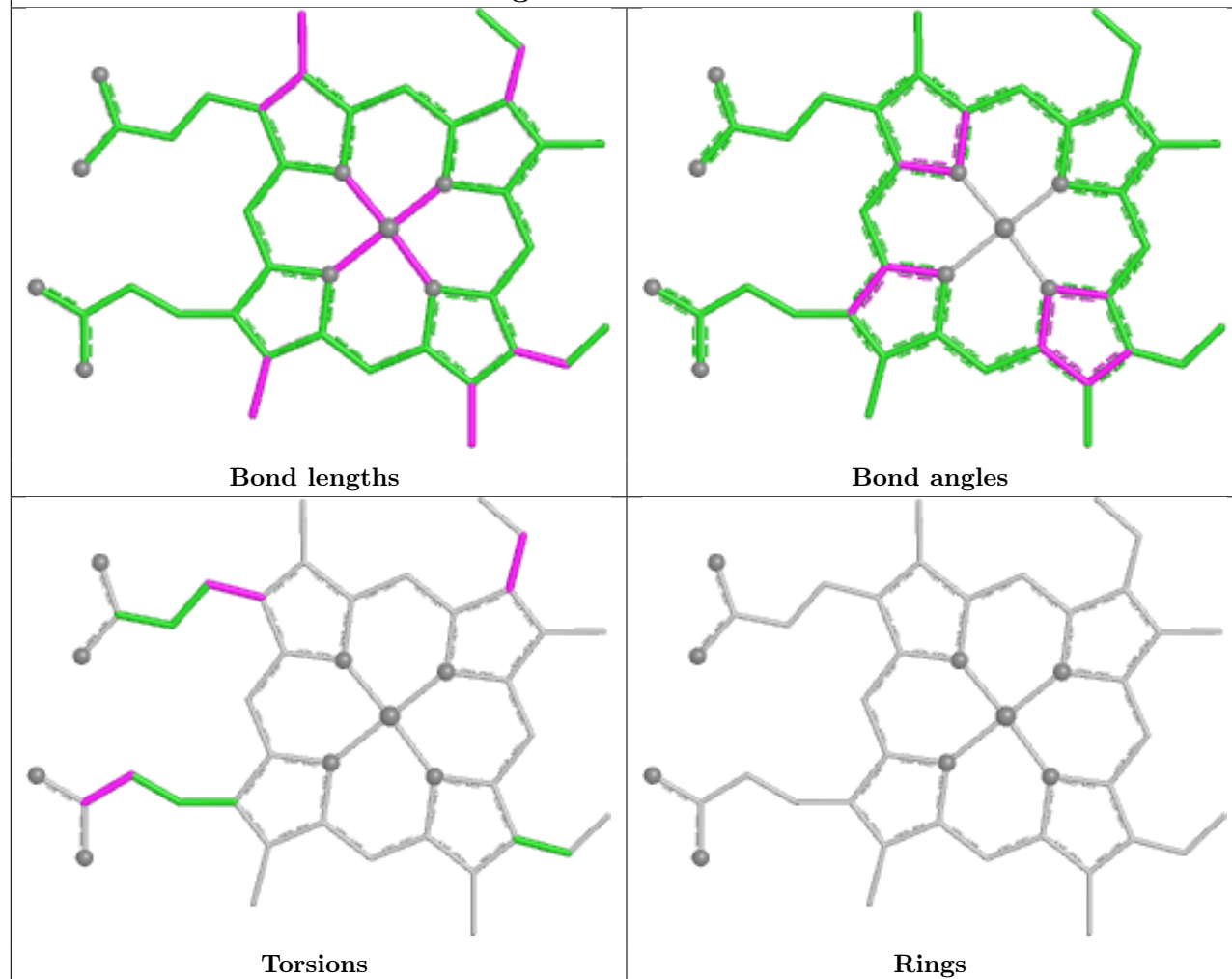
Ligand CLA H 101



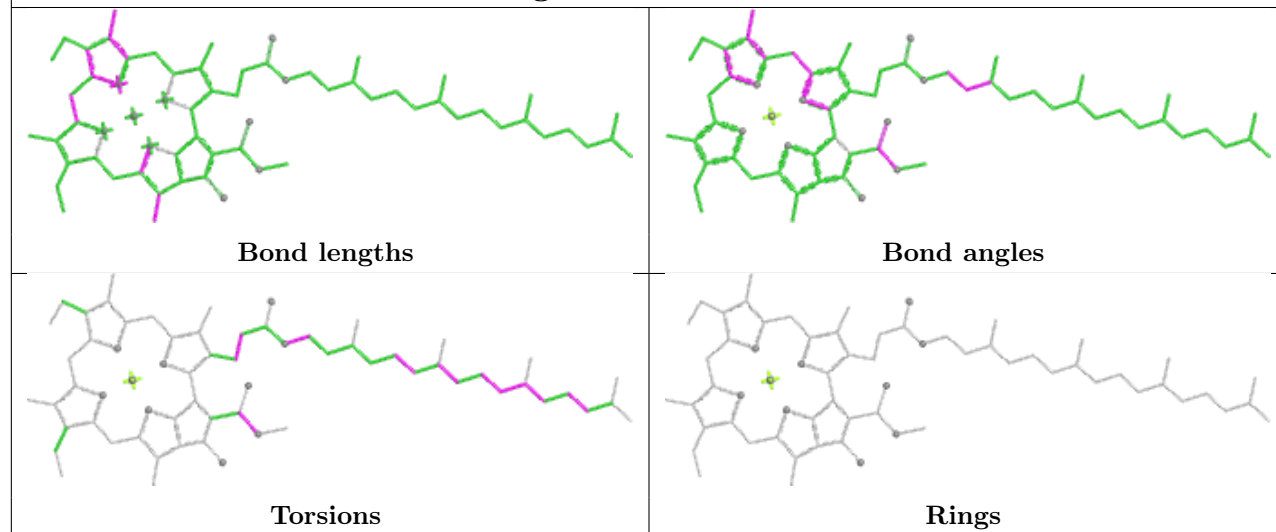
Ligand CLA b 610

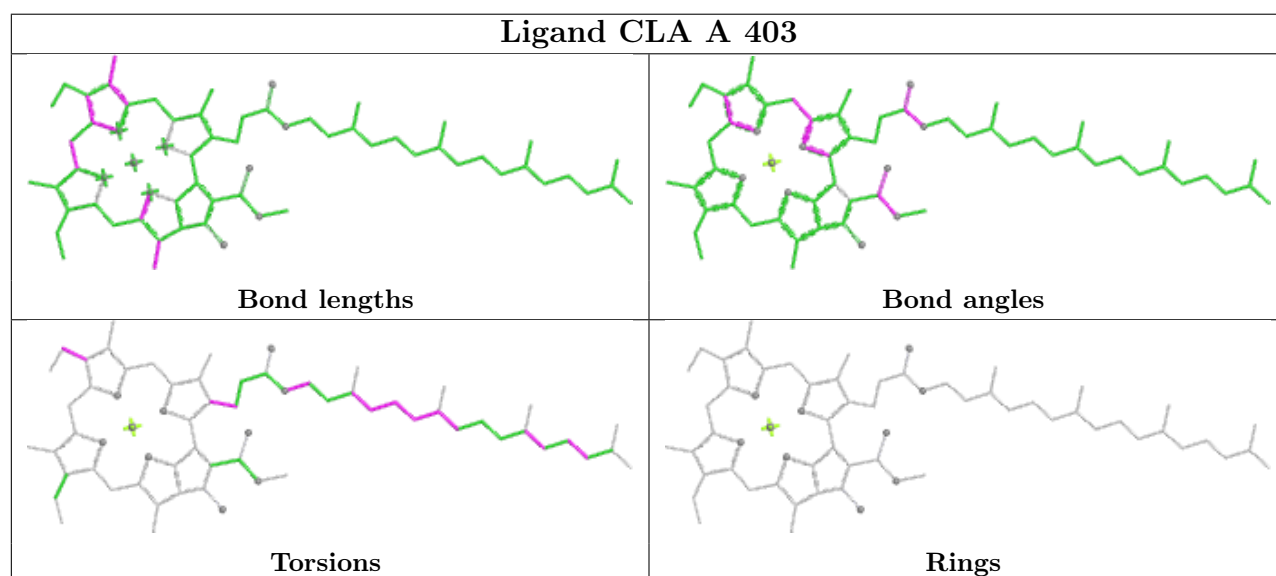
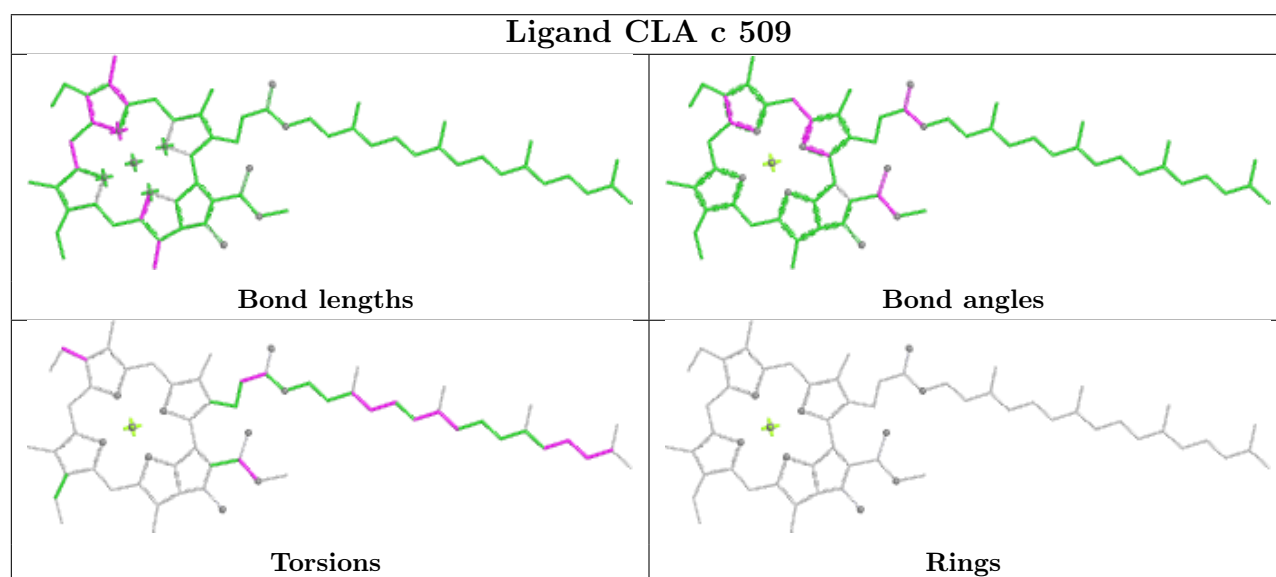
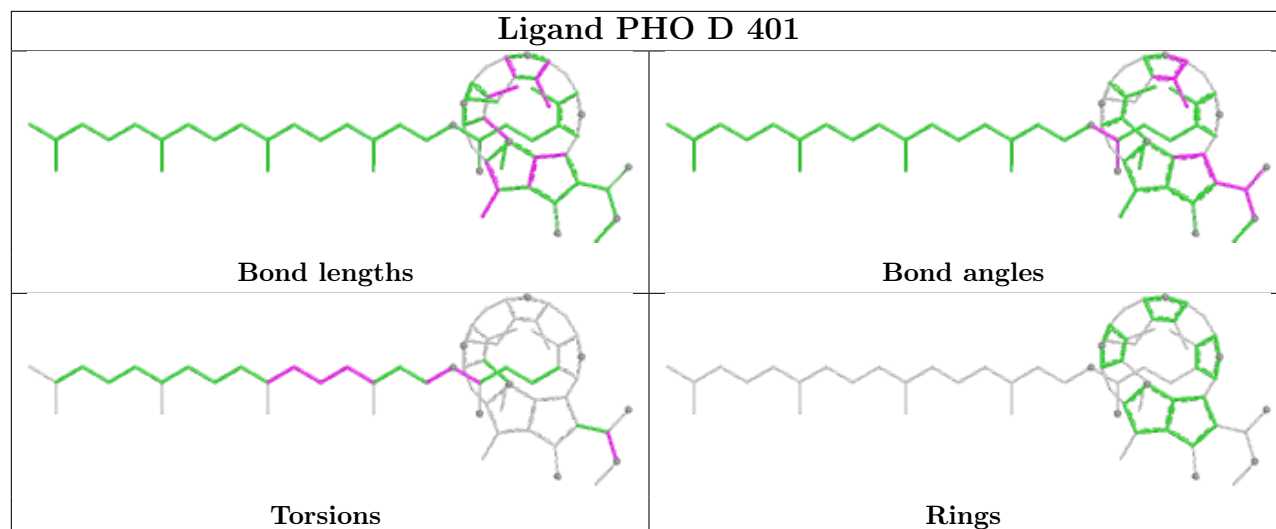


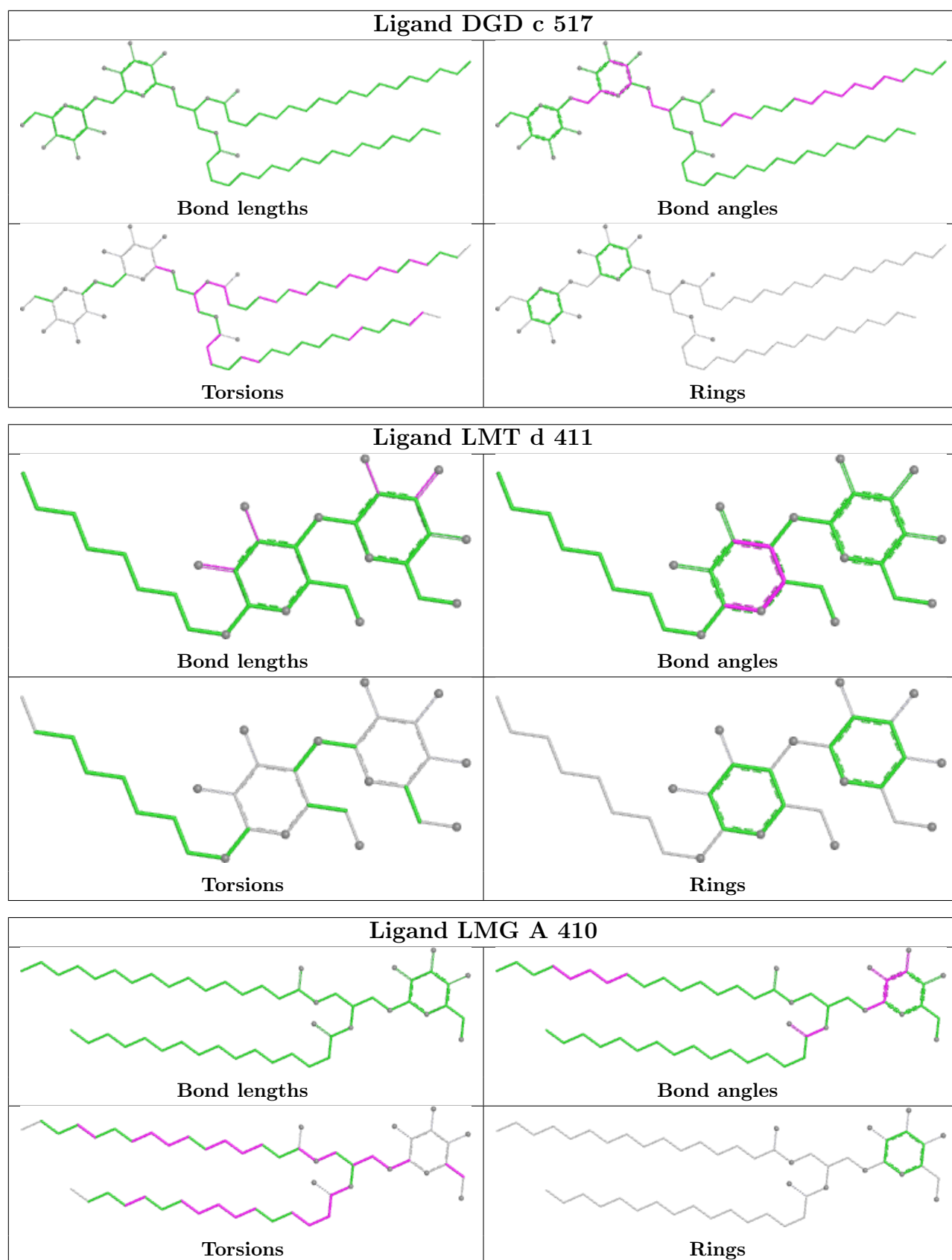
Ligand HEM v 201



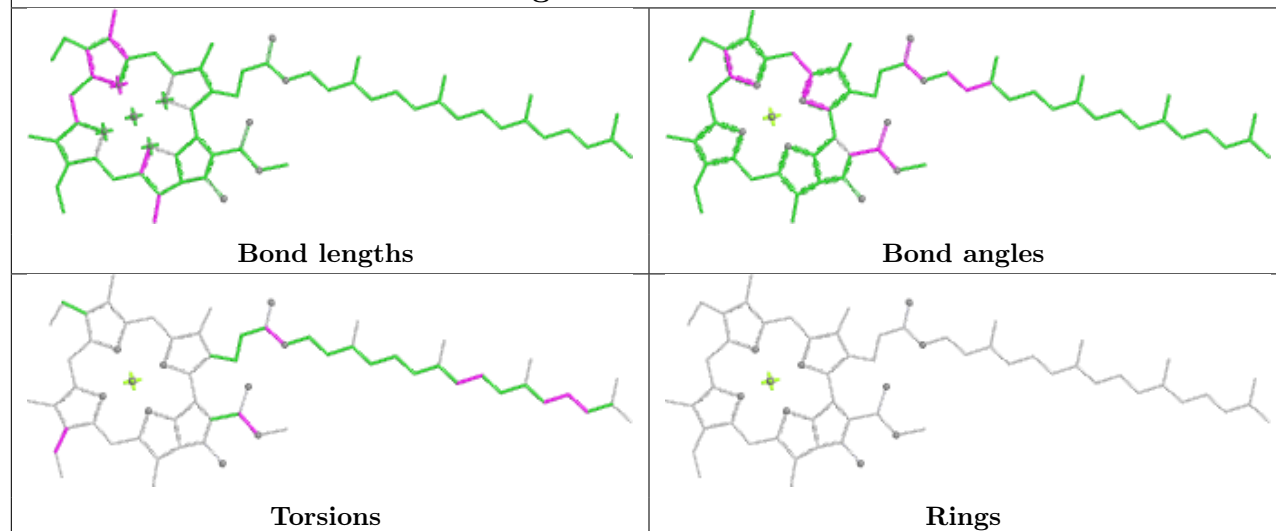
Ligand CLA C 507



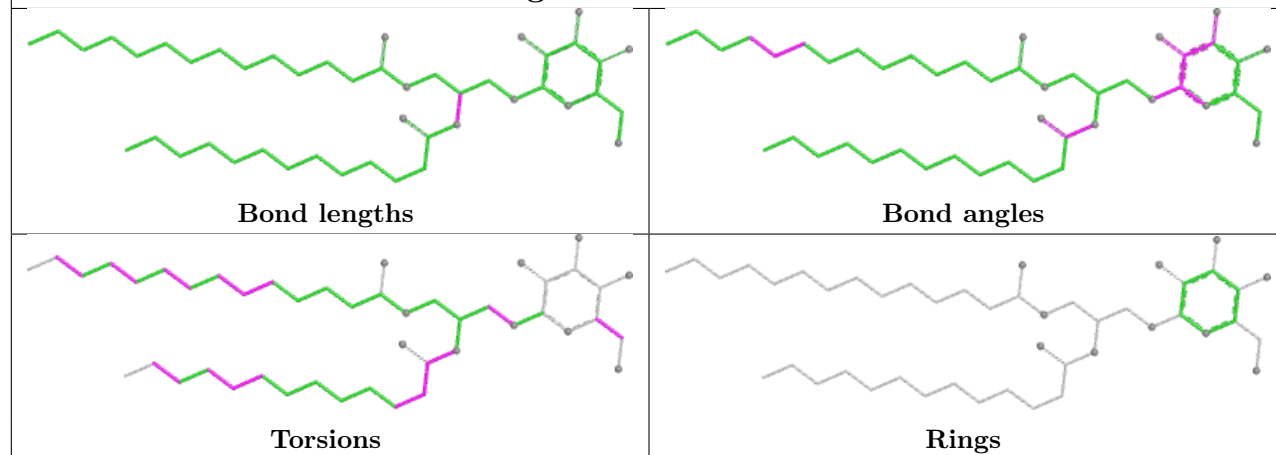




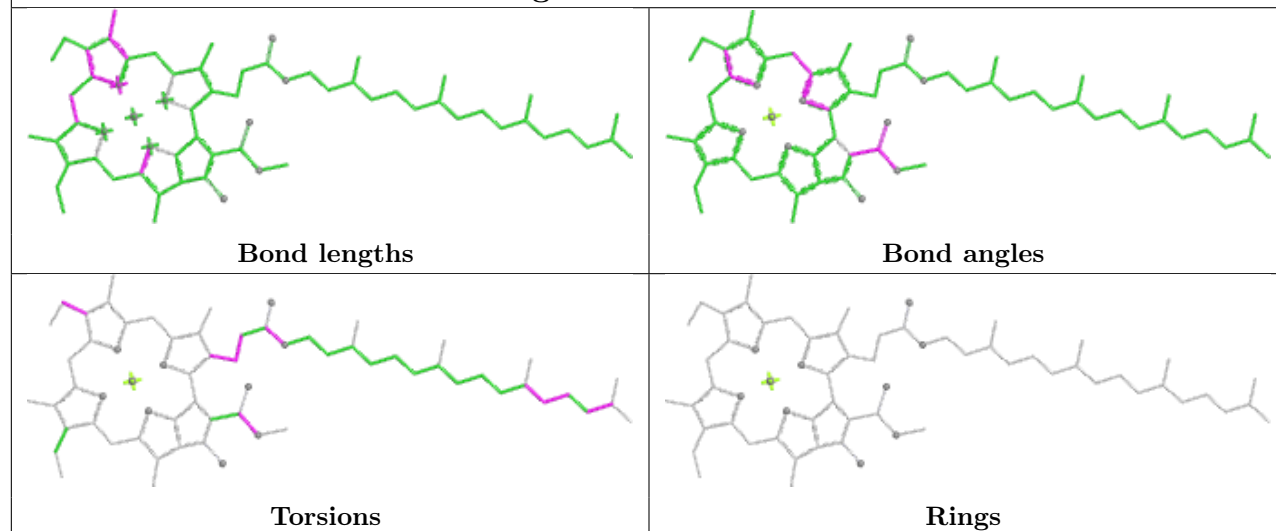
Ligand CLA B 603

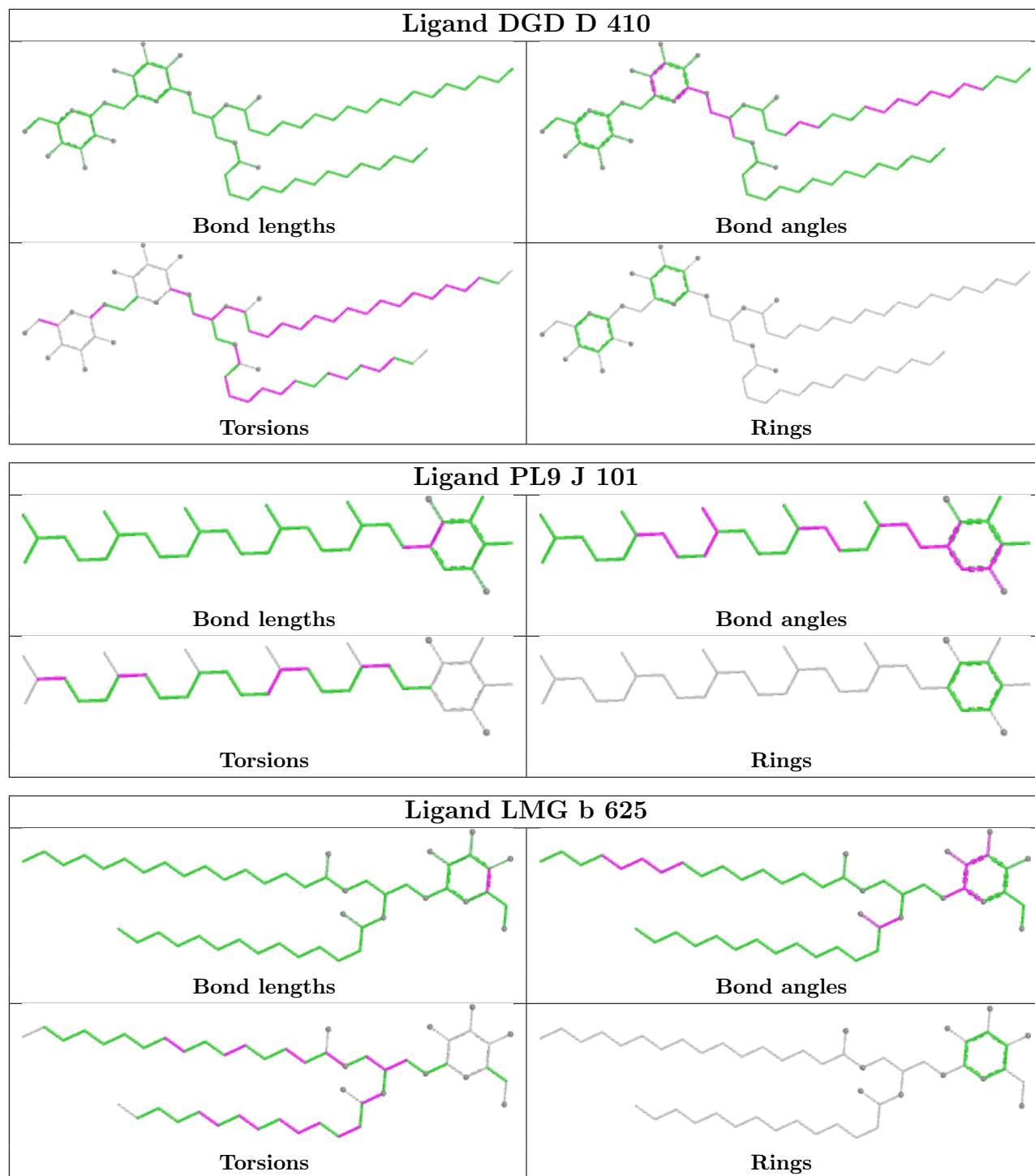


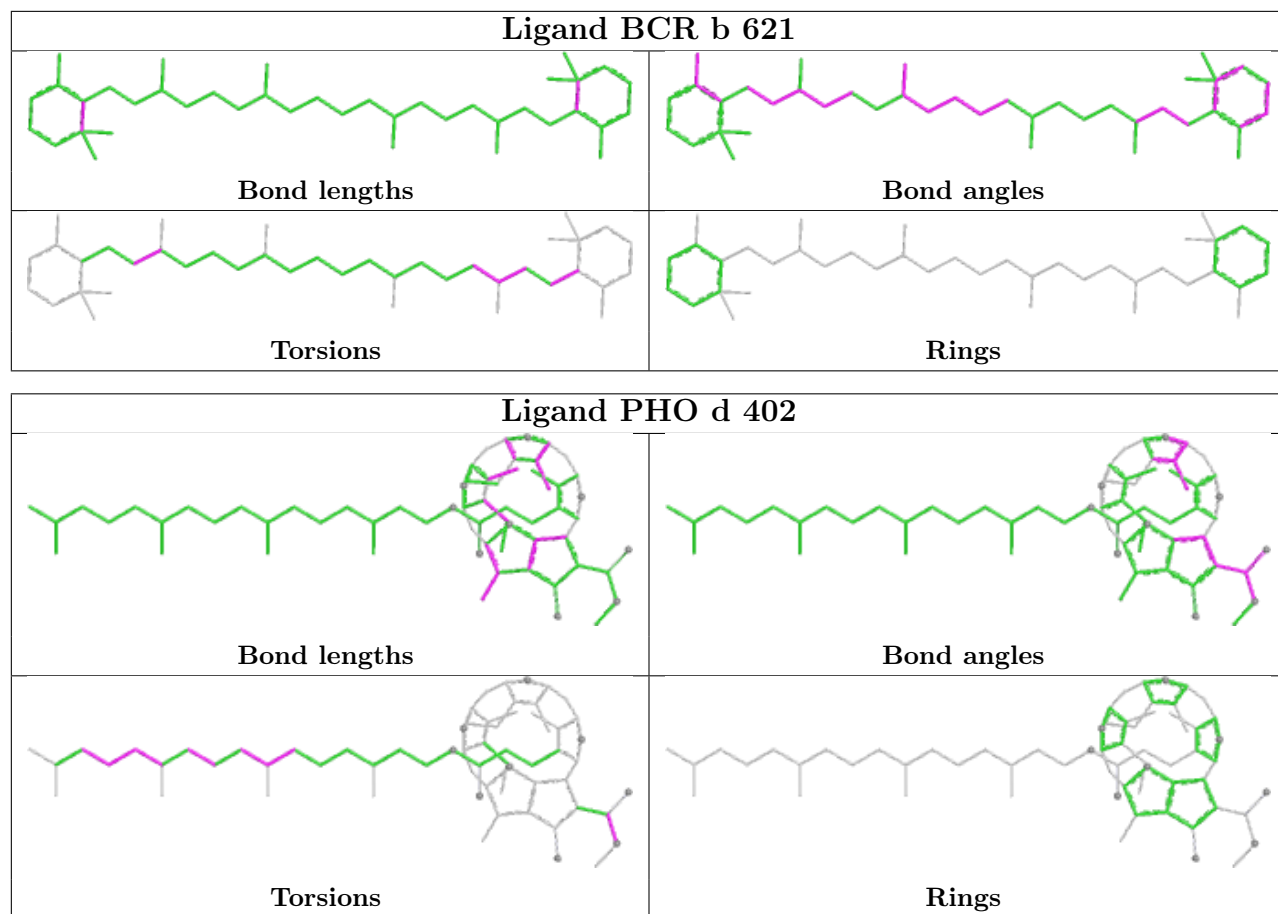
Ligand LMG D 412

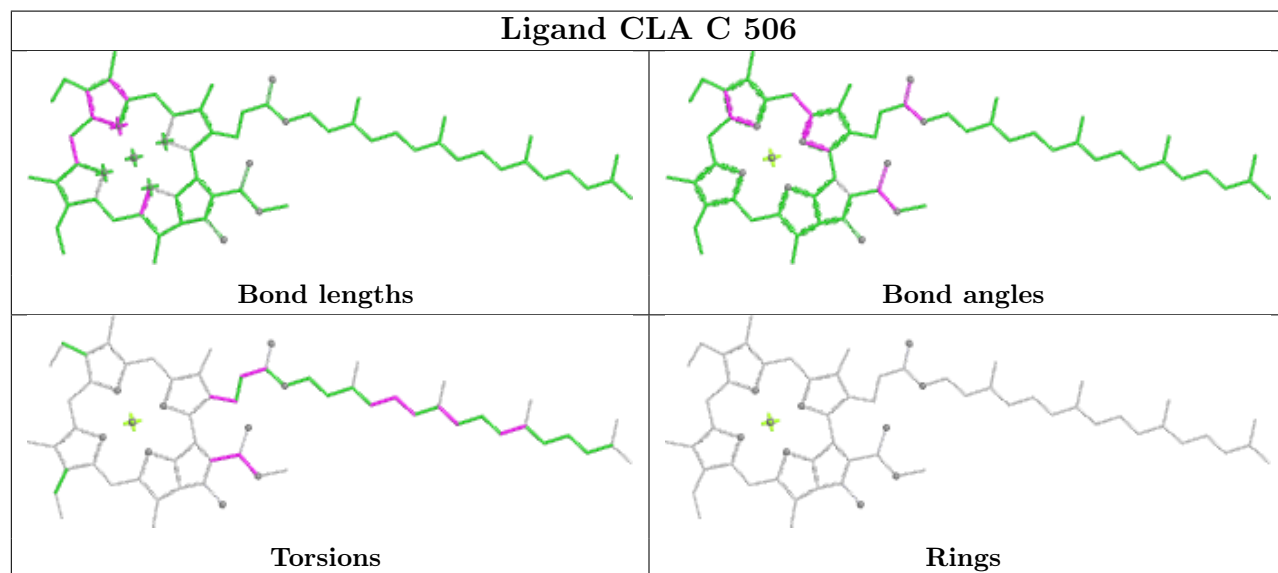
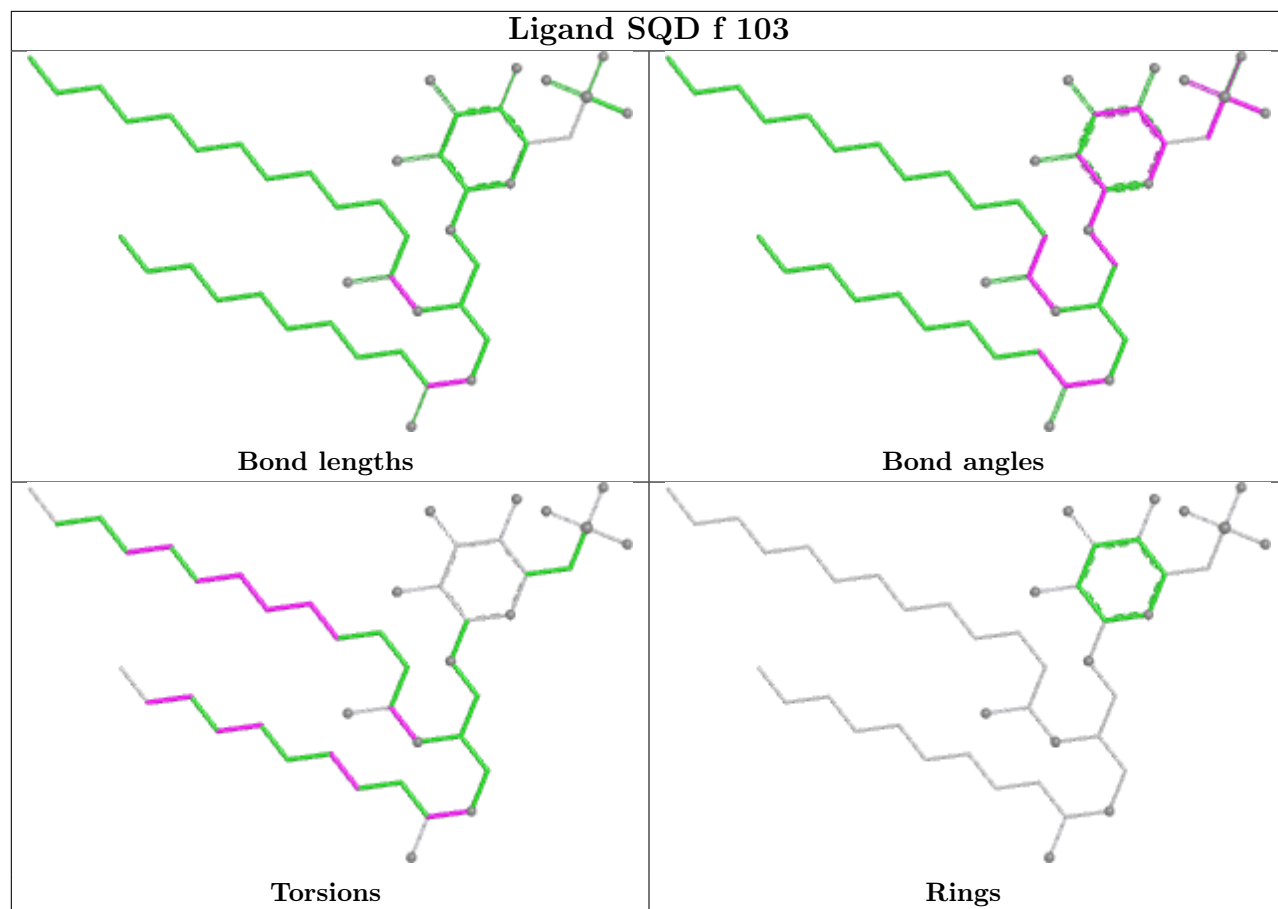


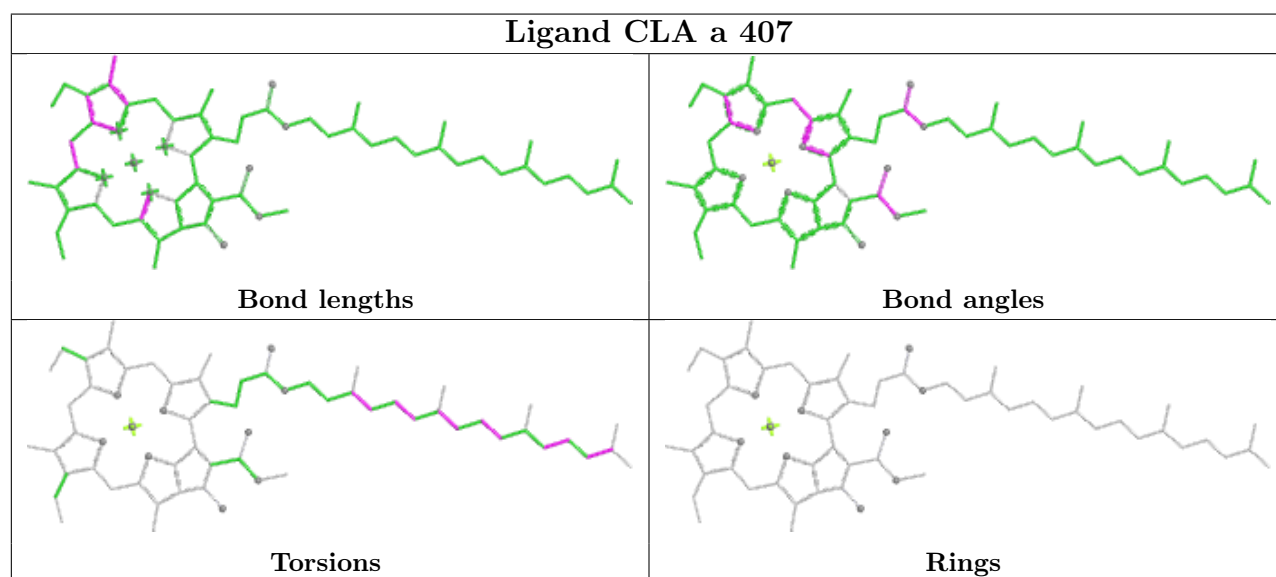
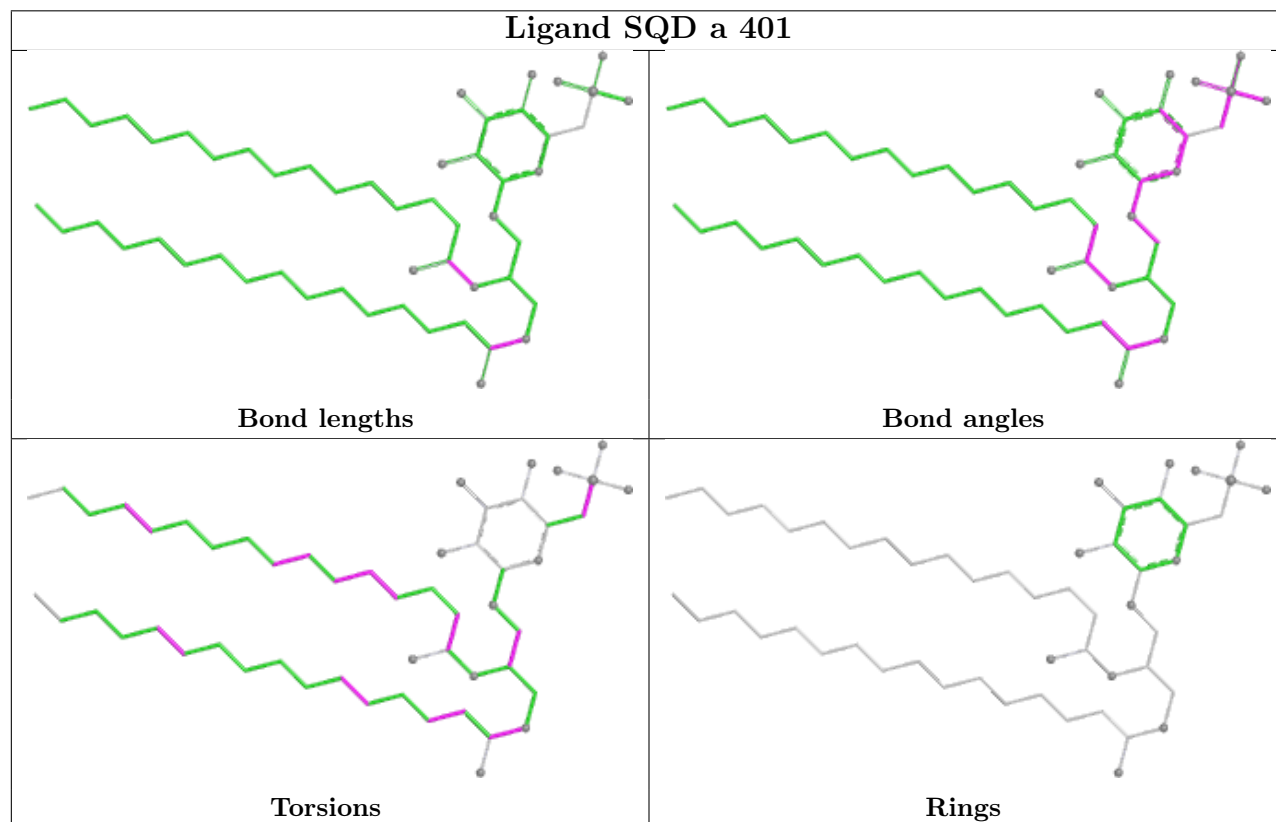
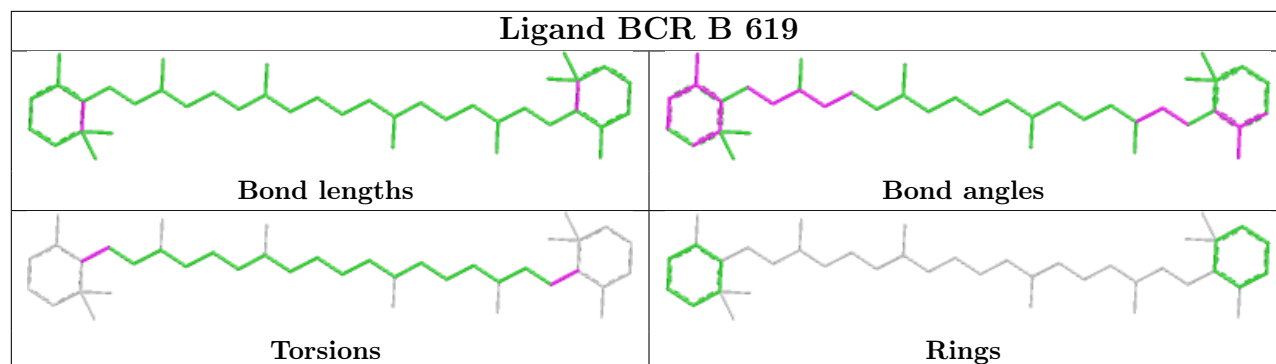
Ligand CLA B 605



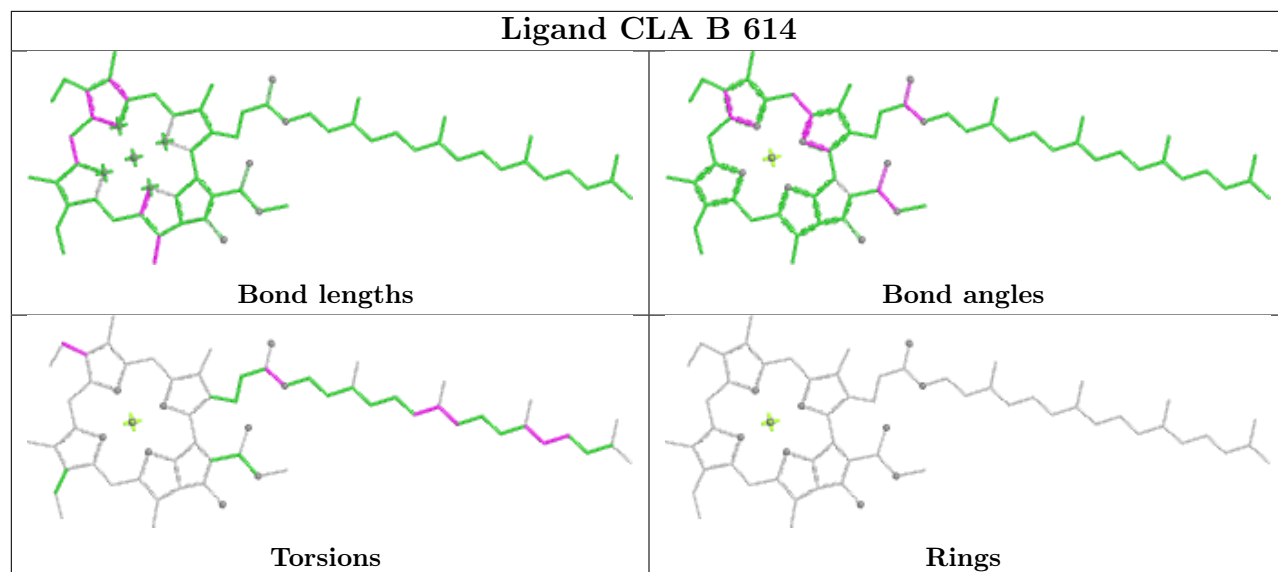




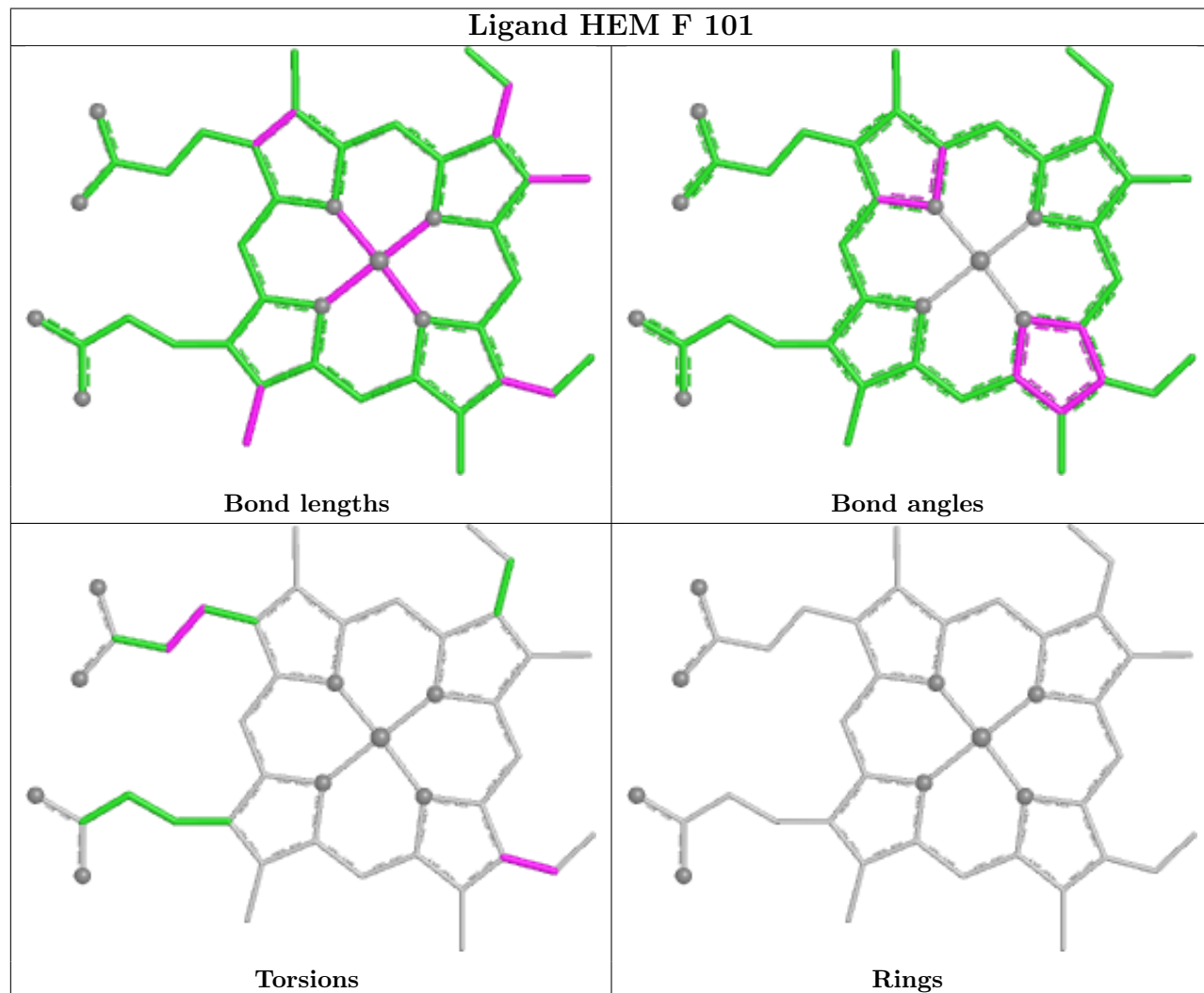


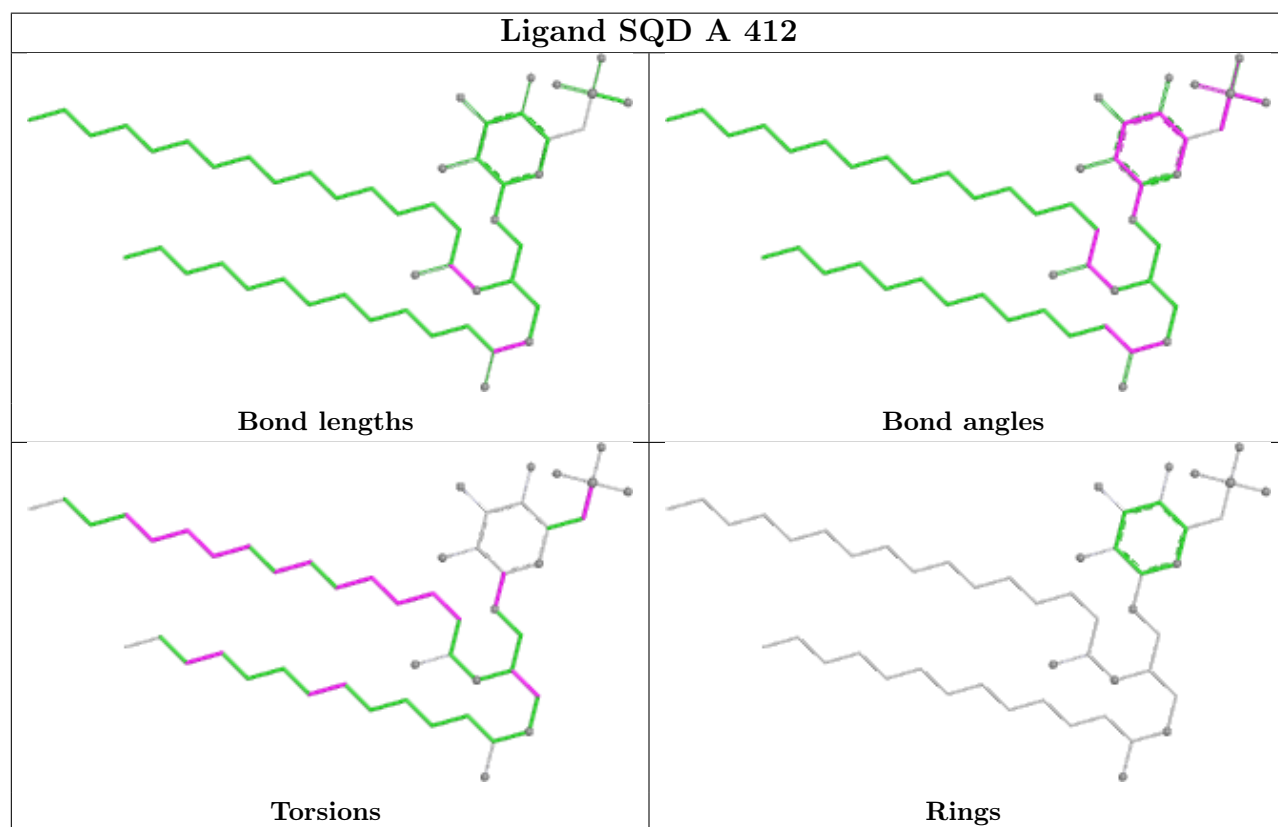
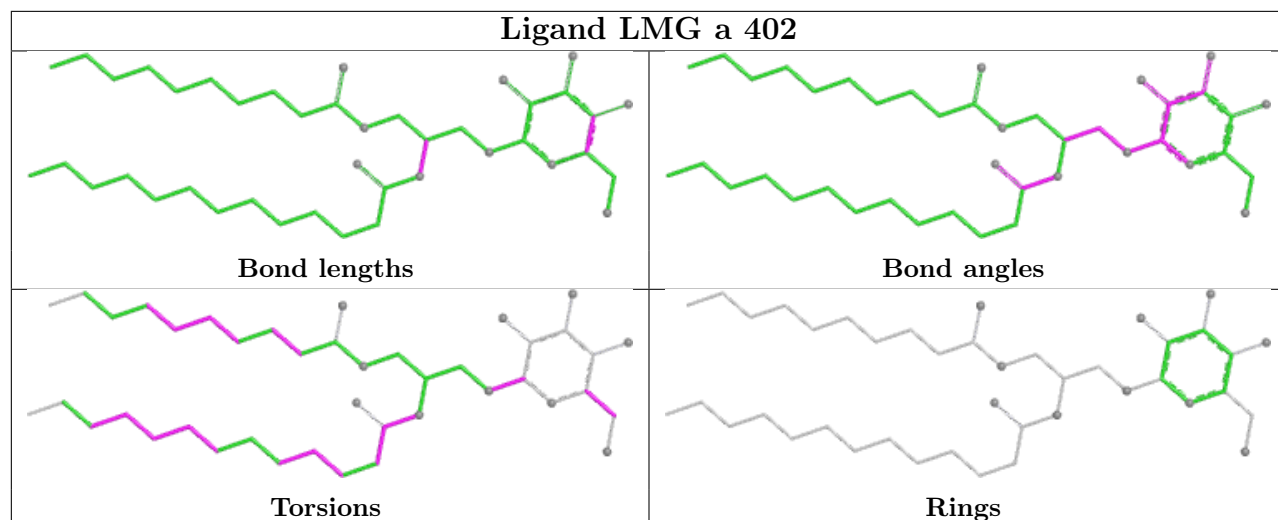


