



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 07:43 AM EDT

PDB ID : 5KAI / pdb_00005kai
Title : NH3-bound RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 2.8 Å resolution
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2016-06-01
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

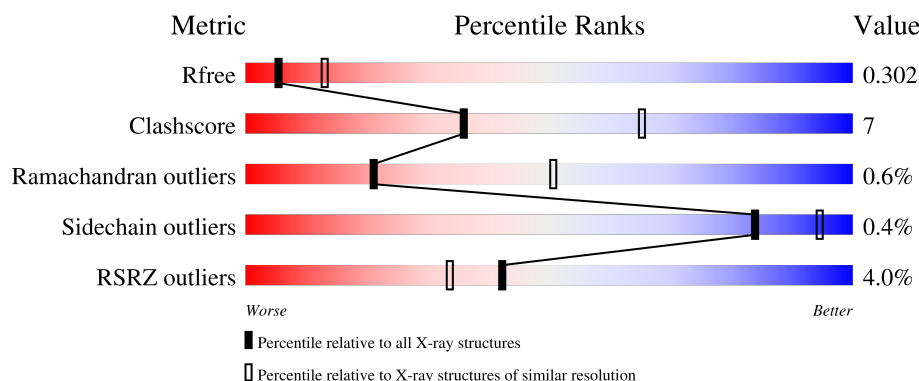
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

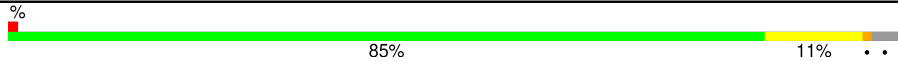
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	63	
7	h	63	
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	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	BCT	A	615	-	X	-	-
31	BCT	a	706	-	X	-	-
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 50284 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 II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			
1	a	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	1	0
			3968	2605	661	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			
4	d	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			661	432	107	122			
5	e	82	Total	C	N	O	0	0	0
			665	434	108	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	expression tag	UNP Q8DJZ6
i	1	FME	-	expression tag	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	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			
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	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			
12	m	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	expression tag	UNP Q8DHA7
m	1	FME	-	expression tag	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	expression tag	UNP Q8DIQ0
t	1	FME	-	expression tag	UNP Q8DIQ0

- 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
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			200	131	35	31	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			281	188	45	48				
18	x	38	Total	C	N	O		0	0	0
			279	187	45	47				

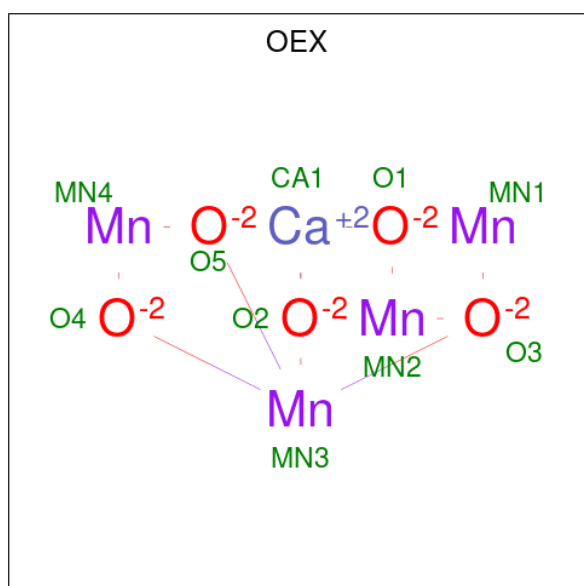
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			478	328	72	76	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			273	186	47	40				
20	r	34	Total	C	N	O		0	0	0
			270	183	47	40				

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



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

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

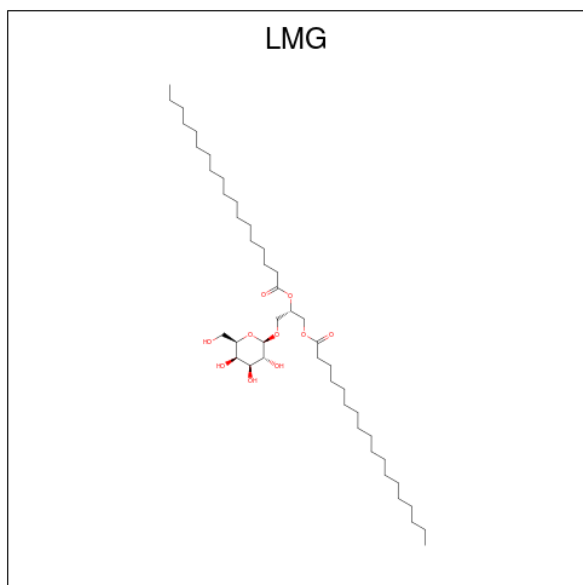
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	D	1	Total	C	O	0	0
			51	41	10		
23	M	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C	O	0	0
			51	41	10		

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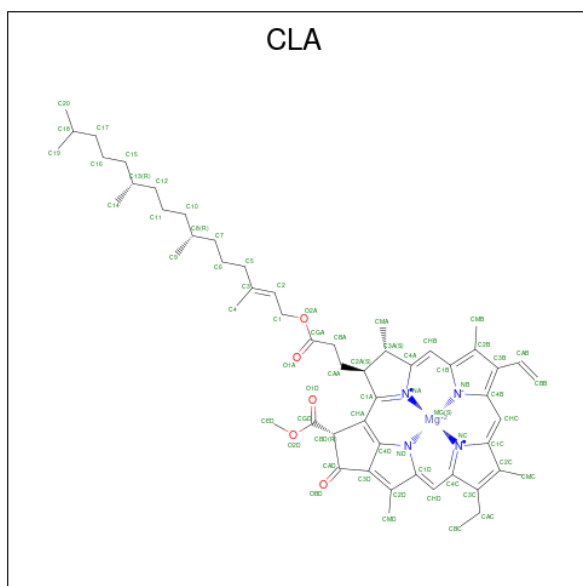
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	b	1	Total C O 51 41 10	0	0
23	b	1	Total C 9 9	0	0
23	c	1	Total C O 51 41 10	0	0
23	c	1	Total C O 51 41 10	0	0
23	d	1	Total C O 40 35 5	0	0
23	f	1	Total C O 51 41 10	0	0

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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

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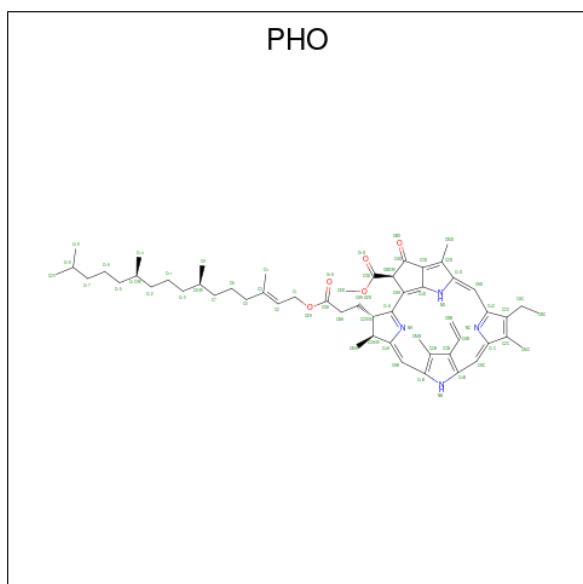
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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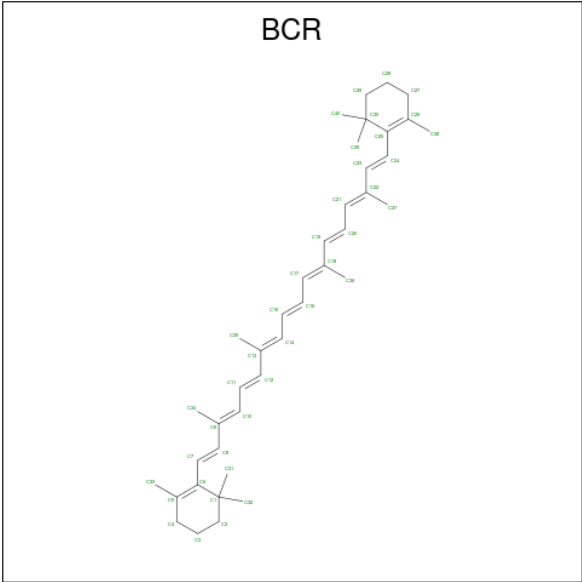
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



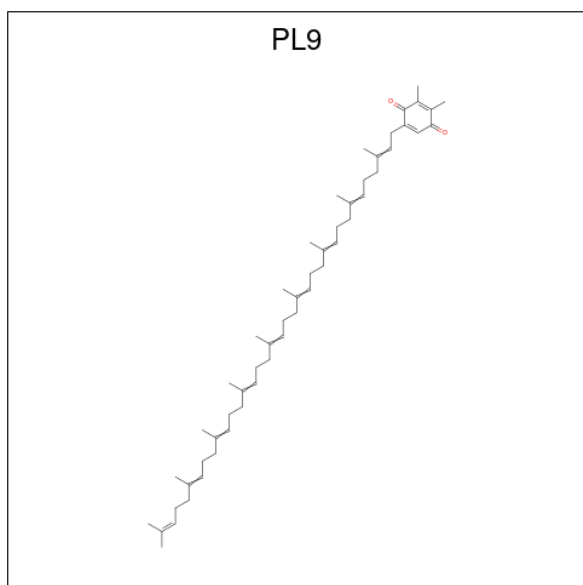
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0

- Molecule 28 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).



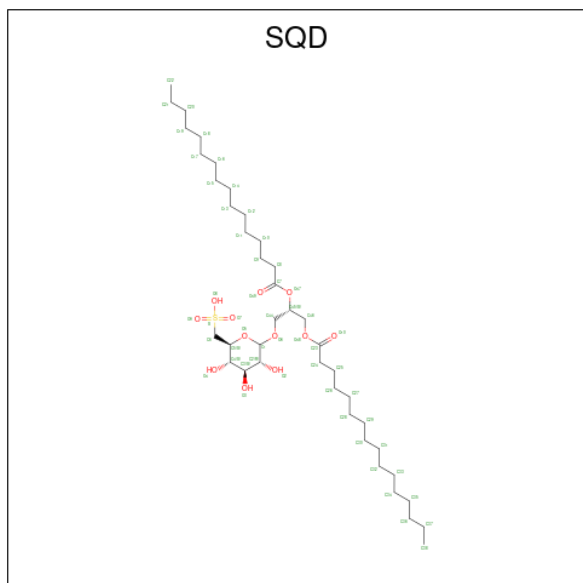
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).

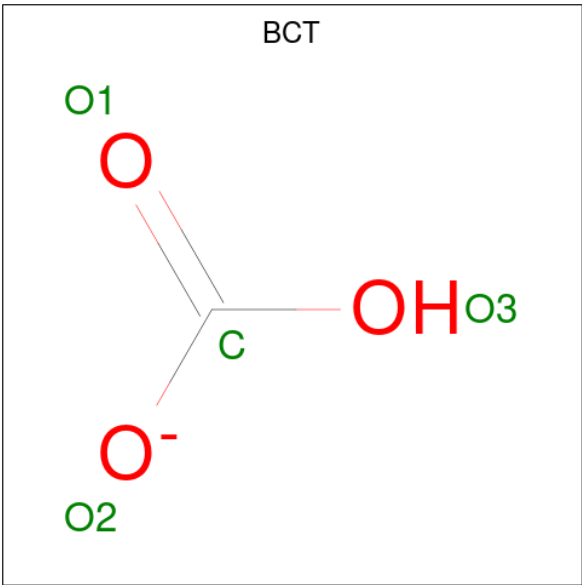


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			40	35	5			
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	I	1	Total	C	O		0	0
			40	35	5			
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O	S	0	0
			54	41	12	1		
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

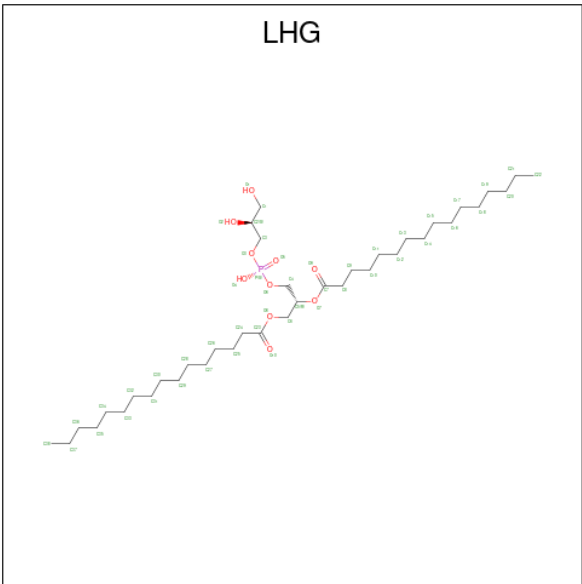
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C 7 7	0	0
30	B	3	Total C 29 29	0	0
30	H	1	Total C 8 8	0	0
30	I	1	Total C 9 9	0	0
30	M	2	Total C 22 22	0	0
30	a	3	Total C 24 24	0	0
30	b	4	Total C 48 48	0	0
30	d	1	Total C 22 22	0	0
30	i	1	Total C 22 22	0	0
30	j	1	Total C 9 9	0	0
30	m	2	Total C 17 17	0	0
30	t	2	Total C 15 15	0	0
30	z	1	Total C 11 11	0	0

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



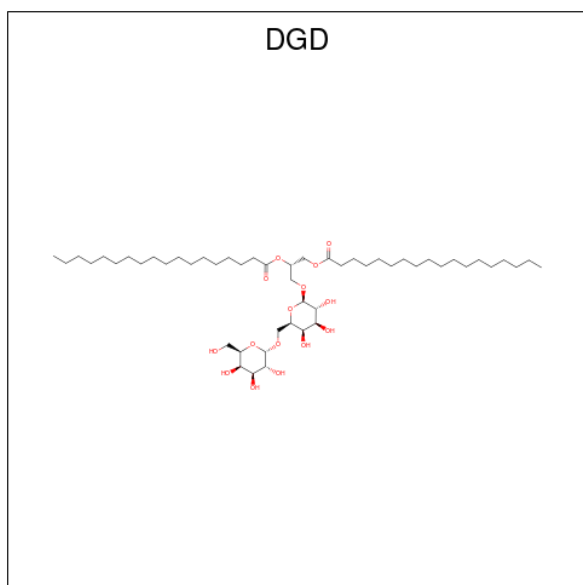
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			49	38	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	a	1	Total	C	O	P	0	0
			39	28	10	1		
32	b	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		

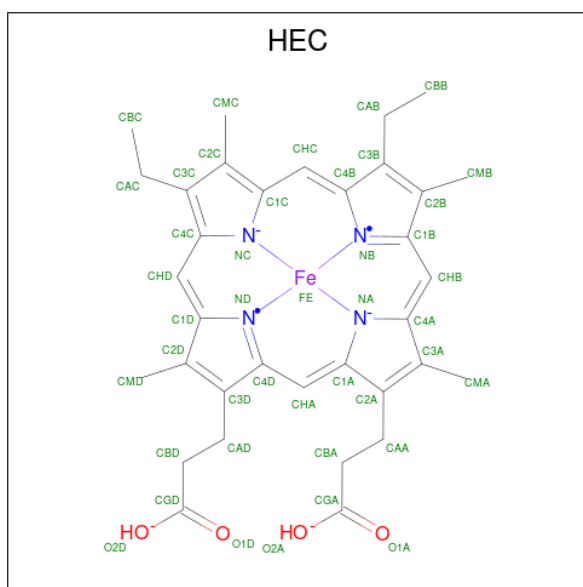
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total 62	C 47	O 15	0	0
33	H	1	Total 62	C 47	O 15	0	0
33	c	1	Total 62	C 47	O 15	0	0
33	c	1	Total 62	C 47	O 15	0	0
33	c	1	Total 62	C 47	O 15	0	0
33	h	1	Total 62	C 47	O 15	0	0

- # HEM

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
34	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	14	Total	O		
			14	14	0	0
36	B	5	Total	O		
			5	5	0	0
36	C	2	Total	O		
			2	2	0	0
36	D	5	Total	O		
			5	5	0	0
36	H	1	Total	O		
			1	1	0	0
36	K	1	Total	O		
			1	1	0	0
36	L	1	Total	O		
			1	1	0	0
36	M	1	Total	O		
			1	1	0	0
36	O	9	Total	O		
			9	9	0	0
36	U	1	Total	O		
			1	1	0	0

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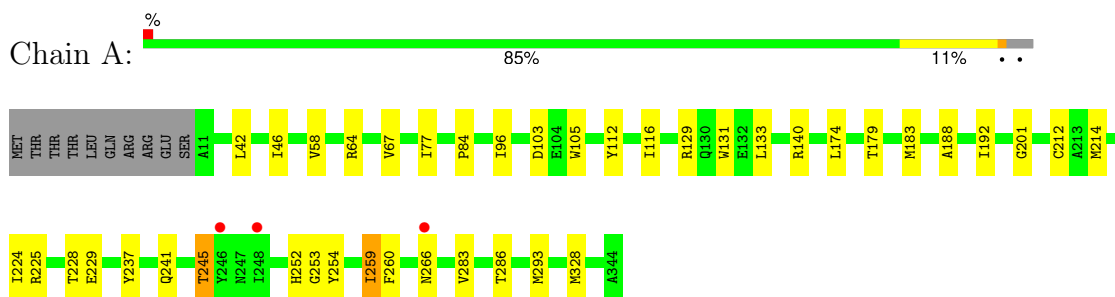
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	V	6	Total 6	O 6	0	0
36	a	13	Total 13	O 13	0	0
36	b	12	Total 12	O 12	0	0
36	c	8	Total 8	O 8	0	0
36	d	11	Total 11	O 11	0	0
36	e	1	Total 1	O 1	0	0
36	h	1	Total 1	O 1	0	0
36	l	1	Total 1	O 1	0	0
36	o	5	Total 5	O 5	0	0
36	u	5	Total 5	O 5	0	0
36	v	3	Total 3	O 3	0	0
36	z	1	Total 1	O 1	0	0

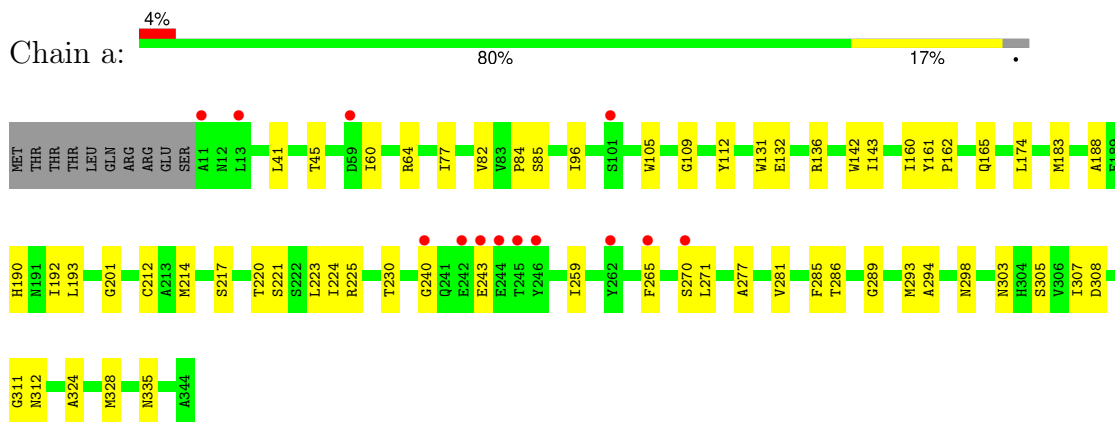
3 Residue-property plots

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

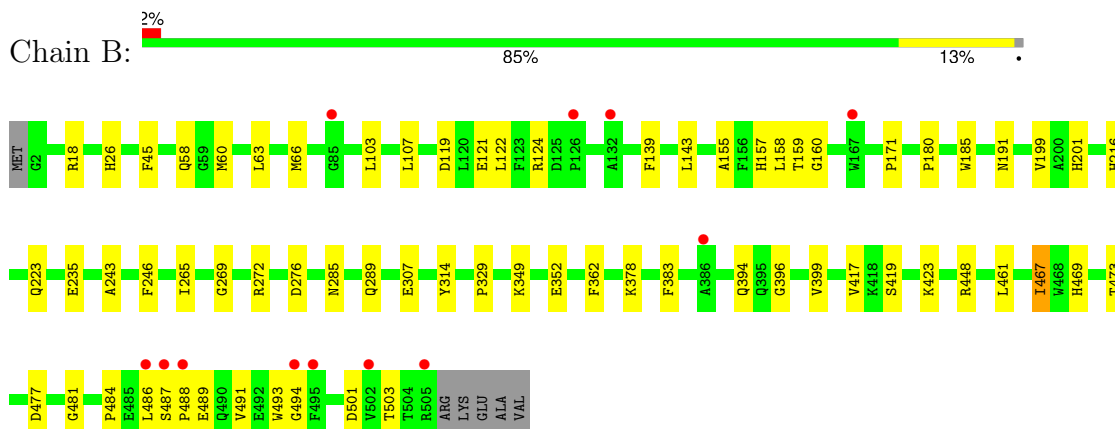
• Molecule 1: Photosystem II protein D1 1



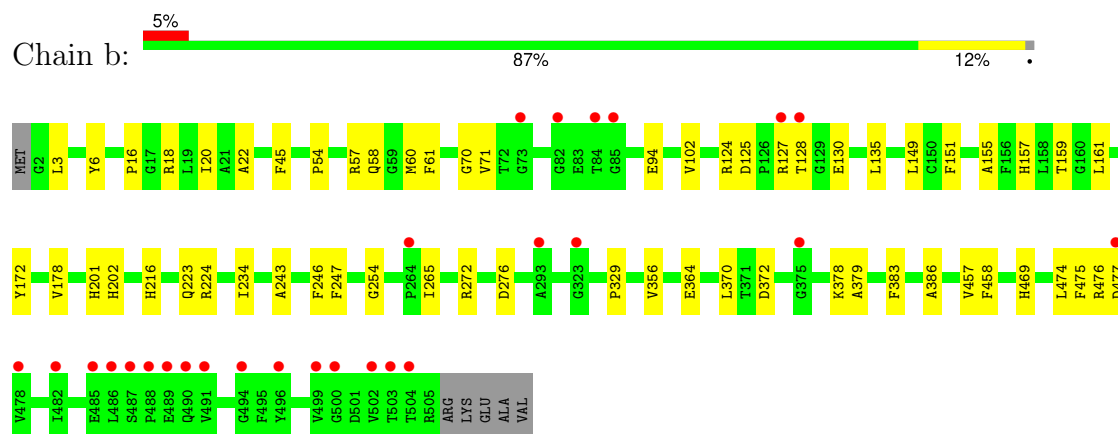
• Molecule 1: Photosystem II protein D1 1



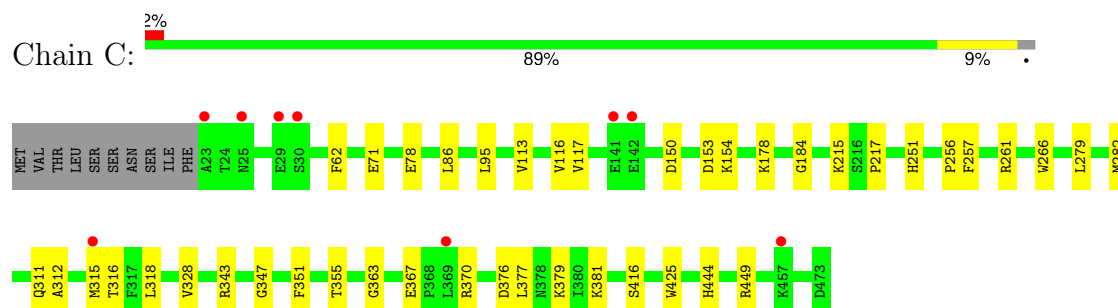
• Molecule 2: Photosystem II CP47 reaction center protein



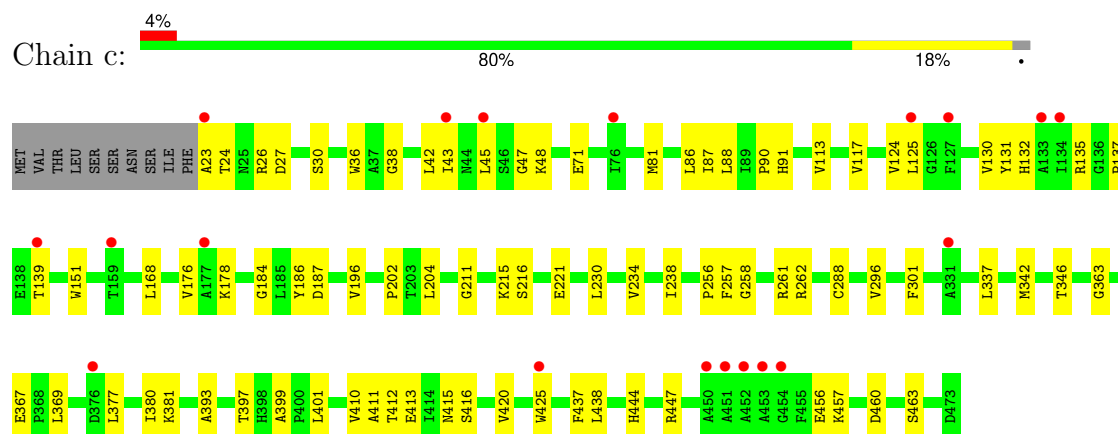
- Molecule 2: Photosystem II CP47 reaction center protein



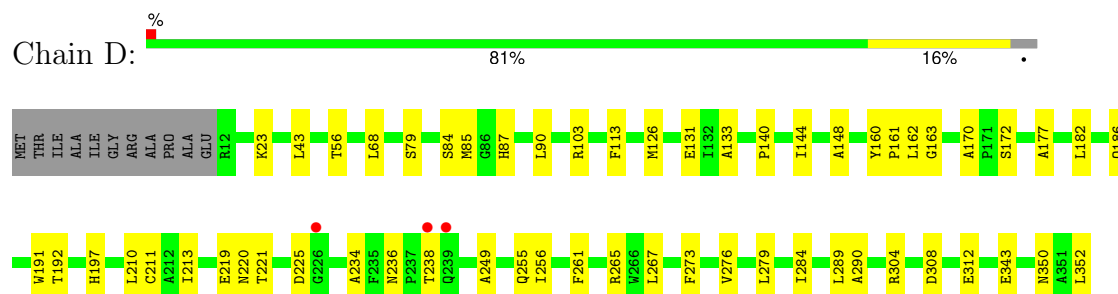
- Molecule 3: Photosystem II CP43 reaction center protein



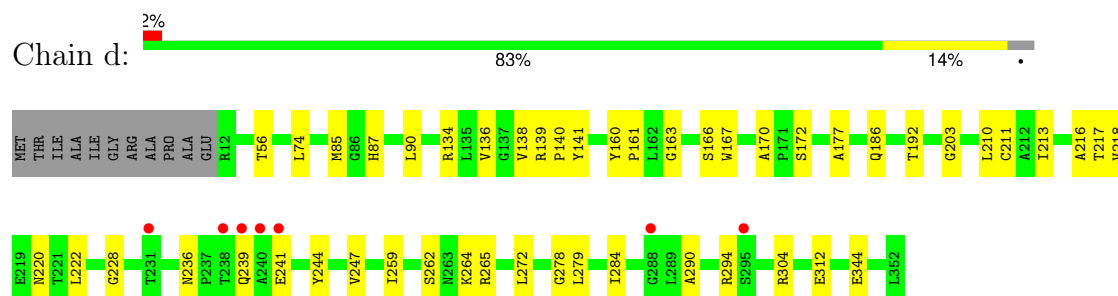
- Molecule 3: Photosystem II CP43 reaction center protein



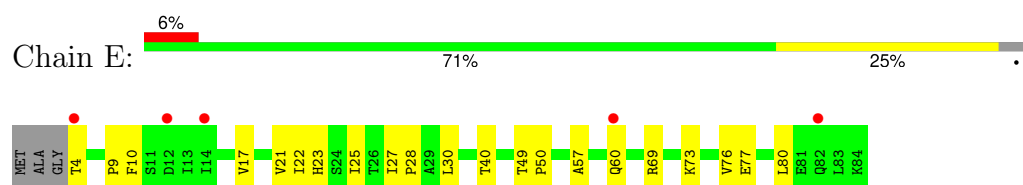
- Molecule 4: Photosystem II D2 protein



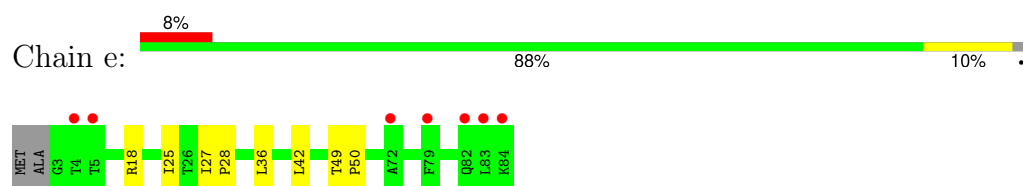
- Molecule 4: Photosystem II D2 protein



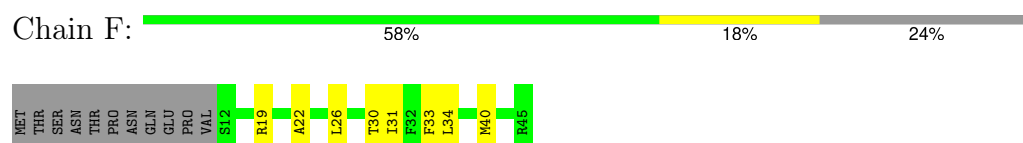
- Molecule 5: Cytochrome b559 subunit alpha



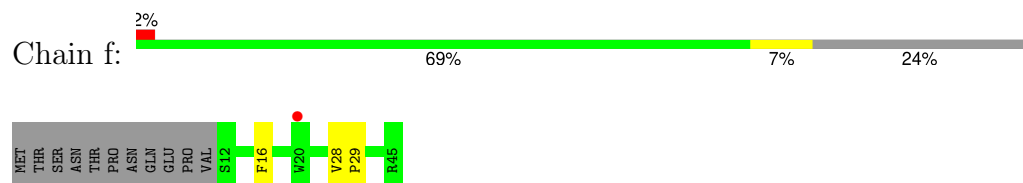
- Molecule 5: Cytochrome b559 subunit alpha



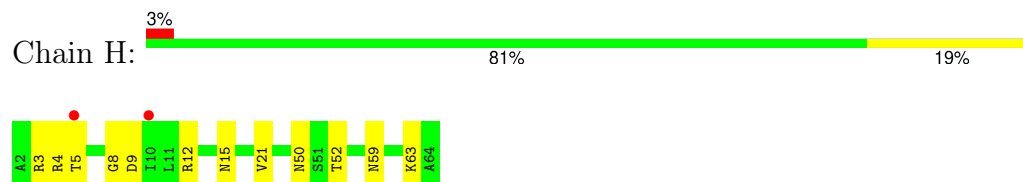
- Molecule 6: Cytochrome b559 subunit beta



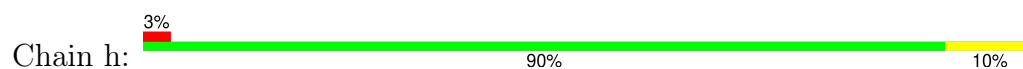
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

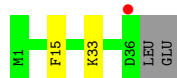
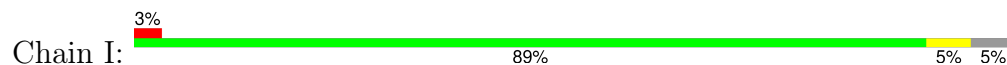


- Molecule 7: Photosystem II reaction center protein H

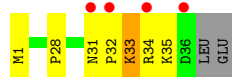
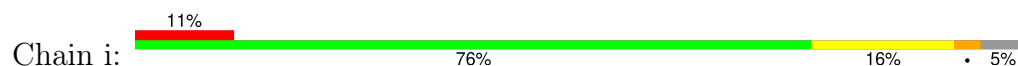




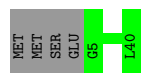
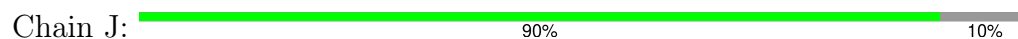
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



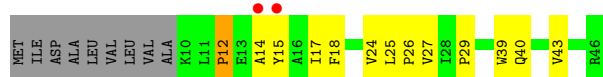
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 11% 3%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  92% 8% 3%



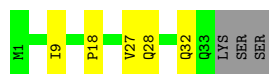
- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 14% 8% 3%



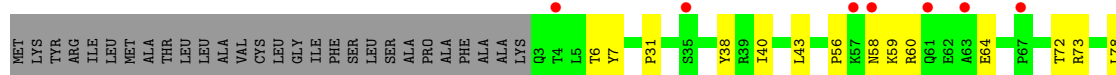
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% 8%



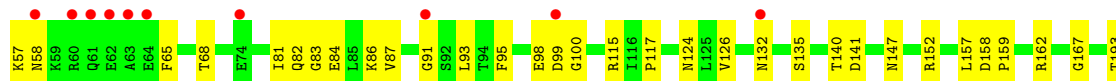
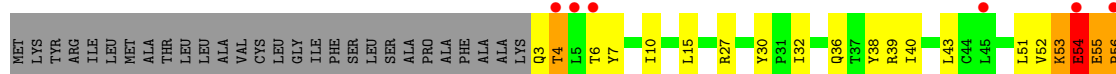
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  77% 12% 10% 4%



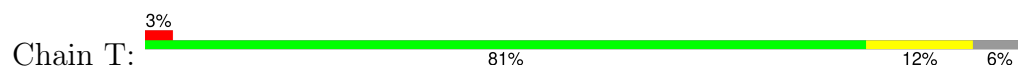
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  67% 21% 10% 6%

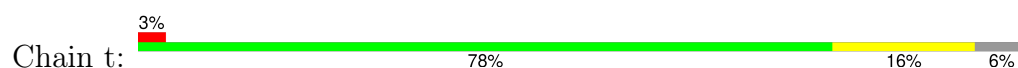




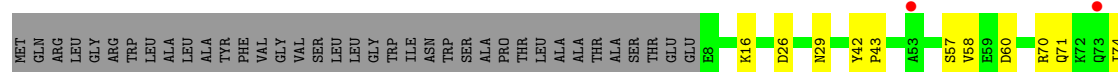
- Molecule 14: Photosystem II reaction center protein T



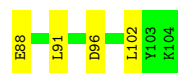
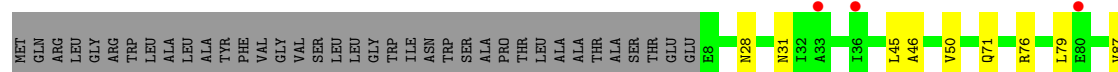
- Molecule 14: Photosystem II reaction center protein T



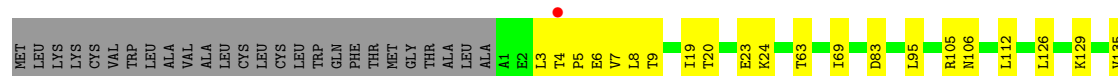
- Molecule 15: Photosystem II 12 kDa extrinsic protein



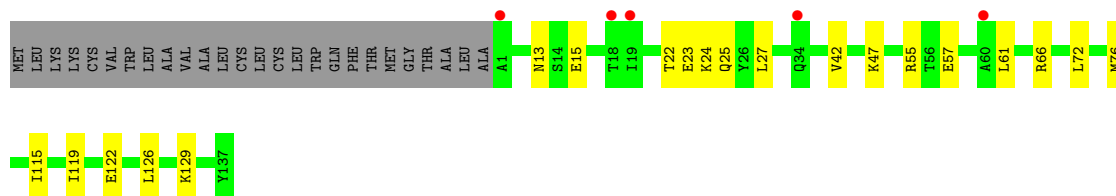
- Molecule 15: Photosystem II 12 kDa extrinsic protein



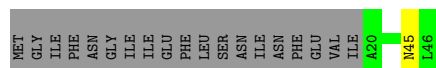
- Molecule 16: Cytochrome c-550



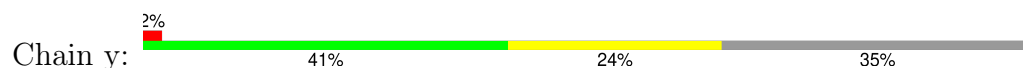
- Molecule 16: Cytochrome c-550



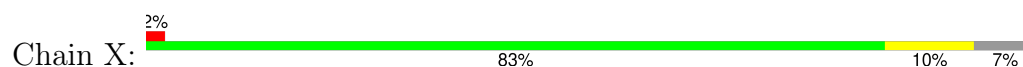
• Molecule 17: Photosystem II reaction center protein Ycf12



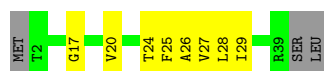
• Molecule 17: Photosystem II reaction center protein Ycf12



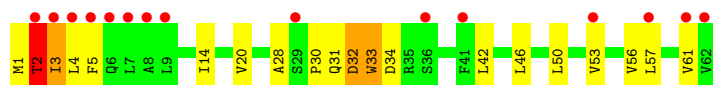
• Molecule 18: Photosystem II reaction center X protein



• Molecule 18: Photosystem II reaction center X protein

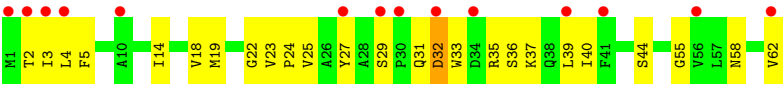


• Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.91Å 224.27Å 331.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.57 – 2.80 43.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.57-2.80) 87.6 (43.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.81Å)	Xtriage
Refinement program	PHENIX dev_2411	Depositor
R, R_{free}	0.250 , 0.300 0.253 , 0.302	Depositor DCC
R_{free} test set	1792 reflections (0.83%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50284	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: PHO, HEM, UNL, FME, BCR, DGD, LHG, CL, PL9, HEC, LMG, FE2, SQD, BCT, OEX, CLA

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	0.13	0/2707	0.30	0/3692
1	a	0.09	0/2707	0.28	0/3692
2	B	0.11	0/4109	0.29	0/5600
2	b	0.11	0/4111	0.27	0/5603
3	C	0.09	0/3599	0.25	0/4900
3	c	0.15	0/3599	0.32	0/4900
4	D	0.10	0/2811	0.27	0/3830
4	d	0.09	0/2811	0.27	0/3830
5	E	0.18	0/680	0.34	0/928
5	e	0.21	0/684	0.29	0/933
6	F	0.11	0/284	0.28	0/387
6	f	0.08	0/284	0.24	0/387
7	H	0.18	0/511	0.34	0/697
7	h	0.11	0/511	0.25	0/697
8	I	0.16	0/293	0.34	0/396
8	i	0.51	1/293 (0.3%)	0.47	0/396
9	J	0.08	0/263	0.23	0/356
9	j	0.10	0/263	0.25	0/356
10	K	0.18	0/303	0.52	0/416
10	k	0.34	0/303	0.38	0/416
11	L	0.17	0/311	0.38	0/422
11	l	0.09	0/311	0.26	0/422
12	M	0.09	0/253	0.25	0/346
12	m	0.14	0/253	0.29	0/346
13	O	0.12	0/1905	0.30	0/2583
13	o	0.18	0/1905	0.46	2/2583 (0.1%)
14	T	0.10	0/257	0.27	0/349
14	t	0.09	0/257	0.24	0/349
15	U	0.11	0/785	0.31	0/1064
15	u	0.22	0/785	0.35	0/1064
16	V	0.13	0/1085	0.27	0/1473
16	v	0.12	0/1085	0.28	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.11	0/201	0.35	0/268
17	y	0.20	0/225	0.40	0/301
18	X	0.11	0/284	0.26	0/384
18	x	0.10	0/282	0.28	0/381
19	Z	0.28	0/490	0.57	2/669 (0.3%)
19	z	0.24	0/489	0.46	0/669
20	R	0.17	0/279	0.44	0/383
20	r	0.19	0/276	0.44	0/379
All	All	0.14	1/42844 (0.0%)	0.31	4/58320 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	33	LYS	CB-CG	-5.42	1.36	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	54	GLU	CA-C-N	7.99	136.08	121.70
13	o	54	GLU	C-N-CA	7.99	136.08	121.70
19	Z	2	THR	CA-C-N	5.79	132.12	121.70
19	Z	2	THR	C-N-CA	5.79	132.12	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	4	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	0	2519	39	0
1	a	2622	0	2519	48	0
2	B	3969	0	3828	53	0
2	b	3968	0	3829	50	0
3	C	3486	0	3407	31	0
3	c	3486	0	3407	59	0
4	D	2716	0	2621	44	0
4	d	2716	0	2621	43	0
5	E	661	0	648	23	0
5	e	665	0	651	7	0
6	F	275	0	282	9	0
6	f	275	0	282	2	0
7	H	498	0	518	13	0
7	h	498	0	518	6	0
8	I	296	0	311	2	0
8	i	296	0	311	5	0
9	J	257	0	268	0	0
9	j	257	0	268	4	0
10	K	293	0	305	5	0
10	k	293	0	305	9	0
11	L	304	0	316	5	0
11	l	304	0	316	3	0
12	M	260	0	275	4	0
12	m	260	0	275	4	0
13	O	1874	0	1846	25	0
13	o	1874	0	1846	46	0
14	T	258	0	261	3	0
14	t	258	0	261	5	0
15	U	774	0	773	10	0
15	u	774	0	773	9	0
16	V	1064	0	1073	16	0
16	v	1064	0	1073	18	0
17	Y	200	0	226	1	0
17	y	224	0	252	8	0
18	X	281	0	312	4	0
18	x	279	0	307	7	0
19	Z	479	0	516	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	478	0	516	28	0
20	R	273	0	305	13	0
20	r	270	0	296	12	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	51	0	72	3	0
23	B	51	0	72	1	0
23	C	153	0	216	1	0
23	D	51	0	72	3	0
23	M	51	0	72	3	0
23	a	102	0	144	3	0
23	b	111	0	158	3	0
23	c	102	0	144	2	0
23	d	40	0	61	2	0
23	f	51	0	72	2	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	184	0	192	4	0
25	B	1040	0	1152	32	0
25	C	845	0	936	23	0
25	D	195	0	216	6	0
25	a	260	0	288	13	0
25	b	1022	0	1115	31	0
25	c	838	0	919	25	0
25	d	130	0	144	8	0
26	A	64	0	74	1	0
26	D	64	0	74	2	0
26	a	128	0	148	8	0
27	A	40	0	56	4	0
27	B	120	0	168	5	0
27	C	80	0	112	5	0
27	D	40	0	56	4	0
27	H	40	0	56	3	0
27	K	40	0	56	0	0
27	Y	40	0	56	0	0
27	a	40	0	56	2	0
27	b	160	0	224	11	0
27	c	80	0	112	1	0
27	d	40	0	56	0	0
27	h	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	k	80	0	112	6	0
27	t	40	0	56	6	0
28	A	55	0	80	5	0
28	D	55	0	80	2	0
28	a	55	0	80	4	0
28	d	55	0	80	0	0
29	A	92	0	138	3	0
29	B	101	0	135	7	0
29	D	43	0	53	4	0
29	I	40	0	67	3	0
29	a	54	0	78	1	0
29	b	54	0	77	3	0
29	f	41	0	49	1	0
30	A	7	0	0	0	0
30	B	29	0	0	0	0
30	H	8	0	0	0	0
30	I	9	0	0	0	0
30	M	22	0	0	0	0
30	a	24	0	0	0	0
30	b	48	0	0	0	0
30	d	22	0	0	0	0
30	i	22	0	0	0	0
30	j	9	0	0	0	0
30	m	17	0	0	0	0
30	t	15	0	0	0	0
30	z	11	0	0	0	0
31	A	4	0	0	0	0
31	a	4	0	0	1	0
32	B	49	0	74	2	0
32	D	98	0	148	7	0
32	E	49	0	74	3	0
32	L	49	0	74	4	0
32	a	39	0	51	1	0
32	b	49	0	74	1	0
32	d	98	0	148	6	0
32	e	42	0	57	2	0
33	C	186	0	246	5	0
33	H	62	0	82	0	0
33	c	186	0	246	4	0
33	h	62	0	82	3	0
34	E	43	0	30	3	0
34	e	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	V	43	0	30	1	0
35	v	43	0	30	0	0
36	A	14	0	0	0	0
36	B	5	0	0	0	0
36	C	2	0	0	0	0
36	D	5	0	0	0	0
36	H	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	O	9	0	0	2	0
36	U	1	0	0	0	0
36	V	6	0	0	1	0
36	a	13	0	0	2	0
36	b	12	0	0	0	0
36	c	8	0	0	0	0
36	d	11	0	0	1	0
36	e	1	0	0	0	0
36	h	1	0	0	0	0
36	l	1	0	0	0	0
36	o	5	0	0	0	0
36	u	5	0	0	0	0
36	v	3	0	0	0	0
36	z	1	0	0	0	0
All	All	50284	0	51202	742	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 7.

All (742) 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)
7:H:4:ARG:NH2	7:H:9:ASP:OD2	1.66	1.23
13:o:54:GLU:HA	13:o:55:GLU:HB2	1.42	1.02
3:c:38:GLY:HA3	25:c:511:CLA:HMD2	1.52	0.91
1:A:225:ARG:HD3	2:B:484:PRO:HD3	1.58	0.83
13:o:55:GLU:OE1	13:o:56:PRO:HD3	1.79	0.81
2:B:269:GLY:O	2:B:448:ARG:NH2	2.13	0.80
19:z:36:SER:HA	19:z:39:LEU:HD21	1.63	0.80
2:b:125:ASP:OD2	2:b:127:ARG:NH1	2.15	0.80
4:d:141:TYR:OH	32:d:406:LHG:O4	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:608:CLA:HAC2	27:t:103:BCR:H272	1.64	0.79
2:B:157:HIS:HE1	25:B:607:CLA:NA	1.81	0.78
23:A:603:LMG:H412	27:b:602:BCR:HC7	1.65	0.78
19:Z:2:THR:N	19:Z:3:ILE:O	2.17	0.78
6:F:31:ILE:HA	6:F:34:LEU:HD23	1.65	0.77
2:B:18:ARG:NH2	29:B:626:SQD:O8	2.14	0.77
13:O:40:ILE:HD13	13:O:243:ILE:HD13	1.67	0.77
1:A:237:TYR:HB2	1:A:245:THR:HG21	1.66	0.76
34:E:102:HEM:HHD	34:E:102:HEM:HBC2	1.70	0.74
2:b:124:ARG:O	7:h:12:ARG:NH2	2.18	0.74
3:c:42:LEU:HD23	3:c:45:LEU:HD12	1.70	0.73
34:e:102:HEM:HHD	34:e:102:HEM:HBC2	1.69	0.73
34:e:102:HEM:HHC	34:e:102:HEM:HBB2	1.69	0.73
2:b:155:ALA:O	2:b:159:THR:OG1	2.07	0.73
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.69	0.72
2:B:307:GLU:OE1	13:o:58:ASN:ND2	2.21	0.72
29:B:626:SQD:O10	11:l:14:ARG:NH2	2.22	0.72
14:t:15:ALA:HB2	27:t:103:BCR:H14C	1.70	0.72
5:E:27:ILE:HG23	5:E:28:PRO:HD3	1.71	0.72
25:C:504:CLA:H172	25:C:511:CLA:HBB2	1.73	0.71
4:d:236:ASN:H	4:d:239:GLN:HE22	1.38	0.70
1:a:240:GLY:HA3	14:t:29:ILE:HG23	1.73	0.70
2:B:349:LYS:HG2	2:B:396:GLY:HA3	1.73	0.70
29:D:410:SQD:H252	18:X:31:ILE:HD13	1.72	0.69
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.73	0.69
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.73	0.69
3:c:26:ARG:NH2	17:y:46:LEU:OXT	2.26	0.69
2:b:18:ARG:NH1	29:b:601:SQD:O8	2.27	0.68
4:D:192:THR:HG23	25:D:403:CLA:HBC2	1.76	0.68
4:D:279:LEU:HD22	26:D:401:PHO:HBC3	1.76	0.68
10:K:13:GLU:OE2	10:K:14:ALA:N	2.27	0.68
2:b:157:HIS:HE1	25:b:612:CLA:NA	1.91	0.68
2:b:172:TYR:OH	7:h:63:LYS:NZ	2.26	0.67
25:C:509:CLA:H92	32:D:408:LHG:H371	1.75	0.67
7:H:5:THR:HG23	7:H:8:GLY:H	1.60	0.67
3:c:135:ARG:NH1	19:z:27:TYR:CD2	2.62	0.67
3:C:116:VAL:HG21	27:C:515:BCR:H312	1.77	0.67
2:b:474:LEU:O	4:d:134:ARG:NH1	2.27	0.67
26:a:710:PHO:HBC3	4:d:279:LEU:HD22	1.77	0.67
12:M:24:ILE:HG23	12:m:27:VAL:HG21	1.77	0.66
36:a:802:HOH:O	4:d:264:LYS:NZ	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:425:TRP:CD1	25:C:505:CLA:H3A	2.31	0.66
19:z:31:GLN:HG3	19:z:32:ASP:HB2	1.78	0.66
5:E:57:ALA:HB3	5:E:60:GLN:HB2	1.77	0.65
1:a:142:TRP:CZ2	3:c:447:ARG:HG3	2.30	0.65
1:a:225:ARG:NH2	2:b:477:ASP:O	2.29	0.65
5:E:10:PHE:N	32:E:101:LHG:O4	2.29	0.65
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.78	0.65
32:D:408:LHG:H352	32:D:408:LHG:H172	1.79	0.64
32:D:408:LHG:H372	32:D:408:LHG:H141	1.79	0.64
33:C:518:DGD:HO3D	33:C:519:DGD:HO5E	1.40	0.64
20:r:14:LEU:H	20:r:14:LEU:HD23	1.63	0.64
19:z:23:VAL:HG23	19:z:27:TYR:CE1	2.34	0.63
16:v:24:LYS:H	16:v:24:LYS:HD2	1.63	0.63
1:A:241:GLN:NE2	1:A:245:THR:HG23	2.12	0.63
1:a:217:SER:O	1:a:221:SER:OG	2.15	0.63
13:o:53:LYS:NZ	13:o:55:GLU:OE2	2.22	0.63
3:c:410:VAL:HG13	3:c:412:THR:H	1.62	0.63
19:z:19:MET:O	19:z:23:VAL:HG12	1.99	0.63
27:B:619:BCR:H363	27:t:103:BCR:H19C	1.81	0.62
4:d:192:THR:HG23	25:d:402:CLA:HBC2	1.79	0.62
19:z:24:PRO:HA	19:z:27:TYR:HB2	1.81	0.62
2:B:18:ARG:CZ	11:L:4:ASN:HD22	2.12	0.62
31:a:706:BCT:O1	36:a:802:HOH:O	2.16	0.62
29:A:612:SQD:H251	32:D:408:LHG:H121	1.81	0.61
20:R:6:LEU:HD13	20:R:10:LEU:HD21	1.82	0.61
2:B:216:HIS:HE1	25:B:610:CLA:NA	1.97	0.61
16:v:55:ARG:NH1	16:v:57:GLU:OE1	2.33	0.61
3:c:137:PRO:HB2	3:c:139:THR:O	2.00	0.61
15:u:76:ARG:HA	15:u:79:LEU:HD23	1.83	0.61
29:B:626:SQD:O7	11:L:7:ARG:NH2	2.32	0.61
19:Z:32:ASP:O	19:Z:34:ASP:N	2.32	0.61
19:z:19:MET:O	19:z:22:GLY:N	2.33	0.61
20:R:16:ALA:O	20:R:20:VAL:HG23	2.01	0.61
13:o:87:VAL:HG22	13:o:93:LEU:HD22	1.82	0.61
19:z:23:VAL:HG13	19:z:24:PRO:HD3	1.83	0.61
3:C:154:LYS:HE3	3:C:261:ARG:HD2	1.83	0.60
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.83	0.60
19:Z:3:ILE:O	19:Z:5:PHE:N	2.33	0.60
13:o:54:GLU:CA	13:o:55:GLU:HB2	2.26	0.60
3:c:135:ARG:NH1	19:z:27:TYR:CE2	2.69	0.60
5:E:77:GLU:HA	5:E:80:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:18:PHE:HB2	27:b:602:BCR:HC8	1.83	0.60
17:y:42:ARG:NH1	19:z:31:GLN:OE1	2.34	0.60
19:z:39:LEU:H	19:z:39:LEU:HD23	1.66	0.60
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.82	0.60
2:B:216:HIS:HE1	25:B:610:CLA:C1A	2.14	0.60
4:D:186:GLN:HB2	25:D:403:CLA:HBC1	1.84	0.60
13:o:99:ASP:OD1	13:o:100:GLY:N	2.34	0.60
4:d:56:THR:HB	5:e:49:THR:HG23	1.83	0.60
8:i:28:PRO:O	8:i:31:ASN:ND2	2.34	0.60
2:B:272:ARG:NH1	2:B:276:ASP:OD2	2.35	0.59
16:V:105:ARG:NH2	36:V:301:HOH:O	2.35	0.59
13:o:84:GLU:OE2	13:o:86:LYS:NZ	2.35	0.59
4:D:163:GLY:HA3	4:D:290:ALA:HB1	1.84	0.59
16:V:5:PRO:HA	16:V:8:LEU:HD12	1.84	0.59
2:b:254:GLY:HA3	33:h:102:DGD:HB61	1.84	0.59
19:Z:2:THR:H	19:Z:3:ILE:C	2.09	0.59
3:c:43:ILE:O	3:c:151:TRP:NE1	2.29	0.59
17:y:39:LEU:HD21	19:z:25:VAL:HG13	1.83	0.59
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.67	0.59
2:b:216:HIS:HE1	25:b:615:CLA:C1A	2.16	0.59
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.84	0.59
1:a:308:ASP:OD1	1:a:312:ASN:N	2.34	0.59
19:z:25:VAL:O	19:z:29:SER:OG	2.15	0.59
16:v:15:GLU:OE1	16:v:15:GLU:N	2.27	0.58
13:O:153:THR:HG22	13:O:154:ALA:H	1.68	0.58
1:a:265:PHE:HB2	1:a:271:LEU:HD12	1.83	0.58
25:B:617:CLA:H171	7:H:3:ARG:NH1	2.19	0.58
1:a:143:ILE:HD11	4:d:217:THR:HA	1.85	0.58
15:U:29:ASN:HD21	15:U:87:VAL:HA	1.67	0.58
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.85	0.58
13:O:158:ASP:OD1	13:O:162:ARG:N	2.34	0.58
1:a:243:GLU:OE1	1:a:243:GLU:N	2.31	0.58
25:b:612:CLA:H72	27:b:625:BCR:H311	1.85	0.57
13:O:64:GLU:N	13:O:64:GLU:OE1	2.37	0.57
7:h:12:ARG:O	7:h:16:SER:OG	2.21	0.57
2:B:469:HIS:CE1	25:B:612:CLA:NA	2.72	0.57
3:C:311:GLN:NE2	3:C:355:THR:OG1	2.36	0.57
25:B:616:CLA:H2	25:B:617:CLA:HBB2	1.87	0.57
3:c:135:ARG:HH21	3:c:135:ARG:HG3	1.70	0.57
1:A:84:PRO:HA	1:A:112:TYR:CG	2.39	0.56
3:C:113:VAL:HA	3:C:116:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:711:CLA:H172	25:c:505:CLA:H141	1.87	0.56
1:A:253:GLY:HA2	2:B:493:TRP:CH2	2.40	0.56
2:B:185:TRP:HD1	23:B:621:LMG:HC2	1.69	0.56
19:z:32:ASP:HB3	19:z:35:ARG:HB3	1.87	0.56
19:z:33:TRP:O	19:z:37:LYS:HB2	2.05	0.56
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.88	0.56
17:Y:45:ASN:HB3	19:Z:28:ALA:HB1	1.87	0.56
3:c:87:ILE:HG13	3:c:88:LEU:HG	1.86	0.56
25:C:505:CLA:H51	33:C:519:DGD:HB62	1.86	0.56
13:o:27:ARG:NH2	13:o:202:ALA:O	2.37	0.56
2:b:22:ALA:HB1	25:b:618:CLA:HBB1	1.88	0.56
1:a:303:ASN:O	3:c:415:ASN:ND2	2.37	0.56
5:e:18:ARG:HH21	34:e:102:HEM:CGA	2.19	0.56
3:C:370:ARG:HD3	13:O:7:TYR:CE2	2.41	0.56
9:j:9:PRO:HD2	9:j:12:ILE:HD12	1.87	0.56
2:B:487:SER:O	2:B:489:GLU:N	2.35	0.56
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.87	0.56
25:D:404:CLA:H61	18:X:14:LEU:HD12	1.86	0.56
4:d:186:GLN:HB2	25:d:402:CLA:HBC1	1.88	0.55
5:E:76:VAL:O	5:E:80:LEU:HD22	2.05	0.55
27:B:618:BCR:H383	29:B:626:SQD:H91	1.88	0.55
25:b:607:CLA:H12	25:b:607:CLA:H71	1.88	0.55
25:B:602:CLA:HAC1	27:H:102:BCR:H383	1.88	0.55
2:b:102:VAL:HG23	25:b:612:CLA:H102	1.87	0.55
2:b:216:HIS:HE1	25:b:615:CLA:NA	2.01	0.55
3:c:204:LEU:HD22	3:c:238:ILE:HD11	1.88	0.55
1:A:131:TRP:CH2	25:C:506:CLA:HAA2	2.42	0.55
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.88	0.55
29:B:626:SQD:H382	27:t:103:BCR:H362	1.89	0.55
4:D:221:THR:HG21	4:D:249:ALA:HB2	1.89	0.55
34:E:102:HEM:HBB2	34:E:102:HEM:HMB2	1.88	0.55
6:F:26:LEU:O	6:F:30:THR:OG1	2.12	0.55
11:l:24:ILE:HD12	12:m:18:PRO:HG2	1.89	0.55
2:b:457:VAL:HG13	4:d:284:ILE:HD12	1.89	0.55
3:c:438:LEU:HD11	25:c:505:CLA:HBB1	1.88	0.55
13:o:40:ILE:HD13	13:o:243:ILE:HG22	1.89	0.55
1:a:64:ARG:O	13:o:152:ARG:NH1	2.40	0.55
13:o:201:VAL:HG12	13:o:239:PHE:HZ	1.72	0.55
25:B:617:CLA:OBD	7:H:5:THR:OG1	2.15	0.54
19:Z:2:THR:HB	19:Z:3:ILE:HB	1.87	0.54
26:a:710:PHO:H3A	25:d:402:CLA:H142	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ILE:HA	2:B:448:ARG:HH22	1.72	0.54
25:B:617:CLA:H143	23:a:701:LMG:HC62	1.88	0.54
25:C:509:CLA:H202	10:K:33:LEU:HD22	1.90	0.54
16:V:4:THR:HG23	16:V:6:GLU:H	1.72	0.54
16:V:4:THR:HG22	16:V:7:VAL:HG13	1.89	0.54
2:b:149:LEU:HD23	25:b:609:CLA:HBC1	1.89	0.54
10:k:25:LEU:HD22	27:k:101:BCR:H332	1.87	0.54
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.90	0.54
4:D:343:GLU:HG2	16:V:135:VAL:HG11	1.89	0.54
1:a:193:LEU:HD11	25:a:707:CLA:HMC2	1.89	0.54
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.90	0.54
16:V:24:LYS:HD2	16:V:24:LYS:N	2.21	0.54
1:a:136:ARG:O	8:i:32:PRO:HG3	2.07	0.54
3:c:202:PRO:HB3	3:c:234:VAL:HG12	1.88	0.54
13:o:53:LYS:HE2	13:o:231:HIS:HA	1.90	0.54
16:v:13:ASN:CG	16:v:15:GLU:OE1	2.50	0.54
4:d:304:ARG:NH1	36:d:502:HOH:O	2.41	0.54
25:b:614:CLA:H142	7:h:39:LEU:HD11	1.90	0.54
19:z:19:MET:O	19:z:23:VAL:N	2.35	0.54
2:b:272:ARG:NH1	2:b:276:ASP:OD2	2.41	0.54
19:z:23:VAL:CG2	19:z:27:TYR:CE1	2.91	0.54
2:B:103:LEU:HB2	25:B:607:CLA:H62	1.90	0.54
1:A:214:MET:HB3	28:A:611:PL9:H103	1.90	0.53
2:B:223:GLN:HA	7:H:21:VAL:HG21	1.90	0.53
4:D:304:ARG:NH2	4:D:308:ASP:OD2	2.41	0.53
13:o:124:ASN:HB2	13:o:147:ASN:HD22	1.73	0.53
18:X:31:ILE:HA	18:X:34:ILE:HG22	1.90	0.53
2:b:476:ARG:HG3	2:b:477:ASP:N	2.24	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.43	0.53
1:A:241:GLN:HE22	1:A:245:THR:HG23	1.71	0.53
6:F:30:THR:HG22	6:F:34:LEU:HD21	1.90	0.53
2:b:383:PHE:N	4:d:344:GLU:O	2.35	0.53
15:u:31:ASN:ND2	15:u:96:ASP:O	2.42	0.53
20:R:24:LEU:HD12	20:R:27:ALA:HB3	1.90	0.53
16:v:122:GLU:HG3	16:v:126:LEU:HD12	1.91	0.53
3:C:377:LEU:HG	3:C:381:LYS:HE3	1.90	0.53
1:a:223:LEU:HD23	4:d:139:ARG:HH11	1.72	0.53
9:j:21:VAL:O	9:j:25:VAL:HG12	2.08	0.53
2:B:314:TYR:OH	13:O:176:GLN:NE2	2.42	0.52
29:A:612:SQD:H311	25:C:509:CLA:H71	1.90	0.52
2:B:307:GLU:CD	13:o:58:ASN:HD21	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:t:18:PHE:HB2	27:t:103:BCR:HC8	1.91	0.52
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.44	0.52
2:b:364:GLU:OE1	4:d:294:ARG:NH2	2.40	0.52
2:b:372:ASP:HB3	2:b:378:LYS:HD2	1.90	0.52
19:Z:50:LEU:HA	19:Z:53:VAL:HG12	1.90	0.52
1:a:41:LEU:O	1:a:45:THR:HG23	2.09	0.52
3:c:178:LYS:NZ	3:c:184:GLY:O	2.42	0.52
1:A:237:TYR:CB	1:A:245:THR:HG21	2.39	0.52
3:c:413:GLU:OE2	16:v:47:LYS:NZ	2.41	0.52
5:e:25:ILE:HG21	20:r:18:TRP:CD1	2.45	0.52
25:C:512:CLA:H171	19:Z:20:VAL:HG22	1.92	0.52
2:b:45:PHE:HD1	2:b:60:MET:HE3	1.74	0.52
13:o:10:ILE:HG23	13:o:15:LEU:HB2	1.91	0.52
2:b:370:LEU:HB2	2:b:379:ALA:HB3	1.92	0.52
9:j:21:VAL:HA	9:j:24:ILE:HG22	1.91	0.52
3:c:456:GLU:HG2	3:c:457:LYS:HG3	1.92	0.52
20:r:11:PRO:HA	20:r:14:LEU:HD21	1.91	0.52
4:D:312:GLU:HB2	13:O:159:PRO:HG3	1.92	0.52
20:r:23:ILE:O	20:r:27:ALA:N	2.42	0.52
1:A:224:ILE:O	4:D:265:ARG:NH2	2.42	0.52
3:C:312:ALA:O	3:C:316:THR:OG1	2.24	0.51
25:c:501:CLA:H203	25:c:507:CLA:H13	1.93	0.51
25:d:403:CLA:H2	18:x:17:GLY:HA3	1.90	0.51
13:o:52:VAL:HG23	13:o:68:THR:HG21	1.92	0.51
19:z:23:VAL:O	19:z:27:TYR:HD1	1.94	0.51
5:E:30:LEU:CD2	20:R:12:VAL:HG22	2.40	0.51
5:e:42:LEU:HD12	20:r:4:ARG:HB2	1.91	0.51
15:u:88:GLU:HG3	15:u:91:LEU:HD23	1.91	0.51
2:b:6:TYR:OH	32:b:629:LHG:O5	2.24	0.51
25:C:506:CLA:H43	27:C:516:BCR:HC7	1.91	0.51
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.93	0.51
23:b:627:LMG:O5	23:b:627:LMG:O4	2.26	0.51
25:C:509:CLA:H193	33:C:518:DGD:HAW2	1.93	0.51
16:V:4:THR:O	16:V:7:VAL:HG22	2.11	0.51
2:b:469:HIS:HE1	25:b:617:CLA:NA	2.06	0.51
3:c:135:ARG:NH2	19:z:27:TYR:O	2.44	0.51
27:D:405:BCR:H383	23:D:409:LMG:H161	1.92	0.51
6:F:30:THR:O	6:F:33:PHE:N	2.44	0.51
4:d:161:PRO:HB3	4:d:170:ALA:HB2	1.92	0.51
15:U:29:ASN:ND2	15:U:88:GLU:H	2.09	0.51
13:o:210:GLU:OE1	13:o:240:TYR:OH	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:122:GLU:HG3	16:v:126:LEU:CD1	2.41	0.51
10:K:27:VAL:O	10:K:30:VAL:HG12	2.11	0.50
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.93	0.50
3:c:131:TYR:HA	19:z:27:TYR:HE2	1.76	0.50
3:c:296:VAL:HG11	25:c:501:CLA:HMA2	1.92	0.50
4:d:236:ASN:HB3	4:d:239:GLN:NE2	2.26	0.50
4:d:312:GLU:HB2	13:o:159:PRO:HG3	1.93	0.50
15:U:71:GLN:O	15:U:75:LEU:HD12	2.11	0.50
2:b:128:THR:OG1	2:b:130:GLU:OE1	2.23	0.50
3:c:87:ILE:O	3:c:91:HIS:ND1	2.44	0.50
13:o:53:LYS:HZ1	13:o:231:HIS:HA	1.76	0.50
28:A:611:PL9:H221	26:D:401:PHO:HMA2	1.93	0.50
2:B:487:SER:C	2:B:489:GLU:H	2.19	0.50
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.92	0.50
26:a:710:PHO:HBA2	25:d:402:CLA:H142	1.93	0.50
2:B:26:HIS:HB2	25:B:613:CLA:HMB1	1.94	0.50
2:b:201:HIS:HB2	25:b:608:CLA:C1B	2.41	0.50
13:O:58:ASN:O	13:O:60:ARG:N	2.44	0.50
1:a:45:THR:HG22	26:a:709:PHO:H93	1.94	0.50
1:a:142:TRP:HZ2	3:c:447:ARG:HG3	1.75	0.50
13:O:38:TYR:OH	36:O:301:HOH:O	2.19	0.50
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.94	0.50
13:o:55:GLU:HB3	13:o:56:PRO:CD	2.42	0.50
13:o:158:ASP:OD1	13:o:162:ARG:N	2.43	0.50
1:a:201:GLY:HA3	1:a:286:THR:HB	1.94	0.49
26:a:710:PHO:HBA1	28:a:713:PL9:H252	1.94	0.49
10:k:14:ALA:HB1	19:z:5:PHE:CE2	2.47	0.49
1:a:183:MET:HA	25:a:707:CLA:HMD1	1.93	0.49
3:c:176:VAL:HG23	3:c:234:VAL:HG13	1.92	0.49
1:A:201:GLY:HA3	1:A:286:THR:HB	1.93	0.49
29:A:614:SQD:H101	2:b:94:GLU:HG2	1.94	0.49
25:B:612:CLA:H142	32:L:101:LHG:H361	1.93	0.49
3:C:444:HIS:CE1	25:C:509:CLA:NA	2.80	0.49
7:H:50:ASN:OD1	7:H:52:THR:OG1	2.25	0.49
2:b:155:ALA:O	2:b:161:LEU:HD12	2.11	0.49
28:A:611:PL9:H403	6:F:22:ALA:HB2	1.94	0.49
25:D:402:CLA:HED1	28:D:406:PL9:H371	1.95	0.49
1:A:64:ARG:NH1	13:O:105:PRO:O	2.44	0.49
4:d:56:THR:HG21	5:e:50:PRO:HD3	1.94	0.49
4:d:222:LEU:HA	4:d:244:TYR:HA	1.93	0.49
5:E:23:HIS:O	5:E:27:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.95	0.49
18:x:25:PHE:O	18:x:28:LEU:N	2.41	0.49
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.95	0.49
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.94	0.49
1:a:160:ILE:HD11	33:c:516:DGD:HBT2	1.94	0.49
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.47	0.49
23:f:101:LMG:H342	23:f:101:LMG:H231	1.94	0.49
8:i:31:ASN:O	8:i:35:LYS:NZ	2.40	0.49
19:z:23:VAL:HG23	19:z:27:TYR:HE1	1.78	0.49
16:V:23:GLU:HG2	16:V:24:LYS:NZ	2.27	0.49
23:a:715:LMG:H382	33:c:516:DGD:HA81	1.94	0.49
33:h:102:DGD:O4E	33:h:102:DGD:O5E	2.25	0.49
4:d:259:ILE:HD13	32:d:407:LHG:H262	1.95	0.49
5:E:25:ILE:HD11	20:R:18:TRP:CD1	2.48	0.48
15:u:76:ARG:HA	15:u:79:LEU:CD2	2.43	0.48
2:B:121:GLU:O	7:H:12:ARG:NH2	2.46	0.48
2:b:356:VAL:HG22	2:b:370:LEU:HD22	1.94	0.48
13:o:30:TYR:CD2	13:o:243:ILE:HD11	2.47	0.48
25:B:614:CLA:H192	32:B:625:LHG:H223	1.95	0.48
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.95	0.48
3:c:47:GLY:HA3	3:c:137:PRO:O	2.14	0.48
25:c:511:CLA:H162	27:k:102:BCR:H19C	1.95	0.48
23:c:519:LMG:H192	10:k:27:VAL:HG11	1.94	0.48
4:d:236:ASN:N	4:d:239:GLN:HE22	2.09	0.48
4:D:236:ASN:CG	4:D:238:THR:HG22	2.38	0.48
3:c:216:SER:HB3	3:c:221:GLU:HG3	1.94	0.48
16:V:19:ILE:HG21	16:V:69:ILE:HG13	1.95	0.48
2:B:139:PHE:CZ	2:B:143:LEU:HD12	2.48	0.48
2:B:352:GLU:OE2	2:B:378:LYS:NZ	2.35	0.48
35:V:201:HEC:HBC2	35:V:201:HEC:HHD	1.95	0.48
26:a:710:PHO:H61	25:d:402:CLA:H111	1.95	0.48
4:d:134:ARG:HG2	23:d:408:LMG:H302	1.96	0.48
16:v:13:ASN:OD1	16:v:15:GLU:CD	2.56	0.48
3:c:425:TRP:CD1	25:c:504:CLA:H3A	2.47	0.48
10:k:12:PRO:CB	10:k:15:TYR:HD2	2.26	0.48
16:v:13:ASN:OD1	16:v:15:GLU:OE1	2.32	0.48
16:v:72:LEU:O	16:v:76:MET:HG3	2.13	0.48
2:B:467:ILE:HD13	4:D:126:MET:HE1	1.95	0.48
5:E:40:THR:HB	20:R:4:ARG:HG2	1.95	0.48
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.95	0.48
19:z:14:ILE:O	19:z:18:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.48	0.48
5:E:9:PRO:HB3	32:E:101:LHG:HC31	1.95	0.48
11:L:22:LEU:O	11:L:26:VAL:HG13	2.14	0.48
25:b:612:CLA:H93	25:b:612:CLA:H112	1.73	0.48
16:v:57:GLU:O	16:v:61:LEU:HD12	2.13	0.48
2:B:501:ASP:OD1	2:B:503:THR:OG1	2.32	0.47
1:a:132:GLU:O	1:a:136:ARG:HG2	2.13	0.47
1:a:277:ALA:O	1:a:281:VAL:HG12	2.13	0.47
25:c:508:CLA:HBC3	25:c:510:CLA:H92	1.96	0.47
3:C:217:PRO:HB2	33:C:517:DGD:HA32	1.96	0.47
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.97	0.47
2:B:171:PRO:HB3	7:H:63:LYS:HA	1.96	0.47
3:c:399:ALA:O	3:c:401:LEU:N	2.44	0.47
3:c:23:ALA:O	3:c:26:ARG:N	2.47	0.47
15:u:46:ALA:O	15:u:50:VAL:HG22	2.15	0.47
16:v:23:GLU:O	16:v:27:LEU:HG	2.15	0.47
13:O:96:VAL:HG13	13:O:126:VAL:HG22	1.95	0.47
6:f:16:PHE:HB2	29:f:102:SQD:H82	1.96	0.47
1:A:42:LEU:HD13	27:A:610:BCR:H353	1.96	0.47
1:A:140:ARG:NE	4:D:219:GLU:O	2.46	0.47
3:C:376:ASP:HB3	3:C:379:LYS:HB2	1.95	0.47
2:b:102:VAL:HA	27:b:624:BCR:H402	1.97	0.47
3:c:176:VAL:HG11	3:c:238:ILE:HG22	1.96	0.47
1:A:283:VAL:HA	1:A:286:THR:HG22	1.96	0.47
2:B:45:PHE:HD1	2:B:60:MET:HE3	1.79	0.47
25:B:605:CLA:H121	25:B:616:CLA:H42	1.96	0.47
15:U:70:ARG:O	15:U:74:ILE:HG13	2.15	0.47
25:B:609:CLA:HMC2	25:B:610:CLA:H142	1.96	0.47
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.49	0.47
5:E:27:ILE:CG2	5:E:28:PRO:HD3	2.43	0.47
3:c:460:ASP:OD1	3:c:463:SER:OG	2.32	0.47
4:d:85:MET:HE2	4:d:90:LEU:HD21	1.96	0.47
14:t:1:FME:HE3	14:t:1:FME:HB2	1.74	0.47
20:r:24:LEU:HD22	20:r:24:LEU:H	1.80	0.47
13:O:40:ILE:CD1	13:O:243:ILE:HD13	2.42	0.47
19:z:58:ASN:O	19:z:62:VAL:HG23	2.14	0.47
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.98	0.46
25:C:507:CLA:H141	25:C:507:CLA:H162	1.64	0.46
4:d:166:SER:OG	4:d:167:TRP:N	2.47	0.46
1:A:67:VAL:HG22	4:D:312:GLU:HG2	1.96	0.46
1:A:254:TYR:HE1	4:D:133:ALA:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:617:CLA:HMD3	7:H:5:THR:HG21	1.97	0.46
13:O:31:PRO:O	36:O:301:HOH:O	2.20	0.46
3:C:318:LEU:HD21	3:C:328:VAL:HG21	1.97	0.46
7:H:5:THR:CG2	7:H:8:GLY:H	2.26	0.46
1:a:190:HIS:O	1:a:298:ASN:HB3	2.14	0.46
1:a:230:THR:O	2:b:3:LEU:HD23	2.15	0.46
2:B:191:ASN:ND2	7:H:59:ASN:O	2.47	0.46
3:c:113:VAL:O	3:c:117:VAL:HG23	2.15	0.46
3:c:130:VAL:HG21	25:c:511:CLA:H161	1.97	0.46
15:u:28:ASN:HB3	15:u:87:VAL:HG22	1.96	0.46
16:V:95:LEU:HD11	16:V:112:LEU:HD11	1.96	0.46
25:b:609:CLA:HAB	25:b:611:CLA:H151	1.98	0.46
8:i:31:ASN:OD1	8:i:33:LYS:HB2	2.16	0.46
18:x:24:THR:O	18:x:28:LEU:HD12	2.15	0.46
25:b:607:CLA:H141	25:b:607:CLA:H161	1.67	0.46
3:c:444:HIS:CE1	25:c:508:CLA:NA	2.84	0.46
13:o:6:THR:OG1	13:o:7:TYR:N	2.49	0.46
25:B:606:CLA:H92	25:B:606:CLA:H62	1.76	0.46
27:B:620:BCR:H20C	27:B:620:BCR:H361	1.81	0.46
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.97	0.46
19:Z:56:VAL:HG23	19:Z:57:LEU:HD12	1.97	0.46
1:a:286:THR:OG1	25:a:707:CLA:O1D	2.31	0.46
27:h:101:BCR:H15C	27:h:101:BCR:H351	1.83	0.46
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.97	0.46
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.97	0.46
27:A:610:BCR:H24C	27:A:610:BCR:H371	1.79	0.46
25:B:605:CLA:H141	25:B:605:CLA:H161	1.62	0.46
8:i:33:LYS:HB3	8:i:34:ARG:H	1.51	0.46
2:B:119:ASP:OD1	2:B:124:ARG:NH2	2.49	0.45
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.98	0.45
3:c:27:ASP:OD1	3:c:30:SER:OG	2.26	0.45
3:c:393:ALA:O	3:c:397:THR:HG23	2.16	0.45
13:o:53:LYS:NZ	13:o:231:HIS:HA	2.31	0.45
23:A:603:LMG:H342	23:A:603:LMG:H312	1.69	0.45
25:B:615:CLA:H61	25:B:615:CLA:H41	1.67	0.45
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.98	0.45
3:c:81:MET:HB3	3:c:86:LEU:HD12	1.97	0.45
3:c:410:VAL:HG22	3:c:411:ALA:H	1.81	0.45
27:C:516:BCR:H15C	27:C:516:BCR:H351	1.84	0.45
4:D:261:PHE:CG	4:D:267:LEU:HD12	2.52	0.45
25:c:503:CLA:H62	25:c:503:CLA:H101	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:VAL:HG23	3:C:117:VAL:HG13	1.98	0.45
1:a:60:ILE:HD12	1:a:84:PRO:HD2	1.97	0.45
25:b:607:CLA:HED1	23:b:627:LMG:HC61	1.98	0.45
13:o:95:PHE:O	13:o:126:VAL:HA	2.16	0.45
2:B:329:PRO:HD3	23:M:101:LMG:HC61	1.99	0.45
3:C:256:PRO:HA	25:C:507:CLA:HED2	1.98	0.45
27:H:102:BCR:H24C	27:H:102:BCR:H371	1.74	0.45
25:a:719:CLA:H202	25:a:719:CLA:H162	1.69	0.45
4:d:210:LEU:HA	4:d:213:ILE:HG22	1.99	0.45
1:A:174:LEU:HD22	26:A:608:PHO:H151	1.98	0.45
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.52	0.45
3:C:370:ARG:HD3	13:O:7:TYR:CD2	2.52	0.45
13:O:58:ASN:C	13:O:60:ARG:H	2.24	0.45
25:a:711:CLA:H41	25:a:711:CLA:H61	1.56	0.45
13:o:40:ILE:HG13	13:o:95:PHE:CD1	2.52	0.45
1:a:214:MET:HE1	26:a:710:PHO:O2D	2.16	0.45
23:b:627:LMG:H221	23:b:627:LMG:H191	1.67	0.45
27:c:515:BCR:H15C	27:c:515:BCR:H351	1.85	0.45
13:o:53:LYS:CE	13:o:231:HIS:HA	2.47	0.45
1:a:271:LEU:HD11	28:a:713:PL9:C4	2.46	0.45
3:c:363:GLY:O	3:c:367:GLU:HG2	2.17	0.45
25:c:509:CLA:H192	25:c:512:CLA:HAC1	1.99	0.45
10:k:17:ILE:HG23	10:k:18:PHE:CD1	2.51	0.45
1:A:131:TRP:HZ2	3:C:449:ARG:HD2	1.81	0.45
25:b:607:CLA:C4D	25:b:607:CLA:H72	2.47	0.45
32:e:101:LHG:H302	32:e:101:LHG:H271	1.64	0.45
2:B:235:GLU:HB3	2:B:473:THR:HG22	1.99	0.45
13:O:72:THR:C	13:O:73:ARG:HG3	2.41	0.45
16:V:4:THR:HG23	16:V:6:GLU:N	2.32	0.45
25:a:708:CLA:HAB	25:d:402:CLA:H72	1.98	0.45
4:d:136:VAL:HG23	4:d:138:VAL:HG13	1.99	0.45
15:U:29:ASN:HD21	15:U:88:GLU:H	1.65	0.44
20:R:24:LEU:O	20:R:28:VAL:HG12	2.17	0.44
1:a:217:SER:HA	4:d:272:LEU:HD12	1.98	0.44
3:c:90:PRO:HB3	3:c:301:PHE:HB3	2.00	0.44
18:x:24:THR:O	18:x:27:VAL:HG22	2.17	0.44
19:z:19:MET:C	19:z:23:VAL:HG12	2.42	0.44
2:B:58:GLN:C	2:B:329:PRO:HB3	2.42	0.44
29:B:626:SQD:H202	29:B:626:SQD:H171	1.74	0.44
3:C:363:GLY:O	3:C:367:GLU:HG2	2.18	0.44
5:E:17:VAL:O	5:E:21:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:26:ASP:OD2	15:U:85:THR:OG1	2.28	0.44
17:y:23:THR:O	17:y:27:MET:HG3	2.18	0.44
1:A:253:GLY:HA3	2:B:491:VAL:CG1	2.47	0.44
2:B:122:LEU:O	7:H:15:ASN:ND2	2.50	0.44
3:C:78:GLU:HG2	16:V:106:ASN:HD21	1.83	0.44
12:M:8:LEU:HG	12:m:9:ILE:HD12	2.00	0.44
13:o:30:TYR:CE2	13:o:243:ILE:HD11	2.52	0.44
18:x:25:PHE:O	18:x:27:VAL:N	2.51	0.44
25:A:607:CLA:H193	23:D:409:LMG:H401	1.99	0.44
2:B:285:ASN:O	2:B:289:GLN:HG2	2.18	0.44
3:c:257:PHE:O	3:c:261:ARG:HG3	2.17	0.44
3:c:337:LEU:HD22	3:c:342:MET:HE3	1.98	0.44
33:c:518:DGD:HA62	4:d:74:LEU:HD21	2.00	0.44
25:B:602:CLA:H111	25:B:602:CLA:H91	1.74	0.44
25:B:610:CLA:H91	25:B:610:CLA:H112	1.86	0.44
3:C:343:ARG:NH1	3:C:347:GLY:O	2.51	0.44
8:I:15:PHE:CZ	29:I:102:SQD:H381	2.53	0.44
25:a:711:CLA:H151	25:c:506:CLA:H13	1.98	0.44
25:a:711:CLA:H162	25:c:506:CLA:H101	2.00	0.44
2:b:18:ARG:NH2	29:b:601:SQD:O8	2.51	0.44
3:c:369:LEU:HD22	3:c:380:ILE:HD13	1.99	0.44
20:r:28:VAL:O	20:r:32:GLN:HG2	2.18	0.44
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.44
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.87	0.44
12:M:17:VAL:HG21	23:M:101:LMG:H401	1.99	0.44
15:U:16:LYS:HE3	15:U:88:GLU:HB2	2.00	0.44
1:a:165:GLN:NE2	1:a:294:ALA:O	2.50	0.44
3:c:42:LEU:HD22	3:c:48:LYS:HB3	2.00	0.44
3:c:256:PRO:HA	25:c:506:CLA:HED2	2.00	0.44
11:l:10:VAL:O	12:m:28:GLN:NE2	2.47	0.44
19:z:3:ILE:O	19:z:5:PHE:N	2.41	0.44
20:r:10:LEU:HA	20:r:13:LEU:HD23	2.00	0.44
1:a:85:SER:HA	1:a:109:GLY:HA3	1.98	0.44
2:b:223:GLN:HE21	2:b:224:ARG:HG2	1.83	0.44
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.53	0.44
25:c:512:CLA:H111	25:c:512:CLA:H142	1.72	0.44
4:D:225:ASP:HB2	4:D:234:ALA:HB1	2.00	0.44
25:d:403:CLA:H143	25:d:403:CLA:H162	1.79	0.44
27:k:101:BCR:H20C	27:k:101:BCR:H361	1.84	0.44
13:o:53:LYS:HD3	13:o:232:GLU:H	1.82	0.44
3:C:315:MET:HB2	3:C:351:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:42:LEU:O	19:Z:46:LEU:N	2.47	0.44
1:A:46:ILE:HD12	27:A:610:BCR:H15C	2.00	0.43
28:D:406:PL9:H371	28:D:406:PL9:H351	1.63	0.43
27:H:102:BCR:H15C	27:H:102:BCR:H351	1.87	0.43
11:L:2:GLU:CD	11:L:2:GLU:H	2.26	0.43
13:O:6:THR:OG1	13:O:7:TYR:N	2.51	0.43
1:a:212:CYS:HB2	4:d:211:CYS:HB2	2.00	0.43
4:d:241:GLU:N	4:d:241:GLU:OE2	2.50	0.43
16:v:13:ASN:OD1	16:v:13:ASN:N	2.50	0.43
4:D:140:PRO:O	4:D:144:ILE:HG12	2.18	0.43
5:E:25:ILE:C	5:E:28:PRO:HD2	2.43	0.43
13:o:36:GLN:HB3	13:o:38:TYR:CE2	2.53	0.43
25:C:509:CLA:H171	25:C:509:CLA:H13	1.84	0.43
18:x:25:PHE:O	18:x:29:ILE:HD12	2.19	0.43
28:A:611:PL9:H121	28:A:611:PL9:HC8	1.53	0.43
3:C:257:PHE:O	3:C:261:ARG:HG3	2.19	0.43
25:D:402:CLA:H141	25:D:402:CLA:H162	1.69	0.43
5:E:27:ILE:HG13	6:F:31:ILE:HG21	2.00	0.43
6:F:31:ILE:HD13	6:F:34:LEU:HD23	2.00	0.43
20:R:10:LEU:O	20:R:14:LEU:N	2.29	0.43
1:a:77:ILE:HD11	14:t:6:TYR:HB3	2.00	0.43
13:o:39:ARG:NH2	13:o:82:GLN:OE1	2.51	0.43
2:B:201:HIS:HE2	25:B:604:CLA:C2B	2.31	0.43
25:C:504:CLA:H193	25:C:504:CLA:H161	1.85	0.43
27:D:405:BCR:H15C	27:D:405:BCR:H351	1.88	0.43
16:V:3:LEU:HG	16:V:8:LEU:HD21	1.99	0.43
2:b:386:ALA:HB3	15:u:102:LEU:HD22	2.00	0.43
8:I:33:LYS:NZ	8:I:33:LYS:HB3	2.33	0.43
3:c:186:TYR:HA	3:c:196:VAL:HA	2.00	0.43
2:B:63:LEU:HA	2:B:66:MET:HE3	2.01	0.43
2:B:469:HIS:HE1	25:B:612:CLA:NA	2.16	0.43
25:B:604:CLA:H192	25:B:604:CLA:H162	1.81	0.43
27:B:618:BCR:H11C	27:B:618:BCR:H341	1.87	0.43
25:C:514:CLA:H92	25:C:514:CLA:H62	1.79	0.43
33:C:517:DGD:HAT2	33:C:517:DGD:HAH1	1.73	0.43
17:y:24:MET:HG2	17:y:27:MET:HE2	2.00	0.43
2:B:419:SER:O	2:B:423:LYS:HG2	2.19	0.43
4:D:43:LEU:HD23	4:D:113:PHE:HZ	1.84	0.43
4:D:84:SER:O	5:E:69:ARG:HB2	2.18	0.43
32:D:408:LHG:H372	32:D:408:LHG:H122	2.00	0.43
15:U:58:VAL:HG12	15:U:79:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.01	0.43
1:A:228:THR:CG2	1:A:229:GLU:H	2.32	0.43
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.43
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.52	0.43
25:b:620:CLA:H93	25:b:620:CLA:H111	1.90	0.43
25:c:509:CLA:H142	25:c:509:CLA:H112	1.82	0.43
16:v:24:LYS:HD2	16:v:24:LYS:N	2.32	0.43
27:C:516:BCR:H24C	27:C:516:BCR:H371	1.84	0.43
25:b:619:CLA:H51	32:d:406:LHG:H361	1.99	0.43
13:o:140:THR:O	13:o:201:VAL:HG22	2.19	0.43
17:y:24:MET:O	17:y:28:ILE:HG12	2.18	0.43
1:a:307:ILE:HD11	1:a:311:GLY:O	2.18	0.42
3:c:168:LEU:HD11	25:c:509:CLA:H61	2.01	0.42
4:d:216:ALA:O	4:d:220:ASN:ND2	2.47	0.42
2:B:265:ILE:HA	2:B:448:ARG:NH2	2.34	0.42
4:D:350:ASN:O	4:D:352:LEU:N	2.45	0.42
23:D:409:LMG:H161	23:D:409:LMG:H192	1.54	0.42
13:O:59:LYS:HB3	13:O:60:ARG:HH11	1.84	0.42
2:b:135:LEU:HD11	2:b:234:ILE:HA	2.01	0.42
3:c:437:PHE:HA	25:c:508:CLA:HMC2	2.01	0.42
4:d:163:GLY:HA3	4:d:290:ALA:HB1	2.02	0.42
16:v:22:THR:H	16:v:25:GLN:NE2	2.17	0.42
20:r:10:LEU:HB3	20:r:11:PRO:HD3	2.00	0.42
28:A:611:PL9:H512	29:D:410:SQD:H331	2.01	0.42
3:C:154:LYS:HD3	3:C:266:TRP:CE2	2.54	0.42
13:O:207:ARG:HE	13:O:207:ARG:HB3	1.67	0.42
1:a:305:SER:HA	9:j:39:SER:HB3	2.01	0.42
2:b:61:PHE:CZ	25:b:610:CLA:HMA1	2.54	0.42
3:c:71:GLU:HB3	3:c:86:LEU:HD22	2.01	0.42
3:c:288:CYS:SG	33:c:516:DGD:HB32	2.59	0.42
17:y:38:LEU:O	17:y:41:VAL:HG22	2.19	0.42
19:z:40:ILE:O	19:z:44:SER:OG	2.25	0.42
20:r:9:LEU:HD22	20:r:9:LEU:HA	1.88	0.42
3:C:95:LEU:HD21	25:C:502:CLA:OBD	2.19	0.42
1:a:324:ALA:O	1:a:328:MET:HG3	2.19	0.42
25:a:719:CLA:H92	25:a:719:CLA:H62	1.86	0.42
2:b:475:PHE:CD1	4:d:140:PRO:HG3	2.54	0.42
27:b:602:BCR:H15C	27:b:602:BCR:H351	1.92	0.42
3:c:211:GLY:O	3:c:215:LYS:HG3	2.20	0.42
23:c:520:LMG:O2	23:c:520:LMG:HC71	2.18	0.42
25:C:512:CLA:H152	25:C:512:CLA:H112	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:LYS:NZ	4:D:131:GLU:OE1	2.52	0.42
15:U:57:SER:OG	15:U:60:ASP:OD2	2.32	0.42
3:c:258:GLY:O	3:c:262:ARG:HG2	2.19	0.42
13:o:53:LYS:HE2	13:o:231:HIS:CA	2.50	0.42
27:B:619:BCR:H20C	27:B:619:BCR:H361	1.83	0.42
3:C:178:LYS:NZ	3:C:184:GLY:O	2.53	0.42
16:V:63:THR:HB	16:V:83:ASP:HA	2.00	0.42
25:b:616:CLA:H162	25:b:616:CLA:H202	1.83	0.42
27:b:625:BCR:H20C	27:b:625:BCR:H361	1.83	0.42
3:c:125:LEU:HA	25:c:513:CLA:HMC1	2.02	0.42
3:c:187:ASP:HB2	3:c:230:LEU:HD12	2.01	0.42
27:k:102:BCR:H371	27:k:102:BCR:H24C	1.81	0.42
23:A:603:LMG:H341	23:A:603:LMG:H372	1.91	0.42
32:B:625:LHG:H152	32:L:101:LHG:H281	2.01	0.42
29:D:410:SQD:H272	29:D:410:SQD:H242	1.88	0.42
1:a:223:LEU:HD23	4:d:139:ARG:NH1	2.35	0.42
25:b:612:CLA:H52	27:b:625:BCR:H321	2.01	0.42
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.01	0.42
23:f:101:LMG:H351	23:f:101:LMG:H382	1.88	0.42
13:o:193:THR:HG21	13:o:220:LEU:HD12	2.02	0.42
2:B:486:LEU:HD23	2:B:487:SER:N	2.34	0.42
25:B:607:CLA:H193	25:B:607:CLA:H161	1.83	0.42
25:B:615:CLA:H143	25:B:615:CLA:H111	1.88	0.42
25:C:502:CLA:H202	25:C:502:CLA:H161	1.85	0.42
11:L:7:ARG:H	11:L:7:ARG:HG2	1.67	0.42
1:a:335:ASN:HD21	13:o:157:LEU:H	1.67	0.42
28:a:713:PL9:H28	32:e:101:LHG:H223	2.01	0.42
27:b:602:BCR:H20C	27:b:602:BCR:H361	1.89	0.42
4:d:134:ARG:HG2	23:d:408:LMG:O10	2.19	0.42
20:r:20:VAL:O	20:r:24:LEU:HD22	2.20	0.42
29:B:623:SQD:H82	29:B:623:SQD:H242	2.01	0.42
25:a:711:CLA:H102	25:a:711:CLA:H62	1.80	0.42
2:b:70:GLY:HA2	2:b:178:VAL:HG11	2.02	0.42
4:d:218:VAL:O	4:d:222:LEU:HG	2.20	0.42
2:B:494:GLY:HA3	5:E:4:THR:O	2.20	0.41
3:C:425:TRP:NE1	25:C:505:CLA:H3A	2.33	0.41
23:M:101:LMG:H392	23:M:101:LMG:H421	1.94	0.41
1:a:285:PHE:O	1:a:289:GLY:N	2.52	0.41
2:b:151:PHE:HA	2:b:202:HIS:O	2.20	0.41
15:u:45:LEU:HD11	15:u:71:GLN:HB2	2.02	0.41
20:R:4:ARG:C	20:R:6:LEU:H	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.55	0.41
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.02	0.41
1:A:112:TYR:O	1:A:116:ILE:HG23	2.20	0.41
1:A:133:LEU:HD23	4:D:256:ILE:HG12	2.02	0.41
1:A:228:THR:CG2	1:A:229:GLU:N	2.83	0.41
25:C:505:CLA:H62	25:C:505:CLA:H41	1.91	0.41
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.54	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.55	0.41
32:D:408:LHG:H291	32:D:408:LHG:H321	1.89	0.41
25:a:711:CLA:HAA2	23:a:715:LMG:H112	2.02	0.41
10:k:24:VAL:HB	17:y:25:ILE:HD13	2.02	0.41
13:o:52:VAL:CG2	13:o:68:THR:HG21	2.50	0.41
19:z:55:GLY:O	19:z:58:ASN:HB3	2.21	0.41
1:A:179:THR:O	1:A:183:MET:HG3	2.20	0.41
1:A:228:THR:HG22	1:A:229:GLU:N	2.35	0.41
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.02	0.41
29:D:410:SQD:H301	29:D:410:SQD:H271	1.89	0.41
16:V:9:THR:HG22	16:V:20:THR:HG23	2.01	0.41
18:X:27:VAL:O	18:X:31:ILE:HG13	2.20	0.41
2:b:201:HIS:HB2	25:b:608:CLA:NB	2.35	0.41
25:b:610:CLA:H62	25:b:610:CLA:H41	1.72	0.41
32:d:407:LHG:HC82	32:d:407:LHG:H112	1.88	0.41
15:u:88:GLU:CG	15:u:91:LEU:HD23	2.50	0.41
2:B:155:ALA:O	2:B:159:THR:OG1	2.36	0.41
25:B:603:CLA:H111	25:B:603:CLA:H152	1.83	0.41
25:B:604:CLA:H62	25:B:604:CLA:H41	1.82	0.41
4:D:85:MET:HE2	4:D:90:LEU:HD21	2.02	0.41
13:O:78:LEU:HD13	13:O:122:VAL:HG22	2.02	0.41
2:b:16:PRO:O	2:b:20:ILE:HG12	2.20	0.41
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.03	0.41
1:a:224:ILE:O	4:d:265:ARG:NH2	2.52	0.41
25:c:503:CLA:H161	25:c:503:CLA:H193	1.87	0.41
13:o:32:ILE:HG22	13:o:135:SER:HA	2.03	0.41
1:A:259:ILE:HB	1:A:260:PHE:H	1.74	0.41
25:B:611:CLA:H202	25:B:611:CLA:H161	1.85	0.41
25:B:613:CLA:H8	25:B:613:CLA:H122	1.88	0.41
3:C:251:HIS:HE1	25:C:507:CLA:NA	2.16	0.41
2:b:71:VAL:HG23	25:b:612:CLA:HMA2	2.02	0.41
25:b:607:CLA:H62	27:h:101:BCR:H402	2.03	0.41
27:b:624:BCR:H15C	27:b:624:BCR:H351	1.84	0.41
5:e:27:ILE:HB	5:e:28:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:26:PRO:O	10:k:29:PRO:HD2	2.20	0.41
27:k:101:BCR:H11C	27:k:101:BCR:H341	1.97	0.41
13:o:115:ARG:O	13:o:117:PRO:HD3	2.21	0.41
27:t:103:BCR:H20C	27:t:103:BCR:H361	1.87	0.41
1:A:225:ARG:HG2	2:B:481:GLY:C	2.45	0.41
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.41
3:C:62:PHE:CZ	10:K:28:ILE:HD11	2.55	0.41
25:C:505:CLA:OBD	23:C:520:LMG:O2	2.36	0.41
27:D:405:BCR:H11C	27:D:405:BCR:H341	1.92	0.41
34:E:102:HEM:CGD	6:F:19:ARG:HH21	2.34	0.41
4:d:203:GLY:HA3	4:d:278:GLY:HA3	2.03	0.41
5:e:36:LEU:HD13	20:r:7:VAL:HG12	2.03	0.41
13:o:224:ASP:HB3	13:o:227:ALA:HB3	2.03	0.41
16:v:115:ILE:O	16:v:119:ILE:HG13	2.21	0.41
1:A:252:HIS:CE1	1:A:266:ASN:HB3	2.55	0.41
27:A:610:BCR:H15C	27:A:610:BCR:H351	1.87	0.41
2:B:121:GLU:CD	7:H:12:ARG:HH21	2.29	0.41
2:B:477:ASP:OD1	2:B:477:ASP:N	2.52	0.41
25:B:605:CLA:H142	25:B:616:CLA:H62	2.02	0.41
3:C:71:GLU:HB3	3:C:86:LEU:HD22	2.02	0.41
3:C:215:LYS:HE2	3:C:215:LYS:HB3	1.92	0.41
3:C:279:LEU:HD23	3:C:282:MET:HE3	2.03	0.41
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.55	0.41
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.84	0.41
13:O:180:GLU:CD	13:O:180:GLU:H	2.29	0.41
15:U:42:TYR:HA	15:U:43:PRO:HA	1.83	0.41
20:R:10:LEU:HD22	20:R:10:LEU:H	1.86	0.41
1:a:220:THR:HA	1:a:223:LEU:HD21	2.03	0.41
26:a:709:PHO:H161	26:a:709:PHO:H141	1.65	0.41
27:a:712:BCR:H11C	27:a:712:BCR:H341	1.93	0.41
27:a:712:BCR:H24C	27:a:712:BCR:H371	1.79	0.41
2:b:58:GLN:C	2:b:329:PRO:HB3	2.46	0.41
25:b:607:CLA:HAC1	27:h:101:BCR:H383	2.03	0.41
3:c:124:VAL:O	25:c:513:CLA:HAC1	2.21	0.41
4:d:87:HIS:HB2	33:h:102:DGD:HG11	2.02	0.41
4:d:262:SER:OG	32:d:407:LHG:O4	2.26	0.41
27:k:102:BCR:H20C	27:k:102:BCR:H361	1.84	0.41
16:v:42:VAL:HG12	16:v:47:LYS:HE2	2.02	0.41
1:A:183:MET:HA	25:A:606:CLA:HMD1	2.02	0.41
4:D:273:PHE:CE2	32:L:101:LHG:H112	2.56	0.41
32:D:407:LHG:O1	32:L:101:LHG:O4	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:707:CLA:H202	32:d:407:LHG:H161	2.03	0.41
29:a:714:SQD:H223	29:a:714:SQD:H192	1.85	0.41
2:b:247:PHE:HB2	25:b:614:CLA:HBC1	2.03	0.41
2:b:458:PHE:HB3	25:b:610:CLA:HBC2	2.03	0.41
18:x:20:VAL:O	18:x:24:THR:OG1	2.26	0.41
1:A:103:ASP:OD1	1:A:103:ASP:N	2.54	0.40
25:A:609:CLA:HBC1	29:I:102:SQD:H182	2.02	0.40
4:D:68:LEU:HD13	6:F:40:MET:HE2	2.03	0.40
10:K:40:GLN:HA	10:K:43:VAL:HG22	2.04	0.40
20:R:6:LEU:CD1	20:R:10:LEU:HD21	2.48	0.40
2:b:265:ILE:HD11	7:h:62:TRP:CH2	2.56	0.40
10:k:40:GLN:HA	10:k:43:VAL:HG22	2.02	0.40
4:D:56:THR:HB	5:E:49:THR:HG23	2.02	0.40
4:D:79:SER:HA	4:D:172:SER:HB3	2.02	0.40
29:I:102:SQD:H182	29:I:102:SQD:H212	1.81	0.40
19:Z:33:TRP:CG	19:Z:33:TRP:O	2.73	0.40
32:a:720:LHG:HC31	3:c:36:TRP:CZ3	2.56	0.40
25:b:615:CLA:H161	25:b:615:CLA:H141	1.67	0.40
25:b:621:CLA:H61	25:b:621:CLA:H92	1.89	0.40
3:c:132:HIS:CE1	25:c:513:CLA:NA	2.88	0.40
25:c:511:CLA:H2	10:k:39:TRP:NE1	2.36	0.40
1:A:129:ARG:NH2	4:D:255:GLN:O	2.54	0.40
19:Z:14:ILE:HD13	19:Z:14:ILE:HA	1.94	0.40
27:b:625:BCR:H11C	27:b:625:BCR:H341	1.95	0.40
3:c:457:LYS:HE3	4:d:228:GLY:O	2.22	0.40
25:D:402:CLA:H91	25:D:402:CLA:H112	1.91	0.40
27:D:405:BCR:H20C	27:D:405:BCR:H361	1.85	0.40
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.03	0.40
29:b:601:SQD:H161	29:b:601:SQD:H131	1.90	0.40
13:o:3:GLN:O	13:o:4:THR:HG23	2.20	0.40
25:A:607:CLA:HMD3	4:D:182:LEU:HD11	2.03	0.40
5:E:22:ILE:HA	20:R:18:TRP:HE1	1.87	0.40
32:E:101:LHG:H261	32:E:101:LHG:H291	1.71	0.40
1:a:271:LEU:HD11	28:a:713:PL9:C3	2.52	0.40
25:b:620:CLA:H111	25:b:620:CLA:H142	1.87	0.40
27:b:623:BCR:H351	27:b:623:BCR:H15C	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	324 (98%)	7 (2%)	1 (0%)	36	66
1	a	332/344 (96%)	325 (98%)	6 (2%)	1 (0%)	36	66
2	B	502/510 (98%)	482 (96%)	19 (4%)	1 (0%)	43	72
2	b	503/510 (99%)	484 (96%)	19 (4%)	0	100	100
3	C	449/461 (97%)	431 (96%)	17 (4%)	1 (0%)	43	72
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	30	60
4	D	339/352 (96%)	325 (96%)	14 (4%)	0	100	100
4	d	339/352 (96%)	323 (95%)	16 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
7	h	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	29 (85%)	5 (15%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	13
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	3	13
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	3	13
11	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	3	11
12	m	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	3	11
13	O	242/272 (89%)	230 (95%)	10 (4%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	223 (92%)	15 (6%)	4 (2%)	7	25
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	88 (93%)	7 (7%)	0	100	100
16	V	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	36/41 (88%)	32 (89%)	3 (8%)	1 (3%)	4	14
19	Z	60/62 (97%)	51 (85%)	1 (2%)	8 (13%)	0	0
19	z	60/62 (97%)	53 (88%)	4 (7%)	3 (5%)	1	5
20	R	32/41 (78%)	29 (91%)	3 (9%)	0	100	100
20	r	32/41 (78%)	30 (94%)	1 (3%)	1 (3%)	3	12
All	All	5237/5694 (92%)	4987 (95%)	220 (4%)	30 (1%)	21	51

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	Z	30	PRO
19	Z	31	GLN
19	Z	33	TRP
19	Z	61	VAL
3	c	24	THR
10	k	12	PRO
13	o	53	LYS
13	o	55	GLU
19	z	32	ASP
3	C	416	SER
10	K	14	ALA
12	M	32	GLN
19	Z	3	ILE
19	Z	32	ASP
3	c	416	SER
18	x	26	ALA
13	O	132	ASN

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Mol	Chain	Res	Type
19	Z	2	THR
13	o	54	GLU
1	a	259	ILE
19	z	2	THR
19	z	4	LEU
20	r	21	ARG
13	O	56	PRO
19	Z	4	LEU
12	m	32	GLN
2	B	488	PRO
9	j	6	GLY
1	A	259	ILE
13	o	56	PRO

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	270/280 (96%)	268 (99%)	2 (1%)	76	91
1	a	270/280 (96%)	269 (100%)	1 (0%)	84	94
2	B	402/407 (99%)	398 (99%)	4 (1%)	68	88
2	b	402/407 (99%)	402 (100%)	0	100	100
3	C	352/362 (97%)	352 (100%)	0	100	100
3	c	352/362 (97%)	350 (99%)	2 (1%)	78	92
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	276/283 (98%)	275 (100%)	1 (0%)	84	94
5	E	72/73 (99%)	72 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	53/53 (100%)	53 (100%)	0	100	100
7	h	53/53 (100%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
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	73
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	207/228 (91%)	207 (100%)	0	100	100
13	o	207/228 (91%)	205 (99%)	2 (1%)	68	88
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	116 (99%)	1 (1%)	70	89
17	Y	20/37 (54%)	20 (100%)	0	100	100
17	y	23/37 (62%)	22 (96%)	1 (4%)	26	60
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	30/34 (88%)	30 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	81
19	z	52/52 (100%)	52 (100%)	0	100	100
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	28/33 (85%)	27 (96%)	1 (4%)	31	66
All	All	4339/4650 (93%)	4322 (100%)	17 (0%)	84	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	245	THR

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Mol	Chain	Res	Type
2	B	107	LEU
2	B	362	PHE
2	B	394	GLN
2	B	467	ILE
11	L	26	VAL
19	Z	1	MET
1	a	270	SER
3	c	346	THR
3	c	420	VAL
4	d	247	VAL
13	o	57	LYS
13	o	141	ASP
16	v	66	ARG
17	y	17	GLU
20	r	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	241	GLN
1	A	247	ASN
1	A	252	HIS
2	B	53	ASN
2	B	216	HIS
2	B	331	ASN
2	B	409	GLN
3	C	201	ASN
3	C	311	GLN
3	C	322	GLN
3	C	415	ASN
4	D	98	GLN
4	D	224	GLN
5	E	60	GLN
5	E	74	GLN
5	E	82	GLN
11	L	8	GLN
13	O	82	GLN
13	O	130	GLN
15	U	29	ASN
15	U	78	ASN
16	V	106	ASN

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Mol	Chain	Res	Type
16	V	118	HIS
20	R	32	GLN
1	a	165	GLN
1	a	261	GLN
1	a	296	ASN
1	a	335	ASN
2	b	216	HIS
2	b	223	GLN
2	b	317	ASN
2	b	331	ASN
2	b	343	HIS
2	b	490	GLN
3	c	322	GLN
4	d	186	GLN
4	d	239	GLN
4	d	338	ASN
5	e	74	GLN
10	k	40	GLN
12	m	5	GLN
13	o	46	GLN
13	o	61	GLN
13	o	147	ASN
13	o	231	HIS
13	o	236	GLN
16	v	25	GLN
16	v	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	T	1	14	8,9,10	0.98	0	8,9,11	1.15	1 (12%)
8	FME	i	1	8	8,9,10	0.97	0	8,9,11	1.10	1 (12%)
8	FME	I	1	8	8,9,10	0.99	0	8,9,11	1.19	0
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	1.03	0
14	FME	t	1	14	8,9,10	0.97	0	8,9,11	1.03	0
12	FME	M	1	12	8,9,10	0.94	0	8,9,11	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	2.25	114.62	110.52
8	i	1	FME	CB-CA-N	2.06	114.27	110.52

