



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:07 PM UTC

PDB ID : 4PJ0 / pdb_00004pj0
Title : Structure of T.elongatus Photosystem II, rows of dimers crystal packing
Authors : Hellmich, J.; Bommer, M.; Burkhardt, A.; Ibrahim, M.; Kern, J.; Meents, A.; Mueh, F.; Dobbek, H.; Zouni, A.
Deposited on : 2014-05-10
Resolution : 2.44 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

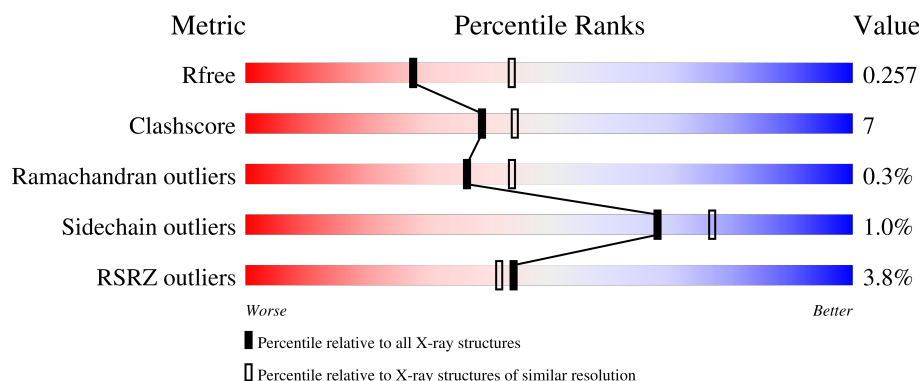
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	0% 85% 12% .
1	a	344	2% 83% 14% .
2	B	510	4% 87% 11% ..
2	b	510	3% 85% 13% ..
3	C	461	2% 82% 15% .

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Mol	Chain	Length	Quality of chain
3	c	461	2% 81% 16% .
4	D	352	% 84% 13% .
4	d	352	% 81% 15% .
5	E	84	13% 83% 14% .
5	e	84	6% 76% 18% 6%
6	F	45	64% 9% 27%
6	f	45	2% 69% . 27%
7	H	66	2% 86% 9% 5%
7	h	66	5% 91% 5% 5%
8	I	38	3% 82% 5% 13%
8	i	38	79% 13% 8%
9	J	40	2% 82% . 15%
9	j	40	80% . 18%
10	K	46	13% 63% 15% 22%
10	k	46	2% 72% 7% 22%
11	L	37	86% 11% .
11	l	37	78% 19% .
12	M	36	72% 17% 11%
12	m	36	86% . 11%
13	O	272	4% 77% 12% 11%
13	o	272	4% 75% 14% 11%
14	T	32	6% 66% 25% 9%
14	t	32	9% 81% 9% 9%
15	U	134	% 61% 10% . 28%
15	u	134	59% 13% 28%

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Mol	Chain	Length	Quality of chain
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
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	0	0
			3980	2611	665	691	13			
2	b	503	Total	C	N	O	S	0	0	0
			3958	2599	657	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			
3	c	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			661	431	107	123			
5	e	79	Total	C	N	O	0	0	0
			645	422	104	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	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	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	36	Total	C	N	O	0	0	0
			284	198	41	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			284	198	41	45			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			
12	m	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1859	1162	314	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	0	0
			249	176	35	36	2			
14	t	29	Total	C	N	O	S	0	0	0
			249	176	35	36	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	96	Total	C	N	O	0	0	0
			765	486	128	151			

- 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	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

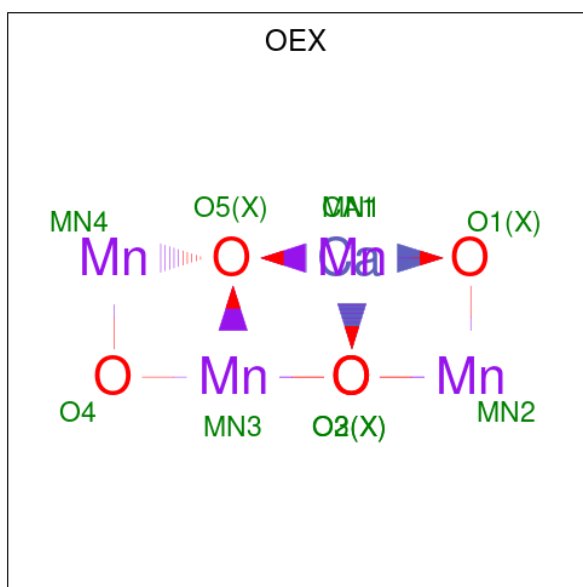
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			479	328	72	77	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	33	Total	C	N	O	0	0	0
			265	182	46	37			

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

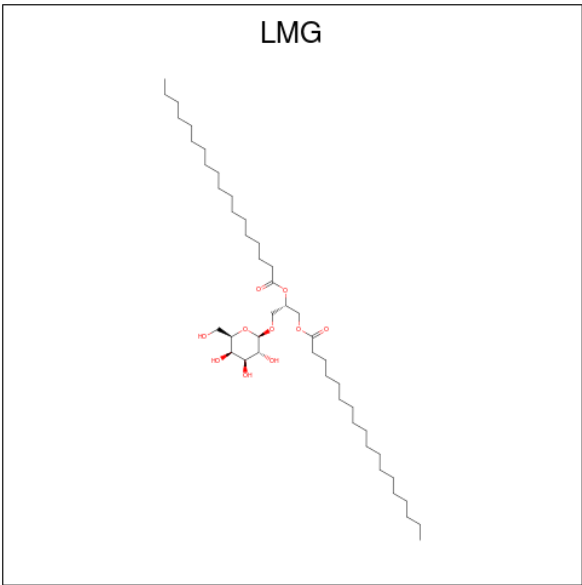


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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

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

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

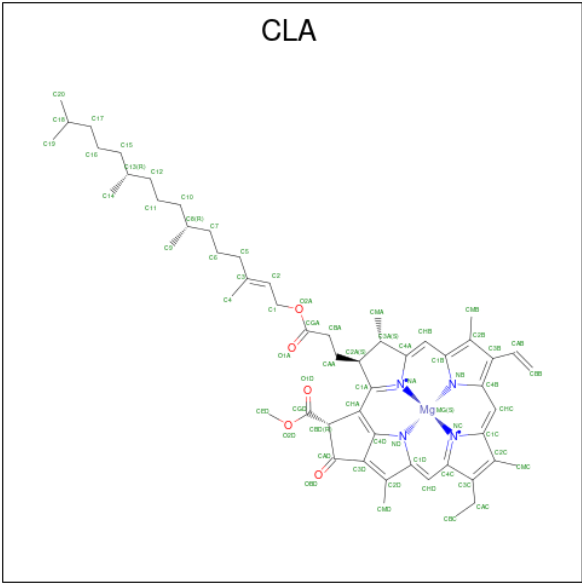


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			51	41	10		
23	A	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	D	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total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

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

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

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



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 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
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	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	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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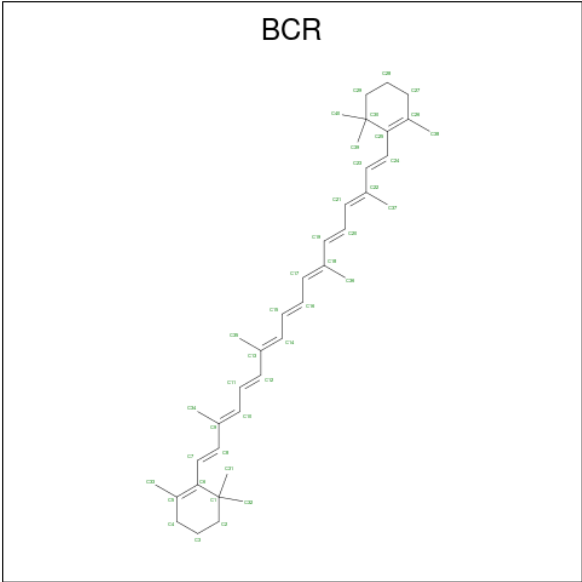
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	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	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	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 BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



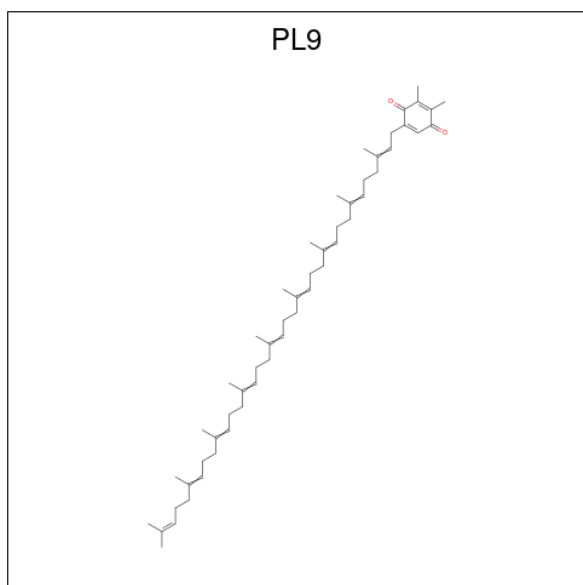
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

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

- Molecule 27 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).



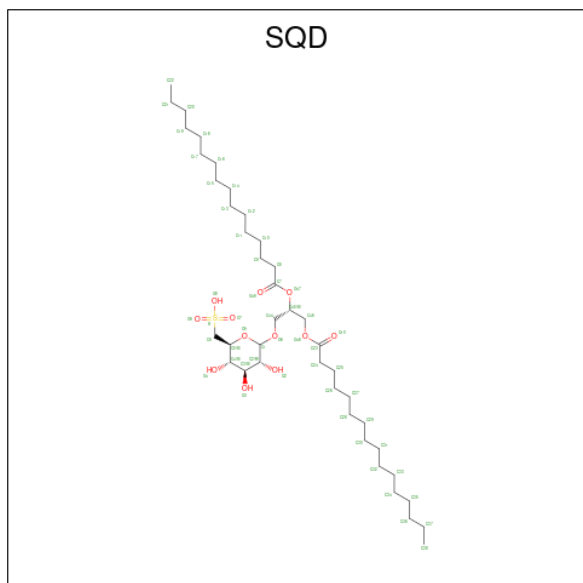
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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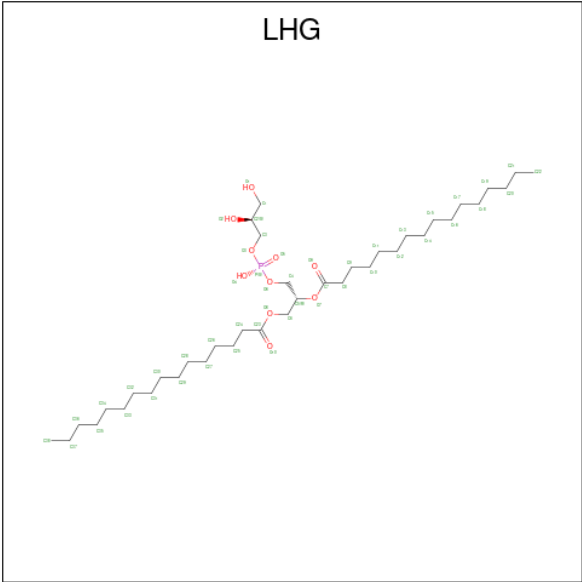
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



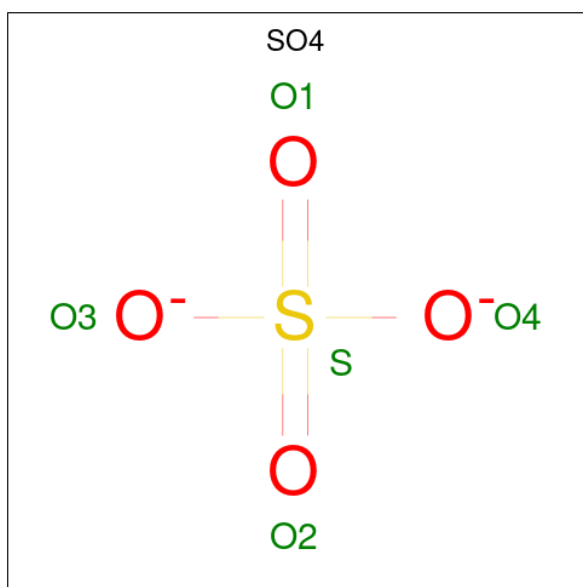
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			43	30	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



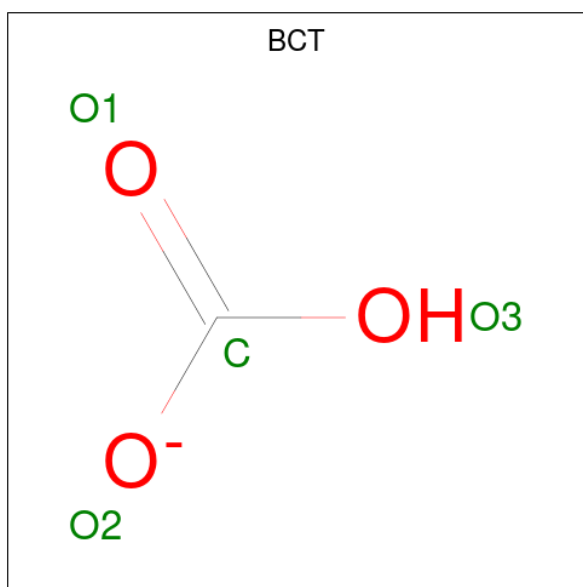
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	E	1	Total	C	O	P	0	0
			42	31	10	1		
29	L	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			42	31	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 30 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	O	S	0	0
			5	4	1		
30	O	1	Total	O	S	0	0
			5	4	1		
30	O	1	Total	O	S	0	0
			5	4	1		
30	U	1	Total	O	S	0	0
			5	4	1		
30	V	1	Total	O	S	0	0
			5	4	1		
30	a	1	Total	O	S	0	0
			5	4	1		
30	d	1	Total	O	S	0	0
			5	4	1		
30	o	1	Total	O	S	0	0
			5	4	1		
30	u	1	Total	O	S	0	0
			5	4	1		
30	u	1	Total	O	S	0	0
			5	4	1		

- 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 UNKNOWN LIGAND (CCD ID: UNL) (formula:).

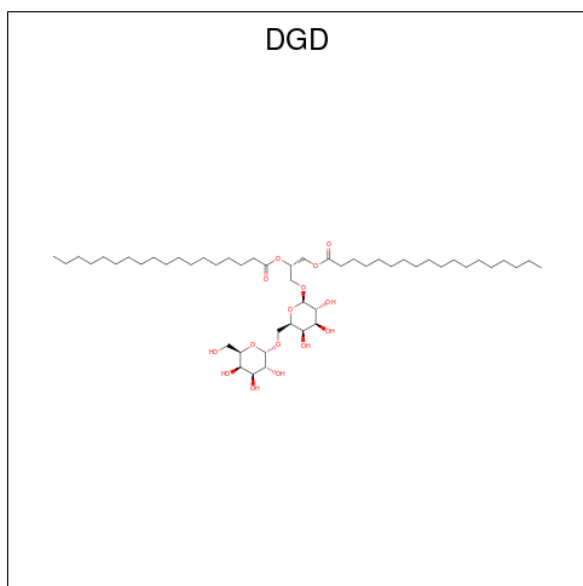
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	6	Total	C	0	0
			68	68		
32	C	1	Total	C	0	0
			15	15		
32	D	1	Total	C	0	0
			15	15		
32	I	1	Total	C	0	0
			14	14		
32	J	1	Total	C	0	0
			11	11		
32	M	2	Total	C	0	0
			26	26		
32	T	2	Total	C	0	0
			27	27		
32	X	1	Total	C	0	0
			10	10		
32	b	5	Total	C	0	0
			60	60		
32	c	1	Total	C	0	0
			15	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	d	1	Total C 15 15	0	0
32	i	1	Total C 16 16	0	0
32	j	1	Total C 15 15	0	0
32	k	1	Total C 9 9	0	0
32	m	2	Total C 25 25	0	0
32	t	1	Total C 15 15	0	0
32	x	1	Total C 16 16	0	0

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



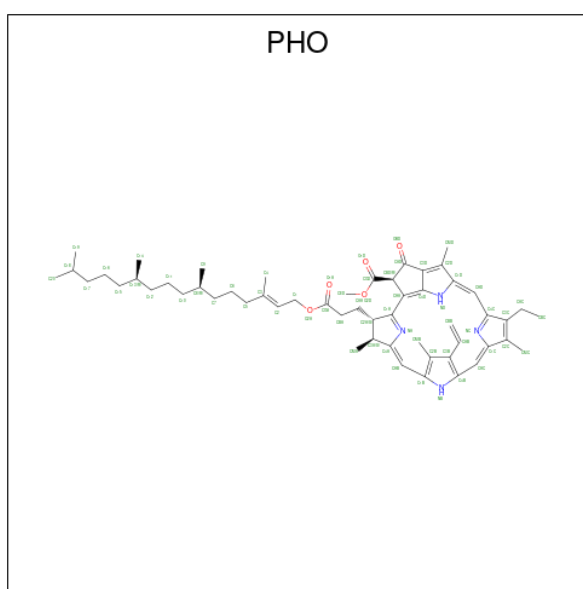
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	H	1	Total C O 62 47 15	0	0

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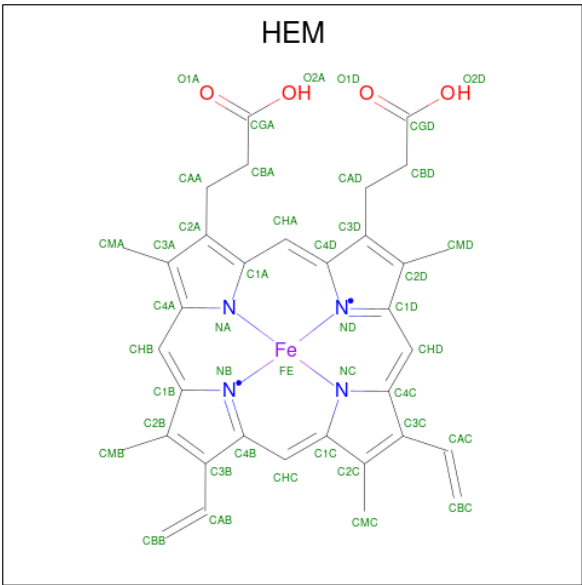
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



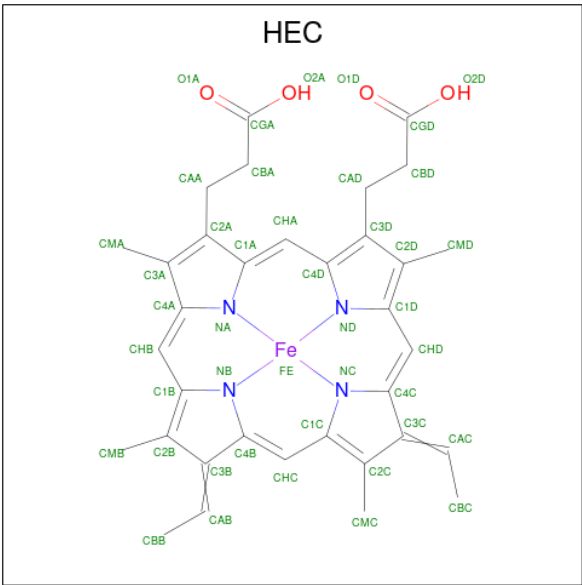
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	N	O	0	0
			64	55	4	5		
34	D	1	Total	C	N	O	0	0
			64	55	4	5		
34	a	1	Total	C	N	O	0	0
			64	55	4	5		
34	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	33	Total O 33 33	0	0
37	B	42	Total O 42 42	0	0
37	C	24	Total O 24 24	0	0
37	D	27	Total O 27 27	0	0
37	E	2	Total O 2 2	0	0
37	H	8	Total O 8 8	0	0
37	L	1	Total O 1 1	0	0
37	O	15	Total O 15 15	0	0
37	T	3	Total O 3 3	0	0
37	U	6	Total O 6 6	0	0
37	V	9	Total O 9 9	0	0
37	X	1	Total O 1 1	0	0
37	a	24	Total O 24 24	0	0
37	b	37	Total O 37 37	0	0
37	c	26	Total O 26 26	0	0
37	d	17	Total O 17 17	0	0
37	h	1	Total O 1 1	0	0
37	i	1	Total O 1 1	0	0
37	j	1	Total O 1 1	0	0
37	l	3	Total O 3 3	0	0
37	m	1	Total O 1 1	0	0

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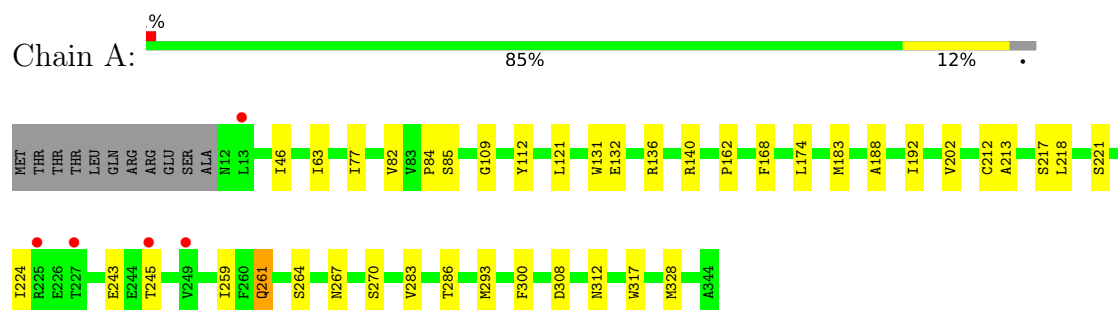
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	o	11	Total 11	O 11	0	0
37	t	1	Total 1	O 1	0	0
37	u	7	Total 7	O 7	0	0
37	v	3	Total 3	O 3	0	0

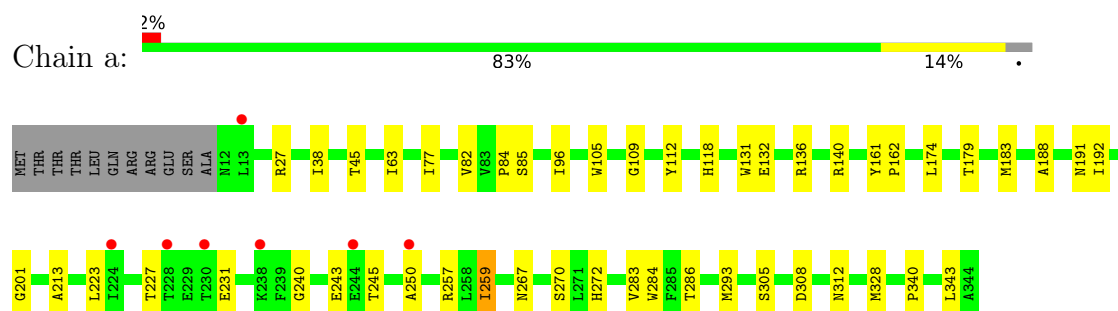
3 Residue-property plots [i](#)

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

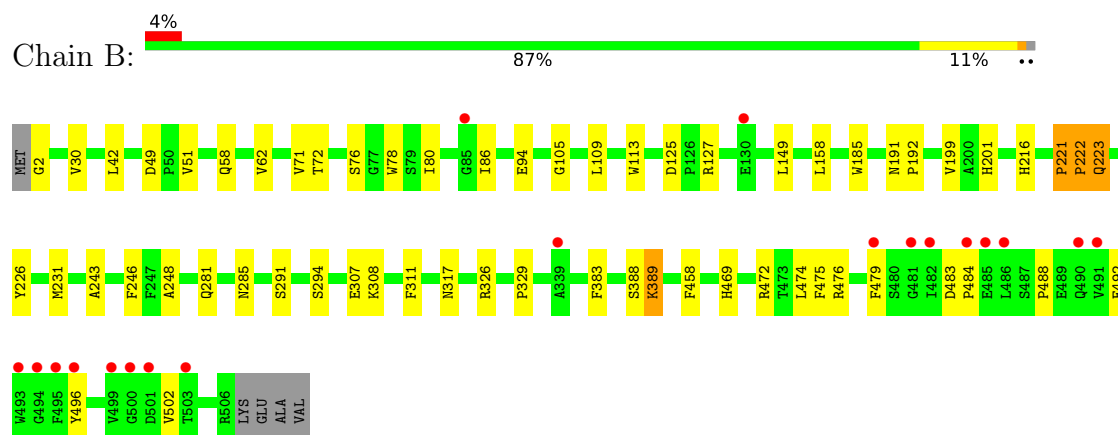
• Molecule 1: Photosystem Q(B) protein 1



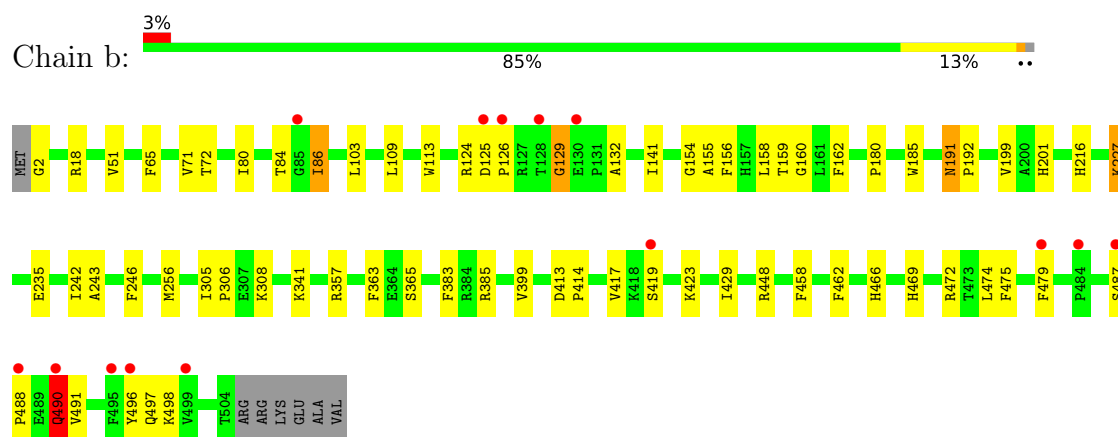
• Molecule 1: Photosystem Q(B) protein 1



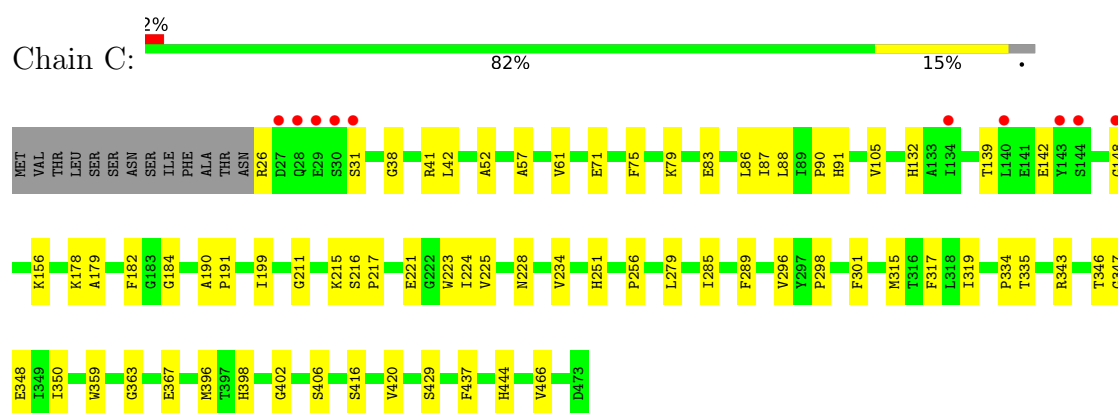
• Molecule 2: CP47 protein



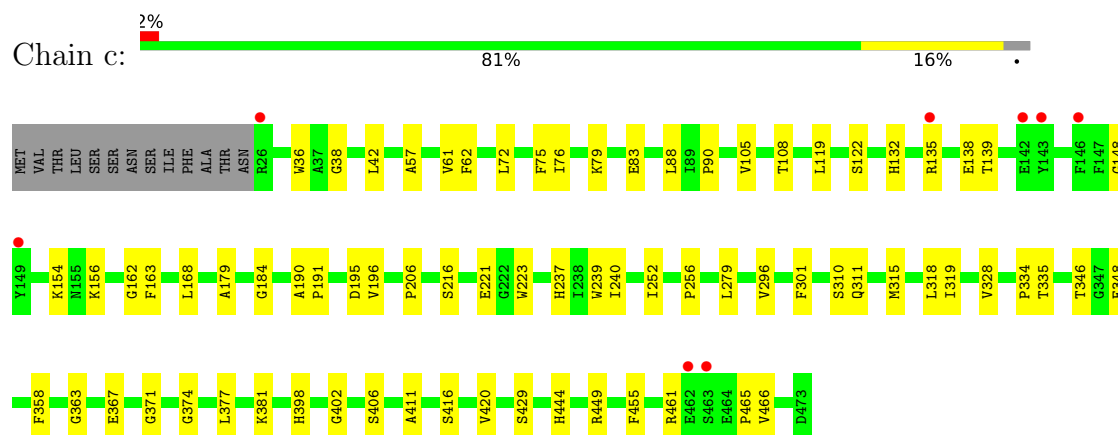
• Molecule 2: CP47 protein



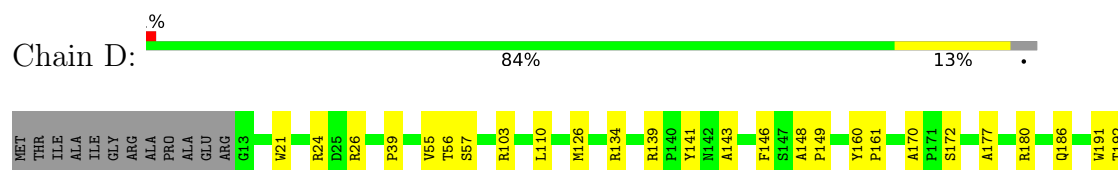
• Molecule 3: Photosystem II CP43 protein



• Molecule 3: Photosystem II CP43 protein

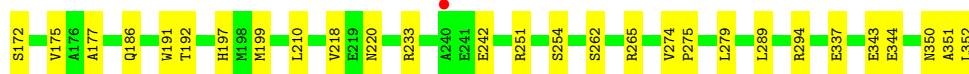
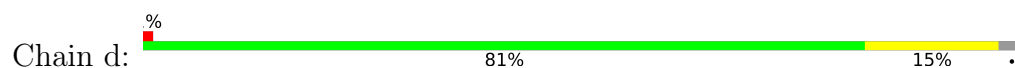


• Molecule 4: Photosystem II D2 protein

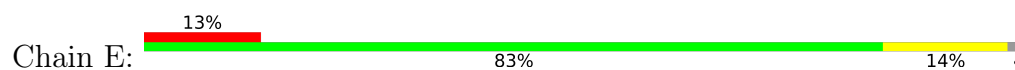




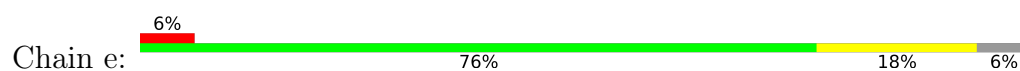
• Molecule 4: Photosystem II D2 protein



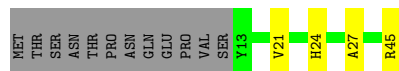
• Molecule 5: Cytochrome b559 subunit alpha



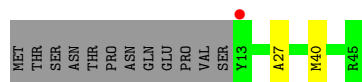
• Molecule 5: Cytochrome b559 subunit alpha



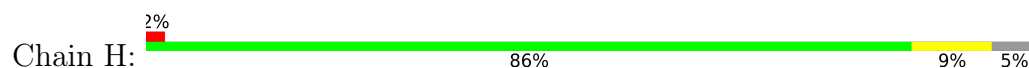
• Molecule 6: Cytochrome b559 subunit beta



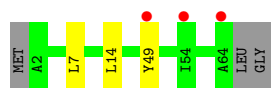
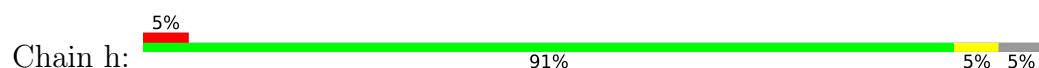
• Molecule 6: Cytochrome b559 subunit beta



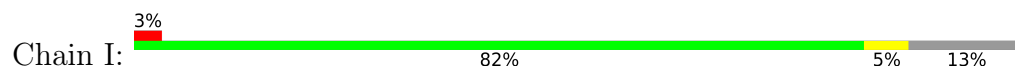
• Molecule 7: Photosystem II reaction center protein H



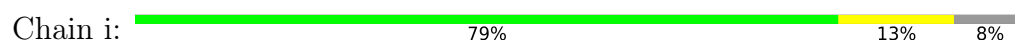
- Molecule 7: Photosystem II reaction center protein H



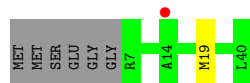
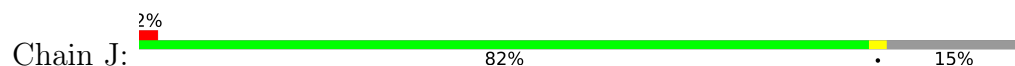
- Molecule 8: Photosystem II reaction center protein I



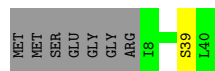
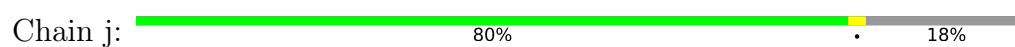
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

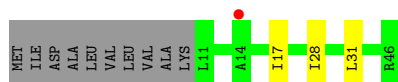


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K





- Molecule 11: Photosystem II reaction center protein L

Chain L: 86% 11% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 78% 19% .



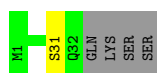
- Molecule 12: Photosystem II reaction center protein M

Chain M: 72% 17% 11%



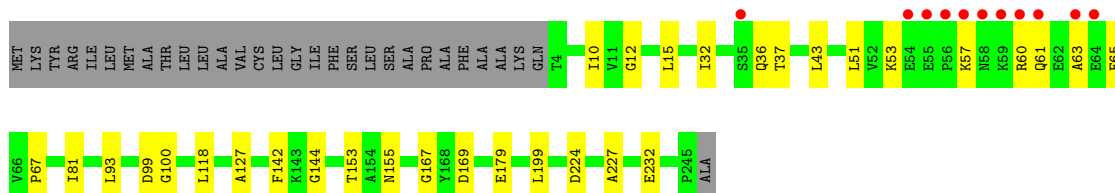
- Molecule 12: Photosystem II reaction center protein M

Chain m: 86% . 11%



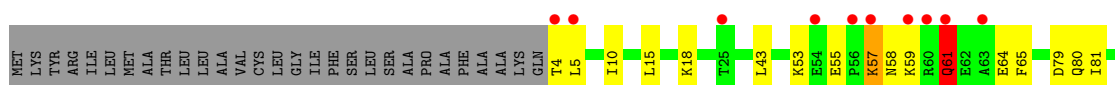
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 4% 77% 12% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 4% 75% 14% 11%

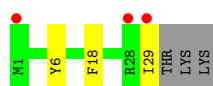
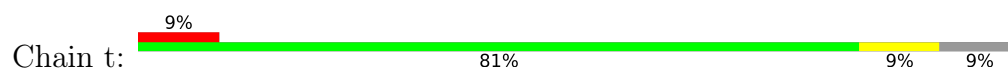




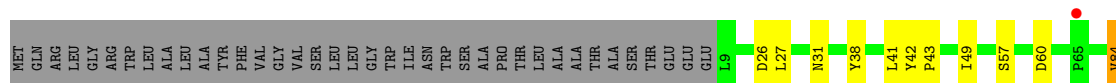
- Molecule 14: Photosystem II reaction center protein T



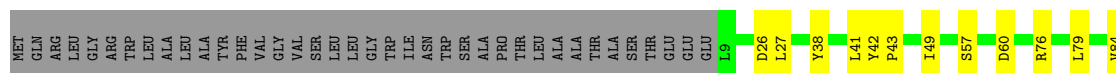
- Molecule 14: Photosystem II reaction center protein T



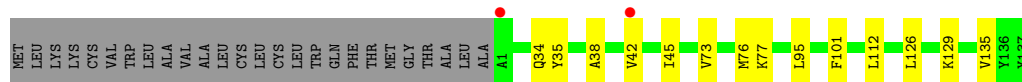
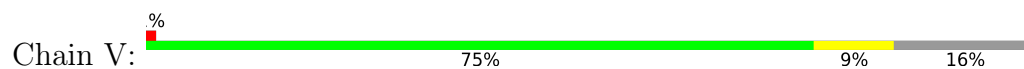
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

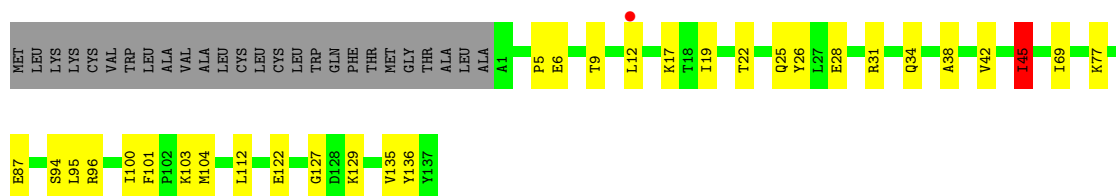


- Molecule 16: Cytochrome c-550

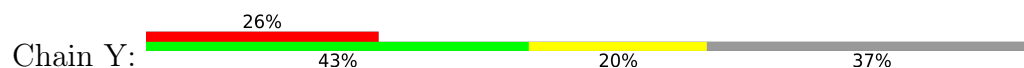


- Molecule 16: Cytochrome c-550

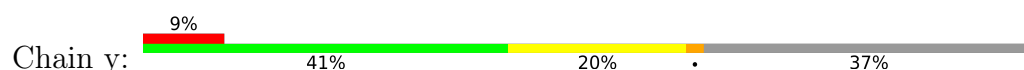




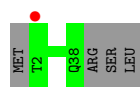
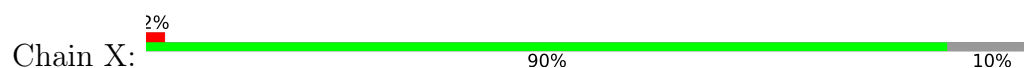
- Molecule 17: Photosystem II reaction center protein Ycf12



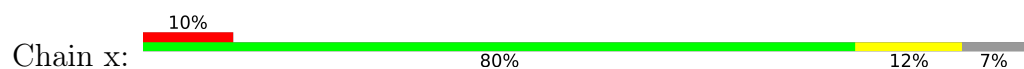
- Molecule 17: Photosystem II reaction center protein Ycf12



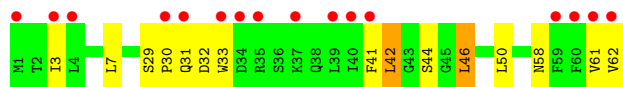
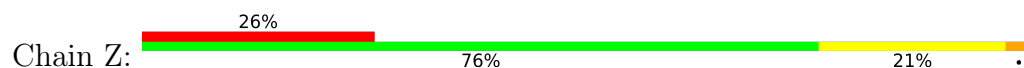
- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein

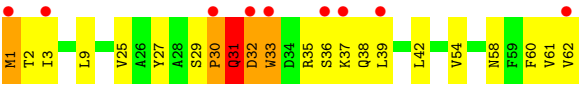


- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z

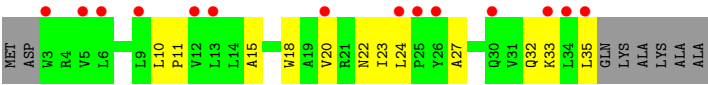




● Molecule 20: Photosystem II protein Y



● 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	116.45Å 218.89Å 302.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.44 49.12 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.12-2.44) 98.3 (49.12-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.216 , 0.256 0.218 , 0.257	Depositor DCC
R_{free} test set	14111 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	50236	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: FE, UNL, HEM, CL, CLA, SQD, LMG, BCT, PL9, HEC, OEX, DGD, PHO, SO4, LHG, BCR