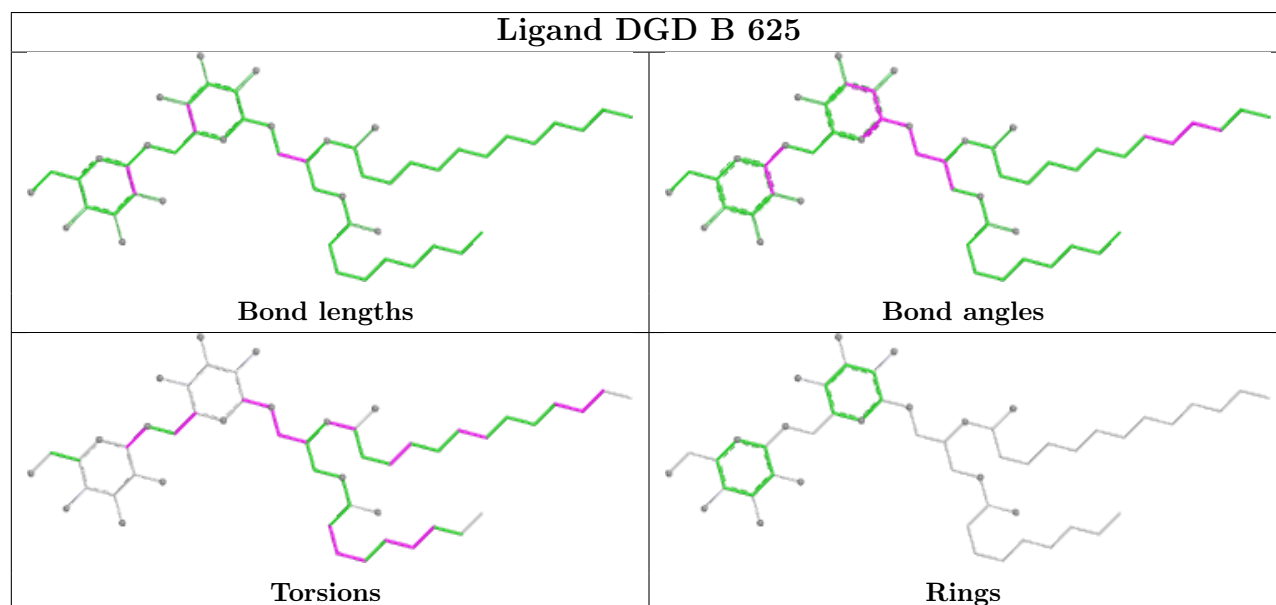
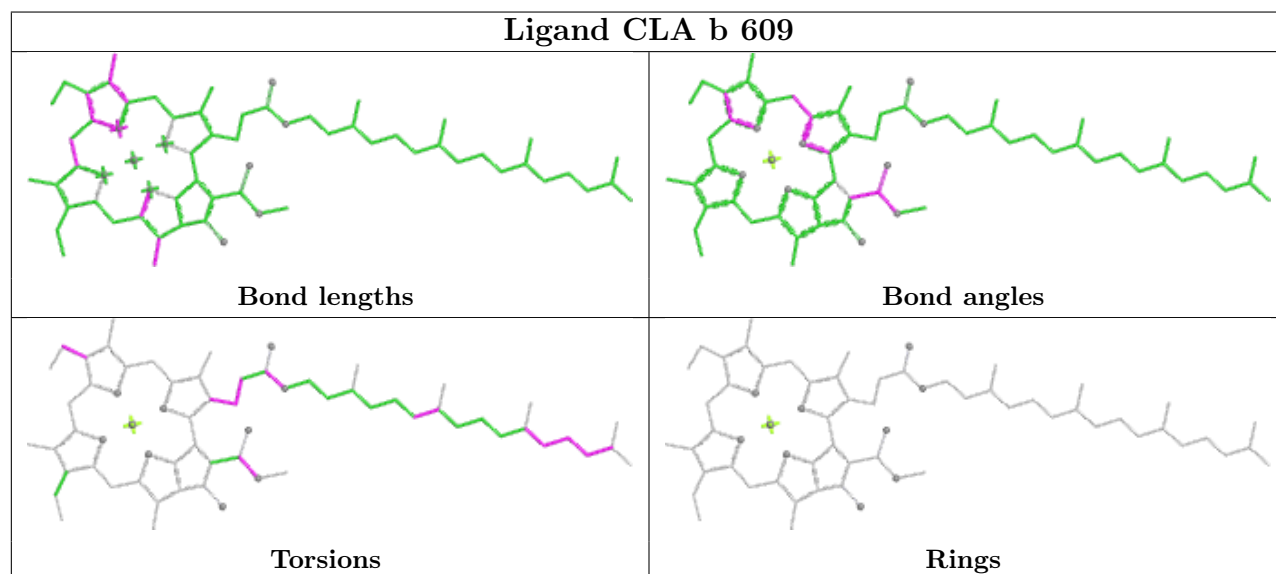
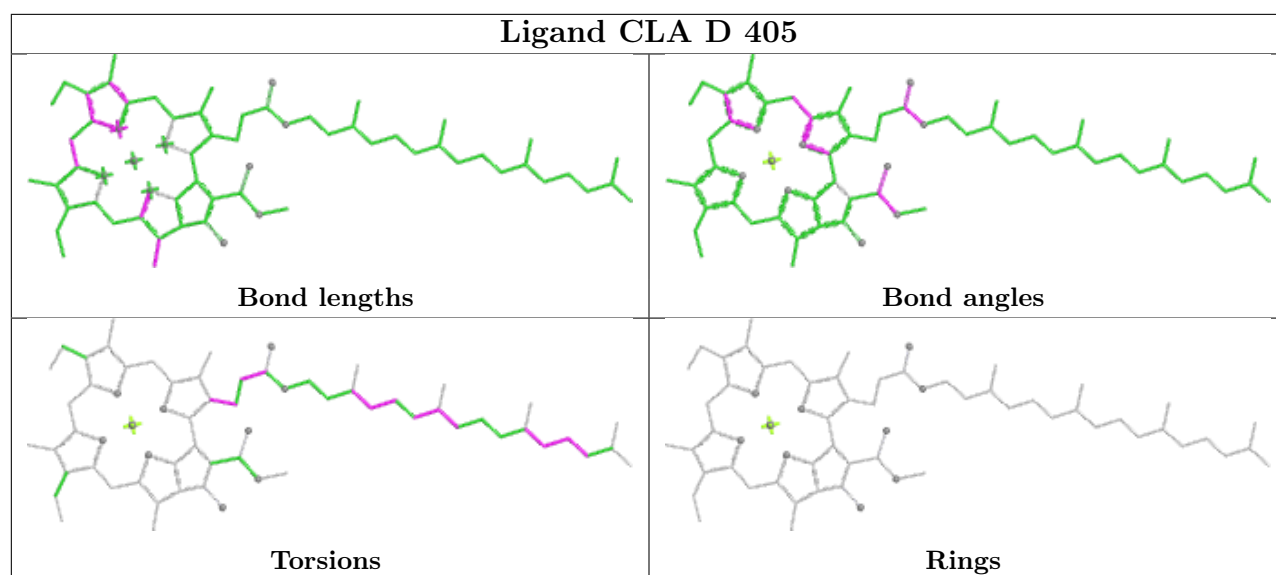
Ligand CLA B 614

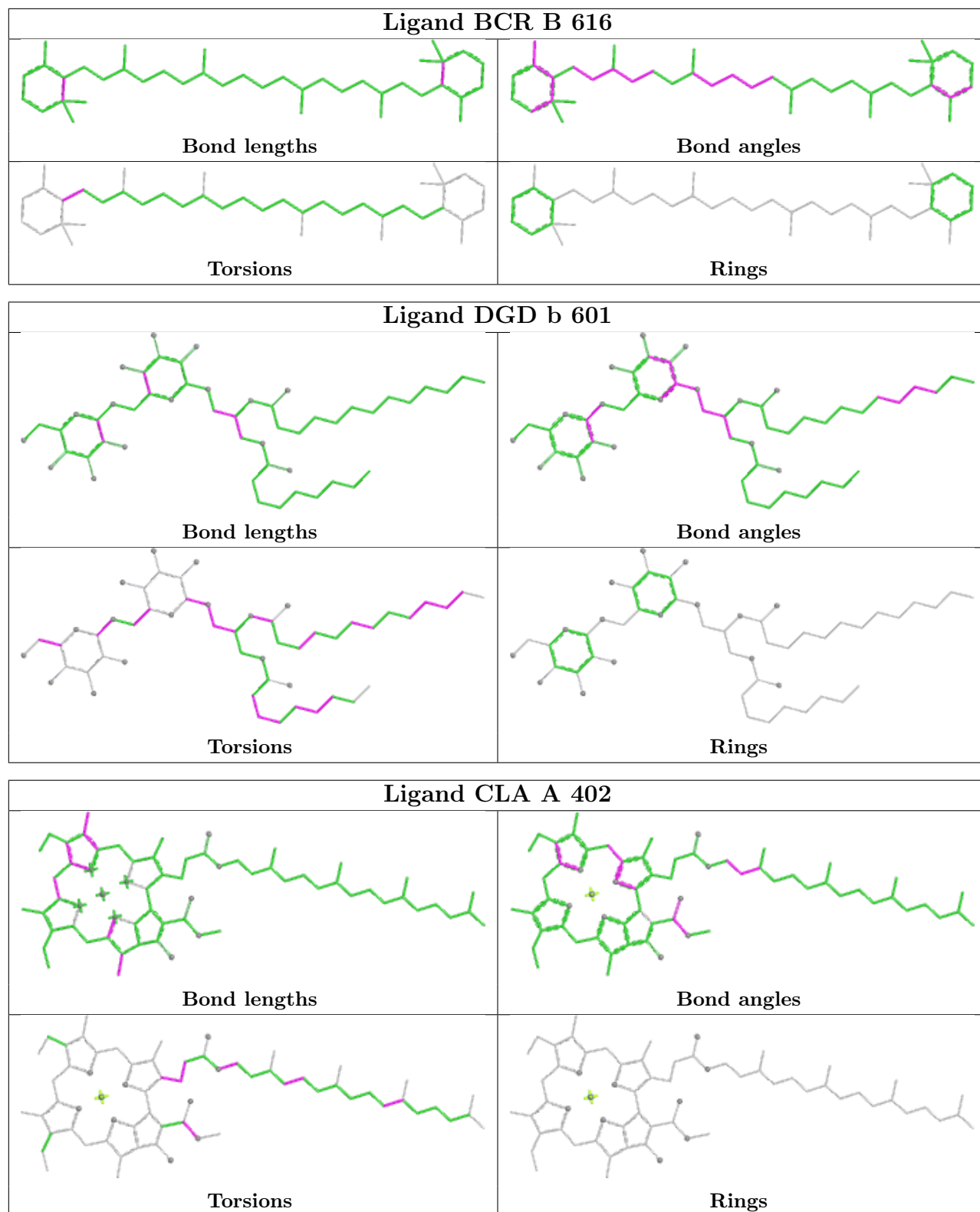


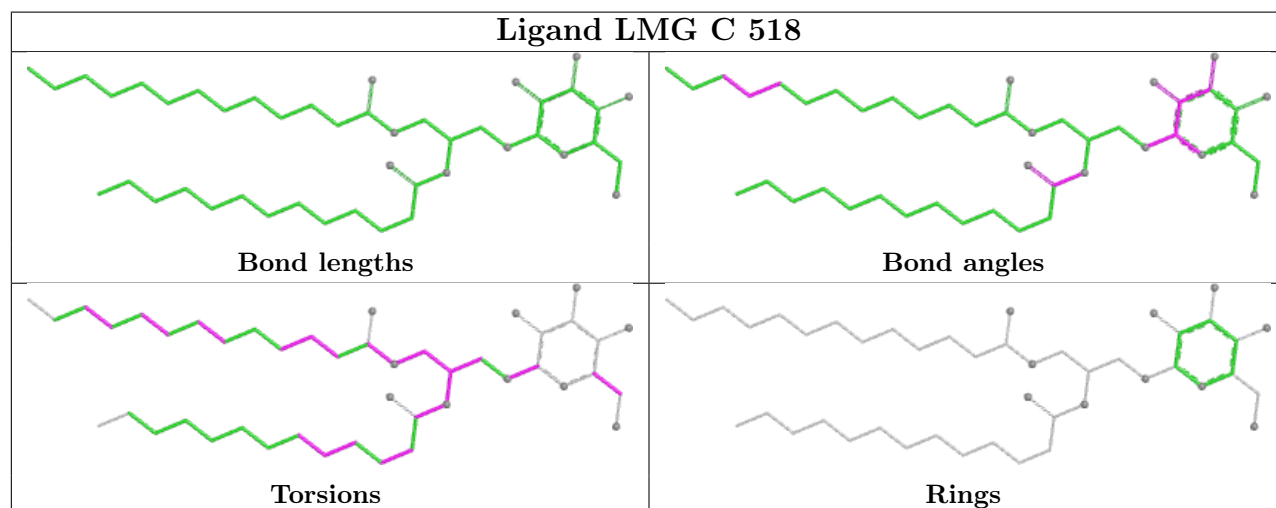
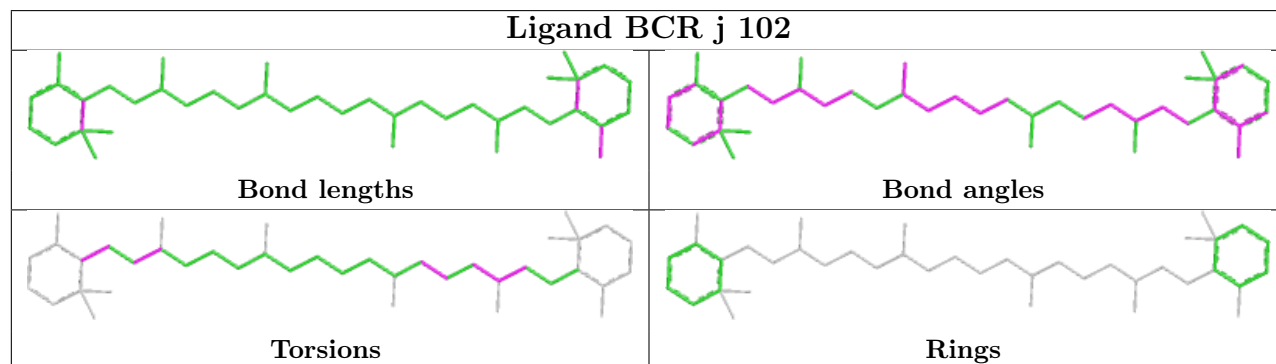
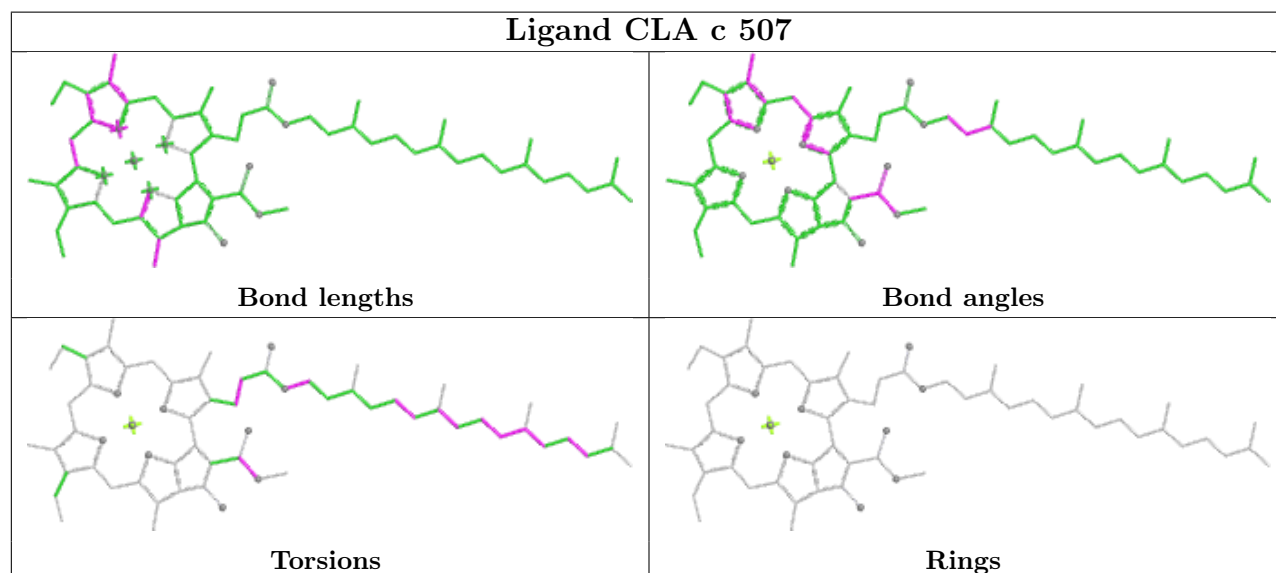
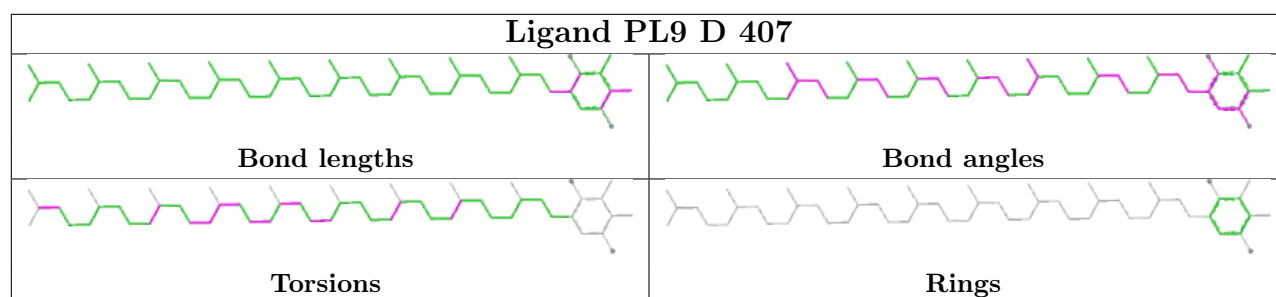
Ligand HEM F 101



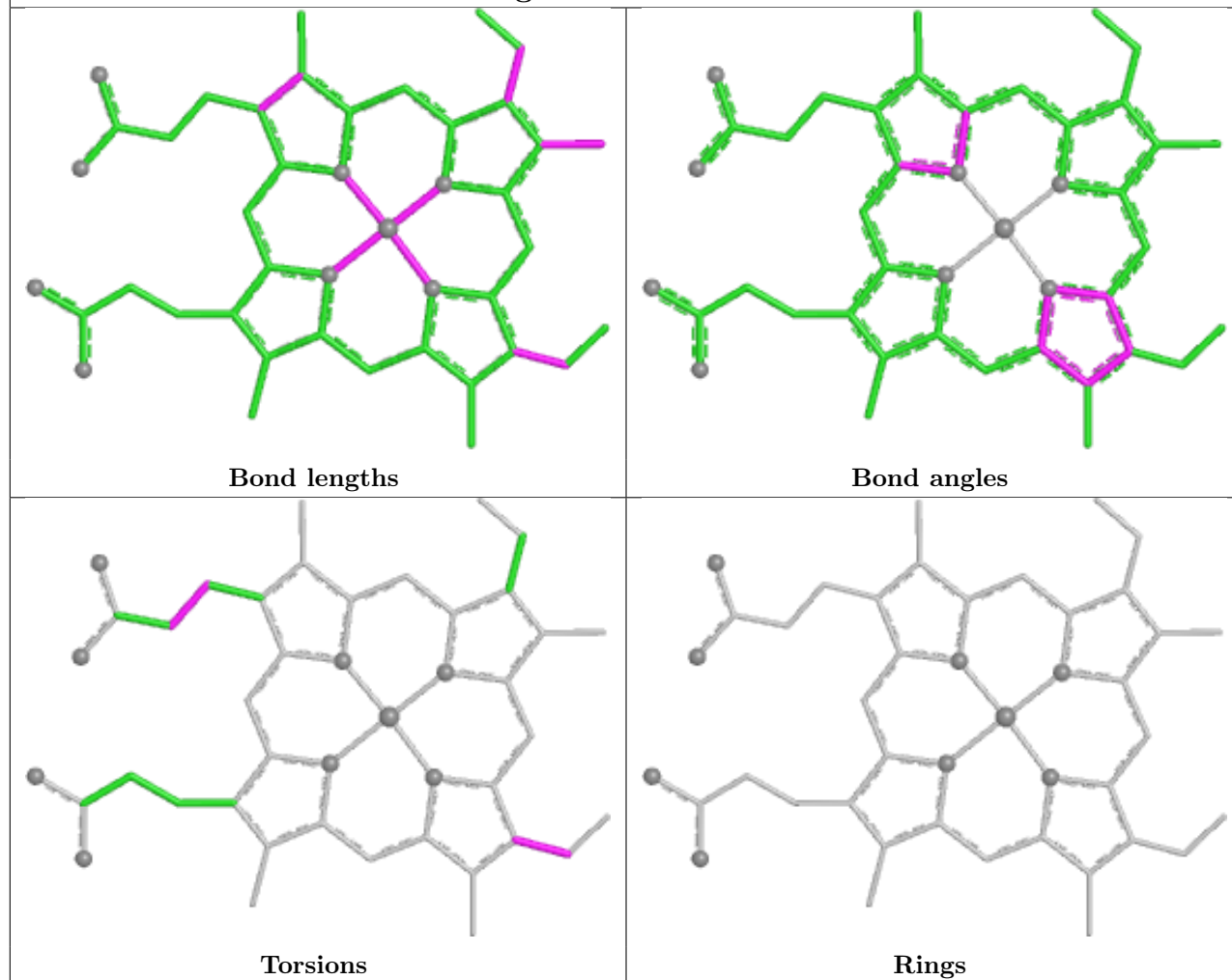




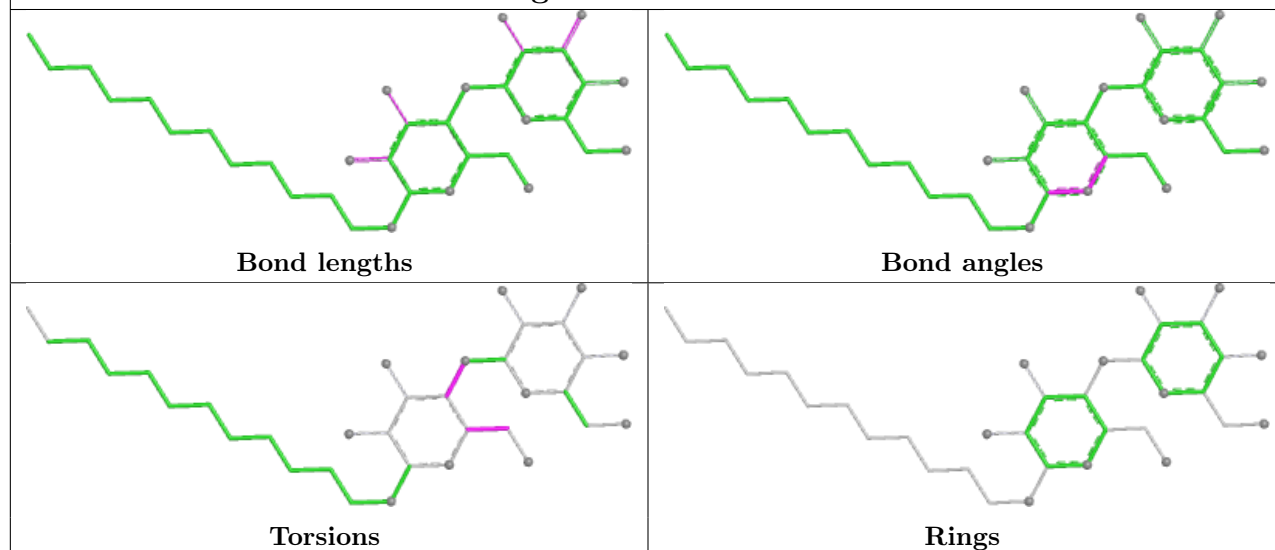




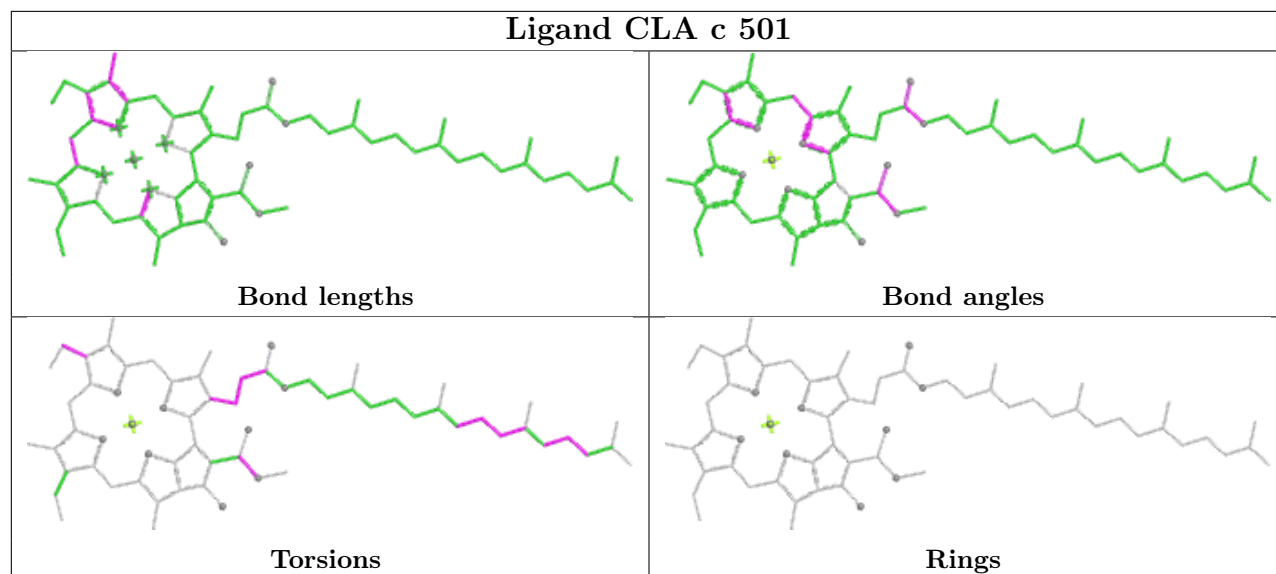
Ligand HEM f 101



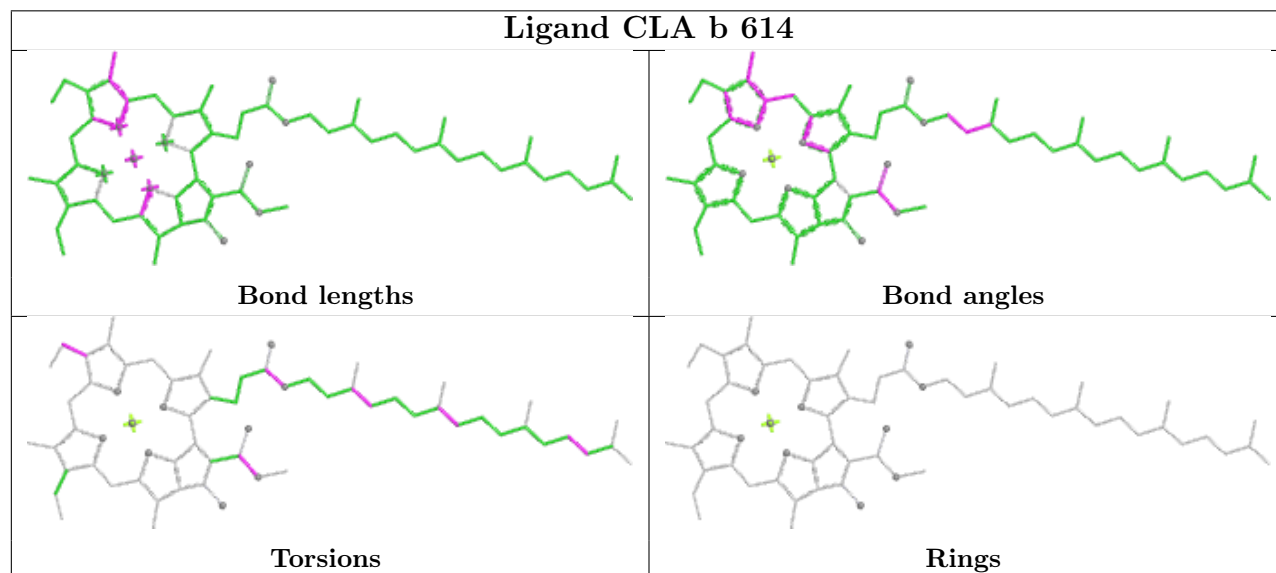
Ligand LMT b 603



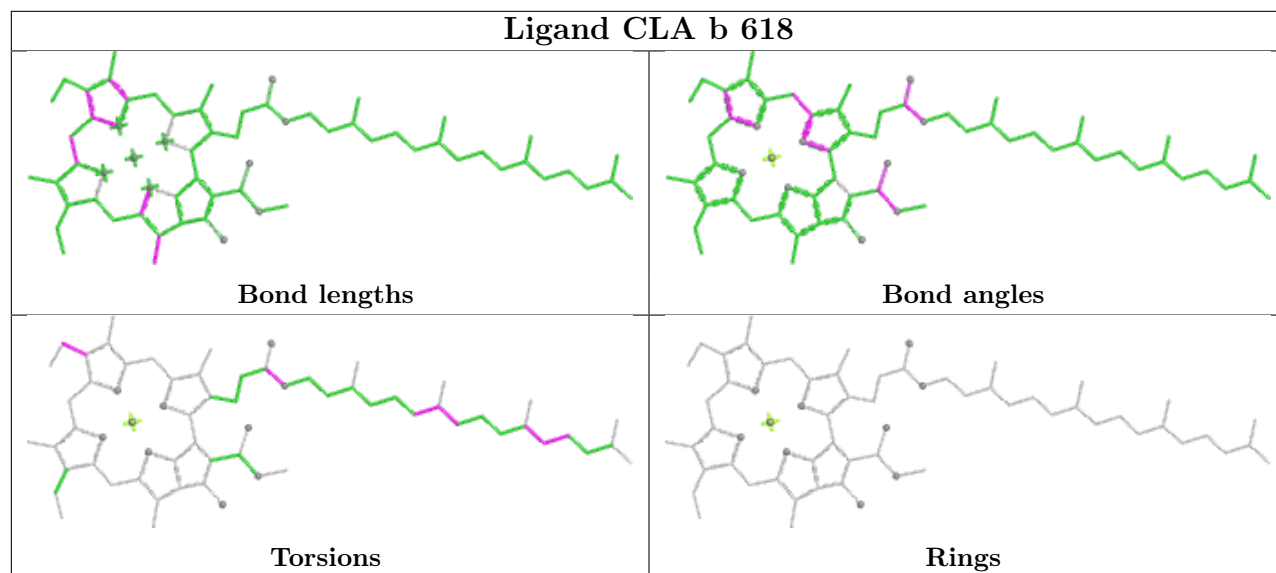
Ligand CLA c 501



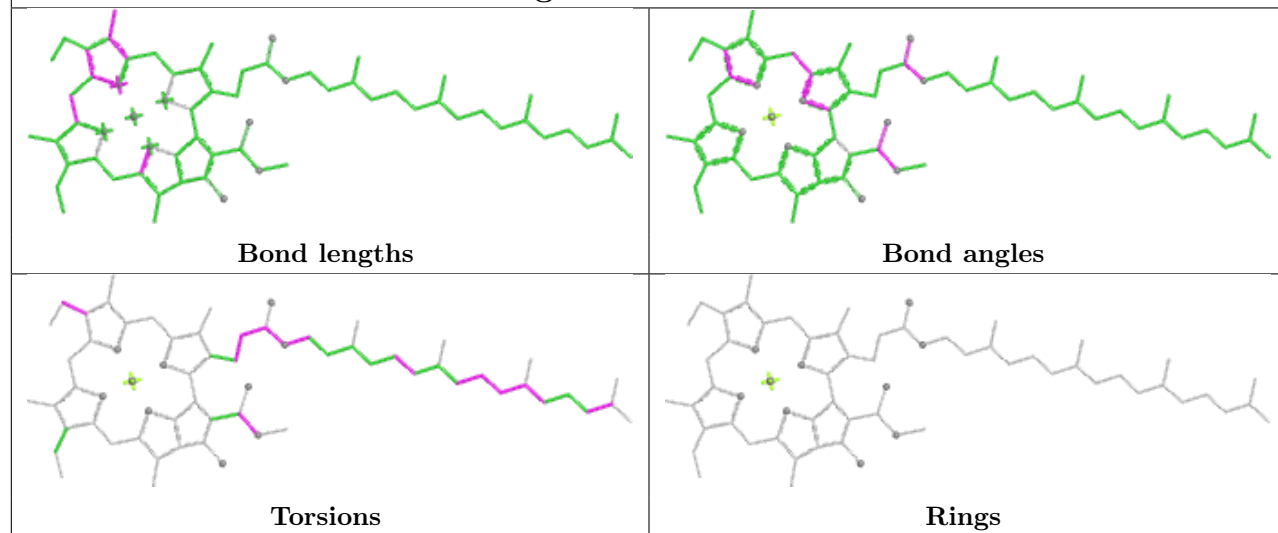
Ligand CLA b 614



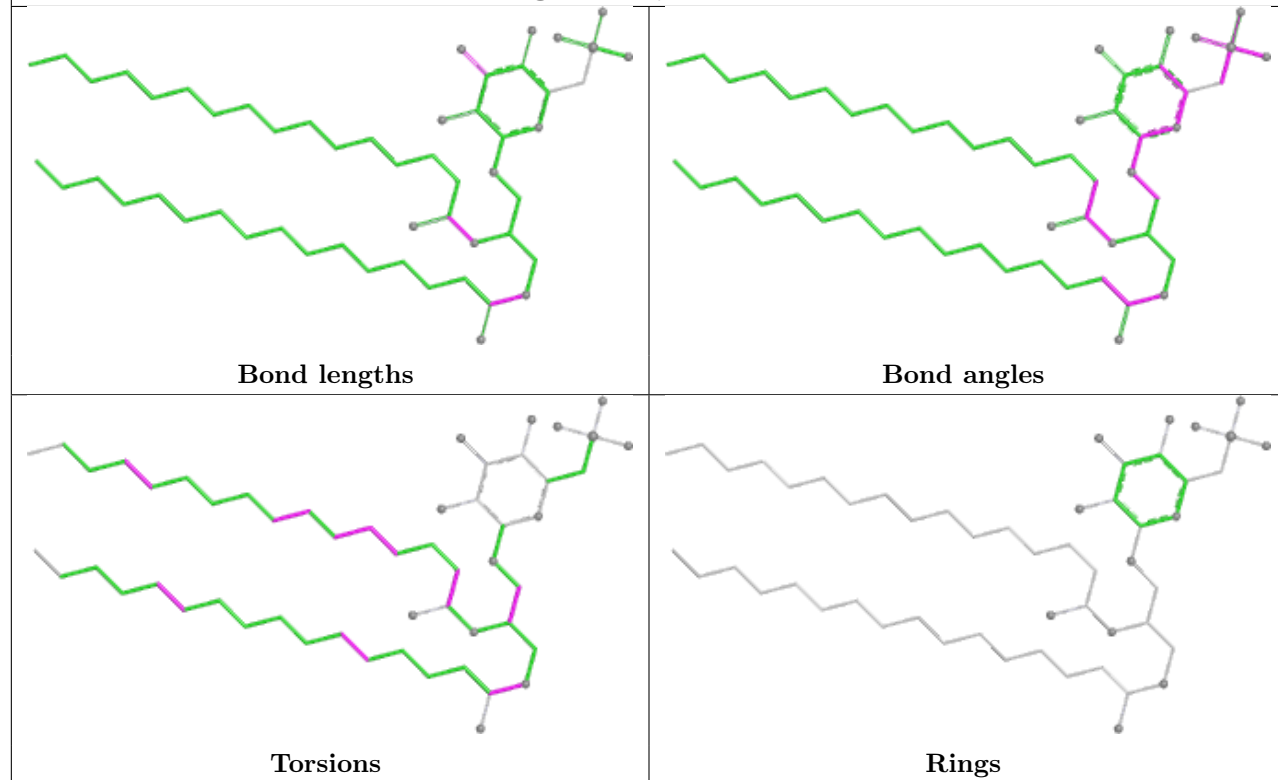
Ligand CLA b 618



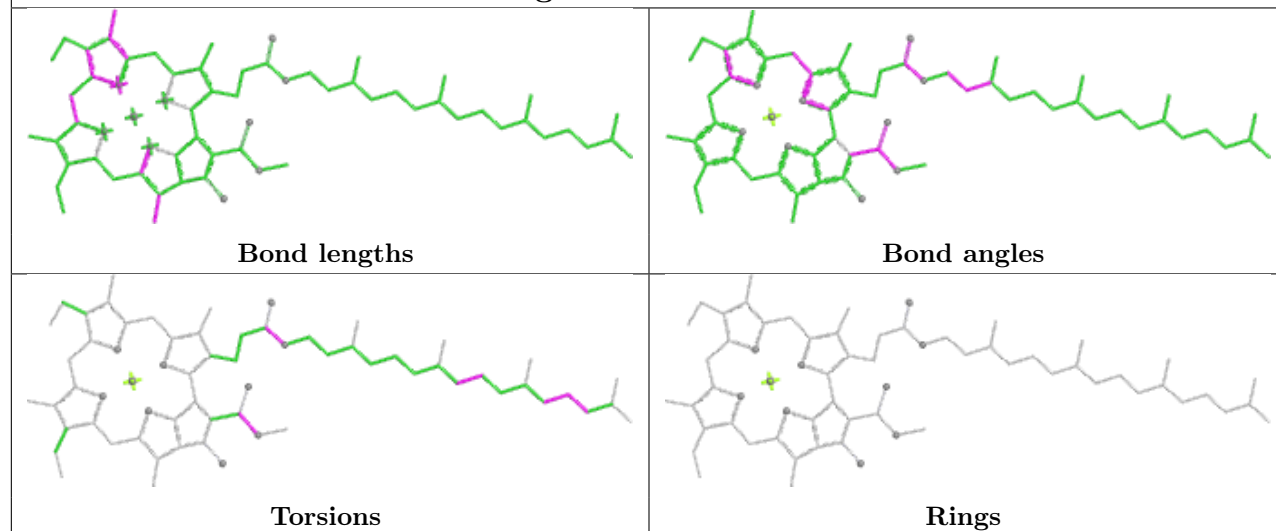
Ligand CLA b 613



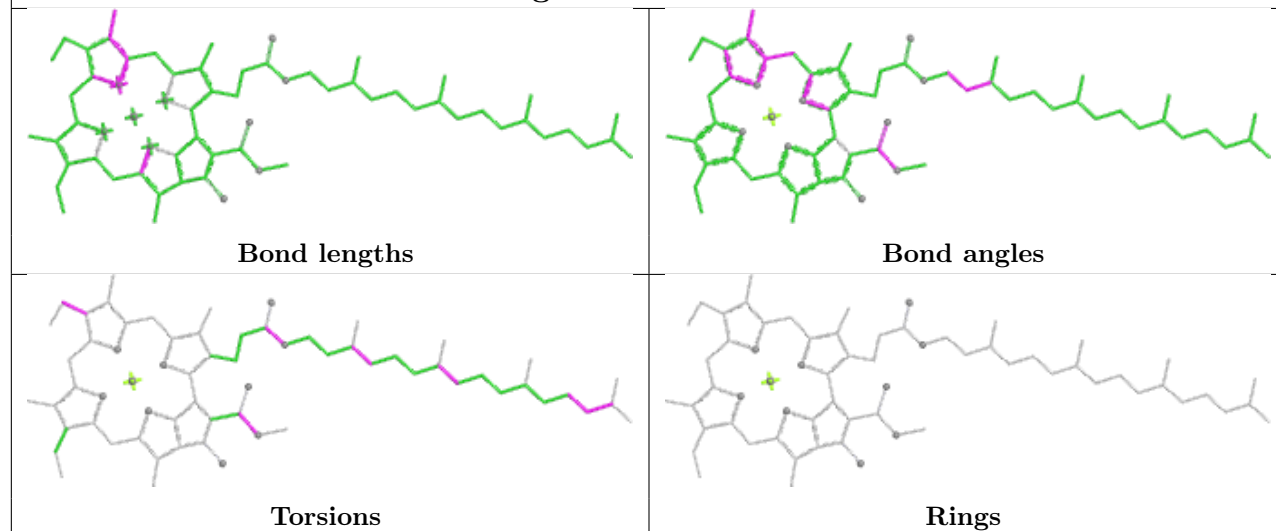
Ligand SQD A 413

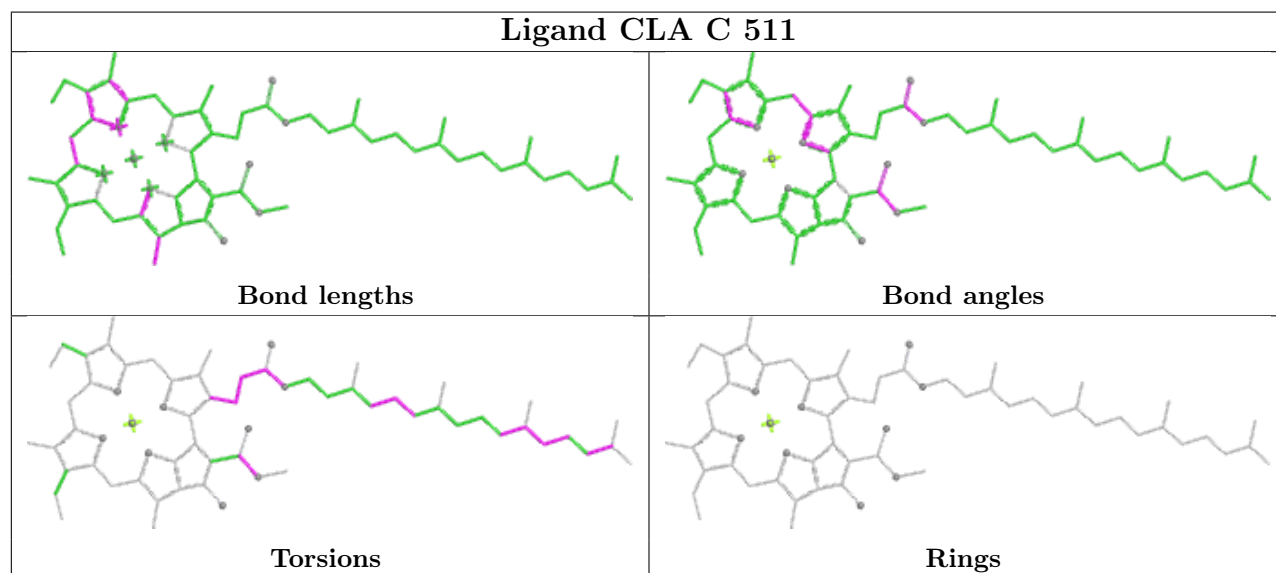
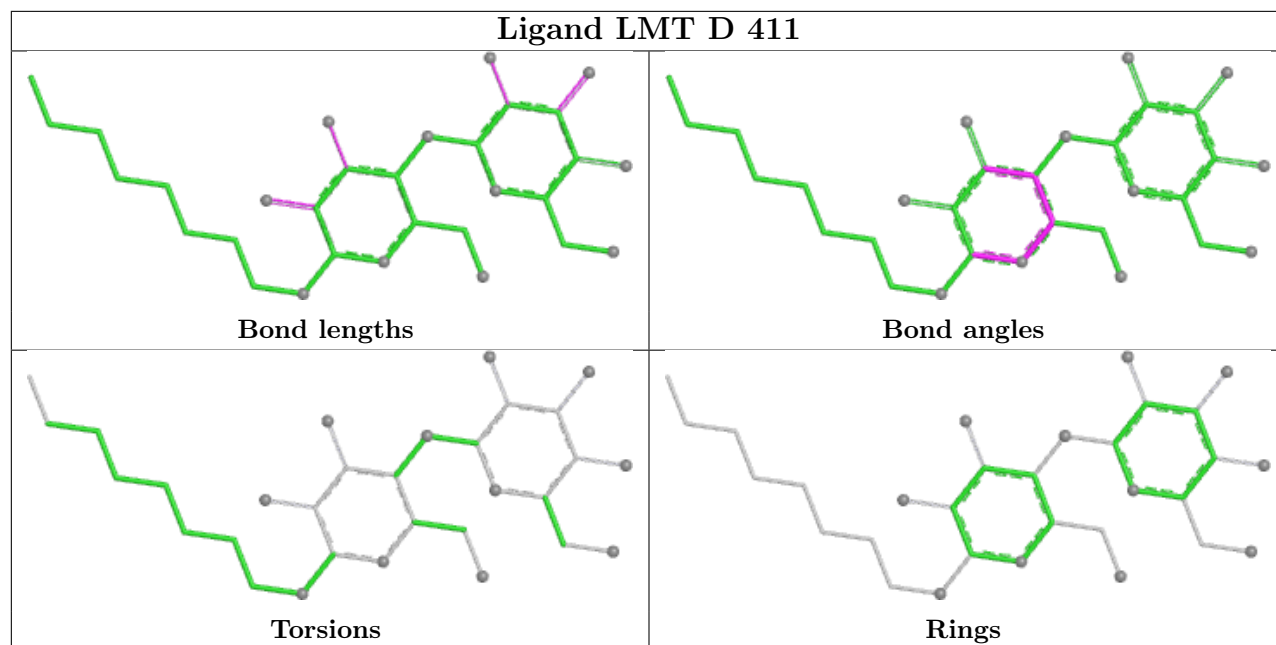


Ligand CLA b 607

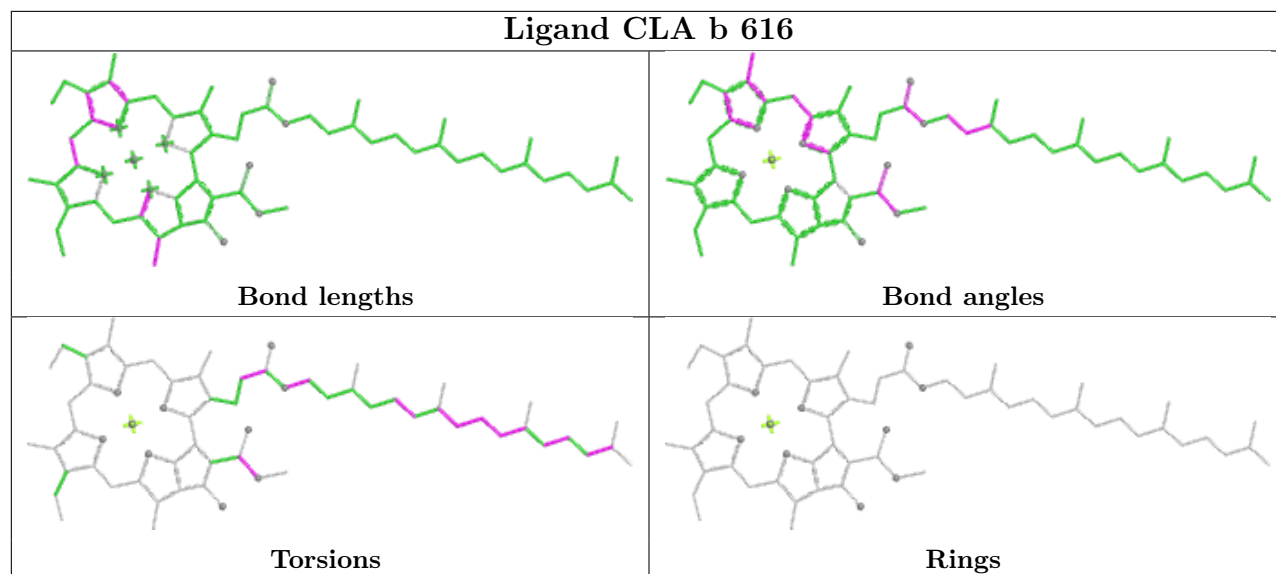


Ligand CLA B 610

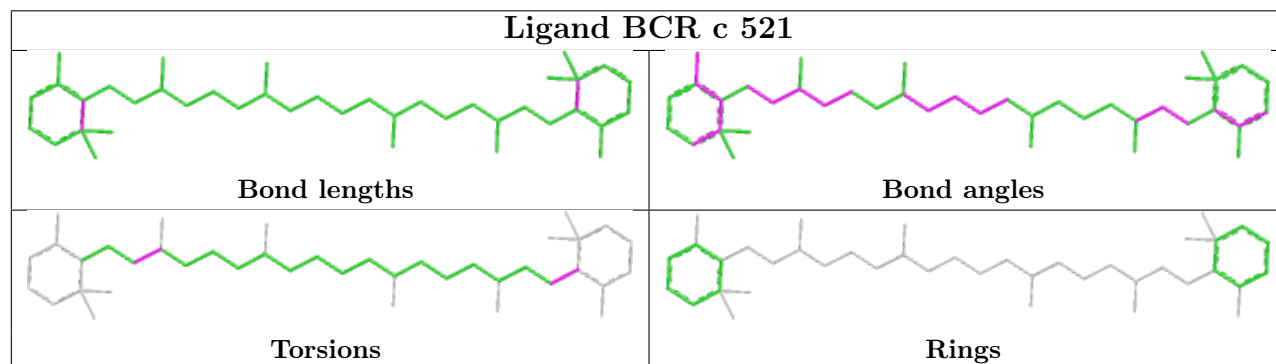




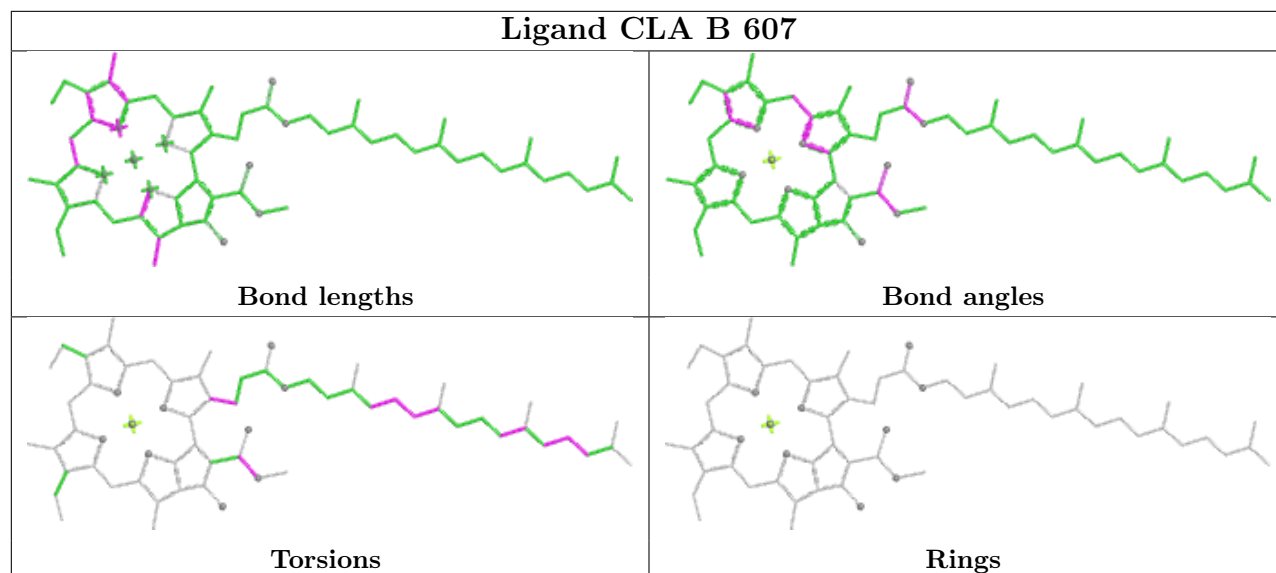
Ligand CLA b 616



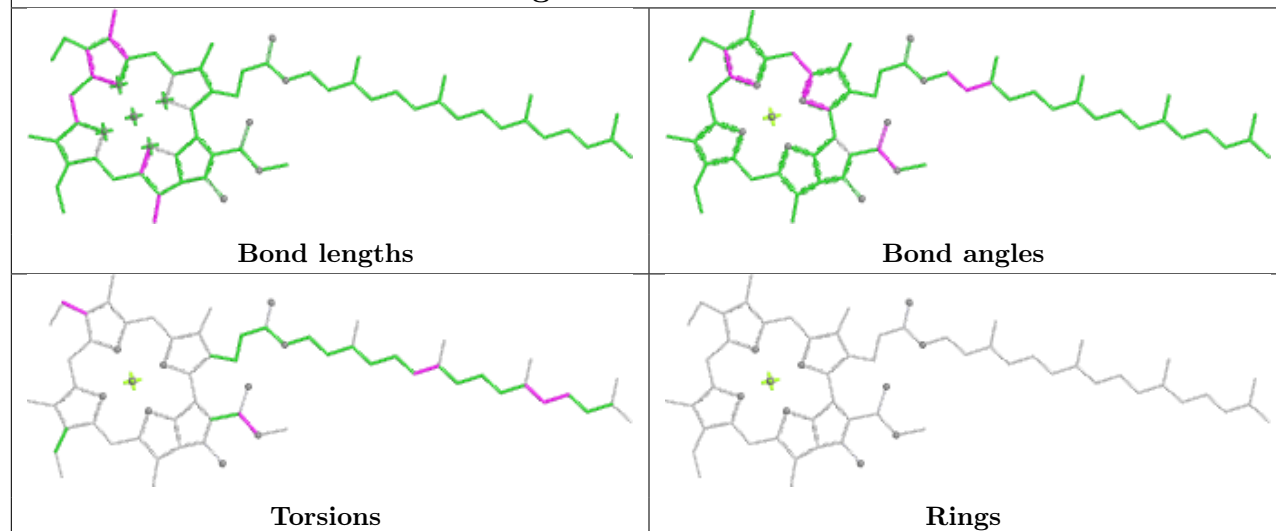
Ligand BCR c 521



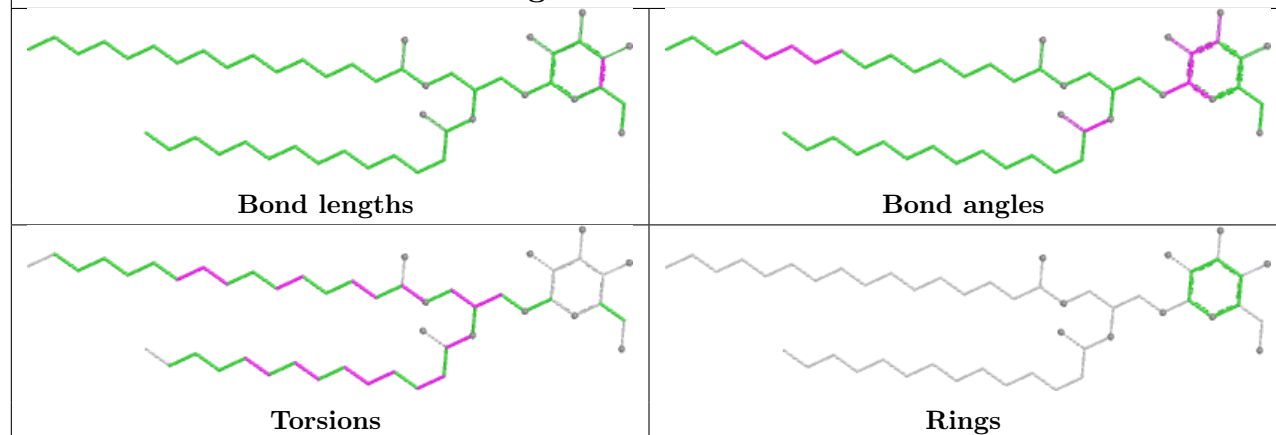
Ligand CLA B 607



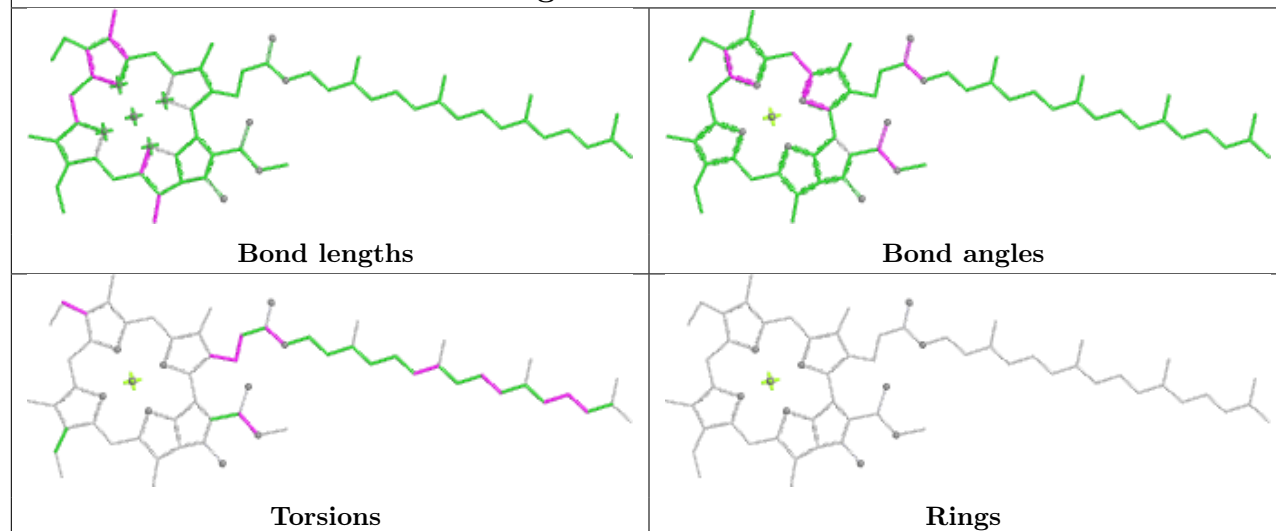
Ligand CLA B 608

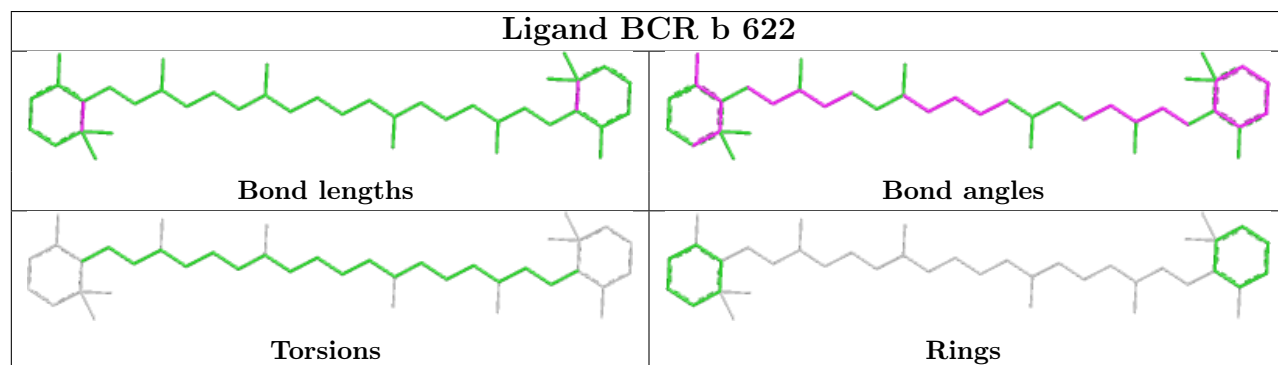
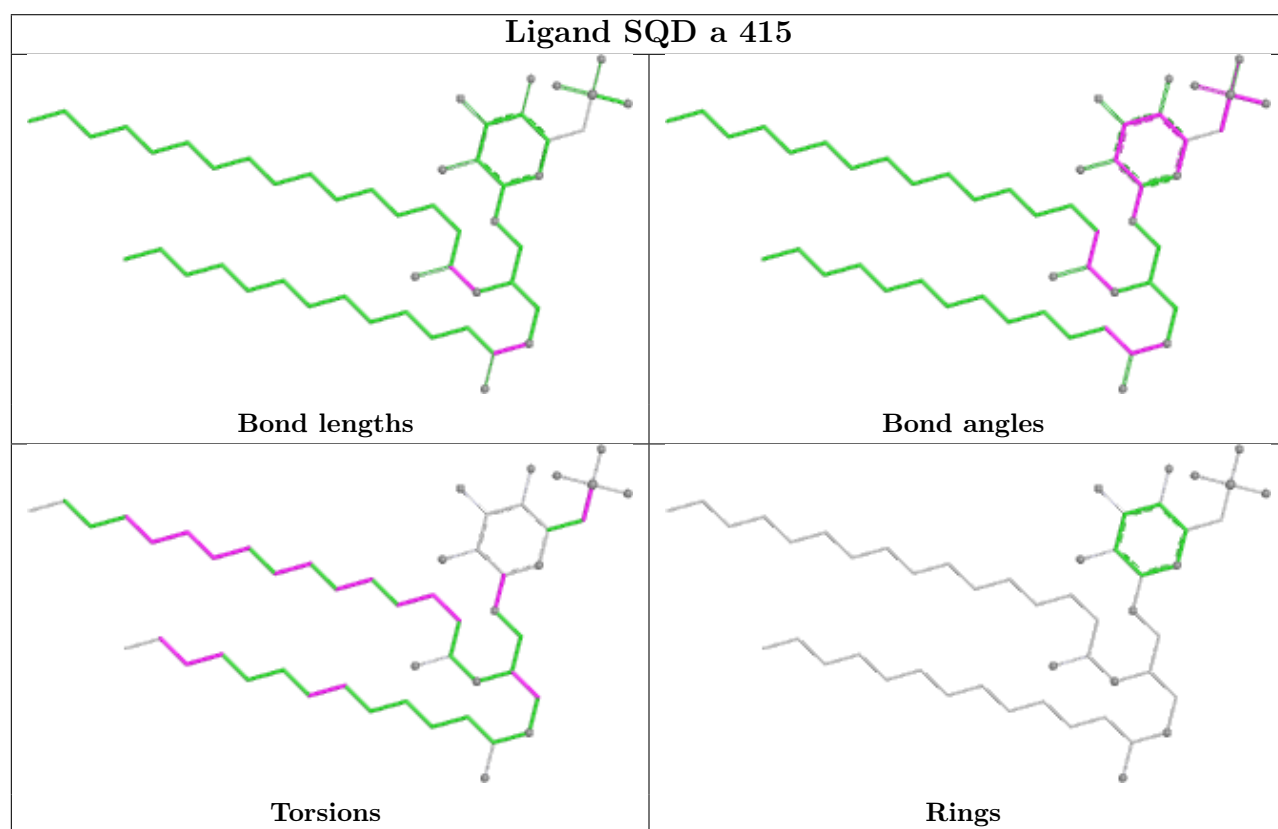
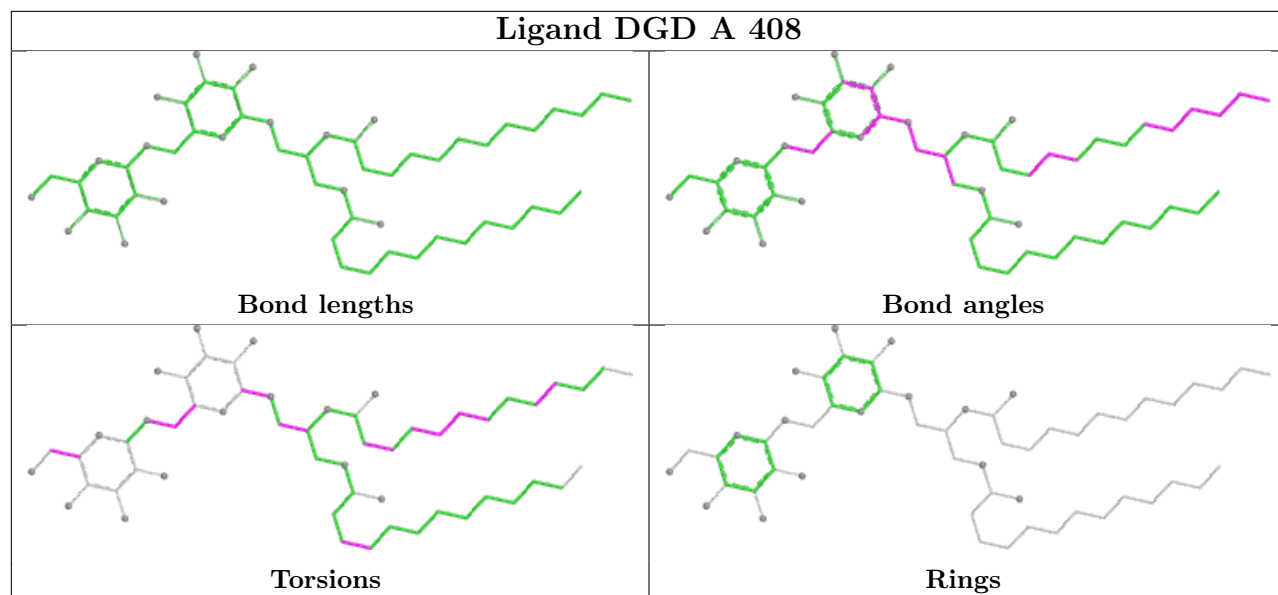