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	t	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 6 are monoatomic and 23 are unknown - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	CLA	b	614	2	69,73,73	1.12	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	C	504	3	69,73,73	1.14	6 (8%)	82,113,113	1.24	5 (6%)
25	CLA	d	403	4	69,73,73	1.12	5 (7%)	82,113,113	1.19	8 (9%)
25	CLA	C	512	3	69,73,73	1.14	5 (7%)	82,113,113	1.24	6 (7%)
26	PHO	D	401	-	58,69,69	2.17	9 (15%)	55,99,99	1.45	7 (12%)
29	SQD	D	410	-	41,43,54	1.07	3 (7%)	51,54,65	1.57	10 (19%)
25	CLA	c	513	3	69,73,73	1.12	5 (7%)	82,113,113	1.23	9 (10%)
27	BCR	b	602	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	7 (12%)
25	CLA	B	613	2	69,73,73	1.13	7 (10%)	82,113,113	1.23	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.41	9 (11%)
23	LMG	b	627	-	51,51,55	0.77	0	59,59,63	1.27	4 (6%)
31	BCT	a	706	22	3,3,3	3.22	1 (33%)	2,3,3	2.78	2 (100%)
27	BCR	k	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.14	2 (3%)
33	DGD	c	517	-	63,63,67	0.95	4 (6%)	77,77,81	1.40	9 (11%)
28	PL9	a	713	-	55,55,55	0.96	4 (7%)	68,69,69	1.49	12 (17%)
34	HEM	e	102	5,6	50,50,50	1.51	8 (16%)	67,82,82	1.24	5 (7%)
25	CLA	c	504	36	62,66,73	1.19	8 (12%)	73,104,113	1.25	7 (9%)
23	LMG	b	626	-	51,51,55	0.80	3 (5%)	59,59,63	1.54	9 (15%)
25	CLA	C	513	3	69,73,73	1.13	6 (8%)	82,113,113	1.28	5 (6%)
25	CLA	C	503	3	69,73,73	1.13	6 (8%)	82,113,113	1.20	6 (7%)
29	SQD	A	612	-	50,52,54	0.97	3 (6%)	60,63,65	1.61	12 (20%)
32	LHG	E	101	-	48,48,48	0.68	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	D	404	4	69,73,73	1.13	6 (8%)	82,113,113	1.18	5 (6%)
25	CLA	B	603	2	69,73,73	1.13	6 (8%)	82,113,113	1.16	6 (7%)
27	BCR	a	712	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	6 (10%)
25	CLA	B	602	36	69,73,73	1.13	7 (10%)	82,113,113	1.21	5 (6%)
25	CLA	b	621	2	69,73,73	1.13	6 (8%)	82,113,113	1.24	6 (7%)
25	CLA	c	506	3	69,73,73	1.12	5 (7%)	82,113,113	1.15	5 (6%)
25	CLA	c	508	3	69,73,73	1.13	5 (7%)	82,113,113	1.19	6 (7%)
25	CLA	b	619	2	69,73,73	1.13	6 (8%)	82,113,113	1.25	7 (8%)
25	CLA	b	615	2	69,73,73	1.13	7 (10%)	82,113,113	1.20	6 (7%)
27	BCR	B	620	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	5 (8%)
25	CLA	c	511	3	69,73,73	1.14	7 (10%)	82,113,113	1.22	5 (6%)
25	CLA	b	609	2	69,73,73	1.13	6 (8%)	82,113,113	1.10	5 (6%)
27	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	8 (14%)
25	CLA	a	708	36	69,73,73	1.13	7 (10%)	82,113,113	1.17	6 (7%)
21	OEX	a	702	3,1,36	0,14,14	-	-	-	-	-
25	CLA	B	608	36	69,73,73	1.13	6 (8%)	82,113,113	1.13	5 (6%)
32	LHG	b	629	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
33	DGD	H	103	-	63,63,67	0.87	1 (1%)	77,77,81	1.34	7 (9%)
25	CLA	a	711	1	69,73,73	1.13	6 (8%)	82,113,113	1.17	6 (7%)
28	PL9	d	405	-	55,55,55	0.94	4 (7%)	68,69,69	1.49	13 (19%)
25	CLA	B	610	2	69,73,73	1.15	6 (8%)	82,113,113	1.19	6 (7%)
27	BCR	H	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMG	a	701	-	51,51,55	0.79	0	59,59,63	1.33	7 (11%)
25	CLA	b	611	2	69,73,73	1.13	6 (8%)	82,113,113	1.17	6 (7%)
27	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
27	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	8 (14%)
28	PL9	D	406	-	55,55,55	0.97	4 (7%)	68,69,69	1.50	12 (17%)
23	LMG	B	621	-	51,51,55	0.73	0	59,59,63	1.37	8 (13%)
23	LMG	b	628	-	8,8,55	0.14	0	7,7,63	0.93	0
23	LMG	A	603	-	51,51,55	0.94	3 (5%)	59,59,63	1.41	8 (13%)
26	PHO	A	608	-	58,69,69	2.19	9 (15%)	55,99,99	1.44	7 (12%)
32	LHG	L	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
23	LMG	C	520	-	51,51,55	0.74	1 (1%)	59,59,63	1.31	5 (8%)
27	BCR	k	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	6 (10%)
25	CLA	B	611	36	69,73,73	1.13	6 (8%)	82,113,113	1.19	6 (7%)
25	CLA	B	612	2	69,73,73	1.13	6 (8%)	82,113,113	1.23	7 (8%)
27	BCR	C	516	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
25	CLA	B	609	2	69,73,73	1.12	6 (8%)	82,113,113	1.12	6 (7%)
23	LMG	C	501	-	51,51,55	0.73	1 (1%)	59,59,63	1.32	5 (8%)
27	BCR	b	623	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	7 (12%)
25	CLA	B	614	2	69,73,73	1.14	6 (8%)	82,113,113	1.21	5 (6%)
29	SQD	f	102	-	39,41,54	1.09	3 (7%)	49,52,65	1.50	9 (18%)
25	CLA	a	707	1	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
31	BCT	A	615	22	3,3,3	3.24	1 (33%)	2,3,3	2.73	2 (100%)
23	LMG	f	101	-	51,51,55	0.71	1 (1%)	59,59,63	1.36	7 (11%)
35	HEC	v	201	16	50,50,50	1.56	8 (16%)	68,82,82	1.48	9 (13%)
25	CLA	C	509	3	69,73,73	1.12	6 (8%)	82,113,113	1.22	7 (8%)
25	CLA	A	607	36	69,73,73	1.14	6 (8%)	82,113,113	1.19	7 (8%)
23	LMG	D	409	-	51,51,55	0.72	1 (1%)	59,59,63	1.30	5 (8%)
27	BCR	t	103	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	5 (8%)
28	PL9	A	611	-	55,55,55	1.01	4 (7%)	68,69,69	1.49	13 (19%)
27	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	C	508	36	69,73,73	1.14	6 (8%)	82,113,113	1.26	4 (4%)
25	CLA	b	616	36	69,73,73	1.14	7 (10%)	82,113,113	1.15	4 (4%)
25	CLA	b	618	2	69,73,73	1.13	6 (8%)	82,113,113	1.22	5 (6%)
25	CLA	c	505	3	69,73,73	1.13	7 (10%)	82,113,113	1.12	4 (4%)
26	PHO	a	710	-	58,69,69	2.17	9 (15%)	55,99,99	1.43	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	D	405	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
25	CLA	B	604	2	69,73,73	1.12	6 (8%)	82,113,113	1.16	5 (6%)
27	BCR	b	625	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	8 (14%)
29	SQD	A	614	-	39,39,54	0.89	2 (5%)	41,41,65	1.21	3 (7%)
25	CLA	C	510	3	69,73,73	1.14	6 (8%)	82,113,113	1.20	4 (4%)
25	CLA	b	622	2	51,55,73	1.29	7 (13%)	60,91,113	1.33	6 (10%)
33	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.40	11 (14%)
33	DGD	h	102	-	63,63,67	0.88	1 (1%)	77,77,81	1.29	7 (9%)
23	LMG	a	715	-	51,51,55	0.75	0	59,59,63	1.32	6 (10%)
25	CLA	C	514	3	69,73,73	1.12	5 (7%)	82,113,113	1.22	8 (9%)
21	OEX	A	601	3,1,36	0,14,14	-	-	-	-	-
25	CLA	B	607	2	69,73,73	1.14	7 (10%)	82,113,113	1.19	4 (4%)
25	CLA	c	503	3	69,73,73	1.14	6 (8%)	82,113,113	1.24	6 (7%)
23	LMG	c	520	-	51,51,55	0.82	1 (1%)	59,59,63	1.36	5 (8%)
23	LMG	M	101	-	51,51,55	0.74	0	59,59,63	1.33	5 (8%)
27	BCR	Y	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.17	5 (8%)
32	LHG	d	406	-	48,48,48	0.62	2 (4%)	51,54,54	1.30	7 (13%)
25	CLA	c	501	3	69,73,73	1.13	7 (10%)	82,113,113	1.19	6 (7%)
27	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	6 (10%)
25	CLA	b	608	2	69,73,73	1.13	6 (8%)	82,113,113	1.10	5 (6%)
27	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	7 (12%)
25	CLA	c	509	3	69,73,73	1.14	5 (7%)	82,113,113	1.24	6 (7%)
29	SQD	I	102	-	39,39,54	0.87	2 (5%)	41,41,65	1.23	2 (4%)
25	CLA	c	502	3	69,73,73	1.12	7 (10%)	82,113,113	1.21	5 (6%)
33	DGD	C	518	-	63,63,67	0.92	4 (6%)	77,77,81	1.43	10 (12%)
25	CLA	C	505	36	69,73,73	1.12	5 (7%)	82,113,113	1.16	7 (8%)
27	BCR	b	624	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
32	LHG	D	407	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
34	HEM	E	102	5,6	50,50,50	1.50	8 (16%)	67,82,82	1.14	6 (8%)
27	BCR	d	404	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	8 (14%)
25	CLA	C	502	3	69,73,73	1.13	7 (10%)	82,113,113	1.20	6 (7%)
25	CLA	A	609	1	58,62,73	1.23	6 (10%)	68,99,113	1.25	6 (8%)
25	CLA	C	507	3	69,73,73	1.14	7 (10%)	82,113,113	1.14	5 (6%)
25	CLA	c	510	3	69,73,73	1.13	6 (8%)	82,113,113	1.20	6 (7%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	h	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
32	LHG	D	408	-	48,48,48	0.61	0	51,54,54	1.27	6 (11%)
33	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.41	9 (11%)
33	DGD	c	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	10 (12%)
25	CLA	B	606	2	69,73,73	1.13	7 (10%)	82,113,113	1.14	4 (4%)
23	LMG	d	408	-	39,39,55	0.54	1 (2%)	41,41,63	1.30	4 (9%)
25	CLA	b	610	2	69,73,73	1.14	5 (7%)	82,113,113	1.31	7 (8%)
25	CLA	b	620	2	69,73,73	1.13	5 (7%)	82,113,113	1.13	6 (7%)
29	SQD	B	626	-	52,54,54	0.95	3 (5%)	62,65,65	1.64	9 (14%)
25	CLA	a	719	36	69,73,73	1.13	7 (10%)	82,113,113	1.15	7 (8%)
35	HEC	V	201	16	50,50,50	1.56	8 (16%)	68,82,82	1.46	10 (14%)
25	CLA	B	605	2	69,73,73	1.14	7 (10%)	82,113,113	1.33	7 (8%)
29	SQD	b	601	-	52,54,54	0.94	3 (5%)	62,65,65	1.63	10 (16%)
25	CLA	c	507	36	69,73,73	1.14	5 (7%)	82,113,113	1.24	4 (4%)
26	PHO	a	709	-	58,69,69	2.18	9 (15%)	55,99,99	1.41	7 (12%)
25	CLA	b	617	2	69,73,73	1.12	7 (10%)	82,113,113	1.24	7 (8%)
25	CLA	C	511	3	69,73,73	1.13	6 (8%)	82,113,113	1.21	6 (7%)
25	CLA	A	606	1	69,73,73	1.13	6 (8%)	82,113,113	1.11	6 (7%)
25	CLA	b	612	2	69,73,73	1.13	6 (8%)	82,113,113	1.17	7 (8%)
32	LHG	d	407	-	48,48,48	0.63	1 (2%)	51,54,54	1.27	7 (13%)
23	LMG	c	519	-	51,51,55	0.71	0	59,59,63	1.32	5 (8%)
25	CLA	C	506	3	69,73,73	1.13	7 (10%)	82,113,113	1.18	5 (6%)
25	CLA	c	512	3	69,73,73	1.12	6 (8%)	82,113,113	1.23	6 (7%)
32	LHG	B	625	-	48,48,48	0.64	2 (4%)	51,54,54	1.30	6 (11%)
32	LHG	a	720	-	38,38,48	0.69	0	41,44,54	1.20	3 (7%)
25	CLA	B	617	2	69,73,73	1.13	7 (10%)	82,113,113	1.21	7 (8%)
29	SQD	B	623	-	45,47,54	1.01	2 (4%)	55,58,65	1.77	13 (23%)
25	CLA	D	402	36	69,73,73	1.12	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	B	615	2	69,73,73	1.13	6 (8%)	82,113,113	1.18	6 (7%)
25	CLA	D	403	4	69,73,73	1.14	6 (8%)	82,113,113	1.13	5 (6%)
32	LHG	e	101	-	41,41,48	0.69	2 (4%)	44,47,54	1.34	7 (15%)
25	CLA	d	402	4	69,73,73	1.13	6 (8%)	82,113,113	1.14	5 (6%)
25	CLA	b	607	36	69,73,73	1.13	7 (10%)	82,113,113	1.24	6 (7%)
25	CLA	B	616	2	69,73,73	1.15	6 (8%)	82,113,113	1.23	4 (4%)
25	CLA	b	613	36	69,73,73	1.13	6 (8%)	82,113,113	1.11	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	a	714	-	52,54,54	0.95	3 (5%)	62,65,65	1.57	12 (19%)
23	LMG	C	521	-	51,51,55	0.79	1 (1%)	59,59,63	1.36	6 (10%)

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
25	CLA	b	614	2	-	3/39/115/115	-
25	CLA	C	504	3	-	11/39/115/115	-
25	CLA	d	403	4	-	8/39/115/115	-
25	CLA	C	512	3	-	14/39/115/115	-
26	PHO	D	401	-	-	6/37/103/103	0/5/6/6
29	SQD	D	410	-	-	16/38/58/69	0/1/1/1
25	CLA	c	513	3	-	17/39/115/115	-
27	BCR	b	602	-	-	6/29/63/63	0/2/2/2
25	CLA	B	613	2	-	8/39/115/115	-
33	DGD	C	517	-	-	18/51/91/95	0/2/2/2
23	LMG	b	627	-	-	19/46/66/70	0/1/1/1
27	BCR	k	101	-	-	6/29/63/63	0/2/2/2
33	DGD	c	517	-	-	19/51/91/95	0/2/2/2
28	PL9	a	713	-	-	13/53/73/73	0/1/1/1
34	HEM	e	102	5,6	-	7/14/54/54	-
25	CLA	c	504	36	-	4/31/107/115	-
23	LMG	b	626	-	-	16/46/66/70	0/1/1/1
25	CLA	C	513	3	-	10/39/115/115	-
25	CLA	C	503	3	-	18/39/115/115	-
29	SQD	A	612	-	-	17/47/67/69	0/1/1/1
32	LHG	E	101	-	-	26/53/53/53	-
25	CLA	D	404	4	-	16/39/115/115	-
25	CLA	B	603	2	-	8/39/115/115	-
27	BCR	a	712	-	-	4/29/63/63	0/2/2/2
25	CLA	B	602	36	-	14/39/115/115	-
25	CLA	b	621	2	-	9/39/115/115	-
25	CLA	c	506	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	508	3	-	10/39/115/115	-
25	CLA	b	619	2	-	10/39/115/115	-
25	CLA	b	615	2	-	12/39/115/115	-
27	BCR	B	620	-	-	6/29/63/63	0/2/2/2
25	CLA	c	511	3	-	7/39/115/115	-
25	CLA	b	609	2	-	14/39/115/115	-
27	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	CLA	a	708	36	-	7/39/115/115	-
25	CLA	B	608	36	-	8/39/115/115	-
32	LHG	b	629	-	-	18/53/53/53	-
33	DGD	H	103	-	-	10/51/91/95	0/2/2/2
25	CLA	a	711	1	-	13/39/115/115	-
28	PL9	d	405	-	-	7/53/73/73	0/1/1/1
25	CLA	B	610	2	-	12/39/115/115	-
27	BCR	H	102	-	-	5/29/63/63	0/2/2/2
23	LMG	a	701	-	-	25/46/66/70	0/1/1/1
25	CLA	b	611	2	-	12/39/115/115	-
27	BCR	K	101	-	-	3/29/63/63	0/2/2/2
27	BCR	C	515	-	-	1/29/63/63	0/2/2/2
28	PL9	D	406	-	-	9/53/73/73	0/1/1/1
23	LMG	B	621	-	-	19/46/66/70	0/1/1/1
23	LMG	b	628	-	-	3/6/6/70	-
23	LMG	A	603	-	-	24/46/66/70	0/1/1/1
26	PHO	A	608	-	-	9/37/103/103	0/5/6/6
32	LHG	L	101	-	-	17/53/53/53	-
23	LMG	C	520	-	-	25/46/66/70	0/1/1/1
27	BCR	k	102	-	-	3/29/63/63	0/2/2/2
25	CLA	B	611	36	-	12/39/115/115	-
25	CLA	B	612	2	-	5/39/115/115	-
27	BCR	C	516	-	-	4/29/63/63	0/2/2/2
25	CLA	B	609	2	-	11/39/115/115	-
23	LMG	C	501	-	-	22/46/66/70	0/1/1/1
27	BCR	b	623	-	-	3/29/63/63	0/2/2/2
25	CLA	B	614	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	f	102	-	-	13/36/56/69	0/1/1/1
25	CLA	a	707	1	-	6/39/115/115	-
35	HEC	v	201	16	1/1/3/7	4/14/54/54	-
23	LMG	f	101	-	-	16/46/66/70	0/1/1/1
25	CLA	C	509	3	-	5/39/115/115	-
25	CLA	A	607	36	-	8/39/115/115	-
23	LMG	D	409	-	-	19/46/66/70	0/1/1/1
27	BCR	t	103	-	-	8/29/63/63	0/2/2/2
28	PL9	A	611	-	-	8/53/73/73	0/1/1/1
27	BCR	c	515	-	-	5/29/63/63	0/2/2/2
25	CLA	C	508	36	-	11/39/115/115	-
25	CLA	b	616	36	-	6/39/115/115	-
25	CLA	b	618	2	-	11/39/115/115	-
25	CLA	c	505	3	-	8/39/115/115	-
26	PHO	a	710	-	-	7/37/103/103	0/5/6/6
27	BCR	D	405	-	-	8/29/63/63	0/2/2/2
25	CLA	B	604	2	-	17/39/115/115	-
27	BCR	b	625	-	-	7/29/63/63	0/2/2/2
29	SQD	A	614	-	-	21/41/41/69	-
25	CLA	C	510	3	-	17/39/115/115	-
25	CLA	b	622	2	-	2/18/94/115	-
33	DGD	c	518	-	-	11/51/91/95	0/2/2/2
33	DGD	h	102	-	-	16/51/91/95	0/2/2/2
23	LMG	a	715	-	-	25/46/66/70	0/1/1/1
25	CLA	C	514	3	-	5/39/115/115	-
25	CLA	B	607	2	-	16/39/115/115	-
25	CLA	c	503	3	-	8/39/115/115	-
23	LMG	c	520	-	-	16/46/66/70	0/1/1/1
23	LMG	M	101	-	-	13/46/66/70	0/1/1/1
27	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
32	LHG	d	406	-	-	17/53/53/53	-
25	CLA	c	501	3	-	9/39/115/115	-
27	BCR	B	619	-	-	5/29/63/63	0/2/2/2
25	CLA	b	608	2	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	c	514	-	-	5/29/63/63	0/2/2/2
25	CLA	c	509	3	-	4/39/115/115	-
29	SQD	I	102	-	-	25/41/41/69	-
25	CLA	c	502	3	-	12/39/115/115	-
33	DGD	C	518	-	-	23/51/91/95	0/2/2/2
25	CLA	C	505	36	-	12/39/115/115	-
27	BCR	b	624	-	-	7/29/63/63	0/2/2/2
32	LHG	D	407	-	-	17/53/53/53	-
34	HEM	E	102	5,6	-	4/14/54/54	-
27	BCR	d	404	-	-	7/29/63/63	0/2/2/2
25	CLA	C	502	3	-	12/39/115/115	-
25	CLA	A	609	1	-	2/26/102/115	-
25	CLA	C	507	3	-	14/39/115/115	-
25	CLA	c	510	3	-	16/39/115/115	-
27	BCR	A	610	-	-	3/29/63/63	0/2/2/2
27	BCR	h	101	-	-	6/29/63/63	0/2/2/2
32	LHG	D	408	-	-	23/53/53/53	-
33	DGD	C	519	-	-	16/51/91/95	0/2/2/2
33	DGD	c	516	-	-	16/51/91/95	0/2/2/2
25	CLA	B	606	2	-	16/39/115/115	-
23	LMG	d	408	-	-	19/41/41/70	-
25	CLA	b	610	2	-	9/39/115/115	-
25	CLA	b	620	2	-	11/39/115/115	-
29	SQD	B	626	-	-	23/49/69/69	0/1/1/1
35	HEC	V	201	16	1/1/3/7	6/14/54/54	-
25	CLA	a	719	36	-	8/39/115/115	-
25	CLA	B	605	2	-	12/39/115/115	-
29	SQD	b	601	-	-	25/49/69/69	0/1/1/1
25	CLA	c	507	36	-	9/39/115/115	-
26	PHO	a	709	-	-	5/37/103/103	0/5/6/6
25	CLA	b	617	2	-	11/39/115/115	-
25	CLA	C	511	3	-	11/39/115/115	-
25	CLA	A	606	1	-	1/39/115/115	-
25	CLA	b	612	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	d	407	-	-	13/53/53/53	-
23	LMG	c	519	-	-	22/46/66/70	0/1/1/1
25	CLA	C	506	3	-	7/39/115/115	-
25	CLA	c	512	3	-	14/39/115/115	-
32	LHG	B	625	-	-	19/53/53/53	-
32	LHG	a	720	-	-	18/43/43/53	-
25	CLA	B	617	2	-	12/39/115/115	-
29	SQD	B	623	-	-	25/42/62/69	0/1/1/1
25	CLA	D	402	36	-	4/39/115/115	-
25	CLA	B	615	2	-	16/39/115/115	-
25	CLA	D	403	4	-	12/39/115/115	-
32	LHG	e	101	-	-	22/46/46/53	-
25	CLA	d	402	4	-	10/39/115/115	-
25	CLA	b	607	36	-	15/39/115/115	-
25	CLA	B	616	2	-	13/39/115/115	-
25	CLA	b	613	36	-	8/39/115/115	-
29	SQD	a	714	-	-	17/49/69/69	0/1/1/1
23	LMG	C	521	-	-	18/46/66/70	0/1/1/1

All (630) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	C1B-C2B	9.71	1.50	1.39
26	a	709	PHO	C1B-C2B	9.68	1.50	1.39
26	a	710	PHO	C1B-C2B	9.68	1.50	1.39
26	D	401	PHO	C1B-C2B	9.65	1.50	1.39
26	A	608	PHO	C3B-C4B	8.73	1.50	1.41
26	a	710	PHO	C3B-C4B	8.72	1.50	1.41
26	D	401	PHO	C3B-C4B	8.62	1.50	1.41
26	a	709	PHO	C3B-C4B	8.56	1.50	1.41
31	A	615	BCT	O1-C	5.33	1.44	1.25
31	a	706	BCT	O1-C	5.30	1.44	1.25
26	a	710	PHO	C1D-C2D	4.35	1.44	1.39
26	A	608	PHO	C1D-C2D	4.29	1.44	1.39
26	a	709	PHO	C1D-C2D	4.29	1.44	1.39
26	D	401	PHO	C1D-C2D	4.27	1.44	1.39
35	V	201	HEC	CBC-CAC	-4.13	1.33	1.51
35	v	201	HEC	CBC-CAC	-4.10	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	102	HEM	FE-ND	4.07	2.07	1.94
35	V	201	HEC	CBB-CAB	-4.05	1.34	1.51
35	v	201	HEC	CBB-CAB	-4.04	1.34	1.51
27	d	404	BCR	C1-C6	-4.00	1.48	1.53
34	e	102	HEM	FE-NB	3.99	2.07	1.94
27	D	405	BCR	C30-C25	-3.93	1.48	1.53
26	a	709	PHO	C4D-CHA	3.91	1.45	1.39
27	D	405	BCR	C1-C6	-3.84	1.48	1.53
27	b	623	BCR	C1-C6	-3.82	1.48	1.53
34	e	102	HEM	FE-ND	3.81	2.06	1.94
26	A	608	PHO	C4D-CHA	3.80	1.45	1.39
26	D	401	PHO	C4D-CHA	3.78	1.45	1.39
27	k	101	BCR	C1-C6	-3.74	1.49	1.53
27	c	515	BCR	C1-C6	-3.74	1.49	1.53
27	C	516	BCR	C1-C6	-3.72	1.49	1.53
27	Y	101	BCR	C1-C6	-3.69	1.49	1.53
27	t	103	BCR	C1-C6	-3.69	1.49	1.53
26	a	710	PHO	C4D-CHA	3.68	1.45	1.39
27	b	602	BCR	C1-C6	-3.68	1.49	1.53
27	B	620	BCR	C1-C6	-3.68	1.49	1.53
27	a	712	BCR	C1-C6	-3.65	1.49	1.53
25	B	610	CLA	C1D-ND	3.64	1.42	1.37
25	C	508	CLA	C1D-ND	3.64	1.42	1.37
27	c	514	BCR	C30-C25	-3.63	1.49	1.53
25	B	605	CLA	C1D-ND	3.62	1.42	1.37
27	b	624	BCR	C1-C6	-3.62	1.49	1.53
27	B	618	BCR	C1-C6	-3.62	1.49	1.53
27	k	102	BCR	C1-C6	-3.62	1.49	1.53
27	K	101	BCR	C1-C6	-3.61	1.49	1.53
27	b	625	BCR	C1-C6	-3.60	1.49	1.53
27	c	514	BCR	C1-C6	-3.60	1.49	1.53
25	B	614	CLA	C1D-ND	3.59	1.42	1.37
25	B	617	CLA	C1D-ND	3.59	1.42	1.37
25	c	509	CLA	C1D-ND	3.58	1.42	1.37
25	b	615	CLA	C1D-ND	3.57	1.42	1.37
25	c	507	CLA	C1D-ND	3.57	1.42	1.37
27	B	619	BCR	C1-C6	-3.57	1.49	1.53
25	B	616	CLA	C1D-ND	3.56	1.42	1.37
25	C	510	CLA	C1D-ND	3.56	1.42	1.37
25	B	611	CLA	C1D-ND	3.56	1.42	1.37
25	b	622	CLA	C1D-ND	3.55	1.42	1.37
25	D	404	CLA	C1D-ND	3.55	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	619	CLA	C1D-ND	3.55	1.42	1.37
27	b	623	BCR	C30-C25	-3.54	1.49	1.53
25	b	616	CLA	C1D-ND	3.54	1.42	1.37
25	c	511	CLA	C1D-ND	3.53	1.42	1.37
34	E	102	HEM	FE-NB	3.53	2.05	1.94
25	B	603	CLA	C1D-ND	3.53	1.42	1.37
34	e	102	HEM	FE-NA	3.52	2.06	1.95
23	A	603	LMG	C4-C5	3.52	1.60	1.53
25	B	602	CLA	C1D-ND	3.52	1.42	1.37
25	C	507	CLA	C1D-ND	3.51	1.42	1.37
25	b	610	CLA	C1D-ND	3.51	1.42	1.37
25	C	513	CLA	C1D-ND	3.51	1.42	1.37
25	C	512	CLA	C1D-ND	3.50	1.42	1.37
25	B	606	CLA	C1D-ND	3.50	1.42	1.37
25	B	613	CLA	C1D-ND	3.50	1.42	1.37
25	a	719	CLA	C1D-ND	3.50	1.42	1.37
25	A	606	CLA	C1D-ND	3.50	1.42	1.37
27	A	610	BCR	C1-C6	-3.49	1.49	1.53
25	c	504	CLA	C1D-ND	3.48	1.42	1.37
25	b	611	CLA	C1D-ND	3.48	1.42	1.37
25	A	607	CLA	C1D-ND	3.48	1.42	1.37
25	D	403	CLA	C1D-ND	3.47	1.42	1.37
25	c	503	CLA	C1D-ND	3.47	1.42	1.37
25	a	711	CLA	C1D-ND	3.47	1.42	1.37
25	C	511	CLA	C1D-ND	3.47	1.42	1.37
25	b	608	CLA	C1D-ND	3.47	1.42	1.37
25	c	501	CLA	C1D-ND	3.47	1.42	1.37
25	B	615	CLA	C1D-ND	3.47	1.42	1.37
25	C	509	CLA	C1D-ND	3.46	1.42	1.37
25	C	504	CLA	C1D-ND	3.46	1.42	1.37
25	a	708	CLA	C1D-ND	3.45	1.42	1.37
25	C	506	CLA	C1D-ND	3.45	1.42	1.37
25	A	609	CLA	C1D-ND	3.45	1.42	1.37
25	b	618	CLA	C1D-ND	3.44	1.42	1.37
25	d	403	CLA	C1D-ND	3.44	1.42	1.37
25	D	402	CLA	C1D-ND	3.44	1.42	1.37
25	B	607	CLA	C1D-ND	3.43	1.42	1.37
25	c	513	CLA	C1D-ND	3.43	1.42	1.37
25	d	402	CLA	C1D-ND	3.42	1.42	1.37
25	b	621	CLA	C1D-ND	3.42	1.42	1.37
25	C	502	CLA	C1D-ND	3.42	1.42	1.37
34	E	102	HEM	FE-NC	3.42	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	C1D-ND	3.42	1.42	1.37
25	c	508	CLA	C1D-ND	3.41	1.42	1.37
27	b	625	BCR	C30-C25	-3.41	1.49	1.53
25	c	510	CLA	C1D-ND	3.41	1.42	1.37
35	v	201	HEC	FE-NB	3.41	2.05	1.94
25	a	707	CLA	C1D-ND	3.41	1.42	1.37
25	c	505	CLA	C1D-ND	3.41	1.42	1.37
25	c	512	CLA	C1D-ND	3.40	1.42	1.37
25	b	607	CLA	C1D-ND	3.40	1.42	1.37
35	V	201	HEC	FE-ND	3.40	2.05	1.94
25	b	613	CLA	C1D-ND	3.39	1.42	1.37
25	B	608	CLA	C1D-ND	3.39	1.42	1.37
25	C	503	CLA	C1D-ND	3.39	1.42	1.37
25	c	502	CLA	C1D-ND	3.38	1.42	1.37
27	C	515	BCR	C30-C25	-3.38	1.49	1.53
25	b	617	CLA	C1D-ND	3.38	1.42	1.37
25	b	614	CLA	C1D-ND	3.38	1.42	1.37
25	c	506	CLA	C1D-ND	3.36	1.42	1.37
25	b	609	CLA	C1D-ND	3.36	1.42	1.37
25	b	620	CLA	C1D-ND	3.36	1.42	1.37
25	B	604	CLA	C1D-ND	3.36	1.42	1.37
35	V	201	HEC	FE-NC	3.36	2.06	1.95
25	B	609	CLA	C1D-ND	3.36	1.42	1.37
25	C	514	CLA	C1D-ND	3.36	1.42	1.37
27	C	515	BCR	C1-C6	-3.35	1.49	1.53
25	b	612	CLA	C1D-ND	3.34	1.42	1.37
25	C	505	CLA	C1D-ND	3.34	1.42	1.37
27	C	516	BCR	C30-C25	-3.33	1.49	1.53
34	E	102	HEM	FE-NA	3.33	2.06	1.95
27	B	620	BCR	C30-C25	-3.32	1.49	1.53
27	c	515	BCR	C30-C25	-3.29	1.49	1.53
29	A	614	SQD	O48-C23	3.29	1.42	1.33
35	v	201	HEC	FE-NC	3.29	2.06	1.95
27	H	102	BCR	C1-C6	-3.28	1.49	1.53
34	e	102	HEM	FE-NC	3.28	2.06	1.95
27	b	624	BCR	C30-C25	-3.27	1.49	1.53
27	a	712	BCR	C30-C25	-3.27	1.49	1.53
27	d	404	BCR	C30-C25	-3.27	1.49	1.53
27	Y	101	BCR	C30-C25	-3.26	1.49	1.53
25	B	610	CLA	C4B-NB	3.25	1.42	1.37
25	C	507	CLA	C4B-NB	3.23	1.42	1.37
25	c	505	CLA	C4B-NB	3.22	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	403	CLA	C4B-NB	3.21	1.42	1.37
25	b	615	CLA	C4B-NB	3.20	1.42	1.37
27	B	619	BCR	C30-C25	-3.18	1.49	1.53
25	C	506	CLA	C4B-NB	3.18	1.42	1.37
35	v	201	HEC	FE-ND	3.18	2.04	1.94
25	d	402	CLA	C4B-NB	3.18	1.42	1.37
35	V	201	HEC	FE-NB	3.18	2.04	1.94
27	h	101	BCR	C1-C6	-3.18	1.49	1.53
27	k	102	BCR	C30-C25	-3.17	1.49	1.53
27	A	610	BCR	C30-C25	-3.17	1.49	1.53
25	b	609	CLA	C4B-NB	3.17	1.42	1.37
25	B	607	CLA	C4B-NB	3.17	1.42	1.37
29	D	410	SQD	O48-C23	3.17	1.42	1.33
27	b	602	BCR	C30-C25	-3.16	1.49	1.53
29	a	714	SQD	O48-C23	3.16	1.42	1.33
29	B	623	SQD	O48-C23	3.15	1.42	1.33
27	h	101	BCR	C30-C25	-3.15	1.49	1.53
29	f	102	SQD	O48-C23	3.15	1.42	1.33
35	v	201	HEC	FE-NA	3.14	2.05	1.95
25	A	609	CLA	C4B-NB	3.14	1.42	1.37
25	c	506	CLA	C4B-NB	3.14	1.42	1.37
25	b	612	CLA	C4B-NB	3.13	1.42	1.37
28	A	611	PL9	C7-C3	-3.12	1.47	1.51
35	V	201	HEC	FE-NA	3.12	2.05	1.95
25	B	616	CLA	C4B-NB	3.12	1.42	1.37
27	B	618	BCR	C30-C25	-3.12	1.49	1.53
27	k	101	BCR	C30-C25	-3.11	1.49	1.53
25	B	606	CLA	C4B-NB	3.11	1.41	1.37
25	b	608	CLA	C4B-NB	3.11	1.41	1.37
25	a	711	CLA	C4B-NB	3.10	1.41	1.37
25	B	615	CLA	C4B-NB	3.10	1.41	1.37
29	B	626	SQD	O48-C23	3.10	1.42	1.33
29	I	102	SQD	O48-C23	3.10	1.42	1.33
34	E	102	HEM	CAB-C3B	3.09	1.55	1.47
25	B	603	CLA	C4B-NB	3.09	1.41	1.37
25	a	719	CLA	C4B-NB	3.09	1.41	1.37
27	K	101	BCR	C30-C25	-3.09	1.49	1.53
29	A	612	SQD	O48-C23	3.09	1.42	1.33
25	D	404	CLA	C4B-NB	3.08	1.41	1.37
25	b	611	CLA	C4B-NB	3.08	1.41	1.37
29	b	601	SQD	O48-C23	3.08	1.42	1.33
25	B	604	CLA	C4B-NB	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	620	CLA	C4B-NB	3.08	1.41	1.37
25	c	508	CLA	C4B-NB	3.07	1.41	1.37
27	H	102	BCR	C30-C25	-3.07	1.49	1.53
25	b	614	CLA	C4B-NB	3.07	1.41	1.37
27	t	103	BCR	C30-C25	-3.07	1.49	1.53
25	a	707	CLA	C4B-NB	3.06	1.41	1.37
25	C	504	CLA	C4B-NB	3.05	1.41	1.37
25	b	621	CLA	C4B-NB	3.04	1.41	1.37
25	c	507	CLA	C4B-NB	3.04	1.41	1.37
25	b	616	CLA	C4B-NB	3.03	1.41	1.37
25	B	602	CLA	C4B-NB	3.03	1.41	1.37
25	B	611	CLA	C4B-NB	3.03	1.41	1.37
25	C	509	CLA	C4B-NB	3.02	1.41	1.37
25	C	508	CLA	C4B-NB	3.02	1.41	1.37
25	C	513	CLA	C4B-NB	3.02	1.41	1.37
34	e	102	HEM	CAC-C3C	3.02	1.55	1.47
25	d	403	CLA	C4B-NB	3.02	1.41	1.37
25	C	503	CLA	C4B-NB	3.02	1.41	1.37
25	b	607	CLA	C4B-NB	3.02	1.41	1.37
25	b	618	CLA	C4B-NB	3.02	1.41	1.37
34	E	102	HEM	CAC-C3C	3.01	1.55	1.47
25	b	610	CLA	C4B-NB	3.00	1.41	1.37
29	A	614	SQD	O47-C7	3.00	1.42	1.34
25	B	608	CLA	C4B-NB	3.00	1.41	1.37
25	A	606	CLA	C4B-NB	3.00	1.41	1.37
29	B	623	SQD	O47-C7	2.99	1.42	1.34
25	B	617	CLA	C4B-NB	2.99	1.41	1.37
25	c	512	CLA	C4B-NB	2.99	1.41	1.37
25	c	503	CLA	C4B-NB	2.98	1.41	1.37
25	C	505	CLA	C4B-NB	2.98	1.41	1.37
23	A	603	LMG	C4-C3	2.98	1.60	1.52
25	b	613	CLA	C4B-NB	2.97	1.41	1.37
25	B	614	CLA	C4B-NB	2.97	1.41	1.37
25	C	512	CLA	C4B-NB	2.97	1.41	1.37
25	c	509	CLA	C4B-NB	2.97	1.41	1.37
25	B	609	CLA	C4B-NB	2.97	1.41	1.37
25	B	605	CLA	C4B-NB	2.95	1.41	1.37
25	C	502	CLA	C4B-NB	2.95	1.41	1.37
25	c	501	CLA	C4B-NB	2.95	1.41	1.37
25	B	612	CLA	C4B-NB	2.95	1.41	1.37
25	b	622	CLA	C4B-NB	2.94	1.41	1.37
25	A	607	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	406	PL9	C3-C4	-2.93	1.45	1.49
25	c	511	CLA	C4B-NB	2.93	1.41	1.37
25	B	613	CLA	C4B-NB	2.93	1.41	1.37
25	C	511	CLA	C4B-NB	2.93	1.41	1.37
25	D	402	CLA	C4B-NB	2.92	1.41	1.37
29	I	102	SQD	O47-C7	2.91	1.42	1.34
25	b	619	CLA	C4B-NB	2.91	1.41	1.37
25	C	510	CLA	C4B-NB	2.91	1.41	1.37
28	A	611	PL9	C3-C4	-2.90	1.45	1.49
34	e	102	HEM	CAB-C3B	2.90	1.55	1.47
25	c	502	CLA	C4B-NB	2.90	1.41	1.37
25	b	621	CLA	C1B-C2B	2.89	1.49	1.43
25	a	719	CLA	C1B-C2B	2.89	1.49	1.43
25	a	708	CLA	C4B-NB	2.88	1.41	1.37
29	f	102	SQD	O47-C7	2.88	1.42	1.34
25	c	504	CLA	C4B-NB	2.87	1.41	1.37
25	c	510	CLA	C1B-C2B	2.86	1.49	1.43
29	B	626	SQD	O47-C7	2.86	1.42	1.34
25	b	617	CLA	C4B-NB	2.85	1.41	1.37
25	b	619	CLA	C1B-C2B	2.85	1.49	1.43
29	D	410	SQD	O47-C7	2.84	1.42	1.34
25	B	604	CLA	C1B-C2B	2.84	1.49	1.43
29	A	612	SQD	O47-C7	2.84	1.42	1.34
25	b	608	CLA	C1B-C2B	2.84	1.49	1.43
25	B	610	CLA	C1B-C2B	2.84	1.49	1.43
25	B	605	CLA	C1B-C2B	2.84	1.49	1.43
25	b	618	CLA	C1B-C2B	2.83	1.49	1.43
25	c	511	CLA	C1B-C2B	2.83	1.49	1.43
25	b	612	CLA	C1B-C2B	2.83	1.49	1.43
25	c	513	CLA	C1B-C2B	2.83	1.49	1.43
25	c	510	CLA	C4B-NB	2.83	1.41	1.37
25	D	403	CLA	C1B-C2B	2.82	1.49	1.43
25	C	514	CLA	C4B-NB	2.82	1.41	1.37
25	A	606	CLA	C1B-C2B	2.82	1.49	1.43
29	a	714	SQD	O47-C7	2.82	1.42	1.34
25	B	602	CLA	C1B-C2B	2.82	1.49	1.43
25	c	508	CLA	C1B-C2B	2.82	1.49	1.43
25	a	707	CLA	C1B-C2B	2.82	1.49	1.43
25	C	511	CLA	C1B-C2B	2.81	1.49	1.43
25	C	514	CLA	C1B-C2B	2.81	1.49	1.43
25	B	612	CLA	C1B-C2B	2.81	1.49	1.43
25	c	504	CLA	C1B-C2B	2.81	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	505	CLA	C1B-C2B	2.81	1.49	1.43
25	c	513	CLA	C4B-NB	2.81	1.41	1.37
25	B	615	CLA	C1B-C2B	2.80	1.49	1.43
25	C	502	CLA	C1B-C2B	2.80	1.49	1.43
25	b	610	CLA	C1B-C2B	2.80	1.49	1.43
25	C	512	CLA	C1B-C2B	2.79	1.49	1.43
25	A	607	CLA	C1B-C2B	2.79	1.49	1.43
25	B	606	CLA	C1B-C2B	2.79	1.49	1.43
25	b	622	CLA	C1B-C2B	2.79	1.49	1.43
25	c	502	CLA	C1B-C2B	2.79	1.49	1.43
29	b	601	SQD	O47-C7	2.79	1.42	1.34
25	B	616	CLA	C1B-C2B	2.79	1.49	1.43
25	B	614	CLA	C1B-C2B	2.79	1.49	1.43
25	C	503	CLA	C1B-C2B	2.79	1.49	1.43
25	B	617	CLA	C1B-C2B	2.78	1.49	1.43
25	B	609	CLA	C1B-C2B	2.78	1.49	1.43
25	C	509	CLA	C1B-C2B	2.78	1.49	1.43
25	c	509	CLA	C1B-C2B	2.78	1.49	1.43
25	b	607	CLA	C1B-C2B	2.78	1.49	1.43
25	d	402	CLA	C1B-C2B	2.77	1.49	1.43
25	b	616	CLA	C1B-C2B	2.77	1.49	1.43
25	b	615	CLA	C1B-C2B	2.77	1.49	1.43
25	c	507	CLA	C1B-C2B	2.77	1.49	1.43
25	C	508	CLA	C1B-C2B	2.77	1.49	1.43
25	C	510	CLA	C1B-C2B	2.77	1.49	1.43
25	B	603	CLA	C1B-C2B	2.76	1.49	1.43
25	D	404	CLA	C1B-C2B	2.76	1.49	1.43
25	b	614	CLA	C1B-C2B	2.76	1.49	1.43
25	C	513	CLA	C1B-C2B	2.76	1.49	1.43
25	c	503	CLA	C1B-C2B	2.76	1.49	1.43
25	b	617	CLA	C1B-C2B	2.75	1.49	1.43
25	B	611	CLA	C1B-C2B	2.75	1.49	1.43
25	B	607	CLA	C1B-C2B	2.75	1.49	1.43
25	a	711	CLA	C1B-C2B	2.75	1.49	1.43
25	b	611	CLA	C1B-C2B	2.75	1.49	1.43
25	C	504	CLA	C1B-C2B	2.75	1.49	1.43
25	c	501	CLA	C1B-C2B	2.75	1.49	1.43
25	b	609	CLA	C1B-C2B	2.75	1.49	1.43
25	B	608	CLA	C1B-C2B	2.74	1.49	1.43
25	c	512	CLA	C1B-C2B	2.74	1.49	1.43
25	a	708	CLA	C1B-C2B	2.74	1.49	1.43
25	d	403	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	402	CLA	C1B-C2B	2.73	1.49	1.43
25	C	505	CLA	C1B-C2B	2.73	1.49	1.43
25	A	609	CLA	C1B-C2B	2.73	1.49	1.43
25	B	613	CLA	C1B-C2B	2.73	1.49	1.43
25	c	506	CLA	C1B-C2B	2.73	1.49	1.43
28	a	713	PL9	C7-C3	-2.73	1.47	1.51
25	C	506	CLA	C1B-C2B	2.72	1.49	1.43
25	C	507	CLA	C1B-C2B	2.71	1.49	1.43
25	b	620	CLA	C1B-C2B	2.71	1.49	1.43
28	d	405	PL9	C3-C4	-2.71	1.45	1.49
25	b	613	CLA	C1B-C2B	2.70	1.49	1.43
28	a	713	PL9	C3-C4	-2.67	1.45	1.49
26	A	608	PHO	C3D-C4D	2.62	1.44	1.41
26	D	401	PHO	C3D-C4D	2.58	1.44	1.41
26	a	710	PHO	CMC-C2C	-2.56	1.46	1.50
26	a	709	PHO	CMC-C2C	-2.54	1.46	1.50
26	a	709	PHO	C3D-C4D	2.54	1.44	1.41
26	A	608	PHO	CMC-C2C	-2.52	1.46	1.50
26	a	710	PHO	C3D-C4D	2.51	1.44	1.41
28	D	406	PL9	C7-C3	-2.51	1.47	1.51
26	D	401	PHO	CMC-C2C	-2.50	1.46	1.50
25	b	607	CLA	C3B-C4B	2.50	1.50	1.42
25	b	616	CLA	C3B-C4B	2.45	1.49	1.42
23	c	520	LMG	C1-C2	2.44	1.59	1.52
26	D	401	PHO	CMD-C2D	-2.44	1.46	1.51
25	B	611	CLA	C3B-C4B	2.44	1.49	1.42
26	a	709	PHO	CMB-C2B	-2.43	1.46	1.51
26	a	710	PHO	CMD-C2D	-2.43	1.46	1.51
25	c	503	CLA	CHC-C1C	2.42	1.43	1.38
25	B	609	CLA	CHC-C1C	2.42	1.43	1.38
25	B	609	CLA	C3B-C4B	2.42	1.49	1.42
25	C	504	CLA	C3B-C4B	2.42	1.49	1.42
25	C	512	CLA	C3B-C4B	2.42	1.49	1.42
25	b	613	CLA	C3B-C4B	2.41	1.49	1.42
26	a	709	PHO	CMD-C2D	-2.41	1.46	1.51
25	c	503	CLA	C3B-C4B	2.41	1.49	1.42
23	C	521	LMG	C1-C2	2.40	1.59	1.52
25	B	613	CLA	CHC-C1C	2.40	1.43	1.38
25	b	611	CLA	C3B-C4B	2.40	1.49	1.42
26	A	608	PHO	CMD-C2D	-2.40	1.46	1.51
25	b	620	CLA	CHC-C1C	2.40	1.43	1.38
25	B	615	CLA	CHC-C1C	2.40	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	518	DGD	O2G-C2G	-2.40	1.41	1.46
33	c	517	DGD	O2G-C2G	-2.40	1.41	1.46
25	C	513	CLA	C3B-C4B	2.39	1.49	1.42
25	d	403	CLA	C3B-C4B	2.39	1.49	1.42
25	B	614	CLA	C3B-C4B	2.38	1.49	1.42
25	B	613	CLA	C3B-C4B	2.38	1.49	1.42
25	c	511	CLA	C3B-C4B	2.38	1.49	1.42
26	A	608	PHO	CMB-C2B	-2.38	1.46	1.51
33	c	517	DGD	O1G-C1G	-2.38	1.39	1.45
25	C	509	CLA	C3B-C4B	2.38	1.49	1.42
25	A	607	CLA	CHC-C1C	2.38	1.43	1.38
25	C	512	CLA	CHC-C1C	2.38	1.43	1.38
25	C	507	CLA	C3B-C4B	2.37	1.49	1.42
25	C	511	CLA	C3B-C4B	2.37	1.49	1.42
25	c	501	CLA	C3B-C4B	2.37	1.49	1.42
25	C	504	CLA	CHC-C1C	2.37	1.43	1.38
25	C	509	CLA	CHC-C1C	2.37	1.43	1.38
25	c	509	CLA	C3B-C4B	2.37	1.49	1.42
25	b	613	CLA	CHC-C1C	2.37	1.43	1.38
25	c	508	CLA	C3B-C4B	2.37	1.49	1.42
25	b	620	CLA	C3B-C4B	2.36	1.49	1.42
25	b	609	CLA	CHC-C1C	2.36	1.43	1.38
25	C	506	CLA	C3B-C4B	2.36	1.49	1.42
33	C	518	DGD	O1G-C1G	-2.36	1.39	1.45
25	d	403	CLA	CHC-C1C	2.36	1.43	1.38
25	c	506	CLA	C3B-C4B	2.36	1.49	1.42
26	D	401	PHO	CMB-C2B	-2.36	1.46	1.51
25	C	511	CLA	CHC-C1C	2.36	1.43	1.38
25	c	508	CLA	CHC-C1C	2.36	1.43	1.38
25	b	614	CLA	C3B-C4B	2.36	1.49	1.42
26	a	709	PHO	CAC-C3C	-2.36	1.47	1.51
25	b	614	CLA	CHC-C1C	2.36	1.43	1.38
25	B	614	CLA	CHC-C1C	2.35	1.43	1.38
25	C	503	CLA	C3B-C4B	2.35	1.49	1.42
25	c	511	CLA	CHC-C1C	2.35	1.43	1.38
25	B	615	CLA	C3B-C4B	2.35	1.49	1.42
25	c	504	CLA	C3B-C4B	2.35	1.49	1.42
25	b	611	CLA	CHC-C1C	2.35	1.43	1.38
25	B	607	CLA	CHC-C1C	2.35	1.43	1.38
25	D	402	CLA	C3B-C4B	2.34	1.49	1.42
25	b	609	CLA	C3B-C4B	2.34	1.49	1.42
25	B	602	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	CHC-C1C	2.34	1.43	1.38
25	b	618	CLA	CHC-C1C	2.34	1.43	1.38
25	B	602	CLA	C3B-C4B	2.34	1.49	1.42
25	B	607	CLA	C3B-C4B	2.34	1.49	1.42
25	A	609	CLA	CHC-C1C	2.34	1.43	1.38
25	B	603	CLA	CHC-C1C	2.34	1.43	1.38
25	B	612	CLA	C3B-C4B	2.34	1.49	1.42
25	b	622	CLA	C3B-C4B	2.33	1.49	1.42
26	A	608	PHO	CAC-C3C	-2.33	1.47	1.51
25	c	509	CLA	CHC-C1C	2.33	1.43	1.38
25	B	604	CLA	C3B-C4B	2.33	1.49	1.42
25	b	616	CLA	CHC-C1C	2.33	1.43	1.38
25	A	607	CLA	C3B-C4B	2.33	1.49	1.42
25	c	510	CLA	C3B-C4B	2.33	1.49	1.42
25	C	502	CLA	C3B-C4B	2.33	1.49	1.42
25	C	506	CLA	CHC-C1C	2.33	1.43	1.38
25	a	711	CLA	C3B-C4B	2.33	1.49	1.42
25	C	514	CLA	CHC-C1C	2.33	1.43	1.38
25	B	608	CLA	C3B-C4B	2.33	1.49	1.42
25	b	610	CLA	C3B-C4B	2.33	1.49	1.42
25	C	505	CLA	C3B-C4B	2.33	1.49	1.42
25	b	618	CLA	C3B-C4B	2.33	1.49	1.42
26	a	710	PHO	CMB-C2B	-2.32	1.47	1.51
32	E	101	LHG	P-O6	2.32	1.68	1.59
25	C	503	CLA	CHC-C1C	2.32	1.43	1.38
25	B	617	CLA	C3B-C4B	2.32	1.49	1.42
25	c	505	CLA	C3B-C4B	2.32	1.49	1.42
25	A	606	CLA	CHC-C1C	2.32	1.43	1.38
32	b	629	LHG	O7-C5	-2.32	1.41	1.46
25	b	615	CLA	C3B-C4B	2.32	1.49	1.42
25	D	403	CLA	CHC-C1C	2.32	1.43	1.38
25	A	606	CLA	C3B-C4B	2.32	1.49	1.42
25	c	502	CLA	C3B-C4B	2.32	1.49	1.42
25	d	402	CLA	CHC-C1C	2.32	1.43	1.38
25	b	612	CLA	C3B-C4B	2.32	1.49	1.42
25	c	502	CLA	CHC-C1C	2.32	1.43	1.38
25	D	403	CLA	C3B-C4B	2.32	1.49	1.42
25	a	707	CLA	C3B-C4B	2.32	1.49	1.42
25	a	708	CLA	C3B-C4B	2.32	1.49	1.42
25	c	507	CLA	C3B-C4B	2.32	1.49	1.42
25	c	506	CLA	CHC-C1C	2.32	1.43	1.38
25	A	609	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	719	CLA	C3B-C4B	2.32	1.49	1.42
25	C	505	CLA	CHC-C1C	2.32	1.43	1.38
25	C	514	CLA	C3B-C4B	2.32	1.49	1.42
25	C	510	CLA	C3B-C4B	2.31	1.49	1.42
32	D	407	LHG	O7-C5	-2.31	1.41	1.46
25	d	402	CLA	C3B-C4B	2.31	1.49	1.42
25	a	708	CLA	CHC-C1C	2.31	1.43	1.38
32	L	101	LHG	O7-C5	-2.31	1.41	1.46
28	d	405	PL9	C7-C3	-2.31	1.48	1.51
25	b	619	CLA	C3B-C4B	2.31	1.49	1.42
25	D	402	CLA	CHC-C1C	2.31	1.43	1.38
25	B	606	CLA	C3B-C4B	2.31	1.49	1.42
25	B	616	CLA	C3B-C4B	2.30	1.49	1.42
25	b	617	CLA	C3B-C4B	2.30	1.49	1.42
25	c	512	CLA	C3B-C4B	2.30	1.49	1.42
25	a	711	CLA	CHC-C1C	2.30	1.43	1.38
25	C	513	CLA	CHC-C1C	2.30	1.43	1.38
33	H	103	DGD	O2G-C2G	-2.30	1.41	1.46
25	a	719	CLA	CHC-C1C	2.30	1.43	1.38
25	B	603	CLA	C3B-C4B	2.30	1.49	1.42
25	B	610	CLA	CHC-C1C	2.29	1.43	1.38
25	c	510	CLA	CHC-C1C	2.29	1.43	1.38
25	B	610	CLA	C3B-C4B	2.29	1.49	1.42
25	b	608	CLA	C3B-C4B	2.29	1.49	1.42
25	B	606	CLA	CHC-C1C	2.29	1.43	1.38
25	B	616	CLA	CHC-C1C	2.29	1.43	1.38
25	b	622	CLA	CHC-C1C	2.29	1.43	1.38
25	c	505	CLA	CHC-C1C	2.29	1.43	1.38
25	C	502	CLA	CHC-C1C	2.28	1.43	1.38
25	a	707	CLA	CHC-C1C	2.28	1.43	1.38
25	c	504	CLA	CHC-C1C	2.28	1.43	1.38
25	C	510	CLA	CHC-C1C	2.28	1.43	1.38
25	b	615	CLA	CHC-C1C	2.28	1.43	1.38
25	b	607	CLA	CHC-C1C	2.28	1.43	1.38
25	B	612	CLA	CHC-C1C	2.28	1.43	1.38
25	B	617	CLA	CHC-C1C	2.28	1.43	1.38
32	d	407	LHG	O7-C5	-2.28	1.41	1.46
25	b	617	CLA	CHC-C1C	2.27	1.43	1.38
25	b	621	CLA	C3B-C4B	2.27	1.49	1.42
25	c	513	CLA	C3B-C4B	2.27	1.49	1.42
25	B	611	CLA	CHC-C1C	2.27	1.43	1.38
26	a	710	PHO	CAC-C3C	-2.27	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	CHC-C1C	2.27	1.43	1.38
25	b	610	CLA	CHC-C1C	2.27	1.43	1.38
26	D	401	PHO	CAC-C3C	-2.27	1.47	1.51
25	c	501	CLA	CHC-C1C	2.26	1.43	1.38
25	b	619	CLA	CHC-C1C	2.26	1.43	1.38
25	B	608	CLA	CHC-C1C	2.26	1.43	1.38
25	C	508	CLA	C3B-C4B	2.25	1.49	1.42
25	D	404	CLA	C3B-C4B	2.25	1.49	1.42
25	c	512	CLA	CHC-C1C	2.24	1.43	1.38
25	c	507	CLA	CHC-C1C	2.24	1.43	1.38
25	B	605	CLA	C3B-C4B	2.24	1.49	1.42
32	B	625	LHG	O7-C5	-2.24	1.41	1.46
25	B	604	CLA	CHC-C1C	2.24	1.43	1.38
25	c	513	CLA	CHC-C1C	2.23	1.43	1.38
25	D	404	CLA	CHC-C1C	2.22	1.42	1.38
25	c	510	CLA	CMD-C2D	-2.22	1.46	1.50
25	b	612	CLA	CHC-C1C	2.22	1.42	1.38
33	C	518	DGD	O6D-C5D	-2.21	1.39	1.44
25	c	505	CLA	CMD-C2D	-2.20	1.46	1.50
33	c	516	DGD	O2G-C2G	-2.20	1.41	1.46
33	C	517	DGD	O1G-C1G	-2.20	1.40	1.45
25	C	508	CLA	CHC-C1C	2.19	1.42	1.38
32	e	101	LHG	P-O6	2.19	1.68	1.59
33	C	518	DGD	O5D-C6D	-2.18	1.40	1.43
25	b	621	CLA	CHC-C1C	2.17	1.42	1.38
25	C	506	CLA	CMD-C2D	-2.16	1.46	1.50
28	A	611	PL9	C6-C1	-2.15	1.45	1.48
33	C	517	DGD	O2G-C2G	-2.15	1.41	1.46
23	b	626	LMG	O6-C1	2.14	1.47	1.41
25	B	604	CLA	CMD-C2D	-2.14	1.46	1.50
33	c	518	DGD	O2G-C2G	-2.14	1.41	1.46
33	c	516	DGD	O1G-C1G	-2.14	1.40	1.45
34	E	102	HEM	CMD-C2D	2.14	1.55	1.50
25	b	618	CLA	CMD-C2D	-2.13	1.46	1.50
25	B	605	CLA	CHC-C1C	2.13	1.42	1.38
34	E	102	HEM	CMB-C2B	2.13	1.55	1.50
25	a	707	CLA	CMD-C2D	-2.13	1.46	1.50
33	h	102	DGD	O2G-C2G	-2.12	1.41	1.46
29	A	612	SQD	O2-C2	-2.11	1.37	1.43
25	B	617	CLA	CMC-C2C	-2.11	1.46	1.50
28	d	405	PL9	C53-C6	-2.11	1.46	1.50
32	e	101	LHG	O7-C5	-2.11	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	606	CLA	CMD-C2D	-2.11	1.46	1.50
25	c	501	CLA	CMB-C2B	-2.10	1.46	1.50
32	d	406	LHG	O7-C5	-2.10	1.41	1.46
25	C	507	CLA	CMB-C2B	-2.10	1.46	1.50
28	D	406	PL9	C6-C1	-2.10	1.45	1.48
29	a	714	SQD	O2-C2	-2.09	1.37	1.43
28	A	611	PL9	C53-C6	-2.09	1.46	1.50
25	b	609	CLA	CMD-C2D	-2.09	1.46	1.50
25	c	503	CLA	CMD-C2D	-2.09	1.46	1.50
25	d	402	CLA	CMD-C2D	-2.09	1.46	1.50
25	D	403	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.08	1.46	1.50
23	d	408	LMG	C7-C8	2.08	1.56	1.51
34	e	102	HEM	CMD-C2D	2.08	1.55	1.50
28	a	713	PL9	C53-C6	-2.08	1.46	1.50
25	b	611	CLA	CMD-C2D	-2.08	1.46	1.50
35	V	201	HEC	CMB-C2B	2.07	1.55	1.50
28	D	406	PL9	C53-C6	-2.07	1.46	1.50
25	c	512	CLA	CMD-C2D	-2.07	1.46	1.50
33	c	518	DGD	O1G-C1G	-2.07	1.40	1.45
25	B	609	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	617	CLA	CMB-C2B	-2.07	1.46	1.50
23	C	520	LMG	O7-C8	-2.07	1.41	1.46
25	b	607	CLA	CMB-C2B	-2.07	1.46	1.50
23	b	626	LMG	O7-C8	-2.06	1.41	1.46
28	d	405	PL9	C6-C1	-2.06	1.45	1.48
25	C	504	CLA	CMD-C2D	-2.06	1.46	1.50
23	b	626	LMG	O8-C9	-2.06	1.40	1.45
29	D	410	SQD	O2-C2	-2.06	1.37	1.43
25	b	615	CLA	CMB-C2B	-2.06	1.46	1.50
25	a	708	CLA	CMB-C2B	-2.06	1.46	1.50
33	C	519	DGD	O1G-C1G	-2.06	1.40	1.45
29	b	601	SQD	O2-C2	-2.06	1.37	1.43
23	f	101	LMG	O7-C8	-2.06	1.41	1.46
25	b	616	CLA	CMB-C2B	-2.06	1.46	1.50
32	B	625	LHG	P-O6	2.05	1.67	1.59
25	C	502	CLA	CMD-C2D	-2.05	1.46	1.50
25	C	503	CLA	CMD-C2D	-2.05	1.46	1.50
25	b	621	CLA	CMC-C2C	-2.05	1.46	1.50
25	B	605	CLA	CMB-C2B	-2.05	1.46	1.50
29	f	102	SQD	O2-C2	-2.05	1.37	1.43
25	b	612	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	CMB-C2B	-2.05	1.46	1.50
33	C	519	DGD	O2G-C2G	-2.05	1.41	1.46
25	B	613	CLA	CMC-C2C	-2.05	1.46	1.50
25	a	708	CLA	CMD-C2D	-2.05	1.46	1.50
29	B	626	SQD	O2-C2	-2.05	1.37	1.43
33	c	517	DGD	O6E-C5E	-2.04	1.39	1.44
25	B	614	CLA	CMD-C2D	-2.04	1.46	1.50
25	a	711	CLA	CMB-C2B	-2.04	1.46	1.50
25	c	502	CLA	CMD-C2D	-2.04	1.46	1.50
23	C	501	LMG	O7-C8	-2.04	1.41	1.46
25	C	510	CLA	CMB-C2B	-2.04	1.46	1.50
35	v	201	HEC	CMB-C2B	2.04	1.54	1.50
25	B	602	CLA	CMD-C2D	-2.04	1.46	1.50
25	B	606	CLA	CMB-C2B	-2.04	1.46	1.50
25	B	615	CLA	CMD-C2D	-2.03	1.46	1.50
25	b	619	CLA	CMD-C2D	-2.03	1.46	1.50
25	D	404	CLA	CMD-C2D	-2.03	1.46	1.50
25	C	509	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	610	CLA	CMD-C2D	-2.03	1.46	1.50
32	d	406	LHG	P-O6	2.03	1.67	1.59
25	c	501	CLA	CMD-C2D	-2.03	1.46	1.50
25	C	507	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	602	CLA	CMB-C2B	-2.03	1.46	1.50
25	B	613	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	606	CLA	CMD-C2D	-2.02	1.46	1.50
25	C	511	CLA	CMD-C2D	-2.02	1.46	1.50
25	B	608	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	608	CLA	CMD-C2D	-2.02	1.46	1.50
25	c	511	CLA	CMB-C2B	-2.02	1.46	1.50
25	b	616	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	622	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	504	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	504	CLA	CMD-C2D	-2.02	1.46	1.50
25	B	603	CLA	CMB-C2B	-2.02	1.46	1.50
34	e	102	HEM	CMA-C3A	2.02	1.54	1.50
27	d	404	BCR	C33-C5	-2.02	1.47	1.50
25	b	607	CLA	CMD-C2D	-2.01	1.46	1.50
23	A	603	LMG	O7-C8	-2.01	1.41	1.46
25	b	614	CLA	CMB-C2B	-2.01	1.46	1.50
25	a	719	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	613	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	615	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	605	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	508	CLA	CMD-C2D	-2.01	1.46	1.50
35	V	201	HEC	CMC-C2C	2.01	1.54	1.50
25	B	607	CLA	CMD-C2D	-2.01	1.46	1.50
25	a	719	CLA	CMB-C2B	-2.01	1.46	1.50
25	B	611	CLA	CMB-C2B	-2.01	1.46	1.50
27	b	623	BCR	C33-C5	-2.01	1.47	1.50
25	B	607	CLA	CMB-C2B	-2.01	1.46	1.50
23	D	409	LMG	O7-C8	-2.01	1.41	1.46
25	B	616	CLA	CMC-C2C	-2.01	1.46	1.50
25	C	502	CLA	CMB-C2B	-2.01	1.46	1.50
25	C	513	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	505	CLA	CMB-C2B	-2.01	1.46	1.50
25	D	402	CLA	CMD-C2D	-2.01	1.46	1.50
35	v	201	HEC	CMD-C2D	2.01	1.54	1.50
25	B	617	CLA	CMD-C2D	-2.00	1.46	1.50
25	C	506	CLA	CMB-C2B	-2.00	1.46	1.50
33	c	517	DGD	C1E-C2E	2.00	1.58	1.52
25	c	504	CLA	CMB-C2B	-2.00	1.46	1.50
25	A	607	CLA	CMD-C2D	-2.00	1.46	1.50
25	b	617	CLA	CMD-C2D	-2.00	1.46	1.50
25	b	622	CLA	CMD-C2D	-2.00	1.46	1.50
25	c	502	CLA	CMB-C2B	-2.00	1.46	1.50
28	a	713	PL9	C6-C1	-2.00	1.45	1.48
27	Y	101	BCR	C33-C5	-2.00	1.47	1.50
25	A	609	CLA	CMB-C2B	-2.00	1.46	1.50

All (957) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	605	CLA	C4A-NA-C1A	6.58	109.68	106.68
25	b	610	CLA	C4A-NA-C1A	6.37	109.58	106.68
25	C	508	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	C	513	CLA	C4A-NA-C1A	6.26	109.53	106.68
25	b	619	CLA	C4A-NA-C1A	6.18	109.50	106.68
25	b	621	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	c	507	CLA	C4A-NA-C1A	6.10	109.46	106.68
25	C	504	CLA	C4A-NA-C1A	6.06	109.44	106.68
25	c	509	CLA	C4A-NA-C1A	6.05	109.44	106.68
26	A	608	PHO	C4D-CHA-CBD	-6.03	105.56	108.45
25	c	511	CLA	C4A-NA-C1A	6.03	109.43	106.68
25	c	513	CLA	C4A-NA-C1A	6.01	109.42	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	503	CLA	C4A-NA-C1A	6.00	109.42	106.68
25	c	512	CLA	C4A-NA-C1A	5.94	109.39	106.68
26	D	401	PHO	C4D-CHA-CBD	-5.94	105.61	108.45
25	b	615	CLA	C4A-NA-C1A	5.90	109.37	106.68
25	C	510	CLA	C4A-NA-C1A	5.89	109.36	106.68
26	a	709	PHO	C4D-CHA-CBD	-5.88	105.63	108.45
25	B	616	CLA	C4A-NA-C1A	5.87	109.36	106.68
25	B	610	CLA	C4A-NA-C1A	5.87	109.36	106.68
25	C	512	CLA	C4A-NA-C1A	5.84	109.34	106.68
25	b	607	CLA	C4A-NA-C1A	5.83	109.34	106.68
25	B	617	CLA	C4A-NA-C1A	5.81	109.33	106.68
25	B	613	CLA	C4A-NA-C1A	5.77	109.31	106.68
25	c	502	CLA	C4A-NA-C1A	5.77	109.31	106.68
26	a	710	PHO	C4D-CHA-CBD	-5.77	105.69	108.45
25	b	618	CLA	C4A-NA-C1A	5.76	109.31	106.68
25	B	612	CLA	C4A-NA-C1A	5.72	109.29	106.68
25	C	506	CLA	C4A-NA-C1A	5.71	109.28	106.68
25	B	602	CLA	C4A-NA-C1A	5.71	109.28	106.68
25	b	622	CLA	C4A-NA-C1A	5.66	109.26	106.68
25	B	614	CLA	C4A-NA-C1A	5.65	109.26	106.68
25	C	502	CLA	C4A-NA-C1A	5.62	109.24	106.68
25	C	503	CLA	C4A-NA-C1A	5.57	109.22	106.68
25	d	402	CLA	C4A-NA-C1A	5.54	109.21	106.68
25	c	510	CLA	C4A-NA-C1A	5.53	109.20	106.68
25	B	607	CLA	C4A-NA-C1A	5.49	109.18	106.68
25	C	509	CLA	C4A-NA-C1A	5.44	109.16	106.68
25	D	404	CLA	C4A-NA-C1A	5.43	109.16	106.68
25	C	507	CLA	C4A-NA-C1A	5.41	109.15	106.68
25	C	514	CLA	C4A-NA-C1A	5.40	109.14	106.68
25	c	501	CLA	C4A-NA-C1A	5.39	109.14	106.68
25	C	511	CLA	C4A-NA-C1A	5.37	109.13	106.68
25	b	617	CLA	C4A-NA-C1A	5.35	109.12	106.68
25	B	606	CLA	C4A-NA-C1A	5.34	109.11	106.68
25	c	508	CLA	C4A-NA-C1A	5.31	109.10	106.68
25	a	711	CLA	C4A-NA-C1A	5.26	109.08	106.68
25	D	403	CLA	C4A-NA-C1A	5.25	109.07	106.68
28	a	713	PL9	C7-C3-C4	5.22	121.21	116.91
25	A	609	CLA	C4A-NA-C1A	5.22	109.06	106.68
25	b	611	CLA	C4A-NA-C1A	5.20	109.05	106.68
25	c	504	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	d	403	CLA	C4A-NA-C1A	5.16	109.03	106.68
25	B	611	CLA	C4A-NA-C1A	5.12	109.02	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C4A-NA-C1A	5.12	109.02	106.68
25	c	506	CLA	C4A-NA-C1A	5.12	109.01	106.68
25	B	615	CLA	C4A-NA-C1A	5.12	109.01	106.68
28	d	405	PL9	C7-C3-C4	5.12	121.12	116.91
25	c	505	CLA	C4A-NA-C1A	5.07	108.99	106.68
25	b	614	CLA	C4A-NA-C1A	5.00	108.96	106.68
28	D	406	PL9	C7-C3-C4	4.98	121.01	116.91
29	b	601	SQD	O6-C1-C2	4.97	115.82	108.27
25	b	616	CLA	C4A-NA-C1A	4.92	108.92	106.68
25	A	607	CLA	C4A-NA-C1A	4.91	108.92	106.68
25	B	603	CLA	C4A-NA-C1A	4.90	108.91	106.68
28	A	611	PL9	C7-C3-C4	4.90	120.94	116.91
25	a	708	CLA	C4A-NA-C1A	4.88	108.91	106.68
25	b	612	CLA	C4A-NA-C1A	4.86	108.89	106.68
25	D	402	CLA	C4A-NA-C1A	4.73	108.84	106.68
25	a	719	CLA	C4A-NA-C1A	4.72	108.83	106.68
35	v	201	HEC	CBB-CAB-C3B	4.69	125.13	112.42
35	V	201	HEC	CBB-CAB-C3B	4.67	125.07	112.42
25	a	707	CLA	C4A-NA-C1A	4.62	108.79	106.68
29	B	626	SQD	O5-C5-C4	4.57	117.93	109.70
29	B	626	SQD	O9-S-C6	4.53	113.53	106.76
29	B	623	SQD	C4-C3-C2	4.45	118.64	110.83
32	D	408	LHG	O4-P-O5	4.42	133.01	112.44
29	b	601	SQD	O7-S-C6	4.41	113.34	106.76
32	B	625	LHG	O4-P-O5	4.41	132.94	112.44
32	L	101	LHG	O4-P-O5	4.41	132.94	112.44
32	d	407	LHG	O4-P-O5	4.40	132.91	112.44
32	d	406	LHG	O4-P-O5	4.40	132.91	112.44
32	b	629	LHG	O4-P-O5	4.40	132.90	112.44
32	a	720	LHG	O4-P-O5	4.39	132.89	112.44
32	D	407	LHG	O4-P-O5	4.39	132.88	112.44
32	e	101	LHG	O4-P-O5	4.37	132.79	112.44
32	E	101	LHG	O4-P-O5	4.34	132.62	112.44
25	B	608	CLA	C4A-NA-C1A	4.32	108.65	106.68
33	C	519	DGD	O3G-C3G-C2G	-4.32	100.32	110.82
25	b	608	CLA	C4A-NA-C1A	4.22	108.61	106.68
33	C	517	DGD	O3G-C3G-C2G	-4.22	100.56	110.82
29	a	714	SQD	O5-C5-C4	4.21	117.28	109.70
33	c	516	DGD	O3G-C3G-C2G	-4.20	100.60	110.82
25	C	505	CLA	C4A-NA-C1A	4.16	108.58	106.68
33	C	518	DGD	O3G-C3G-C2G	-4.16	100.70	110.82
25	b	620	CLA	C4A-NA-C1A	4.15	108.57	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	518	DGD	O3G-C3G-C2G	-4.13	100.78	110.82
28	a	713	PL9	C7-C3-C2	-4.12	118.53	123.39
33	c	517	DGD	O3G-C3G-C2G	-4.11	100.82	110.82
29	I	102	SQD	O47-C7-C8	4.09	120.33	111.48
23	b	626	LMG	O6-C1-C2	4.08	118.76	110.37
29	A	612	SQD	O9-S-O7	-4.08	100.56	113.82
29	B	626	SQD	O6-C1-C2	4.07	114.46	108.27
29	D	410	SQD	O6-C1-C2	4.07	114.46	108.27
23	c	520	LMG	O6-C1-O1	-4.07	100.42	110.04
29	B	626	SQD	O9-S-O7	-4.05	100.66	113.82
29	A	612	SQD	O5-C5-C4	4.04	116.99	109.70
29	B	623	SQD	O9-S-O7	-3.99	100.84	113.82
29	A	612	SQD	O9-S-C6	3.99	112.71	106.76
28	A	611	PL9	C7-C3-C2	-3.98	118.70	123.39
28	D	406	PL9	C7-C3-C2	-3.94	118.75	123.39
27	H	102	BCR	C2-C1-C6	3.94	116.16	110.44
25	A	606	CLA	C4A-NA-C1A	3.94	108.47	106.68
28	d	405	PL9	C7-C3-C2	-3.92	118.77	123.39
29	f	102	SQD	O9-S-O7	-3.90	101.13	113.82
29	D	410	SQD	O9-S-O7	-3.88	101.21	113.82
23	C	521	LMG	O6-C1-O1	-3.86	100.91	110.04
29	a	714	SQD	O9-S-O7	-3.83	101.37	113.82
25	B	609	CLA	C4A-NA-C1A	3.79	108.41	106.68
35	v	201	HEC	CBC-CAC-C3C	3.79	122.69	112.42
26	A	608	PHO	C2B-C1B-NB	-3.76	106.71	109.43
33	H	103	DGD	O3G-C3G-C2G	-3.74	101.71	110.82
25	b	609	CLA	C4A-NA-C1A	3.74	108.38	106.68
29	B	623	SQD	O47-C7-C8	3.73	119.54	111.48
29	b	601	SQD	O9-S-C6	3.72	112.31	106.76
29	A	612	SQD	O47-C7-C8	3.69	119.47	111.48
29	B	623	SQD	O5-C5-C4	3.66	116.29	109.70
23	b	626	LMG	O6-C5-C4	3.65	116.28	109.70
26	a	709	PHO	C2B-C1B-NB	-3.63	106.81	109.43
29	A	614	SQD	O47-C7-C8	3.58	119.24	111.48
26	D	401	PHO	C2B-C1B-NB	-3.57	106.85	109.43
35	V	201	HEC	CBC-CAC-C3C	3.54	122.01	112.42
33	C	519	DGD	O6D-C1D-O3G	-3.52	101.72	110.04
25	b	613	CLA	C4A-NA-C1A	3.52	108.29	106.68
29	a	714	SQD	O47-C7-C8	3.51	119.06	111.48
29	B	626	SQD	O7-S-C6	3.48	111.96	106.76
29	A	612	SQD	O6-C1-C2	3.48	113.56	108.27
33	c	518	DGD	O6D-C1D-O3G	-3.47	101.85	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	714	SQD	O7-S-C6	3.45	111.91	106.76
29	b	601	SQD	O9-S-O7	-3.45	102.61	113.82
33	c	517	DGD	O6D-C1D-O3G	-3.43	101.94	110.04
29	D	410	SQD	O47-C7-C8	3.42	118.89	111.48
29	B	623	SQD	C3-C4-C5	3.40	116.41	110.23
33	C	518	DGD	O6D-C1D-O3G	-3.40	102.02	110.04
33	h	102	DGD	O3G-C3G-C2G	-3.39	102.56	110.82
29	b	601	SQD	O47-C7-C8	3.39	118.81	111.48
29	f	102	SQD	O7-S-C6	3.37	111.79	106.76
33	C	517	DGD	O6D-C1D-O3G	-3.36	102.09	110.04
33	c	516	DGD	O6D-C1D-O3G	-3.36	102.10	110.04
29	B	626	SQD	O47-C7-C8	3.36	118.75	111.48
26	a	710	PHO	C2B-C1B-NB	-3.35	107.01	109.43
26	a	710	PHO	O1D-CGD-CBD	3.35	129.80	124.72
29	D	410	SQD	O7-S-C6	3.34	111.75	106.76
31	a	706	BCT	O2-C-O1	-3.33	111.16	119.68
29	D	410	SQD	O9-S-C6	3.30	111.68	106.76
29	f	102	SQD	O9-S-C6	3.30	111.68	106.76
29	f	102	SQD	O6-C1-C2	3.29	113.27	108.27
29	a	714	SQD	C3-C4-C5	3.27	116.15	110.23
26	D	401	PHO	O1D-CGD-CBD	3.25	129.66	124.72
23	B	621	LMG	O6-C1-O1	-3.24	102.39	110.04
27	C	516	BCR	C15-C16-C17	-3.23	116.91	123.52
26	a	709	PHO	O1D-CGD-CBD	3.22	129.61	124.72
31	A	615	BCT	O2-C-O1	-3.21	111.46	119.68
29	a	714	SQD	O9-S-C6	3.18	111.51	106.76
27	h	101	BCR	C2-C1-C6	3.17	115.05	110.44
33	H	103	DGD	O6D-C1D-O3G	-3.17	102.55	110.04
29	a	714	SQD	O6-C1-C2	3.17	113.09	108.27
25	b	607	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
29	B	626	SQD	C1-O5-C5	3.13	119.82	113.72
29	D	410	SQD	O5-C5-C4	3.12	115.33	109.70
25	B	602	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
29	B	623	SQD	O9-S-C6	3.09	111.36	106.76
25	C	505	CLA	CHB-C4A-NA	3.08	128.85	124.40
26	a	710	PHO	CMB-C2B-C3B	3.08	130.84	124.68
25	C	513	CLA	CHB-C4A-NA	3.08	128.84	124.40
25	b	612	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
25	B	607	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
25	B	605	CLA	CHB-C4A-NA	3.06	128.82	124.40
25	D	402	CLA	CHB-C4A-NA	3.06	128.81	124.40
25	B	608	CLA	CHB-C4A-NA	3.05	128.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	612	SQD	O7-S-C6	3.05	111.31	106.76
23	b	626	LMG	C1-O6-C5	3.04	119.65	113.72
25	B	604	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
25	b	610	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
25	b	621	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
29	B	623	SQD	C1-O5-C5	3.00	119.58	113.72
29	A	612	SQD	C3-C4-C5	3.00	115.67	110.23
25	a	708	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
25	A	606	CLA	CHB-C4A-NA	2.99	128.71	124.40
25	C	502	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
33	h	102	DGD	O6D-C1D-O3G	-2.98	103.00	110.04
25	C	508	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
26	A	608	PHO	O1D-CGD-CBD	2.98	129.24	124.72
25	D	402	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	D	404	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	B	605	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
27	H	102	BCR	C24-C23-C22	-2.97	121.85	126.23
27	c	515	BCR	C15-C16-C17	-2.97	117.45	123.52
25	c	504	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	b	613	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
25	C	506	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
25	c	508	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
26	D	401	PHO	CMB-C2B-C3B	2.95	130.59	124.68
25	A	607	CLA	C3B-C4B-NB	-2.95	107.90	110.53
27	d	404	BCR	C27-C26-C25	2.95	126.69	122.70
25	b	613	CLA	CHB-C4A-NA	2.94	128.65	124.40
25	b	610	CLA	CHB-C4A-NA	2.94	128.64	124.40
33	C	518	DGD	O5D-C6D-C5D	-2.94	102.80	109.42
32	a	720	LHG	O8-C23-C24	2.94	120.78	111.83
25	c	507	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	B	605	CLA	C1-C2-C3	-2.93	121.39	126.20
25	c	501	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	c	502	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	C	509	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
32	B	625	LHG	O8-C23-C24	2.93	120.76	111.83
25	C	513	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
27	b	625	BCR	C27-C26-C25	2.92	126.66	122.70
27	b	602	BCR	C33-C5-C6	-2.92	121.29	124.48
27	t	103	BCR	C33-C5-C6	-2.92	121.30	124.48
25	C	505	CLA	C3B-C4B-NB	-2.92	107.92	110.53
35	V	201	HEC	CAC-C3C-C4C	2.92	128.92	124.91
25	A	607	CLA	O2D-CGD-O1D	-2.91	118.17	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	t	103	BCR	C15-C14-C13	-2.91	123.19	127.28
25	b	617	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
27	B	620	BCR	C27-C26-C25	2.91	126.64	122.70
25	B	616	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
25	C	503	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
25	c	504	CLA	CHB-C4A-NA	2.90	128.59	124.40
25	A	607	CLA	CHB-C4A-NA	2.90	128.59	124.40
25	a	719	CLA	CHB-C4A-NA	2.90	128.59	124.40
25	c	505	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
28	A	611	PL9	C7-C8-C9	-2.89	121.85	126.83
25	B	603	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	C	505	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
25	b	617	CLA	C1-C2-C3	-2.89	121.47	126.20
25	a	711	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
27	B	618	BCR	C15-C16-C17	-2.89	117.61	123.52
25	b	618	CLA	C3B-C4B-NB	-2.89	107.95	110.53
26	a	710	PHO	O2D-CGD-O1D	-2.88	118.24	123.85
25	C	508	CLA	CHB-C4A-NA	2.88	128.56	124.40
32	D	407	LHG	O8-C23-C24	2.88	120.62	111.83
25	B	609	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	d	403	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
25	b	609	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
25	b	620	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
25	C	510	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
27	B	618	BCR	C29-C30-C25	2.87	114.61	110.44
27	b	623	BCR	C27-C26-C25	2.87	126.58	122.70
25	a	719	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
25	c	507	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	a	709	PHO	CMB-C2B-C3B	2.87	130.41	124.68
25	c	512	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	C	514	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
25	b	618	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	d	402	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
26	A	608	PHO	O2D-CGD-O1D	-2.86	118.29	123.85
25	a	708	CLA	C3B-C4B-NB	-2.86	107.98	110.53
29	B	623	SQD	O7-S-C6	2.86	111.02	106.76
25	A	609	CLA	CHB-C4A-NA	2.85	128.52	124.40
23	A	603	LMG	O6-C5-C4	2.85	114.84	109.70
25	B	616	CLA	CHB-C4A-NA	2.85	128.52	124.40
25	C	502	CLA	C3B-C4B-NB	-2.85	107.98	110.53
27	C	515	BCR	C2-C1-C6	2.85	114.58	110.44
25	B	613	CLA	O2D-CGD-O1D	-2.85	118.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	501	CLA	C3B-C4B-NB	-2.85	107.99	110.53
25	b	620	CLA	CHB-C4A-NA	2.85	128.51	124.40
25	B	615	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	A	609	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
32	E	101	LHG	O8-C23-C24	2.85	120.51	111.83
25	c	511	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
25	b	620	CLA	C3B-C4B-NB	-2.84	107.99	110.53
23	A	603	LMG	O6-C1-O1	-2.84	103.33	110.04
25	B	604	CLA	CHB-C4A-NA	2.84	128.50	124.40
25	C	510	CLA	C3B-C4B-NB	-2.84	108.00	110.53
28	A	611	PL9	C22-C23-C24	-2.84	121.13	127.62
35	v	201	HEC	CAC-C3C-C4C	2.84	128.81	124.91
29	B	626	SQD	C3-C4-C5	2.83	115.37	110.23
33	h	102	DGD	CDB-CCB-CBB	-2.83	100.04	114.37
25	b	611	CLA	C3B-C4B-NB	-2.83	108.01	110.53
29	f	102	SQD	O5-C5-C4	2.82	114.79	109.70
34	e	102	HEM	C3B-C4B-NB	-2.82	107.44	109.47
25	C	511	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
28	d	405	PL9	C40-C39-C41	2.82	120.13	115.23
27	b	623	BCR	C15-C16-C17	-2.82	117.75	123.52
25	b	616	CLA	C3B-C4B-NB	-2.82	108.01	110.53
27	c	514	BCR	C27-C26-C25	2.82	126.51	122.70
32	d	406	LHG	O8-C23-C24	2.82	120.42	111.83
25	B	613	CLA	CHB-C4A-NA	2.82	128.46	124.40
33	c	517	DGD	CDB-CCB-CBB	-2.82	100.14	114.37
27	b	602	BCR	C15-C14-C13	-2.82	123.33	127.28
25	a	711	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	b	616	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	c	502	CLA	C3B-C4B-NB	-2.81	108.02	110.53
28	A	611	PL9	C40-C39-C41	2.81	120.11	115.23
25	a	707	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	b	614	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	C	504	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	B	611	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	c	513	CLA	CHB-C4A-NA	2.81	128.45	124.40
25	B	609	CLA	CHB-C4A-NA	2.81	128.45	124.40
25	c	503	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
25	b	613	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	b	618	CLA	CHB-C4A-NA	2.80	128.45	124.40
27	D	405	BCR	C27-C26-C25	2.80	126.49	122.70
27	b	624	BCR	C27-C26-C25	2.80	126.49	122.70
25	b	621	CLA	CHB-C4A-NA	2.80	128.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	616	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
27	b	623	BCR	C33-C5-C6	-2.80	121.43	124.48
25	C	509	CLA	CHB-C4A-NA	2.80	128.44	124.40
25	c	509	CLA	CHB-C4A-NA	2.80	128.43	124.40
35	v	201	HEC	C2A-C1A-NA	-2.80	107.63	110.32
25	b	607	CLA	CHB-C4A-NA	2.79	128.43	124.40
25	c	510	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
33	C	519	DGD	CDB-CCB-CBB	-2.79	100.28	114.37
23	b	626	LMG	C4-C3-C2	-2.78	105.94	110.83
32	d	407	LHG	O8-C23-C24	2.78	120.33	111.83
25	D	403	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
27	t	103	BCR	C15-C16-C17	-2.78	117.83	123.52
25	b	608	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	b	622	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	B	612	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	B	603	CLA	CHB-C4A-NA	2.78	128.41	124.40
25	a	708	CLA	CHB-C4A-NA	2.77	128.40	124.40
25	B	614	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
33	C	518	DGD	CDB-CCB-CBB	-2.77	100.38	114.37
25	b	619	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
25	c	512	CLA	CHB-C4A-NA	2.76	128.39	124.40
27	b	602	BCR	C15-C16-C17	-2.76	117.87	123.52
25	B	608	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	C	504	CLA	CHB-C4A-NA	2.75	128.37	124.40
27	B	619	BCR	C27-C26-C25	2.75	126.42	122.70
25	C	504	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
33	c	516	DGD	CDB-CCB-CBB	-2.75	100.48	114.37
25	b	609	CLA	CHB-C4A-NA	2.75	128.36	124.40
25	c	506	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	B	618	BCR	C33-C5-C6	-2.75	121.49	124.48
26	D	401	PHO	O2D-CGD-O1D	-2.74	118.51	123.85
25	C	512	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
25	B	610	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
25	B	602	CLA	CHB-C4A-NA	2.74	128.35	124.40
25	B	614	CLA	C3B-C4B-NB	-2.74	108.09	110.53
35	V	201	HEC	C2A-C1A-NA	-2.74	107.68	110.32
25	b	607	CLA	C3B-C4B-NB	-2.74	108.09	110.53
27	h	101	BCR	C27-C26-C25	2.74	126.40	122.70
25	b	619	CLA	CHB-C4A-NA	2.73	128.34	124.40
26	A	608	PHO	CMB-C2B-C3B	2.73	130.14	124.68
25	B	617	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	c	503	CLA	C3B-C4B-NB	-2.73	108.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	408	LHG	C11-C10-C9	-2.73	100.59	114.37
25	c	508	CLA	CHB-C4A-NA	2.73	128.33	124.40
25	b	614	CLA	CHB-C4A-NA	2.72	128.33	124.40
23	f	101	LMG	O6-C1-O1	-2.72	103.61	110.04
25	C	509	CLA	C3B-C4B-NB	-2.72	108.10	110.53
29	I	102	SQD	O48-C23-C24	2.72	120.14	111.83
27	k	101	BCR	C33-C5-C6	-2.72	121.52	124.48
27	B	618	BCR	C11-C10-C9	-2.72	123.47	127.28
25	C	511	CLA	C3B-C4B-NB	-2.72	108.11	110.53
27	c	515	BCR	C27-C26-C25	2.71	126.37	122.70
33	c	518	DGD	CDB-CCB-CBB	-2.71	100.66	114.37
25	B	611	CLA	CHB-C4A-NA	2.71	128.31	124.40
33	H	103	DGD	CDB-CCB-CBB	-2.71	100.69	114.37
25	c	501	CLA	CHB-C4A-NA	2.71	128.30	124.40
33	C	519	DGD	C3G-C2G-C1G	-2.70	105.48	111.78
25	B	606	CLA	CHB-C4A-NA	2.70	128.30	124.40
35	v	201	HEC	C3D-C4D-ND	-2.70	107.74	110.35
25	c	503	CLA	CHB-C4A-NA	2.70	128.30	124.40
28	a	713	PL9	C22-C23-C24	-2.70	121.44	127.62
32	L	101	LHG	O8-C23-C24	2.70	120.06	111.83
25	C	510	CLA	CHB-C4A-NA	2.70	128.29	124.40
27	b	623	BCR	C15-C14-C13	-2.69	123.50	127.28
28	D	406	PL9	C27-C28-C29	-2.69	121.46	127.62
25	B	615	CLA	C3B-C4B-NB	-2.69	108.13	110.53
35	v	201	HEC	C1D-ND-C4D	2.69	108.39	105.21
27	a	712	BCR	C27-C26-C25	2.69	126.34	122.70
25	c	513	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
27	D	405	BCR	C33-C5-C6	-2.68	121.56	124.48
29	B	623	SQD	O48-C23-C24	2.68	120.01	111.83
25	C	514	CLA	CHB-C4A-NA	2.68	128.27	124.40
25	B	611	CLA	C3B-C4B-NB	-2.68	108.14	110.53
29	b	601	SQD	C44-O6-C1	2.68	119.54	113.80
25	B	612	CLA	CHB-C4A-NA	2.68	128.26	124.40
34	e	102	HEM	C3B-C2B-C1B	2.68	108.42	106.41
25	d	403	CLA	CHB-C4A-NA	2.67	128.26	124.40
28	d	405	PL9	C22-C23-C24	-2.67	121.50	127.62
25	c	513	CLA	C3B-C4B-NB	-2.67	108.15	110.53
27	c	515	BCR	C15-C14-C13	-2.66	123.54	127.28
25	B	607	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	B	615	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	b	611	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	B	614	CLA	CHB-C4A-NA	2.66	128.24	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	617	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	C	512	CLA	C3B-C4B-NB	-2.66	108.16	110.53
27	K	101	BCR	C27-C26-C25	2.66	126.30	122.70
25	B	617	CLA	CHB-C4A-NA	2.66	128.23	124.40
25	b	615	CLA	CHB-C4A-NA	2.66	128.23	124.40
25	c	506	CLA	CHB-C4A-NA	2.66	128.23	124.40
23	b	627	LMG	O6-C1-O1	-2.66	103.77	110.04
27	C	515	BCR	C11-C10-C9	-2.66	123.55	127.28
27	H	102	BCR	C27-C26-C25	2.66	126.29	122.70
25	c	509	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
29	A	612	SQD	O48-C23-C24	2.65	119.92	111.83
23	A	603	LMG	O6-C1-C2	-2.65	104.92	110.37
25	c	502	CLA	CHB-C4A-NA	2.65	128.22	124.40
29	a	714	SQD	O48-C23-C24	2.65	119.91	111.83
25	c	509	CLA	C3B-C4B-NB	-2.65	108.17	110.53
25	C	507	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
25	b	612	CLA	CHB-C4A-NA	2.65	128.22	124.40
25	B	613	CLA	C3B-C4B-NB	-2.64	108.17	110.53
28	a	713	PL9	C40-C39-C41	2.64	119.82	115.23
25	c	504	CLA	C3B-C4B-NB	-2.64	108.17	110.53
25	C	503	CLA	CHB-C4A-NA	2.64	128.21	124.40
28	d	405	PL9	C27-C28-C29	-2.64	121.58	127.62
25	b	611	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	c	510	CLA	CHB-C4A-NA	2.64	128.21	124.40
29	A	614	SQD	O48-C23-C24	2.64	119.87	111.83
27	k	102	BCR	C29-C30-C25	2.63	114.27	110.44
25	b	614	CLA	C3B-C4B-NB	-2.63	108.18	110.53
25	B	606	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
27	B	620	BCR	C33-C5-C6	-2.63	121.61	124.48
23	a	701	LMG	O6-C1-O1	-2.63	103.84	110.04
27	Y	101	BCR	C33-C5-C6	-2.62	121.62	124.48
25	C	511	CLA	CHB-C4A-NA	2.62	128.18	124.40
27	C	515	BCR	C27-C26-C25	2.62	126.25	122.70
25	c	511	CLA	CHB-C4A-NA	2.62	128.18	124.40
29	B	626	SQD	O48-C23-C24	2.61	119.81	111.83
26	a	709	PHO	O2D-CGD-O1D	-2.61	118.76	123.85
27	b	625	BCR	C33-C5-C6	-2.61	121.64	124.48
25	C	503	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	t	103	BCR	C24-C23-C22	-2.60	122.38	126.23
25	B	607	CLA	C3B-C4B-NB	-2.60	108.21	110.53
33	C	517	DGD	CDB-CCB-CBB	-2.60	101.22	114.37
28	D	406	PL9	C40-C39-C41	2.60	119.74	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	508	CLA	C3B-C4B-NB	-2.60	108.21	110.53
25	C	507	CLA	CHB-C4A-NA	2.59	128.14	124.40
28	D	406	PL9	C7-C8-C9	-2.59	122.36	126.83
35	V	201	HEC	C1D-ND-C4D	2.59	108.28	105.21
27	Y	101	BCR	C27-C26-C25	2.59	126.20	122.70
27	b	624	BCR	C15-C16-C17	-2.59	118.22	123.52
32	b	629	LHG	O8-C23-C24	2.59	119.73	111.83
34	e	102	HEM	C1B-NB-C4B	2.59	108.27	105.21
32	D	408	LHG	O8-C23-C24	2.59	119.72	111.83
25	C	514	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	b	608	CLA	CHB-C4A-NA	2.58	128.13	124.40
27	D	405	BCR	C24-C23-C22	-2.58	122.42	126.23
27	A	610	BCR	C27-C26-C25	2.58	126.19	122.70
27	D	405	BCR	C15-C16-C17	-2.58	118.25	123.52
27	c	514	BCR	C33-C5-C6	-2.57	121.68	124.48
27	C	516	BCR	C15-C14-C13	-2.57	123.67	127.28
25	C	512	CLA	CHB-C4A-NA	2.57	128.11	124.40
27	A	610	BCR	C24-C23-C22	-2.57	122.44	126.23
28	A	611	PL9	C27-C28-C29	-2.57	121.75	127.62
29	b	601	SQD	C4-C3-C2	2.57	115.33	110.83
25	B	610	CLA	CHB-C4A-NA	2.57	128.10	124.40
23	c	519	LMG	O6-C1-O1	-2.56	103.99	110.04
32	B	625	LHG	C11-C10-C9	-2.56	101.42	114.37
25	B	612	CLA	C1-C2-C3	-2.56	122.00	126.20
25	B	616	CLA	C3B-C4B-NB	-2.56	108.24	110.53
25	D	404	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	B	602	CLA	C3B-C4B-NB	-2.56	108.25	110.53
25	C	502	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	c	511	CLA	C3B-C4B-NB	-2.56	108.25	110.53
33	c	518	DGD	C3G-C2G-C1G	-2.55	105.84	111.78
35	V	201	HEC	C3C-C4C-NC	-2.55	107.32	110.15
25	C	513	CLA	C3B-C4B-NB	-2.55	108.25	110.53
29	B	623	SQD	O8-S-C6	2.55	110.89	105.97
32	d	406	LHG	C11-C10-C9	-2.55	101.50	114.37
27	C	516	BCR	C33-C5-C6	-2.55	121.71	124.48
25	C	506	CLA	CHB-C4A-NA	2.55	128.07	124.40
25	b	622	CLA	CHB-C4A-NA	2.55	128.07	124.40
25	b	615	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
23	M	101	LMG	O6-C1-O1	-2.54	104.04	110.04
27	c	515	BCR	C33-C5-C6	-2.54	121.71	124.48
27	c	514	BCR	C15-C16-C17	-2.54	118.32	123.52
27	C	516	BCR	C27-C26-C25	2.54	126.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	D	403	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	a	711	CLA	C3B-C4B-NB	-2.54	108.27	110.53
23	a	715	LMG	O6-C1-O1	-2.53	104.06	110.04
27	k	101	BCR	C27-C26-C25	2.53	126.12	122.70
25	c	510	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	B	606	CLA	C3B-C4B-NB	-2.52	108.28	110.53
33	C	517	DGD	C3G-C2G-C1G	-2.52	105.91	111.78
32	L	101	LHG	C11-C10-C9	-2.52	101.63	114.37
25	A	606	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
23	a	701	LMG	C38-C37-C36	-2.52	101.63	114.37
29	a	714	SQD	C4-C3-C2	2.52	115.25	110.83
25	C	511	CLA	C1-C2-C3	-2.52	122.07	126.20
23	C	501	LMG	C38-C37-C36	-2.52	101.64	114.37
23	a	701	LMG	C40-C39-C38	-2.51	101.67	114.37
25	C	508	CLA	C3B-C4B-NB	-2.50	108.30	110.53
27	h	101	BCR	C15-C14-C13	-2.50	123.78	127.28
32	b	629	LHG	C11-C10-C9	-2.49	101.78	114.37
23	C	501	LMG	O6-C1-O1	-2.49	104.16	110.04
25	a	707	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
32	e	101	LHG	O8-C23-C24	2.49	119.42	111.83
27	b	624	BCR	C15-C14-C13	-2.49	123.79	127.28
25	d	403	CLA	C3B-C4B-NB	-2.48	108.31	110.53
27	k	102	BCR	C33-C5-C6	-2.48	121.77	124.48
27	K	101	BCR	C24-C23-C22	-2.48	122.56	126.23
23	M	101	LMG	C38-C37-C36	-2.48	101.83	114.37
28	a	713	PL9	C7-C8-C9	-2.48	122.56	126.83
27	c	514	BCR	C11-C10-C9	-2.48	123.80	127.28
27	d	404	BCR	C7-C8-C9	-2.47	122.57	126.23
27	t	103	BCR	C27-C26-C25	2.47	126.05	122.70
35	v	201	HEC	C3C-C4C-NC	-2.47	107.41	110.15
27	b	602	BCR	C27-C26-C25	2.47	126.04	122.70
27	a	712	BCR	C24-C23-C22	-2.47	122.58	126.23
27	k	102	BCR	C27-C26-C25	2.47	126.03	122.70
27	h	101	BCR	C24-C23-C22	-2.46	122.59	126.23
25	b	619	CLA	C3B-C4B-NB	-2.46	108.33	110.53
29	B	623	SQD	C1-C2-C3	2.46	115.18	110.01
23	D	409	LMG	O6-C1-O1	-2.46	104.24	110.04
23	d	408	LMG	O7-C10-O9	-2.45	117.97	123.70
27	d	404	BCR	C2-C3-C4	2.45	116.67	111.28
32	D	408	LHG	C20-C19-C18	-2.45	101.98	114.37
27	c	514	BCR	C24-C23-C22	-2.45	122.61	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	405	PL9	C20-C19-C21	2.45	119.48	115.23
29	B	623	SQD	C44-O6-C1	2.44	119.04	113.80
28	D	406	PL9	C22-C23-C24	-2.44	122.03	127.62
25	B	609	CLA	C3B-C4B-NB	-2.44	108.35	110.53
25	b	610	CLA	C3B-C4B-NB	-2.44	108.35	110.53
23	b	626	LMG	O2-C2-C1	-2.44	104.26	110.08
27	B	618	BCR	C15-C14-C13	-2.44	123.86	127.28
28	a	713	PL9	O2-C1-C6	2.44	124.36	120.48
32	D	407	LHG	C20-C19-C18	-2.44	102.03	114.37
32	d	406	LHG	C20-C19-C18	-2.44	102.04	114.37
28	A	611	PL9	O2-C1-C6	2.44	124.36	120.48
33	c	518	DGD	O5D-C6D-C5D	-2.44	103.93	109.42
32	D	407	LHG	C11-C10-C9	-2.43	102.06	114.37
25	a	719	CLA	C3B-C4B-NB	-2.43	108.36	110.53
23	C	520	LMG	O6-C1-O1	-2.43	104.30	110.04
27	a	712	BCR	C33-C5-C6	-2.43	121.83	124.48
23	M	101	LMG	C40-C39-C38	-2.43	102.08	114.37
32	d	407	LHG	C20-C19-C18	-2.43	102.08	114.37
25	b	610	CLA	C1-C2-C3	-2.43	122.22	126.20
33	c	516	DGD	O5D-C6D-C5D	-2.43	103.95	109.42
27	c	514	BCR	C15-C14-C13	-2.43	123.88	127.28
23	f	101	LMG	C40-C39-C38	-2.42	102.12	114.37
28	D	406	PL9	C20-C19-C21	2.42	119.43	115.23
27	b	624	BCR	C33-C5-C6	-2.42	121.84	124.48
23	C	501	LMG	C40-C39-C38	-2.42	102.15	114.37
32	B	625	LHG	C20-C19-C18	-2.42	102.15	114.37
23	A	603	LMG	C40-C39-C38	-2.42	102.15	114.37
23	B	621	LMG	O7-C10-O9	-2.41	118.06	123.70
27	h	101	BCR	C11-C10-C9	-2.41	123.89	127.28
27	K	101	BCR	C33-C5-C6	-2.41	121.85	124.48
23	B	621	LMG	C38-C37-C36	-2.41	102.18	114.37
27	a	712	BCR	C15-C16-C17	-2.41	118.59	123.52
25	A	609	CLA	C3B-C4B-NB	-2.41	108.38	110.53
28	D	406	PL9	O2-C1-C6	2.41	124.31	120.48
25	b	618	CLA	C1-C2-C3	-2.41	122.25	126.20
25	b	617	CLA	C3B-C4B-NB	-2.41	108.38	110.53
27	K	101	BCR	C15-C14-C13	-2.41	123.90	127.28
28	d	405	PL9	O2-C1-C6	2.41	124.31	120.48
27	B	619	BCR	C33-C5-C6	-2.40	121.86	124.48
25	D	402	CLA	C3B-C4B-NB	-2.40	108.39	110.53
23	C	521	LMG	C40-C39-C38	-2.40	102.23	114.37
23	B	621	LMG	C40-C39-C38	-2.40	102.24	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	e	101	LHG	C11-C10-C9	-2.40	102.24	114.37
27	b	625	BCR	C24-C23-C22	-2.39	122.69	126.23
35	V	201	HEC	C3D-C4D-ND	-2.39	108.04	110.35
23	B	621	LMG	O1-C7-C8	-2.39	105.01	110.82
23	b	627	LMG	C38-C37-C36	-2.39	102.30	114.37
25	c	507	CLA	C3B-C4B-NB	-2.39	108.40	110.53
23	c	520	LMG	C40-C39-C38	-2.39	102.30	114.37
23	c	519	LMG	C40-C39-C38	-2.38	102.31	114.37
33	c	516	DGD	C3G-C2G-C1G	-2.38	106.23	111.78
27	K	101	BCR	C15-C16-C17	-2.38	118.65	123.52
23	a	715	LMG	C40-C39-C38	-2.38	102.34	114.37
23	D	409	LMG	C40-C39-C38	-2.38	102.35	114.37
27	C	515	BCR	C33-C5-C6	-2.38	121.89	124.48
35	V	201	HEC	CAC-C3C-C2C	-2.38	123.13	126.89
23	b	627	LMG	C40-C39-C38	-2.38	102.36	114.37
32	L	101	LHG	C20-C19-C18	-2.37	102.36	114.37
27	A	610	BCR	C33-C5-C6	-2.37	121.90	124.48
28	a	713	PL9	C27-C28-C29	-2.37	122.20	127.62
32	d	407	LHG	C11-C10-C9	-2.37	102.38	114.37
25	b	615	CLA	C1-C2-C3	-2.37	122.31	126.20
32	e	101	LHG	C20-C19-C18	-2.37	102.40	114.37
27	A	610	BCR	C15-C16-C17	-2.37	118.68	123.52
32	b	629	LHG	C20-C19-C18	-2.37	102.41	114.37
25	B	612	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	c	505	CLA	CHB-C4A-NA	2.36	127.81	124.40
25	b	621	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	b	607	CLA	O2D-CGD-CBD	2.36	115.36	111.23
25	B	611	CLA	C1-C2-C3	-2.36	122.33	126.20
27	Y	101	BCR	C15-C16-C17	-2.36	118.69	123.52
23	b	626	LMG	O3-C3-C2	-2.36	104.82	110.38
23	c	519	LMG	C38-C37-C36	-2.36	102.45	114.37
25	b	617	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
25	d	403	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
27	b	623	BCR	C11-C10-C9	-2.35	123.98	127.28
27	A	610	BCR	C15-C14-C13	-2.35	123.98	127.28
29	f	102	SQD	O48-C23-C24	2.35	119.00	111.83
25	A	606	CLA	C3B-C4B-NB	-2.35	108.43	110.53
25	B	602	CLA	O2D-CGD-CBD	2.34	115.33	111.23
32	E	101	LHG	C20-C19-C18	-2.34	102.53	114.37
25	B	605	CLA	C3B-C4B-NB	-2.34	108.44	110.53
32	e	101	LHG	C5-O7-C7	-2.34	112.20	117.80
25	B	608	CLA	C3B-C4B-NB	-2.34	108.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	405	PL9	C7-C8-C9	-2.34	122.81	126.83
27	b	625	BCR	C15-C16-C17	-2.34	118.74	123.52
23	b	626	LMG	C40-C39-C38	-2.33	102.58	114.37
25	B	603	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	c	506	CLA	C3B-C4B-NB	-2.33	108.45	110.53
27	B	620	BCR	C24-C23-C22	-2.33	122.79	126.23
29	f	102	SQD	C44-O6-C1	2.33	118.79	113.80
23	f	101	LMG	C38-C37-C36	-2.33	102.60	114.37
27	H	102	BCR	C15-C14-C13	-2.33	124.01	127.28
27	d	404	BCR	C1-C6-C5	-2.33	119.45	122.64
28	D	406	PL9	C37-C38-C39	-2.33	122.30	127.62
29	D	410	SQD	C3-C4-C5	2.32	114.45	110.23
23	a	715	LMG	C38-C37-C36	-2.32	102.62	114.37
25	b	612	CLA	C3B-C4B-NB	-2.32	108.46	110.53
27	k	102	BCR	C15-C16-C17	-2.32	118.77	123.52
29	A	612	SQD	C1-O5-C5	2.32	118.25	113.72
34	E	102	HEM	C4D-ND-C1D	2.32	107.95	105.21
27	C	515	BCR	C15-C14-C13	-2.32	124.03	127.28
27	b	602	BCR	C11-C10-C9	-2.32	124.03	127.28
25	C	514	CLA	CMB-C2B-C1B	-2.31	121.89	125.42
27	C	515	BCR	C15-C16-C17	-2.31	118.79	123.52
27	B	618	BCR	C7-C8-C9	-2.31	122.82	126.23
27	k	102	BCR	C24-C23-C22	-2.31	122.82	126.23
29	b	601	SQD	O5-C5-C4	2.30	113.85	109.70
27	Y	101	BCR	C24-C23-C22	-2.30	122.83	126.23
23	c	520	LMG	C38-C37-C36	-2.30	102.76	114.37
27	a	712	BCR	C15-C14-C13	-2.30	124.06	127.28
25	B	617	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
23	C	520	LMG	C38-C37-C36	-2.30	102.76	114.37
23	A	603	LMG	C38-C37-C36	-2.29	102.77	114.37
23	C	521	LMG	C38-C37-C36	-2.29	102.77	114.37
27	c	514	BCR	C2-C1-C6	2.29	113.77	110.44
35	v	201	HEC	C4B-NB-C1B	2.29	107.92	105.21
25	A	607	CLA	C1-C2-C3	-2.28	122.45	126.20
23	A	603	LMG	O3-C3-C2	-2.28	104.99	110.38
27	B	619	BCR	C15-C16-C17	-2.28	118.85	123.52
27	B	619	BCR	C15-C14-C13	-2.28	124.08	127.28
33	h	102	DGD	C3G-C2G-C1G	-2.28	106.47	111.78
27	D	405	BCR	C7-C8-C9	-2.28	122.86	126.23
33	c	517	DGD	CBB-CAB-C9B	-2.28	102.84	114.37
27	H	102	BCR	C3-C4-C5	-2.28	109.99	114.06
23	A	603	LMG	C1-C2-C3	-2.28	105.22	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	520	LMG	C40-C39-C38	-2.28	102.86	114.37
33	C	519	DGD	O5D-C6D-C5D	-2.27	104.29	109.42
23	D	409	LMG	C38-C37-C36	-2.27	102.88	114.37
23	B	621	LMG	O3-C3-C2	-2.27	105.02	110.38
34	E	102	HEM	C3C-C2C-C1C	2.27	109.19	107.05
32	d	406	LHG	C18-C17-C16	-2.27	102.89	114.37
34	E	102	HEM	CHC-C1C-NC	2.26	126.92	124.45
27	d	404	BCR	C24-C23-C22	-2.26	122.89	126.23
25	B	604	CLA	C3B-C4B-NB	-2.26	108.51	110.53
25	C	507	CLA	C3B-C4B-NB	-2.26	108.51	110.53
33	c	518	DGD	C3D-C4D-C5D	-2.26	106.13	110.23
23	C	520	LMG	O3-C3-C2	-2.26	105.06	110.38
25	B	612	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
27	B	618	BCR	C27-C26-C25	2.25	125.75	122.70
25	D	403	CLA	C3B-C4B-NB	-2.25	108.52	110.53
29	b	601	SQD	O48-C23-O10	-2.25	117.99	123.63
27	d	404	BCR	C11-C10-C9	-2.25	124.12	127.28
35	v	201	HEC	CAC-C3C-C2C	-2.25	123.33	126.89
34	e	102	HEM	C4D-ND-C1D	2.25	107.87	105.21
25	B	613	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
29	f	102	SQD	O47-C7-C8	2.24	119.18	110.93
23	f	101	LMG	O1-C7-C8	-2.24	105.37	110.82
27	H	102	BCR	C11-C10-C9	-2.24	124.14	127.28
25	a	707	CLA	C3B-C4B-NB	-2.24	108.53	110.53
23	d	408	LMG	O1-C7-C8	-2.24	106.02	111.77
23	a	701	LMG	O1-C7-C8	-2.24	105.38	110.82
25	c	512	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
27	h	101	BCR	C15-C16-C17	-2.24	118.94	123.52
33	c	517	DGD	O5D-C6D-C5D	-2.23	104.38	109.42
25	C	512	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
23	b	626	LMG	O6-C1-O1	-2.23	104.77	110.04
28	d	405	PL9	O1-C4-C3	-2.23	118.38	120.73
33	H	103	DGD	C3G-C2G-C1G	-2.23	106.58	111.78
23	f	101	LMG	O3-C3-C2	-2.23	105.12	110.38
25	C	504	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
33	C	517	DGD	O6E-C5E-C4E	2.23	113.71	109.70
29	a	714	SQD	C44-O6-C1	2.23	118.57	113.80
25	B	605	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
29	D	410	SQD	O48-C23-C24	2.22	118.62	111.83
34	E	102	HEM	C1B-NB-C4B	2.22	107.84	105.21
33	C	517	DGD	O5D-C6D-C5D	-2.22	104.41	109.42
25	c	508	CLA	C1-C2-C3	-2.22	122.56	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	626	LMG	C38-C37-C36	-2.22	103.14	114.37
25	C	509	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
26	a	709	PHO	C1-C2-C3	-2.22	122.57	126.20
28	a	713	PL9	C37-C38-C39	-2.22	122.55	127.62
25	C	507	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
27	B	618	BCR	C24-C23-C22	-2.22	122.96	126.23
25	b	617	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
25	b	619	CLA	C1-C2-C3	-2.21	122.58	126.20
35	V	201	HEC	C4B-NB-C1B	2.21	107.82	105.21
27	b	624	BCR	C11-C10-C9	-2.21	124.18	127.28
32	D	408	LHG	C18-C17-C16	-2.21	103.22	114.37
25	b	622	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
33	c	516	DGD	O6E-C5E-C4E	2.20	113.67	109.70
34	e	102	HEM	C2A-C1A-NA	-2.20	107.71	110.15
27	b	625	BCR	C2-C1-C6	2.20	113.64	110.44
25	C	509	CLA	C1-C2-C3	-2.20	122.59	126.20
26	A	608	PHO	C1-C2-C3	-2.20	122.59	126.20
25	D	404	CLA	C3B-C4B-NB	-2.20	108.56	110.53
23	a	701	LMG	C1-O6-C5	-2.20	109.42	113.72
25	B	610	CLA	C3B-C4B-NB	-2.20	108.57	110.53
28	A	611	PL9	O1-C4-C3	-2.20	118.42	120.73
29	A	614	SQD	C45-O47-C7	2.20	123.05	117.80
32	D	408	LHG	C27-C26-C25	-2.19	103.28	114.37
28	D	406	PL9	O1-C4-C3	-2.19	118.42	120.73
32	L	101	LHG	C18-C17-C16	-2.19	103.30	114.37
28	a	713	PL9	C20-C19-C21	2.19	119.03	115.23
25	c	508	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
25	C	503	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
25	a	719	CLA	C1-C2-C3	-2.19	122.62	126.20
32	e	101	LHG	C27-C26-C25	-2.19	103.32	114.37
25	B	608	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
28	a	713	PL9	O1-C4-C3	-2.18	118.43	120.73
27	H	102	BCR	C20-C21-C22	-2.18	124.21	127.28
32	B	625	LHG	C27-C26-C25	-2.18	103.33	114.37
25	B	610	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
25	D	404	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
32	L	101	LHG	C27-C26-C25	-2.18	103.33	114.37
23	f	101	LMG	O2-C2-C1	-2.18	104.87	110.08
25	B	612	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
32	E	101	LHG	C11-C10-C9	-2.18	103.35	114.37
23	c	519	LMG	O3-C3-C2	-2.18	105.24	110.38
25	B	610	CLA	C1-C2-C3	-2.18	122.63	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	629	LHG	C18-C17-C16	-2.18	103.35	114.37
25	A	606	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
33	C	518	DGD	C3D-C4D-C5D	-2.18	106.28	110.23
23	a	715	LMG	O3-C3-C2	-2.18	105.24	110.38
25	c	512	CLA	C3B-C4B-NB	-2.18	108.59	110.53
32	d	406	LHG	C27-C26-C25	-2.18	103.37	114.37
23	C	521	LMG	O3-C3-C2	-2.17	105.25	110.38
32	B	625	LHG	C18-C17-C16	-2.17	103.38	114.37
25	B	617	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
27	d	404	BCR	C33-C5-C6	-2.17	122.11	124.48
23	f	101	LMG	O1-C1-C2	-2.17	104.98	108.27
25	B	614	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	C	514	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	c	503	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	c	502	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
33	c	517	DGD	C3G-C2G-C1G	-2.17	106.73	111.78
23	a	701	LMG	O2-C2-C1	-2.17	104.91	110.08
27	C	516	BCR	C11-C10-C9	-2.17	124.24	127.28
28	a	713	PL9	O2-C1-C2	-2.17	116.90	121.83
33	C	518	DGD	CBB-CAB-C9B	-2.17	103.42	114.37
26	D	401	PHO	C1-C2-C3	-2.17	122.65	126.20
25	C	505	CLA	CHD-C1D-ND	-2.16	121.76	124.80
25	C	511	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
32	a	720	LHG	C27-C26-C25	-2.16	103.43	114.37
33	c	517	DGD	O3E-C3E-C2E	-2.16	105.28	110.38
25	C	513	CLA	C1-C2-C3	-2.16	122.66	126.20
27	C	515	BCR	C24-C23-C22	-2.16	123.04	126.23
33	c	516	DGD	CBB-CAB-C9B	-2.16	103.46	114.37
25	A	609	CLA	C1-C2-C3	-2.16	122.66	126.20
27	C	515	BCR	C7-C8-C9	-2.15	123.05	126.23
33	C	518	DGD	C3G-C2G-C1G	-2.15	106.76	111.78
32	d	407	LHG	C18-C17-C16	-2.15	103.48	114.37
32	e	101	LHG	C18-C17-C16	-2.15	103.48	114.37
34	E	102	HEM	C2A-C1A-NA	-2.15	107.76	110.15
23	C	501	LMG	O3-C3-C2	-2.15	105.30	110.38
33	C	519	DGD	CAB-C9B-C8B	-2.15	103.49	114.37
23	C	520	LMG	O2-C2-C1	-2.15	104.95	110.08
25	b	608	CLA	C3B-C4B-NB	-2.15	108.61	110.53
25	C	512	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
25	b	619	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
25	b	619	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
25	b	615	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	611	PL9	C20-C19-C21	2.15	118.96	115.23
25	c	513	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
25	c	504	CLA	C1-C2-C3	-2.15	122.68	126.20
25	B	617	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	b	625	BCR	C15-C14-C13	-2.14	124.27	127.28
23	M	101	LMG	O3-C3-C2	-2.14	105.33	110.38
27	k	102	BCR	C15-C14-C13	-2.14	124.27	127.28
25	c	506	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
23	M	101	LMG	O2-C2-C1	-2.14	104.97	110.08
28	A	611	PL9	O2-C1-C2	-2.14	116.96	121.83
23	C	521	LMG	O2-C2-C3	-2.14	105.34	110.38
31	A	615	BCT	O3-C-O1	-2.14	114.21	119.68
28	d	405	PL9	C37-C38-C39	-2.14	122.73	127.62
25	C	505	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
25	A	609	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
27	d	404	BCR	C16-C15-C14	-2.13	119.15	123.52
25	B	605	CLA	O2D-CGD-CBD	2.13	114.96	111.23
23	b	627	LMG	O2-C2-C1	-2.13	104.99	110.08
25	a	707	CLA	O1D-CGD-CBD	2.13	128.72	124.52
33	C	517	DGD	CAB-C9B-C8B	-2.13	103.59	114.37
32	d	407	LHG	C27-C26-C25	-2.13	103.59	114.37
25	c	504	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
28	D	406	PL9	O2-C1-C2	-2.13	116.99	121.83
25	B	613	CLA	C1-C2-C3	-2.13	122.71	126.20
23	a	715	LMG	O2-C2-C1	-2.13	105.01	110.08
27	b	623	BCR	C24-C23-C22	-2.13	123.09	126.23
27	D	405	BCR	C11-C10-C9	-2.12	124.30	127.28
25	B	613	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
33	C	519	DGD	O6E-C1E-O5D	-2.12	105.03	110.04
25	b	621	CLA	O2D-CGD-CBD	2.12	114.94	111.23
32	b	629	LHG	C27-C26-C25	-2.12	103.65	114.37
29	A	612	SQD	O48-C23-O10	-2.12	118.33	123.63
33	H	103	DGD	CBB-CAB-C9B	-2.12	103.66	114.37
25	b	609	CLA	C3B-C4B-NB	-2.12	108.64	110.53
25	A	607	CLA	CHD-C1D-ND	-2.12	121.82	124.80
25	B	603	CLA	C1-C2-C3	-2.12	122.73	126.20
25	C	514	CLA	CMB-C2B-C3B	2.12	131.53	126.55
33	h	102	DGD	C1D-C2D-C3D	-2.12	105.56	110.01
25	D	402	CLA	CHD-C1D-ND	-2.12	121.83	124.80
33	c	518	DGD	CBB-CAB-C9B	-2.11	103.68	114.37
28	d	405	PL9	O2-C1-C2	-2.11	117.02	121.83
23	D	409	LMG	O2-C2-C1	-2.11	105.04	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
32	D	407	LHG	C27-C26-C25	-2.11	103.69	114.37
25	b	615	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
25	A	607	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
29	b	601	SQD	O8-S-C6	2.11	110.05	105.97
25	c	503	CLA	C1-C2-C3	-2.11	122.74	126.20
27	D	405	BCR	C15-C14-C13	-2.11	124.32	127.28
27	b	602	BCR	C7-C8-C9	-2.11	123.12	126.23
33	c	518	DGD	CAB-C9B-C8B	-2.11	103.72	114.37
25	b	610	CLA	O2D-CGD-CBD	2.11	114.91	111.23
27	c	515	BCR	C11-C10-C9	-2.10	124.33	127.28
32	E	101	LHG	C18-C17-C16	-2.10	103.73	114.37
26	D	401	PHO	O2A-CGA-O1A	-2.10	118.36	123.63
27	b	623	BCR	C7-C8-C9	-2.10	123.12	126.23
27	Y	101	BCR	C15-C14-C13	-2.10	124.33	127.28
31	a	706	BCT	O3-C-O1	-2.10	114.30	119.68
25	C	503	CLA	C1-C2-C3	-2.10	122.75	126.20
27	b	625	BCR	C11-C10-C9	-2.10	124.33	127.28
27	B	620	BCR	C2-C1-C6	2.10	113.49	110.44
28	a	713	PL9	C32-C33-C34	-2.10	122.81	127.62
27	B	619	BCR	C24-C23-C22	-2.10	123.13	126.23
25	b	613	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	B	603	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	b	607	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
23	B	621	LMG	C3-C4-C5	-2.10	106.43	110.23
25	d	402	CLA	C3B-C4B-NB	-2.10	108.66	110.53
23	c	520	LMG	O2-C2-C3	-2.10	105.43	110.38
25	b	614	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	b	610	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
33	h	102	DGD	CBB-CAB-C9B	-2.09	103.78	114.37
25	a	719	CLA	CHD-C1D-ND	-2.09	121.86	124.80
32	D	407	LHG	C18-C17-C16	-2.09	103.79	114.37
25	b	621	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
25	d	403	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
25	b	612	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
23	c	520	LMG	O3-C3-C2	-2.09	105.46	110.38
25	a	711	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
33	c	518	DGD	O2D-C2D-C1D	-2.08	105.11	110.08
25	b	612	CLA	CHD-C1D-ND	-2.08	121.87	124.80
25	B	609	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
33	H	103	DGD	CAB-C9B-C8B	-2.08	103.87	114.37
33	C	518	DGD	CAB-C9B-C8B	-2.08	103.88	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
25	d	402	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
33	c	517	DGD	CAB-C9B-C8B	-2.07	103.89	114.37
25	C	505	CLA	C1-C2-C3	-2.07	122.80	126.20
25	c	510	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
25	b	611	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	B	617	CLA	CMB-C2B-C3B	2.07	131.42	126.55
33	c	518	DGD	O6E-C1E-O5D	-2.07	105.15	110.04
23	c	519	LMG	O2-C2-C1	-2.07	105.14	110.08
25	C	506	CLA	C1-C2-C3	-2.07	122.81	126.20
33	H	103	DGD	C1D-C2D-C3D	-2.07	105.66	110.01
27	b	625	BCR	C38-C26-C25	-2.07	122.23	124.48
28	A	611	PL9	C37-C38-C39	-2.07	122.89	127.62
25	A	606	CLA	O1D-CGD-CBD	2.07	128.60	124.52
33	C	517	DGD	CBB-CAB-C9B	-2.07	103.91	114.37
25	d	403	CLA	C1-C2-C3	-2.07	122.81	126.20
32	E	101	LHG	C27-C26-C25	-2.07	103.93	114.37
25	b	620	CLA	CHD-C1D-ND	-2.06	121.90	124.80
25	d	403	CLA	CMB-C2B-C3B	2.06	131.41	126.55
25	D	402	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
29	D	410	SQD	C4-C3-C2	2.06	114.45	110.83
29	D	410	SQD	O8-S-C6	2.06	109.95	105.97
25	b	622	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
25	b	613	CLA	CHD-C1D-ND	-2.06	121.91	124.80
23	C	521	LMG	O7-C10-O9	-2.06	118.89	123.70
27	a	712	BCR	C11-C10-C9	-2.06	124.39	127.28
25	C	502	CLA	CHD-C1D-ND	-2.06	121.91	124.80
25	a	719	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
25	b	620	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
25	c	512	CLA	CMB-C2B-C3B	2.05	131.38	126.55
25	b	614	CLA	CHD-C1D-ND	-2.05	121.91	124.80
25	a	711	CLA	C1-C2-C3	-2.05	122.83	126.20
25	B	611	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	B	604	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
25	B	615	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
25	c	501	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
25	c	509	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
23	a	715	LMG	C1-C2-C3	-2.05	105.71	110.01
33	c	516	DGD	CAB-C9B-C8B	-2.04	104.03	114.37
26	a	710	PHO	C1-C2-C3	-2.04	122.85	126.20
23	d	408	LMG	C38-C37-C36	-2.04	104.03	114.37
28	A	611	PL9	C32-C33-C34	-2.04	122.95	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	V	201	HEC	C2D-C1D-ND	-2.04	107.49	109.84
25	b	612	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
23	D	409	LMG	O3-C3-C2	-2.04	105.56	110.38
25	b	622	CLA	CMB-C2B-C3B	2.04	131.35	126.55
25	b	611	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
25	c	501	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	c	504	CLA	CHD-C1D-ND	-2.04	121.93	124.80
23	a	701	LMG	O7-C10-O9	-2.04	118.94	123.70
26	A	608	PHO	O2A-CGA-O1A	-2.04	118.53	123.63
27	B	620	BCR	C38-C26-C25	-2.04	122.26	124.48
33	h	102	DGD	CAB-C9B-C8B	-2.04	104.07	114.37
32	d	406	LHG	C5-O7-C7	-2.04	112.92	117.80
23	d	408	LMG	C40-C39-C38	-2.04	104.08	114.37
25	c	509	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
33	C	517	DGD	C5B-C4B-C3B	-2.04	104.08	114.37
26	a	709	PHO	O2A-CGA-O1A	-2.04	118.54	123.63
33	c	516	DGD	C5B-C4B-C3B	-2.03	104.08	114.37
33	C	518	DGD	O3E-C3E-C2E	-2.03	105.58	110.38
28	A	611	PL9	C12-C13-C14	-2.03	122.97	127.62
27	b	602	BCR	C24-C23-C22	-2.03	123.23	126.23
28	D	406	PL9	C36-C34-C33	-2.03	116.61	121.17
29	A	612	SQD	O8-S-C6	2.03	109.89	105.97
25	b	609	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	B	609	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	a	708	CLA	C1-C2-C3	-2.03	122.88	126.20
25	a	707	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
25	a	708	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
25	c	505	CLA	C3B-C4B-NB	-2.03	108.72	110.53
25	D	403	CLA	C1-C2-C3	-2.02	122.88	126.20
27	K	101	BCR	C11-C10-C9	-2.02	124.44	127.28
25	C	514	CLA	CHD-C1D-ND	-2.02	121.95	124.80
28	d	405	PL9	C32-C33-C34	-2.02	122.99	127.62
25	c	513	CLA	O1D-CGD-CBD	2.02	128.51	124.52
33	C	519	DGD	C5B-C4B-C3B	-2.02	104.15	114.37
25	B	615	CLA	CHD-C1D-ND	-2.02	121.96	124.80
25	c	513	CLA	C1-C2-C3	-2.02	122.89	126.20
33	C	519	DGD	CBB-CAB-C9B	-2.02	104.16	114.37
27	B	619	BCR	C8-C7-C6	-2.02	121.60	127.00
33	C	518	DGD	O2D-C2D-C1D	-2.02	105.26	110.08
25	c	510	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	C	506	CLA	C3B-C4B-NB	-2.02	108.73	110.53
23	C	501	LMG	C1-C2-C3	-2.02	105.76	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	516	DGD	O2D-C2D-C1D	-2.02	105.27	110.08
23	B	621	LMG	O2-C2-C1	-2.02	105.27	110.08
25	C	509	CLA	CHD-C1D-ND	-2.02	121.96	124.80
34	E	102	HEM	C3D-C4D-ND	-2.02	107.96	110.17
27	h	101	BCR	C33-C5-C6	-2.02	122.28	124.48
29	f	102	SQD	O8-S-C6	2.02	109.86	105.97
33	c	518	DGD	C5B-C4B-C3B	-2.01	104.19	114.37
27	C	516	BCR	C7-C8-C9	-2.01	123.26	126.23
25	b	608	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
33	c	517	DGD	C3D-C4D-C5D	-2.01	106.59	110.23
25	c	513	CLA	CMB-C2B-C3B	2.01	131.27	126.55
28	d	405	PL9	C12-C13-C14	-2.01	123.03	127.62
25	a	707	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
23	A	603	LMG	O2-C2-C1	-2.00	105.30	110.08
32	d	407	LHG	C5-O7-C7	-2.00	113.00	117.80
25	C	502	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
29	a	714	SQD	C1-O5-C5	2.00	117.63	113.72
29	B	623	SQD	C45-O47-C7	2.00	122.58	117.80
25	b	613	CLA	O2D-CGD-CBD	2.00	114.73	111.23
29	A	612	SQD	C4-C3-C2	2.00	114.34	110.83
29	a	714	SQD	O8-S-C6	2.00	109.83	105.97