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	0.29	0/2702	0.74	1/3685 (0.0%)
1	a	0.28	0/2702	0.71	0/3685
2	B	0.29	0/4120	0.74	7/5614 (0.1%)
2	b	0.28	0/4098	0.73	4/5586 (0.1%)
3	C	0.27	0/3579	0.71	0/4872
3	c	0.28	0/3579	0.73	3/4872 (0.1%)
4	D	0.27	0/2801	0.69	0/3818
4	d	0.28	0/2801	0.70	0/3818
5	E	0.28	0/680	0.76	0/929
5	e	0.29	0/664	0.72	0/907
6	F	0.33	0/278	0.77	0/379
6	f	0.32	0/278	0.77	0/379
7	H	0.28	0/511	0.69	0/697
7	h	0.27	0/511	0.69	0/697
8	I	0.29	0/273	0.71	0/370
8	i	0.33	0/293	0.81	0/395
9	J	0.27	0/255	0.73	0/346
9	j	0.26	0/244	0.73	0/332
10	K	0.43	0/294	0.97	2/405 (0.5%)
10	k	0.40	0/294	0.81	0/405
11	L	0.27	0/303	0.65	0/412
11	l	0.27	0/303	0.64	0/412
12	M	0.31	0/252	0.80	0/344
12	m	0.32	0/252	0.78	0/344
13	O	0.26	0/1890	0.67	0/2564
13	o	0.27	0/1896	0.72	2/2571 (0.1%)
14	T	0.26	0/258	0.69	0/349
14	t	0.27	0/258	0.68	0/349
15	U	0.26	0/776	0.65	0/1052
15	u	0.25	0/776	0.64	0/1052
16	V	0.29	0/1085	0.73	2/1473 (0.1%)
16	v	0.28	0/1085	0.73	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.29	0/216	0.73	0/289
17	y	0.33	0/216	0.87	0/289
18	X	0.27	0/273	0.71	0/370
18	x	0.27	0/284	0.70	0/384
19	Z	0.32	0/490	0.78	0/669
19	z	0.50	0/490	1.00	2/669 (0.3%)
20	R	0.32	0/279	0.74	0/383
20	r	0.35	0/271	0.86	1/372 (0.3%)
All	All	0.28	0/42610	0.73	24/58011 (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
2	B	0	1
19	z	0	1
All	All	0	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	GLN	N-CA-C	-12.26	96.61	111.69
2	b	490	GLN	N-CA-C	-8.50	102.91	113.28
2	b	129	GLY	N-CA-C	-7.30	104.65	114.95
19	z	32	ASP	N-CA-C	7.05	120.89	111.30
10	K	19	ASP	CA-C-N	-6.65	111.52	119.84
10	K	19	ASP	C-N-CA	-6.65	111.52	119.84
2	b	191	ASN	CA-C-N	6.33	126.82	119.47
2	b	191	ASN	C-N-CA	6.33	126.82	119.47
19	z	36	SER	N-CA-C	6.11	122.62	114.12
2	B	483	ASP	CA-C-N	6.01	125.49	119.24
2	B	483	ASP	C-N-CA	6.01	125.49	119.24
1	A	261	GLN	N-CA-C	5.99	119.42	111.75
3	c	76	ILE	CA-C-N	5.95	125.43	119.24
3	c	76	ILE	C-N-CA	5.95	125.43	119.24
2	B	221	PRO	CA-C-N	5.80	126.13	119.92
2	B	221	PRO	C-N-CA	5.80	126.13	119.92
13	o	55	GLU	CA-C-N	5.43	126.63	119.84
13	o	55	GLU	C-N-CA	5.43	126.63	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	223	TRP	CB-CA-C	-5.39	110.38	116.63
16	V	101	PHE	CA-C-N	5.33	125.00	119.56
16	V	101	PHE	C-N-CA	5.33	125.00	119.56
20	r	33	LYS	N-CA-C	-5.32	106.05	112.54
2	B	125	ASP	CA-C-N	5.13	125.17	119.32
2	B	125	ASP	C-N-CA	5.13	125.17	119.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	PRO	Peptide
19	z	31	GLN	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	2617	0	2514	33	0
1	a	2617	0	2514	38	0
2	B	3980	0	3841	49	0
2	b	3958	0	3815	58	0
3	C	3466	0	3389	49	0
3	c	3466	0	3389	49	0
4	D	2706	0	2608	38	0
4	d	2706	0	2608	46	0
5	E	661	0	643	9	0
5	e	645	0	628	13	0
6	F	269	0	277	5	0
6	f	269	0	277	2	0
7	H	498	0	518	5	0
7	h	498	0	518	4	0
8	I	266	0	282	2	0
8	i	286	0	308	4	0
9	J	249	0	262	0	0
9	j	238	0	249	1	0
10	K	284	0	292	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	284	0	292	2	0
11	L	296	0	304	3	0
11	l	296	0	304	9	0
12	M	249	0	268	6	0
12	m	249	0	268	2	0
13	O	1859	0	1833	18	0
13	o	1865	0	1838	23	0
14	T	249	0	255	8	0
14	t	249	0	255	4	0
15	U	765	0	767	8	0
15	u	765	0	767	10	0
16	V	1064	0	1073	9	0
16	v	1064	0	1073	19	0
17	Y	215	0	246	5	0
17	y	215	0	246	7	0
18	X	270	0	299	0	0
18	x	281	0	312	5	0
19	Z	479	0	516	7	0
19	z	479	0	516	20	0
20	R	273	0	305	7	0
20	r	265	0	301	6	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	102	0	144	1	0
23	B	102	0	144	3	0
23	C	102	0	144	4	0
23	D	51	0	72	0	0
23	a	102	0	144	2	0
23	b	102	0	144	1	0
23	c	102	0	144	5	0
23	d	51	0	72	2	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	195	0	216	7	0
25	B	1040	0	1152	34	0
25	C	845	0	936	36	0
25	D	195	0	216	10	0
25	a	260	0	288	11	0
25	b	1040	0	1152	32	0
25	c	845	0	936	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	d	130	0	144	4	0
26	A	40	0	56	3	0
26	B	120	0	168	14	0
26	C	120	0	168	8	0
26	D	40	0	56	2	0
26	H	40	0	56	2	0
26	K	40	0	56	4	0
26	T	40	0	56	6	0
26	a	40	0	56	3	0
26	b	120	0	168	6	0
26	c	80	0	112	5	0
26	d	40	0	56	4	0
26	h	40	0	56	4	0
26	k	40	0	56	3	0
26	t	40	0	56	5	0
26	z	40	0	56	10	0
27	A	55	0	80	6	0
27	D	55	0	80	3	0
27	a	55	0	80	6	0
27	d	55	0	80	4	0
28	A	54	0	78	2	0
28	F	43	0	53	2	0
28	L	108	0	156	10	0
28	a	54	0	78	5	0
28	f	43	0	53	0	0
29	A	98	0	148	13	0
29	D	49	0	74	5	0
29	E	42	0	57	0	0
29	L	49	0	74	4	0
29	a	91	0	131	6	0
29	d	98	0	148	11	0
29	l	49	0	74	3	0
30	A	5	0	0	0	0
30	O	10	0	0	0	0
30	U	5	0	0	0	0
30	V	5	0	0	0	0
30	a	5	0	0	0	0
30	d	5	0	0	0	0
30	o	5	0	0	0	0
30	u	10	0	0	0	0
31	A	4	0	0	0	0
31	a	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B	68	0	0	0	0
32	C	15	0	0	0	0
32	D	15	0	0	0	0
32	I	14	0	0	0	0
32	J	11	0	0	0	0
32	M	26	0	0	0	0
32	T	27	0	0	0	0
32	X	10	0	0	0	0
32	b	60	0	0	0	0
32	c	15	0	0	0	0
32	d	15	0	0	0	0
32	i	16	0	0	0	0
32	j	15	0	0	0	0
32	k	9	0	0	0	0
32	m	25	0	0	0	0
32	t	15	0	0	0	0
32	x	16	0	0	0	0
33	C	186	0	246	9	0
33	H	62	0	82	0	0
33	c	186	0	246	3	0
33	h	62	0	82	2	0
34	D	128	0	148	6	0
34	a	64	0	74	2	0
34	d	64	0	74	1	0
35	E	43	0	30	3	0
35	e	43	0	30	5	0
36	V	43	0	30	0	0
36	v	43	0	30	0	0
37	A	33	0	0	0	0
37	B	42	0	0	1	0
37	C	24	0	0	0	0
37	D	27	0	0	0	0
37	E	2	0	0	0	0
37	H	8	0	0	0	0
37	L	1	0	0	0	0
37	O	15	0	0	0	0
37	T	3	0	0	1	0
37	U	6	0	0	0	0
37	V	9	0	0	0	0
37	X	1	0	0	0	0
37	a	24	0	0	0	0
37	b	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	c	26	0	0	0	0
37	d	17	0	0	0	0
37	h	1	0	0	0	0
37	i	1	0	0	0	0
37	j	1	0	0	0	0
37	l	3	0	0	0	0
37	m	1	0	0	0	0
37	o	11	0	0	0	0
37	t	1	0	0	0	0
37	u	7	0	0	0	0
37	v	3	0	0	0	0
All	All	50236	0	50766	684	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 (684) 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)
17:y:18:VAL:HG23	17:y:19:ILE:HD12	1.61	0.83
25:B:604:CLA:H93	25:B:605:CLA:HAB	1.66	0.77
3:c:79:LYS:HG3	16:v:103:LYS:HD3	1.68	0.75
25:C:503:CLA:H172	25:C:510:CLA:HBB2	1.68	0.74
25:A:607:CLA:HAB	25:D:404:CLA:H72	1.69	0.73
25:C:501:CLA:H71	25:C:501:CLA:HBB1	1.71	0.72
10:K:21:LEU:HD13	17:Y:24:MET:HE3	1.71	0.71
26:K:101:BCR:H10C	17:Y:28:ILE:HG23	1.70	0.71
19:z:31:GLN:HA	19:z:31:GLN:NE2	2.07	0.69
4:d:192:THR:HG23	25:d:401:CLA:HBC2	1.75	0.69
4:D:192:THR:HG23	25:D:404:CLA:HBC2	1.74	0.69
29:A:614:LHG:H151	29:A:614:LHG:H352	1.76	0.68
23:b:624:LMG:H232	23:b:624:LMG:H402	1.76	0.67
25:c:503:CLA:H172	25:c:510:CLA:HBB2	1.75	0.67
25:c:510:CLA:H2	25:c:510:CLA:HED2	1.77	0.67
4:D:279:LEU:HD22	34:D:402:PHO:HBC3	1.76	0.67
25:c:513:CLA:HAB	26:z:101:BCR:H24C	1.77	0.66
3:C:148:GLY:O	3:C:156:LYS:NZ	2.28	0.66
25:c:508:CLA:H201	23:c:518:LMG:H242	1.77	0.66
14:t:18:PHE:HD1	26:t:102:BCR:HC7	1.61	0.66
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.77	0.66
2:B:469:HIS:HE1	25:B:611:CLA:NA	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:613:SQD:H62	4:d:233:ARG:HE	1.61	0.65
25:c:502:CLA:HBB2	25:c:510:CLA:H151	1.77	0.65
19:z:31:GLN:HA	19:z:31:GLN:HE21	1.62	0.64
28:L:103:SQD:O7	11:l:7:ARG:NH1	2.30	0.64
3:c:148:GLY:O	3:c:156:LYS:NZ	2.28	0.64
19:z:29:SER:OG	19:z:32:ASP:OD2	2.15	0.64
25:c:501:CLA:H203	25:c:507:CLA:H13	1.78	0.64
26:B:617:BCR:H383	28:L:101:SQD:H81	1.80	0.64
4:D:199:MET:HG2	27:D:407:PL9:H321	1.80	0.64
29:L:102:LHG:H271	12:M:22:LEU:HD21	1.78	0.64
2:B:216:HIS:HE1	25:B:609:CLA:C1A	2.11	0.63
23:a:614:LMG:H242	25:c:505:CLA:HBB2	1.81	0.63
2:b:71:VAL:HG23	25:b:606:CLA:HMA2	1.81	0.63
3:c:138:GLU:HG3	3:c:139:THR:HG23	1.80	0.63
25:A:608:CLA:H193	25:C:505:CLA:H13	1.79	0.63
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.80	0.63
23:B:620:LMG:H401	12:M:17:VAL:HG21	1.79	0.63
3:C:315:MET:HE3	3:C:319:ILE:HD11	1.80	0.63
17:y:42:ARG:NH1	19:z:32:ASP:OD2	2.28	0.63
28:A:611:SQD:H131	29:A:614:LHG:H142	1.81	0.62
4:d:279:LEU:HD22	34:d:402:PHO:HBC3	1.81	0.62
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.79	0.62
29:A:614:LHG:H112	29:A:614:LHG:H382	1.81	0.62
2:B:216:HIS:HE1	25:B:609:CLA:NA	1.91	0.62
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.81	0.62
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.81	0.62
35:e:101:HEM:HBC2	35:e:101:HEM:HHD	1.82	0.62
2:b:216:HIS:HE1	25:b:609:CLA:C1A	2.13	0.62
2:b:357:ARG:NH2	4:d:337:GLU:O	2.33	0.62
25:c:505:CLA:HAB	25:c:505:CLA:H71	1.82	0.62
2:B:192:PRO:HG2	7:H:49:TYR:CD1	2.35	0.61
3:C:251:HIS:HE1	25:C:506:CLA:NA	1.97	0.61
20:r:18:TRP:O	20:r:22:ASN:ND2	2.25	0.61
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.83	0.61
28:L:103:SQD:S	11:l:7:ARG:NH1	2.74	0.61
2:b:192:PRO:HG3	7:h:49:TYR:CD1	2.36	0.61
13:o:10:ILE:HG23	13:o:15:LEU:HB2	1.83	0.61
3:c:83:GLU:OE2	3:c:398:HIS:NE2	2.30	0.61
1:a:38:ILE:HG23	23:a:603:LMG:H191	1.83	0.61
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.84	0.60
19:z:39:LEU:HA	19:z:42:LEU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:343:GLU:HG2	16:v:135:VAL:HG11	1.83	0.60
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.83	0.60
25:B:602:CLA:H101	25:B:609:CLA:H18	1.83	0.60
3:c:315:MET:HE3	3:c:319:ILE:HD11	1.83	0.60
4:d:199:MET:HG2	27:d:405:PL9:H321	1.83	0.60
2:b:2:GLY:N	11:l:11:GLU:OE2	2.34	0.60
2:B:76:SER:HG	2:B:78:TRP:CD1	2.20	0.60
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.84	0.60
6:F:21:VAL:HG21	28:F:101:SQD:H242	1.82	0.59
2:B:475:PHE:HB2	2:B:479:PHE:CE1	2.37	0.59
28:a:613:SQD:H252	29:d:407:LHG:H122	1.84	0.59
2:b:124:ARG:NH1	2:b:129:GLY:O	2.35	0.59
4:D:21:TRP:O	4:D:26:ARG:NH1	2.35	0.59
1:a:85:SER:HA	1:a:109:GLY:HA3	1.83	0.59
25:C:513:CLA:HAB	26:C:514:BCR:H24C	1.84	0.59
4:D:343:GLU:HG2	16:V:135:VAL:HG11	1.84	0.59
13:o:142:PHE:HB2	13:o:199:LEU:HB2	1.84	0.59
3:c:239:TRP:HH2	23:c:520:LMG:H291	1.67	0.59
29:a:615:LHG:O4	4:d:141:TYR:OH	2.16	0.58
2:B:71:VAL:HG23	25:B:606:CLA:HMA2	1.85	0.58
2:B:383:PHE:N	4:D:344:GLU:O	2.33	0.58
25:C:505:CLA:H141	8:I:16:VAL:HG22	1.85	0.58
2:b:469:HIS:HE1	25:b:611:CLA:NA	1.95	0.58
15:u:26:ASP:OD2	15:u:85:THR:OG1	2.17	0.58
20:r:32:GLN:HA	20:r:35:LEU:HB3	1.85	0.58
19:z:61:VAL:HG23	19:z:62:VAL:HG13	1.85	0.58
25:B:614:CLA:H43	28:L:101:SQD:H112	1.84	0.58
2:B:488:PRO:O	2:B:492:GLU:HG2	2.03	0.57
25:c:505:CLA:H141	8:i:16:VAL:HG22	1.86	0.57
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.86	0.57
3:C:26:ARG:NH1	25:C:511:CLA:O1A	2.37	0.57
4:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.85	0.57
34:D:402:PHO:HBA2	25:D:404:CLA:H142	1.86	0.57
19:Z:41:PHE:HA	19:Z:44:SER:HB2	1.87	0.57
2:B:248:ALA:HA	25:B:603:CLA:H42	1.86	0.57
26:B:617:BCR:H14C	29:L:102:LHG:H381	1.87	0.57
2:b:458:PHE:HB3	25:b:604:CLA:HBC2	1.87	0.57
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.40	0.57
5:e:26:THR:HB	35:e:101:HEM:HAB	1.87	0.57
13:O:10:ILE:HG23	13:O:15:LEU:HB2	1.86	0.56
1:a:245:THR:HG1	4:d:265:ARG:HE	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HA	1:A:112:TYR:CG	2.40	0.56
3:c:346:THR:OG1	3:c:348:GLU:OE2	2.23	0.56
3:C:217:PRO:HB2	33:C:516:DGD:HA32	1.88	0.56
2:b:185:TRP:HB3	25:b:601:CLA:HMA3	1.87	0.56
5:E:26:THR:HB	35:E:102:HEM:HAB	1.88	0.56
25:c:506:CLA:H43	26:c:514:BCR:HC8	1.87	0.56
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.87	0.56
16:V:77:LYS:HG2	16:V:95:LEU:HD12	1.87	0.56
29:a:615:LHG:H223	25:b:613:CLA:H192	1.87	0.56
2:b:216:HIS:HE1	25:b:609:CLA:NA	1.99	0.56
2:B:185:TRP:HB3	25:B:601:CLA:HMA3	1.89	0.55
4:D:274:VAL:HG22	27:D:407:PL9:H222	1.87	0.55
15:U:26:ASP:OD2	15:U:85:THR:OG1	2.21	0.55
33:C:517:DGD:HAH2	33:C:517:DGD:HA81	1.88	0.55
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.42	0.55
25:B:612:CLA:H171	25:B:613:CLA:HBB2	1.87	0.55
25:a:610:CLA:H152	25:c:506:CLA:H142	1.89	0.55
2:b:497:GLN:HE22	18:x:38:GLN:HB3	1.71	0.55
25:B:611:CLA:H71	29:L:102:LHG:H321	1.89	0.55
3:c:38:GLY:HA3	25:c:511:CLA:HMD2	1.87	0.55
2:B:49:ASP:CG	13:o:57:LYS:HD2	2.32	0.55
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.89	0.55
28:a:613:SQD:H182	29:d:407:LHG:H212	1.89	0.55
3:c:465:PRO:HB3	8:i:32:PRO:HB3	1.89	0.55
2:B:105:GLY:HA3	26:B:618:BCR:H282	1.89	0.54
13:O:155:ASN:ND2	15:U:100:ASN:O	2.38	0.54
2:b:383:PHE:N	4:d:344:GLU:O	2.41	0.54
19:z:32:ASP:HB2	19:z:35:ARG:CZ	2.38	0.54
4:d:186:GLN:HB2	25:d:401:CLA:HBC1	1.88	0.54
2:B:201:HIS:HE1	25:B:602:CLA:ND	2.02	0.54
13:O:53:LYS:NZ	13:O:63:ALA:O	2.41	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.54
15:u:57:SER:OG	15:u:60:ASP:OD2	2.22	0.54
13:o:57:LYS:HB2	13:o:61:GLN:HE22	1.72	0.54
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.88	0.54
16:V:95:LEU:HD11	16:V:112:LEU:HD11	1.89	0.54
4:d:262:SER:OG	29:d:406:LHG:O4	2.23	0.54
10:K:17:ILE:HD12	10:K:17:ILE:H	1.71	0.53
14:T:15:ALA:HA	26:T:101:BCR:H12C	1.90	0.53
26:T:101:BCR:H272	25:b:607:CLA:HAC2	1.89	0.53
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.90	0.53
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.89	0.53
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.91	0.53
2:b:155:ALA:O	2:b:159:THR:OG1	2.22	0.53
29:A:614:LHG:H132	29:A:614:LHG:H372	1.90	0.53
7:H:17:GLU:OE1	7:H:20:LYS:NZ	2.29	0.53
28:L:103:SQD:O9	2:b:18:ARG:NH2	2.41	0.53
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.89	0.53
25:b:611:CLA:H142	29:l:101:LHG:H361	1.90	0.53
17:y:42:ARG:HH22	19:z:35:ARG:NH1	2.07	0.53
2:b:383:PHE:O	2:b:385:ARG:NH2	2.41	0.53
2:b:256:MET:O	2:b:448:ARG:NH1	2.41	0.53
26:d:404:BCR:H372	23:d:408:LMG:H301	1.91	0.53
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.90	0.53
25:b:608:CLA:H162	25:d:403:CLA:H3A	1.91	0.52
5:E:42:LEU:HA	20:R:4:ARG:HH21	1.74	0.52
28:L:103:SQD:H342	14:T:12:CYS:HB3	1.91	0.52
4:d:24:ARG:HD3	18:x:37:VAL:HG22	1.89	0.52
3:C:444:HIS:HE1	25:C:508:CLA:NA	2.05	0.52
11:L:7:ARG:NH2	28:L:101:SQD:O9	2.43	0.52
13:O:53:LYS:HB3	13:O:232:GLU:HB2	1.91	0.52
2:B:311:PHE:O	2:B:317:ASN:ND2	2.43	0.52
15:u:27:LEU:HD22	15:u:49:ILE:HG21	1.91	0.52
3:c:72:LEU:HD11	3:c:108:THR:HB	1.92	0.52
1:A:131:TRP:CH2	25:C:505:CLA:HAA2	2.45	0.52
13:O:32:ILE:HG21	13:O:93:LEU:HD21	1.91	0.52
1:a:257:ARG:NH1	2:b:491:VAL:O	2.38	0.52
1:A:140:ARG:HH22	29:A:614:LHG:HC41	1.74	0.52
3:C:38:GLY:HA3	25:C:511:CLA:HMD2	1.91	0.52
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.92	0.52
25:a:608:CLA:HAB	25:d:401:CLA:H72	1.91	0.51
3:c:163:PHE:CD2	25:c:512:CLA:HAB	2.45	0.51
3:c:461:ARG:NH1	4:d:242:GLU:O	2.33	0.51
3:C:139:THR:OG1	3:C:142:GLU:OE1	2.23	0.51
13:o:152:ARG:HB2	13:o:225:MET:HE2	1.93	0.51
16:v:28:GLU:HG3	16:v:31:ARG:HE	1.75	0.51
2:B:458:PHE:HB3	25:B:604:CLA:HBC2	1.92	0.51
13:O:36:GLN:OE1	13:O:37:THR:N	2.35	0.51
16:V:38:ALA:O	16:V:42:VAL:HG23	2.10	0.51
2:B:2:GLY:N	11:L:11:GLU:OE2	2.43	0.51
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:33:TRP:CZ3	19:z:37:LYS:HB2	2.44	0.51
3:c:90:PRO:HB3	3:c:301:PHE:HB3	1.92	0.51
7:h:49:TYR:CE2	33:h:102:DGD:HG32	2.45	0.51
13:o:103:PHE:HB3	13:o:123:LYS:HE2	1.93	0.51
25:B:607:CLA:HAC2	26:t:102:BCR:H272	1.93	0.51
27:a:612:PL9:H371	4:d:38:PHE:HB3	1.92	0.51
1:a:267:ASN:HB3	1:a:270:SER:HB3	1.93	0.51
13:o:15:LEU:HA	13:o:18:LYS:HG3	1.93	0.51
3:C:429:SER:HB3	33:C:517:DGD:HBT2	1.93	0.50
1:A:224:ILE:HG23	2:B:484:PRO:HA	1.94	0.50
1:A:308:ASP:OD1	1:A:312:ASN:N	2.45	0.50
3:c:216:SER:HB3	3:c:221:GLU:HG3	1.94	0.50
25:a:610:CLA:H193	25:c:505:CLA:H13	1.92	0.50
14:t:18:PHE:CD1	26:t:102:BCR:HC7	2.45	0.50
4:d:350:ASN:O	4:d:352:LEU:N	2.44	0.50
2:B:62:VAL:HB	25:B:605:CLA:HED3	1.92	0.50
2:B:474:LEU:O	4:D:134:ARG:NH1	2.44	0.50
25:C:501:CLA:H203	25:C:507:CLA:H13	1.92	0.50
3:C:285:ILE:HA	33:C:516:DGD:HB31	1.94	0.50
25:c:502:CLA:H61	25:c:512:CLA:H42	1.92	0.50
5:e:26:THR:HA	20:r:15:ALA:HB1	1.94	0.50
16:v:5:PRO:O	16:v:9:THR:OG1	2.26	0.50
2:b:201:HIS:HE1	25:b:602:CLA:ND	2.10	0.50
33:C:517:DGD:HB22	23:C:519:LMG:H302	1.94	0.50
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.49
3:C:132:HIS:HE1	25:C:513:CLA:NA	2.08	0.49
3:c:406:SER:HA	3:c:420:VAL:HG23	1.94	0.49
14:T:15:ALA:HB2	26:T:101:BCR:H14C	1.94	0.49
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.94	0.49
3:c:402:GLY:HA3	3:c:420:VAL:HG22	1.95	0.49
20:r:20:VAL:O	20:r:24:LEU:N	2.44	0.49
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.49
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.93	0.49
14:T:18:PHE:HB2	26:T:101:BCR:HC8	1.93	0.49
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.46	0.49
15:u:57:SER:HA	15:u:84:VAL:HG21	1.94	0.49
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.40	0.49
2:B:479:PHE:O	4:D:139:ARG:NH2	2.46	0.49
13:O:60:ARG:HG3	13:O:60:ARG:O	2.12	0.49
25:c:513:CLA:H8	26:z:101:BCR:H23C	1.94	0.49
16:v:22:THR:HG23	16:v:25:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:24:HIS:HA	6:F:27:ALA:HB3	1.95	0.49
2:b:475:PHE:HB2	2:b:479:PHE:HE2	1.78	0.49
3:c:154:LYS:HB3	3:c:256:PRO:HG2	1.94	0.49
13:o:90:ASP:OD1	13:o:92:SER:N	2.38	0.49
13:o:155:ASN:ND2	15:u:100:ASN:O	2.46	0.49
2:B:476:ARG:NH1	37:B:733:HOH:O	2.42	0.49
2:B:475:PHE:HB2	2:B:479:PHE:HE1	1.76	0.48
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.94	0.48
2:b:399:VAL:HG12	2:b:417:VAL:HG22	1.95	0.48
3:c:195:ASP:OD1	3:c:196:VAL:N	2.46	0.48
10:K:25:LEU:HD22	26:K:101:BCR:H332	1.94	0.48
1:a:259:ILE:HA	29:a:616:LHG:H211	1.96	0.48
25:b:601:CLA:H122	26:h:101:BCR:H19C	1.95	0.48
13:O:224:ASP:HB3	13:O:227:ALA:HB3	1.94	0.48
25:b:601:CLA:HBD	25:b:601:CLA:H42	1.95	0.48
3:c:311:GLN:NE2	3:c:358:PHE:O	2.44	0.48
10:K:31:LEU:HD22	26:K:101:BCR:H363	1.94	0.48
3:c:455:PHE:HD2	8:i:33:LYS:HD3	1.78	0.48
29:A:614:LHG:H383	25:C:510:CLA:H43	1.95	0.48
3:C:52:ALA:HB1	25:C:509:CLA:HBB1	1.96	0.48
3:C:444:HIS:HE1	25:C:508:CLA:C1A	2.27	0.48
2:B:113:TRP:CD1	25:B:616:CLA:HBA2	2.49	0.48
3:c:119:LEU:O	3:c:122:SER:OG	2.26	0.48
17:y:39:LEU:HD21	19:z:25:VAL:HA	1.95	0.48
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.96	0.48
29:A:613:LHG:HC82	29:A:613:LHG:H371	1.95	0.48
25:c:503:CLA:HAB	25:c:512:CLA:H41	1.96	0.48
16:v:22:THR:H	16:v:25:GLN:NE2	2.12	0.48
3:C:71:GLU:HB3	3:C:86:LEU:HD22	1.95	0.48
5:E:36:LEU:HD13	20:R:7:VAL:HG12	1.96	0.48
5:E:57:ALA:H	5:E:60:GLN:HG2	1.78	0.48
1:a:191:ASN:HB2	3:c:411:ALA:HB1	1.96	0.48
19:Z:29:SER:O	19:Z:33:TRP:NE1	2.47	0.48
1:a:132:GLU:O	1:a:136:ARG:HG2	2.13	0.48
3:c:444:HIS:HE1	25:c:508:CLA:NA	2.10	0.48
12:M:31:SER:HG	12:m:31:SER:HG	1.62	0.47
16:V:34:GLN:HA	16:V:38:ALA:HB2	1.96	0.47
1:A:245:THR:HG1	4:D:265:ARG:HE	1.59	0.47
27:a:612:PL9:H161	29:a:616:LHG:H302	1.95	0.47
2:b:474:LEU:O	4:d:134:ARG:NH1	2.47	0.47
2:b:498:LYS:HE3	4:d:23:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:318:LEU:HD21	3:c:328:VAL:HG21	1.96	0.47
26:A:609:BCR:H15C	26:A:609:BCR:H351	1.73	0.47
3:C:88:LEU:HB3	25:C:503:CLA:HED3	1.96	0.47
3:c:466:VAL:HG13	4:d:251:ARG:HD2	1.96	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.96	0.47
1:A:270:SER:OG	28:A:611:SQD:O49	2.24	0.47
25:b:605:CLA:HBB1	25:b:606:CLA:H51	1.96	0.47
2:b:86:ILE:H	2:b:86:ILE:HG13	1.56	0.47
25:c:513:CLA:H91	26:z:101:BCR:H21C	1.96	0.47
3:C:317:PHE:HE2	3:C:396:MET:HE1	1.79	0.47
34:D:402:PHO:HBA2	34:D:402:PHO:H3A	1.69	0.47
5:E:26:THR:HA	20:R:15:ALA:HB1	1.97	0.47
2:b:103:LEU:HB2	25:b:606:CLA:H62	1.97	0.47
2:b:154:GLY:HA2	2:b:158:LEU:HD12	1.97	0.47
2:b:242:ILE:HG23	2:b:462:PHE:HD2	1.79	0.47
2:B:496:TYR:CZ	2:B:502:VAL:HA	2.50	0.47
4:D:270:PHE:HZ	27:D:407:PL9:H203	1.79	0.47
28:L:101:SQD:H461	28:L:101:SQD:H92	1.96	0.47
25:b:614:CLA:H62	25:b:614:CLA:H41	1.53	0.47
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.95	0.47
3:c:237:HIS:HA	3:c:240:ILE:HG22	1.96	0.47
4:d:274:VAL:HG22	27:d:405:PL9:H222	1.96	0.47
35:e:101:HEM:CAC	6:f:27:ALA:HB1	2.44	0.47
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.49	0.47
25:D:403:CLA:H92	29:D:408:LHG:H172	1.95	0.47
27:a:612:PL9:H172	27:a:612:PL9:H13	1.58	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.46	0.47
1:a:223:LEU:HD13	4:d:265:ARG:HD3	1.96	0.47
1:a:63:ILE:HB	3:c:335:THR:HG21	1.97	0.47
1:a:284:TRP:HZ3	29:d:407:LHG:H332	1.80	0.47
4:d:103:ARG:HH21	5:e:77:GLU:HG2	1.80	0.47
13:o:4:THR:OG1	13:o:5:LEU:N	2.45	0.47
2:B:281:GLN:O	2:B:285:ASN:ND2	2.38	0.46
1:a:201:GLY:HA3	1:a:286:THR:HB	1.97	0.46
1:a:308:ASP:OD1	1:a:312:ASN:N	2.47	0.46
3:c:57:ALA:O	3:c:61:VAL:HG23	2.15	0.46
5:e:56:TYR:C	5:e:83:LEU:HD21	2.41	0.46
27:A:610:PL9:H502	4:D:39:PRO:HG3	1.98	0.46
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.96	0.46
2:B:388:SER:O	2:B:389:LYS:HD3	2.14	0.46
19:Z:29:SER:OG	19:Z:32:ASP:OD2	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:206:PRO:HG3	23:c:520:LMG:H292	1.97	0.46
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.98	0.46
1:A:286:THR:HG21	25:A:606:CLA:HMA2	1.96	0.46
3:C:57:ALA:O	3:C:61:VAL:HG23	2.15	0.46
15:U:31:ASN:ND2	15:U:96:ASP:O	2.46	0.46
1:a:305:SER:HA	9:j:39:SER:HB3	1.97	0.46
26:c:514:BCR:H11C	26:c:514:BCR:H341	1.80	0.46
4:d:19:ASP:O	4:d:23:LYS:HG2	2.15	0.46
27:d:405:PL9:H412	11:l:29:LEU:HD23	1.98	0.46
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.98	0.46
29:A:614:LHG:H121	29:A:614:LHG:H312	1.97	0.46
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.98	0.46
19:Z:3:ILE:O	19:Z:7:LEU:HB2	2.14	0.46
1:a:27:ARG:NH1	4:d:254:SER:O	2.44	0.46
1:a:213:ALA:HB2	4:d:275:PRO:HG2	1.97	0.46
26:b:619:BCR:H351	26:b:619:BCR:H15C	1.78	0.46
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.96	0.46
4:d:78:VAL:HG11	4:d:114:ILE:HD12	1.97	0.46
16:v:77:LYS:HG2	16:v:95:LEU:HD12	1.98	0.46
19:z:33:TRP:HZ3	19:z:37:LYS:HG3	1.79	0.46
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.50	0.46
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.81	0.46
3:c:279:LEU:HD22	25:c:509:CLA:HED2	1.98	0.46
25:B:616:CLA:H11	25:B:616:CLA:H52	1.74	0.46
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.97	0.46
25:c:513:CLA:HMB3	26:z:101:BCR:H402	1.98	0.46
1:A:283:VAL:HA	1:A:286:THR:HG22	1.97	0.46
25:B:608:CLA:H162	25:D:405:CLA:H3A	1.98	0.46
4:D:149:PRO:HB3	25:D:404:CLA:H41	1.98	0.46
26:T:101:BCR:H15C	26:T:101:BCR:H351	1.71	0.46
26:B:618:BCR:H11C	26:B:618:BCR:H341	1.81	0.46
3:C:79:LYS:HD2	16:V:35:TYR:HE1	1.81	0.46
25:c:503:CLA:H192	25:c:509:CLA:H12	1.96	0.46
19:Z:42:LEU:HD12	19:Z:42:LEU:HA	1.81	0.46
1:a:140:ARG:NH2	29:d:407:LHG:HC41	2.31	0.46
25:b:612:CLA:H171	25:b:613:CLA:HBB2	1.97	0.46
14:T:24:ARG:NH1	37:T:202:HOH:O	2.34	0.45
15:U:57:SER:HA	15:U:84:VAL:HG21	1.98	0.45
29:a:615:LHG:H361	25:b:613:CLA:H51	1.97	0.45
13:o:158:ASP:OD2	13:o:162:ARG:HB2	2.15	0.45
19:z:1:MET:HE3	19:z:60:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.99	0.45
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.97	0.45
26:D:406:BCR:H15C	26:D:406:BCR:H351	1.75	0.45
35:E:102:HEM:C3C	6:F:27:ALA:HB1	2.51	0.45
2:b:109:LEU:O	26:b:619:BCR:H21C	2.16	0.45
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.80	0.45
26:d:404:BCR:H15C	26:d:404:BCR:H351	1.79	0.45
2:B:149:LEU:HD22	25:B:604:CLA:H152	1.97	0.45
3:C:343:ARG:NH1	3:C:347:GLY:O	2.49	0.45
2:b:113:TRP:CD1	25:b:616:CLA:HBA2	2.52	0.45
25:b:605:CLA:H62	25:b:605:CLA:H41	1.75	0.45
25:b:613:CLA:HBB1	25:b:613:CLA:HMB1	1.97	0.45
26:B:617:BCR:HC32	23:B:620:LMG:H322	1.99	0.45
23:B:620:LMG:H411	12:M:17:VAL:HG11	1.98	0.45
2:b:125:ASP:HB2	2:b:132:ALA:HB3	1.98	0.45
26:k:102:BCR:H10C	17:y:28:ILE:HG23	1.99	0.45
13:o:127:ALA:HA	13:o:144:GLY:HA3	1.99	0.45
1:A:308:ASP:O	6:F:45:ARG:NH1	2.46	0.45
3:C:199:ILE:HG13	3:C:234:VAL:HG21	1.97	0.45
3:C:406:SER:HA	3:C:420:VAL:HG23	1.99	0.45
2:b:475:PHE:HB2	2:b:479:PHE:CE2	2.52	0.45
3:c:168:LEU:HD21	25:c:509:CLA:H61	1.97	0.45
25:c:501:CLA:C2D	25:c:503:CLA:H2	2.47	0.45
4:d:103:ARG:HE	5:e:77:GLU:HG3	1.81	0.45
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.45
25:c:508:CLA:H151	23:c:518:LMG:H382	1.98	0.45
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.52	0.45
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.99	0.45
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.50	0.45
13:O:127:ALA:HA	13:O:144:GLY:HA3	1.99	0.45
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.99	0.45
19:Z:58:ASN:O	19:Z:61:VAL:HG12	2.17	0.45
26:h:101:BCR:H11C	26:h:101:BCR:H341	1.81	0.45
13:o:99:ASP:OD1	13:o:100:GLY:N	2.48	0.45
1:A:221:SER:HB2	4:D:139:ARG:O	2.17	0.45
26:A:609:BCR:H24C	26:A:609:BCR:H371	1.82	0.45
2:B:30:VAL:HG12	25:B:605:CLA:HHD	1.98	0.45
25:C:506:CLA:H62	25:C:506:CLA:H41	1.74	0.45
26:a:611:BCR:H15C	26:a:611:BCR:H351	1.75	0.45
29:A:613:LHG:O4	4:D:141:TYR:OH	2.18	0.45
2:B:307:GLU:OE1	13:o:59:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:E:102:HEM:CAC	6:F:27:ALA:HB1	2.47	0.45
4:d:74:LEU:HD22	4:d:175:VAL:HG11	1.99	0.45
13:o:118:LEU:HD22	13:o:233:VAL:HG11	1.99	0.45
25:A:606:CLA:H151	25:D:403:CLA:H151	1.98	0.44
3:C:251:HIS:HE1	25:C:506:CLA:C1A	2.30	0.44
25:C:512:CLA:H93	25:C:513:CLA:H202	1.99	0.44
25:a:610:CLA:H61	25:a:610:CLA:H41	1.87	0.44
11:l:26:VAL:HG11	29:l:101:LHG:H201	1.98	0.44
16:v:19:ILE:HD11	16:v:69:ILE:HG13	1.99	0.44
26:B:619:BCR:H11C	26:B:619:BCR:H341	1.79	0.44
1:a:118:HIS:HE1	25:a:610:CLA:C4D	2.29	0.44
3:c:162:GLY:HA3	3:c:252:ILE:HG13	1.99	0.44
3:c:179:ALA:HA	3:c:184:GLY:HA2	1.98	0.44
3:c:371:GLY:N	3:c:374:GLY:O	2.38	0.44
19:z:33:TRP:HZ3	19:z:37:LYS:HB2	1.81	0.44
25:C:507:CLA:H62	25:C:507:CLA:H41	1.86	0.44
26:C:514:BCR:H15C	26:C:514:BCR:H351	1.75	0.44
3:c:429:SER:HB3	33:c:516:DGD:HBT2	1.99	0.44
4:d:79:SER:HA	4:d:172:SER:HB3	2.00	0.44
5:e:61:ARG:HH12	16:v:127:GLY:HA3	1.82	0.44
15:u:38:TYR:HB2	15:u:41:LEU:HD12	2.00	0.44
27:A:610:PL9:H252	34:D:402:PHO:HBA1	1.99	0.44
26:b:619:BCR:H11C	26:b:619:BCR:H341	1.79	0.44
3:c:36:TRP:CE3	29:d:407:LHG:H111	2.52	0.44
16:v:34:GLN:HA	16:v:38:ALA:HB2	1.99	0.44
19:z:27:TYR:C	19:z:29:SER:H	2.24	0.44
2:B:149:LEU:HD23	25:B:603:CLA:HBC1	1.99	0.44
26:C:514:BCR:H24C	26:C:514:BCR:H371	1.84	0.44
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.44
2:b:227:LYS:HA	2:b:227:LYS:HD3	1.62	0.44
2:b:235:GLU:OE1	2:b:472:ARG:NH2	2.50	0.44
29:d:407:LHG:H131	29:d:407:LHG:H372	1.99	0.44
26:k:102:BCR:H15C	26:k:102:BCR:H351	1.82	0.44
16:v:129:LYS:HG2	16:v:136:TYR:HB3	2.00	0.44
2:b:72:THR:HG22	2:b:80:ILE:HD11	1.99	0.44
2:b:413:ASP:HA	2:b:414:PRO:HD3	1.87	0.44
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.00	0.44
13:o:199:LEU:HD23	13:o:215:PHE:HB3	2.00	0.44
26:a:611:BCR:H11C	26:a:611:BCR:H341	1.82	0.44
2:b:65:PHE:HE1	25:b:604:CLA:HED2	1.82	0.44
16:v:12:LEU:HD12	16:v:69:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:PRO:HG2	7:H:49:TYR:CE1	2.53	0.44
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.90	0.44
26:B:617:BCR:H351	26:B:617:BCR:H15C	1.76	0.44
13:o:79:ASP:OD1	13:o:80:GLN:N	2.48	0.44
19:z:25:VAL:O	19:z:29:SER:HB2	2.18	0.44
26:z:101:BCR:H24C	26:z:101:BCR:H371	1.81	0.44
25:B:614:CLA:HBA1	28:L:101:SQD:H82	2.00	0.44
4:D:126:MET:HE3	4:D:143:ALA:O	2.18	0.44
13:O:169:ASP:OD1	13:O:169:ASP:N	2.51	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.44
3:c:239:TRP:CH2	23:c:520:LMG:H291	2.50	0.44
26:d:404:BCR:H20C	26:d:404:BCR:H361	1.90	0.44
2:B:291:SER:O	2:B:294:SER:OG	2.32	0.43
3:C:179:ALA:HA	3:C:184:GLY:HA2	1.98	0.43
26:H:101:BCR:H361	26:H:101:BCR:H20C	1.84	0.43
17:Y:18:VAL:O	17:Y:21:GLN:HB3	2.18	0.43
3:c:190:ALA:HA	3:c:191:PRO:HD3	1.91	0.43
15:u:76:ARG:HA	15:u:79:LEU:HG	2.00	0.43
29:A:613:LHG:H223	25:B:613:CLA:H192	1.98	0.43
3:C:228:ASN:HB3	33:C:516:DGD:HE62	1.99	0.43
16:V:42:VAL:O	16:V:45:ILE:HG12	2.18	0.43
2:b:357:ARG:NH1	37:b:720:HOH:O	2.51	0.43
25:c:508:CLA:H13	25:c:510:CLA:H202	2.00	0.43
16:v:87:GLU:OE1	16:v:96:ARG:NH1	2.50	0.43
1:A:140:ARG:NH2	29:A:614:LHG:HC41	2.32	0.43
1:a:283:VAL:HA	1:a:286:THR:HG22	2.00	0.43
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.43
4:d:161:PRO:HB3	4:d:170:ALA:HB2	1.99	0.43
3:C:402:GLY:HA3	3:C:420:VAL:HG22	2.01	0.43
4:D:24:ARG:HB2	4:D:26:ARG:HE	1.82	0.43
1:a:286:THR:HG21	25:a:606:CLA:HMA2	2.00	0.43
33:c:516:DGD:HA31	33:c:516:DGD:HA62	1.77	0.43
3:C:334:PRO:HA	13:O:153:THR:OG1	2.19	0.43
26:C:514:BCR:H11C	26:C:514:BCR:H341	1.75	0.43
4:D:342:PRO:O	4:D:345:VAL:HG22	2.18	0.43
26:D:406:BCR:H11C	26:D:406:BCR:H341	1.78	0.43
1:a:131:TRP:HZ2	3:c:449:ARG:HG3	1.82	0.43
1:a:340:PRO:HD3	15:u:103:TYR:CZ	2.53	0.43
35:e:101:HEM:HBA2	35:e:101:HEM:HHA	2.01	0.43
8:i:2:GLU:O	8:i:6:ILE:HG12	2.19	0.43
11:l:4:ASN:O	11:l:7:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:408:LMG:H221	23:d:408:LMG:H192	1.81	0.43
26:z:101:BCR:H11C	26:z:101:BCR:H341	1.81	0.43
2:B:42:LEU:HD13	2:B:94:GLU:HG3	2.01	0.43
26:B:619:BCR:H24C	26:B:619:BCR:H371	1.84	0.43
3:C:211:GLY:O	3:C:215:LYS:HG3	2.18	0.43
26:C:522:BCR:H351	26:C:522:BCR:H15C	1.76	0.43
2:b:497:GLN:HE22	18:x:38:GLN:CB	2.32	0.43
3:c:88:LEU:HB3	25:c:503:CLA:HED3	1.99	0.43
4:d:126:MET:HE3	4:d:143:ALA:O	2.18	0.43
13:o:86:LYS:HD2	13:o:86:LYS:HA	1.75	0.43
19:z:33:TRP:HZ3	19:z:37:LYS:CB	2.31	0.43
1:A:264:SER:OG	27:A:610:PL9:O2	2.32	0.43
1:A:300:PHE:HZ	33:C:518:DGD:HB61	1.84	0.43
2:B:191:ASN:HB2	7:H:58:VAL:HG13	2.01	0.43
3:C:279:LEU:HD22	25:C:509:CLA:HED2	2.01	0.43
25:C:513:CLA:C4B	26:C:514:BCR:H383	2.49	0.43
19:Z:46:LEU:HD23	19:Z:50:LEU:HG	2.00	0.43
1:a:343:LEU:HD12	3:c:310:SER:HA	2.01	0.43
4:d:27:PHE:HD2	4:d:28:VAL:HG23	1.84	0.43
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.43
25:B:613:CLA:H191	26:B:618:BCR:H333	2.01	0.43
3:C:31:SER:HB3	3:C:41:ARG:HG2	2.01	0.43
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.53	0.43
26:c:514:BCR:H15C	26:c:514:BCR:H351	1.76	0.43
10:k:31:LEU:HD22	26:k:102:BCR:H363	2.01	0.43
20:r:10:LEU:HB3	20:r:11:PRO:HD3	2.00	0.43
26:C:515:BCR:H24C	26:C:515:BCR:H371	1.85	0.43
4:D:146:PHE:C	4:D:149:PRO:HD2	2.44	0.43
34:D:401:PHO:H61	34:D:401:PHO:H2	1.82	0.43
13:O:99:ASP:OD1	13:O:100:GLY:N	2.44	0.43
17:Y:19:ILE:HD12	17:Y:19:ILE:H	1.84	0.43
25:a:607:CLA:H142	34:a:609:PHO:H172	2.00	0.43
17:y:44:GLY:HA2	19:z:30:PRO:HD3	2.01	0.43
2:b:51:VAL:HG13	2:b:308:LYS:HB2	2.01	0.42
3:c:363:GLY:O	3:c:367:GLU:HG2	2.18	0.42
25:c:507:CLA:HAA2	25:c:507:CLA:HBD	2.00	0.42
25:c:513:CLA:C4B	26:z:101:BCR:H383	2.49	0.42
3:C:42:LEU:HD21	25:C:511:CLA:H2A	2.01	0.42
25:C:501:CLA:H71	25:C:501:CLA:CBB	2.45	0.42
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.54	0.42
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG11	25:A:607:CLA:C3D	2.50	0.42
27:A:610:PL9:H151	27:A:610:PL9:H171	1.71	0.42
25:C:508:CLA:H141	25:C:510:CLA:H18	2.01	0.42
27:a:612:PL9:H451	18:x:28:LEU:HD21	2.00	0.42
1:A:46:ILE:HD13	23:A:603:LMG:H421	2.01	0.42
26:A:609:BCR:H11C	26:A:609:BCR:H341	1.85	0.42
3:C:346:THR:OG1	3:C:348:GLU:OE2	2.27	0.42
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.84	0.42
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.01	0.42
1:a:179:THR:O	1:a:183:MET:HG3	2.20	0.42
2:b:479:PHE:O	4:d:139:ARG:NH2	2.52	0.42
26:h:101:BCR:H15C	26:h:101:BCR:H351	1.77	0.42
1:A:217:SER:HA	4:D:272:LEU:HD12	2.00	0.42
2:B:30:VAL:HG13	25:B:613:CLA:HMC2	2.00	0.42
25:B:614:CLA:H72	26:B:617:BCR:H362	2.01	0.42
3:C:216:SER:HB3	3:C:221:GLU:HG3	2.00	0.42
23:C:521:LMG:H391	23:C:521:LMG:H362	1.75	0.42
34:D:402:PHO:H3A	25:D:404:CLA:H142	2.00	0.42
2:b:363:PHE:HB3	2:b:365:SER:O	2.19	0.42
2:b:490:GLN:HB3	2:b:496:TYR:HE2	1.84	0.42
25:b:605:CLA:H122	25:b:610:CLA:HMA2	2.02	0.42
5:e:8:ARG:HA	5:e:9:PRO:HD3	1.95	0.42
3:C:256:PRO:HA	25:C:506:CLA:HED2	2.02	0.42
25:C:501:CLA:C2D	25:C:503:CLA:H2	2.50	0.42
12:M:32:GLN:HG3	12:m:31:SER:HB2	2.01	0.42
1:a:45:THR:HG23	25:a:607:CLA:H201	2.01	0.42
1:a:227:THR:HB	1:a:231:GLU:HG3	2.02	0.42
25:a:607:CLA:H2	34:a:609:PHO:C2B	2.50	0.42
2:b:141:ILE:HD11	7:h:14:LEU:HD22	2.00	0.42
26:d:404:BCR:H341	26:d:404:BCR:H11C	1.76	0.42
15:u:42:TYR:HA	15:u:43:PRO:HA	1.81	0.42
25:D:403:CLA:H91	29:D:408:LHG:H191	2.02	0.42
16:V:73:VAL:HA	16:V:76:MET:HE3	2.01	0.42
25:c:505:CLA:H43	26:c:514:BCR:HC7	2.01	0.42
25:c:506:CLA:C3D	25:c:507:CLA:H193	2.49	0.42
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.00	0.42
2:B:109:LEU:O	26:B:619:BCR:H21C	2.19	0.42
25:B:605:CLA:H62	25:B:605:CLA:H41	1.75	0.42
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.01	0.42
3:C:363:GLY:O	3:C:367:GLU:HG2	2.19	0.42
13:O:67:PRO:HD2	2:b:84:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:607:CLA:H152	29:d:406:LHG:H212	2.01	0.42
28:a:613:SQD:H161	29:d:407:LHG:H181	2.02	0.42
2:B:469:HIS:HE1	25:B:611:CLA:C1A	2.32	0.42
26:B:617:BCR:H24C	26:B:617:BCR:H371	1.81	0.42
25:C:503:CLA:HMD1	25:C:503:CLA:H191	2.02	0.42
5:E:14:ILE:O	5:E:20:TRP:NE1	2.44	0.42
25:b:603:CLA:H61	25:b:603:CLA:H41	1.88	0.42
26:b:617:BCR:H15C	26:b:617:BCR:H351	1.80	0.42
26:h:101:BCR:H371	26:h:101:BCR:H24C	1.79	0.42
26:t:102:BCR:H11C	26:t:102:BCR:H341	1.80	0.42
16:v:26:TYR:OH	16:v:122:GLU:OE2	2.21	0.42
18:x:3:ILE:HA	18:x:7:LEU:HD23	2.02	0.42
25:B:615:CLA:H2	25:B:616:CLA:HBB2	2.01	0.42
4:D:56:THR:OG1	4:D:57:SER:N	2.52	0.42
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.91	0.42
15:U:27:LEU:HD22	15:U:49:ILE:HG21	2.01	0.42
25:a:606:CLA:HMB1	25:a:606:CLA:HBB1	2.01	0.42
2:b:141:ILE:HG21	25:b:615:CLA:HBB1	2.02	0.42
2:b:201:HIS:HB2	25:b:602:CLA:CHB	2.49	0.42
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.42
4:d:68:LEU:HD13	6:f:40:MET:HE2	2.01	0.42
29:A:613:LHG:H101	29:A:613:LHG:H351	2.02	0.41
25:C:504:CLA:C1D	33:C:517:DGD:HB21	2.50	0.41
25:C:504:CLA:H62	25:C:504:CLA:H41	1.91	0.41
16:v:45:ILE:H	16:v:45:ILE:HG13	1.65	0.41
1:A:121:LEU:HD11	25:C:505:CLA:H171	2.03	0.41
3:C:437:PHE:HA	25:C:508:CLA:HMC2	2.01	0.41
15:U:42:TYR:HA	15:U:43:PRO:HA	1.80	0.41
2:b:466:HIS:HE1	25:b:608:CLA:C4D	2.33	0.41
25:b:604:CLA:H62	25:b:604:CLA:H41	1.86	0.41
26:z:101:BCR:H20C	26:z:101:BCR:H361	1.88	0.41
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.41
26:b:619:BCR:H24C	26:b:619:BCR:H371	1.83	0.41
25:c:506:CLA:H192	25:c:506:CLA:H13	2.01	0.41
4:d:210:LEU:CD2	27:d:405:PL9:H13	2.50	0.41
1:A:136:ARG:NH1	8:I:27:ASP:OD1	2.49	0.41
1:A:218:LEU:HD12	27:A:610:PL9:C3	2.51	0.41
27:A:610:PL9:H121	27:A:610:PL9:HC8	1.72	0.41
25:C:502:CLA:H61	25:C:512:CLA:H42	2.01	0.41
26:a:611:BCR:H24C	26:a:611:BCR:H371	1.83	0.41
2:b:341:LYS:HD2	2:b:429:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:11:SER:O	5:e:15:THR:OG1	2.27	0.41
20:r:23:ILE:O	20:r:27:ALA:N	2.49	0.41
26:z:101:BCR:H15C	26:z:101:BCR:H351	1.72	0.41
25:B:616:CLA:H142	26:B:619:BCR:H14C	2.02	0.41
17:Y:34:MET:HE2	17:Y:34:MET:HB2	1.88	0.41
2:b:487:SER:HA	2:b:488:PRO:HD3	1.89	0.41
25:c:513:CLA:HAB	26:z:101:BCR:H371	2.02	0.41
2:B:472:ARG:HA	2:B:479:PHE:CE1	2.55	0.41
25:B:601:CLA:C4D	25:B:601:CLA:H8	2.50	0.41
28:L:101:SQD:H241	11:l:18:TYR:OH	2.21	0.41
15:U:57:SER:OG	15:U:60:ASP:OD2	2.27	0.41
29:a:615:LHG:HC82	29:a:615:LHG:H371	2.00	0.41
5:e:57:ALA:HB3	5:e:60:GLN:HB2	2.01	0.41
5:e:61:ARG:NH1	16:v:127:GLY:HA3	2.36	0.41
1:A:183:MET:HA	25:A:606:CLA:HMD2	2.03	0.41
3:C:87:ILE:O	3:C:91:HIS:ND1	2.47	0.41
2:b:216:HIS:HE1	25:b:609:CLA:CHA	2.34	0.41
11:l:26:VAL:HG21	29:l:101:LHG:H192	2.02	0.41
20:R:18:TRP:O	20:R:22:ASN:ND2	2.35	0.41
29:A:613:LHG:H361	25:B:613:CLA:H51	2.02	0.41
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.83	0.41
2:b:419:SER:O	2:b:423:LYS:HG2	2.21	0.41
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.85	0.41
4:d:191:TRP:CZ2	4:d:197:HIS:HB2	2.56	0.41
19:z:58:ASN:O	19:z:62:VAL:HG22	2.20	0.41
25:A:608:CLA:H202	25:C:506:CLA:H101	2.01	0.41
25:B:607:CLA:H41	25:B:607:CLA:H62	1.85	0.41
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.96	0.41
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.03	0.41
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.92	0.41
7:H:22:ALA:HA	7:H:23:PRO:HD3	1.91	0.41
26:H:101:BCR:H341	26:H:101:BCR:H11C	1.79	0.41
27:a:612:PL9:H121	27:a:612:PL9:HC8	1.78	0.41
2:b:191:ASN:HA	2:b:192:PRO:HD2	1.76	0.41
25:c:504:CLA:H202	29:d:407:LHG:H192	2.02	0.41
5:e:19:TYR:HE1	35:e:101:HEM:C3D	2.39	0.41
16:v:100:ILE:HG13	16:v:101:PHE:CD2	2.56	0.41
20:R:8:VAL:O	20:R:11:PRO:HD2	2.21	0.41
17:y:20:ALA:O	17:y:24:MET:HG2	2.21	0.41
3:C:296:VAL:C	3:C:298:PRO:HD3	2.46	0.41
25:C:512:CLA:O2D	25:C:513:CLA:HBB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:408:LHG:H201	14:T:13:ILE:HG21	2.01	0.41
12:M:23:ILE:O	12:M:27:VAL:HG23	2.21	0.41
25:b:612:CLA:H61	25:b:612:CLA:H102	1.94	0.41
20:R:20:VAL:O	20:R:24:LEU:N	2.51	0.41
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.02	0.40
33:C:516:DGD:HAT2	33:C:516:DGD:HAH1	1.88	0.40
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.03	0.40
5:E:9:PRO:O	5:E:13:ILE:HG13	2.21	0.40
14:T:26:PRO:HA	14:T:27:PRO:HD2	1.98	0.40
25:c:508:CLA:H203	33:c:516:DGD:HA92	2.03	0.40
26:c:521:BCR:H351	26:c:521:BCR:H15C	1.78	0.40
4:d:23:LYS:HE2	4:d:23:LYS:HB3	1.93	0.40
4:d:87:HIS:HB2	33:h:102:DGD:HG11	2.03	0.40
29:d:406:LHG:HC62	11:l:15:THR:HG23	2.03	0.40
13:o:53:LYS:HB2	13:o:65:PHE:CE1	2.56	0.40
2:B:201:HIS:HE2	25:B:603:CLA:C2B	2.34	0.40
3:C:346:THR:HG21	13:O:12:GLY:HA2	2.02	0.40
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.03	0.40
4:D:261:PHE:CZ	29:D:408:LHG:HC81	2.56	0.40
29:D:408:LHG:H142	29:D:408:LHG:H171	1.93	0.40
26:b:618:BCR:H341	26:b:618:BCR:H11C	1.80	0.40
25:C:505:CLA:H43	26:C:515:BCR:HC7	2.04	0.40
23:C:521:LMG:O2	23:C:521:LMG:HC71	2.21	0.40
23:C:521:LMG:H411	23:C:521:LMG:H382	1.74	0.40
26:T:101:BCR:H11C	26:T:101:BCR:H341	1.76	0.40
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.04	0.40
3:c:296:VAL:HG11	25:c:501:CLA:HMA2	2.02	0.40
25:c:508:CLA:H72	25:c:510:CLA:HED3	2.04	0.40
26:t:102:BCR:H15C	26:t:102:BCR:H351	1.74	0.40
16:v:94:SER:HA	16:v:104:MET:HE2	2.02	0.40
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.40
3:C:90:PRO:HB3	3:C:301:PHE:HB3	2.04	0.40
11:L:22:LEU:HG	29:L:102:LHG:H181	2.03	0.40
1:a:240:GLY:HA3	14:t:29:ILE:HG23	2.04	0.40
2:b:156:PHE:HB3	2:b:162:PHE:HB3	2.03	0.40
3:c:132:HIS:HE1	25:c:513:CLA:NA	2.17	0.40
4:d:56:THR:OG1	4:d:57:SER:N	2.53	0.40
19:z:38:GLN:O	19:z:42:LEU:N	2.52	0.40
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.47	0.40
3:C:350:ILE:HG21	3:C:359:TRP:HB2	2.04	0.40
28:F:101:SQD:H361	28:F:101:SQD:H332	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:612:PL9:H221	27:a:612:PL9:H201	1.95	0.40
28:a:613:SQD:H321	25:c:508:CLA:H102	2.03	0.40
2:b:305:ILE:HA	2:b:306:PRO:HD3	1.96	0.40
25:b:615:CLA:H161	7:h:7:LEU:HD21	2.04	0.40
3:c:62:PHE:HZ	10:k:28:ILE:HD12	1.87	0.40
5:e:80:LEU:HD23	5:e:80:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	36	44
1	a	331/344 (96%)	324 (98%)	6 (2%)	1 (0%)	36	44
2	B	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
2	b	501/510 (98%)	482 (96%)	18 (4%)	1 (0%)	43	53
3	C	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	43	53
3	c	446/461 (97%)	435 (98%)	9 (2%)	2 (0%)	30	36
4	D	338/352 (96%)	326 (96%)	12 (4%)	0	100	100
4	d	338/352 (96%)	323 (96%)	14 (4%)	1 (0%)	36	44
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	31/38 (82%)	31 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/40 (80%)	32 (100%)	0	0	100	100
9	j	31/40 (78%)	31 (100%)	0	0	100	100
10	K	34/46 (74%)	31 (91%)	3 (9%)	0	100	100
10	k	34/46 (74%)	34 (100%)	0	0	100	100
11	L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	228 (95%)	11 (5%)	1 (0%)	30	36
13	o	241/272 (89%)	225 (93%)	13 (5%)	3 (1%)	10	10
14	T	27/32 (84%)	27 (100%)	0	0	100	100
14	t	27/32 (84%)	26 (96%)	1 (4%)	0	100	100
15	U	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
15	u	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
16	v	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	21
17	Y	27/46 (59%)	26 (96%)	1 (4%)	0	100	100
17	y	27/46 (59%)	24 (89%)	2 (7%)	1 (4%)	2	1
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	6
19	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	3	1
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	31/41 (76%)	29 (94%)	2 (6%)	0	100	100
All	All	5199/5700 (91%)	5010 (96%)	173 (3%)	16 (0%)	36	44

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	30	PRO
13	o	57	LYS

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Mol	Chain	Res	Type
3	c	416	SER
13	o	58	ASN
13	o	61	GLN
17	y	21	GLN
19	z	31	GLN
3	C	416	SER
3	c	135	ARG
4	d	351	ALA
2	b	126	PRO
19	z	30	PRO
1	A	259	ILE
1	a	259	ILE
16	v	45	ILE

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	83
1	a	270/280 (96%)	269 (100%)	1 (0%)	84	89
2	B	403/407 (99%)	399 (99%)	4 (1%)	68	77
2	b	401/407 (98%)	398 (99%)	3 (1%)	76	83
3	C	350/362 (97%)	350 (100%)	0	100	100
3	c	350/362 (97%)	350 (100%)	0	100	100
4	D	275/283 (97%)	275 (100%)	0	100	100
4	d	275/283 (97%)	274 (100%)	1 (0%)	84	89
5	E	71/73 (97%)	70 (99%)	1 (1%)	59	70
5	e	70/73 (96%)	69 (99%)	1 (1%)	59	70
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	53 (100%)	0	100	100
7	h	53/55 (96%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	30/35 (86%)	30 (100%)	0	100	100
8	i	32/35 (91%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	37
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	29/37 (78%)	27 (93%)	2 (7%)	14	18
10	k	29/37 (78%)	28 (97%)	1 (3%)	32	45
11	L	34/35 (97%)	33 (97%)	1 (3%)	37	49
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	29 (100%)	0	100	100
13	O	206/228 (90%)	203 (98%)	3 (2%)	57	69
13	o	206/228 (90%)	204 (99%)	2 (1%)	68	77
14	T	26/29 (90%)	26 (100%)	0	100	100
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	82 (99%)	1 (1%)	63	74
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	45
17	Y	22/37 (60%)	19 (86%)	3 (14%)	3	3
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	10
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	48 (92%)	4 (8%)	12	14
19	z	52/52 (100%)	47 (90%)	5 (10%)	8	8
20	R	29/33 (88%)	28 (97%)	1 (3%)	32	45
20	r	28/33 (85%)	28 (100%)	0	100	100
All	All	4318/4660 (93%)	4275 (99%)	43 (1%)	68	77

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
1	A	261	GLN

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Mol	Chain	Res	Type
2	B	86	ILE
2	B	127	ARG
2	B	223	GLN
2	B	389	LYS
5	E	5	THR
9	J	19	MET
10	K	11	LEU
10	K	27	VAL
11	L	2	GLU
13	O	61	GLN
13	O	118	LEU
13	O	179	GLU
15	U	84	VAL
17	Y	22	LEU
17	Y	23	THR
17	Y	25	ILE
19	Z	31	GLN
19	Z	42	LEU
19	Z	46	LEU
19	Z	62	VAL
1	a	243	GLU
2	b	86	ILE
2	b	227	LYS
2	b	490	GLN
4	d	294	ARG
5	e	7	GLU
10	k	17	ILE
13	o	61	GLN
13	o	64	GLU
16	v	6	GLU
16	v	17	LYS
16	v	42	VAL
16	v	45	ILE
20	R	31	VAL
17	y	18	VAL
17	y	22	LEU
19	z	1	MET
19	z	2	THR
19	z	3	ILE
19	z	31	GLN
19	z	33	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26)

such sidechains are listed below:

Mol	Chain	Res	Type
2	B	223	GLN
2	B	331	ASN
2	B	394	GLN
2	B	497	GLN
3	C	311	GLN
3	C	327	ASN
3	C	385	GLN
10	K	40	GLN
11	L	6	ASN
1	a	75	ASN
1	a	312	ASN
2	b	331	ASN
2	b	394	GLN
2	b	490	GLN
3	c	332	GLN
4	d	186	GLN
4	d	250	ASN
4	d	255	GLN
4	d	336	HIS
5	e	74	GLN
10	k	40	GLN
13	o	61	GLN
13	o	130	GLN
13	o	132	ASN
16	v	25	GLN
19	z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 191 ligands modelled in this entry, 6 are monoatomic and 29 are unknown - leaving 156 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	$\# Z > 2$
23	LMG	A	612	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	3 (5%)
26	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.83	12 (21%)
25	CLA	b	613	-	69,73,73	1.58	7 (10%)	82,113,113	1.16	9 (10%)
30	SO4	O	301	-	4,4,4	0.23	0	6,6,6	0.08	0
23	LMG	C	519	-	51,51,55	0.95	2 (3%)	59,59,63	0.99	3 (5%)
27	PL9	D	407	-	55,55,55	0.63	2 (3%)	68,69,69	1.69	17 (25%)
30	SO4	o	301	-	4,4,4	0.23	0	6,6,6	0.09	0
30	SO4	V	202	-	4,4,4	0.23	0	6,6,6	0.14	0
26	BCR	T	101	-	41,41,41	0.69	0	56,56,56	2.06	12 (21%)
21	OEX	A	601	1,37,3	0,15,15	-	-	-	-	-
25	CLA	C	504	-	69,73,73	1.61	7 (10%)	82,113,113	1.15	8 (9%)
25	CLA	C	507	-	69,73,73	1.58	7 (10%)	82,113,113	1.16	8 (9%)
33	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	0.95	3 (3%)
25	CLA	b	601	-	69,73,73	1.60	9 (13%)	82,113,113	1.16	9 (10%)
25	CLA	d	403	-	69,73,73	1.59	9 (13%)	82,113,113	1.13	8 (9%)
26	BCR	k	102	-	41,41,41	0.70	0	56,56,56	1.86	17 (30%)
23	LMG	B	620	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)
23	LMG	a	603	-	51,51,55	0.94	2 (3%)	59,59,63	1.09	6 (10%)
25	CLA	c	513	-	69,73,73	1.60	8 (11%)	82,113,113	1.19	9 (10%)
30	SO4	u	202	-	4,4,4	0.24	0	6,6,6	0.08	0
26	BCR	h	101	-	41,41,41	0.68	0	56,56,56	1.98	13 (23%)
23	LMG	A	603	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	3 (5%)
21	OEX	a	601	1,37,3	0,15,15	-	-	-	-	-
30	SO4	a	617	-	4,4,4	0.24	0	6,6,6	0.07	0
23	LMG	C	521	-	51,51,55	0.97	3 (5%)	59,59,63	1.11	4 (6%)
28	SQD	L	103	-	52,54,54	1.12	3 (5%)	62,65,65	1.12	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	503	-	69,73,73	1.57	8 (11%)	82,113,113	1.20	8 (9%)
33	DGD	C	516	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	4 (5%)
34	PHO	D	401	-	58,69,69	1.36	6 (10%)	55,99,99	1.65	4 (7%)
26	BCR	B	618	-	41,41,41	0.67	0	56,56,56	1.87	11 (19%)
26	BCR	K	101	-	41,41,41	0.71	0	56,56,56	1.80	14 (25%)
29	LHG	d	407	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	2 (3%)
25	CLA	b	615	-	69,73,73	1.57	7 (10%)	82,113,113	1.20	8 (9%)
35	HEM	e	101	5,6	50,50,50	1.38	6 (12%)	67,82,82	1.02	3 (4%)
25	CLA	B	609	-	69,73,73	1.60	9 (13%)	82,113,113	1.18	10 (12%)
26	BCR	B	617	-	41,41,41	0.68	0	56,56,56	1.97	17 (30%)
25	CLA	C	505	-	69,73,73	1.59	8 (11%)	82,113,113	1.17	8 (9%)
25	CLA	b	608	-	69,73,73	1.61	8 (11%)	82,113,113	1.17	9 (10%)
23	LMG	b	620	-	51,51,55	0.94	2 (3%)	59,59,63	1.04	5 (8%)
25	CLA	C	501	-	69,73,73	1.59	8 (11%)	82,113,113	1.16	9 (10%)
25	CLA	b	616	-	69,73,73	1.59	9 (13%)	82,113,113	1.21	9 (10%)
29	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
25	CLA	b	607	37	69,73,73	1.58	8 (11%)	82,113,113	1.19	9 (10%)
23	LMG	c	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.05	4 (6%)
25	CLA	b	610	37	69,73,73	1.61	8 (11%)	82,113,113	1.20	9 (10%)
25	CLA	C	508	-	69,73,73	1.59	8 (11%)	82,113,113	1.19	8 (9%)
23	LMG	B	624	-	51,51,55	0.94	2 (3%)	59,59,63	0.98	3 (5%)
25	CLA	a	606	-	69,73,73	1.57	8 (11%)	82,113,113	1.22	9 (10%)
25	CLA	c	501	-	69,73,73	1.58	8 (11%)	82,113,113	1.18	9 (10%)
28	SQD	F	101	-	41,43,54	1.23	3 (7%)	51,54,65	1.25	7 (13%)
27	PL9	A	610	-	55,55,55	0.64	2 (3%)	68,69,69	1.77	20 (29%)
26	BCR	b	618	-	41,41,41	0.63	0	56,56,56	1.97	17 (30%)
25	CLA	c	507	-	69,73,73	1.58	7 (10%)	82,113,113	1.16	8 (9%)
25	CLA	A	606	-	69,73,73	1.59	8 (11%)	82,113,113	1.23	8 (9%)
26	BCR	A	609	-	41,41,41	0.67	0	56,56,56	1.86	12 (21%)
25	CLA	B	611	-	69,73,73	1.59	7 (10%)	82,113,113	1.20	9 (10%)
25	CLA	b	602	-	69,73,73	1.64	9 (13%)	82,113,113	1.25	8 (9%)
23	LMG	b	624	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	3 (5%)
33	DGD	h	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.90	2 (2%)
25	CLA	a	608	-	69,73,73	1.62	9 (13%)	82,113,113	1.18	10 (12%)
26	BCR	c	521	-	41,41,41	0.64	0	56,56,56	2.07	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	612	-	69,73,73	1.59	7 (10%)	82,113,113	1.19	9 (10%)
25	CLA	B	605	-	69,73,73	1.58	8 (11%)	82,113,113	1.20	8 (9%)
25	CLA	B	614	-	69,73,73	1.59	8 (11%)	82,113,113	1.21	9 (10%)
30	SO4	A	615	-	4,4,4	0.24	0	6,6,6	0.09	0
25	CLA	B	602	-	69,73,73	1.60	8 (11%)	82,113,113	1.23	9 (10%)
33	DGD	c	517	-	63,63,67	0.87	2 (3%)	77,77,81	0.90	3 (3%)
29	LHG	a	616	-	41,41,48	1.01	2 (4%)	44,47,54	1.11	3 (6%)
25	CLA	c	508	-	69,73,73	1.58	8 (11%)	82,113,113	1.19	9 (10%)
29	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.09	4 (7%)
25	CLA	B	615	-	69,73,73	1.56	8 (11%)	82,113,113	1.20	8 (9%)
26	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
25	CLA	b	614	-	69,73,73	1.59	8 (11%)	82,113,113	1.22	8 (9%)
25	CLA	C	513	-	69,73,73	1.59	8 (11%)	82,113,113	1.18	9 (10%)
25	CLA	b	609	-	69,73,73	1.60	9 (13%)	82,113,113	1.16	9 (10%)
27	PL9	d	405	-	55,55,55	0.63	2 (3%)	68,69,69	1.70	19 (27%)
33	DGD	c	515	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	4 (5%)
33	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	0.89	3 (3%)
25	CLA	B	603	-	69,73,73	1.58	8 (11%)	82,113,113	1.21	9 (10%)
25	CLA	B	607	37	69,73,73	1.60	8 (11%)	82,113,113	1.19	9 (10%)
25	CLA	C	503	-	69,73,73	1.57	7 (10%)	82,113,113	1.18	9 (10%)
25	CLA	c	511	3	69,73,73	1.58	8 (11%)	82,113,113	1.13	10 (12%)
33	DGD	c	516	-	63,63,67	0.88	2 (3%)	77,77,81	0.93	4 (5%)
28	SQD	f	101	-	41,43,54	1.26	3 (7%)	51,54,65	1.28	6 (11%)
31	BCT	A	616	22	3,3,3	0.58	0	2,3,3	0.23	0
26	BCR	t	102	-	41,41,41	0.67	0	56,56,56	2.07	14 (25%)
29	LHG	A	614	-	48,48,48	0.95	2 (4%)	51,54,54	1.02	2 (3%)
25	CLA	C	502	-	69,73,73	1.60	8 (11%)	82,113,113	1.17	9 (10%)
25	CLA	C	509	-	69,73,73	1.59	8 (11%)	82,113,113	1.15	9 (10%)
29	LHG	A	613	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
30	SO4	d	410	-	4,4,4	0.23	0	6,6,6	0.07	0
23	LMG	a	614	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	3 (5%)
25	CLA	c	502	-	69,73,73	1.61	8 (11%)	82,113,113	1.17	9 (10%)
25	CLA	c	510	-	69,73,73	1.58	7 (10%)	82,113,113	1.20	9 (10%)
29	LHG	L	102	-	48,48,48	0.93	2 (4%)	51,54,54	1.11	4 (7%)
27	PL9	a	612	-	55,55,55	0.65	2 (3%)	68,69,69	1.69	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SO4	O	302	-	4,4,4	0.23	0	6,6,6	0.07	0
23	LMG	D	409	-	51,51,55	0.95	2 (3%)	59,59,63	0.99	3 (5%)
29	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
25	CLA	B	604	-	69,73,73	1.57	7 (10%)	82,113,113	1.18	10 (12%)
26	BCR	D	406	-	41,41,41	0.69	0	56,56,56	2.23	15 (26%)
28	SQD	L	101	-	52,54,54	1.15	3 (5%)	62,65,65	3.07	8 (12%)
25	CLA	a	607	37	69,73,73	1.62	8 (11%)	82,113,113	1.22	9 (10%)
30	SO4	u	201	-	4,4,4	0.24	0	6,6,6	0.07	0
31	BCT	a	618	22	3,3,3	0.59	0	2,3,3	0.74	0
26	BCR	H	101	-	41,41,41	0.65	0	56,56,56	2.05	13 (23%)
25	CLA	D	403	37	69,73,73	1.61	8 (11%)	82,113,113	1.23	9 (10%)
26	BCR	C	514	-	41,41,41	0.67	0	56,56,56	1.94	14 (25%)
26	BCR	b	619	-	41,41,41	0.71	0	56,56,56	1.94	13 (23%)
25	CLA	D	404	-	69,73,73	1.60	8 (11%)	82,113,113	1.18	8 (9%)
28	SQD	a	613	-	52,54,54	1.11	3 (5%)	62,65,65	1.19	7 (11%)
34	PHO	d	402	-	58,69,69	1.32	6 (10%)	55,99,99	1.70	4 (7%)
35	HEM	E	102	5,6	50,50,50	1.38	6 (12%)	67,82,82	0.99	2 (2%)
25	CLA	C	512	-	69,73,73	1.57	8 (11%)	82,113,113	1.15	8 (9%)
34	PHO	a	609	-	58,69,69	1.34	6 (10%)	55,99,99	1.64	3 (5%)
23	LMG	d	408	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)
25	CLA	B	608	-	69,73,73	1.59	8 (11%)	82,113,113	1.16	9 (10%)
25	CLA	A	607	-	69,73,73	1.61	8 (11%)	82,113,113	1.17	9 (10%)
25	CLA	B	601	-	69,73,73	1.61	9 (13%)	82,113,113	1.16	8 (9%)
25	CLA	B	610	-	69,73,73	1.62	8 (11%)	82,113,113	1.21	9 (10%)
25	CLA	A	608	-	69,73,73	1.60	8 (11%)	82,113,113	1.17	8 (9%)
25	CLA	D	405	-	69,73,73	1.59	9 (13%)	82,113,113	1.16	9 (10%)
26	BCR	z	101	-	41,41,41	0.68	0	56,56,56	1.87	10 (17%)
36	HEC	V	201	16	46,50,50	1.35	4 (8%)	58,82,82	1.67	3 (5%)
25	CLA	c	512	-	69,73,73	1.58	8 (11%)	82,113,113	1.14	8 (9%)
25	CLA	c	505	-	69,73,73	1.61	8 (11%)	82,113,113	1.17	7 (8%)
25	CLA	b	611	-	69,73,73	1.60	8 (11%)	82,113,113	1.19	9 (10%)
25	CLA	B	613	-	69,73,73	1.58	7 (10%)	82,113,113	1.18	9 (10%)
25	CLA	C	506	-	69,73,73	1.61	7 (10%)	82,113,113	1.17	9 (10%)
25	CLA	B	616	-	69,73,73	1.58	9 (13%)	82,113,113	1.28	9 (10%)
25	CLA	C	511	3	69,73,73	1.57	7 (10%)	82,113,113	1.15	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	a	615	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
33	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	0.91	3 (3%)
25	CLA	b	604	-	69,73,73	1.57	7 (10%)	82,113,113	1.18	10 (12%)
25	CLA	d	401	-	69,73,73	1.61	8 (11%)	82,113,113	1.18	8 (9%)
25	CLA	c	506	-	69,73,73	1.61	9 (13%)	82,113,113	1.19	8 (9%)
34	PHO	D	402	-	58,69,69	1.31	6 (10%)	55,99,99	1.66	4 (7%)
26	BCR	d	404	-	41,41,41	0.73	0	56,56,56	2.04	13 (23%)
25	CLA	c	509	-	69,73,73	1.58	8 (11%)	82,113,113	1.16	9 (10%)
28	SQD	A	611	-	52,54,54	1.10	3 (5%)	62,65,65	1.21	6 (9%)
26	BCR	b	617	-	41,41,41	0.67	0	56,56,56	2.03	15 (26%)
26	BCR	C	522	-	41,41,41	0.64	0	56,56,56	2.08	15 (26%)
26	BCR	a	611	-	41,41,41	0.68	0	56,56,56	1.80	12 (21%)
29	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.10	3 (6%)
25	CLA	b	603	-	69,73,73	1.60	8 (11%)	82,113,113	1.18	9 (10%)
36	HEC	v	201	16	46,50,50	1.36	4 (8%)	58,82,82	1.72	3 (5%)
25	CLA	b	606	-	69,73,73	1.59	8 (11%)	82,113,113	1.17	7 (8%)
30	SO4	U	201	-	4,4,4	0.24	0	6,6,6	0.08	0
23	LMG	c	518	-	51,51,55	0.94	2 (3%)	59,59,63	0.98	3 (5%)
26	BCR	B	619	-	41,41,41	0.74	0	56,56,56	1.94	16 (28%)
25	CLA	C	510	-	69,73,73	1.60	7 (10%)	82,113,113	1.21	9 (10%)
25	CLA	a	610	-	69,73,73	1.60	8 (11%)	82,113,113	1.18	9 (10%)
25	CLA	b	605	-	69,73,73	1.59	8 (11%)	82,113,113	1.19	8 (9%)
25	CLA	B	612	-	69,73,73	1.59	8 (11%)	82,113,113	1.17	9 (10%)
25	CLA	c	504	-	69,73,73	1.59	8 (11%)	82,113,113	1.16	9 (10%)
25	CLA	B	606	-	69,73,73	1.59	8 (11%)	82,113,113	1.20	9 (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
23	LMG	A	612	-	-	11/46/66/70	0/1/1/1
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	CLA	b	613	-	1/1/15/20	1/39/115/115	-
23	LMG	C	519	-	-	9/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	D	407	-	-	8/53/73/73	0/1/1/1
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
25	CLA	C	507	-	1/1/15/20	5/39/115/115	-
25	CLA	C	504	-	1/1/15/20	6/39/115/115	-
33	DGD	C	517	-	-	12/51/91/95	0/2/2/2
25	CLA	b	601	-	1/1/15/20	7/39/115/115	-
25	CLA	d	403	-	1/1/15/20	2/39/115/115	-
26	BCR	k	102	-	-	4/29/63/63	0/2/2/2
23	LMG	B	620	-	-	4/46/66/70	0/1/1/1
23	LMG	a	603	-	-	11/46/66/70	0/1/1/1
25	CLA	c	513	-	1/1/15/20	3/39/115/115	-
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
23	LMG	A	603	-	-	15/46/66/70	0/1/1/1
23	LMG	C	521	-	-	17/46/66/70	0/1/1/1
28	SQD	L	103	-	-	18/49/69/69	0/1/1/1
25	CLA	c	503	-	1/1/15/20	4/39/115/115	-
33	DGD	C	516	-	-	8/51/91/95	0/2/2/2
34	PHO	D	401	-	-	5/37/103/103	0/5/6/6
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
29	LHG	d	407	-	-	16/53/53/53	-
25	CLA	b	615	-	1/1/15/20	4/39/115/115	-
35	HEM	e	101	5,6	-	7/14/54/54	-
25	CLA	B	609	-	1/1/15/20	5/39/115/115	-
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	CLA	C	505	-	1/1/15/20	2/39/115/115	-
25	CLA	b	608	-	1/1/15/20	2/39/115/115	-
25	CLA	C	501	-	1/1/15/20	0/39/115/115	-
23	LMG	b	620	-	-	4/46/66/70	0/1/1/1
25	CLA	b	616	-	1/1/15/20	4/39/115/115	-
29	LHG	D	408	-	-	5/53/53/53	-
25	CLA	b	607	37	1/1/15/20	5/39/115/115	-
25	CLA	b	610	37	1/1/15/20	3/39/115/115	-
23	LMG	c	520	-	-	13/46/66/70	0/1/1/1
25	CLA	C	508	-	1/1/15/20	0/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMG	B	624	-	-	10/46/66/70	0/1/1/1
25	CLA	a	606	-	1/1/15/20	1/39/115/115	-
25	CLA	c	501	-	1/1/15/20	2/39/115/115	-
28	SQD	F	101	-	-	5/38/58/69	0/1/1/1
27	PL9	A	610	-	-	8/53/73/73	0/1/1/1
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	CLA	c	507	-	1/1/15/20	7/39/115/115	-
25	CLA	A	606	-	1/1/15/20	1/39/115/115	-
26	BCR	A	609	-	-	0/29/63/63	0/2/2/2
25	CLA	B	611	-	1/1/15/20	1/39/115/115	-
25	CLA	b	602	-	1/1/15/20	2/39/115/115	-
23	LMG	b	624	-	-	9/46/66/70	0/1/1/1
33	DGD	h	102	-	-	7/51/91/95	0/2/2/2
25	CLA	a	608	-	1/1/15/20	2/39/115/115	-
26	BCR	c	521	-	-	0/29/63/63	0/2/2/2
25	CLA	b	612	-	1/1/15/20	0/39/115/115	-
25	CLA	B	605	-	1/1/15/20	6/39/115/115	-
25	CLA	B	614	-	1/1/15/20	7/39/115/115	-
25	CLA	B	602	-	1/1/15/20	8/39/115/115	-
33	DGD	c	517	-	-	1/51/91/95	0/2/2/2
29	LHG	a	616	-	-	8/46/46/53	-
25	CLA	c	508	-	1/1/15/20	0/39/115/115	-
29	LHG	l	101	-	-	17/53/53/53	-
25	CLA	B	615	-	1/1/15/20	5/39/115/115	-
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
25	CLA	b	614	-	1/1/15/20	10/39/115/115	-
25	CLA	C	513	-	1/1/15/20	2/39/115/115	-
25	CLA	b	609	-	1/1/15/20	4/39/115/115	-
27	PL9	d	405	-	-	8/53/73/73	0/1/1/1
33	DGD	c	515	-	-	8/51/91/95	0/2/2/2
33	DGD	H	102	-	-	5/51/91/95	0/2/2/2
25	CLA	B	603	-	1/1/15/20	1/39/115/115	-
25	CLA	B	607	37	1/1/15/20	7/39/115/115	-
25	CLA	C	503	-	1/1/15/20	1/39/115/115	-
25	CLA	c	511	3	1/1/15/20	0/39/115/115	-
33	DGD	c	516	-	-	8/51/91/95	0/2/2/2
28	SQD	f	101	-	-	11/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	t	102	-	-	8/29/63/63	0/2/2/2
29	LHG	A	614	-	-	4/53/53/53	-
25	CLA	C	502	-	1/1/15/20	3/39/115/115	-
25	CLA	C	509	-	1/1/15/20	0/39/115/115	-
29	LHG	A	613	-	-	6/53/53/53	-
23	LMG	a	614	-	-	5/46/66/70	0/1/1/1
25	CLA	c	502	-	1/1/15/20	2/39/115/115	-
25	CLA	c	510	-	1/1/15/20	4/39/115/115	-
29	LHG	L	102	-	-	15/53/53/53	-
27	PL9	a	612	-	-	7/53/73/73	0/1/1/1
23	LMG	D	409	-	-	3/46/66/70	0/1/1/1
29	LHG	d	406	-	-	4/53/53/53	-
25	CLA	B	604	-	1/1/15/20	0/39/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
28	SQD	L	101	-	-	16/49/69/69	0/1/1/1
25	CLA	a	607	37	1/1/15/20	3/39/115/115	-
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
25	CLA	D	403	37	1/1/15/20	3/39/115/115	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	CLA	D	404	-	1/1/15/20	2/39/115/115	-
28	SQD	a	613	-	-	7/49/69/69	0/1/1/1
34	PHO	d	402	-	-	1/37/103/103	0/5/6/6
35	HEM	E	102	5,6	-	8/14/54/54	-
25	CLA	C	512	-	1/1/15/20	4/39/115/115	-
34	PHO	a	609	-	-	6/37/103/103	0/5/6/6
23	LMG	d	408	-	-	3/46/66/70	0/1/1/1
25	CLA	B	608	-	1/1/15/20	1/39/115/115	-
25	CLA	A	607	-	1/1/15/20	3/39/115/115	-
25	CLA	B	610	-	1/1/15/20	3/39/115/115	-
25	CLA	B	601	-	1/1/15/20	8/39/115/115	-
25	CLA	A	608	-	1/1/15/20	6/39/115/115	-
25	CLA	D	405	-	1/1/15/20	2/39/115/115	-
26	BCR	z	101	-	-	1/29/63/63	0/2/2/2
36	HEC	V	201	16	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	512	-	1/1/15/20	6/39/115/115	-
25	CLA	c	505	-	1/1/15/20	2/39/115/115	-
25	CLA	b	611	-	1/1/15/20	2/39/115/115	-
25	CLA	B	613	-	1/1/15/20	1/39/115/115	-
25	CLA	C	506	-	1/1/15/20	8/39/115/115	-
25	CLA	B	616	-	1/1/15/20	2/39/115/115	-
25	CLA	C	511	3	1/1/15/20	0/39/115/115	-
29	LHG	a	615	-	-	7/53/53/53	-
33	DGD	C	518	-	-	4/51/91/95	0/2/2/2
25	CLA	b	604	-	1/1/15/20	3/39/115/115	-
25	CLA	d	401	-	1/1/15/20	0/39/115/115	-
25	CLA	c	506	-	1/1/15/20	2/39/115/115	-
34	PHO	D	402	-	-	1/37/103/103	0/5/6/6
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	1/39/115/115	-
28	SQD	A	611	-	-	5/49/69/69	0/1/1/1
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
26	BCR	C	522	-	-	0/29/63/63	0/2/2/2
26	BCR	a	611	-	-	0/29/63/63	0/2/2/2
29	LHG	E	101	-	-	9/46/46/53	-
25	CLA	b	603	-	1/1/15/20	4/39/115/115	-
36	HEC	v	201	16	-	3/14/54/54	-
25	CLA	b	606	-	1/1/15/20	4/39/115/115	-
23	LMG	c	518	-	-	8/46/66/70	0/1/1/1
26	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	CLA	C	510	-	1/1/15/20	3/39/115/115	-
25	CLA	a	610	-	1/1/15/20	6/39/115/115	-
25	CLA	b	605	-	1/1/15/20	4/39/115/115	-
25	CLA	B	612	-	1/1/15/20	0/39/115/115	-
25	CLA	c	504	-	1/1/15/20	3/39/115/115	-
25	CLA	B	606	-	1/1/15/20	3/39/115/115	-