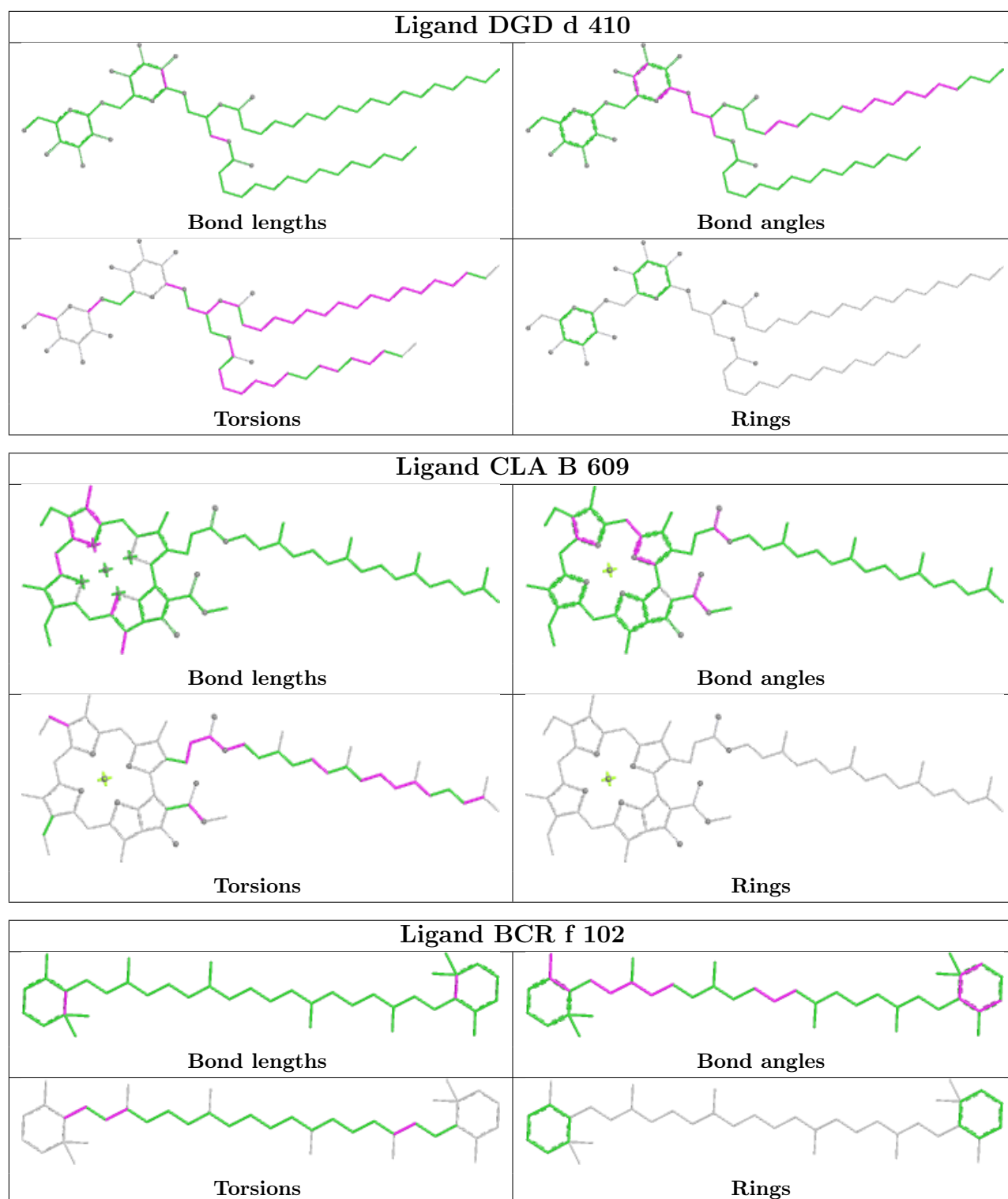
Ligand LMG B 621

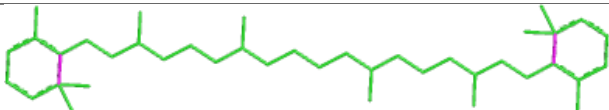
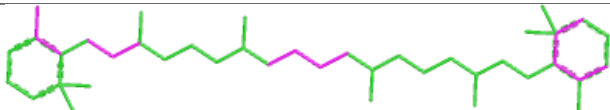
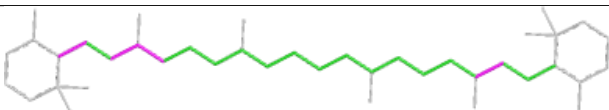
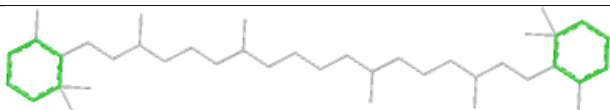


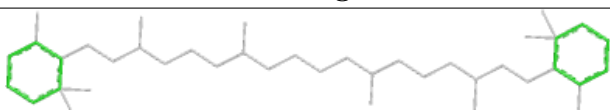
Ligand CLA c 520

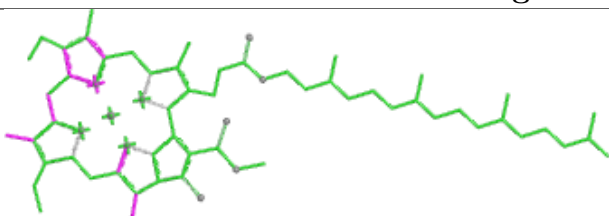
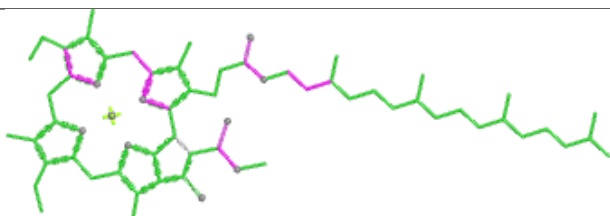
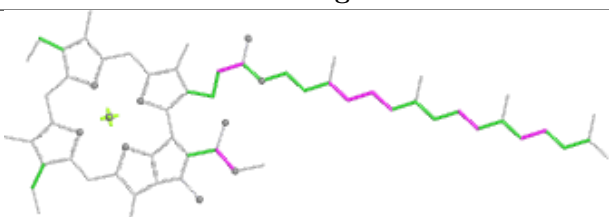
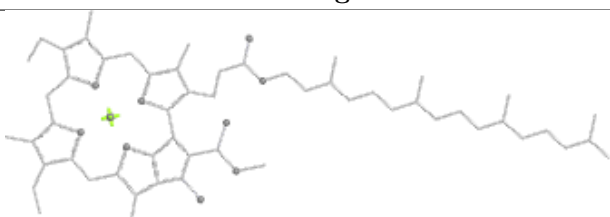


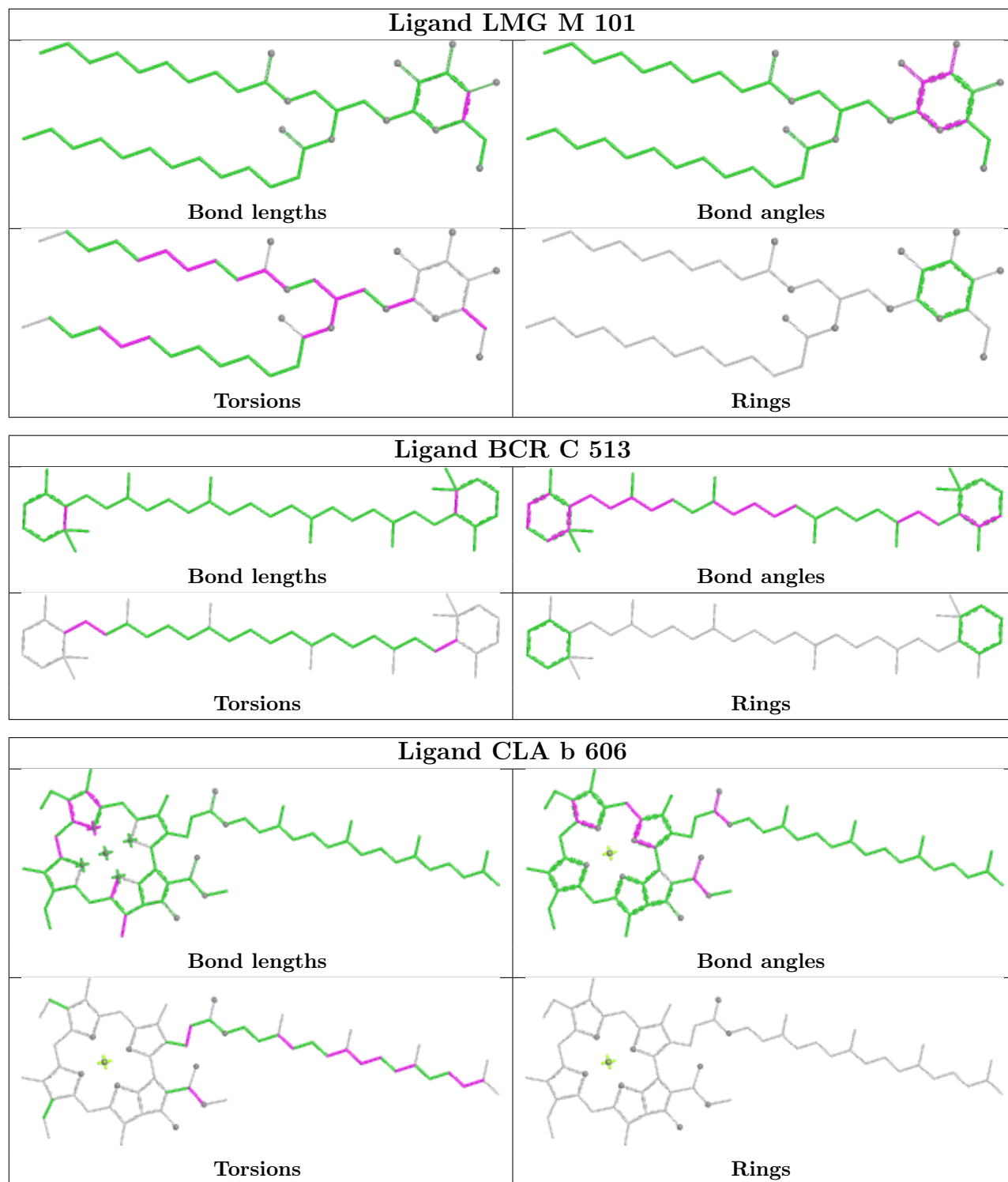




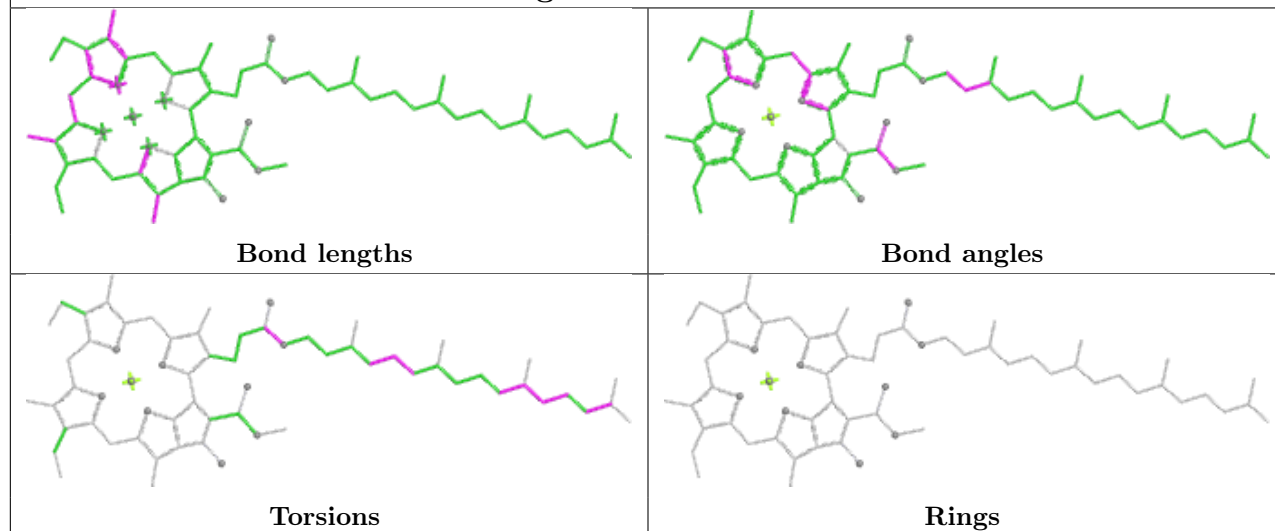
Ligand BCR H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

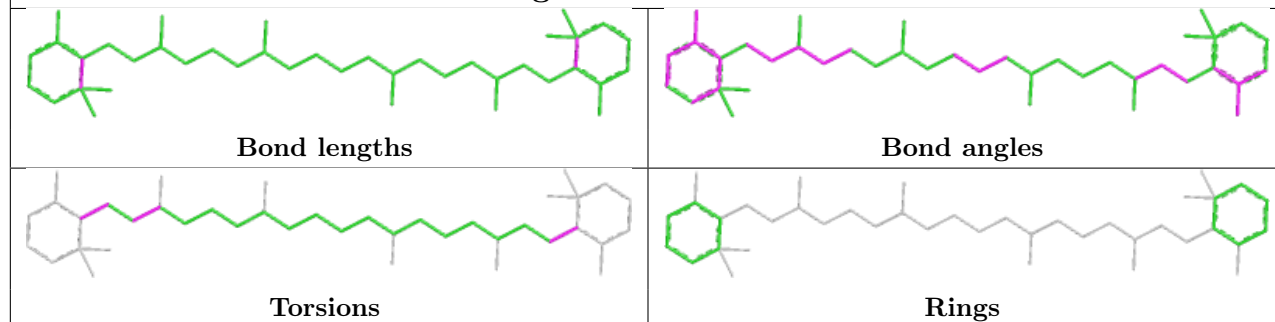
Ligand CLA b 615	
	
Bond lengths	Bond angles
	
Torsions	Rings



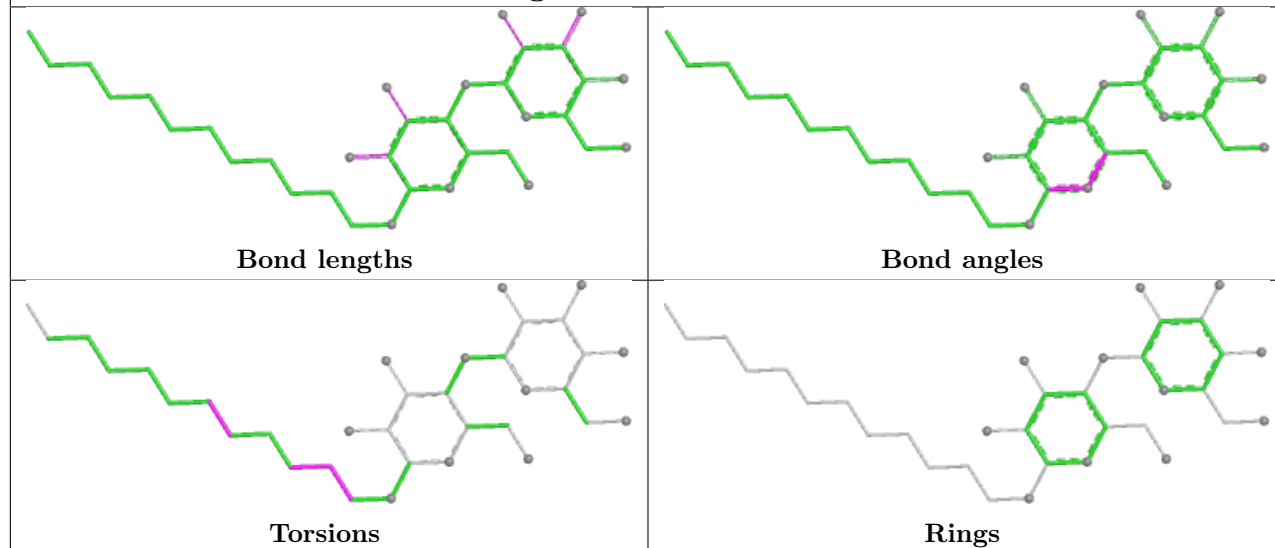
Ligand CLA c 502



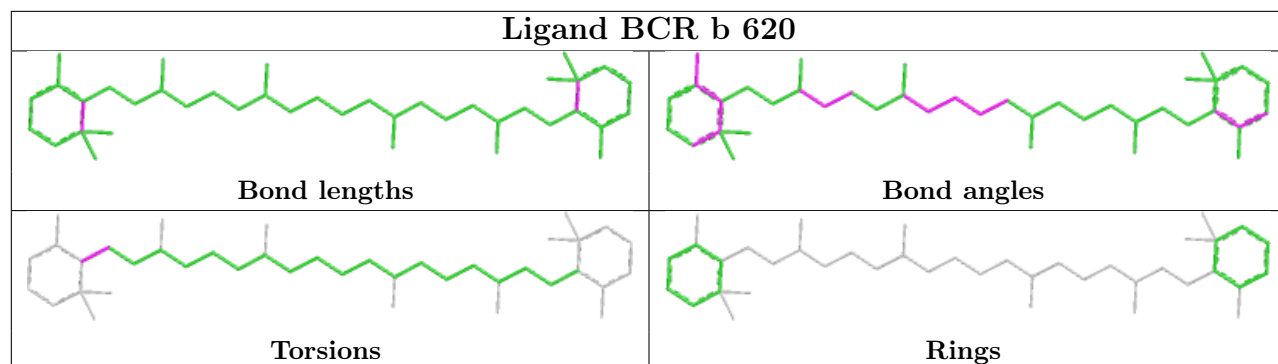
Ligand BCR b 623



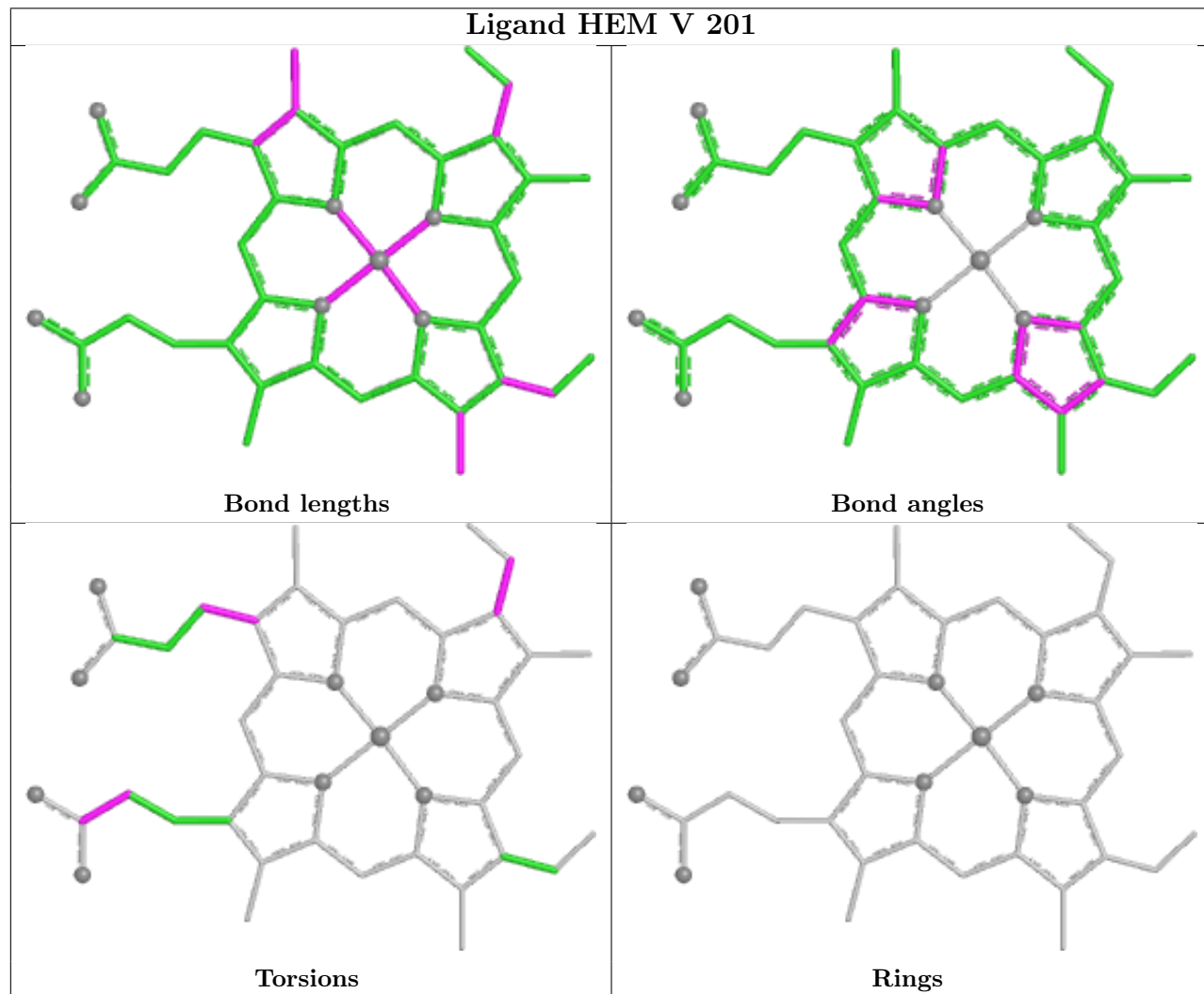
Ligand LMT B 623



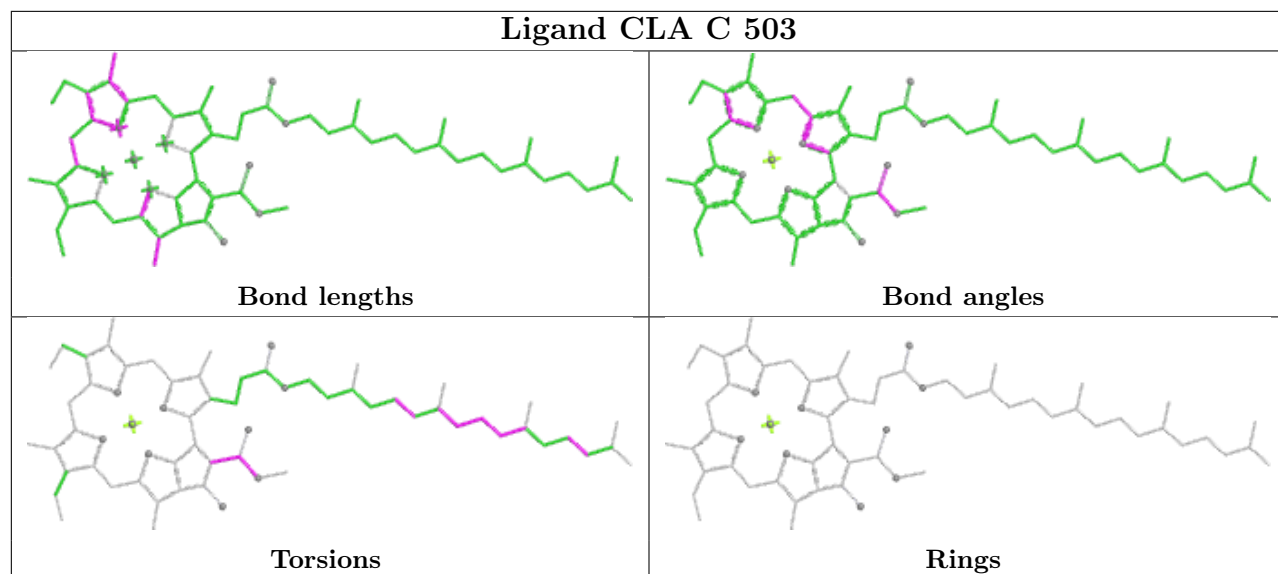
Ligand BCR b 620



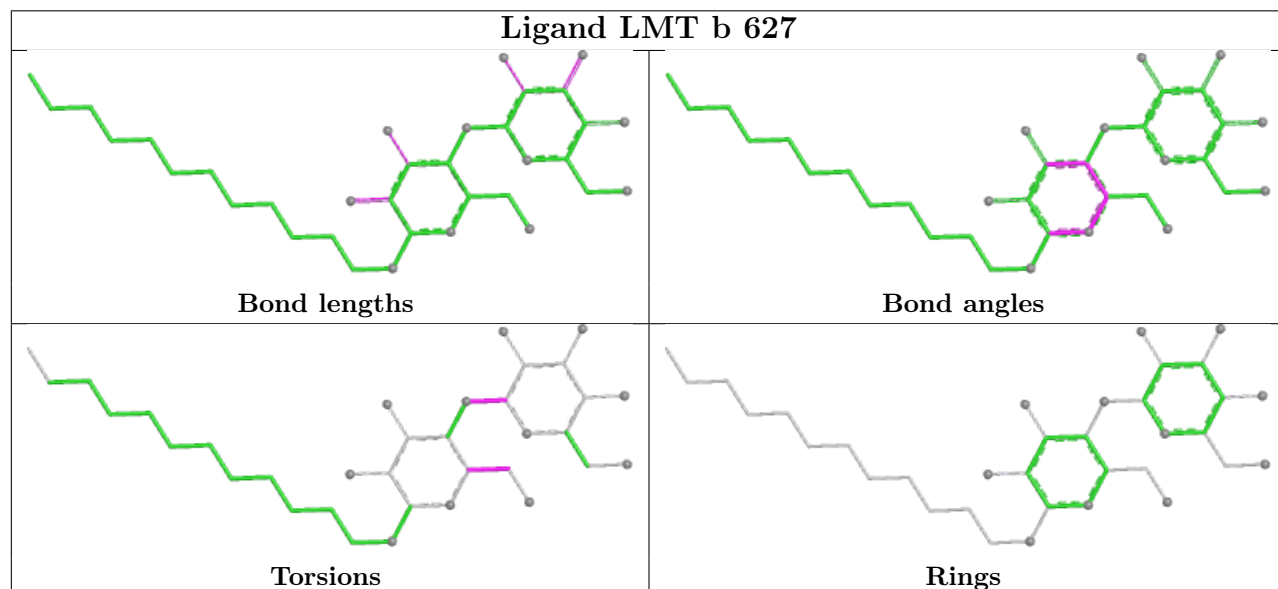
Ligand HEM V 201



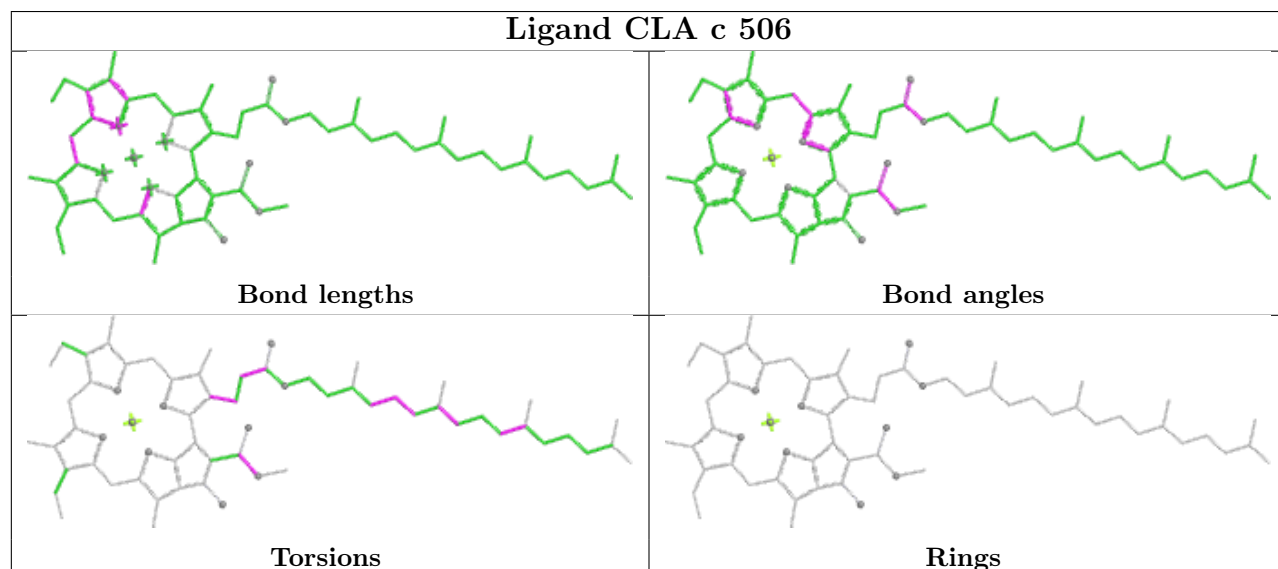
Ligand CLA C 503

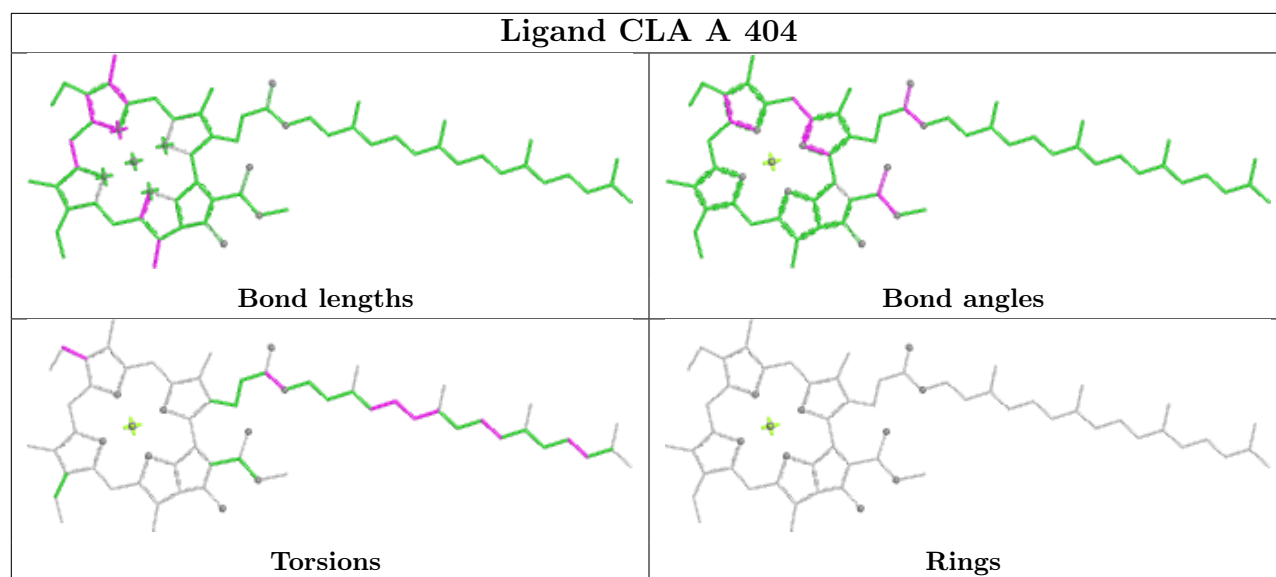
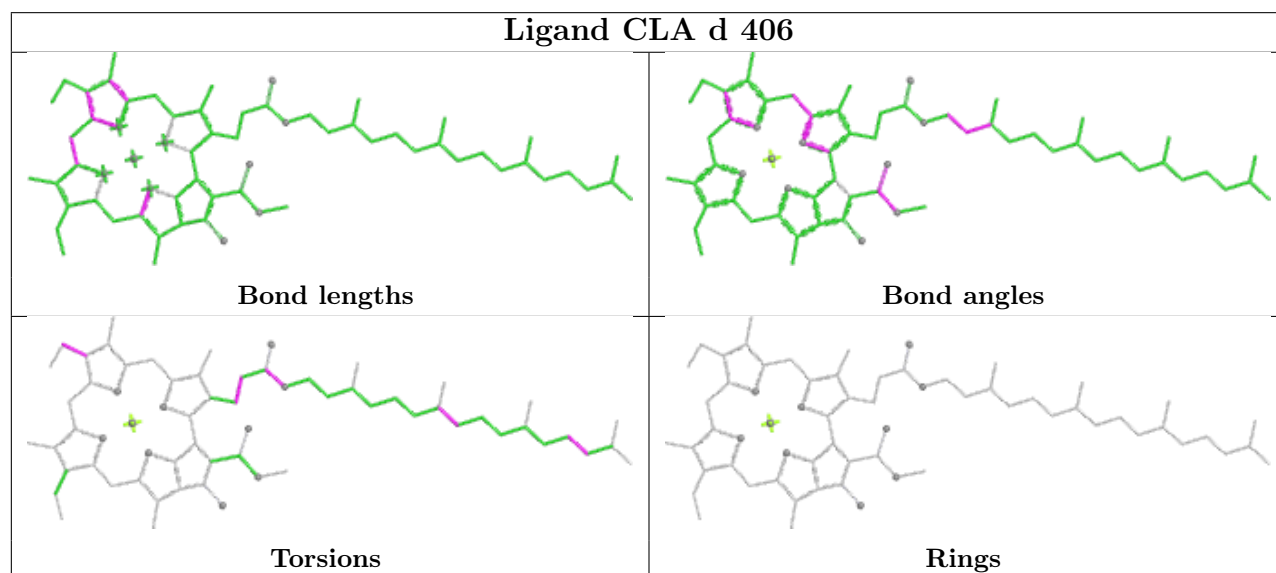
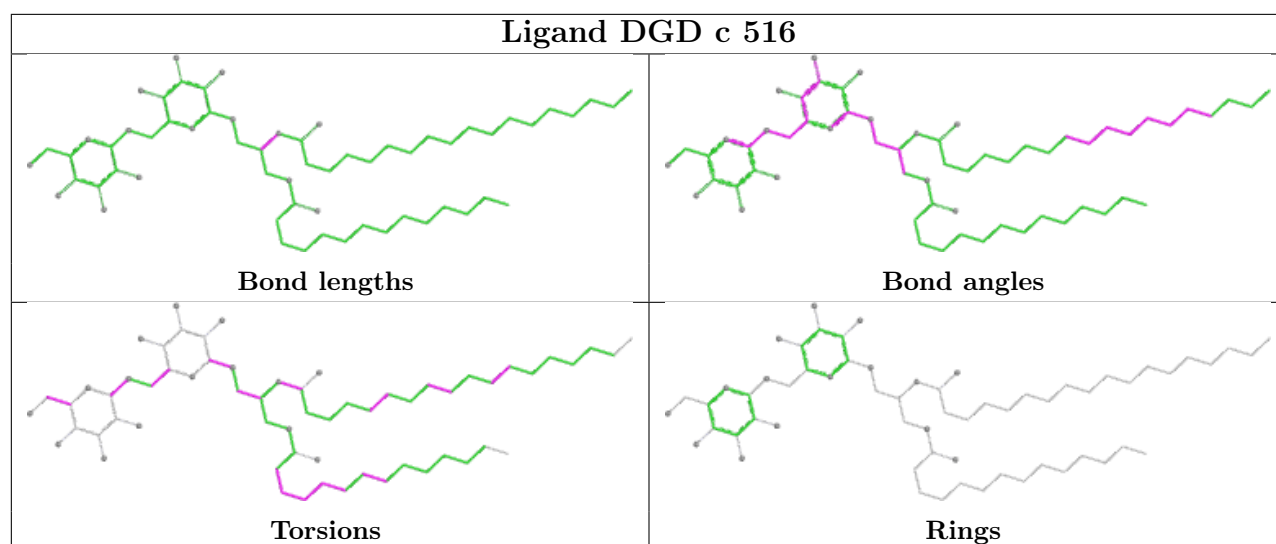


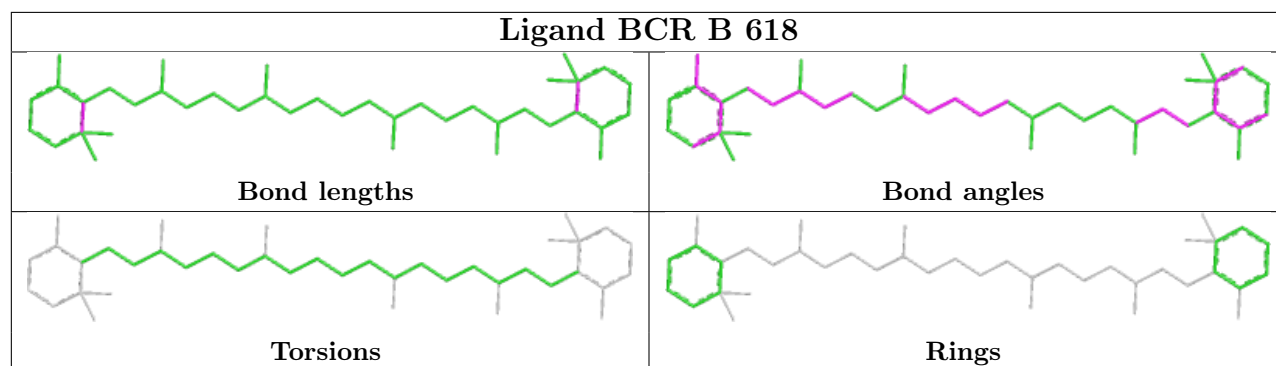
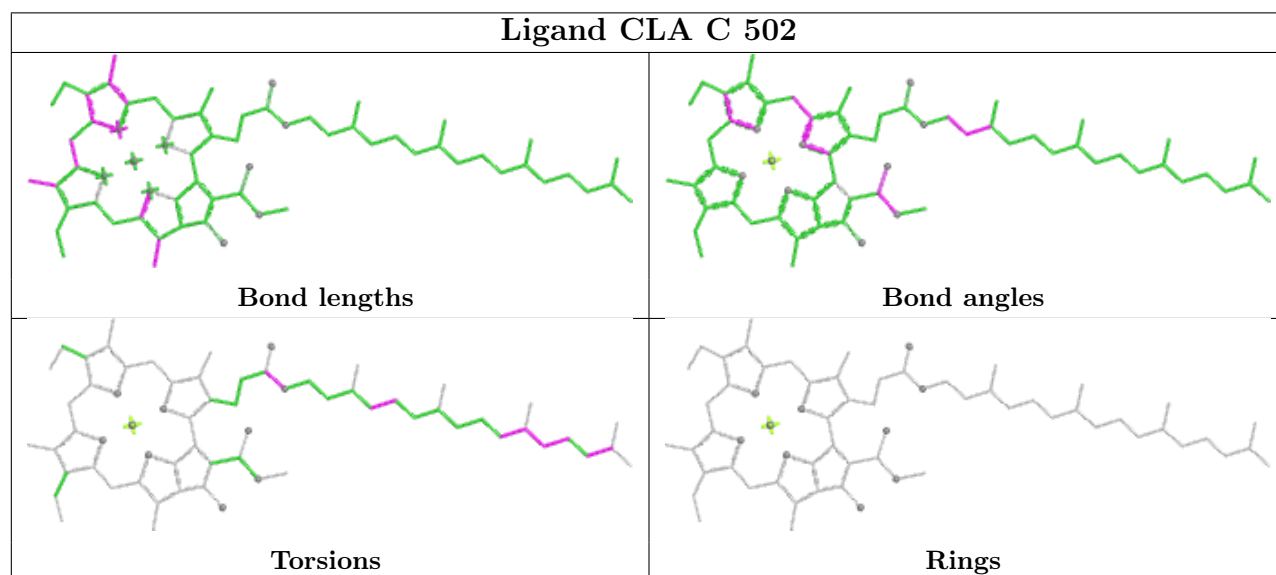
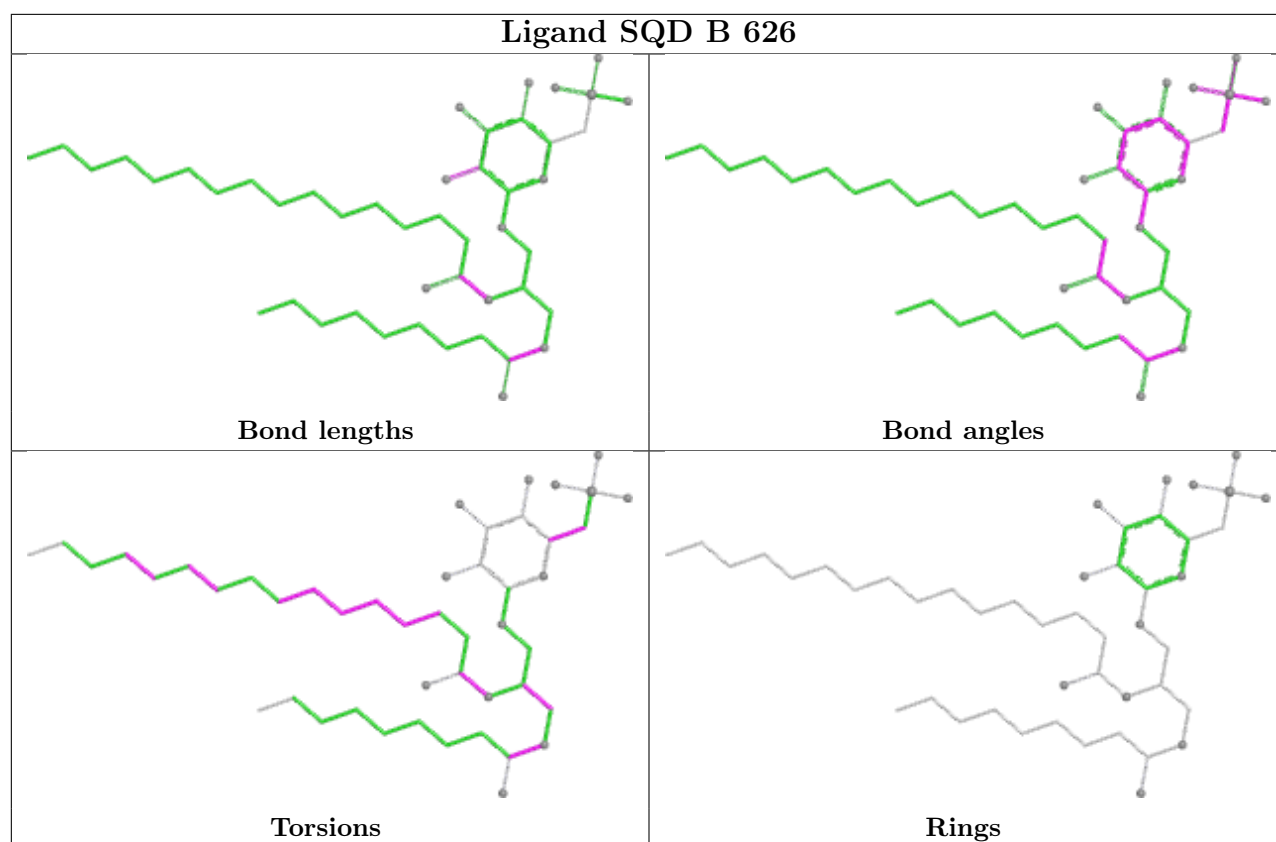
Ligand LMT b 627

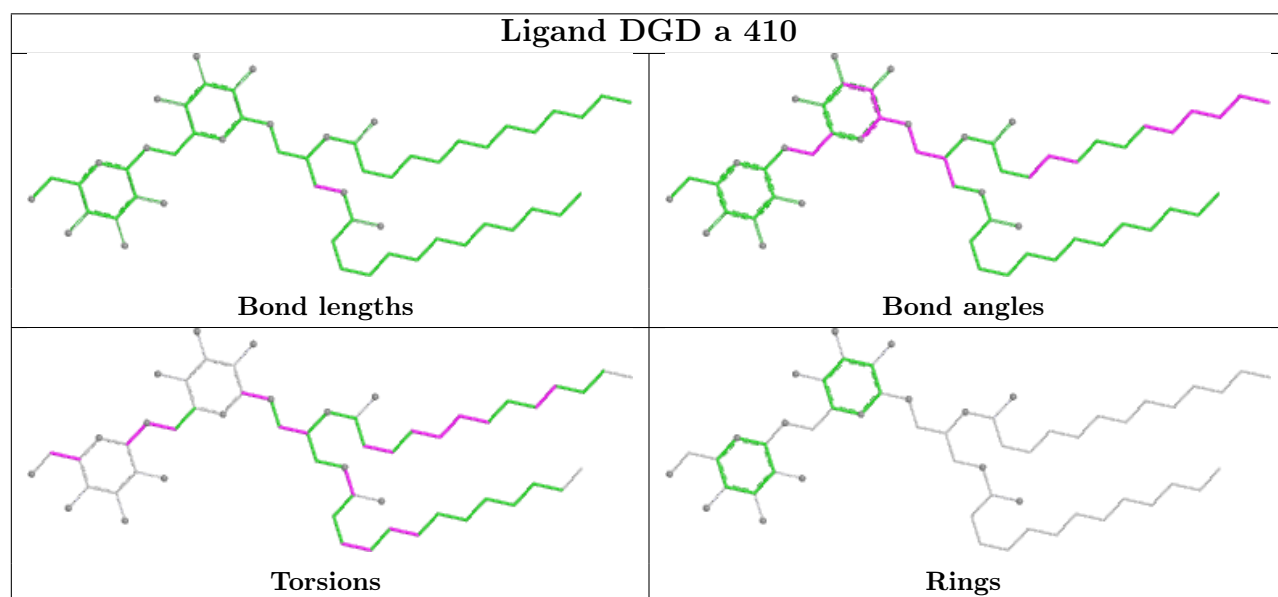
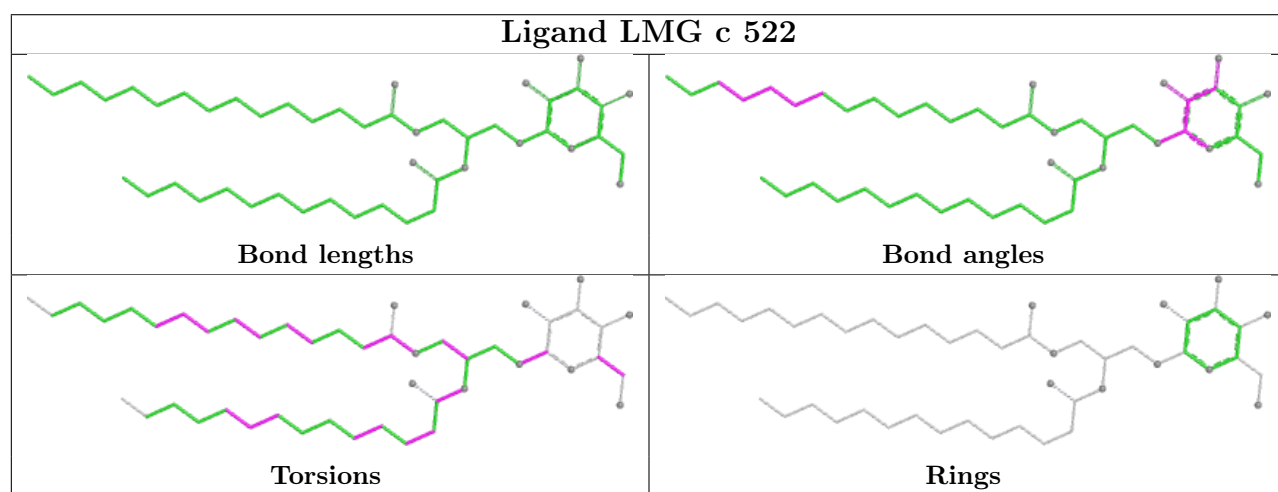
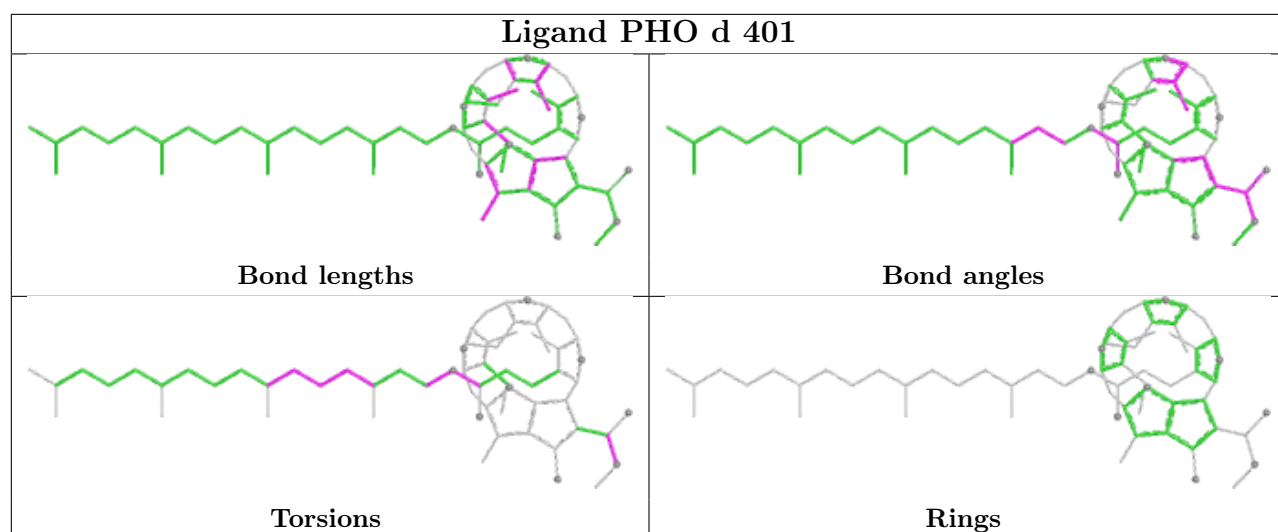