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	V	201	HEC	NA
35	v	201	HEC	NA

All (1703) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	621	LMG	C2-C1-O1-C7
23	B	621	LMG	O6-C1-O1-C7
23	C	521	LMG	O6-C1-O1-C7
23	c	520	LMG	O6-C1-O1-C7
23	d	408	LMG	C11-C10-O7-C8
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	602	CLA	C2B-C3B-CAB-CBB
25	B	602	CLA	C4B-C3B-CAB-CBB
25	B	602	CLA	CAD-CBD-CGD-O1D
25	B	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C11-C10-C8-C9
25	B	603	CLA	C4-C3-C5-C6
25	B	608	CLA	CAD-CBD-CGD-O1D
25	B	608	CLA	CAD-CBD-CGD-O2D
25	B	616	CLA	C2B-C3B-CAB-CBB
25	B	616	CLA	C4B-C3B-CAB-CBB
25	C	503	CLA	CAD-CBD-CGD-O1D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	CHA-CBD-CGD-O1D
25	C	510	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	C11-C10-C8-C9
25	a	707	CLA	CBD-CGD-O2D-CED
25	a	708	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	CAD-CBD-CGD-O2D
25	b	613	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C3A-C2A-CAA-CBA
25	b	620	CLA	CAD-CBD-CGD-O1D
25	b	620	CLA	CAD-CBD-CGD-O2D
25	c	501	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	C6-C7-C8-C9
25	d	402	CLA	CBD-CGD-O2D-CED
27	D	405	BCR	C7-C8-C9-C10
27	D	405	BCR	C21-C22-C23-C24
27	H	102	BCR	C7-C8-C9-C34
27	b	602	BCR	C5-C6-C7-C8
27	b	602	BCR	C7-C8-C9-C34
27	b	602	BCR	C21-C22-C23-C24
27	b	624	BCR	C7-C8-C9-C10
27	b	624	BCR	C7-C8-C9-C34
27	h	101	BCR	C7-C8-C9-C10
27	h	101	BCR	C7-C8-C9-C34
27	k	101	BCR	C20-C21-C22-C37
27	t	103	BCR	C21-C22-C23-C24
28	D	406	PL9	C35-C34-C36-C37
29	A	612	SQD	C5-C6-S-O7
29	A	612	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
29	A	612	SQD	C5-C6-S-O9
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O5-C5-C6-S
29	B	626	SQD	O5-C1-O6-C44
29	B	626	SQD	O49-C7-O47-C45
29	B	626	SQD	O10-C23-O48-C46
29	D	410	SQD	C8-C7-O47-C45
29	I	102	SQD	O6-C44-C45-O47
29	I	102	SQD	C8-C7-O47-C45
29	a	714	SQD	C5-C6-S-O7
29	b	601	SQD	O5-C1-O6-C44
29	b	601	SQD	C8-C7-O47-C45
29	b	601	SQD	C4-C5-C6-S
32	B	625	LHG	C3-O3-P-O6
32	B	625	LHG	C4-O6-P-O5
32	D	407	LHG	O1-C1-C2-C3
32	D	407	LHG	O2-C2-C3-O3
32	D	407	LHG	C3-O3-P-O4
32	D	407	LHG	C4-O6-P-O3
32	D	408	LHG	O1-C1-C2-O2
32	D	408	LHG	O1-C1-C2-C3
32	D	408	LHG	C4-O6-P-O3
32	D	408	LHG	C4-O6-P-O4
32	E	101	LHG	O1-C1-C2-C3
32	E	101	LHG	C3-O3-P-O5
32	E	101	LHG	C4-O6-P-O3
32	a	720	LHG	C3-O3-P-O4
32	a	720	LHG	C4-O6-P-O3
32	a	720	LHG	C4-O6-P-O5
32	b	629	LHG	C4-O6-P-O5
32	d	406	LHG	C3-O3-P-O6
32	d	407	LHG	C4-O6-P-O3
33	C	518	DGD	C2E-C1E-O5D-C6D
25	c	513	CLA	O1D-CGD-O2D-CED
35	V	201	HEC	C4C-C3C-CAC-CBC
25	C	503	CLA	O1D-CGD-O2D-CED
25	B	611	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	b	620	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	CBD-CGD-O2D-CED
35	V	201	HEC	C2C-C3C-CAC-CBC
29	A	614	SQD	C24-C23-O48-C46
29	B	626	SQD	C24-C23-O48-C46
25	B	610	CLA	CBD-CGD-O2D-CED
29	A	614	SQD	O10-C23-O48-C46
29	B	623	SQD	O10-C23-O48-C46
32	e	101	LHG	O10-C23-O8-C6
35	v	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C4C-C3C-CAC-CBC
35	V	201	HEC	C4B-C3B-CAB-CBB
25	c	501	CLA	O1D-CGD-O2D-CED
25	d	402	CLA	O1D-CGD-O2D-CED
35	V	201	HEC	C2B-C3B-CAB-CBB
25	C	510	CLA	O1D-CGD-O2D-CED
25	a	707	CLA	O1D-CGD-O2D-CED
35	v	201	HEC	C4B-C3B-CAB-CBB
35	v	201	HEC	C2B-C3B-CAB-CBB
23	a	701	LMG	O9-C10-O7-C8
29	B	623	SQD	O49-C7-O47-C45
29	I	102	SQD	O49-C7-O47-C45
25	B	602	CLA	C3-C5-C6-C7
25	C	503	CLA	C3-C5-C6-C7
33	C	518	DGD	O6E-C5E-C6E-O5E
25	B	604	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	607	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	CBD-CGD-O2D-CED
25	b	612	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
29	A	614	SQD	C8-C7-O47-C45
29	B	623	SQD	C8-C7-O47-C45
29	B	626	SQD	C8-C7-O47-C45
25	c	506	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
25	B	604	CLA	C4-C3-C5-C6
25	B	615	CLA	C4-C3-C5-C6
25	D	404	CLA	C4-C3-C5-C6
25	a	711	CLA	C4-C3-C5-C6
25	B	603	CLA	C2-C3-C5-C6
25	B	615	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	D	404	CLA	C2-C3-C5-C6
25	a	711	CLA	C2-C3-C5-C6
28	D	406	PL9	C33-C34-C36-C37
25	C	507	CLA	CBD-CGD-O2D-CED
25	B	611	CLA	O1D-CGD-O2D-CED
29	B	623	SQD	C24-C23-O48-C46
28	A	611	PL9	C42-C43-C44-C45
28	A	611	PL9	C42-C43-C44-C46
25	D	404	CLA	O1A-CGA-O2A-C1
23	d	408	LMG	O9-C10-O7-C8
29	A	614	SQD	O49-C7-O47-C45
25	b	613	CLA	O1D-CGD-O2D-CED
25	B	615	CLA	O1D-CGD-O2D-CED
25	b	610	CLA	C3-C5-C6-C7
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	614	CLA	CBD-CGD-O2D-CED
32	d	407	LHG	O2-C2-C3-O3
25	b	620	CLA	O1D-CGD-O2D-CED
23	a	701	LMG	C11-C10-O7-C8
23	a	701	LMG	O6-C5-C6-O5
23	a	715	LMG	O6-C5-C6-O5
23	b	626	LMG	O6-C5-C6-O5
33	C	517	DGD	O6E-C5E-C6E-O5E
33	h	102	DGD	C4E-C5E-C6E-O5E
33	c	517	DGD	O6E-C5E-C6E-O5E
23	b	626	LMG	C4-C5-C6-O5
25	D	404	CLA	CBA-CGA-O2A-C1
32	e	101	LHG	C24-C23-O8-C6
25	b	611	CLA	C4-C3-C5-C6
25	b	611	CLA	C2-C3-C5-C6
28	A	611	PL9	C9-C11-C12-C13
28	A	611	PL9	C24-C26-C27-C28
28	a	713	PL9	C9-C11-C12-C13
25	B	613	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
23	A	603	LMG	O6-C5-C6-O5
33	C	518	DGD	C4E-C5E-C6E-O5E
25	B	607	CLA	C2A-CAA-CBA-CGA
23	b	627	LMG	O10-C28-O8-C9
29	I	102	SQD	O10-C23-O48-C46
32	E	101	LHG	O10-C23-O8-C6
23	C	501	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
29	f	102	SQD	O5-C1-O6-C44
33	C	518	DGD	O6E-C1E-O5D-C6D
23	b	627	LMG	C29-C28-O8-C9
25	c	512	CLA	CBA-CGA-O2A-C1
25	B	614	CLA	CBD-CGD-O2D-CED
25	c	505	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
26	a	710	PHO	CBD-CGD-O2D-CED
25	B	610	CLA	O1D-CGD-O2D-CED
25	b	607	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
33	c	517	DGD	C4E-C5E-C6E-O5E
25	c	512	CLA	O1A-CGA-O2A-C1
32	D	407	LHG	C1-C2-C3-O3
32	d	406	LHG	C1-C2-C3-O3
23	a	701	LMG	C29-C28-O8-C9
25	C	513	CLA	CBA-CGA-O2A-C1
25	b	607	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
29	I	102	SQD	C24-C23-O48-C46
32	E	101	LHG	C24-C23-O8-C6
25	D	404	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	O1D-CGD-O2D-CED
23	a	715	LMG	C4-C5-C6-O5
25	b	609	CLA	C4-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
28	A	611	PL9	C38-C39-C41-C42
25	c	502	CLA	C3-C5-C6-C7
25	B	607	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C10-C8-C9
25	B	617	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C12-C13-C14
25	D	403	CLA	C6-C7-C8-C9
25	b	611	CLA	C14-C13-C15-C16
25	b	612	CLA	C11-C10-C8-C9
25	b	616	CLA	C14-C13-C15-C16
25	c	502	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C10-C8-C9
23	C	501	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
29	f	102	SQD	C2-C1-O6-C44
32	B	625	LHG	C23-C24-C25-C26
25	c	502	CLA	O1D-CGD-O2D-CED
25	b	607	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
27	B	619	BCR	C7-C8-C9-C34
27	B	620	BCR	C7-C8-C9-C34
27	D	405	BCR	C7-C8-C9-C34
27	Y	101	BCR	C7-C8-C9-C34
27	b	602	BCR	C37-C22-C23-C24
27	b	625	BCR	C37-C22-C23-C24
27	c	514	BCR	C7-C8-C9-C34
27	d	404	BCR	C37-C22-C23-C24
27	t	103	BCR	C7-C8-C9-C34
27	b	602	BCR	C7-C8-C9-C10
27	d	404	BCR	C21-C22-C23-C24
27	t	103	BCR	C7-C8-C9-C10
23	a	715	LMG	C10-C11-C12-C13
25	C	513	CLA	O1A-CGA-O2A-C1
33	C	517	DGD	C4E-C5E-C6E-O5E
29	b	601	SQD	O49-C7-O47-C45
32	E	101	LHG	O6-C4-C5-O7
25	b	619	CLA	CBD-CGD-O2D-CED
29	I	102	SQD	C23-C24-C25-C26
25	b	612	CLA	O1D-CGD-O2D-CED
32	D	407	LHG	C28-C29-C30-C31
25	C	510	CLA	C8-C10-C11-C12
25	c	506	CLA	C5-C6-C7-C8
25	d	403	CLA	C3-C5-C6-C7
23	a	701	LMG	C4-C5-C6-O5
32	e	101	LHG	C23-C24-C25-C26
23	c	520	LMG	O6-C5-C6-O5
23	f	101	LMG	O6-C5-C6-O5
25	B	611	CLA	C12-C13-C15-C16
25	C	505	CLA	C12-C13-C15-C16
25	B	607	CLA	O1D-CGD-O2D-CED
23	B	621	LMG	O6-C5-C6-O5
33	H	103	DGD	O6E-C5E-C6E-O5E
25	d	403	CLA	C13-C15-C16-C17
32	a	720	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	A	611	PL9	C44-C46-C47-C48
28	D	406	PL9	C39-C41-C42-C43
28	a	713	PL9	C24-C26-C27-C28
26	a	709	PHO	C13-C15-C16-C17
25	B	604	CLA	O1D-CGD-O2D-CED
23	d	408	LMG	C10-C11-C12-C13
23	d	408	LMG	C28-C29-C30-C31
29	B	623	SQD	C23-C24-C25-C26
32	b	629	LHG	C23-C24-C25-C26
33	C	518	DGD	C1A-C2A-C3A-C4A
25	B	608	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	C15-C16-C17-C18
25	C	512	CLA	C10-C11-C12-C13
25	a	711	CLA	C8-C10-C11-C12
25	c	506	CLA	C15-C16-C17-C18
34	e	102	HEM	C3D-CAD-CBD-CGD
25	B	611	CLA	C2A-CAA-CBA-CGA
25	b	612	CLA	C2A-CAA-CBA-CGA
25	B	604	CLA	C8-C10-C11-C12
25	C	512	CLA	C15-C16-C17-C18
25	C	514	CLA	C15-C16-C17-C18
25	b	607	CLA	C5-C6-C7-C8
25	b	608	CLA	C13-C15-C16-C17
25	b	610	CLA	C10-C11-C12-C13
25	c	505	CLA	C15-C16-C17-C18
33	h	102	DGD	O6E-C5E-C6E-O5E
23	C	501	LMG	C28-C29-C30-C31
23	c	519	LMG	C10-C11-C12-C13
29	A	614	SQD	C7-C8-C9-C10
29	A	614	SQD	C23-C24-C25-C26
29	b	601	SQD	C7-C8-C9-C10
32	E	101	LHG	C23-C24-C25-C26
23	a	715	LMG	O10-C28-O8-C9
25	c	510	CLA	O1A-CGA-O2A-C1
23	C	520	LMG	O6-C1-O1-C7
23	a	715	LMG	O6-C1-O1-C7
23	D	409	LMG	C16-C17-C18-C19
25	B	604	CLA	C15-C16-C17-C18
25	B	607	CLA	C8-C10-C11-C12
25	C	504	CLA	C15-C16-C17-C18
25	a	711	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	b	612	CLA	C8-C10-C11-C12
25	b	612	CLA	C13-C15-C16-C17
25	b	616	CLA	C15-C16-C17-C18
25	b	617	CLA	C8-C10-C11-C12
25	c	503	CLA	C15-C16-C17-C18
25	c	512	CLA	C10-C11-C12-C13
25	d	403	CLA	C15-C16-C17-C18
32	d	406	LHG	O2-C2-C3-O3
26	D	401	PHO	CBD-CGD-O2D-CED
25	C	503	CLA	C13-C15-C16-C17
25	D	404	CLA	C8-C10-C11-C12
25	c	508	CLA	C15-C16-C17-C18
29	D	410	SQD	O49-C7-O47-C45
25	B	607	CLA	C3-C5-C6-C7
25	C	507	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	O1D-CGD-O2D-CED
25	B	604	CLA	C5-C6-C7-C8
25	D	404	CLA	C10-C11-C12-C13
25	b	608	CLA	C10-C11-C12-C13
25	b	608	CLA	C15-C16-C17-C18
25	b	614	CLA	C15-C16-C17-C18
25	c	513	CLA	C13-C15-C16-C17
25	B	609	CLA	C15-C16-C17-C18
25	a	719	CLA	C15-C16-C17-C18
25	b	607	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
25	b	621	CLA	C5-C6-C7-C8
29	f	102	SQD	C24-C23-O48-C46
25	B	605	CLA	CBD-CGD-O2D-CED
23	D	409	LMG	C11-C10-O7-C8
25	c	511	CLA	C15-C16-C17-C18
25	b	615	CLA	C3-C5-C6-C7
32	e	101	LHG	C7-C8-C9-C10
32	d	407	LHG	C1-C2-C3-O3
25	B	605	CLA	CBA-CGA-O2A-C1
25	a	711	CLA	CBA-CGA-O2A-C1
29	D	410	SQD	C24-C23-O48-C46
29	b	601	SQD	C24-C23-O48-C46
25	A	606	CLA	C15-C16-C17-C18
25	B	603	CLA	C5-C6-C7-C8
25	C	512	CLA	C13-C15-C16-C17
25	b	615	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	b	617	CLA	C13-C15-C16-C17
25	c	508	CLA	C8-C10-C11-C12
25	B	602	CLA	C10-C11-C12-C13
25	B	602	CLA	C15-C16-C17-C18
25	B	616	CLA	C5-C6-C7-C8
25	B	616	CLA	C15-C16-C17-C18
25	C	507	CLA	C10-C11-C12-C13
25	b	607	CLA	C8-C10-C11-C12
25	b	609	CLA	O1D-CGD-O2D-CED
25	B	607	CLA	C10-C11-C12-C13
25	C	514	CLA	C13-C15-C16-C17
25	b	607	CLA	C10-C11-C12-C13
25	c	510	CLA	C5-C6-C7-C8
25	c	511	CLA	C8-C10-C11-C12
25	c	511	CLA	C13-C15-C16-C17
23	a	715	LMG	C29-C28-O8-C9
25	C	508	CLA	C4-C3-C5-C6
25	b	610	CLA	C4-C3-C5-C6
25	b	620	CLA	C4-C3-C5-C6
25	B	605	CLA	C13-C15-C16-C17
25	B	615	CLA	C8-C10-C11-C12
25	b	621	CLA	C10-C11-C12-C13
25	c	509	CLA	C13-C15-C16-C17
25	B	609	CLA	CBD-CGD-O2D-CED
23	C	520	LMG	C2-C1-O1-C7
23	a	715	LMG	C2-C1-O1-C7
33	c	517	DGD	C2E-C1E-O5D-C6D
32	d	406	LHG	C23-C24-C25-C26
25	c	504	CLA	CBA-CGA-O2A-C1
33	C	519	DGD	C2A-C1A-O1G-C1G
26	a	709	PHO	C15-C16-C17-C18
27	d	404	BCR	C20-C21-C22-C37
27	D	405	BCR	C37-C22-C23-C24
27	c	515	BCR	C7-C8-C9-C34
27	t	103	BCR	C37-C22-C23-C24
27	H	102	BCR	C7-C8-C9-C10
33	C	518	DGD	O1A-C1A-O1G-C1G
25	b	619	CLA	C8-C10-C11-C12
32	a	720	LHG	O1-C1-C2-C3
32	e	101	LHG	O1-C1-C2-C3
23	a	701	LMG	C7-C8-O7-C10
29	A	614	SQD	C44-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	C46-C45-O47-C7
25	C	507	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
25	B	613	CLA	O1D-CGD-O2D-CED
27	k	101	BCR	C20-C21-C22-C23
23	c	519	LMG	O6-C1-O1-C7
23	C	520	LMG	C28-C29-C30-C31
25	C	512	CLA	O1D-CGD-O2D-CED
25	C	504	CLA	CBA-CGA-O2A-C1
25	b	622	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
25	D	404	CLA	C15-C16-C17-C18
25	B	604	CLA	C16-C17-C18-C20
25	C	507	CLA	C16-C17-C18-C20
25	C	512	CLA	C16-C17-C18-C20
25	b	617	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C20
26	A	608	PHO	C16-C17-C18-C20
23	C	520	LMG	C16-C17-C18-C19
23	D	409	LMG	C17-C18-C19-C20
23	b	627	LMG	C17-C18-C19-C20
29	A	612	SQD	C29-C30-C31-C32
32	d	406	LHG	C32-C33-C34-C35
33	C	518	DGD	C8B-C9B-CAB-CBB
23	B	621	LMG	C18-C19-C20-C21
23	C	521	LMG	C15-C16-C17-C18
23	a	715	LMG	C20-C21-C22-C23
23	b	627	LMG	C29-C30-C31-C32
29	B	623	SQD	C11-C10-C9-C8
29	B	623	SQD	C28-C29-C30-C31
29	B	623	SQD	C30-C31-C32-C33
33	h	102	DGD	C5B-C6B-C7B-C8B
23	A	603	LMG	C10-C11-C12-C13
25	C	507	CLA	C13-C15-C16-C17
23	B	621	LMG	C29-C30-C31-C32
32	e	101	LHG	C15-C16-C17-C18
33	H	103	DGD	C7A-C8A-C9A-CAA
23	C	520	LMG	C15-C16-C17-C18
23	a	715	LMG	C13-C14-C15-C16
23	b	627	LMG	C13-C14-C15-C16
23	c	519	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	B	626	SQD	C13-C14-C15-C16
33	C	519	DGD	C6B-C7B-C8B-C9B
23	C	501	LMG	C18-C19-C20-C21
23	D	409	LMG	C20-C21-C22-C23
23	M	101	LMG	C30-C31-C32-C33
29	b	601	SQD	C12-C13-C14-C15
33	c	516	DGD	C5B-C6B-C7B-C8B
25	B	603	CLA	C4B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB
25	D	403	CLA	C4B-C3B-CAB-CBB
25	c	502	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
23	M	101	LMG	C28-C29-C30-C31
23	b	627	LMG	C28-C29-C30-C31
25	C	505	CLA	C16-C17-C18-C20
25	b	619	CLA	C16-C17-C18-C20
29	f	102	SQD	C27-C28-C29-C30
33	C	518	DGD	C2A-C3A-C4A-C5A
25	B	606	CLA	C15-C16-C17-C18
25	b	607	CLA	C15-C16-C17-C18
25	b	618	CLA	C15-C16-C17-C18
23	C	501	LMG	C31-C32-C33-C34
29	I	102	SQD	C13-C14-C15-C16
32	D	407	LHG	C32-C33-C34-C35
33	c	516	DGD	C4A-C5A-C6A-C7A
25	d	402	CLA	C12-C13-C15-C16
23	b	627	LMG	C14-C15-C16-C17
29	I	102	SQD	C11-C12-C13-C14
29	a	714	SQD	C15-C16-C17-C18
23	c	519	LMG	C32-C33-C34-C35
29	D	410	SQD	C33-C34-C35-C36
29	I	102	SQD	C10-C11-C12-C13
32	e	101	LHG	C18-C19-C20-C21
25	a	711	CLA	O1A-CGA-O2A-C1
25	D	403	CLA	C3A-C2A-CAA-CBA
25	c	511	CLA	O1D-CGD-O2D-CED
29	B	626	SQD	C31-C32-C33-C34
33	C	517	DGD	C5B-C6B-C7B-C8B
33	C	518	DGD	CCA-CDA-CEA-CFA
33	h	102	DGD	C9A-CAA-CBA-CCA
25	B	606	CLA	C8-C10-C11-C12
25	c	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	a	715	LMG	C28-C29-C30-C31
29	I	102	SQD	C7-C8-C9-C10
32	B	625	LHG	C30-C31-C32-C33
25	C	505	CLA	C16-C17-C18-C19
25	b	617	CLA	C16-C17-C18-C20
25	b	619	CLA	C16-C17-C18-C19
25	c	507	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C20
29	B	626	SQD	C14-C15-C16-C17
29	B	626	SQD	C34-C35-C36-C37
23	C	521	LMG	C30-C31-C32-C33
23	b	627	LMG	C34-C35-C36-C37
32	D	408	LHG	C25-C26-C27-C28
32	E	101	LHG	C13-C14-C15-C16
23	C	520	LMG	C29-C28-O8-C9
23	C	521	LMG	C29-C28-O8-C9
25	b	620	CLA	CBA-CGA-O2A-C1
23	M	101	LMG	C35-C36-C37-C38
23	b	627	LMG	C33-C34-C35-C36
23	c	520	LMG	C19-C20-C21-C22
32	D	408	LHG	C17-C18-C19-C20
25	D	404	CLA	C3-C5-C6-C7
26	D	401	PHO	C3-C5-C6-C7
29	D	410	SQD	C23-C24-C25-C26
25	c	513	CLA	C8-C10-C11-C12
23	A	603	LMG	C19-C20-C21-C22
23	C	501	LMG	C17-C18-C19-C20
23	C	521	LMG	C20-C21-C22-C23
23	D	409	LMG	C19-C20-C21-C22
23	b	627	LMG	C37-C38-C39-C40
23	f	101	LMG	C21-C22-C23-C24
29	b	601	SQD	C11-C12-C13-C14
29	f	102	SQD	C32-C33-C34-C35
33	C	519	DGD	CBA-CCA-CDA-CEA
33	c	516	DGD	C4B-C5B-C6B-C7B
25	B	605	CLA	O1A-CGA-O2A-C1
25	b	622	CLA	O1A-CGA-O2A-C1
25	c	504	CLA	O1A-CGA-O2A-C1
23	C	520	LMG	C35-C36-C37-C38
29	I	102	SQD	C9-C10-C11-C12
29	I	102	SQD	C14-C15-C16-C17
25	B	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	a	710	PHO	O1D-CGD-O2D-CED
23	d	408	LMG	C31-C32-C33-C34
29	a	714	SQD	C13-C14-C15-C16
32	D	408	LHG	C30-C31-C32-C33
23	c	520	LMG	C20-C21-C22-C23
29	B	626	SQD	C18-C19-C20-C21
32	b	629	LHG	C10-C11-C12-C13
33	C	517	DGD	C4A-C5A-C6A-C7A
25	c	513	CLA	O1A-CGA-O2A-C1
25	B	606	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
25	a	708	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C2B-C3B-CAB-CBB
27	b	602	BCR	C1-C6-C7-C8
27	b	623	BCR	C1-C6-C7-C8
27	t	103	BCR	C1-C6-C7-C8
27	t	103	BCR	C5-C6-C7-C8
23	A	603	LMG	C18-C19-C20-C21
32	D	408	LHG	C29-C30-C31-C32
25	b	617	CLA	CBD-CGD-O2D-CED
25	a	707	CLA	C13-C15-C16-C17
25	C	507	CLA	C3-C5-C6-C7
23	C	501	LMG	C29-C30-C31-C32
29	A	614	SQD	C13-C14-C15-C16
29	I	102	SQD	C31-C32-C33-C34
25	c	501	CLA	C2A-CAA-CBA-CGA
23	D	409	LMG	C11-C12-C13-C14
23	f	101	LMG	C16-C17-C18-C19
32	b	629	LHG	C34-C35-C36-C37
33	C	518	DGD	CBA-CCA-CDA-CEA
25	C	504	CLA	O1A-CGA-O2A-C1
23	C	501	LMG	C15-C16-C17-C18
23	D	409	LMG	C31-C32-C33-C34
23	d	408	LMG	C30-C31-C32-C33
25	b	610	CLA	C2-C3-C5-C6
28	a	713	PL9	C38-C39-C41-C42
23	a	701	LMG	C31-C32-C33-C34
23	a	701	LMG	C32-C33-C34-C35
23	b	626	LMG	C16-C17-C18-C19
29	A	612	SQD	C25-C26-C27-C28
29	A	614	SQD	C9-C10-C11-C12
29	A	614	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
29	D	410	SQD	C26-C27-C28-C29
25	B	605	CLA	C14-C13-C15-C16
25	B	606	CLA	C14-C13-C15-C16
25	b	617	CLA	C11-C12-C13-C14
26	a	709	PHO	C14-C13-C15-C16
23	c	520	LMG	C14-C15-C16-C17
33	c	517	DGD	C5A-C6A-C7A-C8A
33	c	518	DGD	C2B-C3B-C4B-C5B
25	C	506	CLA	C13-C15-C16-C17
25	D	404	CLA	C5-C6-C7-C8
25	c	505	CLA	O1D-CGD-O2D-CED
32	L	101	LHG	C10-C11-C12-C13
32	L	101	LHG	C32-C33-C34-C35
33	C	519	DGD	O6D-C1D-O3G-C3G
33	c	517	DGD	O6E-C1E-O5D-C6D
32	D	407	LHG	C30-C31-C32-C33
32	E	101	LHG	C32-C33-C34-C35
32	a	720	LHG	C30-C31-C32-C33
32	e	101	LHG	C14-C15-C16-C17
23	c	520	LMG	C2-C1-O1-C7
25	C	510	CLA	C10-C11-C12-C13
25	c	507	CLA	C15-C16-C17-C18
23	b	627	LMG	C35-C36-C37-C38
32	B	625	LHG	C11-C10-C9-C8
32	D	408	LHG	C32-C33-C34-C35
33	H	103	DGD	C5B-C6B-C7B-C8B
23	A	603	LMG	C15-C16-C17-C18
23	B	621	LMG	C33-C34-C35-C36
23	C	521	LMG	C35-C36-C37-C38
23	a	701	LMG	C13-C14-C15-C16
32	b	629	LHG	C32-C33-C34-C35
33	C	519	DGD	C7B-C8B-C9B-CAB
33	c	518	DGD	CBA-CCA-CDA-CEA
23	M	101	LMG	C31-C32-C33-C34
23	a	701	LMG	C30-C31-C32-C33
23	a	715	LMG	C16-C17-C18-C19
23	b	626	LMG	C32-C33-C34-C35
29	B	626	SQD	C24-C25-C26-C27
32	e	101	LHG	C24-C25-C26-C27
33	C	517	DGD	C4B-C5B-C6B-C7B
33	c	517	DGD	C9A-CAA-CBA-CCA
25	C	507	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	c	516	DGD	O6E-C5E-C6E-O5E
25	c	508	CLA	C16-C17-C18-C19
32	E	101	LHG	C8-C7-O7-C5
25	c	504	CLA	O1D-CGD-O2D-CED
23	c	519	LMG	C17-C18-C19-C20
23	b	627	LMG	O9-C10-O7-C8
27	k	101	BCR	C11-C12-C13-C35
29	A	614	SQD	C15-C16-C17-C18
29	b	601	SQD	C23-C24-C25-C26
32	D	408	LHG	C18-C19-C20-C21
25	c	508	CLA	CBA-CGA-O2A-C1
23	D	409	LMG	C15-C16-C17-C18
25	c	512	CLA	C2A-CAA-CBA-CGA
25	B	614	CLA	C16-C17-C18-C19
25	B	614	CLA	C16-C17-C18-C20
25	C	512	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C20
25	c	508	CLA	C16-C17-C18-C20
23	a	701	LMG	C21-C22-C23-C24
29	B	626	SQD	C29-C30-C31-C32
25	B	606	CLA	C4-C3-C5-C6
25	b	609	CLA	C15-C16-C17-C18
23	C	520	LMG	C32-C33-C34-C35
23	C	521	LMG	C21-C22-C23-C24
33	H	103	DGD	C4D-C5D-C6D-O5D
23	a	701	LMG	O10-C28-O8-C9
25	b	620	CLA	O1A-CGA-O2A-C1
29	a	714	SQD	C28-C29-C30-C31
23	c	520	LMG	C32-C33-C34-C35
25	b	607	CLA	O1D-CGD-O2D-CED
23	f	101	LMG	C19-C20-C21-C22
29	a	714	SQD	C9-C10-C11-C12
32	d	406	LHG	C25-C26-C27-C28
32	e	101	LHG	C26-C27-C28-C29
25	B	614	CLA	C13-C15-C16-C17
25	C	513	CLA	C10-C11-C12-C13
25	c	510	CLA	C8-C10-C11-C12
34	E	102	HEM	C4C-C3C-CAC-CBC
25	b	611	CLA	C16-C17-C18-C19
23	C	521	LMG	C38-C39-C40-C41
33	C	517	DGD	C6A-C7A-C8A-C9A
23	A	603	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	a	701	LMG	C28-C29-C30-C31
32	L	101	LHG	C23-C24-C25-C26
23	C	520	LMG	C29-C30-C31-C32
29	I	102	SQD	C30-C31-C32-C33
29	b	601	SQD	C30-C31-C32-C33
32	B	625	LHG	C32-C33-C34-C35
25	C	512	CLA	C3-C5-C6-C7
23	f	101	LMG	C12-C13-C14-C15
33	H	103	DGD	CCA-CDA-CEA-CFA
29	A	612	SQD	C12-C13-C14-C15
32	e	101	LHG	C12-C13-C14-C15
33	H	103	DGD	CBA-CCA-CDA-CEA
23	B	621	LMG	C12-C13-C14-C15
23	C	501	LMG	C32-C33-C34-C35
23	C	520	LMG	C17-C18-C19-C20
29	I	102	SQD	C26-C27-C28-C29
23	d	408	LMG	C11-C12-C13-C14
32	b	629	LHG	C27-C28-C29-C30
33	C	518	DGD	CCB-CDB-CEB-CFB
25	D	404	CLA	O1D-CGD-O2D-CED
23	A	603	LMG	C14-C15-C16-C17
23	B	621	LMG	C30-C31-C32-C33
23	C	521	LMG	C19-C20-C21-C22
23	a	715	LMG	C32-C33-C34-C35
29	b	601	SQD	C24-C25-C26-C27
33	C	518	DGD	C4A-C5A-C6A-C7A
32	e	101	LHG	C9-C10-C11-C12
25	C	508	CLA	C2-C3-C5-C6
25	b	620	CLA	C2-C3-C5-C6
25	b	615	CLA	C15-C16-C17-C18
23	C	520	LMG	C13-C14-C15-C16
29	I	102	SQD	C17-C18-C19-C20
29	I	102	SQD	C27-C28-C29-C30
32	D	408	LHG	C9-C10-C11-C12
33	h	102	DGD	CAA-CBA-CCA-CDA
25	b	620	CLA	C2A-CAA-CBA-CGA
25	C	509	CLA	CBD-CGD-O2D-CED
32	d	407	LHG	C16-C17-C18-C19
32	D	408	LHG	C15-C16-C17-C18
32	D	408	LHG	C11-C12-C13-C14
23	C	520	LMG	C36-C37-C38-C39
29	A	614	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	c	510	CLA	O1D-CGD-O2D-CED
32	E	101	LHG	O1-C1-C2-O2
32	a	720	LHG	O1-C1-C2-O2
32	e	101	LHG	O1-C1-C2-O2
23	A	603	LMG	C32-C33-C34-C35
33	C	519	DGD	CBB-CCB-CDB-CEB
25	C	504	CLA	C1A-C2A-CAA-CBA
25	a	719	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C1A-C2A-CAA-CBA
25	C	504	CLA	C5-C6-C7-C8
32	d	406	LHG	C11-C12-C13-C14
29	B	623	SQD	C32-C33-C34-C35
32	a	720	LHG	C31-C32-C33-C34
33	h	102	DGD	CCA-CDA-CEA-CFA
23	C	521	LMG	O6-C5-C6-O5
23	D	409	LMG	O9-C10-O7-C8
25	c	507	CLA	C3-C5-C6-C7
25	B	604	CLA	C11-C12-C13-C15
25	B	607	CLA	C6-C7-C8-C10
25	B	616	CLA	C11-C12-C13-C15
25	B	616	CLA	C12-C13-C15-C16
25	B	617	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C10-C8-C7
25	C	513	CLA	C11-C10-C8-C7
25	a	711	CLA	C11-C12-C13-C15
25	b	611	CLA	C12-C13-C15-C16
25	b	612	CLA	C6-C7-C8-C10
25	b	621	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	507	CLA	C12-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C10
29	A	614	SQD	C16-C17-C18-C19
25	b	615	CLA	C4-C3-C5-C6
28	a	713	PL9	C43-C44-C46-C47
32	a	720	LHG	C27-C28-C29-C30
29	f	102	SQD	C31-C32-C33-C34
32	E	101	LHG	C28-C29-C30-C31
25	B	604	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	607	CLA	C6-C7-C8-C9
25	B	616	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	509	CLA	C11-C10-C8-C9
25	b	617	CLA	C6-C7-C8-C9
25	b	621	CLA	C11-C10-C8-C9
25	b	621	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
25	c	513	CLA	C11-C12-C13-C14
25	d	403	CLA	C6-C7-C8-C9
29	B	626	SQD	C27-C28-C29-C30
32	a	720	LHG	C25-C26-C27-C28
25	C	511	CLA	CBA-CGA-O2A-C1
25	B	611	CLA	C15-C16-C17-C18
23	b	627	LMG	O6-C5-C6-O5
23	C	521	LMG	C2-C1-O1-C7
23	c	519	LMG	C2-C1-O1-C7
23	D	409	LMG	O6-C5-C6-O5
29	f	102	SQD	C44-C45-C46-O48
32	E	101	LHG	C4-C5-C6-O8
32	e	101	LHG	C4-C5-C6-O8
23	A	603	LMG	C4-C5-C6-O5
23	C	520	LMG	C12-C13-C14-C15
32	E	101	LHG	C24-C25-C26-C27
25	B	608	CLA	O1D-CGD-O2D-CED
25	b	619	CLA	O1D-CGD-O2D-CED
29	I	102	SQD	C25-C26-C27-C28
32	d	406	LHG	C10-C11-C12-C13
25	a	707	CLA	C15-C16-C17-C18
26	A	608	PHO	C15-C16-C17-C18
33	C	518	DGD	C2A-C1A-O1G-C1G
25	C	508	CLA	C16-C17-C18-C19
29	b	601	SQD	C32-C33-C34-C35
25	C	507	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	O1A-CGA-O2A-C1
23	c	519	LMG	C19-C20-C21-C22
23	C	501	LMG	C13-C14-C15-C16
32	d	407	LHG	C34-C35-C36-C37
26	a	710	PHO	CHA-CBD-CGD-O1D
26	a	710	PHO	CHA-CBD-CGD-O2D
25	d	403	CLA	C10-C11-C12-C13
33	C	519	DGD	C2B-C3B-C4B-C5B
23	B	621	LMG	C10-C11-C12-C13
29	B	626	SQD	C7-C8-C9-C10
23	c	519	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
23	d	408	LMG	C18-C19-C20-C21
32	D	408	LHG	C12-C13-C14-C15
25	c	503	CLA	C5-C6-C7-C8
23	a	701	LMG	C17-C18-C19-C20
23	C	521	LMG	C37-C38-C39-C40
23	a	715	LMG	C21-C22-C23-C24
29	A	612	SQD	C30-C31-C32-C33
23	B	621	LMG	C28-C29-C30-C31
23	C	520	LMG	O10-C28-O8-C9
23	M	101	LMG	C16-C17-C18-C19
29	A	612	SQD	C32-C33-C34-C35
23	A	603	LMG	C29-C28-O8-C9
23	c	519	LMG	C29-C28-O8-C9
33	C	519	DGD	C5A-C6A-C7A-C8A
27	h	101	BCR	C18-C19-C20-C21
23	b	628	LMG	C11-C12-C13-C14
23	f	101	LMG	C31-C32-C33-C34
33	C	519	DGD	C4B-C5B-C6B-C7B
29	b	601	SQD	C33-C34-C35-C36
32	D	407	LHG	C34-C35-C36-C37
33	C	518	DGD	C6A-C7A-C8A-C9A
27	t	103	BCR	C22-C23-C24-C25
23	C	520	LMG	C31-C32-C33-C34
23	b	626	LMG	C30-C31-C32-C33
32	b	629	LHG	C33-C34-C35-C36
25	C	502	CLA	O1D-CGD-O2D-CED
26	D	401	PHO	O1D-CGD-O2D-CED
25	c	503	CLA	CBA-CGA-O2A-C1
25	C	506	CLA	CBD-CGD-O2D-CED
32	B	625	LHG	C27-C28-C29-C30
23	C	501	LMG	C22-C23-C24-C25
25	b	620	CLA	C10-C11-C12-C13
25	C	504	CLA	C4-C3-C5-C6
28	D	406	PL9	C30-C29-C31-C32
25	b	615	CLA	C2-C3-C5-C6
33	C	519	DGD	C8A-C9A-CAA-CBA
29	A	614	SQD	C14-C15-C16-C17
29	b	601	SQD	C27-C28-C29-C30
32	e	101	LHG	C19-C20-C21-C22
23	b	626	LMG	C37-C38-C39-C40
23	c	519	LMG	C29-C30-C31-C32
23	f	101	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	E	101	LHG	C31-C32-C33-C34
23	B	621	LMG	O1-C7-C8-O7
23	a	715	LMG	O7-C8-C9-O8
29	a	714	SQD	O6-C44-C45-O47
23	A	603	LMG	C20-C21-C22-C23
25	B	604	CLA	CBA-CGA-O2A-C1
23	C	501	LMG	C38-C39-C40-C41
33	c	517	DGD	C3B-C4B-C5B-C6B
23	f	101	LMG	C33-C34-C35-C36
29	I	102	SQD	C11-C10-C9-C8
23	c	520	LMG	C17-C18-C19-C20
32	B	625	LHG	C10-C11-C12-C13
28	a	713	PL9	C39-C41-C42-C43
25	C	511	CLA	O1A-CGA-O2A-C1
29	D	410	SQD	O48-C23-C24-C25
23	A	603	LMG	C38-C39-C40-C41
23	M	101	LMG	C19-C20-C21-C22
32	b	629	LHG	C9-C10-C11-C12
29	I	102	SQD	C18-C19-C20-C21
23	b	626	LMG	C40-C41-C42-C43
32	e	101	LHG	C28-C29-C30-C31
23	D	409	LMG	C28-C29-C30-C31
28	a	713	PL9	C45-C44-C46-C47
25	C	502	CLA	CBA-CGA-O2A-C1
32	b	629	LHG	C16-C17-C18-C19
33	c	517	DGD	CCB-CDB-CEB-CFB
29	B	626	SQD	C11-C12-C13-C14
32	D	407	LHG	O1-C1-C2-O2
25	B	612	CLA	C14-C13-C15-C16
25	B	616	CLA	C11-C12-C13-C14
25	C	512	CLA	C11-C10-C8-C9
25	C	513	CLA	C11-C10-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	a	711	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C12-C13-C14
25	c	513	CLA	C14-C13-C15-C16
23	b	626	LMG	C31-C32-C33-C34
29	B	626	SQD	C32-C33-C34-C35
33	C	518	DGD	C9B-CAB-CBB-CCB
33	h	102	DGD	CBB-CCB-CDB-CEB
25	B	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C4B-C3B-CAB-CBB
25	B	610	CLA	C4B-C3B-CAB-CBB
25	C	508	CLA	C4B-C3B-CAB-CBB
25	D	404	CLA	C4B-C3B-CAB-CBB
25	b	615	CLA	C4B-C3B-CAB-CBB
25	d	402	CLA	C4B-C3B-CAB-CBB
23	f	101	LMG	C4-C5-C6-O5
32	E	101	LHG	C12-C13-C14-C15
25	B	617	CLA	C15-C16-C17-C18
25	c	507	CLA	C16-C17-C18-C19
29	B	623	SQD	C2-C1-O6-C44
25	B	610	CLA	C15-C16-C17-C18
32	D	407	LHG	C27-C28-C29-C30
32	E	101	LHG	O6-C4-C5-C6
32	b	629	LHG	O6-C4-C5-C6
32	d	407	LHG	O6-C4-C5-C6
23	b	626	LMG	C19-C20-C21-C22
32	D	408	LHG	C19-C20-C21-C22
25	A	607	CLA	C12-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C6-C7-C8-C10
25	B	609	CLA	C11-C12-C13-C15
25	B	612	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C10-C8-C7
25	C	503	CLA	C6-C7-C8-C10
25	C	503	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C12-C13-C15
25	C	512	CLA	C6-C7-C8-C10
25	C	512	CLA	C11-C10-C8-C7
25	C	513	CLA	C12-C13-C15-C16
25	b	617	CLA	C6-C7-C8-C10
25	b	617	CLA	C12-C13-C15-C16
25	b	621	CLA	C12-C13-C15-C16
25	c	513	CLA	C6-C7-C8-C10
25	c	513	CLA	C11-C12-C13-C15
25	c	513	CLA	C12-C13-C15-C16
25	C	503	CLA	C5-C6-C7-C8
25	C	505	CLA	C8-C10-C11-C12
29	f	102	SQD	C35-C36-C37-C38
23	a	715	LMG	C29-C30-C31-C32
33	h	102	DGD	C7A-C8A-C9A-CAA
32	L	101	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
23	B	621	LMG	C40-C41-C42-C43
23	b	626	LMG	C34-C35-C36-C37
25	b	611	CLA	CBA-CGA-O2A-C1
32	D	407	LHG	C14-C15-C16-C17
32	L	101	LHG	C34-C35-C36-C37
33	h	102	DGD	C2B-C3B-C4B-C5B
25	c	505	CLA	C4-C3-C5-C6
28	D	406	PL9	C15-C14-C16-C17
28	a	713	PL9	C15-C14-C16-C17
28	a	713	PL9	C20-C19-C21-C22
25	B	616	CLA	C13-C15-C16-C17
25	b	608	CLA	C8-C10-C11-C12
33	c	518	DGD	C9B-CAB-CBB-CCB
23	d	408	LMG	C12-C13-C14-C15
23	b	626	LMG	C17-C18-C19-C20
25	C	510	CLA	C13-C15-C16-C17
29	A	612	SQD	C9-C10-C11-C12
32	e	101	LHG	C27-C28-C29-C30
25	B	608	CLA	CBA-CGA-O2A-C1
23	C	501	LMG	C21-C22-C23-C24
23	B	621	LMG	O1-C7-C8-C9
23	C	520	LMG	O1-C7-C8-C9
23	a	715	LMG	C7-C8-C9-O8
29	A	614	SQD	C44-C45-C46-O48
29	D	410	SQD	C44-C45-C46-O48
33	c	516	DGD	C1G-C2G-C3G-O3G
29	B	623	SQD	C12-C13-C14-C15
29	a	714	SQD	C14-C15-C16-C17
23	A	603	LMG	C16-C17-C18-C19
23	C	501	LMG	C36-C37-C38-C39
23	c	519	LMG	C30-C31-C32-C33
29	I	102	SQD	O6-C44-C45-C46
23	C	521	LMG	C12-C13-C14-C15
32	L	101	LHG	C31-C32-C33-C34
28	d	405	PL9	C15-C14-C16-C17
23	C	520	LMG	C30-C31-C32-C33
25	c	505	CLA	C2-C3-C5-C6
26	A	608	PHO	C2-C3-C5-C6
23	f	101	LMG	C13-C14-C15-C16
25	B	615	CLA	C16-C17-C18-C20
26	A	608	PHO	C16-C17-C18-C19
32	D	407	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
32	a	720	LHG	O6-C4-C5-O7
32	L	101	LHG	C16-C17-C18-C19
27	B	618	BCR	C1-C6-C7-C8
27	B	620	BCR	C1-C6-C7-C8
27	B	620	BCR	C23-C24-C25-C30
27	D	405	BCR	C1-C6-C7-C8
27	Y	101	BCR	C1-C6-C7-C8
27	b	623	BCR	C5-C6-C7-C8
27	b	625	BCR	C1-C6-C7-C8
27	c	515	BCR	C1-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
23	c	520	LMG	C30-C31-C32-C33
32	B	625	LHG	C11-C12-C13-C14
32	b	629	LHG	C29-C30-C31-C32
23	a	715	LMG	C11-C10-O7-C8
32	D	408	LHG	C24-C23-O8-C6
25	c	506	CLA	C8-C10-C11-C12
33	h	102	DGD	CBA-CCA-CDA-CEA
32	E	101	LHG	C2-C3-O3-P
29	B	623	SQD	C7-C8-C9-C10
33	c	516	DGD	C4D-C5D-C6D-O5D
25	B	616	CLA	C8-C10-C11-C12
33	c	516	DGD	O6D-C5D-C6D-O5D
29	A	612	SQD	C10-C11-C12-C13
25	B	609	CLA	C16-C17-C18-C20
25	C	508	CLA	C16-C17-C18-C20
25	c	508	CLA	C10-C11-C12-C13
23	C	501	LMG	O1-C7-C8-O7
23	a	715	LMG	O1-C7-C8-O7
29	B	623	SQD	O47-C45-C46-O48
29	b	601	SQD	O6-C44-C45-O47
32	E	101	LHG	O7-C5-C6-O8
33	c	516	DGD	O2G-C2G-C3G-O3G
28	d	405	PL9	C4-C3-C7-C8
32	L	101	LHG	C9-C10-C11-C12
33	c	516	DGD	C5A-C6A-C7A-C8A
25	B	611	CLA	C13-C15-C16-C17
25	B	609	CLA	O1D-CGD-O2D-CED
29	B	623	SQD	C33-C34-C35-C36
26	A	608	PHO	C4-C3-C5-C6
23	c	519	LMG	C34-C35-C36-C37
28	D	406	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
28	a	713	PL9	C18-C19-C21-C22
23	c	519	LMG	C14-C15-C16-C17
23	c	519	LMG	C15-C16-C17-C18
23	a	701	LMG	C36-C37-C38-C39
25	b	621	CLA	C15-C16-C17-C18
23	f	101	LMG	C10-C11-C12-C13
25	B	617	CLA	C11-C10-C8-C9
25	C	503	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	514	CLA	C11-C10-C8-C9
25	b	617	CLA	C14-C13-C15-C16
23	C	521	LMG	C36-C37-C38-C39
33	H	103	DGD	C5A-C6A-C7A-C8A
23	C	501	LMG	C16-C17-C18-C19
25	B	604	CLA	C16-C17-C18-C19
23	a	701	LMG	C18-C19-C20-C21
32	d	406	LHG	C18-C19-C20-C21
28	d	405	PL9	C39-C41-C42-C43
23	a	715	LMG	C37-C38-C39-C40
29	a	714	SQD	C16-C17-C18-C19
33	C	517	DGD	C4D-C5D-C6D-O5D
32	a	720	LHG	C9-C10-C11-C12
23	A	603	LMG	C34-C35-C36-C37
33	c	517	DGD	C4B-C5B-C6B-C7B
25	B	607	CLA	C13-C15-C16-C17
25	C	506	CLA	CBA-CGA-O2A-C1
23	M	101	LMG	C38-C39-C40-C41
25	B	615	CLA	C16-C17-C18-C19
29	A	614	SQD	C33-C34-C35-C36
33	C	519	DGD	C3B-C4B-C5B-C6B
23	b	626	LMG	C35-C36-C37-C38
29	B	623	SQD	C31-C32-C33-C34
23	C	520	LMG	C38-C39-C40-C41
25	C	511	CLA	C8-C10-C11-C12
27	C	516	BCR	C16-C17-C18-C36
27	a	712	BCR	C16-C17-C18-C36
25	B	604	CLA	O1A-CGA-O2A-C1
25	C	514	CLA	C8-C10-C11-C12
32	D	407	LHG	O6-C4-C5-C6
25	a	719	CLA	C16-C17-C18-C20
26	a	710	PHO	C16-C17-C18-C20
25	C	509	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	C15-C16-C17-C18
23	D	409	LMG	C30-C31-C32-C33
25	B	617	CLA	C11-C12-C13-C15
25	C	511	CLA	C11-C10-C8-C7
25	C	514	CLA	C11-C10-C8-C7
25	a	708	CLA	C12-C13-C15-C16
25	c	502	CLA	C6-C7-C8-C10
25	c	502	CLA	C11-C10-C8-C7
23	C	521	LMG	C10-C11-C12-C13
23	C	501	LMG	C33-C34-C35-C36
23	f	101	LMG	C14-C15-C16-C17
25	B	602	CLA	C8-C10-C11-C12
25	C	507	CLA	C5-C6-C7-C8
27	Y	101	BCR	C7-C8-C9-C10
27	b	623	BCR	C21-C22-C23-C24
27	c	514	BCR	C21-C22-C23-C24
23	c	520	LMG	C29-C28-O8-C9
23	C	501	LMG	C12-C13-C14-C15
25	c	503	CLA	O1A-CGA-O2A-C1
29	a	714	SQD	C5-C6-S-O8
29	b	601	SQD	C45-C44-O6-C1
25	b	617	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	C10-C11-C12-C13
25	B	609	CLA	C2A-CAA-CBA-CGA
32	D	407	LHG	C11-C10-C9-C8
25	a	711	CLA	C16-C17-C18-C20
23	C	501	LMG	C11-C10-O7-C8
23	d	408	LMG	C20-C21-C22-C23
29	I	102	SQD	C35-C36-C37-C38
25	C	502	CLA	O1A-CGA-O2A-C1
23	C	521	LMG	C39-C40-C41-C42
29	B	626	SQD	C46-C45-O47-C7
25	b	611	CLA	O1A-CGA-O2A-C1
33	c	516	DGD	C2A-C3A-C4A-C5A
25	C	504	CLA	C8-C10-C11-C12
25	B	609	CLA	C16-C17-C18-C19
33	C	517	DGD	O6D-C5D-C6D-O5D
23	A	603	LMG	O10-C28-O8-C9
25	B	605	CLA	O1D-CGD-O2D-CED
23	D	409	LMG	C22-C23-C24-C25
25	C	510	CLA	C5-C6-C7-C8
32	b	629	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
23	a	715	LMG	C33-C34-C35-C36
33	C	518	DGD	C4B-C5B-C6B-C7B
33	c	518	DGD	C7A-C8A-C9A-CAA
29	B	623	SQD	C44-C45-C46-O48
29	a	714	SQD	O6-C44-C45-C46
34	e	102	HEM	C4B-C3B-CAB-CBB
34	e	102	HEM	C4C-C3C-CAC-CBC
23	B	621	LMG	C14-C15-C16-C17
23	B	621	LMG	C34-C35-C36-C37
25	B	606	CLA	C2-C3-C5-C6
29	a	714	SQD	C26-C27-C28-C29
23	c	520	LMG	O7-C8-C9-O8
32	a	720	LHG	O7-C5-C6-O8
25	A	607	CLA	C6-C7-C8-C9
25	B	612	CLA	C11-C12-C13-C14
25	c	505	CLA	C11-C10-C8-C9
25	d	402	CLA	C6-C7-C8-C9
23	B	621	LMG	C39-C40-C41-C42
29	A	612	SQD	C13-C14-C15-C16
25	B	608	CLA	O1A-CGA-O2A-C1
23	D	409	LMG	C18-C19-C20-C21
23	a	715	LMG	C38-C39-C40-C41
32	L	101	LHG	C33-C34-C35-C36
25	c	512	CLA	C5-C6-C7-C8
23	a	715	LMG	C15-C16-C17-C18
23	b	628	LMG	C13-C14-C15-C16
29	A	612	SQD	C14-C15-C16-C17
33	C	519	DGD	CAA-CBA-CCA-CDA
25	C	506	CLA	O1A-CGA-O2A-C1
25	a	711	CLA	C16-C17-C18-C19
25	a	719	CLA	C16-C17-C18-C19
23	a	715	LMG	C36-C37-C38-C39
25	B	611	CLA	C5-C6-C7-C8
25	c	508	CLA	C13-C15-C16-C17
23	M	101	LMG	C40-C41-C42-C43
23	D	409	LMG	C32-C33-C34-C35
32	B	625	LHG	C24-C25-C26-C27
25	C	510	CLA	C16-C17-C18-C20
25	c	513	CLA	C16-C17-C18-C20
25	B	606	CLA	C10-C11-C12-C13
33	h	102	DGD	O1A-C1A-O1G-C1G
25	c	513	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	C	509	CLA	O1D-CGD-O2D-CED
33	c	518	DGD	C4A-C5A-C6A-C7A
25	B	611	CLA	C4B-C3B-CAB-CBB
25	C	502	CLA	C4B-C3B-CAB-CBB
25	D	403	CLA	C1A-C2A-CAA-CBA
25	b	611	CLA	C4B-C3B-CAB-CBB
25	b	616	CLA	C4B-C3B-CAB-CBB
25	c	501	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C4B-C3B-CAB-CBB
25	c	510	CLA	C4-C3-C5-C6
23	C	520	LMG	C11-C12-C13-C14
23	c	520	LMG	C33-C34-C35-C36
25	B	610	CLA	C16-C17-C18-C20
32	e	101	LHG	C25-C26-C27-C28
23	D	409	LMG	C34-C35-C36-C37
29	b	601	SQD	C11-C10-C9-C8
25	A	607	CLA	C6-C7-C8-C10
25	B	615	CLA	C6-C7-C8-C10
25	B	616	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C12-C13-C15
25	b	607	CLA	C11-C12-C13-C15
25	b	609	CLA	C11-C10-C8-C7
25	b	610	CLA	C11-C10-C8-C7
25	b	619	CLA	C6-C7-C8-C10
25	c	509	CLA	C11-C10-C8-C7
26	A	608	PHO	C6-C7-C8-C10
25	C	503	CLA	C16-C17-C18-C20
33	c	517	DGD	CDA-CEA-CFA-CGA
23	f	101	LMG	C18-C19-C20-C21
25	D	404	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C19
23	M	101	LMG	C20-C21-C22-C23
29	b	601	SQD	C26-C27-C28-C29
32	d	407	LHG	O6-C4-C5-O7
25	b	609	CLA	C2A-CAA-CBA-CGA
25	B	609	CLA	C11-C12-C13-C14
25	C	511	CLA	C11-C10-C8-C9
25	a	708	CLA	C14-C13-C15-C16
25	c	502	CLA	C11-C10-C8-C9
29	D	410	SQD	O10-C23-O48-C46
25	a	711	CLA	C10-C11-C12-C13
32	D	408	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	d	404	BCR	C19-C20-C21-C22
26	a	710	PHO	C16-C17-C18-C19
25	B	605	CLA	C10-C11-C12-C13
23	a	701	LMG	C20-C21-C22-C23
23	C	520	LMG	O1-C7-C8-O7
23	a	701	LMG	O1-C7-C8-O7
29	A	614	SQD	O47-C45-C46-O48
29	B	623	SQD	O6-C44-C45-O47
29	D	410	SQD	O47-C45-C46-O48
32	L	101	LHG	O7-C5-C6-O8
32	e	101	LHG	O7-C5-C6-O8
33	C	517	DGD	O2G-C2G-C3G-O3G
32	L	101	LHG	C1-C2-C3-O3
29	D	410	SQD	C2-C1-O6-C44
25	B	613	CLA	C10-C11-C12-C13
23	C	501	LMG	O1-C7-C8-C9
23	a	701	LMG	O1-C7-C8-C9
23	a	715	LMG	O1-C7-C8-C9
23	b	627	LMG	C7-C8-C9-O8
29	b	601	SQD	O6-C44-C45-C46
32	L	101	LHG	C4-C5-C6-O8
32	a	720	LHG	C4-C5-C6-O8
32	b	629	LHG	C4-C5-C6-O8
25	C	504	CLA	C2-C3-C5-C6
32	L	101	LHG	C17-C18-C19-C20
33	c	517	DGD	C6A-C7A-C8A-C9A
25	B	604	CLA	CAD-CBD-CGD-O2D
25	B	606	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	615	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	b	618	CLA	CAD-CBD-CGD-O2D
23	C	521	LMG	O10-C28-O8-C9
23	M	101	LMG	C34-C35-C36-C37
33	c	518	DGD	C6A-C7A-C8A-C9A
25	C	512	CLA	CBA-CGA-O2A-C1
23	M	101	LMG	C32-C33-C34-C35
23	a	701	LMG	C37-C38-C39-C40
25	B	604	CLA	CAD-CBD-CGD-O1D
25	B	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	610	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	615	CLA	CAD-CBD-CGD-O1D
25	B	617	CLA	CHA-CBD-CGD-O1D
25	B	617	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	b	610	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	618	CLA	CAD-CBD-CGD-O1D
25	c	501	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	512	CLA	CHA-CBD-CGD-O1D
25	c	512	CLA	CHA-CBD-CGD-O2D
26	D	401	PHO	CHA-CBD-CGD-O2D
32	B	625	LHG	C3-O3-P-O5
32	D	407	LHG	C4-O6-P-O5
32	E	101	LHG	C4-O6-P-O4
32	E	101	LHG	C4-O6-P-O5
32	L	101	LHG	C4-O6-P-O5
32	a	720	LHG	C3-O3-P-O5
32	a	720	LHG	C3-O3-P-O6
32	d	406	LHG	C3-O3-P-O5
32	d	407	LHG	C3-O3-P-O5
32	d	407	LHG	C4-O6-P-O5
25	D	403	CLA	C3-C5-C6-C7
25	b	618	CLA	CBD-CGD-O2D-CED
32	d	406	LHG	C17-C18-C19-C20
25	B	603	CLA	C2B-C3B-CAB-CBB
25	D	403	CLA	C2B-C3B-CAB-CBB
25	D	404	CLA	C2B-C3B-CAB-CBB
25	b	615	CLA	C2B-C3B-CAB-CBB
25	c	501	CLA	C2B-C3B-CAB-CBB
25	c	502	CLA	C2B-C3B-CAB-CBB
27	B	618	BCR	C5-C6-C7-C8
27	b	625	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
32	D	408	LHG	C13-C14-C15-C16
29	f	102	SQD	C8-C7-O47-C45
23	f	101	LMG	C30-C31-C32-C33
33	c	517	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	C25-C26-C27-C28
23	a	701	LMG	C39-C40-C41-C42
32	d	406	LHG	C27-C28-C29-C30
23	d	408	LMG	C37-C38-C39-C40
25	C	512	CLA	O1A-CGA-O2A-C1
23	c	519	LMG	C37-C38-C39-C40
32	b	629	LHG	C30-C31-C32-C33
28	a	713	PL9	C4-C3-C7-C8
32	d	406	LHG	O1-C1-C2-C3
23	c	520	LMG	C15-C16-C17-C18
23	C	520	LMG	C37-C38-C39-C40
33	C	519	DGD	O6E-C5E-C6E-O5E
25	A	607	CLA	C14-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C14
25	B	617	CLA	C11-C12-C13-C14
25	b	609	CLA	C6-C7-C8-C9
25	c	501	CLA	C11-C12-C13-C14
26	A	608	PHO	C6-C7-C8-C9
25	C	506	CLA	O1D-CGD-O2D-CED
29	b	601	SQD	C18-C19-C20-C21
25	B	607	CLA	C11-C12-C13-C15
25	C	502	CLA	C12-C13-C15-C16
25	b	609	CLA	C6-C7-C8-C10
32	e	101	LHG	O6-C4-C5-O7
25	C	510	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C19
23	C	501	LMG	C29-C28-O8-C9
23	C	520	LMG	C22-C23-C24-C25
33	C	518	DGD	CDA-CEA-CFA-CGA
29	b	601	SQD	C2-C1-O6-C44
33	C	519	DGD	C2D-C1D-O3G-C3G
28	D	406	PL9	C45-C44-C46-C47
25	B	610	CLA	C16-C17-C18-C19
23	a	701	LMG	C15-C16-C17-C18
23	c	519	LMG	C38-C39-C40-C41
23	B	621	LMG	C32-C33-C34-C35
33	H	103	DGD	O2G-C1B-C2B-C3B
25	D	404	CLA	C16-C17-C18-C19
35	V	201	HEC	C3D-CAD-CBD-CGD
32	E	101	LHG	C30-C31-C32-C33
25	B	613	CLA	C13-C15-C16-C17
23	c	520	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C2A-CAA-CBA-CGA
25	D	402	CLA	C15-C16-C17-C18
33	c	516	DGD	C7B-C8B-C9B-CAB
23	c	520	LMG	C31-C32-C33-C34
32	D	408	LHG	C34-C35-C36-C37
23	c	519	LMG	O1-C7-C8-C9
33	C	517	DGD	C1G-C2G-C3G-O3G
25	A	607	CLA	C3-C5-C6-C7
33	h	102	DGD	C4D-C5D-C6D-O5D
32	d	406	LHG	C15-C16-C17-C18
34	e	102	HEM	C2D-C3D-CAD-CBD
25	B	617	CLA	C5-C6-C7-C8
23	C	521	LMG	C8-C7-O1-C1
23	D	409	LMG	C8-C7-O1-C1
25	B	606	CLA	C13-C15-C16-C17
33	C	517	DGD	C3B-C4B-C5B-C6B
25	C	508	CLA	C13-C15-C16-C17
25	c	510	CLA	C2-C3-C5-C6
25	b	618	CLA	O1D-CGD-O2D-CED
32	E	101	LHG	O9-C7-O7-C5
33	C	518	DGD	C1B-C2B-C3B-C4B
25	B	605	CLA	C11-C10-C8-C9
25	B	606	CLA	C6-C7-C8-C9
25	B	616	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	b	609	CLA	C11-C10-C8-C9
25	b	619	CLA	C6-C7-C8-C9
25	c	511	CLA	C6-C7-C8-C9
25	d	402	CLA	C14-C13-C15-C16
25	C	505	CLA	C15-C16-C17-C18
29	f	102	SQD	O10-C23-O48-C46
25	C	505	CLA	C4B-C3B-CAB-CBB
25	B	608	CLA	C16-C17-C18-C20
25	C	513	CLA	C4-C3-C5-C6
33	C	517	DGD	C7A-C8A-C9A-CAA
23	D	409	LMG	C39-C40-C41-C42
33	C	517	DGD	O1A-C1A-O1G-C1G
25	b	611	CLA	C15-C16-C17-C18
32	D	407	LHG	C12-C13-C14-C15
23	C	520	LMG	C20-C21-C22-C23
32	d	406	LHG	C12-C13-C14-C15
25	B	605	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	C6-C7-C8-C10
25	c	506	CLA	C12-C13-C15-C16
25	B	606	CLA	C5-C6-C7-C8
23	a	701	LMG	C34-C35-C36-C37
33	h	102	DGD	CCB-CDB-CEB-CFB
23	b	626	LMG	O8-C28-C29-C30
23	b	627	LMG	O7-C8-C9-O8
23	c	519	LMG	O1-C7-C8-O7
32	b	629	LHG	O7-C5-C6-O8
23	d	408	LMG	C36-C37-C38-C39
23	b	628	LMG	C10-C11-C12-C13
32	d	407	LHG	C25-C26-C27-C28
33	C	517	DGD	C7B-C8B-C9B-CAB
29	A	612	SQD	O5-C1-O6-C44
32	B	625	LHG	C25-C26-C27-C28
25	B	614	CLA	C2-C1-O2A-CGA
33	h	102	DGD	C5A-C6A-C7A-C8A
23	c	519	LMG	C4-C5-C6-O5
33	C	518	DGD	CBB-CCB-CDB-CEB
25	C	502	CLA	C15-C16-C17-C18
27	b	625	BCR	C21-C22-C23-C24
34	E	102	HEM	C3D-CAD-CBD-CGD
25	C	510	CLA	C3-C5-C6-C7
25	B	602	CLA	C16-C17-C18-C20
25	B	613	CLA	C15-C16-C17-C18
33	c	517	DGD	CBA-CCA-CDA-CEA
25	C	502	CLA	C2A-CAA-CBA-CGA
29	A	614	SQD	C34-C35-C36-C37
33	H	103	DGD	O1A-C1A-O1G-C1G
25	B	611	CLA	C11-C12-C13-C14
25	b	613	CLA	C11-C12-C13-C14
25	b	615	CLA	C11-C10-C8-C9
25	c	507	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	512	CLA	C11-C12-C13-C14
26	D	401	PHO	C16-C17-C18-C20
33	c	517	DGD	C8B-C9B-CAB-CBB
29	A	614	SQD	C11-C12-C13-C14
32	d	407	LHG	C32-C33-C34-C35
25	B	615	CLA	C13-C15-C16-C17
33	C	518	DGD	C7B-C8B-C9B-CAB
26	a	709	PHO	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	a	707	CLA	C2A-CAA-CBA-CGA
25	D	404	CLA	C1A-C2A-CAA-CBA
23	d	408	LMG	C29-C30-C31-C32
23	f	101	LMG	C39-C40-C41-C42
32	b	629	LHG	C17-C18-C19-C20
33	c	516	DGD	CAA-CBA-CCA-CDA
25	A	609	CLA	C2B-C3B-CAB-CBB
25	B	607	CLA	C2B-C3B-CAB-CBB
25	B	610	CLA	C2B-C3B-CAB-CBB
25	B	611	CLA	C2B-C3B-CAB-CBB
25	C	503	CLA	C2B-C3B-CAB-CBB
25	C	508	CLA	C2B-C3B-CAB-CBB
25	b	611	CLA	C2B-C3B-CAB-CBB
25	b	616	CLA	C2B-C3B-CAB-CBB
25	b	618	CLA	C2B-C3B-CAB-CBB
25	d	402	CLA	C2B-C3B-CAB-CBB
27	A	610	BCR	C1-C6-C7-C8
27	B	619	BCR	C1-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C30
27	B	620	BCR	C5-C6-C7-C8
27	B	620	BCR	C23-C24-C25-C26
27	C	515	BCR	C1-C6-C7-C8
27	C	516	BCR	C1-C6-C7-C8
27	D	405	BCR	C5-C6-C7-C8
27	D	405	BCR	C23-C24-C25-C30
27	H	102	BCR	C23-C24-C25-C30
27	K	101	BCR	C1-C6-C7-C8
27	Y	101	BCR	C5-C6-C7-C8
27	a	712	BCR	C1-C6-C7-C8
27	b	624	BCR	C1-C6-C7-C8
27	b	625	BCR	C5-C6-C7-C8
27	b	625	BCR	C23-C24-C25-C26
27	c	515	BCR	C5-C6-C7-C8
27	c	515	BCR	C23-C24-C25-C30
27	d	404	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	k	102	BCR	C1-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C30
25	b	615	CLA	CBA-CGA-O2A-C1
25	B	617	CLA	C13-C15-C16-C17
23	d	408	LMG	C14-C15-C16-C17
33	C	518	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
25	a	708	CLA	C16-C17-C18-C19
33	c	518	DGD	O6E-C5E-C6E-O5E
25	B	608	CLA	C12-C13-C15-C16
25	B	610	CLA	C11-C12-C13-C15
25	D	403	CLA	C6-C7-C8-C10
25	D	403	CLA	C11-C12-C13-C15
25	c	510	CLA	C12-C13-C15-C16
25	c	511	CLA	C6-C7-C8-C10
25	B	615	CLA	C2A-CAA-CBA-CGA
29	f	102	SQD	O47-C45-C46-O48
23	a	715	LMG	C22-C23-C24-C25
32	d	407	LHG	C26-C27-C28-C29
32	a	720	LHG	C35-C36-C37-C38
28	A	611	PL9	C4-C3-C7-C8
33	C	519	DGD	CCB-CDB-CEB-CFB
32	b	629	LHG	C11-C10-C9-C8
23	d	408	LMG	C16-C17-C18-C19
27	C	516	BCR	C7-C8-C9-C34
25	C	503	CLA	C4-C3-C5-C6
25	C	505	CLA	C4-C3-C5-C6
25	b	608	CLA	C4-C3-C5-C6
25	d	402	CLA	C4-C3-C5-C6
28	D	406	PL9	C43-C44-C46-C47
23	b	627	LMG	C40-C41-C42-C43
27	B	620	BCR	C7-C8-C9-C10
23	B	621	LMG	C19-C20-C21-C22
32	D	408	LHG	C27-C28-C29-C30
32	E	101	LHG	C10-C11-C12-C13
33	c	517	DGD	C1B-C2B-C3B-C4B
29	B	626	SQD	C10-C11-C12-C13
25	b	609	CLA	C14-C13-C15-C16
25	c	508	CLA	C14-C13-C15-C16
32	d	406	LHG	C33-C34-C35-C36
23	f	101	LMG	C20-C21-C22-C23
25	B	610	CLA	C8-C10-C11-C12
32	E	101	LHG	C26-C27-C28-C29
25	C	513	CLA	C5-C6-C7-C8
25	b	609	CLA	C10-C11-C12-C13
23	b	626	LMG	C20-C21-C22-C23
28	A	611	PL9	C40-C39-C41-C42
25	B	612	CLA	C8-C10-C11-C12
25	B	617	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	d	408	LMG	C15-C16-C17-C18
34	e	102	HEM	C4D-C3D-CAD-CBD
25	b	615	CLA	O1A-CGA-O2A-C1
23	A	603	LMG	C37-C38-C39-C40
23	c	519	LMG	C7-C8-C9-O8
25	c	502	CLA	O1A-CGA-O2A-C1
32	D	408	LHG	C33-C34-C35-C36
23	b	627	LMG	C16-C17-C18-C19
28	d	405	PL9	C35-C34-C36-C37
28	D	406	PL9	C13-C14-C16-C17
23	b	626	LMG	C18-C19-C20-C21
25	A	609	CLA	C4B-C3B-CAB-CBB
25	C	503	CLA	C4B-C3B-CAB-CBB
25	a	711	CLA	C4B-C3B-CAB-CBB
25	a	719	CLA	C4B-C3B-CAB-CBB
29	D	410	SQD	C27-C28-C29-C30
25	B	602	CLA	C16-C17-C18-C19
25	B	603	CLA	C16-C17-C18-C20
26	A	608	PHO	CHA-CBD-CGD-O1D
26	D	401	PHO	CHA-CBD-CGD-O1D
27	b	625	BCR	C20-C21-C22-C37
27	c	514	BCR	C20-C21-C22-C37
23	d	408	LMG	O7-C10-C11-C12
33	c	518	DGD	C5B-C6B-C7B-C8B
33	C	517	DGD	C8A-C9A-CAA-CBA
29	B	626	SQD	O47-C45-C46-O48
23	A	603	LMG	C13-C14-C15-C16
29	A	612	SQD	C34-C35-C36-C37
29	a	714	SQD	O5-C1-O6-C44
25	b	615	CLA	C6-C7-C8-C10
23	d	408	LMG	O9-C10-C11-C12
29	D	410	SQD	C31-C32-C33-C34
25	c	506	CLA	C13-C15-C16-C17
25	B	607	CLA	O1A-CGA-O2A-C1
33	h	102	DGD	C6A-C7A-C8A-C9A
32	L	101	LHG	C28-C29-C30-C31
25	c	502	CLA	CBA-CGA-O2A-C1
25	B	615	CLA	C6-C7-C8-C9
25	C	511	CLA	C6-C7-C8-C9
25	b	610	CLA	C11-C10-C8-C9
25	b	610	CLA	C11-C12-C13-C14
25	c	510	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	B	626	SQD	C26-C27-C28-C29
25	B	609	CLA	C2-C1-O2A-CGA
25	c	512	CLA	C2-C1-O2A-CGA
25	B	607	CLA	CBA-CGA-O2A-C1
29	B	626	SQD	C12-C13-C14-C15
25	c	506	CLA	C3A-C2A-CAA-CBA
26	a	709	PHO	C3A-C2A-CAA-CBA
33	c	517	DGD	CDB-CEB-CFB-CGB
33	h	102	DGD	O2G-C1B-C2B-C3B
33	C	519	DGD	O1A-C1A-O1G-C1G
34	E	102	HEM	CAD-CBD-CGD-O2D
23	C	501	LMG	O8-C28-C29-C30
29	I	102	SQD	C33-C34-C35-C36
27	B	618	BCR	C10-C11-C12-C13
27	b	624	BCR	C10-C11-C12-C13
27	k	101	BCR	C10-C11-C12-C13
27	t	103	BCR	C10-C11-C12-C13
33	c	517	DGD	C4A-C5A-C6A-C7A
35	V	201	HEC	C2D-C3D-CAD-CBD
25	a	719	CLA	C13-C15-C16-C17
33	c	516	DGD	C6A-C7A-C8A-C9A
29	B	626	SQD	C19-C20-C21-C22
23	c	520	LMG	C16-C17-C18-C19
25	b	608	CLA	O1D-CGD-O2D-CED
23	b	627	LMG	O6-C1-O1-C7
25	c	502	CLA	C8-C10-C11-C12
33	c	517	DGD	CBB-CCB-CDB-CEB
23	B	621	LMG	C29-C28-O8-C9
29	b	601	SQD	C31-C32-C33-C34
23	A	603	LMG	C11-C12-C13-C14
25	b	619	CLA	CAA-CBA-CGA-O2A
29	a	714	SQD	C30-C31-C32-C33
25	c	503	CLA	C8-C10-C11-C12
29	A	614	SQD	C10-C11-C12-C13
29	I	102	SQD	C12-C13-C14-C15
23	c	519	LMG	O7-C8-C9-O8
25	B	617	CLA	C10-C11-C12-C13
25	a	708	CLA	C16-C17-C18-C20
23	M	101	LMG	C33-C34-C35-C36
32	B	625	LHG	C9-C10-C11-C12
29	D	410	SQD	C29-C30-C31-C32
25	b	618	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	d	408	LMG	C29-C28-O8-C9
25	C	511	CLA	C4-C3-C5-C6
25	B	606	CLA	C11-C12-C13-C15
25	C	511	CLA	C6-C7-C8-C10
25	b	612	CLA	C11-C10-C8-C7
25	c	508	CLA	C12-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C10
25	d	402	CLA	C11-C10-C8-C7
29	B	623	SQD	C11-C12-C13-C14
25	B	605	CLA	C2B-C3B-CAB-CBB
25	B	615	CLA	C2B-C3B-CAB-CBB
25	C	505	CLA	C2B-C3B-CAB-CBB
25	C	507	CLA	C2B-C3B-CAB-CBB
25	a	711	CLA	C2B-C3B-CAB-CBB
25	a	719	CLA	C2B-C3B-CAB-CBB
25	b	620	CLA	C2B-C3B-CAB-CBB
27	A	610	BCR	C5-C6-C7-C8
27	A	610	BCR	C23-C24-C25-C30
27	B	619	BCR	C5-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C26
27	C	516	BCR	C23-C24-C25-C30
27	D	405	BCR	C23-C24-C25-C26
27	H	102	BCR	C23-C24-C25-C26
27	K	101	BCR	C23-C24-C25-C26
27	K	101	BCR	C23-C24-C25-C30
27	a	712	BCR	C5-C6-C7-C8
27	a	712	BCR	C23-C24-C25-C30
27	b	624	BCR	C5-C6-C7-C8
27	b	624	BCR	C23-C24-C25-C26
27	b	624	BCR	C23-C24-C25-C30
27	c	514	BCR	C5-C6-C7-C8
27	c	515	BCR	C23-C24-C25-C26
27	d	404	BCR	C5-C6-C7-C8
27	h	101	BCR	C23-C24-C25-C26
27	h	101	BCR	C23-C24-C25-C30
27	k	102	BCR	C5-C6-C7-C8
25	C	504	CLA	C2-C1-O2A-CGA
23	A	603	LMG	C22-C23-C24-C25
29	b	601	SQD	O48-C23-C24-C25
23	A	603	LMG	O7-C10-C11-C12
25	B	614	CLA	CAA-CBA-CGA-O2A
25	C	511	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	d	405	PL9	C13-C14-C16-C17
28	d	405	PL9	C28-C29-C31-C32
34	E	102	HEM	CAD-CBD-CGD-O1D
26	a	710	PHO	C8-C10-C11-C12
32	B	625	LHG	C29-C30-C31-C32
25	D	402	CLA	C2C-C3C-CAC-CBC
23	D	409	LMG	C37-C38-C39-C40
32	d	407	LHG	C10-C11-C12-C13
25	B	610	CLA	C13-C15-C16-C17
23	a	701	LMG	C40-C41-C42-C43
29	A	612	SQD	C33-C34-C35-C36
25	D	402	CLA	C4C-C3C-CAC-CBC
34	e	102	HEM	CAD-CBD-CGD-O2D
25	c	510	CLA	CAA-CBA-CGA-O2A
25	C	513	CLA	C2-C3-C5-C6
28	a	713	PL9	C13-C14-C16-C17
28	a	713	PL9	C33-C34-C36-C37
32	B	625	LHG	C28-C29-C30-C31
25	b	621	CLA	C13-C15-C16-C17
23	C	520	LMG	C10-C11-C12-C13
23	c	519	LMG	O10-C28-O8-C9
25	C	510	CLA	C6-C7-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	b	607	CLA	C6-C7-C8-C9
23	A	603	LMG	O8-C28-C29-C30
25	B	605	CLA	C4B-C3B-CAB-CBB
25	C	503	CLA	C1A-C2A-CAA-CBA
25	b	618	CLA	C4B-C3B-CAB-CBB
25	c	506	CLA	C1A-C2A-CAA-CBA
29	D	410	SQD	C7-C8-C9-C10
33	c	516	DGD	O6D-C1D-O3G-C3G
33	c	518	DGD	O6D-C1D-O3G-C3G
25	C	511	CLA	CAA-CBA-CGA-O2A
29	a	714	SQD	O47-C7-C8-C9
27	H	102	BCR	C9-C10-C11-C12
25	C	503	CLA	O1A-CGA-O2A-C1
33	c	518	DGD	C8A-C9A-CAA-CBA
25	b	613	CLA	C10-C11-C12-C13
33	c	516	DGD	CBA-CCA-CDA-CEA
32	L	101	LHG	O7-C7-C8-C9
33	C	517	DGD	O1G-C1A-C2A-C3A
23	b	626	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
29	I	102	SQD	C28-C29-C30-C31
32	a	720	LHG	O6-C4-C5-C6
25	D	403	CLA	CAA-CBA-CGA-O2A
32	b	629	LHG	O7-C7-C8-C9
33	C	517	DGD	C2B-C3B-C4B-C5B
29	A	614	SQD	C25-C26-C27-C28
29	B	623	SQD	C5-C6-S-O9
29	a	714	SQD	C5-C6-S-O9
25	C	507	CLA	C15-C16-C17-C18
25	D	403	CLA	C2-C1-O2A-CGA
25	b	619	CLA	C2-C1-O2A-CGA
25	B	602	CLA	C11-C10-C8-C7
25	B	613	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C10-C8-C7
25	a	719	CLA	C11-C10-C8-C7
25	b	616	CLA	C12-C13-C15-C16
25	c	513	CLA	C11-C10-C8-C7
29	b	601	SQD	C29-C30-C31-C32
25	C	508	CLA	C2A-CAA-CBA-CGA
25	b	616	CLA	C2A-CAA-CBA-CGA
32	e	101	LHG	C11-C12-C13-C14
25	b	609	CLA	C5-C6-C7-C8
25	b	621	CLA	C8-C10-C11-C12
32	D	408	LHG	C2-C3-O3-P
25	B	605	CLA	C2C-C3C-CAC-CBC
29	B	626	SQD	C35-C36-C37-C38
23	C	520	LMG	C14-C15-C16-C17
25	b	618	CLA	CBA-CGA-O2A-C1
32	B	625	LHG	C17-C18-C19-C20
28	d	405	PL9	C11-C12-C13-C14
25	B	614	CLA	CAA-CBA-CGA-O1A
29	B	623	SQD	O49-C7-C8-C9
33	C	518	DGD	O1B-C1B-C2B-C3B
25	C	503	CLA	CBA-CGA-O2A-C1
25	a	708	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	c	512	CLA	C14-C13-C15-C16
29	a	714	SQD	O49-C7-C8-C9
34	e	102	HEM	CAD-CBD-CGD-O1D
23	A	603	LMG	O10-C28-C29-C30
32	D	408	LHG	O10-C23-C24-C25
32	B	625	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	c	501	CLA	C15-C16-C17-C18
29	a	714	SQD	O5-C5-C6-S
29	b	601	SQD	O5-C5-C6-S
25	b	618	CLA	O1A-CGA-O2A-C1
23	M	101	LMG	O10-C28-C29-C30
25	B	603	CLA	C13-C15-C16-C17
27	d	404	BCR	C7-C8-C9-C10
25	C	511	CLA	CAA-CBA-CGA-O1A
25	b	618	CLA	CAA-CBA-CGA-O1A
25	b	619	CLA	CAA-CBA-CGA-O1A
29	A	612	SQD	O49-C7-C8-C9
32	L	101	LHG	O9-C7-C8-C9
32	e	101	LHG	O10-C23-C24-C25
25	B	609	CLA	C13-C15-C16-C17
29	f	102	SQD	C45-C44-O6-C1
33	C	517	DGD	C5D-C6D-O5D-C1E
33	c	516	DGD	C5D-C6D-O5D-C1E
29	f	102	SQD	O6-C44-C45-O47
23	A	603	LMG	O9-C10-C11-C12
33	c	518	DGD	O1G-C1A-C2A-C3A
33	H	103	DGD	C6A-C7A-C8A-C9A
25	b	615	CLA	C16-C17-C18-C20
29	B	623	SQD	O6-C44-C45-C46
32	B	625	LHG	C33-C34-C35-C36
32	E	101	LHG	C29-C30-C31-C32
28	a	713	PL9	C21-C22-C23-C24
23	A	603	LMG	C33-C34-C35-C36
25	B	607	CLA	C15-C16-C17-C18
25	D	402	CLA	C13-C15-C16-C17
25	B	603	CLA	CAA-CBA-CGA-O2A
25	b	607	CLA	CAA-CBA-CGA-O2A
23	a	701	LMG	C22-C23-C24-C25
25	B	609	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
33	C	518	DGD	C5A-C6A-C7A-C8A
27	h	101	BCR	C6-C7-C8-C9
29	D	410	SQD	O5-C1-O6-C44
25	a	707	CLA	C2-C1-O2A-CGA
32	B	625	LHG	O10-C23-C24-C25
29	A	612	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	611	CLA	C2C-C3C-CAC-CBC
25	c	510	CLA	C2A-CAA-CBA-CGA
25	c	510	CLA	CAA-CBA-CGA-O1A
25	C	502	CLA	C13-C15-C16-C17
33	c	517	DGD	C1A-C2A-C3A-C4A
25	B	611	CLA	C11-C10-C8-C7
32	d	406	LHG	C29-C30-C31-C32
25	C	502	CLA	CAA-CBA-CGA-O2A
23	b	627	LMG	C11-C10-O7-C8
25	A	607	CLA	C16-C17-C18-C19
25	D	403	CLA	CAA-CBA-CGA-O1A
25	d	402	CLA	C2C-C3C-CAC-CBC

There are no ring outliers.

129 monomers are involved in 262 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	614	CLA	2	0
25	C	504	CLA	2	0
25	d	403	CLA	2	0
25	C	512	CLA	2	0
26	D	401	PHO	2	0
29	D	410	SQD	4	0
25	c	513	CLA	3	0
27	b	602	BCR	4	0
25	B	613	CLA	2	0
33	C	517	DGD	2	0
23	b	627	LMG	3	0
31	a	706	BCT	1	0
27	k	101	BCR	3	0
28	a	713	PL9	4	0
34	e	102	HEM	3	0
25	c	504	CLA	1	0
29	A	612	SQD	2	0
32	E	101	LHG	3	0
25	D	404	CLA	1	0
25	B	603	CLA	1	0
27	a	712	BCR	2	0
25	B	602	CLA	2	0
25	b	621	CLA	1	0
25	c	506	CLA	3	0
25	c	508	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	619	CLA	1	0
25	b	615	CLA	3	0
27	B	620	BCR	1	0
25	c	511	CLA	4	0
25	b	609	CLA	2	0
27	B	618	BCR	2	0
25	a	708	CLA	1	0
25	B	608	CLA	1	0
32	b	629	LHG	1	0
25	a	711	CLA	6	0
25	B	610	CLA	4	0
27	H	102	BCR	3	0
23	a	701	LMG	1	0
25	b	611	CLA	1	0
27	C	515	BCR	2	0
28	D	406	PL9	2	0
23	B	621	LMG	1	0
23	A	603	LMG	3	0
26	A	608	PHO	1	0
32	L	101	LHG	4	0
23	C	520	LMG	1	0
27	k	102	BCR	3	0
25	B	611	CLA	1	0
25	B	612	CLA	3	0
27	C	516	BCR	3	0
25	B	609	CLA	1	0
27	b	623	BCR	1	0
25	B	614	CLA	1	0
29	f	102	SQD	1	0
25	a	707	CLA	4	0
23	f	101	LMG	2	0
25	C	509	CLA	6	0
25	A	607	CLA	2	0
23	D	409	LMG	3	0
27	t	103	BCR	6	0
28	A	611	PL9	5	0
27	c	515	BCR	1	0
25	b	616	CLA	1	0
25	b	618	CLA	1	0
25	c	505	CLA	3	0
26	a	710	PHO	6	0
27	D	405	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	604	CLA	3	0
27	b	625	BCR	4	0
29	A	614	SQD	1	0
33	c	518	DGD	1	0
33	h	102	DGD	3	0
23	a	715	LMG	2	0
25	C	514	CLA	1	0
25	B	607	CLA	3	0
25	c	503	CLA	2	0
23	c	520	LMG	1	0
23	M	101	LMG	3	0
32	d	406	LHG	2	0
25	c	501	CLA	2	0
27	B	619	BCR	2	0
25	b	608	CLA	2	0
25	c	509	CLA	3	0
29	I	102	SQD	3	0
33	C	518	DGD	2	0
25	C	505	CLA	5	0
27	b	624	BCR	2	0
32	D	407	LHG	1	0
34	E	102	HEM	3	0
25	C	502	CLA	2	0
25	A	609	CLA	1	0
25	C	507	CLA	3	0
25	c	510	CLA	1	0
27	A	610	BCR	4	0
27	h	101	BCR	3	0
32	D	408	LHG	6	0
33	C	519	DGD	2	0
33	c	516	DGD	3	0
25	B	606	CLA	1	0
23	d	408	LMG	2	0
25	b	610	CLA	3	0
25	b	620	CLA	2	0
29	B	626	SQD	6	0
25	a	719	CLA	2	0
35	V	201	HEC	1	0
25	B	605	CLA	3	0
29	b	601	SQD	3	0
25	c	507	CLA	1	0
26	a	709	PHO	2	0

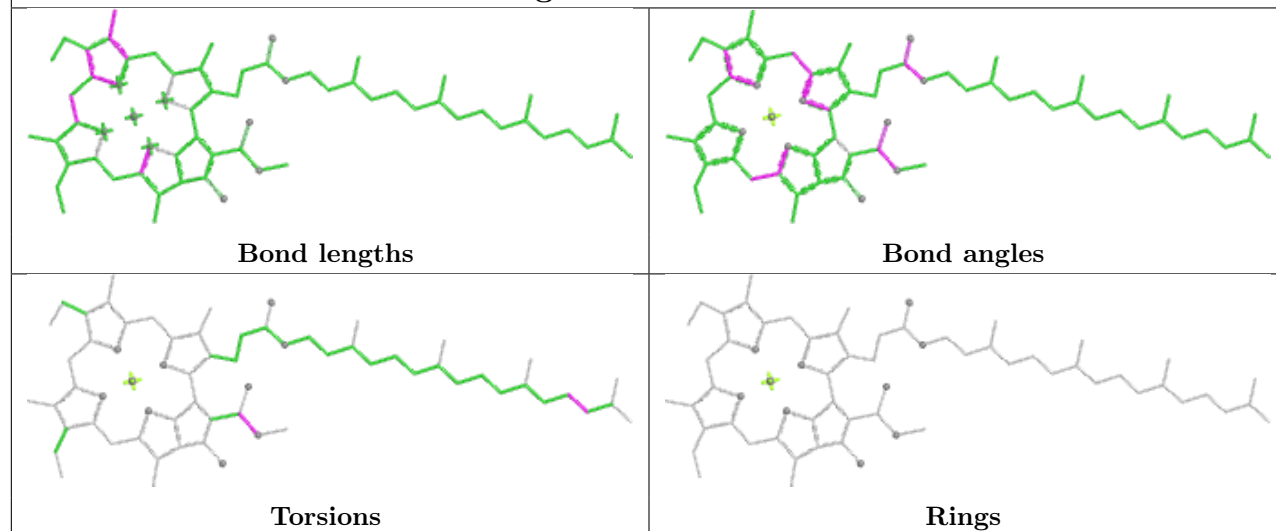
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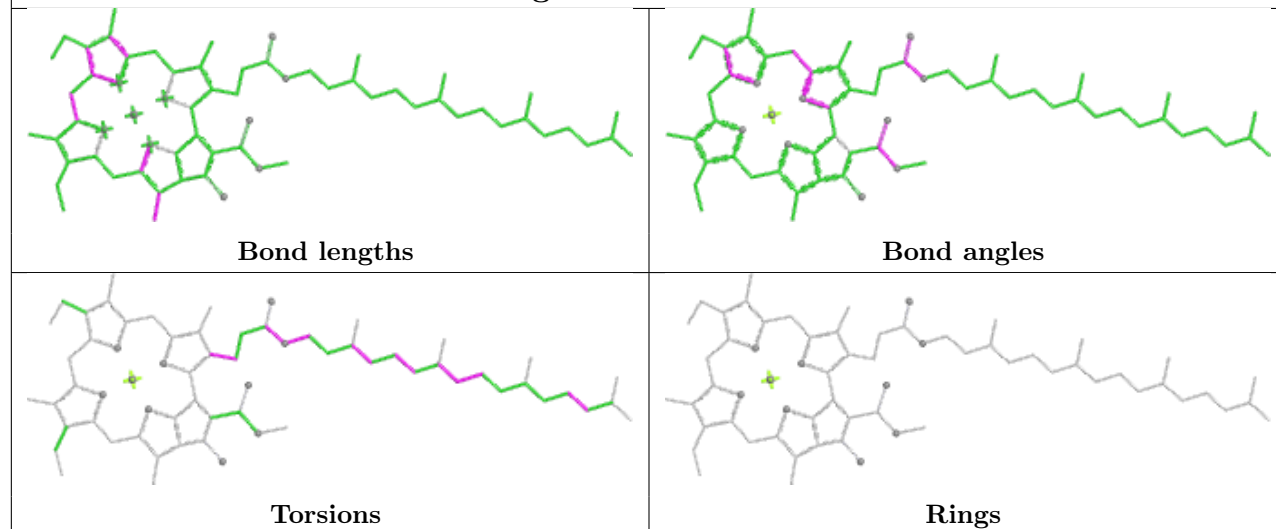
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	617	CLA	1	0
25	C	511	CLA	1	0
25	A	606	CLA	1	0
25	b	612	CLA	6	0
32	d	407	LHG	4	0
23	c	519	LMG	1	0
25	C	506	CLA	2	0
25	c	512	CLA	2	0
32	B	625	LHG	2	0
32	a	720	LHG	1	0
25	B	617	CLA	5	0
29	B	623	SQD	1	0
25	D	402	CLA	3	0
25	B	615	CLA	2	0
25	D	403	CLA	2	0
32	e	101	LHG	2	0
25	d	402	CLA	6	0
25	b	607	CLA	6	0
25	B	616	CLA	3	0
29	a	714	SQD	1	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.