All (691) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	MG-NB	-6.50	1.92	2.05
25	C	506	CLA	MG-NB	-6.47	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	607	CLA	MG-NB	-6.47	1.93	2.05
25	A	607	CLA	MG-NB	-6.44	1.93	2.05
25	C	504	CLA	MG-NB	-6.43	1.93	2.05
25	D	403	CLA	MG-NB	-6.39	1.93	2.05
25	c	506	CLA	MG-NB	-6.36	1.93	2.05
25	b	611	CLA	MG-NB	-6.36	1.93	2.05
25	a	608	CLA	MG-ND	-6.36	1.93	2.05
25	d	403	CLA	MG-NB	-6.34	1.93	2.05
25	b	610	CLA	MG-NB	-6.34	1.93	2.05
25	C	501	CLA	MG-NB	-6.33	1.93	2.05
25	B	612	CLA	MG-NB	-6.32	1.93	2.05
25	D	405	CLA	MG-NB	-6.32	1.93	2.05
25	B	601	CLA	MG-NB	-6.32	1.93	2.05
25	C	509	CLA	MG-NB	-6.32	1.93	2.05
25	c	504	CLA	MG-NB	-6.30	1.93	2.05
25	a	608	CLA	MG-NB	-6.30	1.93	2.05
25	A	606	CLA	MG-NB	-6.30	1.93	2.05
25	B	610	CLA	MG-NB	-6.30	1.93	2.05
25	c	510	CLA	MG-NB	-6.30	1.93	2.05
25	c	505	CLA	MG-NB	-6.28	1.93	2.05
25	C	505	CLA	MG-NB	-6.27	1.93	2.05
25	d	401	CLA	MG-NB	-6.27	1.93	2.05
25	C	510	CLA	MG-ND	-6.27	1.93	2.05
25	C	502	CLA	MG-ND	-6.27	1.93	2.05
25	b	601	CLA	MG-NB	-6.27	1.93	2.05
25	C	510	CLA	MG-NB	-6.26	1.93	2.05
25	C	501	CLA	MG-ND	-6.26	1.93	2.05
25	D	404	CLA	C4B-NB	6.25	1.46	1.37
25	B	602	CLA	MG-NB	-6.25	1.93	2.05
25	b	609	CLA	MG-NB	-6.24	1.93	2.05
25	b	612	CLA	MG-NB	-6.24	1.93	2.05
25	B	608	CLA	MG-NB	-6.24	1.93	2.05
25	b	603	CLA	MG-NB	-6.24	1.93	2.05
25	c	509	CLA	MG-NB	-6.23	1.93	2.05
25	c	511	CLA	MG-NB	-6.23	1.93	2.05
25	b	613	CLA	MG-NB	-6.23	1.93	2.05
25	B	609	CLA	C4B-NB	6.23	1.46	1.37
25	C	504	CLA	MG-ND	-6.23	1.93	2.05
25	A	608	CLA	MG-NB	-6.22	1.93	2.05
25	B	613	CLA	MG-NB	-6.22	1.93	2.05
25	b	613	CLA	MG-ND	-6.21	1.93	2.05
25	c	502	CLA	MG-ND	-6.21	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	501	CLA	MG-NB	-6.21	1.93	2.05
25	c	513	CLA	MG-ND	-6.21	1.93	2.05
25	b	609	CLA	C4B-NB	6.21	1.46	1.37
25	c	503	CLA	C4B-NB	6.21	1.46	1.37
25	b	614	CLA	MG-NB	-6.21	1.93	2.05
25	C	507	CLA	MG-NB	-6.20	1.93	2.05
25	B	613	CLA	MG-ND	-6.20	1.93	2.05
25	B	609	CLA	MG-NB	-6.20	1.93	2.05
25	b	608	CLA	MG-NB	-6.19	1.93	2.05
25	b	607	CLA	MG-NB	-6.19	1.93	2.05
25	c	502	CLA	MG-NB	-6.19	1.93	2.05
25	c	513	CLA	MG-NB	-6.19	1.93	2.05
25	b	608	CLA	MG-ND	-6.19	1.93	2.05
25	C	502	CLA	MG-NB	-6.18	1.93	2.05
25	B	607	CLA	MG-ND	-6.17	1.93	2.05
34	D	401	PHO	C3B-C4B	6.17	1.47	1.41
25	B	610	CLA	MG-ND	-6.17	1.93	2.05
25	C	513	CLA	MG-ND	-6.17	1.93	2.05
25	a	610	CLA	MG-NB	-6.17	1.93	2.05
25	B	615	CLA	MG-NB	-6.16	1.93	2.05
25	b	603	CLA	C4B-NB	6.16	1.46	1.37
25	B	611	CLA	MG-ND	-6.16	1.93	2.05
25	B	614	CLA	C4B-NB	6.15	1.45	1.37
25	B	603	CLA	MG-NB	-6.15	1.93	2.05
25	B	611	CLA	MG-NB	-6.13	1.93	2.05
25	B	607	CLA	MG-NB	-6.13	1.93	2.05
25	B	614	CLA	MG-NB	-6.13	1.93	2.05
25	b	612	CLA	MG-ND	-6.12	1.93	2.05
25	C	509	CLA	MG-ND	-6.12	1.93	2.05
25	C	511	CLA	MG-NB	-6.12	1.93	2.05
25	A	607	CLA	MG-ND	-6.12	1.93	2.05
25	c	501	CLA	MG-ND	-6.12	1.93	2.05
25	C	508	CLA	MG-NB	-6.12	1.93	2.05
25	b	604	CLA	MG-ND	-6.11	1.93	2.05
25	b	616	CLA	MG-NB	-6.11	1.93	2.05
25	b	605	CLA	C4B-NB	6.11	1.45	1.37
25	b	606	CLA	C4B-NB	6.11	1.45	1.37
25	c	502	CLA	C4B-NB	6.11	1.45	1.37
25	b	615	CLA	C4B-NB	6.10	1.45	1.37
25	B	606	CLA	MG-ND	-6.10	1.93	2.05
25	c	507	CLA	MG-NB	-6.10	1.93	2.05
25	B	601	CLA	MG-ND	-6.10	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	607	CLA	MG-ND	-6.10	1.93	2.05
25	c	504	CLA	MG-ND	-6.10	1.93	2.05
25	C	508	CLA	MG-ND	-6.10	1.93	2.05
25	C	511	CLA	MG-ND	-6.10	1.93	2.05
25	C	513	CLA	MG-NB	-6.10	1.93	2.05
25	B	604	CLA	MG-ND	-6.09	1.93	2.05
25	c	509	CLA	MG-ND	-6.09	1.93	2.05
25	c	511	CLA	MG-ND	-6.09	1.93	2.05
25	c	510	CLA	MG-ND	-6.09	1.93	2.05
25	D	404	CLA	MG-NB	-6.08	1.93	2.05
25	D	403	CLA	MG-ND	-6.07	1.93	2.05
25	a	610	CLA	C4B-NB	6.07	1.45	1.37
25	b	606	CLA	MG-NB	-6.07	1.93	2.05
25	b	605	CLA	MG-ND	-6.07	1.93	2.05
25	B	610	CLA	C4B-NB	6.07	1.45	1.37
25	b	604	CLA	C4B-NB	6.06	1.45	1.37
25	c	512	CLA	MG-NB	-6.06	1.93	2.05
25	C	503	CLA	C4B-NB	6.06	1.45	1.37
25	b	601	CLA	MG-ND	-6.06	1.93	2.05
25	B	605	CLA	C4B-NB	6.05	1.45	1.37
25	b	603	CLA	MG-ND	-6.05	1.93	2.05
25	c	506	CLA	C4B-NB	6.05	1.45	1.37
25	B	612	CLA	MG-ND	-6.05	1.93	2.05
25	c	506	CLA	MG-ND	-6.04	1.93	2.05
25	c	508	CLA	MG-NB	-6.04	1.93	2.05
34	D	402	PHO	C3B-C4B	6.04	1.47	1.41
25	c	505	CLA	MG-ND	-6.04	1.93	2.05
25	B	603	CLA	MG-ND	-6.04	1.93	2.05
25	b	606	CLA	MG-ND	-6.04	1.93	2.05
25	b	614	CLA	C4B-NB	6.03	1.45	1.37
25	a	606	CLA	MG-ND	-6.03	1.93	2.05
25	c	512	CLA	MG-ND	-6.03	1.93	2.05
25	b	610	CLA	C4B-NB	6.03	1.45	1.37
25	d	401	CLA	MG-ND	-6.03	1.93	2.05
25	C	506	CLA	C4B-NB	6.03	1.45	1.37
25	c	505	CLA	C4B-NB	6.02	1.45	1.37
25	B	604	CLA	MG-NB	-6.02	1.93	2.05
25	B	606	CLA	MG-NB	-6.02	1.93	2.05
25	d	403	CLA	MG-ND	-6.02	1.93	2.05
25	C	513	CLA	C4B-NB	6.02	1.45	1.37
34	d	402	PHO	C3B-C4B	6.02	1.47	1.41
25	B	616	CLA	MG-NB	-6.02	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	607	CLA	MG-ND	-6.02	1.93	2.05
25	b	601	CLA	C4B-NB	6.02	1.45	1.37
25	B	611	CLA	C4B-NB	6.02	1.45	1.37
25	d	401	CLA	C4B-NB	6.01	1.45	1.37
25	b	610	CLA	MG-ND	-6.01	1.93	2.05
25	C	506	CLA	MG-ND	-6.01	1.93	2.05
25	C	512	CLA	C4B-NB	6.01	1.45	1.37
25	B	606	CLA	C4B-NB	6.00	1.45	1.37
25	C	512	CLA	MG-NB	-6.00	1.93	2.05
25	b	602	CLA	MG-ND	-6.00	1.93	2.05
25	C	503	CLA	MG-NB	-6.00	1.93	2.05
25	c	508	CLA	C4B-NB	6.00	1.45	1.37
25	b	611	CLA	MG-ND	-6.00	1.93	2.05
25	B	601	CLA	C4B-NB	6.00	1.45	1.37
25	b	611	CLA	C4B-NB	5.99	1.45	1.37
25	c	512	CLA	C4B-NB	5.98	1.45	1.37
25	c	503	CLA	MG-NB	-5.98	1.93	2.05
25	C	503	CLA	MG-ND	-5.98	1.93	2.05
25	B	608	CLA	MG-ND	-5.98	1.93	2.05
25	c	507	CLA	MG-ND	-5.98	1.93	2.05
25	b	608	CLA	C4B-NB	5.97	1.45	1.37
25	b	616	CLA	C4B-NB	5.97	1.45	1.37
34	a	609	PHO	C3B-C4B	5.97	1.47	1.41
25	b	609	CLA	MG-ND	-5.97	1.94	2.05
25	C	502	CLA	C4B-NB	5.97	1.45	1.37
25	B	609	CLA	MG-ND	-5.97	1.94	2.05
25	C	507	CLA	MG-ND	-5.97	1.94	2.05
25	A	608	CLA	MG-ND	-5.96	1.94	2.05
25	a	606	CLA	MG-NB	-5.96	1.94	2.05
25	b	605	CLA	MG-NB	-5.96	1.94	2.05
25	C	505	CLA	C4B-NB	5.96	1.45	1.37
25	B	604	CLA	C4B-NB	5.95	1.45	1.37
25	b	607	CLA	C4B-NB	5.95	1.45	1.37
25	c	507	CLA	C4B-NB	5.95	1.45	1.37
25	B	603	CLA	C4B-NB	5.94	1.45	1.37
25	B	605	CLA	MG-ND	-5.94	1.94	2.05
25	b	616	CLA	MG-ND	-5.94	1.94	2.05
25	B	605	CLA	MG-NB	-5.94	1.94	2.05
25	A	608	CLA	C4B-NB	5.94	1.45	1.37
25	b	615	CLA	MG-NB	-5.93	1.94	2.05
25	C	508	CLA	C4B-NB	5.93	1.45	1.37
25	c	501	CLA	C4B-NB	5.93	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	C4B-NB	5.93	1.45	1.37
25	A	607	CLA	C4B-NB	5.93	1.45	1.37
25	c	511	CLA	C4B-NB	5.93	1.45	1.37
25	C	511	CLA	C4B-NB	5.92	1.45	1.37
25	c	508	CLA	MG-ND	-5.92	1.94	2.05
25	A	606	CLA	MG-ND	-5.92	1.94	2.05
25	d	403	CLA	C4B-NB	5.92	1.45	1.37
25	D	404	CLA	MG-ND	-5.91	1.94	2.05
25	B	616	CLA	MG-ND	-5.91	1.94	2.05
25	B	607	CLA	C4B-NB	5.91	1.45	1.37
25	B	616	CLA	C4B-NB	5.91	1.45	1.37
25	B	614	CLA	MG-ND	-5.91	1.94	2.05
25	b	604	CLA	MG-NB	-5.91	1.94	2.05
25	B	608	CLA	C4B-NB	5.91	1.45	1.37
25	B	602	CLA	C4B-NB	5.91	1.45	1.37
25	D	405	CLA	C4B-NB	5.90	1.45	1.37
25	b	614	CLA	MG-ND	-5.90	1.94	2.05
25	C	505	CLA	MG-ND	-5.89	1.94	2.05
25	C	512	CLA	MG-ND	-5.89	1.94	2.05
25	C	507	CLA	C4B-NB	5.88	1.45	1.37
25	b	612	CLA	C4B-NB	5.88	1.45	1.37
25	b	613	CLA	C4B-NB	5.87	1.45	1.37
25	c	513	CLA	C4B-NB	5.87	1.45	1.37
25	D	403	CLA	C4B-NB	5.87	1.45	1.37
25	D	405	CLA	MG-ND	-5.86	1.94	2.05
25	b	615	CLA	MG-ND	-5.86	1.94	2.05
25	b	602	CLA	C4B-NB	5.86	1.45	1.37
25	c	503	CLA	MG-ND	-5.85	1.94	2.05
25	B	615	CLA	C4B-NB	5.85	1.45	1.37
25	a	610	CLA	MG-ND	-5.84	1.94	2.05
25	c	504	CLA	C4B-NB	5.84	1.45	1.37
25	B	613	CLA	C4B-NB	5.83	1.45	1.37
25	C	510	CLA	C4B-NB	5.82	1.45	1.37
25	c	509	CLA	C4B-NB	5.80	1.45	1.37
25	a	607	CLA	C4B-NB	5.78	1.45	1.37
25	c	510	CLA	C4B-NB	5.77	1.45	1.37
25	A	606	CLA	C4B-NB	5.76	1.45	1.37
25	C	504	CLA	C4B-NB	5.76	1.45	1.37
25	B	602	CLA	MG-ND	-5.74	1.94	2.05
25	a	608	CLA	C4B-NB	5.74	1.45	1.37
25	C	509	CLA	C4B-NB	5.73	1.45	1.37
25	B	615	CLA	MG-ND	-5.71	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	606	CLA	C4B-NB	5.70	1.45	1.37
25	C	501	CLA	C4B-NB	5.61	1.45	1.37
34	D	402	PHO	C1B-C2B	5.38	1.45	1.39
34	d	402	PHO	C1B-C2B	5.37	1.45	1.39
34	D	401	PHO	C1B-C2B	5.28	1.45	1.39
34	a	609	PHO	C1B-C2B	5.21	1.45	1.39
36	V	201	HEC	CAB-C3B	4.83	1.50	1.35
28	L	101	SQD	O8-S	4.82	1.65	1.47
36	v	201	HEC	CAB-C3B	4.75	1.50	1.35
28	a	613	SQD	O8-S	4.45	1.64	1.47
28	L	103	SQD	O8-S	4.44	1.63	1.47
28	f	101	SQD	O8-S	4.44	1.63	1.47
28	A	611	SQD	O8-S	4.42	1.63	1.47
36	v	201	HEC	CAC-C3C	4.41	1.49	1.35
28	F	101	SQD	O8-S	4.39	1.63	1.47
28	f	101	SQD	O48-C23	4.34	1.46	1.33
23	C	519	LMG	O8-C28	4.33	1.46	1.33
23	D	409	LMG	O8-C28	4.33	1.46	1.33
23	a	603	LMG	O8-C28	4.32	1.46	1.33
23	d	408	LMG	O8-C28	4.32	1.45	1.33
29	l	101	LHG	O8-C23	4.31	1.45	1.33
23	c	520	LMG	O8-C28	4.30	1.45	1.33
23	A	603	LMG	O8-C28	4.30	1.45	1.33
36	V	201	HEC	CAC-C3C	4.30	1.48	1.35
35	e	101	HEM	FE-ND	4.29	2.08	1.94
23	B	620	LMG	O8-C28	4.29	1.45	1.33
23	C	521	LMG	O8-C28	4.29	1.45	1.33
23	c	518	LMG	O8-C28	4.28	1.45	1.33
23	b	620	LMG	O8-C28	4.28	1.45	1.33
29	A	614	LHG	O8-C23	4.28	1.45	1.33
23	A	612	LMG	O8-C28	4.27	1.45	1.33
23	B	624	LMG	O8-C28	4.27	1.45	1.33
33	c	515	DGD	O1G-C1A	4.27	1.45	1.33
28	L	101	SQD	O47-C7	4.26	1.46	1.34
33	H	102	DGD	O1G-C1A	4.26	1.45	1.33
28	a	613	SQD	O48-C23	4.25	1.45	1.33
23	b	624	LMG	O8-C28	4.25	1.45	1.33
29	E	101	LHG	O8-C23	4.25	1.45	1.33
29	d	406	LHG	O8-C23	4.25	1.45	1.33
35	E	102	HEM	FE-ND	4.25	2.08	1.94
29	d	407	LHG	O8-C23	4.24	1.45	1.33
33	c	516	DGD	O1G-C1A	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	517	DGD	O1G-C1A	4.24	1.45	1.33
33	C	518	DGD	O1G-C1A	4.23	1.45	1.33
28	L	101	SQD	O48-C23	4.23	1.45	1.33
29	a	616	LHG	O8-C23	4.22	1.45	1.33
23	a	614	LMG	O8-C28	4.22	1.45	1.33
28	L	103	SQD	O48-C23	4.22	1.45	1.33
33	c	517	DGD	O1G-C1A	4.22	1.45	1.33
33	C	516	DGD	O1G-C1A	4.21	1.45	1.33
29	L	102	LHG	O8-C23	4.21	1.45	1.33
29	a	615	LHG	O8-C23	4.21	1.45	1.33
29	D	408	LHG	O8-C23	4.18	1.45	1.33
29	A	613	LHG	O8-C23	4.18	1.45	1.33
28	A	611	SQD	O47-C7	4.18	1.46	1.34
23	D	409	LMG	O7-C10	4.18	1.46	1.34
28	f	101	SQD	O47-C7	4.17	1.46	1.34
23	B	620	LMG	O7-C10	4.17	1.46	1.34
28	L	103	SQD	O47-C7	4.17	1.46	1.34
28	A	611	SQD	O48-C23	4.17	1.45	1.33
23	C	521	LMG	O7-C10	4.17	1.46	1.34
33	H	102	DGD	O2G-C1B	4.16	1.46	1.34
29	E	101	LHG	O7-C7	4.16	1.46	1.34
29	A	614	LHG	O7-C7	4.16	1.46	1.34
23	c	520	LMG	O7-C10	4.15	1.46	1.34
28	F	101	SQD	O47-C7	4.15	1.46	1.34
33	h	102	DGD	O2G-C1B	4.15	1.46	1.34
33	c	516	DGD	O2G-C1B	4.14	1.46	1.34
25	c	505	CLA	MG-NC	-4.14	1.96	2.06
23	d	408	LMG	O7-C10	4.14	1.46	1.34
33	C	516	DGD	O2G-C1B	4.13	1.45	1.34
23	b	624	LMG	O7-C10	4.13	1.45	1.34
23	b	620	LMG	O7-C10	4.13	1.45	1.34
23	C	519	LMG	O7-C10	4.12	1.45	1.34
29	d	407	LHG	O7-C7	4.12	1.45	1.34
28	F	101	SQD	O48-C23	4.11	1.45	1.33
23	A	603	LMG	O7-C10	4.11	1.45	1.34
33	C	517	DGD	O2G-C1B	4.11	1.45	1.34
33	c	517	DGD	O2G-C1B	4.11	1.45	1.34
33	C	518	DGD	O2G-C1B	4.10	1.45	1.34
29	l	101	LHG	O7-C7	4.09	1.45	1.34
28	a	613	SQD	O47-C7	4.09	1.45	1.34
25	a	607	CLA	MG-NC	-4.09	1.96	2.06
23	A	612	LMG	O7-C10	4.08	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	603	LMG	O7-C10	4.08	1.45	1.34
23	c	518	LMG	O7-C10	4.08	1.45	1.34
23	B	624	LMG	O7-C10	4.08	1.45	1.34
33	h	102	DGD	O1G-C1A	4.07	1.45	1.33
33	c	515	DGD	O2G-C1B	4.07	1.45	1.34
29	a	616	LHG	O7-C7	4.07	1.45	1.34
29	a	615	LHG	O7-C7	4.06	1.45	1.34
29	L	102	LHG	O7-C7	4.05	1.45	1.34
25	b	602	CLA	MG-NC	-4.05	1.96	2.06
29	d	406	LHG	O7-C7	4.05	1.45	1.34
25	B	602	CLA	MG-NC	-4.04	1.96	2.06
23	a	614	LMG	O7-C10	4.03	1.45	1.34
29	D	408	LHG	O7-C7	3.99	1.45	1.34
29	A	613	LHG	O7-C7	3.98	1.45	1.34
25	d	401	CLA	MG-NC	-3.96	1.96	2.06
25	b	616	CLA	MG-NC	-3.95	1.96	2.06
25	D	403	CLA	MG-NC	-3.95	1.96	2.06
25	C	505	CLA	MG-NC	-3.94	1.96	2.06
25	B	616	CLA	MG-NC	-3.91	1.97	2.06
25	D	404	CLA	MG-NC	-3.91	1.97	2.06
25	A	606	CLA	MG-NC	-3.90	1.97	2.06
25	b	608	CLA	MG-NC	-3.88	1.97	2.06
25	c	506	CLA	MG-NC	-3.85	1.97	2.06
25	A	607	CLA	MG-NC	-3.84	1.97	2.06
25	b	614	CLA	MG-NC	-3.84	1.97	2.06
25	a	610	CLA	MG-NC	-3.84	1.97	2.06
25	B	610	CLA	MG-NC	-3.84	1.97	2.06
25	B	614	CLA	MG-NC	-3.82	1.97	2.06
25	B	608	CLA	MG-NC	-3.81	1.97	2.06
25	B	603	CLA	MG-NC	-3.81	1.97	2.06
25	C	504	CLA	MG-NC	-3.81	1.97	2.06
25	a	606	CLA	MG-NC	-3.81	1.97	2.06
25	c	508	CLA	MG-NC	-3.79	1.97	2.06
25	A	608	CLA	MG-NC	-3.79	1.97	2.06
25	b	610	CLA	MG-NC	-3.79	1.97	2.06
25	B	606	CLA	MG-NC	-3.79	1.97	2.06
25	C	508	CLA	MG-NC	-3.79	1.97	2.06
25	C	506	CLA	MG-NC	-3.78	1.97	2.06
25	b	607	CLA	MG-NC	-3.78	1.97	2.06
25	B	607	CLA	MG-NC	-3.76	1.97	2.06
25	b	606	CLA	MG-NC	-3.76	1.97	2.06
25	c	504	CLA	MG-NC	-3.76	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	MG-NC	-3.76	1.97	2.06
25	B	601	CLA	MG-NC	-3.75	1.97	2.06
25	c	513	CLA	MG-NC	-3.74	1.97	2.06
25	b	601	CLA	MG-NC	-3.72	1.97	2.06
25	c	510	CLA	MG-NC	-3.71	1.97	2.06
25	a	608	CLA	MG-NC	-3.71	1.97	2.06
25	C	507	CLA	MG-NC	-3.71	1.97	2.06
25	b	615	CLA	MG-NC	-3.70	1.97	2.06
25	b	605	CLA	MG-NC	-3.69	1.97	2.06
25	C	510	CLA	MG-NC	-3.69	1.97	2.06
25	c	507	CLA	MG-NC	-3.68	1.97	2.06
25	B	609	CLA	MG-NC	-3.68	1.97	2.06
25	D	405	CLA	MG-NC	-3.67	1.97	2.06
25	B	615	CLA	MG-NC	-3.67	1.97	2.06
25	B	605	CLA	MG-NC	-3.67	1.97	2.06
25	C	502	CLA	MG-NC	-3.65	1.97	2.06
25	b	611	CLA	MG-NC	-3.65	1.97	2.06
25	B	611	CLA	MG-NC	-3.65	1.97	2.06
25	B	613	CLA	MG-NC	-3.65	1.97	2.06
25	c	512	CLA	MG-NC	-3.64	1.97	2.06
25	C	513	CLA	MG-NC	-3.64	1.97	2.06
25	c	502	CLA	MG-NC	-3.64	1.97	2.06
25	b	609	CLA	MG-NC	-3.63	1.97	2.06
25	B	612	CLA	MG-NC	-3.63	1.97	2.06
25	b	612	CLA	MG-NC	-3.62	1.97	2.06
25	c	501	CLA	MG-NC	-3.62	1.97	2.06
25	C	512	CLA	MG-NC	-3.61	1.97	2.06
25	C	509	CLA	MG-NC	-3.59	1.97	2.06
25	b	604	CLA	MG-NC	-3.58	1.97	2.06
25	a	607	CLA	MG-NA	-3.58	1.97	2.06
25	C	501	CLA	MG-NC	-3.56	1.97	2.06
25	c	509	CLA	MG-NC	-3.56	1.97	2.06
25	B	602	CLA	MG-NA	-3.54	1.97	2.06
25	C	511	CLA	MG-NC	-3.54	1.97	2.06
25	d	403	CLA	MG-NC	-3.54	1.97	2.06
25	c	511	CLA	MG-NC	-3.52	1.97	2.06
35	e	101	HEM	FE-NA	3.51	2.06	1.95
25	b	613	CLA	MG-NC	-3.50	1.98	2.06
25	c	503	CLA	MG-NC	-3.49	1.98	2.06
25	b	602	CLA	MG-NA	-3.48	1.98	2.06
25	B	604	CLA	MG-NC	-3.45	1.98	2.06
35	E	102	HEM	FE-NA	3.44	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	503	CLA	MG-NC	-3.44	1.98	2.06
25	a	608	CLA	MG-NA	-3.43	1.98	2.06
25	D	403	CLA	MG-NA	-3.40	1.98	2.06
34	D	401	PHO	C3B-C2B	-3.40	1.35	1.40
25	A	606	CLA	MG-NA	-3.40	1.98	2.06
25	A	607	CLA	MG-NA	-3.39	1.98	2.06
25	C	504	CLA	MG-NA	-3.38	1.98	2.06
25	a	606	CLA	MG-NA	-3.38	1.98	2.06
25	B	612	CLA	MG-NA	-3.33	1.98	2.06
25	c	504	CLA	MG-NA	-3.33	1.98	2.06
25	B	607	CLA	MG-NA	-3.32	1.98	2.06
25	A	608	CLA	MG-NA	-3.30	1.98	2.06
25	d	401	CLA	MG-NA	-3.30	1.98	2.06
35	E	102	HEM	FE-NB	3.29	2.05	1.94
25	B	608	CLA	MG-NA	-3.27	1.98	2.06
25	b	612	CLA	MG-NA	-3.27	1.98	2.06
25	C	510	CLA	MG-NA	-3.26	1.98	2.06
25	c	513	CLA	MG-NA	-3.26	1.98	2.06
25	D	405	CLA	MG-NA	-3.24	1.98	2.06
35	E	102	HEM	C3D-C2D	3.23	1.43	1.36
35	e	101	HEM	FE-NB	3.23	2.04	1.94
25	b	608	CLA	MG-NA	-3.21	1.98	2.06
25	C	508	CLA	MG-NA	-3.20	1.98	2.06
25	b	614	CLA	MG-NA	-3.20	1.98	2.06
25	c	509	CLA	MG-NA	-3.19	1.98	2.06
25	d	403	CLA	MG-NA	-3.18	1.98	2.06
25	c	505	CLA	MG-NA	-3.17	1.98	2.06
35	e	101	HEM	C3D-C2D	3.17	1.43	1.36
25	c	510	CLA	MG-NA	-3.17	1.98	2.06
25	C	513	CLA	MG-NA	-3.16	1.98	2.06
25	B	610	CLA	MG-NA	-3.16	1.98	2.06
25	B	603	CLA	MG-NA	-3.16	1.98	2.06
25	c	508	CLA	MG-NA	-3.15	1.98	2.06
25	a	610	CLA	MG-NA	-3.14	1.98	2.06
25	B	614	CLA	MG-NA	-3.13	1.98	2.06
25	C	509	CLA	MG-NA	-3.13	1.98	2.06
25	b	610	CLA	MG-NA	-3.13	1.98	2.06
25	C	505	CLA	MG-NA	-3.11	1.98	2.06
25	D	404	CLA	MG-NA	-3.10	1.98	2.06
25	b	607	CLA	MG-NA	-3.10	1.98	2.06
25	c	506	CLA	MG-NA	-3.09	1.98	2.06
25	C	502	CLA	MG-NA	-3.08	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	616	CLA	MG-NA	-3.08	1.99	2.06
25	b	601	CLA	MG-NA	-3.07	1.99	2.06
34	a	609	PHO	C3B-C2B	-3.06	1.36	1.40
25	B	616	CLA	MG-NA	-3.06	1.99	2.06
25	C	507	CLA	MG-NA	-3.05	1.99	2.06
25	C	506	CLA	MG-NA	-3.02	1.99	2.06
25	b	603	CLA	MG-NA	-3.02	1.99	2.06
25	B	601	CLA	MG-NA	-3.01	1.99	2.06
25	c	501	CLA	MG-NA	-3.01	1.99	2.06
25	C	501	CLA	MG-NA	-3.01	1.99	2.06
25	B	605	CLA	MG-NA	-3.00	1.99	2.06
25	b	611	CLA	MG-NA	-3.00	1.99	2.06
25	b	615	CLA	MG-NA	-2.99	1.99	2.06
25	B	611	CLA	MG-NA	-2.99	1.99	2.06
25	c	512	CLA	MG-NA	-2.98	1.99	2.06
25	c	502	CLA	MG-NA	-2.96	1.99	2.06
25	c	507	CLA	MG-NA	-2.95	1.99	2.06
25	C	511	CLA	MG-NA	-2.94	1.99	2.06
25	B	613	CLA	MG-NA	-2.92	1.99	2.06
25	C	512	CLA	MG-NA	-2.90	1.99	2.06
25	B	615	CLA	MG-NA	-2.90	1.99	2.06
25	b	613	CLA	MG-NA	-2.89	1.99	2.06
25	c	511	CLA	MG-NA	-2.88	1.99	2.06
25	b	605	CLA	MG-NA	-2.87	1.99	2.06
25	b	609	CLA	MG-NA	-2.86	1.99	2.06
34	a	609	PHO	C4D-CHA	2.83	1.43	1.39
25	B	606	CLA	MG-NA	-2.81	1.99	2.06
35	e	101	HEM	FE-NC	2.81	2.04	1.95
25	B	604	CLA	MG-NA	-2.78	1.99	2.06
25	b	604	CLA	MG-NA	-2.77	1.99	2.06
35	E	102	HEM	FE-NC	2.76	2.04	1.95
25	b	606	CLA	MG-NA	-2.75	1.99	2.06
27	A	610	PL9	C6-C5	2.74	1.48	1.35
27	a	612	PL9	C6-C5	2.74	1.48	1.35
25	B	609	CLA	MG-NA	-2.73	1.99	2.06
27	d	405	PL9	C6-C5	2.72	1.48	1.35
34	a	609	PHO	C3D-C2D	2.72	1.44	1.39
34	D	402	PHO	C3D-C2D	2.72	1.44	1.39
25	C	503	CLA	MG-NA	-2.71	1.99	2.06
27	D	407	PL9	C6-C5	2.71	1.48	1.35
34	d	402	PHO	C4D-CHA	2.71	1.43	1.39
34	D	401	PHO	C3D-C2D	2.71	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	MG-NA	-2.69	1.99	2.06
34	d	402	PHO	C3D-C2D	2.62	1.44	1.39
25	b	606	CLA	C1D-C2D	-2.57	1.40	1.45
25	b	613	CLA	C1D-C2D	-2.55	1.40	1.45
25	B	612	CLA	C1D-C2D	-2.55	1.40	1.45
25	c	503	CLA	C1D-C2D	-2.54	1.40	1.45
25	c	507	CLA	C1D-C2D	-2.54	1.40	1.45
25	C	507	CLA	C1D-C2D	-2.54	1.40	1.45
25	C	512	CLA	C1D-C2D	-2.53	1.40	1.45
25	b	615	CLA	C1D-C2D	-2.53	1.40	1.45
25	B	604	CLA	C1D-C2D	-2.53	1.40	1.45
25	B	606	CLA	C1D-C2D	-2.53	1.40	1.45
25	C	505	CLA	C1D-C2D	-2.53	1.40	1.45
25	B	615	CLA	C1D-C2D	-2.53	1.40	1.45
34	d	402	PHO	C3B-C2B	-2.52	1.37	1.40
35	E	102	HEM	O2D-CGD	-2.52	1.22	1.30
25	b	604	CLA	C1D-C2D	-2.51	1.40	1.45
36	V	201	HEC	O2D-CGD	-2.51	1.22	1.30
25	b	611	CLA	C1D-C2D	-2.51	1.40	1.45
34	D	401	PHO	C4D-CHA	2.51	1.43	1.39
25	B	613	CLA	C1D-C2D	-2.50	1.40	1.45
25	b	612	CLA	C1D-C2D	-2.50	1.40	1.45
36	v	201	HEC	O2D-CGD	-2.50	1.22	1.30
25	B	605	CLA	C1B-NB	2.50	1.41	1.37
25	C	506	CLA	C1D-C2D	-2.50	1.40	1.45
25	B	601	CLA	C1D-C2D	-2.50	1.40	1.45
25	c	511	CLA	C1D-C2D	-2.49	1.40	1.45
25	b	601	CLA	C1D-C2D	-2.49	1.40	1.45
25	B	611	CLA	C1D-C2D	-2.49	1.40	1.45
25	c	509	CLA	C1D-C2D	-2.48	1.40	1.45
25	c	512	CLA	C1D-C2D	-2.48	1.40	1.45
25	c	502	CLA	C1D-C2D	-2.48	1.40	1.45
25	B	603	CLA	C1D-C2D	-2.48	1.40	1.45
25	C	503	CLA	C1D-C2D	-2.48	1.40	1.45
25	B	607	CLA	C1D-C2D	-2.48	1.40	1.45
25	c	504	CLA	C1D-C2D	-2.48	1.40	1.45
25	a	606	CLA	C1D-C2D	-2.47	1.40	1.45
25	C	509	CLA	C1D-C2D	-2.47	1.40	1.45
25	C	504	CLA	C1D-C2D	-2.47	1.40	1.45
25	C	501	CLA	C1D-C2D	-2.47	1.40	1.45
25	C	511	CLA	C1D-C2D	-2.47	1.40	1.45
25	c	508	CLA	C1D-C2D	-2.47	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	505	CLA	C1D-C2D	-2.47	1.40	1.45
25	C	508	CLA	C1D-C2D	-2.46	1.40	1.45
25	b	616	CLA	C1D-C2D	-2.46	1.40	1.45
35	e	101	HEM	O2D-CGD	-2.46	1.22	1.30
25	b	603	CLA	C1D-C2D	-2.46	1.40	1.45
34	D	402	PHO	C4D-CHA	2.46	1.43	1.39
25	b	606	CLA	C1B-NB	2.46	1.41	1.37
25	A	608	CLA	C1D-C2D	-2.45	1.40	1.45
25	D	405	CLA	C1D-C2D	-2.45	1.40	1.45
25	c	510	CLA	C1D-C2D	-2.45	1.40	1.45
25	b	602	CLA	C1B-NB	2.45	1.41	1.37
25	B	614	CLA	C1D-C2D	-2.45	1.40	1.45
25	c	506	CLA	C1D-C2D	-2.45	1.40	1.45
25	b	609	CLA	C1D-C2D	-2.45	1.40	1.45
25	b	610	CLA	C1D-C2D	-2.45	1.40	1.45
25	b	607	CLA	C1D-C2D	-2.45	1.40	1.45
25	B	609	CLA	C1D-C2D	-2.44	1.40	1.45
25	B	605	CLA	C1D-C2D	-2.44	1.40	1.45
25	C	502	CLA	C1D-C2D	-2.44	1.40	1.45
25	b	614	CLA	C1D-C2D	-2.43	1.40	1.45
25	d	403	CLA	C1D-C2D	-2.43	1.40	1.45
25	B	608	CLA	C1D-C2D	-2.43	1.40	1.45
25	B	616	CLA	C1D-C2D	-2.43	1.40	1.45
25	b	605	CLA	C1D-C2D	-2.43	1.40	1.45
25	a	610	CLA	C1D-C2D	-2.42	1.40	1.45
25	B	602	CLA	C1D-C2D	-2.42	1.40	1.45
25	b	608	CLA	C1D-C2D	-2.42	1.40	1.45
25	d	401	CLA	C1D-C2D	-2.41	1.40	1.45
25	B	610	CLA	C1D-C2D	-2.41	1.40	1.45
25	b	602	CLA	C1D-C2D	-2.40	1.40	1.45
25	c	513	CLA	C1D-C2D	-2.40	1.40	1.45
25	C	513	CLA	C1D-C2D	-2.40	1.40	1.45
34	D	401	PHO	CHA-CBD	2.40	1.54	1.51
25	c	501	CLA	C1D-C2D	-2.40	1.40	1.45
25	C	510	CLA	C1D-C2D	-2.40	1.40	1.45
25	B	602	CLA	C1B-NB	2.39	1.41	1.37
25	D	404	CLA	C1D-C2D	-2.39	1.40	1.45
34	a	609	PHO	CHA-CBD	2.39	1.54	1.51
25	a	608	CLA	C1D-C2D	-2.38	1.40	1.45
25	A	607	CLA	C1D-C2D	-2.37	1.40	1.45
25	a	606	CLA	C1B-NB	2.36	1.41	1.37
25	c	513	CLA	C1B-NB	2.35	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	606	CLA	C1D-C2D	-2.35	1.40	1.45
25	D	403	CLA	C1D-C2D	-2.35	1.40	1.45
23	C	521	LMG	O1-C1	2.33	1.44	1.40
36	V	201	HEC	C3C-C2C	-2.33	1.33	1.41
25	a	610	CLA	C1B-NB	2.32	1.40	1.37
25	D	404	CLA	C1B-NB	2.30	1.40	1.37
25	a	608	CLA	C1B-NB	2.29	1.40	1.37
36	v	201	HEC	C3C-C2C	-2.29	1.33	1.41
25	b	614	CLA	C1B-NB	2.29	1.40	1.37
34	d	402	PHO	CHA-CBD	2.29	1.54	1.51
25	B	606	CLA	C1B-NB	2.28	1.40	1.37
25	C	508	CLA	C1B-NB	2.27	1.40	1.37
25	a	607	CLA	C1D-C2D	-2.27	1.40	1.45
34	D	402	PHO	C3B-C2B	-2.27	1.37	1.40
25	A	606	CLA	C1B-NB	2.27	1.40	1.37
25	b	605	CLA	C1B-NB	2.25	1.40	1.37
25	C	513	CLA	C1B-NB	2.25	1.40	1.37
25	a	607	CLA	C1B-NB	2.25	1.40	1.37
25	b	603	CLA	C1B-NB	2.25	1.40	1.37
25	B	603	CLA	C1B-NB	2.24	1.40	1.37
25	C	505	CLA	C1B-NB	2.24	1.40	1.37
25	b	607	CLA	C1B-NB	2.24	1.40	1.37
25	B	614	CLA	C1B-NB	2.24	1.40	1.37
25	b	616	CLA	C1B-NB	2.23	1.40	1.37
25	a	608	CLA	C3D-C4D	-2.22	1.39	1.44
25	B	602	CLA	C3D-C4D	-2.22	1.39	1.44
34	D	402	PHO	CHA-CBD	2.22	1.54	1.51
25	C	501	CLA	C1B-NB	2.21	1.40	1.37
25	b	608	CLA	C1B-NB	2.21	1.40	1.37
25	c	508	CLA	C1B-NB	2.20	1.40	1.37
25	C	510	CLA	C3D-C4D	-2.19	1.39	1.44
25	B	608	CLA	C3D-C4D	-2.19	1.39	1.44
25	D	403	CLA	C1B-NB	2.18	1.40	1.37
25	d	401	CLA	C1B-NB	2.18	1.40	1.37
25	B	605	CLA	C3D-C4D	-2.18	1.39	1.44
25	C	505	CLA	C3D-C4D	-2.18	1.39	1.44
25	c	510	CLA	C3D-C4D	-2.17	1.39	1.44
25	A	608	CLA	C3D-C4D	-2.17	1.39	1.44
25	c	513	CLA	C3D-C4D	-2.17	1.39	1.44
25	a	610	CLA	C3D-C4D	-2.17	1.39	1.44
25	c	508	CLA	C3D-C4D	-2.17	1.39	1.44
25	B	616	CLA	C3D-C4D	-2.16	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	C3D-C4D	-2.16	1.39	1.44
25	c	506	CLA	C3D-C4D	-2.16	1.39	1.44
25	C	508	CLA	C3D-C4D	-2.15	1.39	1.44
25	b	602	CLA	C3D-C4D	-2.15	1.39	1.44
25	C	504	CLA	C3D-C4D	-2.15	1.39	1.44
25	C	513	CLA	C3D-C4D	-2.15	1.39	1.44
25	A	607	CLA	C3D-C4D	-2.15	1.39	1.44
25	B	615	CLA	C3D-C4D	-2.15	1.39	1.44
25	D	403	CLA	C3D-C4D	-2.15	1.39	1.44
25	B	601	CLA	C1B-NB	2.15	1.40	1.37
25	A	606	CLA	C3D-C4D	-2.14	1.39	1.44
25	C	501	CLA	C3D-C4D	-2.14	1.39	1.44
25	b	614	CLA	C3D-C4D	-2.14	1.39	1.44
25	B	603	CLA	C3D-C4D	-2.14	1.39	1.44
25	B	610	CLA	C3D-C4D	-2.14	1.39	1.44
25	b	616	CLA	C3D-C4D	-2.14	1.39	1.44
25	b	605	CLA	C3D-C4D	-2.14	1.39	1.44
25	d	403	CLA	C3D-C4D	-2.13	1.39	1.44
25	C	506	CLA	C3D-C4D	-2.13	1.39	1.44
25	D	404	CLA	C3D-C4D	-2.13	1.39	1.44
25	b	611	CLA	C1B-NB	2.13	1.40	1.37
25	c	504	CLA	C3D-C4D	-2.13	1.39	1.44
25	B	607	CLA	C1B-NB	2.13	1.40	1.37
25	c	503	CLA	C1B-NB	2.13	1.40	1.37
25	B	606	CLA	C3D-C4D	-2.13	1.39	1.44
25	B	614	CLA	C3D-C4D	-2.13	1.39	1.44
25	b	603	CLA	C3D-C4D	-2.13	1.39	1.44
25	C	502	CLA	C3D-C4D	-2.13	1.39	1.44
25	d	401	CLA	C3D-C4D	-2.13	1.39	1.44
25	B	616	CLA	C1B-NB	2.13	1.40	1.37
25	C	502	CLA	C1B-NB	2.13	1.40	1.37
25	B	609	CLA	C3D-C4D	-2.12	1.39	1.44
25	B	607	CLA	C3D-C4D	-2.12	1.39	1.44
25	A	607	CLA	C1B-NB	2.12	1.40	1.37
25	B	611	CLA	C3D-C4D	-2.12	1.39	1.44
25	a	607	CLA	C3D-C4D	-2.12	1.39	1.44
25	b	612	CLA	C3D-C4D	-2.12	1.39	1.44
25	b	609	CLA	C3D-C4D	-2.12	1.39	1.44
25	c	505	CLA	C3D-C4D	-2.12	1.39	1.44
25	C	509	CLA	C3D-C4D	-2.11	1.39	1.44
25	b	610	CLA	C3D-C4D	-2.11	1.39	1.44
25	c	502	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	405	CLA	C3D-C4D	-2.11	1.39	1.44
25	c	502	CLA	C1B-NB	2.11	1.40	1.37
25	c	504	CLA	C1B-NB	2.11	1.40	1.37
25	c	501	CLA	C3D-C4D	-2.11	1.39	1.44
25	c	511	CLA	C3D-C4D	-2.11	1.39	1.44
25	B	612	CLA	C3D-C4D	-2.11	1.39	1.44
25	c	512	CLA	C3D-C4D	-2.10	1.39	1.44
25	b	601	CLA	C1B-NB	2.10	1.40	1.37
25	b	609	CLA	C1B-NB	2.10	1.40	1.37
25	b	607	CLA	C3D-C4D	-2.10	1.39	1.44
25	c	509	CLA	C3D-C4D	-2.10	1.39	1.44
25	c	501	CLA	C1B-NB	2.10	1.40	1.37
25	b	613	CLA	C3D-C4D	-2.10	1.39	1.44
25	b	610	CLA	C1B-NB	2.09	1.40	1.37
25	B	609	CLA	C1D-ND	2.09	1.40	1.37
25	B	613	CLA	C3D-C4D	-2.09	1.39	1.44
25	B	609	CLA	C1B-NB	2.09	1.40	1.37
27	D	407	PL9	C2-C3	2.09	1.39	1.34
25	b	611	CLA	C3D-C4D	-2.09	1.39	1.44
25	b	615	CLA	C3D-C4D	-2.09	1.39	1.44
25	b	609	CLA	C1D-ND	2.09	1.40	1.37
25	b	601	CLA	C1D-ND	2.09	1.40	1.37
25	b	601	CLA	C3D-C4D	-2.08	1.39	1.44
25	A	608	CLA	C1B-NB	2.08	1.40	1.37
25	C	503	CLA	C3D-C4D	-2.08	1.39	1.44
25	c	505	CLA	C1B-NB	2.08	1.40	1.37
27	a	612	PL9	C2-C3	2.08	1.39	1.34
25	B	601	CLA	C3D-C4D	-2.07	1.39	1.44
25	a	606	CLA	C3D-C4D	-2.07	1.39	1.44
25	B	608	CLA	C1B-NB	2.07	1.40	1.37
25	c	506	CLA	C1B-NB	2.07	1.40	1.37
25	C	511	CLA	C3D-C4D	-2.07	1.39	1.44
25	b	602	CLA	C1D-ND	2.07	1.40	1.37
25	c	503	CLA	C3D-C4D	-2.07	1.39	1.44
25	B	610	CLA	C1B-NB	2.06	1.40	1.37
25	C	512	CLA	C3D-C4D	-2.06	1.39	1.44
25	d	403	CLA	C1B-NB	2.06	1.40	1.37
25	b	606	CLA	C3D-C4D	-2.06	1.39	1.44
27	d	405	PL9	C2-C3	2.06	1.39	1.34
27	A	610	PL9	C2-C3	2.06	1.39	1.34
25	B	604	CLA	C3D-C4D	-2.05	1.39	1.44
25	B	615	CLA	C1D-ND	2.04	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C3D-C4D	-2.04	1.39	1.44
25	C	507	CLA	C3D-C4D	-2.03	1.39	1.44
25	D	405	CLA	C1D-ND	2.03	1.40	1.37
25	c	511	CLA	C1D-ND	2.03	1.40	1.37
25	c	509	CLA	C1B-NB	2.02	1.40	1.37
25	b	604	CLA	C3D-C4D	-2.02	1.39	1.44
25	B	616	CLA	C1D-ND	2.02	1.40	1.37
25	B	601	CLA	C1D-ND	2.02	1.40	1.37
25	C	512	CLA	C1B-NB	2.02	1.40	1.37
25	d	403	CLA	C1D-ND	2.02	1.40	1.37
25	c	512	CLA	C1B-NB	2.02	1.40	1.37
25	b	616	CLA	C1D-ND	2.02	1.40	1.37
25	a	608	CLA	C4C-C3C	2.01	1.48	1.45
25	c	506	CLA	C1D-ND	2.01	1.40	1.37
25	B	612	CLA	C1B-NB	2.01	1.40	1.37
25	C	509	CLA	C1B-NB	2.01	1.40	1.37
25	D	405	CLA	C1B-NB	2.00	1.40	1.37