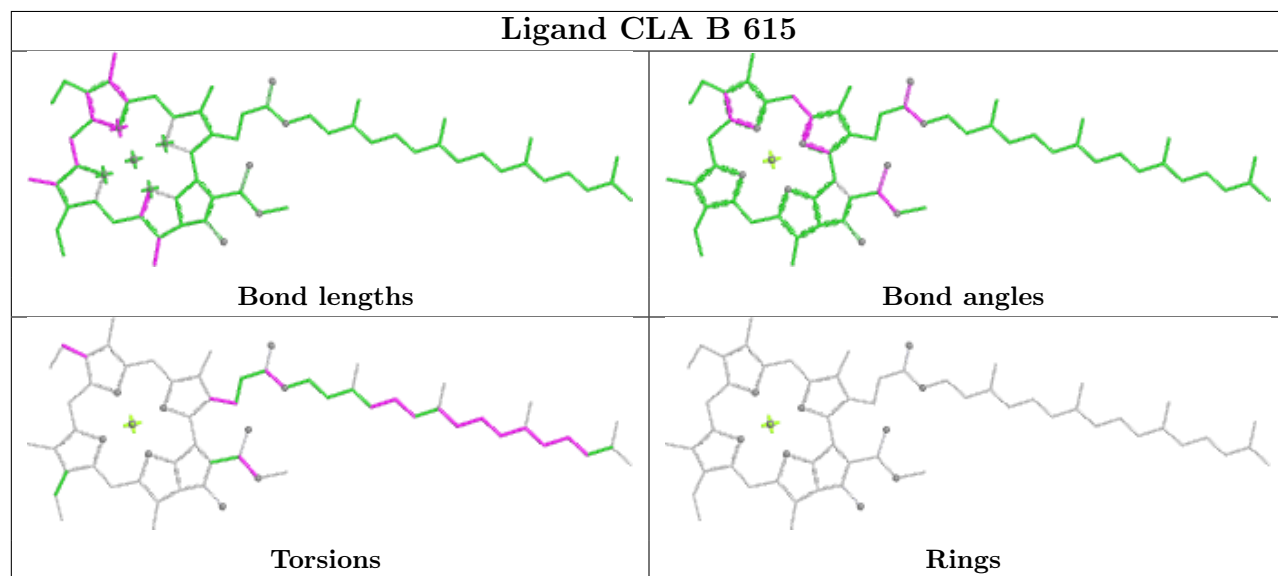
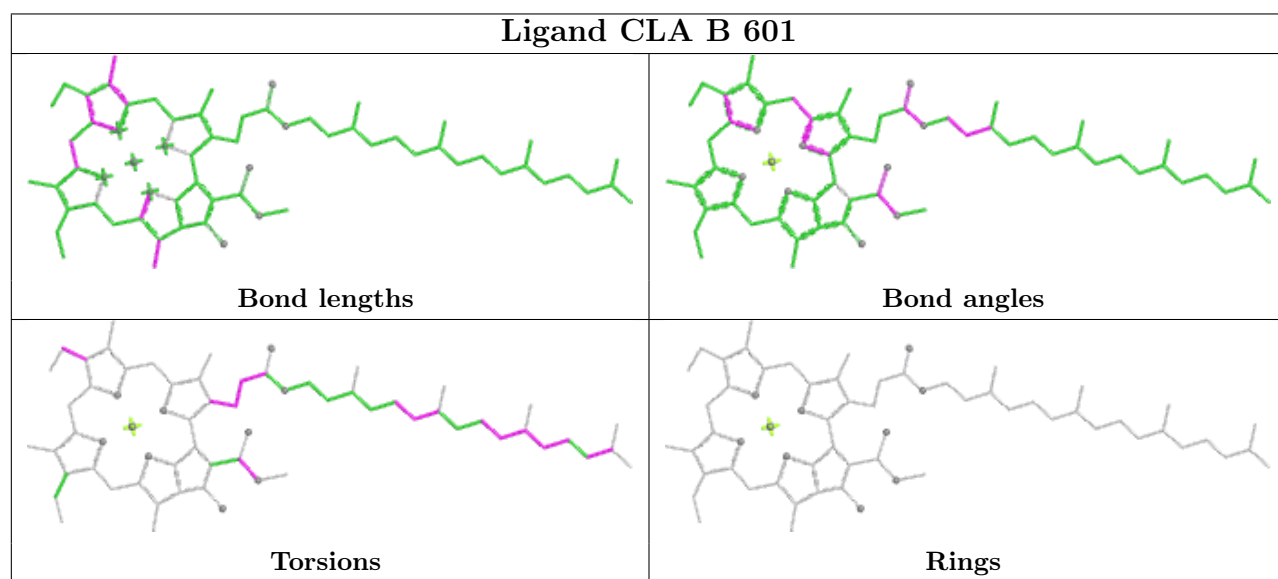
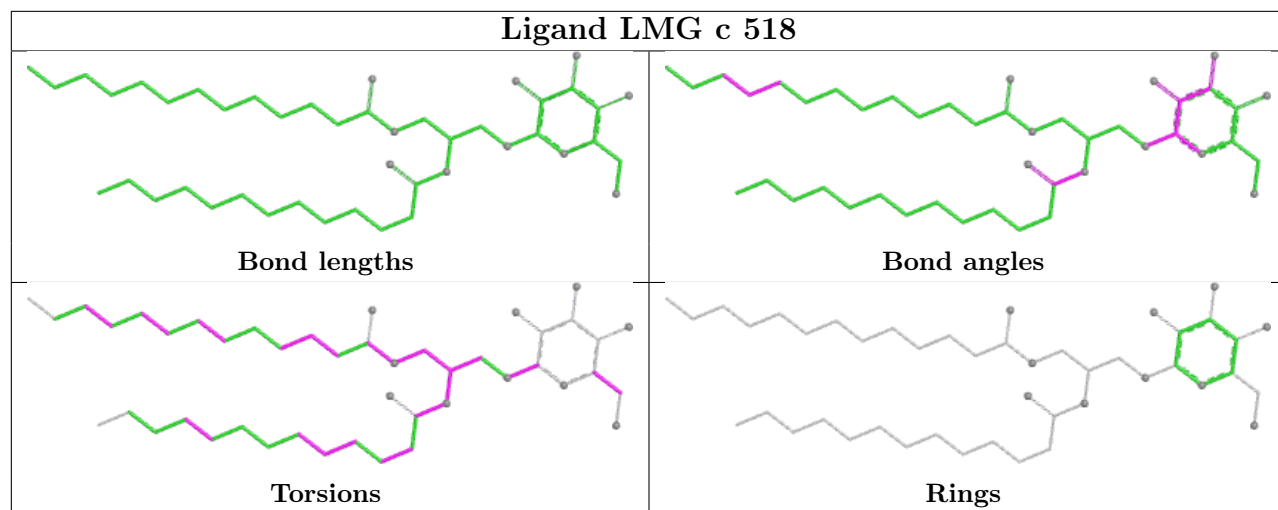
Ligand CLA c 506

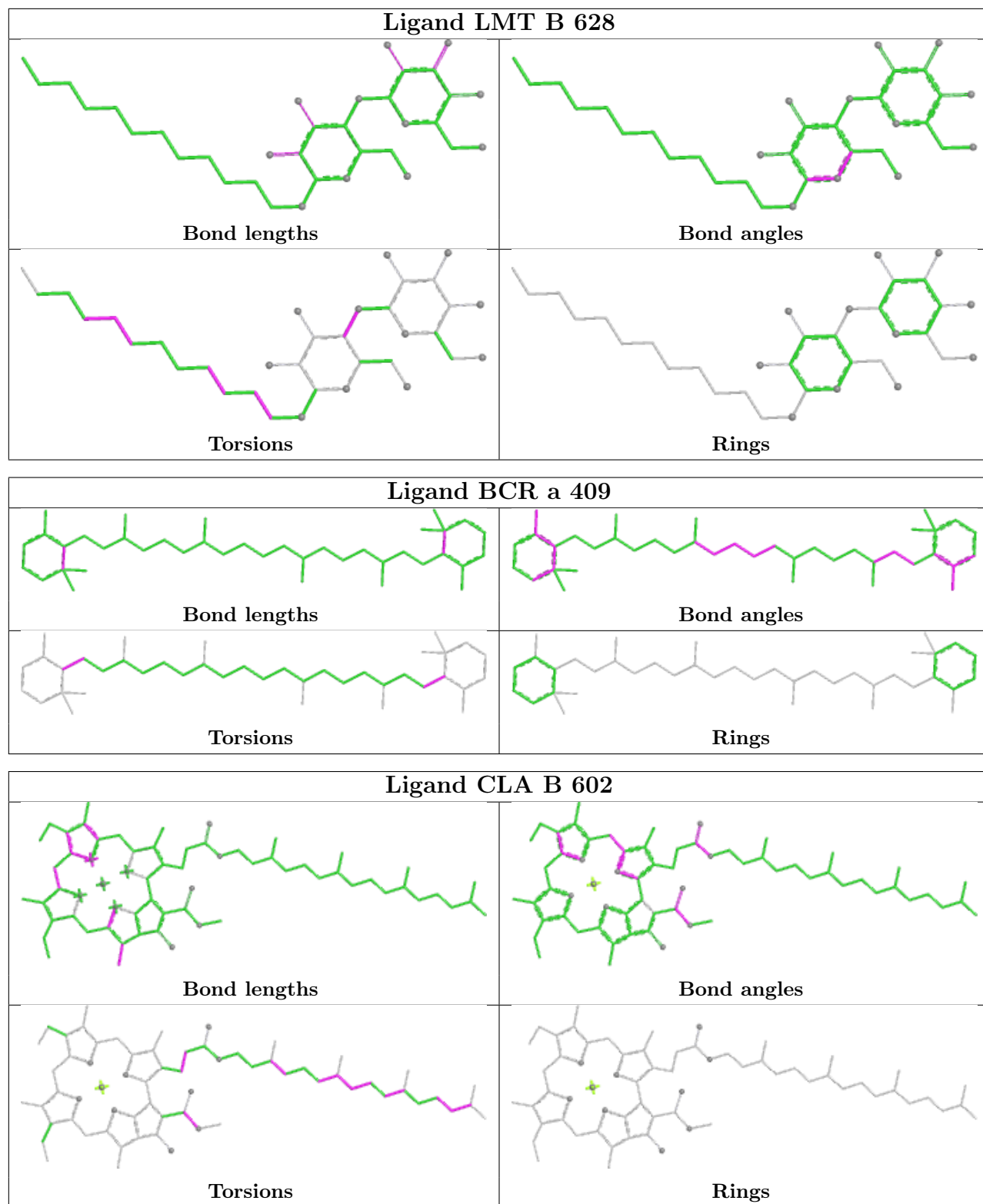


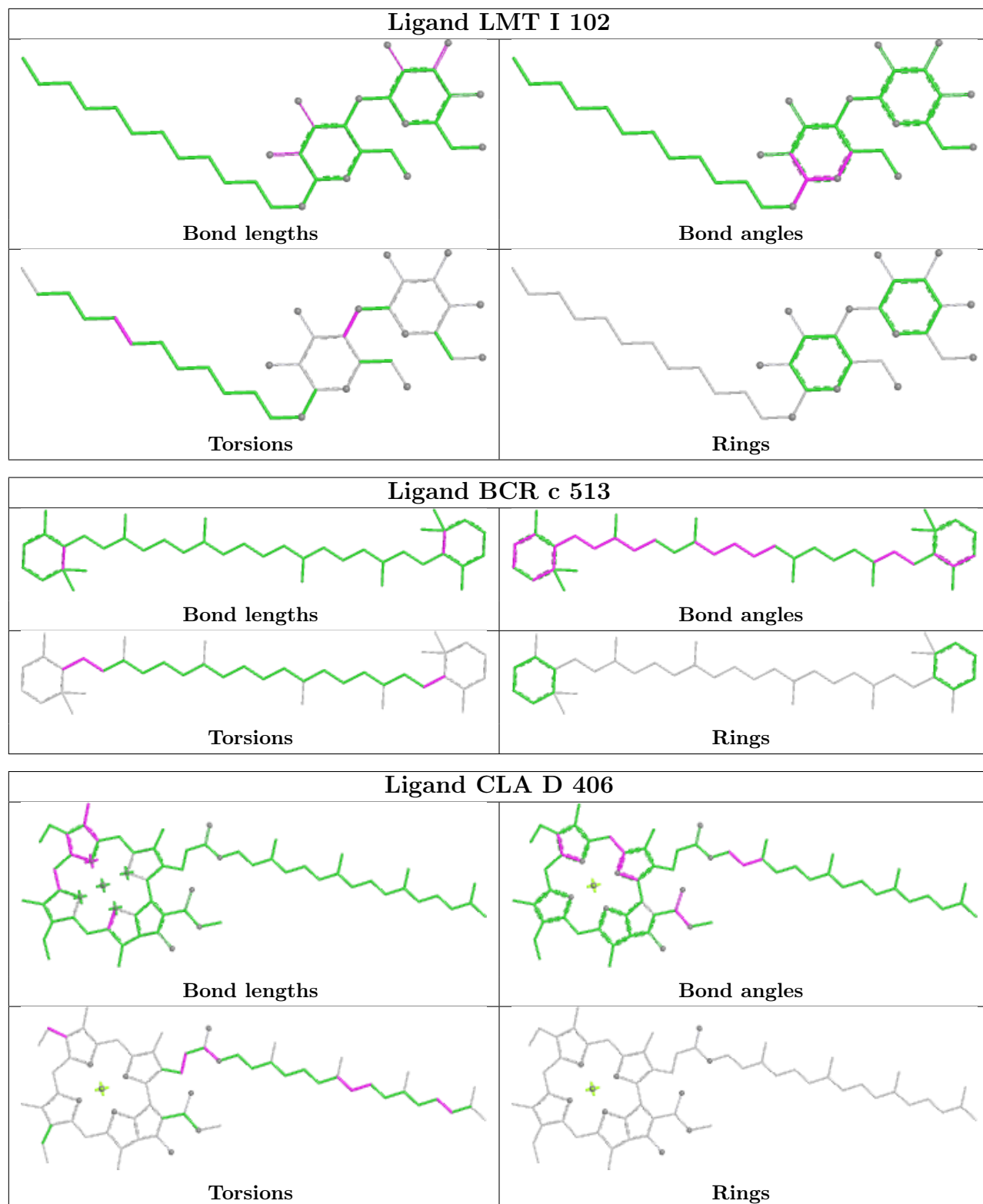


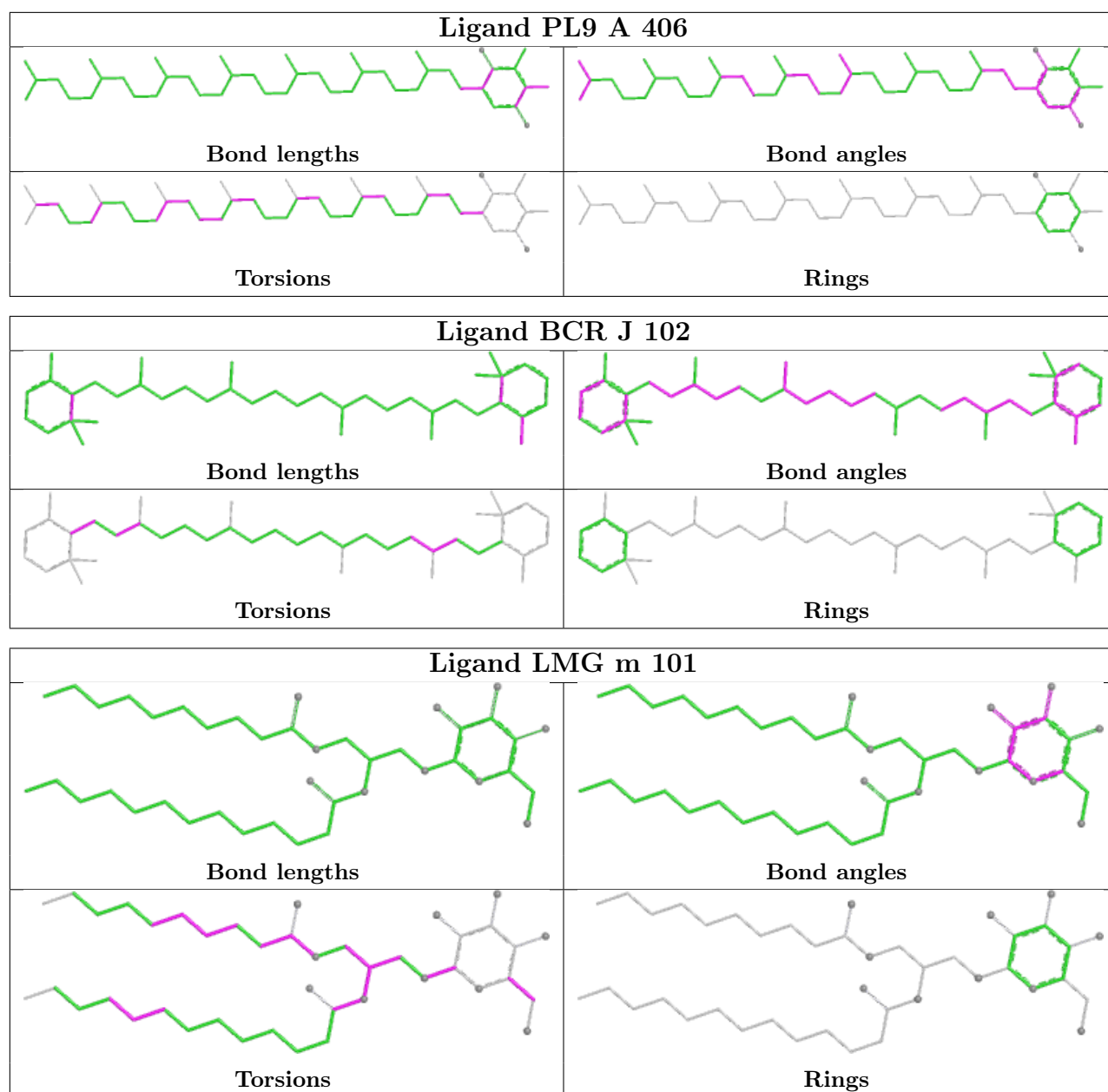


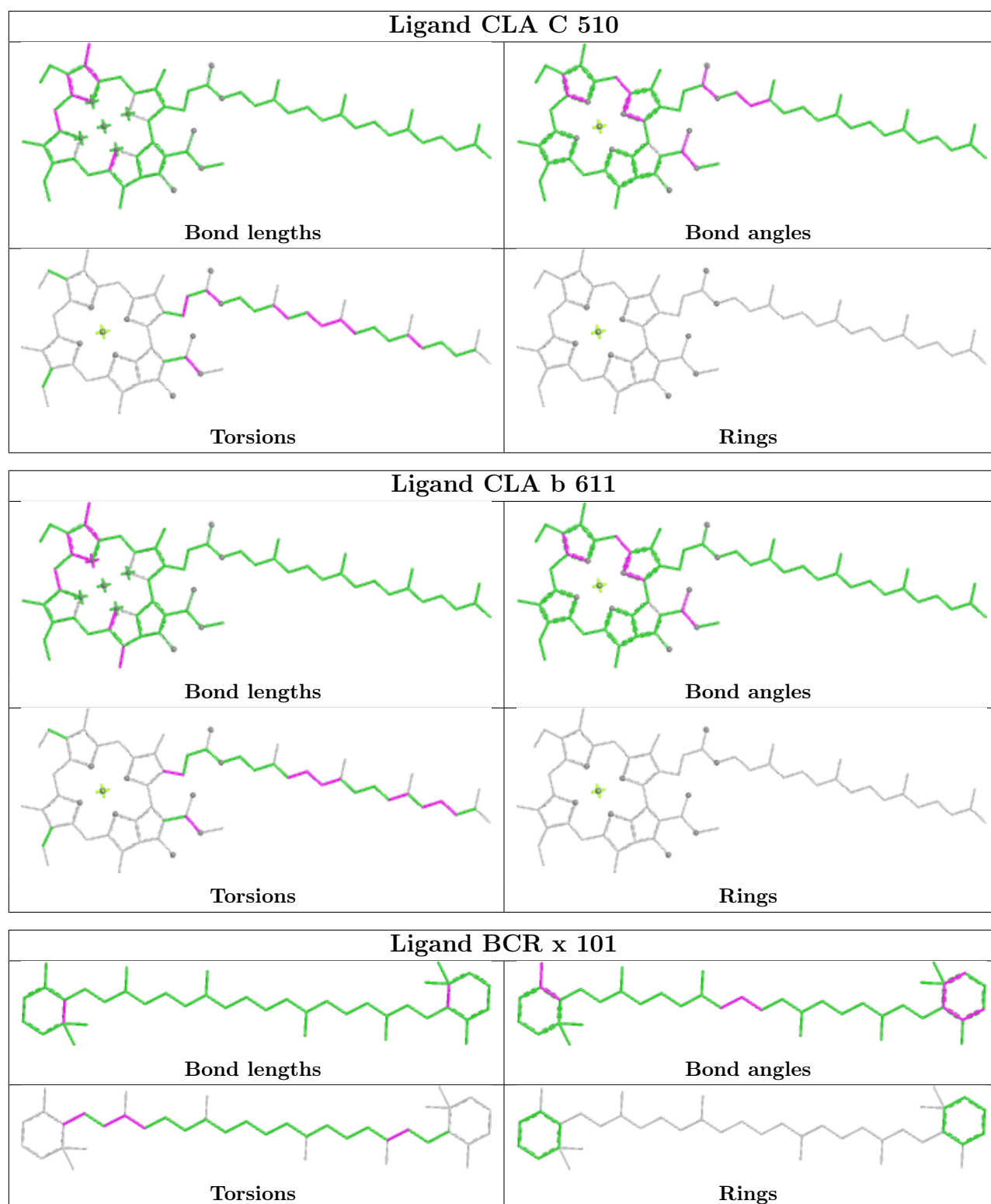


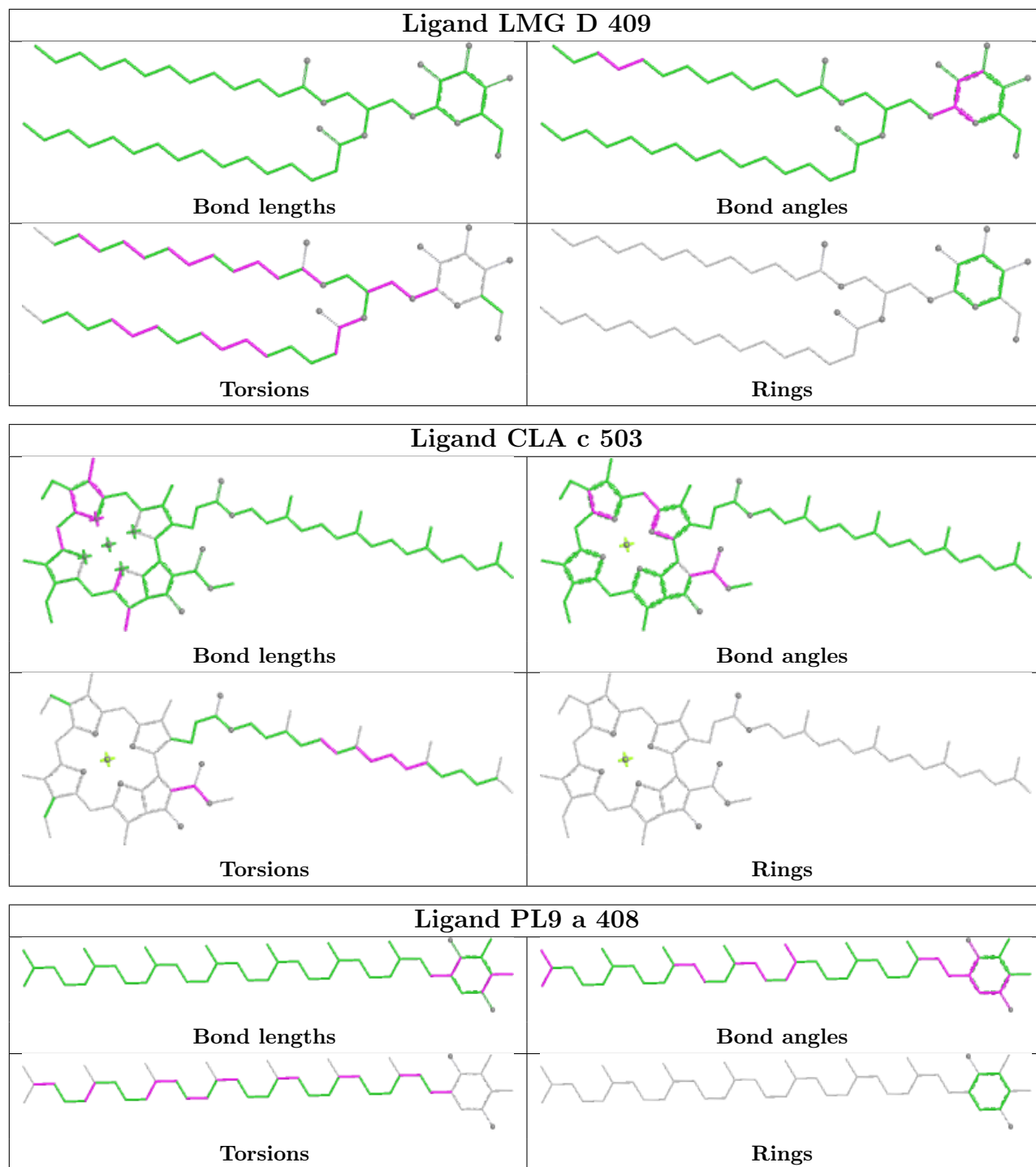


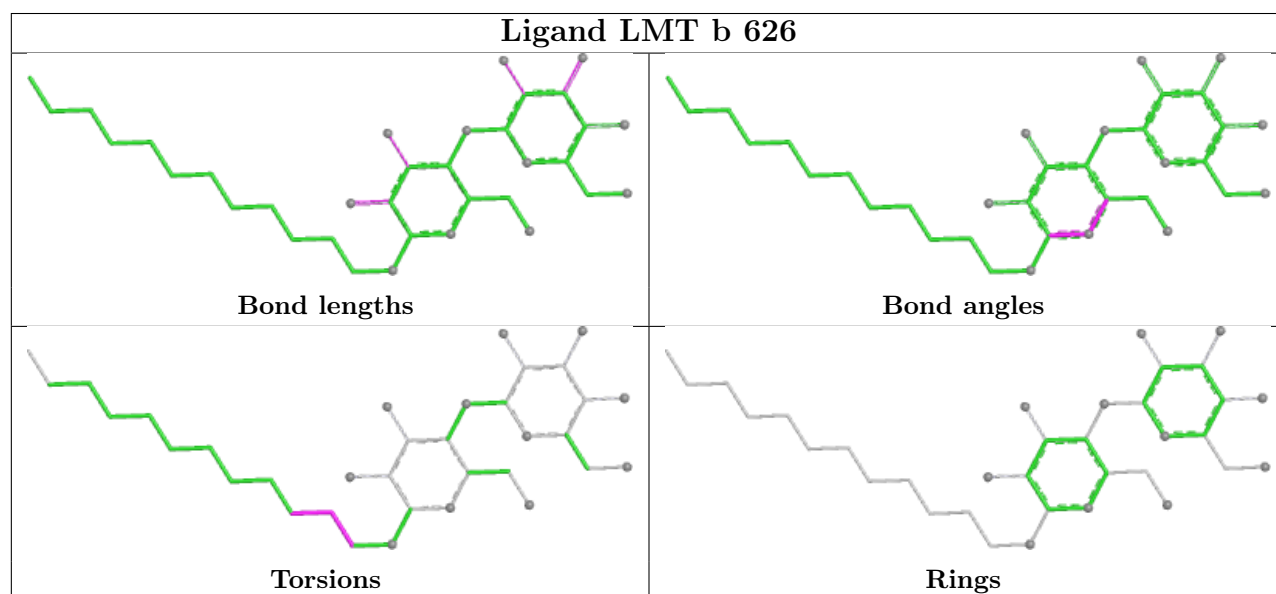
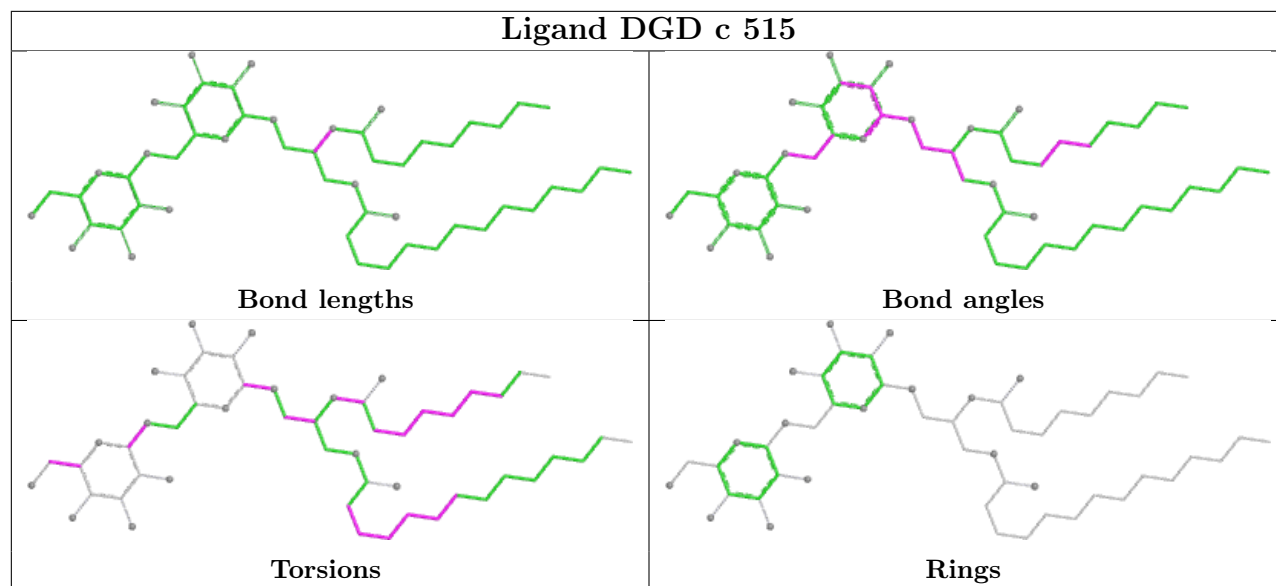




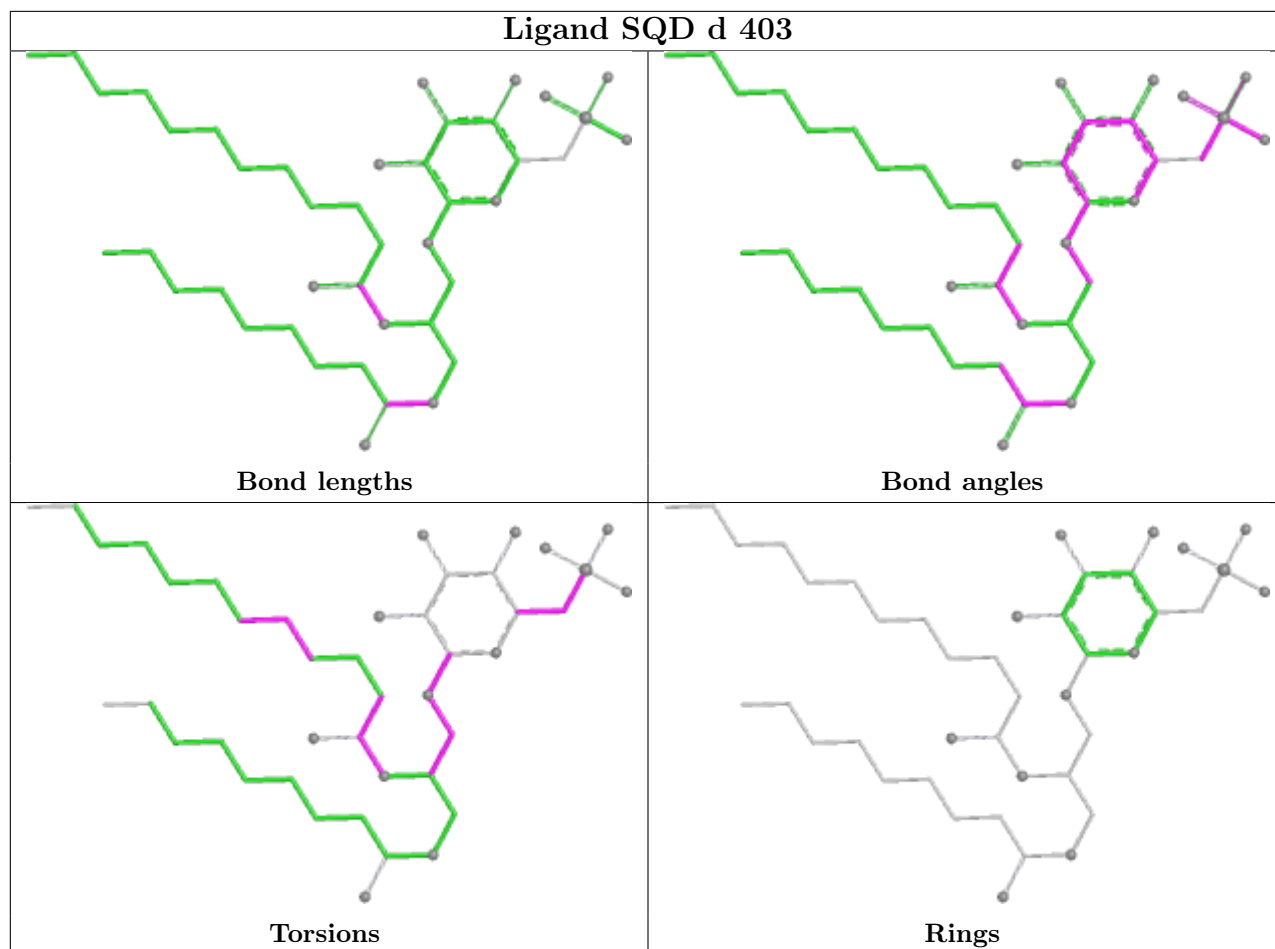




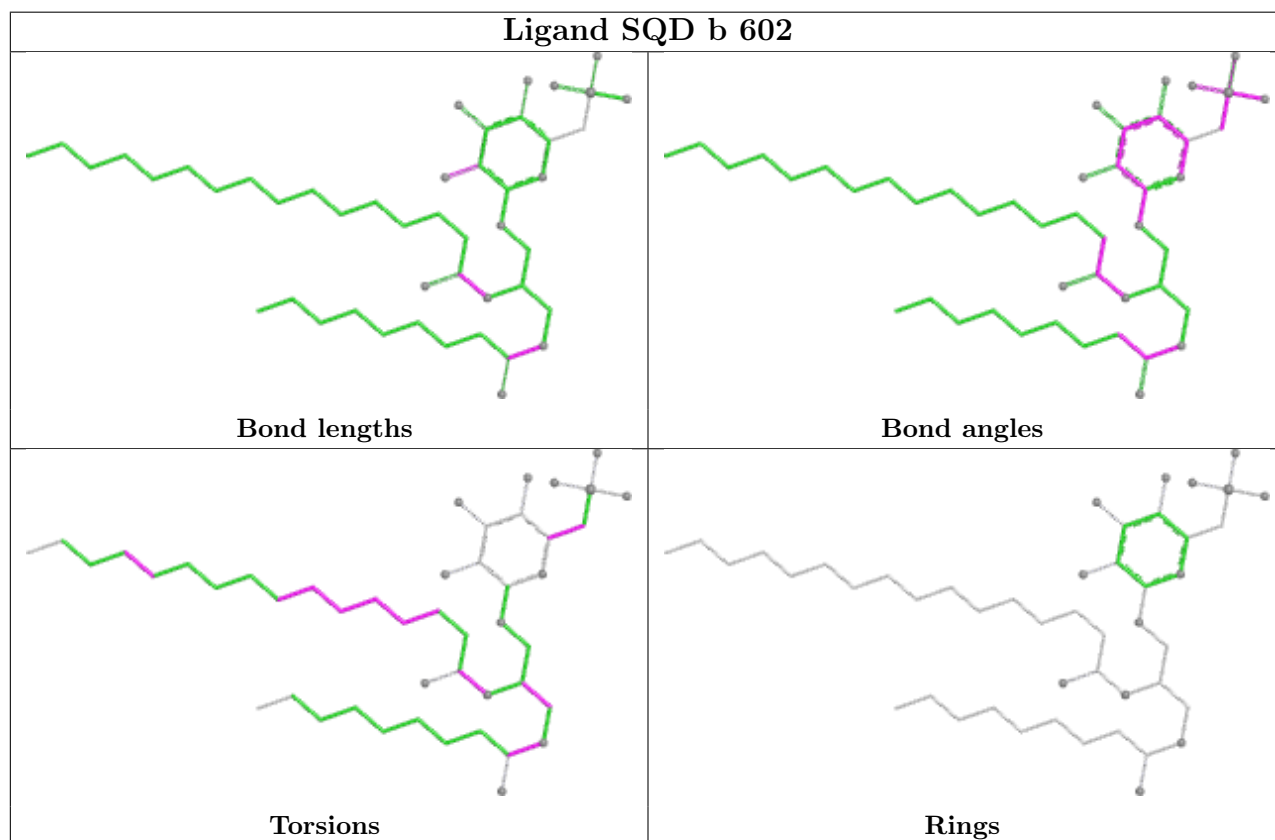


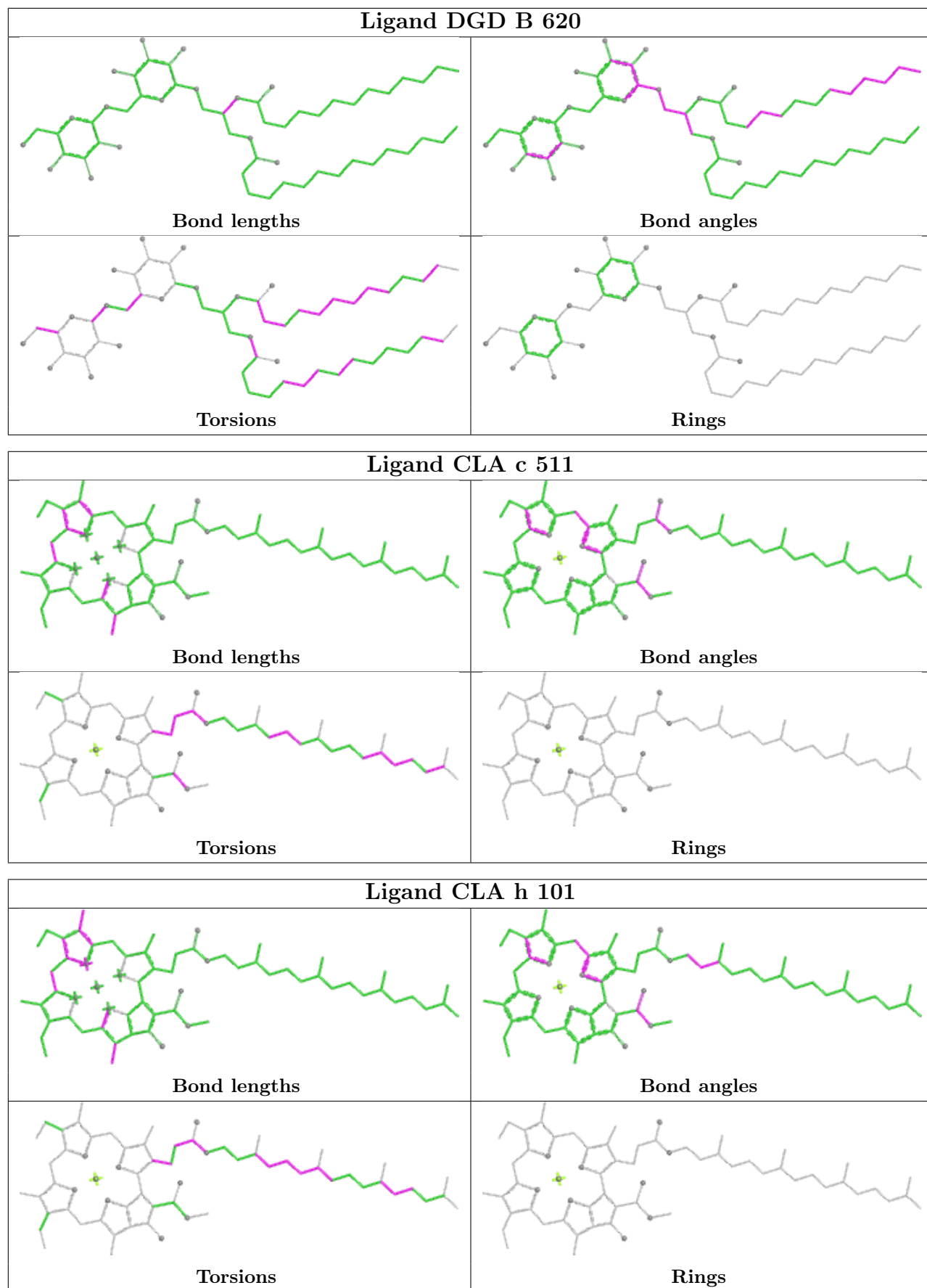


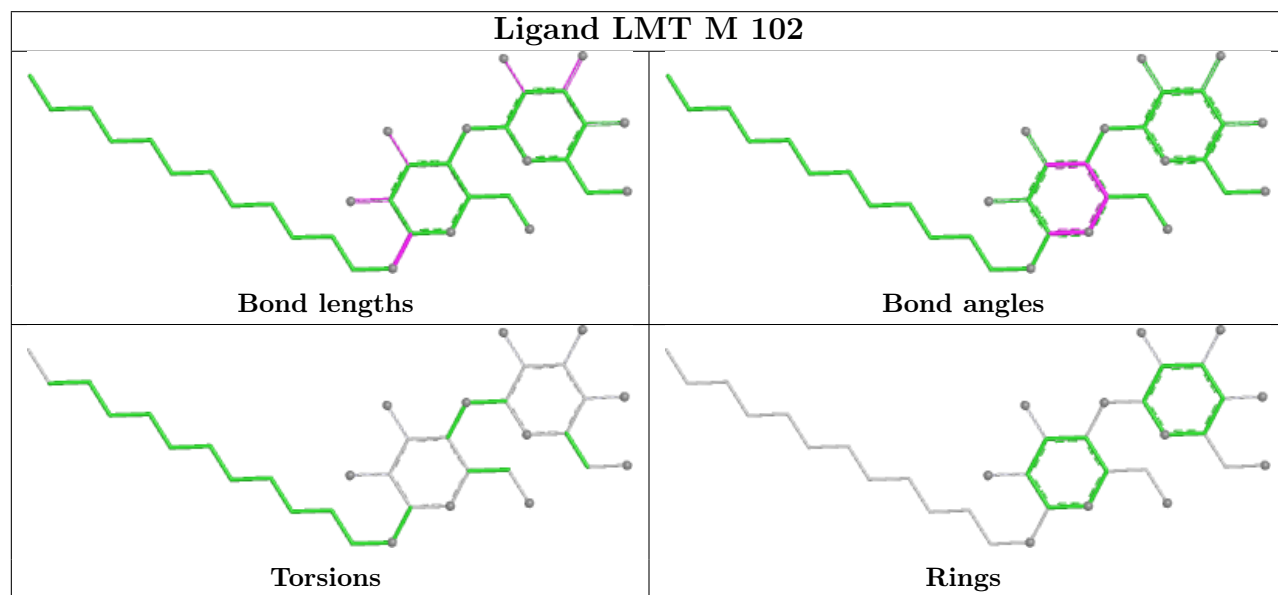
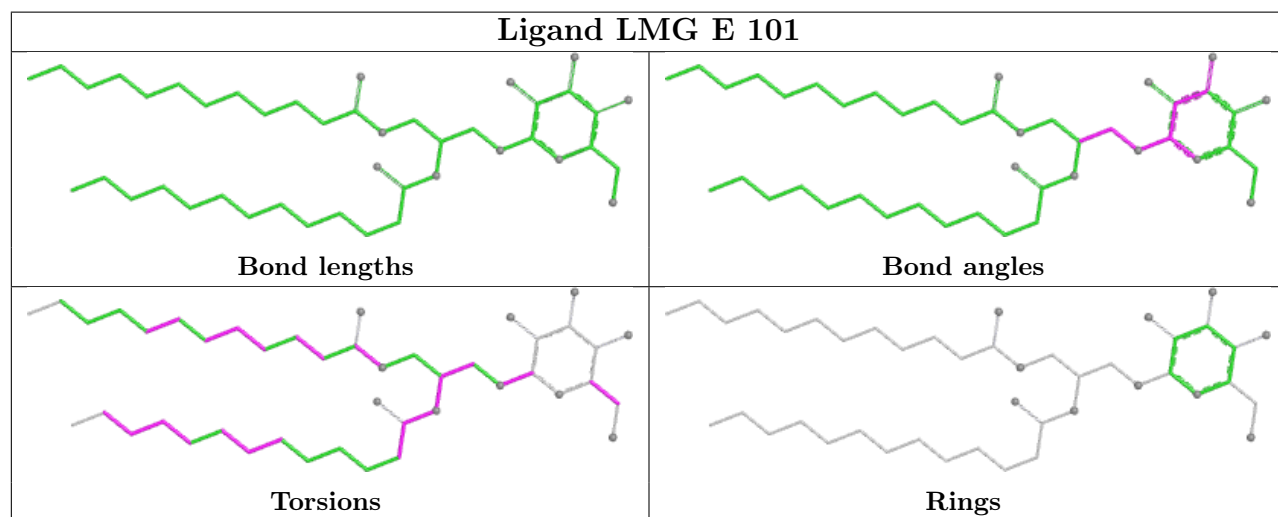
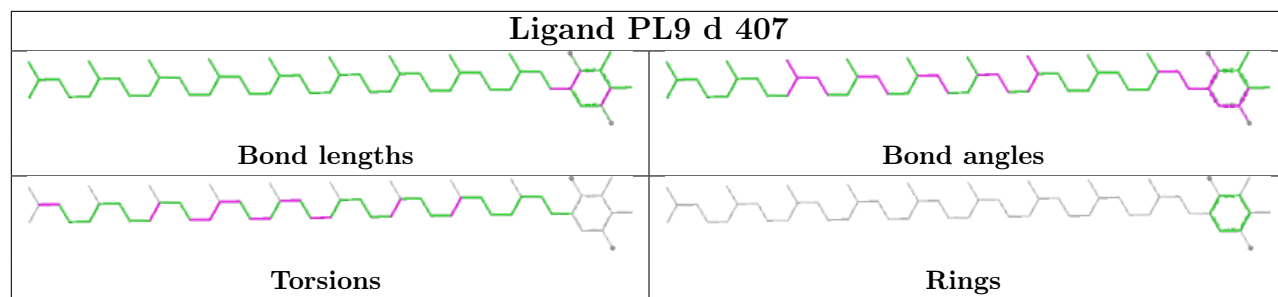
Ligand SQD d 403

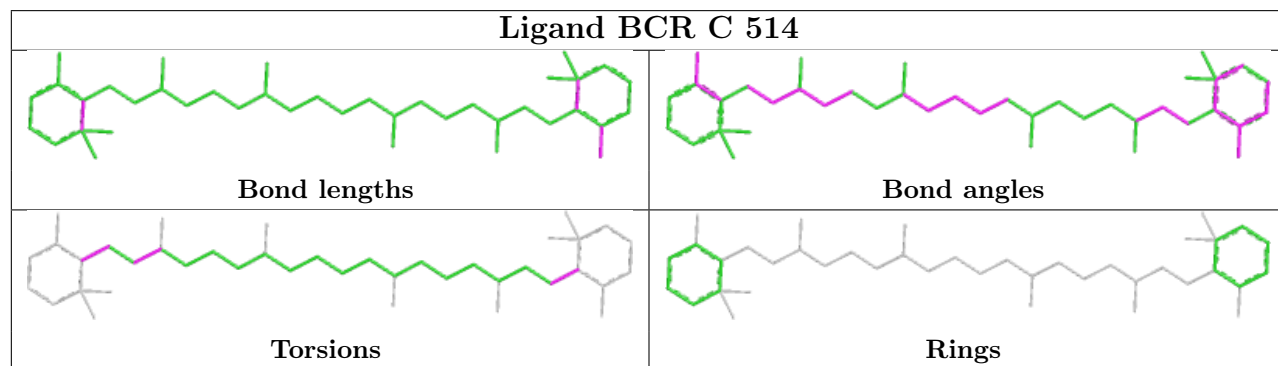
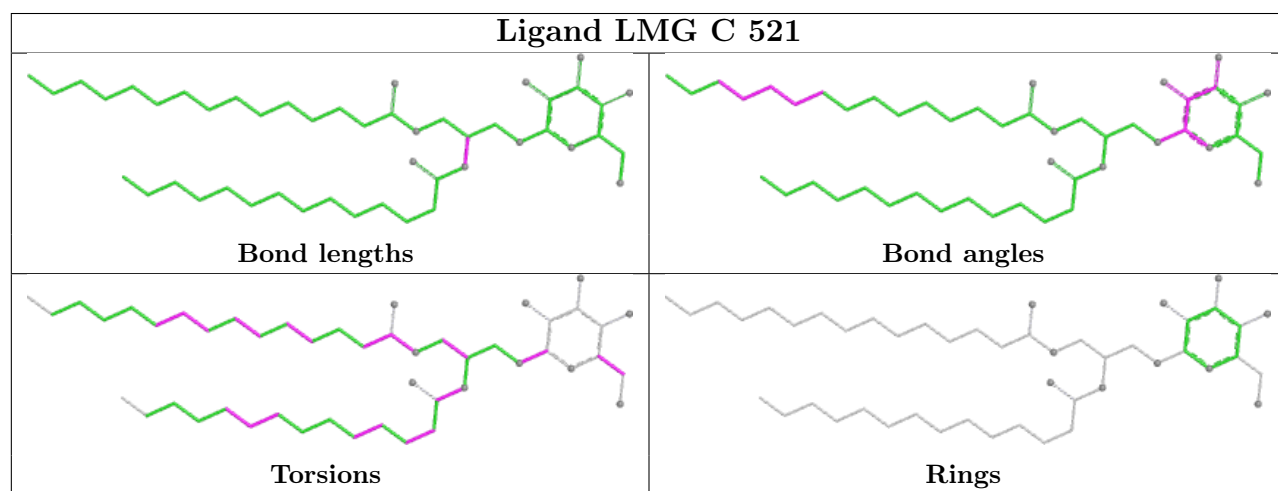
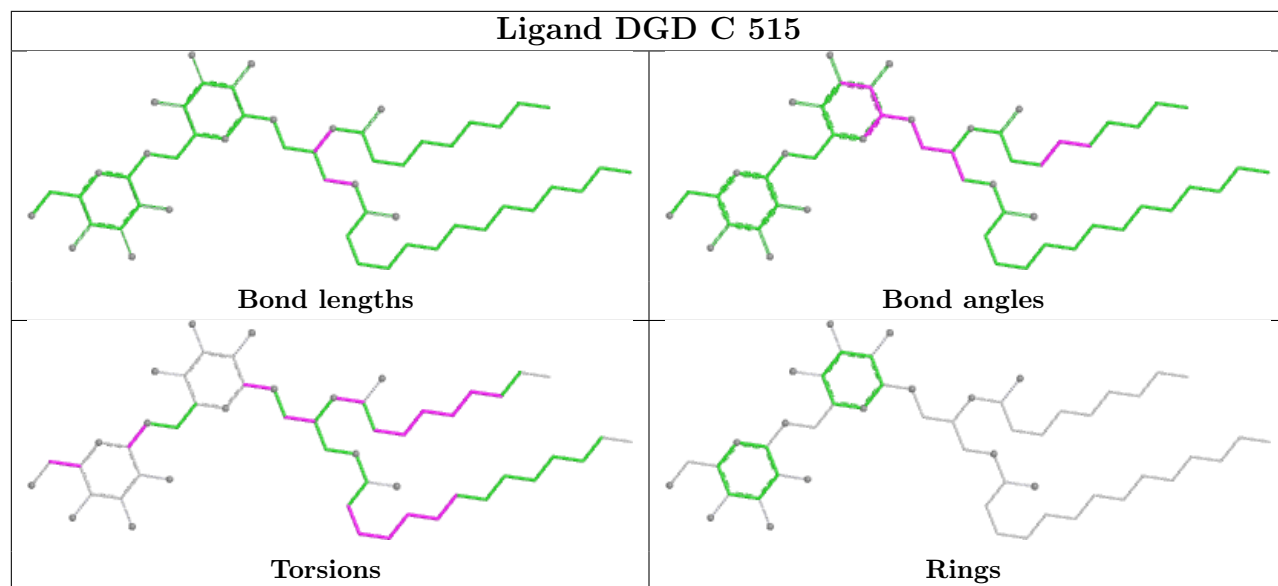