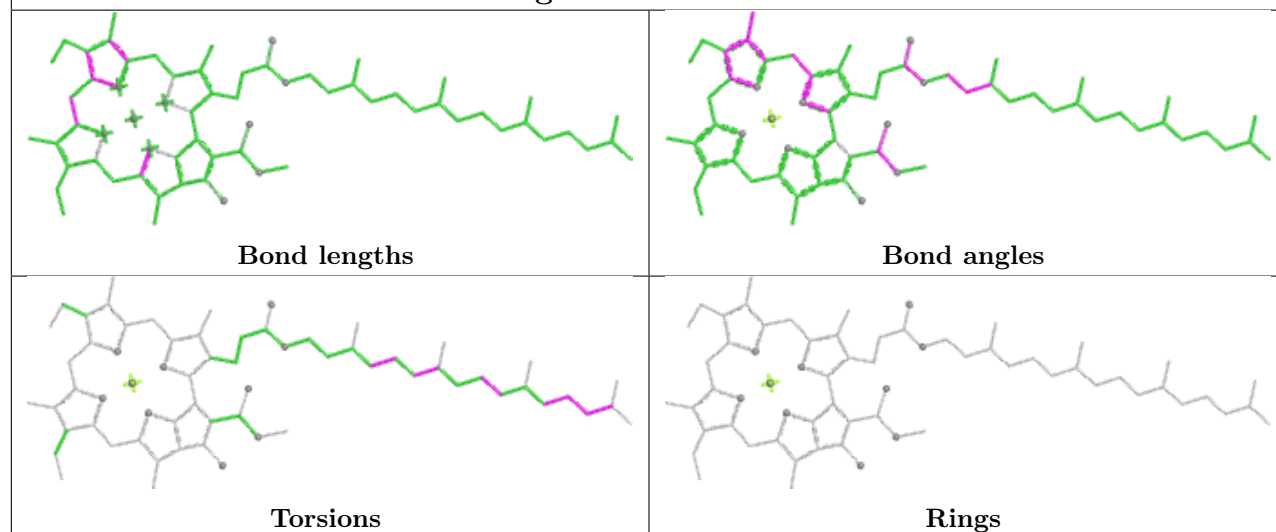
Ligand CLA b 614

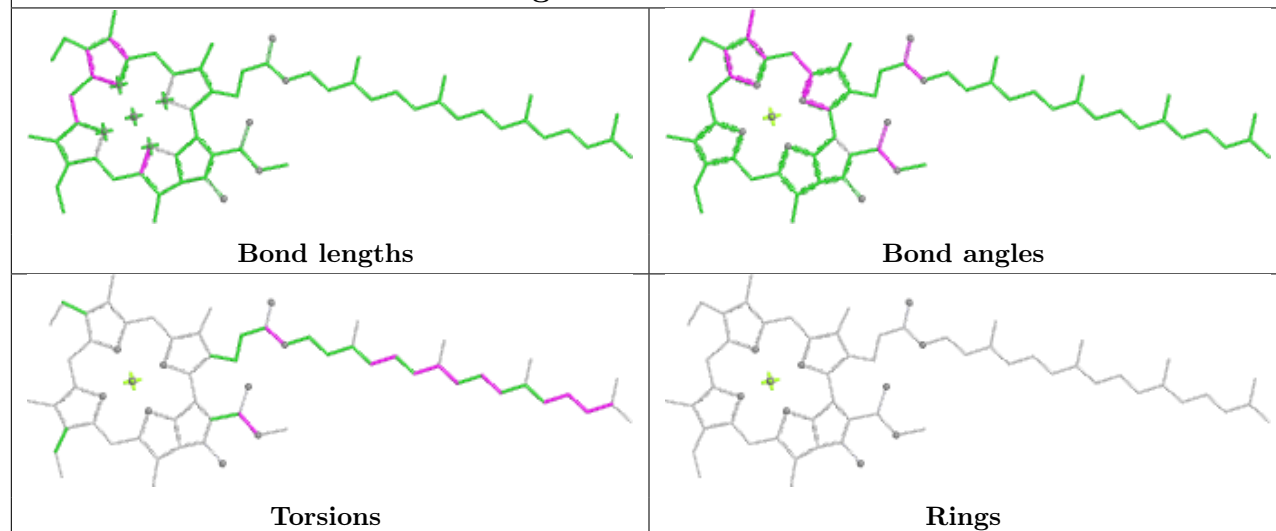
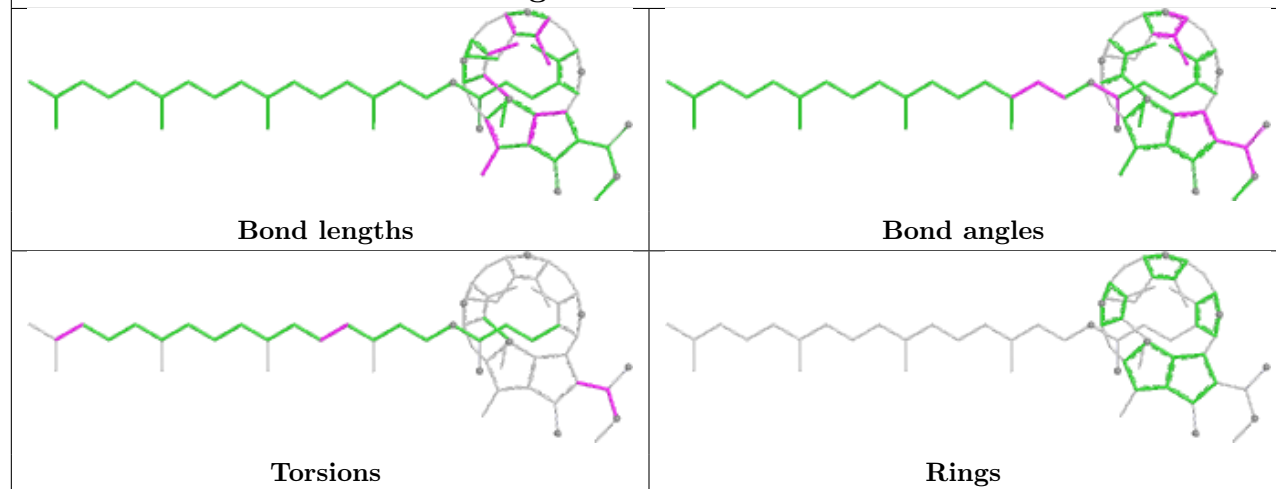


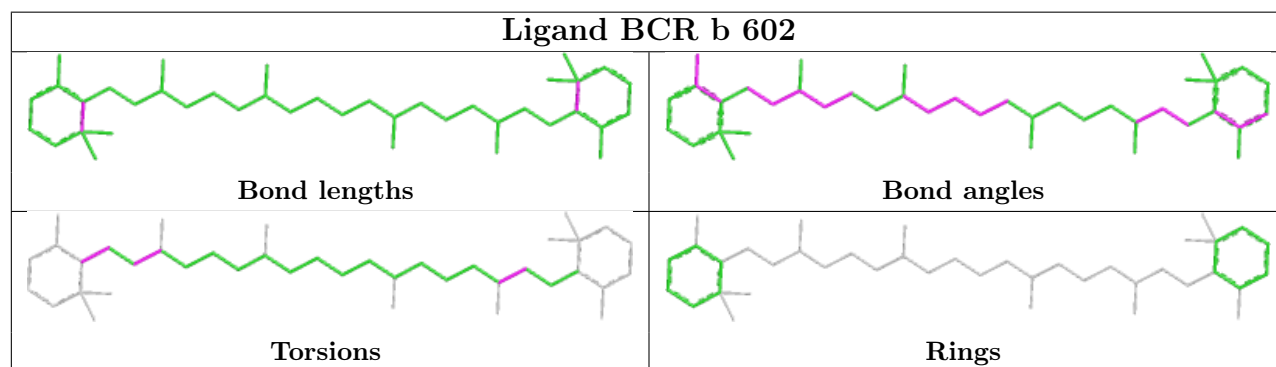
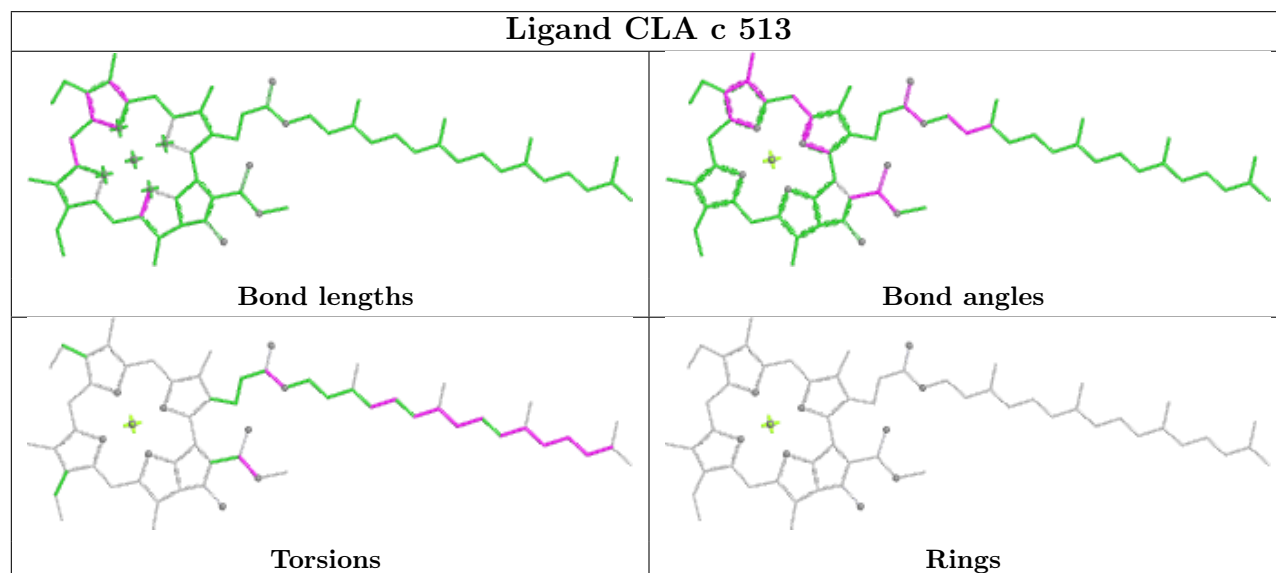
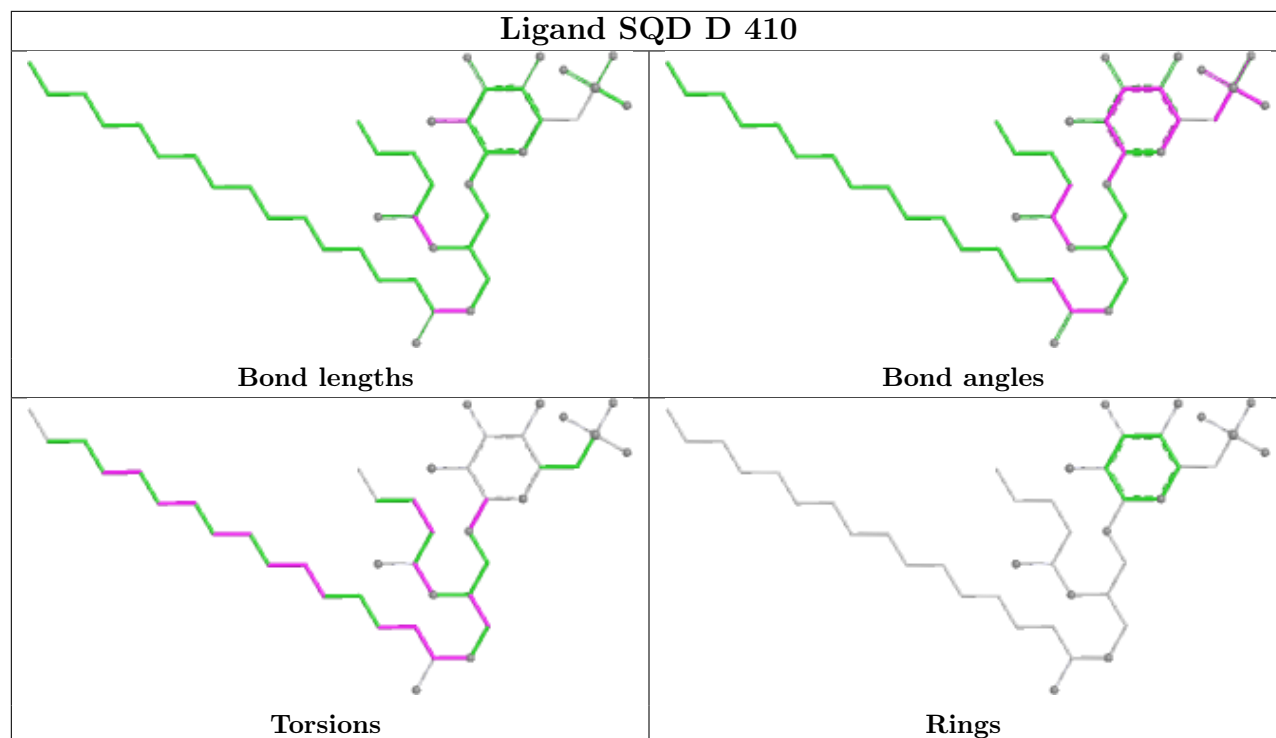
Ligand CLA C 504

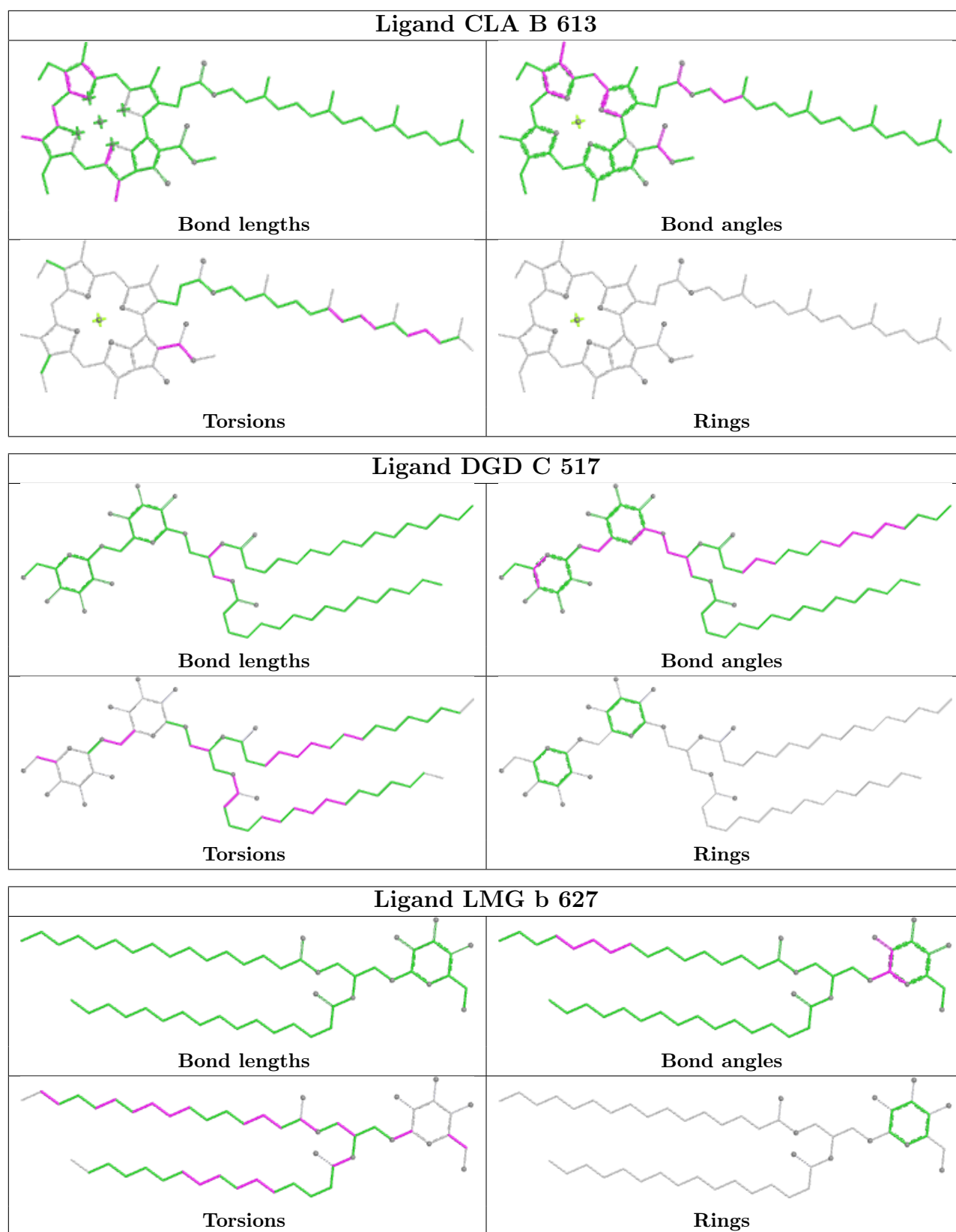


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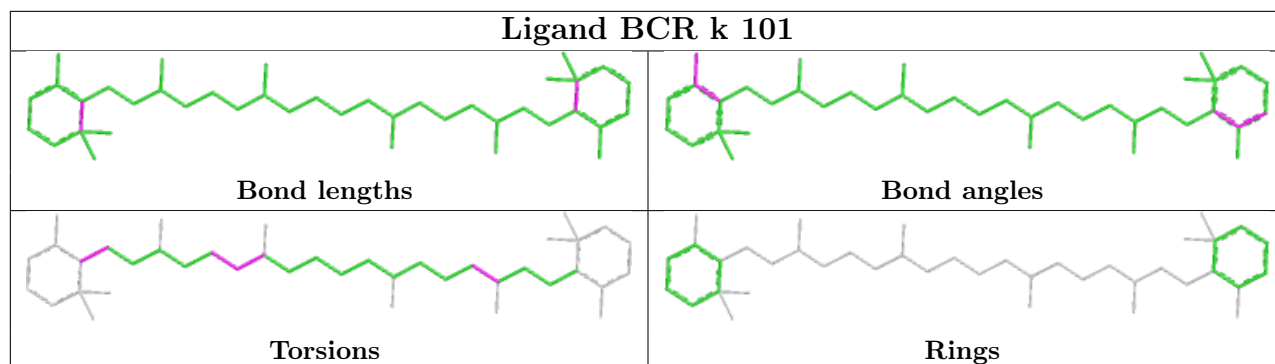


Ligand CLA C 512**Ligand PHO D 401**

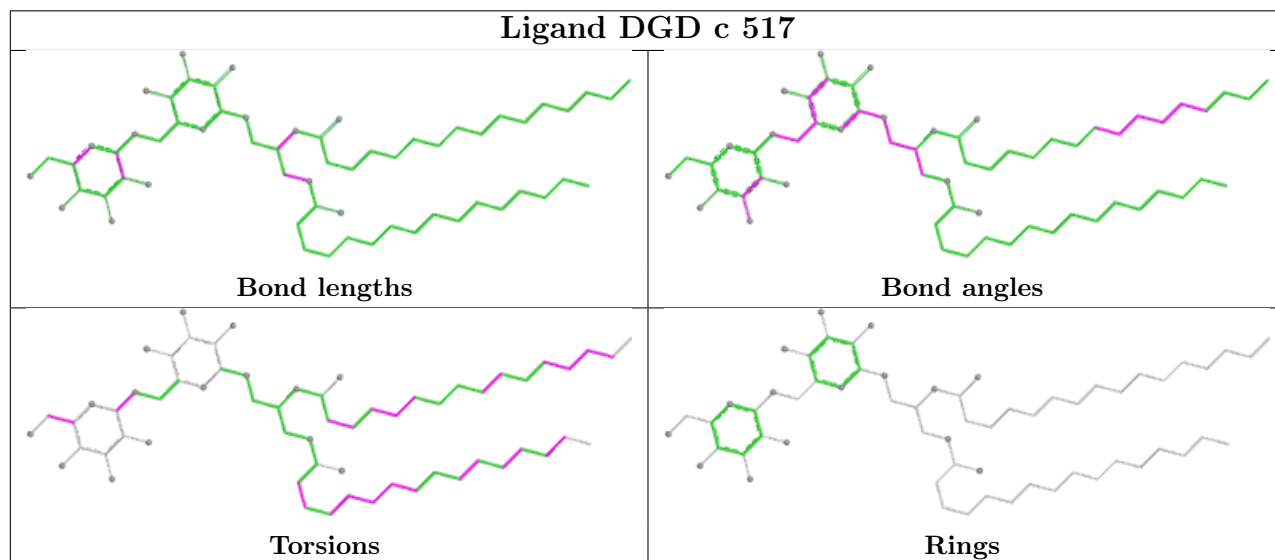




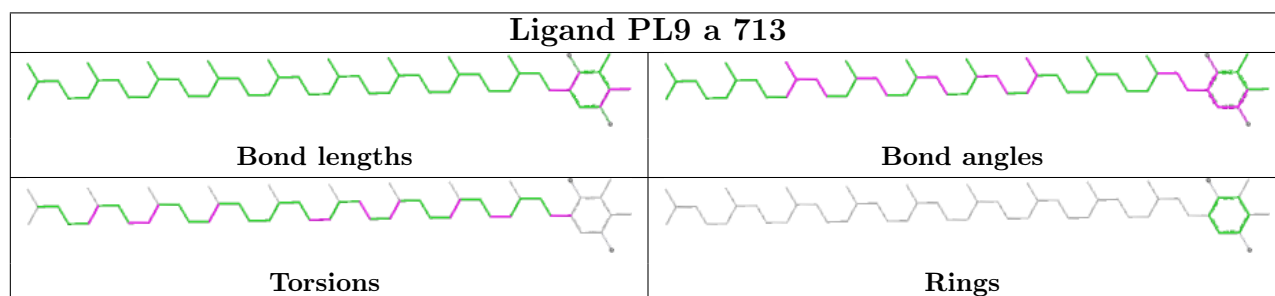
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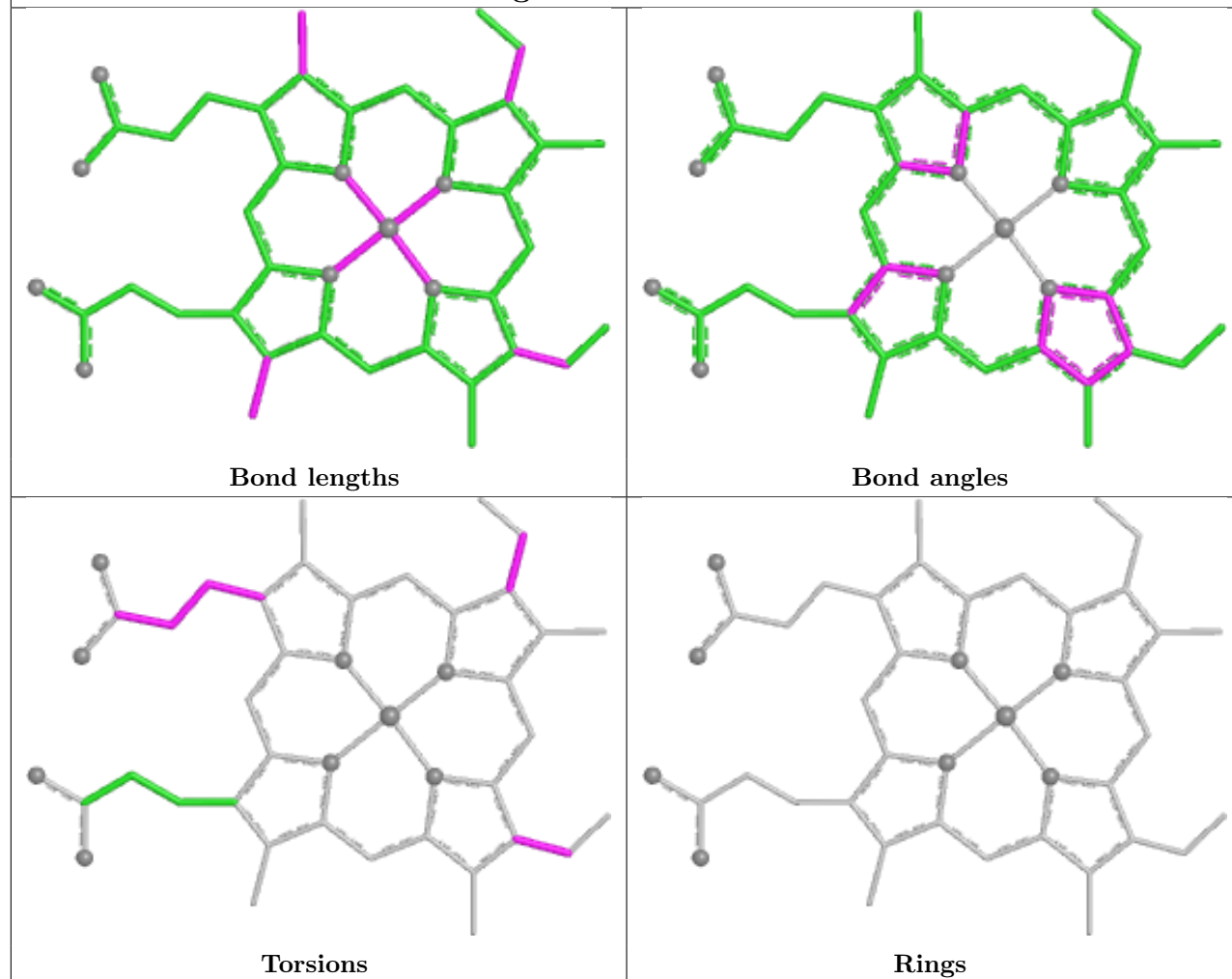
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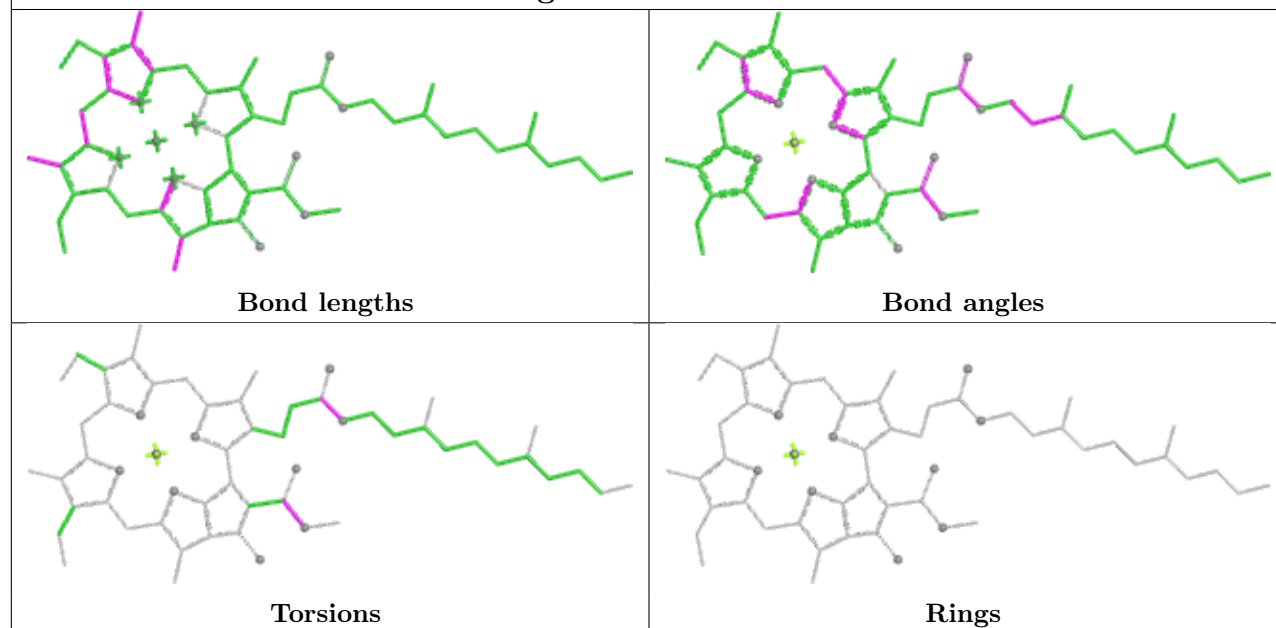
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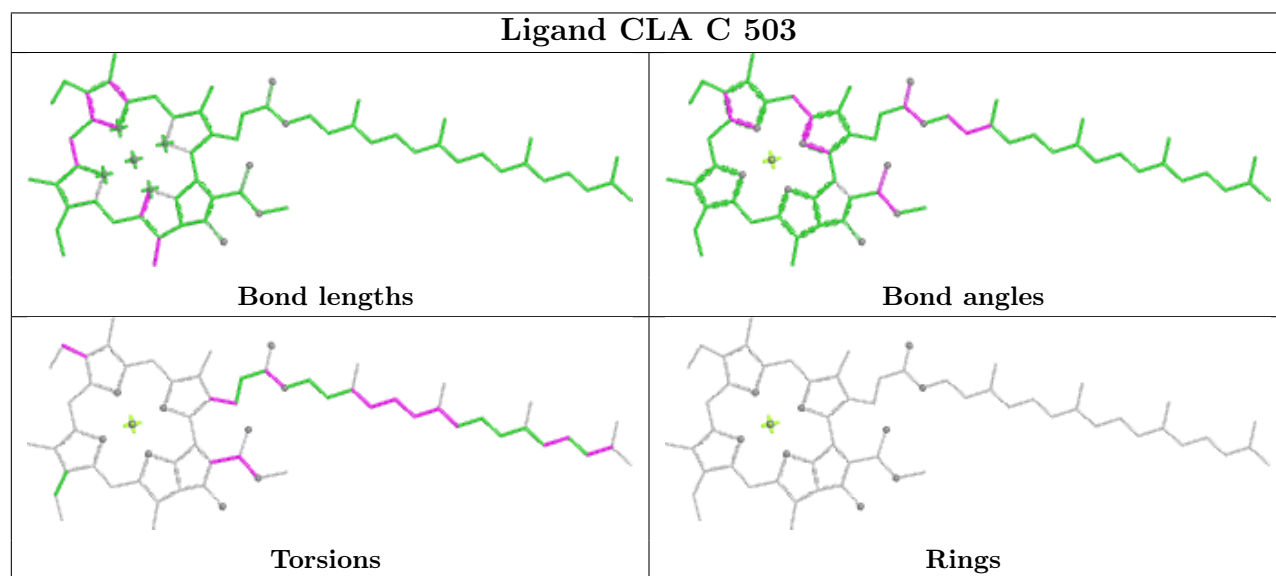
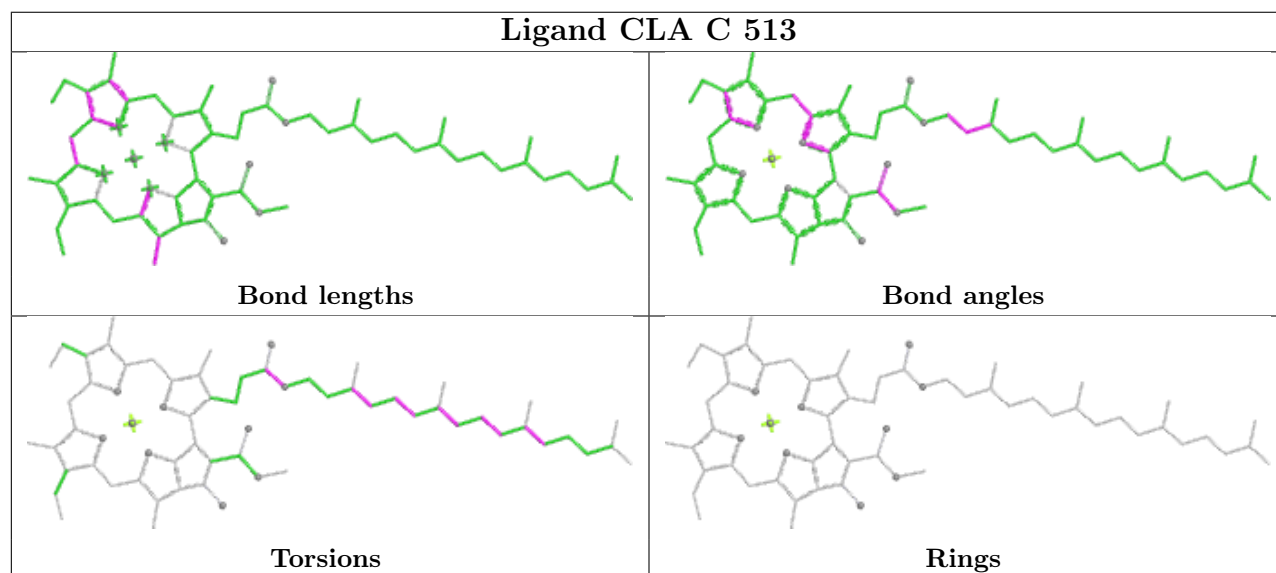
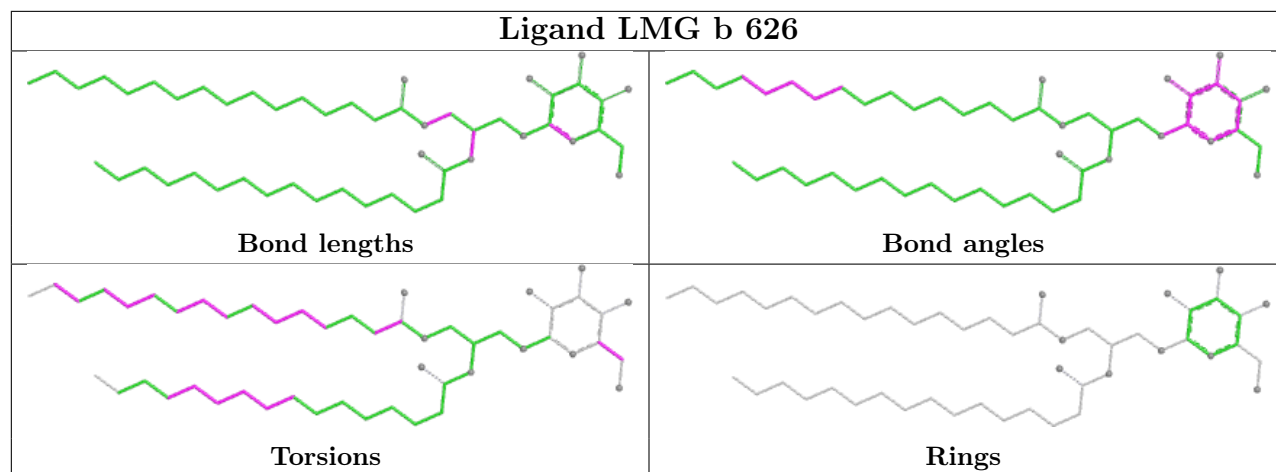


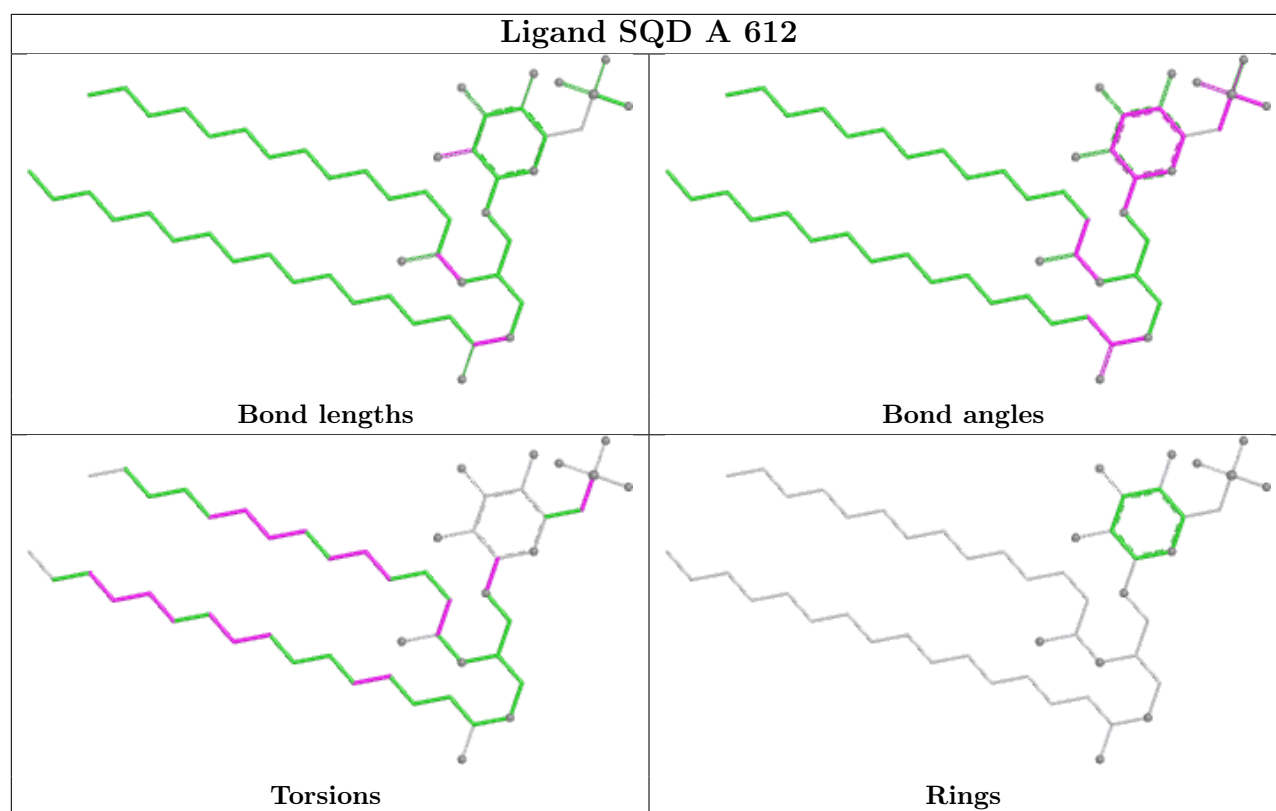
Ligand HEM e 102

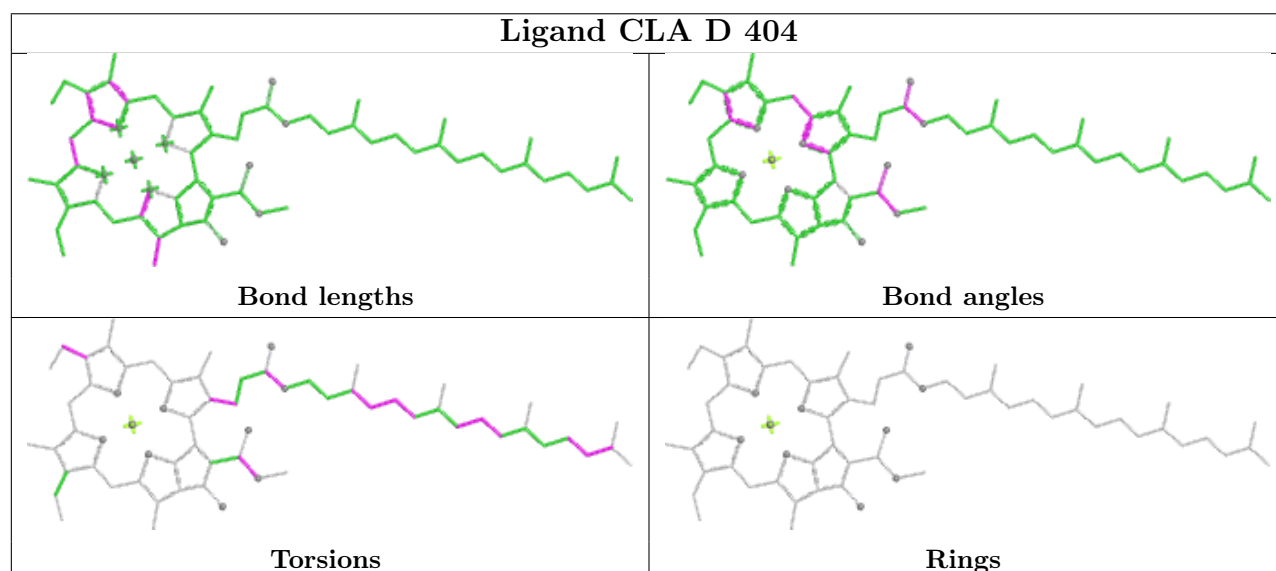
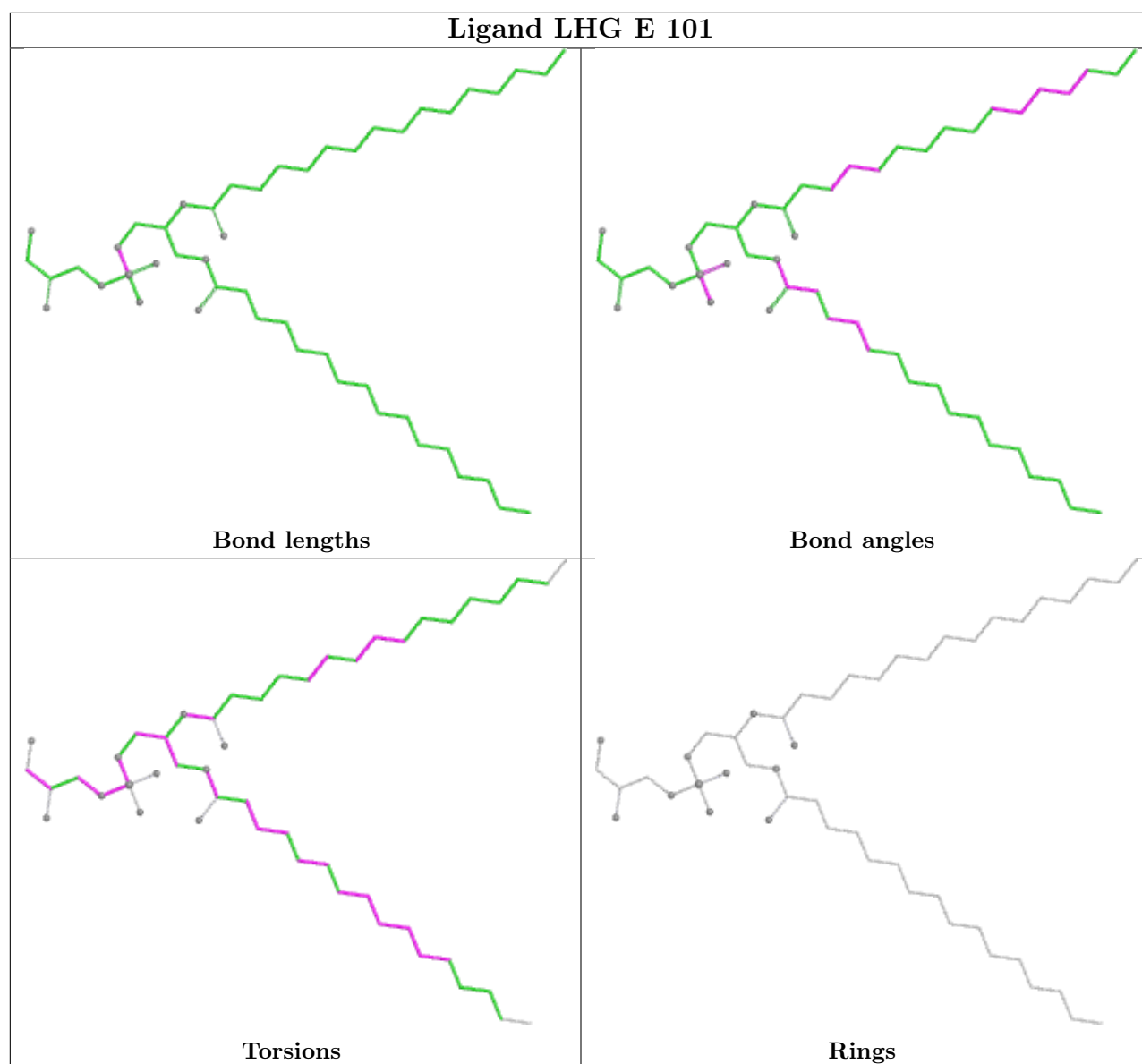


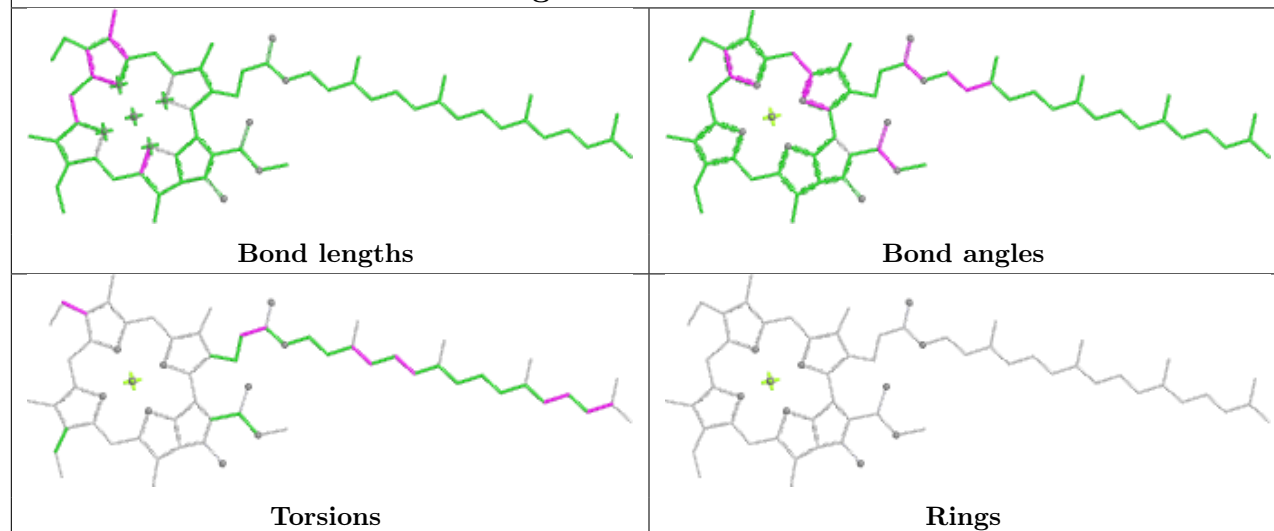
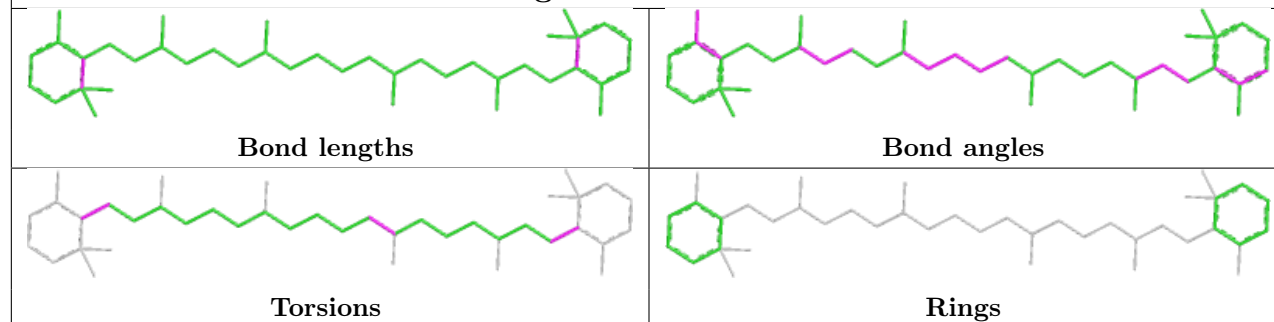
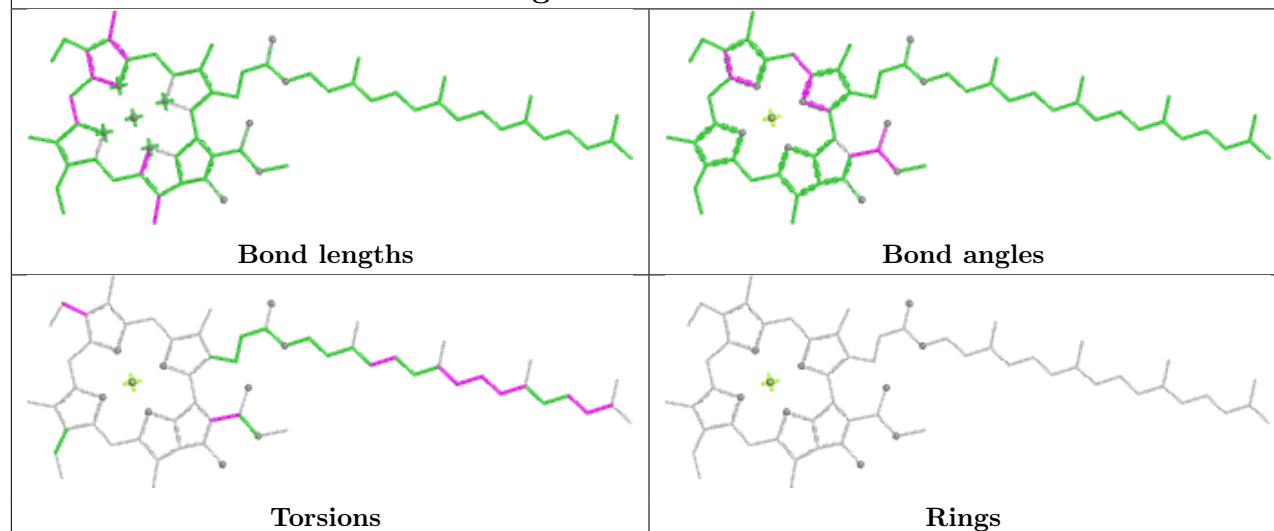
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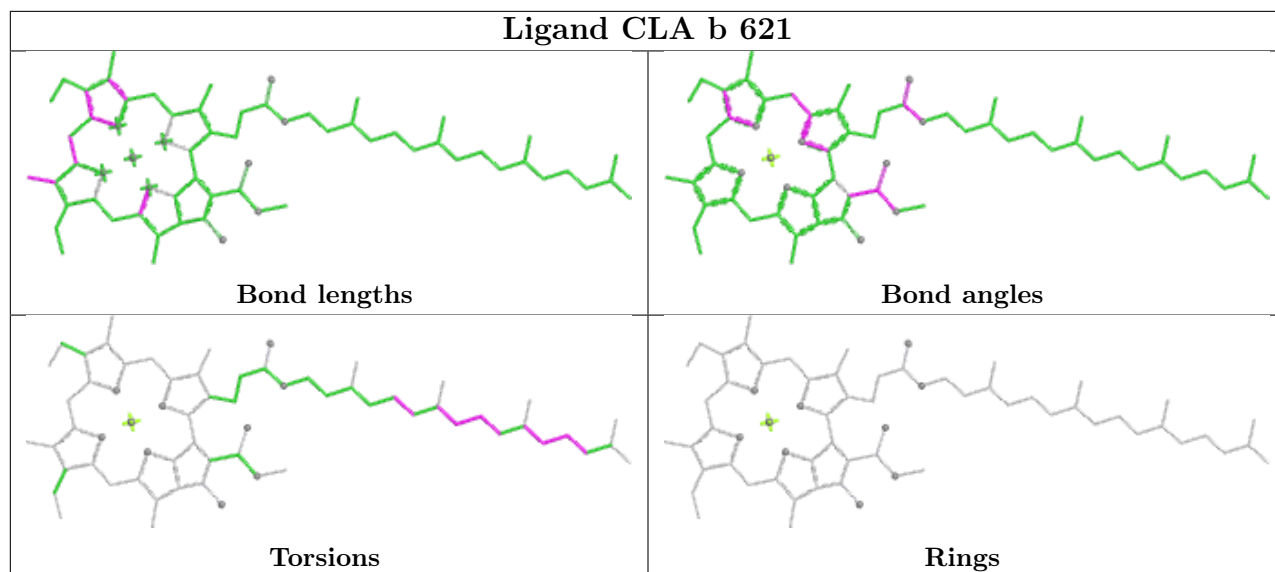




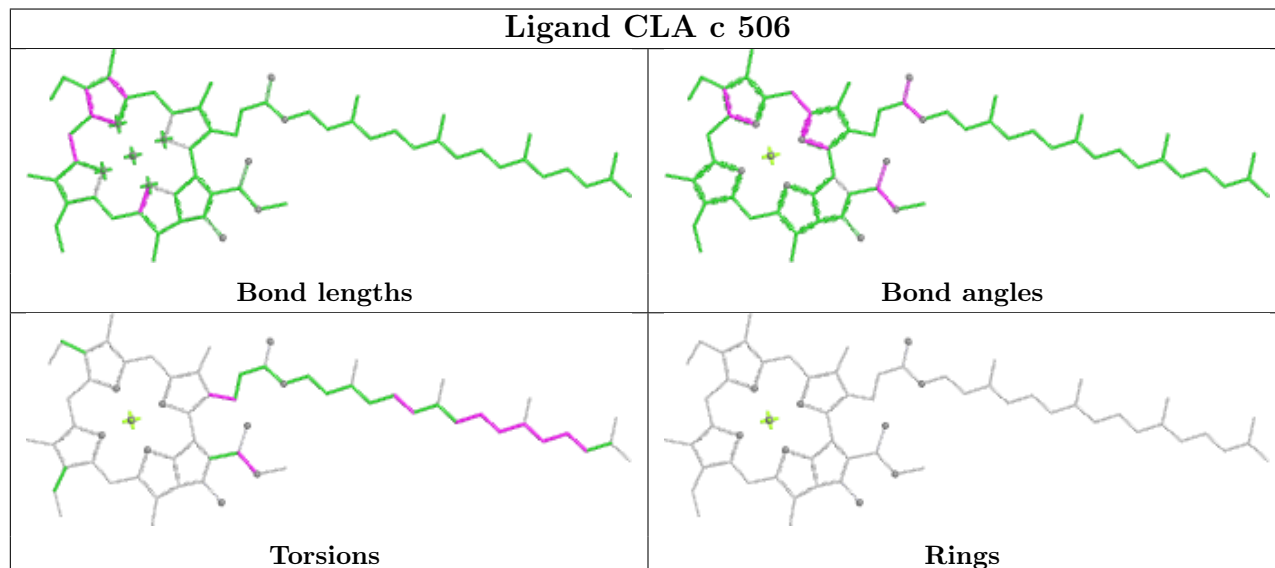


Ligand CLA B 603**Ligand BCR a 712****Ligand CLA B 602**

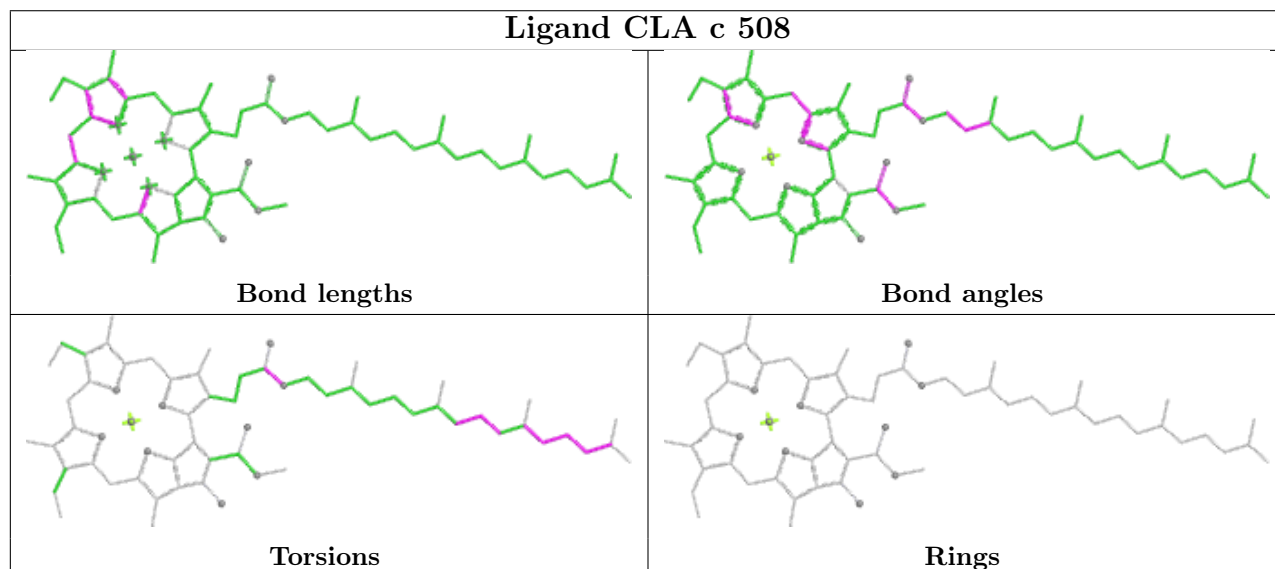
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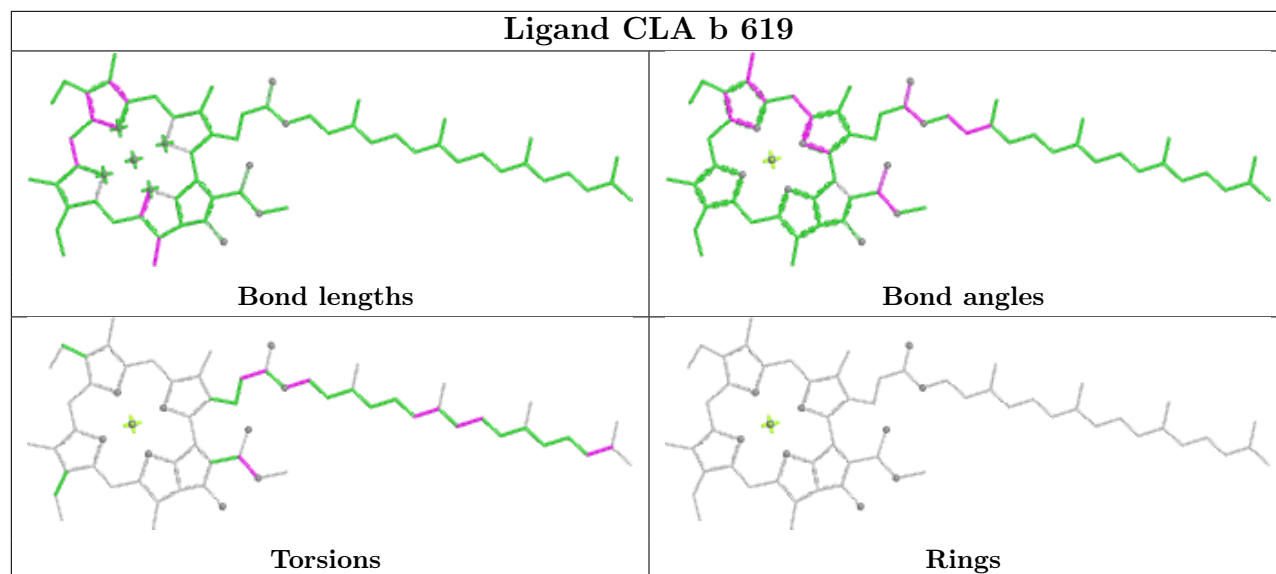
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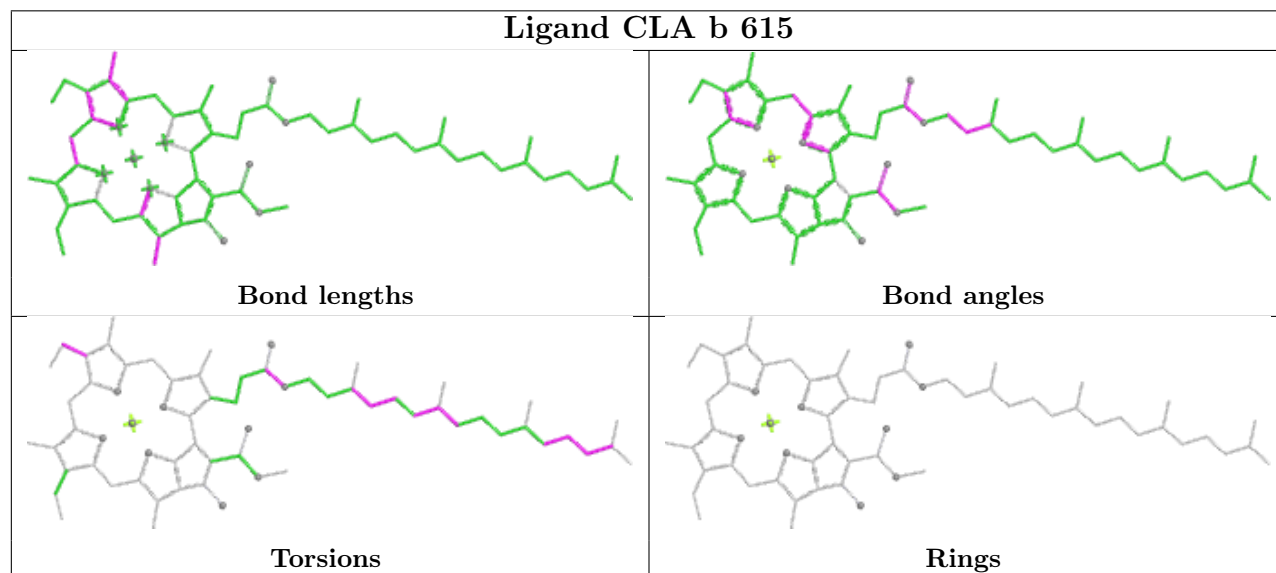
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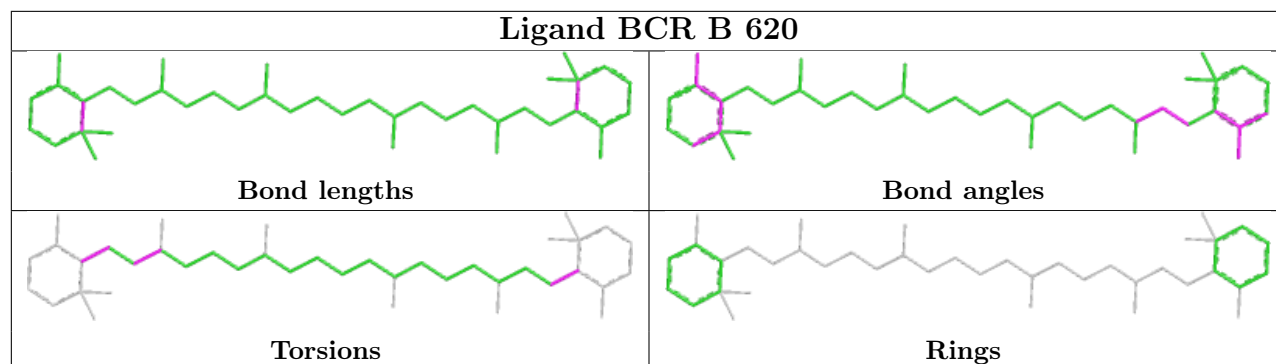
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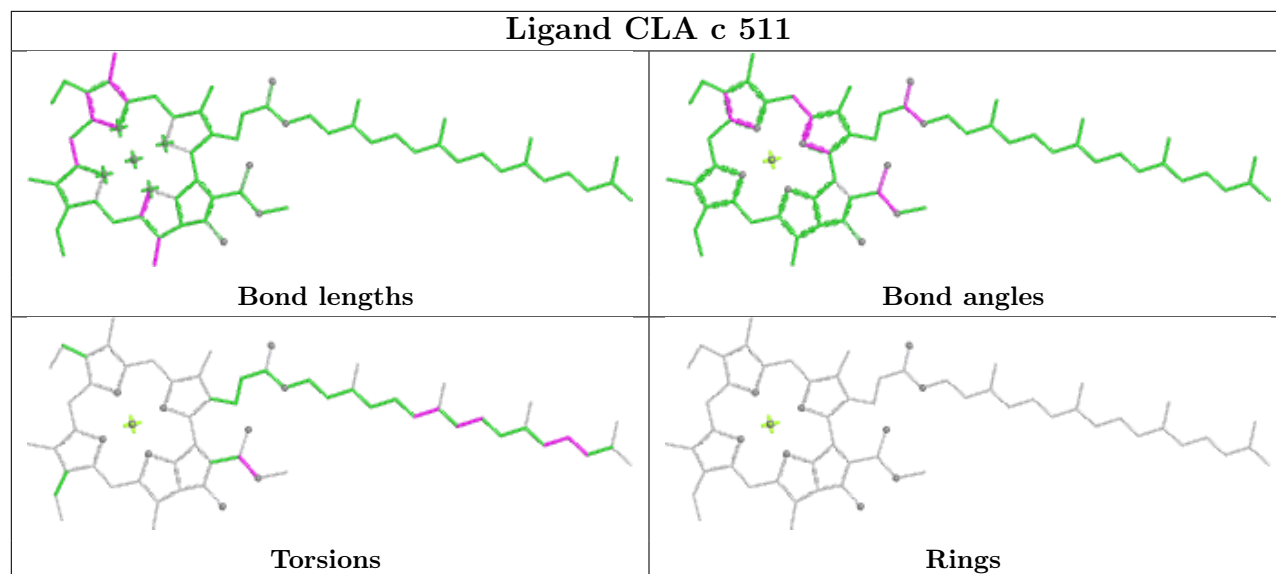
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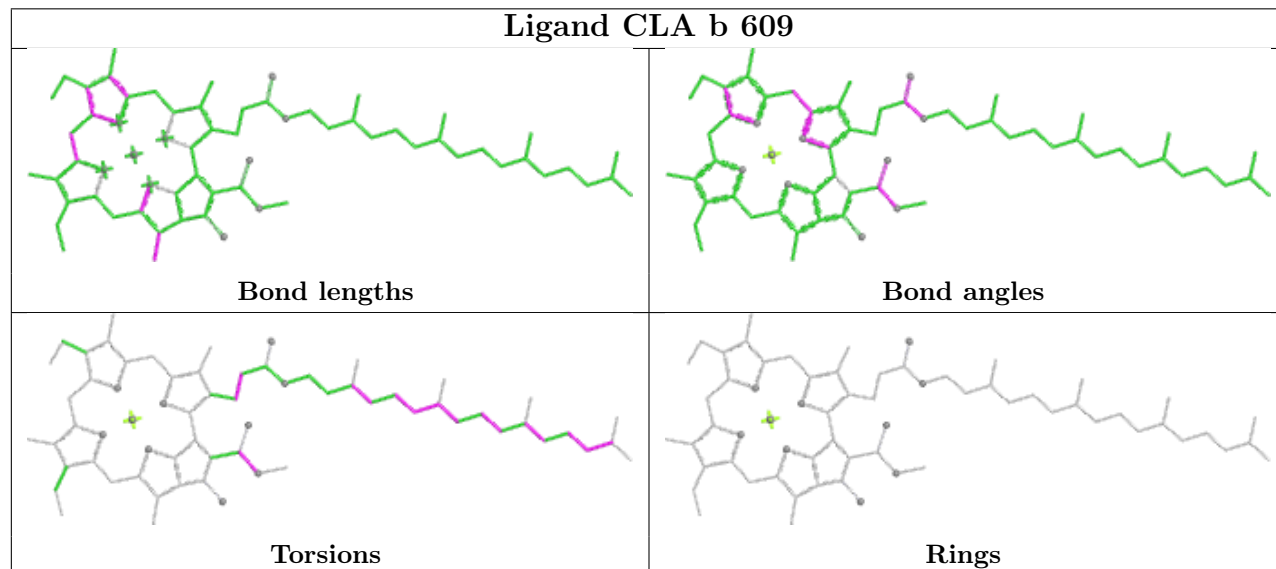
Ligand BCR B 620



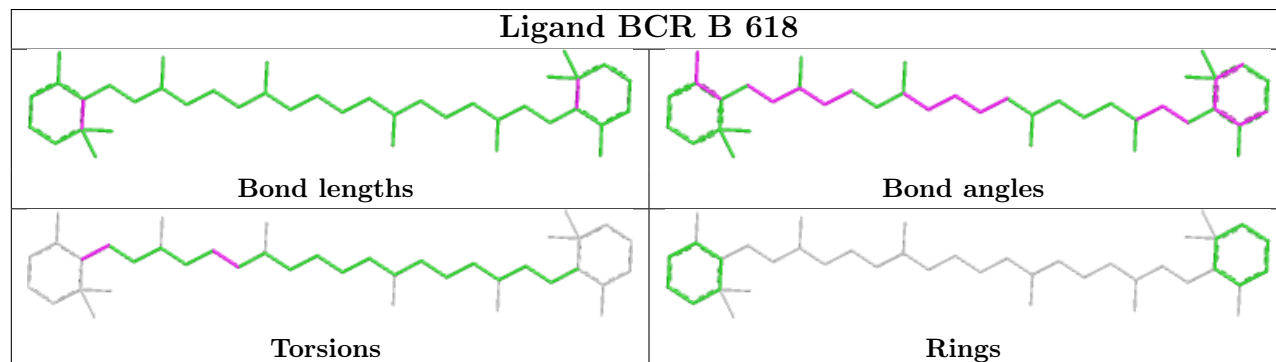
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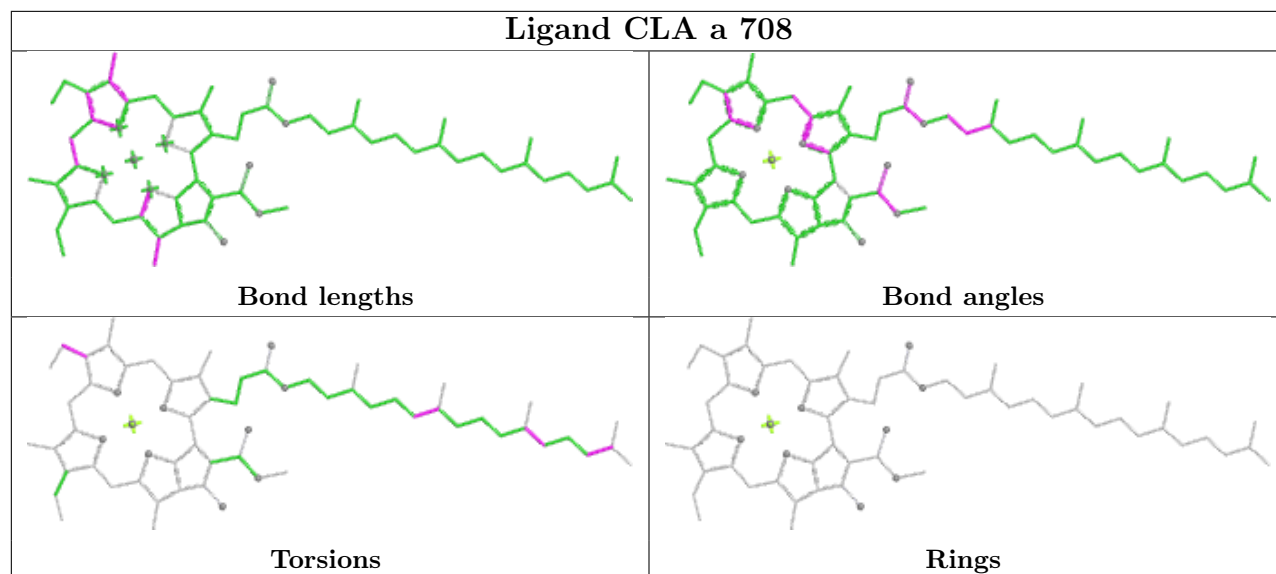
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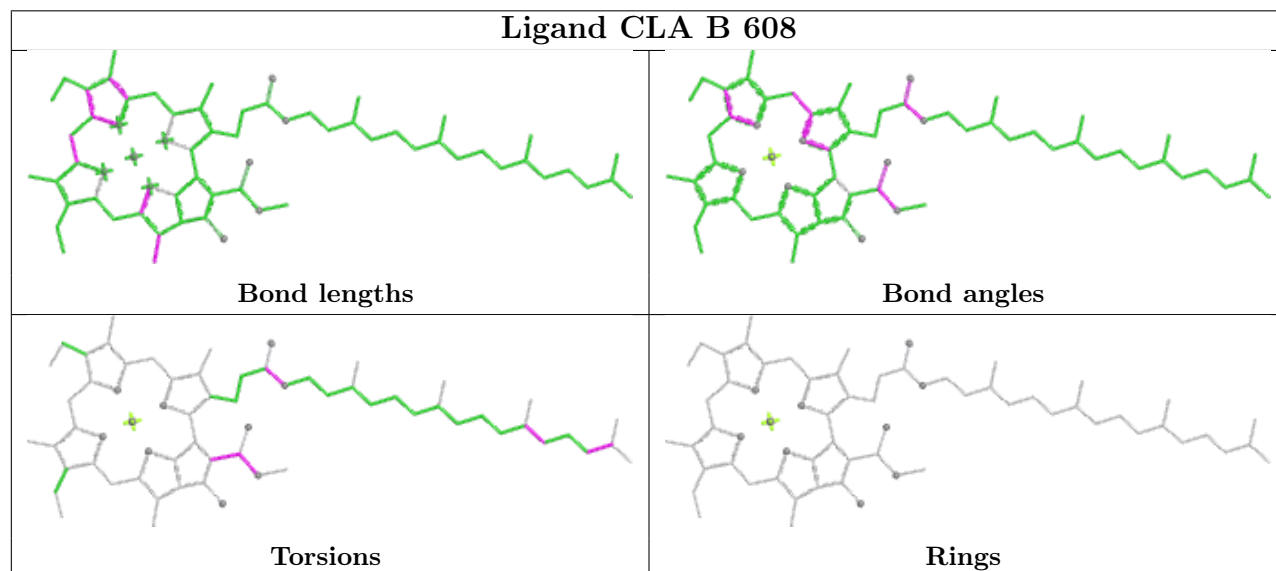
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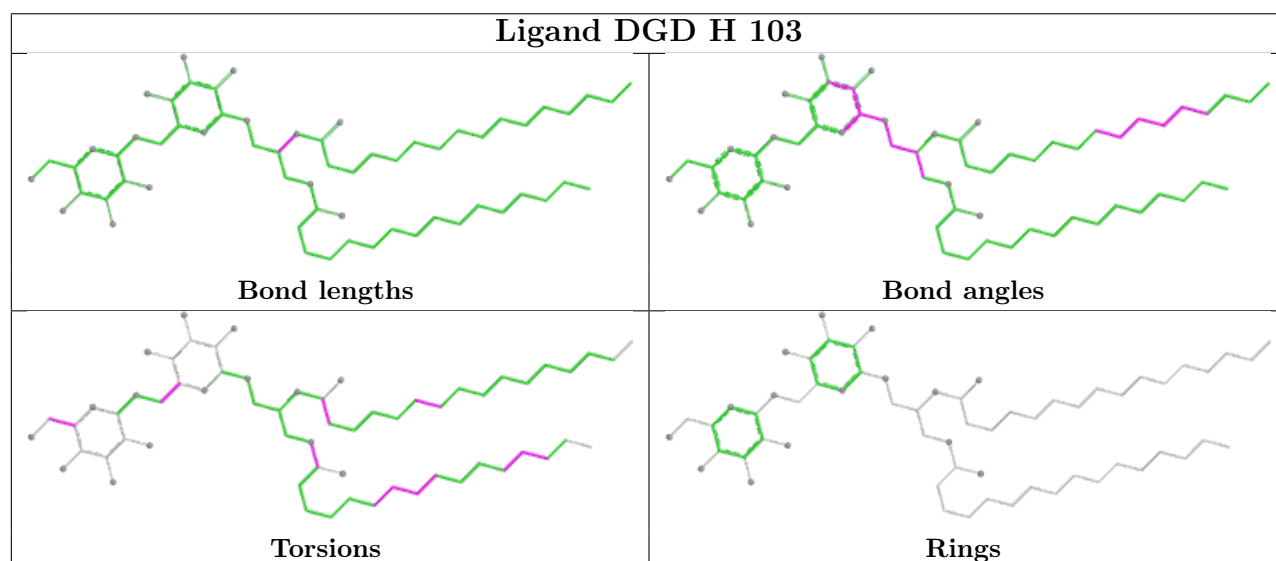
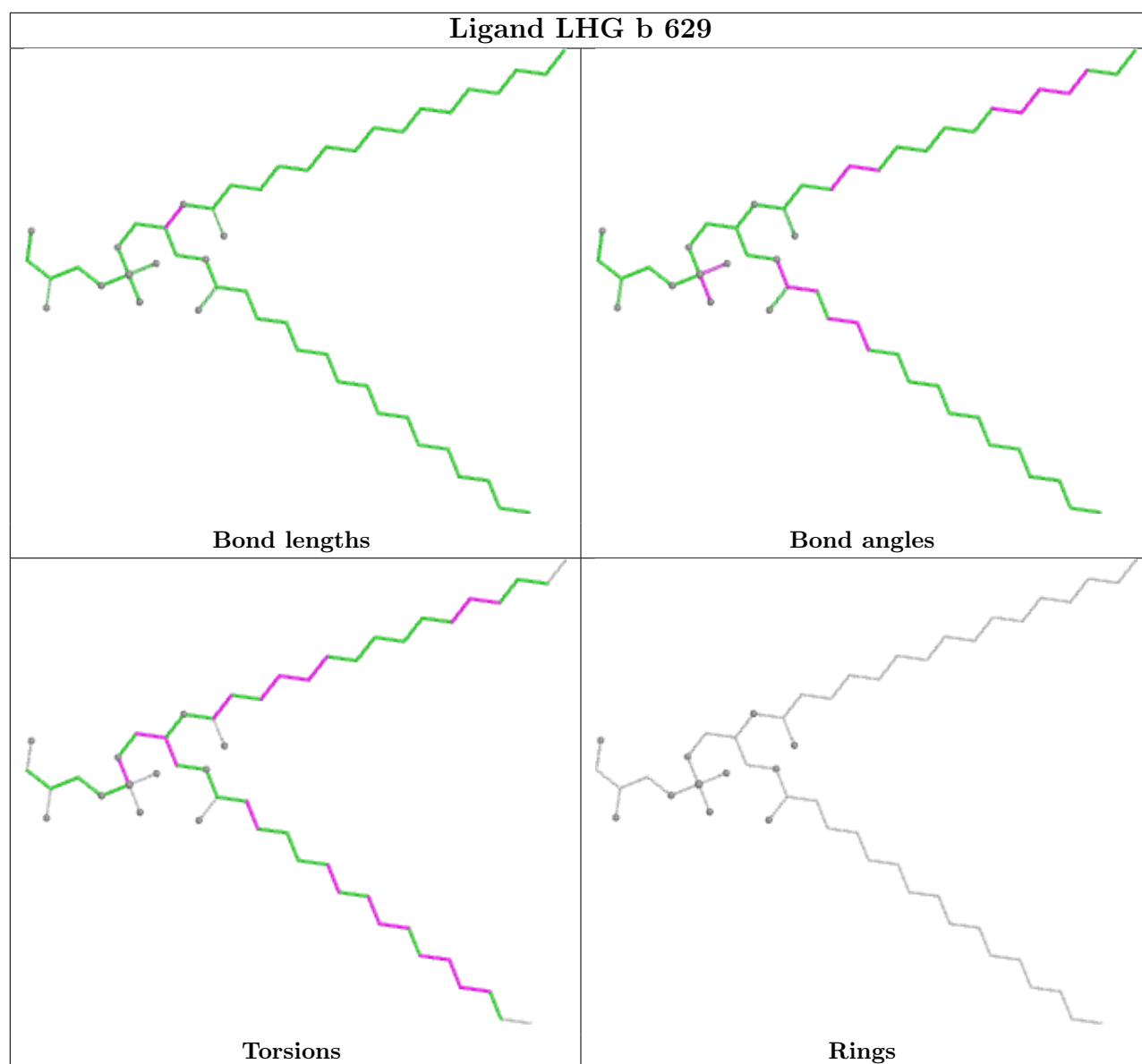


Ligand CLA a 708

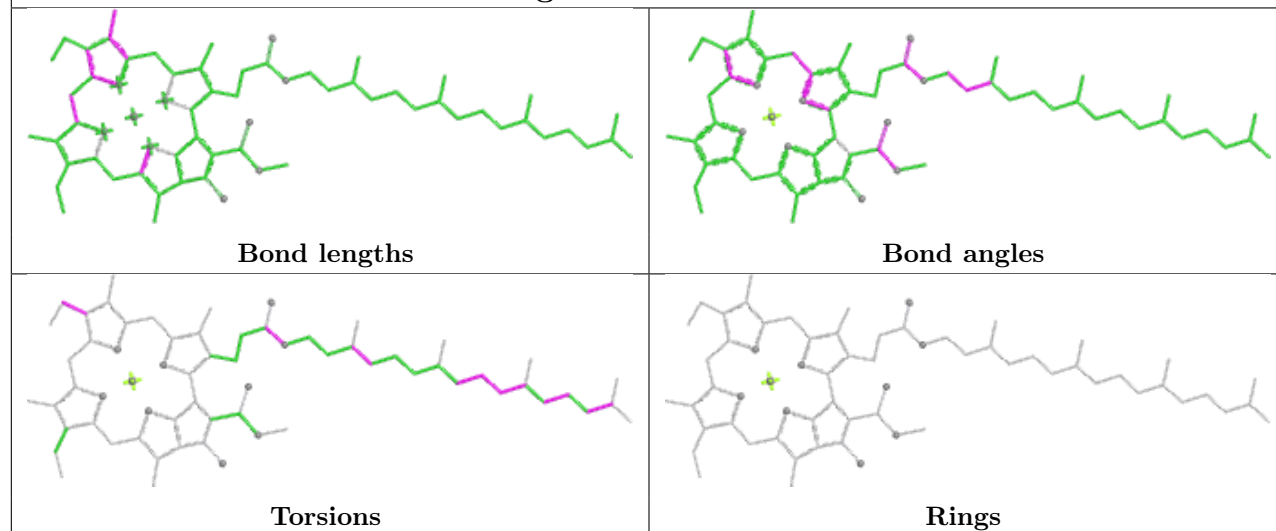


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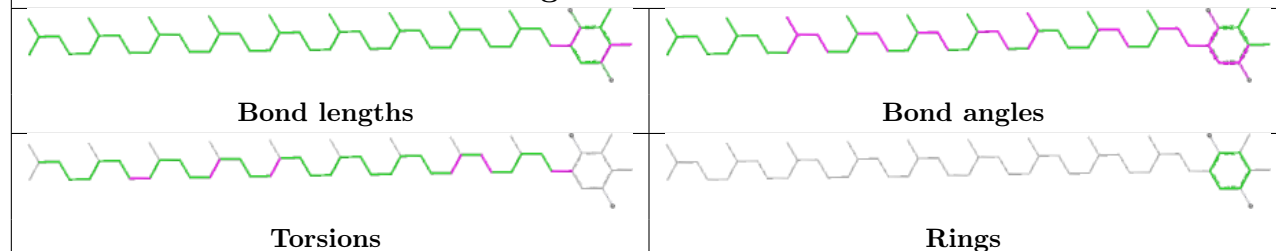




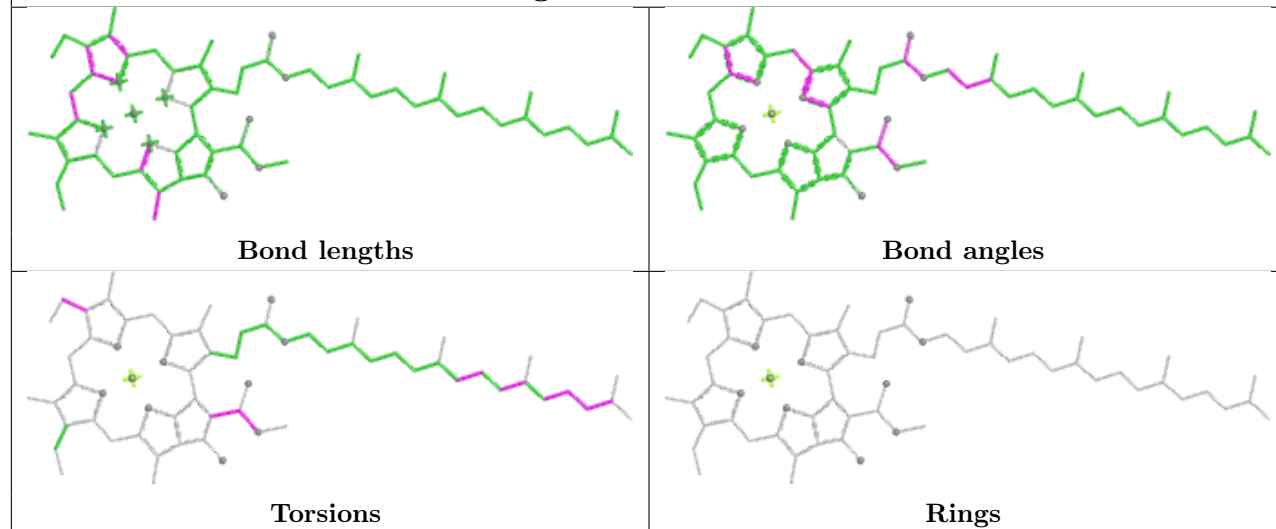
Ligand CLA a 711

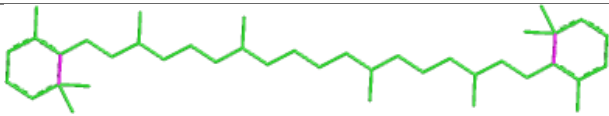
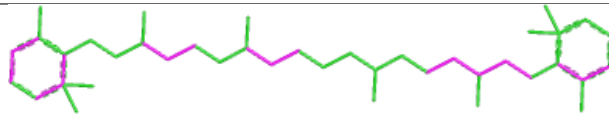
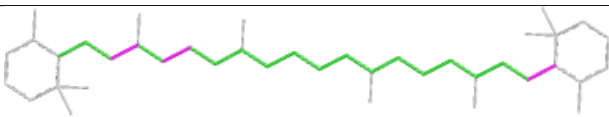
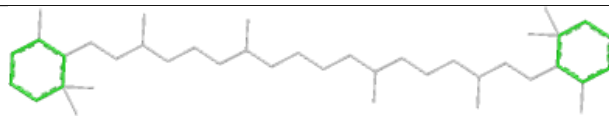


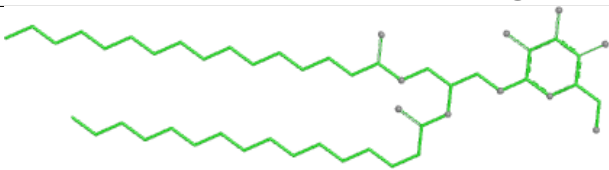
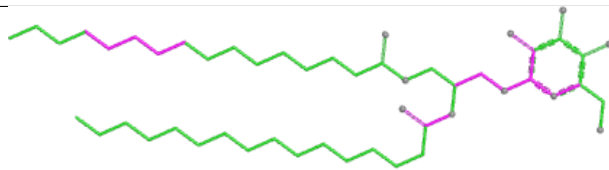
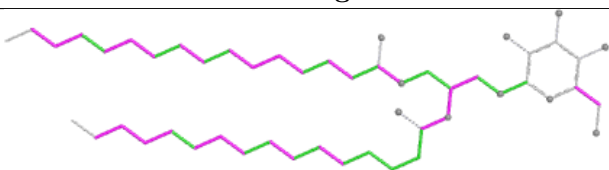
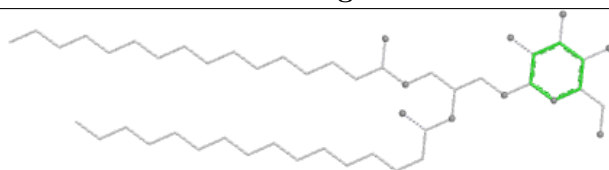
Ligand PL9 d 405

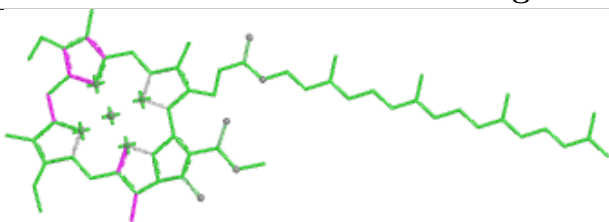
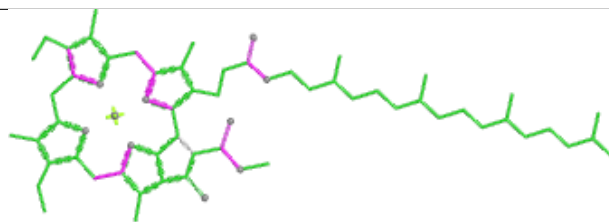
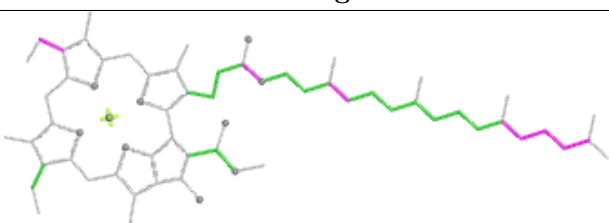
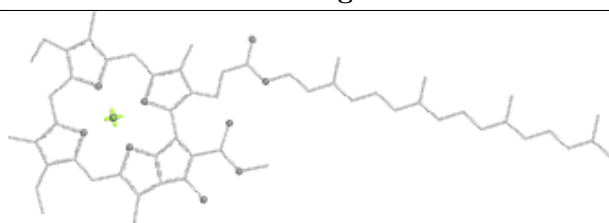


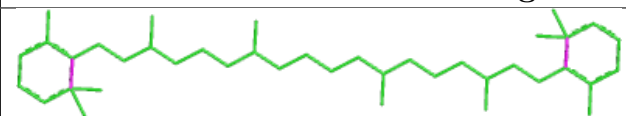
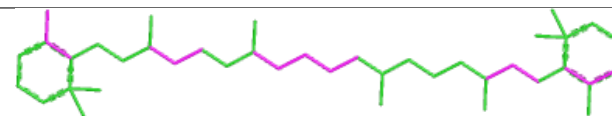
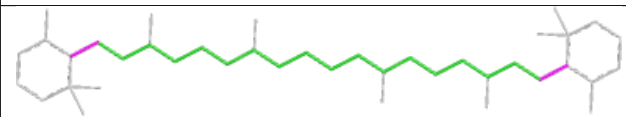
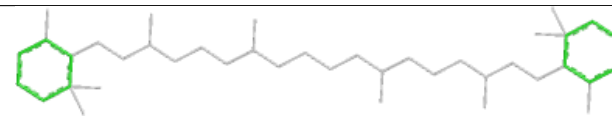
Ligand CLA B 610

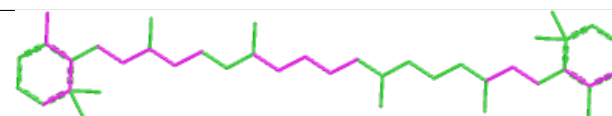
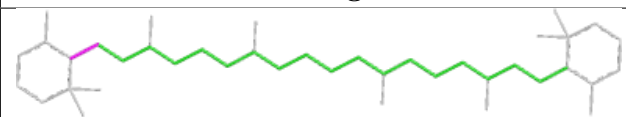
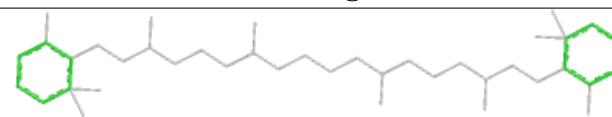


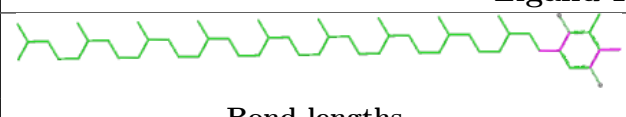
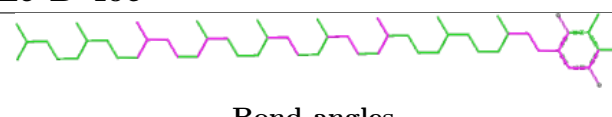
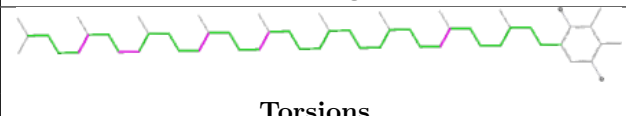
Ligand BCR H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

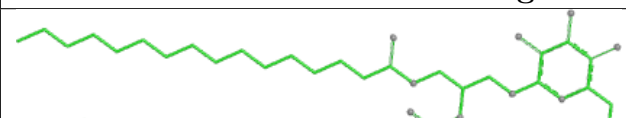
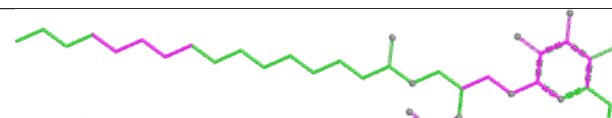
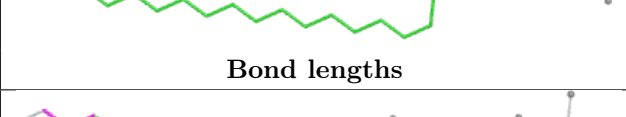
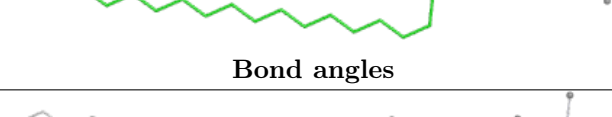
Ligand LMG a 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

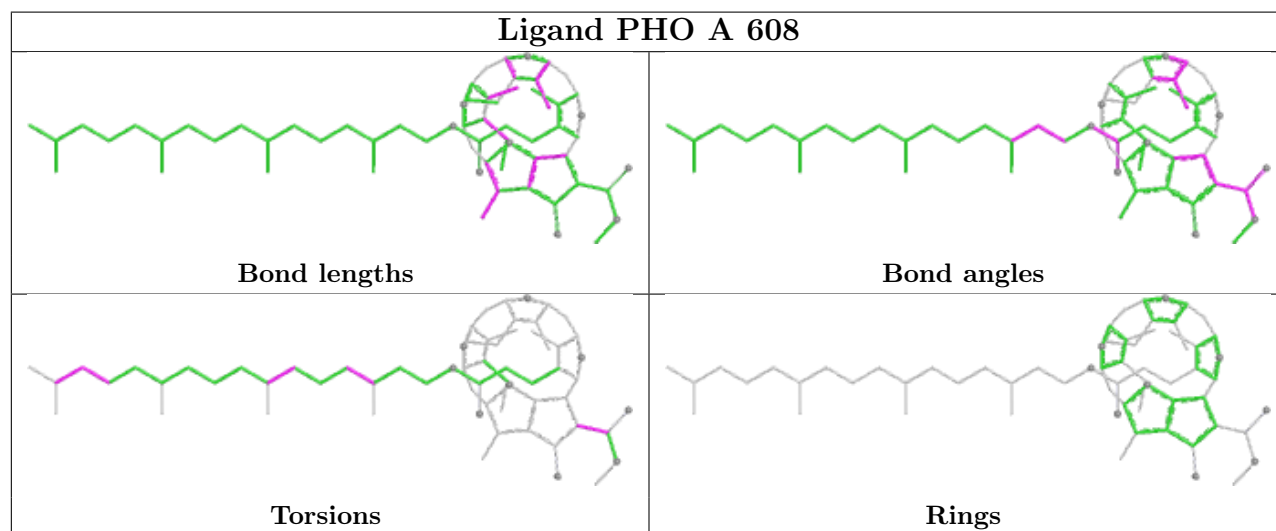
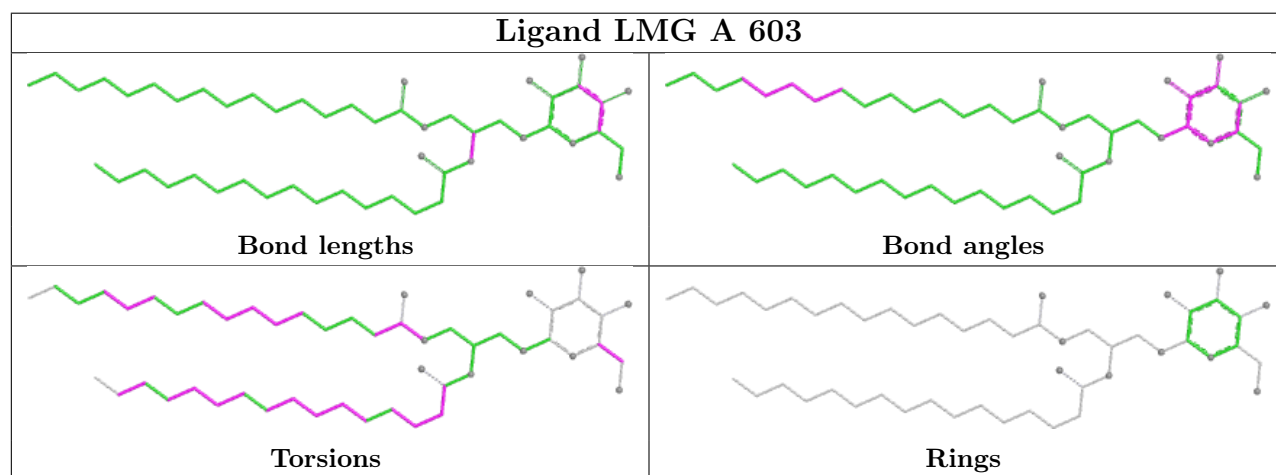
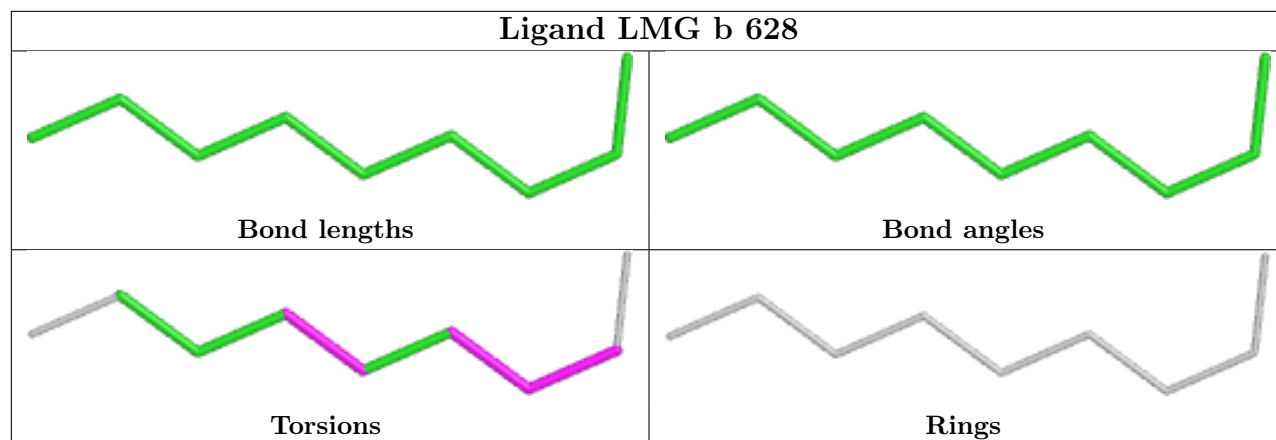
Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

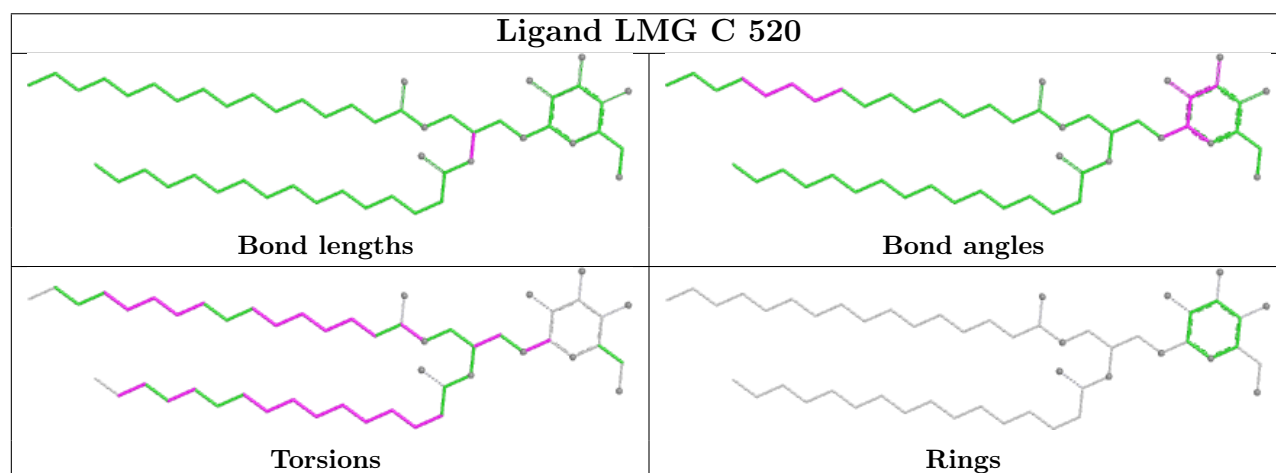
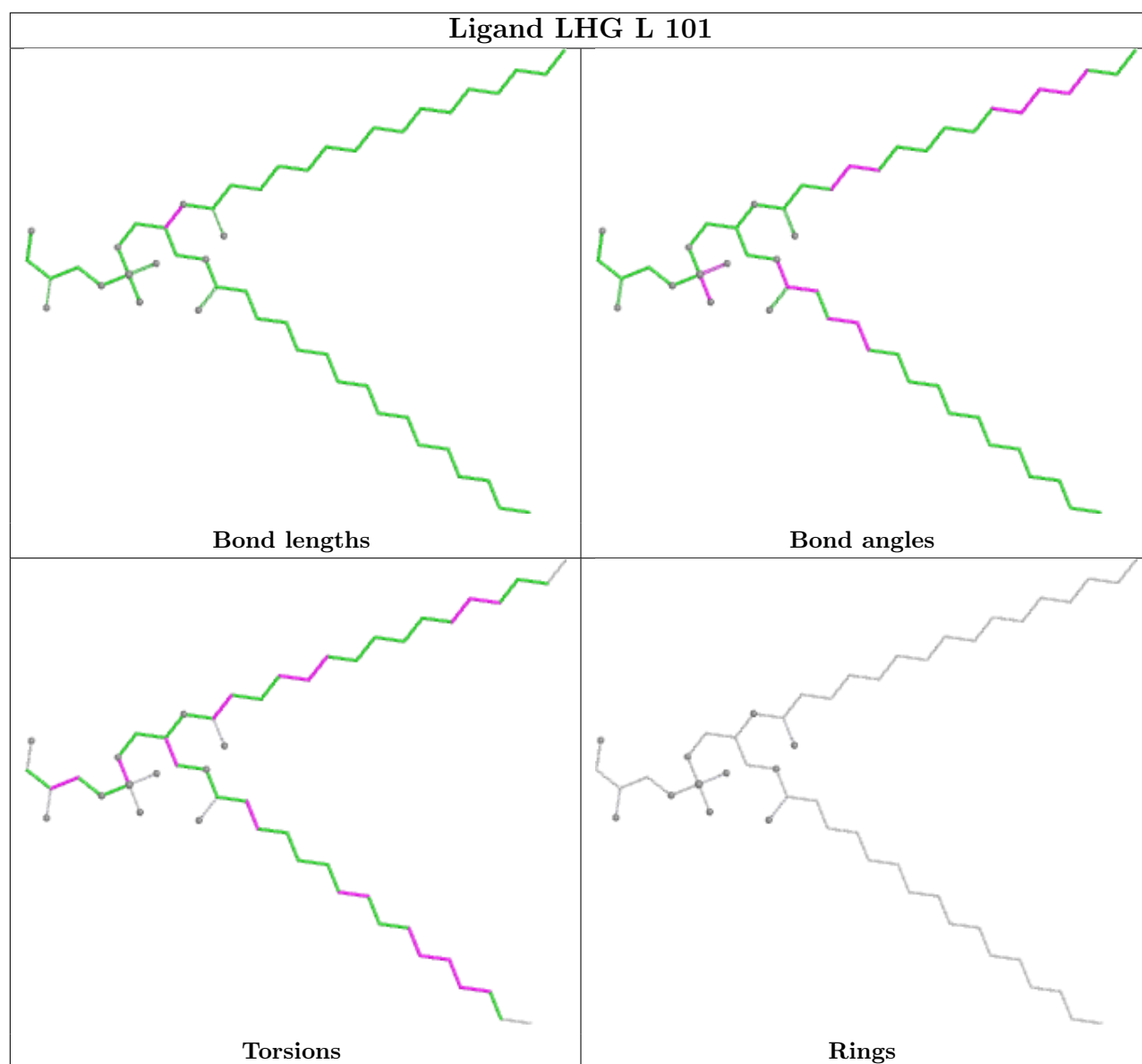
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

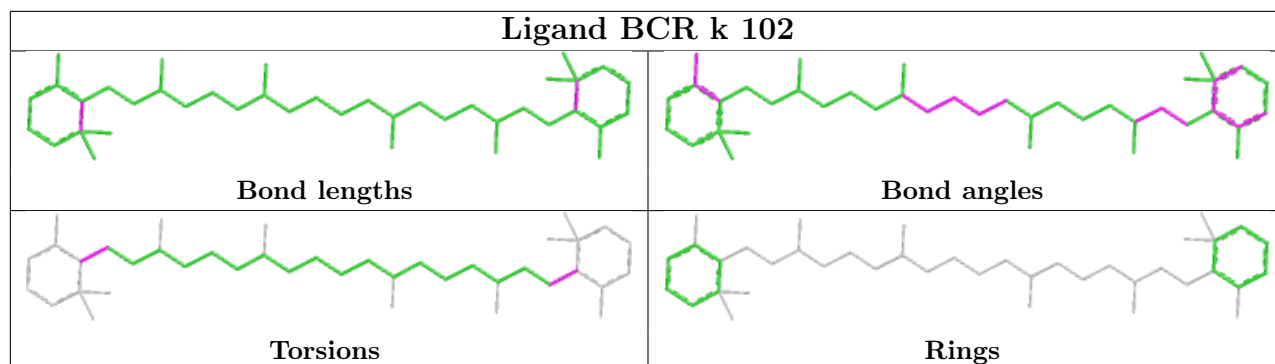
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG B 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