All (1156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	101	SQD	O9-S-C6	-14.06	85.76	106.76
28	L	101	SQD	O8-S-O9	-11.51	82.59	111.40
34	a	609	PHO	C4D-CHA-CBD	-10.48	103.43	108.45
34	d	402	PHO	C4D-CHA-CBD	-10.46	103.44	108.45
34	D	401	PHO	C4D-CHA-CBD	-10.25	103.54	108.45
34	D	402	PHO	C4D-CHA-CBD	-10.06	103.63	108.45
28	L	101	SQD	O9-S-O7	-9.79	81.97	113.82
36	V	201	HEC	CBC-CAC-C3C	-8.12	111.20	127.43
36	v	201	HEC	CBC-CAC-C3C	-8.11	111.22	127.43
28	L	101	SQD	O7-S-C6	7.86	118.49	106.76
36	v	201	HEC	CBB-CAB-C3B	-7.42	112.60	127.43
36	V	201	HEC	CBB-CAB-C3B	-7.02	113.40	127.43
25	A	606	CLA	C4A-NA-C1A	-6.57	103.68	106.68
25	b	602	CLA	C4A-NA-C1A	-6.56	103.69	106.68
26	t	102	BCR	C24-C23-C22	-6.53	116.58	126.23
28	L	101	SQD	O8-S-C6	6.35	118.24	105.97
25	a	606	CLA	C4A-NA-C1A	-6.32	103.80	106.68
25	b	614	CLA	C4A-NA-C1A	-6.29	103.81	106.68
25	B	616	CLA	C4A-NA-C1A	-6.24	103.83	106.68
25	a	607	CLA	C4A-NA-C1A	-6.10	103.90	106.68
25	B	614	CLA	C4A-NA-C1A	-6.06	103.92	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	C4A-NA-C1A	-6.05	103.92	106.68
25	b	616	CLA	C4A-NA-C1A	-6.04	103.92	106.68
25	D	403	CLA	C4A-NA-C1A	-5.99	103.95	106.68
26	d	404	BCR	C7-C8-C9	-5.98	117.38	126.23
25	B	610	CLA	C4A-NA-C1A	-5.98	103.95	106.68
25	B	603	CLA	C4A-NA-C1A	-5.93	103.97	106.68
25	B	605	CLA	C4A-NA-C1A	-5.88	104.00	106.68
25	b	605	CLA	C4A-NA-C1A	-5.84	104.02	106.68
25	B	608	CLA	C4A-NA-C1A	-5.83	104.02	106.68
25	C	508	CLA	C4A-NA-C1A	-5.83	104.02	106.68
25	d	401	CLA	C4A-NA-C1A	-5.80	104.03	106.68
26	t	102	BCR	C20-C21-C22	-5.77	119.19	127.28
25	D	404	CLA	C4A-NA-C1A	-5.76	104.05	106.68
26	D	406	BCR	C7-C8-C9	-5.76	117.72	126.23
25	B	606	CLA	C4A-NA-C1A	-5.75	104.06	106.68
25	b	608	CLA	C4A-NA-C1A	-5.71	104.07	106.68
25	c	508	CLA	C4A-NA-C1A	-5.70	104.08	106.68
25	c	513	CLA	C4A-NA-C1A	-5.69	104.08	106.68
25	c	506	CLA	C4A-NA-C1A	-5.68	104.09	106.68
25	c	505	CLA	C4A-NA-C1A	-5.66	104.10	106.68
25	B	609	CLA	C4A-NA-C1A	-5.65	104.10	106.68
25	C	510	CLA	C4A-NA-C1A	-5.64	104.11	106.68
25	B	615	CLA	C4A-NA-C1A	-5.59	104.13	106.68
25	b	610	CLA	C4A-NA-C1A	-5.58	104.14	106.68
25	C	513	CLA	C4A-NA-C1A	-5.55	104.15	106.68
25	b	606	CLA	C4A-NA-C1A	-5.55	104.15	106.68
25	A	607	CLA	C4A-NA-C1A	-5.54	104.15	106.68
25	b	615	CLA	C4A-NA-C1A	-5.53	104.16	106.68
25	A	608	CLA	C4A-NA-C1A	-5.51	104.17	106.68
25	b	603	CLA	C4A-NA-C1A	-5.50	104.17	106.68
25	b	607	CLA	C4A-NA-C1A	-5.50	104.17	106.68
26	c	521	BCR	C7-C8-C9	-5.44	118.19	126.23
26	h	101	BCR	C7-C8-C9	-5.43	118.20	126.23
25	C	505	CLA	C4A-NA-C1A	-5.39	104.22	106.68
25	B	601	CLA	C4A-NA-C1A	-5.37	104.23	106.68
25	a	610	CLA	C4A-NA-C1A	-5.35	104.24	106.68
25	B	611	CLA	C4A-NA-C1A	-5.34	104.24	106.68
26	H	101	BCR	C11-C10-C9	-5.33	119.80	127.28
25	b	609	CLA	C4A-NA-C1A	-5.30	104.26	106.68
25	B	607	CLA	C4A-NA-C1A	-5.29	104.27	106.68
25	B	613	CLA	C4A-NA-C1A	-5.26	104.28	106.68
25	C	506	CLA	C4A-NA-C1A	-5.23	104.29	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	C4A-NA-C1A	-5.23	104.29	106.68
26	D	406	BCR	C28-C27-C26	-5.22	104.75	114.06
25	D	405	CLA	C4A-NA-C1A	-5.20	104.31	106.68
25	c	503	CLA	C4A-NA-C1A	-5.19	104.31	106.68
25	C	503	CLA	C4A-NA-C1A	-5.12	104.34	106.68
25	b	601	CLA	C4A-NA-C1A	-5.12	104.34	106.68
25	c	501	CLA	C4A-NA-C1A	-5.12	104.34	106.68
26	b	617	BCR	C28-C27-C26	-5.12	104.93	114.06
25	b	611	CLA	C4A-NA-C1A	-5.10	104.35	106.68
25	b	613	CLA	C4A-NA-C1A	-5.07	104.37	106.68
25	C	504	CLA	C4A-NA-C1A	-5.07	104.37	106.68
26	T	101	BCR	C15-C14-C13	-5.07	120.17	127.28
26	T	101	BCR	C7-C8-C9	-5.06	118.75	126.23
25	c	504	CLA	C4A-NA-C1A	-5.05	104.37	106.68
26	D	406	BCR	C15-C14-C13	-5.05	120.19	127.28
26	H	101	BCR	C7-C8-C9	-5.04	118.78	126.23
25	a	608	CLA	C4A-NA-C1A	-5.04	104.38	106.68
25	b	612	CLA	C4A-NA-C1A	-5.02	104.39	106.68
26	z	101	BCR	C15-C14-C13	-5.00	120.26	127.28
26	T	101	BCR	C24-C23-C22	-4.99	118.85	126.23
26	C	515	BCR	C15-C14-C13	-4.99	120.28	127.28
26	c	521	BCR	C11-C10-C9	-4.94	120.35	127.28
26	h	101	BCR	C11-C10-C9	-4.92	120.38	127.28
26	k	102	BCR	C33-C5-C6	-4.91	119.12	124.48
25	C	501	CLA	C4A-NA-C1A	-4.91	104.44	106.68
26	K	101	BCR	C33-C5-C6	-4.90	119.13	124.48
25	C	502	CLA	C4A-NA-C1A	-4.90	104.44	106.68
25	c	502	CLA	C4A-NA-C1A	-4.89	104.45	106.68
26	A	609	BCR	C15-C14-C13	-4.89	120.42	127.28
26	C	522	BCR	C20-C21-C22	-4.89	120.42	127.28
25	c	507	CLA	C4A-NA-C1A	-4.89	104.45	106.68
25	C	509	CLA	C4A-NA-C1A	-4.87	104.45	106.68
25	B	612	CLA	C4A-NA-C1A	-4.87	104.46	106.68
25	c	509	CLA	C4A-NA-C1A	-4.84	104.47	106.68
26	b	618	BCR	C15-C14-C13	-4.80	120.54	127.28
26	t	102	BCR	C15-C14-C13	-4.78	120.57	127.28
26	C	514	BCR	C15-C14-C13	-4.77	120.59	127.28
26	T	101	BCR	C33-C5-C6	-4.76	119.29	124.48
25	b	604	CLA	C4A-NA-C1A	-4.73	104.52	106.68
25	C	512	CLA	C4A-NA-C1A	-4.72	104.53	106.68
26	C	514	BCR	C11-C10-C9	-4.71	120.67	127.28
25	C	507	CLA	C4A-NA-C1A	-4.71	104.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	522	BCR	C15-C14-C13	-4.71	120.68	127.28
26	k	102	BCR	C16-C17-C18	-4.69	120.70	127.28
25	c	512	CLA	C4A-NA-C1A	-4.69	104.54	106.68
26	C	522	BCR	C11-C10-C9	-4.69	120.71	127.28
25	B	604	CLA	C4A-NA-C1A	-4.68	104.55	106.68
26	c	514	BCR	C33-C5-C6	-4.68	119.38	124.48
26	K	101	BCR	C16-C17-C18	-4.67	120.73	127.28
26	T	101	BCR	C20-C21-C22	-4.67	120.73	127.28
26	H	101	BCR	C16-C17-C18	-4.66	120.74	127.28
26	c	521	BCR	C20-C21-C22	-4.63	120.78	127.28
26	T	101	BCR	C11-C10-C9	-4.63	120.78	127.28
26	D	406	BCR	C24-C23-C22	-4.63	119.39	126.23
25	d	403	CLA	C4A-NA-C1A	-4.63	104.57	106.68
26	d	404	BCR	C11-C10-C9	-4.63	120.79	127.28
26	C	515	BCR	C33-C5-C6	-4.62	119.45	124.48
26	t	102	BCR	C33-C5-C6	-4.61	119.46	124.48
26	B	619	BCR	C15-C14-C13	-4.58	120.86	127.28
26	c	514	BCR	C15-C14-C13	-4.57	120.87	127.28
26	B	618	BCR	C15-C14-C13	-4.56	120.88	127.28
26	a	611	BCR	C15-C14-C13	-4.55	120.90	127.28
26	B	617	BCR	C15-C14-C13	-4.54	120.91	127.28
26	C	522	BCR	C7-C8-C9	-4.54	119.52	126.23
25	C	511	CLA	C4A-NA-C1A	-4.53	104.61	106.68
26	B	619	BCR	C38-C26-C25	-4.52	119.56	124.48
27	D	407	PL9	C7-C8-C9	-4.48	119.12	126.83
26	h	101	BCR	C15-C14-C13	-4.47	121.01	127.28
26	d	404	BCR	C24-C23-C22	-4.47	119.62	126.23
26	b	617	BCR	C33-C5-C6	-4.45	119.63	124.48
26	B	617	BCR	C33-C5-C6	-4.44	119.64	124.48
26	b	617	BCR	C15-C14-C13	-4.44	121.05	127.28
26	b	619	BCR	C16-C17-C18	-4.43	121.06	127.28
25	c	511	CLA	C4A-NA-C1A	-4.43	104.66	106.68
26	C	514	BCR	C16-C17-C18	-4.42	121.08	127.28
26	D	406	BCR	C33-C5-C6	-4.41	119.67	124.48
26	c	521	BCR	C24-C23-C22	-4.41	119.72	126.23
26	C	522	BCR	C24-C23-C22	-4.40	119.72	126.23
26	D	406	BCR	C11-C10-C9	-4.40	121.11	127.28
26	B	619	BCR	C7-C8-C9	-4.40	119.73	126.23
26	c	514	BCR	C7-C8-C9	-4.40	119.73	126.23
26	B	617	BCR	C28-C27-C26	-4.38	106.24	114.06
26	T	101	BCR	C16-C17-C18	-4.38	121.13	127.28
27	A	610	PL9	C7-C8-C9	-4.37	119.30	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C15-C14-C13	-4.37	121.15	127.28
26	c	521	BCR	C16-C17-C18	-4.33	121.20	127.28
26	c	521	BCR	C15-C14-C13	-4.31	121.23	127.28
26	b	617	BCR	C11-C10-C9	-4.31	121.23	127.28
26	b	619	BCR	C38-C26-C25	-4.31	119.78	124.48
26	d	404	BCR	C15-C14-C13	-4.29	121.26	127.28
26	d	404	BCR	C33-C5-C6	-4.28	119.81	124.48
27	d	405	PL9	C7-C8-C9	-4.27	119.47	126.83
26	b	619	BCR	C7-C8-C9	-4.25	119.95	126.23
26	d	404	BCR	C38-C26-C25	-4.24	119.85	124.48
26	k	102	BCR	C15-C14-C13	-4.23	121.35	127.28
26	C	515	BCR	C7-C8-C9	-4.23	119.98	126.23
23	a	614	LMG	O7-C10-C11	4.20	120.57	111.48
26	H	101	BCR	C15-C14-C13	-4.19	121.40	127.28
29	l	101	LHG	O7-C7-C8	4.19	120.55	111.48
26	d	404	BCR	C16-C17-C18	-4.18	121.41	127.28
28	a	613	SQD	O47-C7-C8	4.17	120.50	111.48
26	b	619	BCR	C11-C10-C9	-4.17	121.43	127.28
28	L	103	SQD	O47-C7-C8	4.15	120.45	111.48
26	C	514	BCR	C7-C8-C9	-4.14	120.12	126.23
26	z	101	BCR	C16-C17-C18	-4.13	121.48	127.28
26	b	618	BCR	C28-C27-C26	-4.12	106.70	114.06
26	h	101	BCR	C16-C17-C18	-4.12	121.50	127.28
23	c	520	LMG	O7-C10-C11	4.11	120.37	111.48
34	D	401	PHO	C2B-C1B-NB	-4.11	106.46	109.43
26	H	101	BCR	C20-C21-C22	-4.11	121.52	127.28
23	D	409	LMG	O7-C10-C11	4.11	120.36	111.48
29	E	101	LHG	O7-C7-C8	4.10	120.35	111.48
28	A	611	SQD	O47-C7-C8	4.10	120.35	111.48
26	B	617	BCR	C11-C10-C9	-4.10	121.53	127.28
28	f	101	SQD	O47-C7-C8	4.09	120.33	111.48
23	A	612	LMG	O7-C10-C11	4.08	120.32	111.48
26	b	618	BCR	C16-C17-C18	-4.08	121.56	127.28
26	K	101	BCR	C15-C14-C13	-4.08	121.56	127.28
29	L	102	LHG	O7-C7-C8	4.07	120.30	111.48
26	B	619	BCR	C16-C17-C18	-4.07	121.57	127.28
26	B	619	BCR	C11-C10-C9	-4.07	121.58	127.28
23	B	624	LMG	O7-C10-C11	4.06	120.27	111.48
23	b	620	LMG	O7-C10-C11	4.05	120.24	111.48
29	A	614	LHG	O7-C7-C8	4.04	120.22	111.48
26	D	406	BCR	C16-C17-C18	-4.04	121.62	127.28
23	b	624	LMG	O7-C10-C11	4.03	120.21	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	515	DGD	O2G-C1B-C2B	4.03	120.19	111.48
26	b	618	BCR	C11-C10-C9	-4.03	121.63	127.28
29	a	616	LHG	O7-C7-C8	4.02	120.18	111.48
33	C	516	DGD	O2G-C1B-C2B	4.01	120.15	111.48
26	C	522	BCR	C16-C17-C18	-3.99	121.68	127.28
26	c	514	BCR	C11-C10-C9	-3.99	121.68	127.28
26	t	102	BCR	C11-C10-C9	-3.99	121.69	127.28
23	d	408	LMG	O7-C10-C11	3.98	120.10	111.48
33	C	517	DGD	O2G-C1B-C2B	3.98	120.08	111.48
26	z	101	BCR	C11-C10-C9	-3.97	121.72	127.28
28	F	101	SQD	O47-C7-C8	3.97	120.06	111.48
34	D	402	PHO	C2B-C1B-NB	-3.96	106.57	109.43
34	d	402	PHO	C2B-C1B-NB	-3.95	106.58	109.43
33	H	102	DGD	O2G-C1B-C2B	3.91	119.95	111.48
23	a	603	LMG	O7-C10-C11	3.91	119.94	111.48
26	B	618	BCR	C11-C10-C9	-3.90	121.81	127.28
23	A	603	LMG	O7-C10-C11	3.89	119.91	111.48
25	a	610	CLA	C1D-ND-C4D	-3.89	103.58	106.31
26	C	514	BCR	C33-C5-C6	-3.88	120.25	124.48
26	h	101	BCR	C24-C23-C22	-3.88	120.50	126.23
27	a	612	PL9	C7-C8-C9	-3.87	120.16	126.83
26	z	101	BCR	C20-C21-C22	-3.87	121.85	127.28
26	h	101	BCR	C20-C21-C22	-3.87	121.85	127.28
29	d	406	LHG	O7-C7-C8	3.84	119.80	111.48
23	B	620	LMG	O7-C10-C11	3.84	119.79	111.48
33	C	518	DGD	O2G-C1B-C2B	3.83	119.77	111.48
25	b	615	CLA	C1D-ND-C4D	-3.83	103.62	106.31
26	H	101	BCR	C28-C27-C26	-3.83	107.23	114.06
33	c	517	DGD	O2G-C1B-C2B	3.83	119.76	111.48
26	t	102	BCR	C16-C17-C18	-3.82	121.92	127.28
23	c	518	LMG	O7-C10-C11	3.82	119.74	111.48
29	a	615	LHG	O7-C7-C8	3.82	119.74	111.48
26	a	611	BCR	C16-C17-C18	-3.81	121.93	127.28
26	B	618	BCR	C33-C5-C6	-3.81	120.33	124.48
26	H	101	BCR	C24-C23-C22	-3.80	120.61	126.23
33	h	102	DGD	O2G-C1B-C2B	3.80	119.69	111.48
26	b	618	BCR	C3-C4-C5	-3.79	107.29	114.06
29	d	407	LHG	O7-C7-C8	3.78	119.65	111.48
29	D	408	LHG	O7-C7-C8	3.77	119.64	111.48
23	C	519	LMG	O7-C10-C11	3.76	119.61	111.48
25	B	615	CLA	C1D-ND-C4D	-3.74	103.69	106.31
26	B	619	BCR	C24-C23-C22	-3.74	120.70	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	C1D-ND-C4D	-3.73	103.69	106.31
25	A	608	CLA	C1D-ND-C4D	-3.72	103.70	106.31
26	b	617	BCR	C16-C17-C18	-3.72	122.07	127.28
25	b	616	CLA	C1D-ND-C4D	-3.71	103.71	106.31
26	B	618	BCR	C16-C17-C18	-3.69	122.10	127.28
26	z	101	BCR	C24-C23-C22	-3.69	120.77	126.23
25	b	614	CLA	C1D-ND-C4D	-3.69	103.72	106.31
25	D	405	CLA	C1D-ND-C4D	-3.68	103.73	106.31
25	d	403	CLA	C1D-ND-C4D	-3.68	103.73	106.31
26	C	514	BCR	C20-C21-C22	-3.67	122.13	127.28
26	A	609	BCR	C38-C26-C25	-3.67	120.48	124.48
25	B	614	CLA	C1D-ND-C4D	-3.67	103.74	106.31
25	c	503	CLA	C1D-ND-C4D	-3.67	103.74	106.31
26	b	619	BCR	C24-C23-C22	-3.67	120.81	126.23
25	d	401	CLA	C1D-ND-C4D	-3.66	103.74	106.31
25	b	612	CLA	C1D-ND-C4D	-3.66	103.74	106.31
26	B	618	BCR	C7-C8-C9	-3.66	120.82	126.23
29	A	613	LHG	O7-C7-C8	3.65	119.39	111.48
26	a	611	BCR	C11-C10-C9	-3.65	122.16	127.28
25	C	505	CLA	C1D-ND-C4D	-3.65	103.75	106.31
26	B	618	BCR	C24-C23-C22	-3.65	120.84	126.23
25	B	616	CLA	C1D-ND-C4D	-3.64	103.75	106.31
23	C	521	LMG	O7-C10-C11	3.64	119.36	111.48
25	B	612	CLA	C1D-ND-C4D	-3.64	103.76	106.31
25	C	512	CLA	C1D-ND-C4D	-3.64	103.76	106.31
26	b	618	BCR	C20-C21-C22	-3.64	122.18	127.28
25	c	507	CLA	C1D-ND-C4D	-3.63	103.76	106.31
25	b	605	CLA	C1D-ND-C4D	-3.63	103.77	106.31
26	z	101	BCR	C7-C8-C9	-3.62	120.89	126.23
26	B	617	BCR	C24-C23-C22	-3.61	120.89	126.23
25	b	606	CLA	C1D-ND-C4D	-3.61	103.78	106.31
25	D	404	CLA	C1D-ND-C4D	-3.60	103.78	106.31
26	B	618	BCR	C20-C21-C22	-3.60	122.23	127.28
25	C	507	CLA	C1D-ND-C4D	-3.59	103.79	106.31
25	b	610	CLA	C1D-ND-C4D	-3.59	103.79	106.31
25	c	509	CLA	C1D-ND-C4D	-3.59	103.79	106.31
25	C	506	CLA	C1D-ND-C4D	-3.58	103.80	106.31
26	z	101	BCR	C33-C5-C6	-3.58	120.58	124.48
26	B	618	BCR	C28-C27-C26	-3.56	107.71	114.06
26	b	619	BCR	C20-C21-C22	-3.56	122.29	127.28
26	b	618	BCR	C7-C8-C9	-3.55	120.98	126.23
27	D	407	PL9	C37-C38-C39	-3.55	119.49	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	611	CLA	C1D-ND-C4D	-3.55	103.82	106.31
26	C	515	BCR	C11-C10-C9	-3.55	122.30	127.28
25	a	606	CLA	C1D-ND-C4D	-3.55	103.82	106.31
25	c	506	CLA	C1D-ND-C4D	-3.55	103.82	106.31
26	c	521	BCR	C33-C5-C6	-3.54	120.62	124.48
25	B	611	CLA	C1-C2-C3	-3.54	120.39	126.20
25	B	605	CLA	C1D-ND-C4D	-3.54	103.83	106.31
25	B	610	CLA	C1D-ND-C4D	-3.54	103.83	106.31
26	A	609	BCR	C20-C21-C22	-3.54	122.32	127.28
26	A	609	BCR	C7-C8-C9	-3.53	121.01	126.23
26	A	609	BCR	C16-C17-C18	-3.53	122.33	127.28
26	A	609	BCR	C33-C5-C6	-3.53	120.63	124.48
25	A	606	CLA	C1D-ND-C4D	-3.52	103.84	106.31
25	B	603	CLA	C1D-ND-C4D	-3.52	103.84	106.31
25	c	508	CLA	C1D-ND-C4D	-3.51	103.85	106.31
26	D	406	BCR	C20-C21-C22	-3.51	122.36	127.28
26	a	611	BCR	C33-C5-C6	-3.50	120.66	124.48
25	c	512	CLA	C1D-ND-C4D	-3.49	103.86	106.31
26	B	617	BCR	C16-C17-C18	-3.49	122.39	127.28
25	B	609	CLA	C1D-ND-C4D	-3.48	103.87	106.31
34	a	609	PHO	C2B-C1B-NB	-3.48	106.91	109.43
25	b	602	CLA	C1D-ND-C4D	-3.48	103.87	106.31
25	B	606	CLA	C1D-ND-C4D	-3.48	103.87	106.31
25	b	603	CLA	C1D-ND-C4D	-3.47	103.88	106.31
26	A	609	BCR	C24-C23-C22	-3.47	121.10	126.23
25	b	601	CLA	C1D-ND-C4D	-3.47	103.88	106.31
25	c	501	CLA	C1D-ND-C4D	-3.46	103.88	106.31
25	c	511	CLA	C1D-ND-C4D	-3.46	103.88	106.31
26	a	611	BCR	C38-C26-C25	-3.45	120.72	124.48
25	C	503	CLA	C1D-ND-C4D	-3.45	103.89	106.31
25	B	601	CLA	C1D-ND-C4D	-3.45	103.89	106.31
25	b	607	CLA	C1D-ND-C4D	-3.45	103.89	106.31
25	b	611	CLA	C1-C2-C3	-3.45	120.55	126.20
25	C	508	CLA	C1D-ND-C4D	-3.44	103.90	106.31
25	b	609	CLA	C1D-ND-C4D	-3.44	103.90	106.31
33	c	516	DGD	O2G-C1B-C2B	3.43	118.91	111.48
25	B	607	CLA	C1D-ND-C4D	-3.43	103.91	106.31
27	a	612	PL9	C37-C38-C39	-3.43	119.78	127.62
25	c	504	CLA	C1D-ND-C4D	-3.42	103.91	106.31
25	c	505	CLA	C1D-ND-C4D	-3.41	103.92	106.31
27	d	405	PL9	C37-C38-C39	-3.40	119.83	127.62
26	C	514	BCR	C24-C23-C22	-3.40	121.20	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	C1D-ND-C4D	-3.40	103.92	106.31
26	K	101	BCR	C38-C26-C25	-3.39	120.79	124.48
28	L	101	SQD	O47-C7-C8	3.39	118.81	111.48
26	c	521	BCR	C28-C27-C26	-3.39	108.02	114.06
26	C	522	BCR	C3-C4-C5	-3.38	108.02	114.06
26	b	617	BCR	C7-C8-C9	-3.38	121.23	126.23
25	b	608	CLA	C1D-ND-C4D	-3.38	103.94	106.31
25	c	510	CLA	C1-C2-C3	-3.38	120.66	126.20
25	C	511	CLA	C1D-ND-C4D	-3.38	103.94	106.31
25	C	509	CLA	C1D-ND-C4D	-3.37	103.94	106.31
25	C	504	CLA	C1D-ND-C4D	-3.36	103.96	106.31
26	A	609	BCR	C11-C10-C9	-3.35	122.58	127.28
25	B	611	CLA	C1D-ND-C4D	-3.35	103.96	106.31
26	H	101	BCR	C3-C4-C5	-3.33	108.12	114.06
25	D	403	CLA	C1D-ND-C4D	-3.33	103.98	106.31
25	B	604	CLA	C1D-ND-C4D	-3.32	103.98	106.31
25	C	510	CLA	C1D-ND-C4D	-3.32	103.98	106.31
26	a	611	BCR	C7-C8-C9	-3.32	121.32	126.23
25	c	502	CLA	C1D-ND-C4D	-3.32	103.98	106.31
26	k	102	BCR	C38-C26-C25	-3.32	120.86	124.48
25	C	513	CLA	C1D-ND-C4D	-3.32	103.98	106.31
25	A	607	CLA	C1D-ND-C4D	-3.31	103.99	106.31
25	c	503	CLA	C4D-C3D-CAD	3.31	111.70	108.11
25	B	608	CLA	C1D-ND-C4D	-3.31	103.99	106.31
25	C	503	CLA	C4D-C3D-CAD	3.30	111.69	108.11
25	C	505	CLA	C4D-C3D-CAD	3.30	111.69	108.11
26	C	522	BCR	C28-C27-C26	-3.30	108.18	114.06
27	A	610	PL9	C32-C33-C34	-3.29	120.09	127.62
25	C	502	CLA	C1D-ND-C4D	-3.29	104.01	106.31
25	c	513	CLA	C1D-ND-C4D	-3.28	104.01	106.31
25	b	604	CLA	C1D-ND-C4D	-3.28	104.01	106.31
25	c	507	CLA	C4D-C3D-CAD	3.28	111.66	108.11
25	a	608	CLA	C1D-ND-C4D	-3.26	104.02	106.31
26	b	617	BCR	C27-C26-C25	-3.26	118.30	122.70
25	b	613	CLA	C1D-ND-C4D	-3.26	104.03	106.31
25	B	613	CLA	C1D-ND-C4D	-3.26	104.03	106.31
26	B	619	BCR	C20-C21-C22	-3.25	122.72	127.28
25	C	501	CLA	C1D-ND-C4D	-3.24	104.04	106.31
25	B	604	CLA	C4D-C3D-CAD	3.24	111.62	108.11
26	c	514	BCR	C24-C23-C22	-3.24	121.45	126.23
25	B	616	CLA	C1-C2-C3	-3.23	120.90	126.20
23	C	521	LMG	O1-C1-C2	3.23	113.18	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	611	BCR	C24-C23-C22	-3.23	121.45	126.23
25	B	601	CLA	C4D-C3D-CAD	3.23	111.61	108.11
25	C	510	CLA	C1-C2-C3	-3.22	120.92	126.20
27	A	610	PL9	C22-C23-C24	-3.22	120.26	127.62
26	a	611	BCR	C20-C21-C22	-3.22	122.77	127.28
27	d	405	PL9	C27-C28-C29	-3.22	120.26	127.62
25	a	607	CLA	C1D-ND-C4D	-3.22	104.06	106.31
25	c	502	CLA	C1-C2-C3	-3.21	120.94	126.20
25	C	502	CLA	C1-C2-C3	-3.21	120.94	126.20
25	C	507	CLA	C4D-C3D-CAD	3.21	111.59	108.11
26	C	515	BCR	C24-C23-C22	-3.20	121.49	126.23
28	L	101	SQD	O8-S-O7	3.20	119.40	111.40
27	A	610	PL9	C37-C38-C39	-3.20	120.31	127.62
25	b	604	CLA	C4D-C3D-CAD	3.19	111.58	108.11
25	B	612	CLA	C4D-C3D-CAD	3.19	111.57	108.11
25	b	601	CLA	C4D-C3D-CAD	3.18	111.56	108.11
26	C	514	BCR	C38-C26-C25	-3.18	121.01	124.48
26	h	101	BCR	C3-C4-C5	-3.17	108.40	114.06
26	t	102	BCR	C20-C19-C18	-3.17	117.67	126.36
25	b	612	CLA	C4D-C3D-CAD	3.17	111.55	108.11
25	B	614	CLA	C4D-C3D-CAD	3.16	111.54	108.11
25	C	511	CLA	C4D-C3D-CAD	3.16	111.53	108.11
26	b	617	BCR	C29-C30-C25	3.16	115.02	110.44
26	B	617	BCR	C7-C8-C9	-3.15	121.57	126.23
25	C	512	CLA	C4D-C3D-CAD	3.15	111.53	108.11
25	b	614	CLA	C4D-C3D-CAD	3.13	111.51	108.11
25	b	607	CLA	C4D-C3D-CAD	3.13	111.51	108.11
25	b	615	CLA	C4D-C3D-CAD	3.13	111.50	108.11
26	b	617	BCR	C20-C21-C22	-3.13	122.89	127.28
25	c	511	CLA	C4D-C3D-CAD	3.13	111.50	108.11
25	B	605	CLA	C4D-C3D-CAD	3.12	111.50	108.11
26	b	618	BCR	C24-C23-C22	-3.12	121.62	126.23
25	c	505	CLA	C4D-C3D-CAD	3.12	111.49	108.11
25	B	613	CLA	C4D-C3D-CAD	3.11	111.49	108.11
25	b	605	CLA	C4D-C3D-CAD	3.11	111.49	108.11
26	B	617	BCR	C20-C21-C22	-3.11	122.92	127.28
27	D	407	PL9	C20-C19-C21	3.11	120.62	115.23
23	c	520	LMG	O8-C28-C29	3.10	121.29	111.83
25	D	404	CLA	C4D-C3D-CAD	3.10	111.47	108.11
25	c	512	CLA	C4D-C3D-CAD	3.10	111.47	108.11
23	a	603	LMG	O8-C28-C29	3.10	121.28	111.83
25	c	503	CLA	C1-C2-C3	-3.10	121.12	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	BCR	C20-C21-C22	-3.09	122.94	127.28
25	b	610	CLA	C1-C2-C3	-3.09	121.13	126.20
25	c	510	CLA	C4D-C3D-CAD	3.08	111.46	108.11
23	C	519	LMG	O8-C28-C29	3.08	121.23	111.83
25	b	606	CLA	C4D-C3D-CAD	3.08	111.45	108.11
26	c	514	BCR	C16-C17-C18	-3.08	122.97	127.28
26	z	101	BCR	C38-C26-C25	-3.07	121.14	124.48
25	B	606	CLA	C4D-C3D-CAD	3.07	111.44	108.11
25	B	602	CLA	C4D-C3D-CAD	3.06	111.43	108.11
25	b	603	CLA	C4D-C3D-CAD	3.06	111.43	108.11
25	b	610	CLA	C4D-C3D-CAD	3.05	111.42	108.11
25	B	615	CLA	C4D-C3D-CAD	3.05	111.42	108.11
25	A	606	CLA	C4D-C3D-CAD	3.05	111.42	108.11
25	c	506	CLA	C4D-C3D-CAD	3.04	111.41	108.11
26	b	619	BCR	C33-C5-C6	-3.04	121.17	124.48
26	K	101	BCR	C24-C23-C22	-3.03	121.75	126.23
25	B	611	CLA	C4D-C3D-CAD	3.03	111.40	108.11
25	B	607	CLA	C4D-C3D-CAD	3.03	111.40	108.11
28	a	613	SQD	O48-C23-C24	3.03	121.08	111.83
27	A	610	PL9	C7-C3-C2	-3.03	119.82	123.39
26	h	101	BCR	C38-C26-C25	-3.03	121.18	124.48
25	C	501	CLA	C4D-C3D-CAD	3.03	111.39	108.11
34	d	402	PHO	C2D-C1D-ND	-3.02	107.24	109.43
25	B	610	CLA	C1-C2-C3	-3.02	121.24	126.20
25	a	606	CLA	C4D-C3D-CAD	3.02	111.39	108.11
25	b	611	CLA	C4D-C3D-CAD	3.02	111.38	108.11
34	d	402	PHO	C1-C2-C3	-3.01	121.26	126.20
29	L	102	LHG	C5-O7-C7	-3.01	110.58	117.80
26	A	609	BCR	C3-C4-C5	-3.01	108.69	114.06
25	B	616	CLA	C4D-C3D-CAD	3.01	111.37	108.11
25	C	504	CLA	C4D-C3D-CAD	3.01	111.37	108.11
25	b	613	CLA	C4D-C3D-CAD	3.01	111.37	108.11
25	C	510	CLA	C4D-C3D-CAD	3.00	111.37	108.11
27	D	407	PL9	C27-C28-C29	-3.00	120.76	127.62
25	b	616	CLA	C4D-C3D-CAD	3.00	111.36	108.11
23	A	603	LMG	O8-C28-C29	3.00	120.97	111.83
25	c	501	CLA	C4D-C3D-CAD	3.00	111.36	108.11
34	D	401	PHO	C2D-C1D-ND	-2.99	107.27	109.43
27	a	612	PL9	C22-C23-C24	-2.99	120.78	127.62
27	a	612	PL9	C17-C18-C19	-2.99	120.78	127.62
34	a	609	PHO	C2D-C1D-ND	-2.99	107.27	109.43
27	A	610	PL9	C17-C18-C19	-2.98	120.80	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	401	CLA	C4D-C3D-CAD	2.98	111.34	108.11
23	b	620	LMG	O8-C28-C29	2.98	120.91	111.83
25	B	603	CLA	C4D-C3D-CAD	2.97	111.33	108.11
33	c	516	DGD	O1G-C1A-C2A	2.97	120.90	111.83
26	D	406	BCR	C27-C26-C25	-2.97	118.69	122.70
26	C	515	BCR	C20-C21-C22	-2.97	123.11	127.28
25	B	610	CLA	C4D-C3D-CAD	2.97	111.33	108.11
27	a	612	PL9	C42-C43-C44	-2.97	120.83	127.62
34	D	402	PHO	C2D-C1D-ND	-2.96	107.29	109.43
25	d	403	CLA	C4D-C3D-CAD	2.96	111.33	108.11
26	C	515	BCR	C15-C16-C17	-2.96	117.45	123.52
25	c	504	CLA	C4D-C3D-CAD	2.96	111.32	108.11
25	c	513	CLA	C4D-C3D-CAD	2.96	111.32	108.11
26	D	406	BCR	C29-C30-C25	2.96	114.73	110.44
26	D	406	BCR	C38-C26-C27	2.95	119.88	113.60
25	c	509	CLA	C4D-C3D-CAD	2.94	111.30	108.11
28	A	611	SQD	O48-C23-C24	2.94	120.80	111.83
25	b	602	CLA	C4D-C3D-CAD	2.94	111.30	108.11
25	D	403	CLA	C4D-C3D-CAD	2.93	111.29	108.11
25	A	608	CLA	C4D-C3D-CAD	2.93	111.29	108.11
25	c	502	CLA	C4D-C3D-CAD	2.93	111.29	108.11
25	a	610	CLA	C4D-C3D-CAD	2.93	111.29	108.11
27	A	610	PL9	C7-C3-C4	2.93	119.32	116.91
26	b	618	BCR	C2-C1-C6	2.93	114.69	110.44
25	D	403	CLA	C1-C2-C3	-2.93	121.40	126.20
25	B	607	CLA	C1-C2-C3	-2.92	121.42	126.20
27	D	407	PL9	C15-C14-C16	2.91	120.28	115.23
25	C	513	CLA	C4D-C3D-CAD	2.91	111.27	108.11
26	B	619	BCR	C1-C6-C5	-2.91	118.66	122.64
33	C	518	DGD	O1G-C1A-C2A	2.91	120.70	111.83
25	C	502	CLA	C4D-C3D-CAD	2.90	111.26	108.11
25	C	506	CLA	C1-C2-C3	-2.90	121.44	126.20
26	H	101	BCR	C29-C30-C25	2.90	114.65	110.44
25	a	607	CLA	C4D-C3D-CAD	2.89	111.25	108.11
26	C	522	BCR	C33-C5-C6	-2.89	121.33	124.48
27	A	610	PL9	C42-C43-C44	-2.89	121.02	127.62
26	k	102	BCR	C24-C23-C22	-2.88	121.97	126.23
27	d	405	PL9	C20-C19-C21	2.88	120.23	115.23
25	A	607	CLA	C4D-C3D-CAD	2.87	111.22	108.11
25	B	609	CLA	C4D-C3D-CAD	2.87	111.22	108.11
27	a	612	PL9	C32-C33-C34	-2.86	121.07	127.62
23	c	518	LMG	O8-C28-C29	2.86	120.56	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	C4D-C3D-CAD	2.86	111.21	108.11
27	d	405	PL9	C17-C18-C19	-2.86	121.08	127.62
23	B	620	LMG	O8-C28-C29	2.86	120.55	111.83
26	b	617	BCR	C24-C23-C22	-2.85	122.01	126.23
25	C	509	CLA	C4D-C3D-CAD	2.85	111.21	108.11
25	c	508	CLA	C4D-C3D-CAD	2.84	111.19	108.11
26	B	617	BCR	C29-C30-C25	2.84	114.56	110.44
29	A	613	LHG	O8-C23-C24	2.84	120.48	111.83
26	D	406	BCR	C38-C26-C25	-2.83	121.40	124.48
25	a	608	CLA	C1-C2-C3	-2.83	121.56	126.20
27	A	610	PL9	C12-C13-C14	-2.83	121.15	127.62
27	a	612	PL9	C20-C19-C21	2.83	120.14	115.23
23	C	521	LMG	O8-C28-C29	2.82	120.45	111.83
33	C	516	DGD	O1G-C1A-C2A	2.82	120.44	111.83
25	c	507	CLA	C1-C2-C3	-2.82	121.58	126.20
29	l	101	LHG	O8-C23-C24	2.81	120.42	111.83
27	d	405	PL9	C15-C14-C16	2.81	120.11	115.23
29	a	616	LHG	C5-O7-C7	-2.81	111.07	117.80
25	B	604	CLA	C1-C2-C3	-2.81	121.59	126.20
28	L	103	SQD	O48-C23-C24	2.80	120.39	111.83
26	c	521	BCR	C29-C30-C25	2.80	114.51	110.44
29	l	101	LHG	C5-O7-C7	-2.80	111.10	117.80
27	a	612	PL9	C27-C28-C29	-2.80	121.22	127.62
25	C	506	CLA	C4D-C3D-CAD	2.79	111.14	108.11
28	f	101	SQD	O48-C23-C24	2.79	120.35	111.83
33	c	515	DGD	C2G-O2G-C1B	-2.78	111.13	117.80
27	d	405	PL9	C22-C23-C24	-2.78	121.26	127.62
25	a	608	CLA	C4D-C3D-CAD	2.78	111.12	108.11
33	c	517	DGD	O1G-C1A-C2A	2.77	120.29	111.83
27	D	407	PL9	C35-C34-C36	2.77	120.04	115.23
25	b	602	CLA	C1-C2-C3	-2.77	121.66	126.20
23	A	612	LMG	O8-C28-C29	2.77	120.28	111.83
26	C	522	BCR	C29-C30-C25	2.76	114.45	110.44
26	C	515	BCR	C16-C17-C18	-2.76	123.40	127.28
27	A	610	PL9	C45-C44-C46	2.76	120.01	115.23
25	B	604	CLA	C2C-C1C-NC	2.76	112.88	109.98
25	B	613	CLA	C1-C2-C3	-2.75	121.69	126.20
27	d	405	PL9	C25-C24-C26	2.75	120.00	115.23
25	b	608	CLA	C4D-C3D-CAD	2.74	111.08	108.11
25	B	612	CLA	C1-C2-C3	-2.74	121.70	126.20
25	B	608	CLA	C4D-C3D-CAD	2.74	111.08	108.11
23	a	614	LMG	C8-O7-C10	-2.74	111.25	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	102	LHG	O8-C23-C24	2.74	120.18	111.83
25	D	405	CLA	C4D-C3D-CAD	2.73	111.08	108.11
25	C	508	CLA	C4D-C3D-CAD	2.73	111.07	108.11
29	d	406	LHG	C5-O7-C7	-2.73	111.27	117.80
25	c	501	CLA	C1-C2-C3	-2.72	121.73	126.20
28	L	103	SQD	O8-S-C6	2.72	111.23	105.97
33	C	517	DGD	O1G-C1A-C2A	2.72	120.13	111.83
26	B	618	BCR	C38-C26-C25	-2.72	121.52	124.48
25	a	607	CLA	CHD-C1D-ND	-2.72	120.98	124.80
29	a	615	LHG	O8-C23-C24	2.72	120.12	111.83
27	d	405	PL9	C45-C44-C46	2.72	119.94	115.23
27	a	612	PL9	C7-C3-C4	2.71	119.15	116.91
25	D	403	CLA	CHD-C1D-ND	-2.71	120.98	124.80
27	A	610	PL9	C53-C6-C1	2.71	120.83	115.28
27	a	612	PL9	C7-C3-C2	-2.71	120.19	123.39
25	B	606	CLA	C1-C2-C3	-2.71	121.76	126.20
25	C	503	CLA	C1-C2-C3	-2.71	121.76	126.20
25	A	607	CLA	CHD-C1D-ND	-2.71	121.00	124.80
26	b	617	BCR	C38-C26-C27	2.70	119.36	113.60
27	d	405	PL9	C35-C34-C36	2.70	119.91	115.23
27	D	407	PL9	C22-C23-C24	-2.69	121.46	127.62
26	c	514	BCR	C20-C21-C22	-2.69	123.50	127.28
27	a	612	PL9	C45-C44-C46	2.69	119.90	115.23
27	D	407	PL9	C30-C29-C31	2.68	119.88	115.23
26	C	515	BCR	C38-C26-C25	-2.68	121.56	124.48
25	C	501	CLA	C1-C2-C3	-2.67	121.82	126.20
29	A	614	LHG	O8-C23-C24	2.67	119.98	111.83
25	c	508	CLA	C1-C2-C3	-2.67	121.82	126.20
34	D	402	PHO	C1-C2-C3	-2.67	121.82	126.20
27	D	407	PL9	C17-C18-C19	-2.67	121.52	127.62
26	k	102	BCR	C8-C7-C6	-2.66	119.88	127.00
23	A	612	LMG	C8-O7-C10	-2.66	111.42	117.80
33	C	516	DGD	C2G-O2G-C1B	-2.66	111.42	117.80
26	k	102	BCR	C11-C10-C9	-2.66	123.55	127.28
25	a	608	CLA	CHD-C1D-ND	-2.66	121.06	124.80
25	C	504	CLA	CHD-C1D-ND	-2.66	121.06	124.80
29	D	408	LHG	C5-O7-C7	-2.65	111.45	117.80
33	H	102	DGD	O1G-C1A-C2A	2.65	119.92	111.83
25	a	607	CLA	C1-C2-C3	-2.65	121.86	126.20
27	A	610	PL9	C15-C14-C16	2.65	119.83	115.23
26	h	101	BCR	C33-C5-C6	-2.64	121.60	124.48
23	c	520	LMG	C8-O7-C10	-2.64	111.47	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	508	CLA	C1-C2-C3	-2.64	121.87	126.20
25	c	506	CLA	C1-C2-C3	-2.64	121.87	126.20
25	A	606	CLA	CHD-C1D-ND	-2.64	121.09	124.80
25	A	607	CLA	C1-C2-C3	-2.64	121.87	126.20
25	B	602	CLA	CHD-C1D-ND	-2.64	121.09	124.80
26	c	514	BCR	C15-C16-C17	-2.64	118.13	123.52
27	D	407	PL9	C25-C24-C26	2.64	119.80	115.23
27	D	407	PL9	C12-C13-C14	-2.64	121.59	127.62
26	a	611	BCR	C3-C4-C5	-2.64	109.36	114.06
27	a	612	PL9	C53-C6-C1	2.63	120.67	115.28
25	B	603	CLA	C1-C2-C3	-2.63	121.89	126.20
29	E	101	LHG	O8-C23-C24	2.63	119.85	111.83
28	f	101	SQD	C3-C4-C5	2.63	114.99	110.23
26	H	101	BCR	C33-C5-C6	-2.63	121.62	124.48
25	C	513	CLA	CHD-C1D-ND	-2.62	121.11	124.80
26	B	617	BCR	C27-C26-C25	-2.62	119.16	122.70
25	c	504	CLA	CHD-C1D-ND	-2.62	121.12	124.80
27	d	405	PL9	C12-C13-C14	-2.62	121.63	127.62
23	B	624	LMG	C8-O7-C10	-2.62	111.53	117.80
25	a	610	CLA	CHD-C1D-ND	-2.62	121.12	124.80
25	c	508	CLA	CHD-C1D-ND	-2.62	121.12	124.80
25	b	604	CLA	C2C-C1C-NC	2.61	112.73	109.98
27	d	405	PL9	C30-C29-C31	2.61	119.76	115.23
28	F	101	SQD	O6-C1-C2	2.61	112.24	108.27
26	K	101	BCR	C8-C7-C6	-2.61	120.04	127.00
27	d	405	PL9	C53-C6-C1	2.60	120.61	115.28
25	b	602	CLA	CHD-C1D-ND	-2.60	121.14	124.80
29	d	407	LHG	O8-C23-C24	2.60	119.77	111.83
25	c	513	CLA	CHD-C1D-ND	-2.60	121.14	124.80
25	b	608	CLA	C1-C2-C3	-2.60	121.94	126.20
27	A	610	PL9	C25-C24-C26	2.60	119.73	115.23
26	h	101	BCR	C28-C27-C26	-2.59	109.43	114.06
25	b	613	CLA	C1-C2-C3	-2.59	121.96	126.20
26	B	619	BCR	C3-C4-C5	-2.59	109.44	114.06
23	b	624	LMG	C8-O7-C10	-2.59	111.61	117.80
27	A	610	PL9	C27-C28-C29	-2.58	121.71	127.62
25	b	612	CLA	C1-C2-C3	-2.58	121.98	126.20
25	b	604	CLA	C1-C2-C3	-2.57	121.98	126.20
27	a	612	PL9	C25-C24-C26	2.57	119.69	115.23
25	B	614	CLA	CHD-C1D-ND	-2.57	121.18	124.80
25	C	513	CLA	C1-C2-C3	-2.57	121.98	126.20
26	A	609	BCR	C15-C16-C17	-2.57	118.26	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	C1-C2-C3	-2.57	121.99	126.20
27	A	610	PL9	C20-C19-C21	2.56	119.68	115.23
25	C	508	CLA	CHD-C1D-ND	-2.56	121.20	124.80
25	D	405	CLA	C1-C2-C3	-2.56	122.00	126.20
25	C	510	CLA	CHD-C1D-ND	-2.56	121.20	124.80
23	d	408	LMG	C8-O7-C10	-2.56	111.67	117.80
25	b	605	CLA	CHD-C1D-ND	-2.56	121.20	124.80
33	h	102	DGD	O1G-C1A-C2A	2.55	119.62	111.83
25	D	405	CLA	CHD-C1D-ND	-2.55	121.21	124.80
25	b	608	CLA	CHD-C1D-ND	-2.55	121.21	124.80
26	c	521	BCR	C3-C4-C5	-2.55	109.51	114.06
25	a	606	CLA	CHD-C1D-ND	-2.55	121.22	124.80
27	d	405	PL9	C32-C33-C34	-2.55	121.79	127.62
25	C	501	CLA	C2C-C1C-NC	2.55	112.66	109.98
27	D	407	PL9	C53-C6-C1	2.55	120.49	115.28
25	b	614	CLA	CHD-C1D-ND	-2.55	121.22	124.80
27	D	407	PL9	C45-C44-C46	2.55	119.65	115.23
25	d	401	CLA	CHD-C1D-ND	-2.54	121.22	124.80
25	c	501	CLA	CHD-C1D-ND	-2.54	121.22	124.80
27	a	612	PL9	C40-C39-C41	2.54	119.63	115.23
27	a	612	PL9	C12-C13-C14	-2.54	121.82	127.62
23	b	624	LMG	O8-C28-C29	2.54	119.57	111.83
26	c	514	BCR	C21-C20-C19	-2.53	115.86	123.20
28	L	101	SQD	O48-C23-C24	2.53	119.55	111.83
25	a	610	CLA	C1-C2-C3	-2.53	122.05	126.20
26	K	101	BCR	C10-C11-C12	-2.53	115.87	123.20
25	b	604	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
29	a	615	LHG	C5-O7-C7	-2.52	111.76	117.80
26	b	619	BCR	C3-C4-C5	-2.52	109.57	114.06
25	B	616	CLA	CHD-C1D-ND	-2.51	121.26	124.80
33	c	515	DGD	O1G-C1A-C2A	2.51	119.50	111.83
27	A	610	PL9	C10-C9-C11	2.51	119.59	115.23
25	B	610	CLA	CHD-C1D-ND	-2.51	121.27	124.80
27	A	610	PL9	C30-C29-C31	2.51	119.59	115.23
25	B	605	CLA	CHD-C1D-ND	-2.51	121.27	124.80
25	D	404	CLA	CHD-C1D-ND	-2.51	121.27	124.80
25	B	604	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
26	C	515	BCR	C21-C20-C19	-2.51	115.93	123.20
25	a	608	CLA	C2C-C1C-NC	2.51	112.61	109.98
27	D	407	PL9	C32-C33-C34	-2.51	121.89	127.62
25	b	616	CLA	CHD-C1D-ND	-2.50	121.28	124.80
25	c	509	CLA	CHD-C1D-ND	-2.50	121.28	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C29-C30-C25	2.50	114.06	110.44
26	t	102	BCR	C3-C4-C5	-2.50	109.61	114.06
26	K	101	BCR	C7-C8-C9	-2.49	122.55	126.23
25	C	506	CLA	CHD-C1D-ND	-2.49	121.29	124.80
25	d	401	CLA	C1-C2-C3	-2.49	122.11	126.20
27	D	407	PL9	C10-C9-C11	2.49	119.55	115.23
26	K	101	BCR	C20-C21-C22	-2.49	123.79	127.28
25	B	609	CLA	C1-C2-C3	-2.49	122.12	126.20
23	a	614	LMG	O8-C28-C29	2.48	119.41	111.83
35	E	102	HEM	O2D-CGD-CBD	2.48	121.85	114.00
27	A	610	PL9	C40-C39-C41	2.48	119.54	115.23
25	A	608	CLA	CHD-C1D-ND	-2.48	121.31	124.80
28	f	101	SQD	C45-O47-C7	-2.48	111.86	117.80
26	C	522	BCR	C15-C16-C17	-2.48	118.45	123.52
23	B	624	LMG	O8-C28-C29	2.47	119.38	111.83
25	b	607	CLA	C1-C2-C3	-2.47	122.14	126.20
25	c	512	CLA	C2C-C1C-NC	2.47	112.58	109.98
25	B	609	CLA	CHD-C1D-ND	-2.47	121.33	124.80
27	d	405	PL9	C42-C43-C44	-2.47	121.97	127.62
26	B	617	BCR	C38-C26-C27	2.47	118.85	113.60
25	B	603	CLA	CHD-C1D-ND	-2.47	121.33	124.80
25	C	502	CLA	CHD-C1D-ND	-2.46	121.33	124.80
25	d	403	CLA	CHD-C1D-ND	-2.46	121.34	124.80
26	C	522	BCR	C33-C5-C4	2.46	118.85	113.60
25	b	609	CLA	C1-C2-C3	-2.46	122.16	126.20
25	B	607	CLA	C2C-C1C-NC	2.46	112.57	109.98
25	B	615	CLA	C2C-C1C-NC	2.46	112.57	109.98
25	B	613	CLA	C2C-C1C-NC	2.46	112.57	109.98
25	C	507	CLA	C2C-C1C-NC	2.46	112.56	109.98
28	A	611	SQD	O9-S-C6	2.46	110.42	106.76
28	F	101	SQD	C45-O47-C7	-2.46	111.92	117.80
26	k	102	BCR	C16-C15-C14	-2.46	118.49	123.52
25	C	511	CLA	C2C-C1C-NC	2.45	112.56	109.98
29	a	616	LHG	O8-C23-C24	2.45	119.30	111.83
25	B	608	CLA	CHD-C1D-ND	-2.45	121.36	124.80
23	D	409	LMG	C8-O7-C10	-2.45	111.94	117.80
25	c	504	CLA	C2C-C1C-NC	2.44	112.55	109.98
25	c	506	CLA	CHD-C1D-ND	-2.44	121.36	124.80
25	a	608	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
23	D	409	LMG	O8-C28-C29	2.44	119.28	111.83
25	C	503	CLA	C2C-C1C-NC	2.44	112.55	109.98
25	C	501	CLA	CHD-C1D-ND	-2.44	121.37	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C28-C27-C26	-2.44	109.71	114.06
25	B	605	CLA	C2C-C1C-NC	2.44	112.54	109.98
25	B	606	CLA	CHD-C1D-ND	-2.44	121.38	124.80
25	C	511	CLA	C1-C2-C3	-2.44	122.21	126.20
26	t	102	BCR	C28-C27-C26	-2.43	109.72	114.06
29	d	406	LHG	O8-C23-C24	2.43	119.25	111.83
25	c	503	CLA	C2C-C1C-NC	2.43	112.53	109.98
25	c	501	CLA	C2C-C1C-NC	2.43	112.53	109.98
25	c	505	CLA	CHD-C1D-ND	-2.43	121.39	124.80
26	k	102	BCR	C23-C24-C25	-2.42	120.53	127.00
25	C	512	CLA	C2C-C1C-NC	2.42	112.52	109.98
25	c	510	CLA	C2C-C1C-NC	2.42	112.52	109.98
25	C	509	CLA	CHD-C1D-ND	-2.42	121.40	124.80
26	b	618	BCR	C29-C30-C25	2.42	113.95	110.44
28	a	613	SQD	C45-O47-C7	-2.42	112.01	117.80
25	c	510	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	C	509	CLA	C2C-C1C-NC	2.42	112.52	109.98
25	b	606	CLA	CHD-C1D-ND	-2.41	121.41	124.80
33	c	515	DGD	O6D-C5D-C6D	2.41	111.48	106.69
25	B	602	CLA	C1-C2-C3	-2.40	122.26	126.20
25	C	511	CLA	CHD-C1D-ND	-2.40	121.42	124.80
25	b	609	CLA	CHD-C1D-ND	-2.40	121.42	124.80
25	b	611	CLA	CHD-C1D-ND	-2.40	121.42	124.80
29	D	408	LHG	O8-C23-C24	2.40	119.16	111.83
25	d	403	CLA	C2C-C1C-NC	2.40	112.50	109.98
25	B	607	CLA	CHD-C1D-ND	-2.40	121.42	124.80
25	b	615	CLA	CHD-C1D-ND	-2.40	121.42	124.80
27	A	610	PL9	C35-C34-C36	2.40	119.39	115.23
26	k	102	BCR	C20-C21-C22	-2.40	123.92	127.28
25	c	504	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
26	B	619	BCR	C33-C5-C6	-2.39	121.87	124.48
25	c	511	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	C	507	CLA	C1-C2-C3	-2.39	122.28	126.20
25	B	608	CLA	C1-C2-C3	-2.39	122.28	126.20
26	k	102	BCR	C10-C11-C12	-2.39	116.28	123.20
26	k	102	BCR	C21-C20-C19	-2.39	116.28	123.20
25	B	607	CLA	CHC-C1C-C2C	-2.39	120.17	126.95
25	b	603	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	b	610	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	B	601	CLA	CHD-C1D-ND	-2.38	121.45	124.80
25	c	502	CLA	CHD-C1D-ND	-2.38	121.45	124.80
27	d	405	PL9	C10-C9-C11	2.38	119.36	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	101	HEM	O2D-CGD-CBD	2.38	121.52	114.00
25	b	613	CLA	C2C-C1C-NC	2.38	112.48	109.98
25	c	511	CLA	C2C-C1C-NC	2.38	112.48	109.98
26	T	101	BCR	C33-C5-C4	2.38	118.67	113.60
25	b	607	CLA	CHD-C1D-ND	-2.38	121.46	124.80
29	E	101	LHG	C5-O7-C7	-2.37	112.12	117.80
26	k	102	BCR	C7-C8-C9	-2.37	122.72	126.23
25	B	613	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
25	c	509	CLA	C2C-C1C-NC	2.37	112.47	109.98
27	D	407	PL9	C42-C43-C44	-2.37	122.20	127.62
25	b	601	CLA	CHD-C1D-ND	-2.36	121.47	124.80
25	b	611	CLA	C2C-C1C-NC	2.36	112.47	109.98
25	C	511	CLA	CHC-C1C-C2C	-2.36	120.23	126.95
23	a	603	LMG	C8-O7-C10	-2.36	112.14	117.80
25	C	504	CLA	C1-C2-C3	-2.36	122.33	126.20
25	B	613	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	b	609	CLA	C2C-C1C-NC	2.36	112.46	109.98
36	V	201	HEC	O2D-CGD-CBD	2.36	121.45	114.00
25	C	501	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
25	B	615	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
35	e	101	HEM	C3B-C2B-C1B	2.36	108.18	106.41
25	C	507	CLA	CHC-C1C-C2C	-2.35	120.27	126.95
26	t	102	BCR	C8-C7-C6	-2.35	120.72	127.00
25	b	607	CLA	C2C-C1C-NC	2.35	112.45	109.98
26	B	619	BCR	C4-C5-C6	-2.34	119.54	122.70
25	C	504	CLA	C2C-C1C-NC	2.34	112.44	109.98
25	C	505	CLA	CHD-C1D-ND	-2.34	121.50	124.80
25	B	603	CLA	C2C-C1C-NC	2.34	112.44	109.98
26	k	102	BCR	C28-C27-C26	-2.34	109.89	114.06
25	B	606	CLA	C2C-C1C-NC	2.34	112.44	109.98
25	c	501	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
25	C	512	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
25	B	606	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
25	c	512	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
25	C	503	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
25	C	513	CLA	C2C-C1C-NC	2.33	112.43	109.98
25	c	512	CLA	CHD-C1D-ND	-2.33	121.53	124.80
27	a	612	PL9	C10-C9-C11	2.33	119.27	115.23
26	b	619	BCR	C33-C5-C4	2.33	118.56	113.60
25	d	403	CLA	CHC-C1C-C2C	-2.33	120.34	126.95
25	C	509	CLA	CHC-C1C-C2C	-2.33	120.34	126.95
25	C	510	CLA	C2C-C1C-NC	2.32	112.42	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	617	BCR	C38-C26-C25	-2.32	121.95	124.48
26	t	102	BCR	C11-C12-C13	-2.32	120.00	126.36
25	C	507	CLA	CHD-C1D-ND	-2.32	121.53	124.80
25	b	613	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	B	605	CLA	CHC-C1C-C2C	-2.32	120.35	126.95
25	b	606	CLA	CHC-C1C-C2C	-2.32	120.35	126.95
28	a	613	SQD	O6-C1-C2	2.32	111.80	108.27
25	c	507	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	B	611	CLA	C2C-C1C-NC	2.32	112.42	109.98
25	c	513	CLA	C1-C2-C3	-2.32	122.40	126.20
26	T	101	BCR	C20-C19-C18	-2.32	120.01	126.36
25	c	513	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
25	C	513	CLA	CHC-C1C-C2C	-2.32	120.37	126.95
25	b	607	CLA	CHC-C1C-C2C	-2.32	120.37	126.95
26	B	619	BCR	C33-C5-C4	2.31	118.53	113.60
25	C	503	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	C	512	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	C	504	CLA	CHC-C1C-C2C	-2.31	120.37	126.95
26	b	618	BCR	C15-C16-C17	-2.31	118.79	123.52
26	c	514	BCR	C38-C26-C25	-2.31	121.96	124.48
26	B	617	BCR	C15-C16-C17	-2.31	118.79	123.52
26	T	101	BCR	C3-C4-C5	-2.31	109.94	114.06
26	z	101	BCR	C15-C16-C17	-2.31	118.80	123.52
36	v	201	HEC	O2D-CGD-CBD	2.31	121.29	114.00
25	B	611	CLA	CHD-C1D-ND	-2.31	121.56	124.80
25	c	503	CLA	CHD-C1D-ND	-2.30	121.56	124.80
25	b	603	CLA	C2C-C1C-NC	2.30	112.40	109.98
25	c	511	CLA	CHC-C1C-C2C	-2.30	120.40	126.95
25	C	510	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
25	c	510	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
25	B	611	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
25	B	616	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
27	a	612	PL9	C51-C49-C50	2.29	119.87	114.59
28	F	101	SQD	C44-O6-C1	-2.29	108.88	113.80
25	c	509	CLA	CHC-C1C-C2C	-2.29	120.43	126.95
26	b	619	BCR	C23-C24-C25	-2.29	120.87	127.00
23	b	620	LMG	C8-O7-C10	-2.29	112.31	117.80
25	B	603	CLA	CHC-C1C-C2C	-2.29	120.43	126.95
27	a	612	PL9	C30-C29-C31	2.29	119.21	115.23
25	c	513	CLA	C2C-C1C-NC	2.29	112.39	109.98
25	b	603	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
26	K	101	BCR	C23-C24-C25	-2.29	120.88	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	606	CLA	C2C-C1C-NC	2.29	112.39	109.98
25	c	507	CLA	C2C-C1C-NC	2.29	112.38	109.98
25	b	613	CLA	CHC-C1C-C2C	-2.28	120.45	126.95
25	b	603	CLA	C1-C2-C3	-2.28	122.46	126.20
25	B	615	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	D	403	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
25	C	508	CLA	C1D-CHD-C4C	-2.28	121.18	126.02
23	d	408	LMG	O8-C28-C29	2.27	118.77	111.83
25	B	612	CLA	CHD-C1D-ND	-2.27	121.60	124.80
25	c	502	CLA	C2C-C1C-NC	2.27	112.37	109.98
25	b	612	CLA	CHD-C1D-ND	-2.27	121.61	124.80
25	c	503	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
25	b	611	CLA	CHC-C1C-C2C	-2.27	120.50	126.95
25	C	505	CLA	C1D-CHD-C4C	-2.27	121.20	126.02
25	C	509	CLA	C1-C2-C3	-2.26	122.49	126.20
27	a	612	PL9	C35-C34-C36	2.26	119.15	115.23
25	D	405	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
25	C	502	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
25	B	604	CLA	CHD-C1D-ND	-2.26	121.62	124.80
25	b	615	CLA	CHC-C1C-C2C	-2.26	120.53	126.95
25	c	507	CLA	CHC-C1C-C2C	-2.26	120.53	126.95
25	B	615	CLA	C1-C2-C3	-2.25	122.51	126.20
28	F	101	SQD	O48-C23-C24	2.25	118.69	111.83
26	K	101	BCR	C21-C20-C19	-2.25	116.68	123.20
25	c	502	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
27	D	407	PL9	C51-C49-C50	2.25	119.76	114.59
26	d	404	BCR	C38-C26-C27	2.24	118.38	113.60
25	b	601	CLA	CHC-C1C-C2C	-2.24	120.57	126.95
26	B	617	BCR	C8-C7-C6	-2.24	121.01	127.00
33	C	517	DGD	C2G-O2G-C1B	-2.24	112.43	117.80
28	L	103	SQD	O9-S-C6	2.24	110.10	106.76
25	B	609	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
26	K	101	BCR	C16-C15-C14	-2.24	118.94	123.52
25	a	607	CLA	C3D-C2D-C1D	2.24	108.89	105.83
25	B	616	CLA	C2C-C1C-NC	2.24	112.33	109.98
25	c	505	CLA	C3D-C2D-C1D	2.24	108.88	105.83
25	D	403	CLA	C2C-C1C-NC	2.24	112.33	109.98
28	f	101	SQD	O9-S-C6	2.23	110.09	106.76
25	D	405	CLA	C2C-C1C-NC	2.23	112.33	109.98
25	C	508	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
25	C	502	CLA	C2C-C1C-NC	2.23	112.32	109.98
27	A	610	PL9	C51-C49-C50	2.23	119.72	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	CHC-C1C-C2C	-2.23	120.62	126.95
35	E	102	HEM	C3B-C2B-C1B	2.23	108.08	106.41
25	A	608	CLA	CHC-C1C-C2C	-2.23	120.62	126.95
25	a	606	CLA	C1D-CHD-C4C	-2.23	121.29	126.02
25	b	612	CLA	CHC-C1C-C2C	-2.23	120.62	126.95
25	b	615	CLA	C2C-C1C-NC	2.23	112.32	109.98
25	b	604	CLA	CHD-C1D-ND	-2.23	121.67	124.80
25	b	608	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
25	b	601	CLA	C1D-CHD-C4C	-2.22	121.30	126.02
25	a	607	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
25	B	601	CLA	C2C-C1C-NC	2.22	112.31	109.98
25	A	608	CLA	C2C-C1C-NC	2.22	112.31	109.98
25	a	610	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
28	F	101	SQD	O9-S-C6	2.22	110.07	106.76
25	B	615	CLA	C1D-CHD-C4C	-2.22	121.31	126.02
26	b	617	BCR	C23-C24-C25	-2.22	121.08	127.00
23	c	518	LMG	C8-O7-C10	-2.22	112.49	117.80
25	B	601	CLA	CHC-C1C-C2C	-2.21	120.66	126.95
25	B	609	CLA	C2C-C1C-NC	2.21	112.31	109.98
26	B	618	BCR	C15-C16-C17	-2.21	119.00	123.52
25	B	610	CLA	C2C-C1C-NC	2.21	112.30	109.98
25	c	508	CLA	CHC-C1C-C2C	-2.21	120.67	126.95
25	B	614	CLA	C1-C2-C3	-2.21	122.58	126.20
26	c	514	BCR	C28-C27-C26	-2.21	110.12	114.06
25	A	607	CLA	CHC-C1C-C2C	-2.21	120.68	126.95
26	b	617	BCR	C3-C4-C5	-2.20	110.13	114.06
25	B	611	CLA	C1D-CHD-C4C	-2.20	121.34	126.02
25	a	606	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
25	C	509	CLA	C1D-CHD-C4C	-2.20	121.34	126.02
25	D	405	CLA	C1D-CHD-C4C	-2.20	121.34	126.02
25	b	601	CLA	C2C-C1C-NC	2.20	112.29	109.98
25	A	606	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
25	C	510	CLA	C3D-C2D-C1D	2.20	108.83	105.83
25	C	501	CLA	C1D-CHD-C4C	-2.20	121.35	126.02
33	C	518	DGD	C2G-O2G-C1B	-2.20	112.54	117.80
25	b	616	CLA	C1D-CHD-C4C	-2.20	121.35	126.02
25	C	506	CLA	CHC-C1C-C2C	-2.20	120.71	126.95
23	a	603	LMG	C3-C4-C5	2.20	114.21	110.23
23	C	521	LMG	O2-C2-C3	-2.19	105.20	110.38
29	A	613	LHG	C5-O7-C7	-2.19	112.55	117.80
25	c	505	CLA	C1D-CHD-C4C	-2.19	121.36	126.02
25	C	506	CLA	C2C-C1C-NC	2.19	112.28	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	613	CLA	C1D-CHD-C4C	-2.19	121.37	126.02
25	b	612	CLA	C1D-CHD-C4C	-2.19	121.37	126.02
25	b	609	CLA	C1D-CHD-C4C	-2.19	121.37	126.02
25	c	509	CLA	C1-C2-C3	-2.19	122.62	126.20
25	b	610	CLA	C1D-CHD-C4C	-2.19	121.38	126.02
26	k	102	BCR	C38-C26-C27	2.19	118.25	113.60
25	b	605	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
26	B	619	BCR	C23-C24-C25	-2.18	121.18	127.00
25	C	508	CLA	C2C-C1C-NC	2.18	112.27	109.98
25	a	606	CLA	C2C-C1C-NC	2.18	112.27	109.98
25	B	610	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
25	c	506	CLA	C1D-CHD-C4C	-2.18	121.39	126.02
25	b	602	CLA	C1D-CHD-C4C	-2.17	121.40	126.02
25	c	509	CLA	C1D-CHD-C4C	-2.17	121.40	126.02
25	c	504	CLA	C1-C2-C3	-2.17	122.64	126.20
25	C	502	CLA	C1D-CHD-C4C	-2.17	121.40	126.02
25	A	606	CLA	C2C-C1C-NC	2.17	112.26	109.98
25	c	502	CLA	C1D-CHD-C4C	-2.17	121.41	126.02
25	C	505	CLA	C3D-C2D-C1D	2.17	108.79	105.83
25	c	511	CLA	C1-C2-C3	-2.17	122.64	126.20
26	t	102	BCR	C7-C6-C5	-2.17	116.56	121.56
26	c	521	BCR	C33-C5-C4	2.17	118.22	113.60
26	A	609	BCR	C33-C5-C4	2.17	118.22	113.60
25	b	610	CLA	C2C-C1C-NC	2.17	112.26	109.98
25	c	510	CLA	C1D-CHD-C4C	-2.17	121.41	126.02
25	d	403	CLA	C1D-CHD-C4C	-2.17	121.41	126.02
25	B	608	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
25	b	616	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
25	B	612	CLA	C1D-CHD-C4C	-2.17	121.42	126.02
25	A	606	CLA	C1D-CHD-C4C	-2.16	121.42	126.02
25	B	609	CLA	C1D-CHD-C4C	-2.16	121.43	126.02
25	c	508	CLA	C1D-CHD-C4C	-2.16	121.43	126.02
25	a	610	CLA	C2C-C1C-NC	2.16	112.25	109.98
25	a	608	CLA	C1D-CHD-C4C	-2.16	121.43	126.02
25	a	606	CLA	C1-C2-C3	-2.16	122.66	126.20
25	B	601	CLA	C1D-CHD-C4C	-2.16	121.44	126.02
27	d	405	PL9	C40-C39-C41	2.16	118.97	115.23
25	b	603	CLA	C1D-CHD-C4C	-2.16	121.44	126.02
27	d	405	PL9	C51-C49-C50	2.16	119.55	114.59
26	C	514	BCR	C3-C4-C5	-2.16	110.21	114.06
25	C	505	CLA	C1-C2-C3	-2.15	122.67	126.20
26	C	515	BCR	C36-C18-C19	2.15	121.38	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	607	CLA	C2C-C1C-NC	2.15	112.24	109.98
28	A	611	SQD	C45-O47-C7	-2.15	112.64	117.80
33	c	517	DGD	C2G-O2G-C1B	-2.15	112.64	117.80
25	c	507	CLA	C1D-CHD-C4C	-2.15	121.45	126.02
25	C	503	CLA	C1D-CHD-C4C	-2.15	121.45	126.02
25	b	612	CLA	C2C-C1C-NC	2.15	112.24	109.98
25	B	614	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
25	b	604	CLA	C3D-C2D-C1D	2.15	108.76	105.83
25	b	606	CLA	C1D-CHD-C4C	-2.15	121.46	126.02
25	b	607	CLA	C1D-CHD-C4C	-2.15	121.46	126.02
26	b	618	BCR	C21-C20-C19	-2.15	116.98	123.20
25	A	608	CLA	C1D-CHD-C4C	-2.15	121.46	126.02
25	B	612	CLA	CHC-C1C-C2C	-2.14	120.85	126.95
25	b	605	CLA	C2C-C1C-NC	2.14	112.23	109.98
25	c	511	CLA	C1D-CHD-C4C	-2.14	121.46	126.02
23	B	620	LMG	C8-O7-C10	-2.14	112.67	117.80
25	b	611	CLA	C1D-CHD-C4C	-2.14	121.47	126.02
25	b	610	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
25	B	608	CLA	C3D-C2D-C1D	2.14	108.75	105.83
25	B	606	CLA	C1D-CHD-C4C	-2.14	121.48	126.02
25	B	616	CLA	C1D-CHD-C4C	-2.14	121.48	126.02
25	C	510	CLA	C1D-CHD-C4C	-2.14	121.48	126.02
25	B	602	CLA	C1D-CHD-C4C	-2.14	121.48	126.02
25	B	605	CLA	C1D-CHD-C4C	-2.13	121.48	126.02
25	B	607	CLA	C1D-CHD-C4C	-2.13	121.48	126.02
26	C	522	BCR	C4-C5-C6	-2.13	119.82	122.70
25	d	401	CLA	C1D-CHD-C4C	-2.13	121.49	126.02
25	c	513	CLA	C3D-C2D-C1D	2.13	108.74	105.83
26	c	521	BCR	C16-C15-C14	-2.13	119.16	123.52
25	B	608	CLA	C2C-C1C-NC	2.13	112.22	109.98
26	D	406	BCR	C3-C4-C5	-2.13	110.26	114.06
26	C	514	BCR	C28-C27-C26	-2.13	110.26	114.06
28	a	613	SQD	O48-C23-O10	-2.13	118.31	123.63
25	C	507	CLA	C1D-CHD-C4C	-2.13	121.50	126.02
23	b	620	LMG	O7-C10-O9	-2.13	118.73	123.70
26	C	514	BCR	C11-C12-C13	-2.13	120.53	126.36
25	b	608	CLA	C2C-C1C-NC	2.13	112.21	109.98
25	b	605	CLA	C1D-CHD-C4C	-2.12	121.50	126.02
28	a	613	SQD	O9-S-C6	2.12	109.93	106.76
25	B	602	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
23	A	603	LMG	C8-O7-C10	-2.12	112.72	117.80
25	C	513	CLA	C3D-C2D-C1D	2.12	108.73	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	C3D-C2D-C1D	2.12	108.73	105.83
25	a	607	CLA	C1D-CHD-C4C	-2.12	121.51	126.02
26	H	101	BCR	C11-C12-C13	-2.12	120.55	126.36
33	c	516	DGD	O3G-C1D-C2D	2.12	111.49	108.27
25	b	614	CLA	C3D-C2D-C1D	2.12	108.72	105.83
25	D	404	CLA	C1D-CHD-C4C	-2.12	121.52	126.02
25	c	503	CLA	C1D-CHD-C4C	-2.12	121.52	126.02
25	b	608	CLA	C3D-C2D-C1D	2.12	108.72	105.83
25	b	615	CLA	C1D-CHD-C4C	-2.12	121.52	126.02
26	d	404	BCR	C3-C4-C5	-2.12	110.28	114.06
25	c	506	CLA	CHC-C1C-C2C	-2.12	120.93	126.95
25	B	614	CLA	C1D-CHD-C4C	-2.12	121.52	126.02
26	C	522	BCR	C10-C11-C12	-2.12	117.07	123.20
25	A	606	CLA	C3D-C2D-C1D	2.11	108.72	105.83
25	B	601	CLA	C3D-C2D-C1D	2.11	108.72	105.83
25	B	610	CLA	C1D-CHD-C4C	-2.11	121.53	126.02
25	D	403	CLA	C1D-CHD-C4C	-2.11	121.53	126.02
25	D	403	CLA	C3D-C2D-C1D	2.11	108.71	105.83
25	b	615	CLA	C1-C2-C3	-2.11	122.74	126.20
25	A	607	CLA	C1D-CHD-C4C	-2.11	121.53	126.02
25	a	608	CLA	C3D-C2D-C1D	2.11	108.71	105.83
25	c	501	CLA	C1D-CHD-C4C	-2.11	121.53	126.02
26	B	619	BCR	C38-C26-C27	2.11	118.09	113.60
25	b	602	CLA	C3D-C2D-C1D	2.11	108.71	105.83
26	C	514	BCR	C8-C7-C6	-2.11	121.37	127.00
27	d	405	PL9	C7-C3-C2	-2.11	120.90	123.39
33	C	516	DGD	O6D-C5D-C6D	2.11	110.87	106.69
25	C	511	CLA	C1D-CHD-C4C	-2.11	121.54	126.02
25	c	504	CLA	C1D-CHD-C4C	-2.11	121.54	126.02
25	b	611	CLA	C3D-C2D-C1D	2.11	108.70	105.83
25	B	603	CLA	C1D-CHD-C4C	-2.11	121.55	126.02
25	b	604	CLA	CHC-C1C-NC	2.10	127.48	124.31
25	B	604	CLA	C3D-C2D-C1D	2.10	108.70	105.83
26	d	404	BCR	C11-C12-C13	-2.10	120.60	126.36
25	b	609	CLA	CHA-C1A-NA	-2.10	121.63	126.39
25	a	607	CLA	C2C-C1C-NC	2.10	112.19	109.98
25	B	609	CLA	CHA-C1A-NA	-2.10	121.63	126.39
26	B	618	BCR	C38-C26-C27	2.10	118.08	113.60
34	D	401	PHO	C1-C2-C3	-2.10	122.76	126.20
25	a	610	CLA	C1D-CHD-C4C	-2.10	121.56	126.02
25	C	503	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	b	613	CLA	C1D-CHD-C4C	-2.10	121.56	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	618	BCR	C33-C5-C6	-2.10	122.20	124.48
25	b	614	CLA	C1D-CHD-C4C	-2.09	121.57	126.02
25	b	607	CLA	C3D-C2D-C1D	2.09	108.69	105.83
23	C	519	LMG	C8-O7-C10	-2.09	112.78	117.80
26	C	515	BCR	C33-C5-C4	2.09	118.06	113.60
25	b	604	CLA	C1D-CHD-C4C	-2.09	121.57	126.02
26	B	619	BCR	C15-C16-C17	-2.09	119.24	123.52
25	b	603	CLA	C3D-C2D-C1D	2.09	108.69	105.83
26	b	618	BCR	C38-C26-C25	-2.09	122.20	124.48
25	C	512	CLA	C1D-CHD-C4C	-2.09	121.58	126.02
25	c	508	CLA	C2C-C1C-NC	2.09	112.18	109.98
26	a	611	BCR	C15-C16-C17	-2.09	119.25	123.52
25	b	616	CLA	C1-C2-C3	-2.09	122.78	126.20
26	C	522	BCR	C38-C26-C25	-2.09	122.21	124.48
25	C	504	CLA	C1D-CHD-C4C	-2.09	121.59	126.02
25	B	608	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
25	b	616	CLA	C3D-C2D-C1D	2.08	108.68	105.83
26	B	617	BCR	C21-C20-C19	-2.08	117.16	123.20
25	c	513	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
25	C	506	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
25	B	611	CLA	C3D-C2D-C1D	2.08	108.67	105.83
25	d	403	CLA	C3D-C2D-C1D	2.08	108.67	105.83
26	C	515	BCR	C8-C7-C6	-2.08	121.44	127.00
26	h	101	BCR	C2-C1-C6	2.08	113.46	110.44
25	a	606	CLA	C3D-C2D-C1D	2.08	108.67	105.83
25	b	602	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
25	b	614	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
25	c	504	CLA	C3D-C2D-C1D	2.08	108.67	105.83
25	c	505	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
25	c	501	CLA	C3D-C2D-C1D	2.08	108.67	105.83
25	B	612	CLA	C2C-C1C-NC	2.08	112.16	109.98
26	k	102	BCR	C34-C9-C8	2.08	121.26	118.09
26	C	514	BCR	C15-C16-C17	-2.07	119.27	123.52
23	c	520	LMG	O8-C28-O10	-2.07	118.44	123.63
25	A	608	CLA	C3D-C2D-C1D	2.07	108.66	105.83
26	K	101	BCR	C28-C27-C26	-2.07	110.36	114.06
25	b	608	CLA	C1D-CHD-C4C	-2.07	121.62	126.02
29	l	101	LHG	O7-C7-O9	-2.07	118.87	123.70
25	c	512	CLA	C1D-CHD-C4C	-2.07	121.62	126.02
26	z	101	BCR	C28-C27-C26	-2.07	110.37	114.06
25	c	511	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	C	509	CLA	C3D-C2D-C1D	2.07	108.65	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	612	CLA	C3D-C2D-C1D	2.07	108.65	105.83
26	A	609	BCR	C8-C7-C6	-2.06	121.48	127.00
25	A	607	CLA	C3D-C2D-C1D	2.06	108.65	105.83
26	h	101	BCR	C39-C30-C25	-2.06	107.01	110.24
25	B	603	CLA	C3D-C2D-C1D	2.06	108.64	105.83
25	a	610	CLA	C3D-C2D-C1D	2.06	108.64	105.83
26	c	514	BCR	C33-C5-C4	2.06	117.99	113.60
25	c	506	CLA	C3D-C2D-C1D	2.06	108.64	105.83
25	C	505	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
25	B	610	CLA	C3D-C2D-C1D	2.06	108.64	105.83
25	b	612	CLA	C3D-C2D-C1D	2.06	108.64	105.83
25	c	502	CLA	C3D-C2D-C1D	2.06	108.64	105.83
25	B	602	CLA	CAA-C2A-C1A	-2.06	105.23	111.97
26	b	617	BCR	C8-C7-C6	-2.06	121.50	127.00
25	C	512	CLA	C3D-C2D-C1D	2.06	108.64	105.83
26	T	101	BCR	C11-C12-C13	-2.05	120.73	126.36
26	b	618	BCR	C27-C26-C25	-2.05	119.93	122.70
25	B	604	CLA	C1D-CHD-C4C	-2.05	121.66	126.02
29	L	102	LHG	O7-C7-O9	-2.05	118.91	123.70
25	c	509	CLA	C3D-C2D-C1D	2.05	108.63	105.83
26	b	619	BCR	C16-C15-C14	-2.05	119.32	123.52
26	B	617	BCR	C3-C4-C5	-2.05	110.40	114.06
28	a	613	SQD	O47-C7-O49	-2.05	118.91	123.70
26	B	617	BCR	C39-C30-C25	-2.05	107.03	110.24
26	k	102	BCR	C37-C22-C23	2.05	121.22	118.09
35	e	101	HEM	C1B-NB-C4B	2.05	107.63	105.21
33	H	102	DGD	C2G-O2G-C1B	-2.05	112.89	117.80
26	D	406	BCR	C23-C24-C25	-2.05	121.53	127.00
26	d	404	BCR	C16-C15-C14	-2.05	119.33	123.52
25	B	613	CLA	C3D-C2D-C1D	2.05	108.62	105.83
25	b	614	CLA	C1-C2-C3	-2.05	122.84	126.20
25	D	404	CLA	CHC-C1C-C2C	-2.05	121.13	126.95
25	C	501	CLA	C3D-C2D-C1D	2.05	108.62	105.83
25	b	610	CLA	C3D-C2D-C1D	2.05	108.62	105.83
25	b	601	CLA	C3D-C2D-C1D	2.04	108.62	105.83
25	b	605	CLA	C3D-C2D-C1D	2.04	108.62	105.83
25	b	616	CLA	C2C-C1C-NC	2.04	112.13	109.98
25	B	614	CLA	C2C-C1C-NC	2.04	112.13	109.98
28	A	611	SQD	O7-S-C6	2.04	109.81	106.76
25	B	616	CLA	C3D-C2D-C1D	2.04	108.62	105.83
23	a	603	LMG	O6-C5-C4	2.04	113.38	109.70
26	H	101	BCR	C2-C1-C6	2.04	113.40	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C21-C20-C19	-2.04	117.29	123.20
25	d	401	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
25	C	511	CLA	CHA-C1A-NA	-2.04	121.77	126.39
28	f	101	SQD	O47-C7-O49	-2.04	118.94	123.70
25	B	605	CLA	C3D-C2D-C1D	2.04	108.61	105.83
28	A	611	SQD	O48-C23-O10	-2.04	118.54	123.63
25	a	608	CLA	CHC-C1C-NC	2.03	127.38	124.31
26	d	404	BCR	C23-C24-C25	-2.03	121.56	127.00
25	c	508	CLA	C3D-C2D-C1D	2.03	108.61	105.83
25	d	401	CLA	C3D-C2D-C1D	2.03	108.61	105.83
25	B	604	CLA	CHA-C1A-NA	-2.03	121.78	126.39
23	a	603	LMG	O8-C28-O10	-2.03	118.54	123.63
26	b	619	BCR	C21-C20-C19	-2.03	117.31	123.20
25	C	506	CLA	C3D-C2D-C1D	2.03	108.60	105.83
25	b	613	CLA	C3D-C2D-C1D	2.03	108.60	105.83
26	a	611	BCR	C33-C5-C4	2.03	117.92	113.60
25	C	513	CLA	C1D-CHD-C4C	-2.03	121.71	126.02
25	B	609	CLA	C3D-C2D-C1D	2.03	108.60	105.83
26	C	515	BCR	C28-C27-C26	-2.03	110.44	114.06
25	B	606	CLA	C3D-C2D-C1D	2.03	108.60	105.83
25	D	404	CLA	C3D-C2D-C1D	2.03	108.60	105.83
26	b	617	BCR	C21-C20-C19	-2.03	117.33	123.20
25	C	502	CLA	C3D-C2D-C1D	2.02	108.59	105.83
28	F	101	SQD	O7-S-C6	2.02	109.78	106.76
26	H	101	BCR	C27-C26-C25	-2.02	119.97	122.70
26	D	406	BCR	C39-C30-C25	-2.02	107.08	110.24
26	K	101	BCR	C34-C9-C8	2.02	121.17	118.09
25	B	607	CLA	C3D-C2D-C1D	2.02	108.59	105.83
25	D	405	CLA	C3D-C2D-C1D	2.02	108.59	105.83
25	c	511	CLA	C3D-C2D-C1D	2.02	108.58	105.83
26	b	618	BCR	C23-C24-C25	-2.02	121.61	127.00
25	b	601	CLA	C1-C2-C3	-2.02	122.89	126.20
25	C	511	CLA	C3D-C2D-C1D	2.01	108.58	105.83
26	a	611	BCR	C8-C7-C6	-2.01	121.63	127.00
25	B	614	CLA	C3D-C2D-C1D	2.01	108.57	105.83
25	c	512	CLA	C3D-C2D-C1D	2.01	108.57	105.83
26	t	102	BCR	C38-C26-C25	-2.01	122.29	124.48
25	B	602	CLA	C3D-C2D-C1D	2.01	108.57	105.83
26	C	514	BCR	C23-C24-C25	-2.01	121.64	127.00
23	b	620	LMG	O8-C28-O10	-2.01	118.61	123.63
26	b	618	BCR	C38-C26-C27	2.00	117.87	113.60
26	t	102	BCR	C33-C5-C4	2.00	117.87	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	516	DGD	O1G-C1A-O1A	-2.00	118.62	123.63