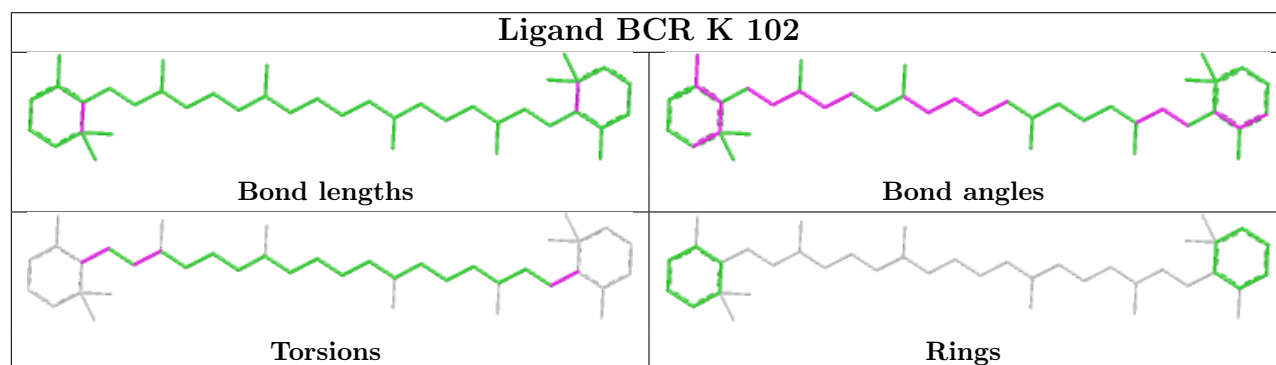
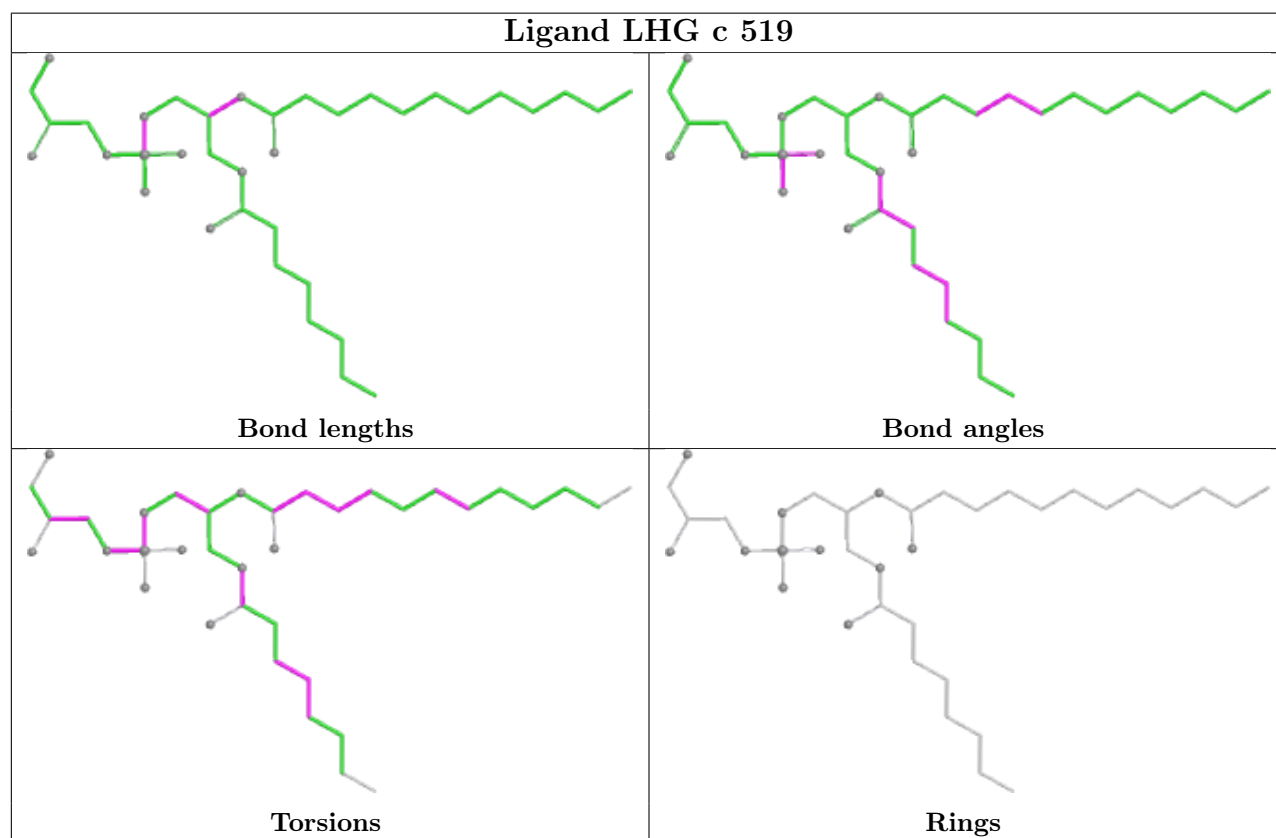
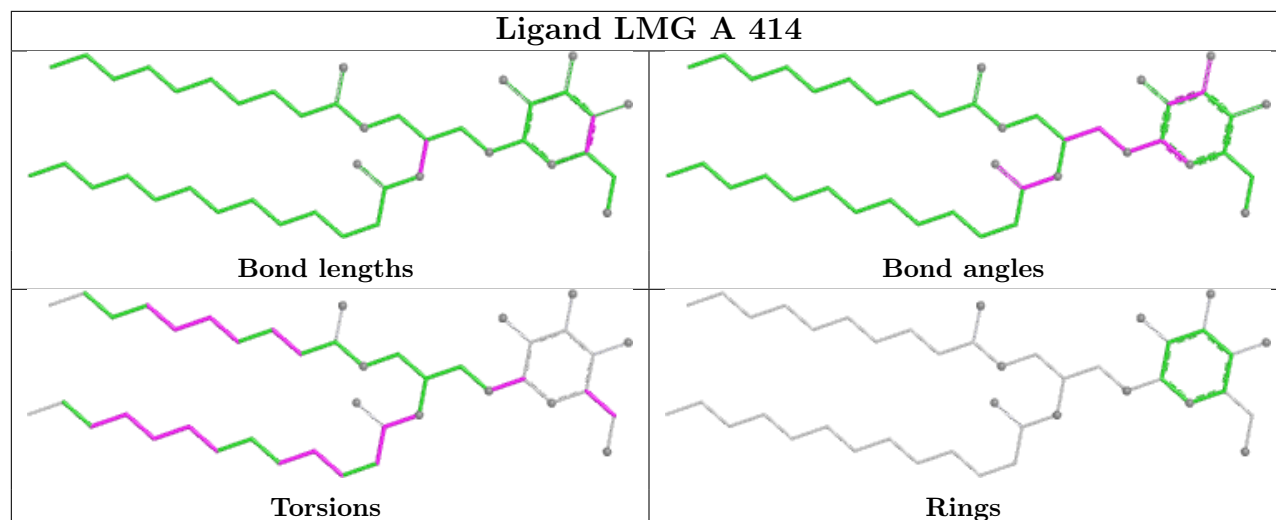
Ligand SQD b 602

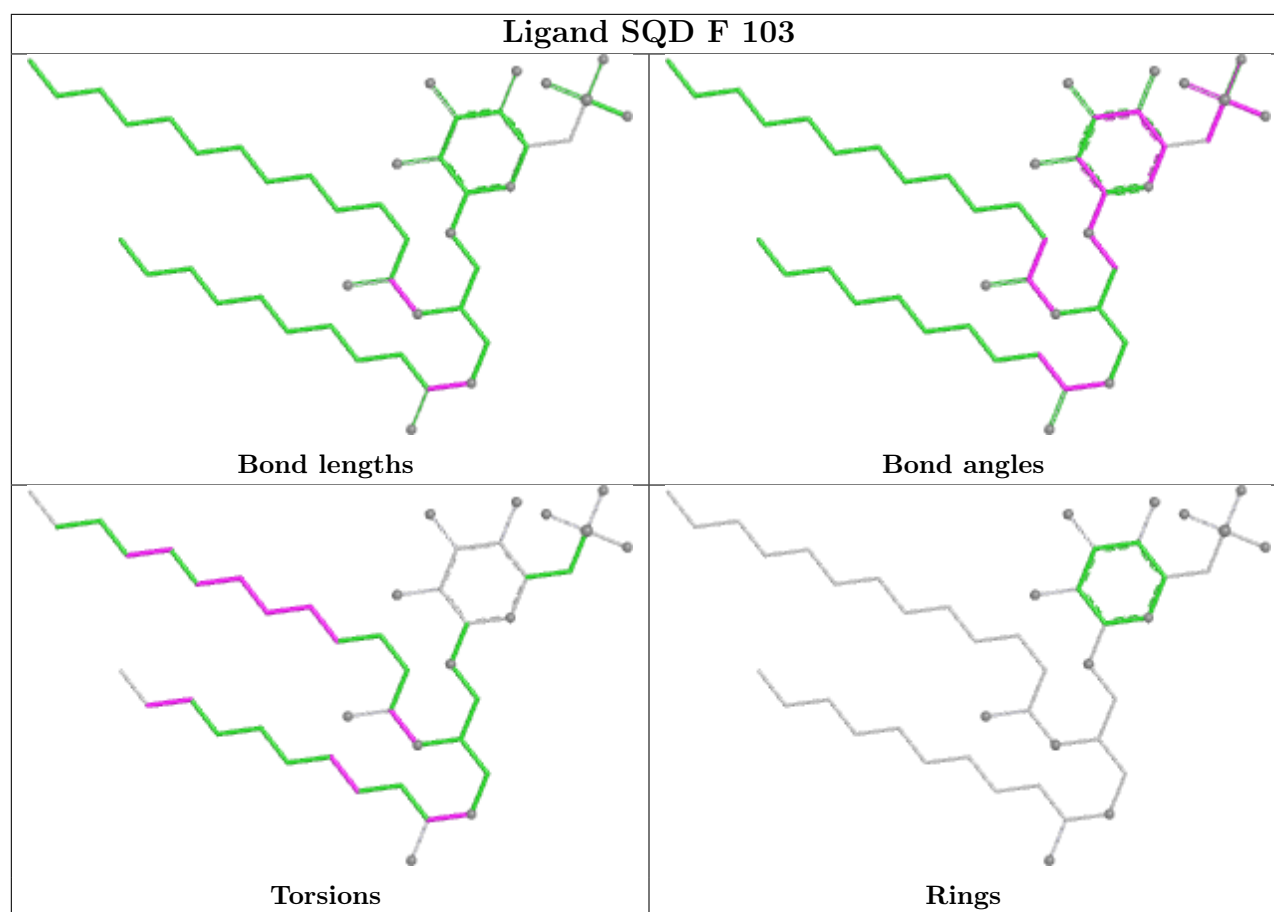












5.7 Other polymers [i](#)

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%)	0.14	8 (2%) 59 48	178, 179, 180, 181	0
1	a	335/344 (97%)	0.00	8 (2%) 59 48	178, 179, 180, 181	0
2	B	490/510 (96%)	0.03	7 (1%) 73 58	178, 179, 180, 181	0
2	b	490/510 (96%)	0.08	12 (2%) 59 48	178, 179, 180, 181	0
3	C	447/461 (96%)	0.05	5 (1%) 78 62	178, 179, 180, 181	0
3	c	447/461 (96%)	-0.05	6 (1%) 75 60	178, 180, 180, 181	0
4	D	340/352 (96%)	0.14	7 (2%) 63 50	177, 179, 180, 181	0
4	d	340/352 (96%)	-0.02	5 (1%) 72 57	177, 179, 180, 181	0
5	E	82/84 (97%)	-0.07	0 100 100	178, 180, 180, 181	0
5	e	82/84 (97%)	-0.04	2 (2%) 59 48	178, 180, 181, 181	0
6	F	35/45 (77%)	0.19	3 (8%) 16 20	179, 179, 180, 180	0
6	f	35/45 (77%)	-0.12	0 100 100	179, 180, 181, 181	0
7	H	65/66 (98%)	0.26	2 (3%) 51 41	179, 180, 180, 181	0
7	h	65/66 (98%)	0.11	2 (3%) 51 41	179, 180, 181, 181	0
8	I	35/38 (92%)	-0.21	0 100 100	178, 179, 180, 181	0
8	i	35/38 (92%)	-0.08	0 100 100	179, 179, 181, 181	0
9	J	34/40 (85%)	-0.13	0 100 100	178, 179, 180, 180	0
9	j	34/40 (85%)	0.06	0 100 100	179, 180, 181, 181	0
10	K	37/46 (80%)	0.03	0 100 100	179, 180, 180, 180	0
10	k	37/46 (80%)	0.04	0 100 100	179, 180, 181, 181	0
11	L	37/37 (100%)	0.12	1 (2%) 56 44	178, 179, 180, 181	0
11	l	37/37 (100%)	-0.07	0 100 100	178, 179, 180, 181	0
12	M	34/36 (94%)	0.27	0 100 100	178, 179, 180, 181	0
12	m	34/36 (94%)	0.09	0 100 100	178, 179, 180, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.13	3 (1%) 76 61	177, 179, 180, 181	0
13	o	243/272 (89%)	0.05	2 (0%) 82 68	177, 179, 181, 181	0
14	T	32/32 (100%)	0.08	0 100 100	178, 179, 181, 181	0
14	t	32/32 (100%)	0.18	1 (3%) 51 41	178, 179, 180, 181	0
15	U	97/134 (72%)	0.29	3 (3%) 51 41	178, 179, 180, 181	0
15	u	97/134 (72%)	0.29	2 (2%) 63 50	178, 179, 180, 181	0
16	V	137/163 (84%)	0.20	5 (3%) 46 39	178, 179, 180, 181	0
16	v	137/163 (84%)	0.02	2 (1%) 72 57	178, 180, 181, 181	0
17	g	28/46 (60%)	0.54	0 100 100	179, 180, 181, 182	0
17	y	28/46 (60%)	-0.13	0 100 100	178, 180, 181, 181	0
18	X	37/41 (90%)	-0.14	0 100 100	179, 179, 181, 181	0
18	x	37/41 (90%)	0.19	0 100 100	179, 180, 180, 181	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	-0.03	1 (1%) 70 55	179, 180, 181, 181	0
20	z	62/62 (100%)	-0.04	1 (1%) 70 55	179, 180, 181, 181	0
All	All	5214/5674 (91%)	0.06	88 (1%) 69 55	177, 179, 180, 182	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	V	47	LEU	5.1
2	b	211	ILE	5.0
2	B	161	LEU	4.5
13	O	195	ASP	4.4
2	b	63	LEU	4.3
1	a	250	ALA	4.3
2	b	443	PHE	4.3
15	U	40	VAL	4.1
20	Z	17	PHE	3.8
13	o	213	VAL	3.8
15	U	39	LEU	3.8
15	u	47	LEU	3.7
2	b	302	TRP	3.4
2	B	411	PHE	3.3
1	A	19	ASN	3.2
2	b	393	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	24	ARG	3.1
2	b	386	ALA	3.1
4	d	181	PHE	3.1
2	B	69	LEU	2.9
7	H	6	TRP	2.9
3	C	140	LEU	2.9
15	U	121	LEU	2.9
2	b	482	ILE	2.8
1	A	61	ASP	2.8
6	F	11	VAL	2.8
16	V	117	VAL	2.8
5	e	84	LYS	2.8
2	b	229	LEU	2.7
3	C	89	ILE	2.6
1	A	274	PHE	2.6
4	D	145	ALA	2.6
3	c	260	ALA	2.6
1	A	263	ALA	2.5
16	v	65	SER	2.5
5	e	82	GLN	2.5
1	a	50	ILE	2.4
1	a	280	VAL	2.4
2	b	78	TRP	2.4
13	o	202	GLN	2.4
4	D	311	PHE	2.3
2	b	64	PRO	2.3
4	d	136	VAL	2.3
3	c	401	LEU	2.3
4	d	122	LEU	2.3
4	D	13	GLY	2.3
4	D	276	VAL	2.3
16	V	69	GLY	2.3
1	A	103	ASP	2.3
1	a	294	ALA	2.2
14	t	29	ILE	2.2
1	A	185	VAL	2.2
3	C	266	TRP	2.2
16	V	52	TYR	2.2
7	H	30	LEU	2.2
13	O	41	LEU	2.2
13	O	141	ARG	2.2
1	A	218	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
11	L	18	TYR	2.2
3	c	375	LEU	2.2
16	v	73	LYS	2.2
2	B	8	VAL	2.2
1	A	188	ALA	2.2
2	b	2	GLY	2.2
1	a	340	PRO	2.2
4	d	334	GLN	2.2
4	d	271	MET	2.2
4	D	203	GLY	2.1
7	h	14	LEU	2.1
1	a	222	SER	2.1
7	h	11	LEU	2.1
15	u	130	ASN	2.1
6	F	38	ALA	2.1
3	C	334	PRO	2.1
3	c	341	LEU	2.1
20	z	17	PHE	2.1
3	c	219	GLY	2.1
6	F	41	GLN	2.1
2	b	175	THR	2.1
1	a	279	PRO	2.1
4	D	274	VAL	2.1
2	B	320	ALA	2.0
3	C	43	ILE	2.0
2	B	472	ARG	2.0
3	c	143	TYR	2.0
1	a	292	THR	2.0
2	B	84	THR	2.0
16	V	147	VAL	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 ⓘ

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
30	LMT	I	102	35/35	0.49	0.17	178,180,182,183	0
30	LMT	d	411	31/35	0.52	0.18	178,181,182,183	0
35	CA	K	101	1/1	0.58	0.18	184,184,184,184	0
30	LMT	i	102	35/35	0.60	0.17	178,181,183,183	0
30	LMT	b	627	35/35	0.60	0.16	178,180,182,182	0
22	CLA	b	605	65/65	0.62	0.22	179,180,182,183	0
30	LMT	D	411	31/35	0.63	0.13	179,180,182,182	0
22	CLA	B	601	65/65	0.63	0.19	177,180,181,182	0
30	LMT	b	626	35/35	0.64	0.14	178,180,182,183	0
30	LMT	b	603	35/35	0.65	0.15	178,179,181,182	0
30	LMT	B	627	35/35	0.65	0.15	178,180,182,182	0
30	LMT	B	628	35/35	0.65	0.21	177,180,182,183	0
30	LMT	B	623	35/35	0.66	0.14	177,181,182,183	0
25	DGD	D	410	63/66	0.70	0.21	178,181,182,183	0
25	DGD	d	410	63/66	0.71	0.23	178,180,183,183	0
23	PL9	J	101	35/55	0.71	0.31	177,180,181,181	0
22	CLA	b	619	65/65	0.72	0.18	177,179,180,181	0
27	LMG	C	518	45/55	0.73	0.17	178,179,180,181	0
24	BCR	J	102	40/40	0.74	0.27	178,180,181,181	0
24	BCR	j	102	40/40	0.75	0.27	179,180,182,183	0
25	DGD	B	625	52/66	0.75	0.19	177,180,182,182	0
29	SQD	B	626	47/54	0.75	0.17	175,179,181,183	0
29	SQD	d	403	43/54	0.75	0.18	178,180,182,186	0
22	CLA	c	512	65/65	0.75	0.16	178,180,181,182	0
26	LHG	C	519	37/49	0.76	0.19	176,180,184,188	0
27	LMG	M	101	42/55	0.77	0.21	178,180,181,182	0
30	LMT	B	624	35/35	0.77	0.15	178,180,182,183	0
25	DGD	b	601	52/66	0.78	0.18	178,180,181,182	0
26	LHG	c	519	37/49	0.78	0.18	178,180,183,187	0
22	CLA	C	506	65/65	0.80	0.18	177,179,180,180	0
27	LMG	A	414	42/55	0.80	0.22	177,179,182,182	0
30	LMT	b	604	35/35	0.81	0.20	177,179,181,182	0
27	LMG	a	402	42/55	0.81	0.23	177,180,181,182	0
27	LMG	I	101	43/55	0.81	0.20	178,180,181,182	0
30	LMT	M	102	35/35	0.82	0.18	178,179,181,182	0
22	CLA	A	405	65/65	0.82	0.17	177,179,180,181	0
23	PL9	A	406	45/55	0.82	0.27	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	DGD	C	516	62/66	0.82	0.15	177,179,180,181	0
29	SQD	b	602	47/54	0.83	0.16	176,179,182,185	0
27	LMG	c	518	45/55	0.83	0.15	178,180,181,181	0
27	LMG	m	101	42/55	0.83	0.20	175,179,181,181	0
25	DGD	c	516	62/66	0.83	0.19	178,179,180,181	0
25	DGD	a	410	56/66	0.84	0.20	178,180,181,182	0
29	SQD	a	415	51/54	0.84	0.18	178,179,181,182	0
24	BCR	b	621	40/40	0.84	0.20	178,178,179,179	0
27	LMG	E	101	44/55	0.84	0.20	176,179,181,182	0
24	BCR	b	623	40/40	0.84	0.18	177,178,180,180	0
29	SQD	A	412	51/54	0.84	0.18	178,179,180,181	0
24	BCR	H	102	40/40	0.85	0.19	178,180,181,182	0
27	LMG	b	625	49/55	0.85	0.20	178,179,180,180	0
25	DGD	A	408	56/66	0.85	0.17	178,179,181,182	0
27	LMG	i	101	43/55	0.85	0.16	177,180,182,184	0
24	BCR	b	622	40/40	0.85	0.27	176,178,179,179	0
23	PL9	j	101	35/55	0.85	0.24	179,180,181,181	0
25	DGD	b	624	58/66	0.86	0.21	177,178,180,180	0
25	DGD	c	515	53/66	0.86	0.20	176,179,181,182	0
24	BCR	a	409	40/40	0.86	0.21	177,178,180,180	0
29	SQD	F	103	45/54	0.86	0.19	178,180,182,182	0
22	CLA	C	512	65/65	0.86	0.13	177,180,181,182	0
27	LMG	e	101	44/55	0.86	0.18	177,179,181,181	0
33	BCT	d	404	4/4	0.86	0.10	178,180,180,180	0
25	DGD	C	517	66/66	0.86	0.18	177,179,180,181	0
35	CA	O	301	1/1	0.86	0.08	182,182,182,182	0
35	CA	k	101	1/1	0.86	0.09	180,180,180,180	0
22	CLA	C	505	65/65	0.87	0.17	177,179,180,181	0
32	CL	D	403	1/1	0.87	0.33	180,180,180,180	0
24	BCR	K	102	40/40	0.87	0.20	178,180,181,182	0
25	DGD	c	517	66/66	0.87	0.17	177,179,181,181	0
24	BCR	c	514	40/40	0.87	0.22	177,179,180,180	0
29	SQD	a	401	54/54	0.87	0.15	178,180,181,183	0
35	CA	o	301	1/1	0.87	0.12	184,184,184,184	0
24	BCR	c	521	40/40	0.88	0.17	178,179,181,181	0
24	BCR	B	619	40/40	0.88	0.16	178,179,180,180	0
22	CLA	c	506	65/65	0.88	0.15	178,179,180,181	0
22	CLA	a	406	65/65	0.88	0.17	177,179,180,181	0
27	LMG	c	522	48/55	0.88	0.21	178,180,180,181	0
22	CLA	C	510	65/65	0.88	0.15	177,179,180,181	0
22	CLA	b	618	65/65	0.88	0.15	177,179,180,180	0
23	PL9	a	408	45/55	0.88	0.19	176,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	PL9	d	407	55/55	0.88	0.17	177,179,180,181	0
22	CLA	C	508	65/65	0.88	0.13	177,179,180,180	0
24	BCR	B	617	40/40	0.88	0.19	177,179,180,180	0
30	LMT	M	103	35/35	0.88	0.17	177,179,180,180	0
26	LHG	A	409	39/49	0.89	0.18	178,179,181,181	0
22	CLA	c	510	65/65	0.89	0.12	178,179,181,181	0
24	BCR	g	101	40/40	0.89	0.16	178,179,180,180	0
24	BCR	x	101	40/40	0.89	0.17	178,179,180,181	0
24	BCR	B	616	40/40	0.89	0.17	176,178,180,180	0
27	LMG	D	409	48/55	0.89	0.16	175,178,180,181	0
22	CLA	b	609	65/65	0.89	0.13	178,179,180,181	0
25	DGD	C	515	53/66	0.89	0.17	177,178,179,180	0
22	CLA	C	520	65/65	0.89	0.15	178,179,180,181	0
24	BCR	b	620	40/40	0.89	0.21	177,179,179,180	0
27	LMG	a	412	51/55	0.89	0.20	177,179,180,180	0
22	CLA	c	502	65/65	0.90	0.18	178,179,180,181	0
22	CLA	c	505	65/65	0.90	0.15	177,179,180,181	0
22	CLA	B	615	65/65	0.90	0.13	176,179,180,181	0
22	CLA	A	404	65/65	0.90	0.19	176,178,180,181	0
22	CLA	B	603	65/65	0.90	0.12	176,179,180,180	0
27	LMG	A	410	51/55	0.90	0.17	177,178,180,181	0
22	CLA	h	101	65/65	0.90	0.15	176,179,180,181	0
27	LMG	B	621	49/55	0.90	0.15	177,179,180,180	0
22	CLA	B	605	65/65	0.90	0.12	178,179,180,180	0
27	LMG	C	521	48/55	0.90	0.16	177,179,180,181	0
27	LMG	D	408	49/55	0.90	0.20	177,178,180,180	0
24	BCR	C	514	40/40	0.90	0.17	178,179,180,181	0
29	SQD	A	413	54/54	0.90	0.14	178,180,182,184	0
22	CLA	b	606	65/65	0.91	0.13	177,179,180,181	0
25	DGD	B	620	58/66	0.91	0.18	176,179,181,182	0
22	CLA	c	503	65/65	0.91	0.13	177,179,180,181	0
29	SQD	f	103	45/54	0.91	0.15	177,179,181,182	0
22	CLA	b	607	65/65	0.91	0.13	177,179,180,181	0
24	BCR	c	513	40/40	0.91	0.15	178,179,180,180	0
31	PHO	D	402	64/64	0.91	0.14	177,179,180,181	0
31	PHO	d	401	64/64	0.91	0.16	178,179,180,180	0
22	CLA	C	509	65/65	0.91	0.15	177,179,180,180	0
22	CLA	a	407	65/65	0.91	0.14	178,179,180,181	0
29	SQD	B	622	43/54	0.91	0.14	177,180,182,185	0
22	CLA	B	613	65/65	0.91	0.13	177,179,180,180	0
24	BCR	A	407	40/40	0.91	0.19	177,179,180,180	0
22	CLA	c	520	65/65	0.91	0.16	177,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	503	65/65	0.92	0.13	177,179,180,180	0
24	BCR	F	102	40/40	0.92	0.18	177,179,180,180	0
27	LMG	D	412	46/55	0.92	0.14	178,179,180,181	0
22	CLA	c	501	65/65	0.92	0.13	177,179,180,181	0
22	CLA	C	507	65/65	0.92	0.17	178,179,180,181	0
22	CLA	C	504	65/65	0.92	0.16	177,179,180,180	0
24	BCR	y	101	40/40	0.92	0.15	177,179,180,180	0
22	CLA	D	405	65/65	0.92	0.13	177,179,180,180	0
31	PHO	D	401	64/64	0.92	0.15	177,179,180,180	0
22	CLA	a	405	65/65	0.92	0.20	174,178,179,180	0
22	CLA	c	508	65/65	0.92	0.11	177,179,180,181	0
22	CLA	c	509	65/65	0.92	0.12	177,179,180,180	0
27	LMG	d	408	49/55	0.92	0.15	178,179,180,180	0
27	LMG	d	409	48/55	0.92	0.14	177,179,180,180	0
22	CLA	b	613	65/65	0.92	0.13	178,179,180,181	0
22	CLA	c	511	65/65	0.92	0.12	178,180,181,182	0
22	CLA	C	501	65/65	0.92	0.12	178,179,180,180	0
22	CLA	B	606	65/65	0.93	0.12	177,179,180,180	0
22	CLA	c	504	65/65	0.93	0.15	177,179,180,180	0
23	PL9	D	407	55/55	0.93	0.18	177,178,179,180	0
22	CLA	B	607	65/65	0.93	0.14	178,179,180,181	0
22	CLA	b	608	65/65	0.93	0.12	178,179,180,181	0
22	CLA	c	507	65/65	0.93	0.14	177,179,180,181	0
22	CLA	H	101	65/65	0.93	0.15	177,179,180,181	0
22	CLA	a	404	65/65	0.93	0.16	177,178,180,180	0
27	LMG	d	412	46/55	0.93	0.13	177,178,180,180	0
22	CLA	B	608	65/65	0.93	0.14	177,179,180,180	0
33	BCT	D	404	4/4	0.93	0.06	178,179,179,179	0
22	CLA	B	604	65/65	0.93	0.10	177,179,180,180	0
22	CLA	C	511	65/65	0.93	0.13	178,179,180,181	0
24	BCR	C	513	40/40	0.93	0.15	177,179,180,180	0
22	CLA	B	602	65/65	0.93	0.13	176,178,180,180	0
22	CLA	d	406	65/65	0.93	0.13	177,179,180,181	0
22	CLA	b	615	65/65	0.94	0.11	177,179,180,180	0
22	CLA	b	617	65/65	0.94	0.17	178,179,180,182	0
26	LHG	a	411	39/49	0.94	0.14	177,179,180,181	0
22	CLA	B	610	65/65	0.94	0.12	177,179,180,180	0
22	CLA	B	612	65/65	0.94	0.14	176,178,180,181	0
31	PHO	d	402	64/64	0.94	0.10	178,179,180,181	0
24	BCR	f	102	40/40	0.94	0.14	177,179,181,181	0
22	CLA	C	502	65/65	0.94	0.14	178,179,180,180	0
22	CLA	D	406	65/65	0.94	0.13	177,179,180,181	0

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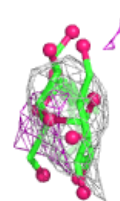
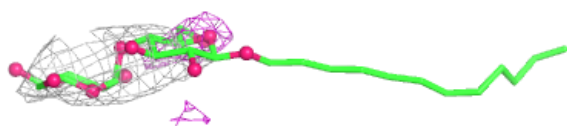
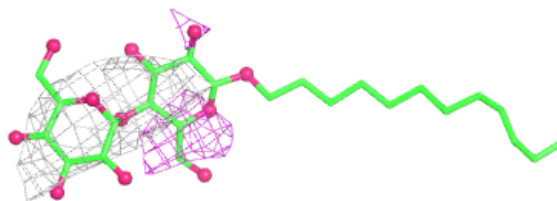
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	HEM	f	101	43/43	0.94	0.12	178,180,180,181	0
22	CLA	b	610	65/65	0.94	0.12	177,179,180,180	0
22	CLA	b	611	65/65	0.94	0.13	177,179,180,180	0
22	CLA	b	612	65/65	0.94	0.13	176,179,181,181	0
22	CLA	B	609	65/65	0.94	0.12	178,179,180,181	0
28	OEX	a	414	10/10	0.95	0.10	174,177,179,182	0
22	CLA	d	405	65/65	0.95	0.15	177,178,179,180	0
22	CLA	B	614	65/65	0.95	0.10	177,179,180,181	0
34	HEM	v	201	43/43	0.95	0.12	177,179,180,180	0
22	CLA	A	402	65/65	0.95	0.14	178,179,180,181	0
22	CLA	A	403	65/65	0.95	0.14	177,179,179,180	0
24	BCR	B	618	40/40	0.95	0.18	177,178,179,179	0
32	CL	a	413	1/1	0.95	0.15	177,177,177,177	0
22	CLA	b	614	65/65	0.96	0.13	178,179,180,180	0
22	CLA	B	611	65/65	0.96	0.12	177,179,180,180	0
28	OEX	A	411	10/10	0.96	0.09	172,175,178,178	0
22	CLA	b	616	65/65	0.96	0.13	177,179,180,180	0
34	HEM	F	101	43/43	0.96	0.11	178,180,181,182	0
34	HEM	V	201	43/43	0.96	0.14	176,178,180,180	0
21	FE2	A	401	1/1	0.97	0.07	176,176,176,176	0
21	FE2	a	403	1/1	0.97	0.10	182,182,182,182	0

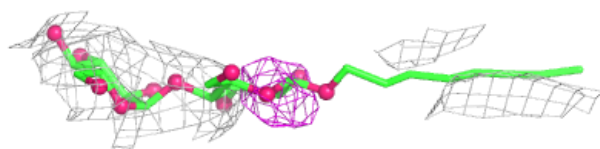
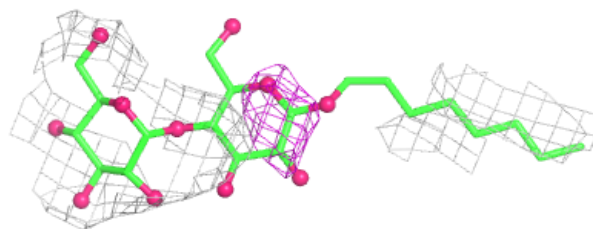
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT I 102:

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

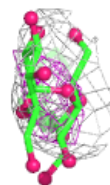
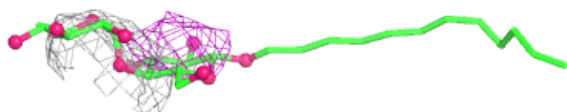
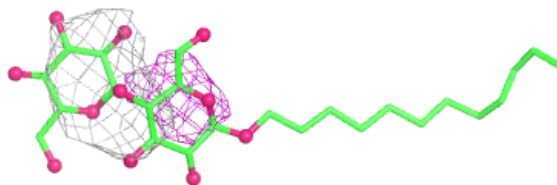
**Electron density around LMT d 411:**

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

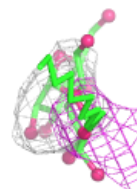
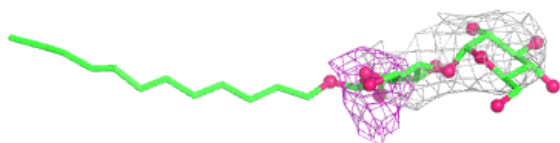
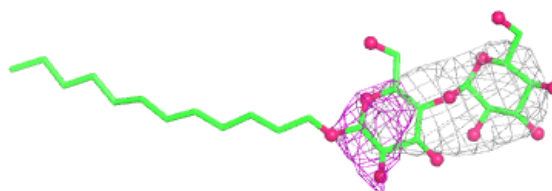


Electron density around LMT i 102:

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

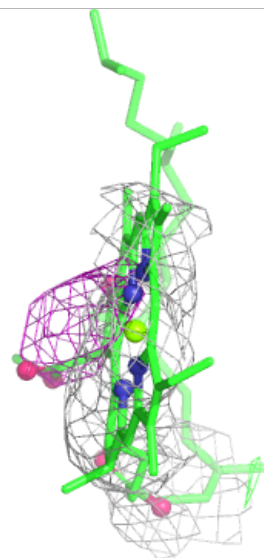
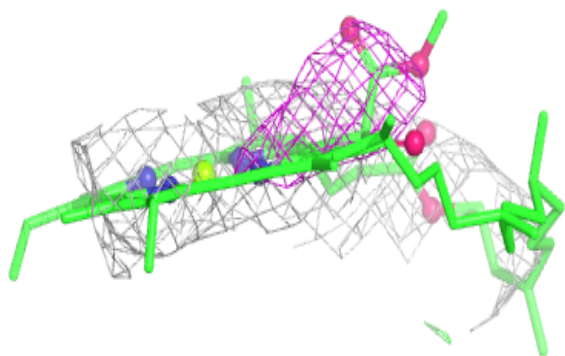
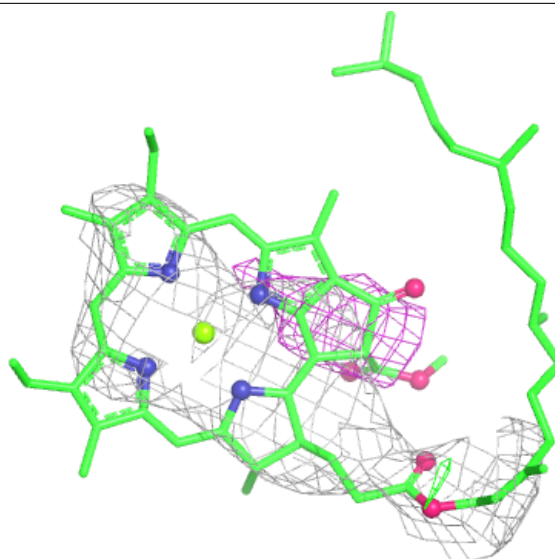
**Electron density around LMT b 627:**

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



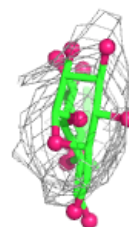
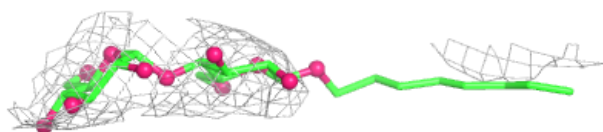
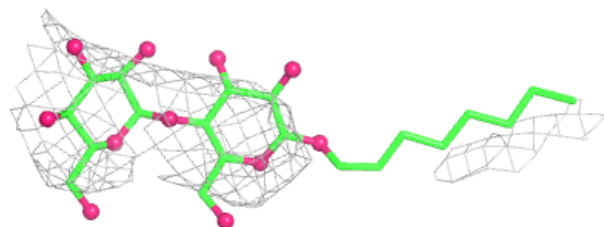
Electron density around CLA b 605:

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



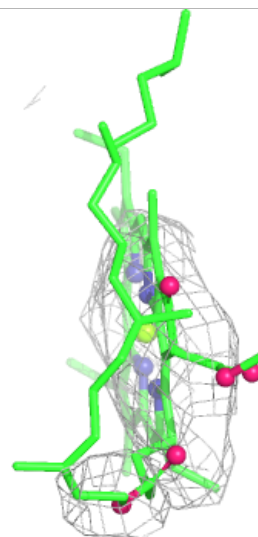
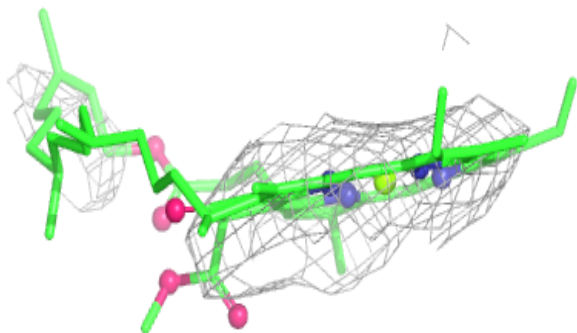
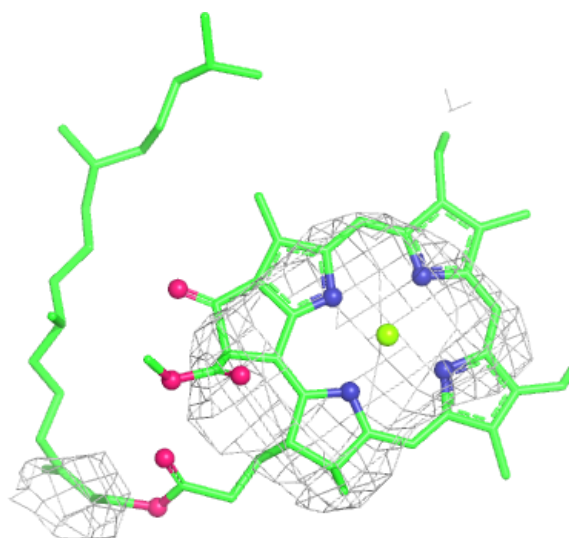
Electron density around LMT D 411:

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



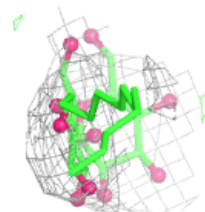
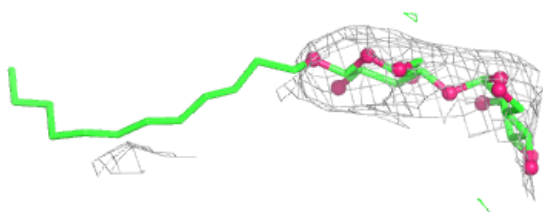
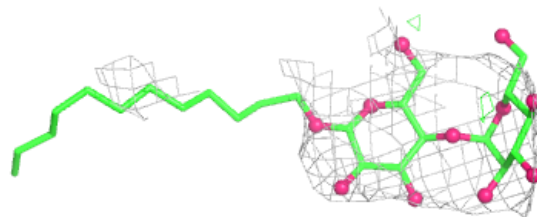
Electron density around CLA B 601:

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

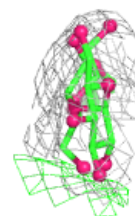
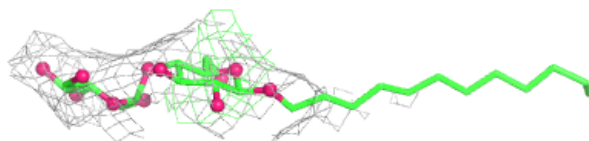
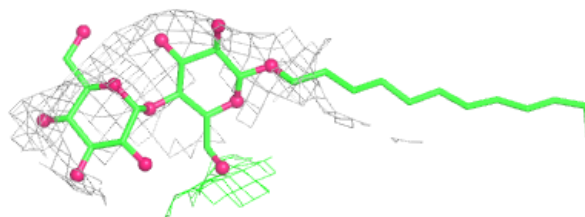


Electron density around LMT b 626:

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

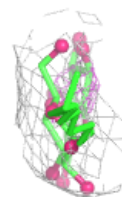
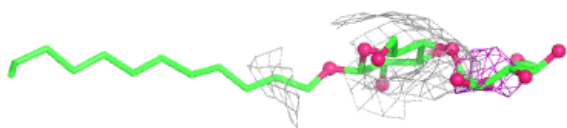
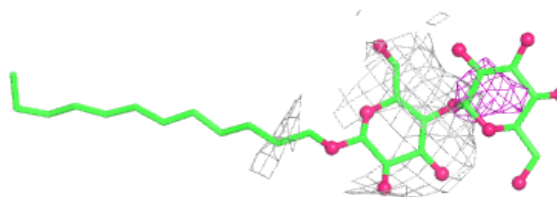
**Electron density around LMT b 603:**

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

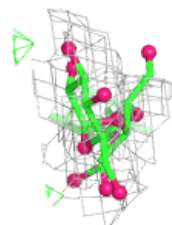
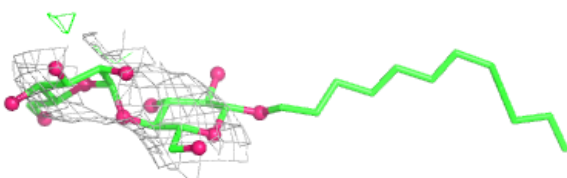
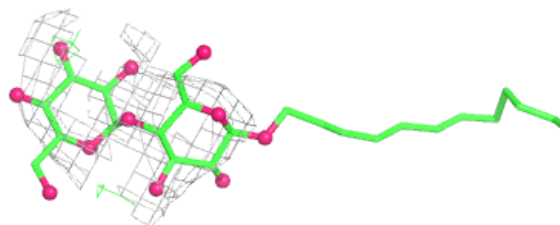


Electron density around LMT B 627:

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

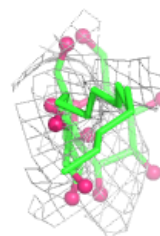
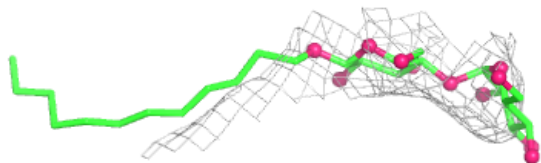
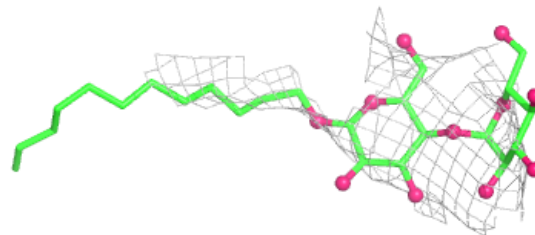
**Electron density around LMT B 628:**

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

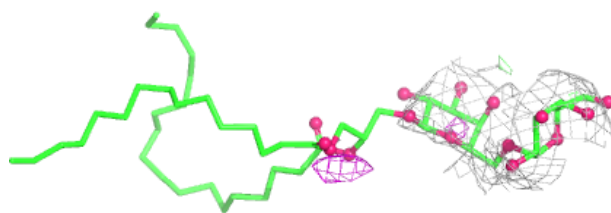
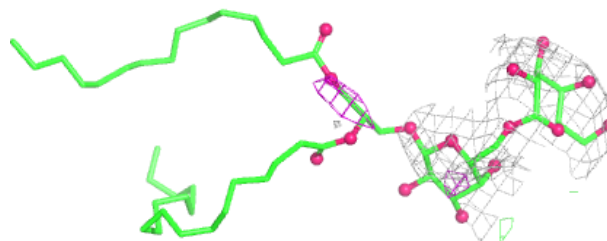


Electron density around LMT B 623:

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

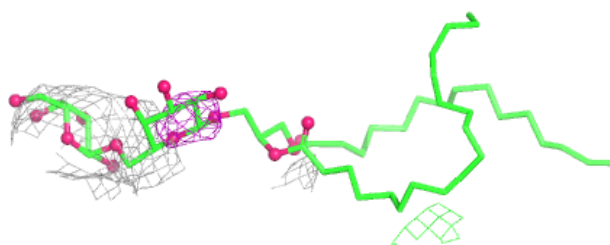
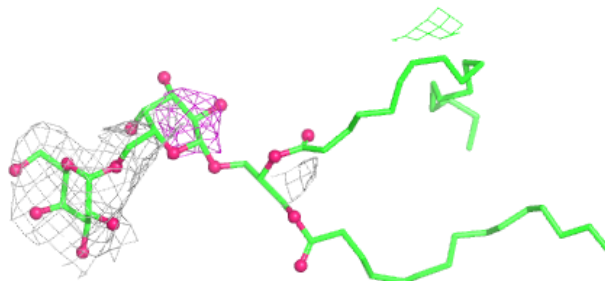
**Electron density around DGD D 410:**

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

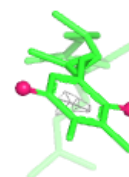
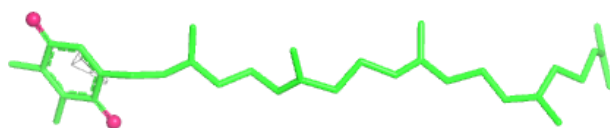
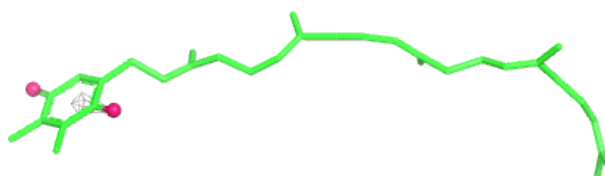


Electron density around DGD d 410:

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

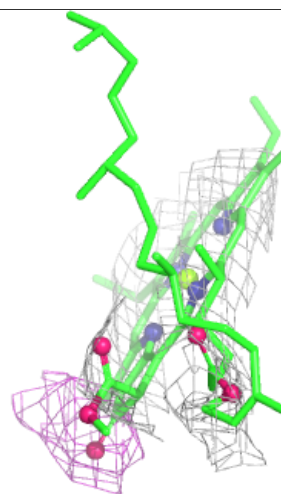
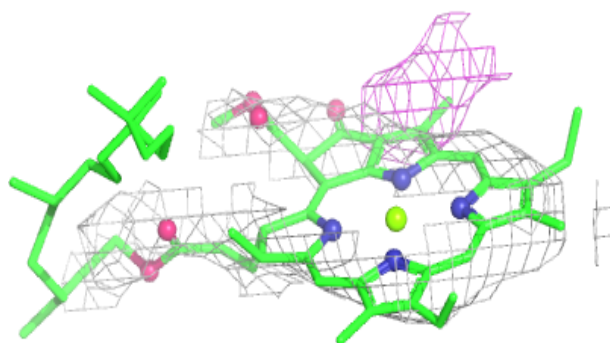
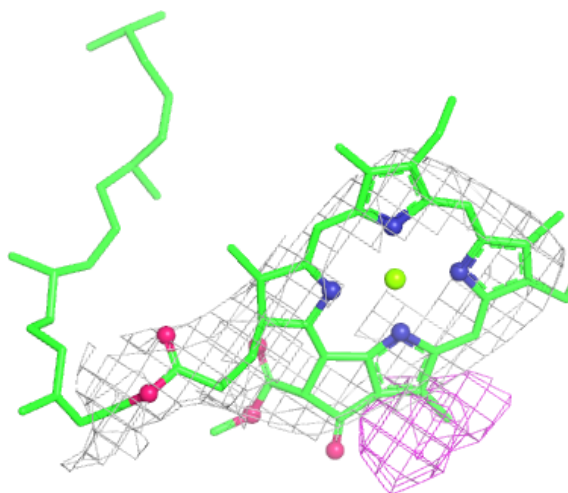
**Electron density around PL9 J 101:**

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



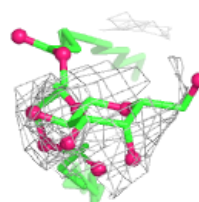
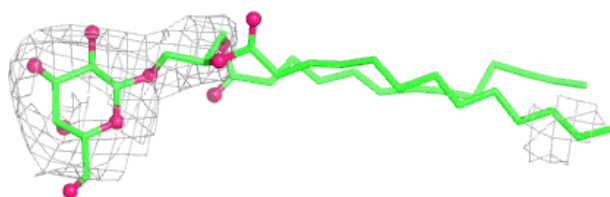
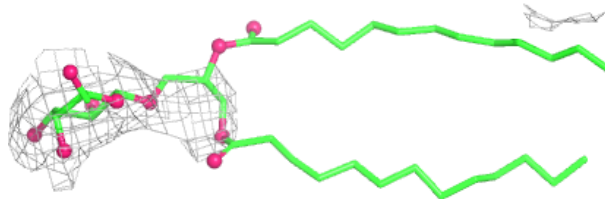
Electron density around CLA b 619:

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

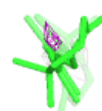
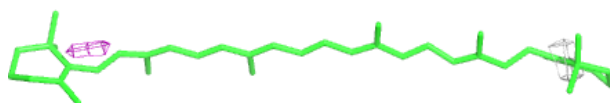
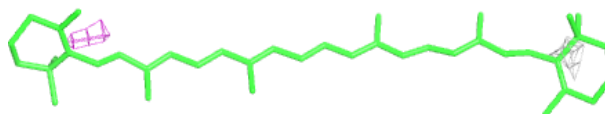


Electron density around LMG C 518:

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

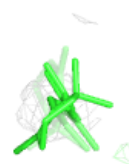
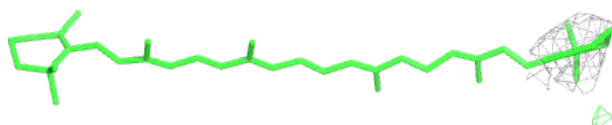
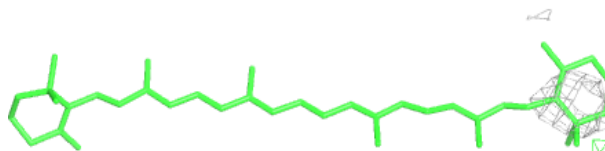
**Electron density around BCR J 102:**

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

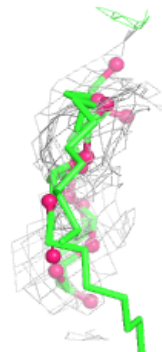
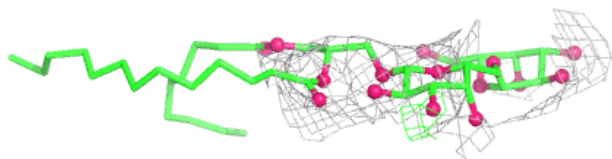
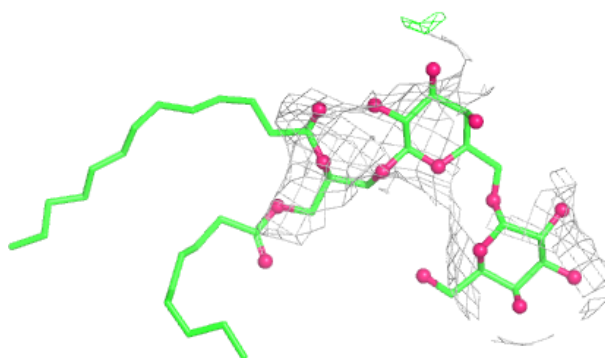


Electron density around BCR j 102:

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

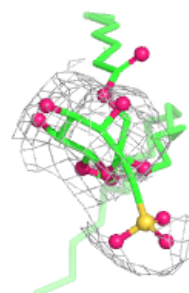
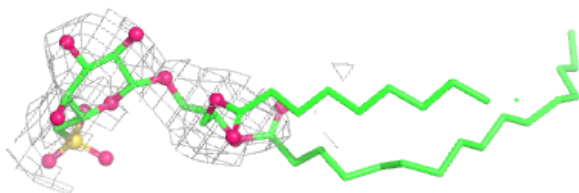
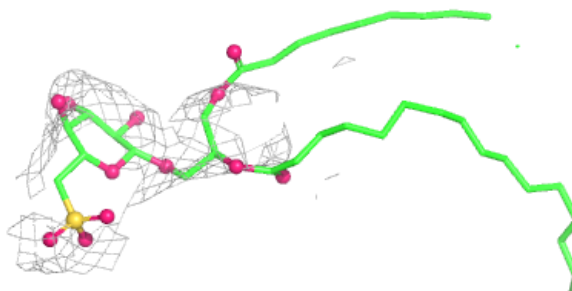
**Electron density around DGD B 625:**

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

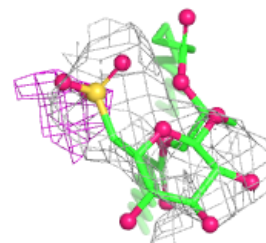
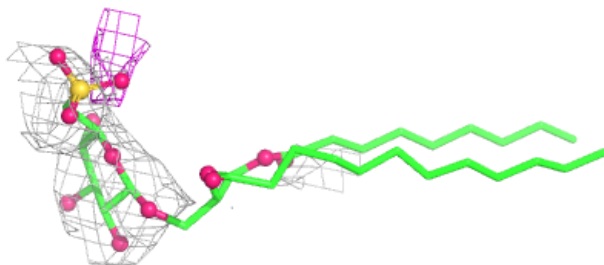
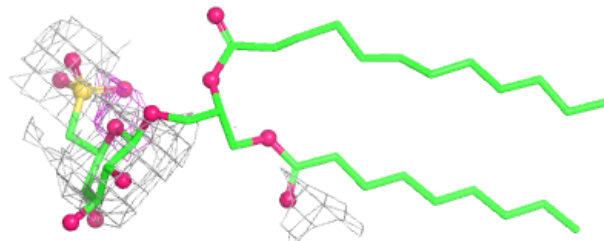


Electron density around SQD B 626:

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

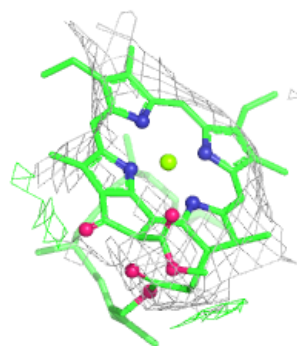
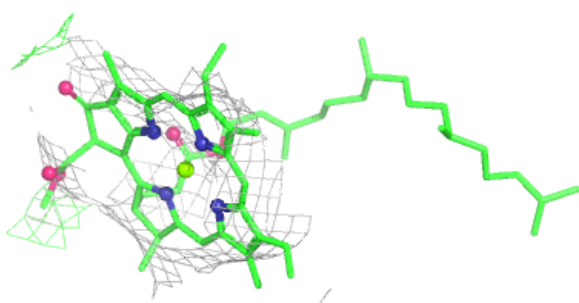
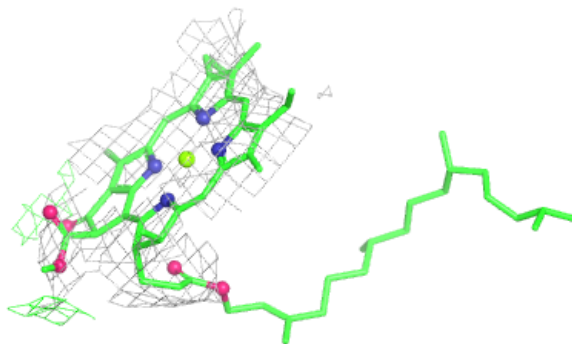
**Electron density around SQD d 403:**

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

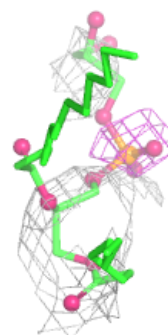
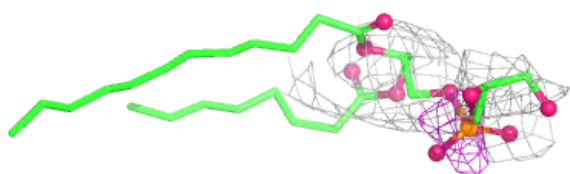
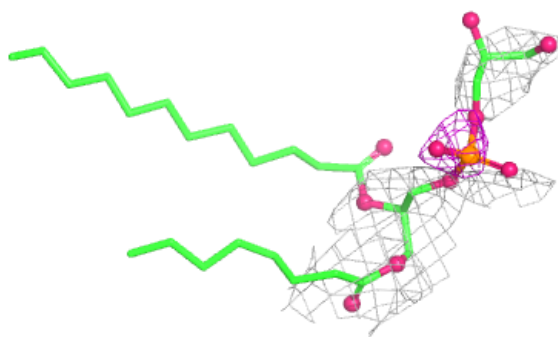


Electron density around CLA c 512:

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

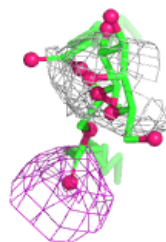
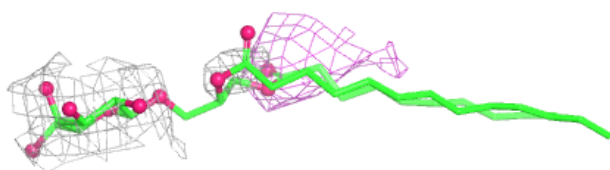
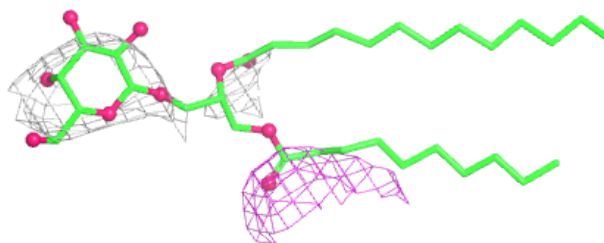
**Electron density around LHG C 519:**

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

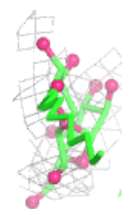
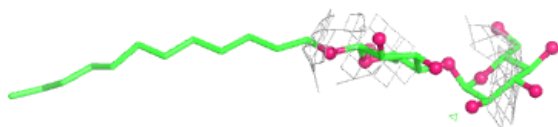
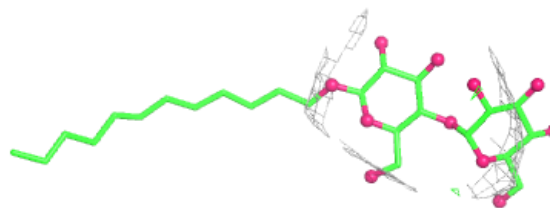