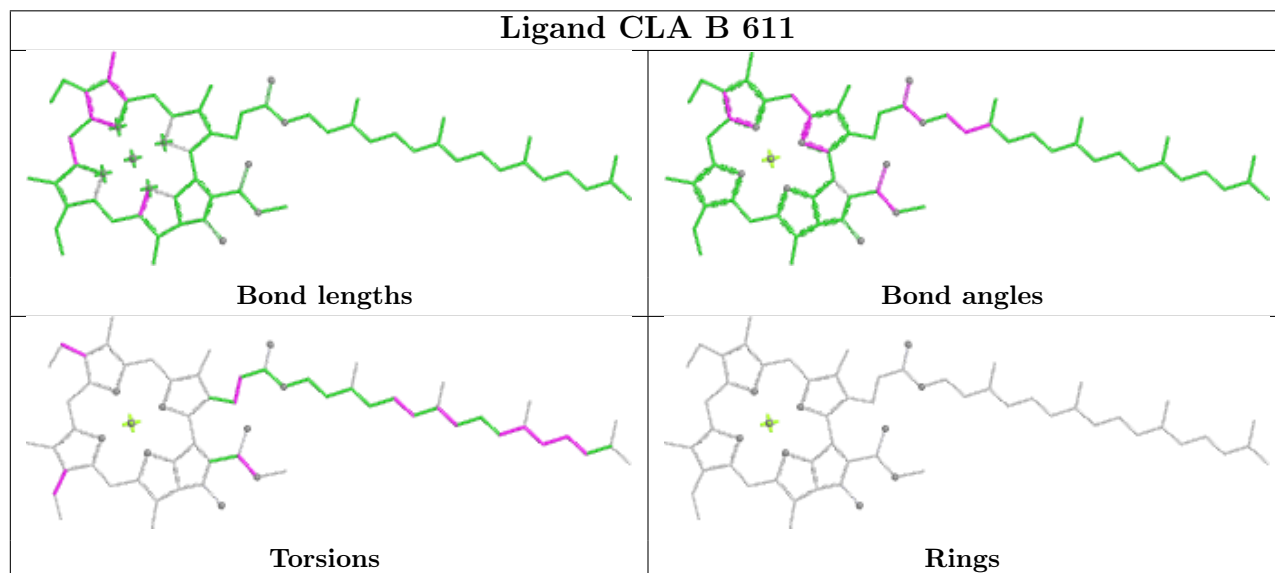




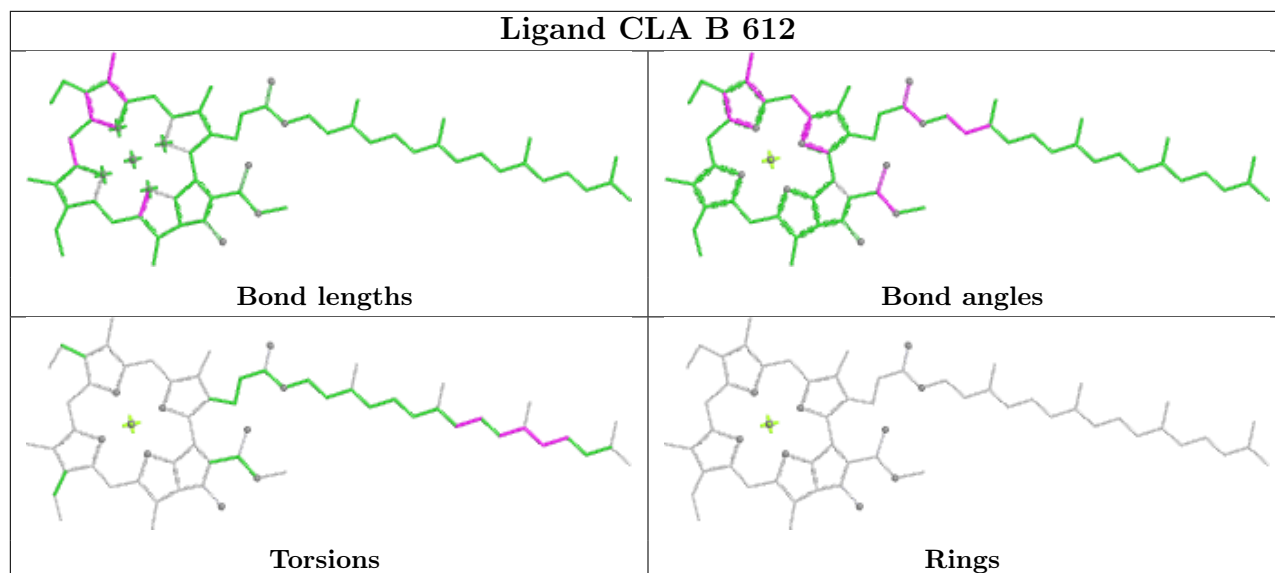
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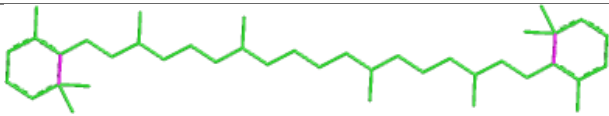
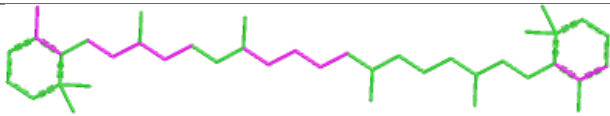
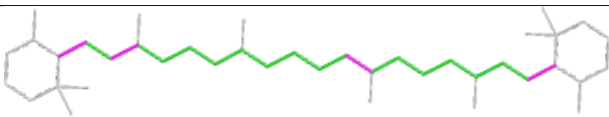
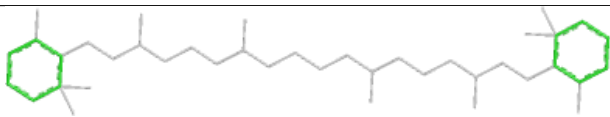


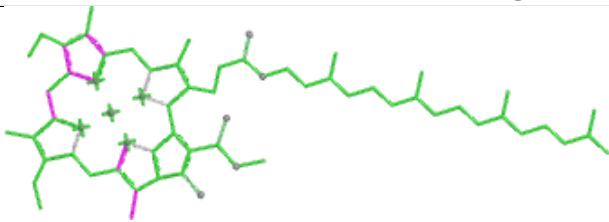
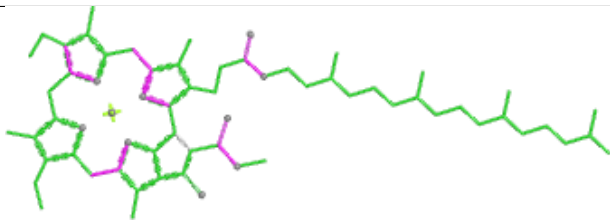
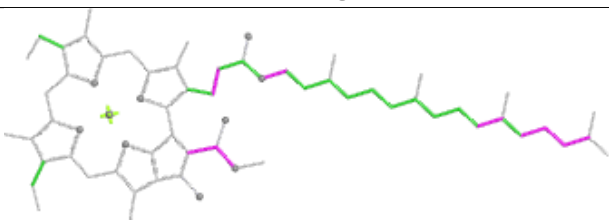
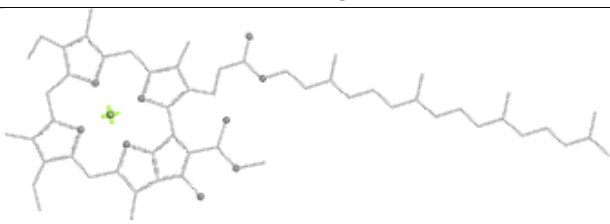
Ligand CLA B 611

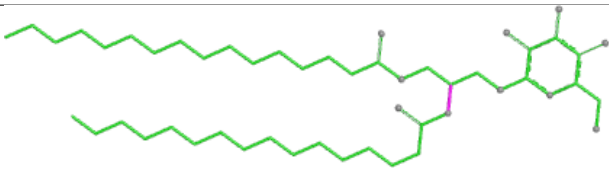
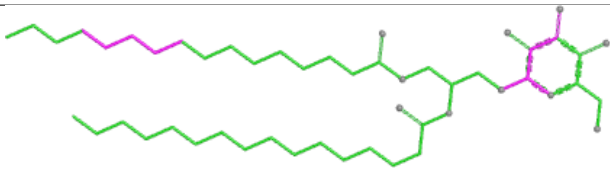
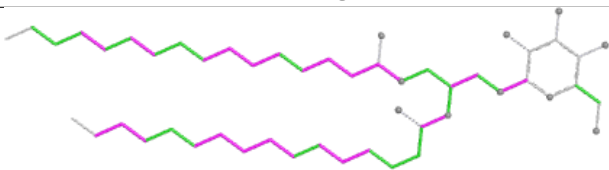
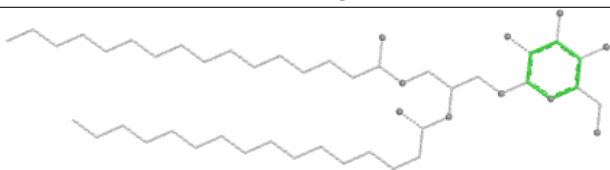


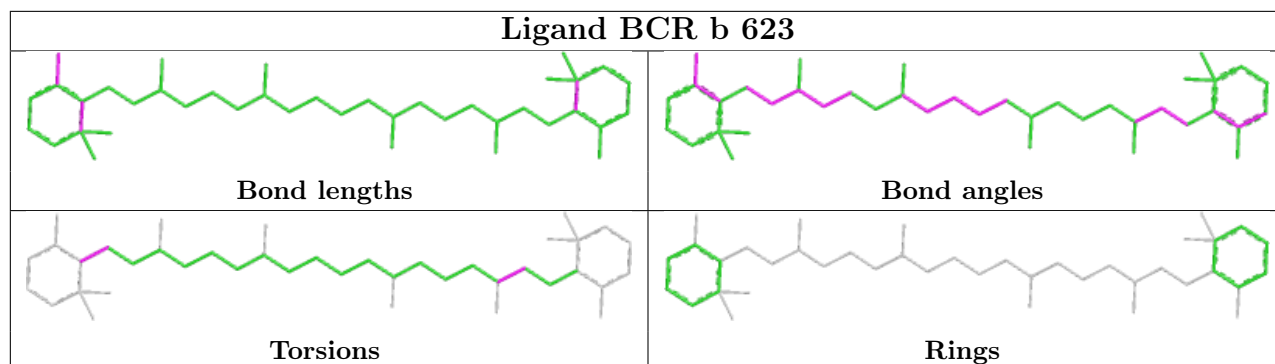
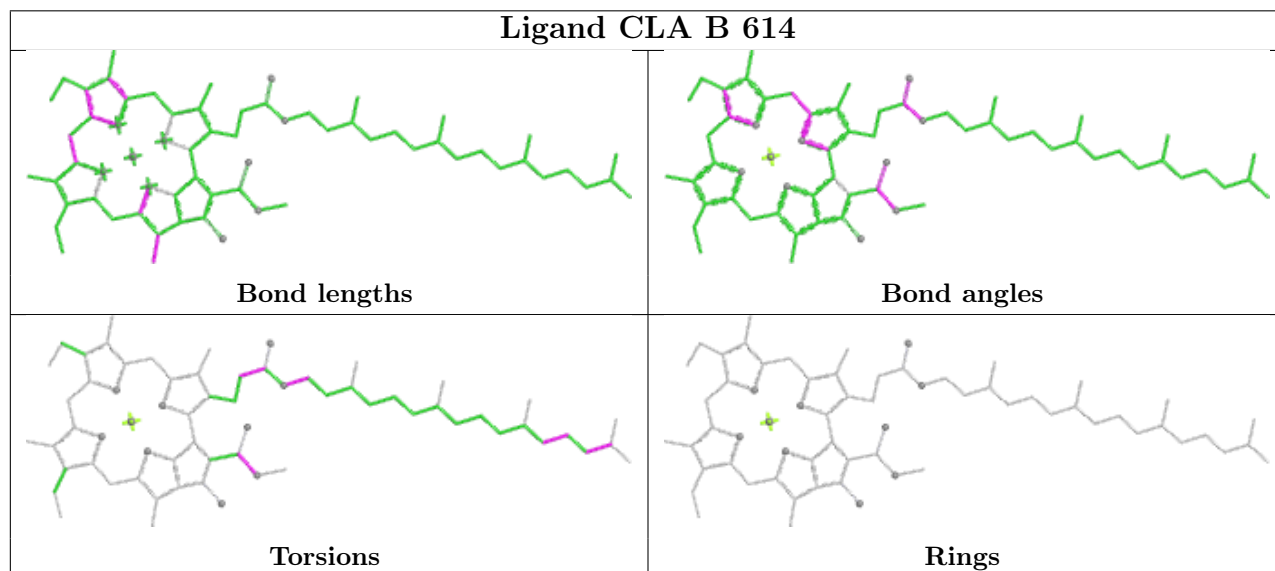
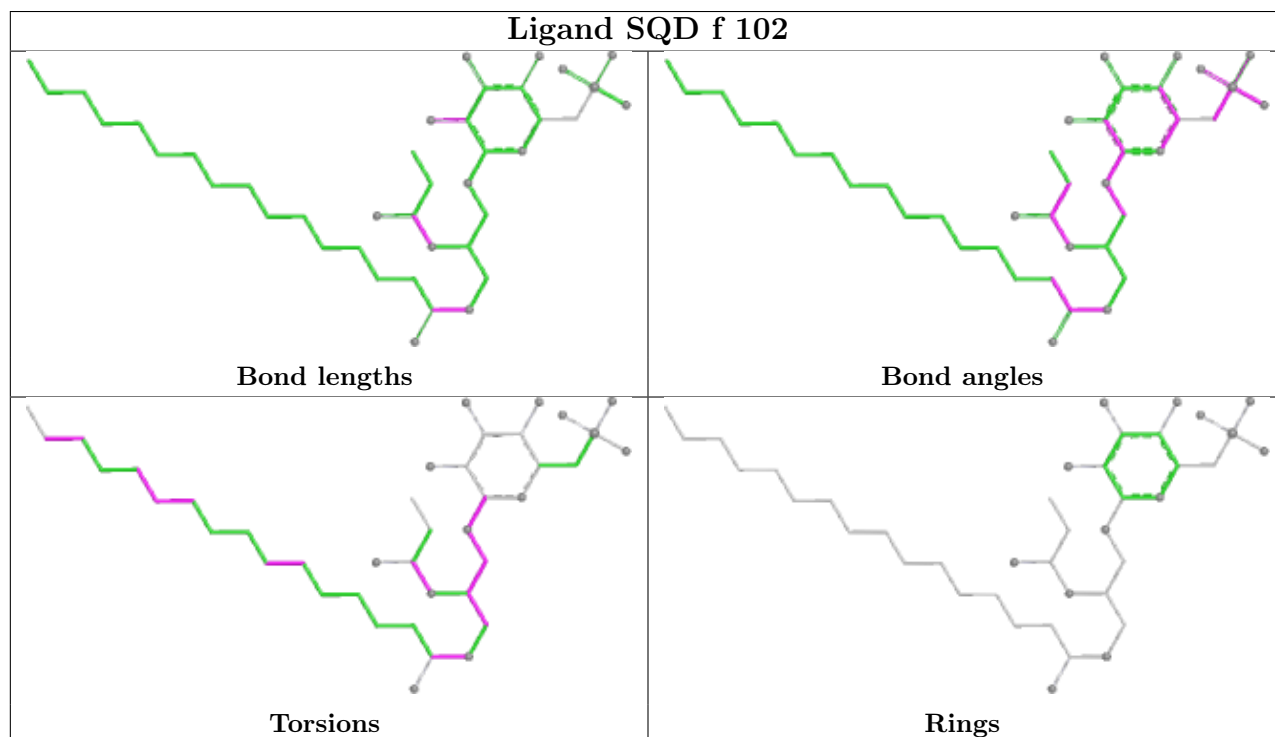
Ligand CLA B 612



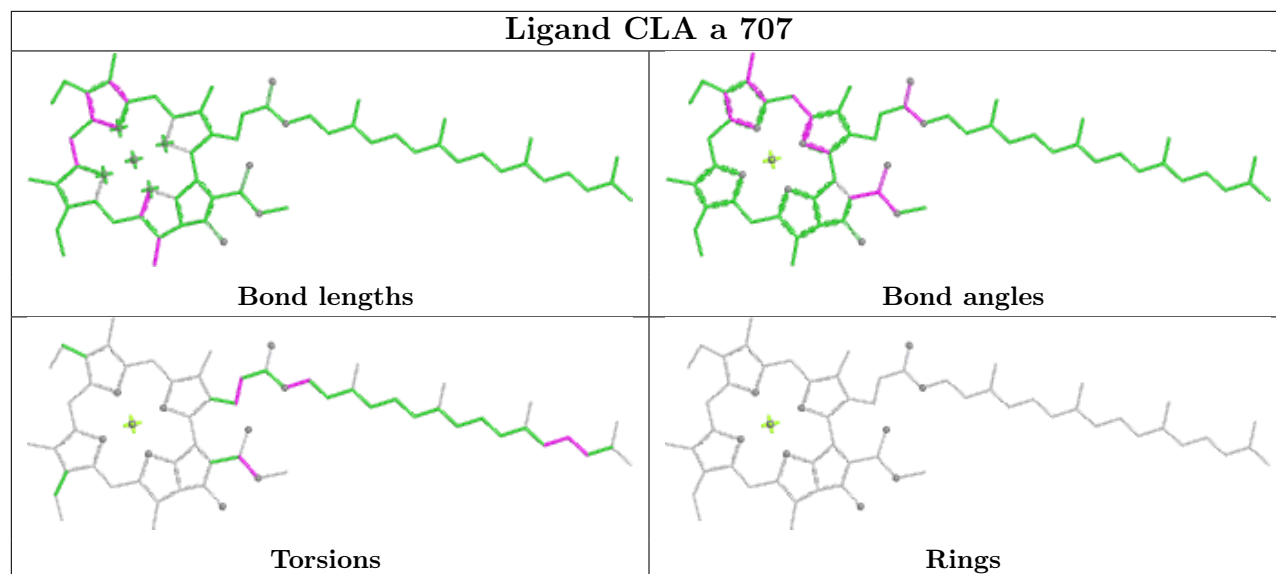
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

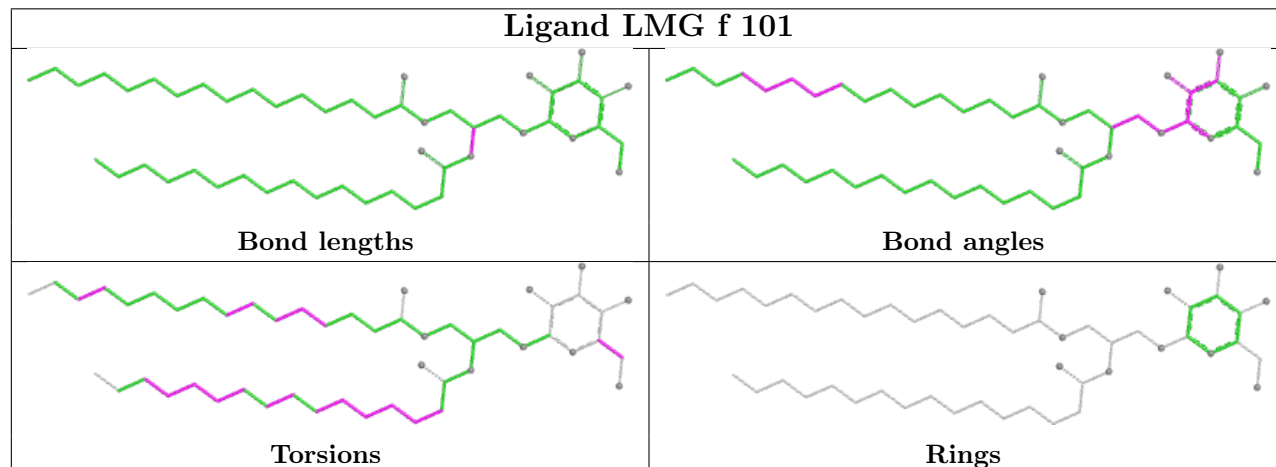
Ligand LMG C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 623**Ligand CLA B 614****Ligand SQD f 102**

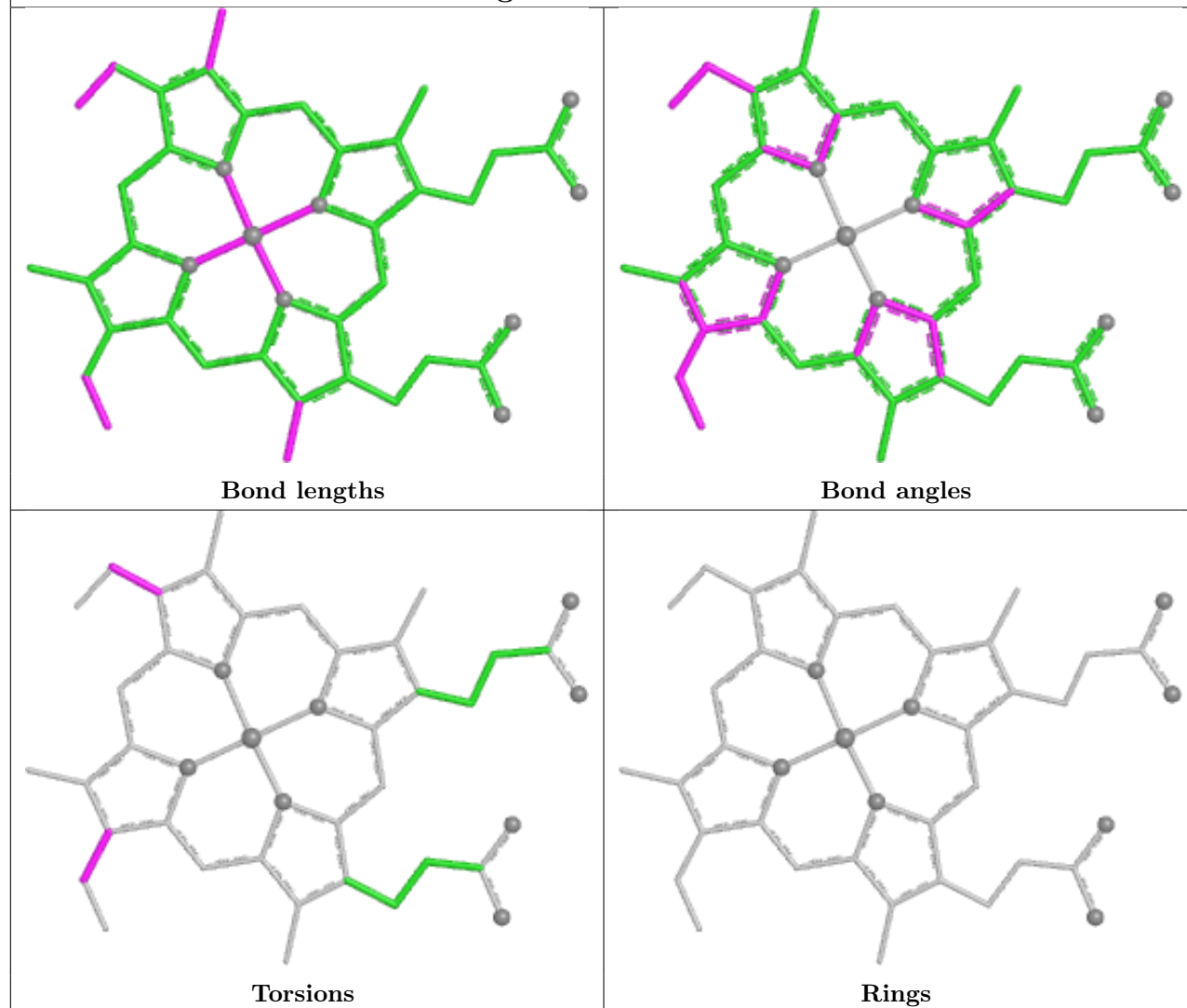
Ligand CLA a 707



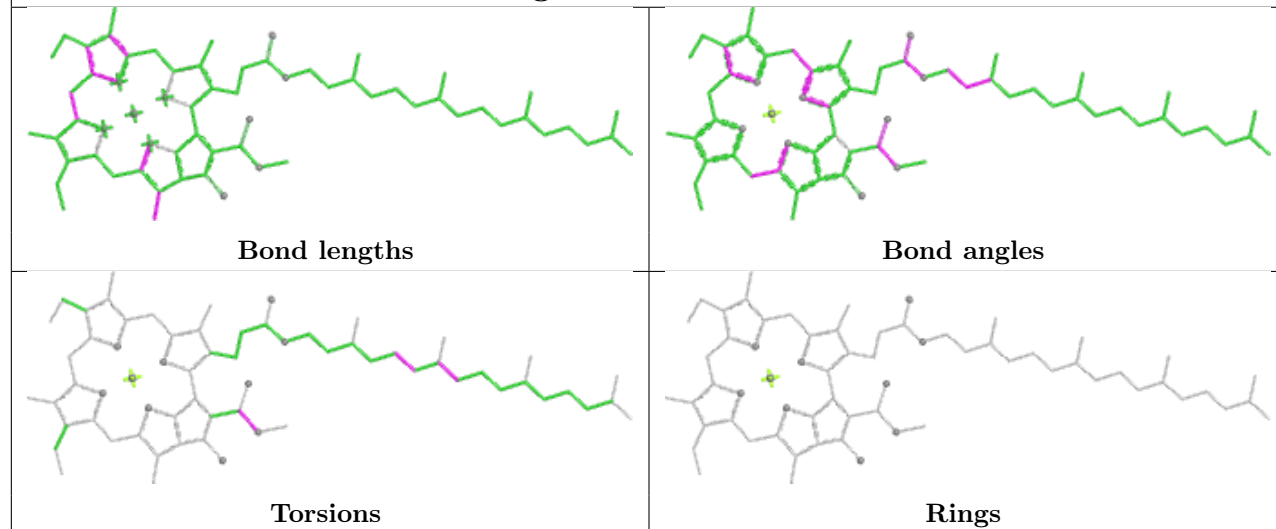
Ligand LMG f 101

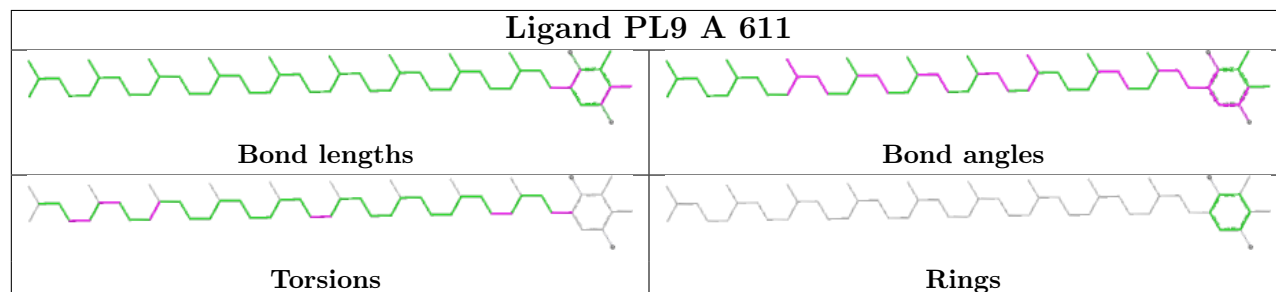
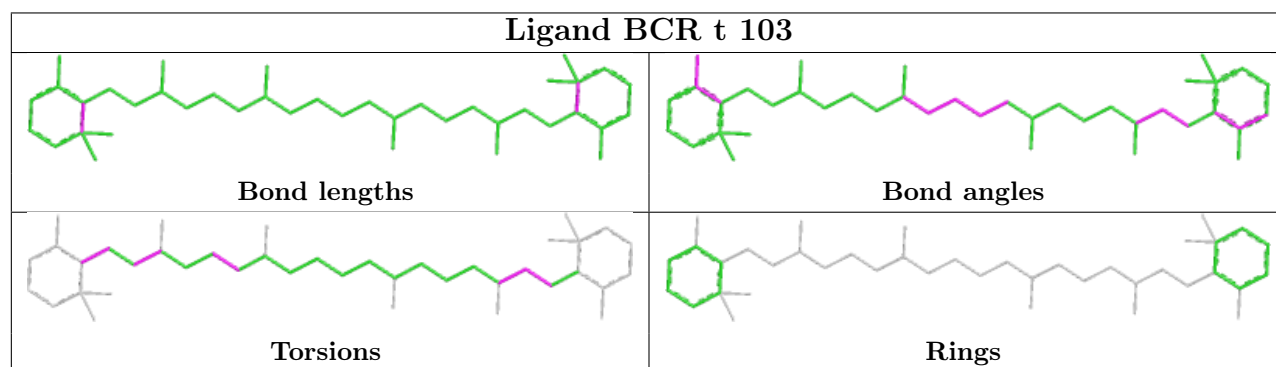
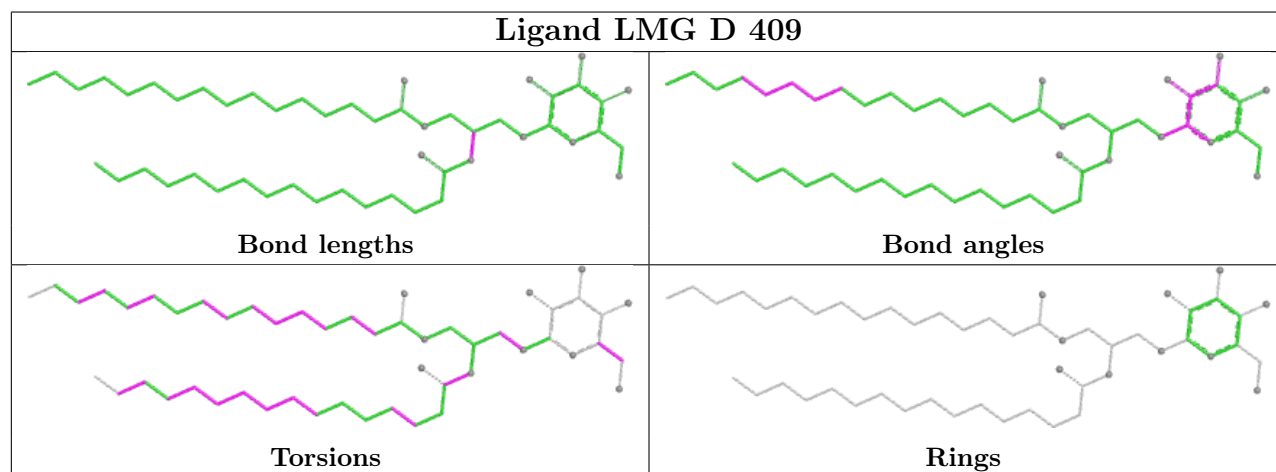
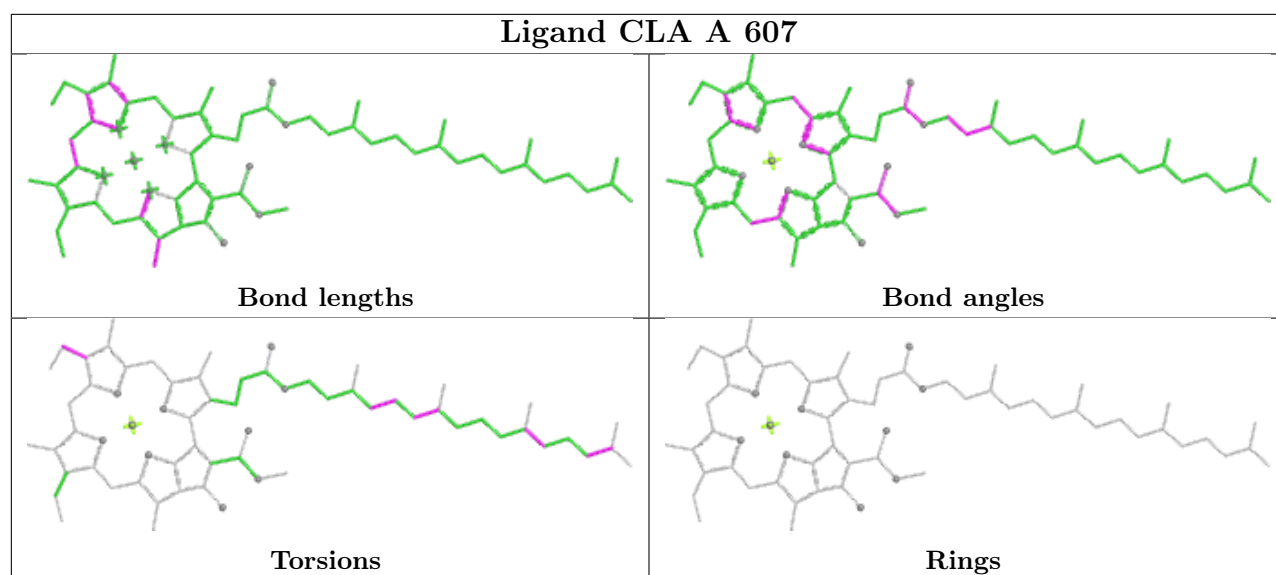


Ligand HEC v 201

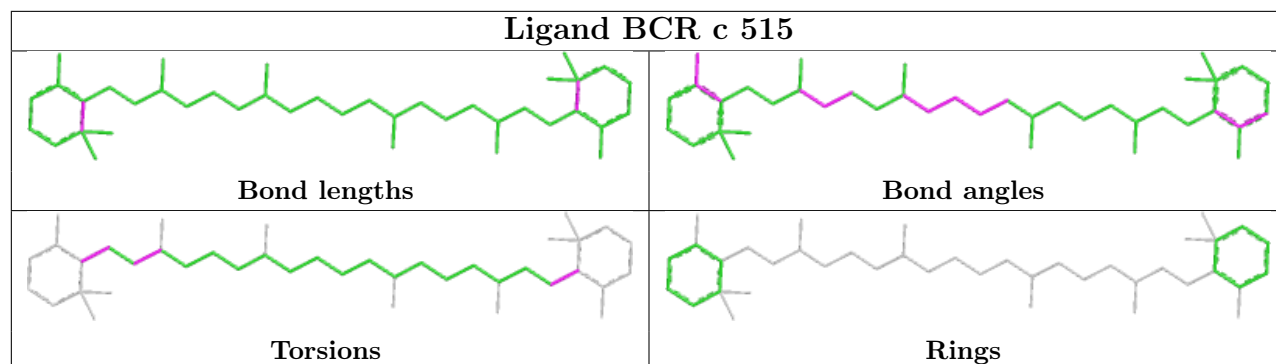


Ligand CLA C 509

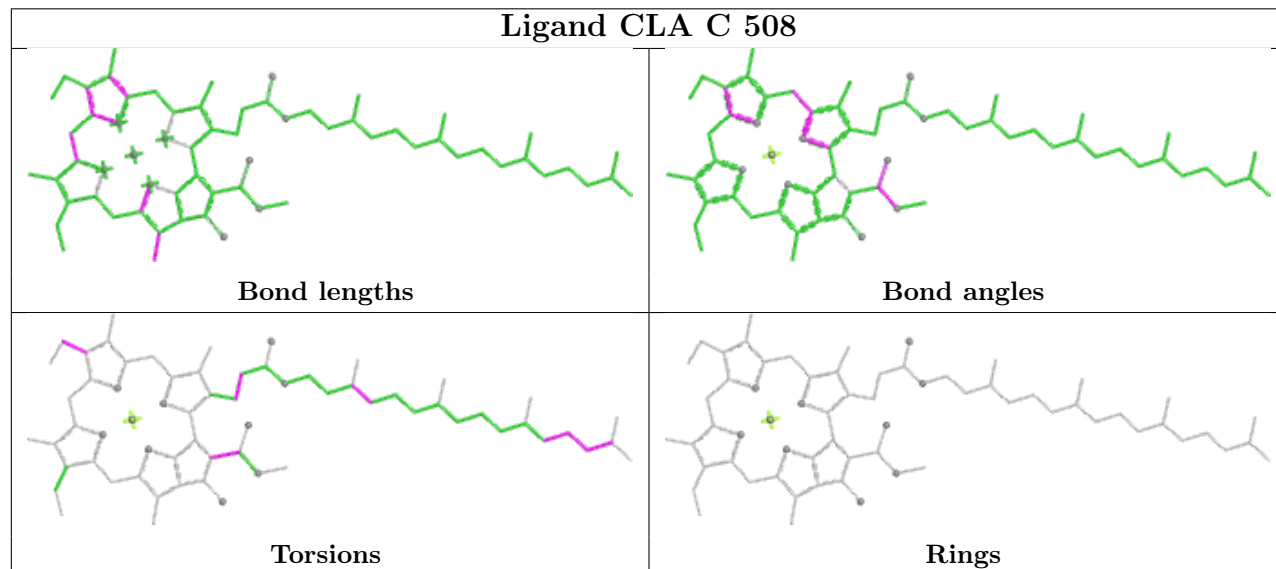




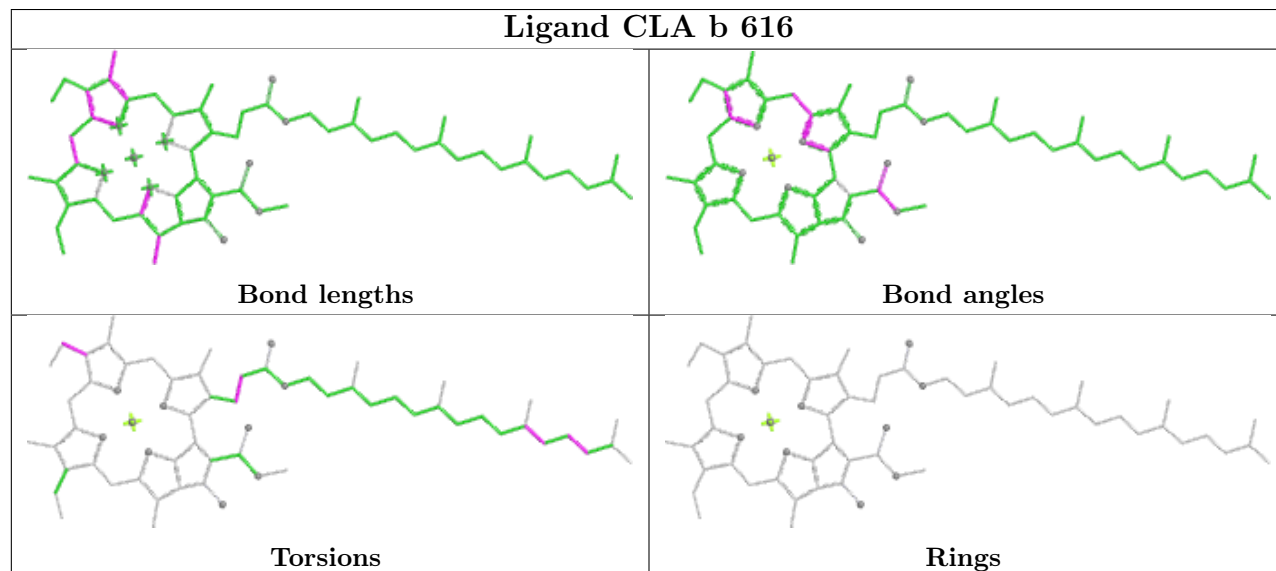
Ligand BCR c 515

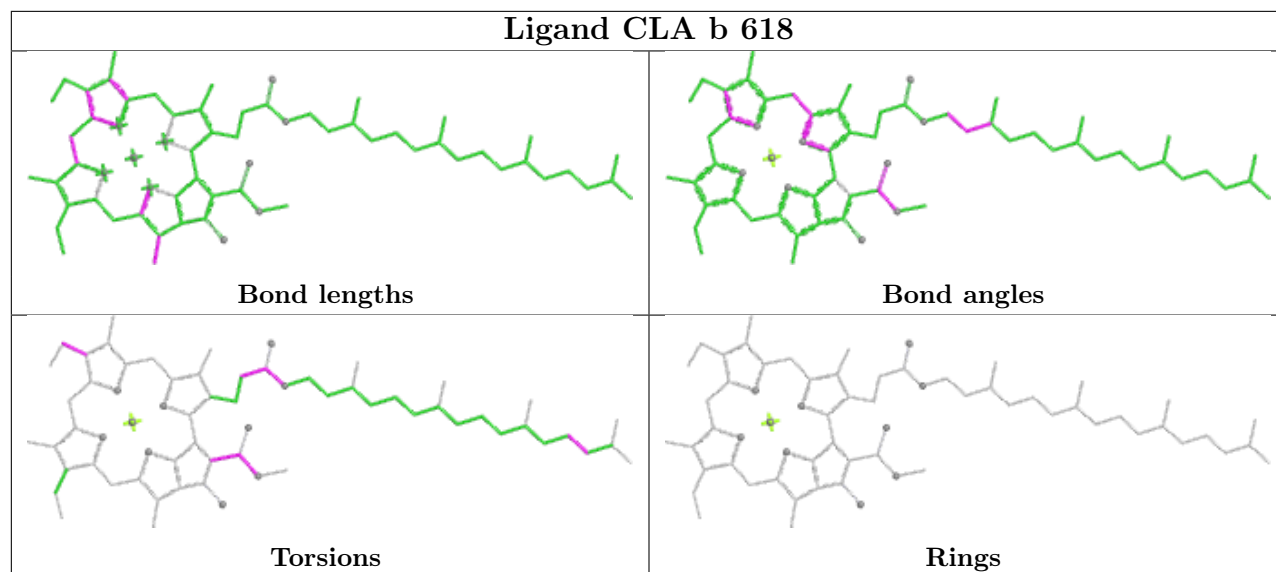
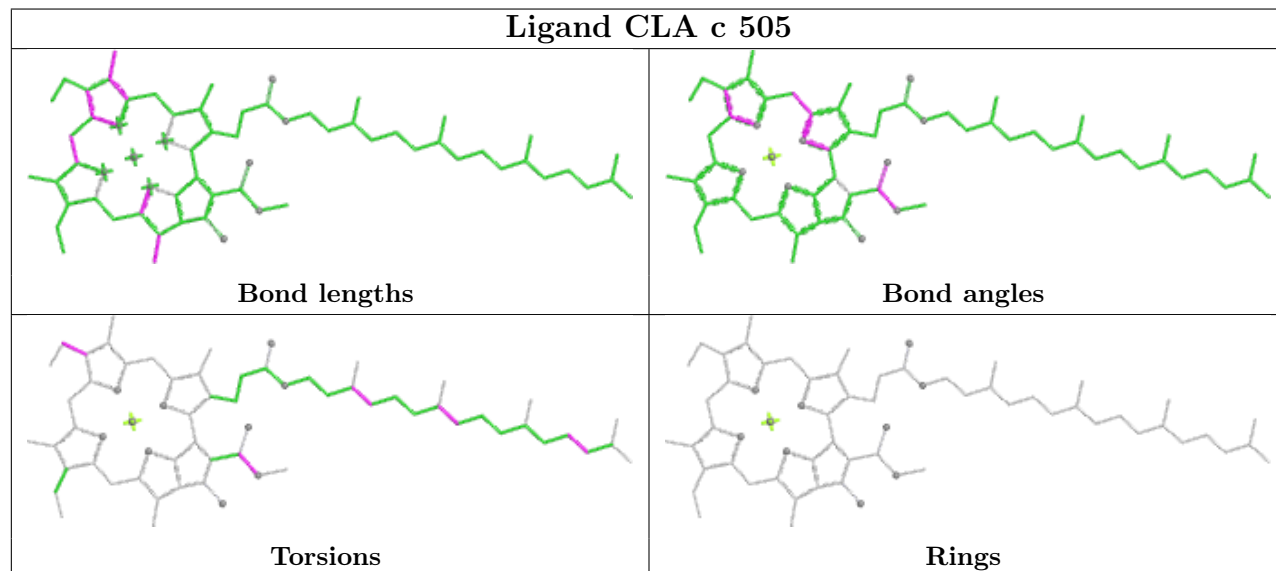
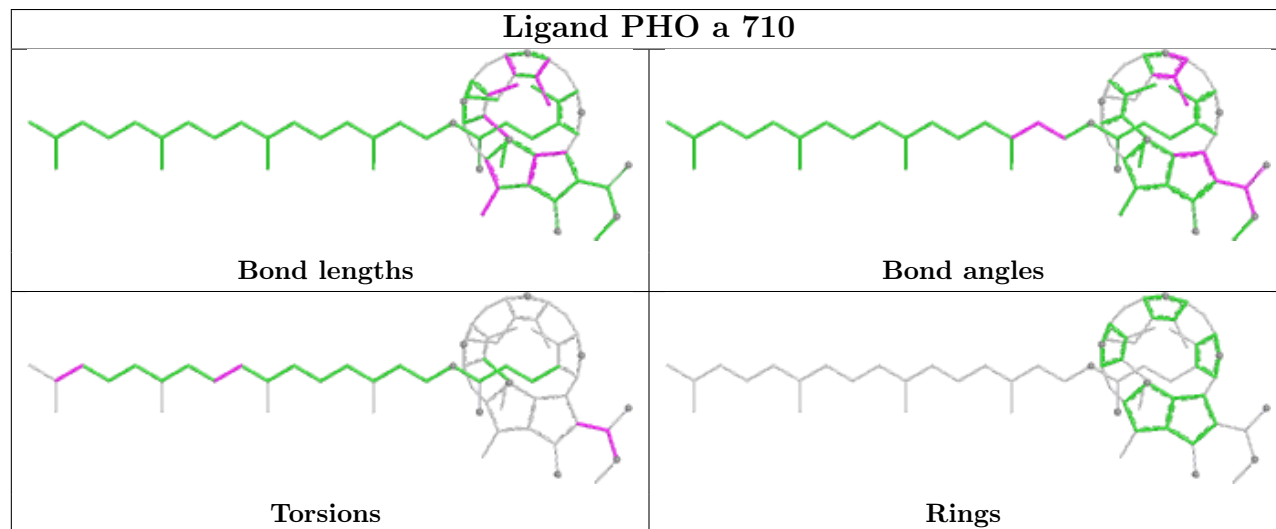


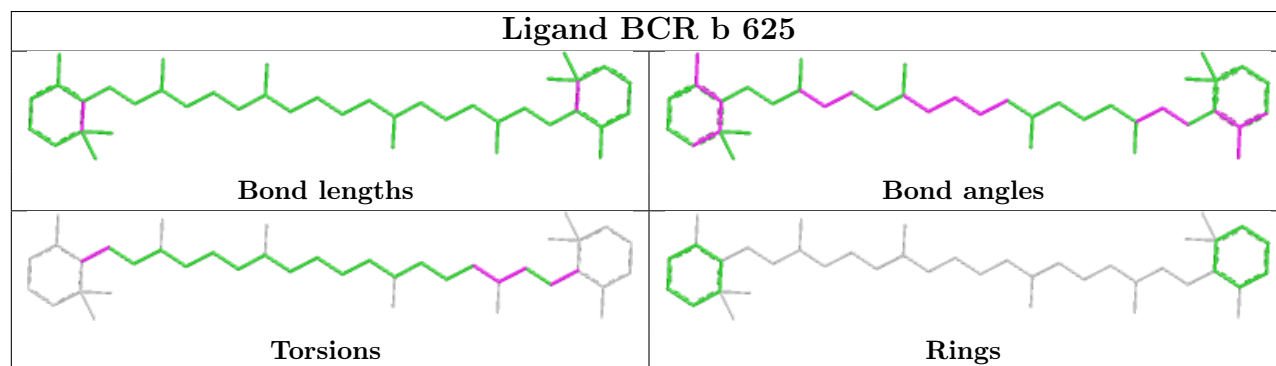
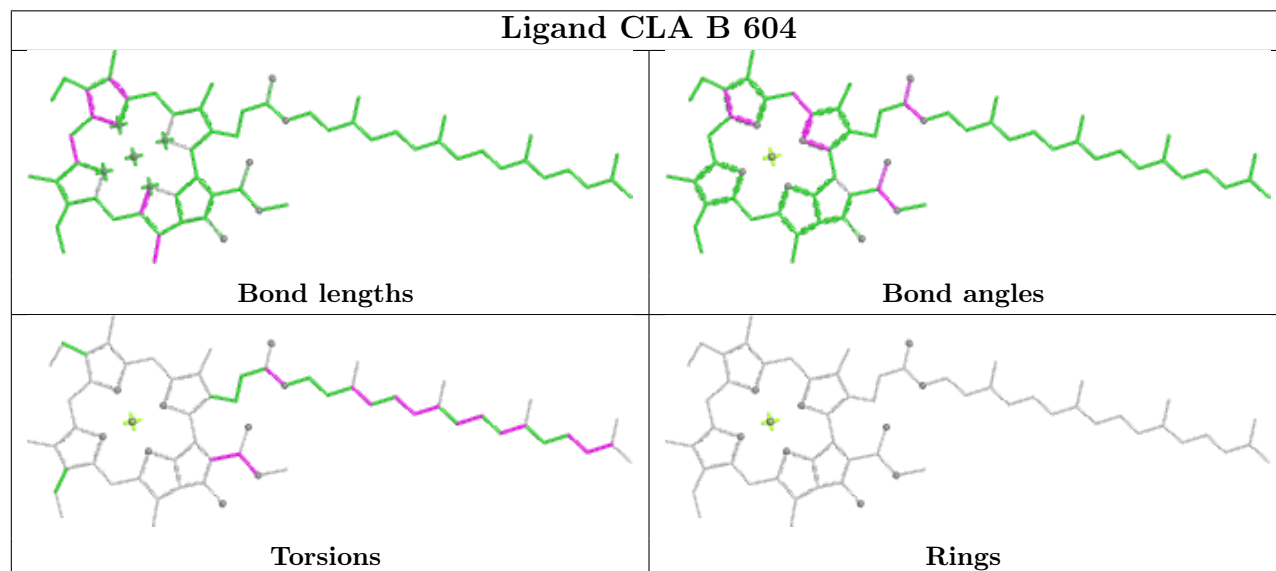
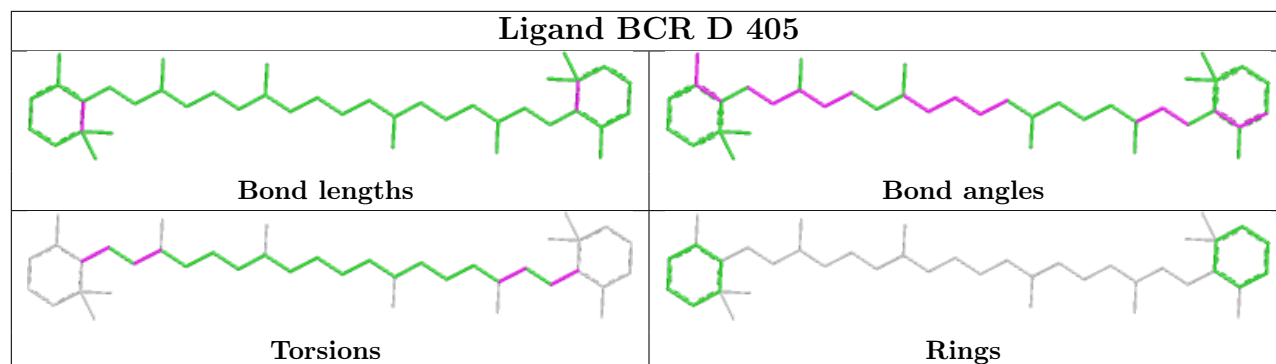
Ligand CLA C 508

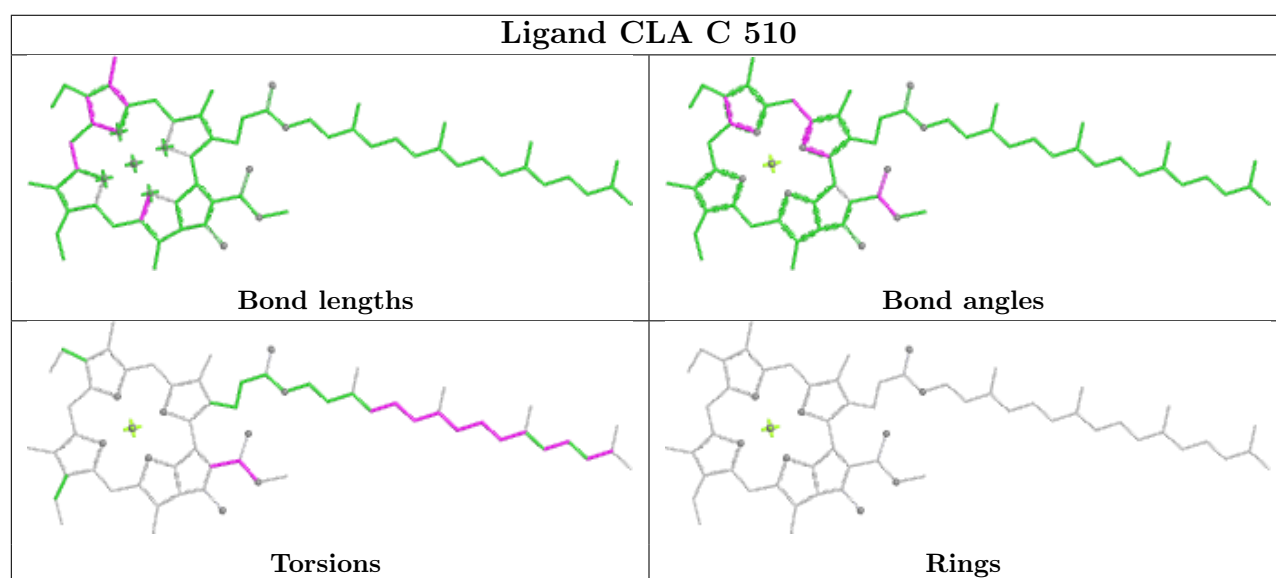
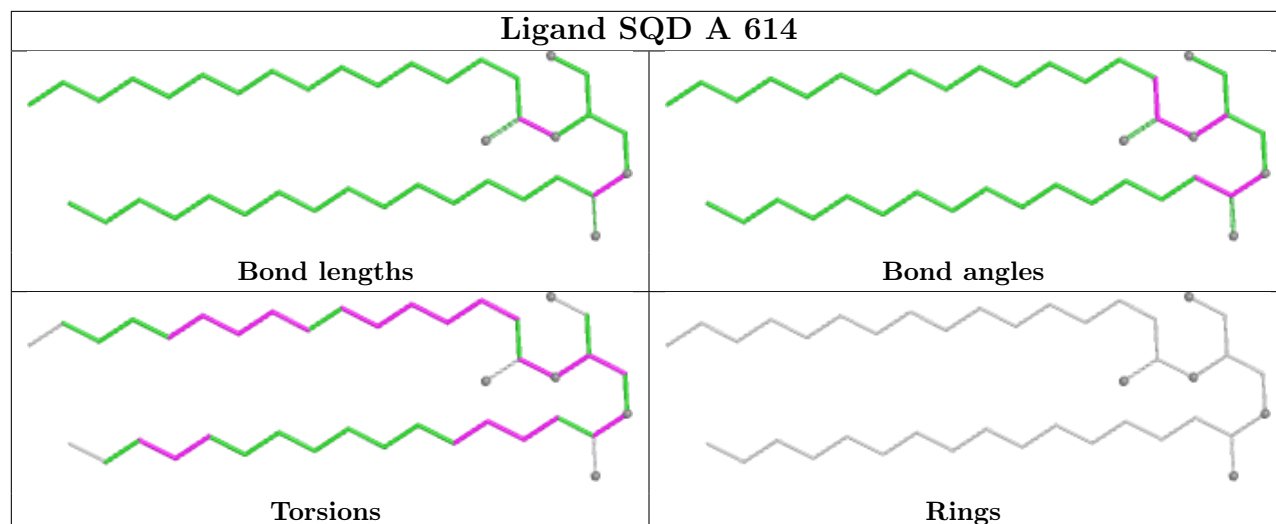


Ligand CLA b 616

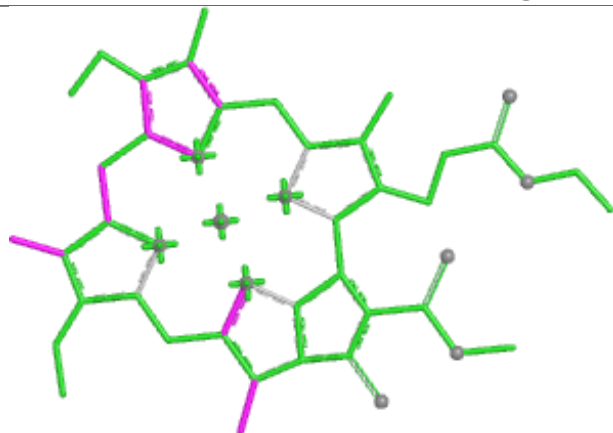


Ligand CLA b 618**Ligand CLA c 505****Ligand PHO a 710**

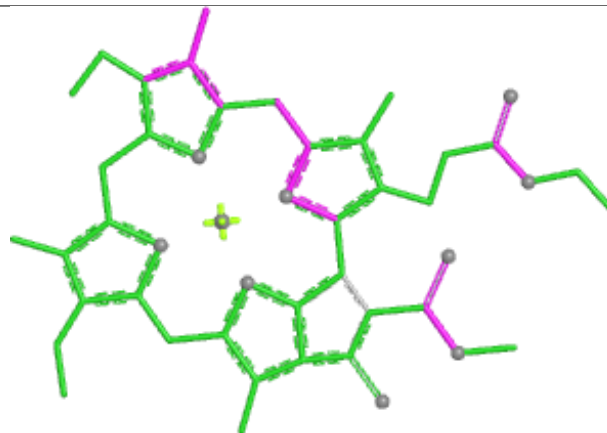




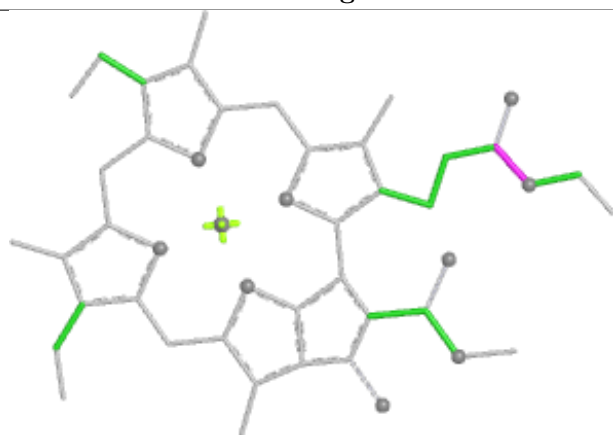
Ligand CLA b 622



Bond lengths



Bond angles

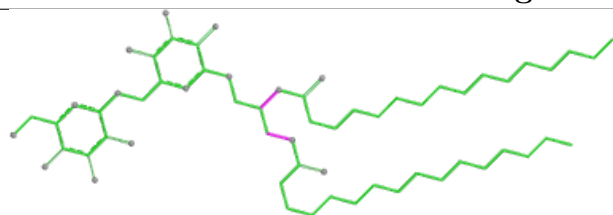


Torsions

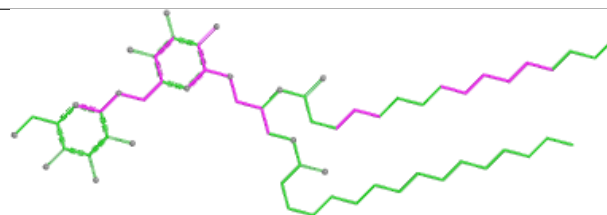


Rings

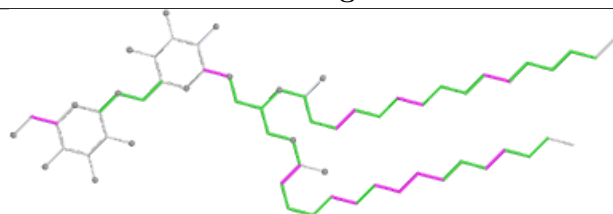
Ligand DGD c 518



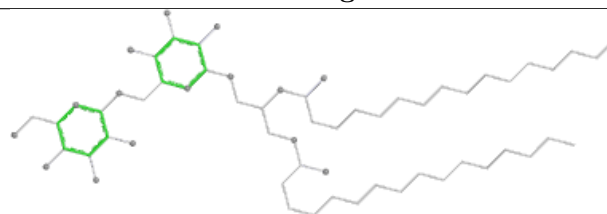
Bond lengths



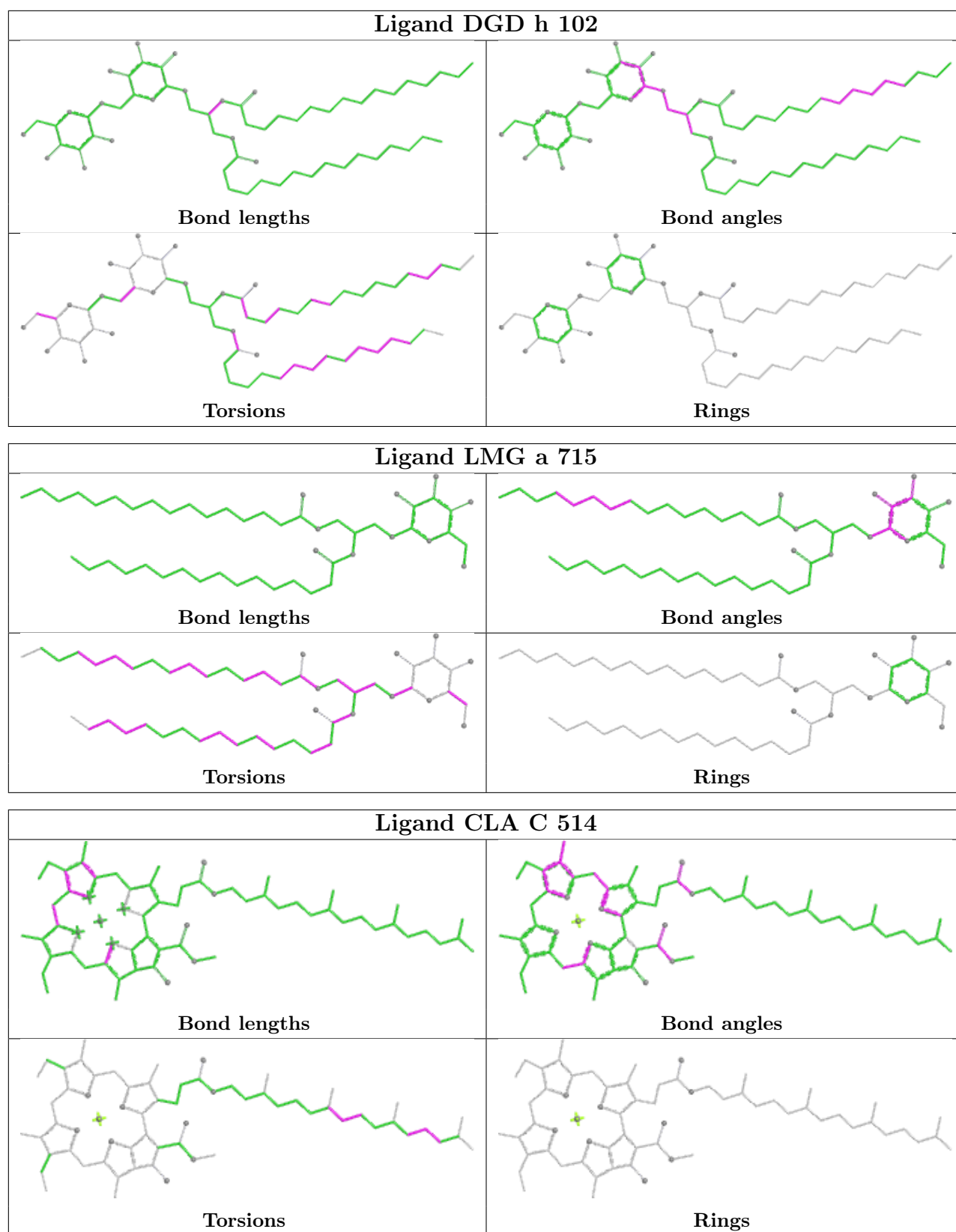
Bond angles



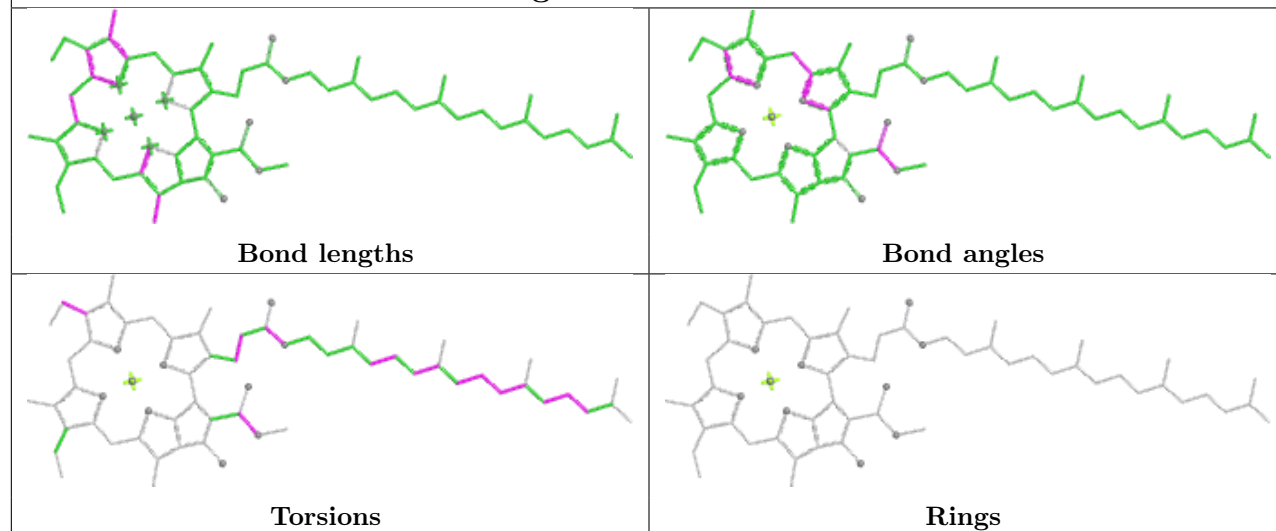
Torsions



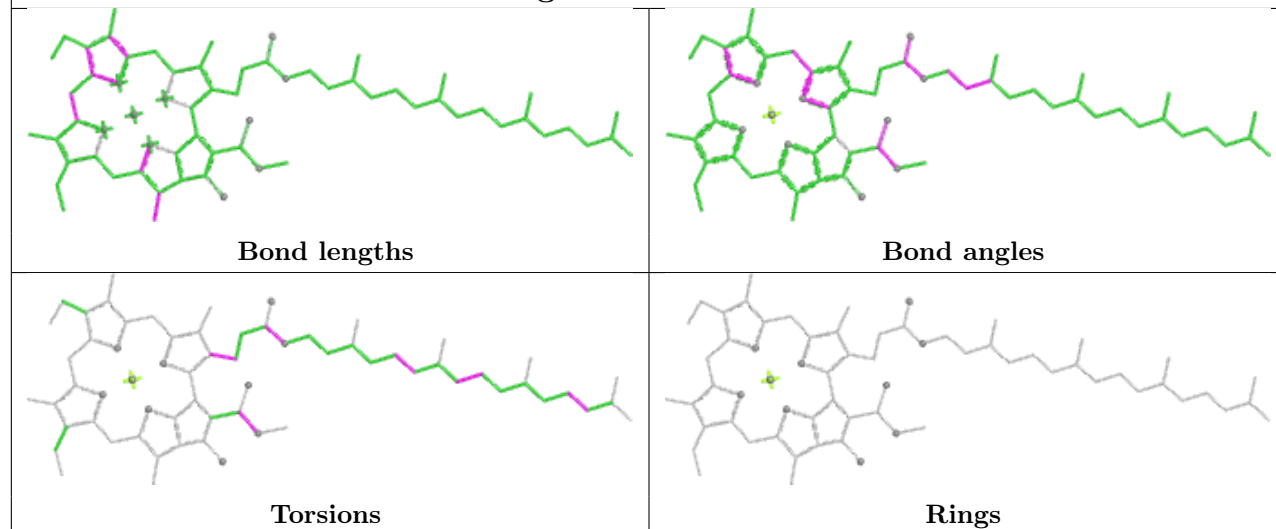
Rings



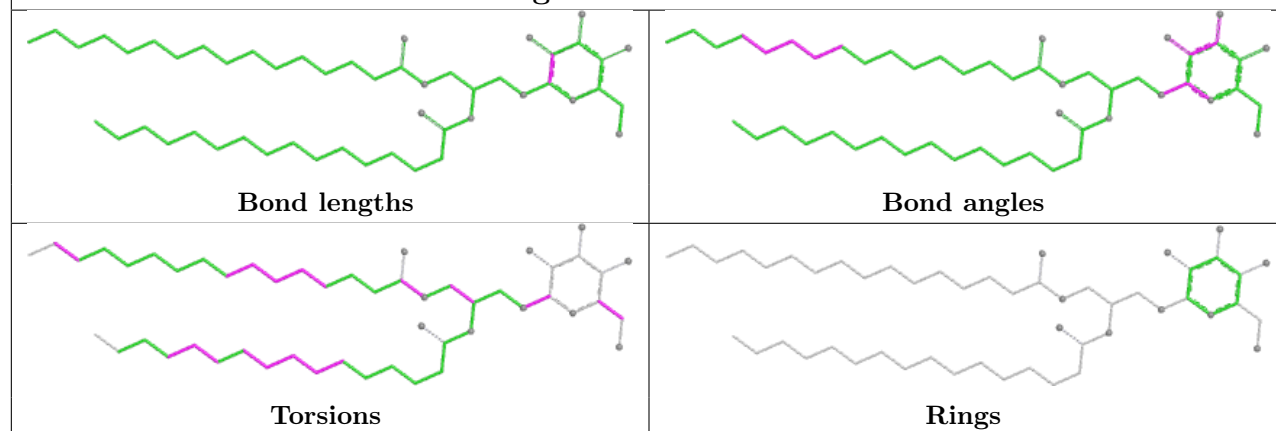
Ligand CLA B 607

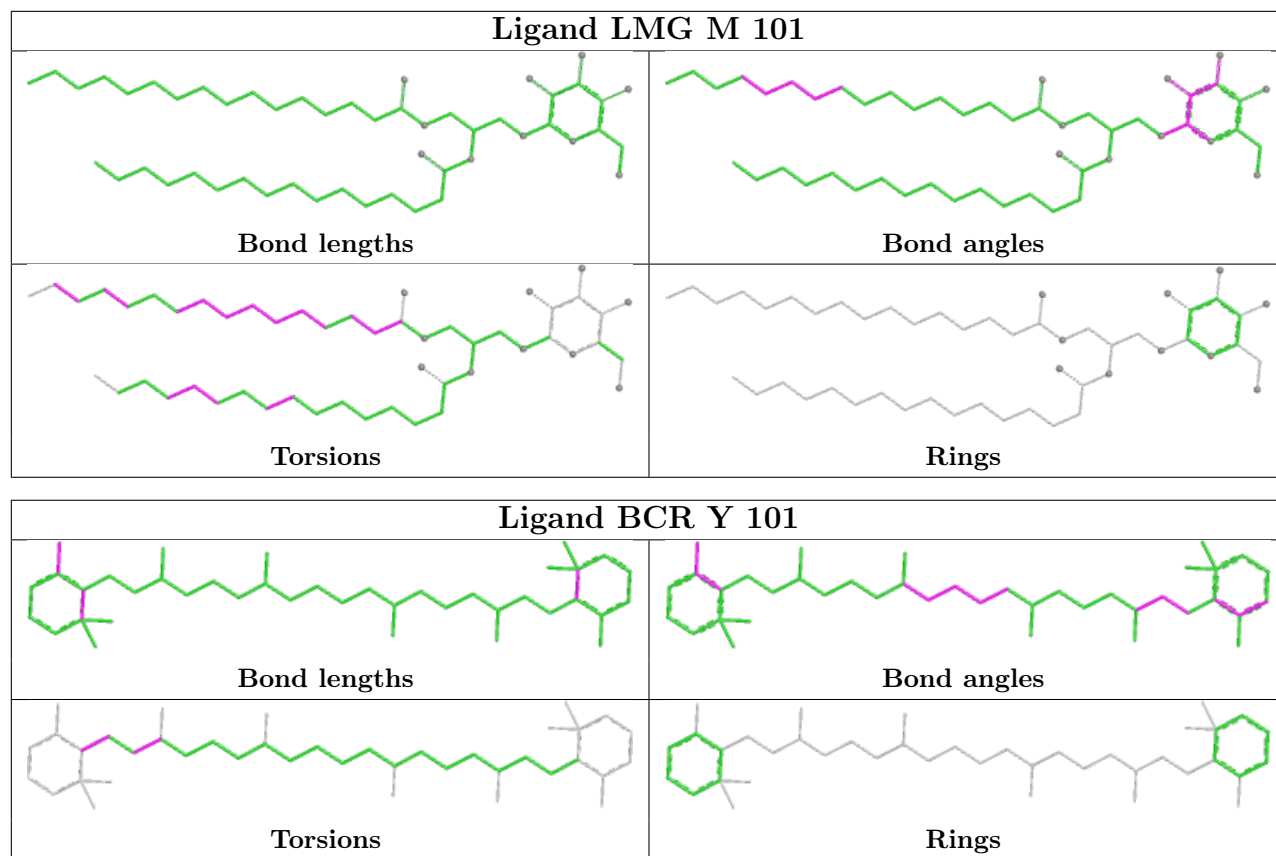


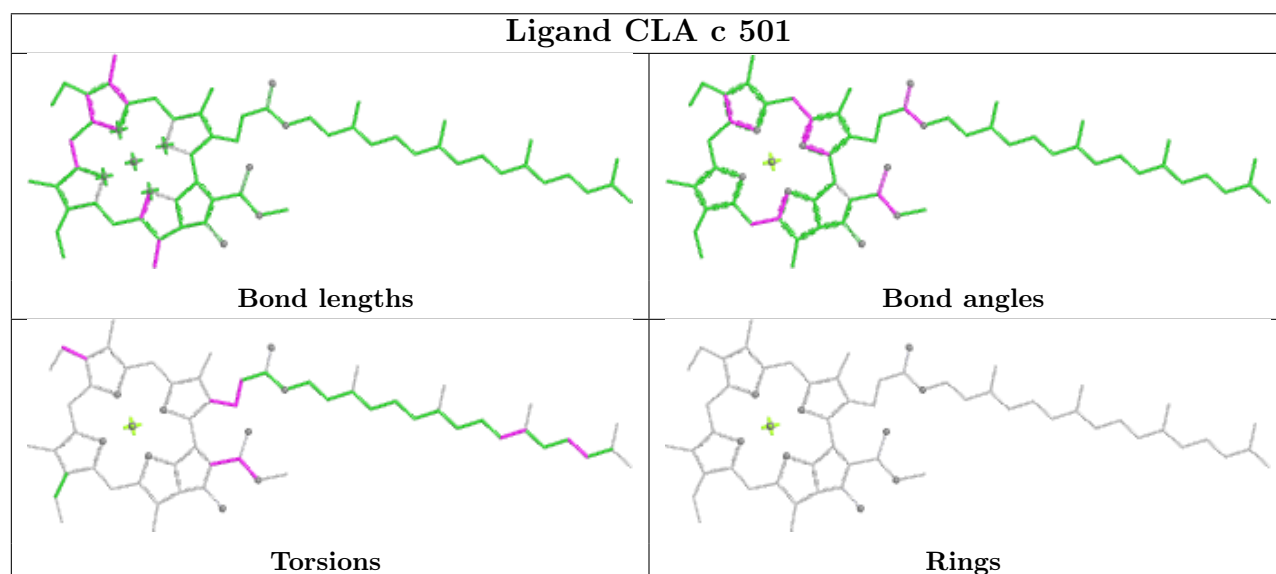
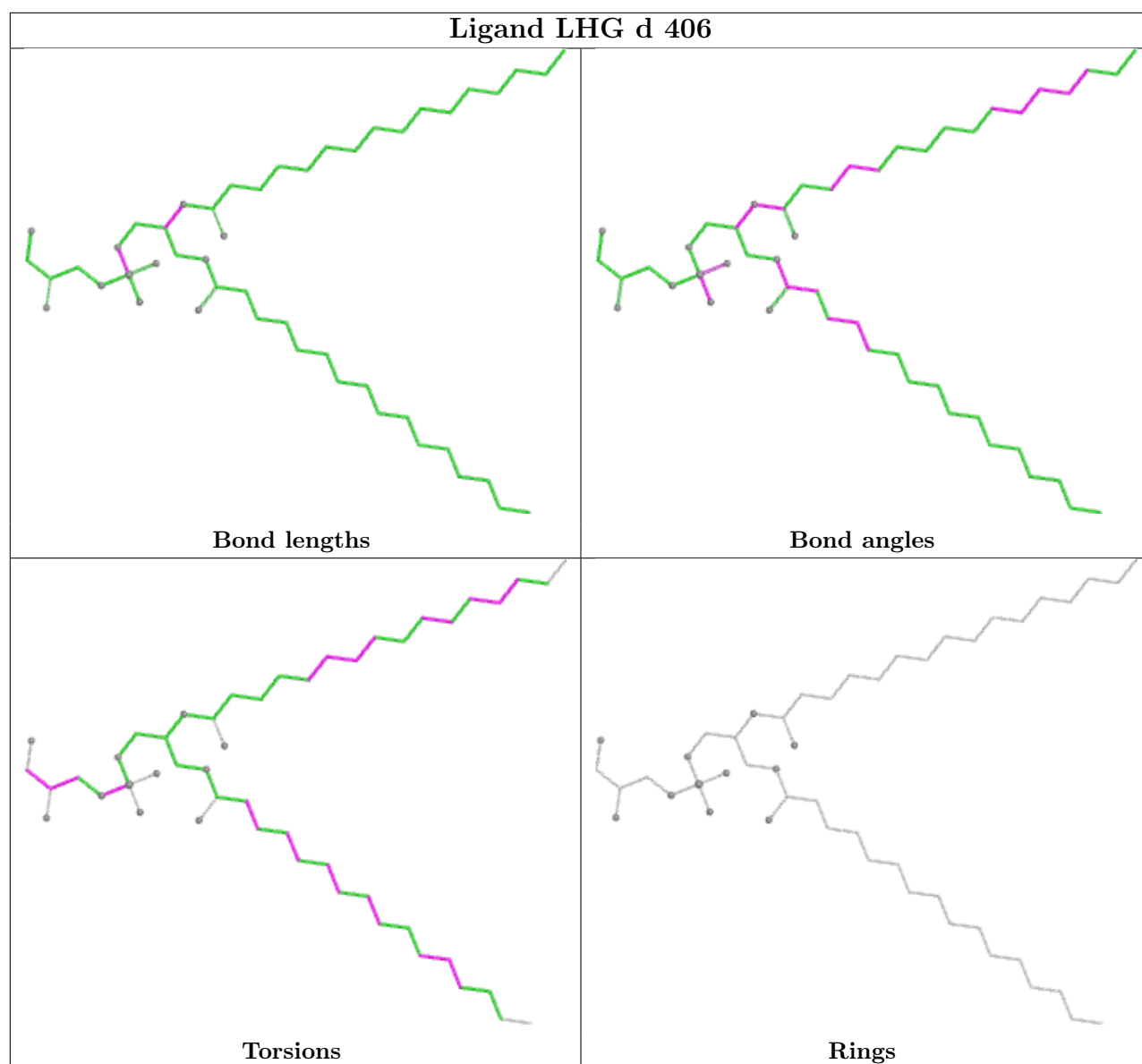
Ligand CLA c 503

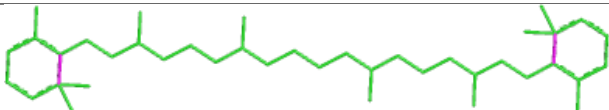
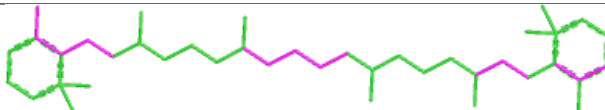
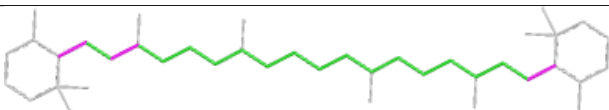
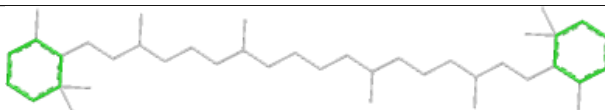


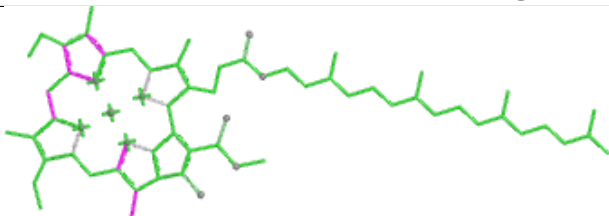
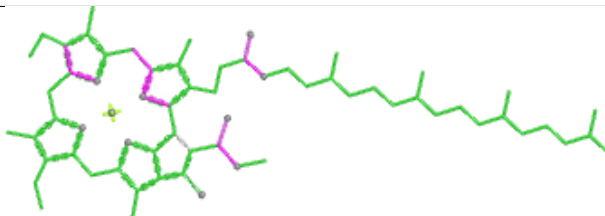
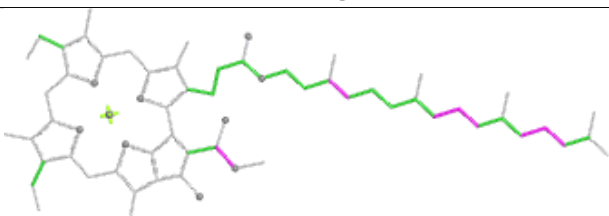
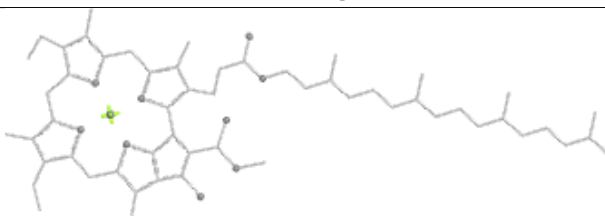
Ligand LMG c 520

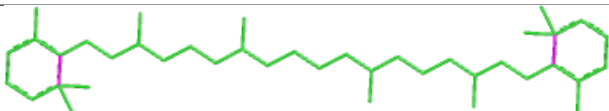
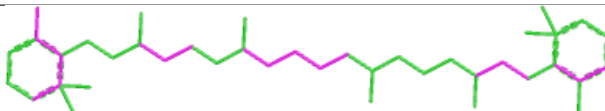
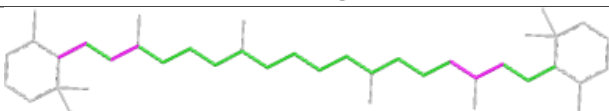
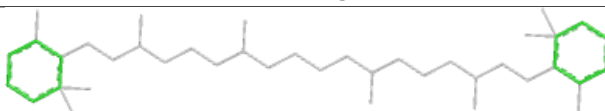




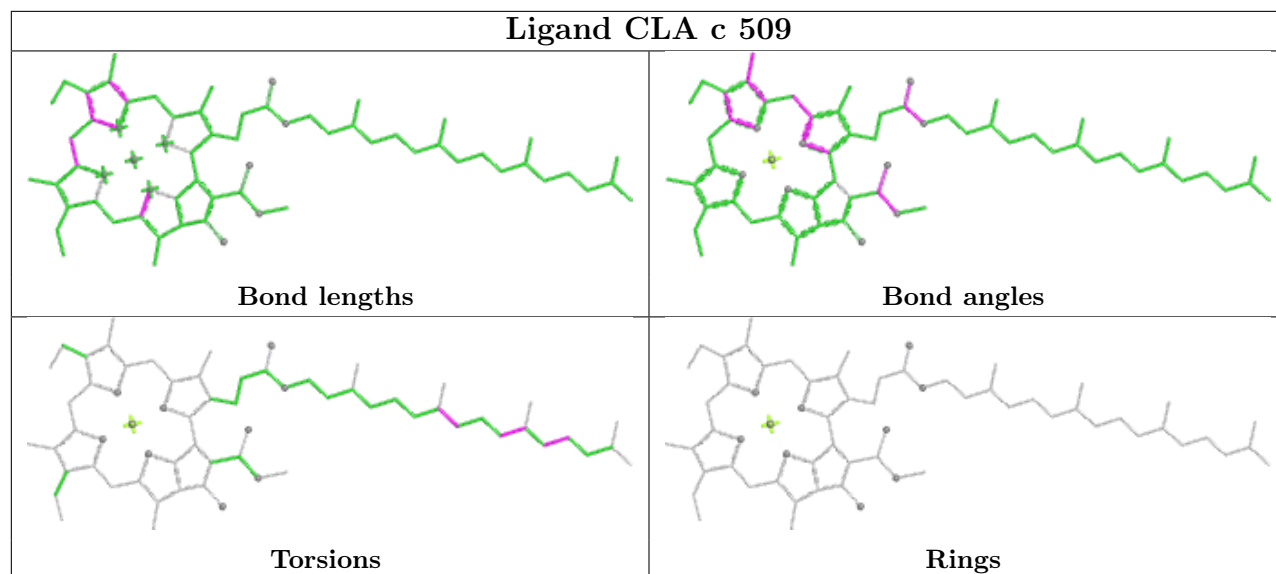


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

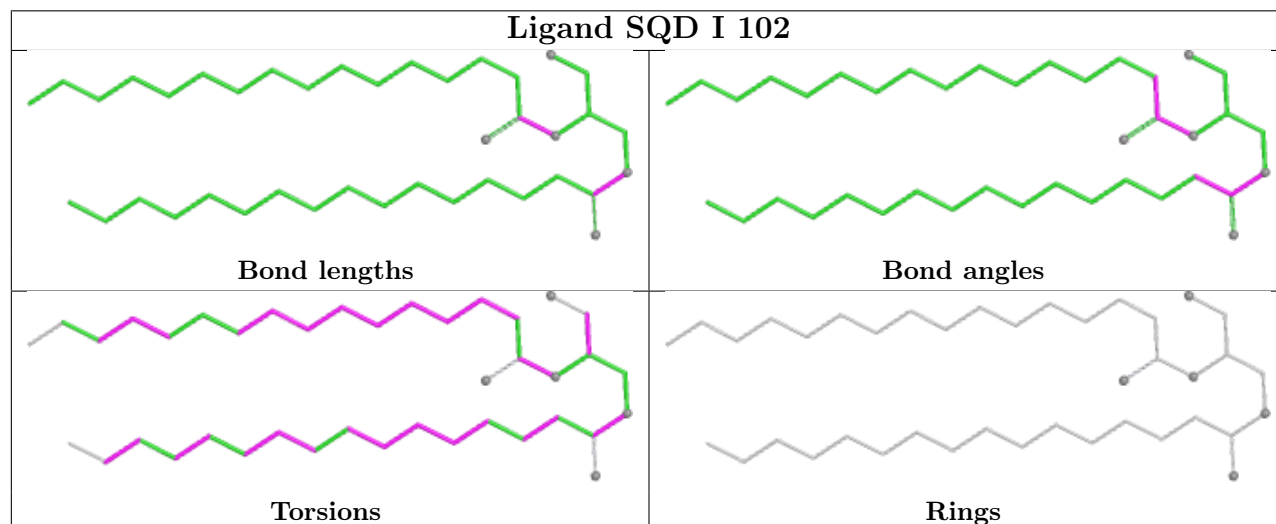
Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

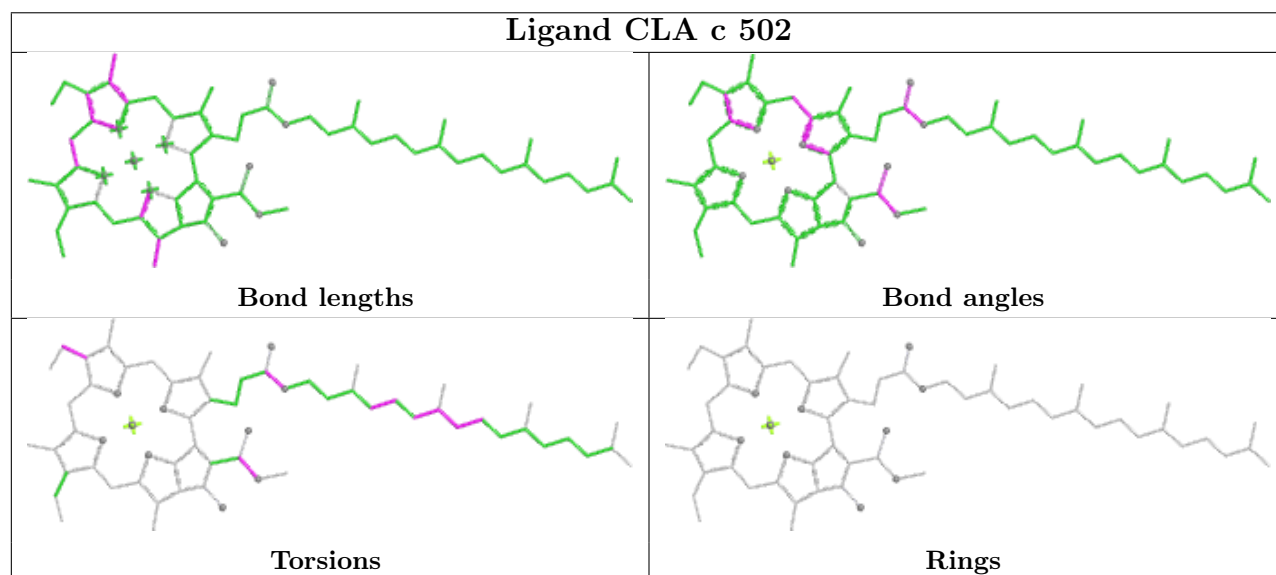
Ligand CLA c 509

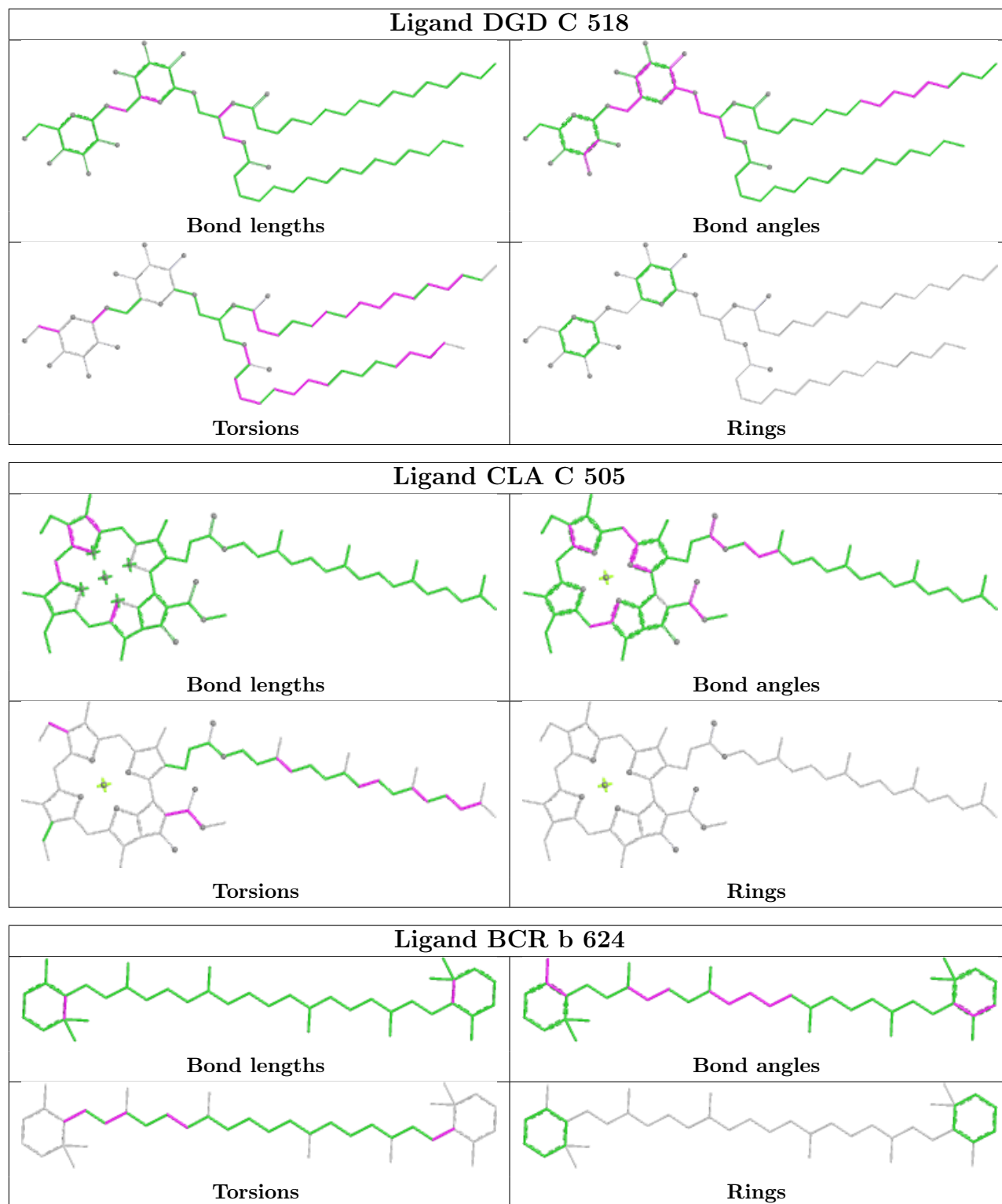


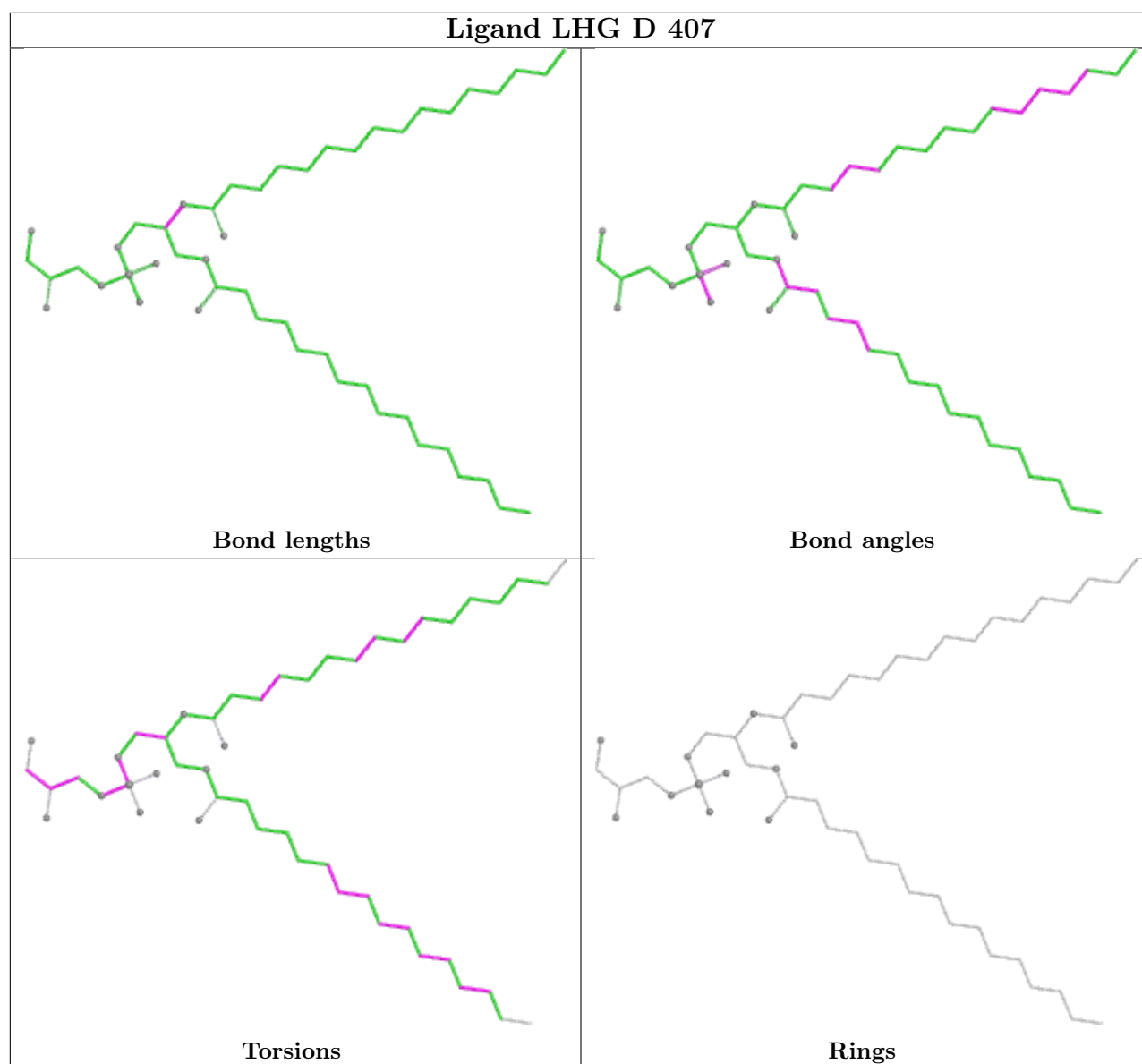
Ligand SQD I 102

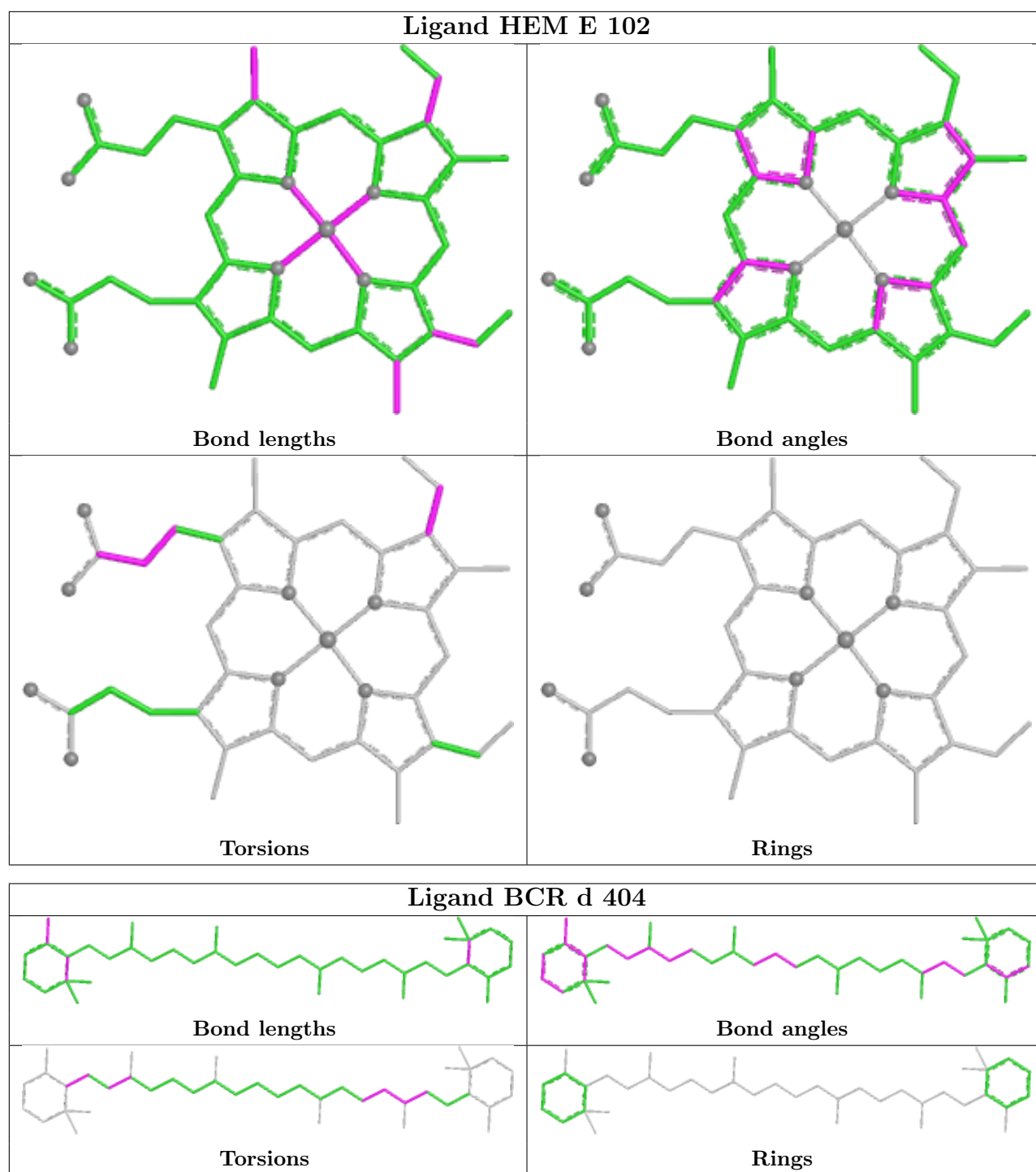


Ligand CLA c 502

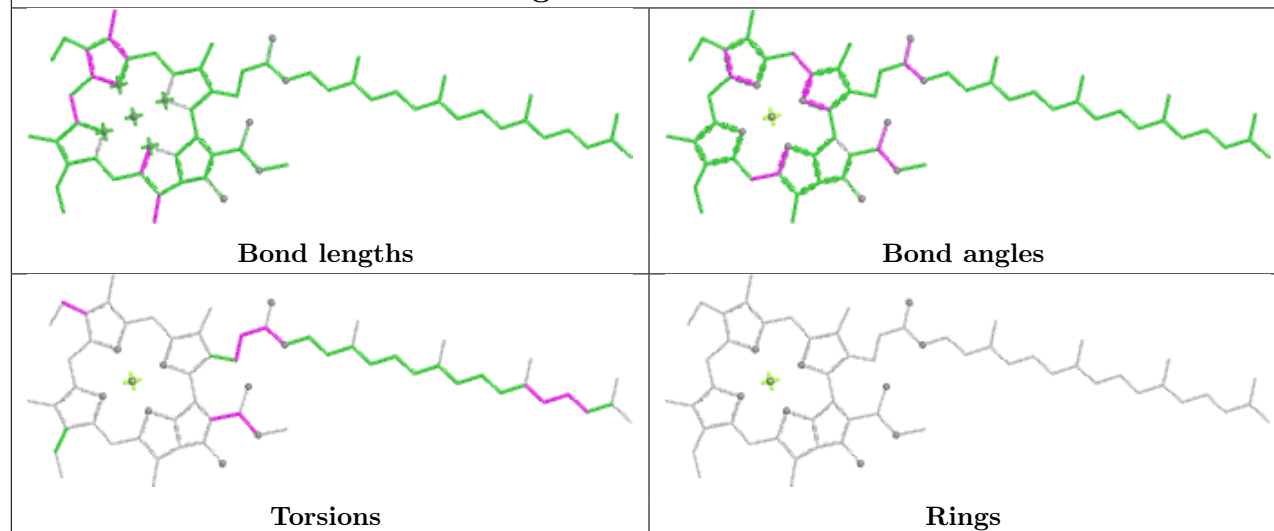




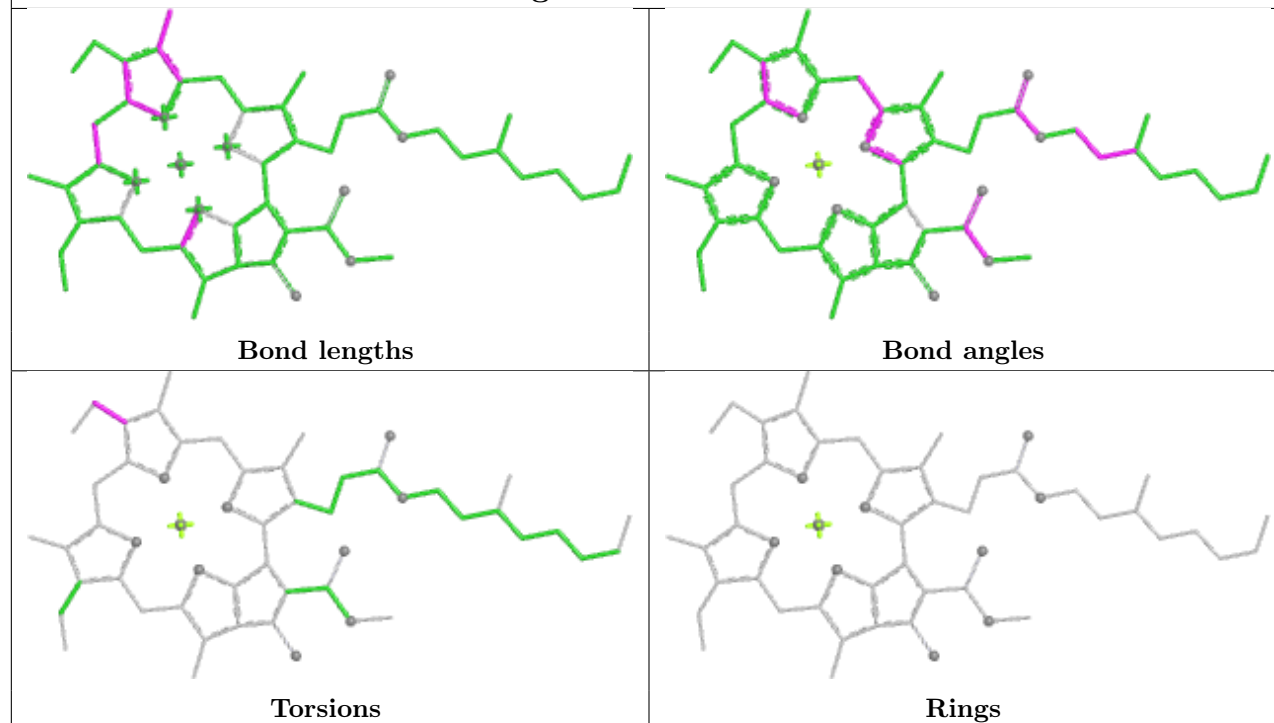




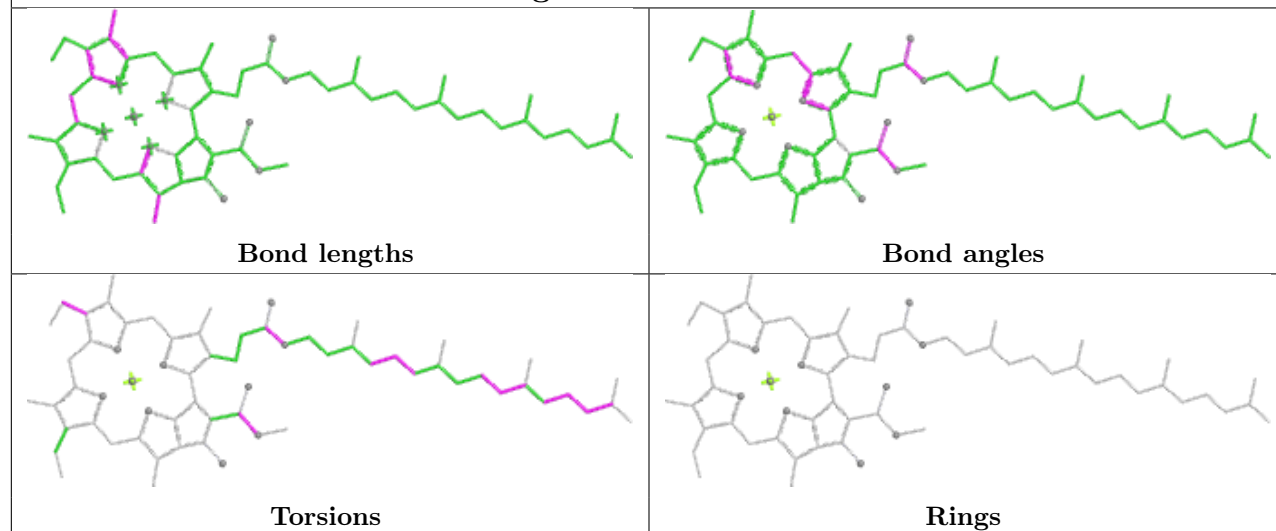
Ligand CLA C 502



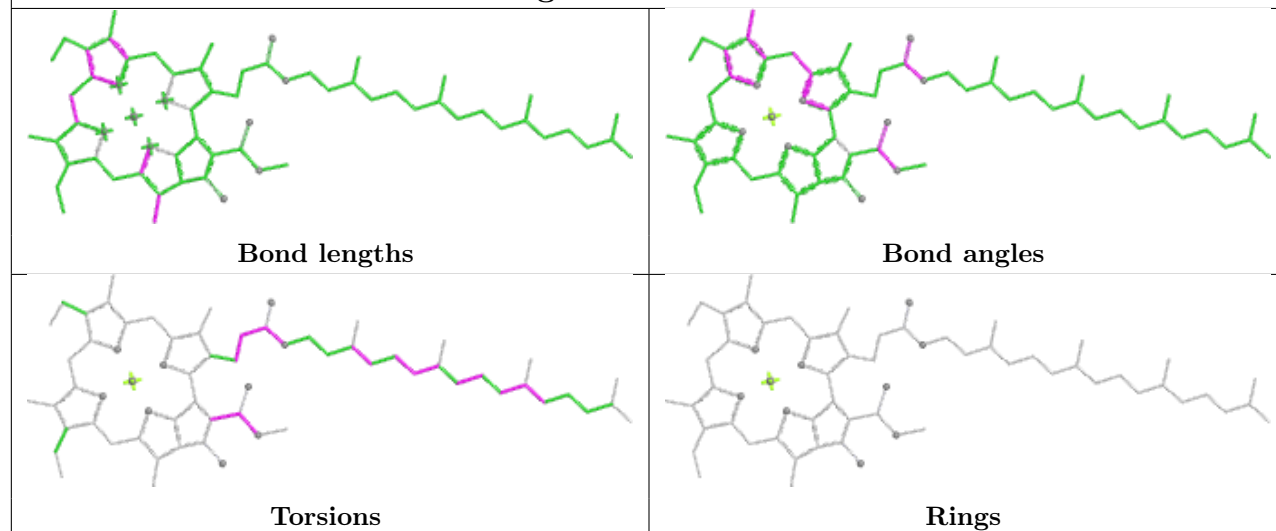
Ligand CLA A 609



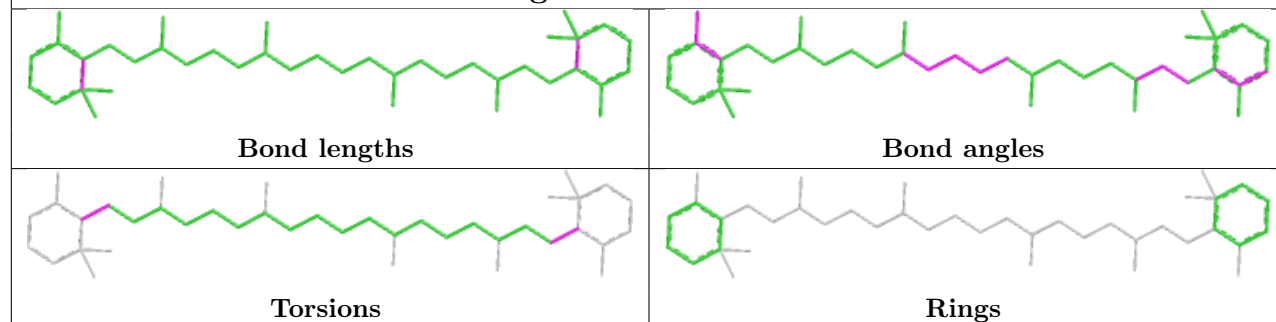
Ligand CLA C 507

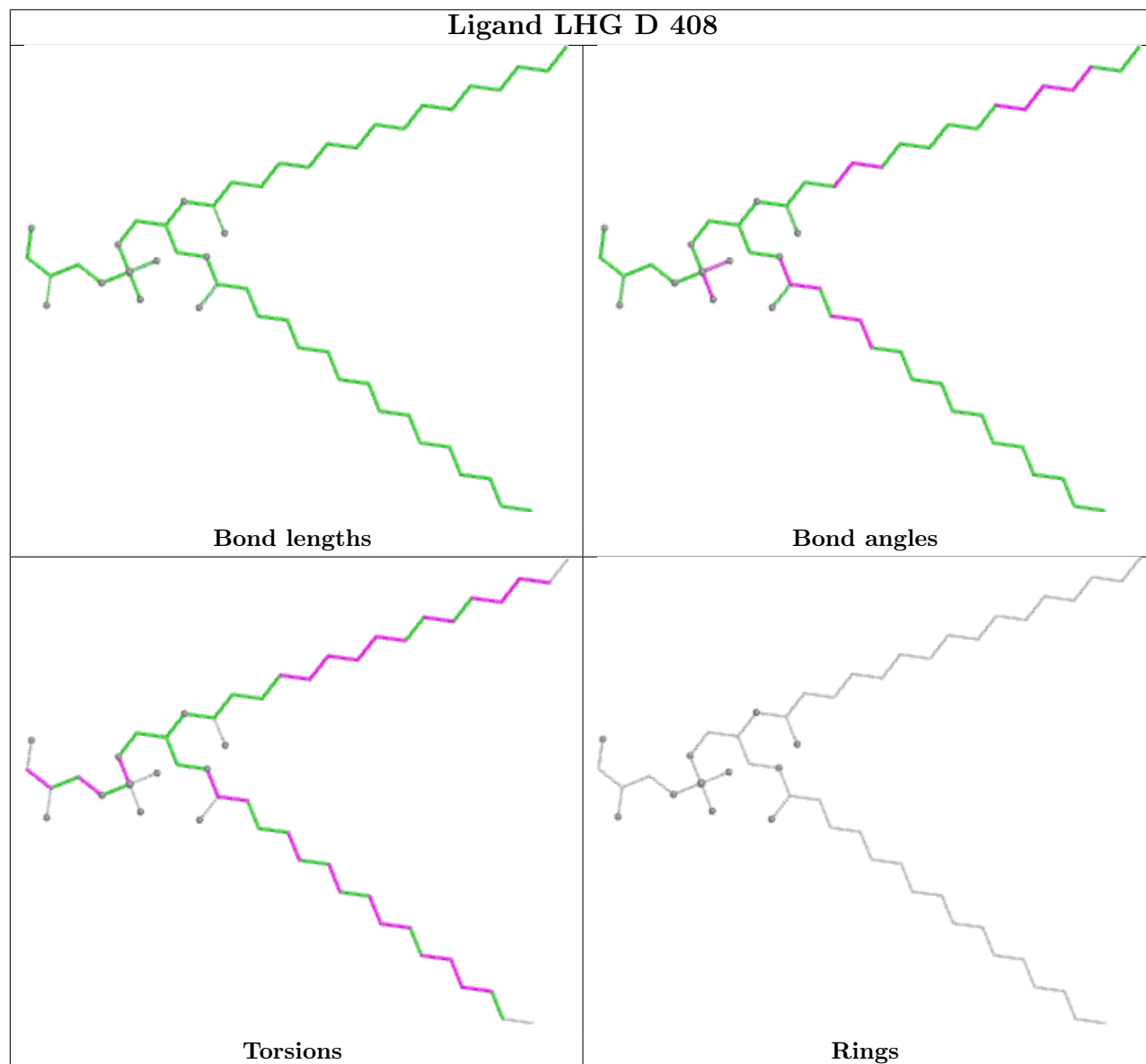
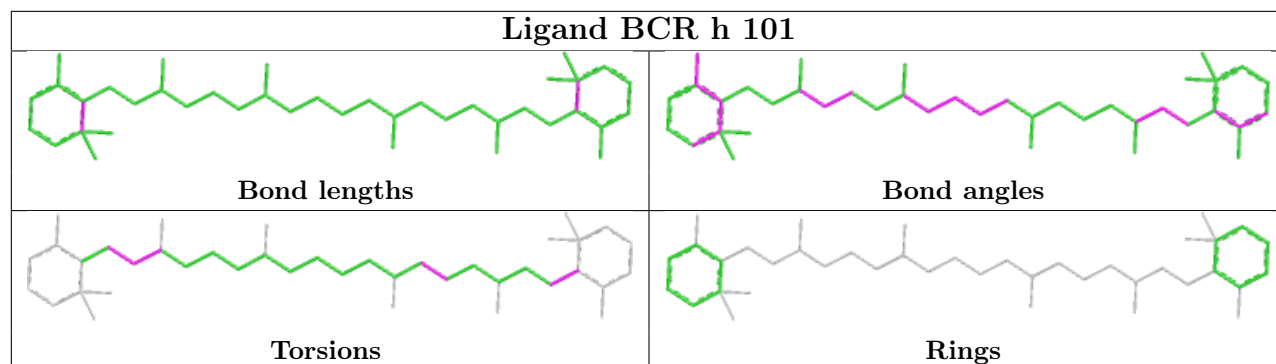