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	608	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	403	CLA	ND
25	D	404	CLA	ND
25	D	405	CLA	ND
25	a	606	CLA	ND
25	a	607	CLA	ND

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Mol	Chain	Res	Type	Atom
25	a	608	CLA	ND
25	a	610	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	401	CLA	ND
25	d	403	CLA	ND

All (662) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	C	521	LMG	O6-C1-O1-C7
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	C2B-C3B-CAB-CBB
25	B	601	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	605	CLA	C4B-C3B-CAB-CBB
25	B	610	CLA	C4B-C3B-CAB-CBB
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	615	CLA	C4B-C3B-CAB-CBB
25	C	507	CLA	CHA-CBD-CGD-O2D
25	a	607	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C2B-C3B-CAB-CBB
25	b	601	CLA	C4B-C3B-CAB-CBB
25	b	603	CLA	C4-C3-C5-C6
25	b	605	CLA	C2B-C3B-CAB-CBB
25	b	605	CLA	C4B-C3B-CAB-CBB
25	b	606	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	C4B-C3B-CAB-CBB
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	615	CLA	C2B-C3B-CAB-CBB
25	b	615	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	512	CLA	C4B-C3B-CAB-CBB
26	B	619	BCR	C7-C8-C9-C10
26	D	406	BCR	C7-C8-C9-C10
26	D	406	BCR	C21-C22-C23-C24
26	H	101	BCR	C7-C8-C9-C10
26	H	101	BCR	C7-C8-C9-C34
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	T	101	BCR	C7-C8-C9-C10
26	T	101	BCR	C7-C8-C9-C34
26	d	404	BCR	C7-C8-C9-C10
26	h	101	BCR	C7-C8-C9-C10
26	h	101	BCR	C7-C8-C9-C34
26	t	102	BCR	C5-C6-C7-C8
26	t	102	BCR	C17-C18-C19-C20
27	a	612	PL9	C18-C19-C21-C22
27	a	612	PL9	C20-C19-C21-C22
28	L	101	SQD	C5-C6-S-O8
28	L	103	SQD	C5-C6-S-O7
28	L	103	SQD	C5-C6-S-O9
28	f	101	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
29	A	613	LHG	C3-O3-P-O5
29	A	613	LHG	C4-O6-P-O3
29	A	613	LHG	C4-O6-P-O5
29	A	614	LHG	O6-C4-C5-O7
29	D	408	LHG	C4-O6-P-O3
29	E	101	LHG	C1-C2-C3-O3
29	E	101	LHG	O2-C2-C3-O3
29	L	102	LHG	C3-O3-P-O4
29	L	102	LHG	C3-O3-P-O5
29	L	102	LHG	C3-O3-P-O6
29	L	102	LHG	C4-O6-P-O3
29	a	615	LHG	C4-O6-P-O3
29	a	615	LHG	C4-O6-P-O4
29	a	615	LHG	C4-O6-P-O5
29	a	616	LHG	C3-O3-P-O4
29	a	616	LHG	C3-O3-P-O6
29	d	406	LHG	C3-O3-P-O4
29	d	406	LHG	C3-O3-P-O6
29	d	407	LHG	C3-O3-P-O5
29	d	407	LHG	C3-O3-P-O6
29	d	407	LHG	C4-O6-P-O3
29	d	407	LHG	C4-O6-P-O4
29	l	101	LHG	C3-O3-P-O4
29	l	101	LHG	C3-O3-P-O5
29	l	101	LHG	C3-O3-P-O6
29	l	101	LHG	C4-O6-P-O3
36	V	201	HEC	C2B-C3B-CAB-CBB
36	V	201	HEC	C4B-C3B-CAB-CBB
28	f	101	SQD	O49-C7-O47-C45
25	B	614	CLA	C3-C5-C6-C7
25	B	605	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
28	L	101	SQD	C8-C7-O47-C45
28	L	103	SQD	C8-C7-O47-C45
25	B	602	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	B	602	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
27	A	610	PL9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
27	a	612	PL9	C9-C11-C12-C13
27	a	612	PL9	C14-C16-C17-C18
35	E	102	HEM	C2A-CAA-CBA-CGA
28	L	103	SQD	O49-C7-O47-C45
29	a	616	LHG	C1-C2-C3-O3
28	F	101	SQD	C24-C23-O48-C46
25	B	605	CLA	C14-C13-C15-C16
25	b	601	CLA	C11-C10-C8-C9
34	D	401	PHO	C14-C13-C15-C16
29	a	616	LHG	O2-C2-C3-O3
26	B	619	BCR	C7-C8-C9-C34
26	D	406	BCR	C7-C8-C9-C34
26	D	406	BCR	C37-C22-C23-C24
26	T	101	BCR	C37-C22-C23-C24
26	d	404	BCR	C7-C8-C9-C34
26	d	404	BCR	C37-C22-C23-C24
26	t	102	BCR	C7-C8-C9-C34
26	t	102	BCR	C36-C18-C19-C20
26	T	101	BCR	C21-C22-C23-C24
26	t	102	BCR	C7-C8-C9-C10
28	L	101	SQD	C24-C23-O48-C46
23	B	624	LMG	C10-C11-C12-C13
28	L	101	SQD	C7-C8-C9-C10
33	h	102	DGD	C1B-C2B-C3B-C4B
28	L	101	SQD	O49-C7-O47-C45
28	L	101	SQD	C23-C24-C25-C26
28	L	101	SQD	O10-C23-O48-C46
36	V	201	HEC	C3D-CAD-CBD-CGD
36	v	201	HEC	C3D-CAD-CBD-CGD
25	b	606	CLA	C2A-CAA-CBA-CGA
23	C	521	LMG	C10-C11-C12-C13
33	c	516	DGD	C1A-C2A-C3A-C4A
33	c	516	DGD	C1B-C2B-C3B-C4B
28	F	101	SQD	O10-C23-O48-C46
23	b	624	LMG	C28-C29-C30-C31
25	c	503	CLA	C15-C16-C17-C18
25	c	506	CLA	C15-C16-C17-C18
33	c	516	DGD	C2E-C1E-O5D-C6D
27	A	610	PL9	C9-C11-C12-C13
29	l	101	LHG	O2-C2-C3-O3
26	t	102	BCR	C37-C22-C23-C24
26	t	102	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
35	E	102	HEM	C3D-CAD-CBD-CGD
25	B	606	CLA	C2A-CAA-CBA-CGA
25	D	405	CLA	C16-C17-C18-C20
33	c	516	DGD	O6E-C1E-O5D-C6D
23	b	624	LMG	C11-C10-O7-C8
25	B	601	CLA	C10-C11-C12-C13
33	C	517	DGD	C6B-C7B-C8B-C9B
33	h	102	DGD	C3B-C4B-C5B-C6B
29	d	407	LHG	C26-C27-C28-C29
23	A	603	LMG	C20-C21-C22-C23
23	A	603	LMG	C30-C31-C32-C33
23	A	612	LMG	C15-C16-C17-C18
23	b	624	LMG	O9-C10-O7-C8
25	B	602	CLA	C4B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB
25	B	609	CLA	C4B-C3B-CAB-CBB
25	C	504	CLA	C4B-C3B-CAB-CBB
25	D	403	CLA	C4B-C3B-CAB-CBB
25	a	608	CLA	C4B-C3B-CAB-CBB
25	a	610	CLA	C4B-C3B-CAB-CBB
25	b	602	CLA	C4B-C3B-CAB-CBB
25	b	609	CLA	C4B-C3B-CAB-CBB
25	c	502	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
25	c	513	CLA	C4B-C3B-CAB-CBB
29	l	101	LHG	C28-C29-C30-C31
23	A	612	LMG	C28-C29-C30-C31
23	a	603	LMG	C31-C32-C33-C34
23	a	603	LMG	O6-C5-C6-O5
23	B	624	LMG	C36-C37-C38-C39
28	L	103	SQD	C11-C12-C13-C14
23	C	521	LMG	C20-C21-C22-C23
33	c	515	DGD	C8A-C9A-CAA-CBA
23	A	612	LMG	C18-C19-C20-C21
28	L	101	SQD	C31-C32-C33-C34
29	a	615	LHG	C25-C26-C27-C28
25	B	605	CLA	C2B-C3B-CAB-CBB
25	B	610	CLA	C2B-C3B-CAB-CBB
25	B	615	CLA	C2B-C3B-CAB-CBB
25	a	607	CLA	C2B-C3B-CAB-CBB
25	b	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C2B-C3B-CAB-CBB
25	b	610	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C1-C6-C7-C8
26	B	617	BCR	C5-C6-C7-C8
26	B	619	BCR	C1-C6-C7-C8
26	B	619	BCR	C5-C6-C7-C8
26	D	406	BCR	C1-C6-C7-C8
26	D	406	BCR	C5-C6-C7-C8
26	K	101	BCR	C1-C6-C7-C8
26	b	617	BCR	C1-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	d	404	BCR	C1-C6-C7-C8
26	d	404	BCR	C5-C6-C7-C8
26	t	102	BCR	C1-C6-C7-C8
35	e	101	HEM	C1A-C2A-CAA-CBA
23	c	520	LMG	C29-C30-C31-C32
23	A	612	LMG	C21-C22-C23-C24
23	a	603	LMG	C13-C14-C15-C16
28	L	101	SQD	C25-C26-C27-C28
28	L	103	SQD	C32-C33-C34-C35
27	A	610	PL9	C15-C14-C16-C17
27	d	405	PL9	C40-C39-C41-C42
23	A	603	LMG	C37-C38-C39-C40
23	a	614	LMG	C20-C21-C22-C23
33	H	102	DGD	C5B-C6B-C7B-C8B
23	c	520	LMG	C29-C28-O8-C9
23	B	624	LMG	C20-C21-C22-C23
33	C	517	DGD	C9A-CAA-CBA-CCA
33	C	516	DGD	O6E-C5E-C6E-O5E
23	a	614	LMG	C10-C11-C12-C13
28	a	613	SQD	C16-C17-C18-C19
23	c	518	LMG	C30-C31-C32-C33
23	A	603	LMG	C36-C37-C38-C39
28	L	103	SQD	C31-C32-C33-C34
29	L	102	LHG	C10-C11-C12-C13
26	d	404	BCR	C21-C22-C23-C24
25	D	405	CLA	C16-C17-C18-C19
25	B	609	CLA	C4-C3-C5-C6
25	C	510	CLA	C4-C3-C5-C6
35	E	102	HEM	C2B-C3B-CAB-CBB
35	E	102	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
35	e	101	HEM	C2B-C3B-CAB-CBB
25	B	601	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
23	C	521	LMG	O6-C5-C6-O5
33	c	516	DGD	CAA-CBA-CCA-CDA
29	d	407	LHG	O6-C4-C5-O7
35	E	102	HEM	C4C-C3C-CAC-CBC
35	e	101	HEM	C4B-C3B-CAB-CBB
23	d	408	LMG	O6-C5-C6-O5
23	C	519	LMG	C31-C32-C33-C34
33	c	515	DGD	O6E-C5E-C6E-O5E
23	A	603	LMG	O1-C7-C8-O7
28	f	101	SQD	O6-C44-C45-O47
23	c	520	LMG	C13-C14-C15-C16
28	A	611	SQD	C11-C10-C9-C8
29	A	614	LHG	C27-C28-C29-C30
29	L	102	LHG	C34-C35-C36-C37
23	B	624	LMG	O6-C5-C6-O5
25	b	609	CLA	C4-C3-C5-C6
25	B	609	CLA	C2-C3-C5-C6
27	d	405	PL9	C38-C39-C41-C42
28	A	611	SQD	C17-C18-C19-C20
23	c	520	LMG	O6-C5-C6-O5
25	D	403	CLA	C1A-C2A-CAA-CBA
25	a	607	CLA	C1A-C2A-CAA-CBA
23	b	624	LMG	O6-C5-C6-O5
25	B	616	CLA	C10-C11-C12-C13
28	L	103	SQD	C25-C26-C27-C28
29	D	408	LHG	O6-C4-C5-C6
29	L	102	LHG	O6-C4-C5-C6
23	c	518	LMG	C14-C15-C16-C17
28	L	101	SQD	C26-C27-C28-C29
25	D	404	CLA	C12-C13-C15-C16
23	C	519	LMG	C10-C11-C12-C13
33	C	516	DGD	C4B-C5B-C6B-C7B
25	c	510	CLA	C4-C3-C5-C6
23	b	624	LMG	C32-C33-C34-C35
25	b	613	CLA	C8-C10-C11-C12
34	a	609	PHO	C14-C13-C15-C16
23	A	612	LMG	C13-C14-C15-C16
23	D	409	LMG	O6-C5-C6-O5
29	A	613	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	A	603	LMG	O1-C7-C8-C9
23	a	603	LMG	O1-C7-C8-C9
23	A	612	LMG	C36-C37-C38-C39
23	C	519	LMG	C20-C21-C22-C23
29	a	615	LHG	C7-C8-C9-C10
23	c	520	LMG	O10-C28-O8-C9
25	C	510	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
25	c	510	CLA	C2-C3-C5-C6
29	l	101	LHG	C10-C11-C12-C13
28	L	101	SQD	C46-C45-O47-C7
23	A	603	LMG	C33-C34-C35-C36
33	c	515	DGD	O6D-C5D-C6D-O5D
23	c	520	LMG	C17-C18-C19-C20
29	a	616	LHG	C9-C10-C11-C12
23	a	603	LMG	C29-C28-O8-C9
25	C	506	CLA	C4-C3-C5-C6
27	A	610	PL9	C13-C14-C16-C17
29	l	101	LHG	C11-C12-C13-C14
23	A	612	LMG	C35-C36-C37-C38
23	C	521	LMG	O1-C7-C8-O7
23	a	603	LMG	O1-C7-C8-O7
28	f	101	SQD	O47-C45-C46-O48
23	A	603	LMG	C19-C20-C21-C22
23	B	624	LMG	C17-C18-C19-C20
23	A	603	LMG	C29-C28-O8-C9
23	B	624	LMG	C22-C23-C24-C25
33	C	517	DGD	C1A-C2A-C3A-C4A
23	c	520	LMG	C32-C33-C34-C35
25	A	608	CLA	C4B-C3B-CAB-CBB
25	C	502	CLA	C4B-C3B-CAB-CBB
25	C	505	CLA	C4B-C3B-CAB-CBB
25	b	603	CLA	C4B-C3B-CAB-CBB
25	b	611	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
23	B	620	LMG	C32-C33-C34-C35
23	C	521	LMG	C2-C1-O1-C7
23	c	520	LMG	C2-C1-O1-C7
29	A	614	LHG	O6-C4-C5-C6
29	d	407	LHG	O6-C4-C5-C6
29	l	101	LHG	O6-C4-C5-C6
33	c	515	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
23	A	603	LMG	C32-C33-C34-C35
23	C	521	LMG	C17-C18-C19-C20
25	b	615	CLA	C12-C13-C15-C16
25	b	616	CLA	C4-C3-C5-C6
27	d	405	PL9	C30-C29-C31-C32
34	D	401	PHO	C2-C3-C5-C6
23	a	603	LMG	C14-C15-C16-C17
33	C	517	DGD	CAA-CBA-CCA-CDA
28	L	103	SQD	C11-C10-C9-C8
23	A	612	LMG	C7-C8-C9-O8
28	L	101	SQD	C44-C45-C46-O48
28	f	101	SQD	O6-C44-C45-C46
23	c	520	LMG	C22-C23-C24-C25
25	c	507	CLA	C4-C3-C5-C6
34	a	609	PHO	C4-C3-C5-C6
27	d	405	PL9	C28-C29-C31-C32
34	a	609	PHO	C2-C3-C5-C6
23	b	620	LMG	C20-C21-C22-C23
29	D	408	LHG	O6-C4-C5-O7
28	f	101	SQD	C32-C33-C34-C35
26	k	102	BCR	C1-C6-C7-C8
33	C	517	DGD	CAB-CBB-CCB-CDB
23	C	521	LMG	C19-C20-C21-C22
28	a	613	SQD	C11-C12-C13-C14
23	C	521	LMG	O7-C8-C9-O8
23	c	520	LMG	O7-C8-C9-O8
28	L	101	SQD	O47-C45-C46-O48
33	C	518	DGD	CBA-CCA-CDA-CEA
27	A	610	PL9	C4-C3-C7-C8
27	D	407	PL9	C4-C3-C7-C8
34	D	401	PHO	C4-C3-C5-C6
23	C	521	LMG	C39-C40-C41-C42
23	B	624	LMG	C31-C32-C33-C34
33	c	516	DGD	C2B-C3B-C4B-C5B
25	C	506	CLA	C11-C10-C8-C9
25	b	615	CLA	C14-C13-C15-C16
27	A	610	PL9	C14-C16-C17-C18
27	d	405	PL9	C9-C11-C12-C13
25	b	616	CLA	C2-C3-C5-C6
29	E	101	LHG	C16-C17-C18-C19
29	E	101	LHG	C11-C12-C13-C14
25	c	506	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C12-C13-C15-C16
25	b	607	CLA	C12-C13-C15-C16
25	b	616	CLA	C11-C12-C13-C15
23	c	518	LMG	C29-C28-O8-C9
23	a	603	LMG	O10-C28-O8-C9
28	L	103	SQD	C5-C6-S-O8
27	D	407	PL9	C30-C29-C31-C32
27	a	612	PL9	C35-C34-C36-C37
23	A	603	LMG	O10-C28-O8-C9
23	C	521	LMG	C15-C16-C17-C18
33	C	517	DGD	C4B-C5B-C6B-C7B
29	l	101	LHG	O6-C4-C5-O7
28	a	613	SQD	O5-C1-O6-C44
33	C	517	DGD	O6E-C1E-O5D-C6D
29	a	616	LHG	C4-C5-C6-O8
25	b	614	CLA	C10-C11-C12-C13
35	E	102	HEM	C4B-C3B-CAB-CBB
35	e	101	HEM	C4C-C3C-CAC-CBC
27	A	610	PL9	C35-C34-C36-C37
23	C	519	LMG	C12-C13-C14-C15
29	A	613	LHG	C25-C26-C27-C28
25	c	513	CLA	C10-C11-C12-C13
25	B	607	CLA	C14-C13-C15-C16
29	A	614	LHG	C12-C13-C14-C15
28	L	101	SQD	C30-C31-C32-C33
33	C	517	DGD	C2E-C1E-O5D-C6D
29	l	101	LHG	C1-C2-C3-O3
33	c	515	DGD	C9A-CAA-CBA-CCA
25	B	616	CLA	C8-C10-C11-C12
33	C	516	DGD	O6D-C5D-C6D-O5D
23	c	518	LMG	C15-C16-C17-C18
27	D	407	PL9	C28-C29-C31-C32
27	a	612	PL9	C33-C34-C36-C37
23	b	624	LMG	C36-C37-C38-C39
33	C	516	DGD	C4D-C5D-C6D-O5D
23	b	620	LMG	C39-C40-C41-C42
29	L	102	LHG	C11-C12-C13-C14
23	c	518	LMG	O10-C28-O8-C9
36	v	201	HEC	C4B-C3B-CAB-CBB
27	A	610	PL9	C33-C34-C36-C37
25	b	616	CLA	C11-C12-C13-C14
28	L	101	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
28	f	101	SQD	O10-C23-O48-C46
23	A	612	LMG	O7-C8-C9-O8
23	C	521	LMG	O1-C7-C8-C9
25	b	606	CLA	C13-C15-C16-C17
23	c	520	LMG	C35-C36-C37-C38
25	B	607	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
28	f	101	SQD	C24-C23-O48-C46
25	B	607	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	512	CLA	CHA-CBD-CGD-O1D
25	C	512	CLA	CHA-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	512	CLA	CHA-CBD-CGD-O1D
25	c	512	CLA	CHA-CBD-CGD-O2D
29	A	613	LHG	C4-O6-P-O4
29	D	408	LHG	C4-O6-P-O5
29	L	102	LHG	C4-O6-P-O5
29	d	407	LHG	C3-O3-P-O4
29	l	101	LHG	C4-O6-P-O5
25	B	602	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	609	CLA	C2B-C3B-CAB-CBB
25	C	504	CLA	C2B-C3B-CAB-CBB
25	D	403	CLA	C2B-C3B-CAB-CBB
25	a	608	CLA	C2B-C3B-CAB-CBB
25	a	610	CLA	C2B-C3B-CAB-CBB
25	b	609	CLA	C2B-C3B-CAB-CBB
25	b	611	CLA	C2B-C3B-CAB-CBB
25	c	502	CLA	C2B-C3B-CAB-CBB
25	c	503	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C2B-C3B-CAB-CBB
25	c	513	CLA	C2B-C3B-CAB-CBB
26	K	101	BCR	C5-C6-C7-C8
23	b	624	LMG	C18-C19-C20-C21
26	b	619	BCR	C7-C8-C9-C34
29	E	101	LHG	C24-C25-C26-C27
23	a	603	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
27	a	612	PL9	C4-C3-C7-C8
23	a	614	LMG	C17-C18-C19-C20
25	C	506	CLA	C2-C3-C5-C6
23	B	620	LMG	C40-C41-C42-C43
29	E	101	LHG	O6-C4-C5-C6
25	B	609	CLA	C14-C13-C15-C16
25	b	607	CLA	C14-C13-C15-C16
25	b	614	CLA	C11-C10-C8-C9
25	c	509	CLA	C11-C10-C8-C9
25	B	614	CLA	C11-C12-C13-C15
25	C	506	CLA	C6-C7-C8-C10
25	a	610	CLA	C11-C10-C8-C7
35	e	101	HEM	C3A-C2A-CAA-CBA
29	L	102	LHG	O6-C4-C5-O7
33	c	517	DGD	O6D-C5D-C6D-O5D
27	D	407	PL9	C40-C39-C41-C42
28	F	101	SQD	C31-C32-C33-C34
23	C	519	LMG	C28-C29-C30-C31
25	B	601	CLA	CAA-CBA-CGA-O2A
28	f	101	SQD	C44-C45-C46-O48
26	k	102	BCR	C7-C8-C9-C34
23	b	624	LMG	C13-C14-C15-C16
23	C	521	LMG	C8-C7-O1-C1
33	c	515	DGD	C5D-C6D-O5D-C1E
25	b	610	CLA	C2A-CAA-CBA-CGA
23	c	520	LMG	O6-C1-O1-C7
33	H	102	DGD	O2G-C1B-C2B-C3B
28	a	613	SQD	C9-C10-C11-C12
25	b	608	CLA	C4B-C3B-CAB-CBB
25	c	504	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C2A-CAA-CBA-CGA
29	d	406	LHG	O6-C4-C5-O7
28	a	613	SQD	C12-C13-C14-C15
25	B	615	CLA	C4-C3-C5-C6
23	a	603	LMG	C33-C34-C35-C36
25	C	507	CLA	C2A-CAA-CBA-CGA
23	a	603	LMG	O6-C1-O1-C7
28	A	611	SQD	C11-C12-C13-C14
28	L	103	SQD	C28-C29-C30-C31
27	d	405	PL9	C45-C44-C46-C47
33	H	102	DGD	O1G-C1G-C2G-C3G
23	a	614	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C11-C10-C8-C9
29	d	407	LHG	C35-C36-C37-C38
28	F	101	SQD	C32-C33-C34-C35
33	c	515	DGD	C5B-C6B-C7B-C8B
28	f	101	SQD	C28-C29-C30-C31
25	C	513	CLA	C4-C3-C5-C6
25	b	614	CLA	C1A-C2A-CAA-CBA
33	c	515	DGD	C4B-C5B-C6B-C7B
25	B	607	CLA	C2B-C3B-CAB-CBB
25	C	505	CLA	C2B-C3B-CAB-CBB
25	b	603	CLA	C2B-C3B-CAB-CBB
25	b	608	CLA	C2B-C3B-CAB-CBB
25	c	504	CLA	C2B-C3B-CAB-CBB
25	c	507	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
26	k	102	BCR	C5-C6-C7-C8
23	c	518	LMG	C10-C11-C12-C13
25	B	608	CLA	C4-C3-C5-C6
29	d	407	LHG	C31-C32-C33-C34
25	B	615	CLA	C2-C3-C5-C6
27	d	405	PL9	C43-C44-C46-C47
25	B	613	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C12-C13-C15
25	b	614	CLA	C2A-CAA-CBA-CGA
28	L	103	SQD	C17-C18-C19-C20
29	a	616	LHG	O7-C5-C6-O8
29	a	615	LHG	C11-C10-C9-C8
33	C	516	DGD	C1B-C2B-C3B-C4B
25	C	504	CLA	C4-C3-C5-C6
25	c	503	CLA	C4-C3-C5-C6
27	D	407	PL9	C20-C19-C21-C22
25	C	513	CLA	C2-C3-C5-C6
27	D	407	PL9	C38-C39-C41-C42
25	B	614	CLA	C2A-CAA-CBA-CGA
34	D	401	PHO	C16-C17-C18-C19
23	B	624	LMG	C30-C31-C32-C33
29	E	101	LHG	C15-C16-C17-C18
25	C	507	CLA	C4-C3-C5-C6
33	h	102	DGD	C7A-C8A-C9A-CAA
25	c	507	CLA	C2-C3-C5-C6
23	b	620	LMG	C7-C8-C9-O8
23	c	520	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
27	D	407	PL9	C9-C11-C12-C13
27	d	405	PL9	C29-C31-C32-C33
35	e	101	HEM	CAA-CBA-CGA-O2A
33	H	102	DGD	CBA-CCA-CDA-CEA
25	b	601	CLA	CAA-CBA-CGA-O2A
29	E	101	LHG	O6-C4-C5-O7
25	A	608	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	a	610	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
23	C	521	LMG	C36-C37-C38-C39
25	B	607	CLA	C4B-C3B-CAB-CBB
23	c	518	LMG	C13-C14-C15-C16
29	d	407	LHG	C1-C2-C3-O3
34	a	609	PHO	CHA-CBD-CGD-O1D
25	c	510	CLA	C3-C5-C6-C7
28	L	103	SQD	C29-C30-C31-C32
29	d	406	LHG	O6-C4-C5-C6
35	E	102	HEM	CAA-CBA-CGA-O2A
29	E	101	LHG	C26-C27-C28-C29
25	b	601	CLA	C10-C11-C12-C13
29	l	101	LHG	C17-C18-C19-C20
25	a	606	CLA	C2-C1-O2A-CGA
25	B	602	CLA	C5-C6-C7-C8
23	A	612	LMG	C32-C33-C34-C35
35	e	101	HEM	CAA-CBA-CGA-O1A
25	C	503	CLA	C10-C11-C12-C13
23	A	612	LMG	C22-C23-C24-C25
29	L	102	LHG	O2-C2-C3-O3
28	L	103	SQD	C16-C17-C18-C19
33	C	518	DGD	O6D-C5D-C6D-O5D
29	a	615	LHG	C33-C34-C35-C36
23	C	521	LMG	C7-C8-C9-O8
23	C	521	LMG	O10-C28-O8-C9
33	C	517	DGD	C4A-C5A-C6A-C7A
33	C	516	DGD	C8A-C9A-CAA-CBA
33	C	517	DGD	C8A-C9A-CAA-CBA
23	C	521	LMG	C29-C28-O8-C9
23	b	620	LMG	C29-C30-C31-C32
23	B	624	LMG	C37-C38-C39-C40
23	b	624	LMG	O1-C7-C8-O7
23	c	518	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C6-C7-C8-C9
25	D	404	CLA	C14-C13-C15-C16
35	E	102	HEM	CAA-CBA-CGA-O1A
23	A	603	LMG	O7-C10-C11-C12
34	D	402	PHO	C16-C17-C18-C20
25	c	501	CLA	C2A-CAA-CBA-CGA
25	A	607	CLA	C12-C13-C15-C16
25	B	610	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C12-C13-C15
34	a	609	PHO	C11-C12-C13-C15
25	A	608	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
26	C	514	BCR	C1-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C26
26	z	101	BCR	C1-C6-C7-C8
25	A	606	CLA	C2-C1-O2A-CGA
33	C	518	DGD	O1A-C1A-O1G-C1G
25	C	512	CLA	CAA-CBA-CGA-O2A
28	L	103	SQD	C26-C27-C28-C29
29	L	102	LHG	O7-C7-C8-C9
29	d	407	LHG	C24-C25-C26-C27
23	a	614	LMG	C22-C23-C24-C25
28	A	611	SQD	O47-C7-C8-C9
25	B	614	CLA	C2-C3-C5-C6
25	C	507	CLA	C2-C3-C5-C6
27	D	407	PL9	C18-C19-C21-C22
23	d	408	LMG	C29-C30-C31-C32
23	B	620	LMG	O8-C28-C29-C30
33	C	517	DGD	O2G-C1B-C2B-C3B
33	C	518	DGD	C2A-C1A-O1G-C1G
23	A	603	LMG	C14-C15-C16-C17
25	B	602	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C12-C13-C14
28	L	103	SQD	O48-C23-C24-C25
25	B	611	CLA	C1A-C2A-CAA-CBA
25	d	403	CLA	C4B-C3B-CAB-CBB
29	D	408	LHG	C28-C29-C30-C31
33	h	102	DGD	CDB-CEB-CFB-CGB
28	a	613	SQD	O6-C44-C45-O47
29	L	102	LHG	O7-C5-C6-O8
29	l	101	LHG	O7-C5-C6-O8
33	c	516	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
26	b	619	BCR	C7-C8-C9-C10
26	k	102	BCR	C7-C8-C9-C10
29	d	407	LHG	C29-C30-C31-C32
25	b	607	CLA	C16-C17-C18-C20
23	C	519	LMG	O7-C10-C11-C12
25	c	512	CLA	CAA-CBA-CGA-O2A
25	C	506	CLA	C16-C17-C18-C20
25	C	506	CLA	C5-C6-C7-C8
23	C	519	LMG	C32-C33-C34-C35
33	H	102	DGD	CDB-CEB-CFB-CGB
29	L	102	LHG	C1-C2-C3-O3
29	a	616	LHG	O1-C1-C2-C3
25	b	614	CLA	C2-C1-O2A-CGA
29	l	101	LHG	O7-C7-C8-C9
29	d	407	LHG	C14-C15-C16-C17
25	c	510	CLA	C8-C10-C11-C12
34	d	402	PHO	C16-C17-C18-C20
25	a	610	CLA	C15-C16-C17-C18
36	V	201	HEC	C4C-C3C-CAC-CBC
36	v	201	HEC	C4C-C3C-CAC-CBC
25	A	608	CLA	C15-C16-C17-C18
25	B	607	CLA	C16-C17-C18-C20
25	C	506	CLA	C16-C17-C18-C19
25	C	504	CLA	C2-C3-C5-C6
29	L	102	LHG	O9-C7-C8-C9
33	h	102	DGD	C4B-C5B-C6B-C7B
25	B	601	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C14-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C9
25	a	610	CLA	C11-C10-C8-C9
23	D	409	LMG	O7-C10-C11-C12
29	l	101	LHG	C12-C13-C14-C15
26	H	101	BCR	C9-C10-C11-C12
33	c	516	DGD	C4A-C5A-C6A-C7A
25	B	605	CLA	C13-C15-C16-C17
23	A	603	LMG	O9-C10-C11-C12
33	h	102	DGD	O2G-C1B-C2B-C3B
28	F	101	SQD	O5-C5-C6-S
28	L	101	SQD	O5-C5-C6-S
25	C	512	CLA	CAA-CBA-CGA-O1A
25	B	602	CLA	C8-C10-C11-C12
33	C	516	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
23	C	519	LMG	O9-C10-C11-C12
28	L	103	SQD	O10-C23-C24-C25
23	C	519	LMG	C21-C22-C23-C24
23	D	409	LMG	C8-C7-O1-C1
33	C	516	DGD	C5D-C6D-O5D-C1E
23	B	624	LMG	O9-C10-O7-C8
28	a	613	SQD	C18-C19-C20-C21
29	d	407	LHG	C32-C33-C34-C35
25	B	603	CLA	C2A-CAA-CBA-CGA
23	A	603	LMG	C35-C36-C37-C38
33	h	102	DGD	C1G-C2G-C3G-O3G
23	B	620	LMG	O10-C28-C29-C30
29	l	101	LHG	O9-C7-C8-C9
25	A	608	CLA	C2-C3-C5-C6
34	D	401	PHO	CAD-CBD-CGD-O2D
28	L	103	SQD	O47-C7-C8-C9
25	c	504	CLA	C2-C1-O2A-CGA
25	c	512	CLA	CAA-CBA-CGA-O1A
28	A	611	SQD	O49-C7-C8-C9
33	C	517	DGD	O1B-C1B-C2B-C3B
25	C	510	CLA	CAA-CBA-CGA-O2A
25	A	608	CLA	C16-C17-C18-C20
34	a	609	PHO	C16-C17-C18-C19
23	d	408	LMG	C11-C12-C13-C14
28	f	101	SQD	O47-C7-C8-C9
29	d	407	LHG	C30-C31-C32-C33
25	c	501	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

130 monomers are involved in 323 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	514	BCR	4	0
25	b	613	CLA	4	0
23	C	519	LMG	1	0
27	D	407	PL9	3	0
26	T	101	BCR	6	0
25	C	504	CLA	2	0
25	C	507	CLA	2	0
33	C	517	DGD	4	0
25	b	601	CLA	3	0
25	d	403	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	k	102	BCR	3	0
23	B	620	LMG	3	0
23	a	603	LMG	1	0
25	c	513	CLA	7	0
26	h	101	BCR	4	0
23	A	603	LMG	1	0
23	C	521	LMG	3	0
28	L	103	SQD	4	0
25	c	503	CLA	5	0
33	C	516	DGD	4	0
34	D	401	PHO	1	0
26	B	618	BCR	4	0
26	K	101	BCR	4	0
29	d	407	LHG	8	0
25	b	615	CLA	3	0
35	e	101	HEM	5	0
25	B	609	CLA	3	0
26	B	617	BCR	6	0
25	C	505	CLA	5	0
25	b	608	CLA	2	0
25	C	501	CLA	4	0
25	b	616	CLA	2	0
29	D	408	LHG	5	0
25	b	607	CLA	1	0
23	c	520	LMG	3	0
25	b	610	CLA	1	0
25	C	508	CLA	4	0
25	a	606	CLA	2	0
25	c	501	CLA	3	0
28	F	101	SQD	2	0
27	A	610	PL9	6	0
26	b	618	BCR	1	0
25	c	507	CLA	3	0
25	A	606	CLA	3	0
26	A	609	BCR	3	0
25	B	611	CLA	3	0
25	b	602	CLA	2	0
23	b	624	LMG	1	0
33	h	102	DGD	2	0
25	a	608	CLA	1	0
26	c	521	BCR	1	0
25	b	612	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	605	CLA	4	0
25	B	614	CLA	3	0
25	B	602	CLA	2	0
29	a	616	LHG	2	0
25	c	508	CLA	7	0
29	l	101	LHG	3	0
25	B	615	CLA	1	0
26	C	515	BCR	2	0
25	b	614	CLA	1	0
25	C	513	CLA	5	0
25	b	609	CLA	3	0
27	d	405	PL9	4	0
25	B	603	CLA	3	0
25	B	607	CLA	2	0
25	C	503	CLA	4	0
25	c	511	CLA	2	0
33	c	516	DGD	3	0
26	t	102	BCR	5	0
29	A	614	LHG	8	0
25	C	502	CLA	1	0
25	C	509	CLA	2	0
29	A	613	LHG	5	0
23	a	614	LMG	1	0
25	c	502	CLA	2	0
25	c	510	CLA	5	0
29	L	102	LHG	4	0
27	a	612	PL9	6	0
29	d	406	LHG	3	0
25	B	604	CLA	3	0
26	D	406	BCR	2	0
28	L	101	SQD	6	0
25	a	607	CLA	4	0
26	H	101	BCR	2	0
25	D	403	CLA	3	0
26	C	514	BCR	5	0
26	b	619	BCR	4	0
25	D	404	CLA	6	0
28	a	613	SQD	5	0
34	d	402	PHO	1	0
35	E	102	HEM	3	0
25	C	512	CLA	3	0
34	a	609	PHO	2	0

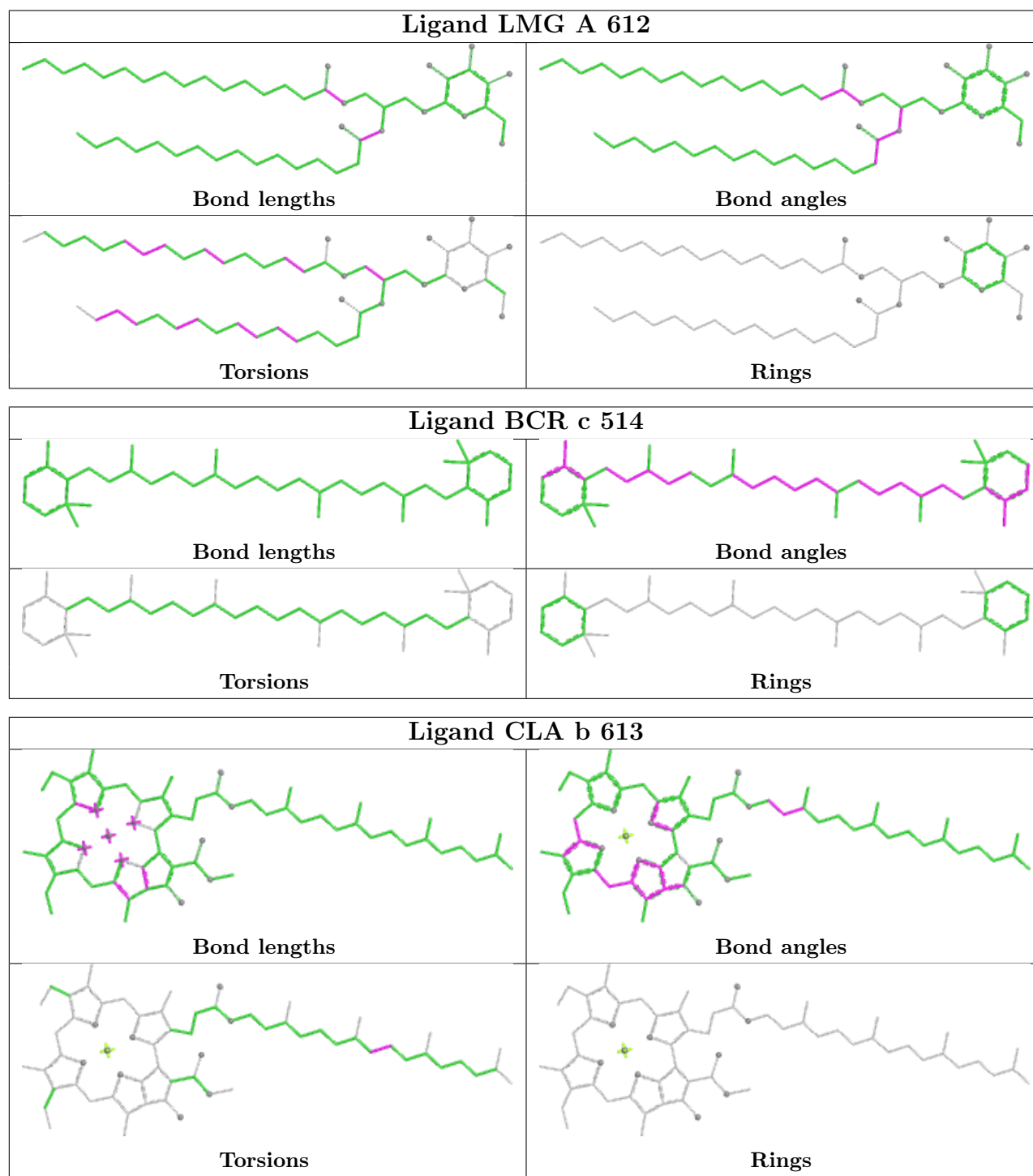
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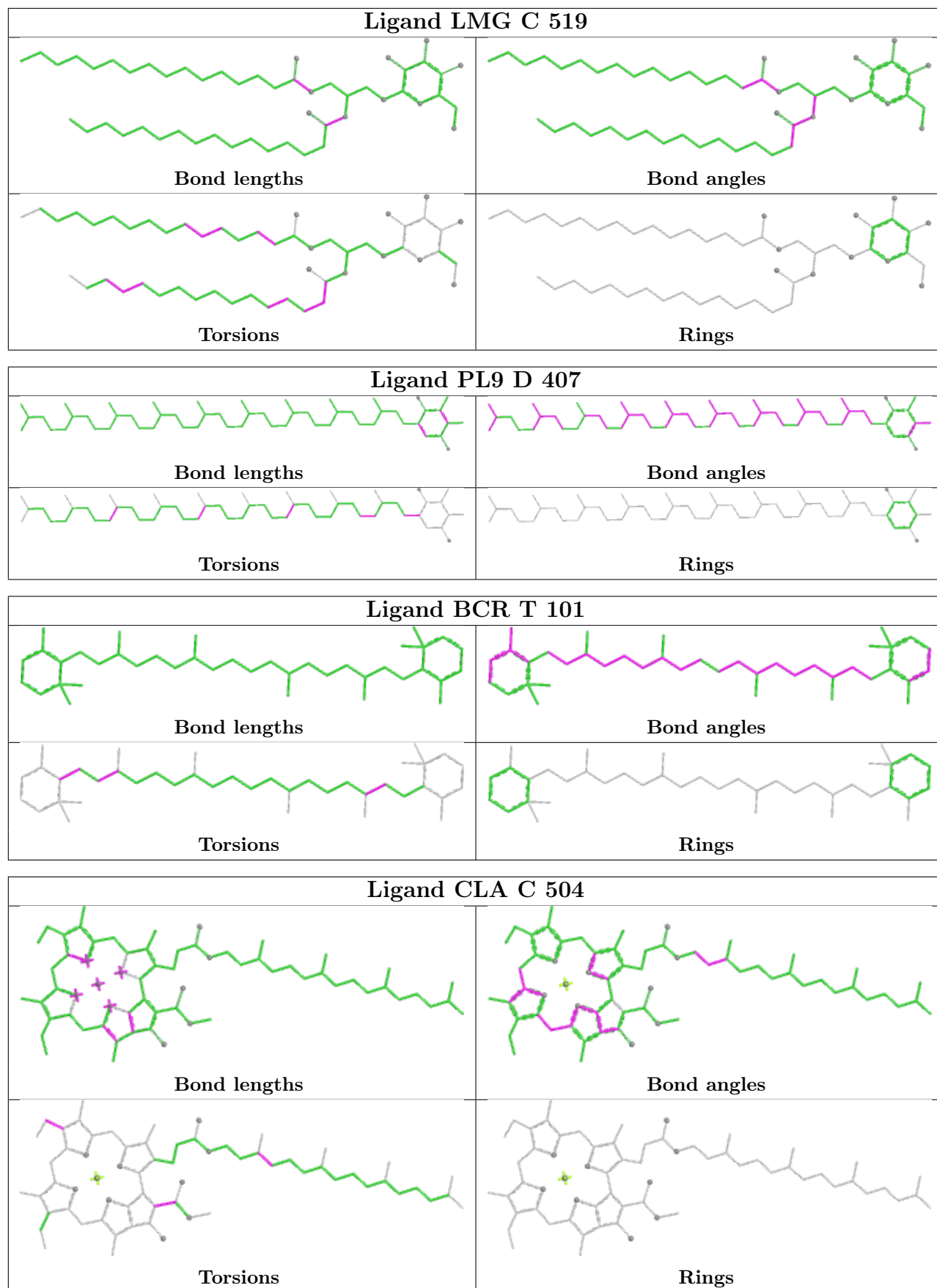
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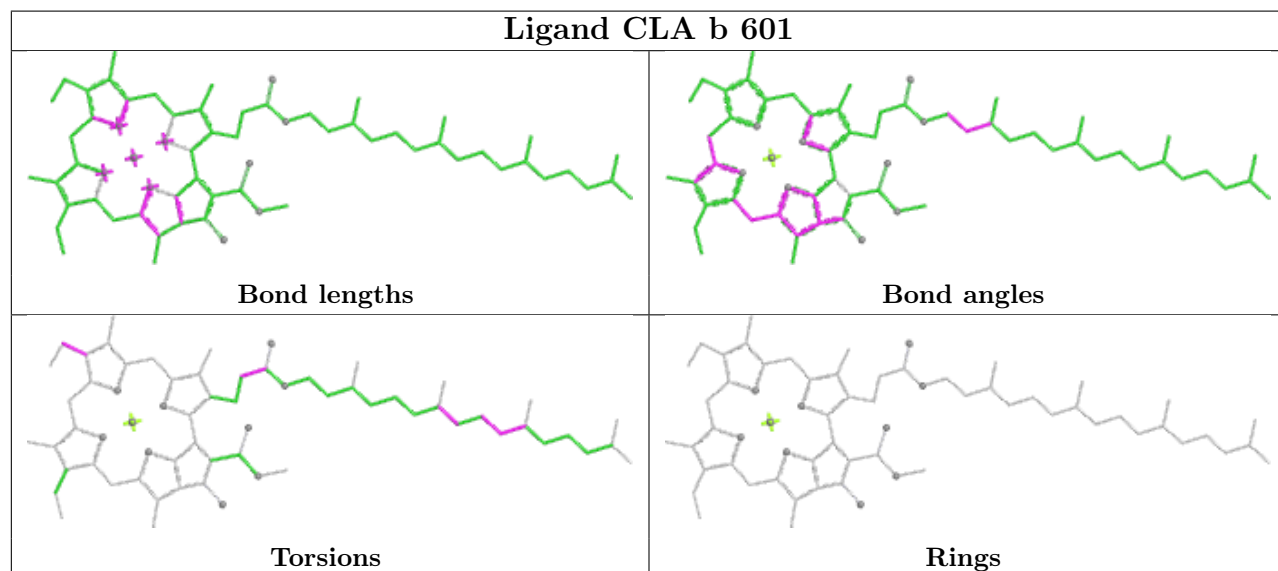
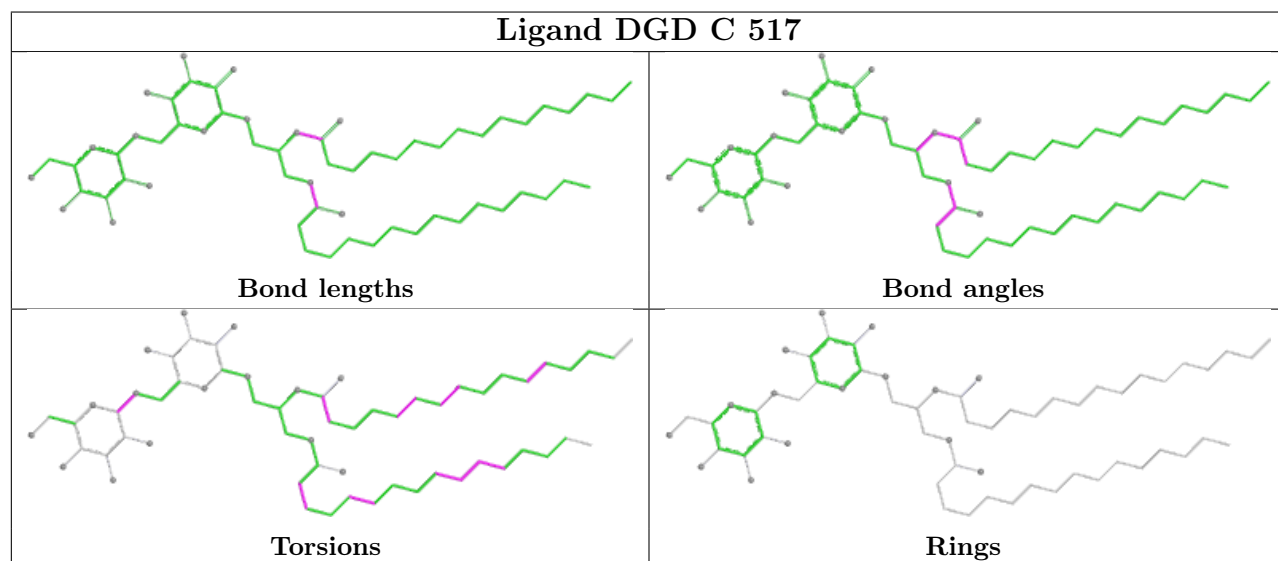
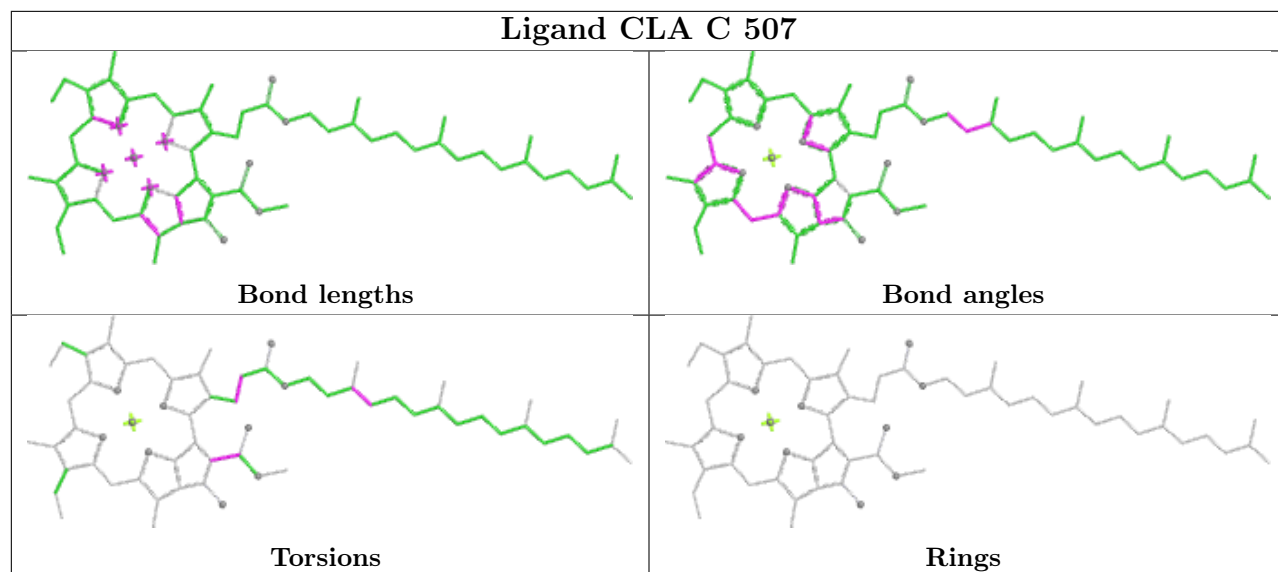
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	408	LMG	2	0
25	B	608	CLA	1	0
25	A	607	CLA	2	0
25	B	601	CLA	2	0
25	A	608	CLA	2	0
25	D	405	CLA	1	0
26	z	101	BCR	10	0
25	c	512	CLA	3	0
25	c	505	CLA	6	0
25	b	611	CLA	2	0
25	B	613	CLA	5	0
25	C	506	CLA	5	0
25	B	616	CLA	4	0
25	C	511	CLA	3	0
29	a	615	LHG	4	0
33	C	518	DGD	1	0
25	b	604	CLA	3	0
25	d	401	CLA	3	0
25	c	506	CLA	4	0
34	D	402	PHO	5	0
26	d	404	BCR	4	0
25	c	509	CLA	3	0
28	A	611	SQD	2	0
26	b	617	BCR	1	0
26	C	522	BCR	1	0
26	a	611	BCR	3	0
25	b	603	CLA	1	0
25	b	606	CLA	3	0
23	c	518	LMG	2	0
26	B	619	BCR	4	0
25	C	510	CLA	3	0
25	a	610	CLA	4	0
25	b	605	CLA	3	0
25	B	612	CLA	1	0
25	c	504	CLA	1	0
25	B	606	CLA	1	0

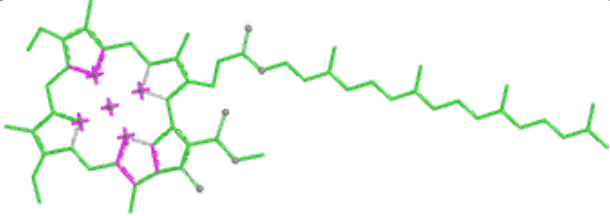
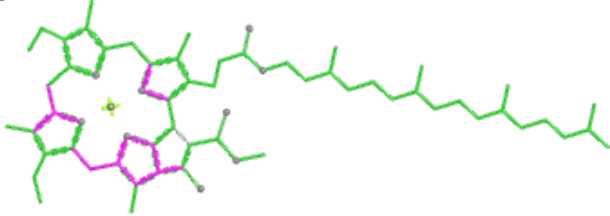
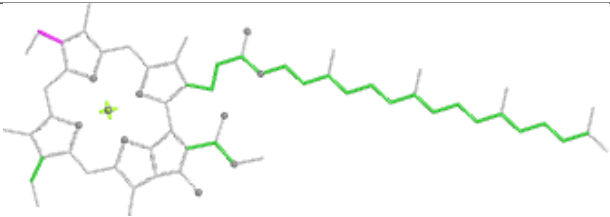
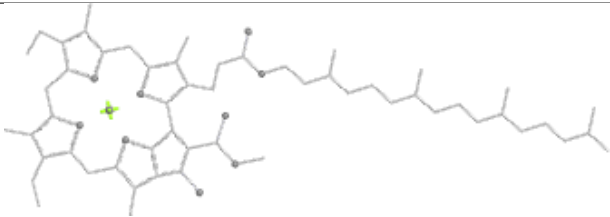
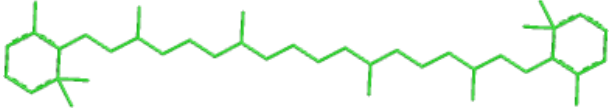
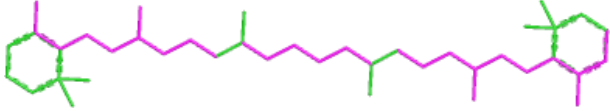
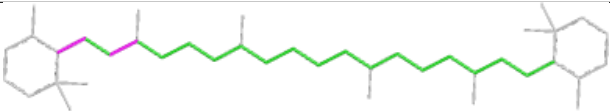
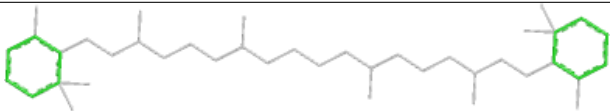
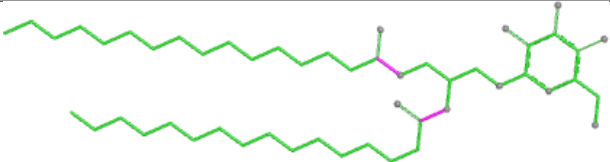
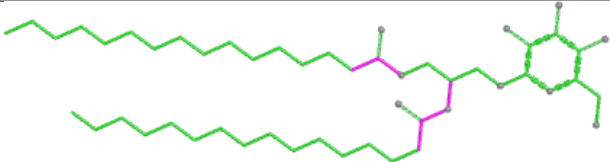
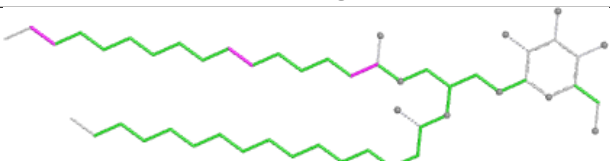
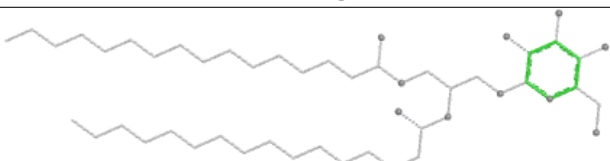
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

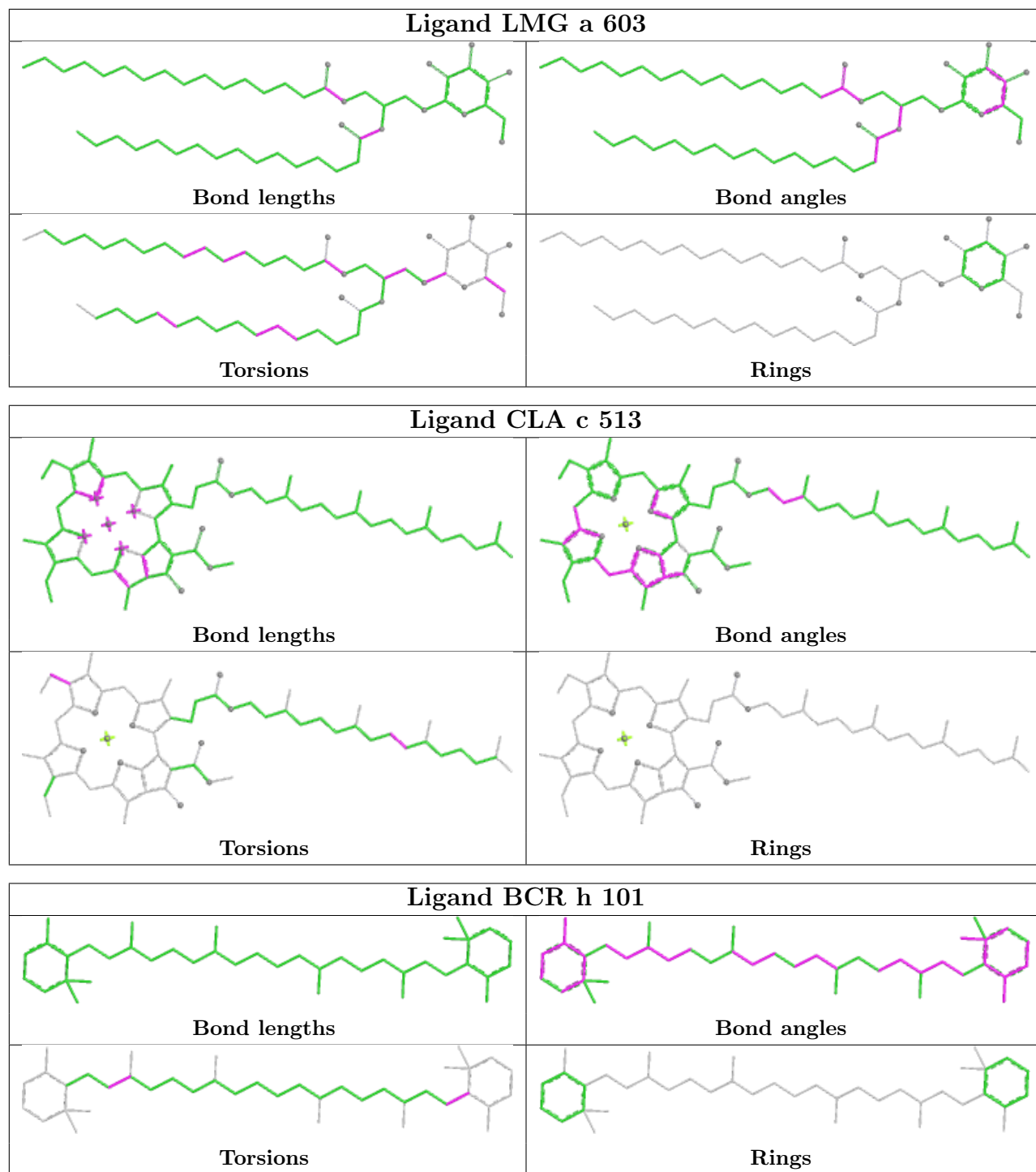
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