Electron density around LMG M 101:

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

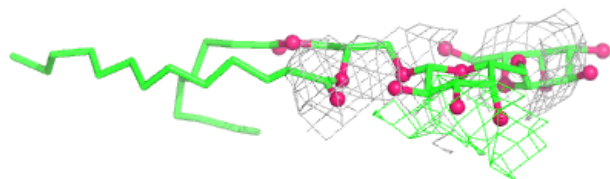
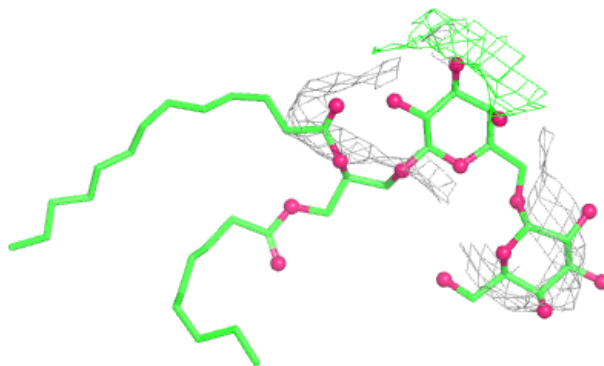
**Electron density around LMT B 624:**

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

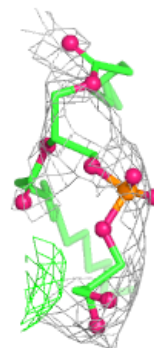
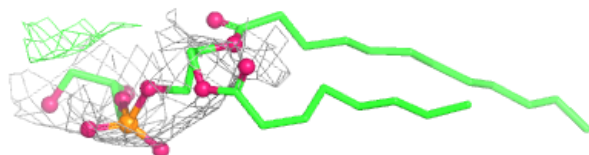
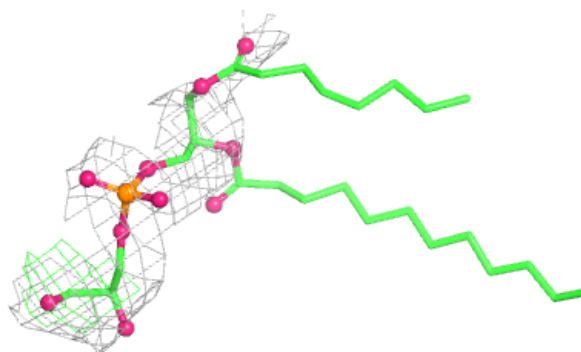


Electron density around DGD b 601:

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

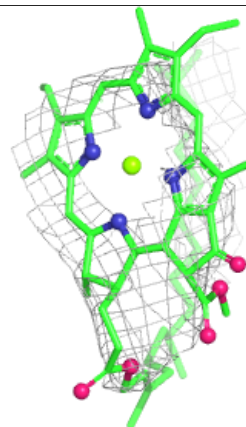
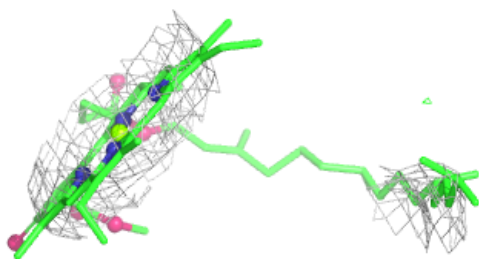
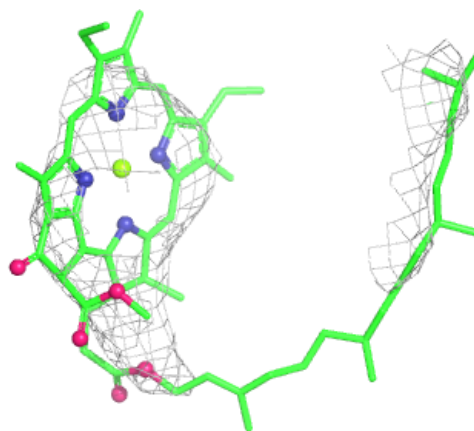
**Electron density around LHG c 519:**

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

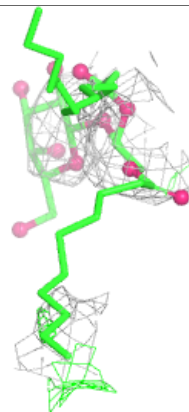
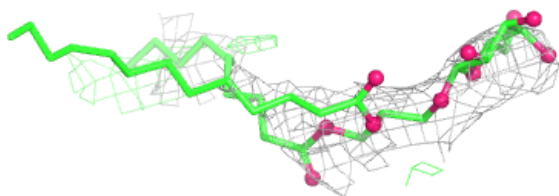


Electron density around CLA C 506:

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

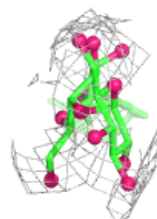
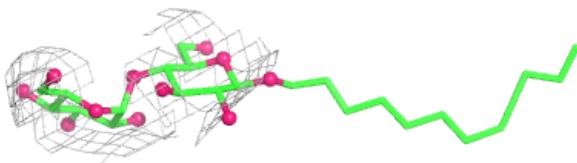
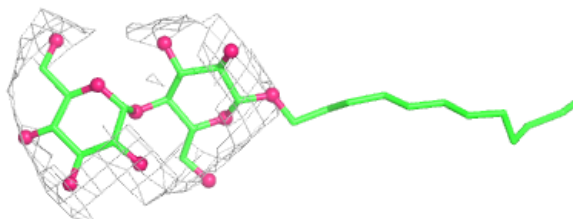
**Electron density around LMG A 414:**

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

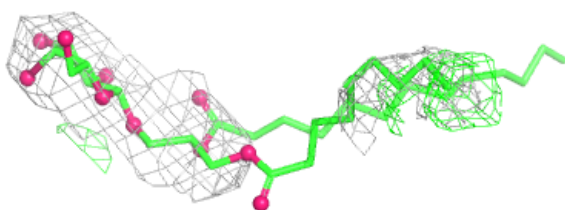
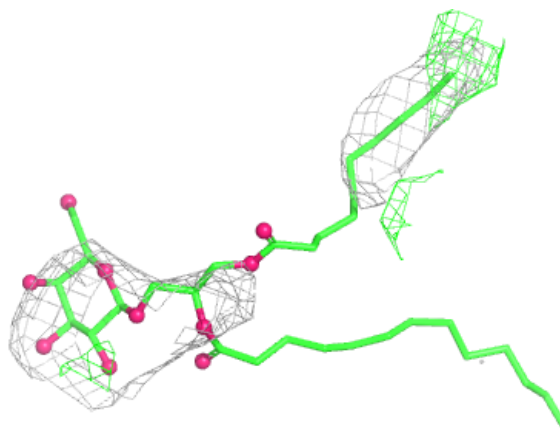


Electron density around LMT b 604:

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

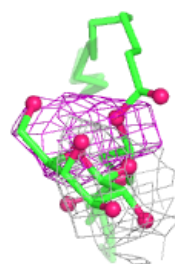
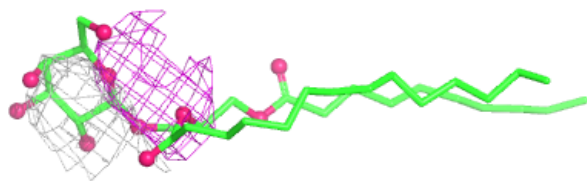
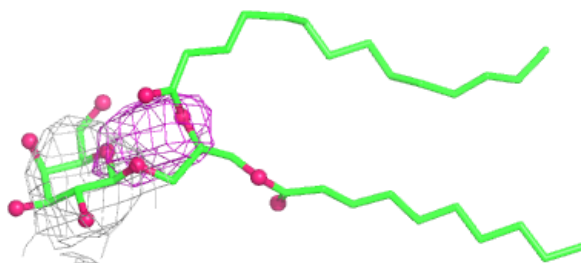
**Electron density around LMG a 402:**

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

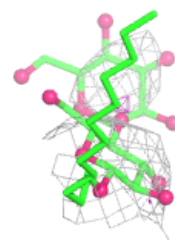
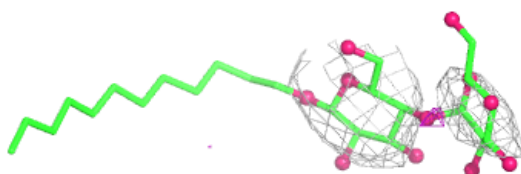
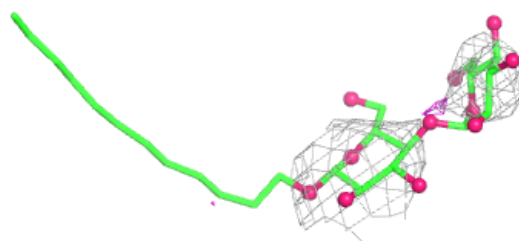


Electron density around LMG I 101:

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

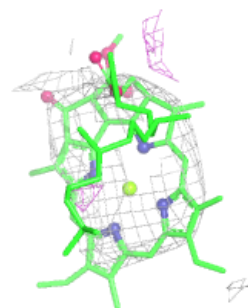
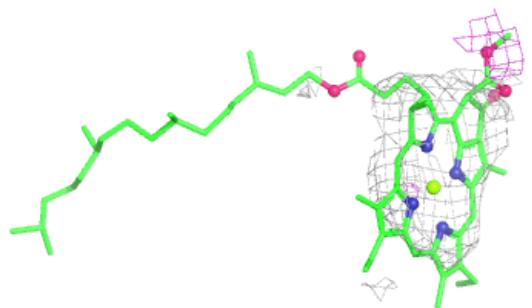
**Electron density around LMT M 102:**

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

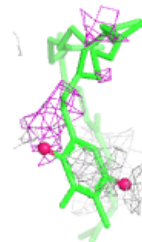
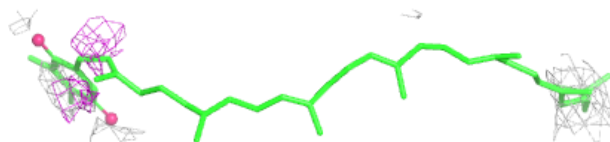
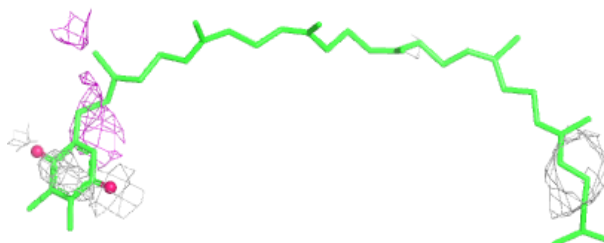


Electron density around CLA A 405:

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

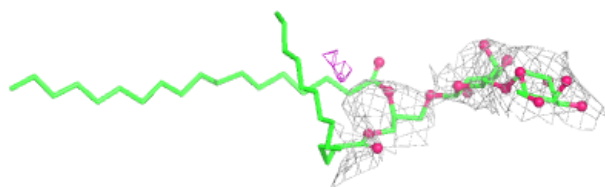
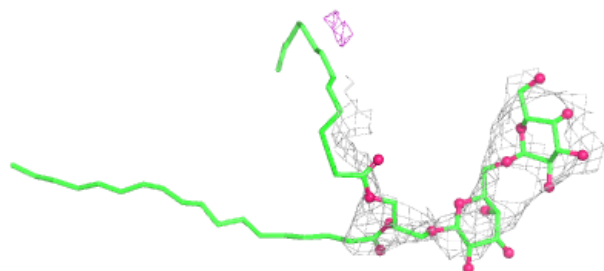
**Electron density around PL9 A 406:**

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

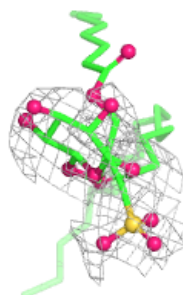
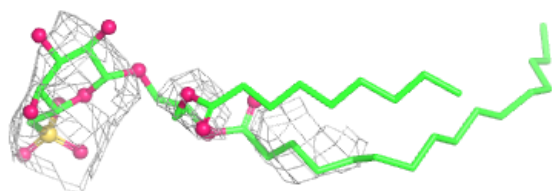


Electron density around DGD C 516:

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

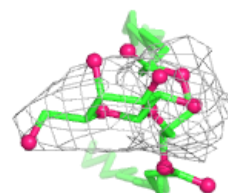
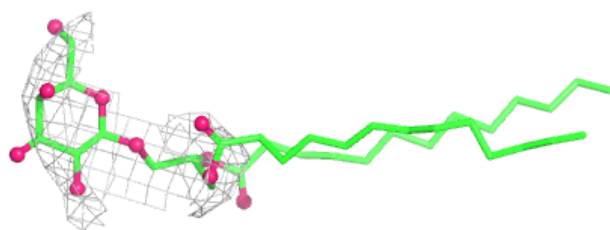
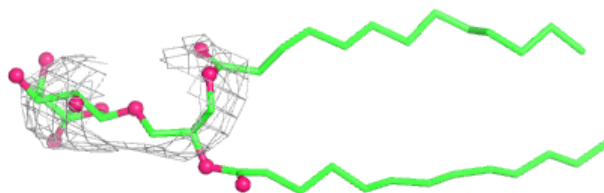
**Electron density around SQD b 602:**

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

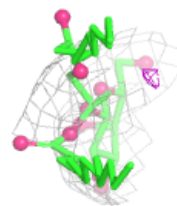
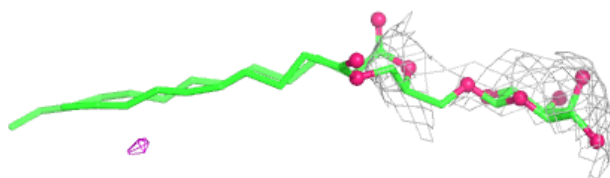
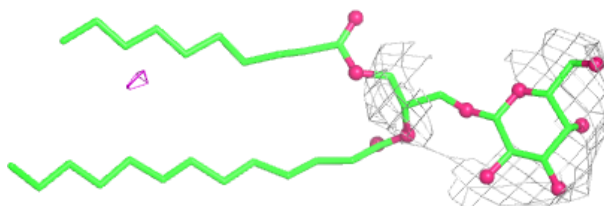


Electron density around LMG c 518:

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

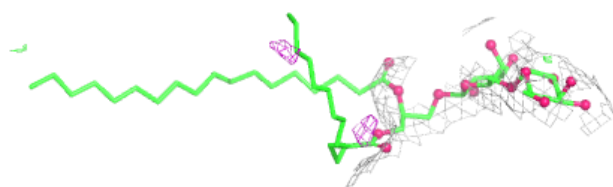
**Electron density around LMG m 101:**

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

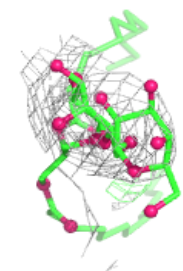
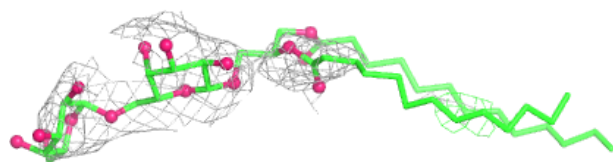


Electron density around DGD c 516:

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

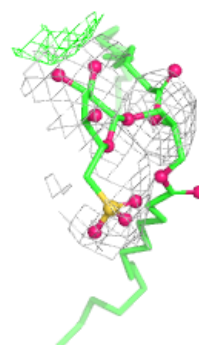
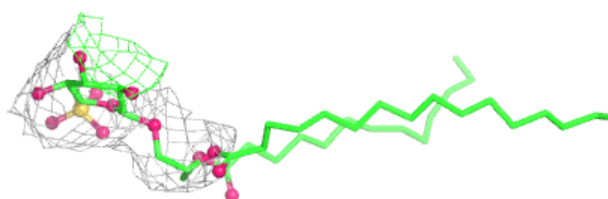
**Electron density around DGD a 410:**

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

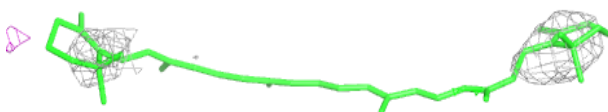
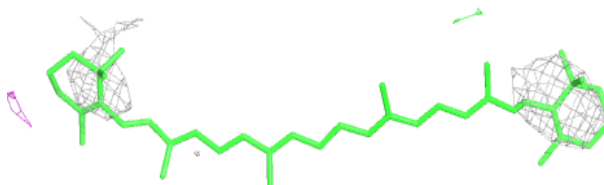


Electron density around SQD a 415:

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

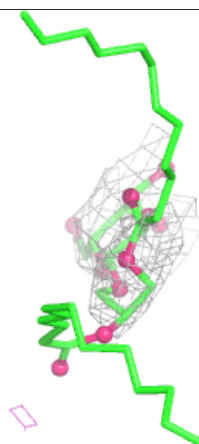
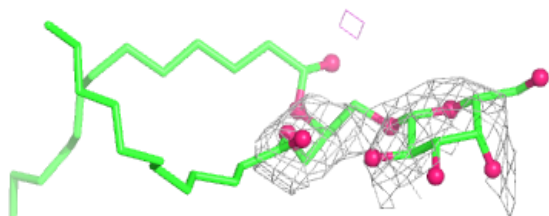
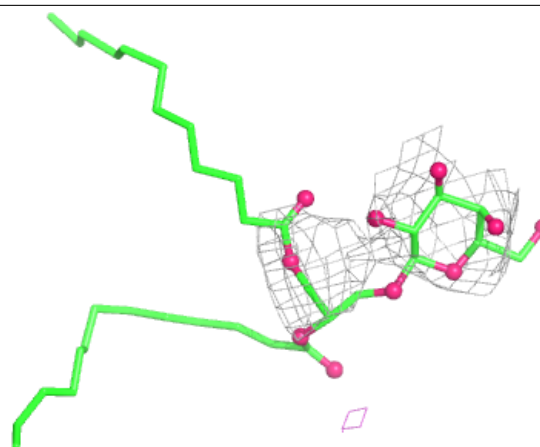
**Electron density around BCR b 621:**

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

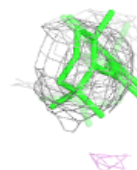
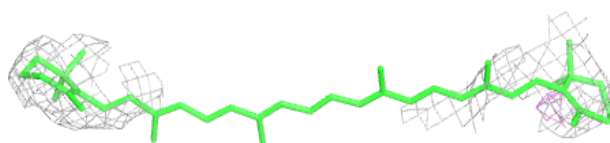
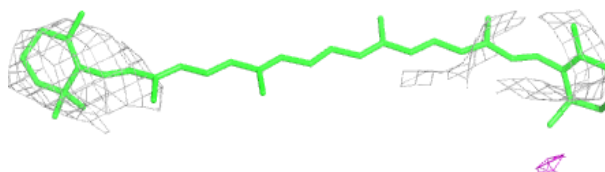


Electron density around LMG E 101:

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

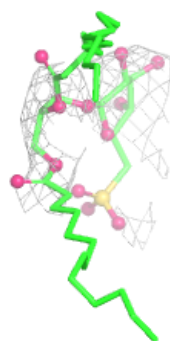
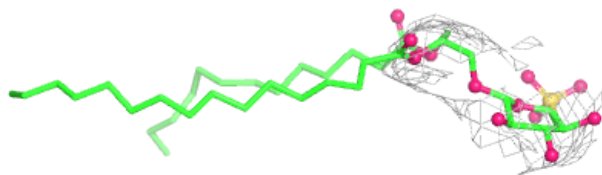
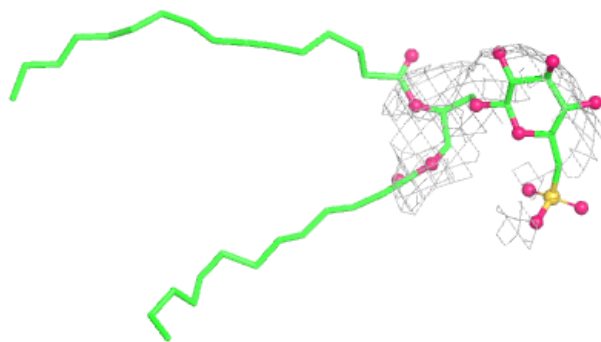
**Electron density around BCR b 623:**

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

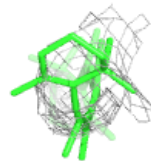
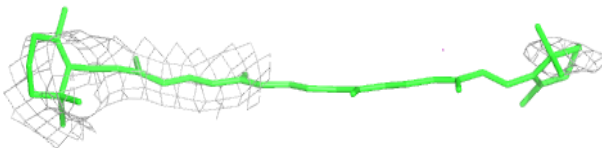
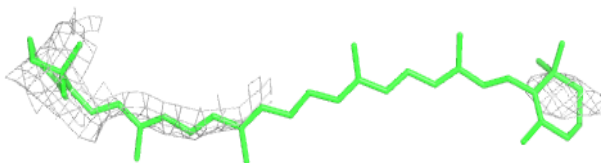


Electron density around SQD A 412:

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

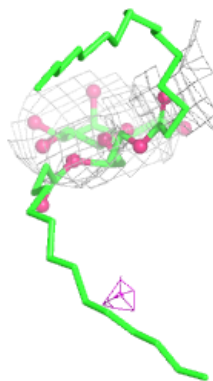
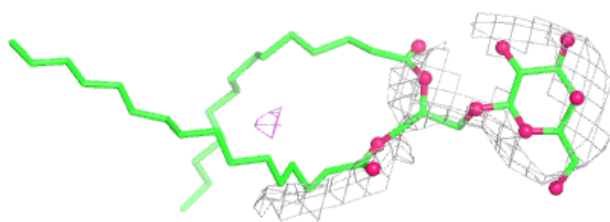
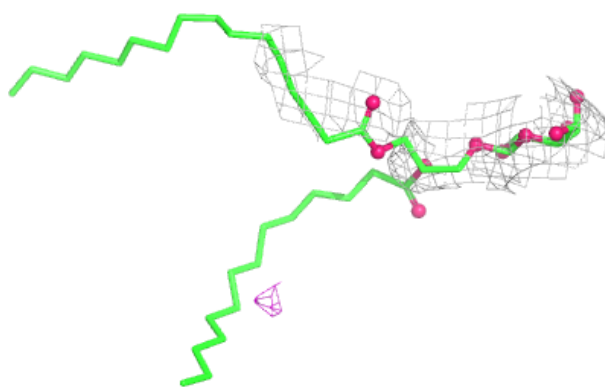
**Electron density around BCR H 102:**

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

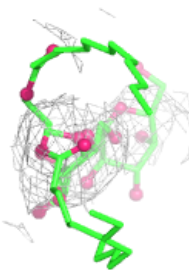
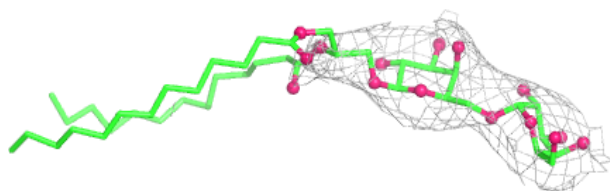
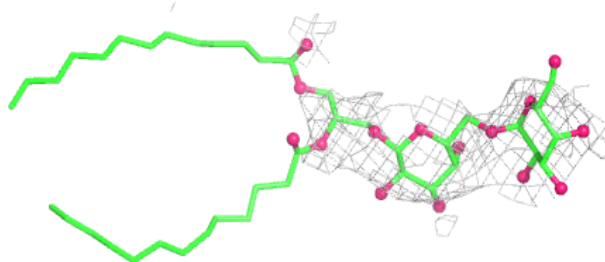


Electron density around LMG b 625:

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

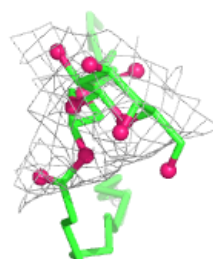
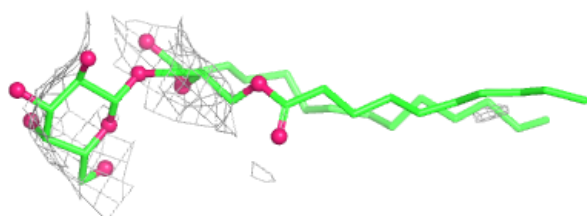
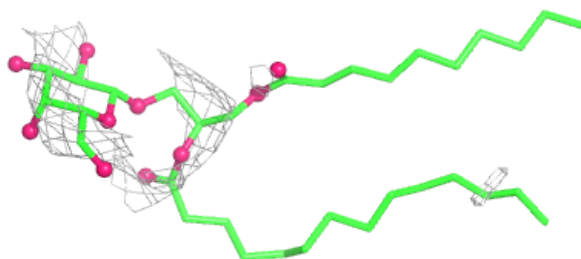
**Electron density around DGD A 408:**

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

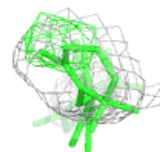
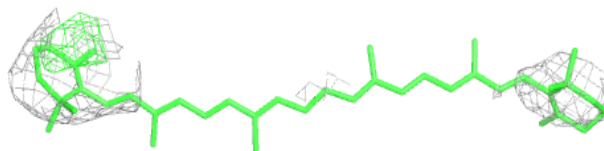


Electron density around LMG i 101:

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

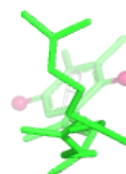
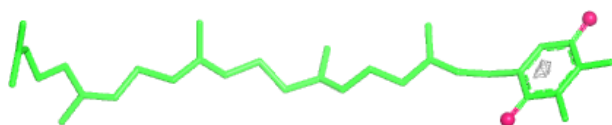
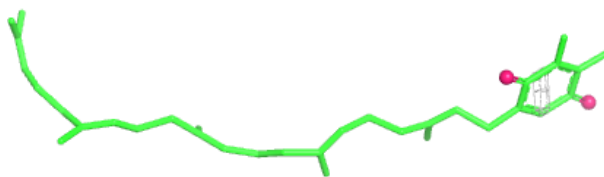
**Electron density around BCR b 622:**

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

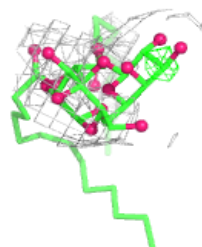
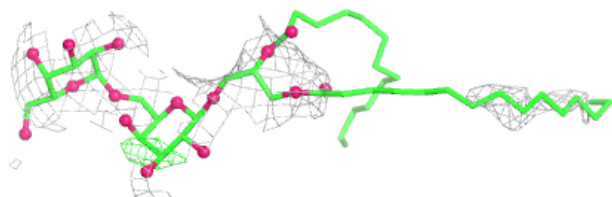


Electron density around PL9 j 101:

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

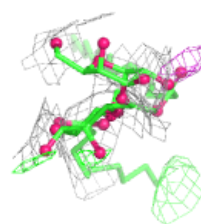
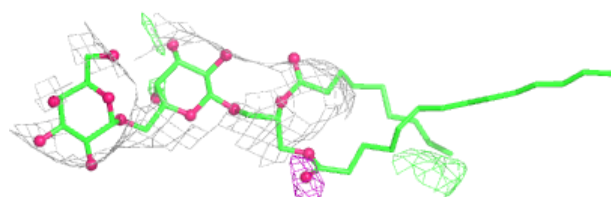
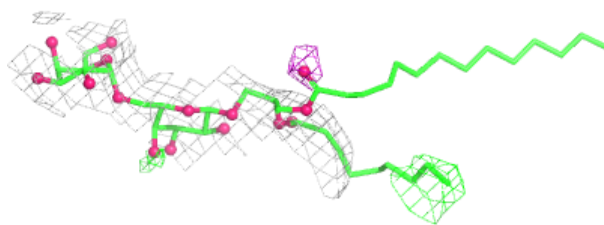
**Electron density around DGD b 624:**

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

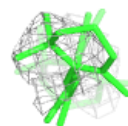
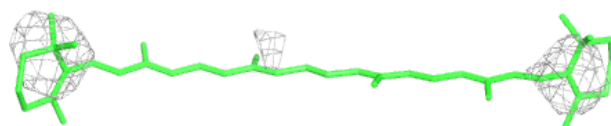
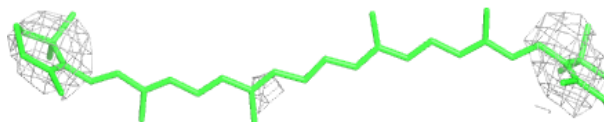


Electron density around DGD c 515:

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

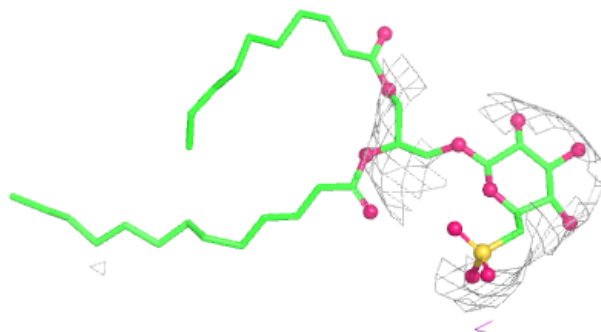
**Electron density around BCR a 409:**

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

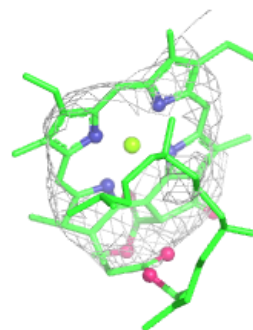
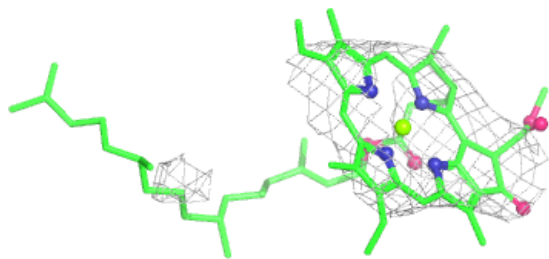
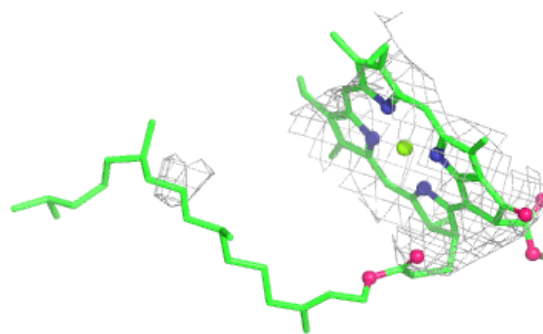


Electron density around SQD F 103:

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

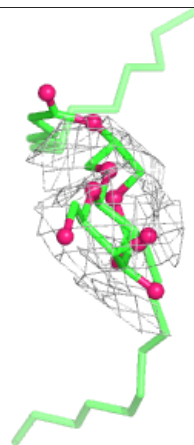
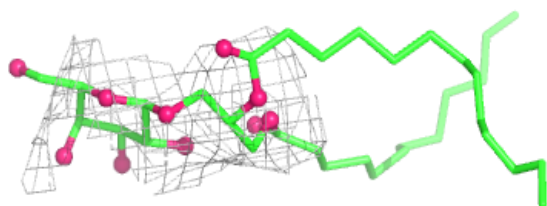
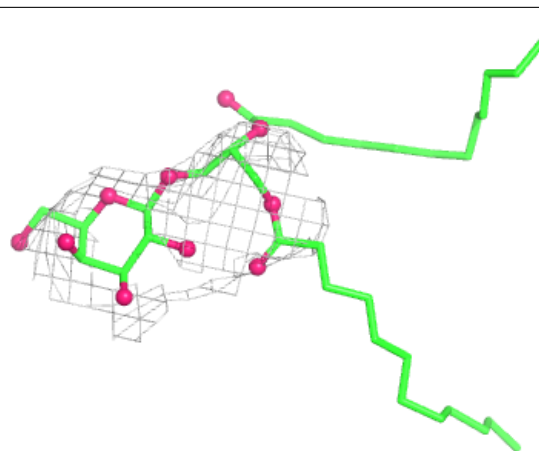
**Electron density around CLA C 512:**

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

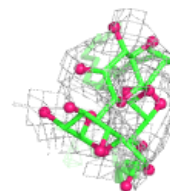
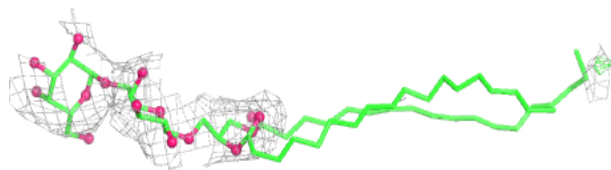


Electron density around LMG e 101:

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

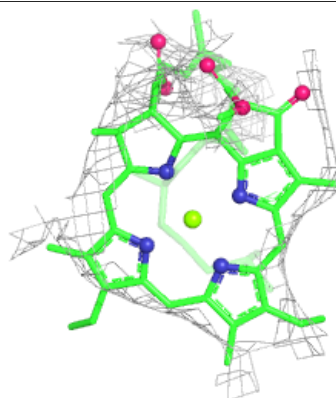
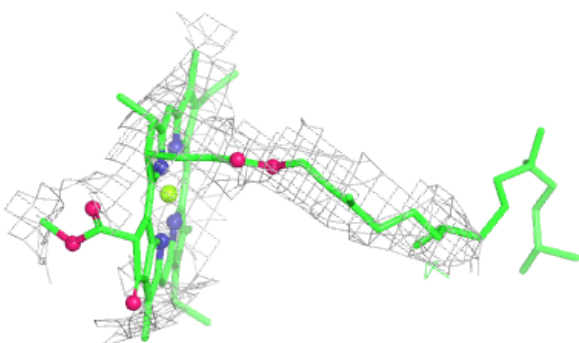
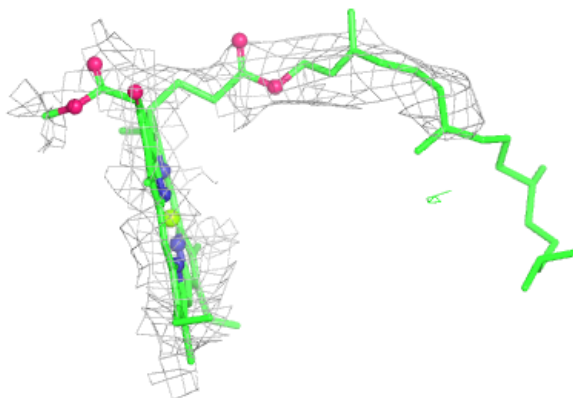
**Electron density around DGD C 517:**

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

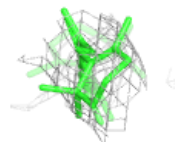
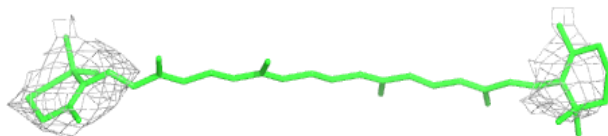
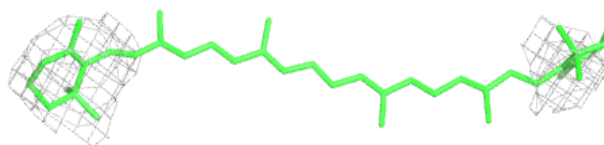


Electron density around CLA C 505:

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

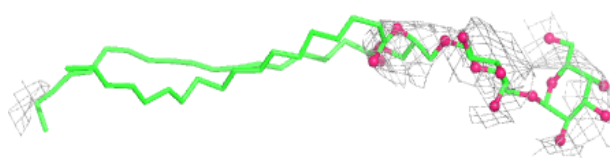
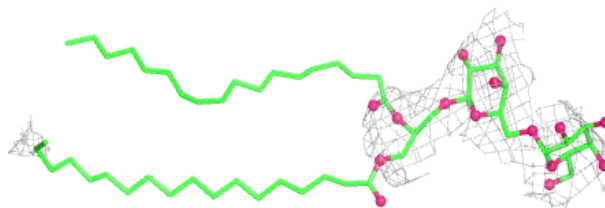
**Electron density around BCR K 102:**

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

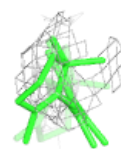
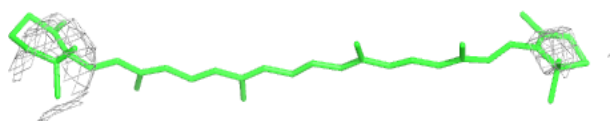
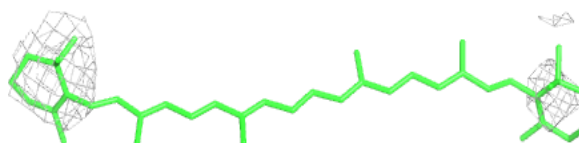


Electron density around DGD c 517:

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

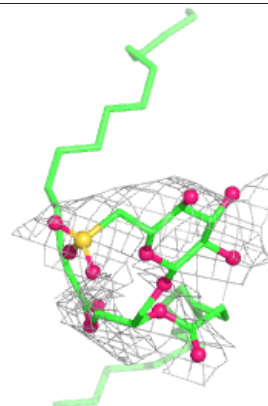
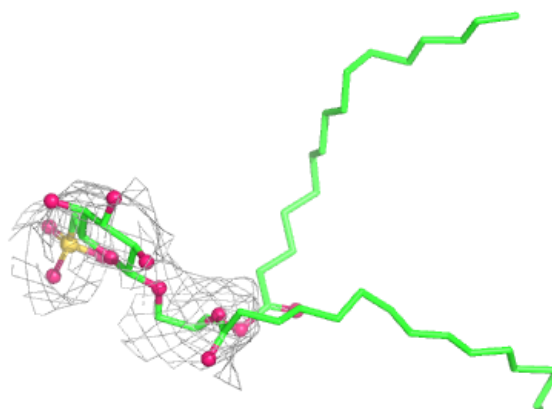
**Electron density around BCR c 514:**

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

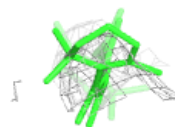
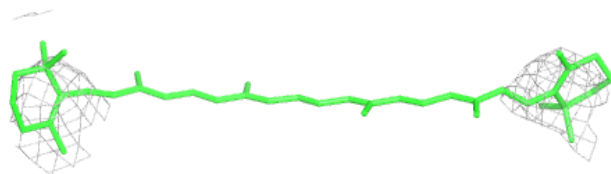
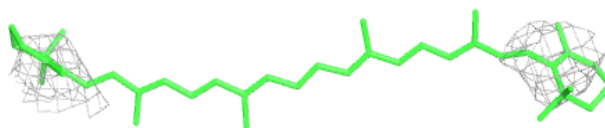


Electron density around SQD a 401:

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

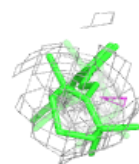
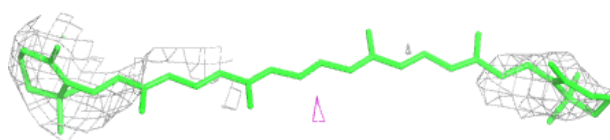
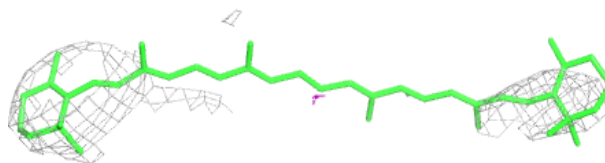
**Electron density around BCR c 521:**

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

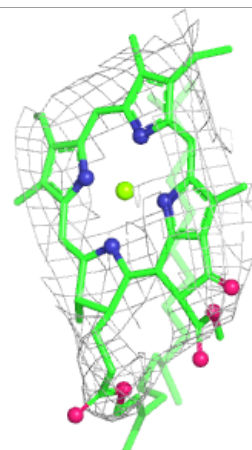
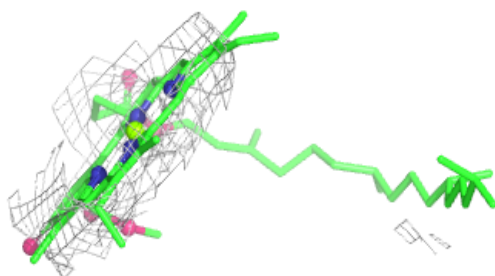
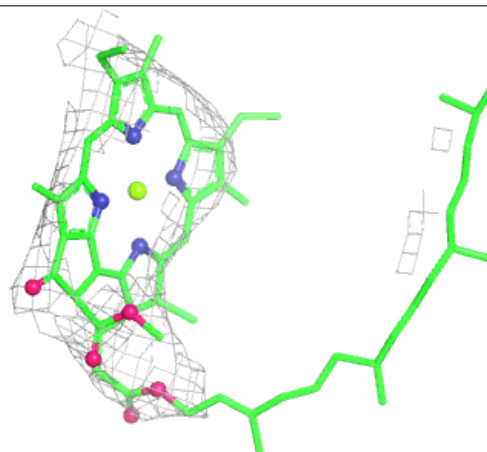


Electron density around BCR B 619:

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

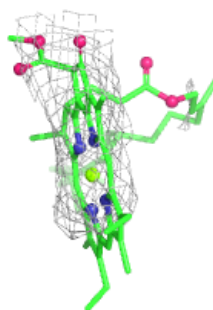
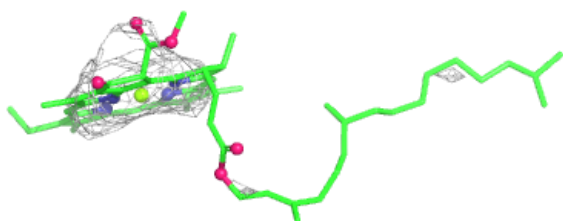
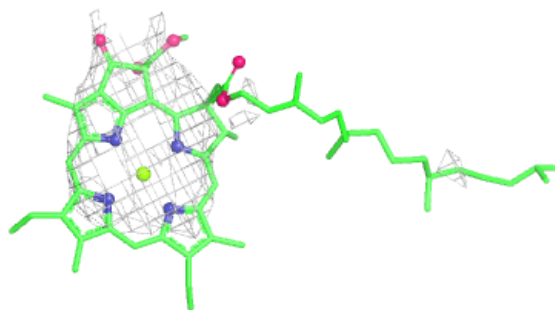
**Electron density around CLA c 506:**

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

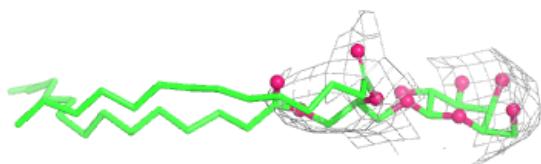


Electron density around CLA a 406:

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

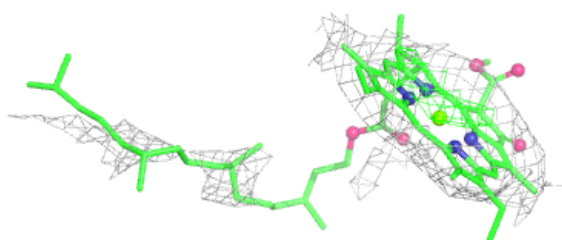
**Electron density around LMG c 522:**

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



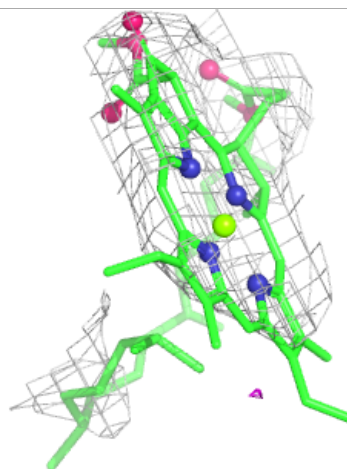
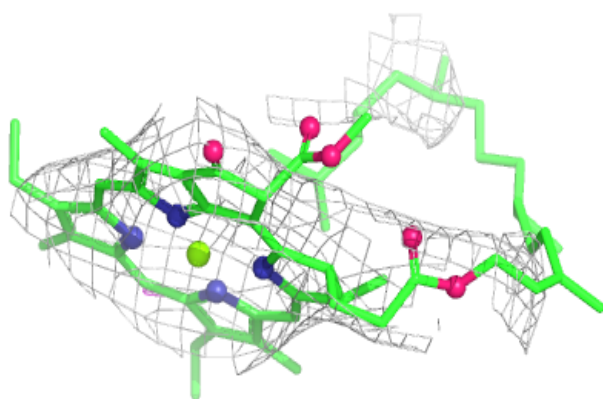
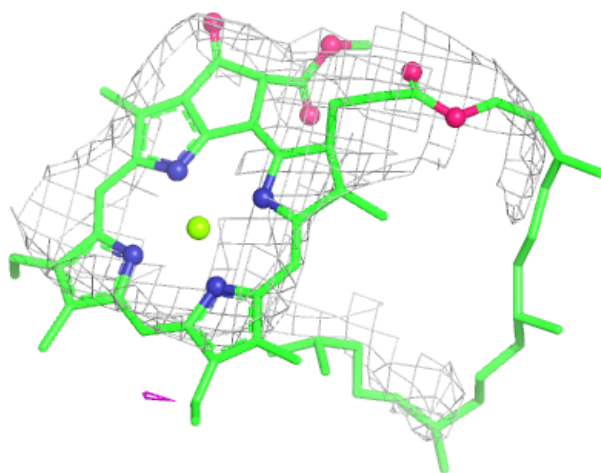
Electron density around CLA C 510:

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



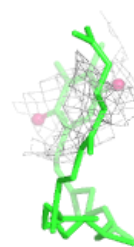
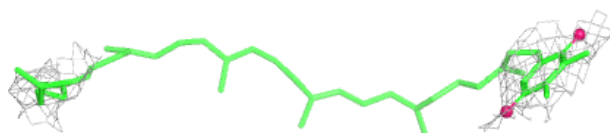
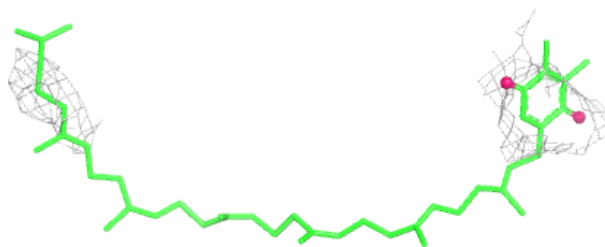
Electron density around CLA b 618:

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

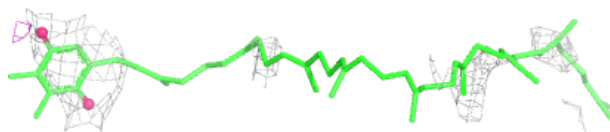
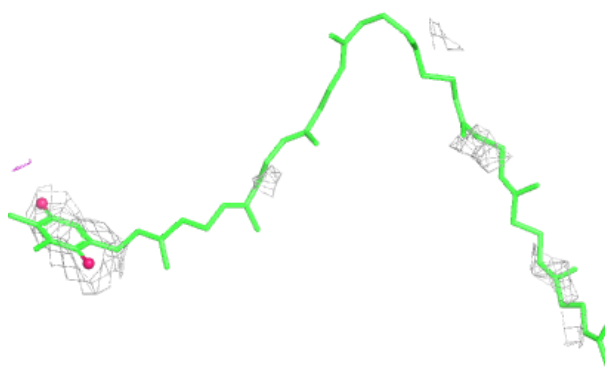


Electron density around PL9 a 408:

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

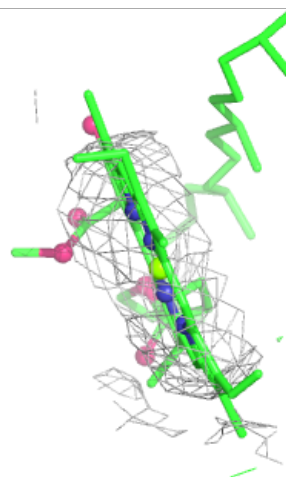
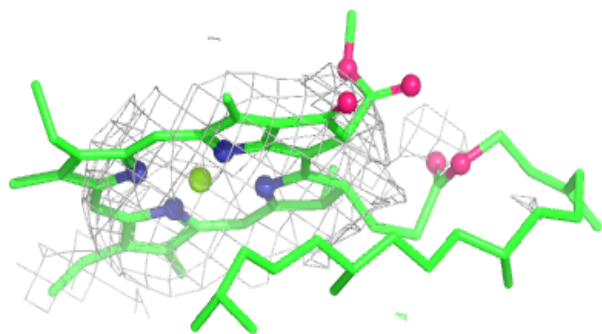
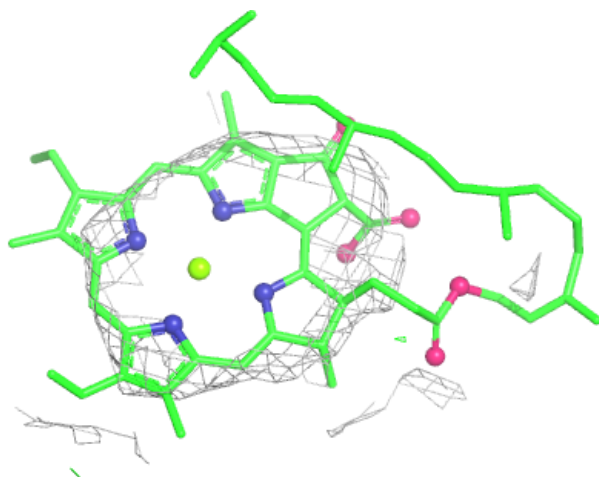
**Electron density around PL9 d 407:**

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



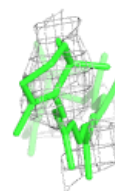
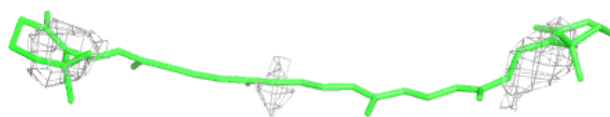
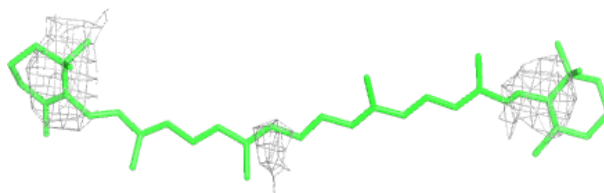
Electron density around CLA C 508:

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

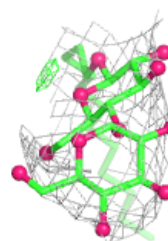
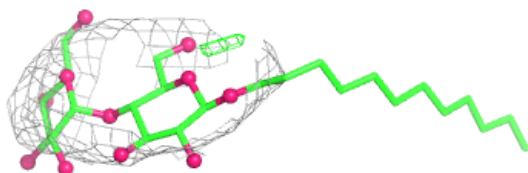
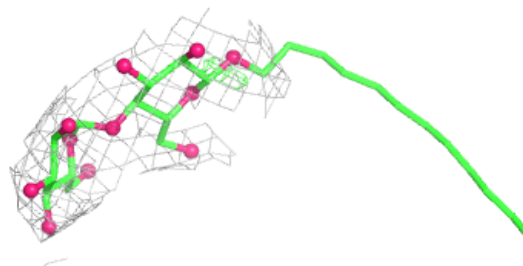


Electron density around BCR B 617:

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

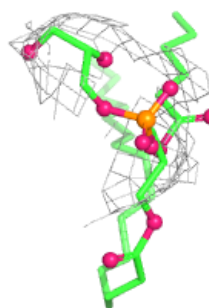
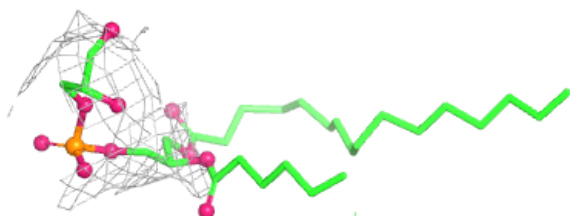
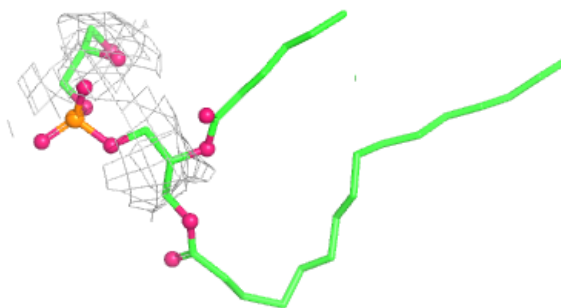
**Electron density around LMT M 103:**

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

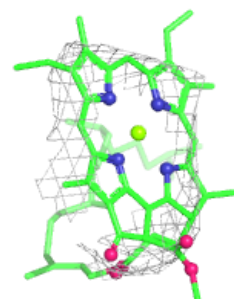
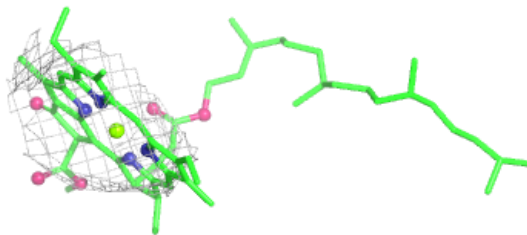
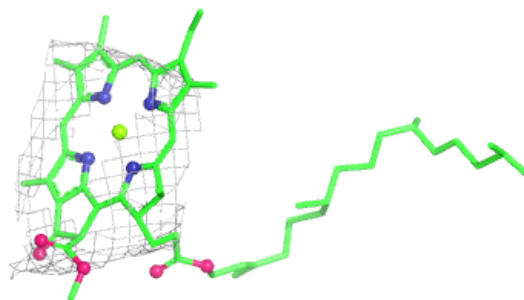


Electron density around LHG A 409:

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

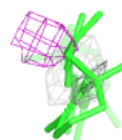
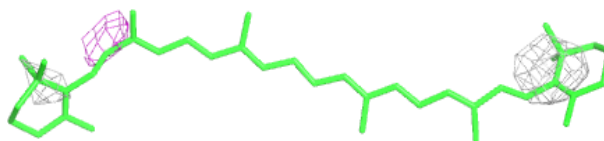
**Electron density around CLA c 510:**

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

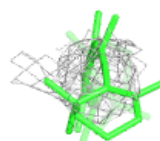
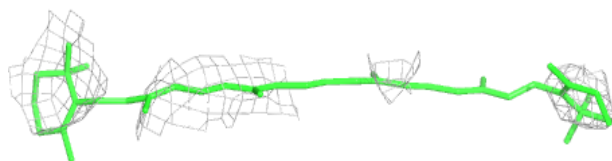
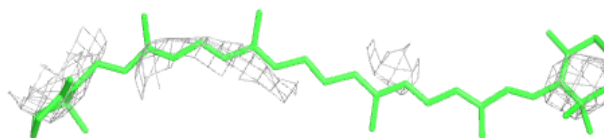


Electron density around BCR g 101:

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

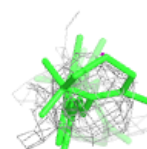
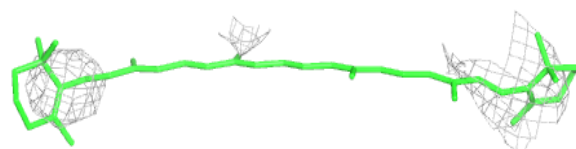
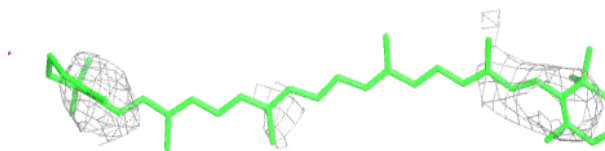
**Electron density around BCR x 101:**