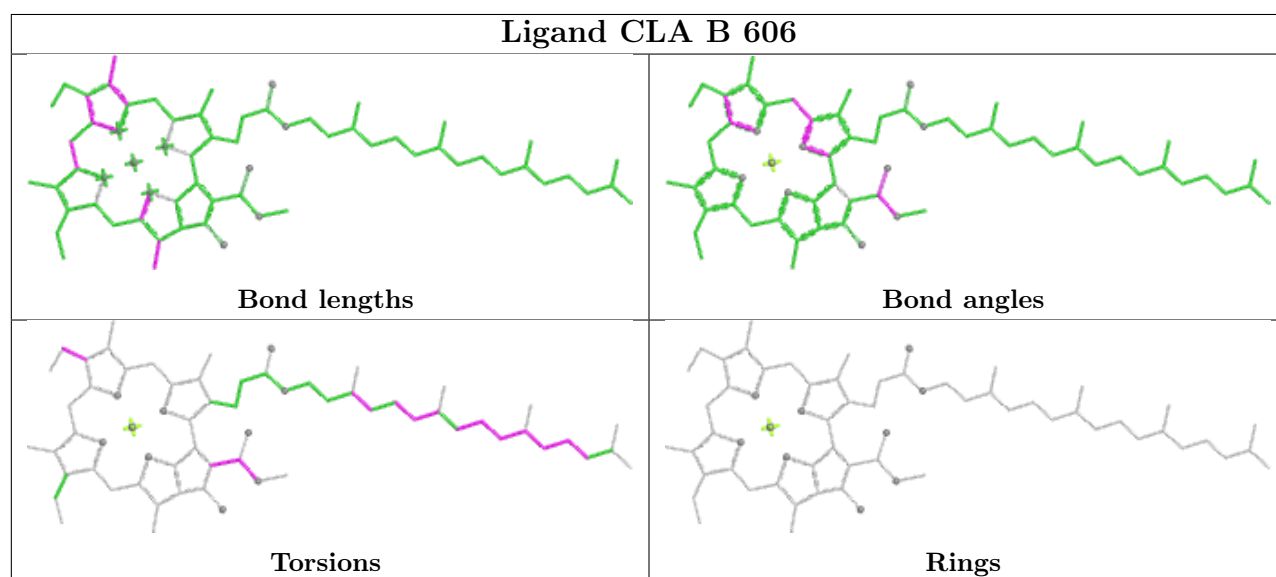
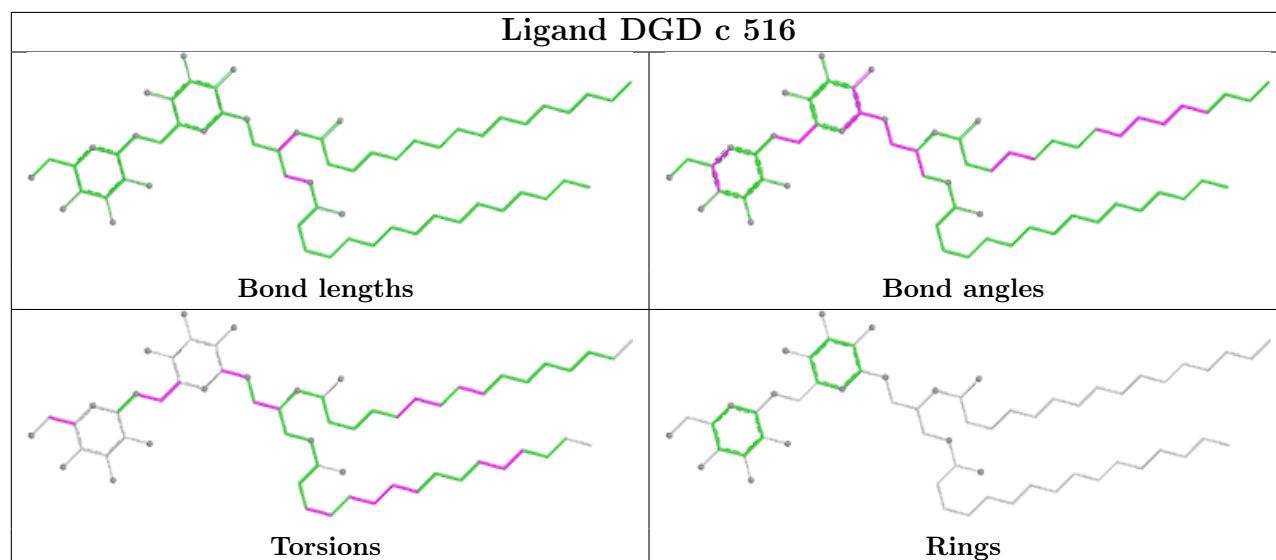
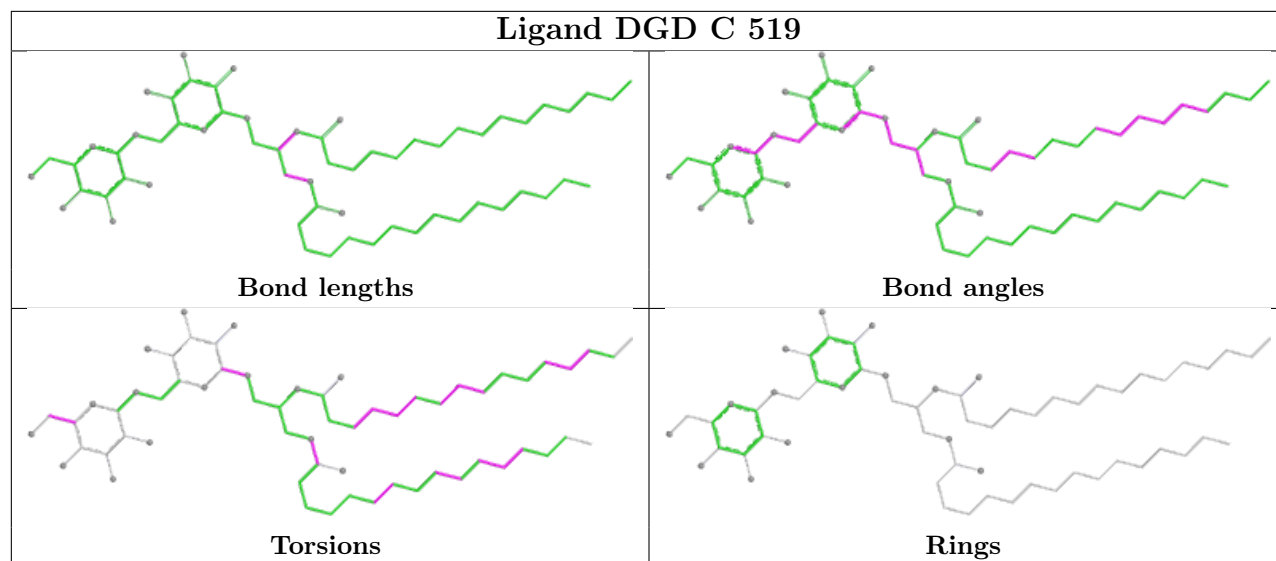
Ligand CLA c 510

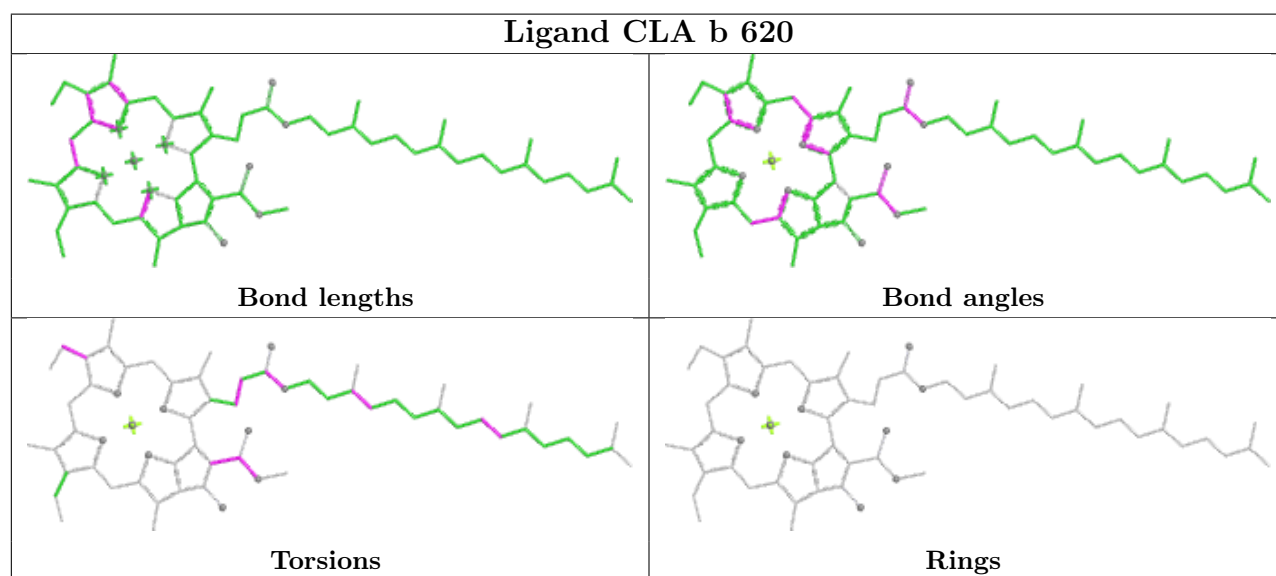
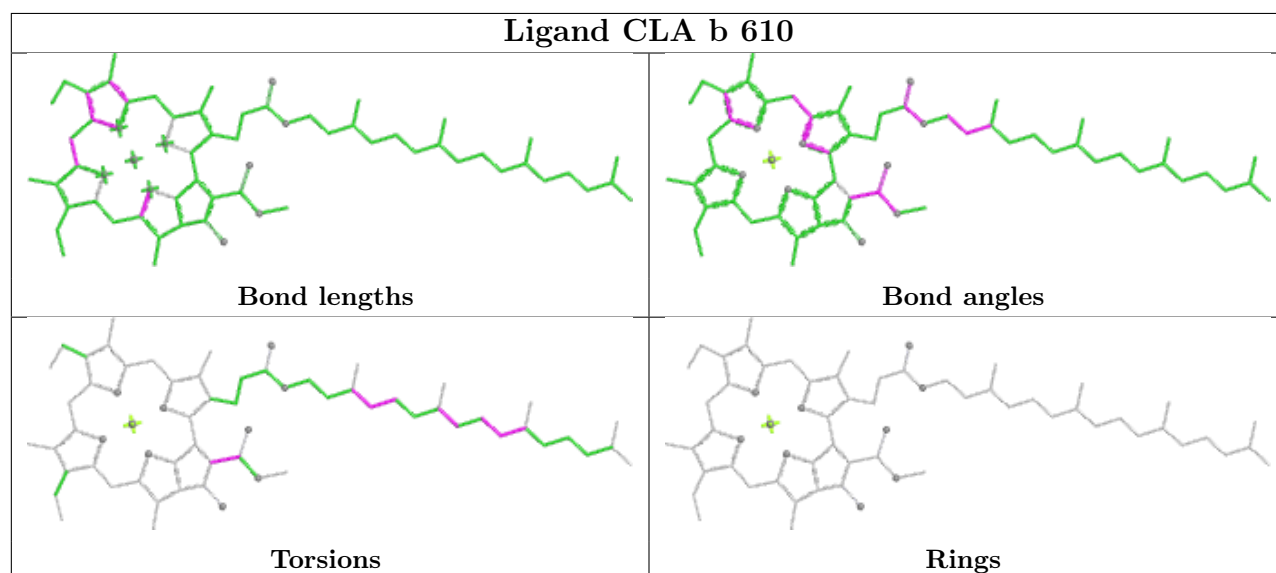
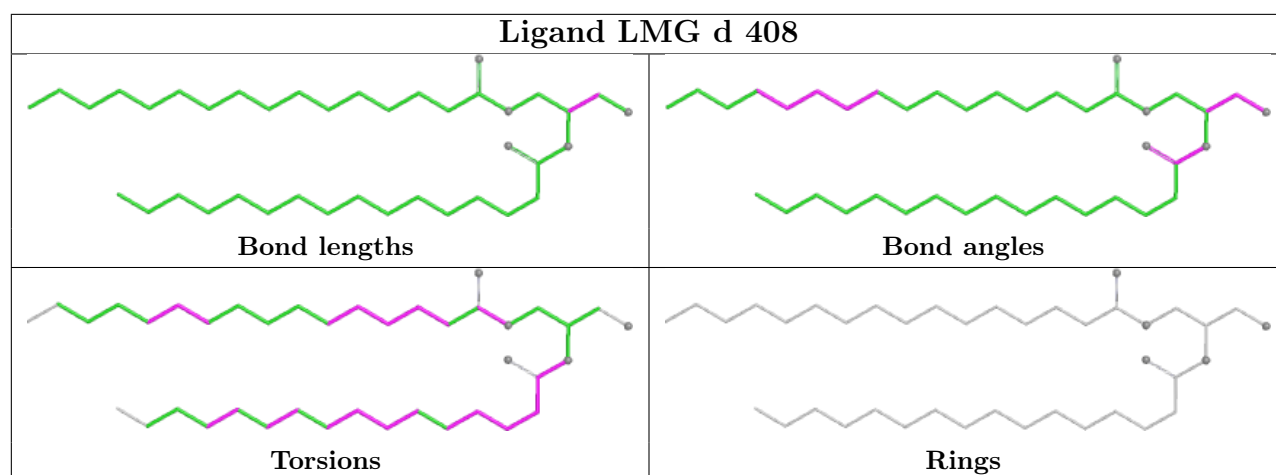


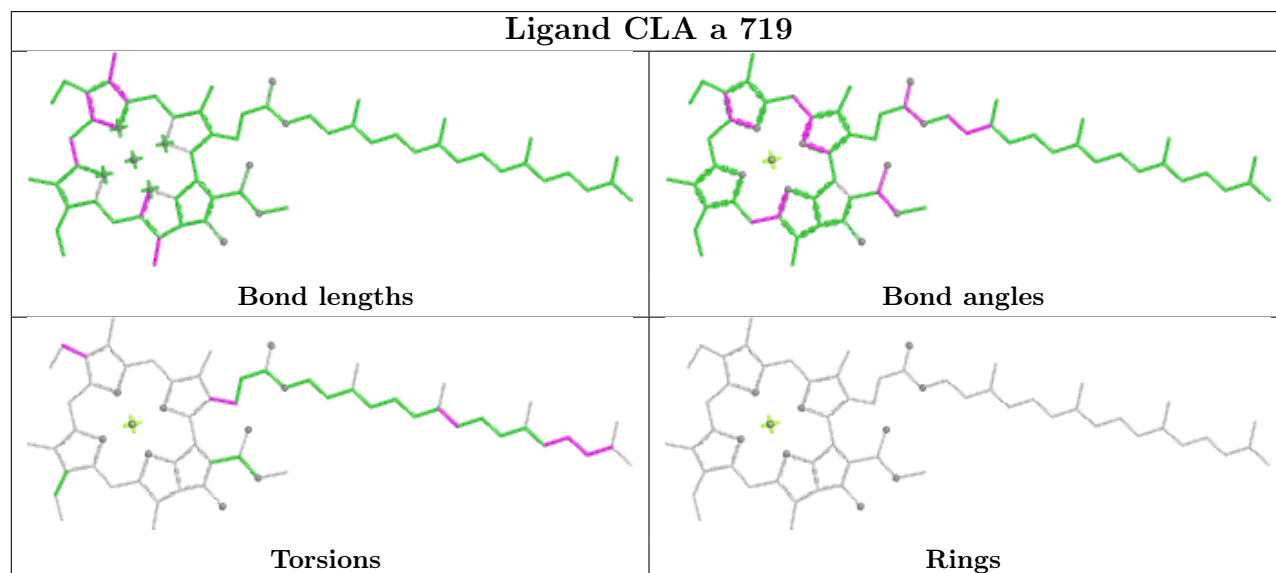
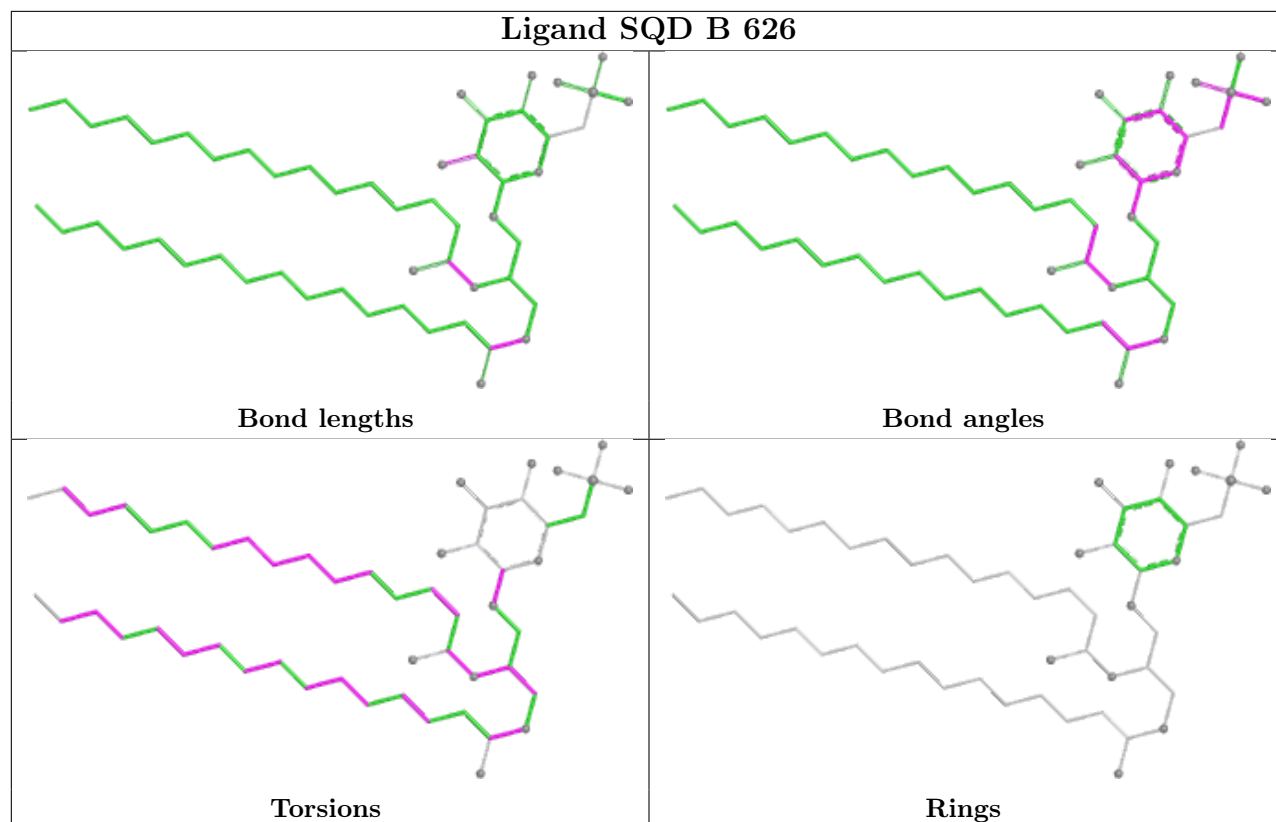
Ligand BCR A 610



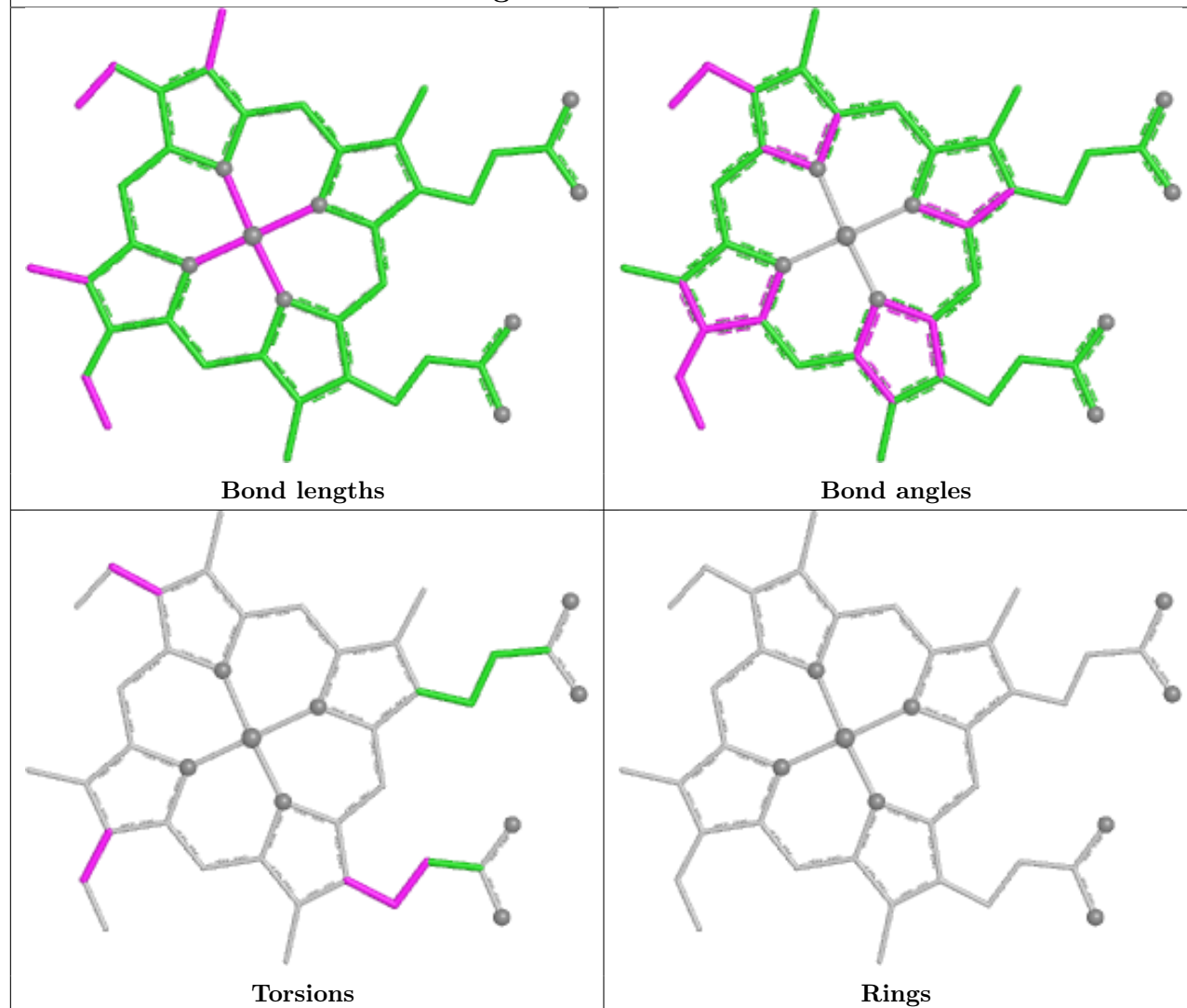




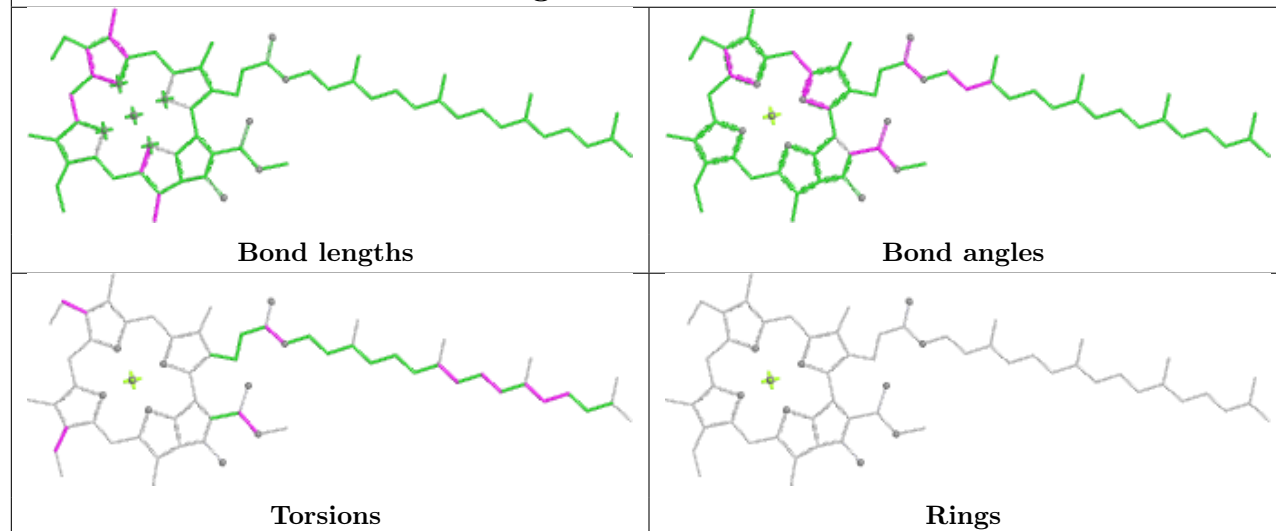


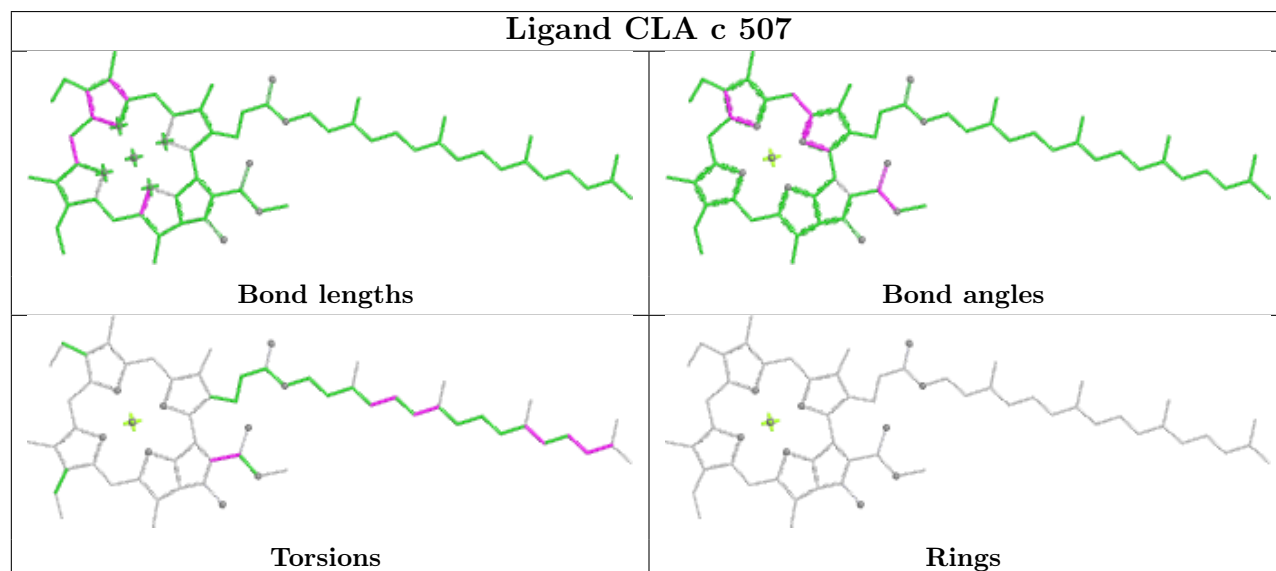
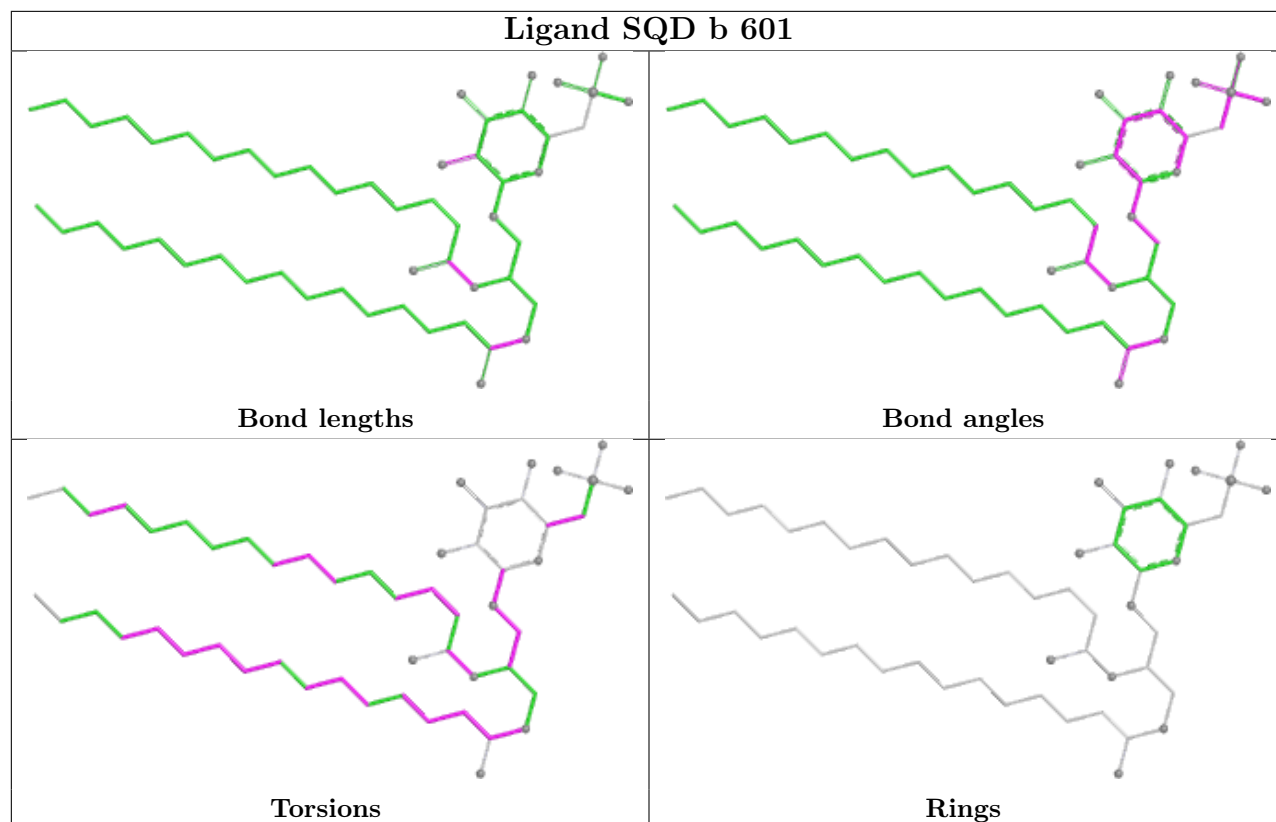


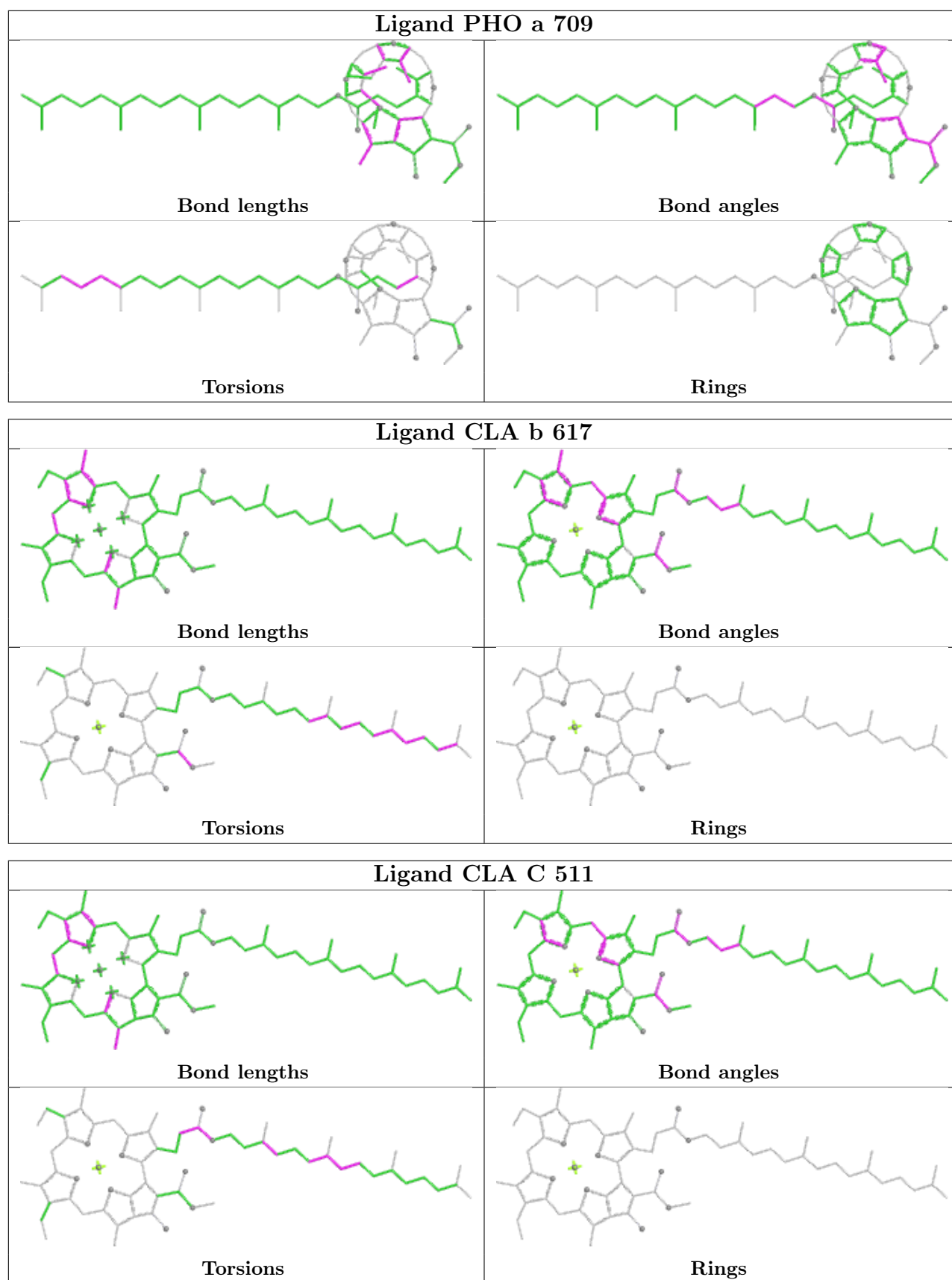
Ligand HEC V 201

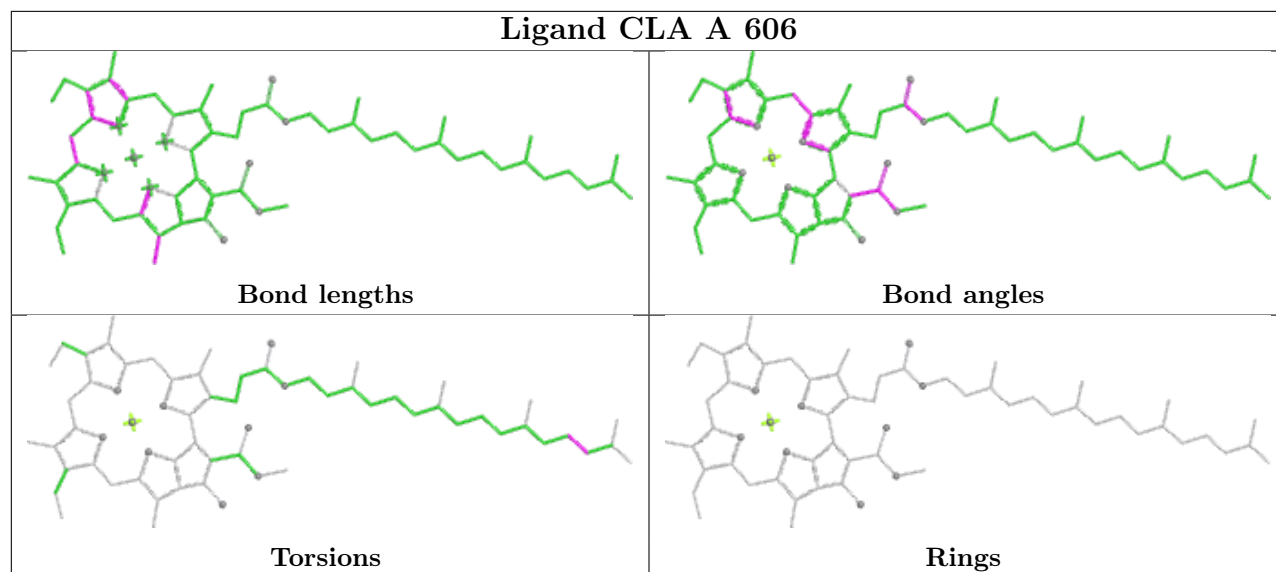
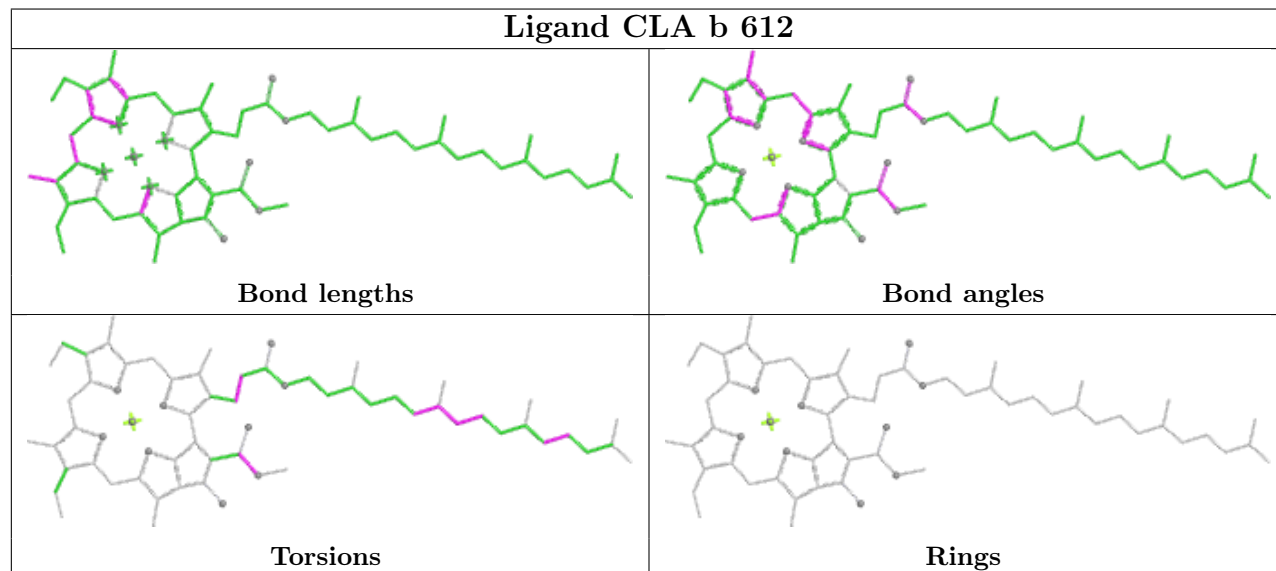


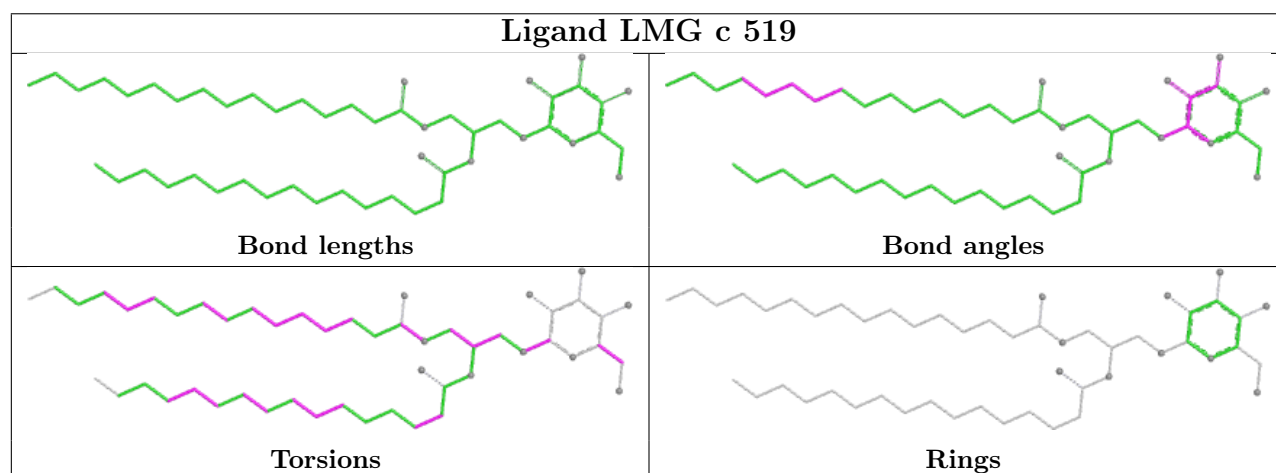
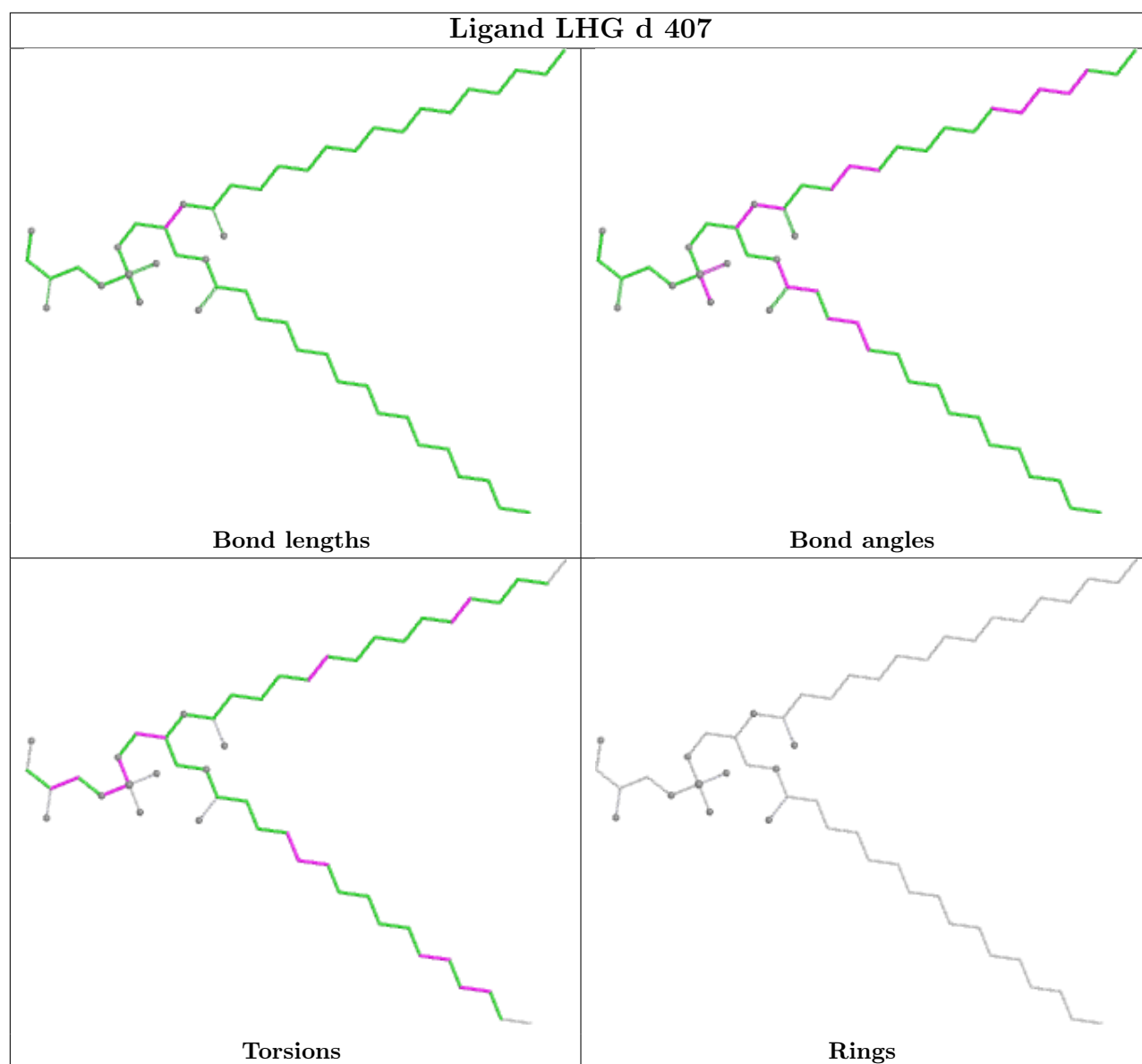
Ligand CLA B 605

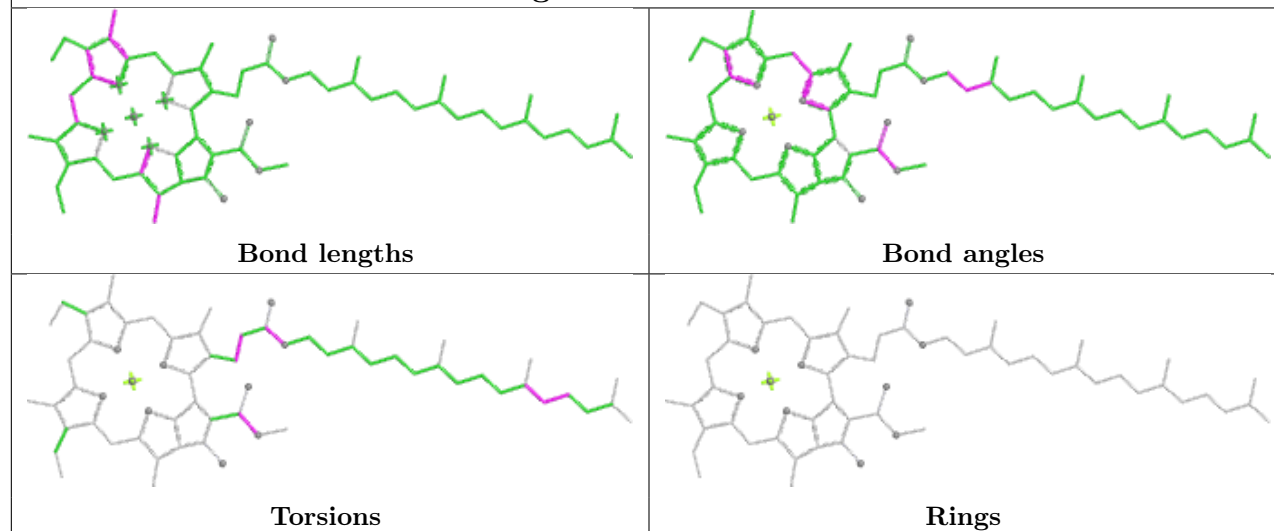
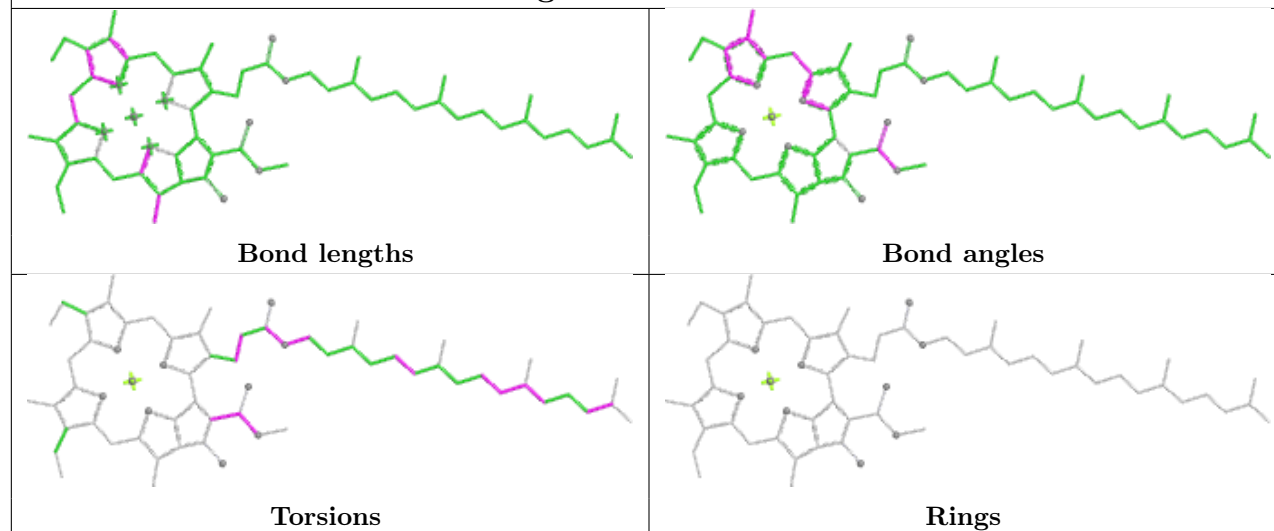


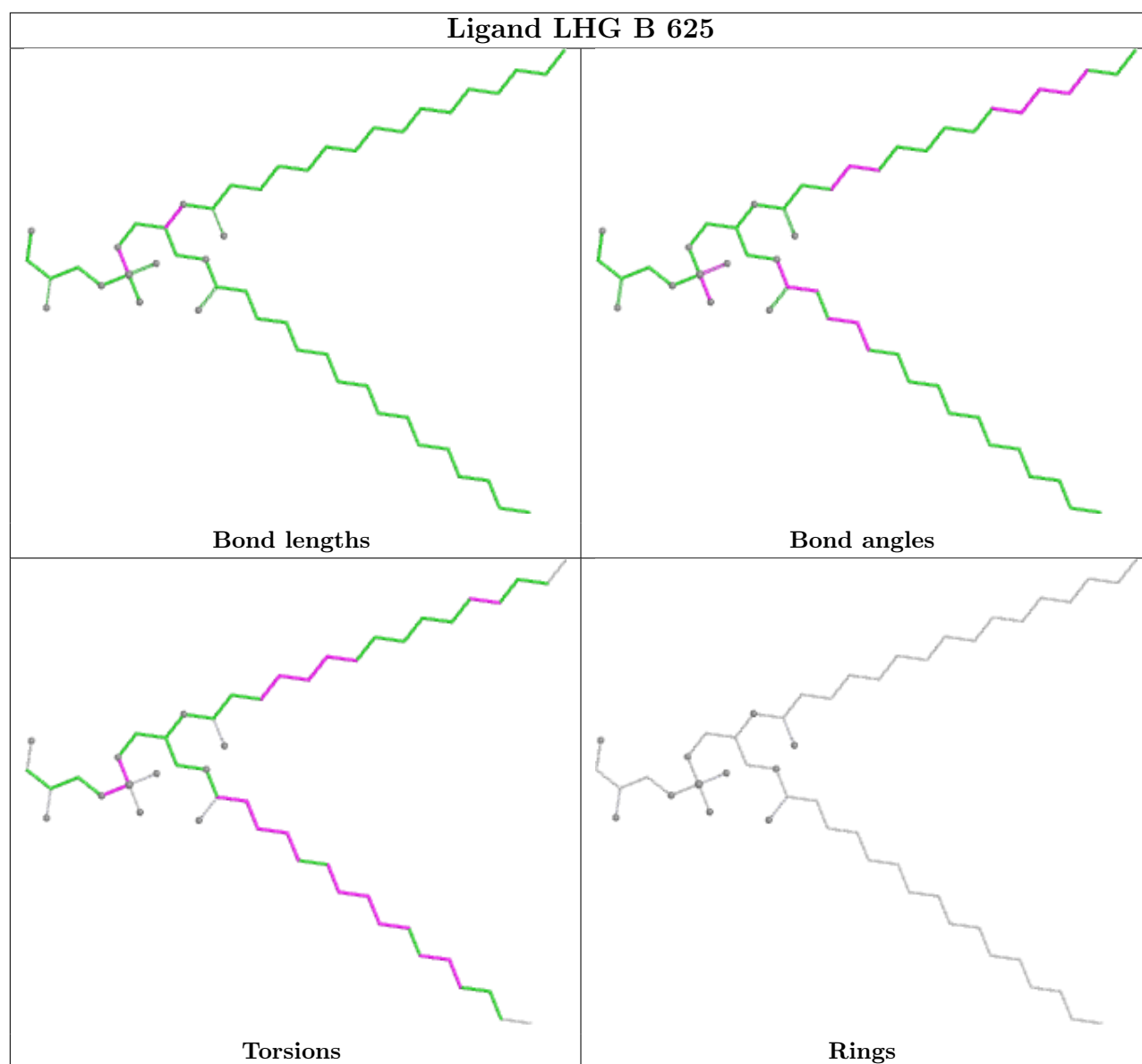


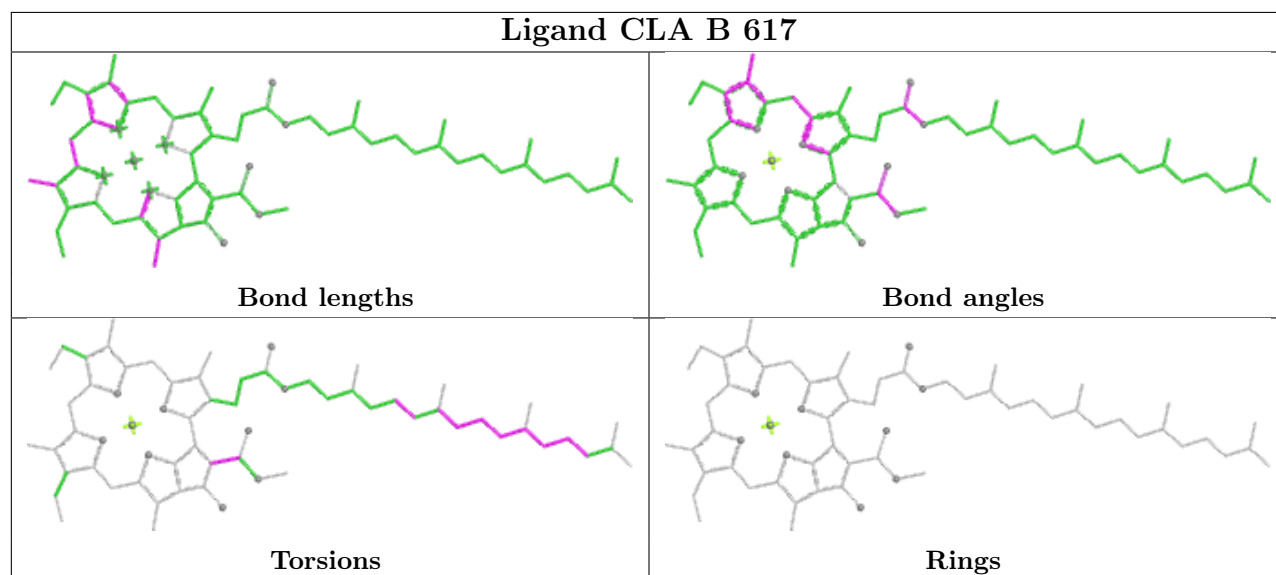
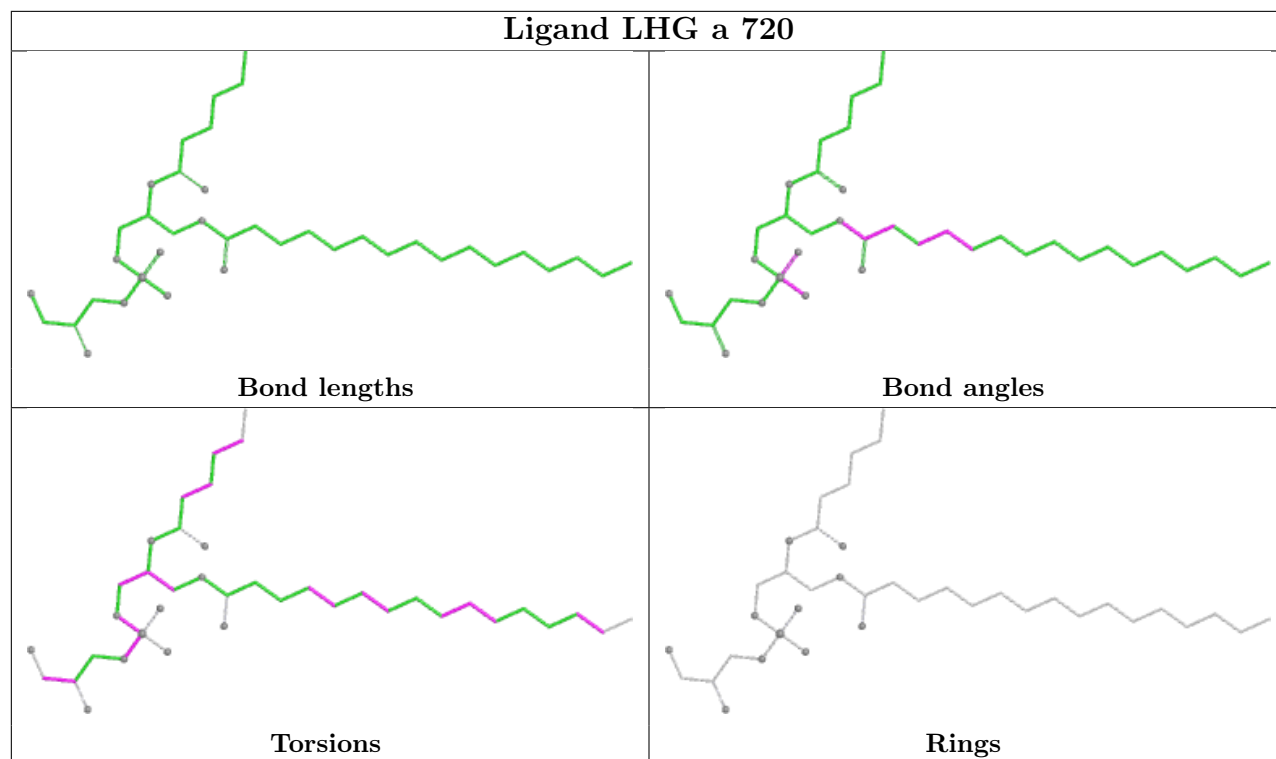


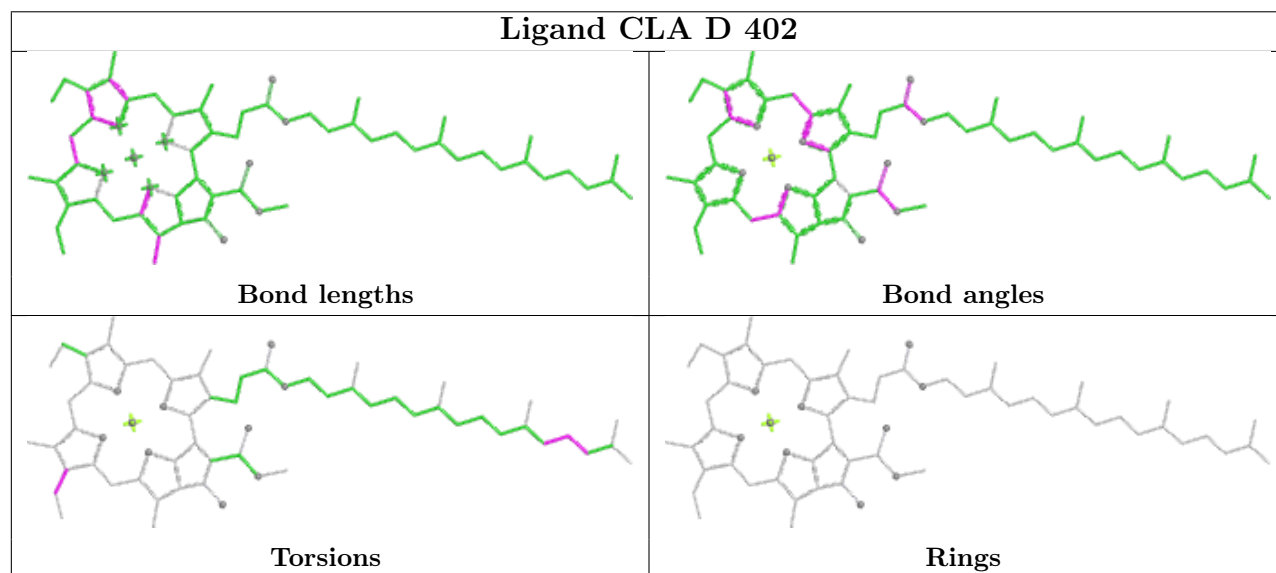
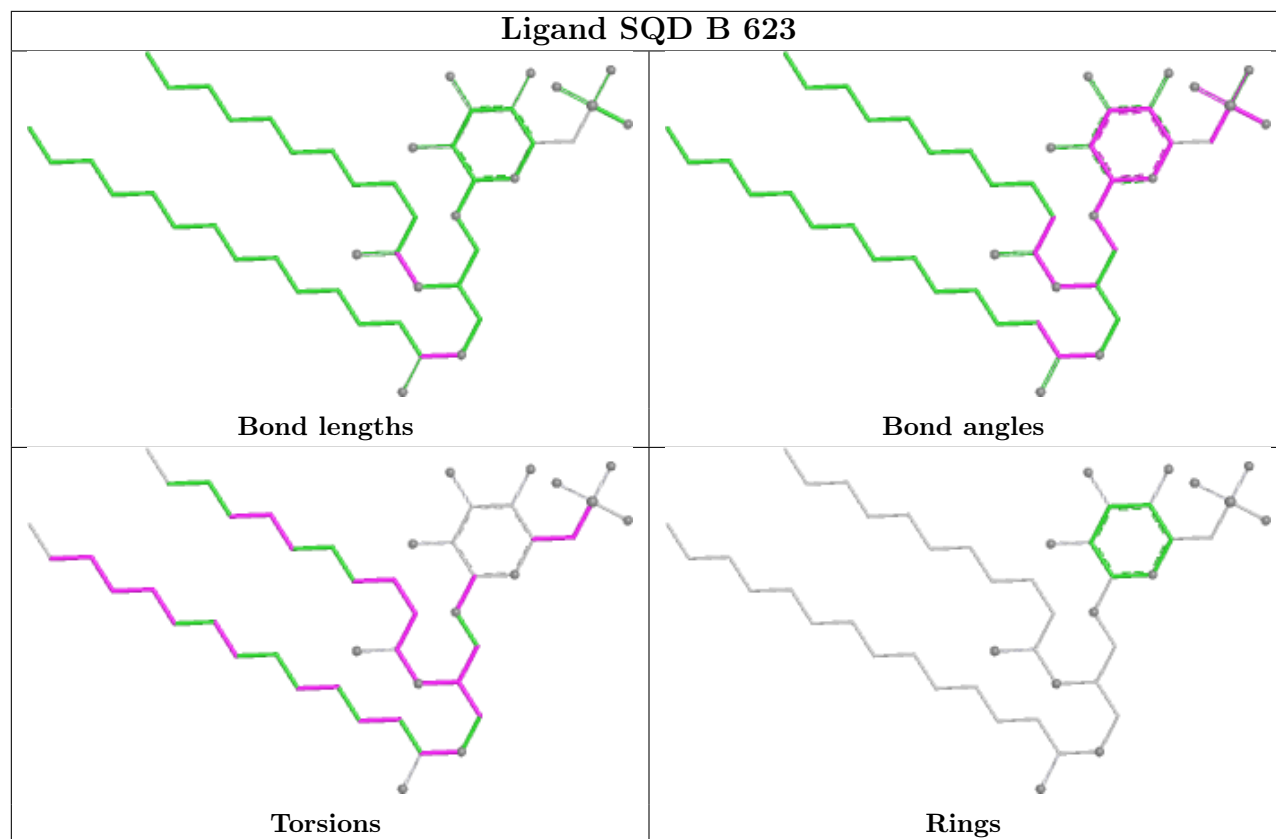
Ligand CLA A 606**Ligand CLA b 612**



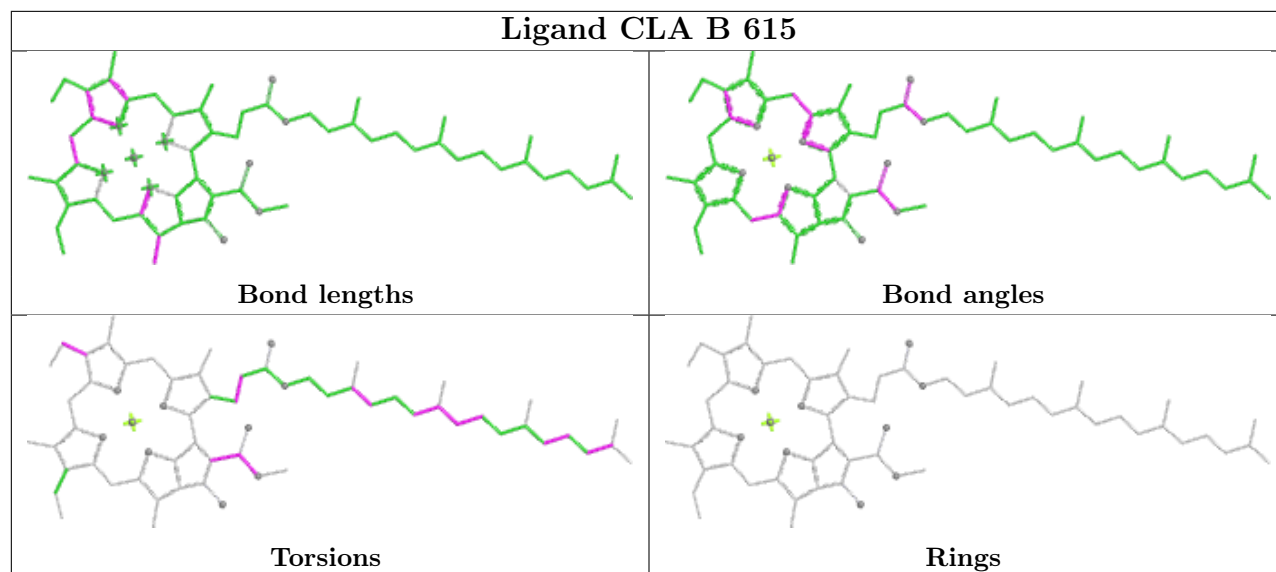
Ligand CLA C 506**Ligand CLA c 512**



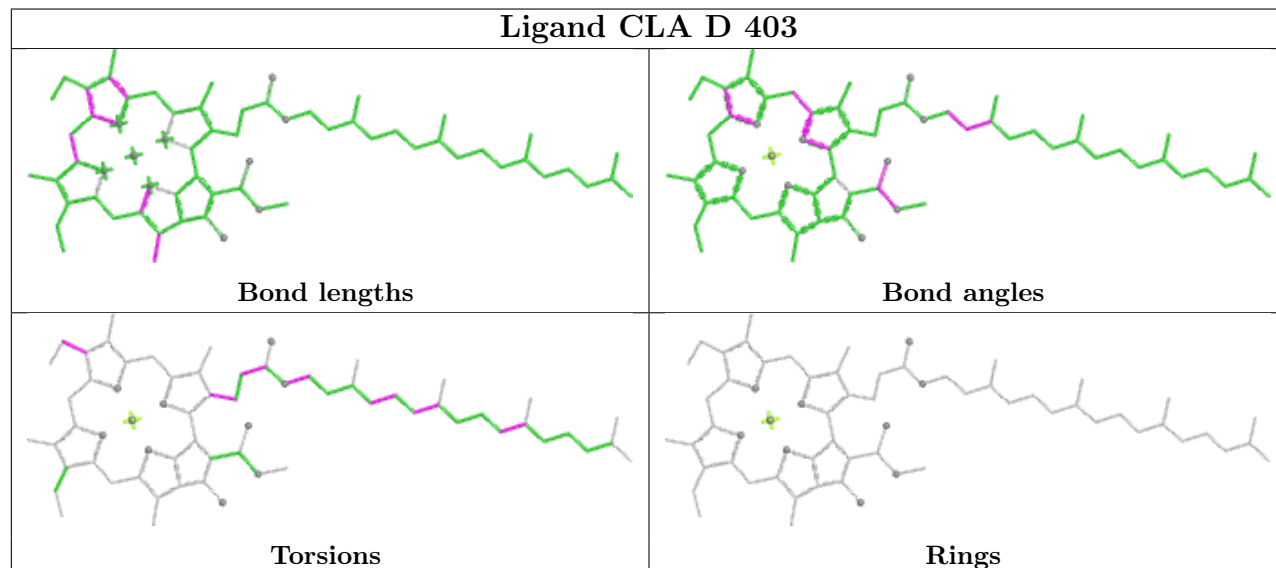


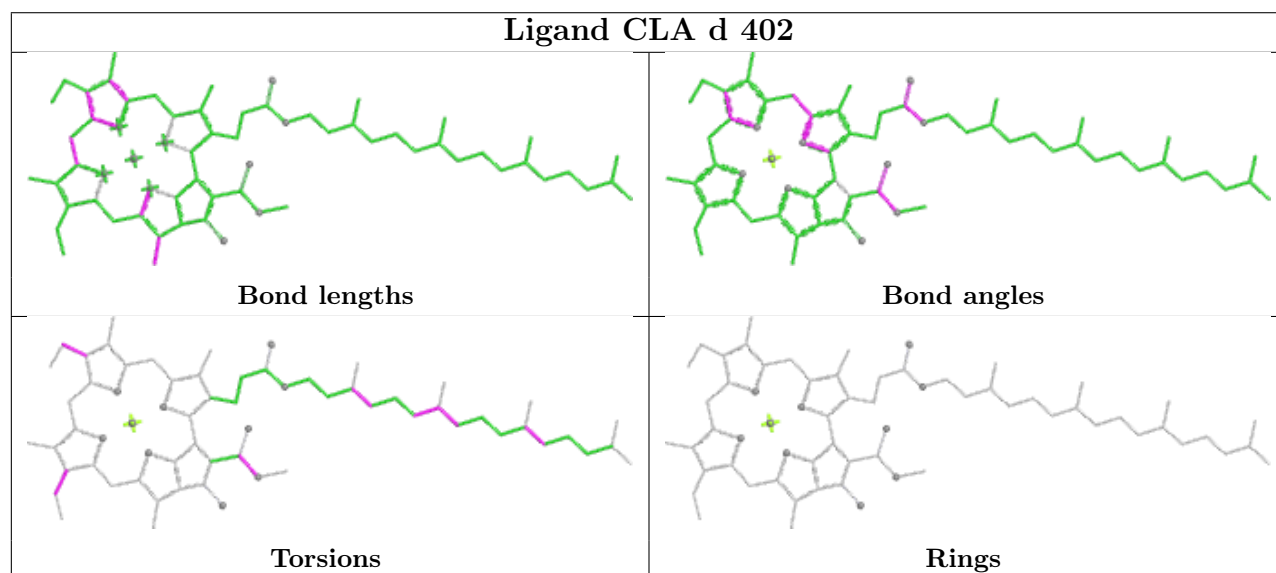
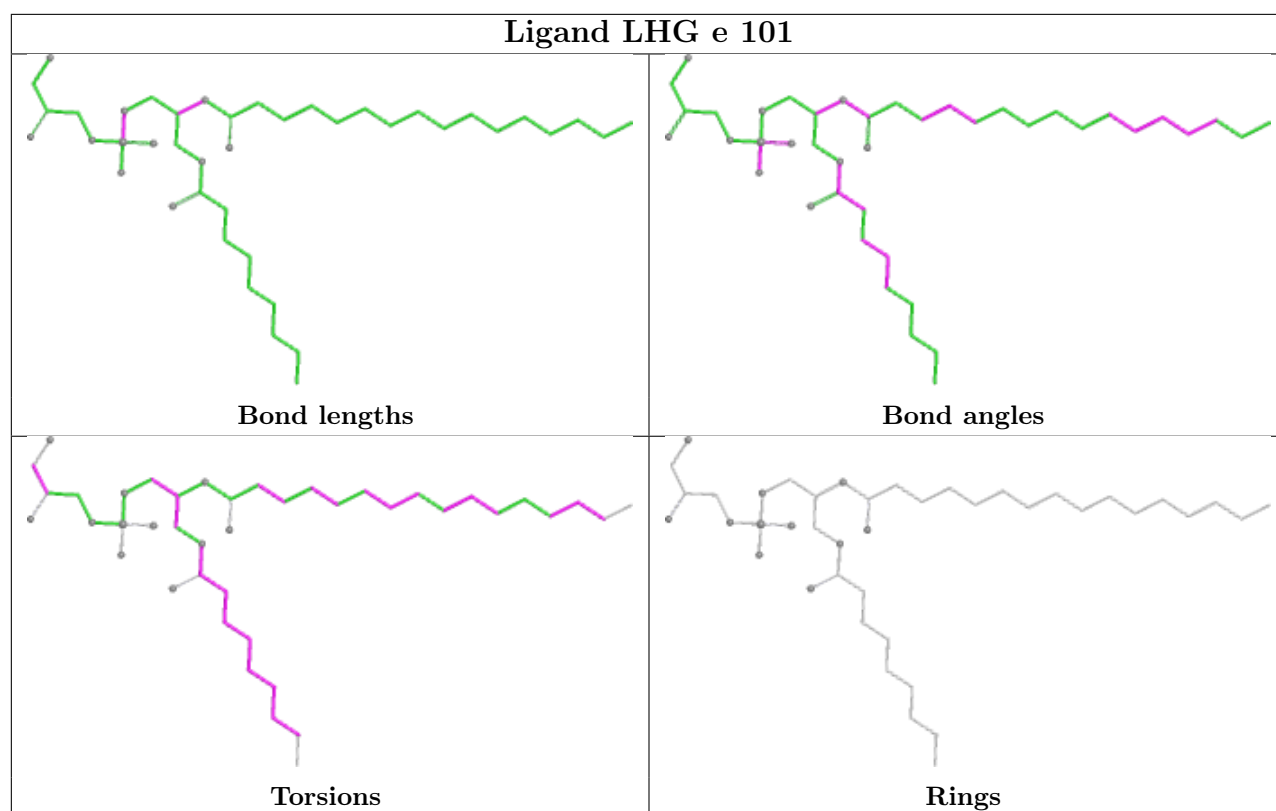


Ligand CLA B 615

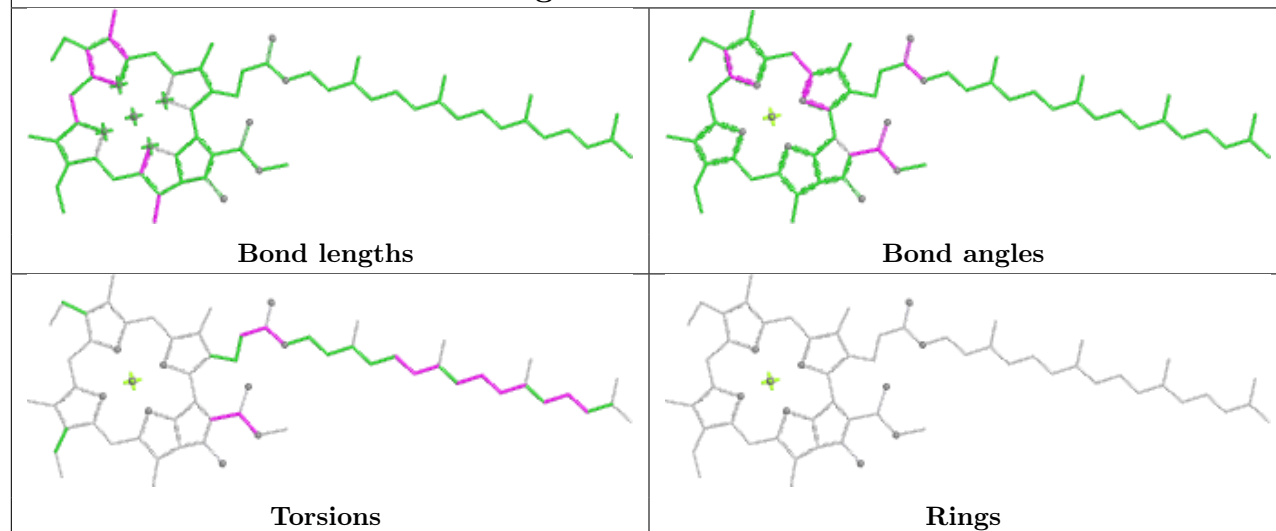


Ligand CLA D 403

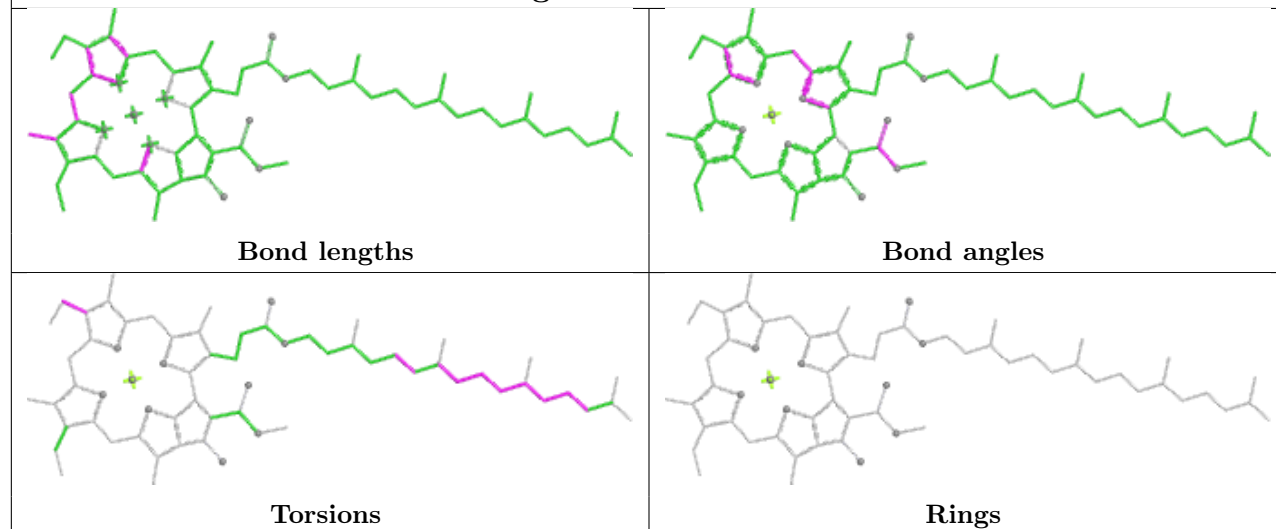




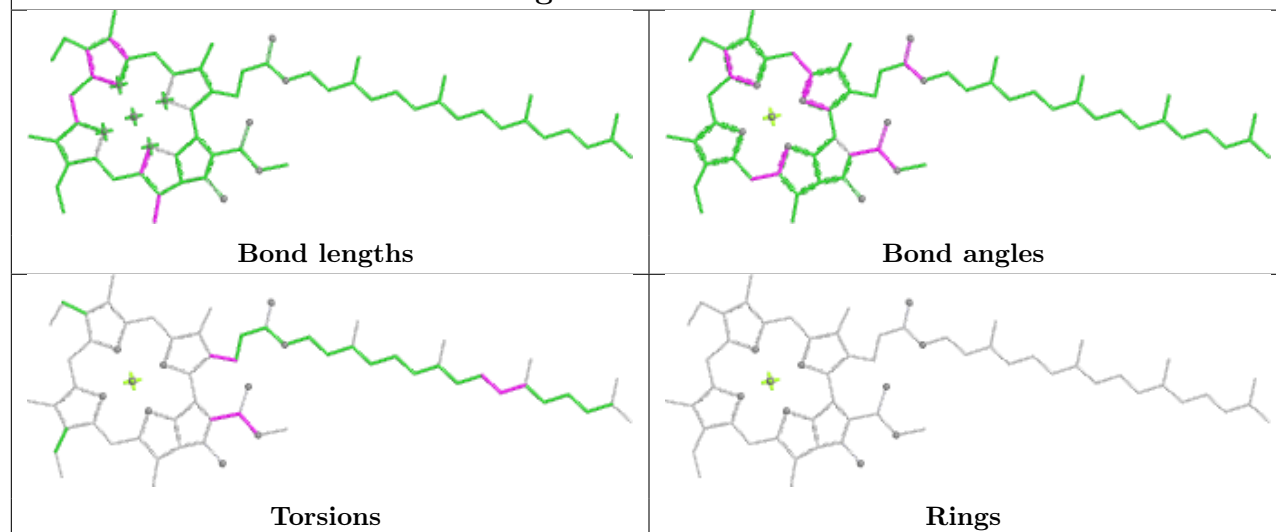
Ligand CLA b 607

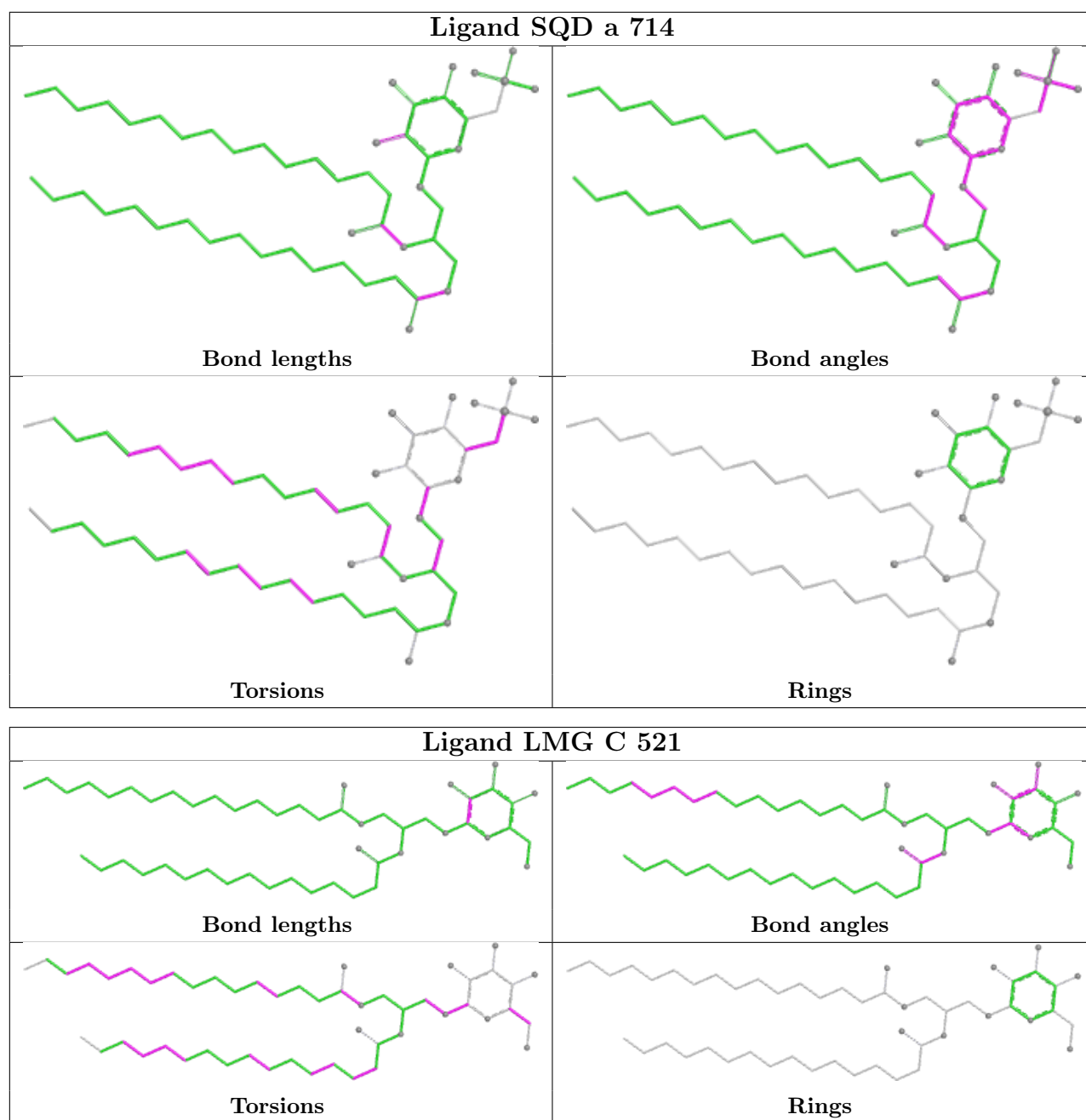


Ligand CLA B 616



Ligand CLA b 613





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	0.33	3 (0%) 81 74	38, 46, 69, 82	0
1	a	334/344 (97%)	0.43	13 (3%) 43 34	35, 48, 71, 82	0
2	B	504/510 (98%)	0.45	12 (2%) 59 49	38, 50, 74, 98	0
2	b	504/510 (98%)	0.51	27 (5%) 31 24	38, 50, 75, 93	1 (0%)
3	C	451/461 (97%)	0.51	9 (1%) 65 56	41, 54, 71, 90	0
3	c	451/461 (97%)	0.71	19 (4%) 40 32	39, 55, 74, 90	0
4	D	341/352 (96%)	0.29	3 (0%) 81 74	37, 48, 63, 82	0
4	d	341/352 (96%)	0.47	7 (2%) 63 54	40, 50, 67, 85	0
5	E	81/84 (96%)	0.85	5 (6%) 26 20	47, 67, 79, 85	0
5	e	82/84 (97%)	1.00	7 (8%) 16 12	52, 70, 85, 87	0
6	F	34/45 (75%)	0.63	0 100 100	54, 64, 78, 84	0
6	f	34/45 (75%)	0.73	1 (2%) 53 43	56, 63, 77, 80	0
7	H	63/63 (100%)	0.52	2 (3%) 50 40	43, 55, 68, 73	0
7	h	63/63 (100%)	0.56	2 (3%) 50 40	48, 56, 64, 68	0
8	I	35/38 (92%)	0.56	1 (2%) 53 43	43, 53, 83, 94	0
8	i	35/38 (92%)	0.60	4 (11%) 10 7	44, 51, 82, 89	0
9	J	36/40 (90%)	0.86	0 100 100	56, 64, 86, 99	0
9	j	36/40 (90%)	0.80	1 (2%) 55 45	55, 66, 85, 89	0
10	K	37/46 (80%)	0.94	2 (5%) 31 24	62, 68, 83, 89	0
10	k	37/46 (80%)	1.01	2 (5%) 31 24	60, 70, 84, 89	0
11	L	37/37 (100%)	0.18	0 100 100	34, 45, 82, 93	0
11	l	37/37 (100%)	0.32	1 (2%) 56 46	36, 47, 81, 90	0
12	M	32/36 (88%)	0.10	1 (3%) 51 41	38, 47, 71, 83	0
12	m	32/36 (88%)	0.15	0 100 100	36, 47, 71, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.62	11 (4%) 38 30	42, 57, 87, 106	0
13	o	244/272 (89%)	0.77	16 (6%) 24 18	43, 56, 89, 116	0
14	T	29/32 (90%)	0.25	1 (3%) 48 39	37, 46, 69, 87	0
14	t	29/32 (90%)	0.39	1 (3%) 48 39	38, 48, 70, 79	0
15	U	97/134 (72%)	0.48	2 (2%) 63 54	45, 58, 75, 86	0
15	u	97/134 (72%)	0.48	3 (3%) 51 41	47, 55, 69, 84	0
16	V	137/163 (84%)	0.58	1 (0%) 84 77	45, 55, 67, 85	0
16	v	137/163 (84%)	0.83	5 (3%) 46 37	49, 63, 79, 100	0
17	Y	27/46 (58%)	1.02	0 100 100	68, 75, 87, 95	0
17	y	30/46 (65%)	1.22	1 (3%) 49 39	69, 79, 89, 90	0
18	X	38/41 (92%)	0.50	1 (2%) 57 47	52, 60, 82, 93	0
18	x	38/41 (92%)	0.81	0 100 100	54, 63, 80, 92	0
19	Z	62/62 (100%)	1.44	15 (24%) 2 1	62, 76, 100, 113	0
19	z	62/62 (100%)	1.28	14 (22%) 2 1	67, 82, 101, 112	0
20	R	34/41 (82%)	1.75	11 (32%) 1 1	70, 82, 94, 95	0
20	r	34/41 (82%)	1.40	7 (20%) 2 2	70, 84, 94, 101	0
All	All	5310/5694 (93%)	0.57	211 (3%) 42 33	34, 53, 81, 116	1 (0%)

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	453	ALA	6.0
3	C	142	GLU	5.7
4	D	238	THR	4.8
2	B	488	PRO	4.7
19	Z	7	LEU	4.7
16	v	18	THR	4.3
2	b	487	SER	4.2
13	o	99	ASP	4.2
13	o	58	ASN	4.0
20	R	5	VAL	4.0
13	O	63	ALA	3.9
2	B	487	SER	3.8
4	d	240	ALA	3.8
2	b	500	GLY	3.7
3	C	23	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
19	Z	9	LEU	3.7
2	b	375	GLY	3.5
4	d	231	THR	3.4
14	t	30	THR	3.4
13	o	56	PRO	3.4
2	b	485	GLU	3.4
19	Z	41	PHE	3.4
3	c	454	GLY	3.3
19	Z	8	ALA	3.3
2	b	496	TYR	3.3
1	A	248	ILE	3.2
14	T	30	THR	3.2
15	u	33	ALA	3.2
5	e	5	THR	3.2
2	b	486	LEU	3.1
8	i	36	ASP	3.1
19	z	39	LEU	3.1
13	o	61	GLN	3.0
2	B	486	LEU	3.0
5	E	60	GLN	3.0
13	O	245	PRO	3.0
1	a	11	ALA	3.0
2	b	489	GLU	3.0
13	O	61	GLN	3.0
15	U	53	ALA	3.0
20	R	9	LEU	2.9
13	O	35	SER	2.9
13	O	98	GLU	2.9
2	b	504	THR	2.9
2	B	505	ARG	2.9
20	R	23	ILE	2.9
3	c	376	ASP	2.9
19	Z	2	THR	2.9
1	A	246	TYR	2.8
3	C	457	LYS	2.8
13	o	54	GLU	2.8
3	c	451	ALA	2.8
2	b	503	THR	2.8
13	o	60	ARG	2.8
2	B	167	TRP	2.8
13	O	244	GLU	2.7
19	Z	61	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	c	331	ALA	2.7
4	D	226	GLY	2.7
19	Z	62	VAL	2.7
5	e	4	THR	2.7
20	R	10	LEU	2.7
2	B	494	GLY	2.7
8	i	31	ASN	2.7
2	b	499	VAL	2.7
20	R	28	VAL	2.7
1	a	270	SER	2.7
5	E	4	THR	2.6
20	r	35	LEU	2.6
16	v	34	GLN	2.6
1	a	101	SER	2.6
13	O	67	PRO	2.6
13	o	91	GLY	2.6
1	a	245	THR	2.6
19	z	62	VAL	2.6
3	C	25	ASN	2.6
2	B	386	ALA	2.6
19	Z	29	SER	2.6
6	f	20	TRP	2.6
10	K	17	ILE	2.6
5	e	72	ALA	2.6
20	R	27	ALA	2.6
4	d	295	SER	2.5
3	C	315	MET	2.5
3	c	76	ILE	2.5
19	z	34	ASP	2.5
19	Z	57	LEU	2.5
2	B	495	PHE	2.5
13	o	4	THR	2.5
13	o	132	ASN	2.5
4	d	288	GLY	2.5
19	z	1	MET	2.5
1	a	243	GLU	2.5
19	z	32	ASP	2.5
11	l	1	MET	2.5
2	b	84	THR	2.5
1	a	13	LEU	2.4
13	o	5	LEU	2.4
16	v	19	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	478	VAL	2.4
1	a	244	GLU	2.4
2	b	127	ARG	2.4
13	O	180	GLU	2.4
20	R	3	TRP	2.4
1	A	266	ASN	2.4
19	z	3	ILE	2.4
1	a	240	GLY	2.4
7	h	64	ALA	2.4
10	k	15	TYR	2.4
13	o	6	THR	2.4
20	r	34	LEU	2.4
2	B	85	GLY	2.4
2	b	477	ASP	2.4
2	b	502	VAL	2.4
20	R	8	VAL	2.4
13	o	45	LEU	2.4
19	Z	3	ILE	2.4
19	z	10	ALA	2.3
2	b	323	GLY	2.3
13	o	62	GLU	2.3
17	y	20	ALA	2.3
18	X	2	THR	2.3
19	z	56	VAL	2.3
2	b	482	ILE	2.3
2	b	128	THR	2.3
2	b	73	GLY	2.3
3	c	23	ALA	2.3
2	b	490	GLN	2.3
13	O	57	LYS	2.3
20	r	25	PRO	2.3
5	e	79	PHE	2.2
19	z	41	PHE	2.2
3	C	29	GLU	2.2
16	v	60	ALA	2.2
3	c	125	LEU	2.2
4	d	239	GLN	2.2
5	e	84	LYS	2.2
15	u	36	ILE	2.2
3	c	425	TRP	2.2
4	d	238	THR	2.2
10	k	14	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
19	Z	4	LEU	2.2
7	H	10	ILE	2.2
20	r	32	GLN	2.2
7	H	5	THR	2.2
13	O	4	THR	2.2
3	c	127	PHE	2.2
3	c	177	ALA	2.2
20	R	13	LEU	2.2
5	E	14	ILE	2.2
5	E	12	ASP	2.2
19	z	30	PRO	2.2
20	r	3	TRP	2.2
3	C	30	SER	2.2
19	z	4	LEU	2.2
3	C	141	GLU	2.2
4	D	239	GLN	2.2
15	U	73	GLN	2.2
3	c	139	THR	2.2
2	b	82	GLY	2.2
1	a	265	PHE	2.2
3	c	45	LEU	2.2
19	Z	36	SER	2.2
16	v	1	ALA	2.2
2	b	264	PRO	2.1
1	a	59	ASP	2.1
8	I	36	ASP	2.1
2	b	494	GLY	2.1
16	V	4	THR	2.1
19	z	29	SER	2.1
13	o	64	GLU	2.1
5	e	82	GLN	2.1
19	Z	6	GLN	2.1
19	Z	53	VAL	2.1
5	e	83	LEU	2.1
19	Z	5	PHE	2.1
2	B	132	ALA	2.1
13	o	74	GLU	2.1
2	b	491	VAL	2.1
13	O	58	ASN	2.1
20	r	8	VAL	2.1
2	b	85	GLY	2.1
3	c	43	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
9	j	30	TYR	2.1
15	u	80	GLU	2.1
20	r	26	TYR	2.1
2	B	126	PRO	2.1
2	b	488	PRO	2.1
7	h	8	GLY	2.1
8	i	34	ARG	2.1
19	z	2	THR	2.1
3	c	134	ILE	2.1
10	K	14	ALA	2.1
1	a	242	GLU	2.1
12	M	31	SER	2.0
2	B	502	VAL	2.0
20	R	7	VAL	2.0
20	R	31	VAL	2.0
8	i	32	PRO	2.0
3	c	159	THR	2.0
13	o	63	ALA	2.0
4	d	241	GLU	2.0
1	a	246	TYR	2.0
19	z	27	TYR	2.0
5	E	82	GLN	2.0
3	C	369	LEU	2.0
2	b	293	ALA	2.0
3	c	133	ALA	2.0
3	c	450	ALA	2.0
3	c	452	ALA	2.0
1	a	262	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.88	0.11	42,56,71,77	0
8	FME	i	1	10/11	0.89	0.13	49,61,69,69	0
8	FME	I	1	10/11	0.89	0.14	50,60,70,76	0
14	FME	T	1	10/11	0.91	0.10	51,58,70,77	0
12	FME	m	1	10/11	0.92	0.11	52,59,74,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.92	0.15	54,63,77,87	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	SQD	I	102	40/54	0.67	0.23	44,69,94,102	0
32	LHG	E	101	49/49	0.69	0.21	48,77,92,95	0
30	UNL	j	101	9/-	0.70	0.28	52,61,65,65	0
30	UNL	b	603	11/-	0.71	0.20	44,54,62,62	0
30	UNL	a	717	7/-	0.72	0.23	48,53,61,67	0
30	UNL	b	606	13/-	0.73	0.22	45,51,57,59	0
29	SQD	B	623	47/54	0.73	0.17	44,61,109,124	0
30	UNL	I	101	9/-	0.73	0.21	44,52,61,61	0
30	UNL	H	101	8/-	0.75	0.21	43,53,58,64	0
23	LMG	b	627	51/55	0.76	0.18	51,70,80,82	0
30	UNL	a	716	4/-	0.76	0.20	31,46,50,51	0
23	LMG	C	521	51/55	0.76	0.19	49,71,81,91	0
30	UNL	z	101	11/-	0.76	0.24	48,65,72,72	0
30	UNL	a	718	13/-	0.76	0.19	45,54,61,62	0
32	LHG	e	101	42/49	0.76	0.18	57,76,98,101	0
30	UNL	A	613	7/-	0.77	0.20	34,49,53,55	0
23	LMG	c	520	51/55	0.77	0.21	61,75,95,100	0
23	LMG	B	621	51/55	0.78	0.18	52,70,78,88	0
23	LMG	C	501	51/55	0.78	0.19	46,67,81,88	0
23	LMG	C	520	51/55	0.78	0.20	43,74,86,89	0
23	LMG	A	603	51/55	0.78	0.19	40,62,77,83	0
30	UNL	B	601	12/-	0.79	0.16	31,49,56,56	0
30	UNL	i	101	22/-	0.79	0.18	36,50,58,62	0
23	LMG	b	626	51/55	0.80	0.17	38,56,72,77	0
29	SQD	b	601	54/54	0.80	0.15	45,66,94,105	0
29	SQD	A	614	40/54	0.80	0.18	47,59,68,72	0
23	LMG	a	701	51/55	0.80	0.16	42,64,87,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	LMG	a	715	51/55	0.81	0.16	47,65,85,91	0
29	SQD	B	626	54/54	0.81	0.16	46,67,90,99	0
23	LMG	d	408	40/55	0.81	0.16	47,61,84,89	0
23	LMG	b	628	9/55	0.81	0.15	36,50,54,54	0
30	UNL	M	102	6/-	0.81	0.19	45,51,51,53	0
28	PL9	a	713	55/55	0.82	0.19	57,68,77,84	0
23	LMG	c	519	51/55	0.82	0.20	42,75,90,91	0
25	CLA	b	607	65/65	0.82	0.16	48,63,81,91	0
30	UNL	t	102	5/-	0.82	0.15	32,38,43,47	0
27	BCR	k	101	40/40	0.82	0.18	53,69,78,78	0
28	PL9	A	611	55/55	0.82	0.19	46,68,78,83	0
30	UNL	b	605	13/-	0.82	0.18	42,54,62,62	0
25	CLA	B	602	65/65	0.83	0.15	44,62,75,80	0
29	SQD	f	102	41/54	0.83	0.17	54,73,85,89	0
27	BCR	D	405	40/40	0.83	0.17	48,61,77,81	0
25	CLA	C	514	65/65	0.83	0.15	44,73,81,89	0
30	UNL	B	622	6/-	0.83	0.19	40,51,56,56	0
27	BCR	b	602	40/40	0.84	0.15	45,53,70,76	0
30	UNL	M	103	16/-	0.84	0.16	41,51,57,58	0
25	CLA	B	617	65/65	0.85	0.15	39,52,80,84	0
27	BCR	t	103	40/40	0.85	0.16	36,47,60,63	0
25	CLA	c	506	65/65	0.85	0.15	47,57,79,92	0
25	CLA	c	512	65/65	0.85	0.17	60,67,89,91	0
25	CLA	c	513	65/65	0.85	0.15	57,68,82,96	0
27	BCR	C	515	40/40	0.85	0.17	53,63,72,76	0
25	CLA	C	505	65/65	0.85	0.16	48,63,71,79	0
29	SQD	D	410	43/54	0.85	0.16	56,75,87,96	0
23	LMG	M	101	51/55	0.85	0.14	34,58,74,77	0
27	BCR	d	404	40/40	0.85	0.17	45,59,70,77	0
33	DGD	c	517	62/66	0.85	0.17	54,61,81,92	0
30	UNL	B	624	11/-	0.86	0.18	34,49,52,53	0
30	UNL	m	101	5/-	0.86	0.13	36,39,42,45	0
30	UNL	m	102	12/-	0.86	0.14	41,47,50,52	0
30	UNL	t	101	10/-	0.86	0.14	26,44,49,50	0
27	BCR	c	514	40/40	0.86	0.17	61,67,74,75	0
27	BCR	H	102	40/40	0.86	0.15	41,54,62,62	0
25	CLA	C	513	65/65	0.86	0.15	52,66,80,86	0
27	BCR	k	102	40/40	0.86	0.18	53,65,81,84	0
29	SQD	a	714	54/54	0.86	0.16	48,68,83,90	0
23	LMG	f	101	51/55	0.87	0.16	48,58,84,93	0
30	UNL	d	401	22/-	0.87	0.16	39,54,63,66	0
25	CLA	c	504	58/65	0.87	0.14	52,59,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	BCR	Y	101	40/40	0.87	0.15	46,66,71,72	0
30	UNL	b	604	11/-	0.87	0.18	38,48,57,59	0
25	CLA	C	507	65/65	0.87	0.14	44,55,75,88	0
25	CLA	C	512	65/65	0.88	0.14	52,60,69,71	0
23	LMG	D	409	51/55	0.88	0.15	39,61,82,88	0
27	BCR	h	101	40/40	0.88	0.15	40,54,68,71	0
25	CLA	c	503	65/65	0.88	0.14	48,61,68,73	0
27	BCR	b	623	40/40	0.88	0.14	42,53,60,61	0
33	DGD	C	518	62/66	0.88	0.13	51,62,81,88	0
27	BCR	b	624	40/40	0.88	0.13	38,49,58,59	0
33	DGD	h	102	62/66	0.88	0.14	41,55,63,66	0
27	BCR	B	618	40/40	0.89	0.13	37,52,60,63	0
27	BCR	B	620	40/40	0.89	0.14	39,48,56,71	0
27	BCR	b	625	40/40	0.89	0.12	36,49,55,58	0
29	SQD	A	612	52/54	0.89	0.16	45,67,80,92	0
25	CLA	C	506	65/65	0.89	0.12	41,51,57,60	0
32	LHG	B	625	49/49	0.89	0.14	41,51,58,61	0
32	LHG	D	408	49/49	0.89	0.15	42,59,72,84	0
27	BCR	c	515	40/40	0.89	0.13	38,53,64,72	0
25	CLA	C	504	65/65	0.89	0.12	43,57,62,68	0
25	CLA	c	511	65/65	0.89	0.14	50,62,71,74	0
33	DGD	H	103	62/66	0.89	0.13	39,49,59,62	0
25	CLA	C	510	65/65	0.89	0.14	45,57,64,68	0
25	CLA	B	605	65/65	0.89	0.13	35,47,62,73	0
25	CLA	B	609	65/65	0.90	0.12	32,45,51,59	0
25	CLA	c	505	65/65	0.90	0.13	41,52,60,69	0
25	CLA	B	615	65/65	0.90	0.12	38,48,67,73	0
25	CLA	a	711	65/65	0.90	0.13	34,46,79,87	0
25	CLA	C	511	65/65	0.90	0.13	44,57,64,70	0
28	PL9	D	406	55/55	0.90	0.14	31,43,52,55	0
25	CLA	b	610	65/65	0.90	0.13	37,47,59,62	0
28	PL9	d	405	55/55	0.90	0.13	32,41,53,56	0
25	CLA	b	612	65/65	0.90	0.13	32,46,56,69	0
33	DGD	C	519	62/66	0.90	0.13	43,56,67,76	0
25	CLA	b	613	65/65	0.90	0.12	37,44,55,58	0
33	DGD	c	516	62/66	0.90	0.14	34,50,68,76	0
25	CLA	B	607	65/65	0.90	0.13	41,50,64,75	0
33	DGD	c	518	62/66	0.90	0.14	44,57,76,81	0
27	BCR	C	516	40/40	0.90	0.13	42,51,58,58	0
27	BCR	B	619	40/40	0.91	0.12	35,47,51,52	0
25	CLA	C	509	65/65	0.91	0.14	46,55,91,100	0
25	CLA	B	616	65/65	0.91	0.11	42,51,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	620	65/65	0.91	0.12	35,52,61,64	0
25	CLA	b	621	65/65	0.91	0.12	38,49,55,60	0
25	CLA	b	622	47/65	0.91	0.11	40,48,58,64	0
27	BCR	K	101	40/40	0.91	0.14	51,60,70,75	0
25	CLA	A	607	65/65	0.91	0.14	31,46,91,99	0
25	CLA	C	503	65/65	0.91	0.12	43,56,62,68	0
25	CLA	B	610	65/65	0.91	0.11	36,51,58,63	0
25	CLA	B	611	65/65	0.91	0.12	40,47,55,60	0
25	CLA	c	507	65/65	0.91	0.11	41,50,61,67	0
25	CLA	c	508	65/65	0.91	0.13	46,57,72,82	0
25	CLA	c	509	65/65	0.91	0.13	49,57,70,73	0
32	LHG	a	720	39/49	0.91	0.13	41,54,65,66	0
25	CLA	c	510	65/65	0.91	0.13	43,54,63,68	0
33	DGD	C	517	62/66	0.91	0.12	36,46,65,71	0
25	CLA	a	707	65/65	0.91	0.11	33,47,51,53	0
25	CLA	B	614	65/65	0.91	0.11	34,43,57,69	0
25	CLA	A	606	65/65	0.91	0.11	29,43,48,53	0
25	CLA	d	402	65/65	0.91	0.12	35,45,51,55	0
25	CLA	d	403	65/65	0.91	0.12	45,54,65,66	0
26	PHO	D	401	64/64	0.91	0.11	37,46,55,59	0
25	CLA	C	508	65/65	0.91	0.12	41,50,57,66	0
26	PHO	a	710	64/64	0.92	0.12	38,46,55,62	0
27	BCR	A	610	40/40	0.92	0.10	31,44,52,56	0
25	CLA	c	502	65/65	0.92	0.12	45,55,67,81	0
25	CLA	B	612	65/65	0.92	0.11	32,42,49,54	0
25	CLA	C	502	65/65	0.92	0.12	38,50,57,64	0
25	CLA	b	608	65/65	0.92	0.12	39,49,60,64	0
25	CLA	A	609	54/65	0.92	0.11	34,43,60,71	0
25	CLA	B	604	65/65	0.92	0.12	33,44,54,57	0
32	LHG	L	101	49/49	0.92	0.11	39,50,57,64	0
25	CLA	D	402	65/65	0.92	0.11	31,41,47,51	0
32	LHG	b	629	49/49	0.92	0.11	36,50,57,64	0
32	LHG	d	406	49/49	0.92	0.12	32,53,61,65	0
25	CLA	b	614	65/65	0.92	0.11	39,48,58,60	0
25	CLA	b	615	65/65	0.92	0.11	42,50,55,60	0
27	BCR	a	712	40/40	0.92	0.12	26,44,53,54	0
25	CLA	b	616	65/65	0.92	0.12	34,42,50,56	0
25	CLA	b	617	65/65	0.92	0.11	36,45,50,57	0
25	CLA	b	619	65/65	0.92	0.11	31,42,59,67	0
25	CLA	D	403	65/65	0.92	0.11	33,42,54,61	0
25	CLA	D	404	65/65	0.92	0.12	34,44,80,84	0
25	CLA	B	608	65/65	0.92	0.11	30,42,52,56	0