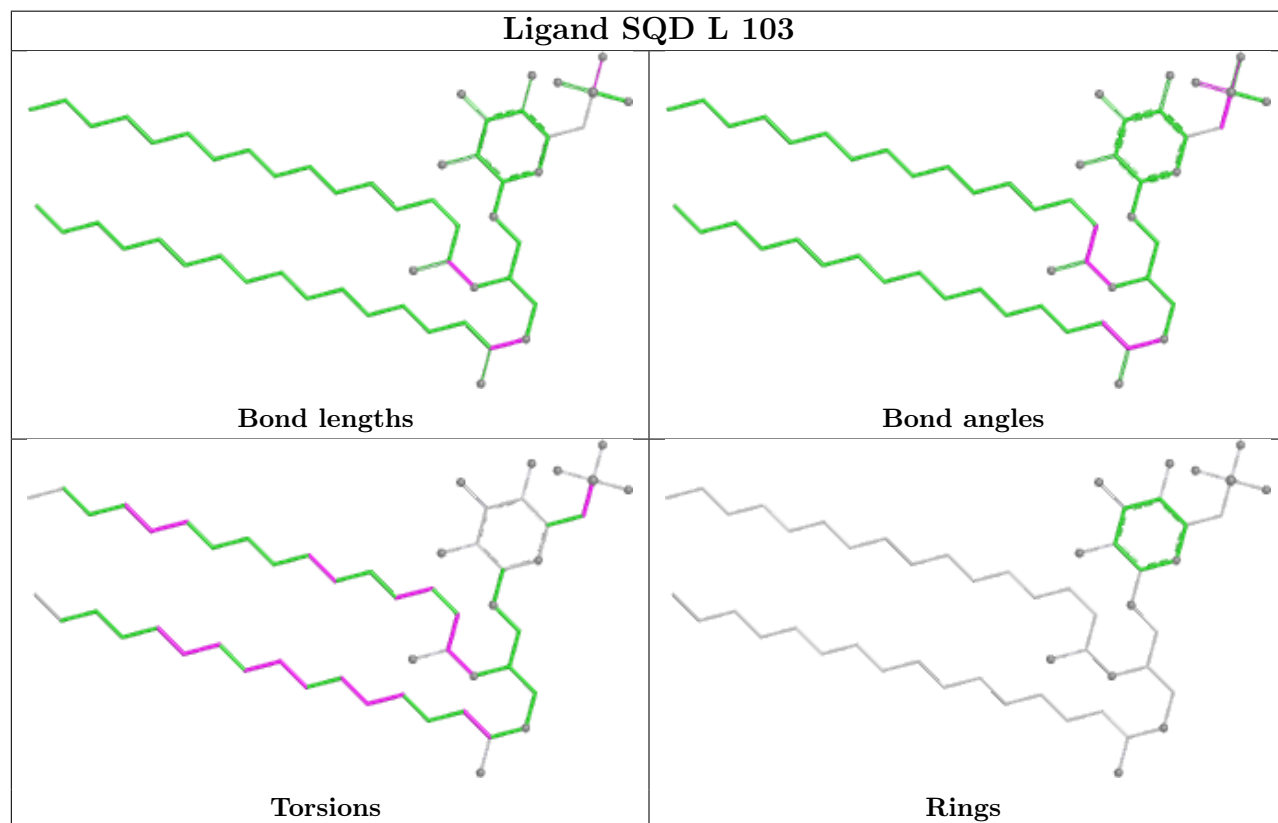
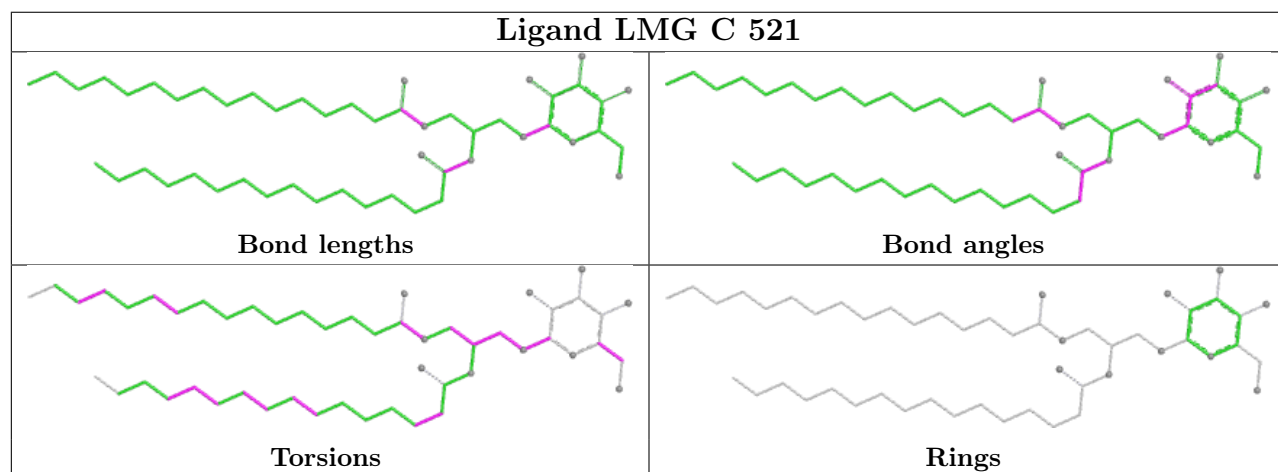
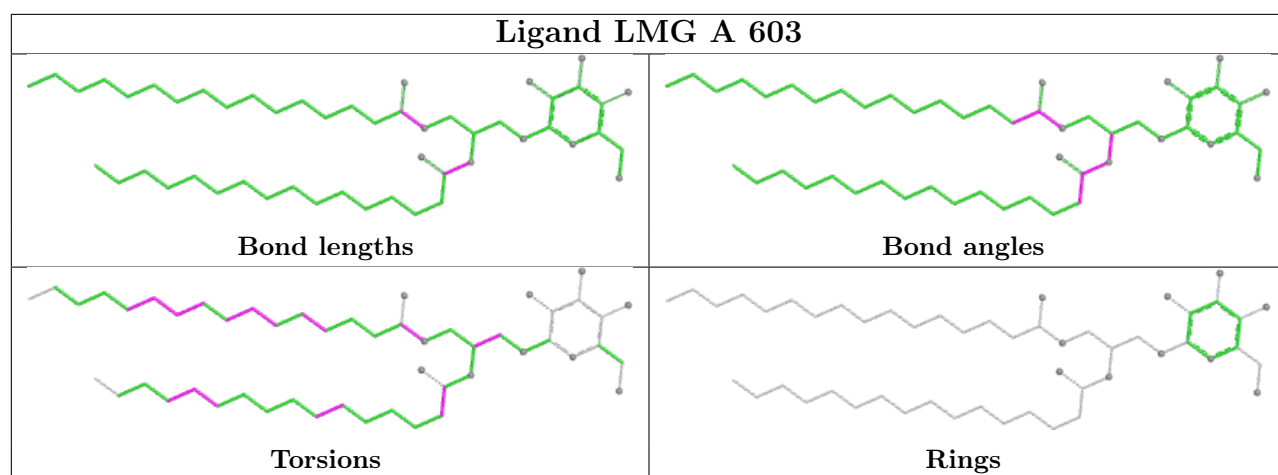


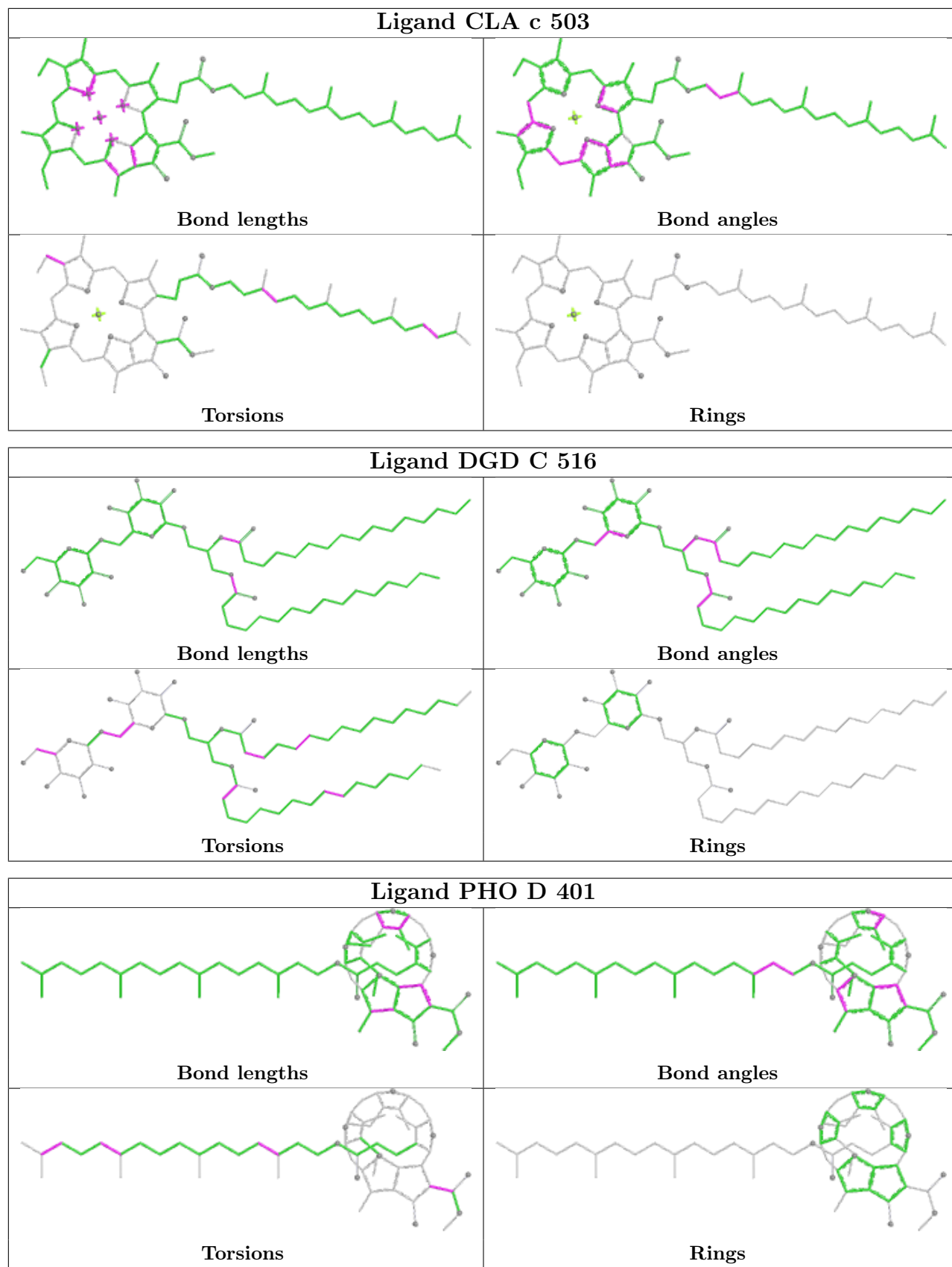


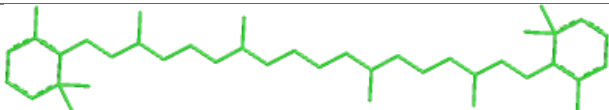
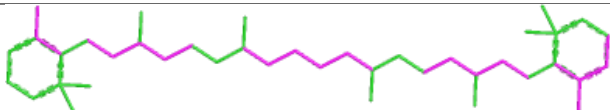
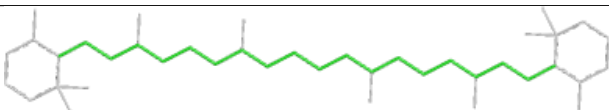
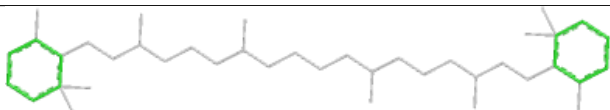


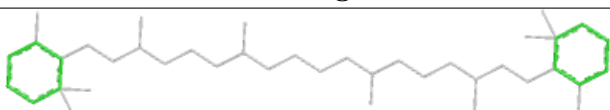
Ligand CLA d 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

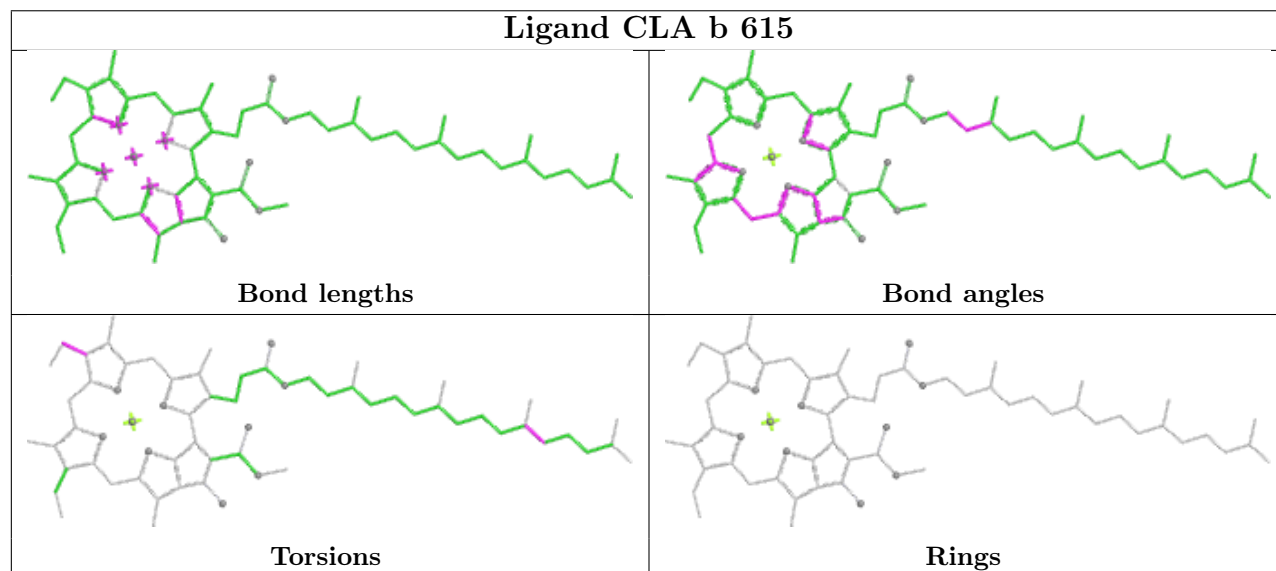
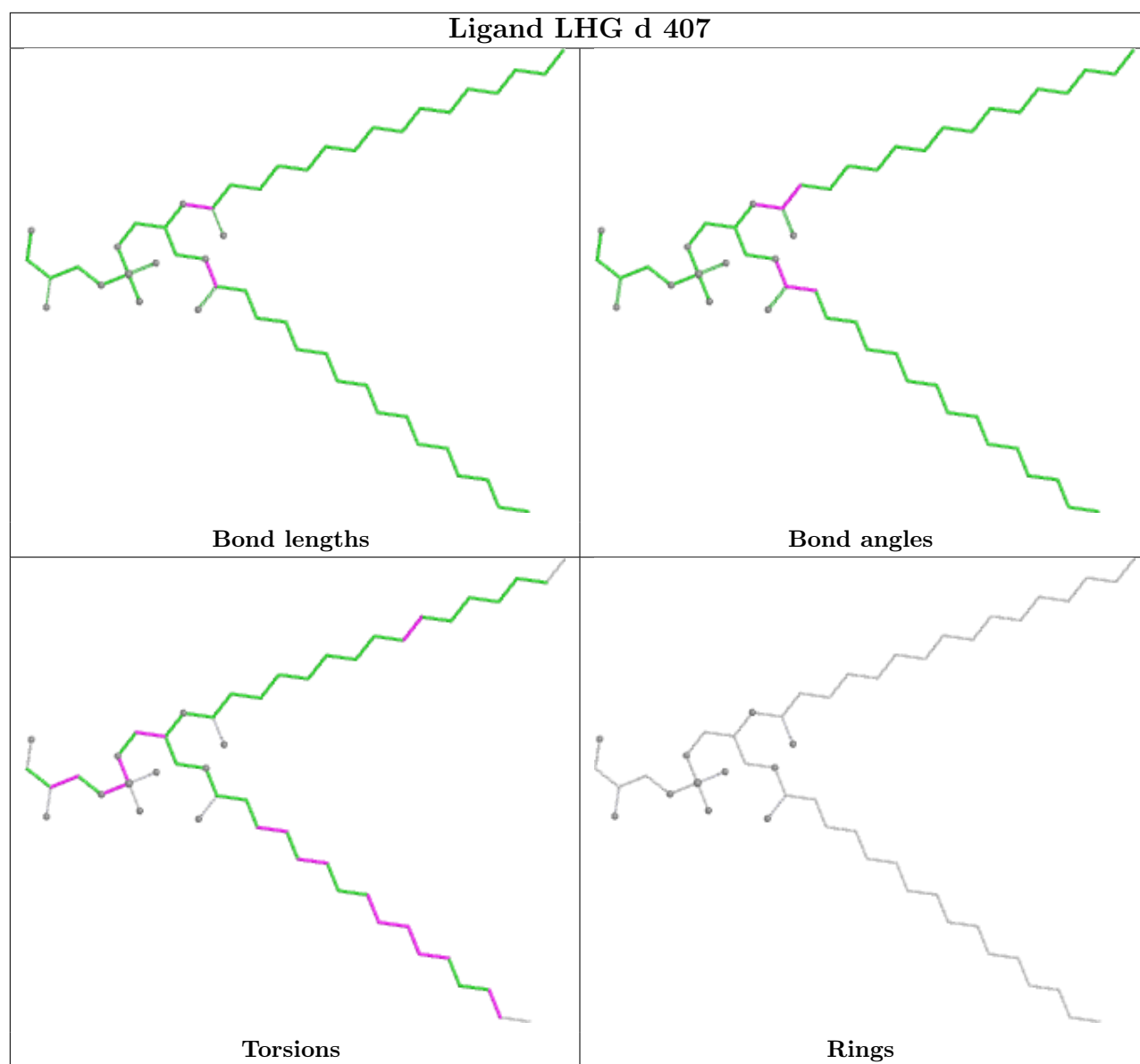




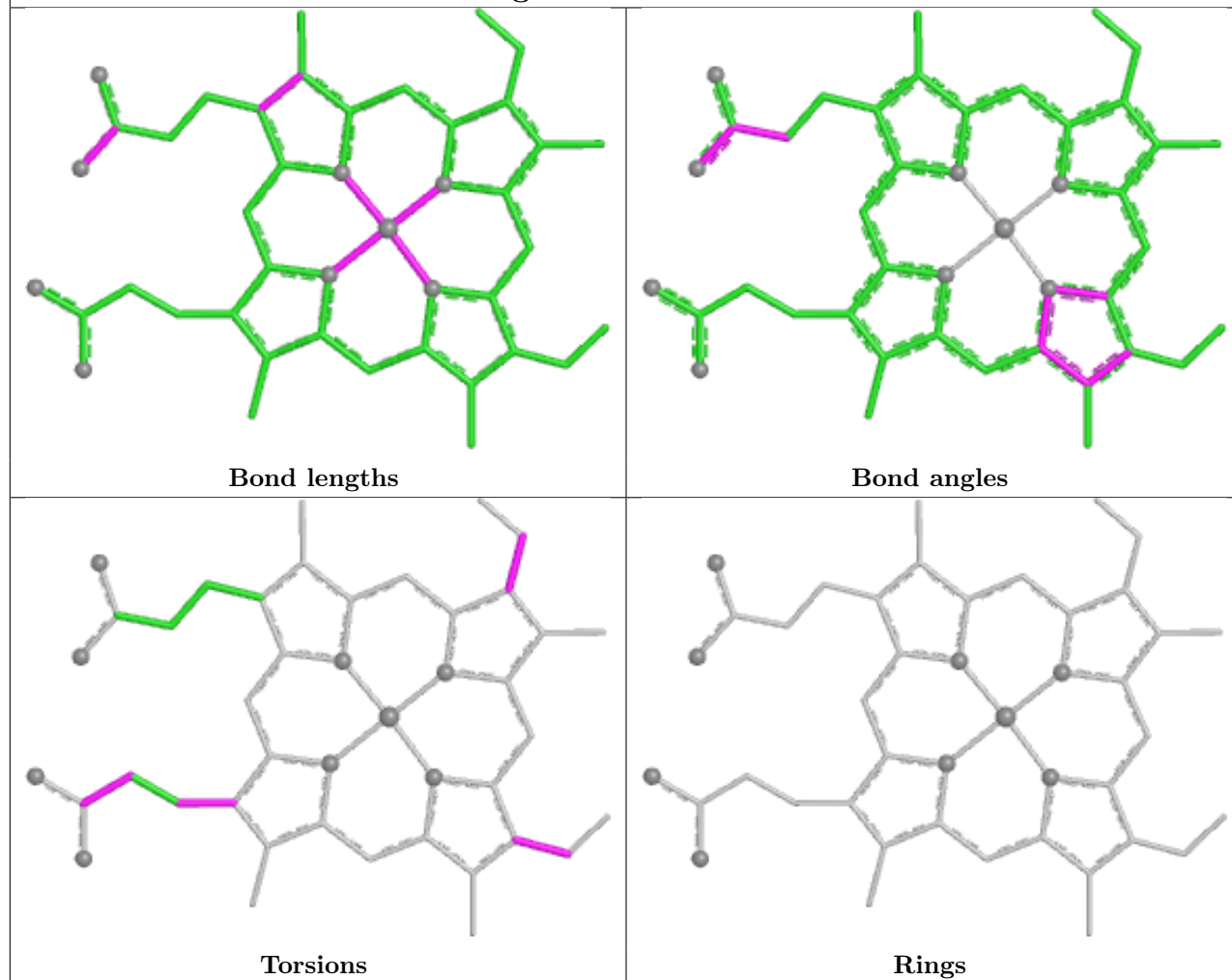


Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

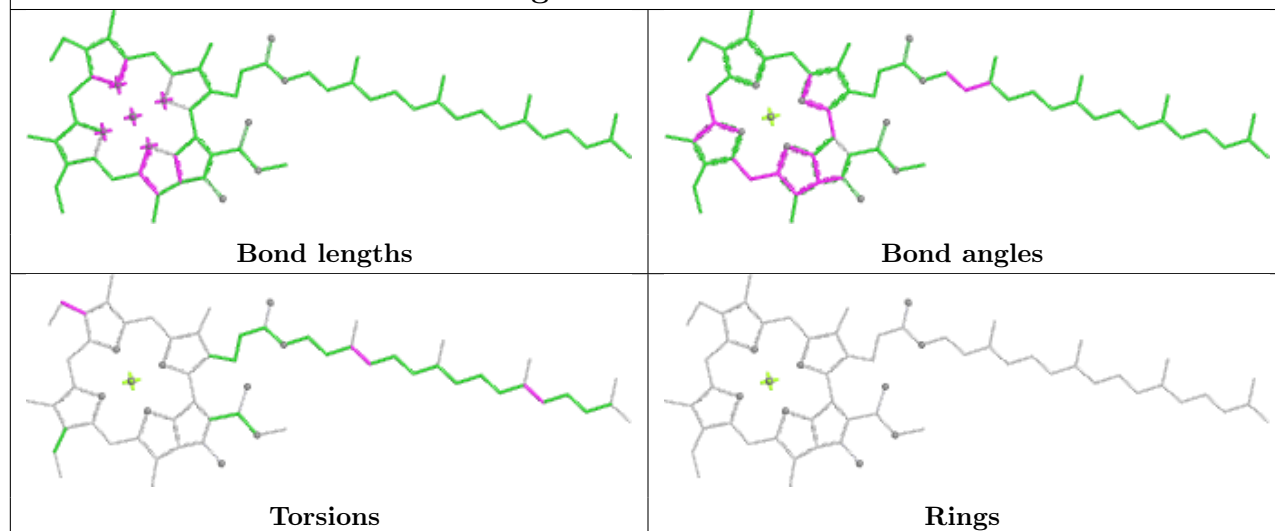
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

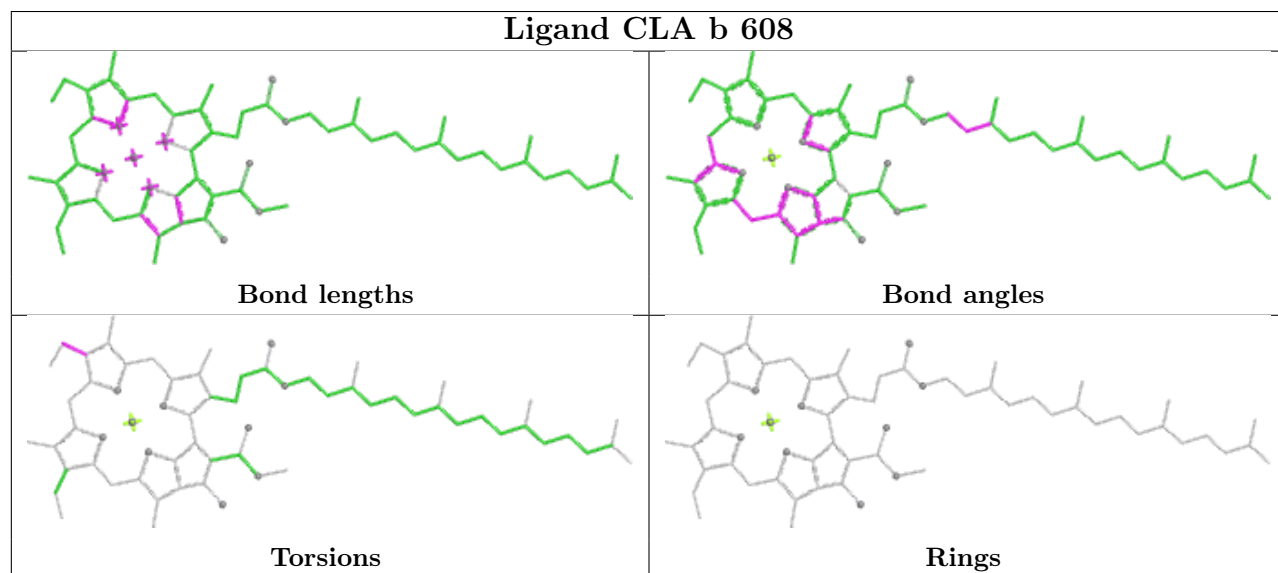
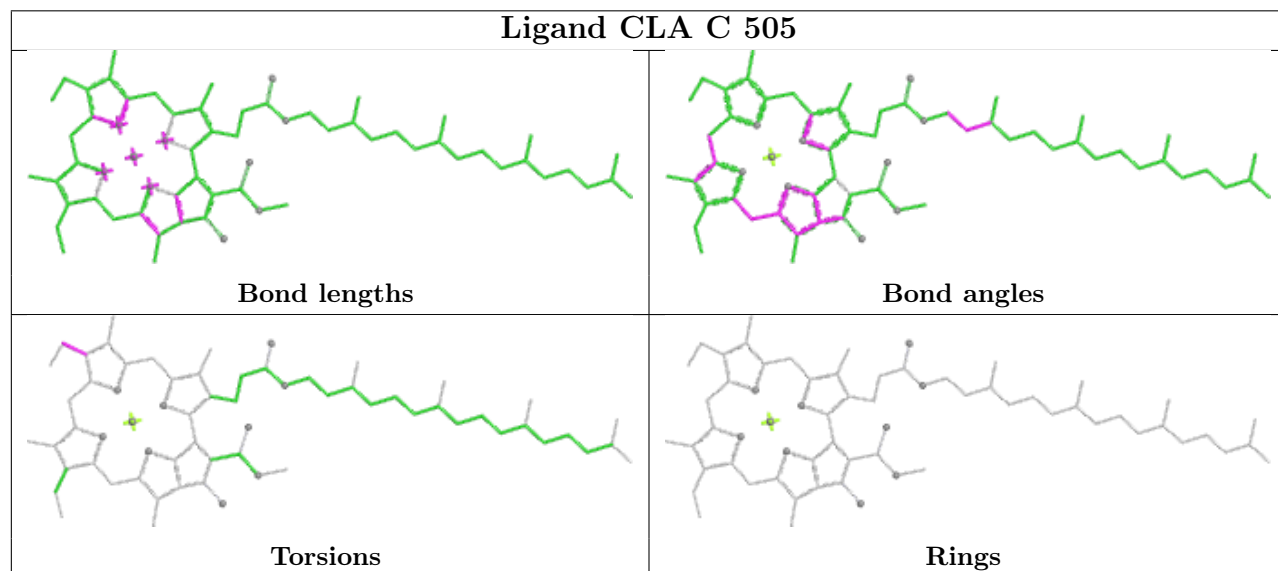
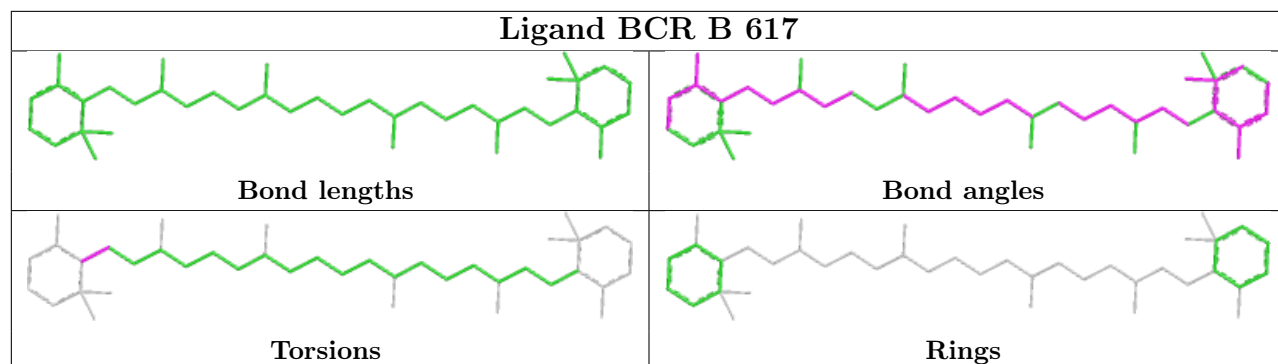


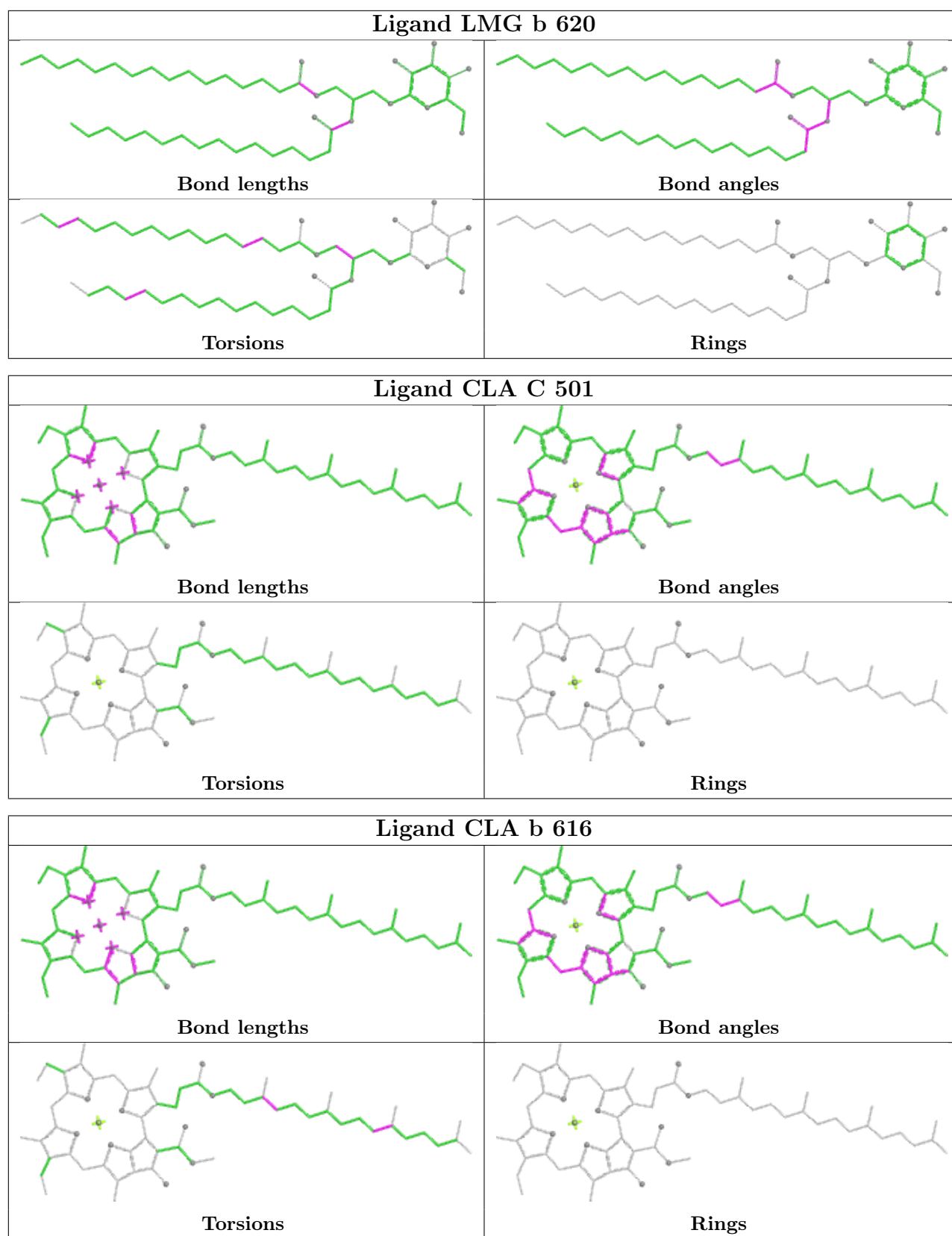
Ligand HEM e 101

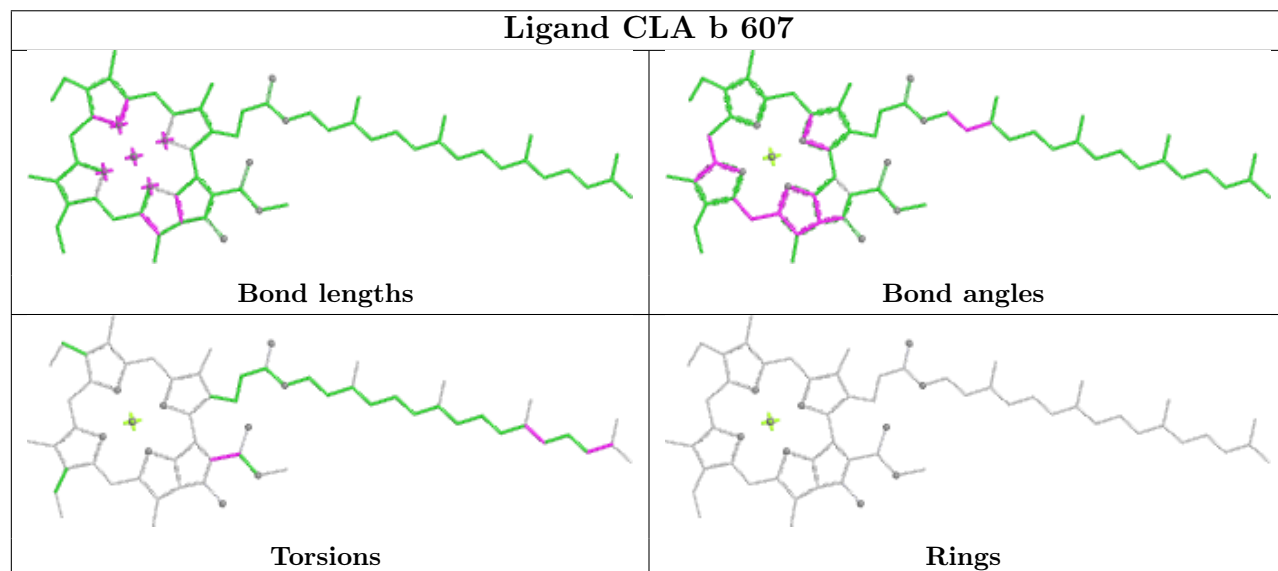
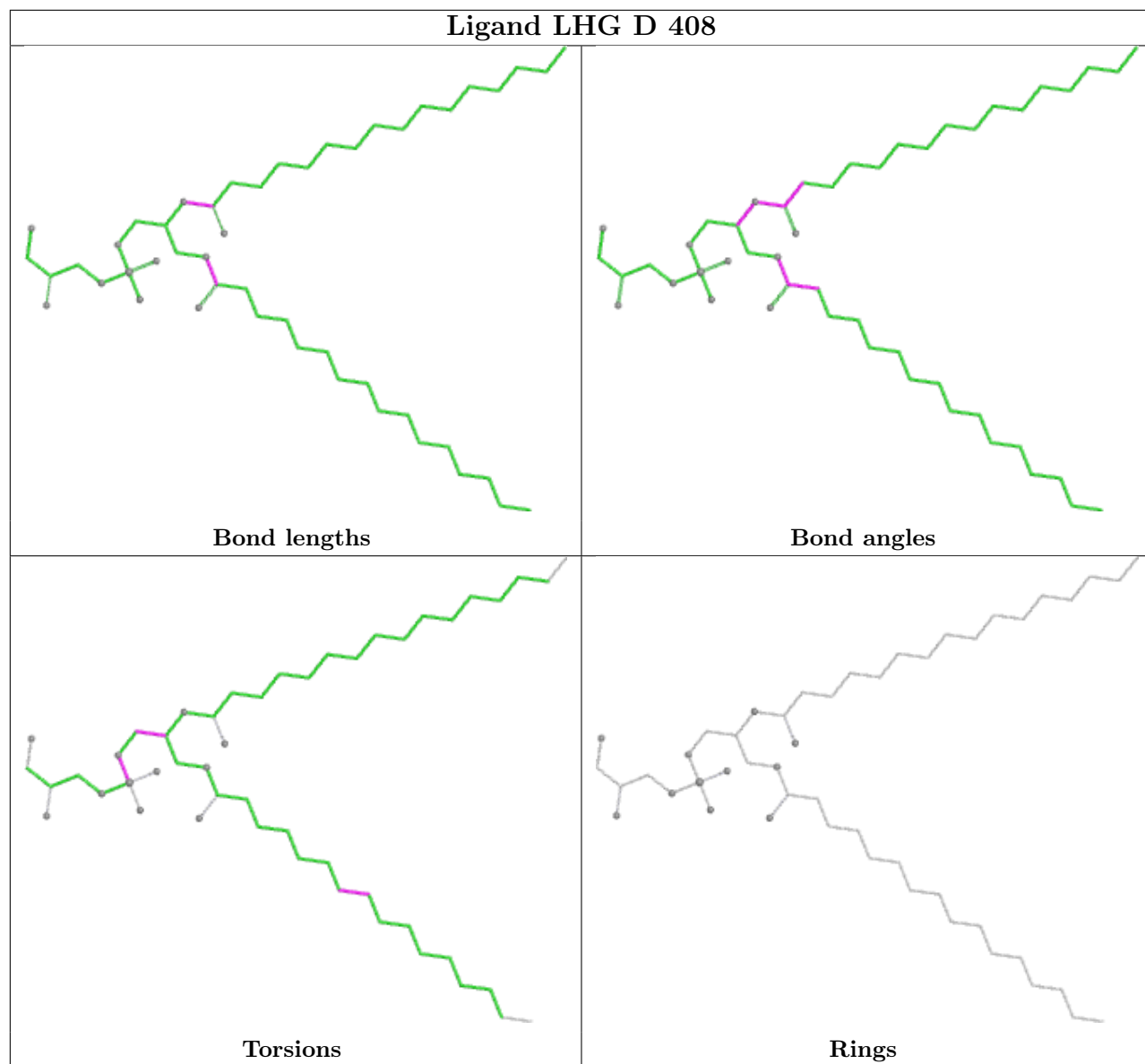


Ligand CLA B 609

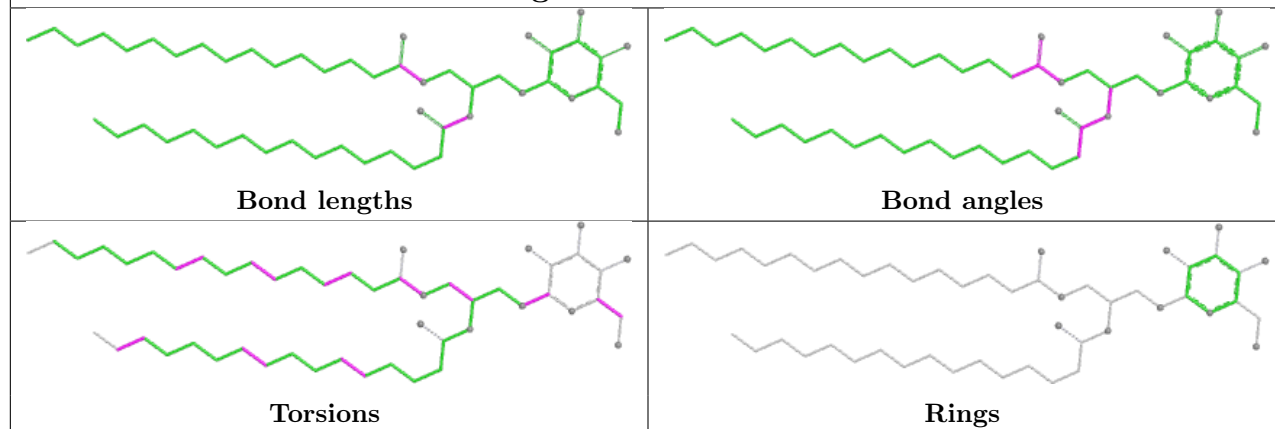




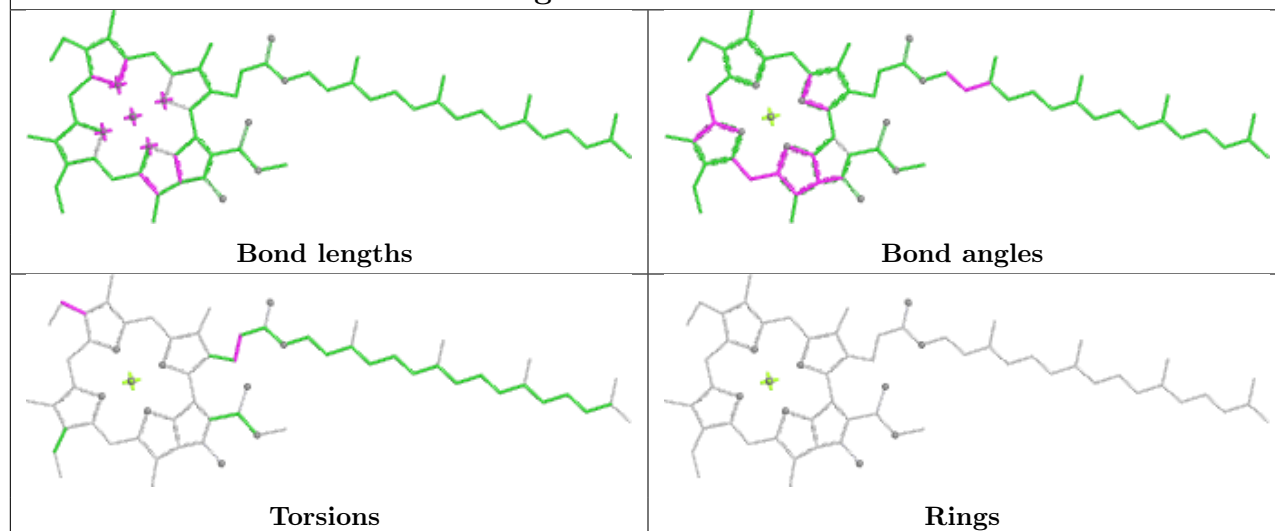




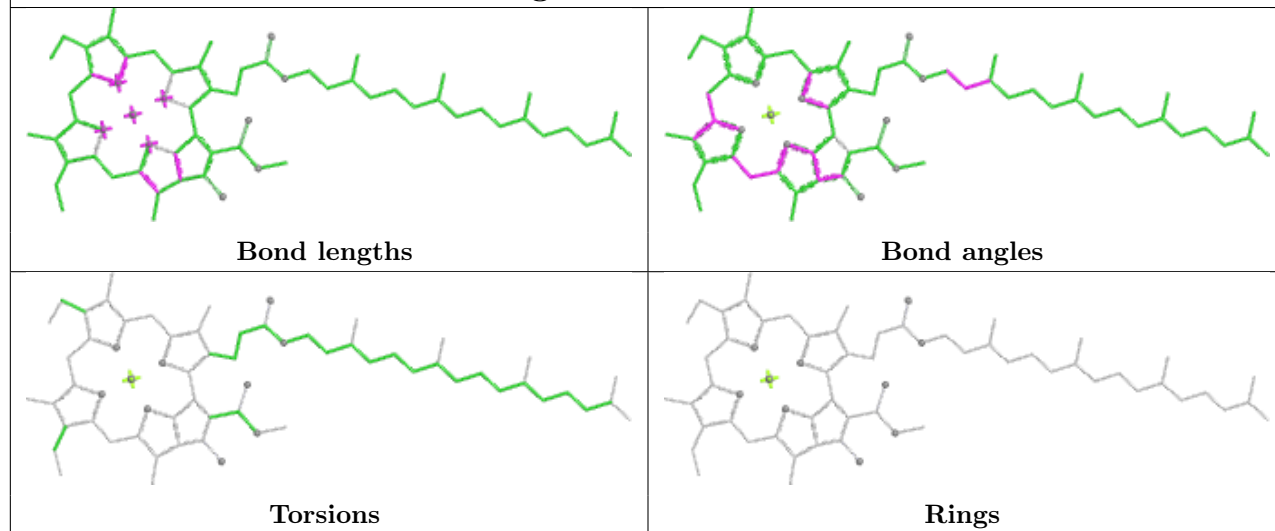
Ligand LMG c 520

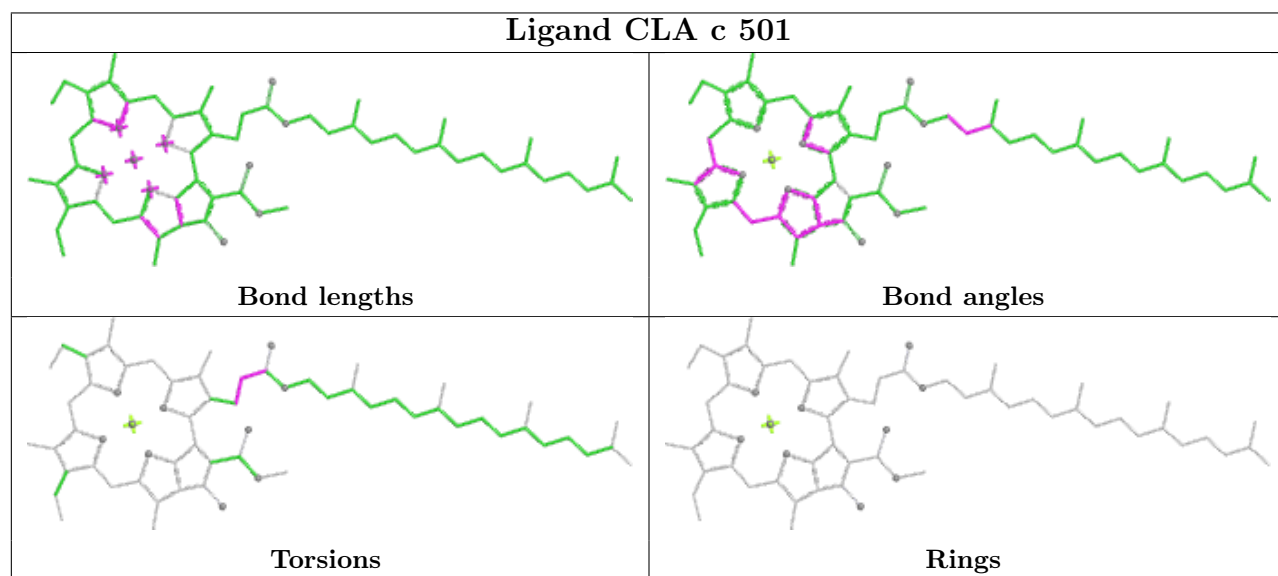
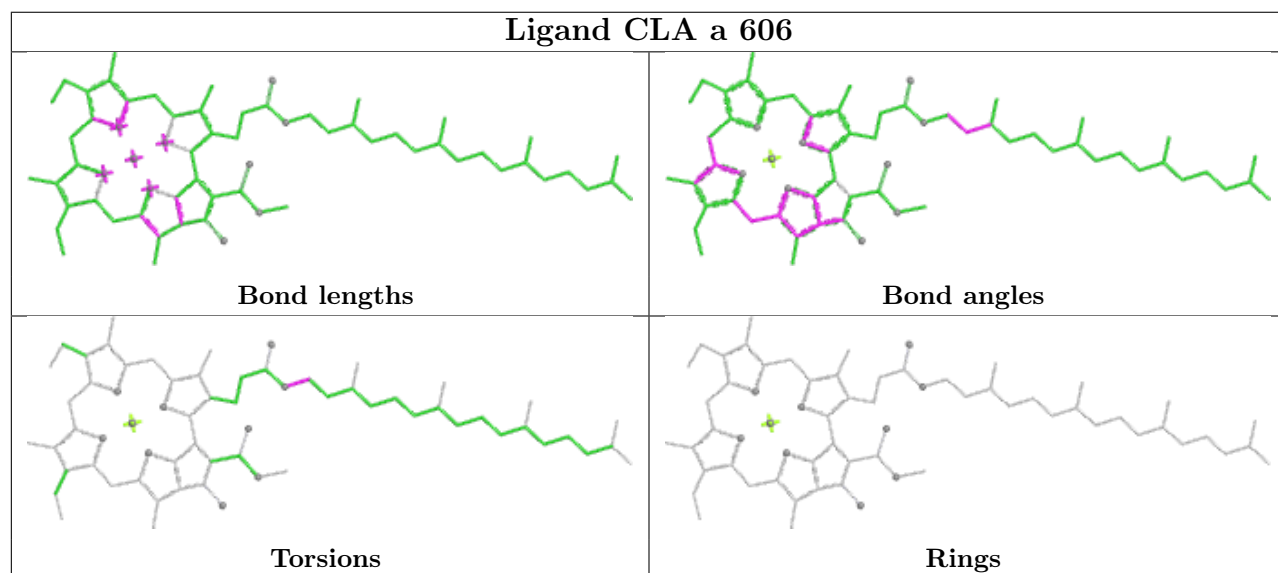
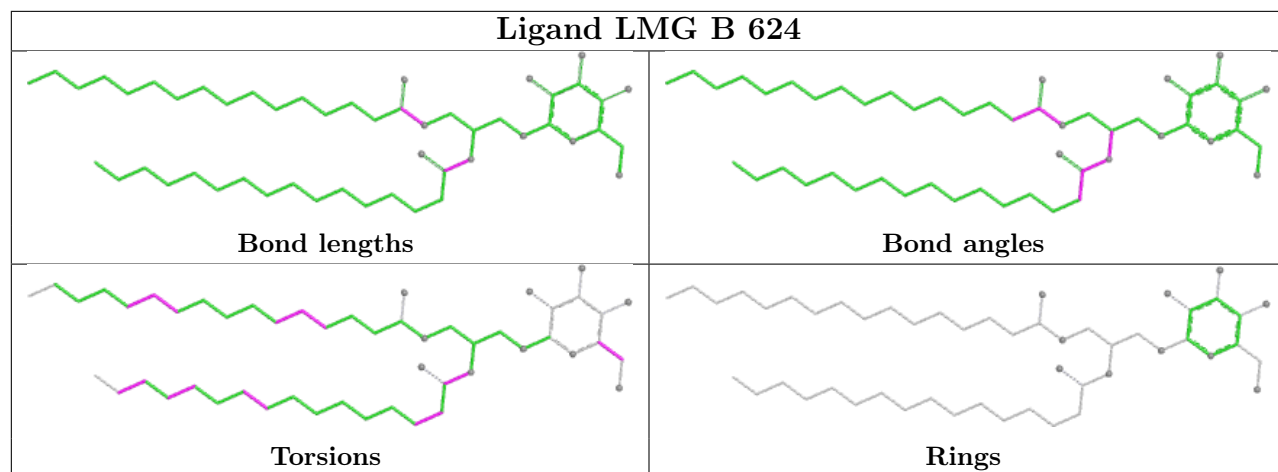


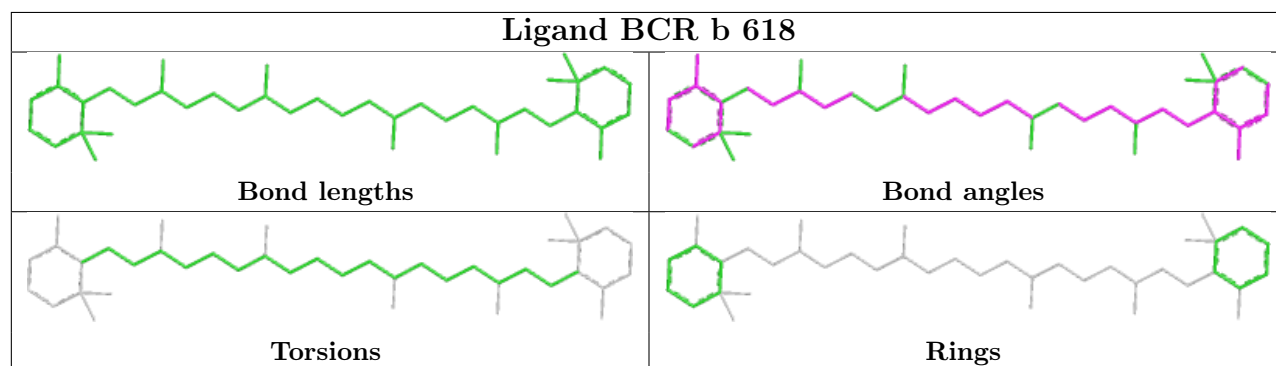
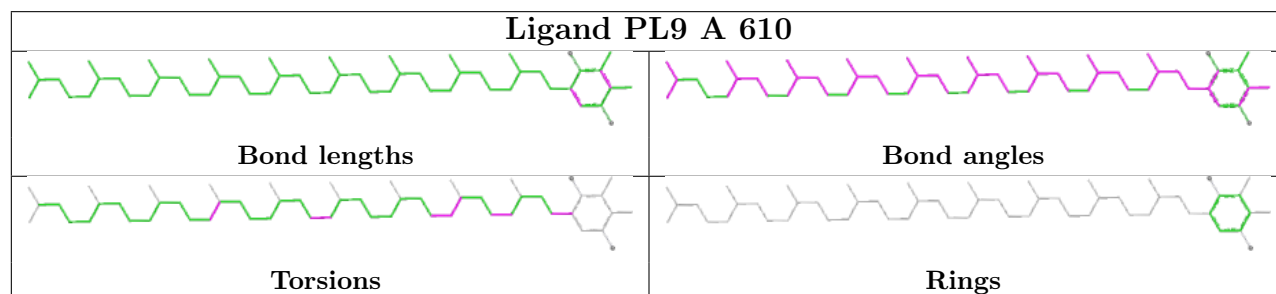
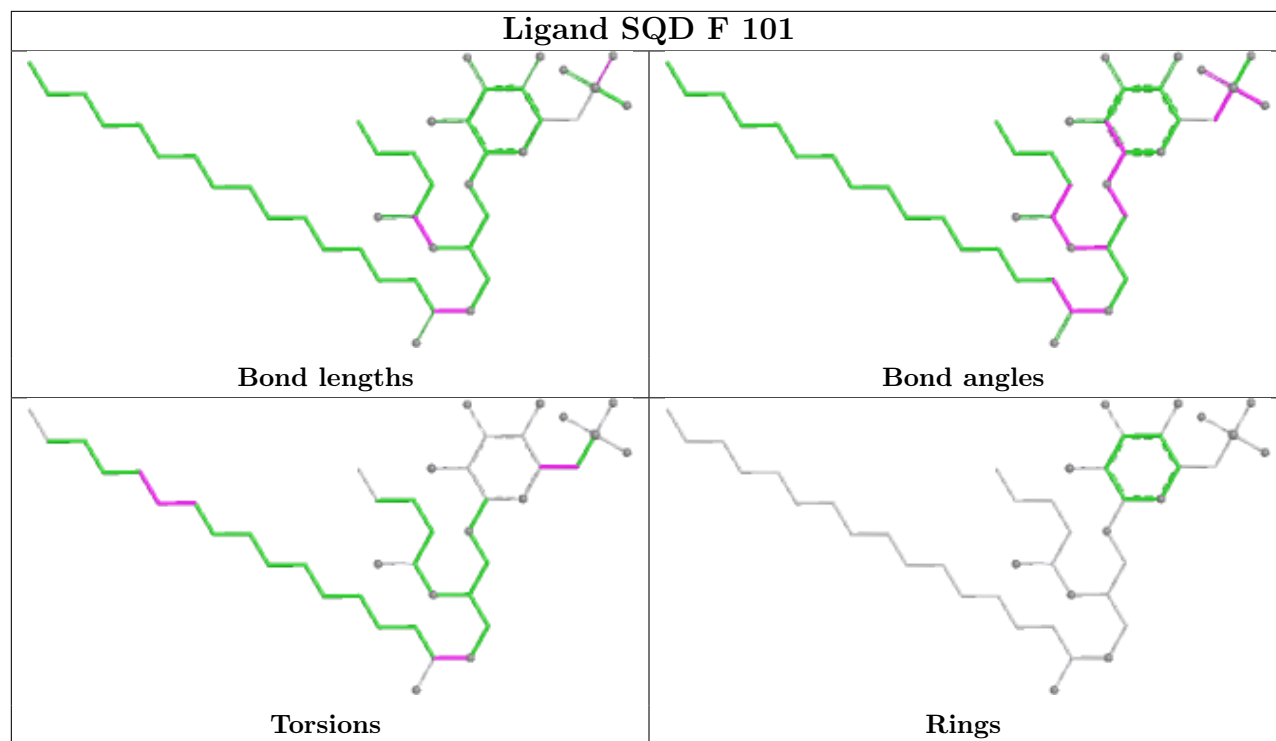
Ligand CLA b 610

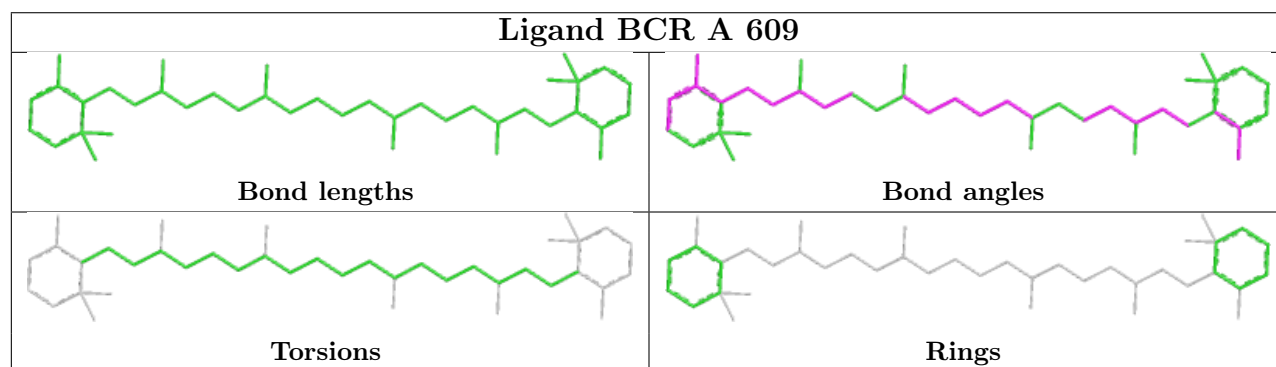
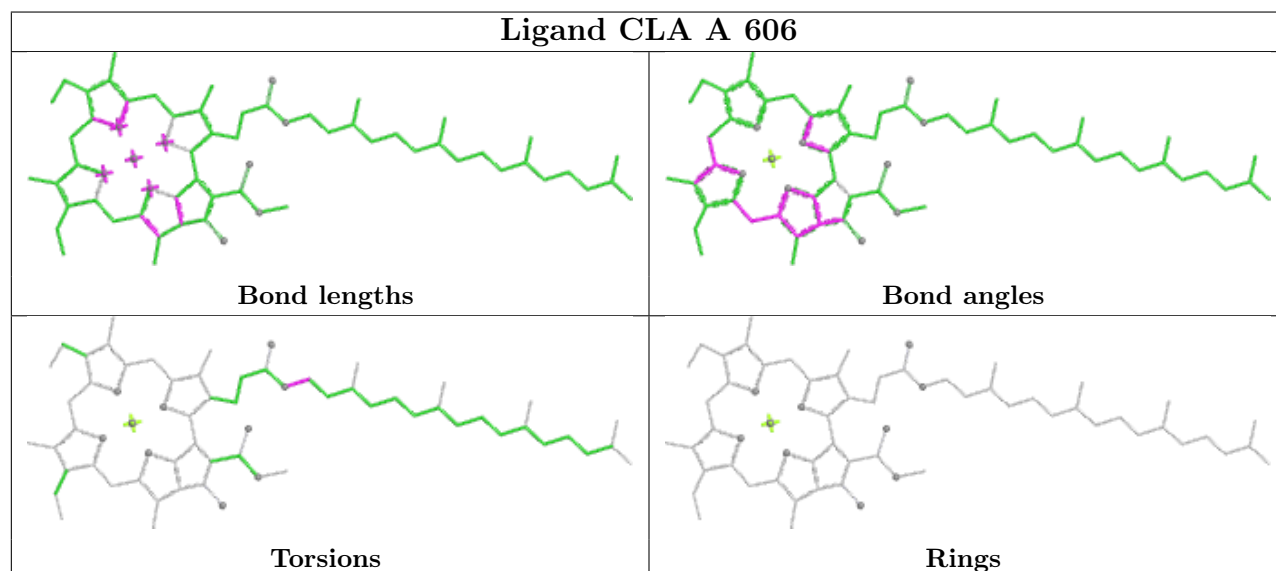
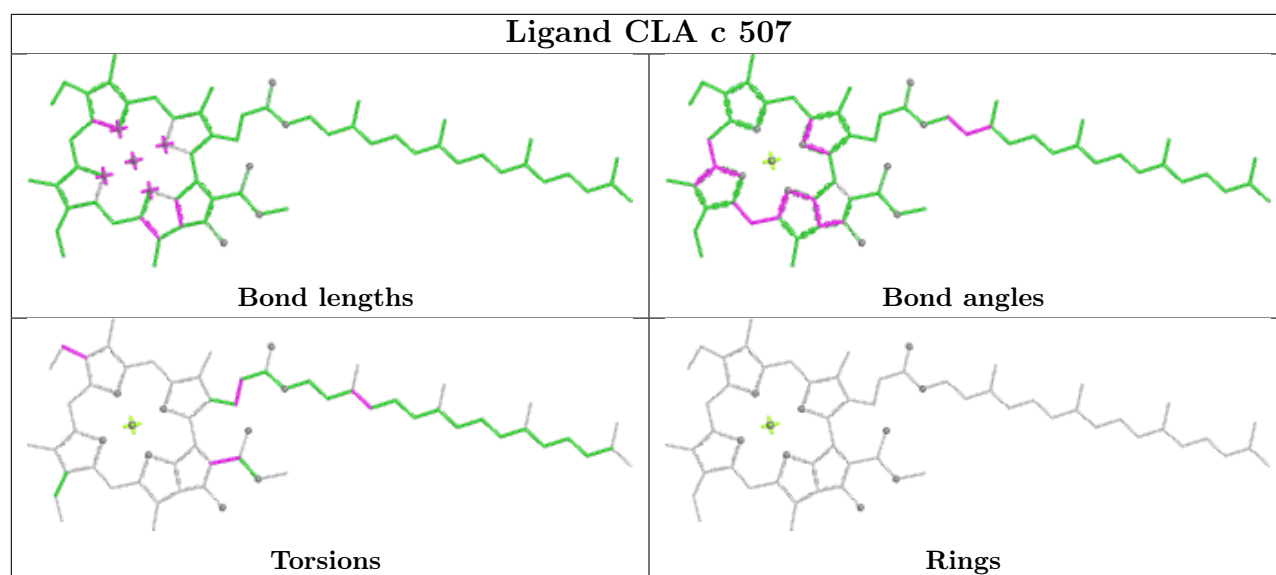