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

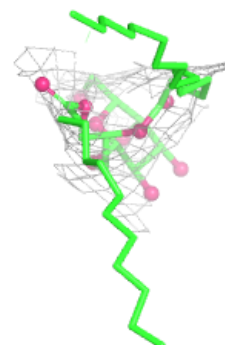
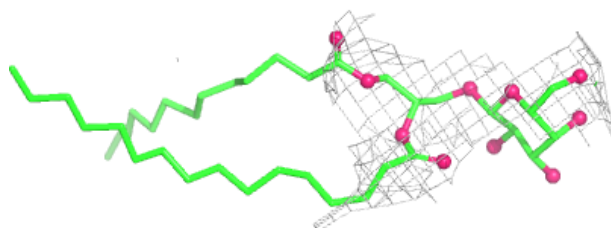
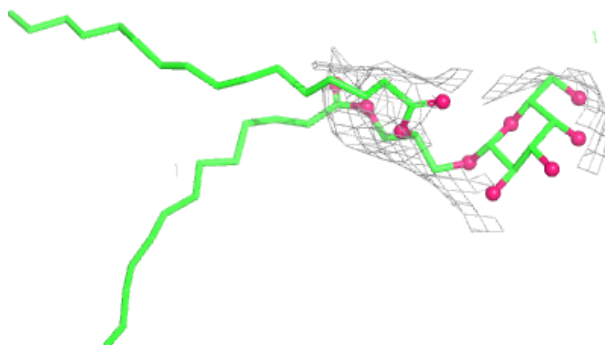


Electron density around BCR B 616:

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

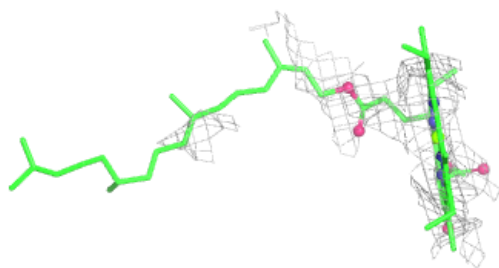
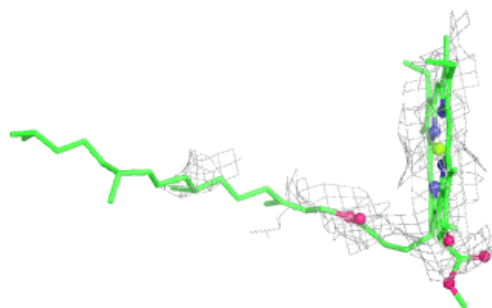
**Electron density around LMG D 409:**

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

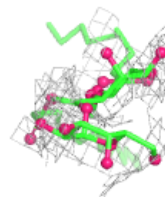
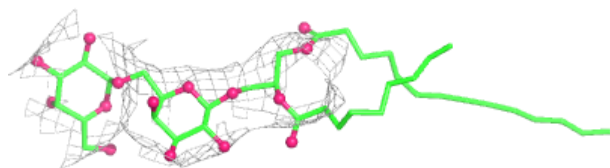


Electron density around CLA b 609:

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

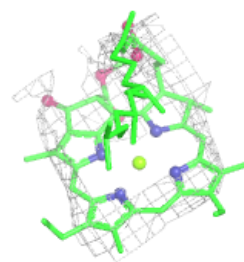
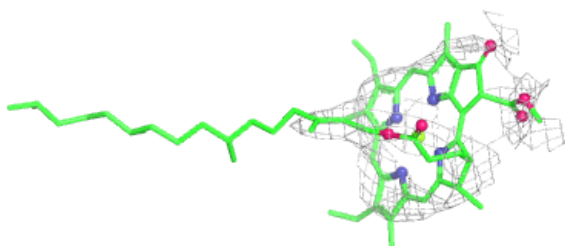
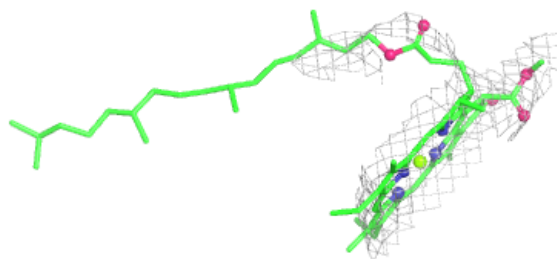
**Electron density around DGD C 515:**

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

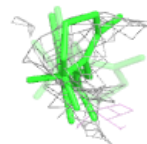
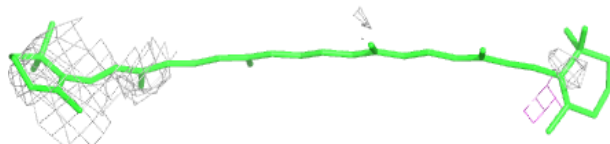
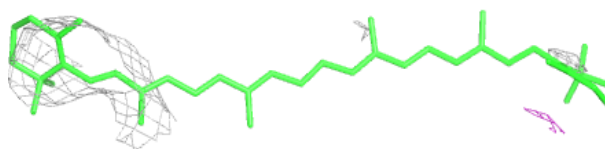


Electron density around CLA C 520:

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

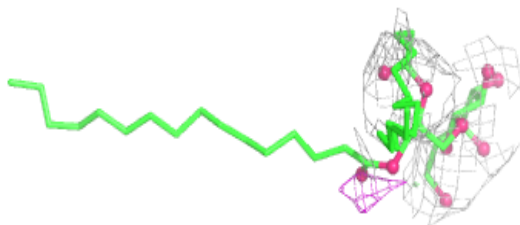
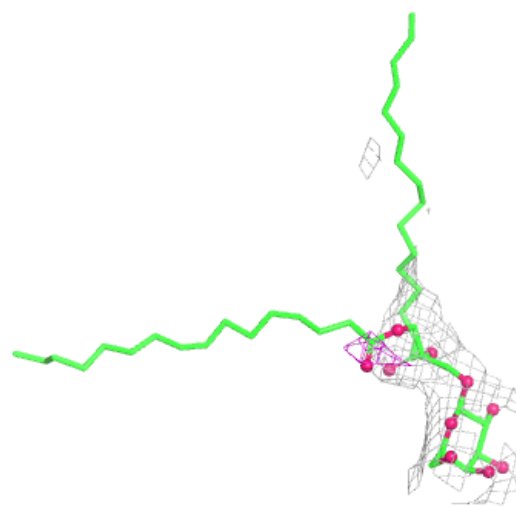
**Electron density around BCR b 620:**

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



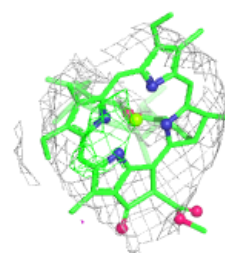
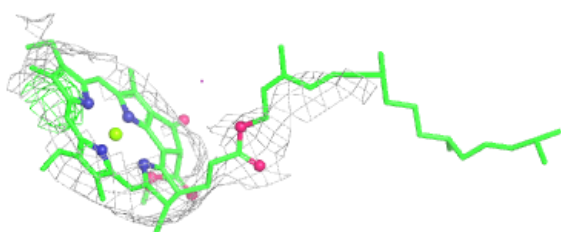
Electron density around LMG a 412:

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

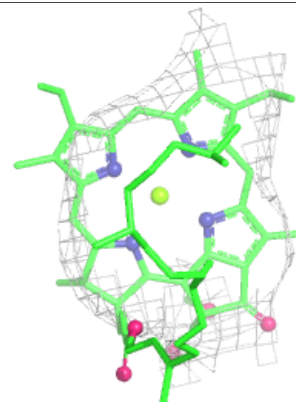
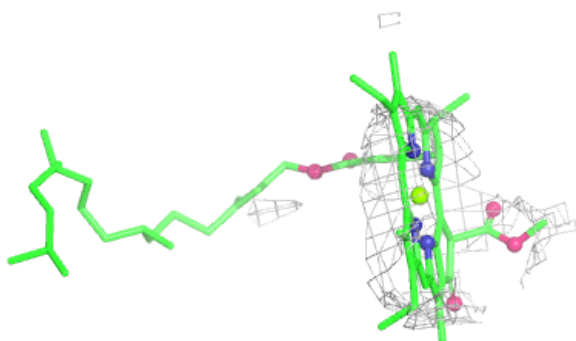
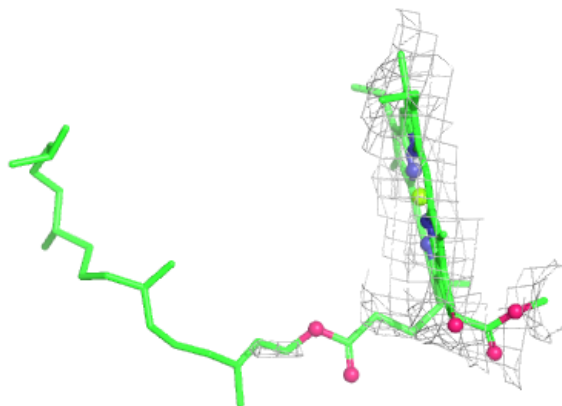


Electron density around CLA c 502:

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

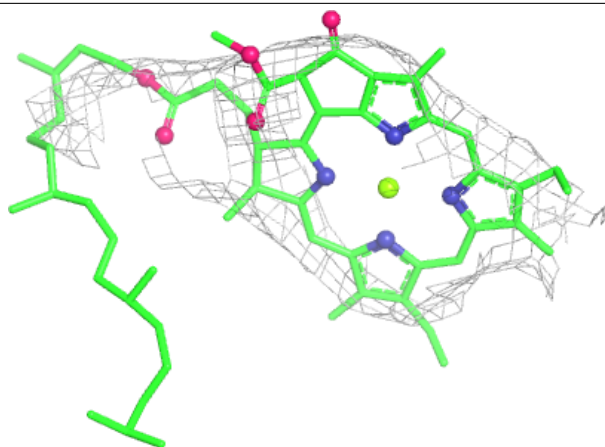
**Electron density around CLA c 505:**

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



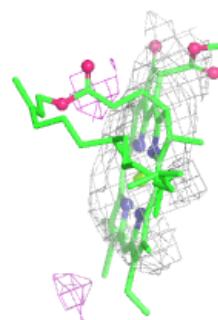
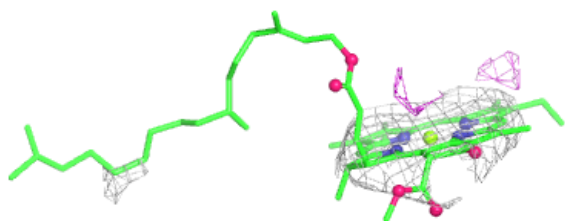
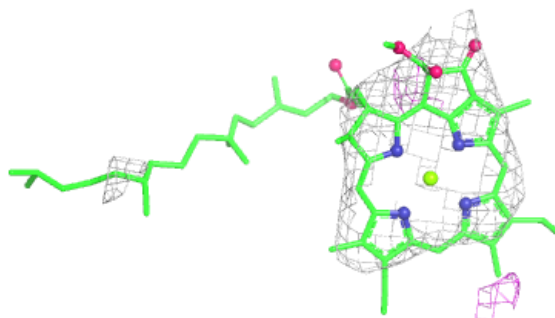
Electron density around CLA B 615:

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

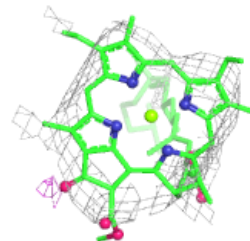
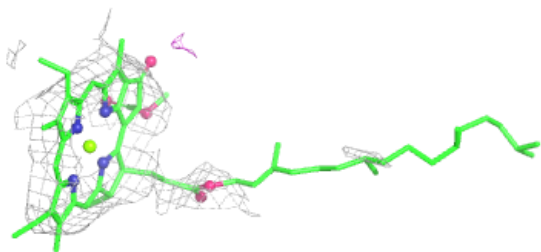
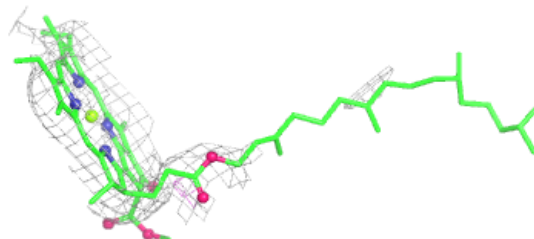


Electron density around CLA A 404:

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

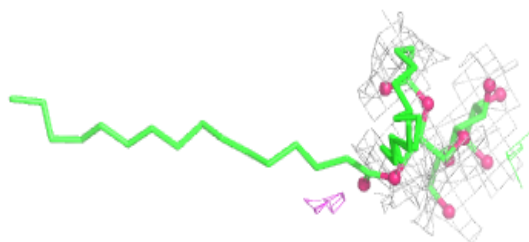
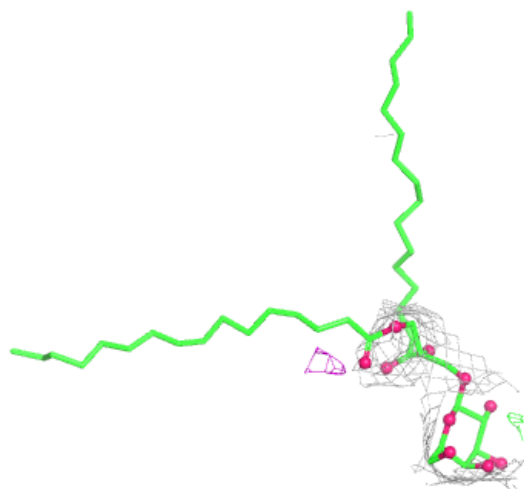
**Electron density around CLA B 603:**

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



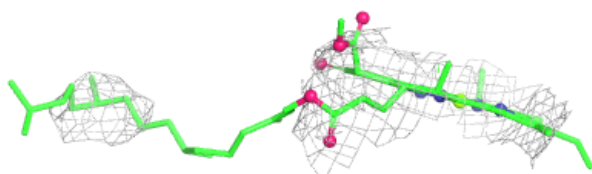
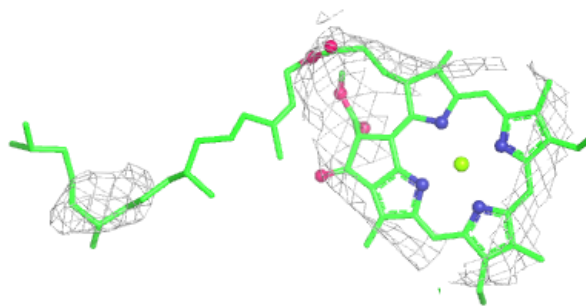
Electron density around LMG A 410:

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

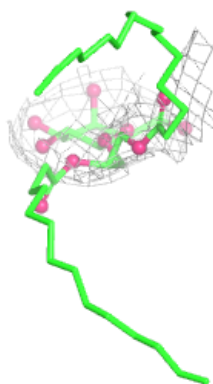


Electron density around CLA h 101:

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

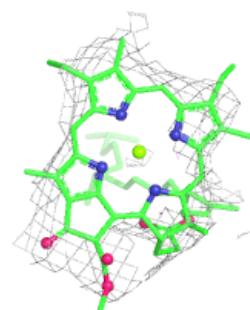
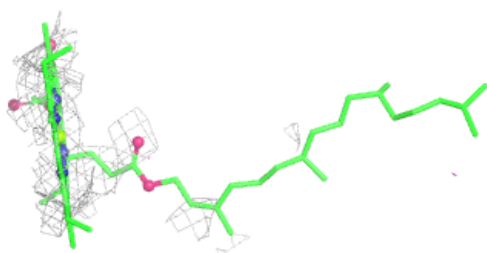
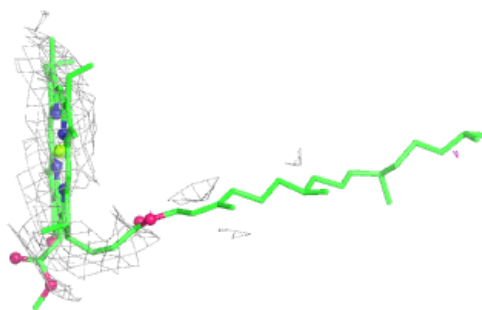
**Electron density around LMG B 621:**

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

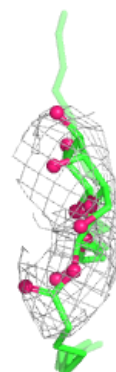
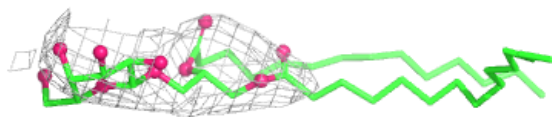
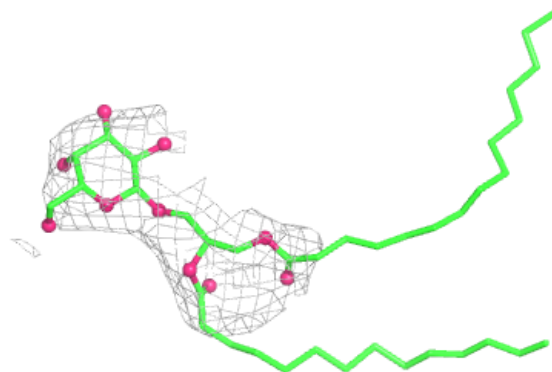


Electron density around CLA B 605:

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

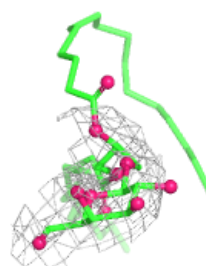
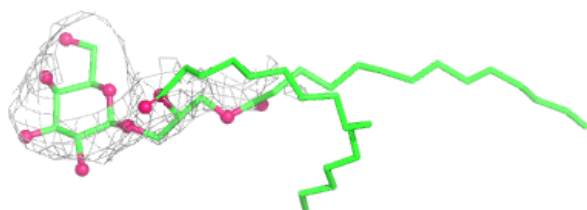
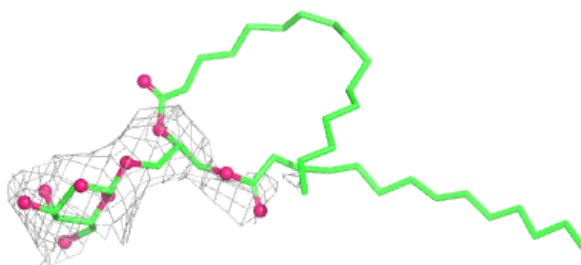
**Electron density around LMG C 521:**

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

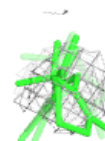
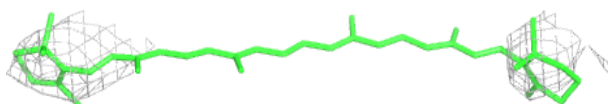
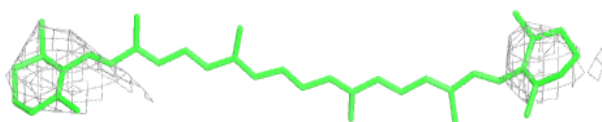


Electron density around LMG D 408:

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

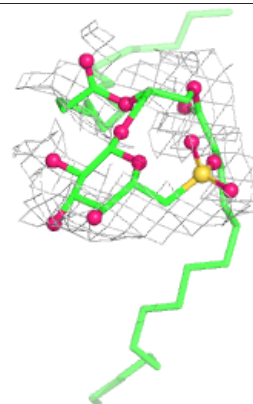
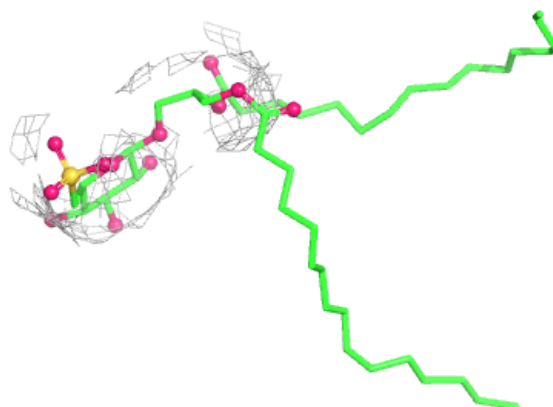
**Electron density around BCR C 514:**

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

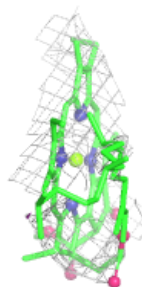
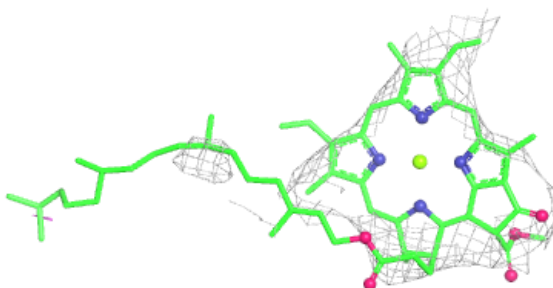


Electron density around SQD A 413:

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

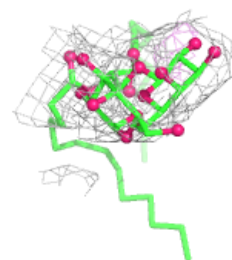
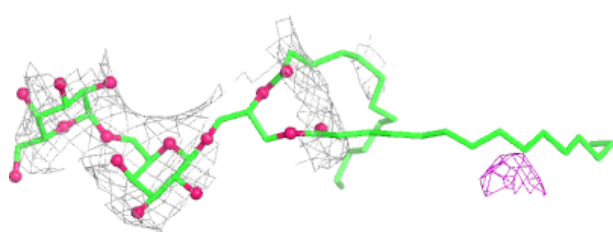
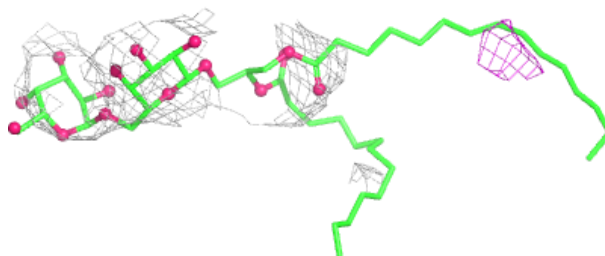
**Electron density around CLA b 606:**

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

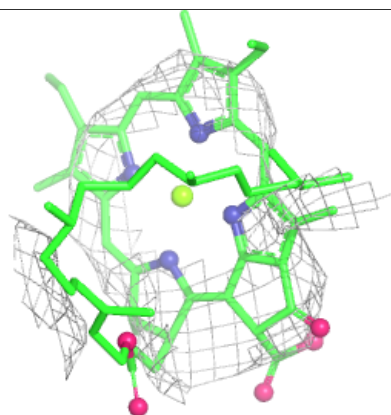
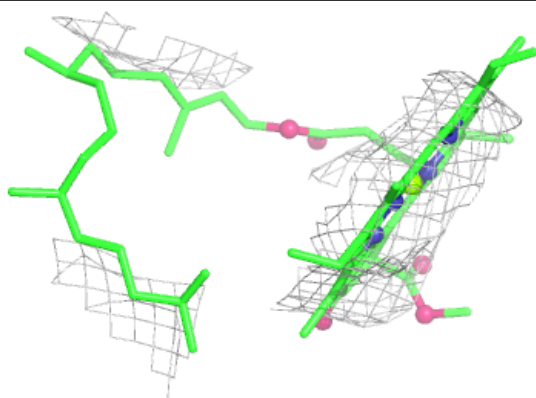
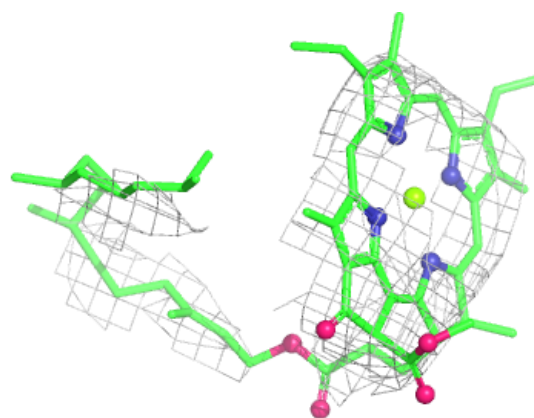


Electron density around DGD B 620:

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

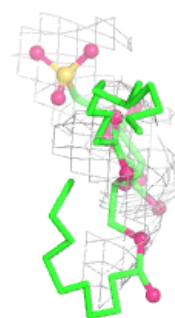
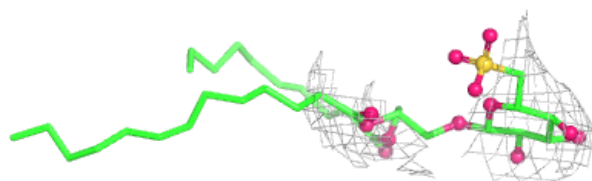
**Electron density around CLA c 503:**

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

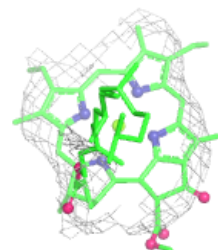


Electron density around SQD f 103:

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

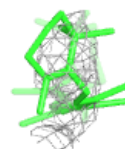
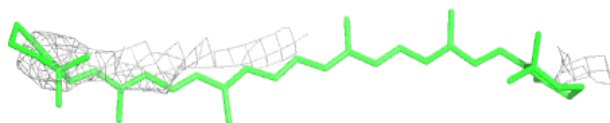
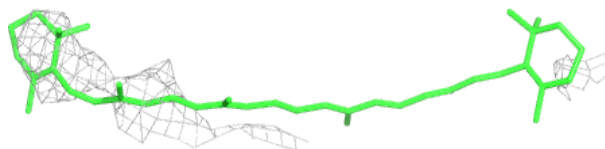
**Electron density around CLA b 607:**

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

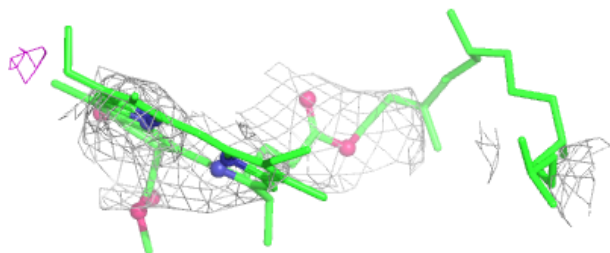
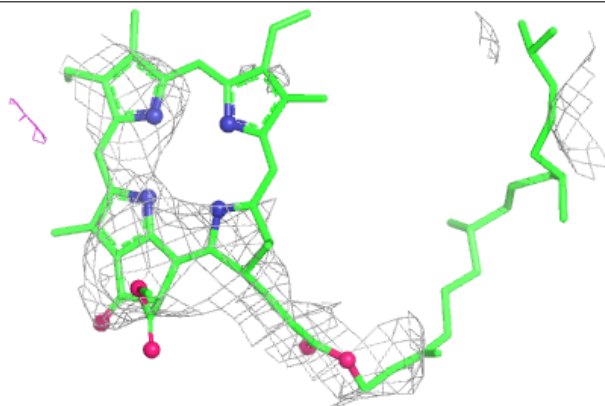


Electron density around BCR c 513:

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

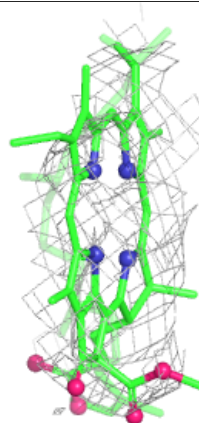
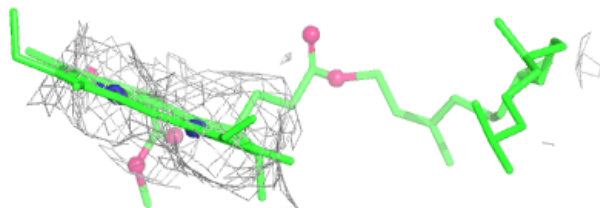
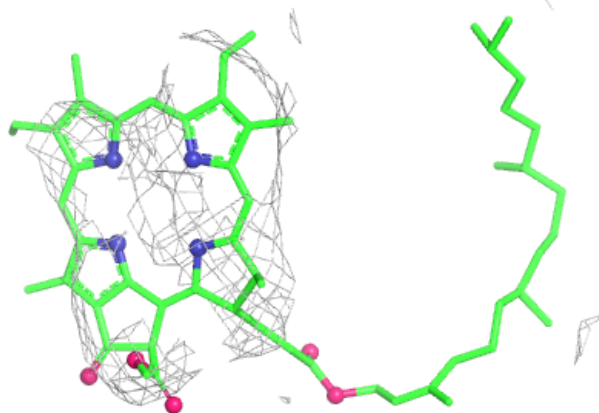
**Electron density around PHO D 402:**

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



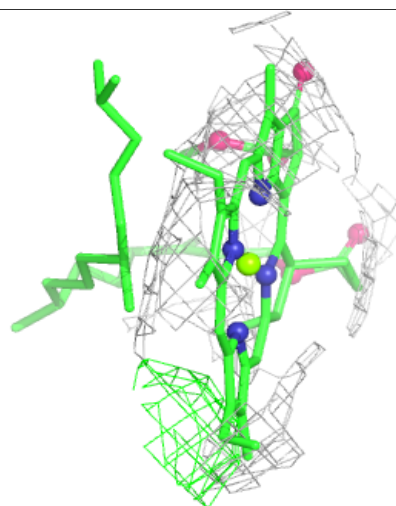
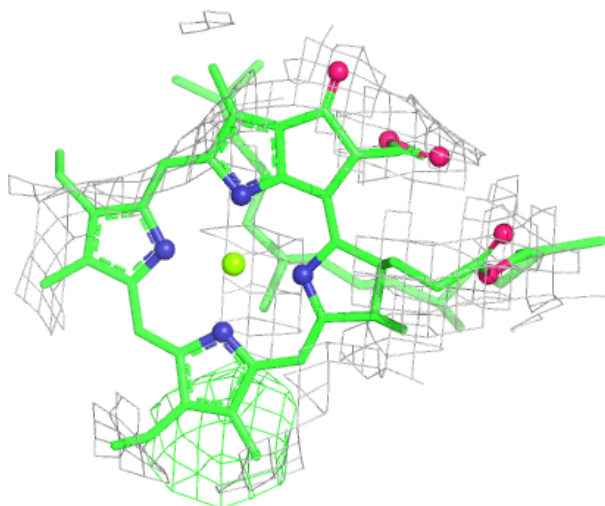
Electron density around PHO d 401:

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



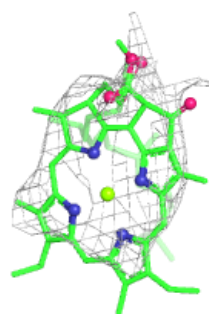
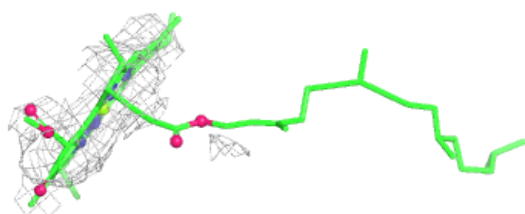
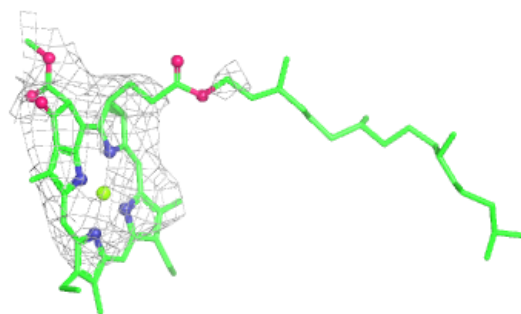
Electron density around CLA C 509:

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

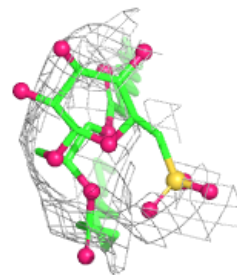
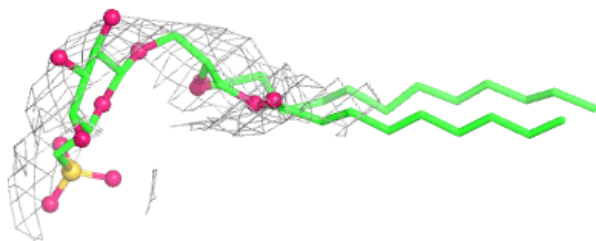


Electron density around CLA a 407:

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

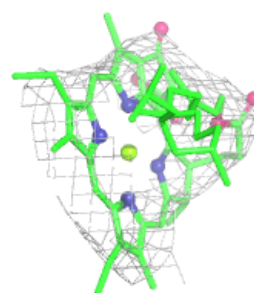
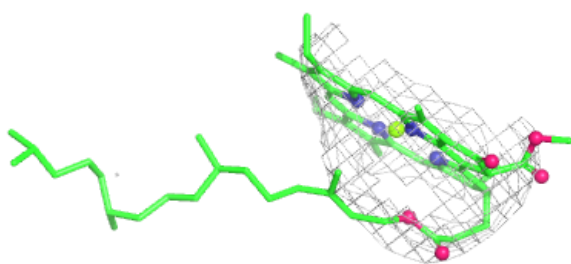
**Electron density around SQD B 622:**

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

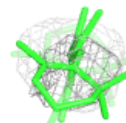
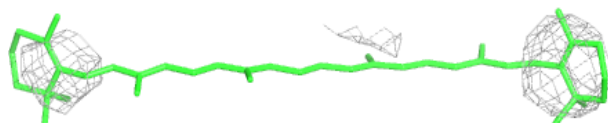
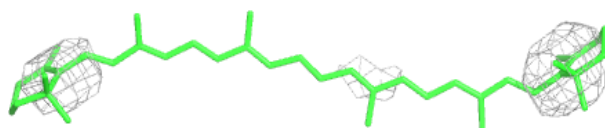


Electron density around CLA B 613:

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

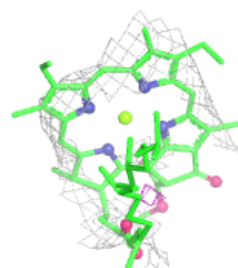
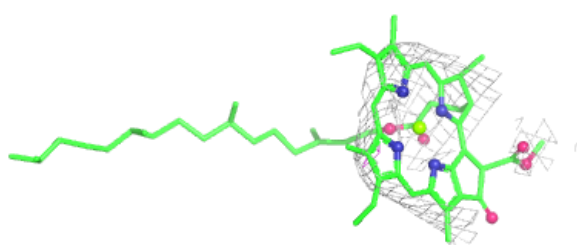
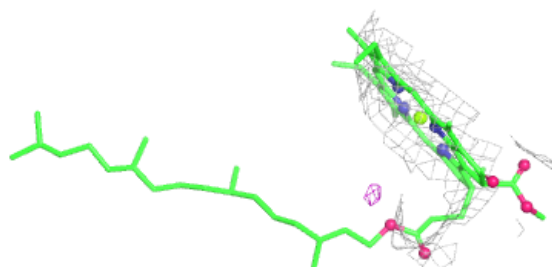
**Electron density around BCR A 407:**

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

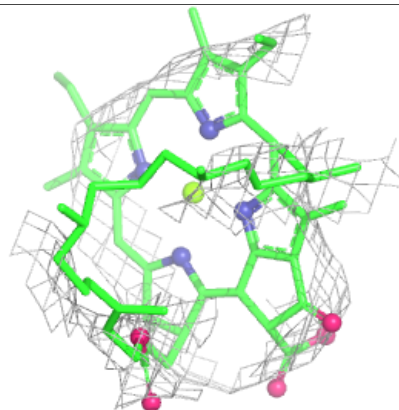
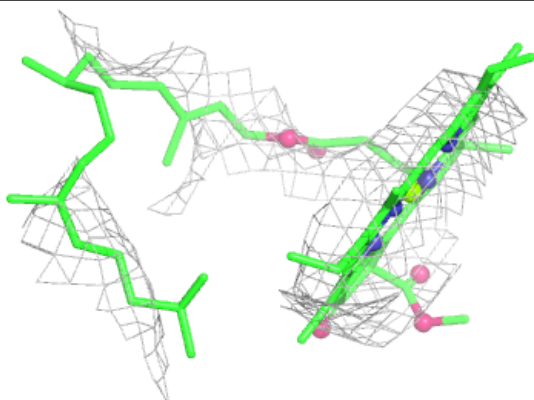
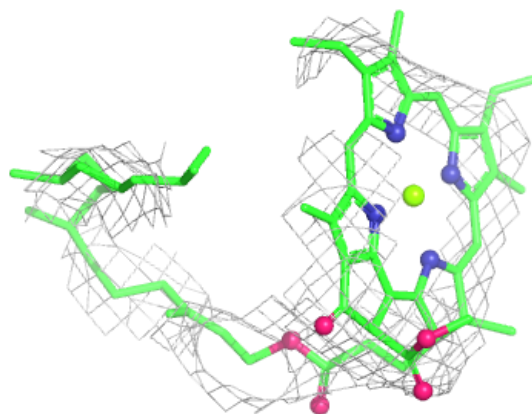


Electron density around CLA c 520:

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

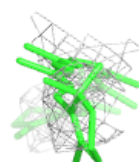
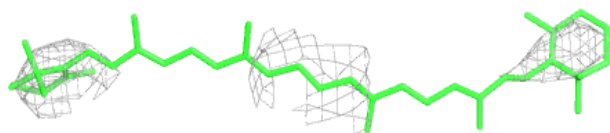
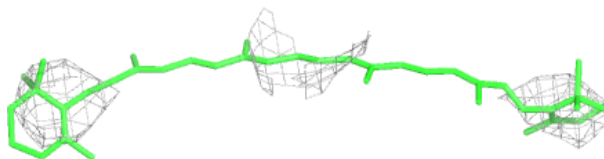
**Electron density around CLA C 503:**

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

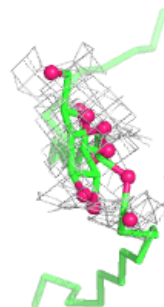
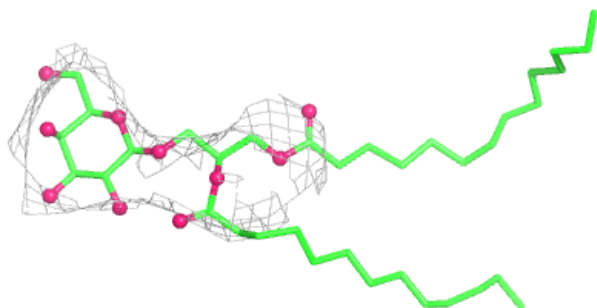


Electron density around BCR F 102:

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

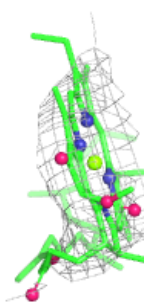
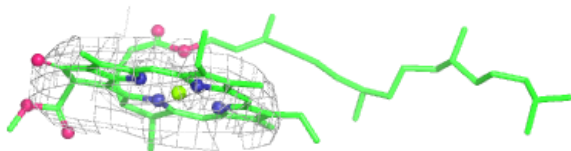
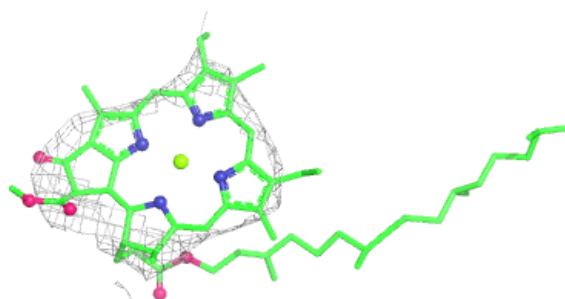
**Electron density around LMG D 412:**

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

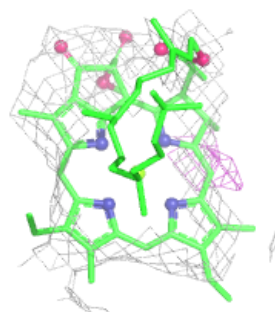
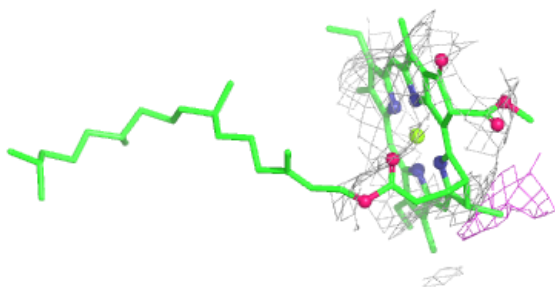
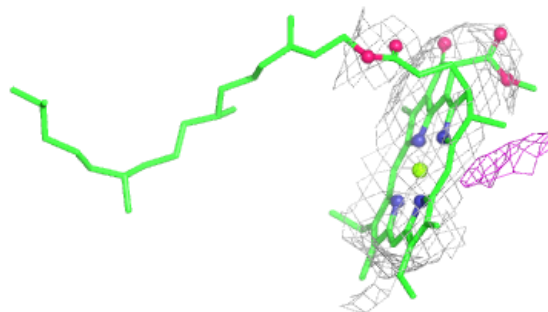


Electron density around CLA c 501:

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

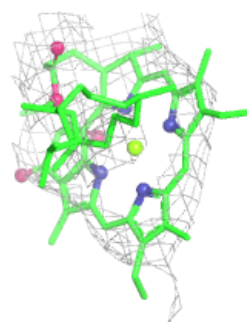
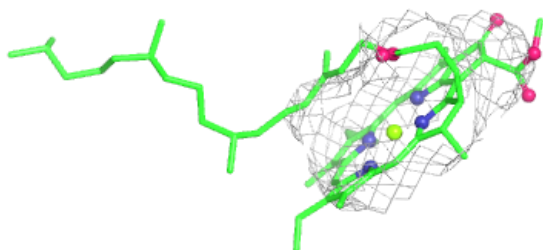
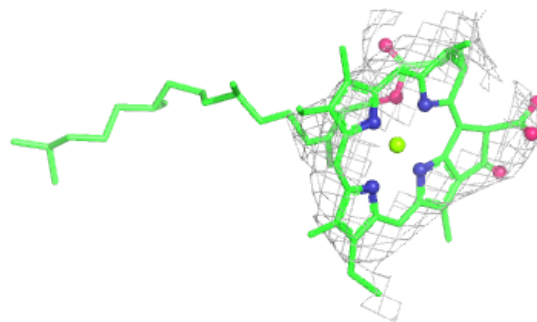
**Electron density around CLA C 507:**

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

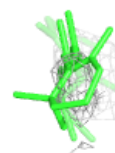
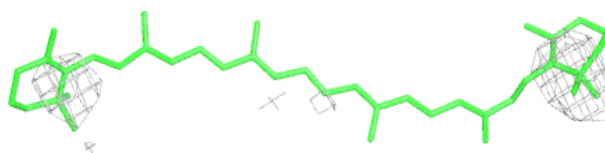


Electron density around CLA C 504:

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

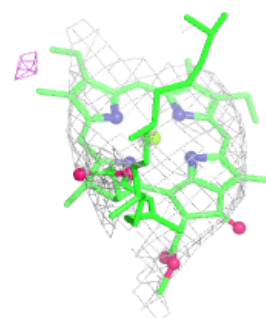
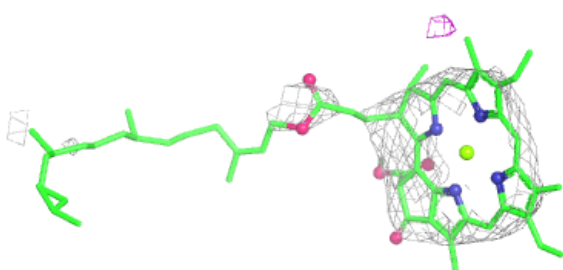
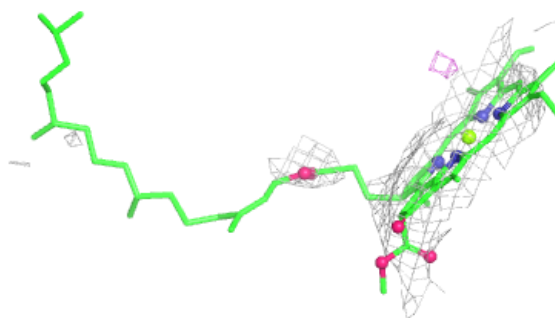
**Electron density around BCR y 101:**

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

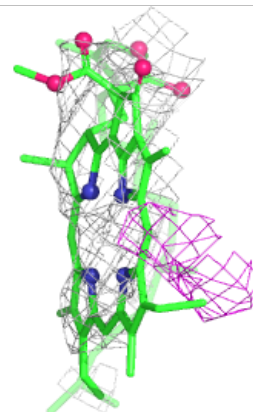
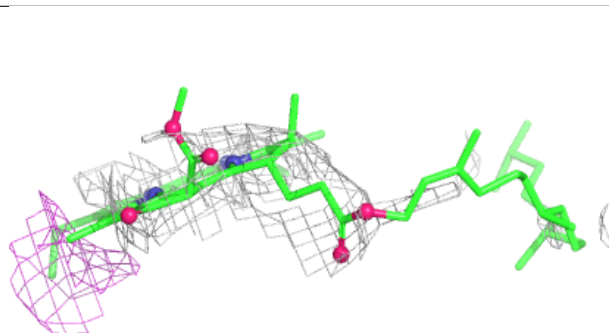
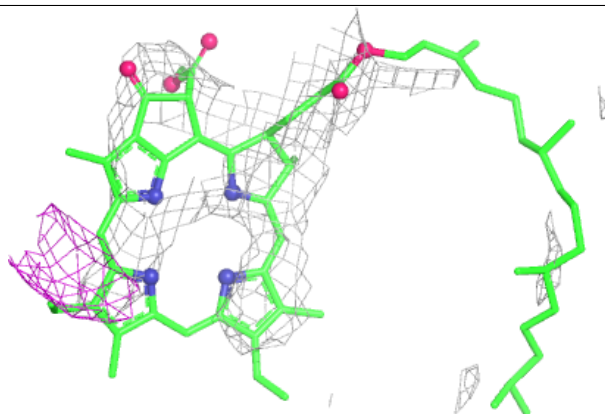


Electron density around CLA D 405:

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

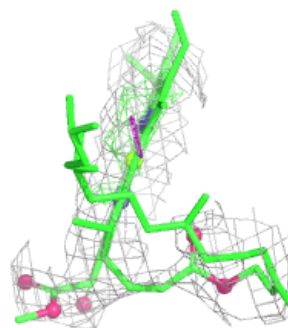
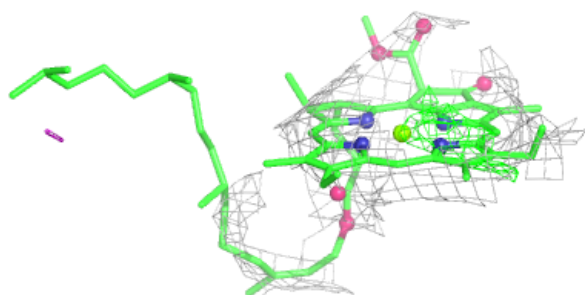
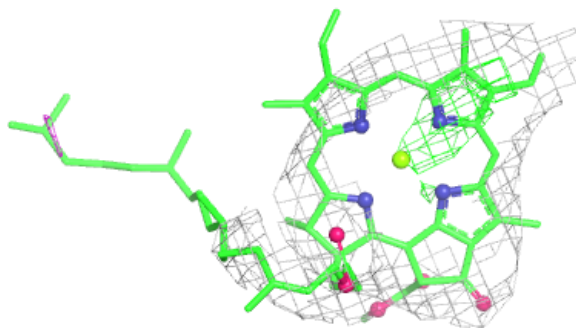
**Electron density around PHO D 401:**

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



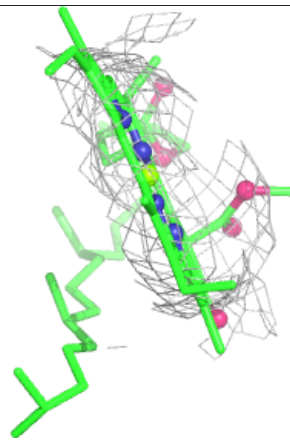
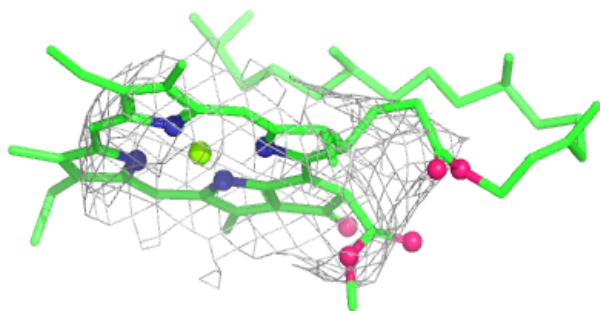
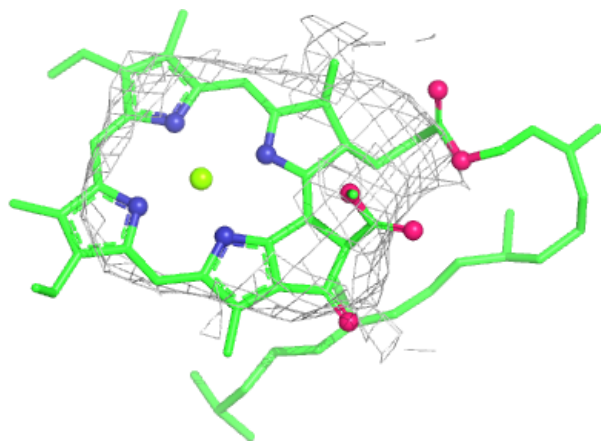
Electron density around CLA a 405:

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



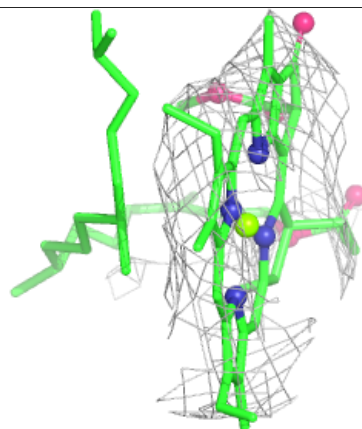
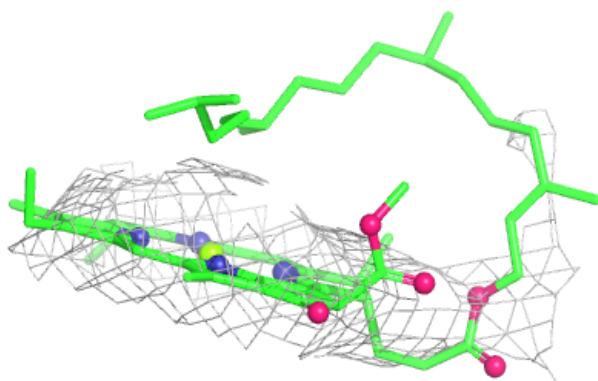
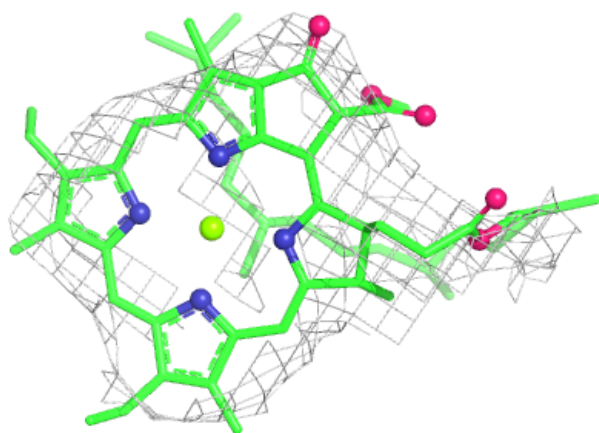
Electron density around CLA c 508:

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

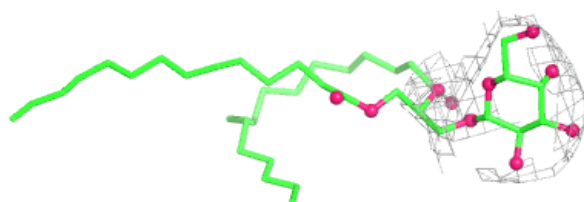
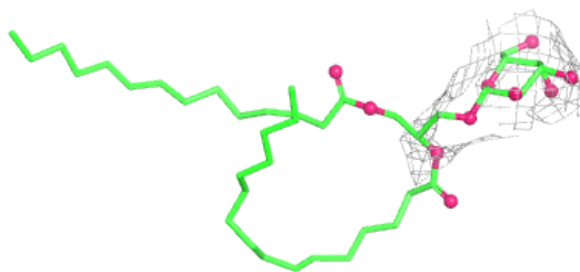


Electron density around CLA c 509:

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

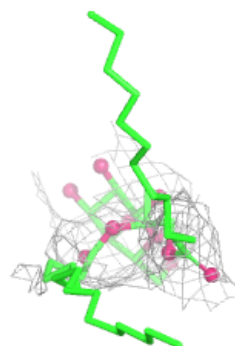
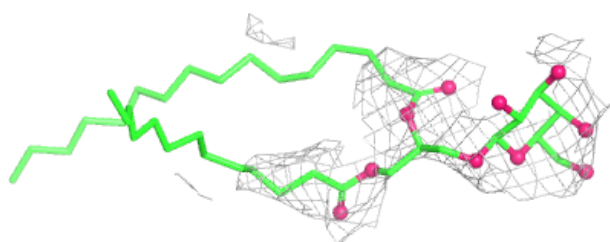
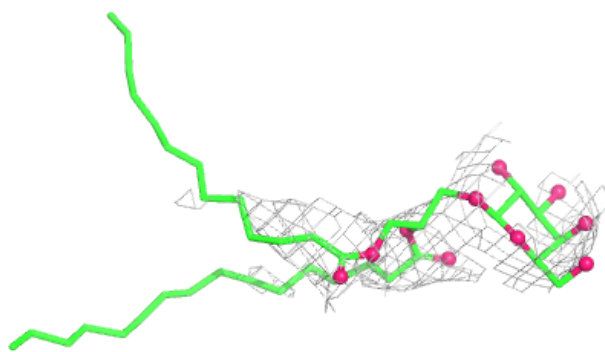
**Electron density around LMG d 408:**

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

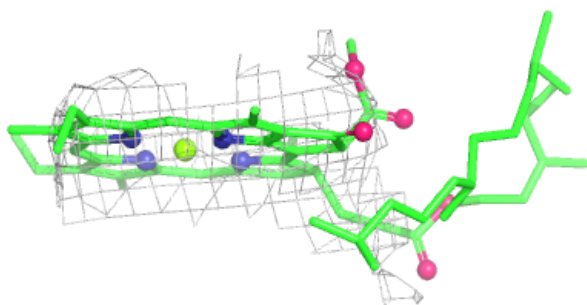
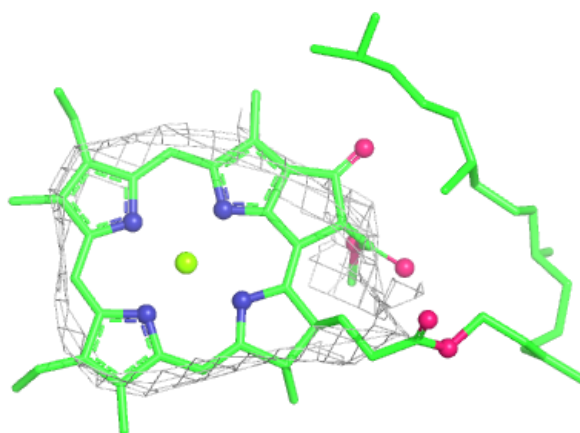


Electron density around LMG d 409:

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

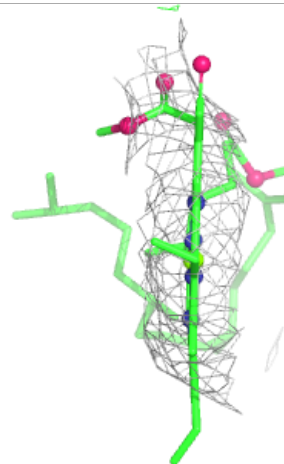
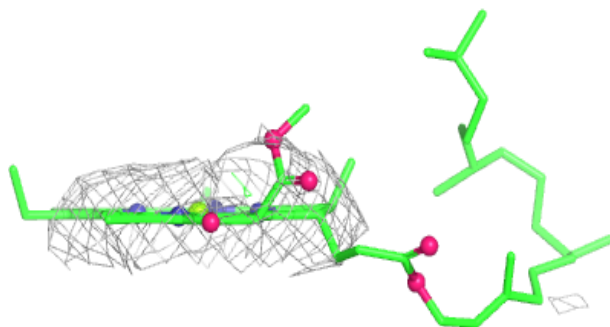
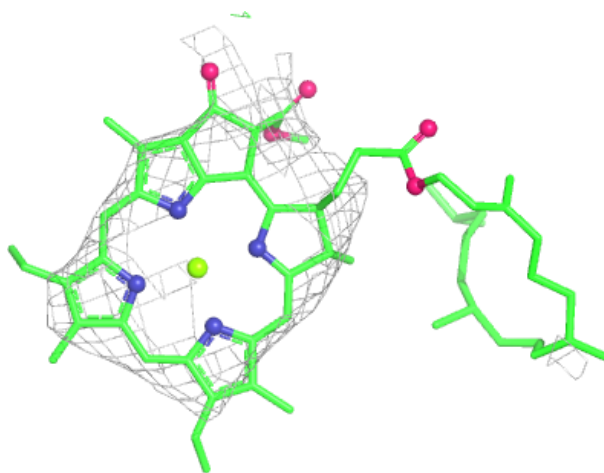
**Electron density around CLA b 613:**