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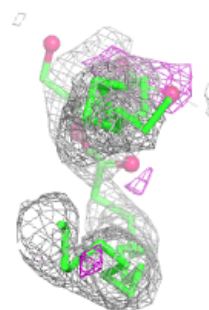
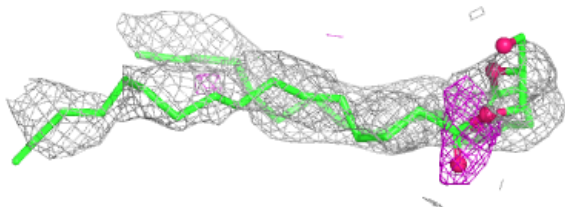
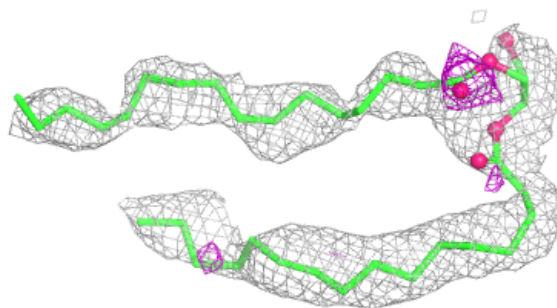
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HEM	E	102	43/43	0.92	0.12	52,66,76,80	0
34	HEM	e	102	43/43	0.92	0.14	60,71,81,91	0
25	CLA	b	611	65/65	0.93	0.10	30,46,52,56	0
32	LHG	d	407	49/49	0.93	0.12	36,46,54,61	0
25	CLA	b	618	65/65	0.93	0.11	32,43,50,52	0
25	CLA	a	719	65/65	0.93	0.11	32,43,49,54	0
31	BCT	A	615	4/4	0.93	0.11	46,49,51,54	0
31	BCT	a	706	4/4	0.93	0.09	50,56,56,59	0
25	CLA	B	606	65/65	0.93	0.11	37,45,52,53	0
32	LHG	D	407	49/49	0.93	0.10	34,49,59,60	0
25	CLA	B	613	65/65	0.93	0.11	36,43,55,59	0
25	CLA	b	609	65/65	0.93	0.11	34,45,55,61	0
26	PHO	a	709	64/64	0.93	0.10	26,41,47,50	0
25	CLA	c	501	65/65	0.93	0.11	37,49,55,59	0
25	CLA	B	603	65/65	0.93	0.11	42,52,59,62	0
26	PHO	A	608	64/64	0.94	0.10	32,40,46,50	0
25	CLA	a	708	65/65	0.94	0.11	37,47,89,101	0
24	CL	A	605	1/1	0.94	0.11	51,51,51,51	0
35	HEC	V	201	43/43	0.94	0.11	41,51,57,63	0
35	HEC	v	201	43/43	0.94	0.11	46,58,64,72	0
24	CL	a	704	1/1	0.95	0.09	59,59,59,59	0
24	CL	a	705	1/1	0.96	0.11	50,50,50,50	0
24	CL	A	604	1/1	0.97	0.07	39,39,39,39	0
22	FE2	a	703	1/1	0.98	0.07	60,60,60,60	0
21	OEX	A	601	10/10	0.98	0.06	42,54,59,60	0
21	OEX	a	702	10/10	0.98	0.05	44,52,59,60	0
22	FE2	A	602	1/1	0.99	0.05	60,60,60,60	0

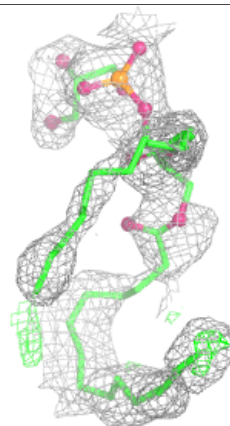
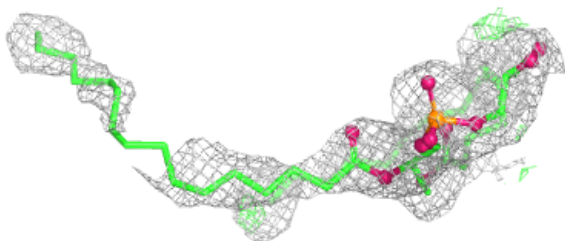
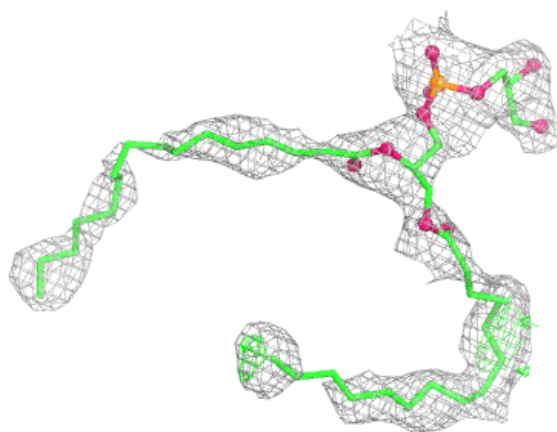
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SQD 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)

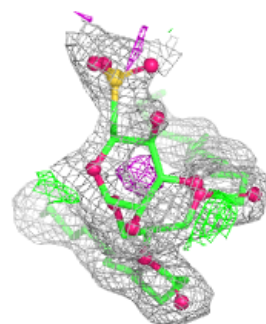
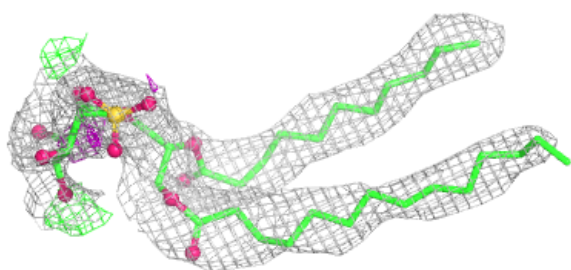
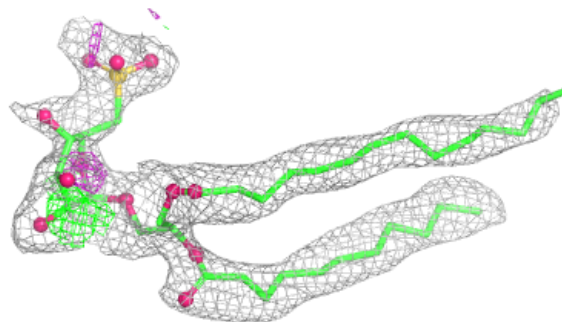
**Electron density around LHG E 101:**

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

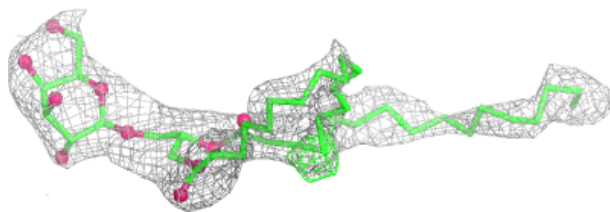
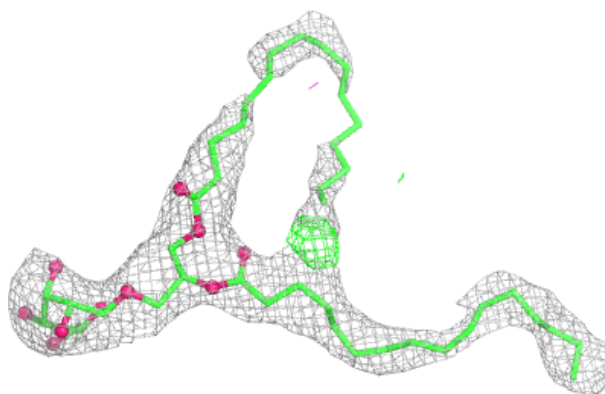


Electron density around SQD B 623:

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

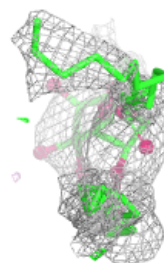
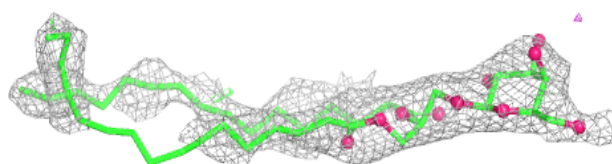
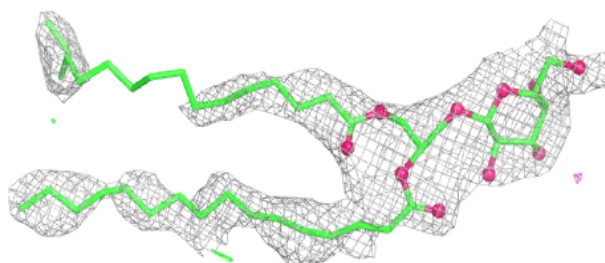
**Electron density around LMG b 627:**

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

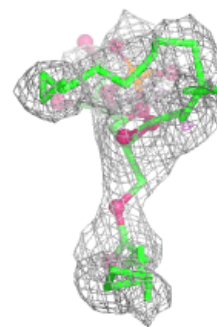
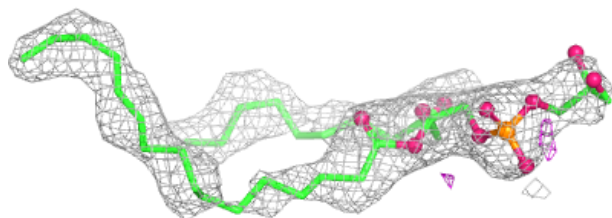
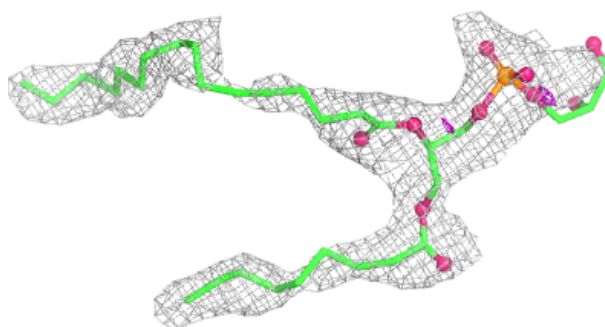


Electron density around LMG C 521:

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

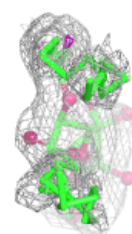
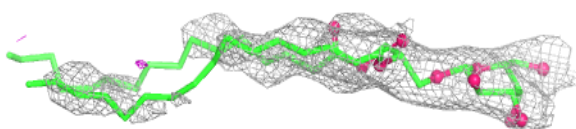
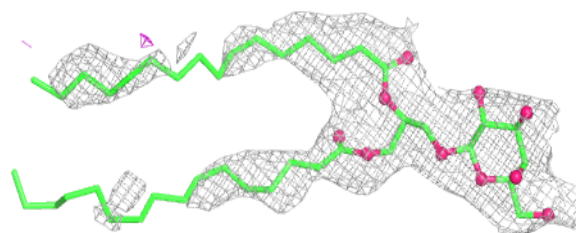
**Electron density around LHG e 101:**

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

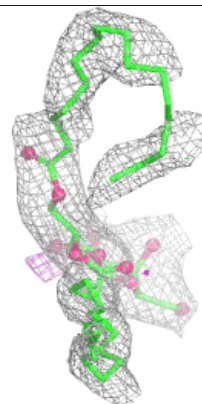
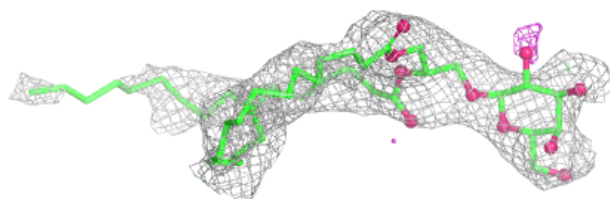
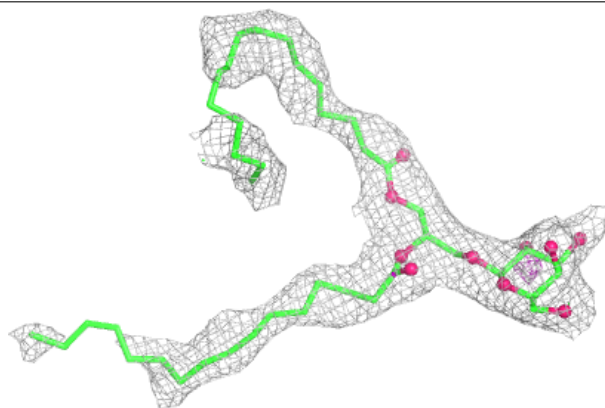


Electron density around LMG c 520:

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

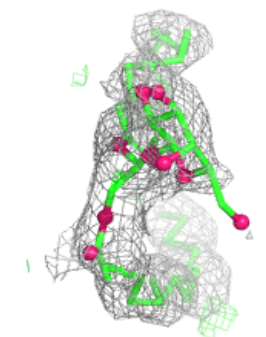
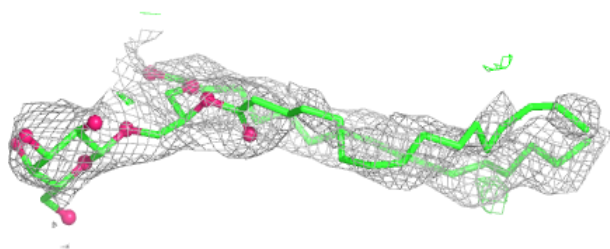
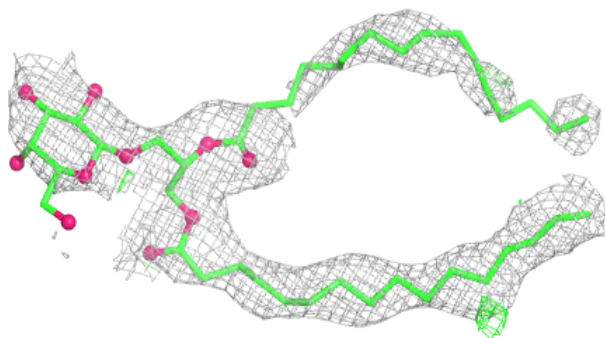
**Electron density around LMG B 621:**

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

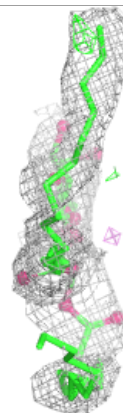
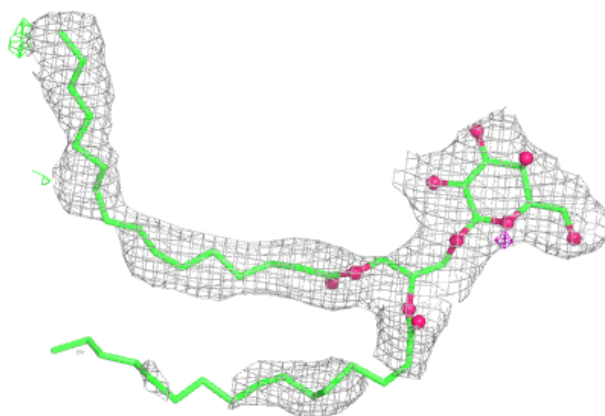


Electron density around LMG C 501:

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

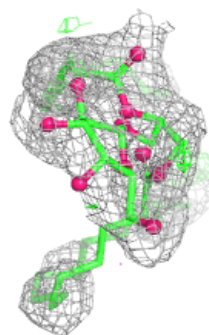
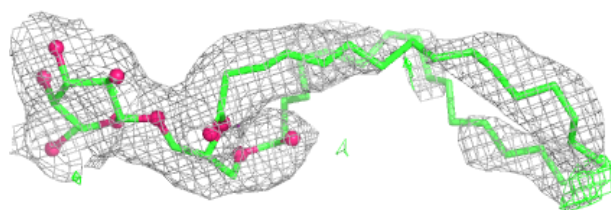
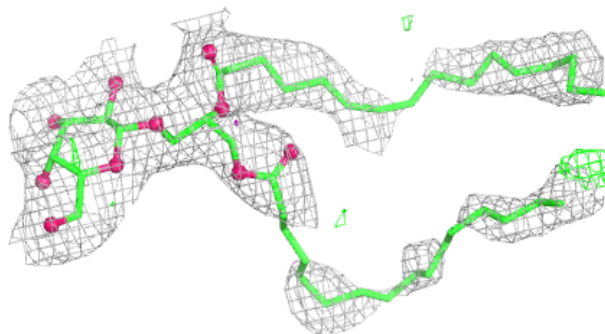
**Electron density around LMG C 520:**

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



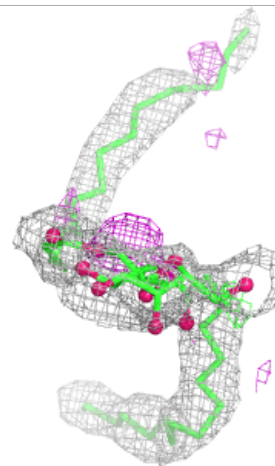
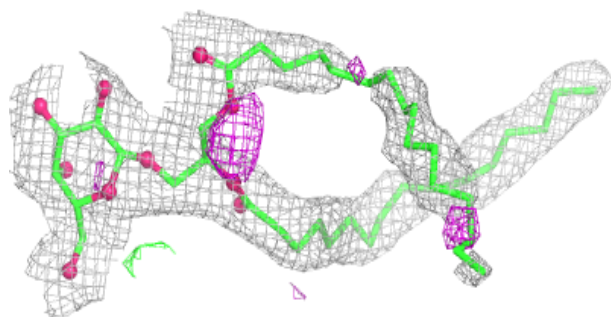
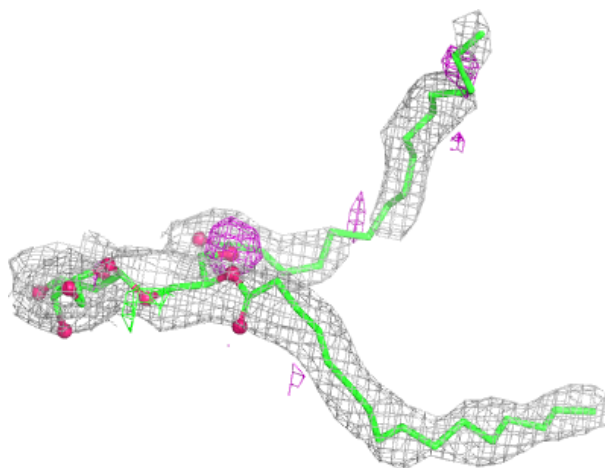
Electron density around LMG A 603:

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



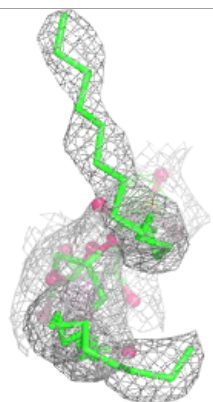
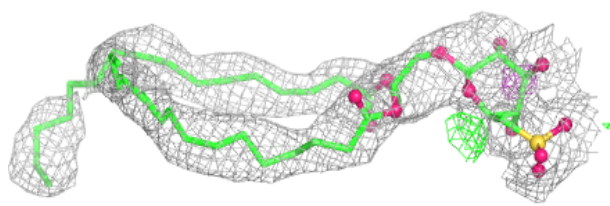
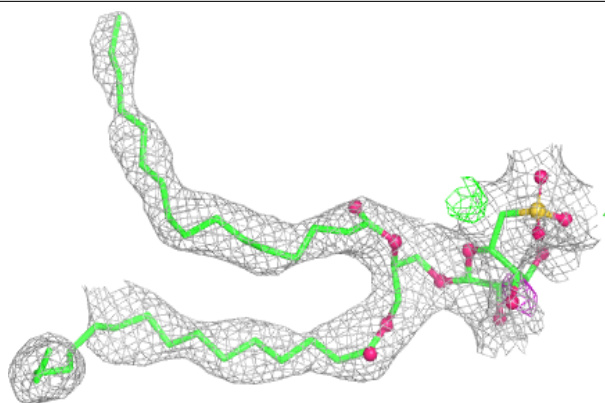
Electron density around LMG b 626:

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

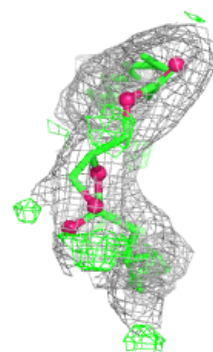
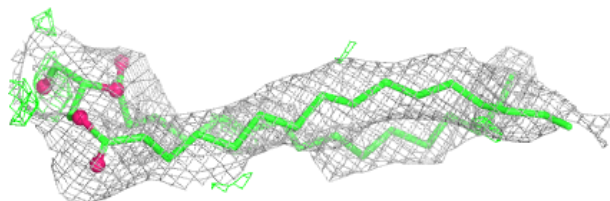
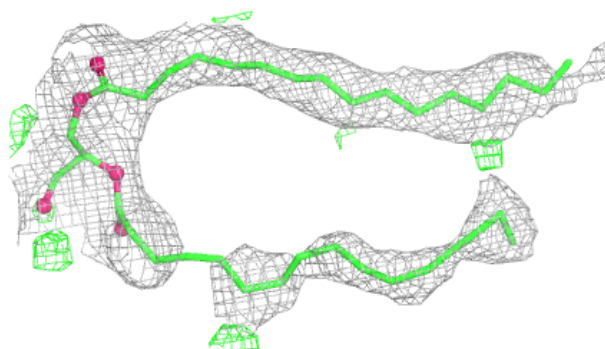


Electron density around SQD b 601:

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

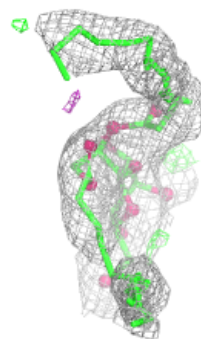
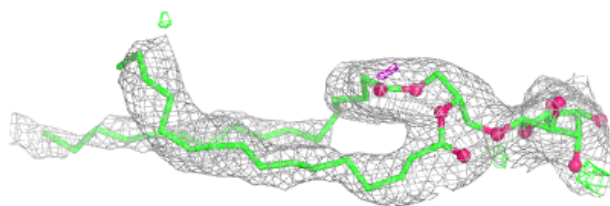
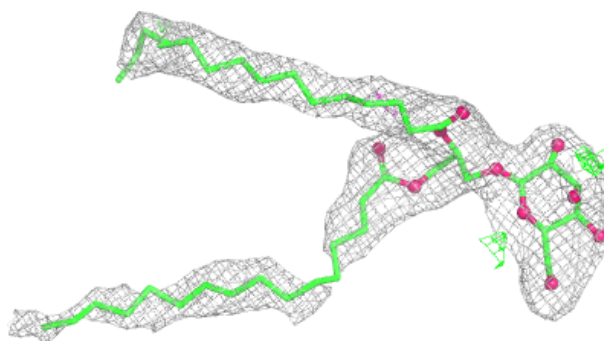
**Electron density around SQD A 614:**

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

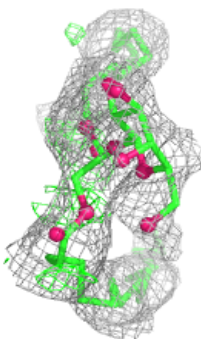
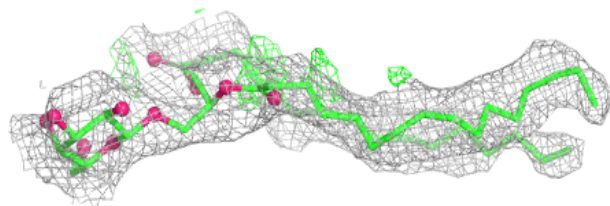
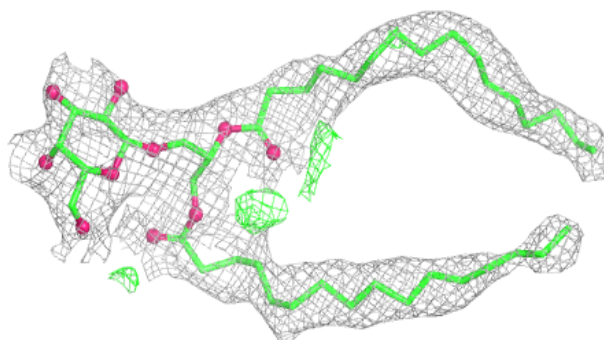


Electron density around LMG a 701:

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

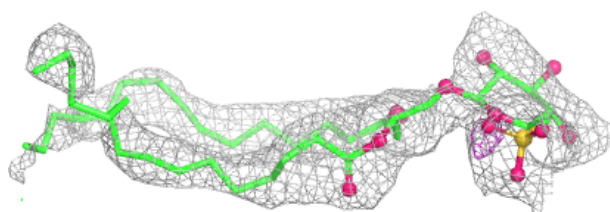
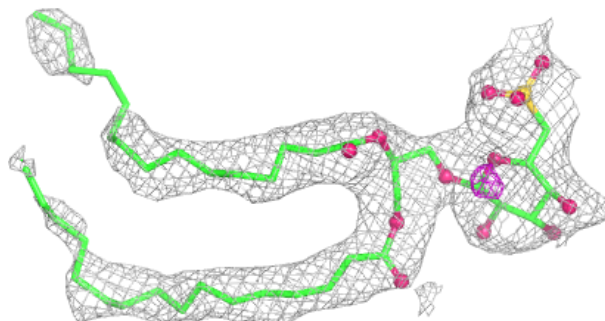
**Electron density around LMG a 715:**

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

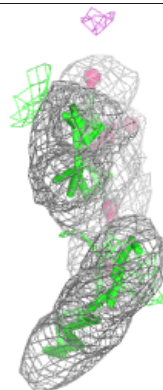
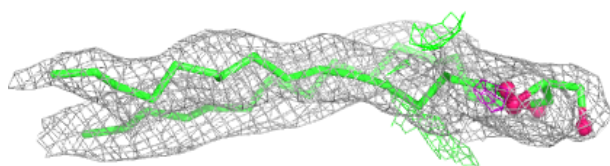
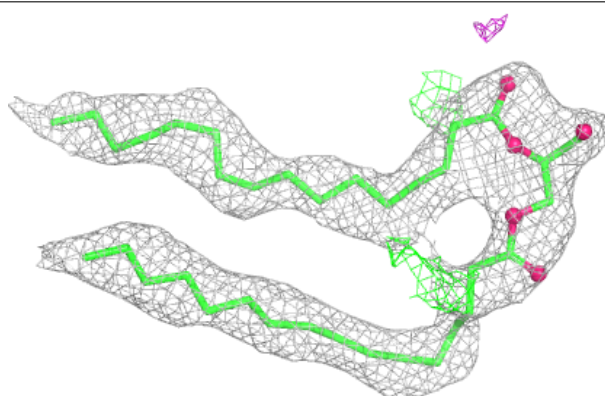


Electron density around SQD B 626:

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

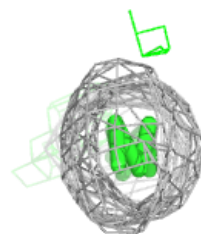
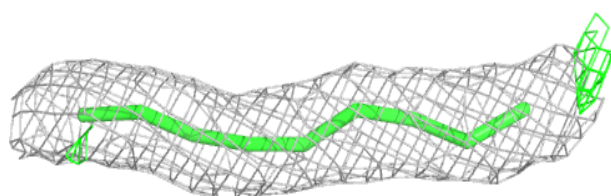
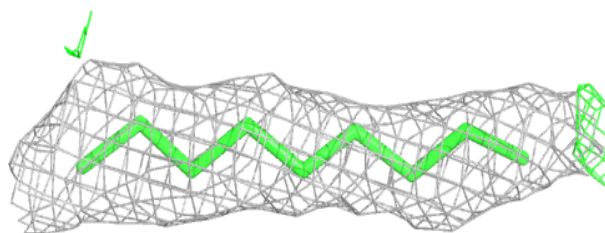
**Electron density around LMG d 408:**

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

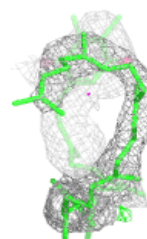
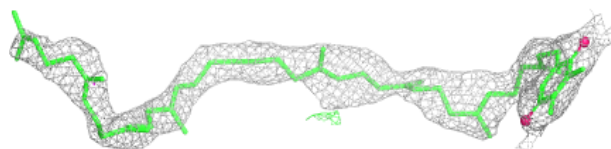
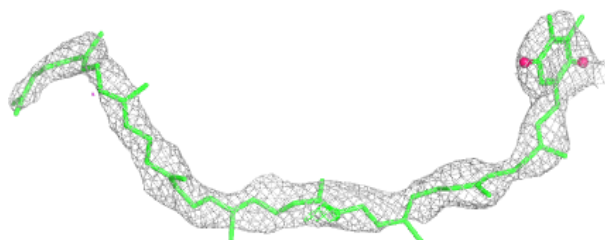


Electron density around LMG b 628:

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

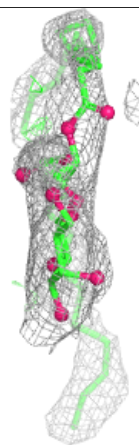
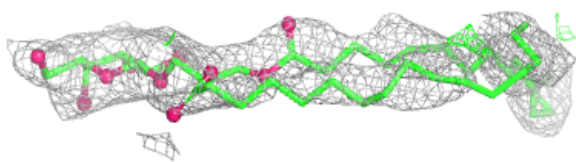
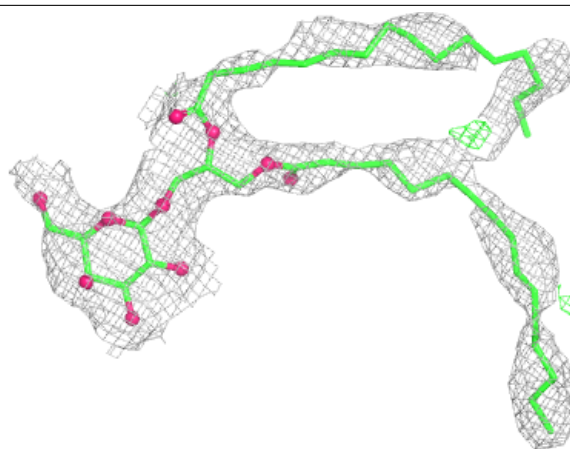
**Electron density around PL9 a 713:**

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



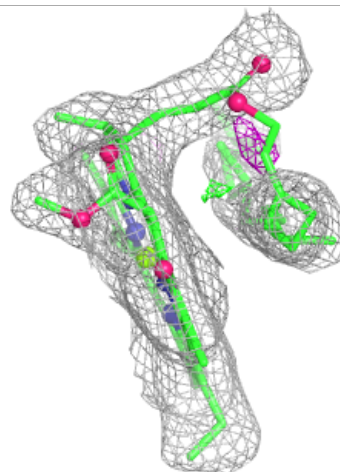
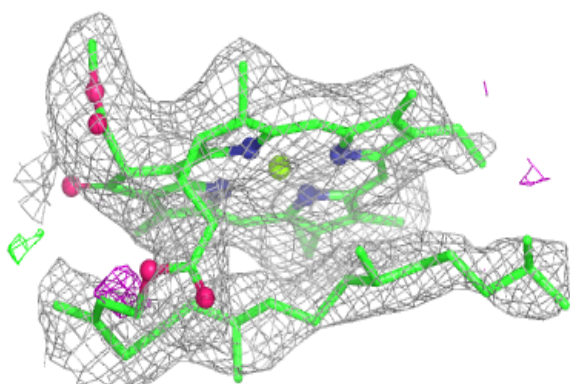
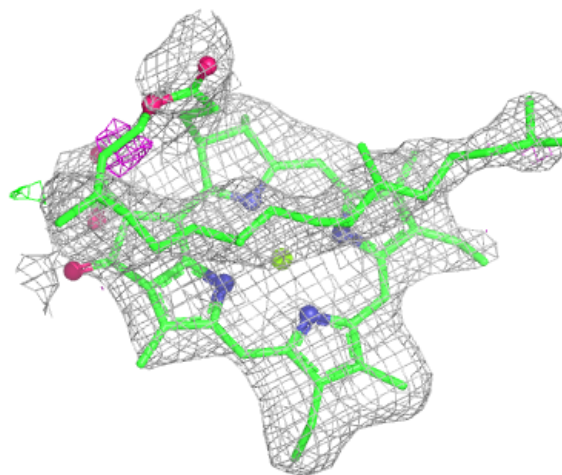
Electron density around LMG c 519:

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



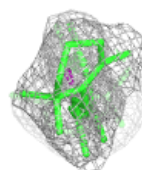
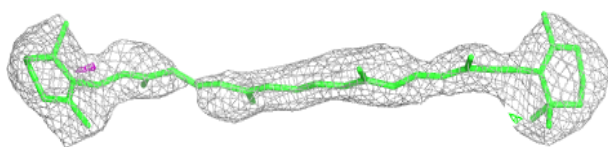
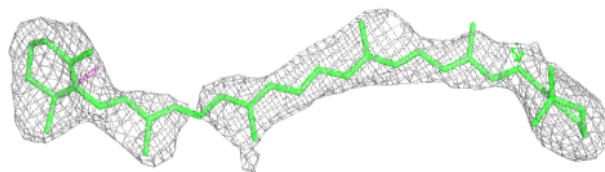
Electron density around CLA b 607:

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

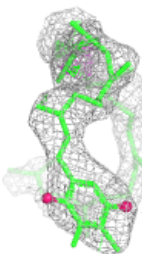
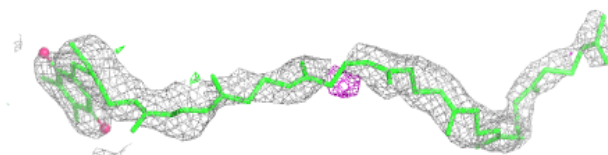
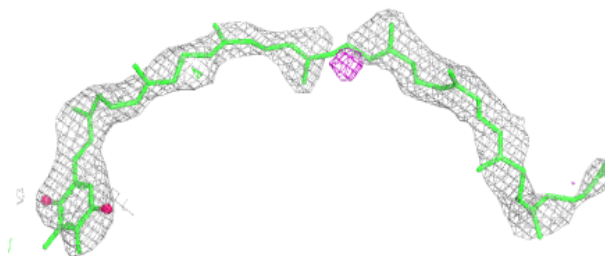


Electron density around BCR k 101:

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

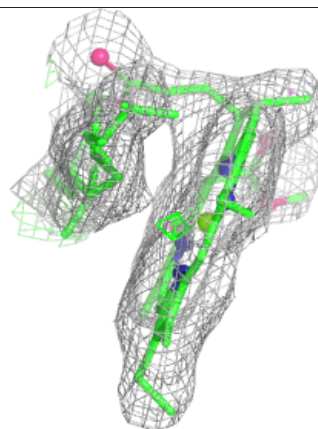
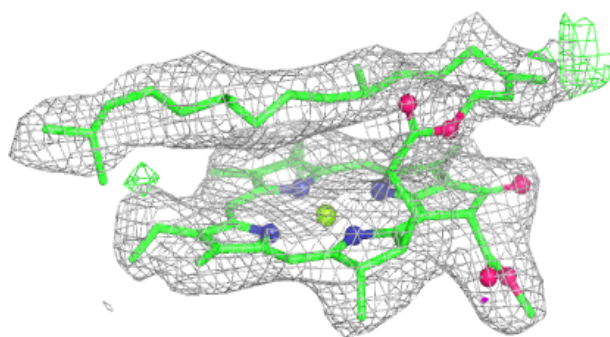
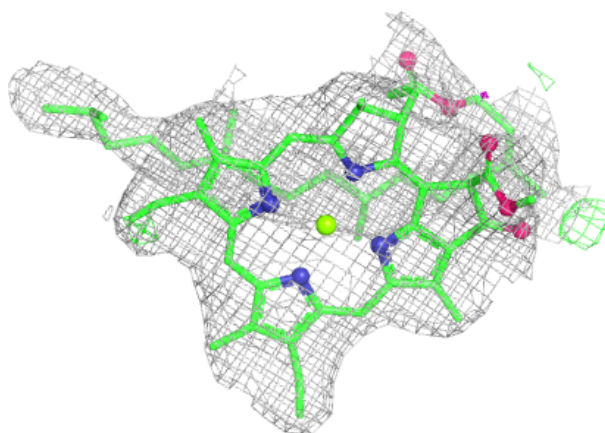
**Electron density around PL9 A 611:**

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

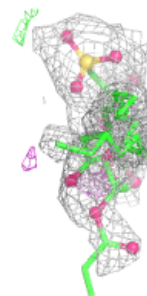
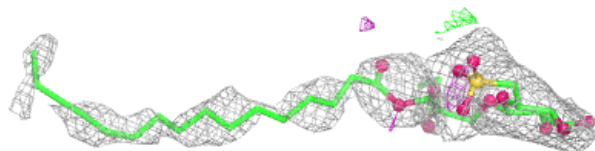
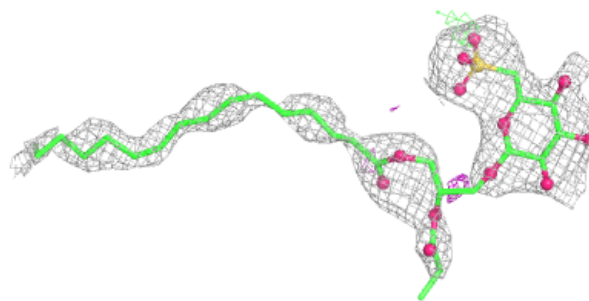


Electron density around CLA B 602:

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

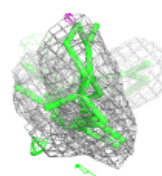
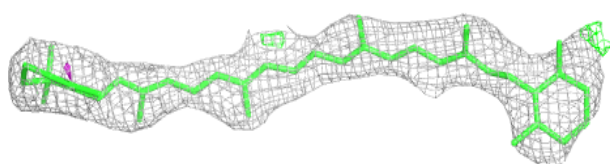
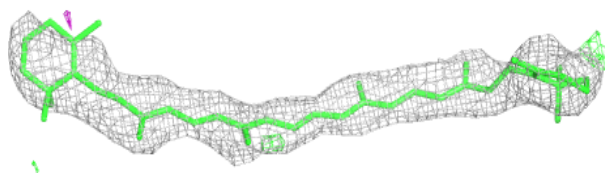
**Electron density around SQD f 102:**

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

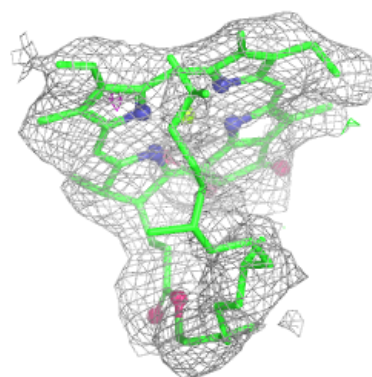
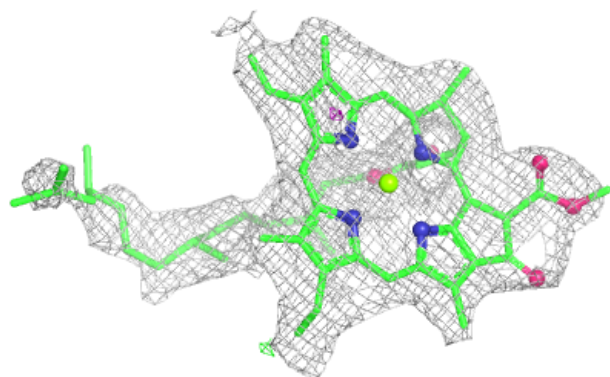
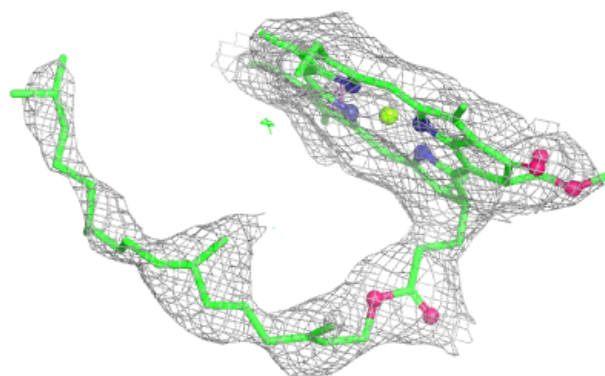


Electron density around BCR D 405:

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

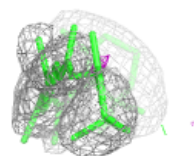
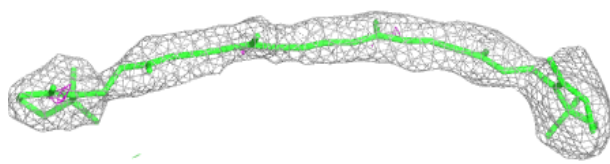
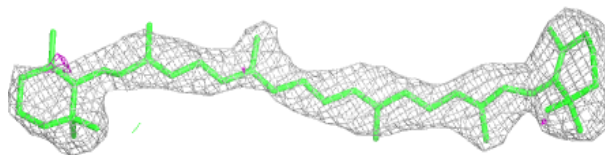
**Electron density around CLA C 514:**

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

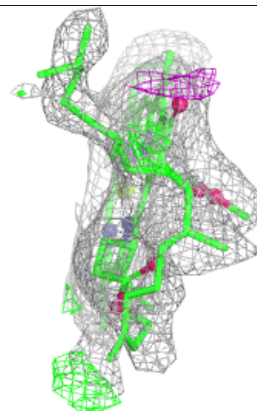
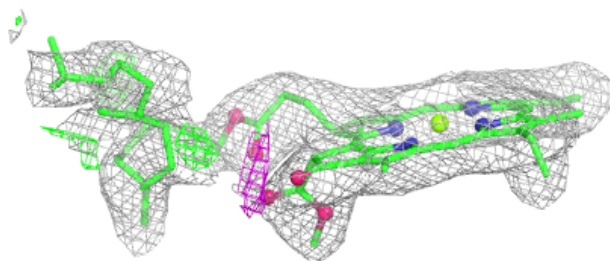
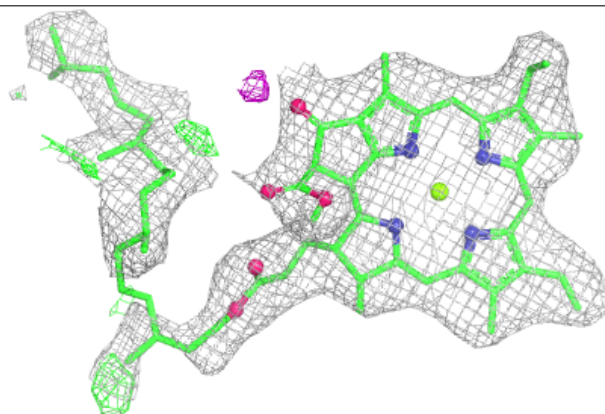


Electron density around BCR b 602:

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

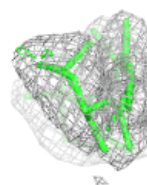
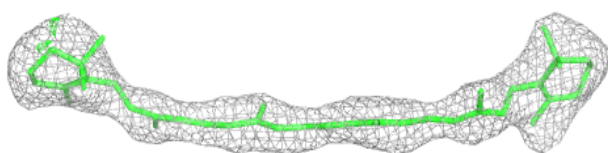
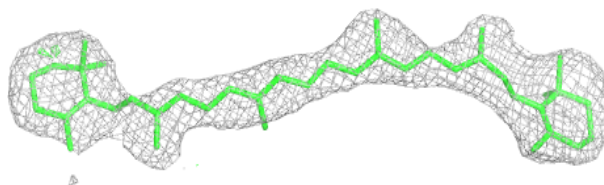
**Electron density around CLA B 617:**

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

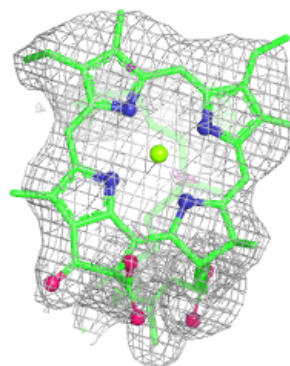
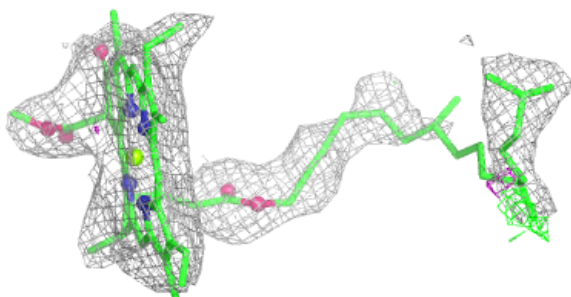
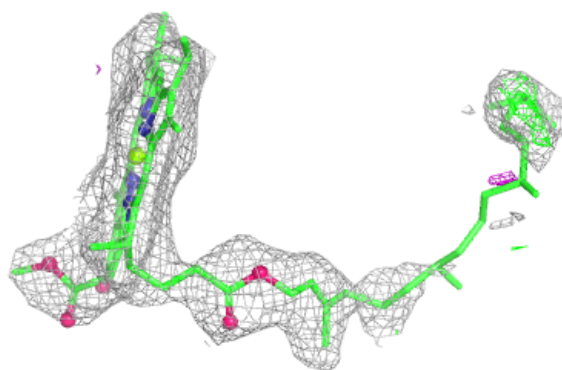


Electron density around BCR t 103:

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

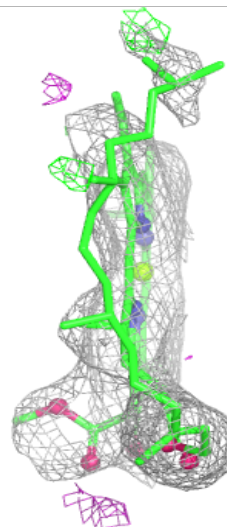
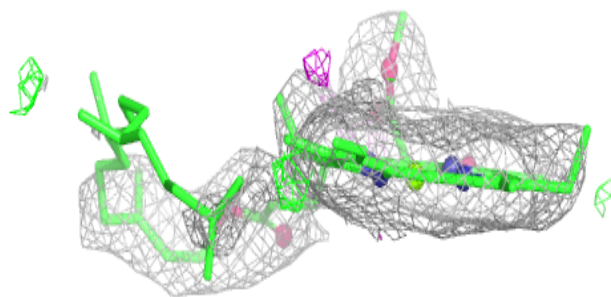
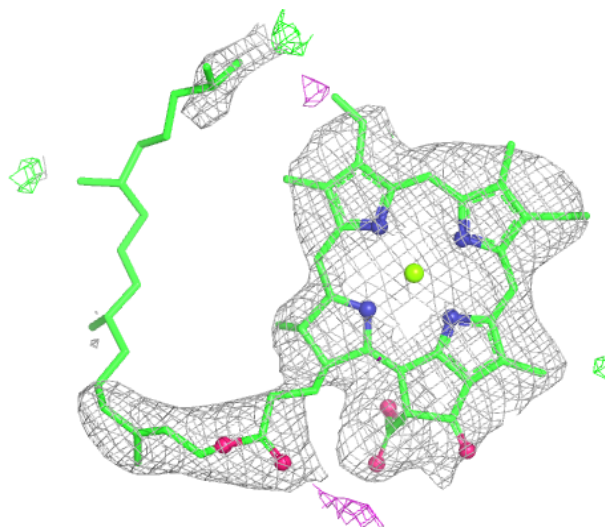
**Electron density around CLA c 506:**

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



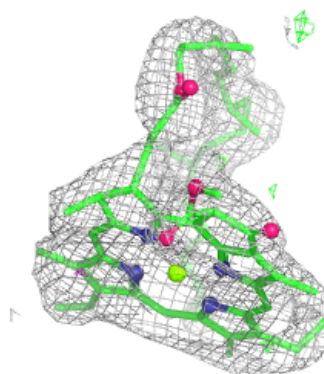
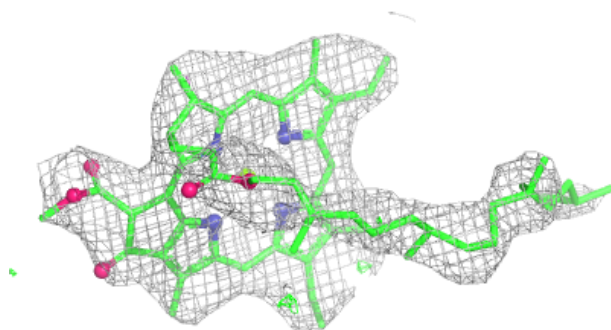
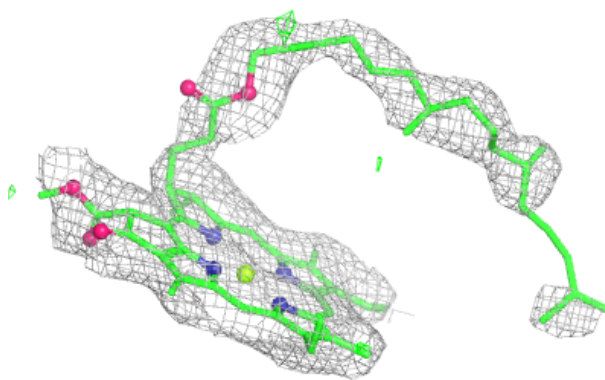
Electron density around CLA c 512:

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

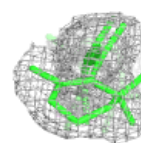
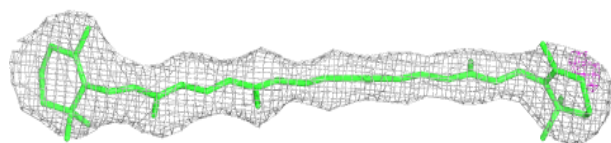
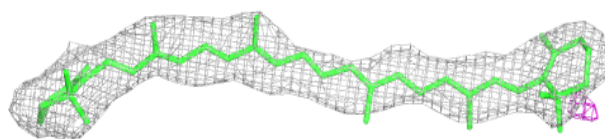


Electron density around CLA c 513:

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

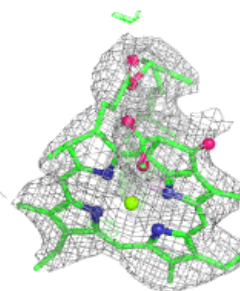
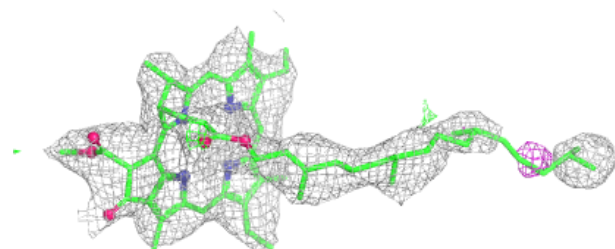
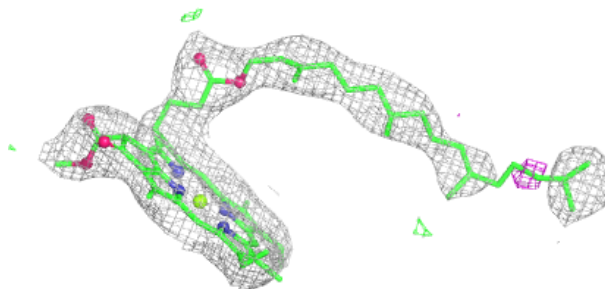
**Electron density around BCR C 515:**

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

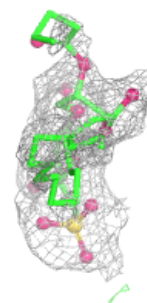
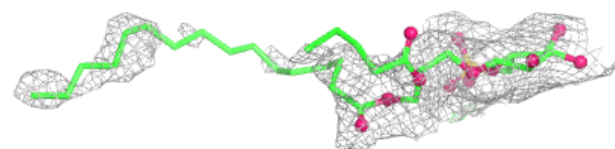
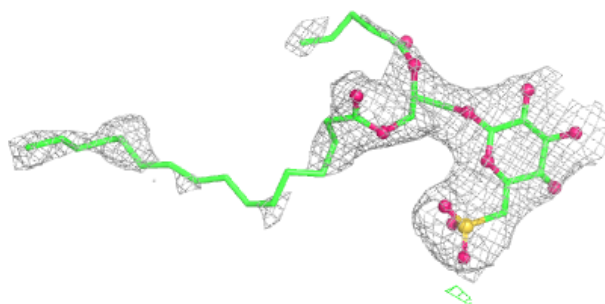


Electron density around CLA C 505:

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

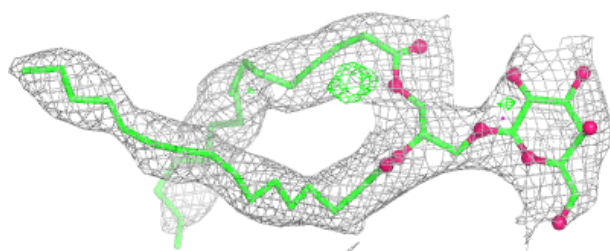
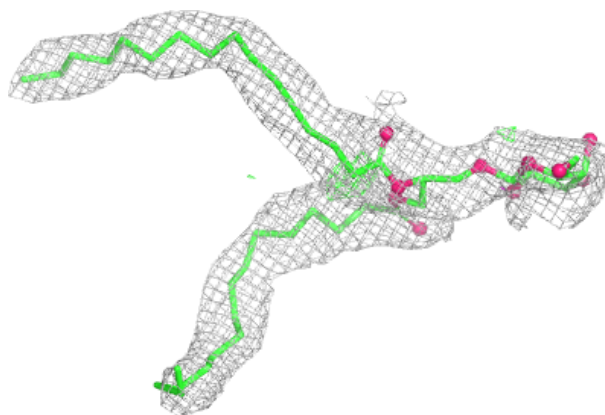
**Electron density around SQD D 410:**

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

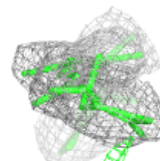
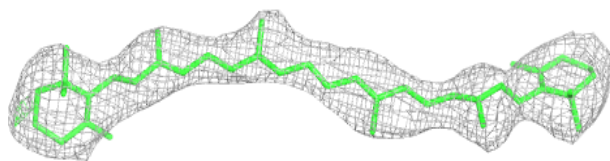
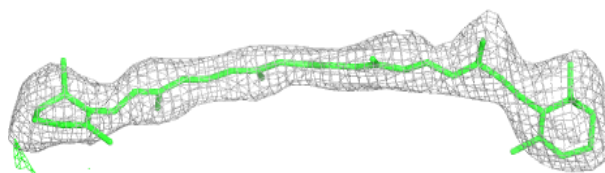


Electron density around LMG M 101:

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

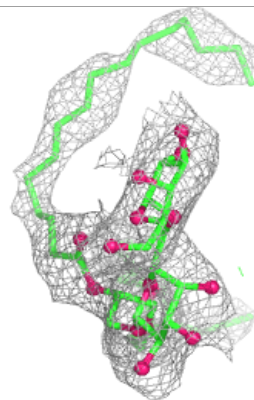
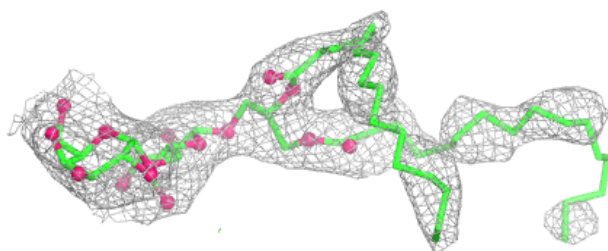
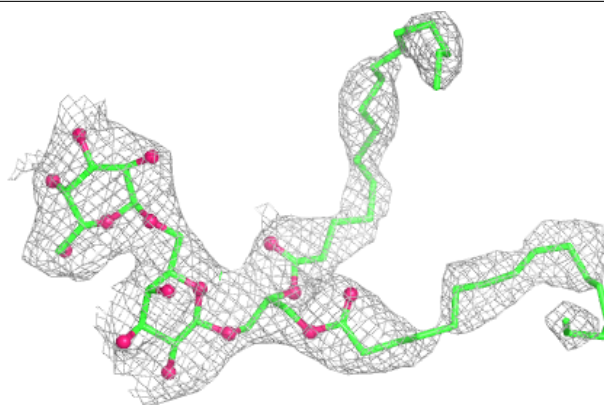
**Electron density around BCR d 404:**

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

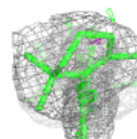
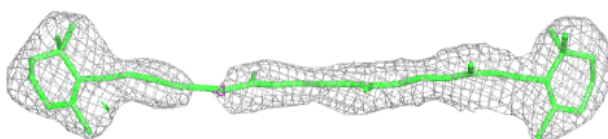
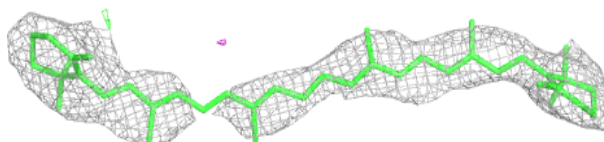


Electron density around DGD c 517:

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

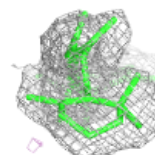
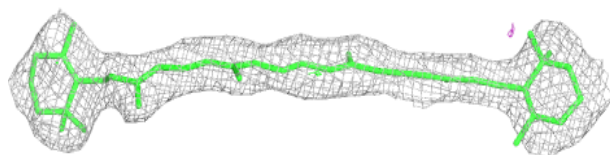
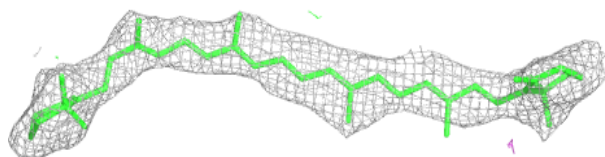
**Electron density around BCR c 514:**

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



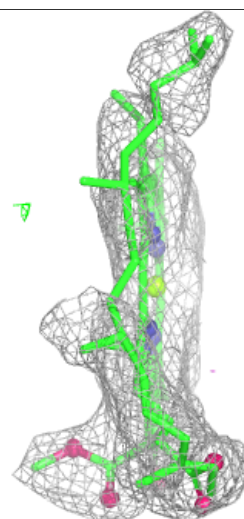
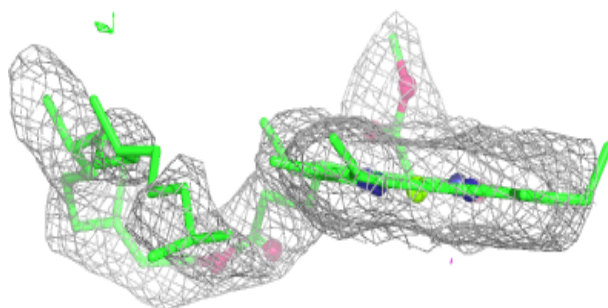
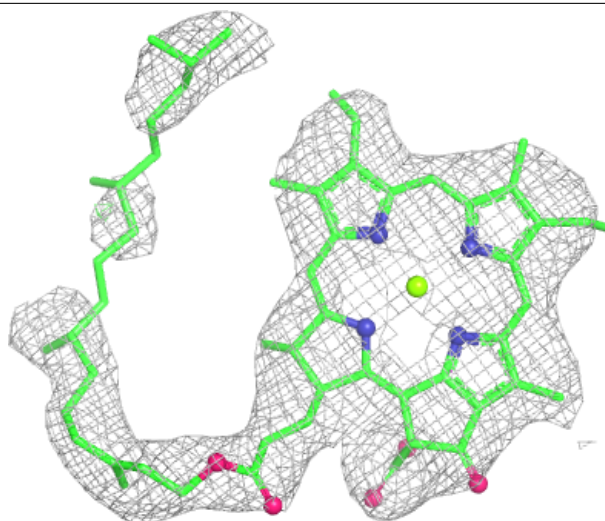
Electron density around BCR H 102:

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



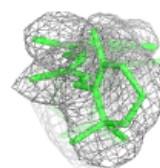
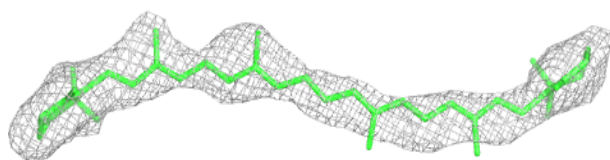
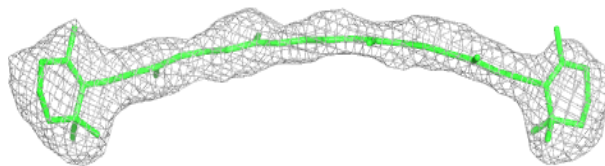
Electron density around CLA C 513:

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

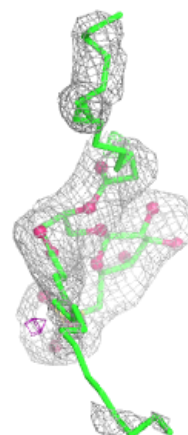
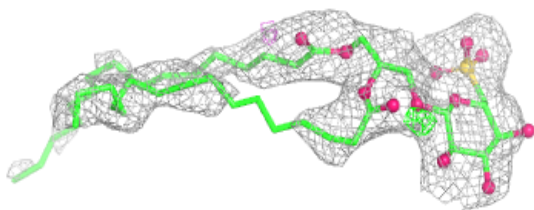
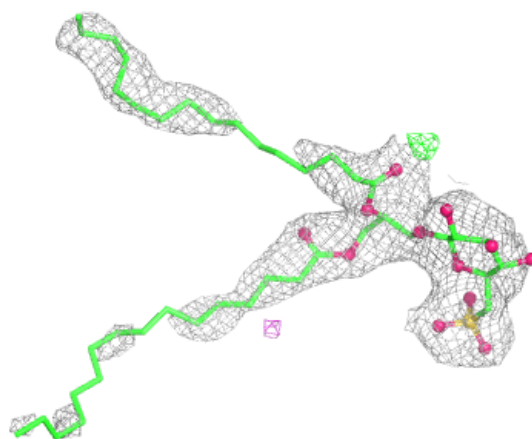


Electron density around BCR k 102:

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

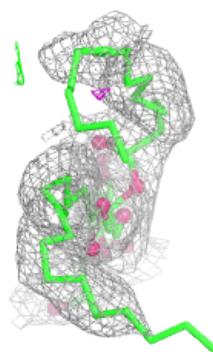
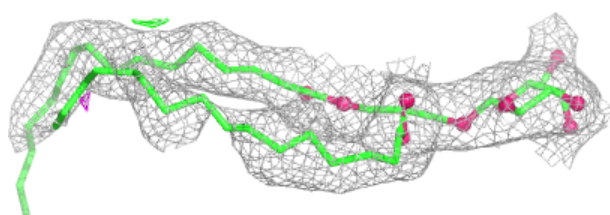
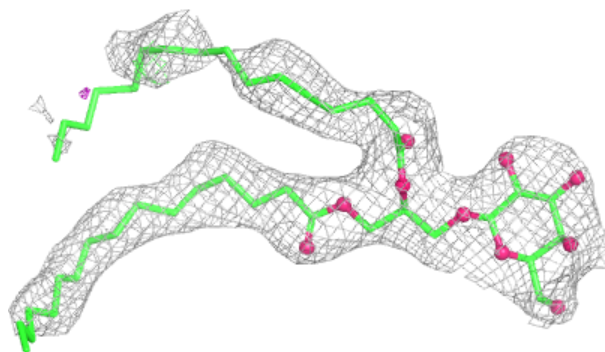
**Electron density around SQD a 714:**

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

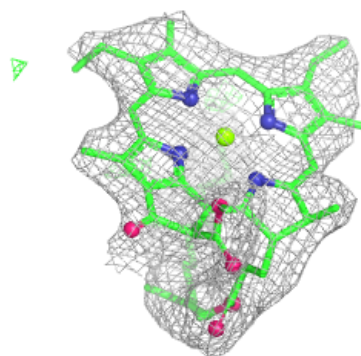
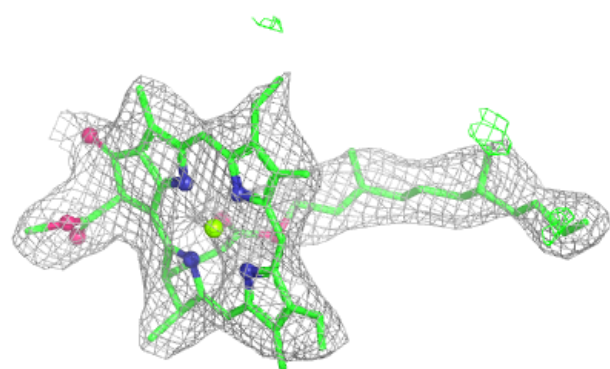
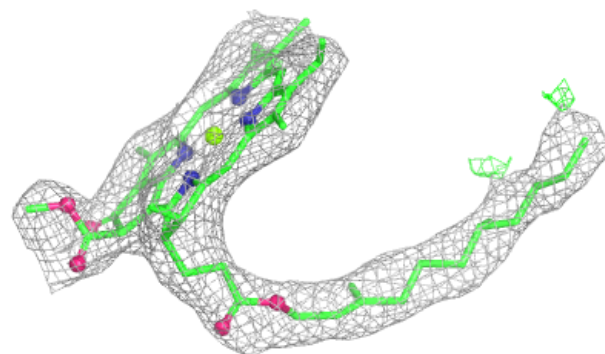


Electron density around LMG f 101:

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

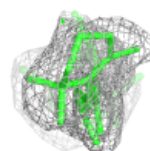
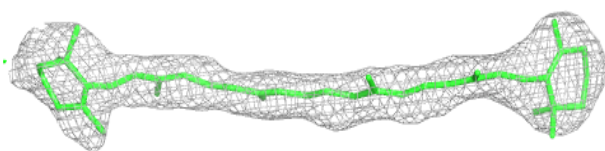
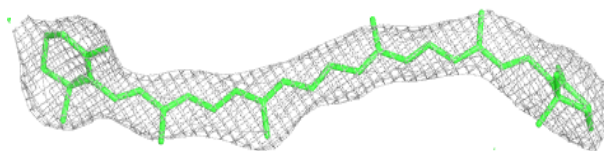
**Electron density around CLA c 504:**

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

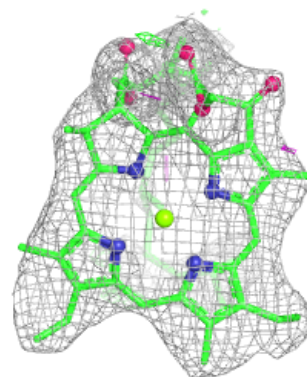
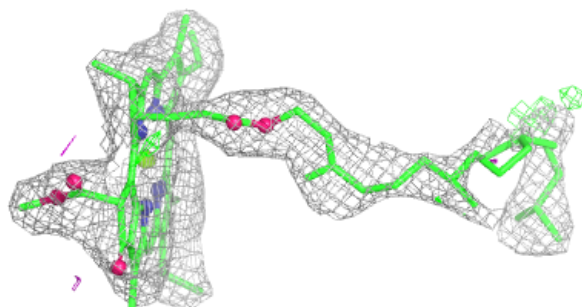
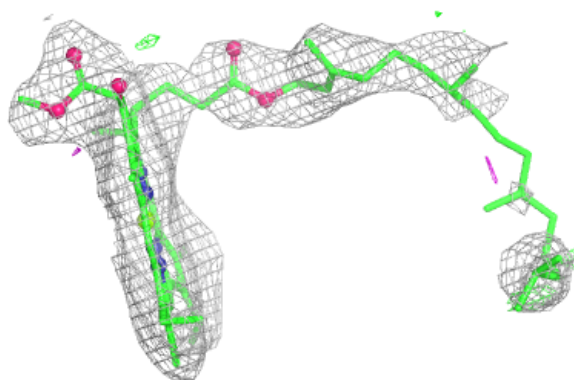


Electron density around BCR Y 101:

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

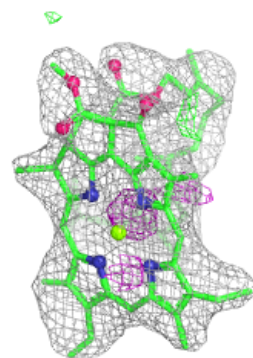
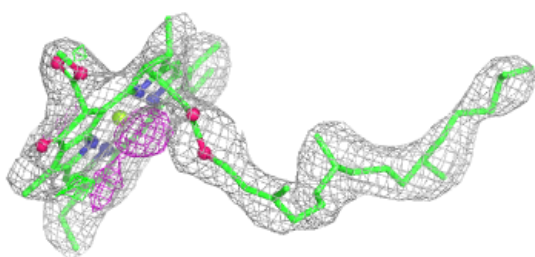
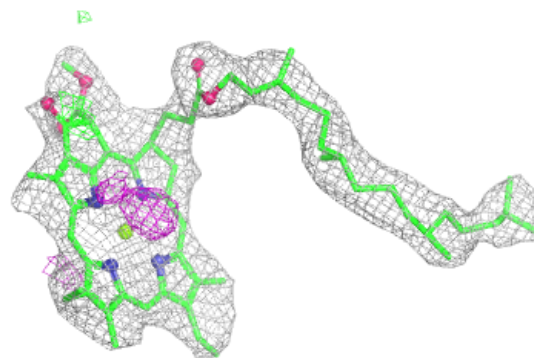
**Electron density around CLA C 507:**

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

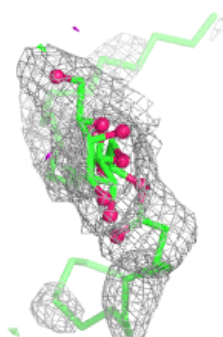
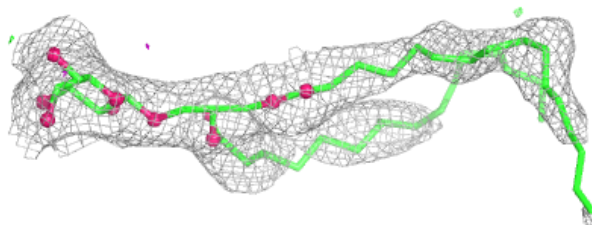
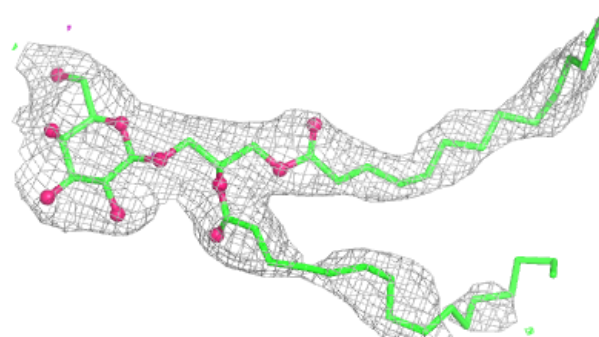


Electron density around CLA C 512:

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

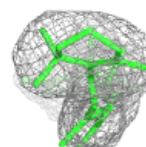
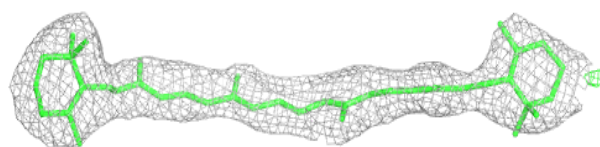
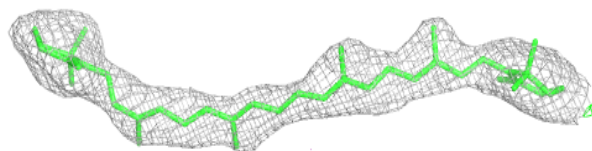
**Electron density around LMG D 409:**

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



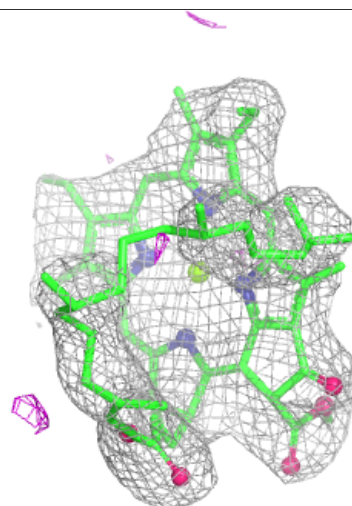
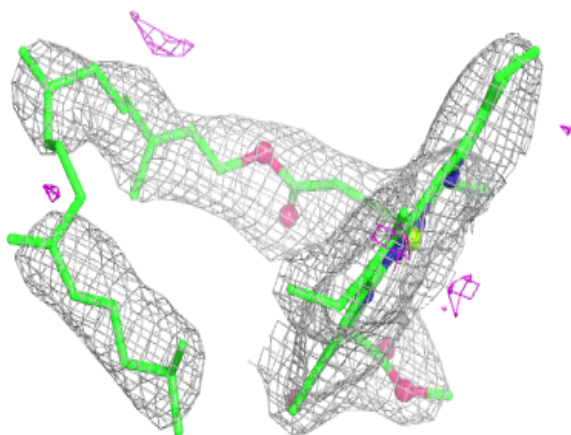
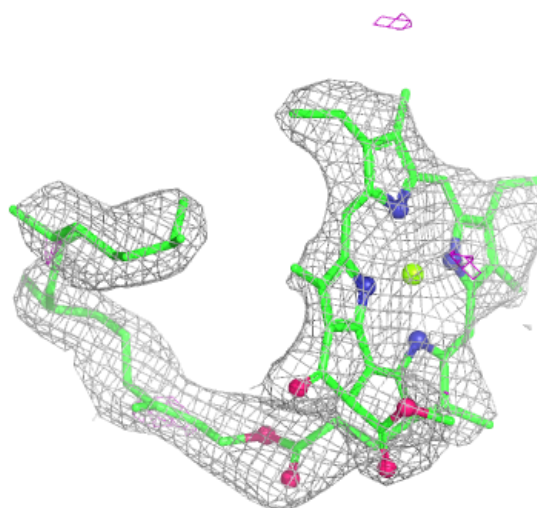
Electron density around BCR h 101:

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



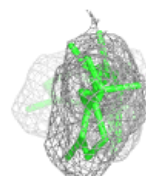
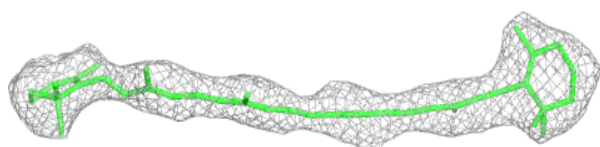
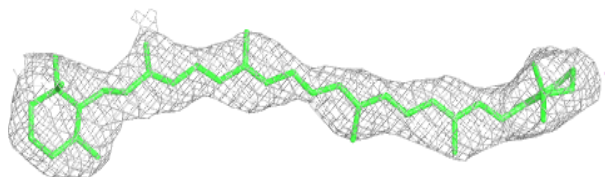
Electron density around CLA c 503:

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

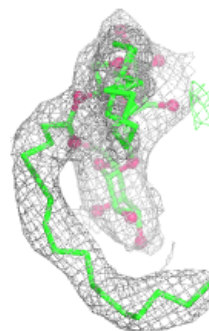
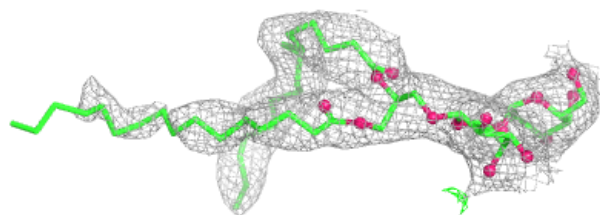
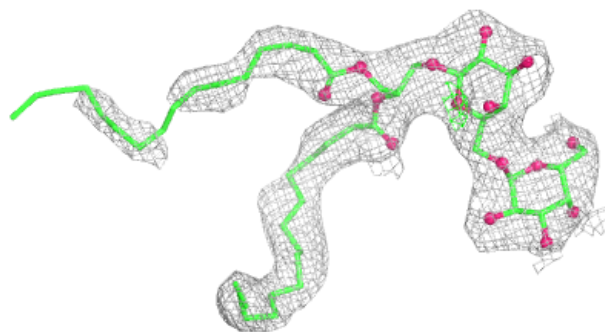


Electron density around BCR b 623:

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

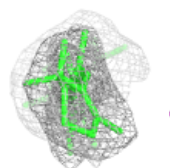
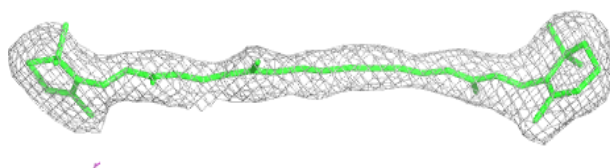
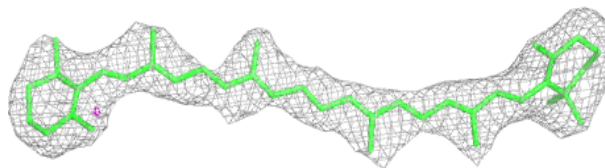
**Electron density around DGD C 518:**

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

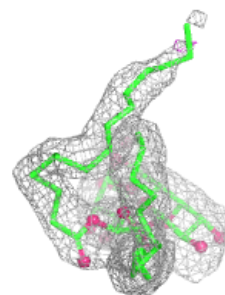
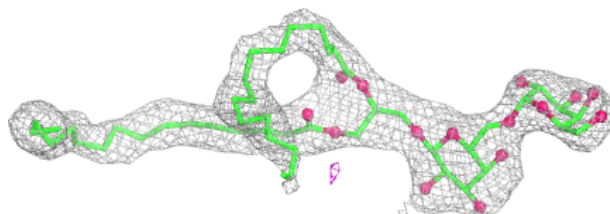


Electron density around BCR b 624:

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

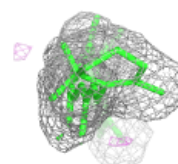
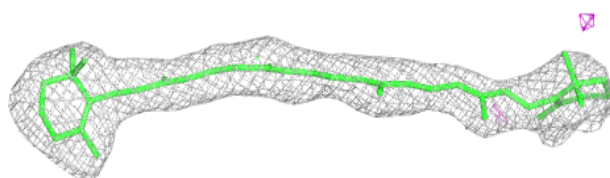
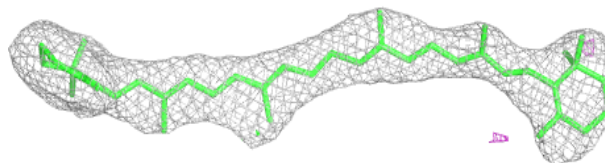
**Electron density around DGD h 102:**

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

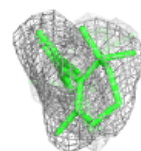
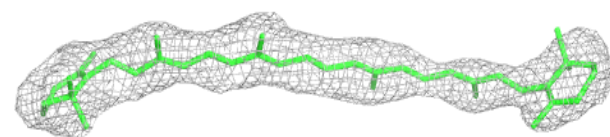
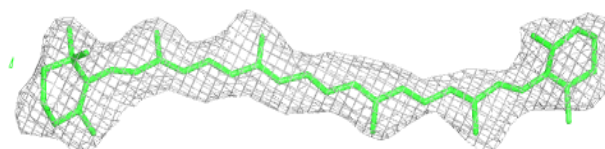


Electron density around BCR B 618:

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

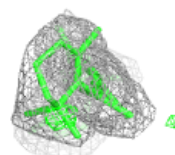
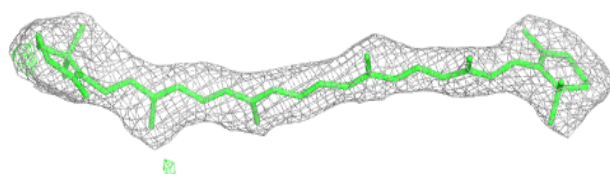
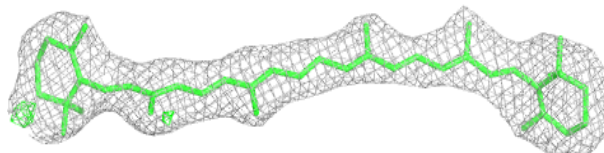
**Electron density around BCR B 620:**

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

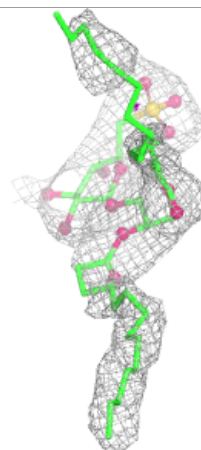
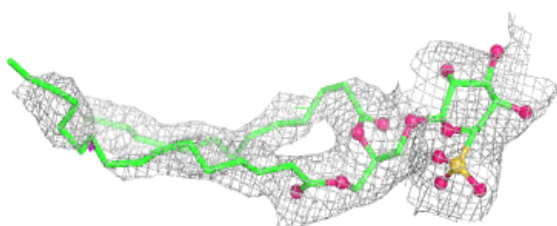
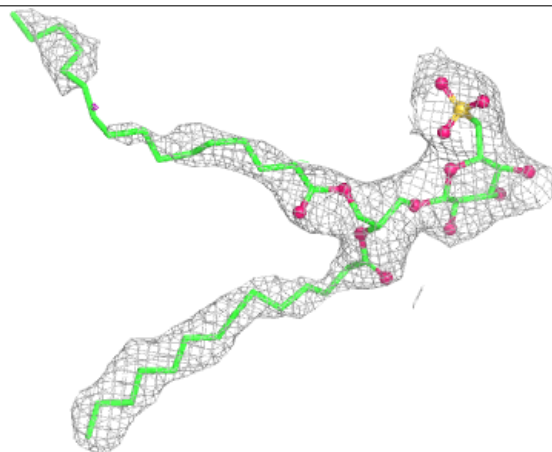


Electron density around BCR b 625:

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

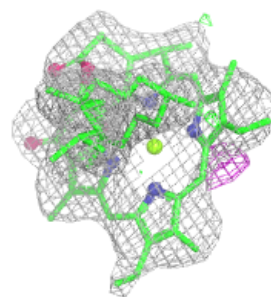
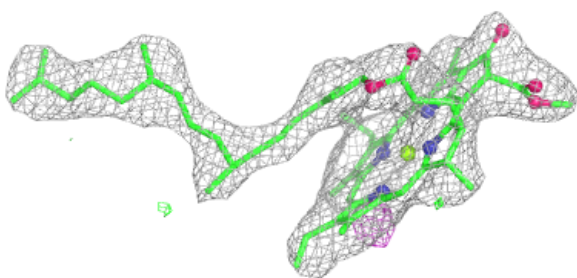
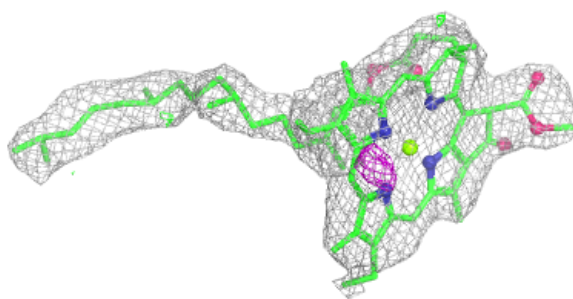
**Electron density around SQD A 612:**

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

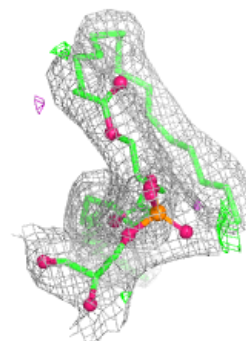
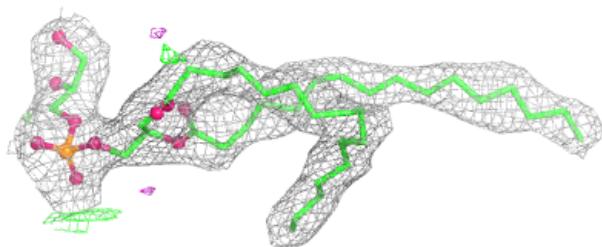
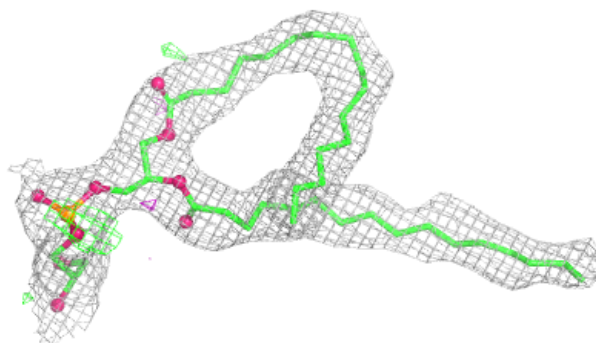


Electron density around CLA C 506:

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

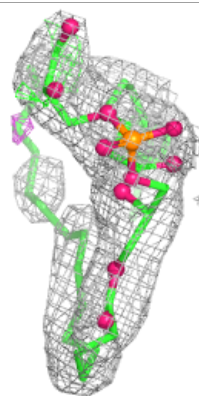
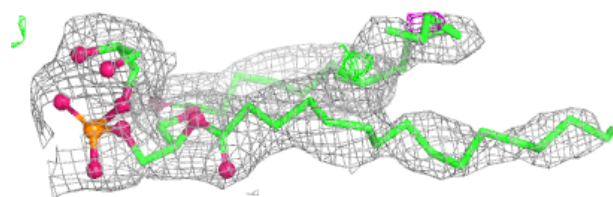
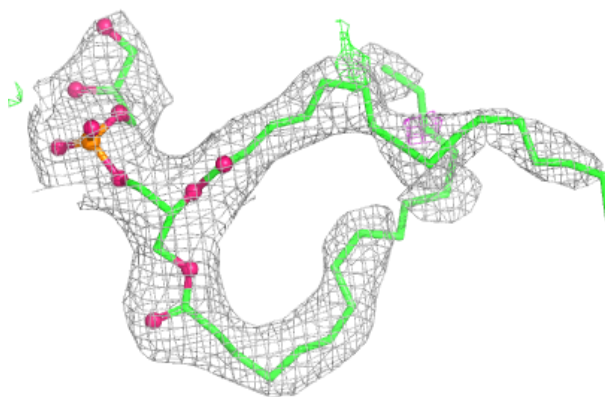
**Electron density around LHG B 625:**

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

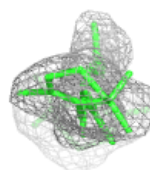
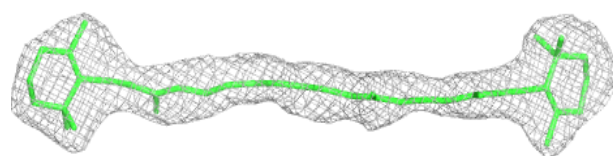
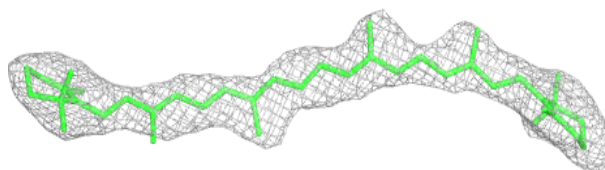


Electron density around LHG D 408:

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

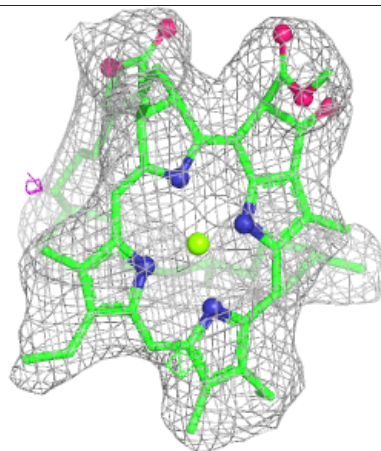
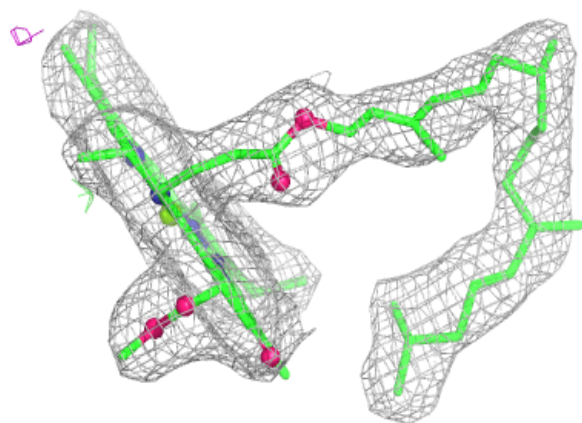
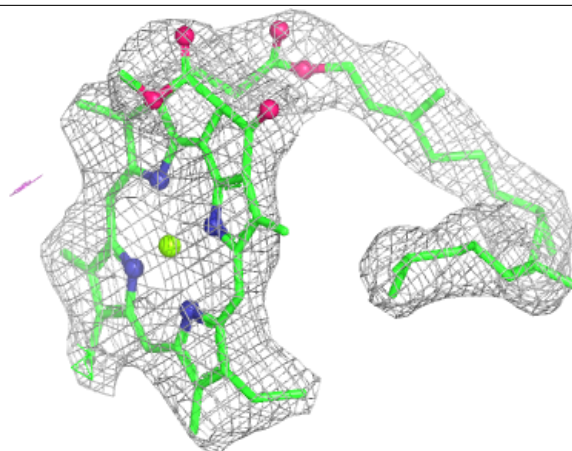
**Electron density around BCR c 515:**

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



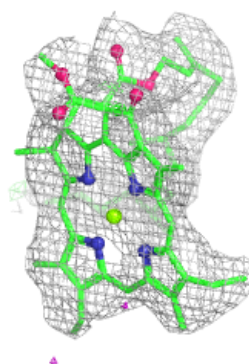
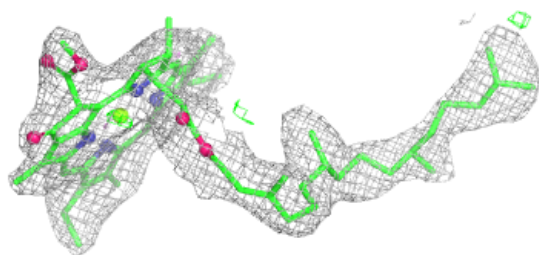
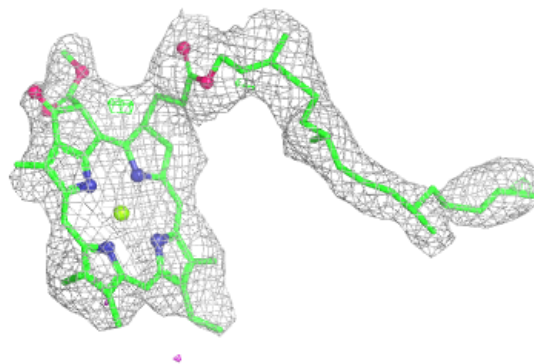
Electron density around CLA C 504:

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

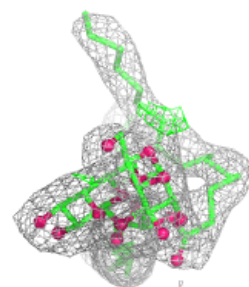
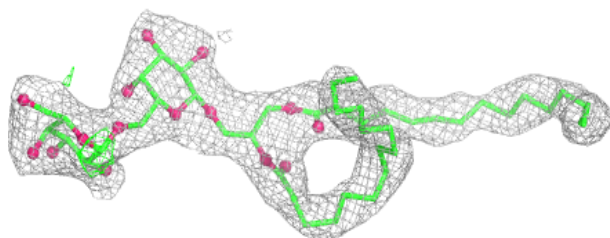
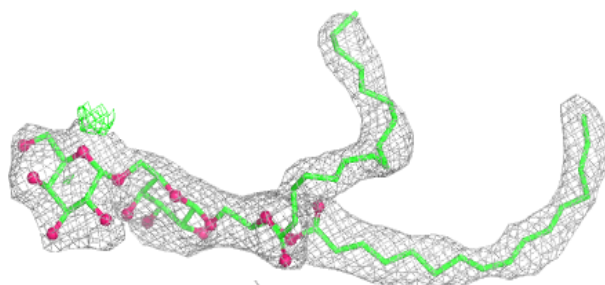


Electron density around CLA c 511:

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

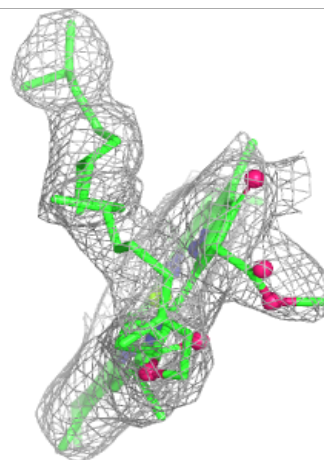
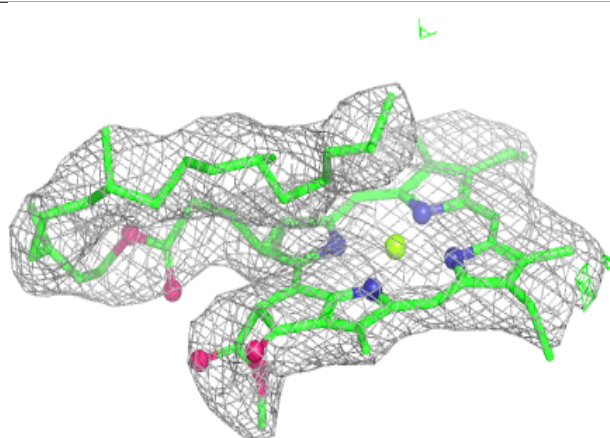
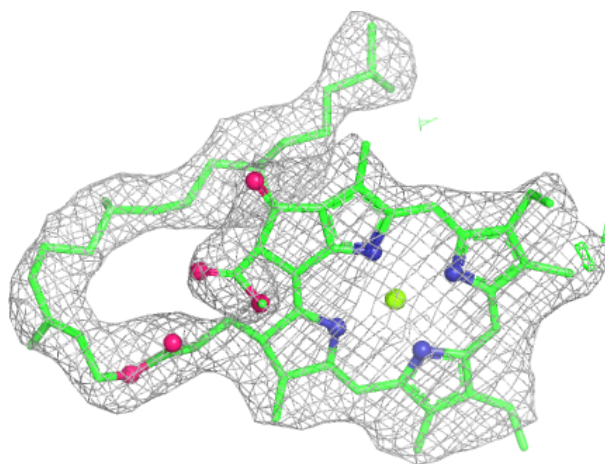
**Electron density around DGD H 103:**

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



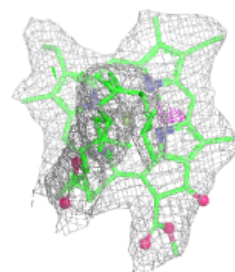
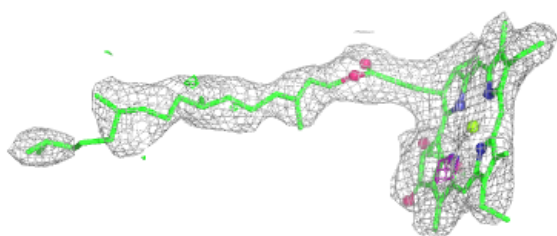
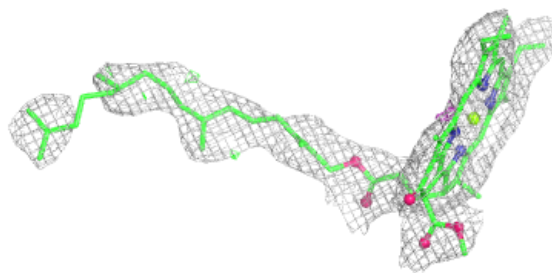
Electron density around CLA C 510:

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

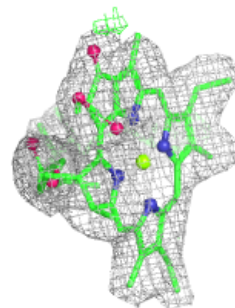
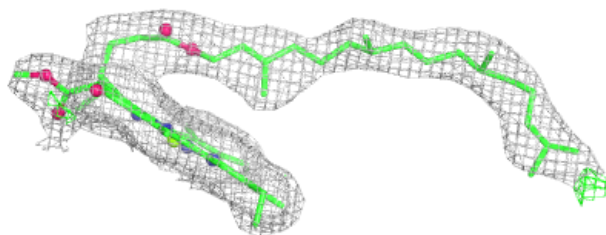
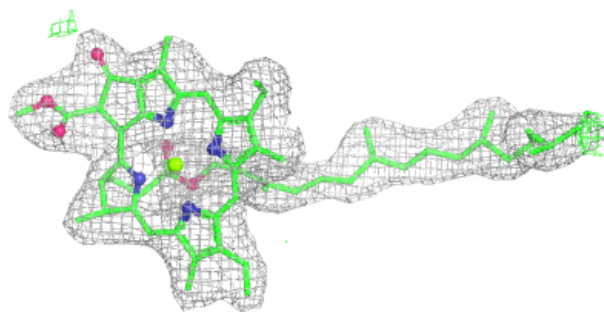


Electron density around CLA B 605:

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

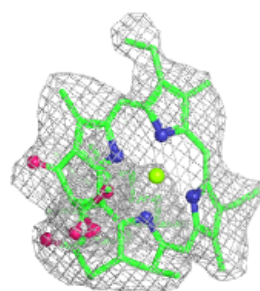
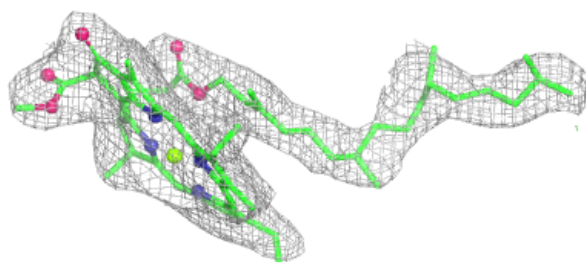
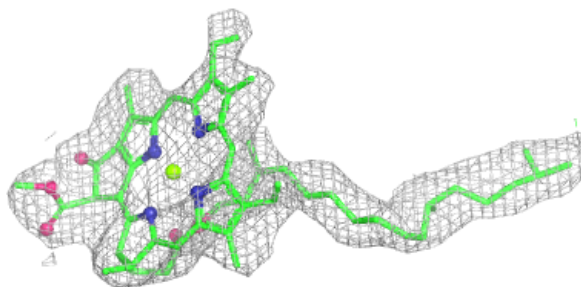
**Electron density around CLA B 609:**

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

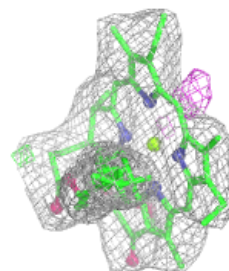
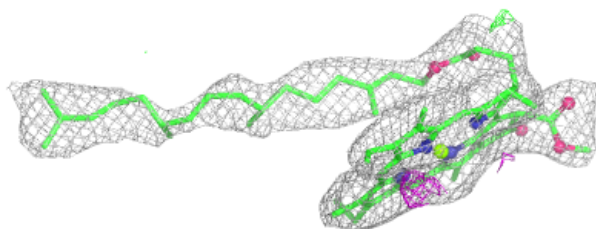
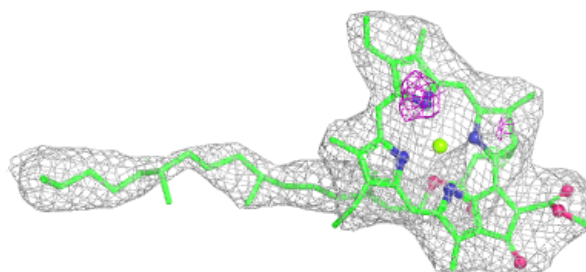


Electron density around CLA c 505:

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

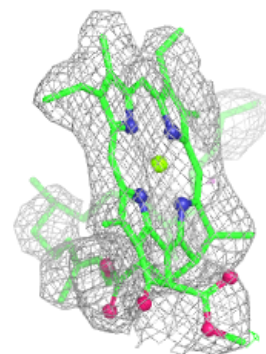
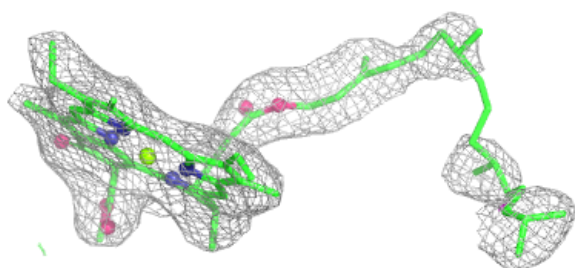
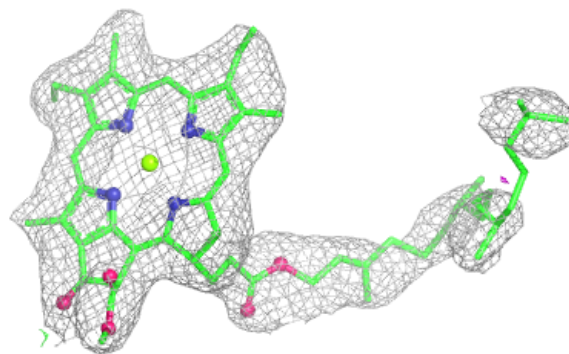
**Electron density around CLA B 615:**

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



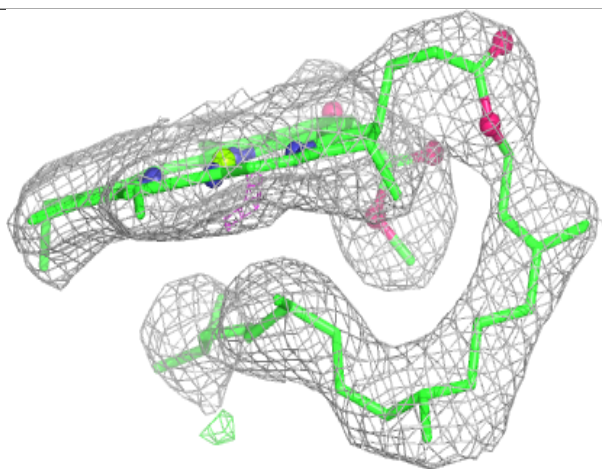
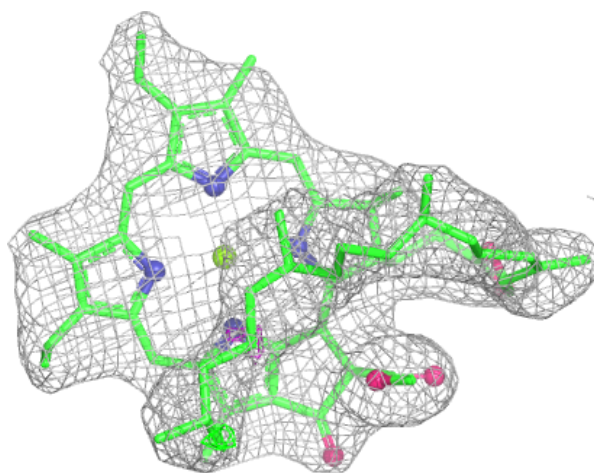
Electron density around CLA a 711:

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



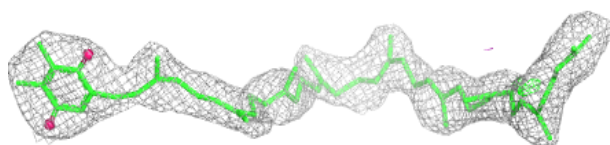
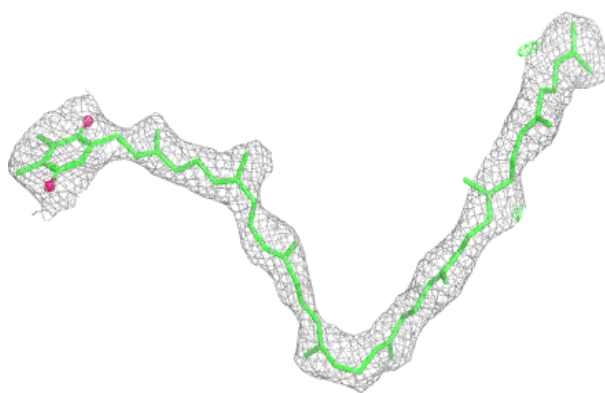
Electron density around CLA C 511:

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

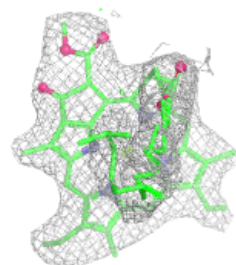
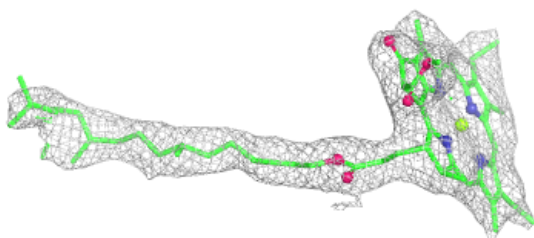
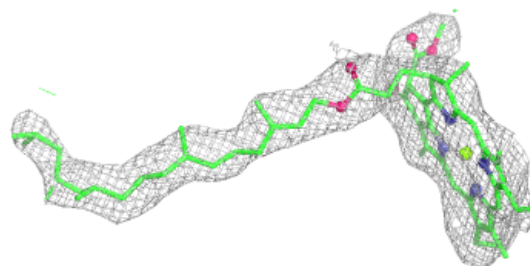


Electron density around PL9 D 406:

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

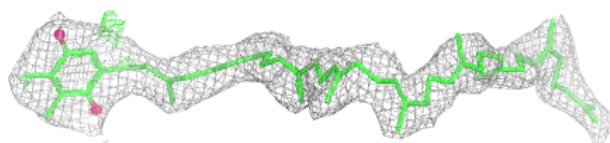
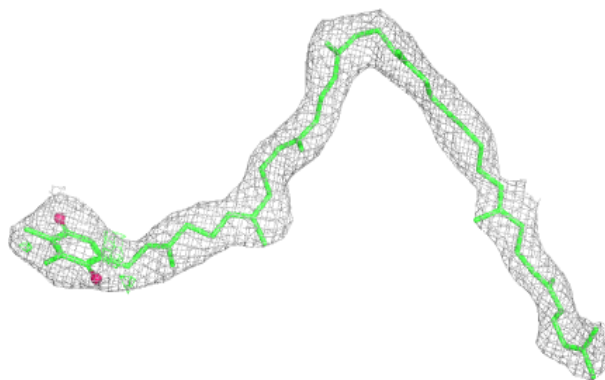
**Electron density around CLA b 610:**

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

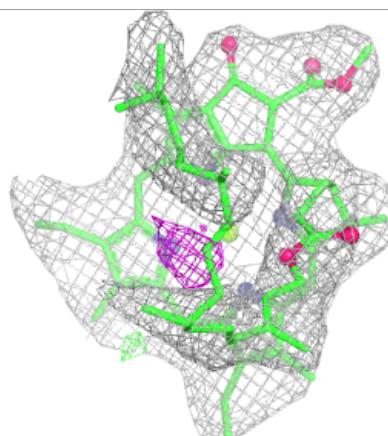
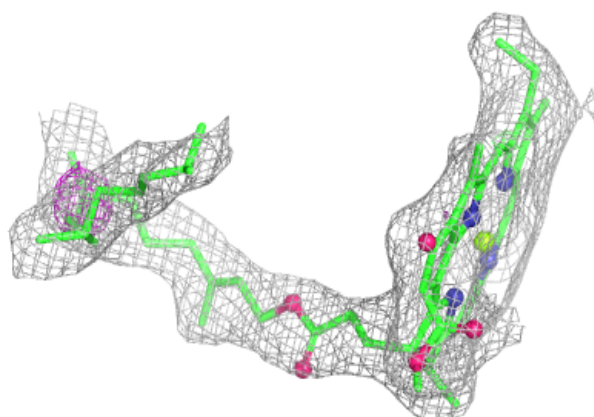
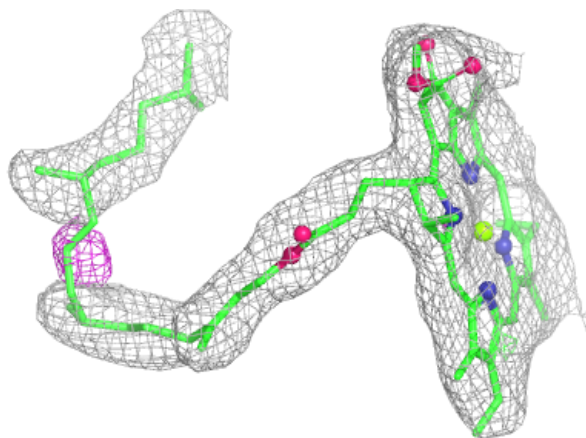


Electron density around PL9 d 405:

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

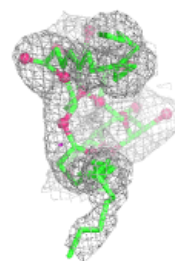
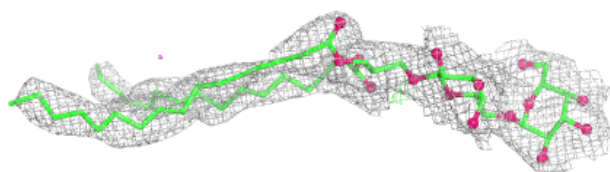
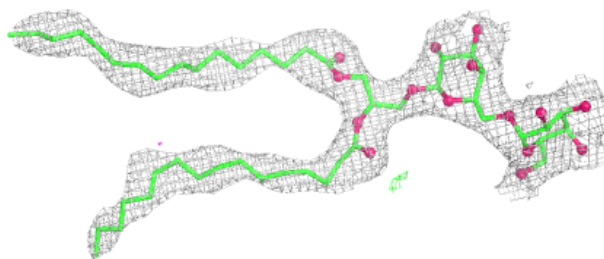
**Electron density around CLA b 612:**

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

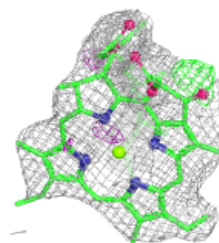
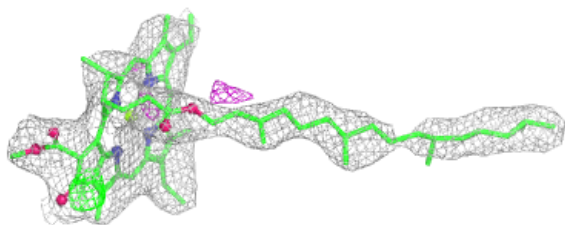
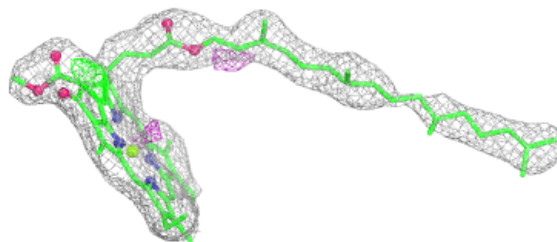


Electron density around DGD C 519:

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

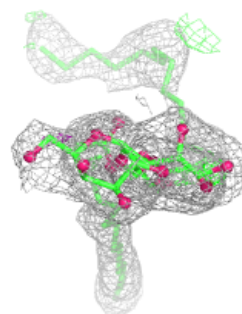
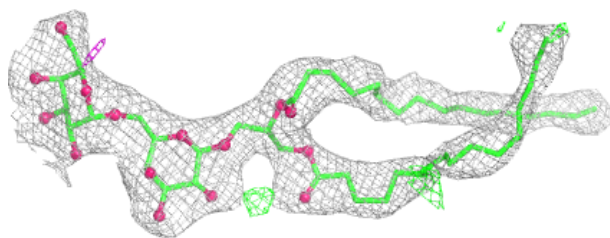
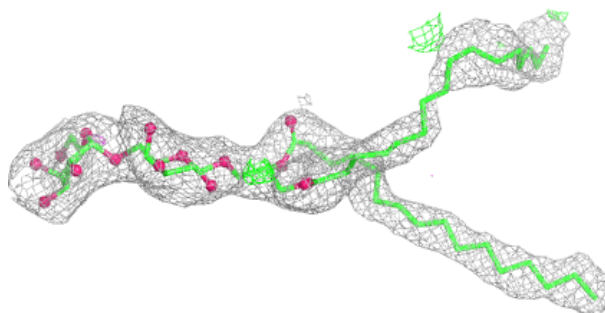
**Electron density around CLA b 613:**

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

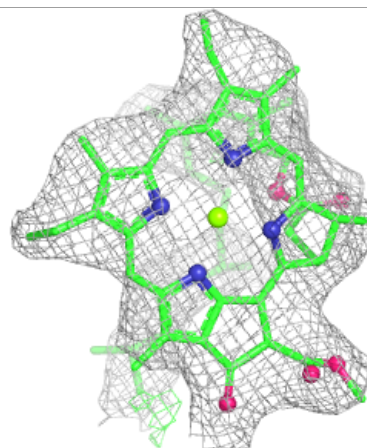
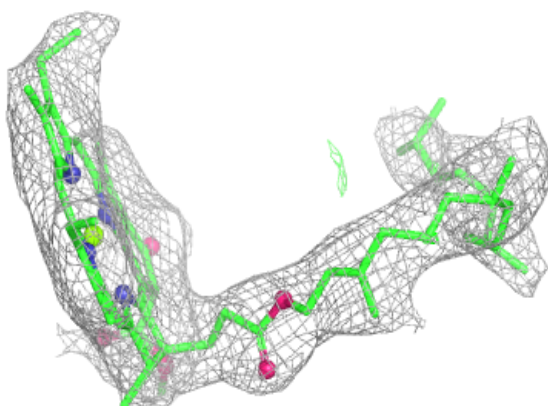
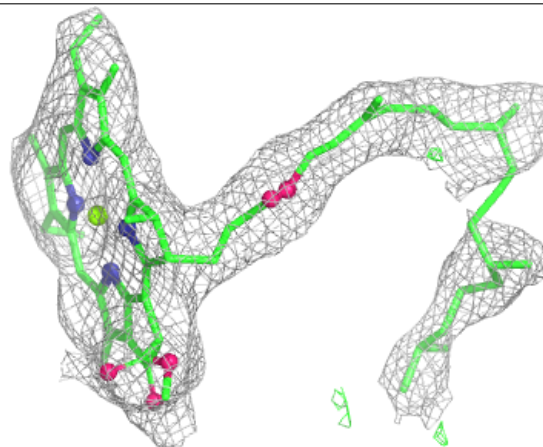


Electron density around DGD c 516:

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

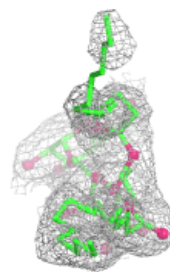
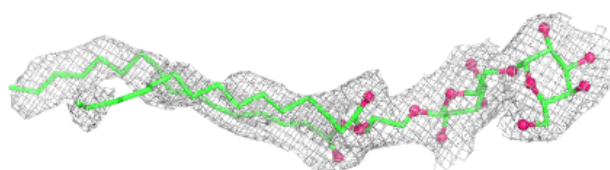
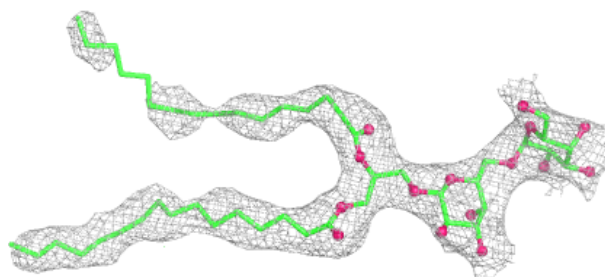
**Electron density around CLA B 607:**

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

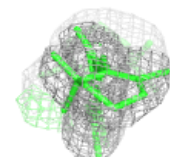
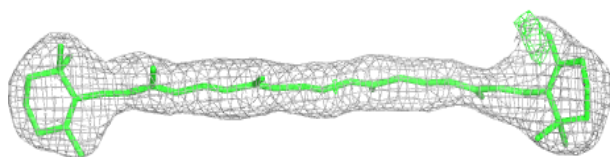


Electron density around DGD c 518:

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

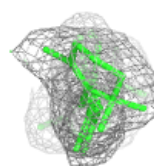
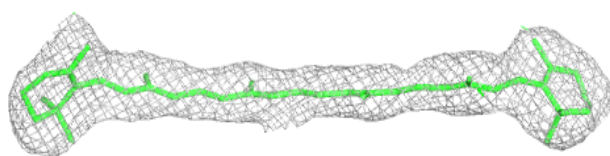
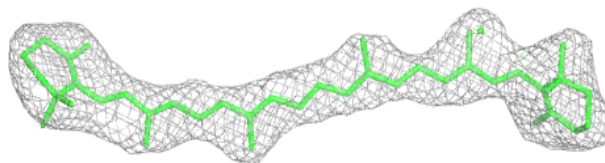
**Electron density around BCR C 516:**

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

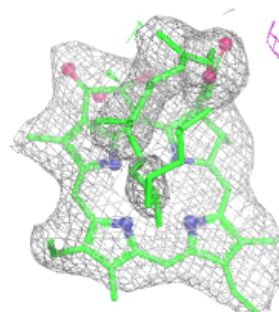
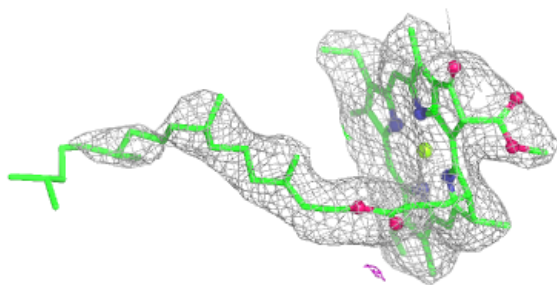
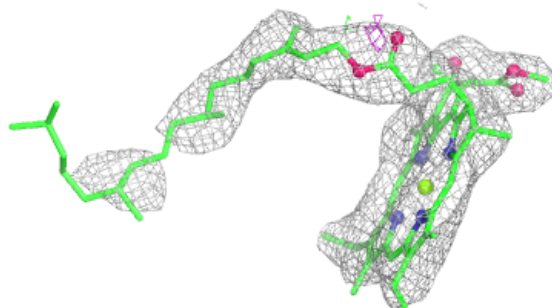


Electron density around BCR B 619:

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

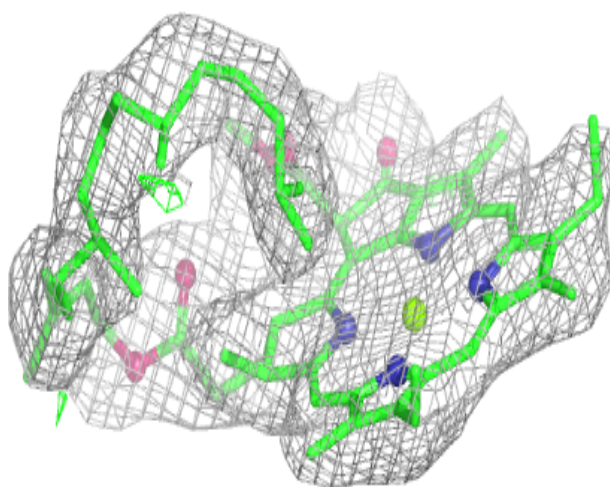
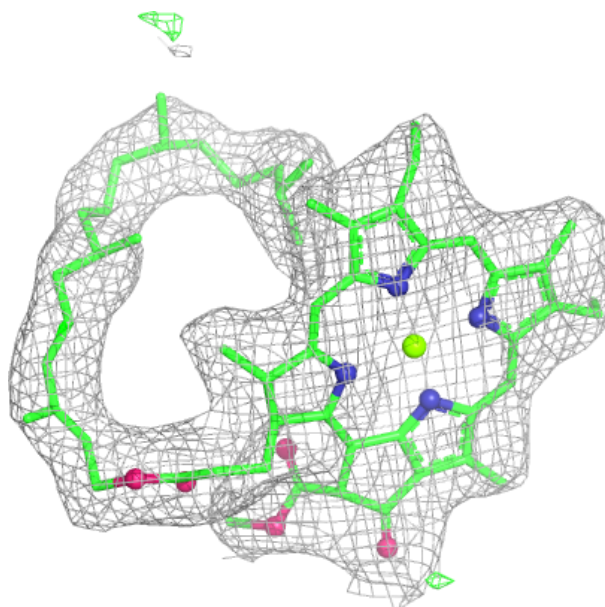
**Electron density around CLA C 509:**

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



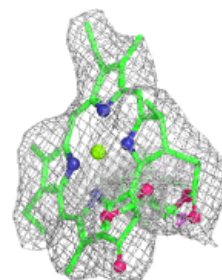
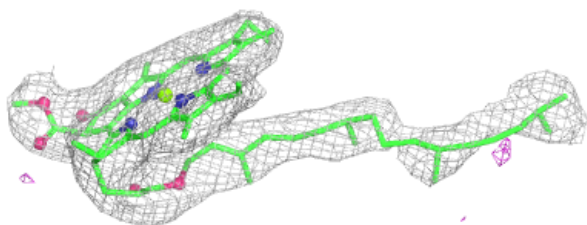
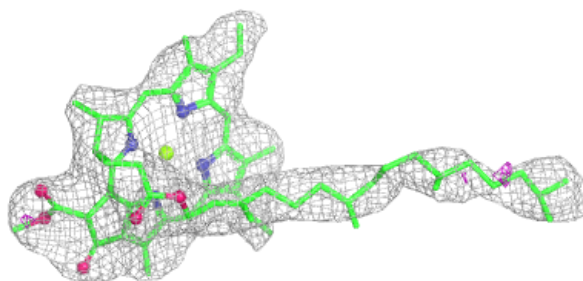
Electron density around CLA B 616:

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



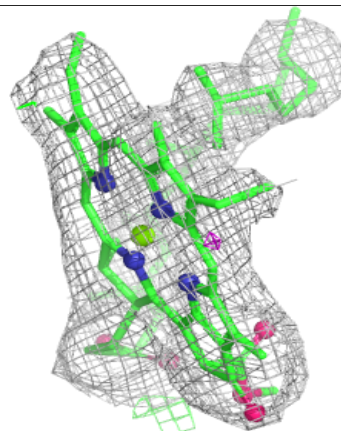
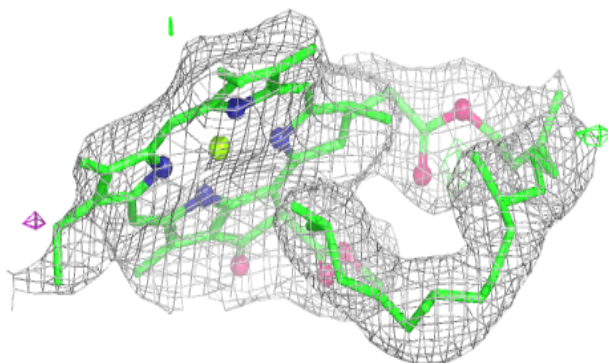
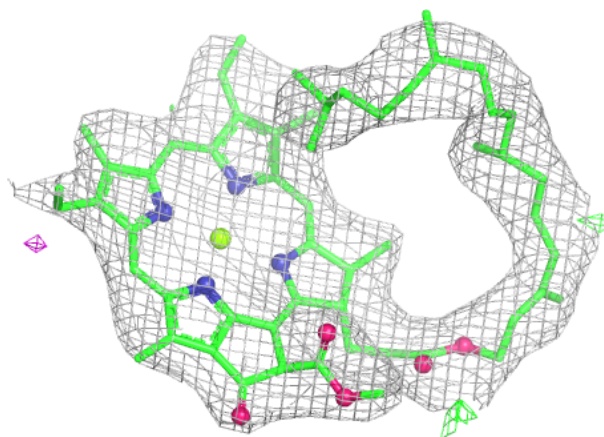
Electron density around CLA b 620:

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



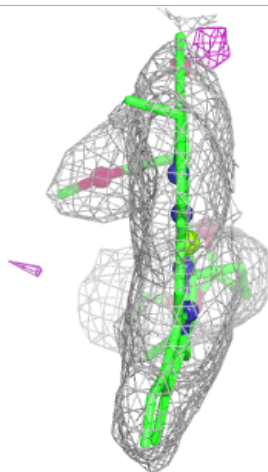
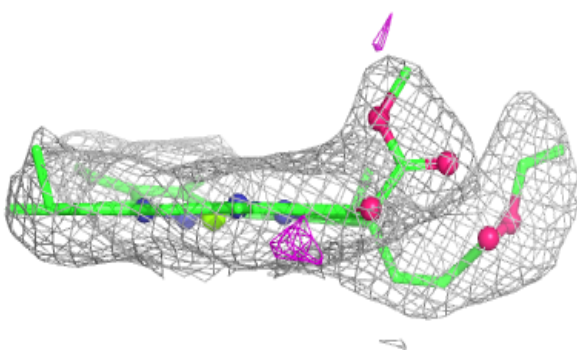
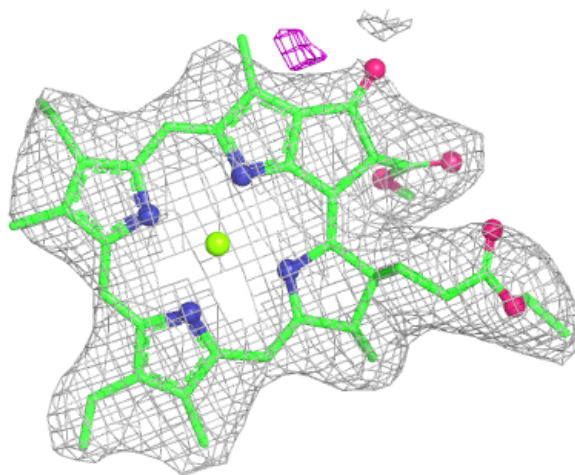
Electron density around CLA b 621:

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



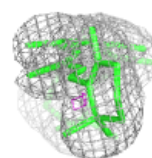
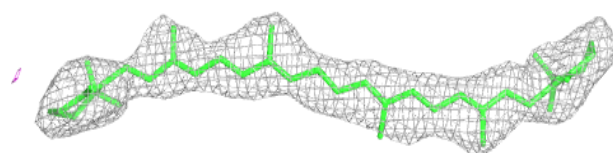
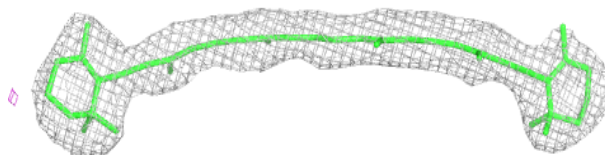
Electron density around CLA b 622:

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

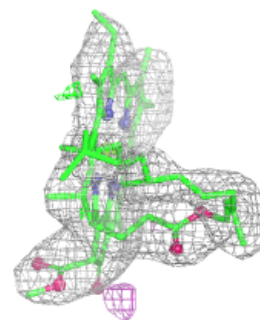
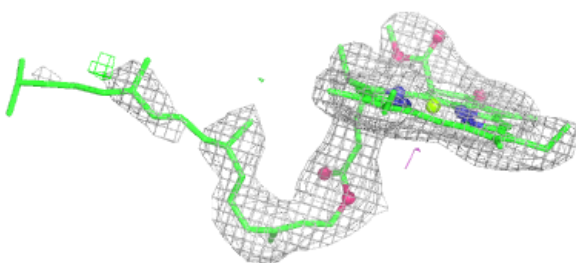
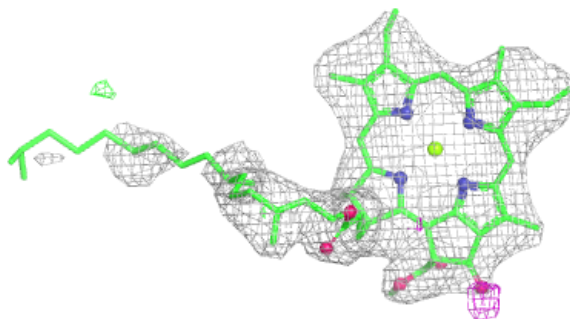


Electron density around BCR K 101:

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

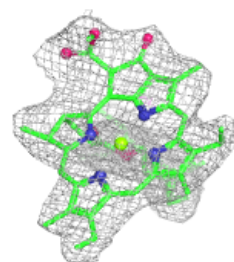
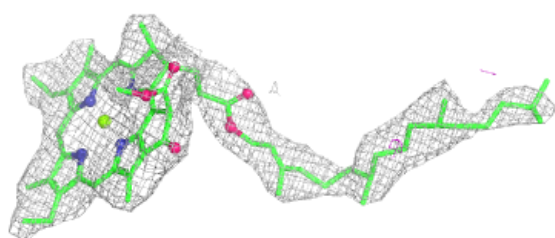
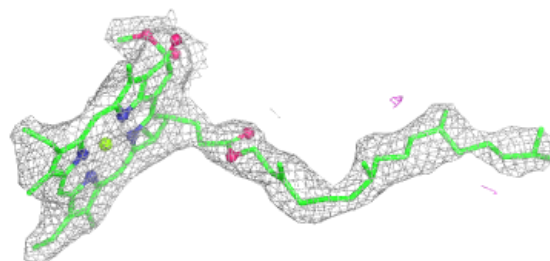
**Electron density around CLA A 607:**

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

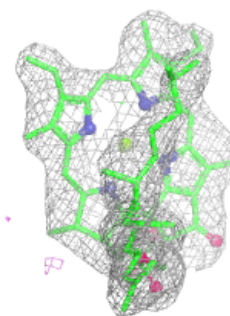
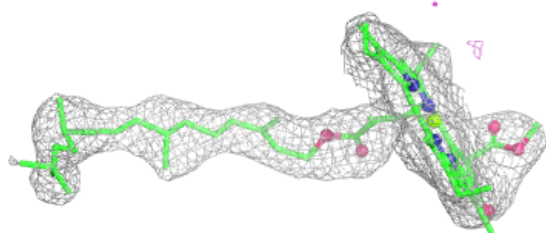
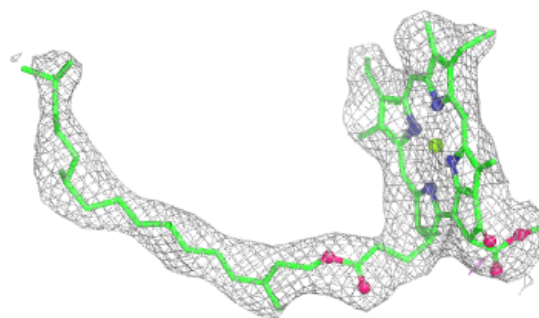


Electron density around CLA C 503:

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

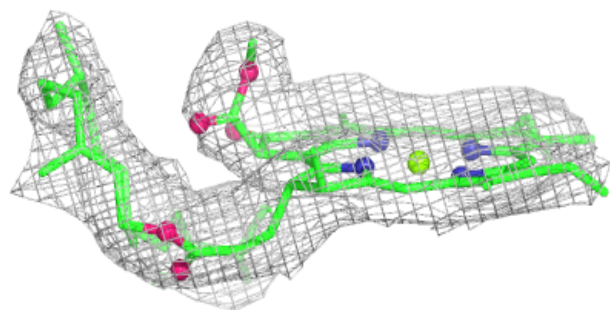
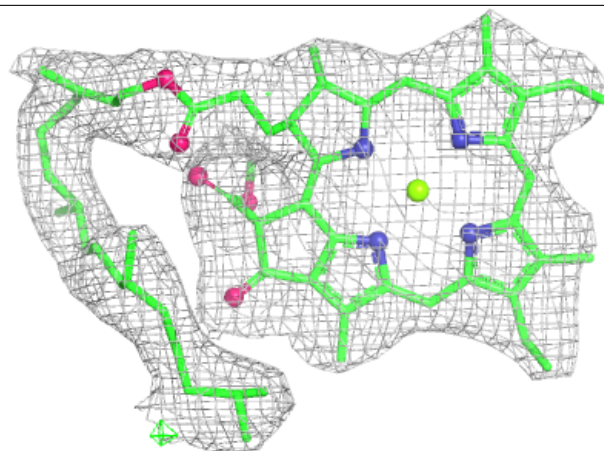
**Electron density around CLA B 610:**

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



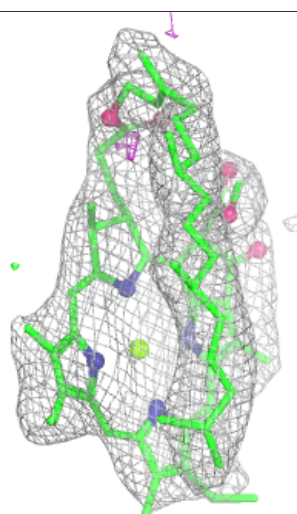
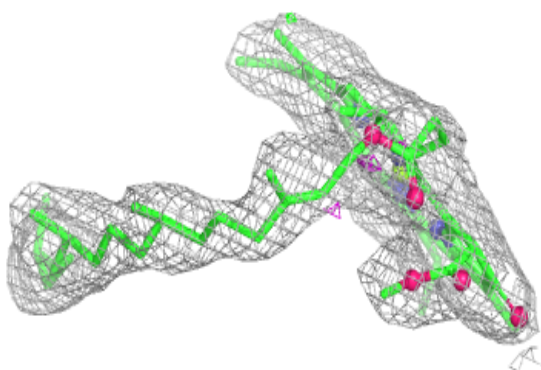
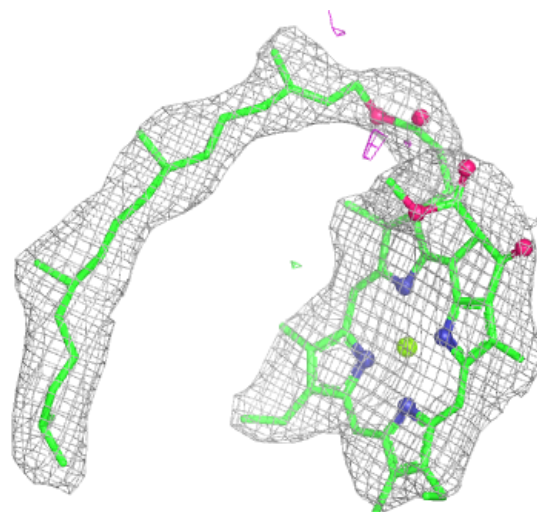
Electron density around CLA B 611:

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



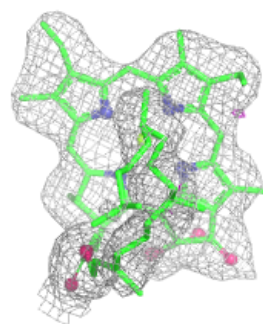
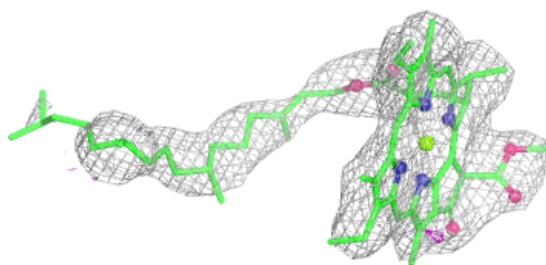
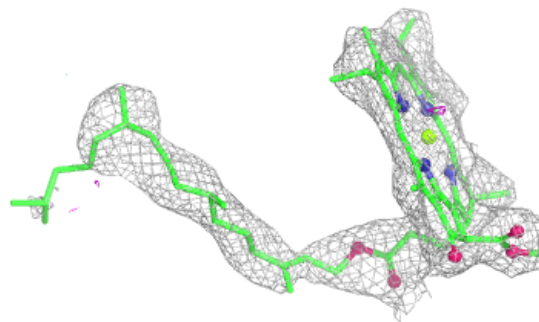
Electron density around CLA c 507:

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



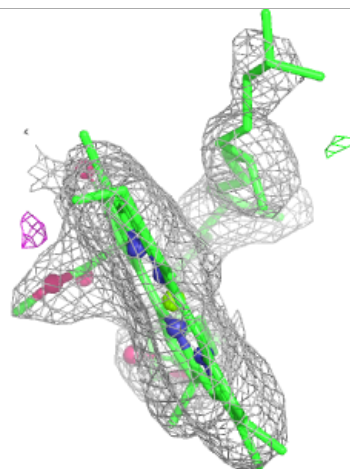
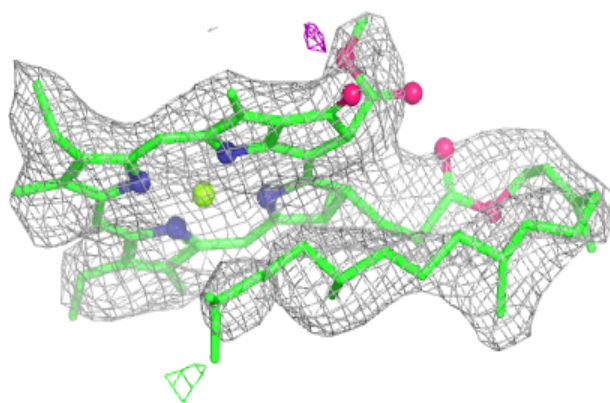
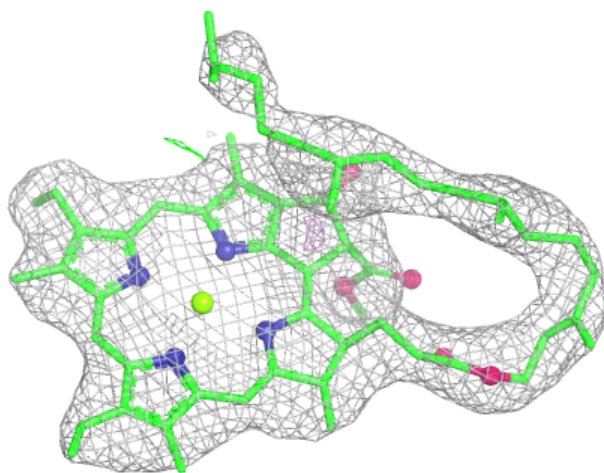
Electron density around CLA c 508:

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



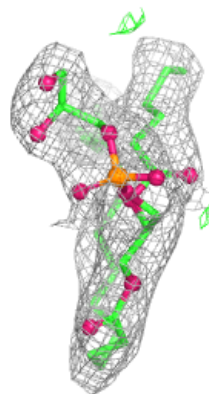
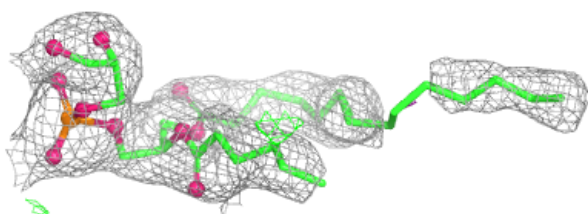
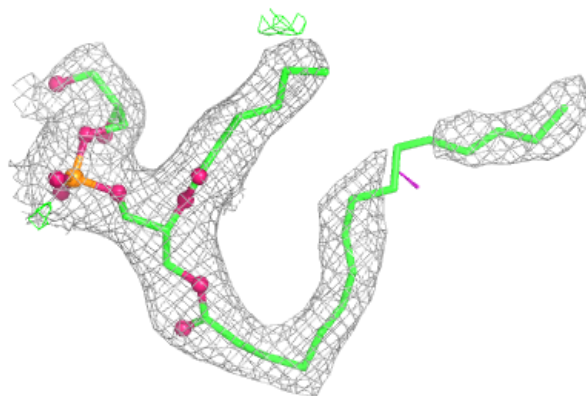
Electron density around CLA c 509:

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

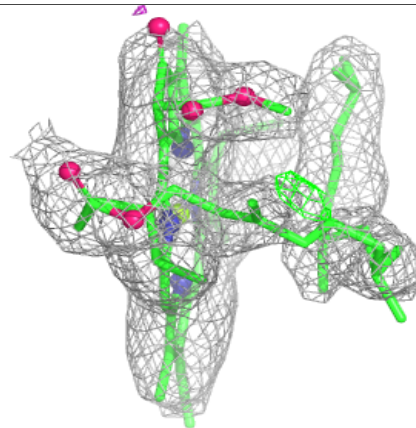
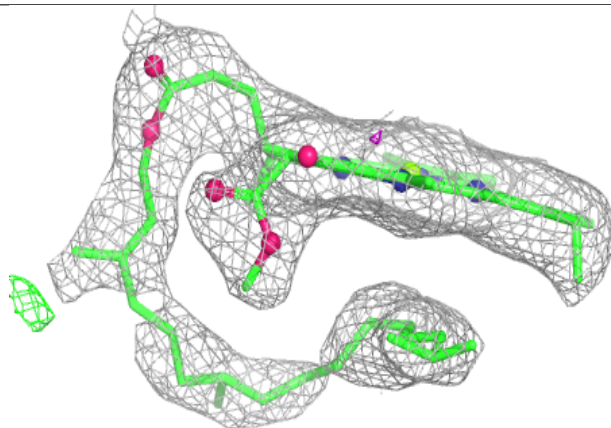
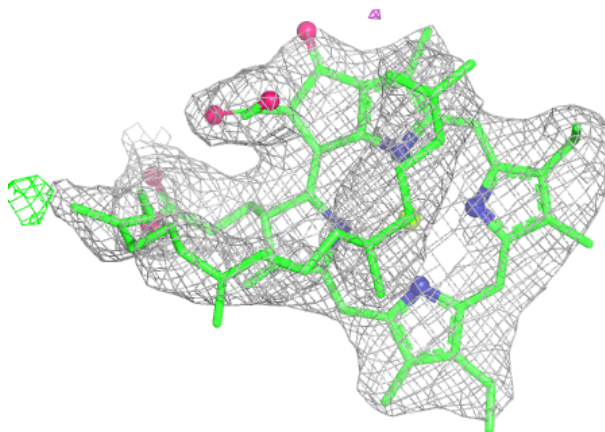


Electron density around LHG a 720:

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

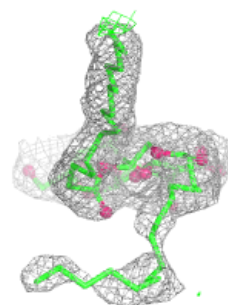
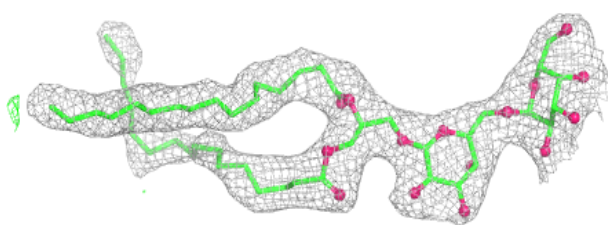
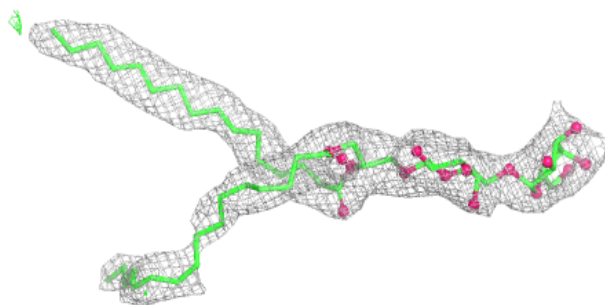
**Electron density around CLA c 510:**

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

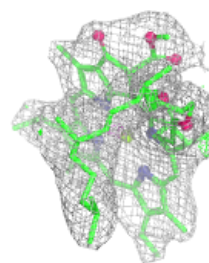
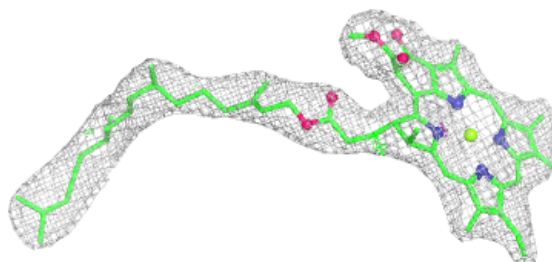


Electron density around DGD C 517:

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

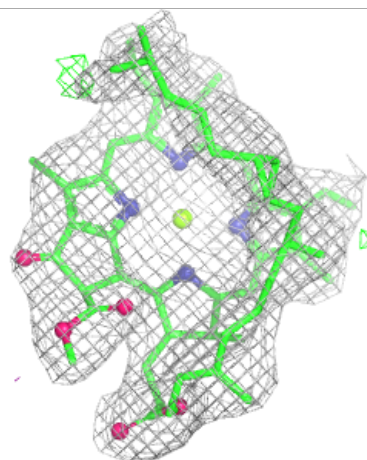
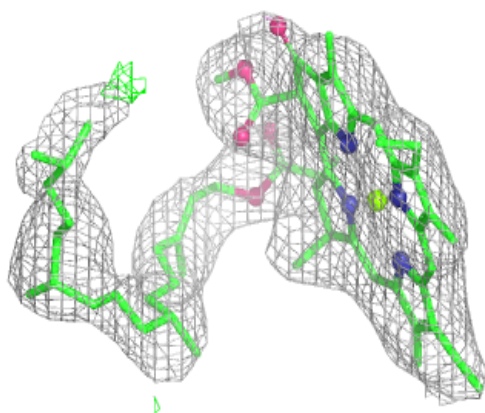
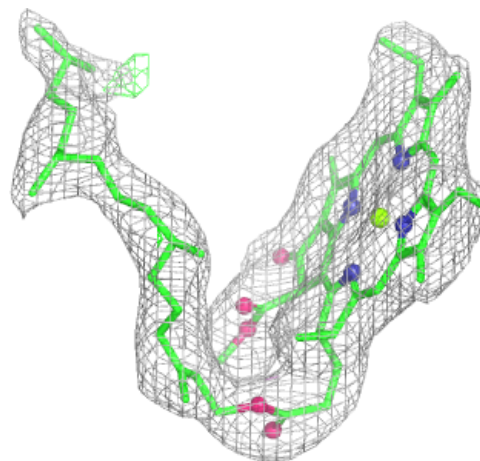
**Electron density around CLA a 707:**

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



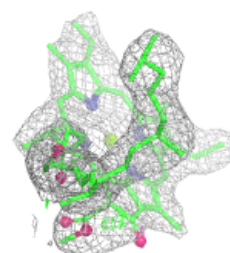
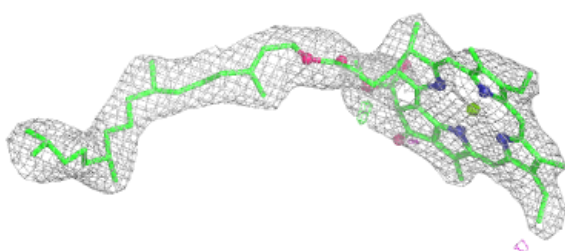
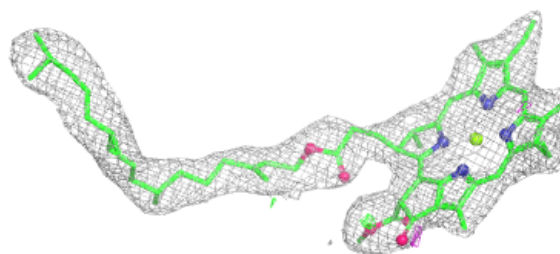
Electron density around CLA B 614:

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

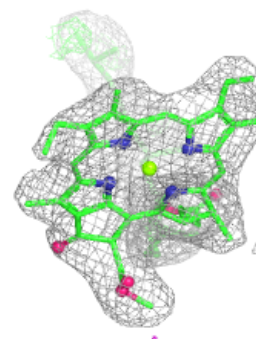
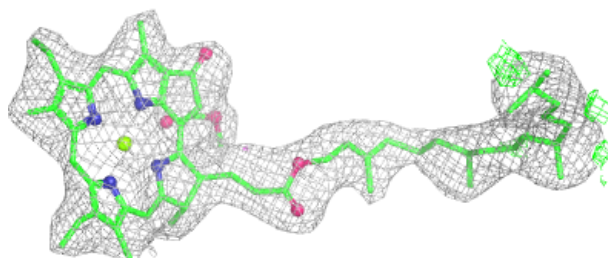
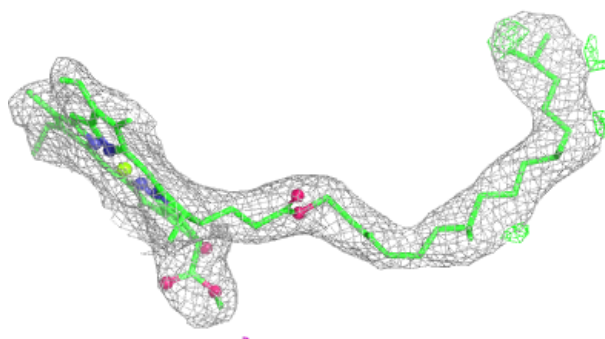


Electron density around CLA A 606:

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

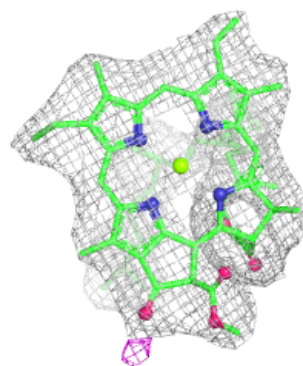
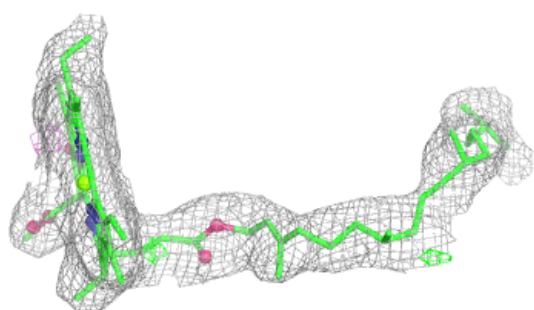
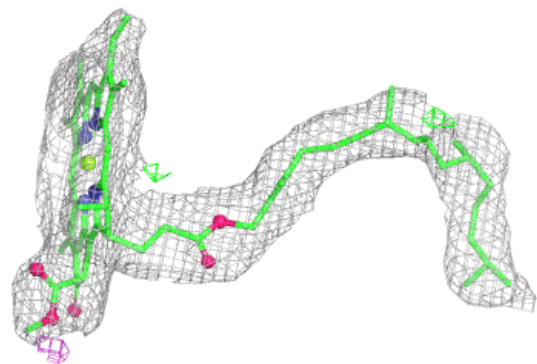
**Electron density around CLA d 402:**

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

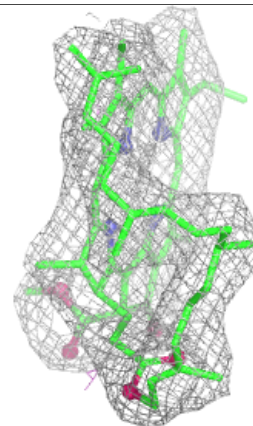
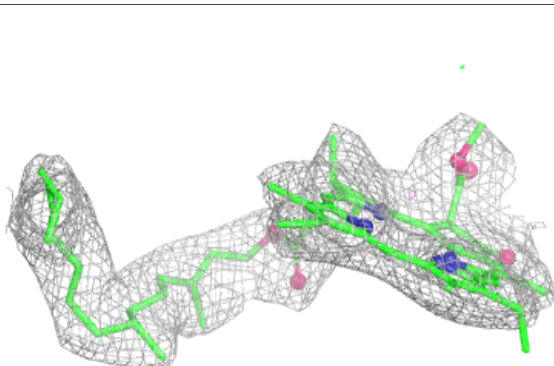
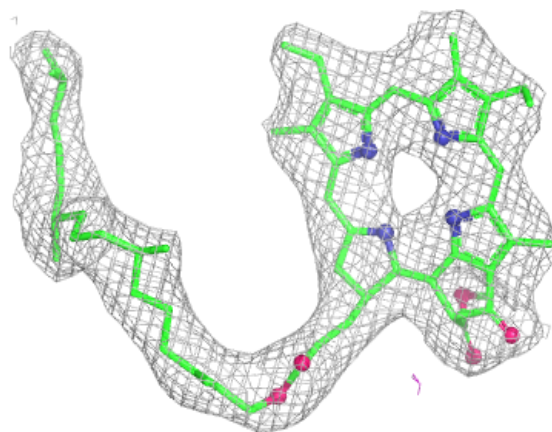


Electron density around CLA d 403:

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

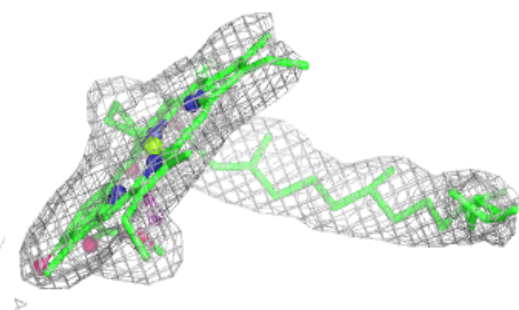
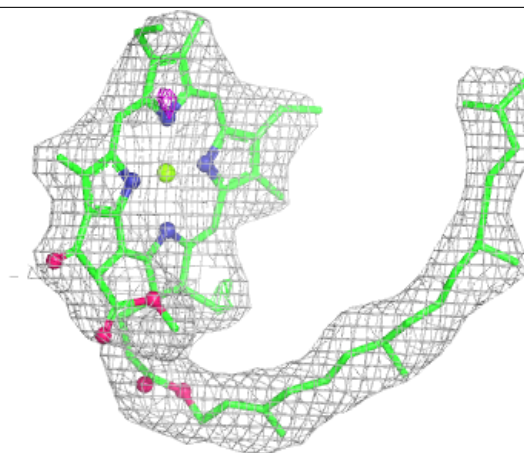
**Electron density around PHO D 401:**

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



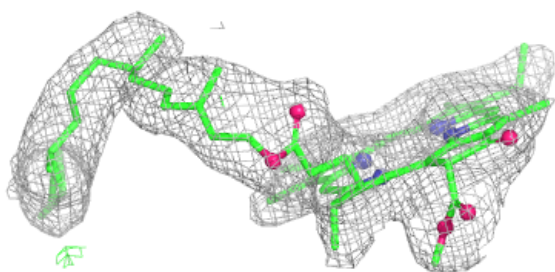
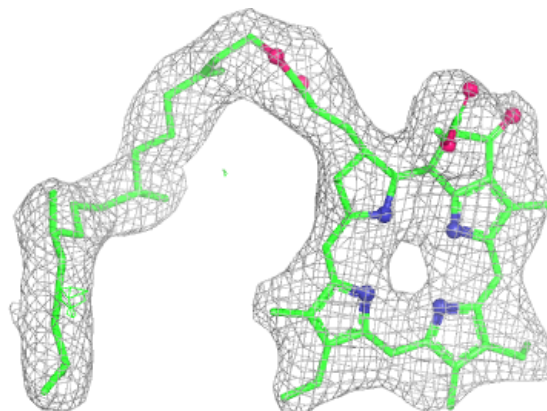
Electron density around CLA C 508:

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

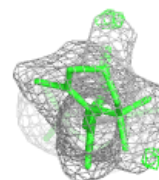
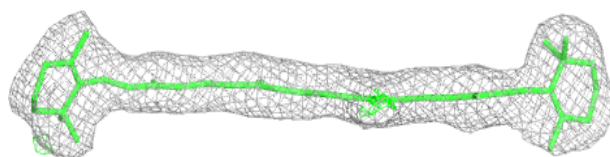
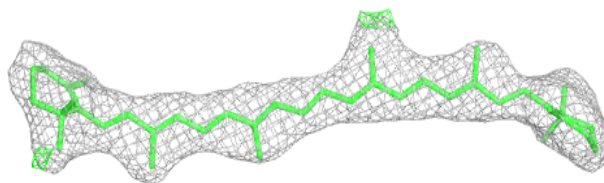


Electron density around PHO a 710:

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

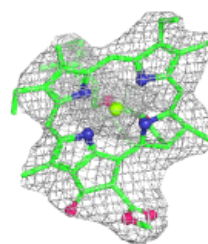
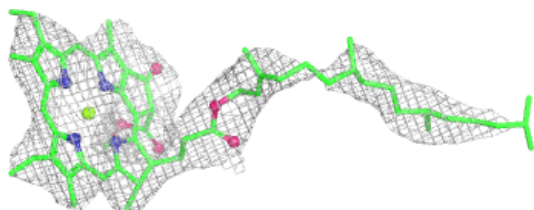
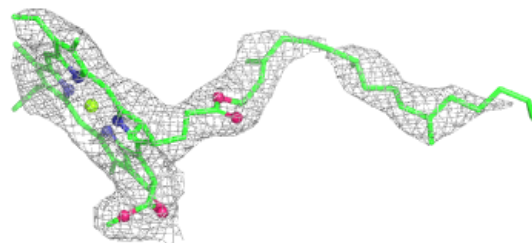
**Electron density around BCR A 610:**

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



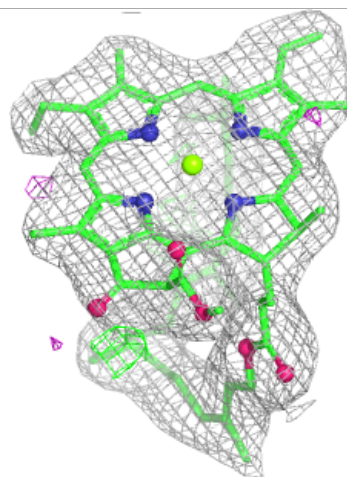
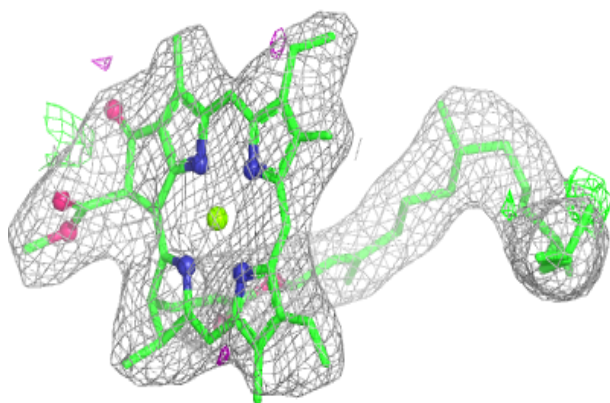
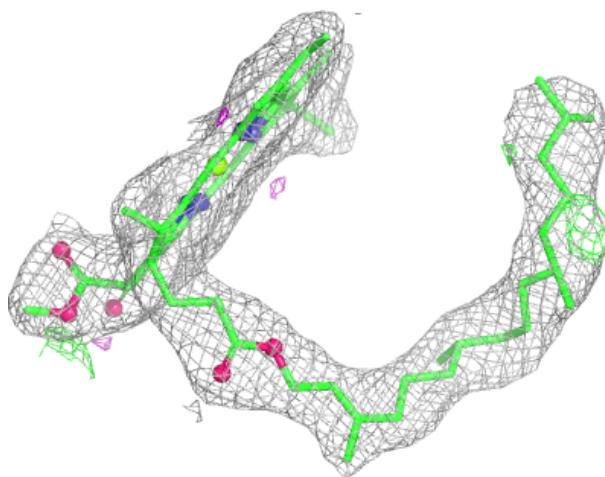
Electron density around CLA c 502:

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



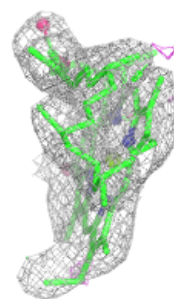
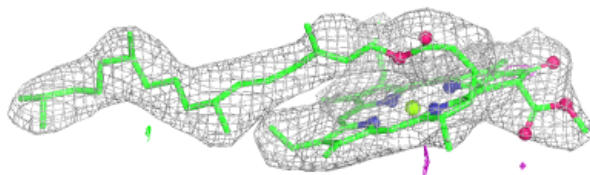
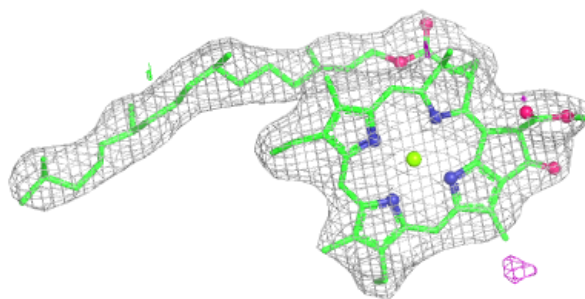
Electron density around CLA B 612:

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

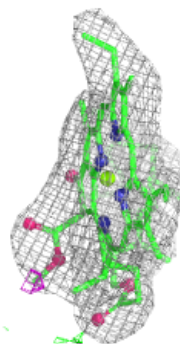
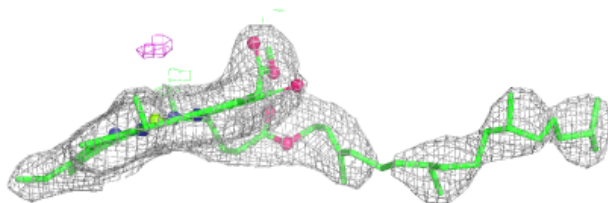
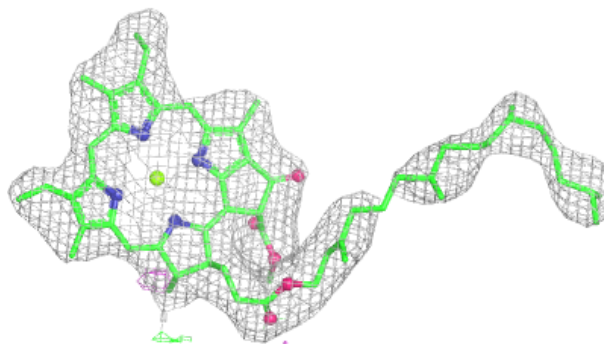


Electron density around CLA C 502:

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

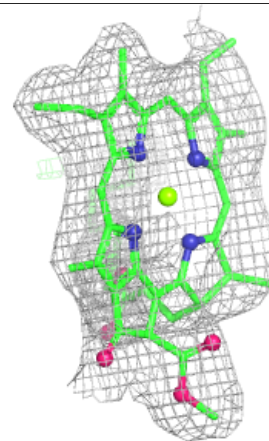
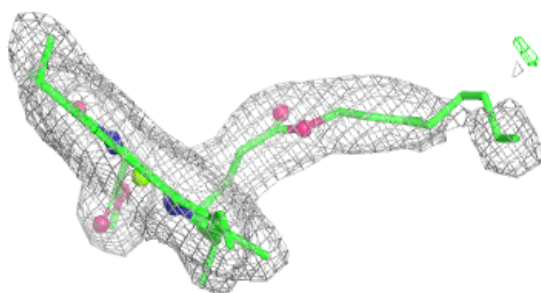
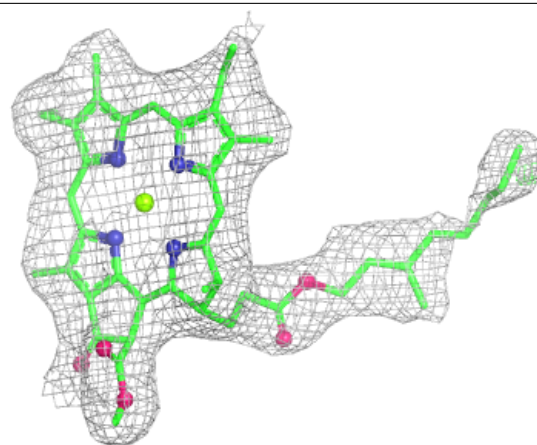
**Electron density around CLA b 608:**

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



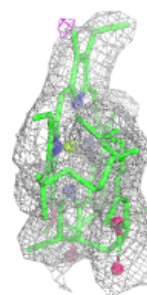
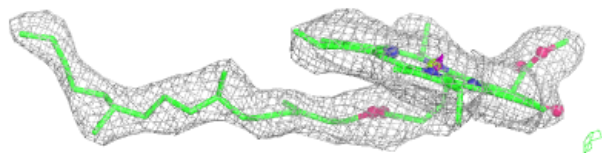
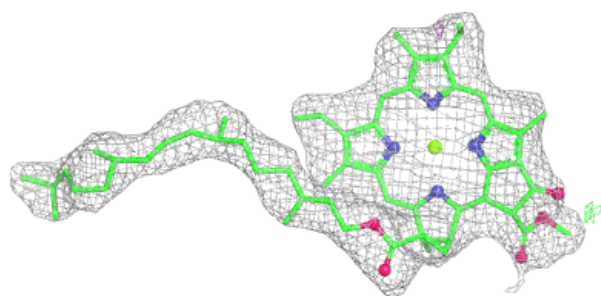
Electron density around CLA A 609:

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



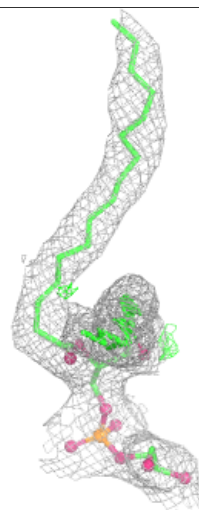
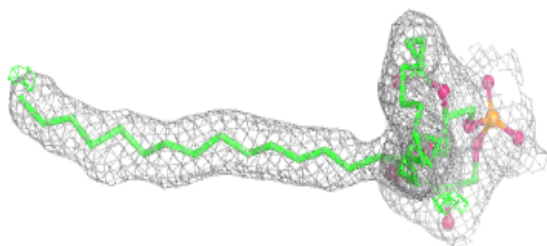
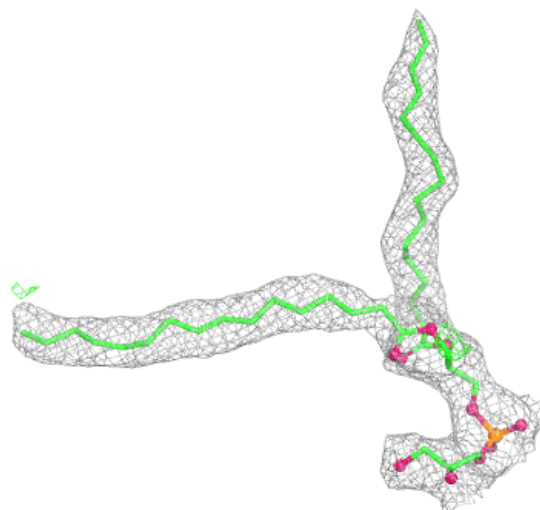
Electron density around CLA B 604:

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



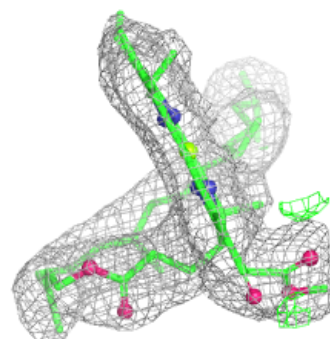
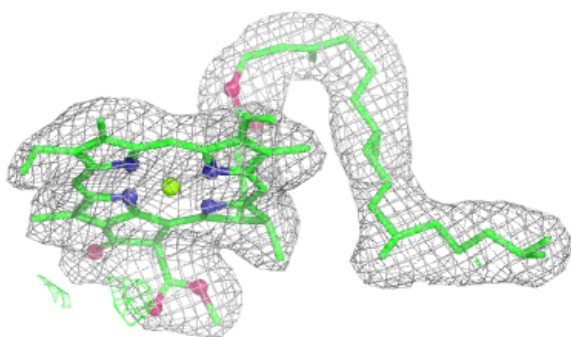
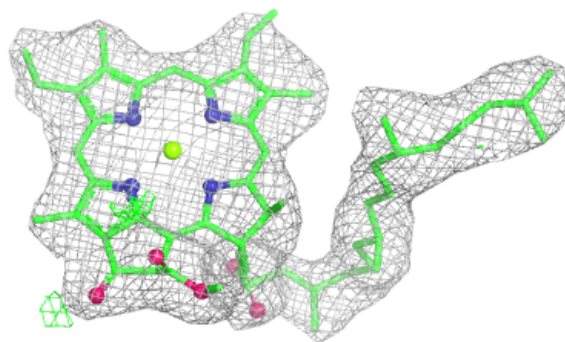
Electron density around LHG L 101:

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



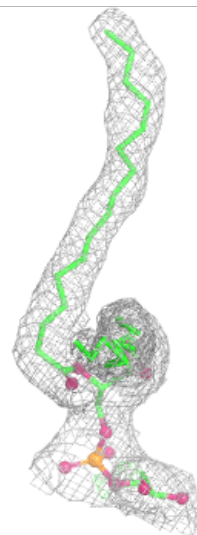
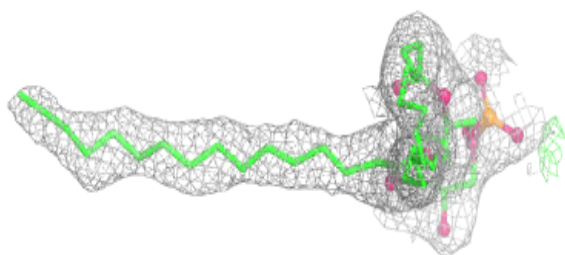
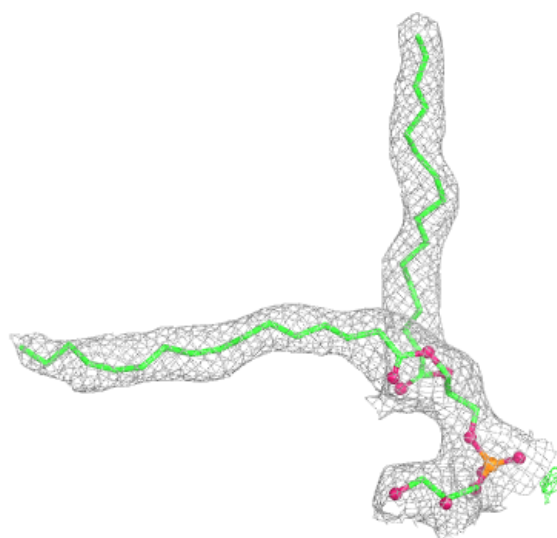
Electron density around CLA D 402:

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



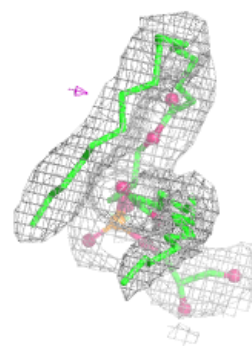
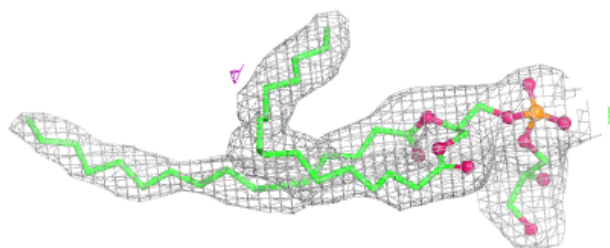
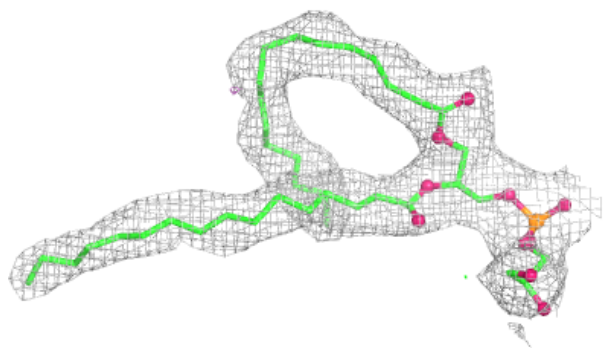
Electron density around LHG b 629:

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

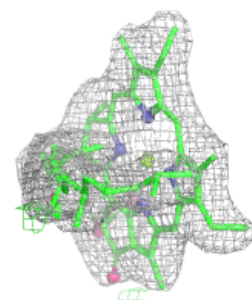
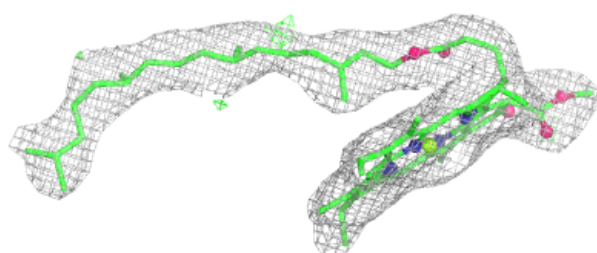
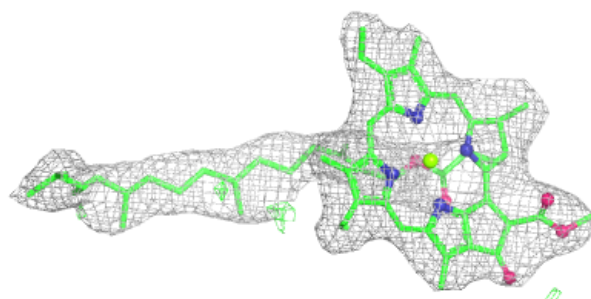


Electron density around LHG d 406:

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

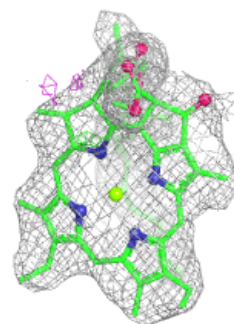
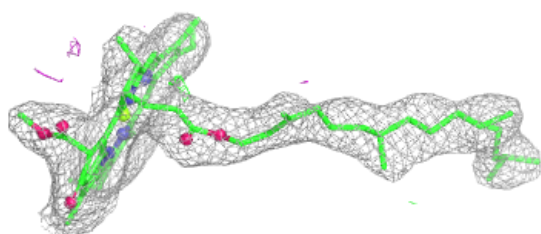
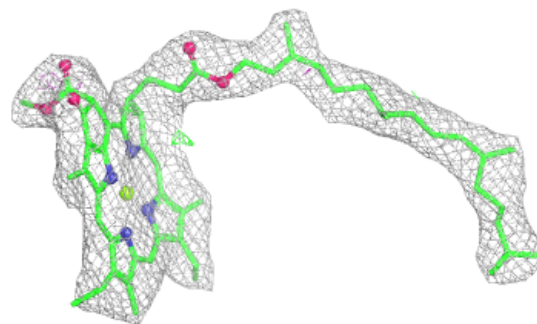
**Electron density around CLA b 614:**

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

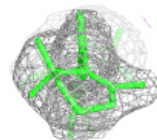
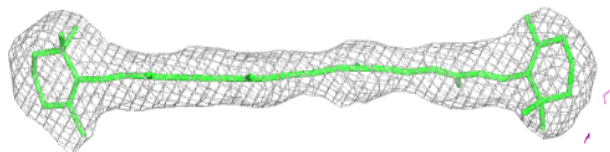
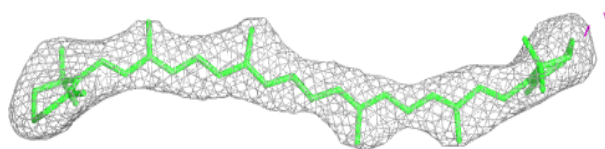


Electron density around CLA b 615:

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

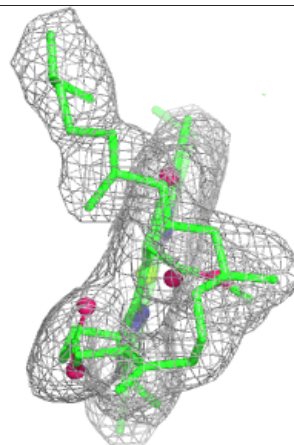
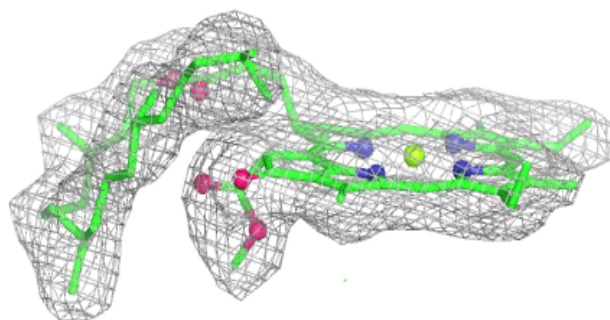
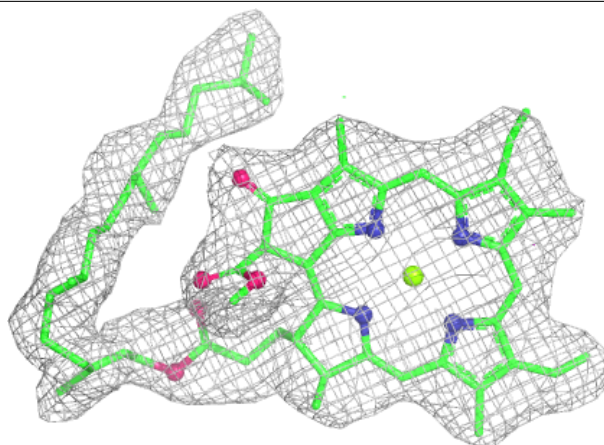
**Electron density around BCR a 712:**

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



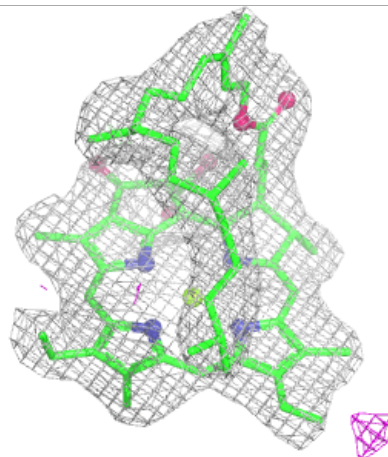
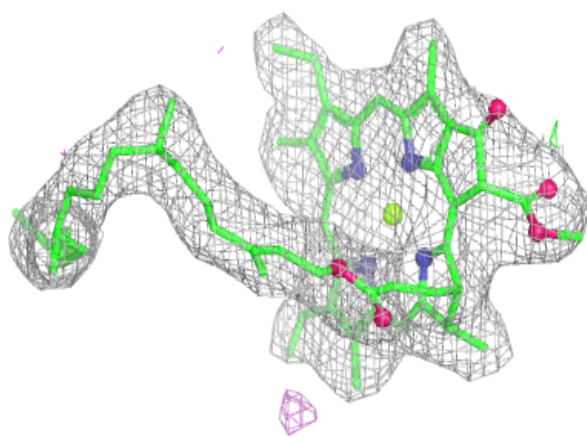
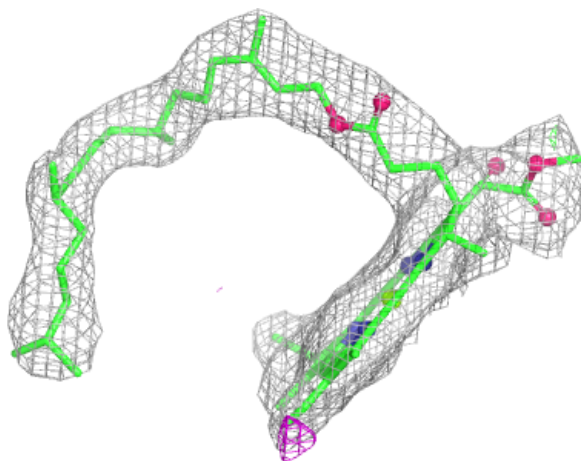
Electron density around CLA b 616:

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



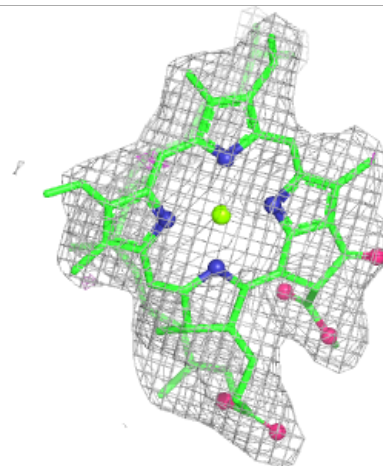
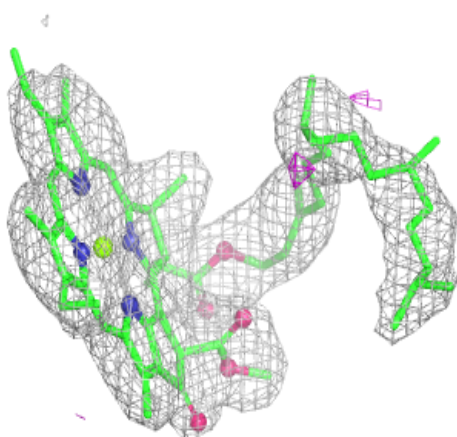
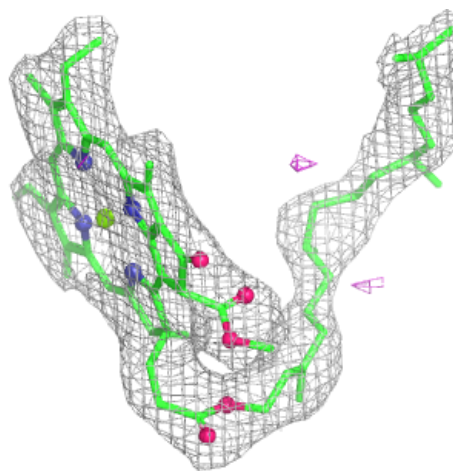
Electron density around CLA b 617:

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



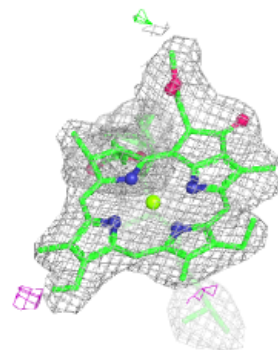
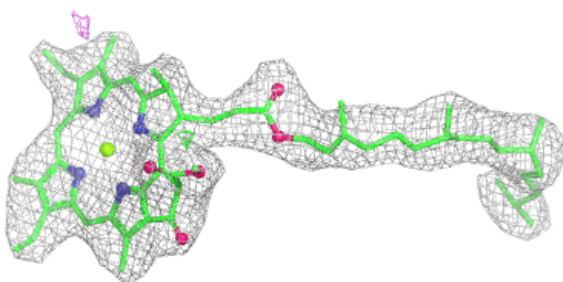
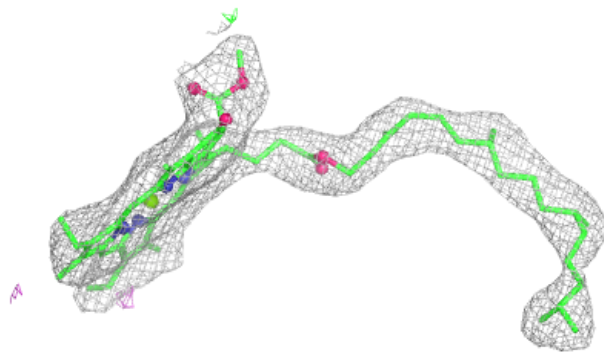
Electron density around CLA b 619:

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

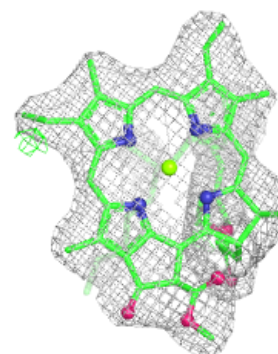
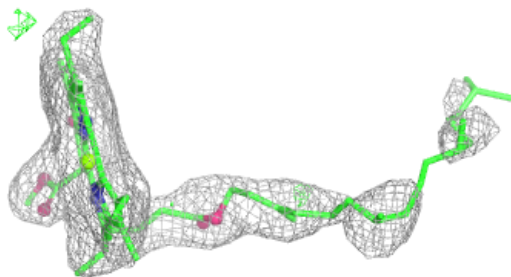
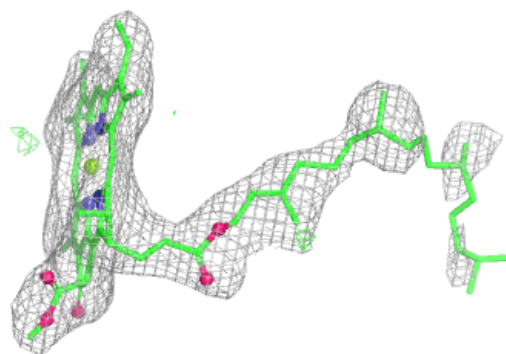


Electron density around CLA D 403:

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

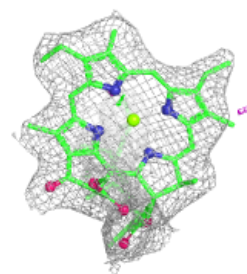
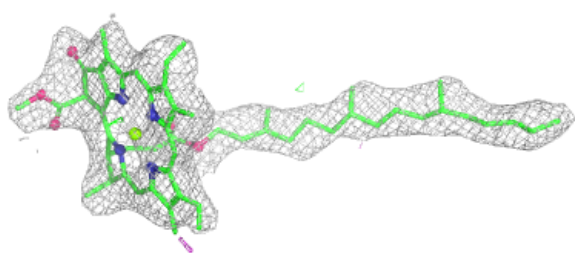
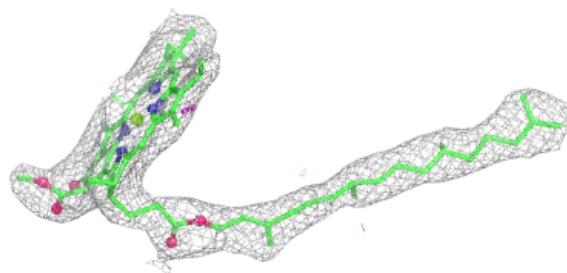
**Electron density around CLA D 404:**

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



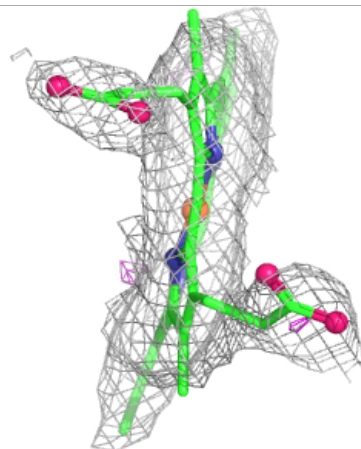
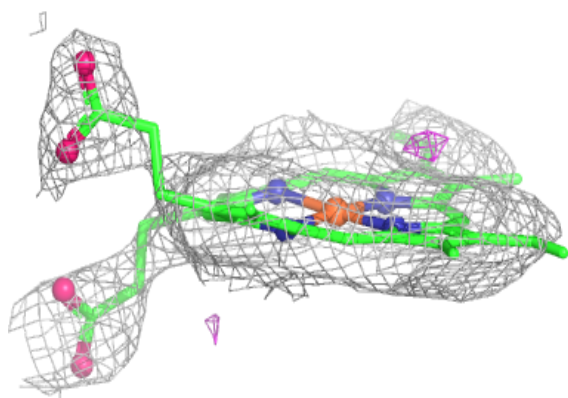
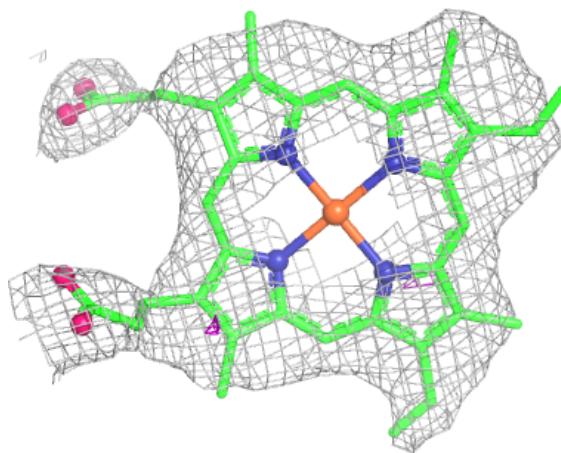
Electron density around CLA B 608:

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



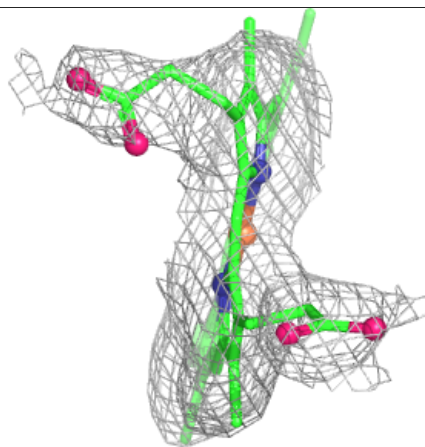
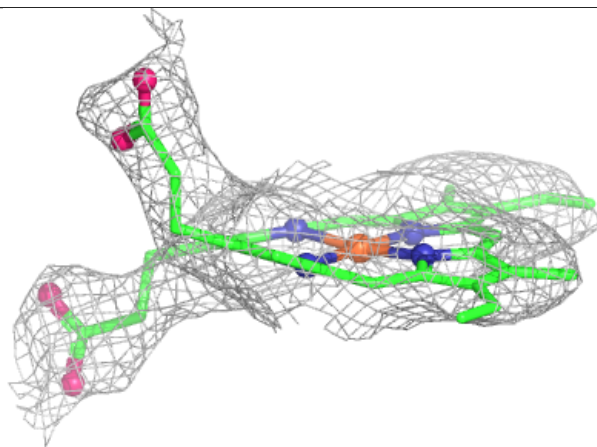
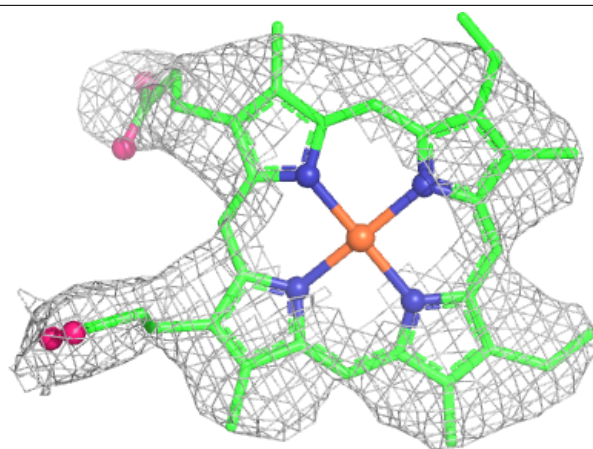
Electron density around HEM E 102:

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



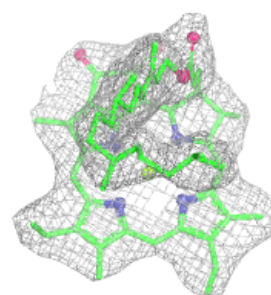
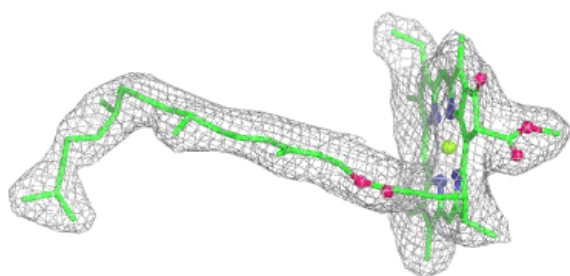
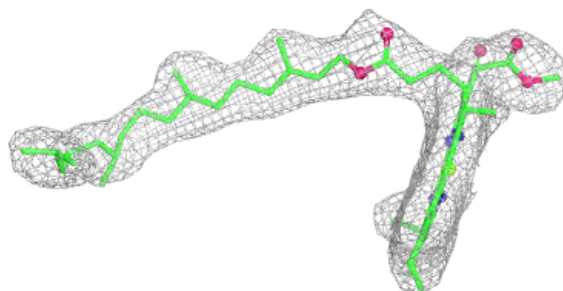
Electron density around HEM e 102:

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

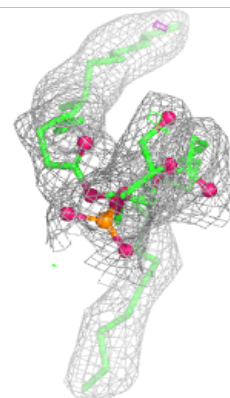
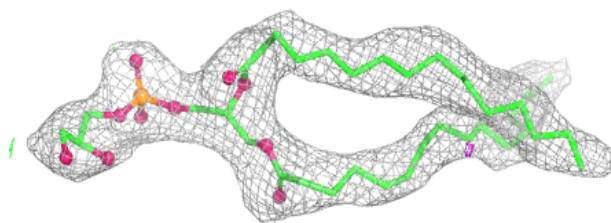
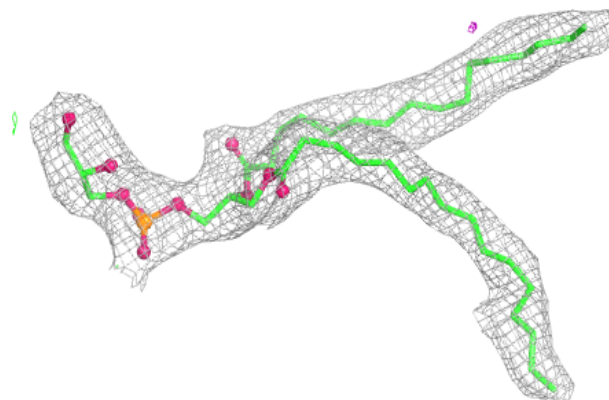


Electron density around CLA b 611:

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

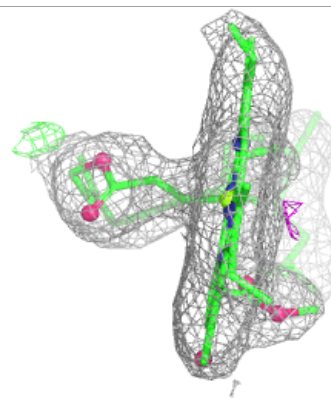
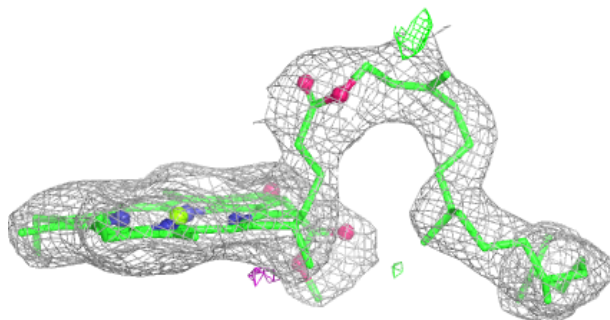
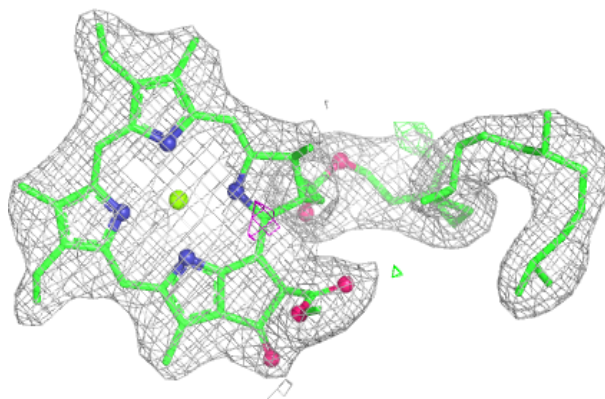
**Electron density around LHG d 407:**

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

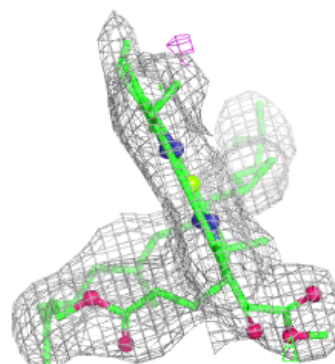
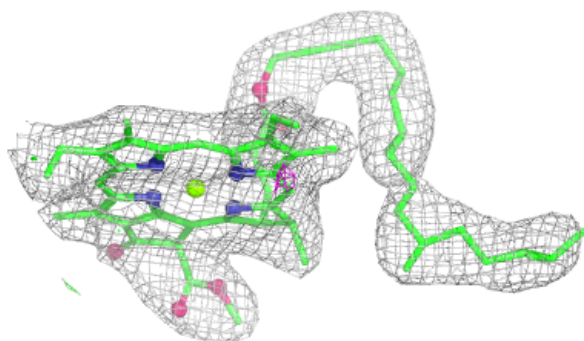
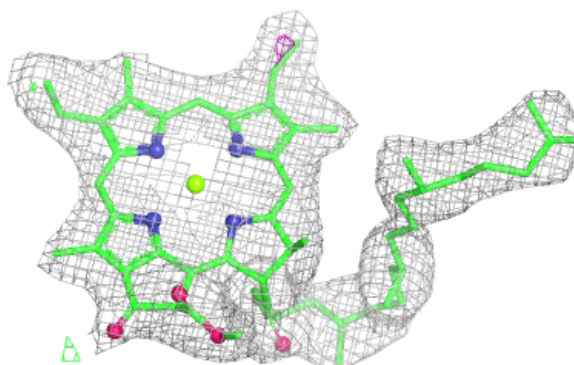


Electron density around CLA b 618:

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

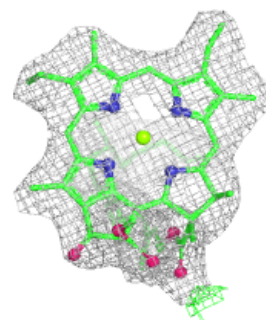
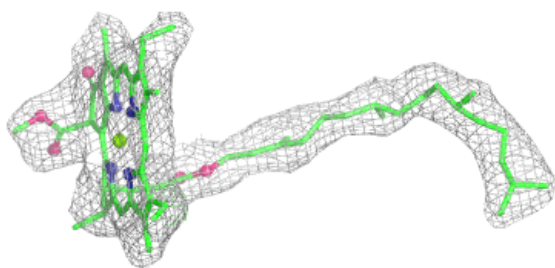
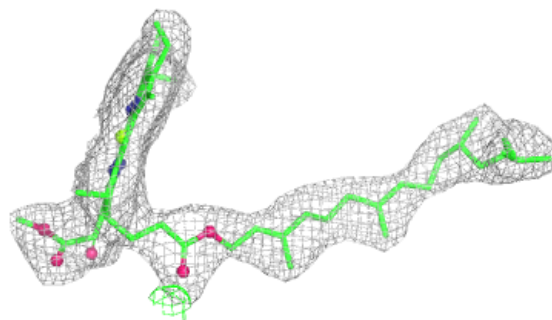
**Electron density around CLA a 719:**

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



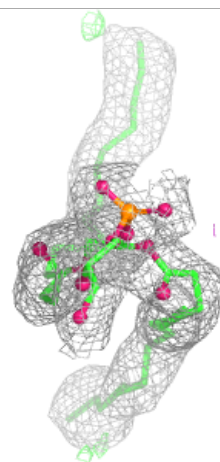
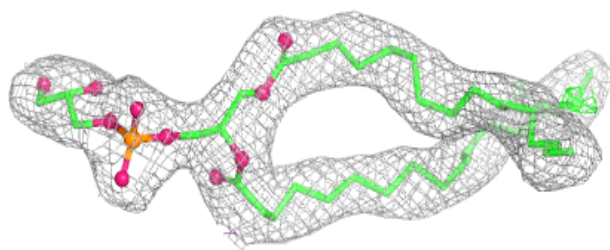
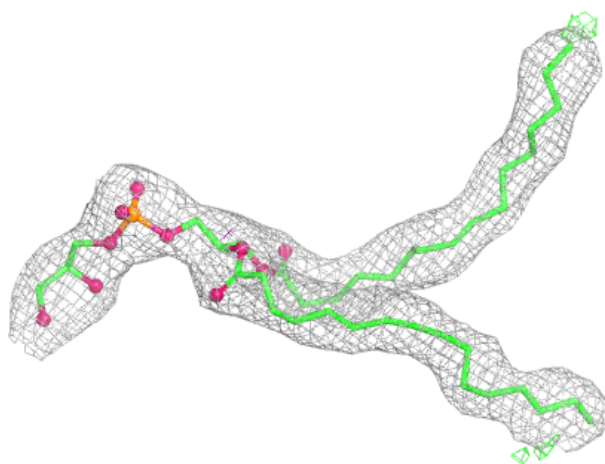
Electron density around CLA B 606:

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



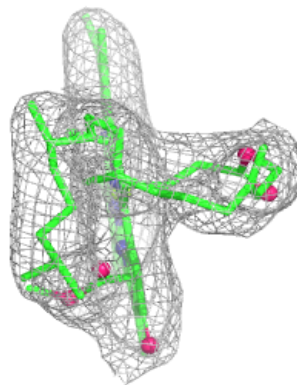
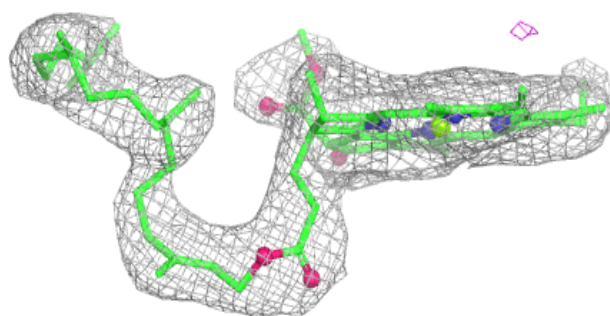
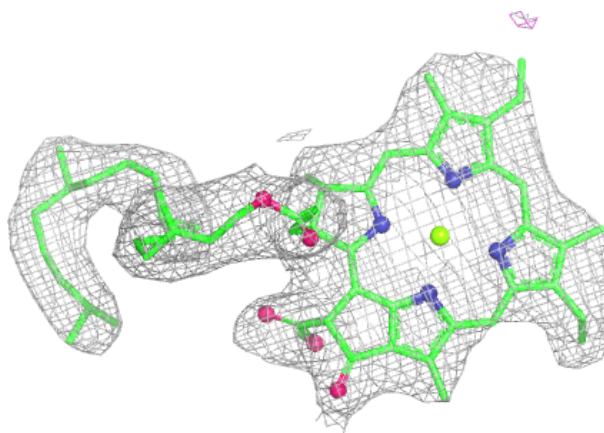
Electron density around LHG D 407:

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

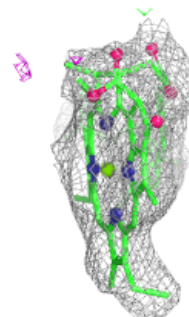
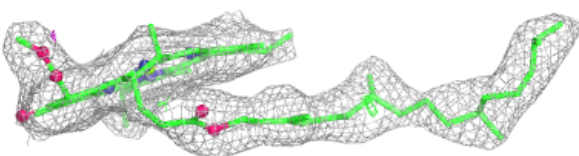
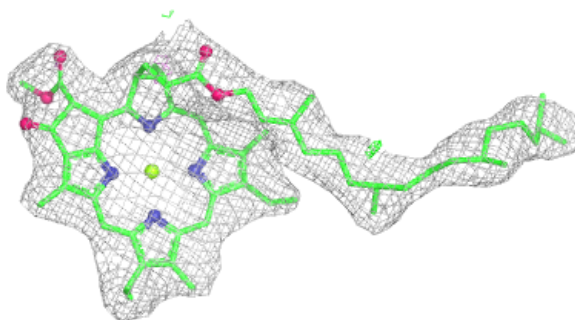


Electron density around CLA B 613:

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

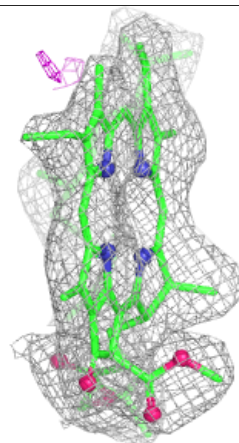
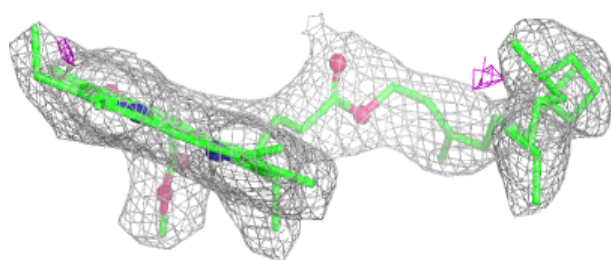
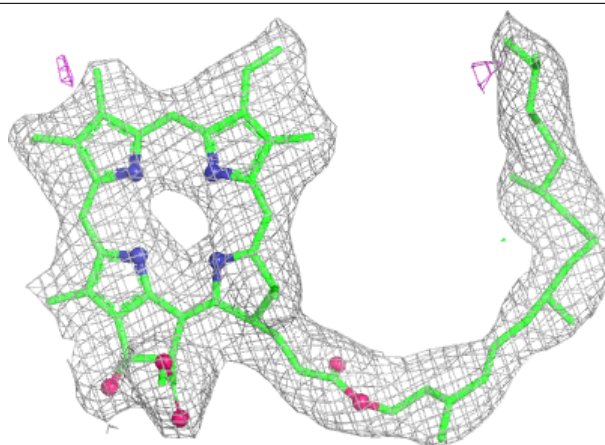
**Electron density around CLA b 609:**

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



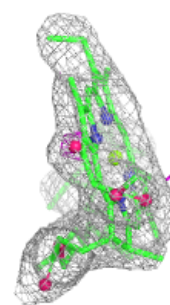
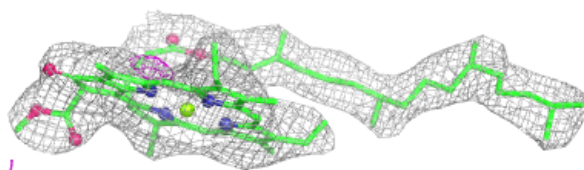
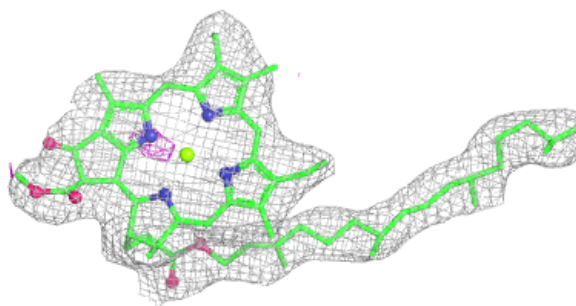
Electron density around PHO a 709:

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

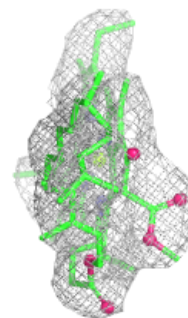
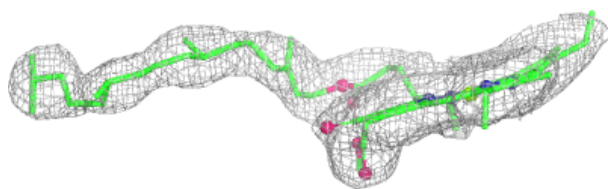
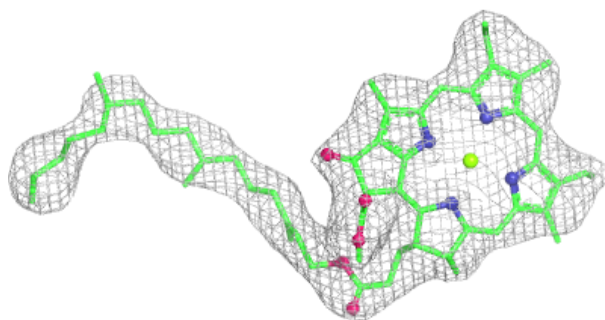


Electron density around CLA c 501:

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

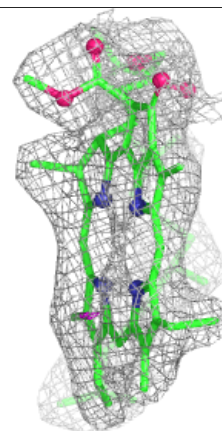
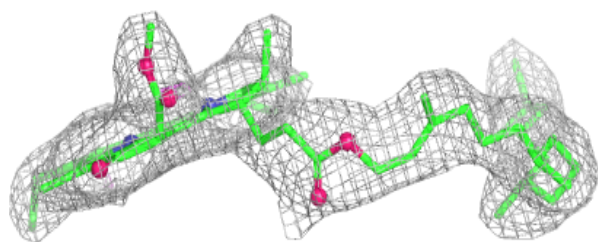
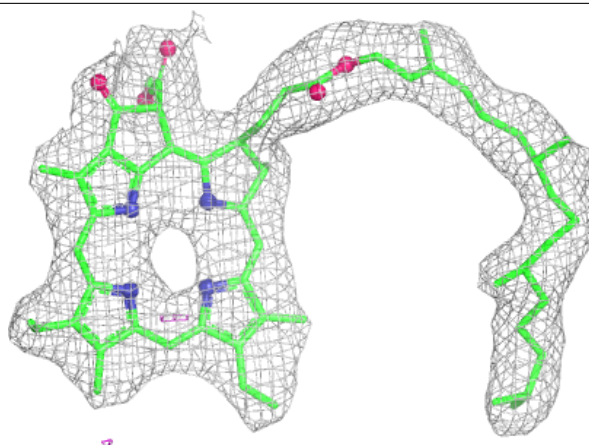
**Electron density around CLA B 603:**

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



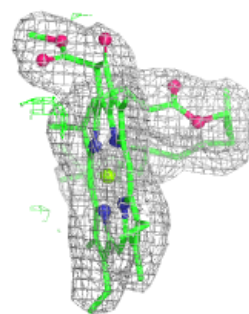
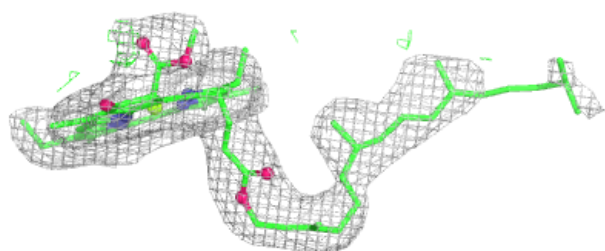
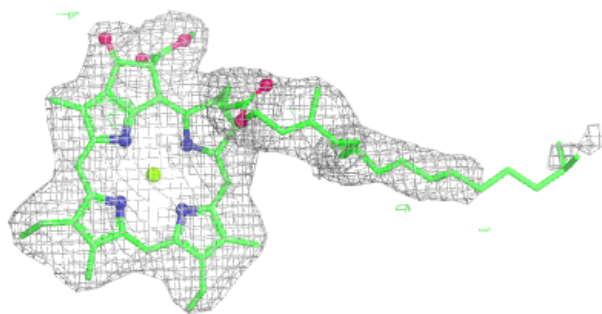
Electron density around PHO A 608:

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



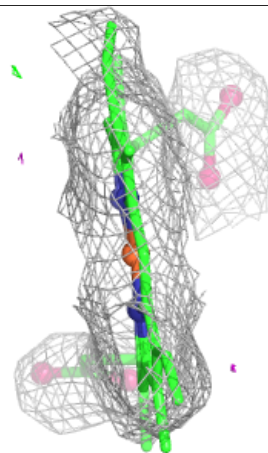
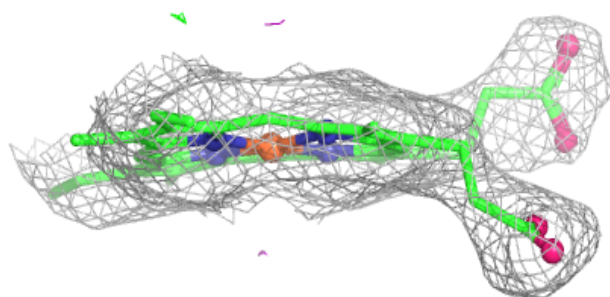
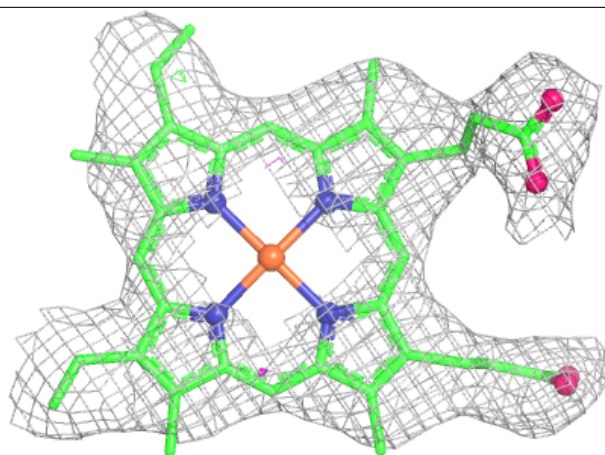
Electron density around CLA a 708:

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



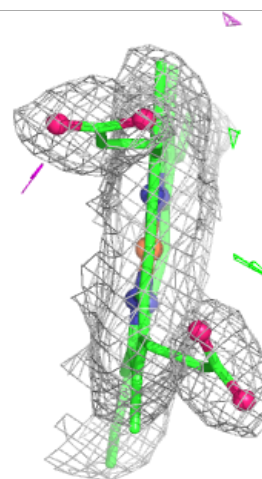
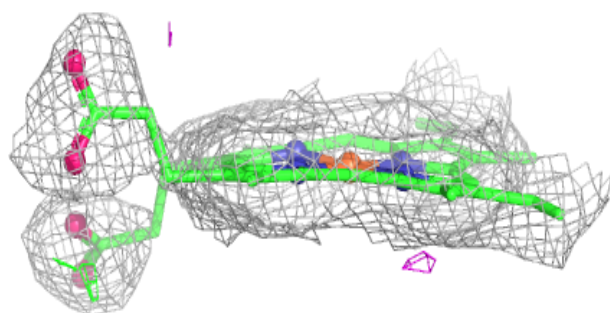
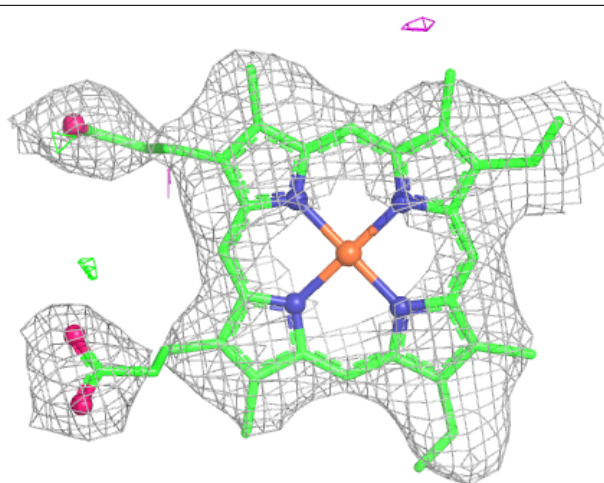
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.