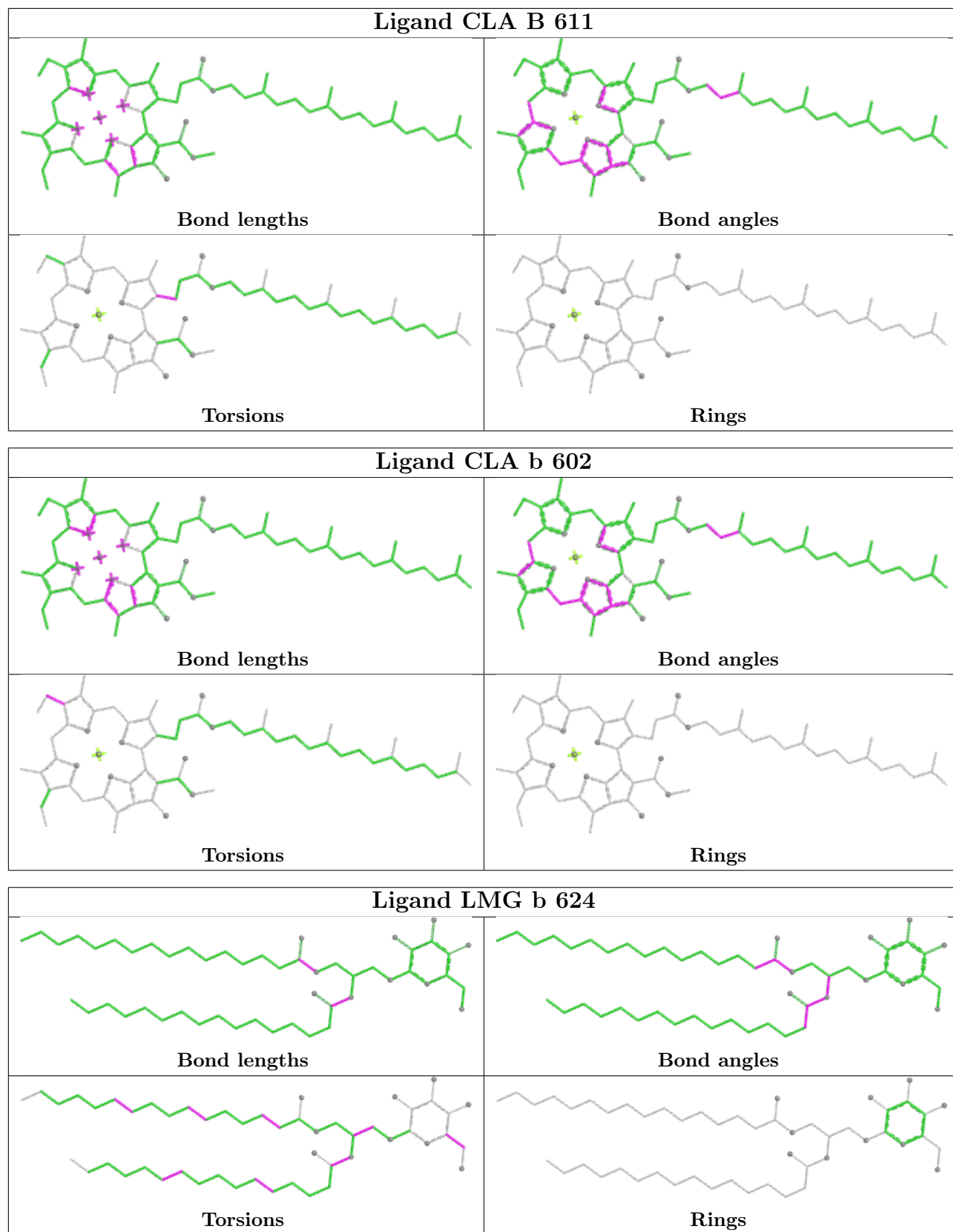
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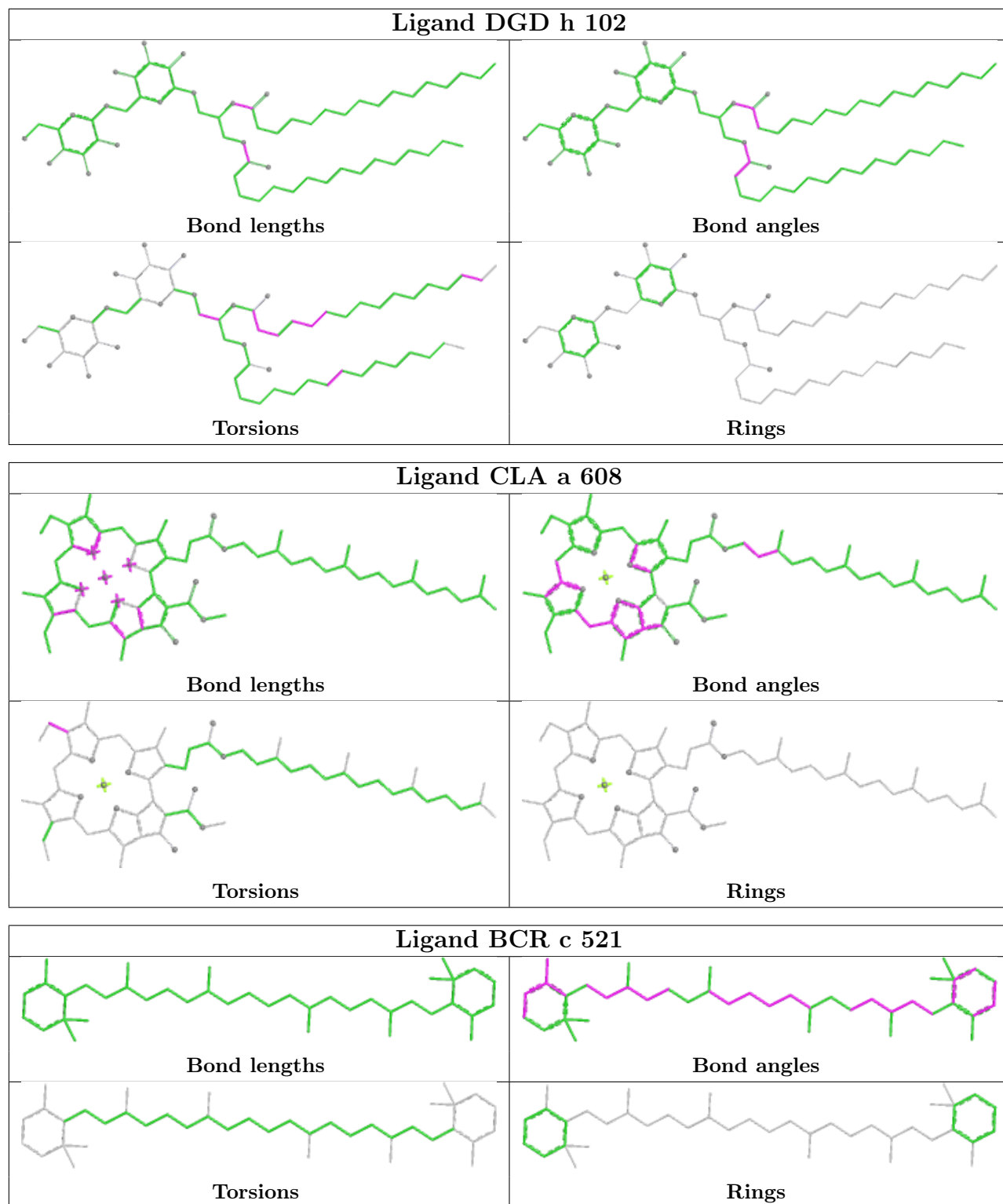


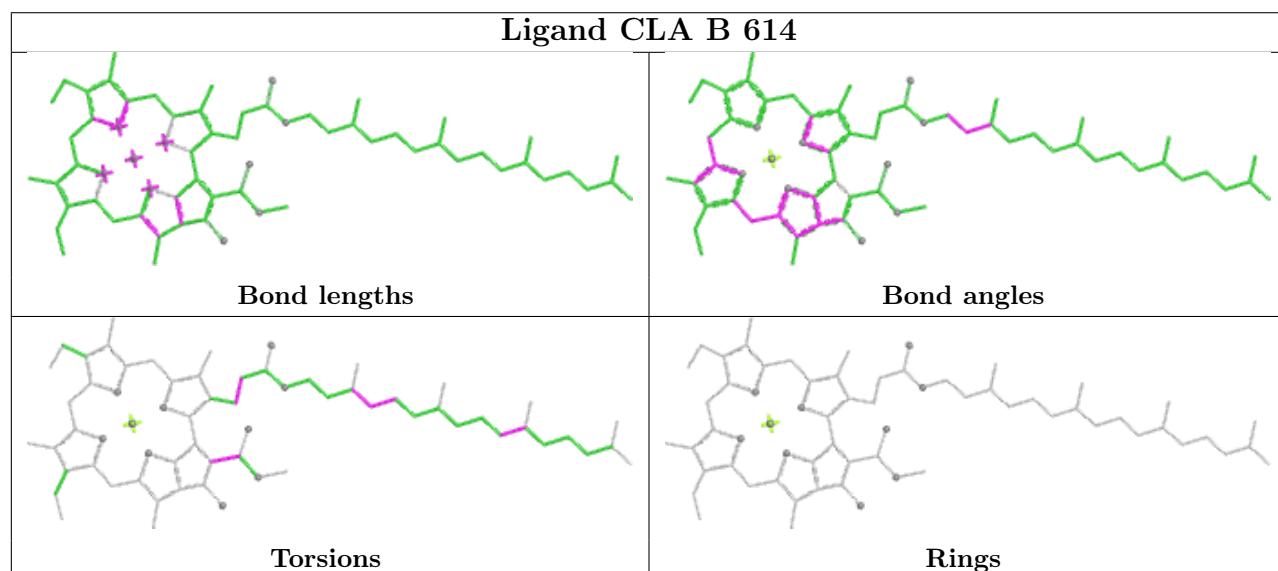
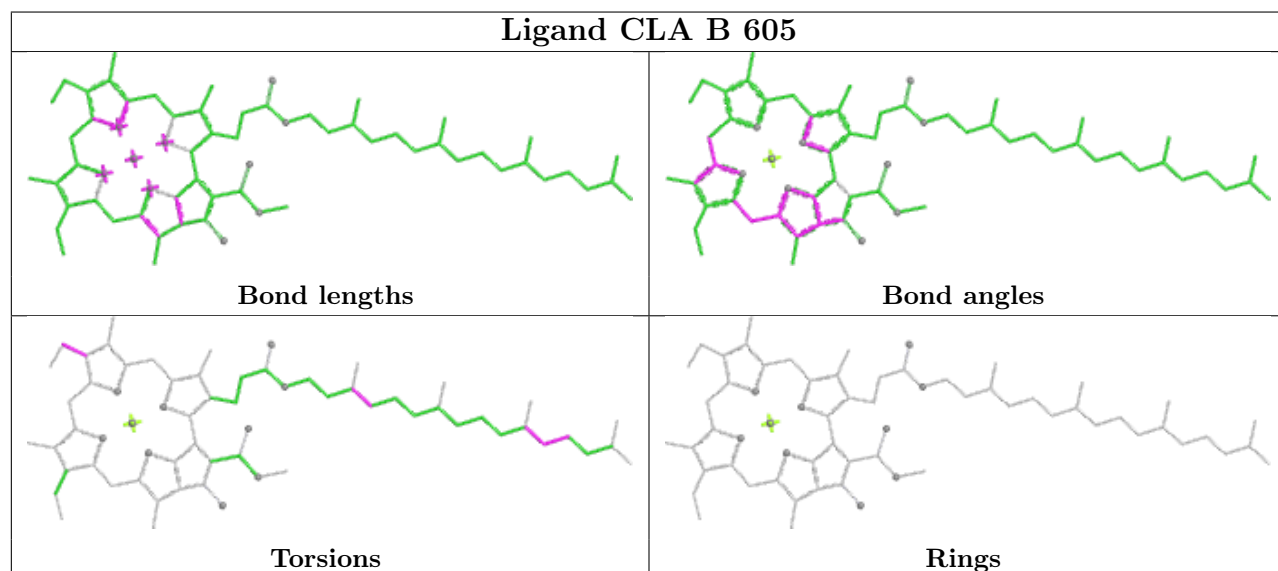
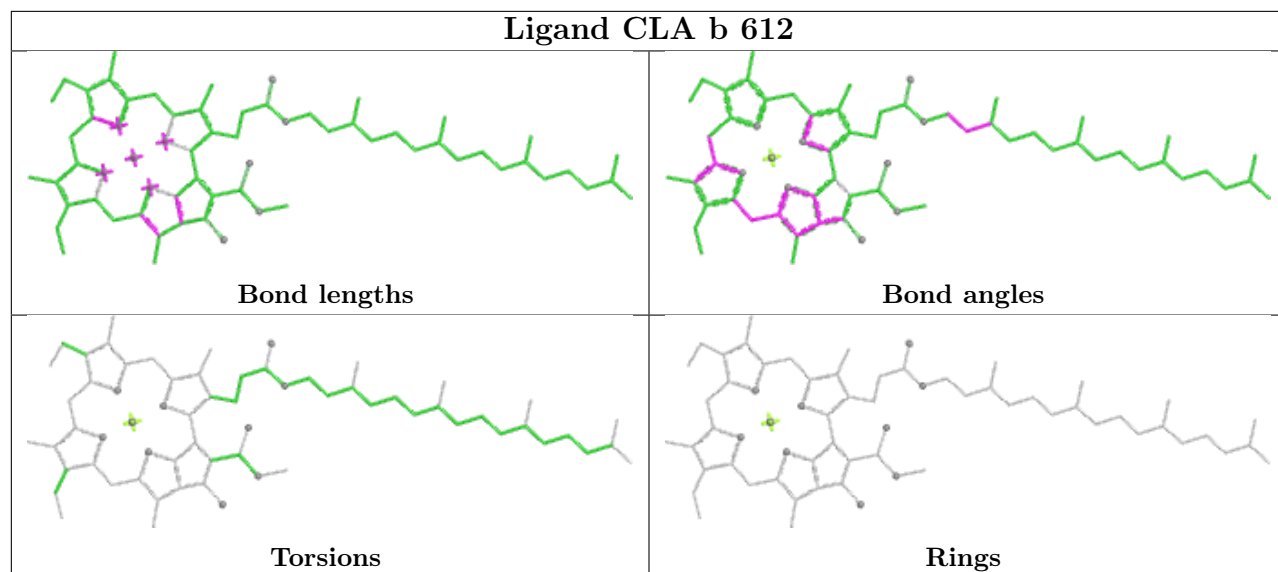


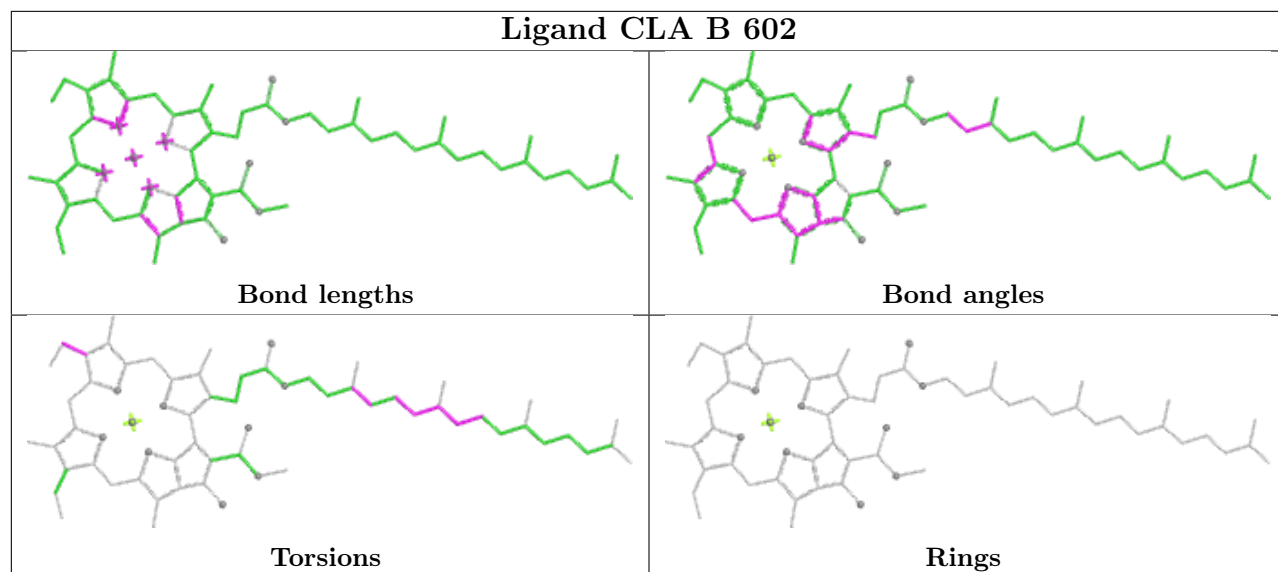
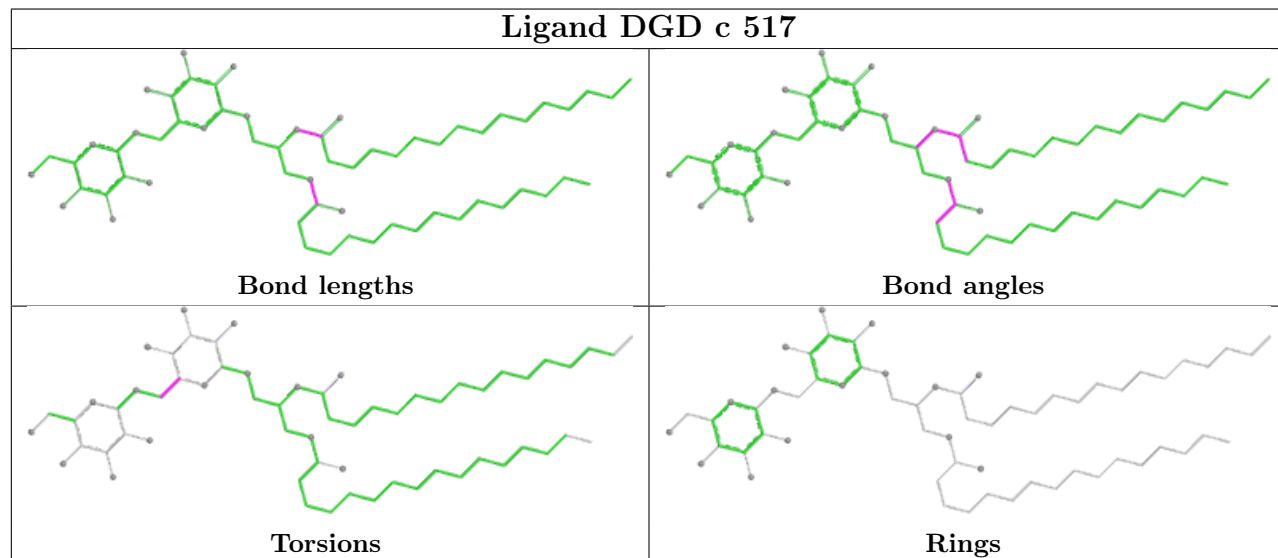


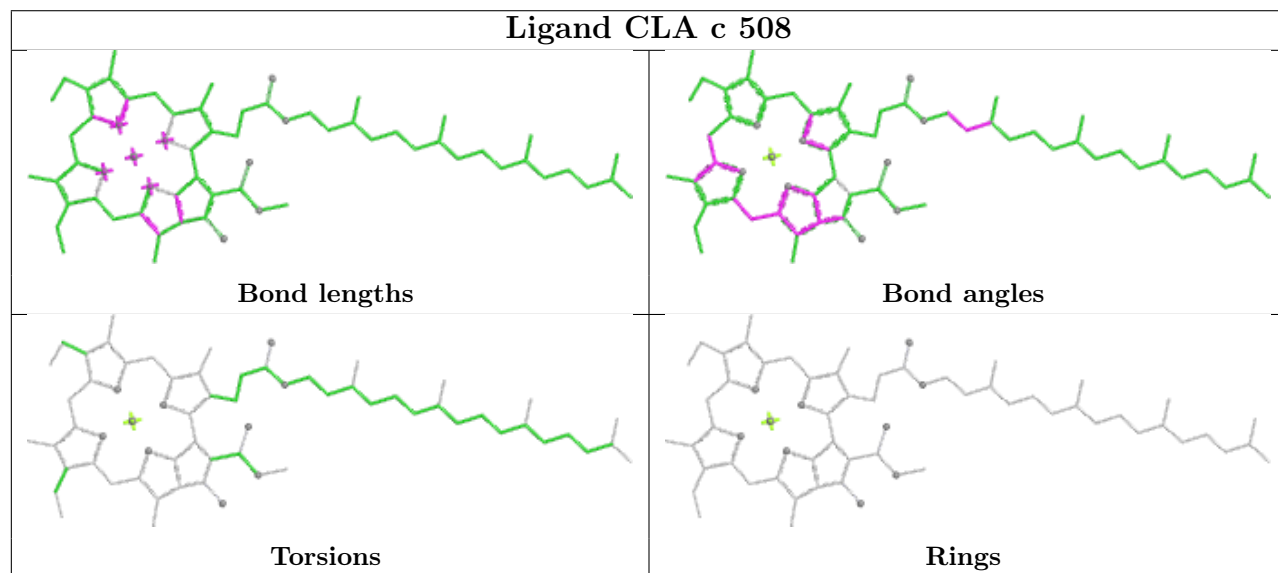
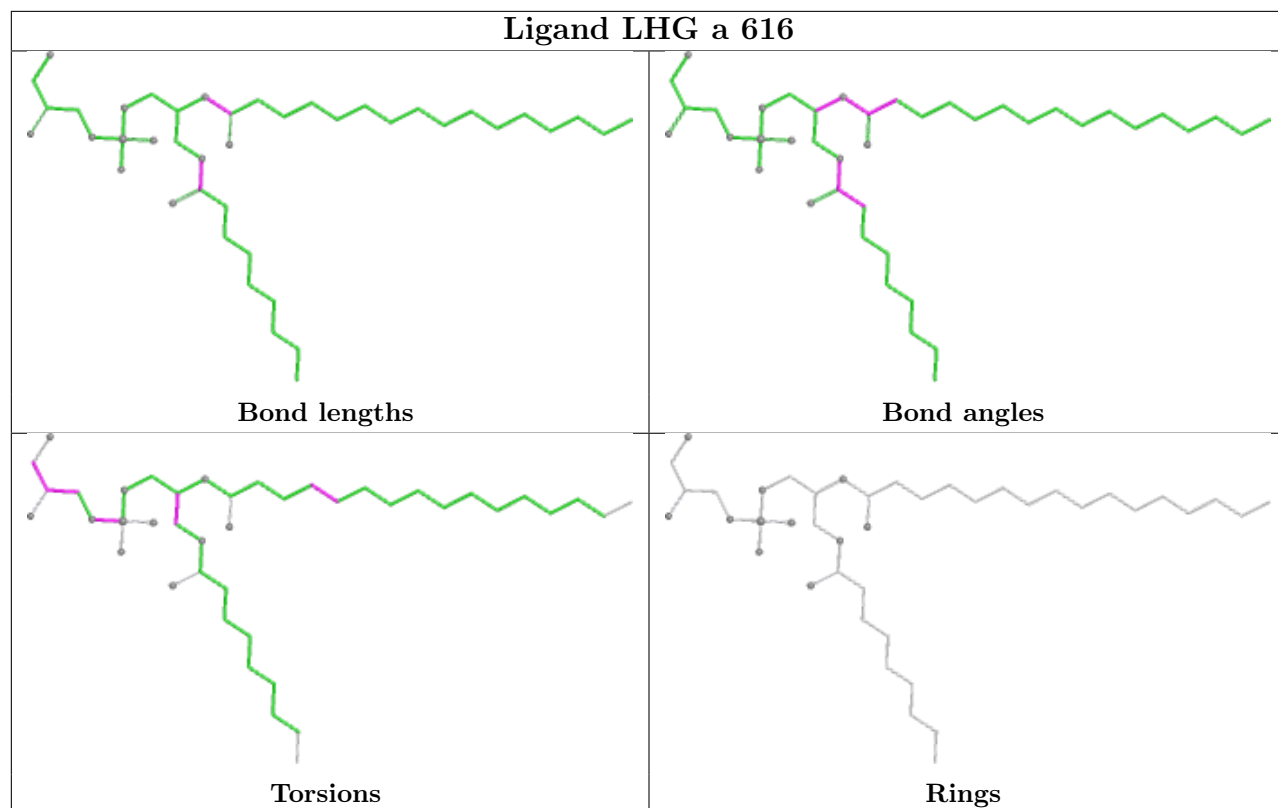




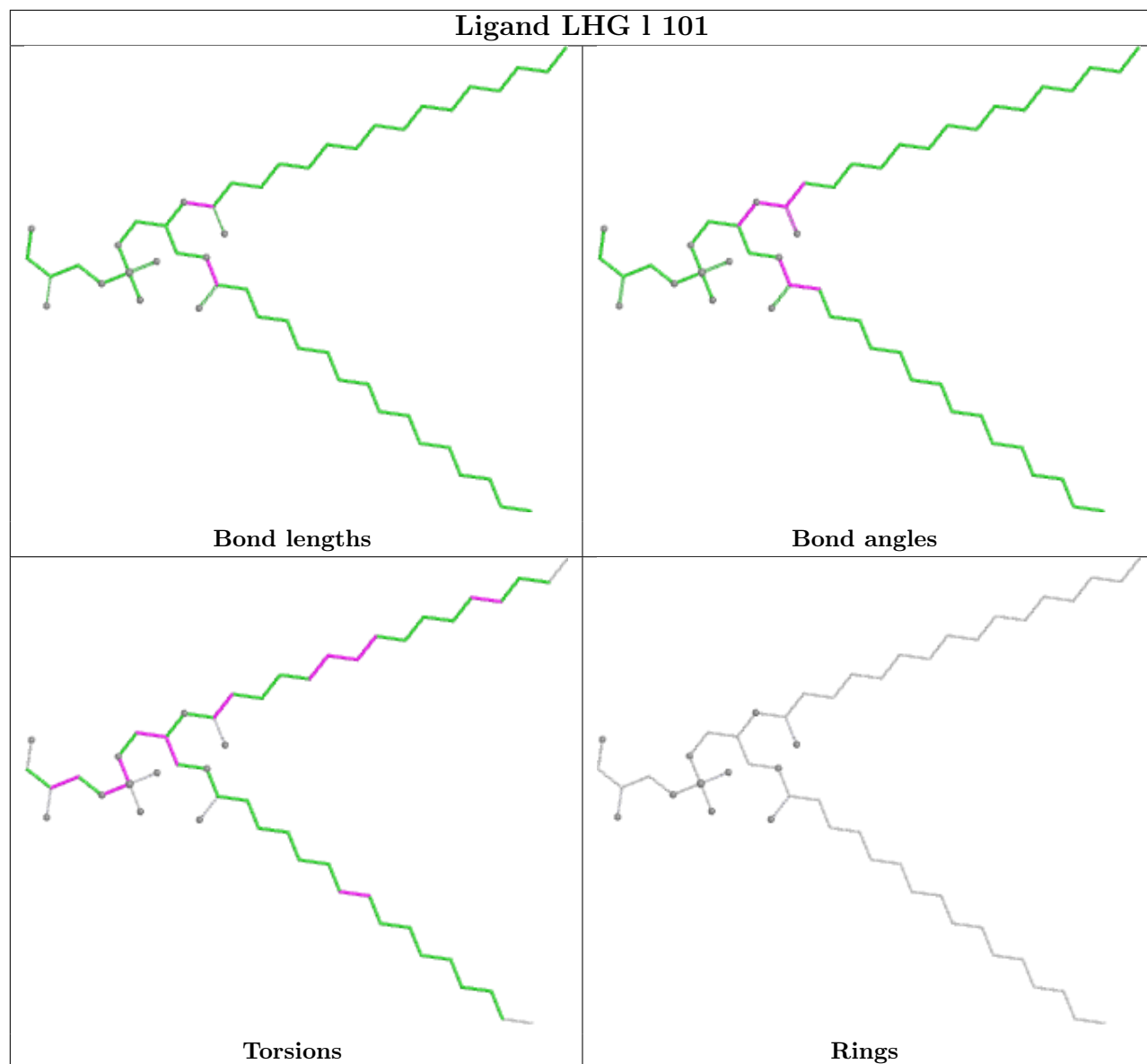




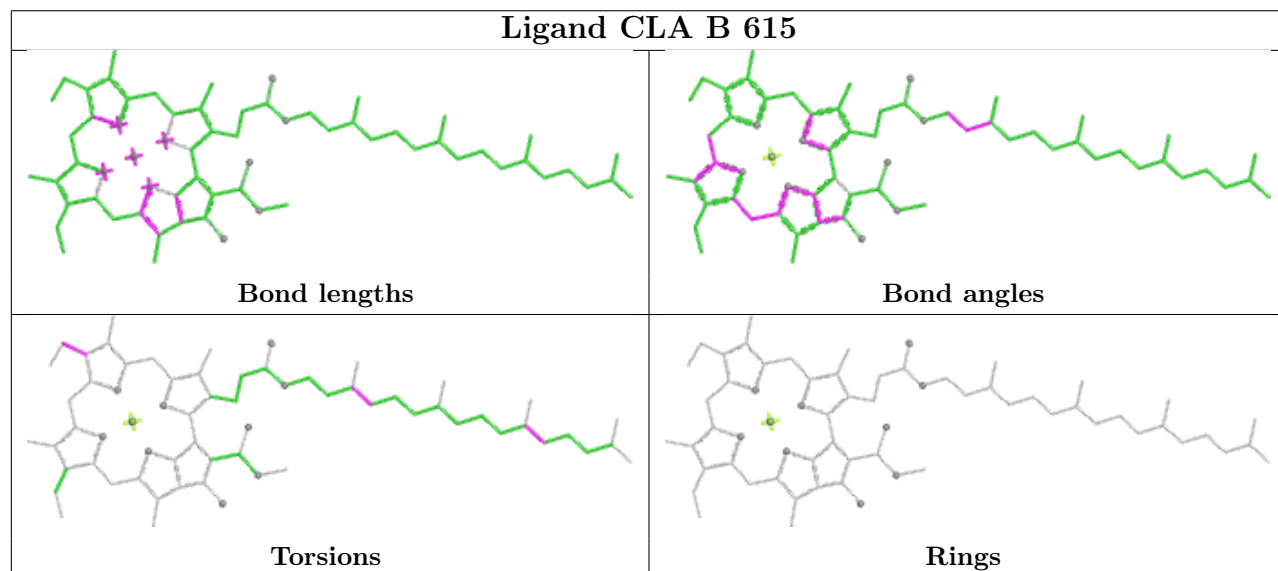
Ligand CLA B 602**Ligand DGD c 517**

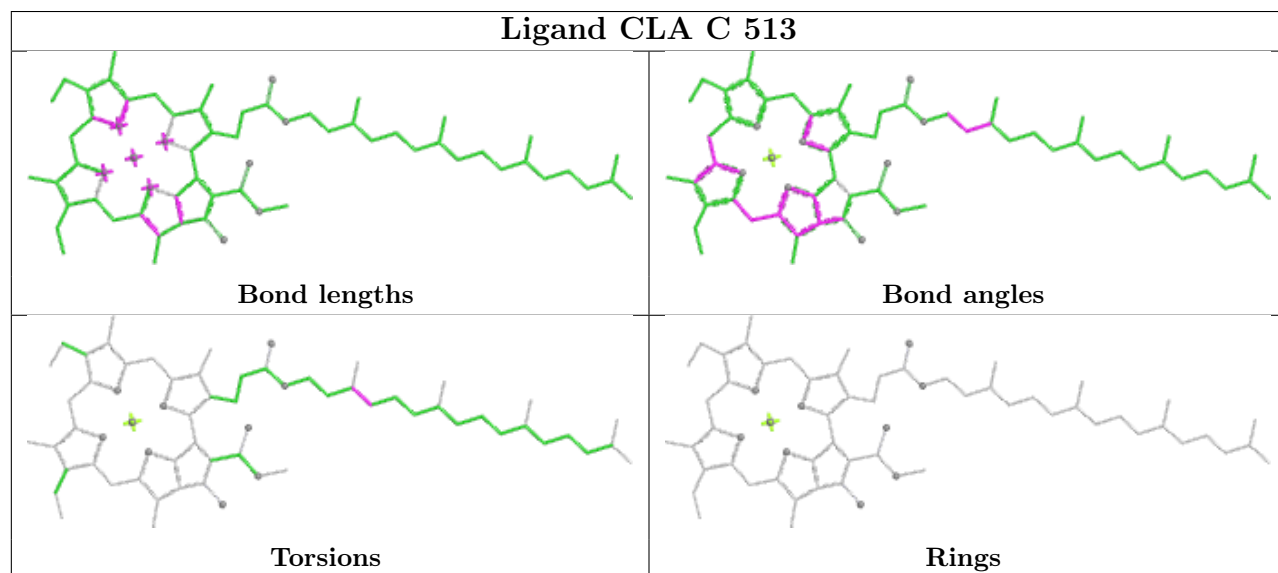
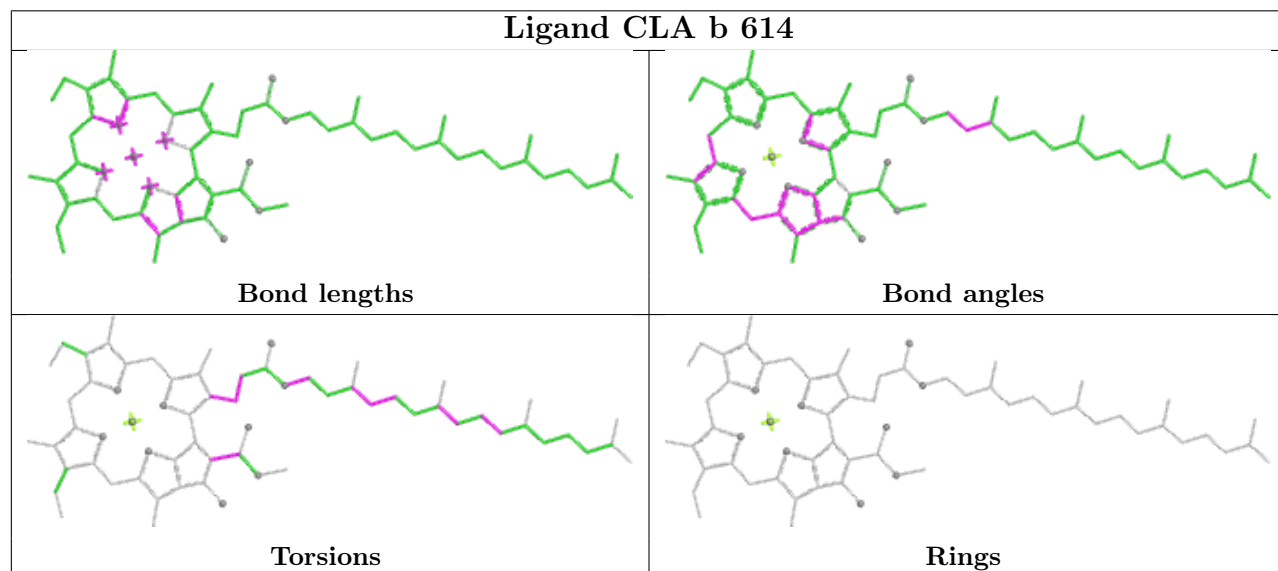
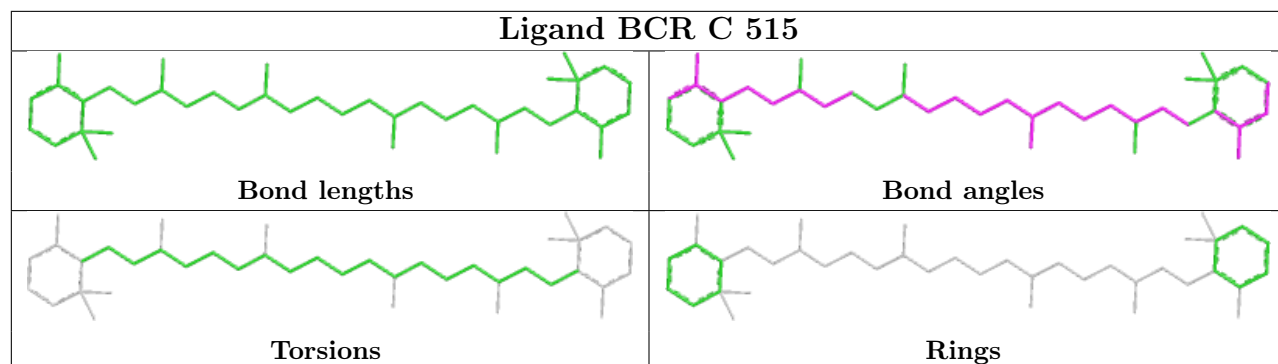


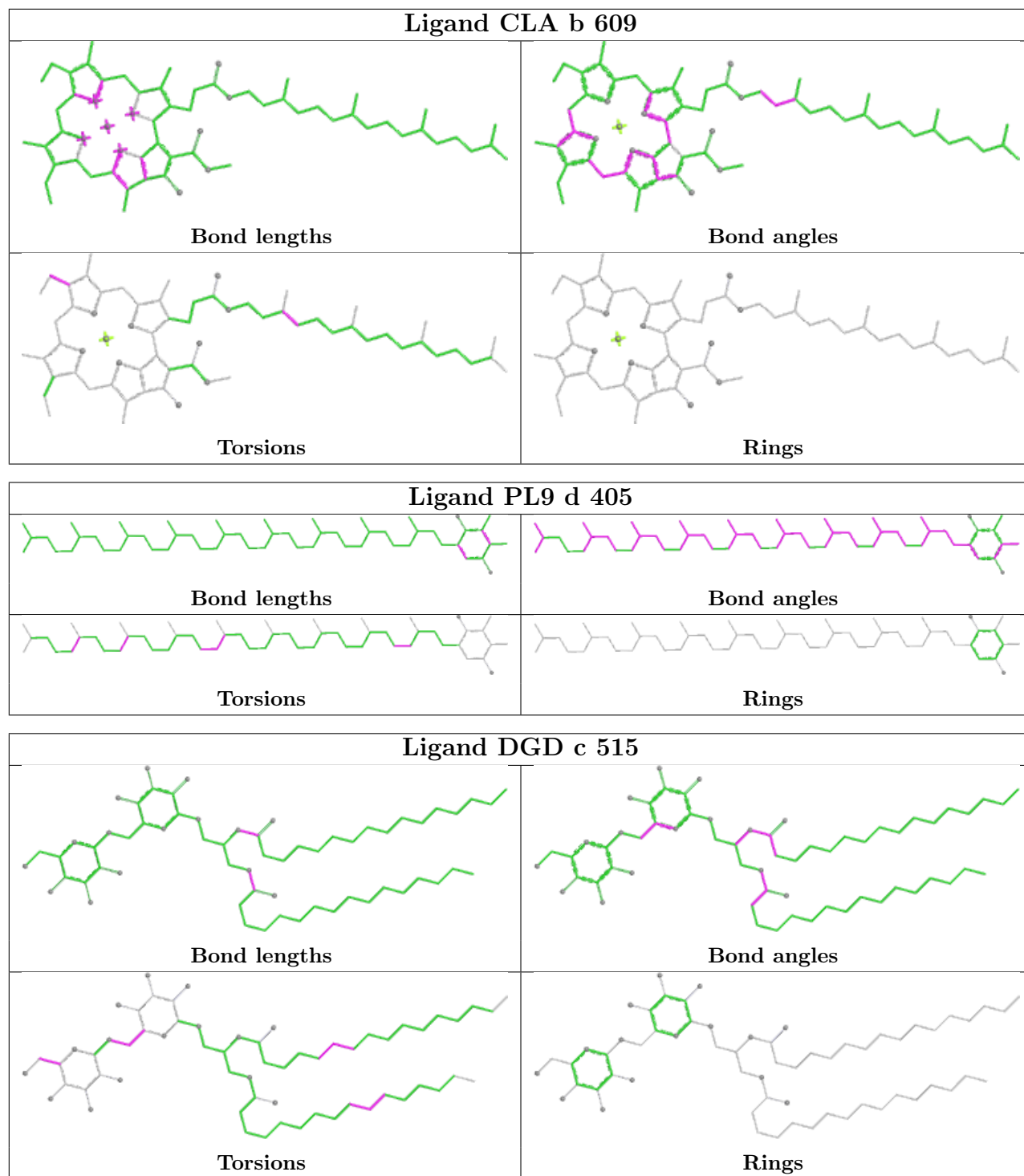
Ligand LHG 1 101

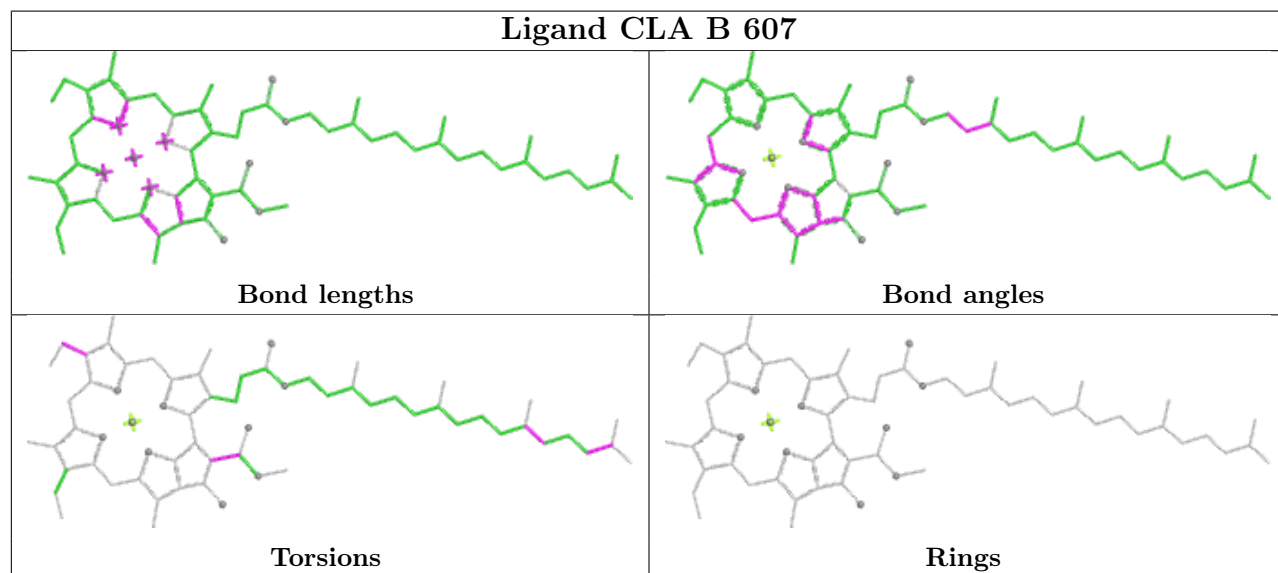
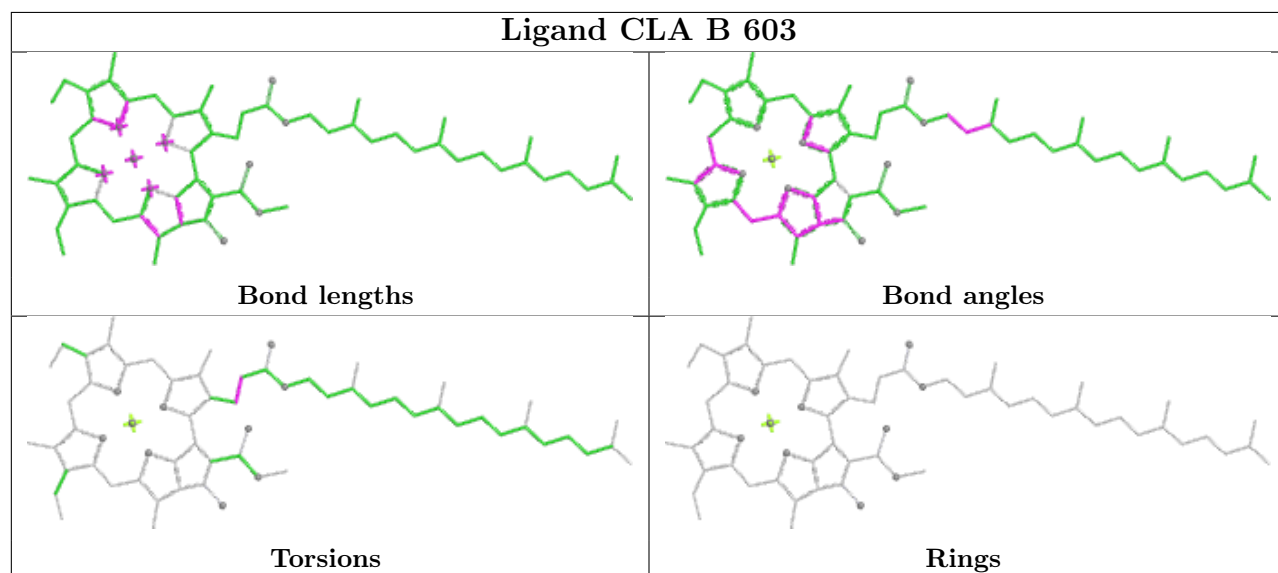
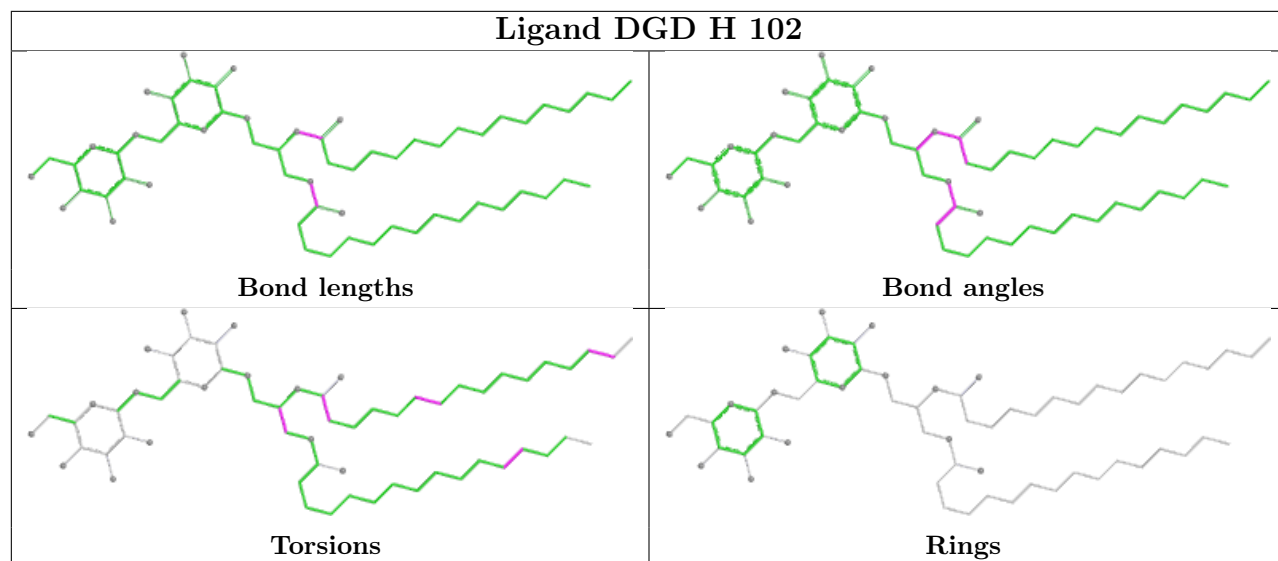


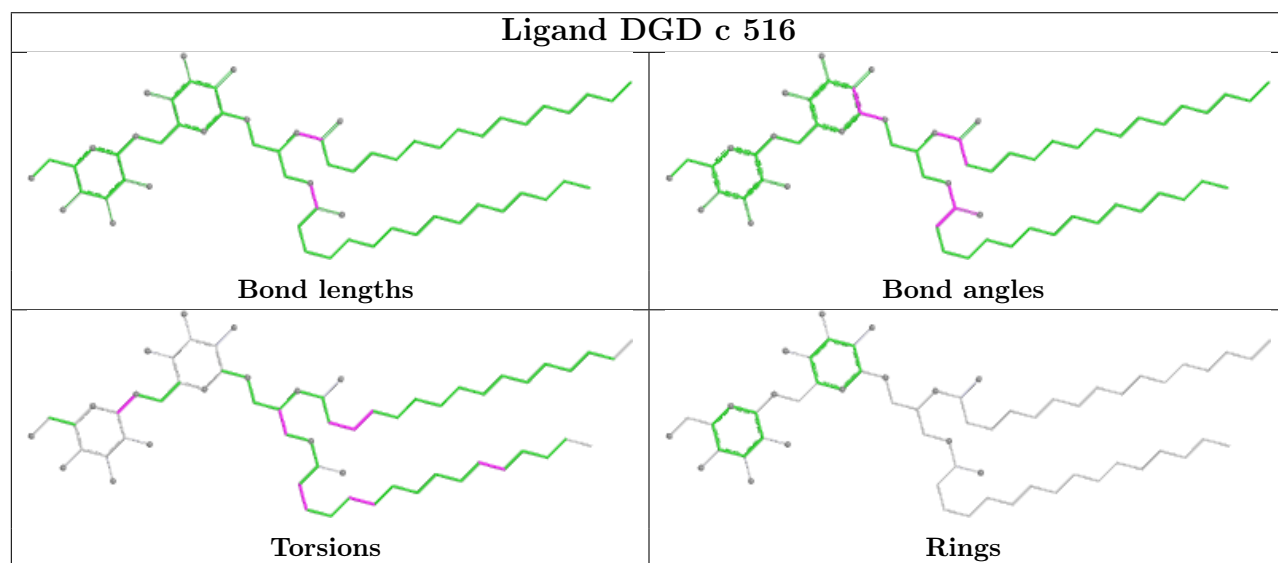
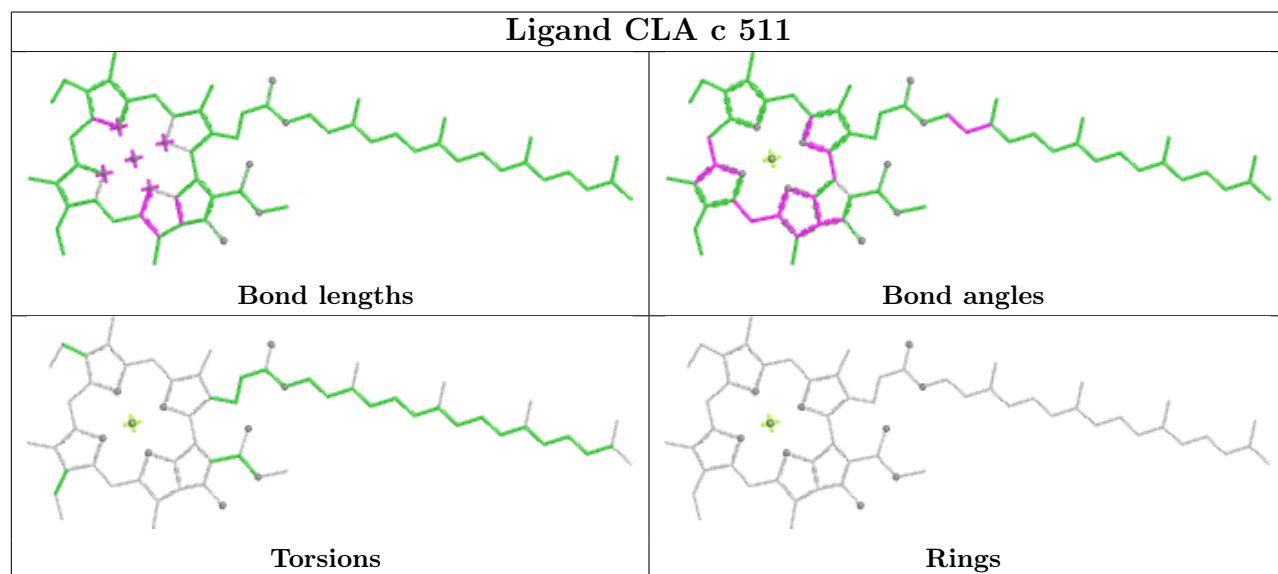
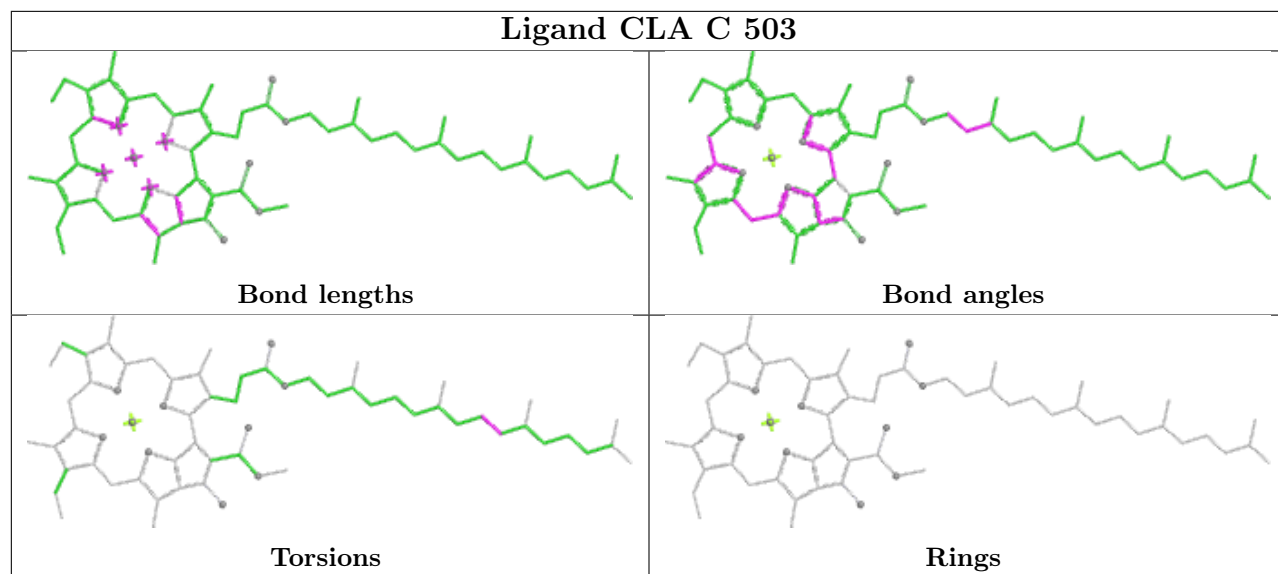
Ligand CLA B 615

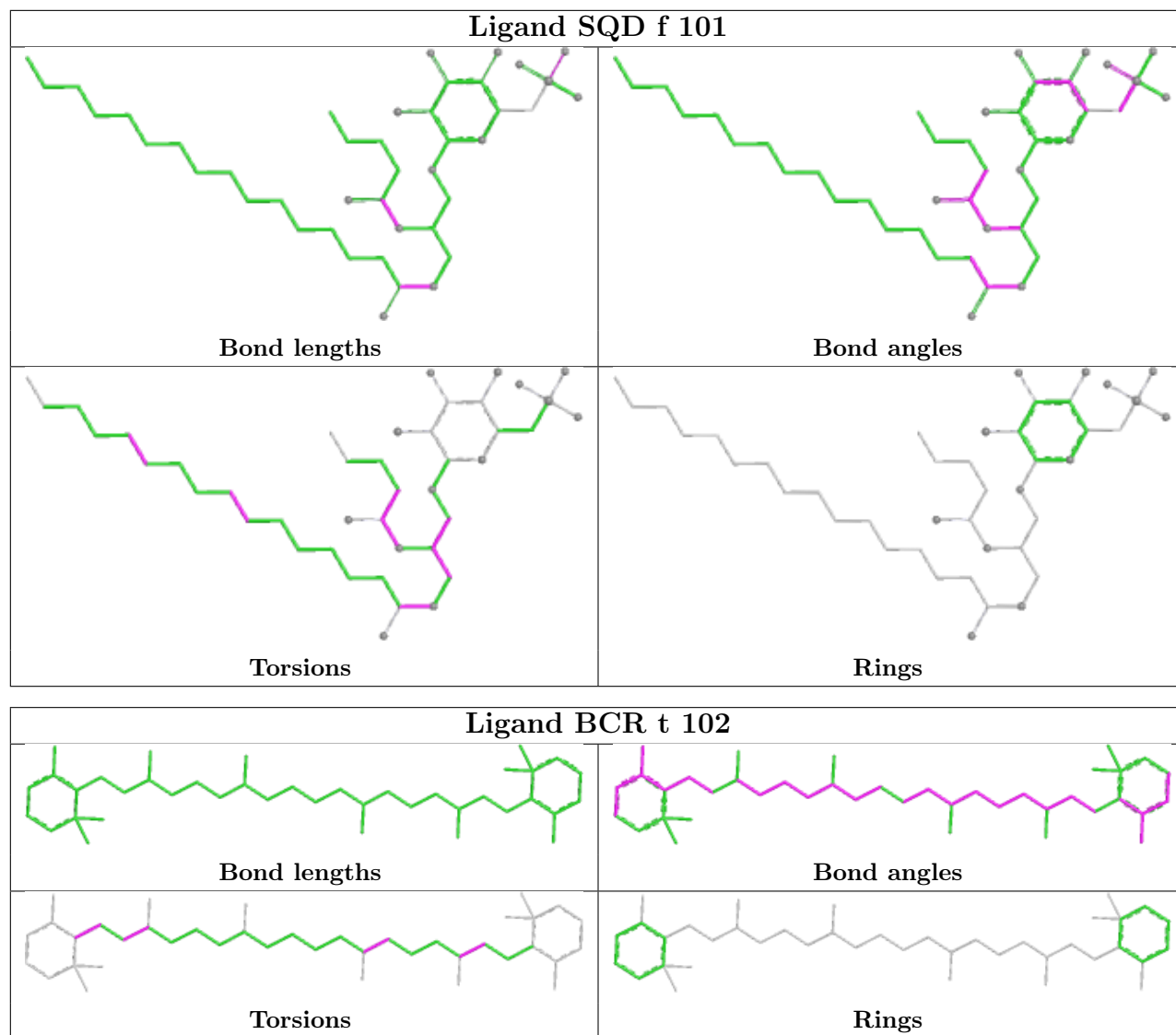


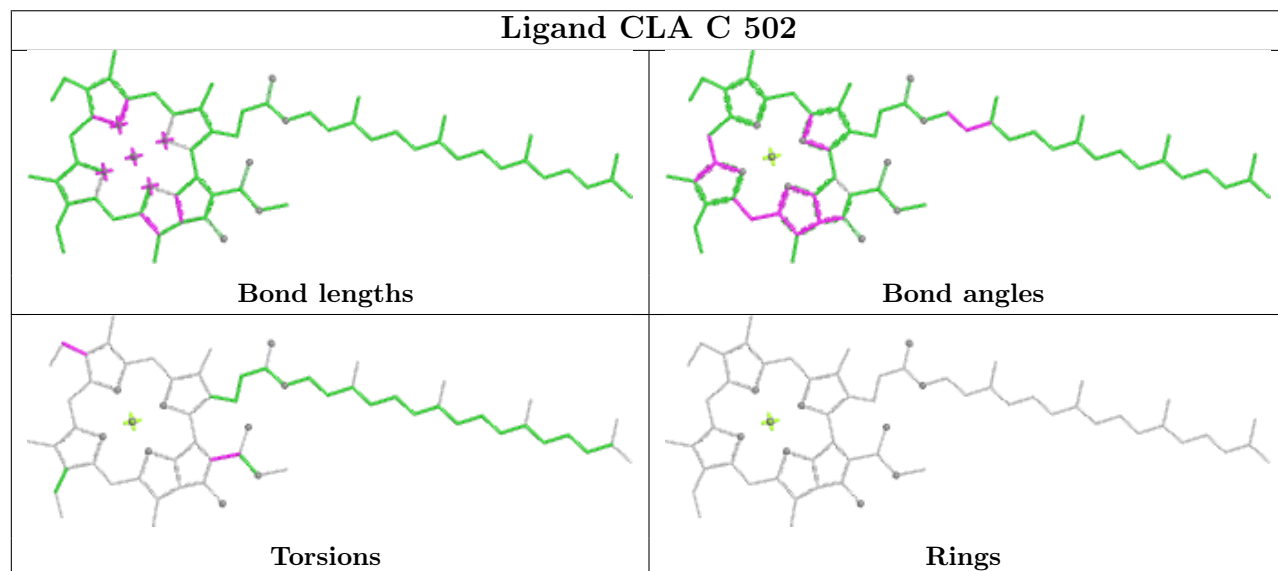
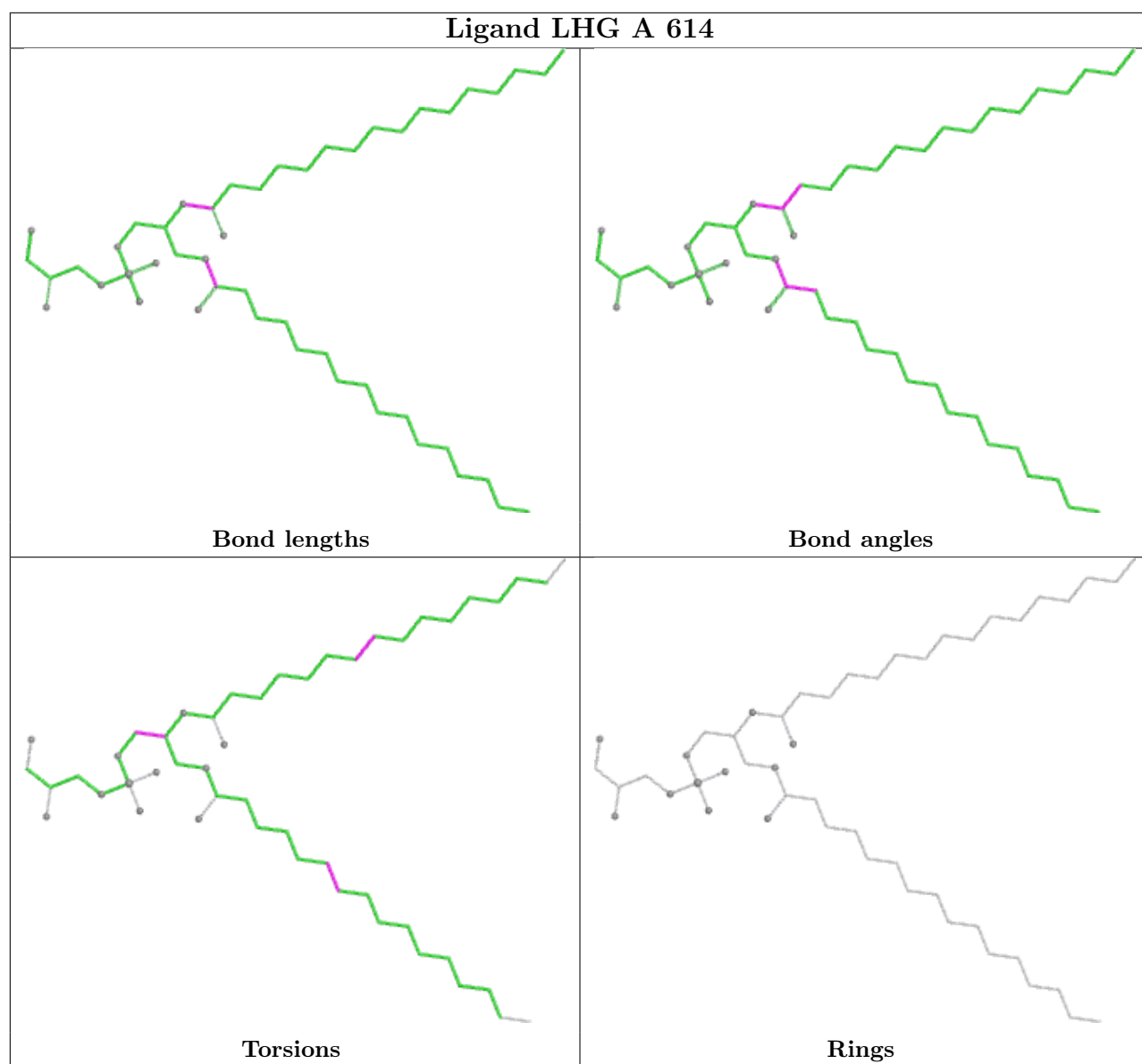