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



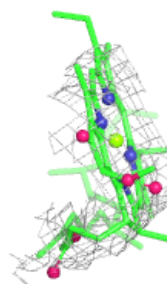
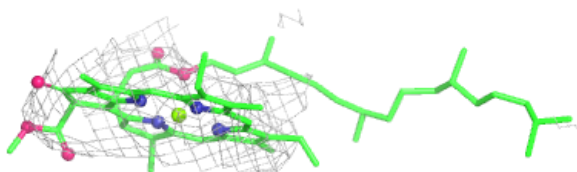
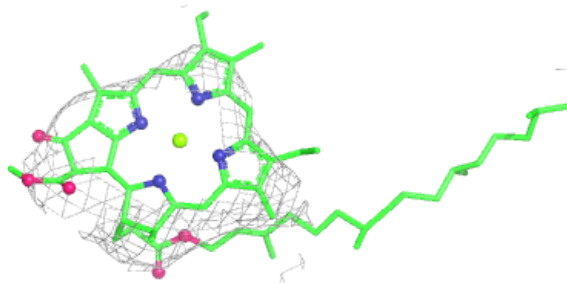
Electron density around CLA c 511:

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

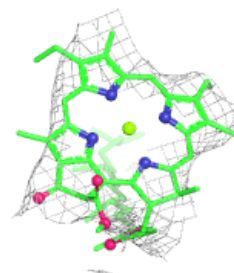
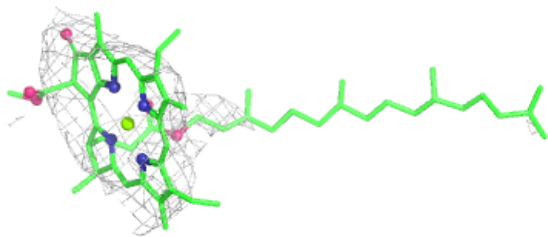
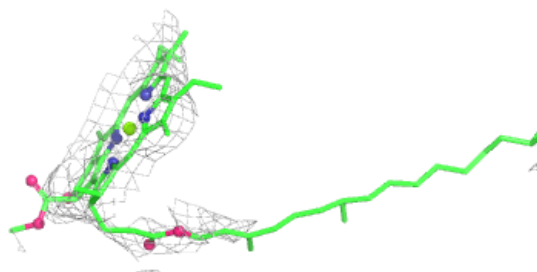


Electron density around CLA C 501:

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

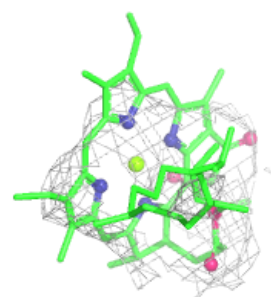
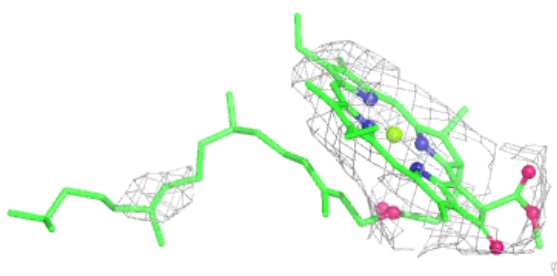
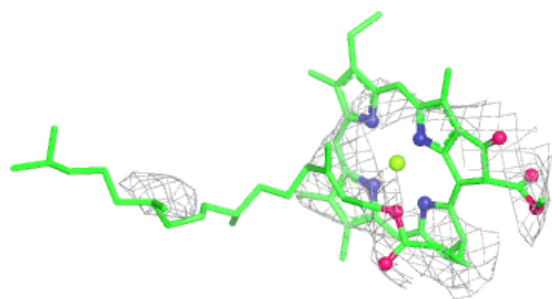
**Electron density around CLA B 606:**

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

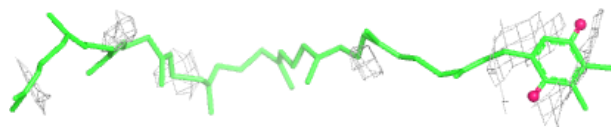
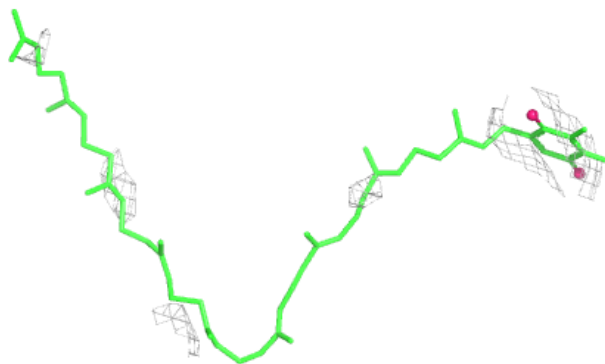


Electron density around CLA c 504:

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

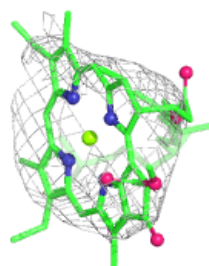
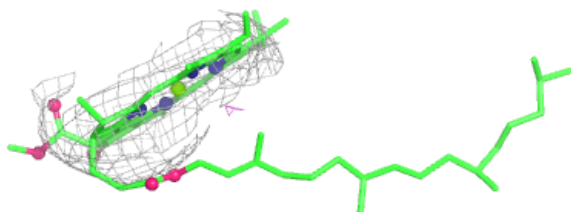
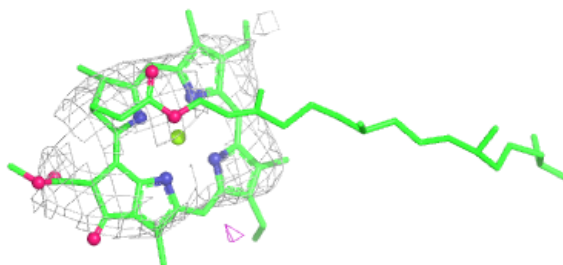
**Electron density around PL9 D 407:**

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

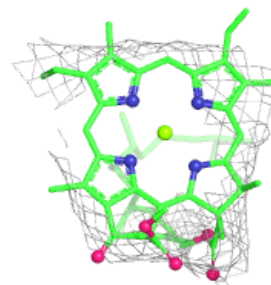
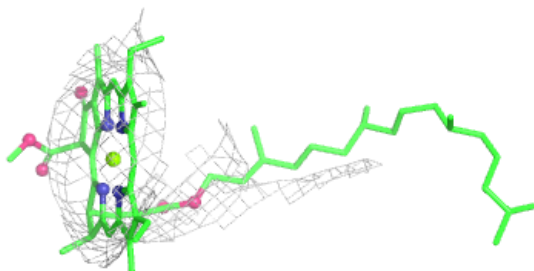
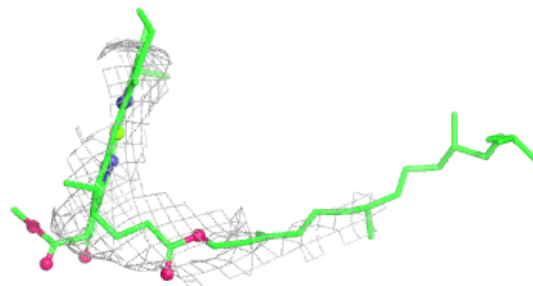


Electron density around CLA B 607:

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

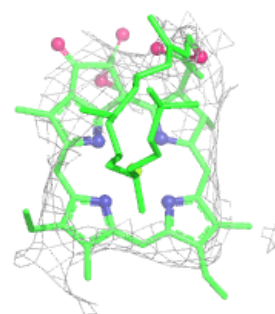
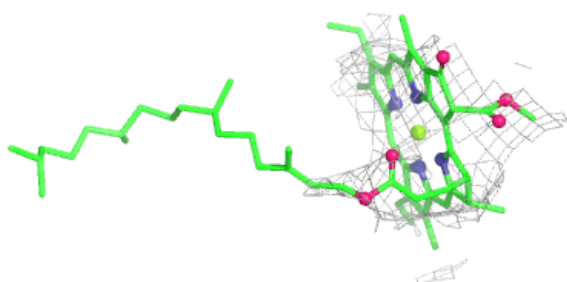
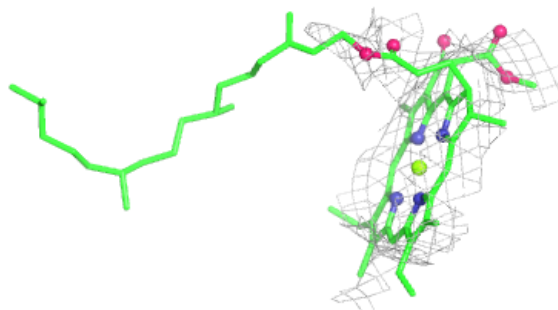
**Electron density around CLA b 608:**

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

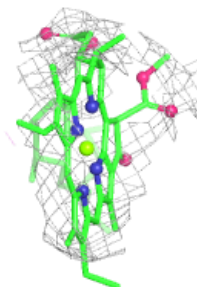
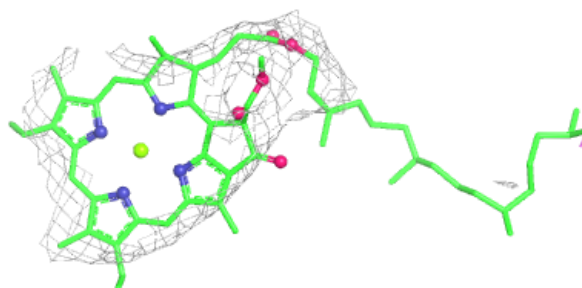


Electron density around CLA c 507:

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

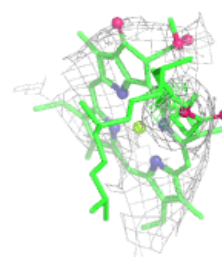
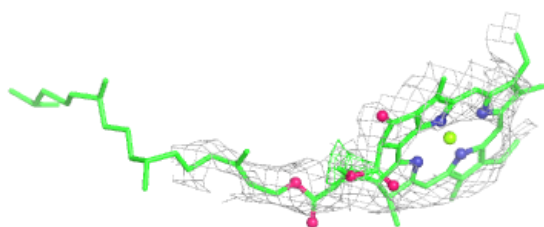
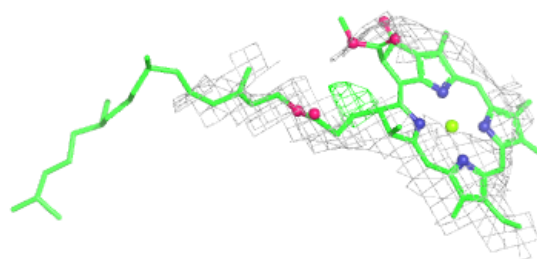
**Electron density around CLA H 101:**

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

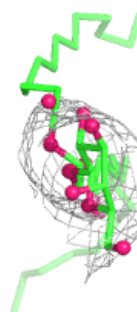
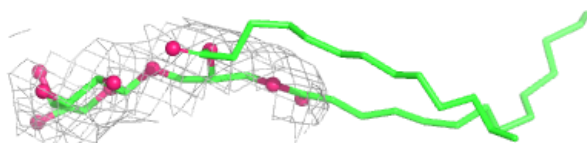
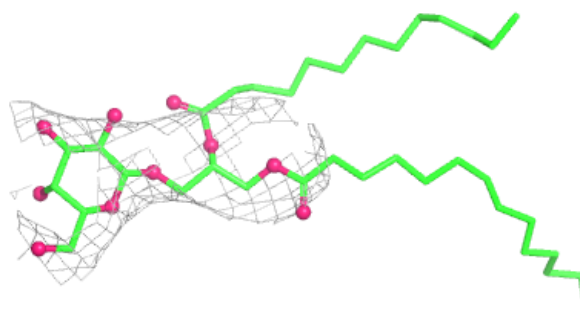


Electron density around CLA a 404:

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

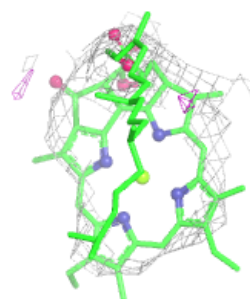
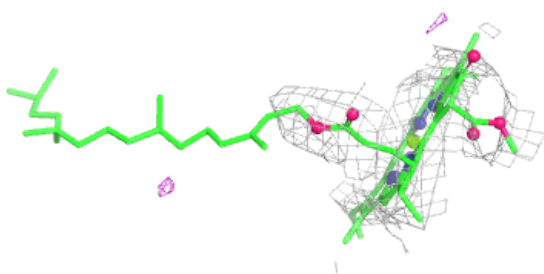
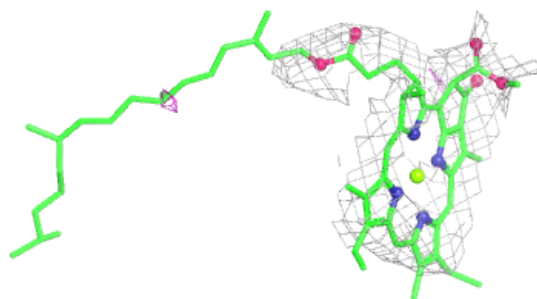
**Electron density around LMG d 412:**

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

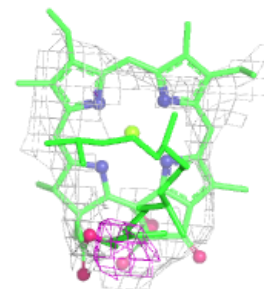
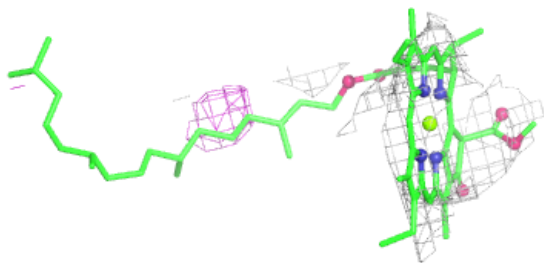
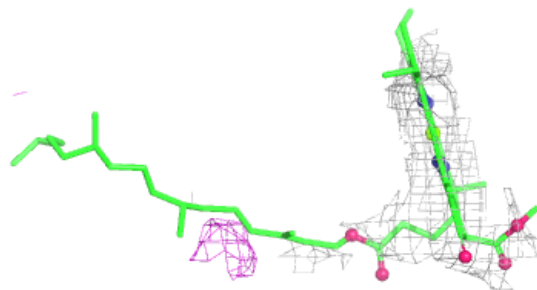


Electron density around CLA B 608:

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

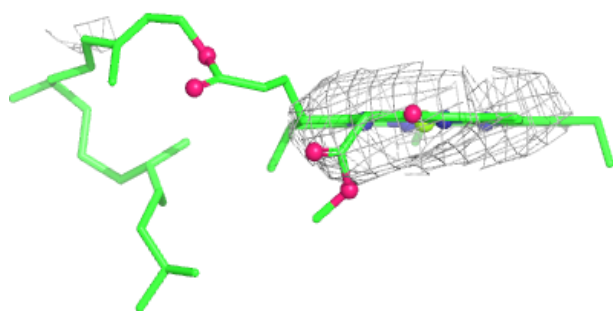
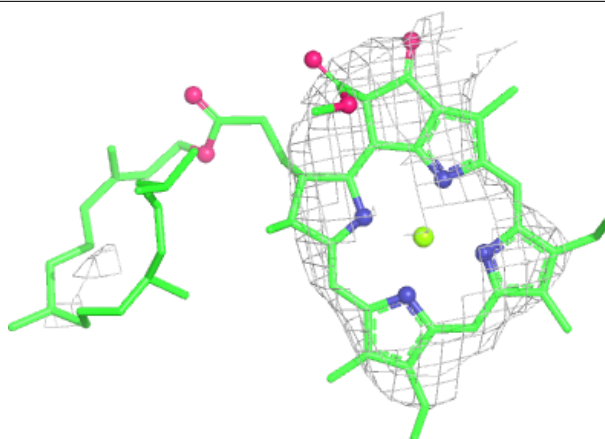
**Electron density around CLA B 604:**

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

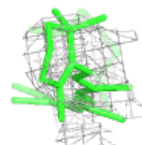
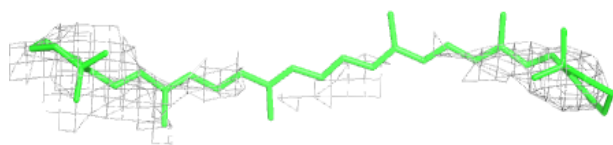
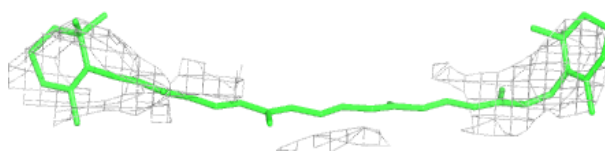


Electron density around CLA C 511:

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

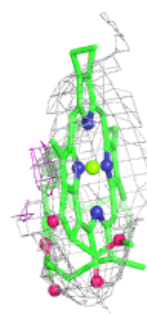
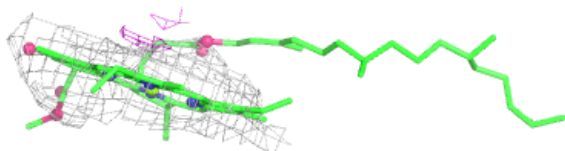
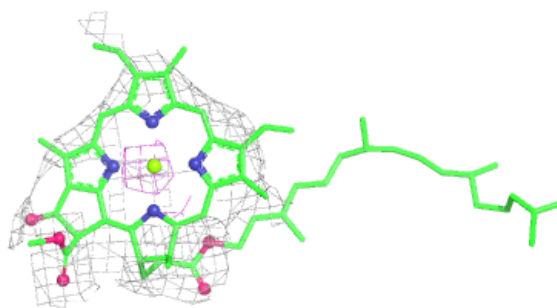
**Electron density around BCR C 513:**

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

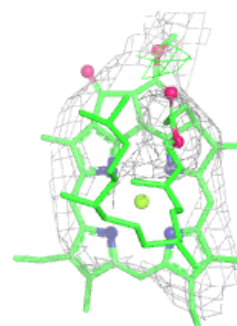
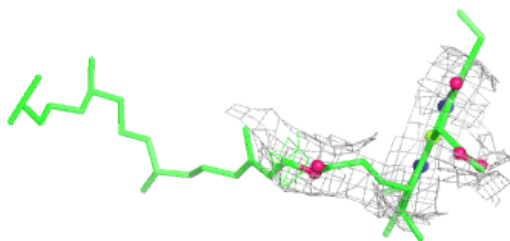
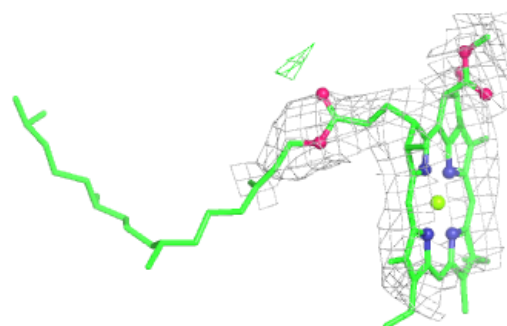


Electron density around CLA B 602:

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

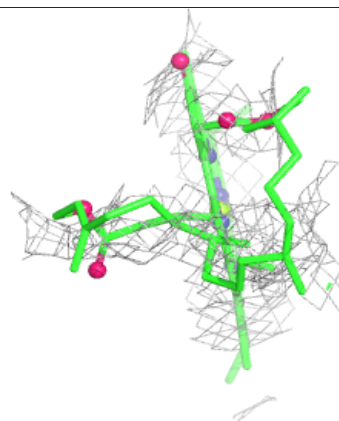
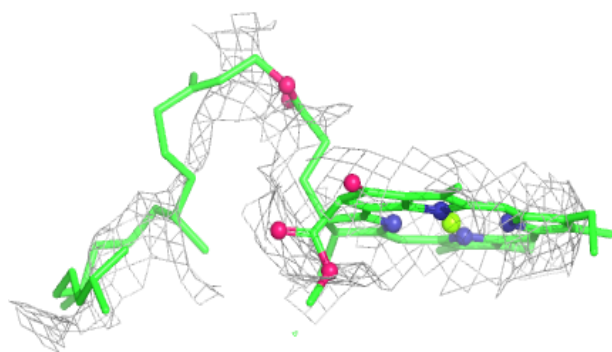
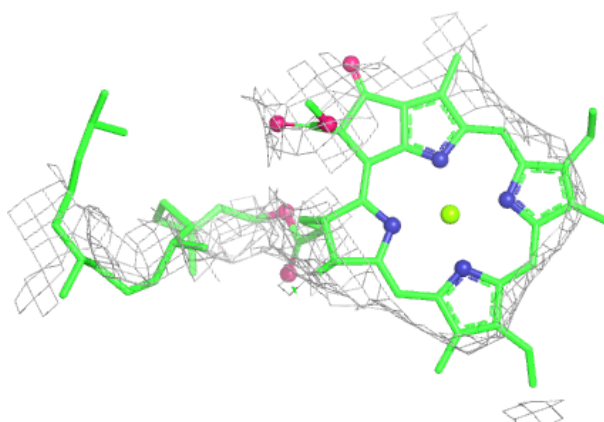
**Electron density around CLA d 406:**

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

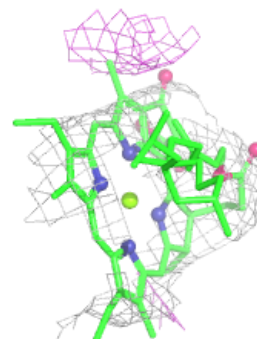
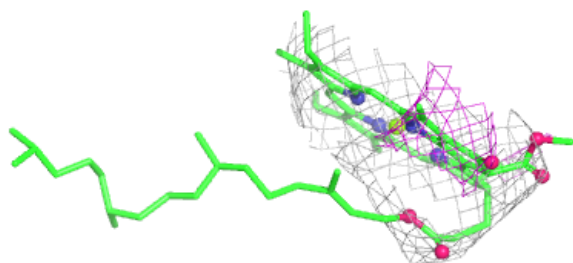
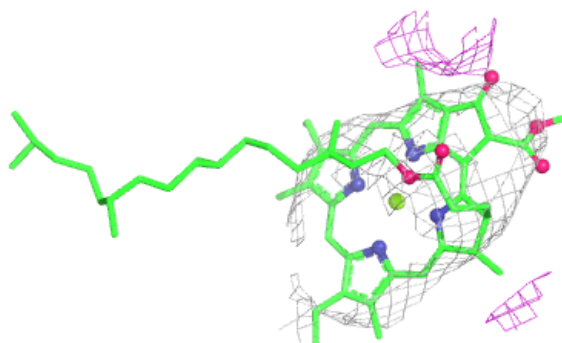


Electron density around CLA b 615:

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

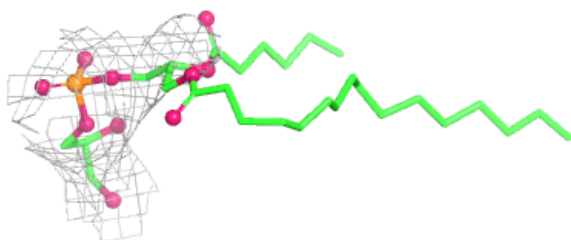
**Electron density around CLA b 617:**

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



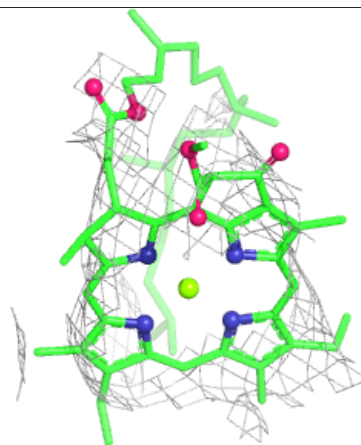
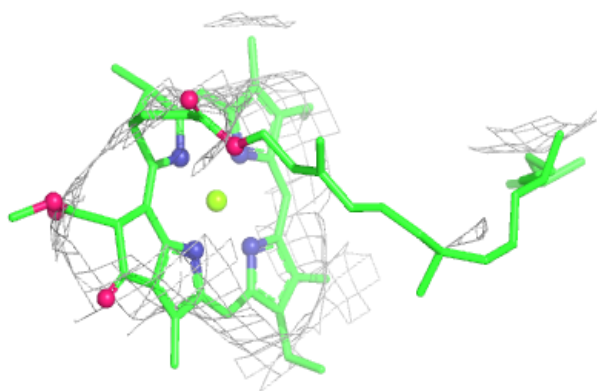
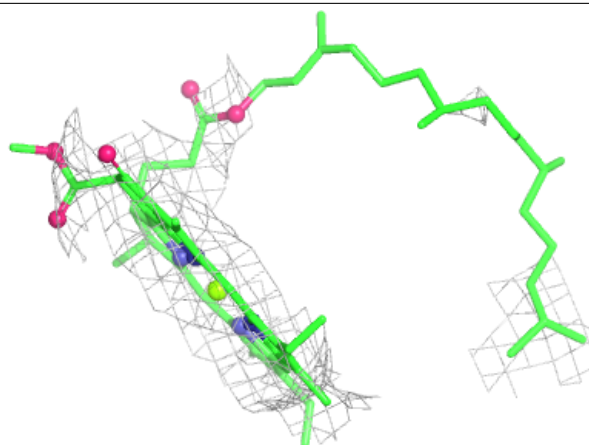
Electron density around LHG a 411:

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



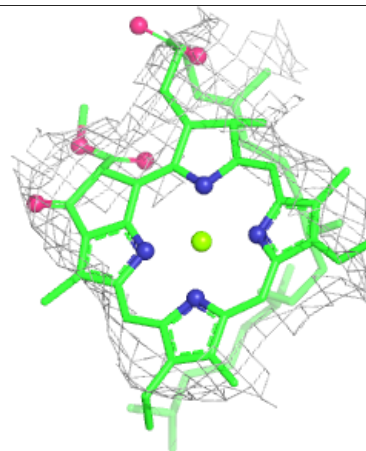
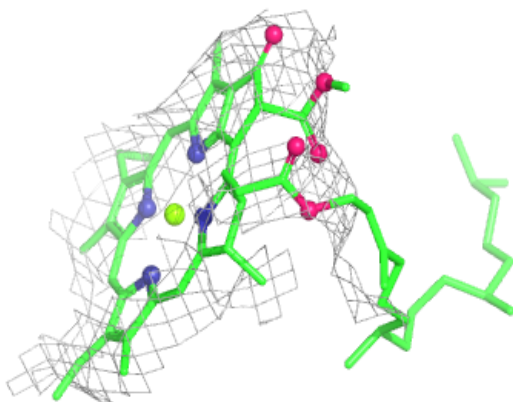
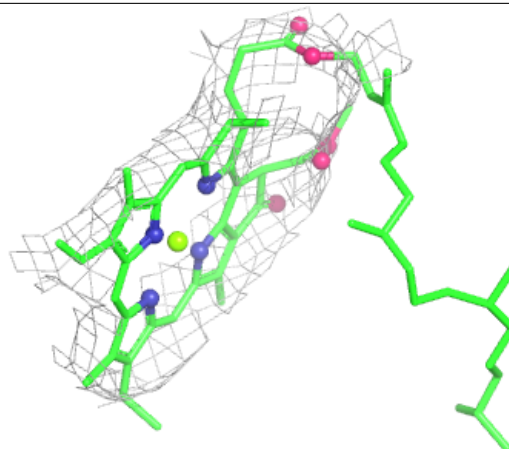
Electron density around CLA B 610:

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



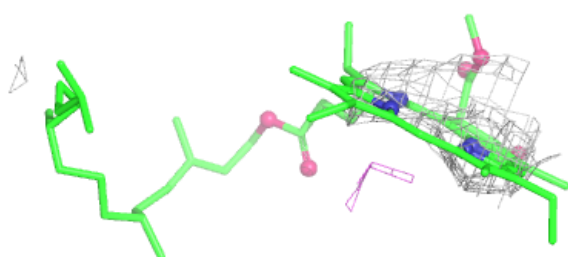
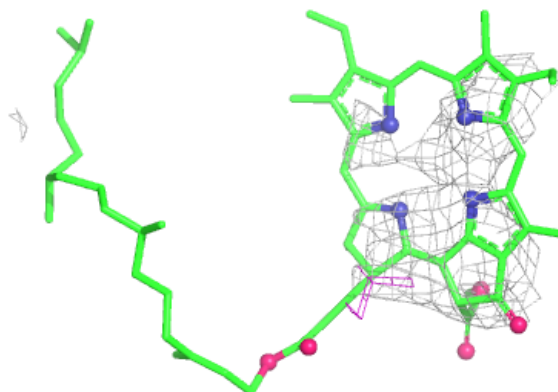
Electron density around CLA B 612:

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

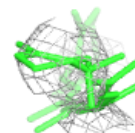
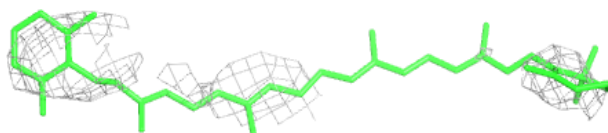
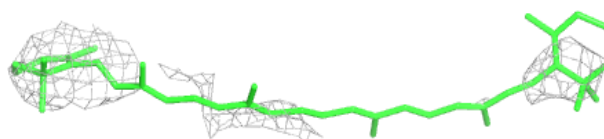


Electron density around PHO d 402:

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

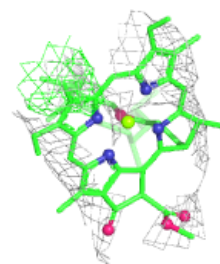
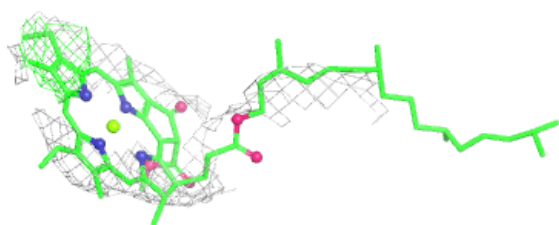
**Electron density around BCR f 102:**

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

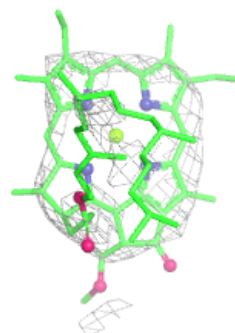
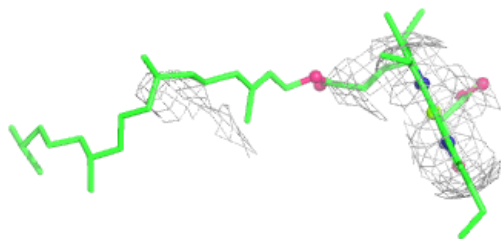
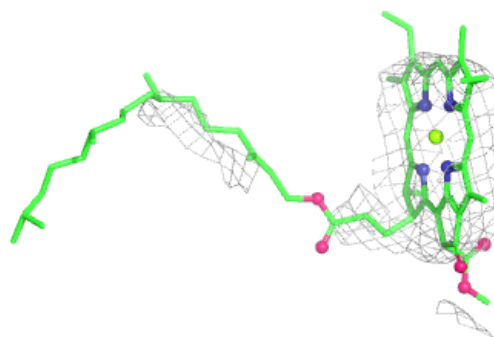


Electron density around CLA C 502:

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

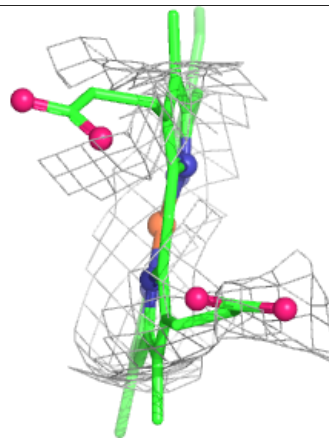
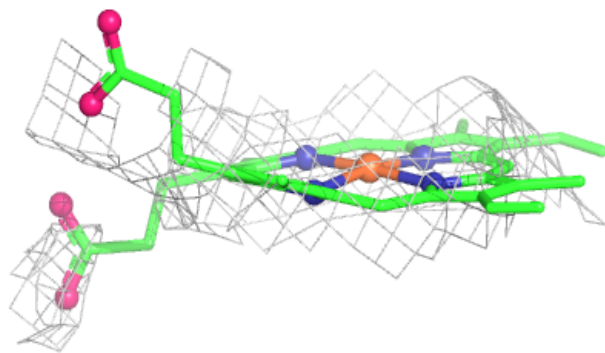
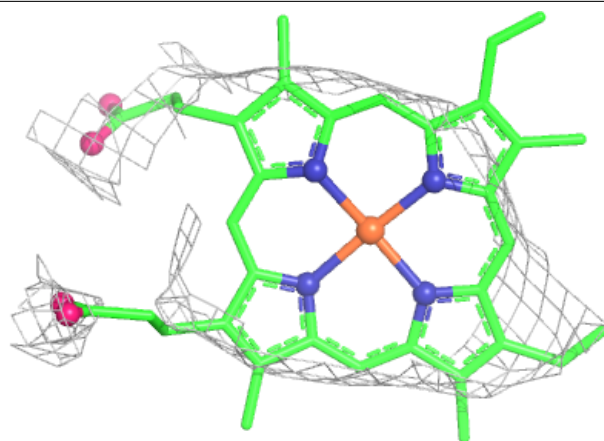
**Electron density around CLA D 406:**

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



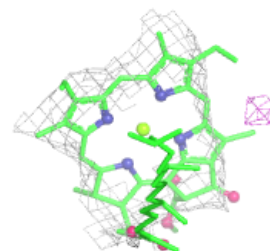
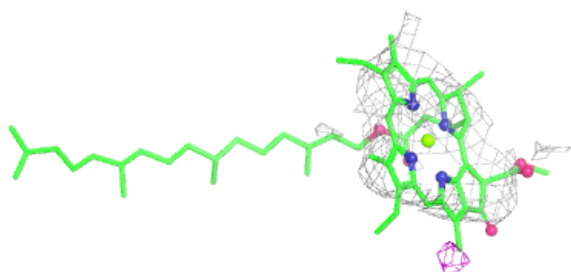
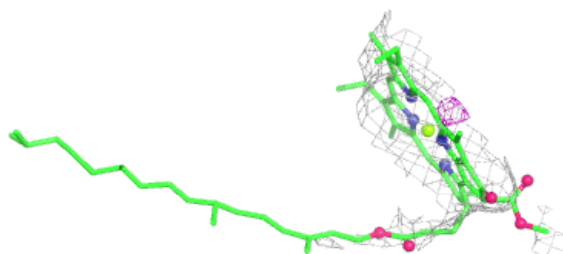
Electron density around HEM f 101:

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

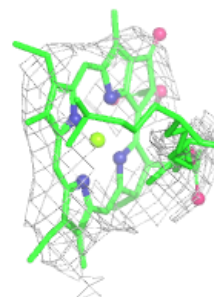
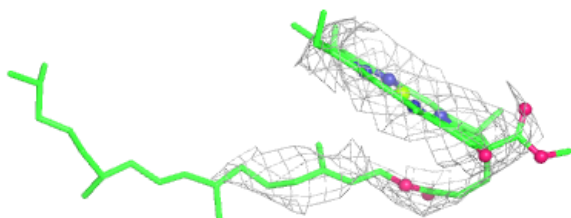
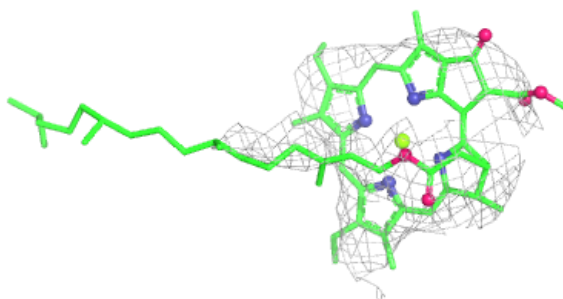


Electron density around CLA b 610:

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

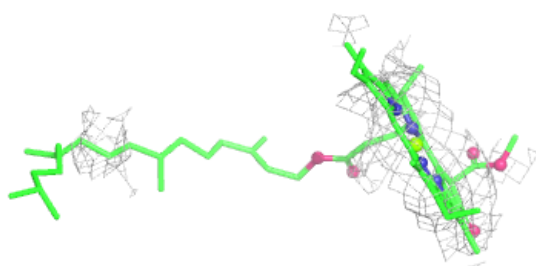
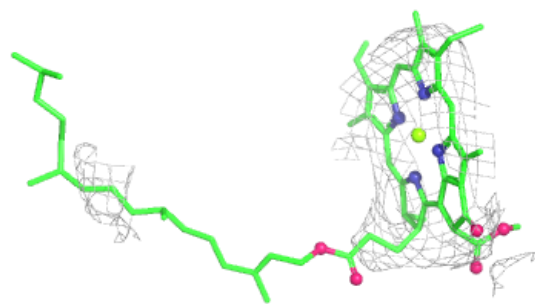
**Electron density around CLA b 611:**

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



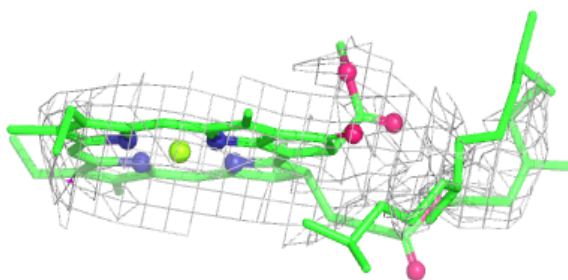
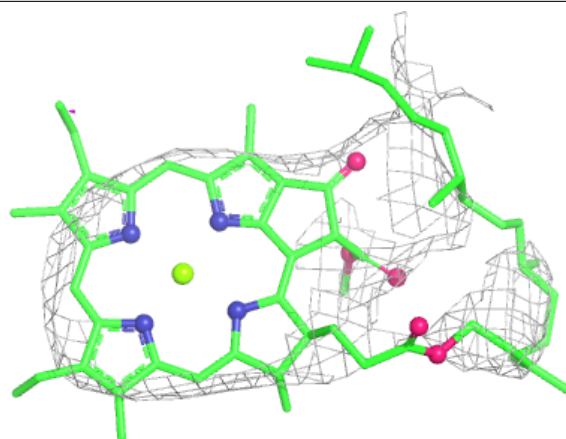
Electron density around CLA b 612:

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



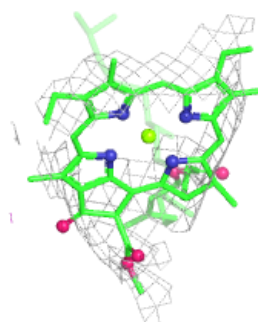
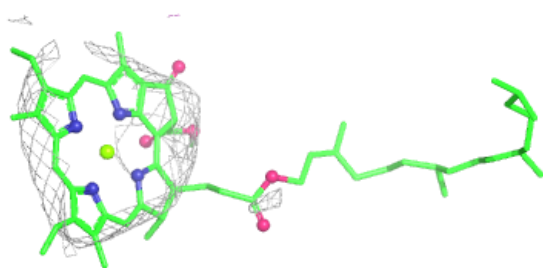
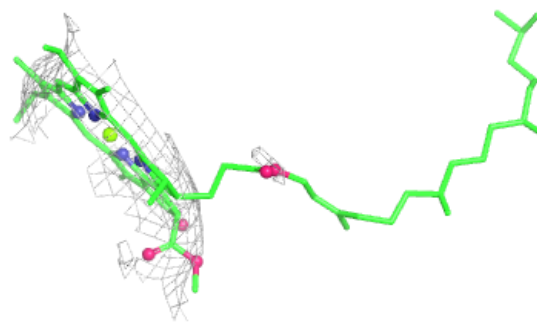
Electron density around CLA B 609:

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



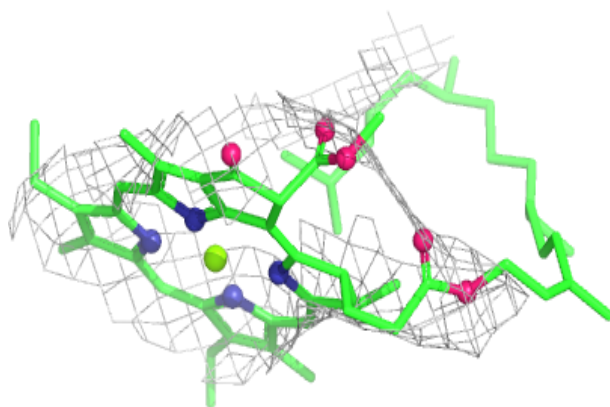
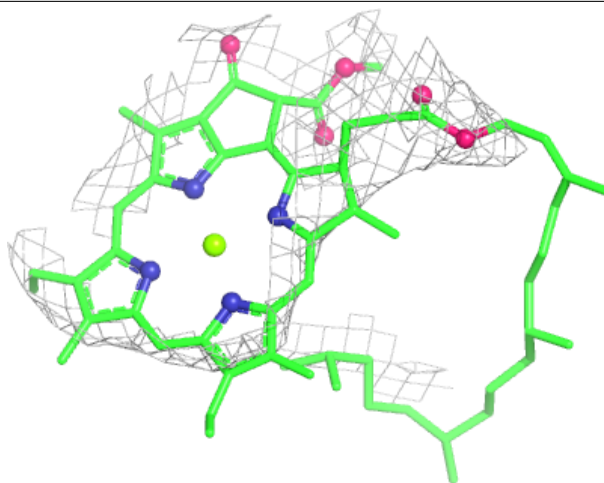
Electron density around CLA d 405:

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



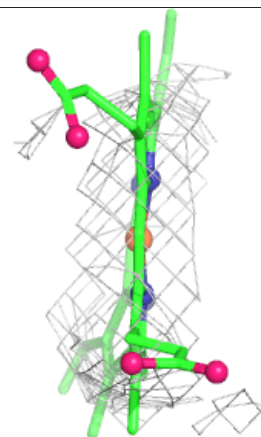
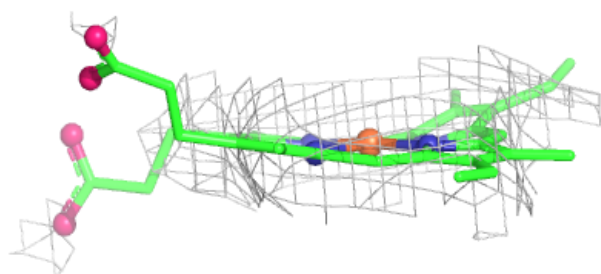
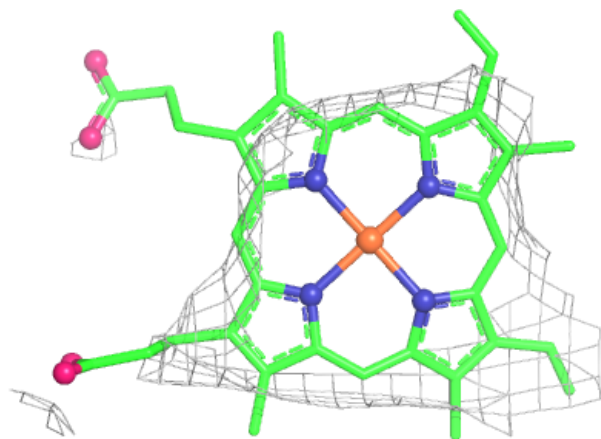
Electron density around CLA B 614:

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



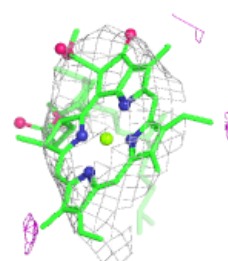
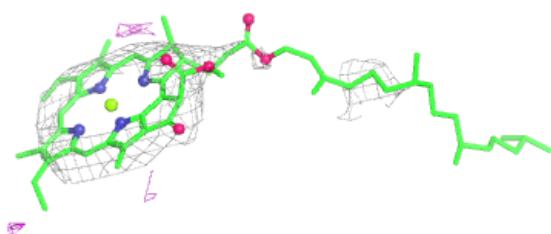
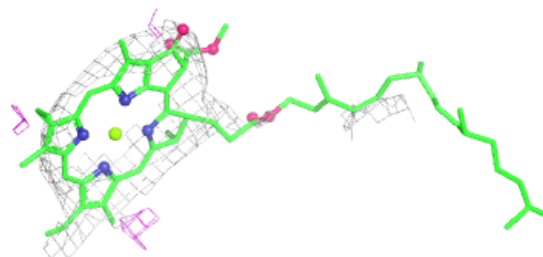
Electron density around HEM v 201:

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

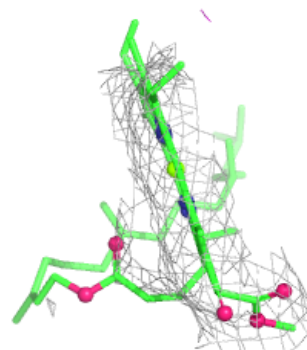
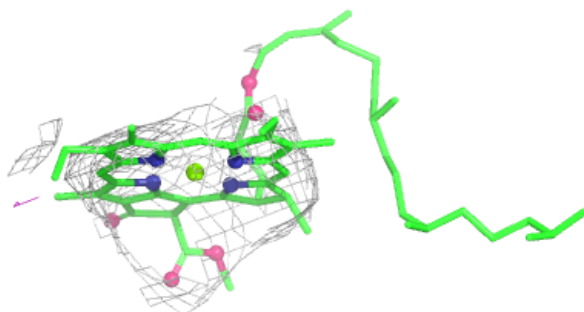
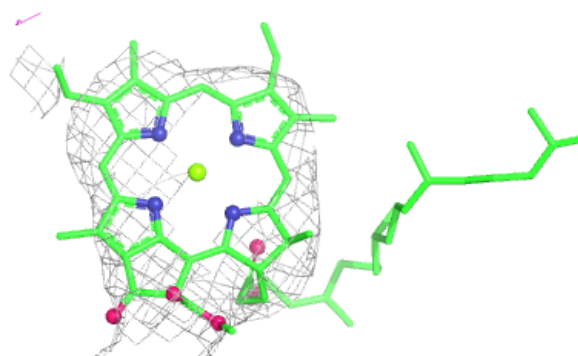


Electron density around CLA A 402:

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

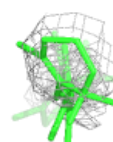
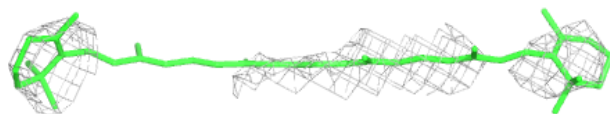
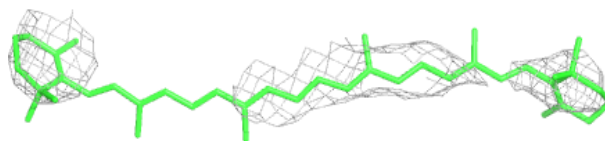
**Electron density around CLA A 403:**

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

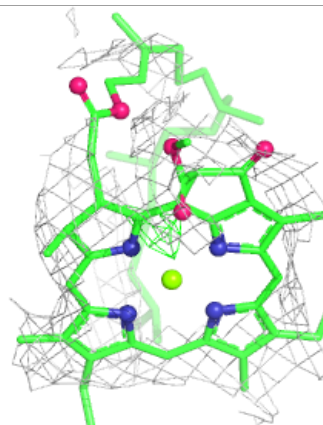
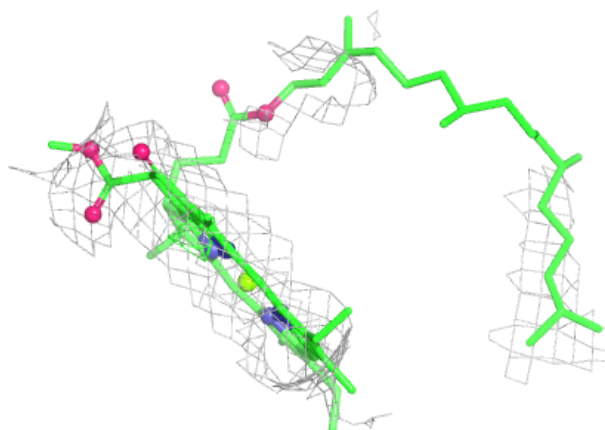


Electron density around BCR B 618:

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

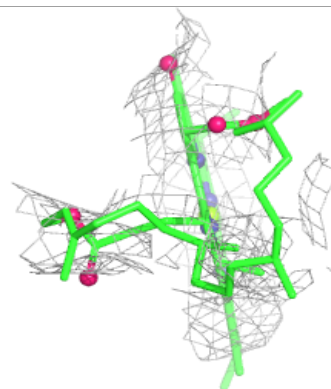
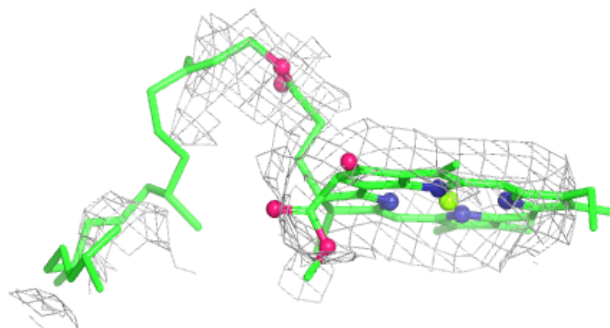
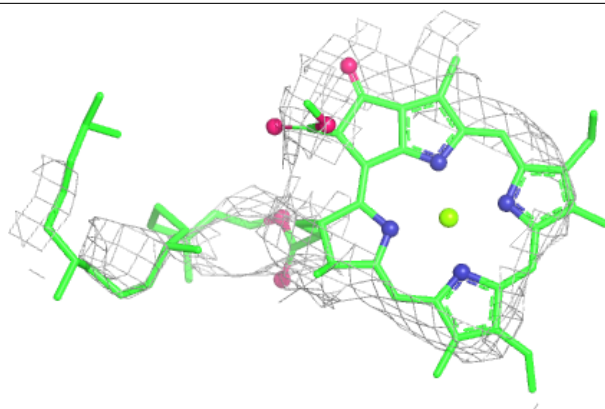
**Electron density around CLA b 614:**

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



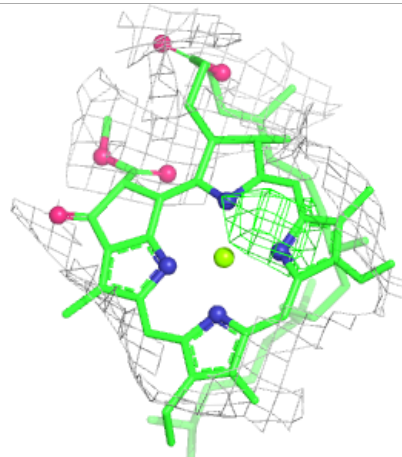
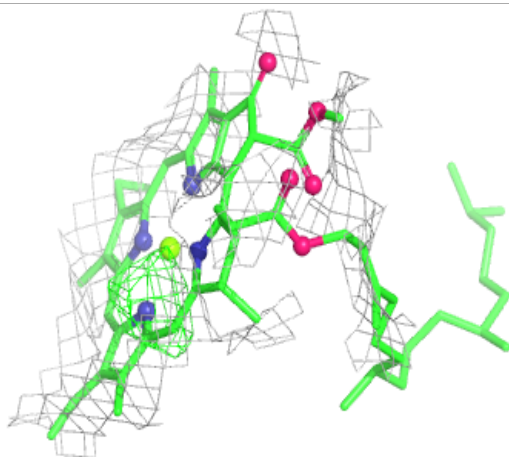
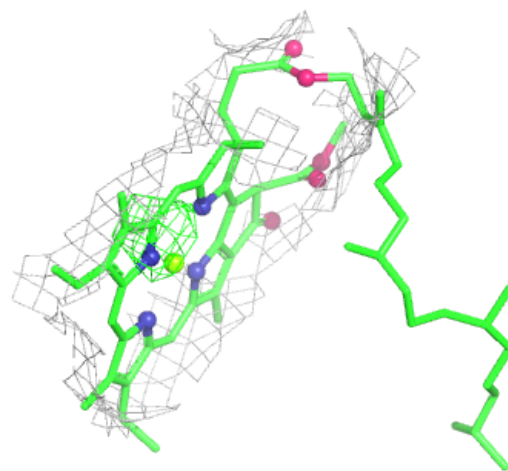
Electron density around CLA B 611:

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



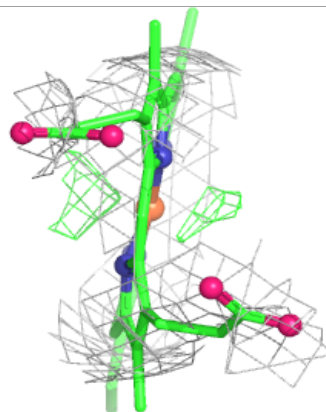
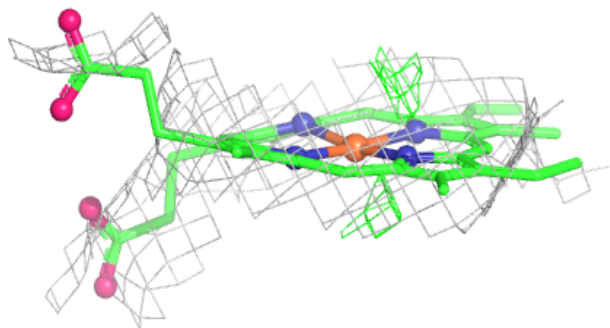
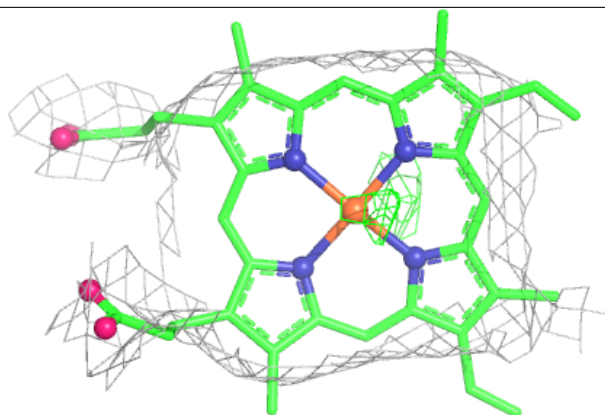
Electron density around CLA b 616:

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

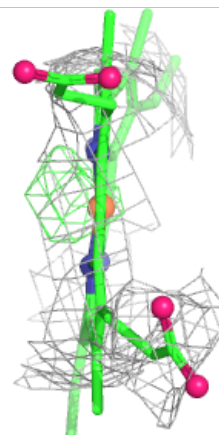
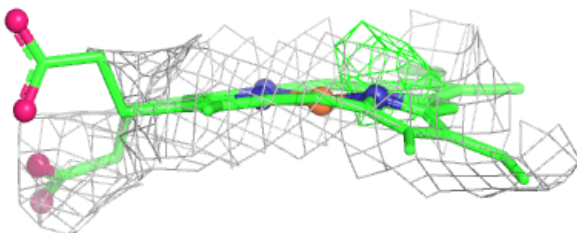
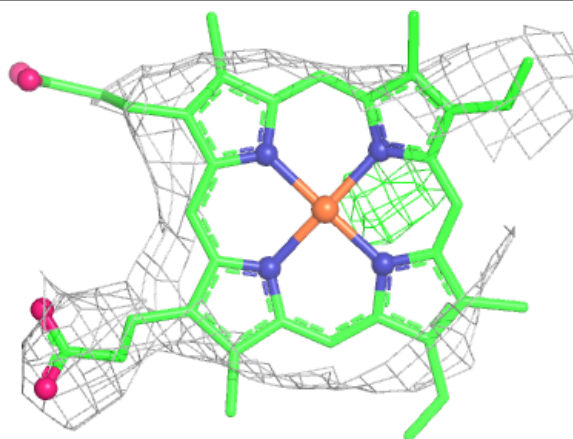


Electron density around HEM F 101:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.