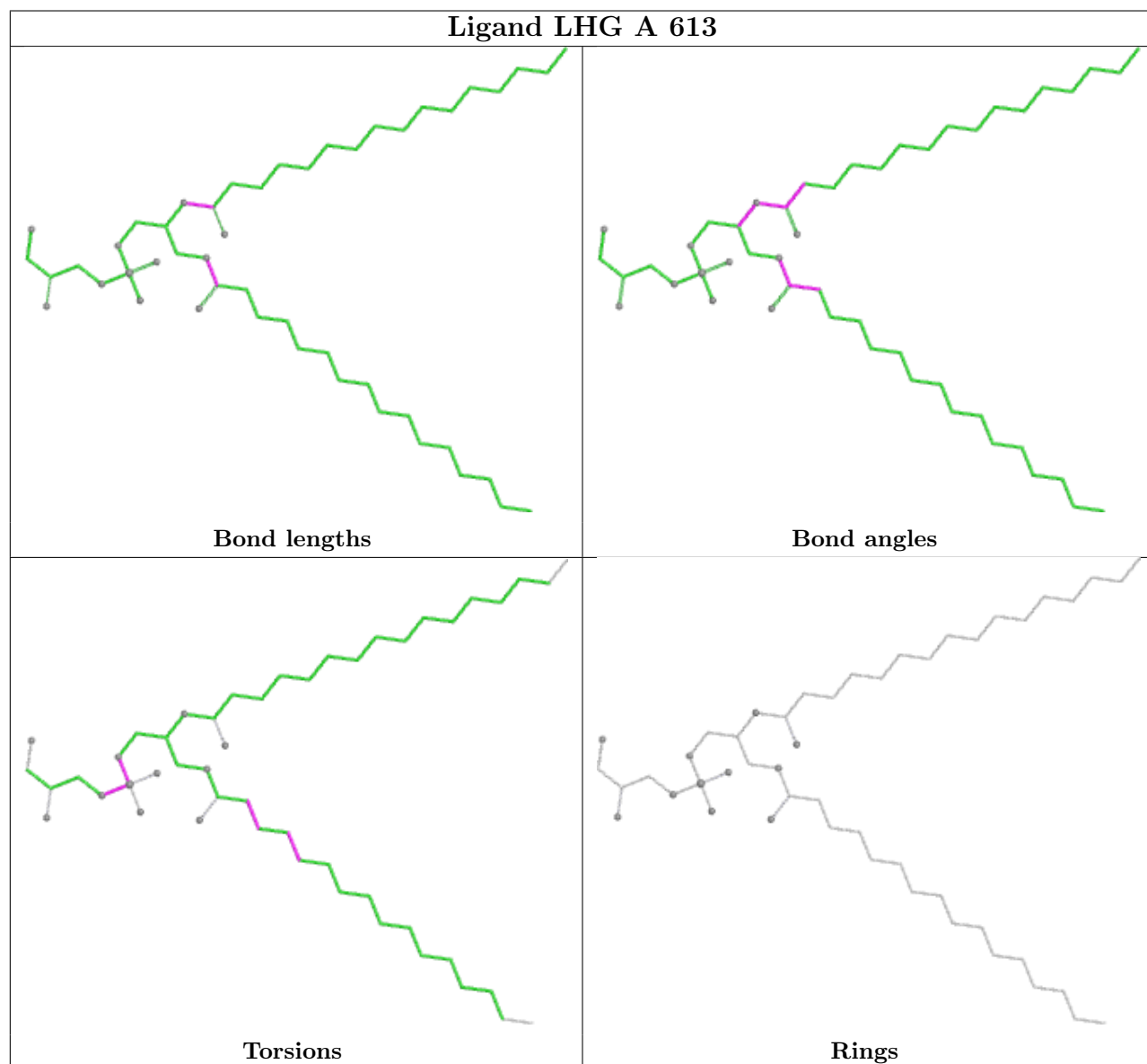
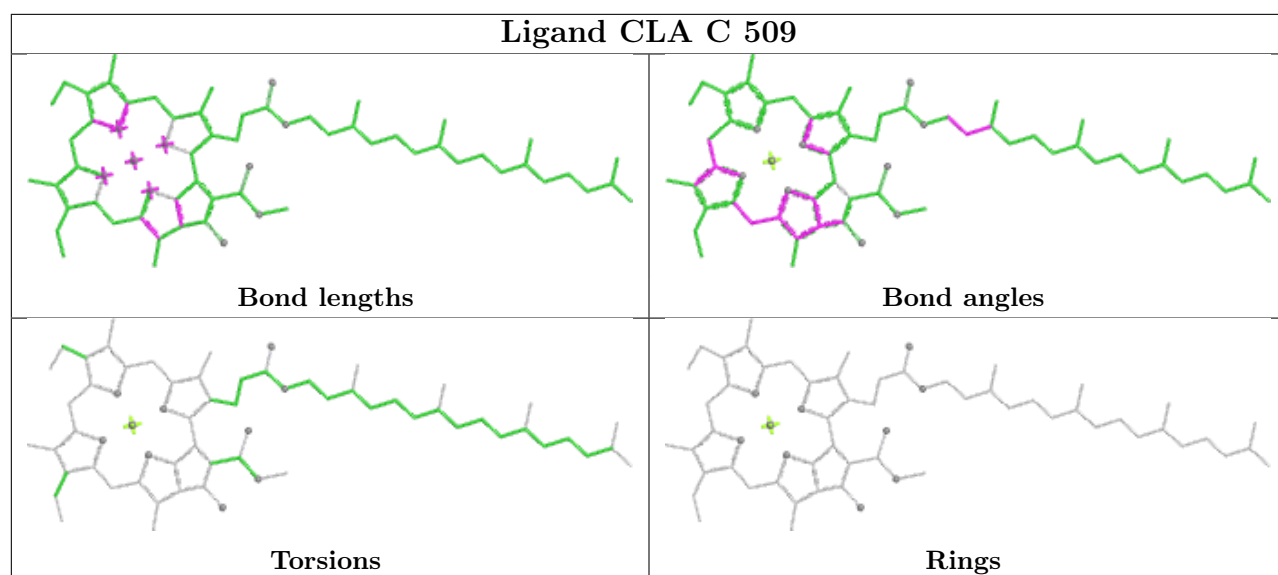


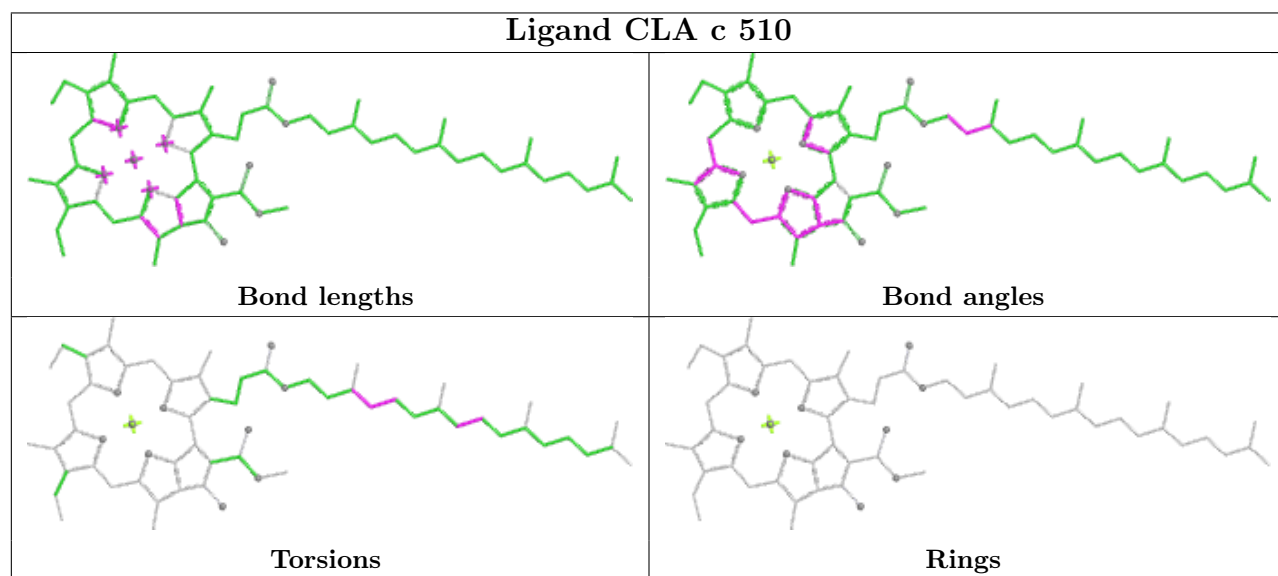
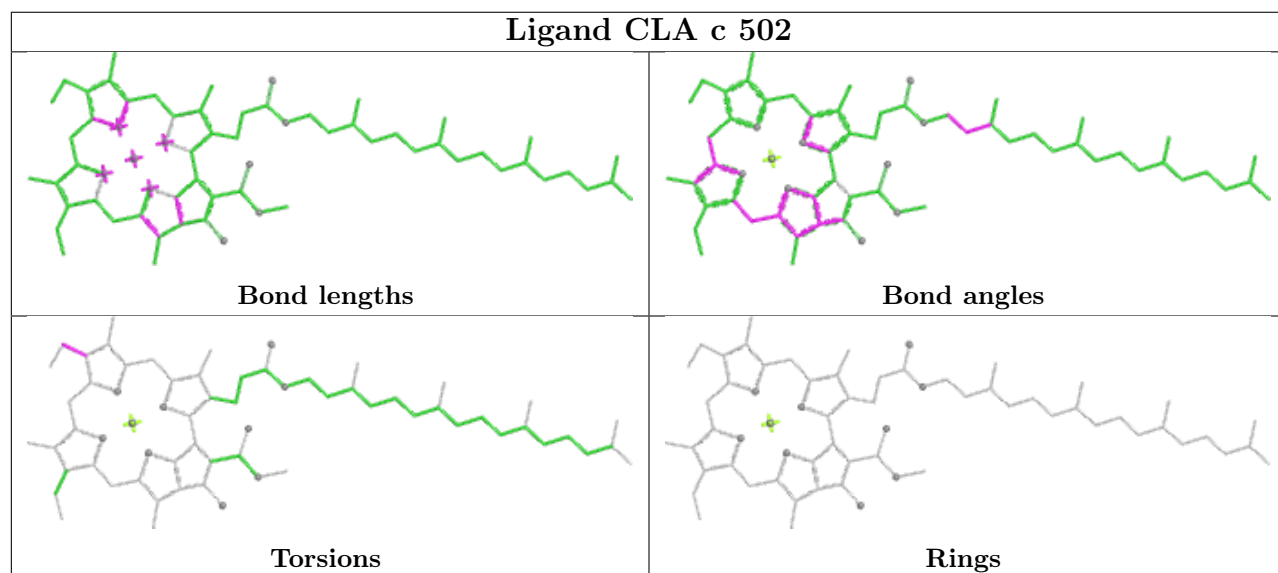
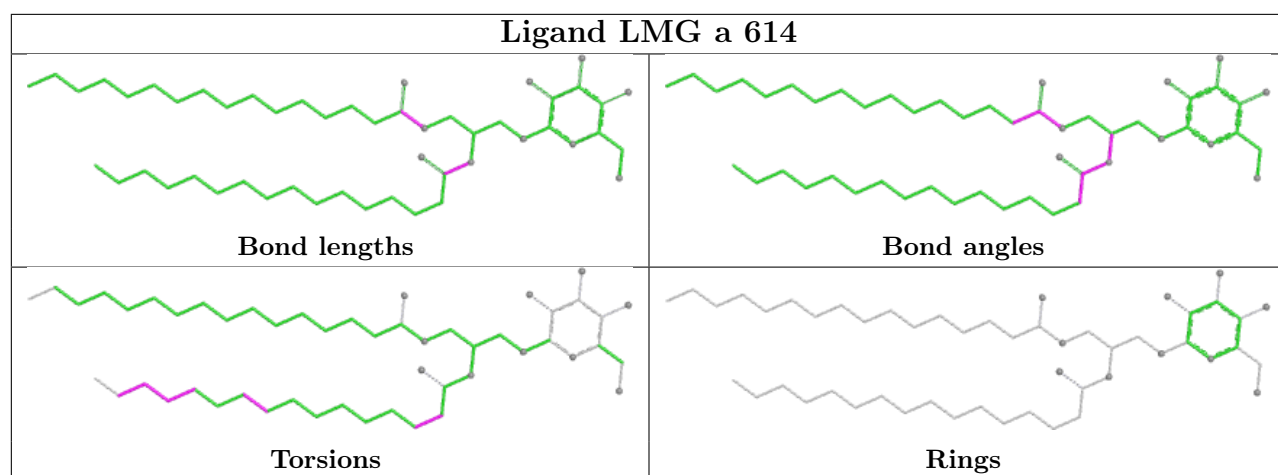


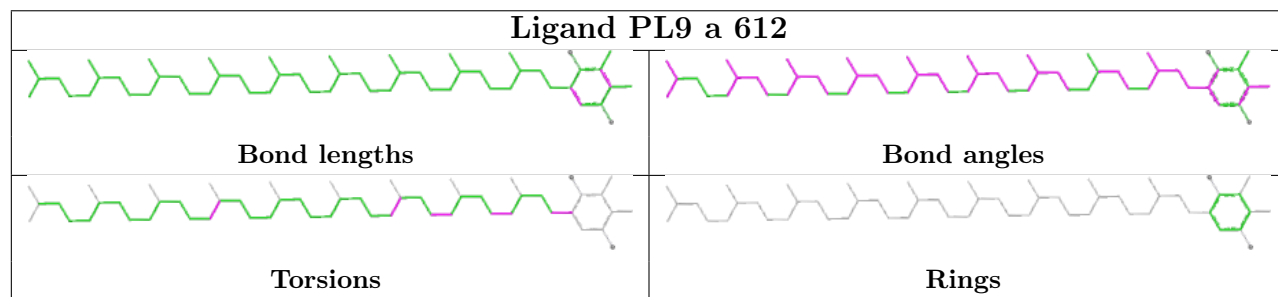
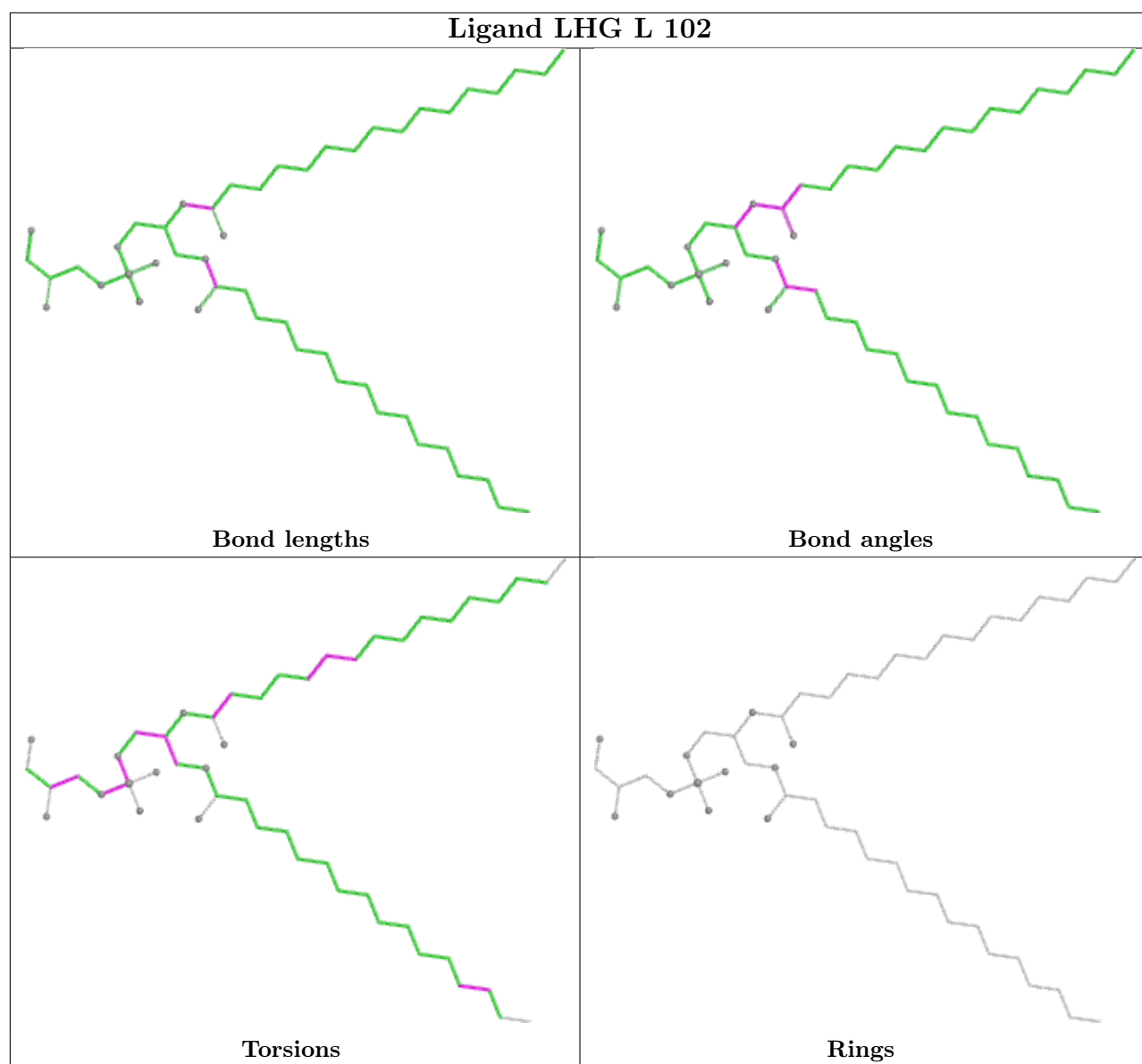


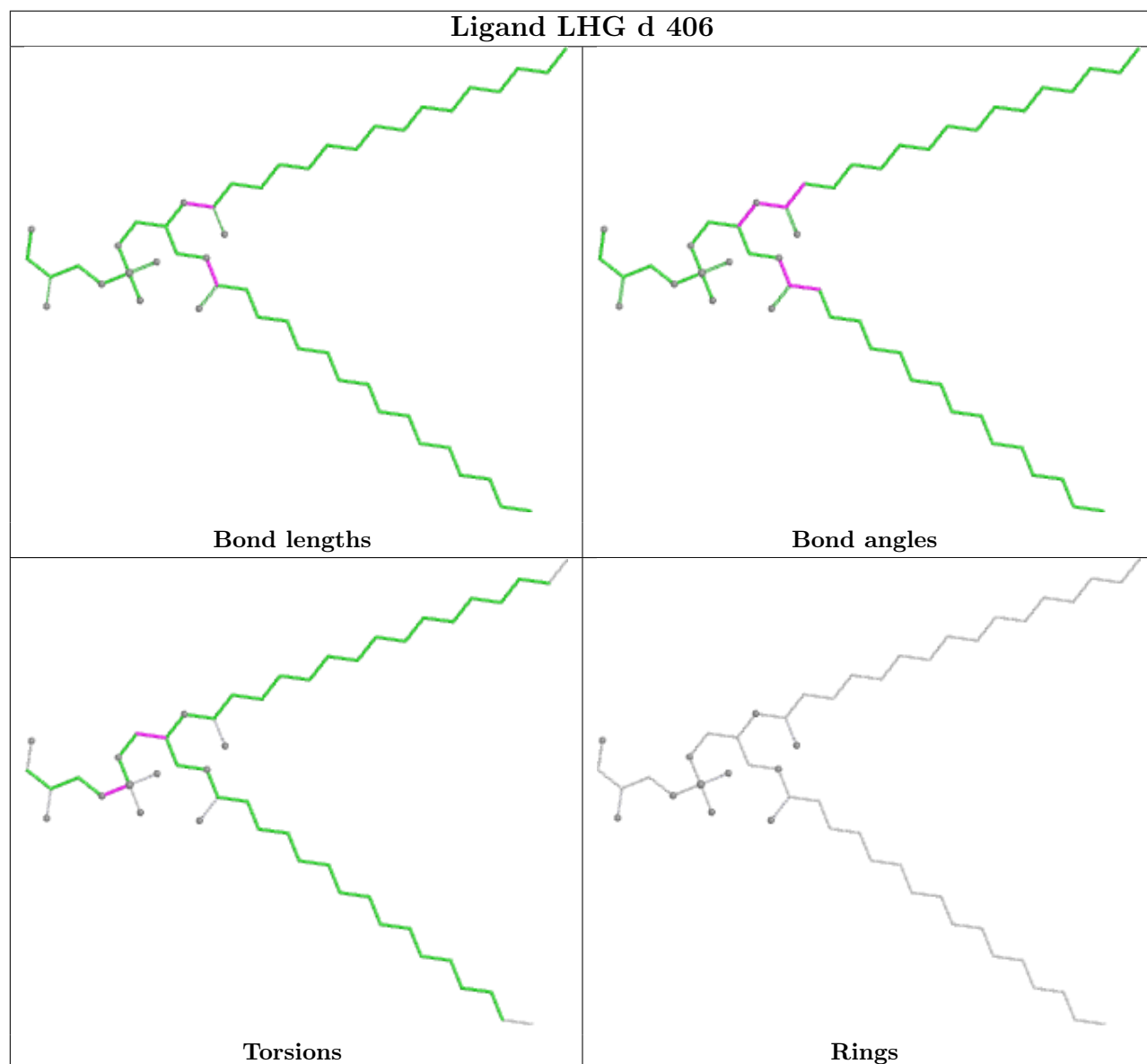
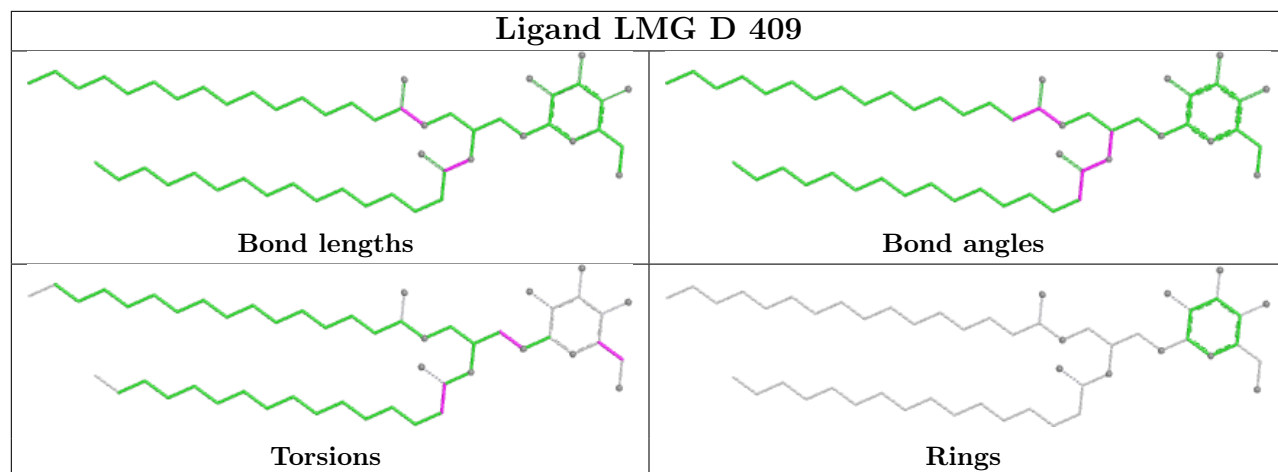


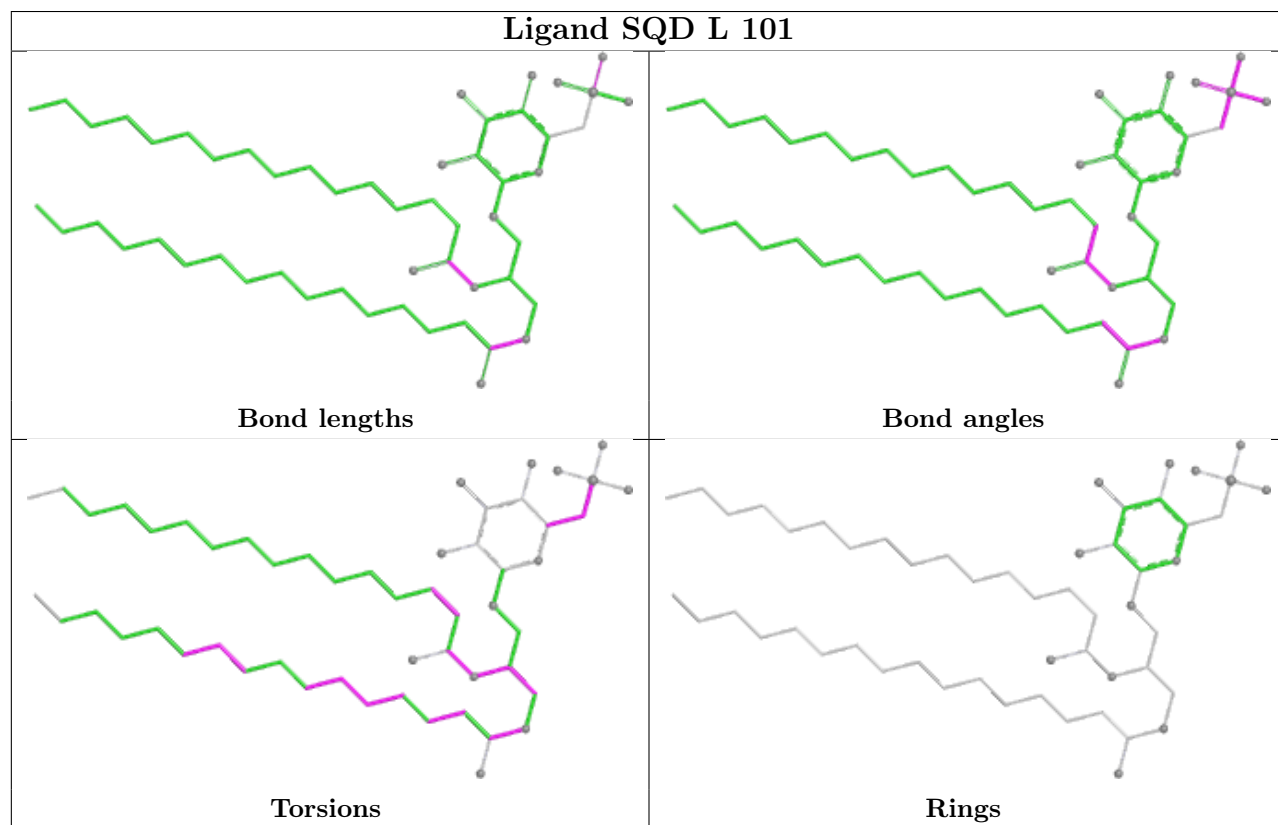
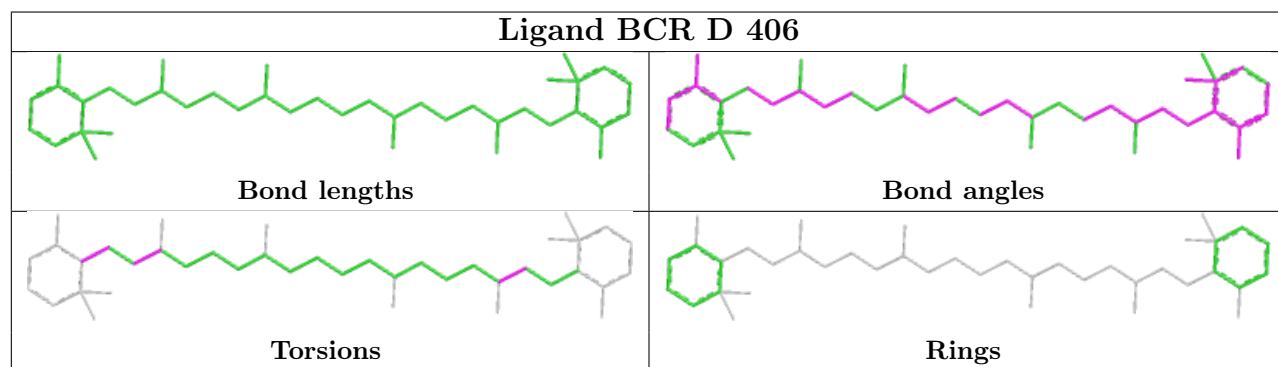
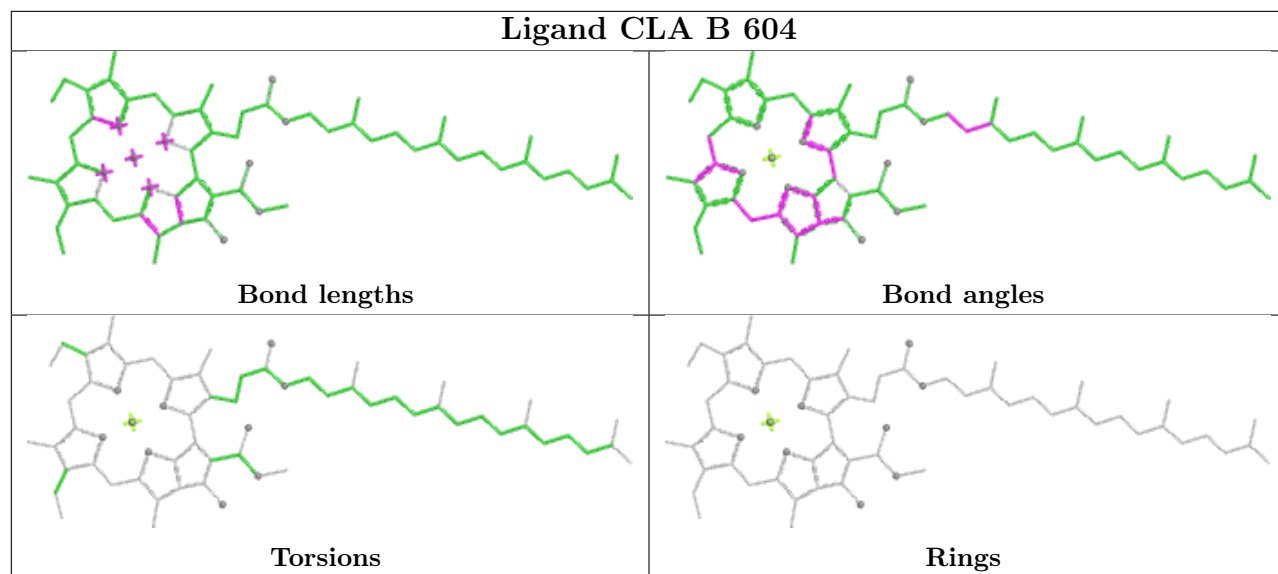


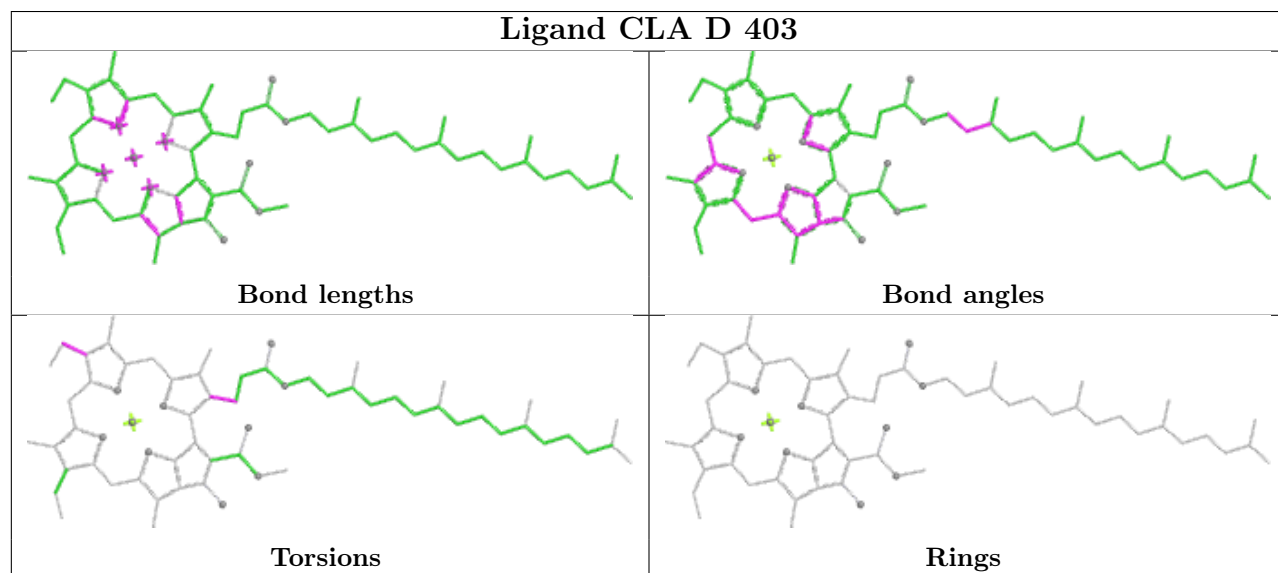
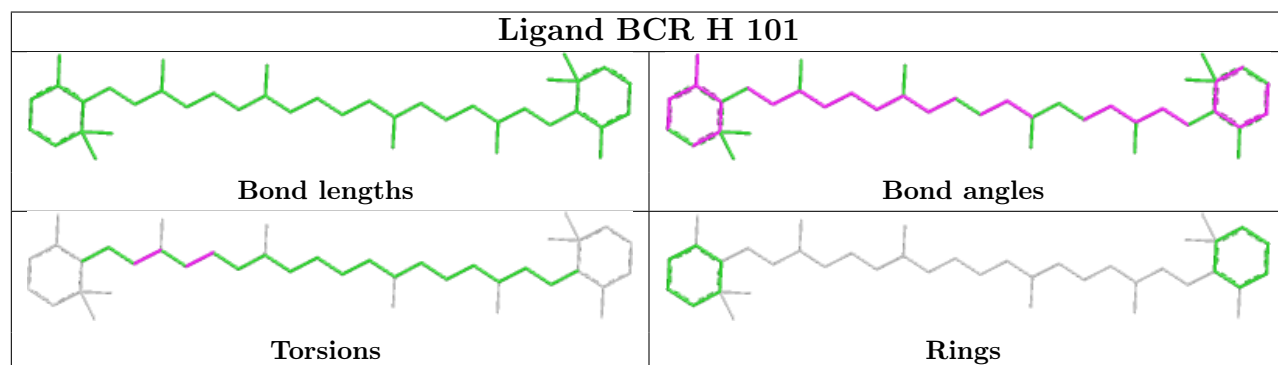
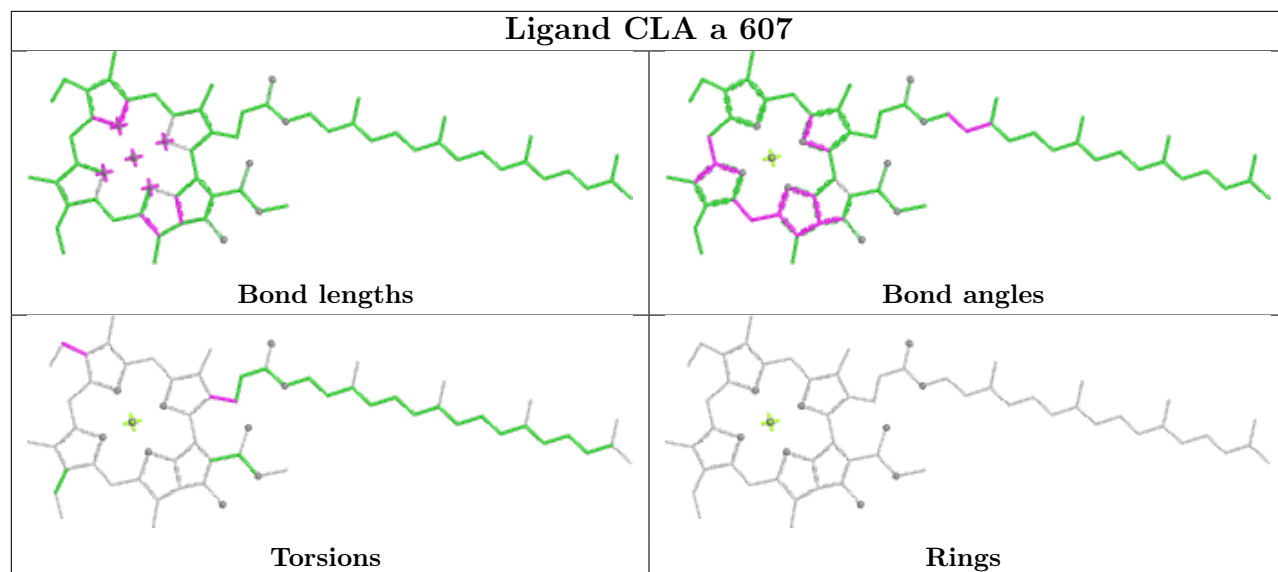


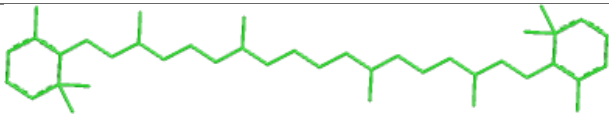
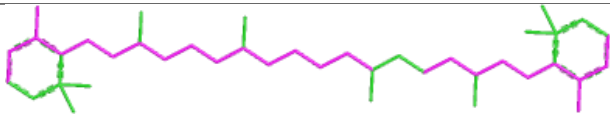
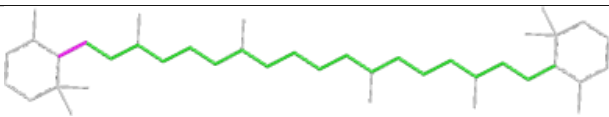
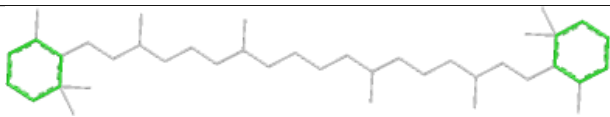


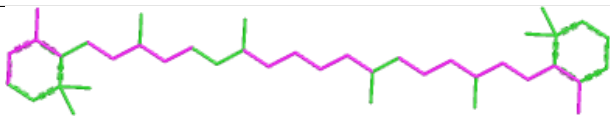
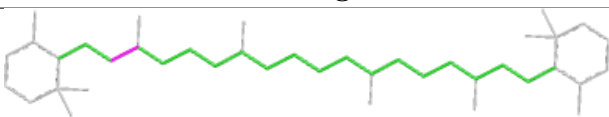
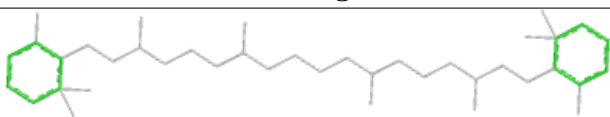


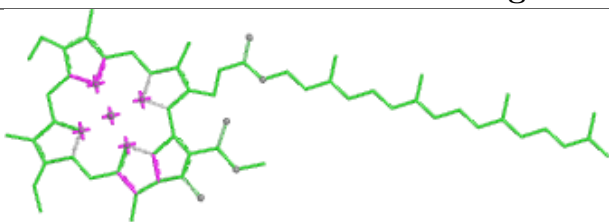
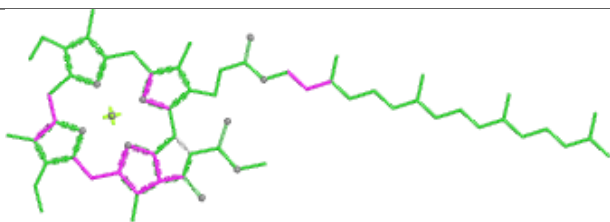
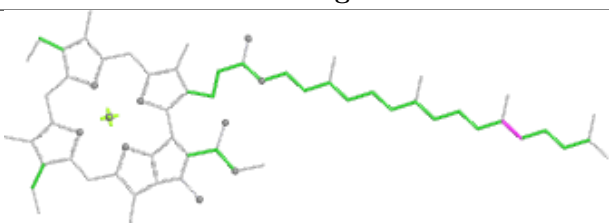
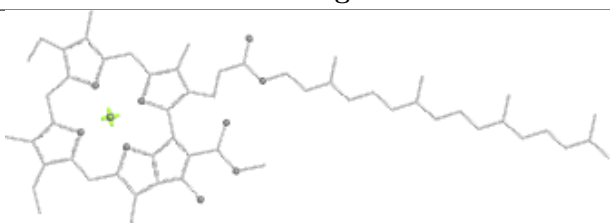


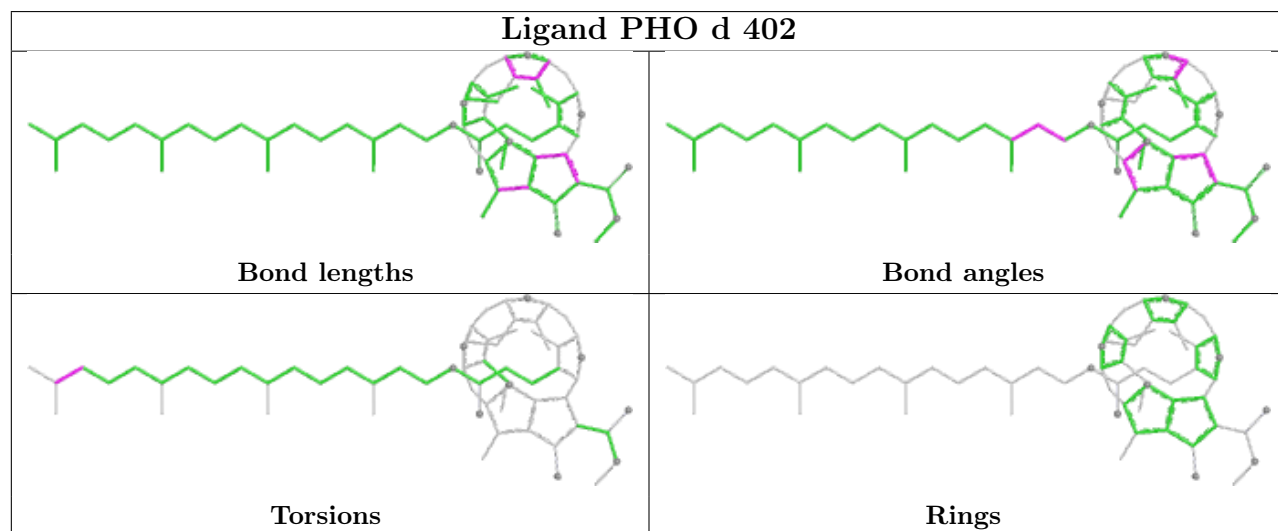
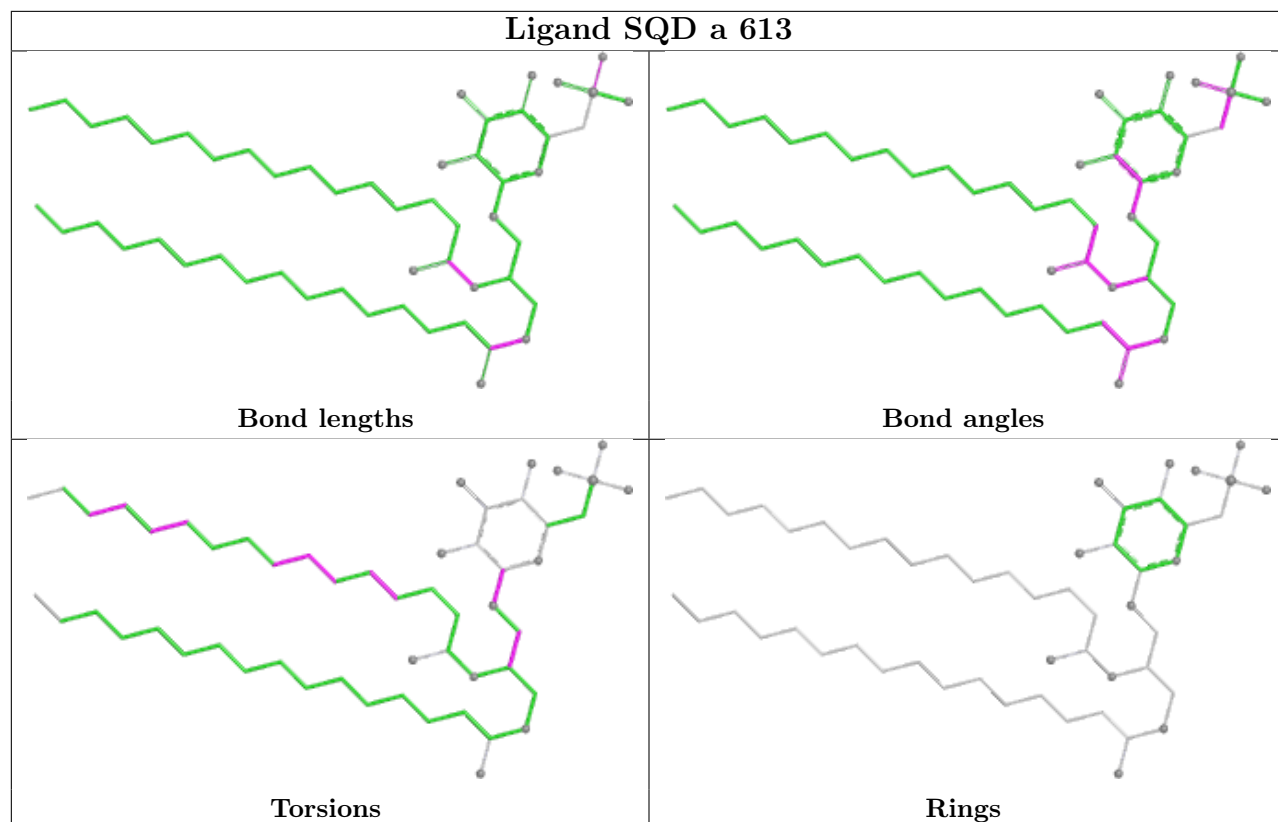


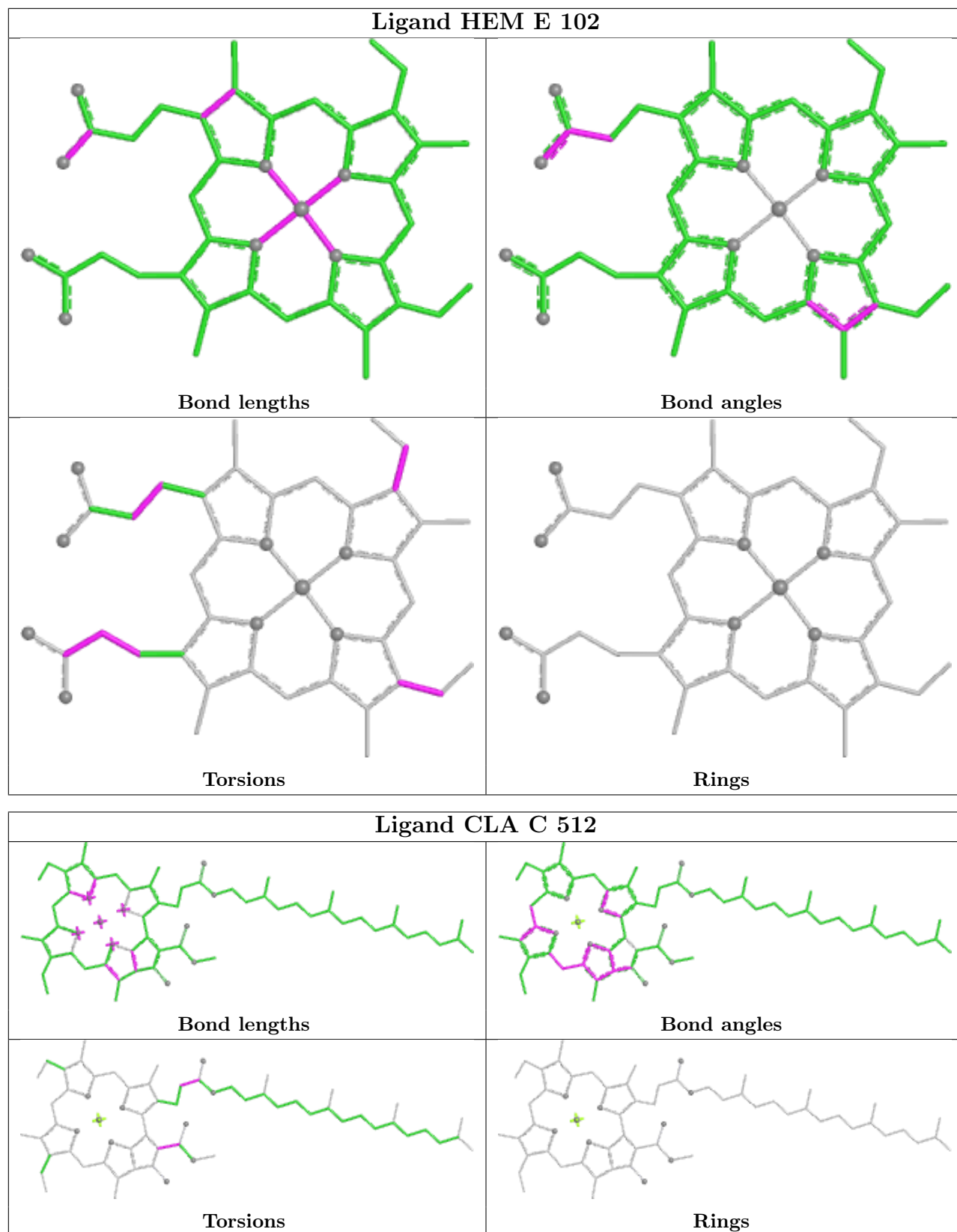


Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

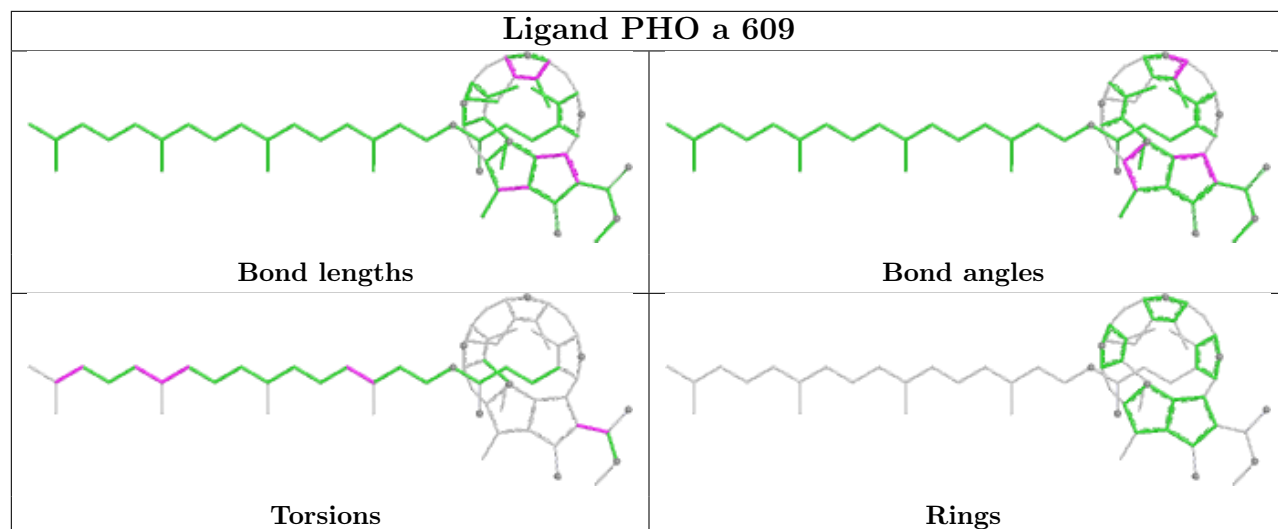
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

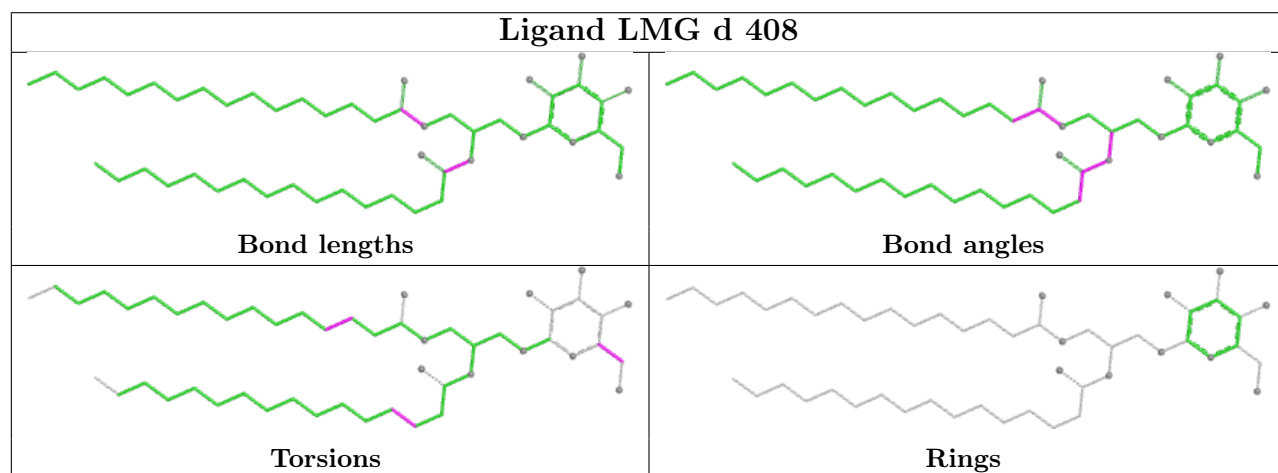




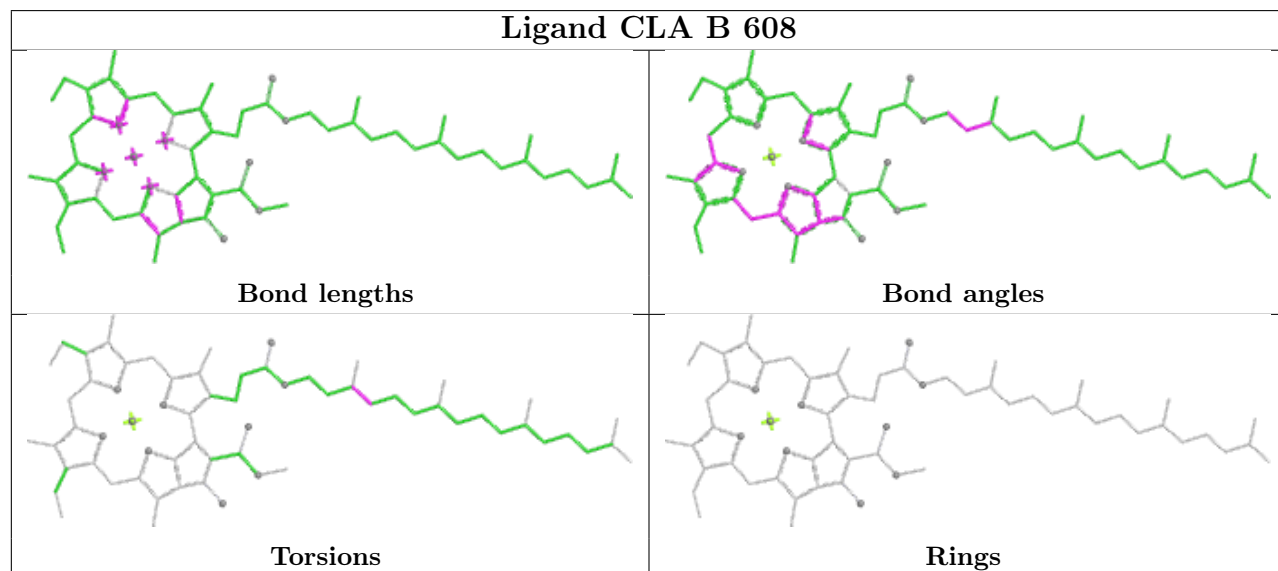
Ligand PHO a 609



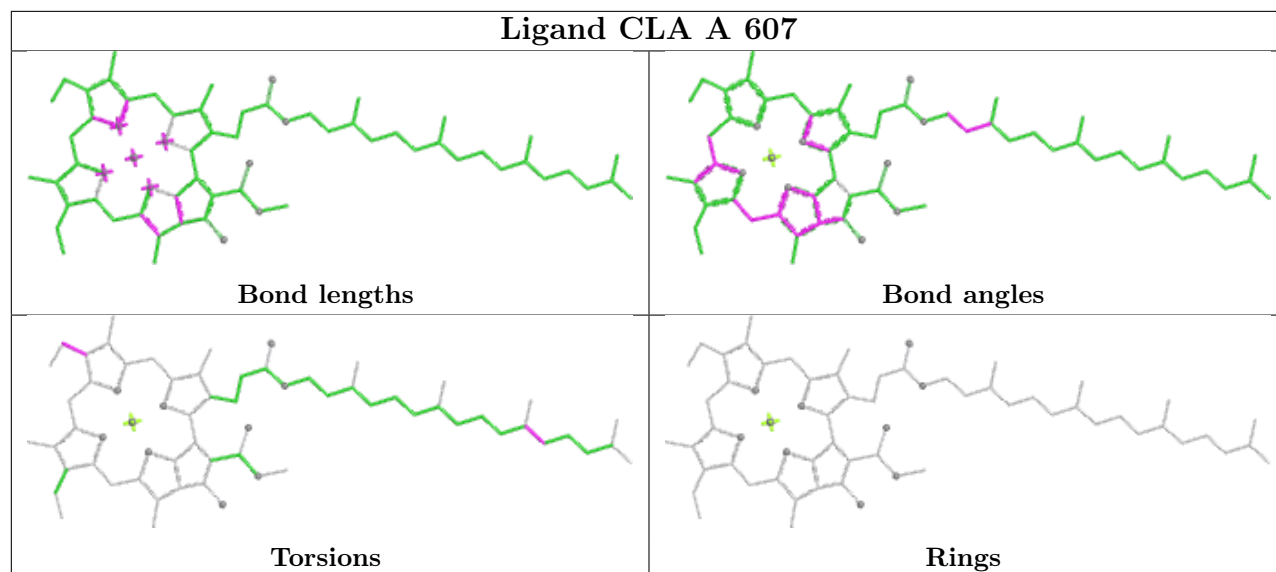
Ligand LMG d 408



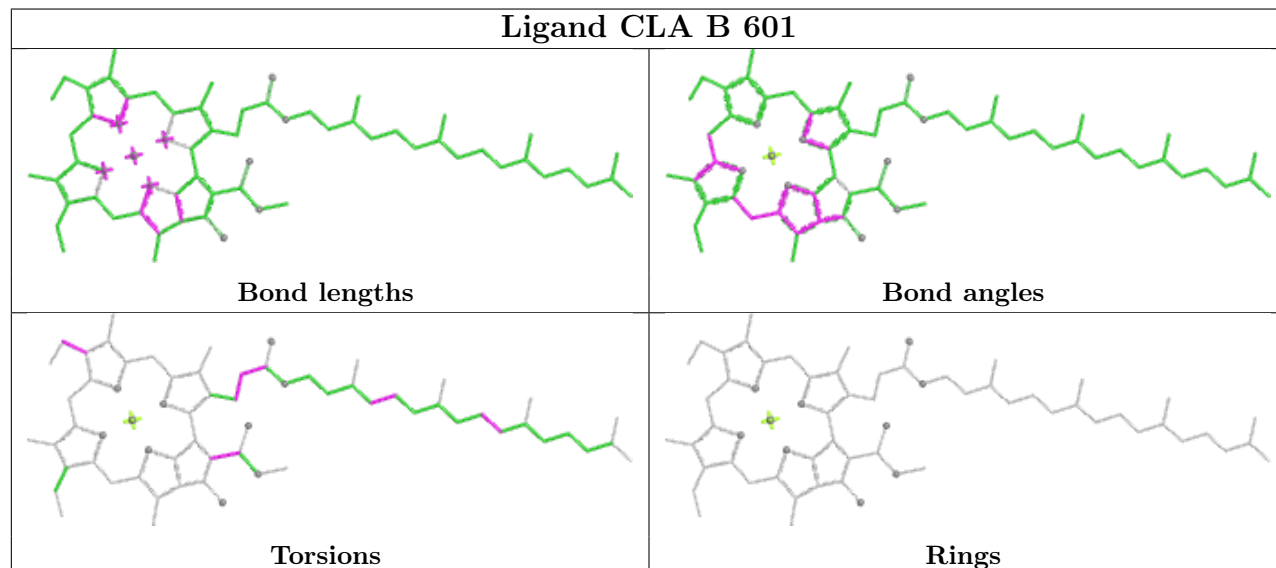
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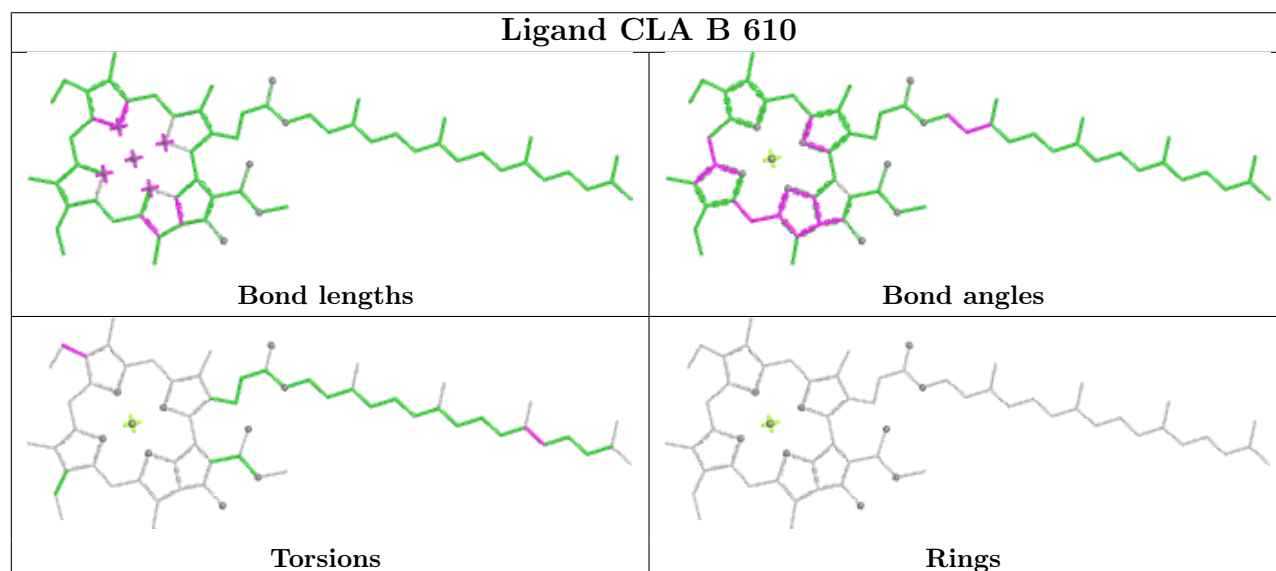
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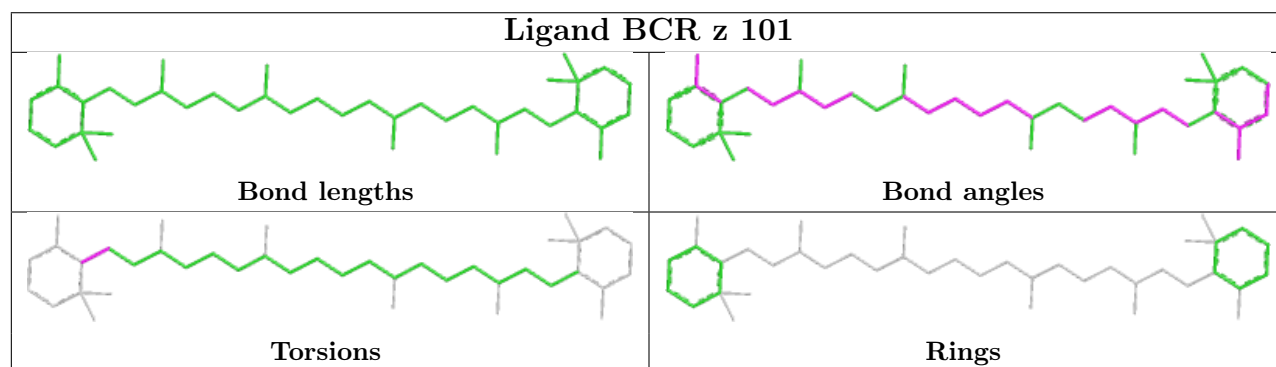
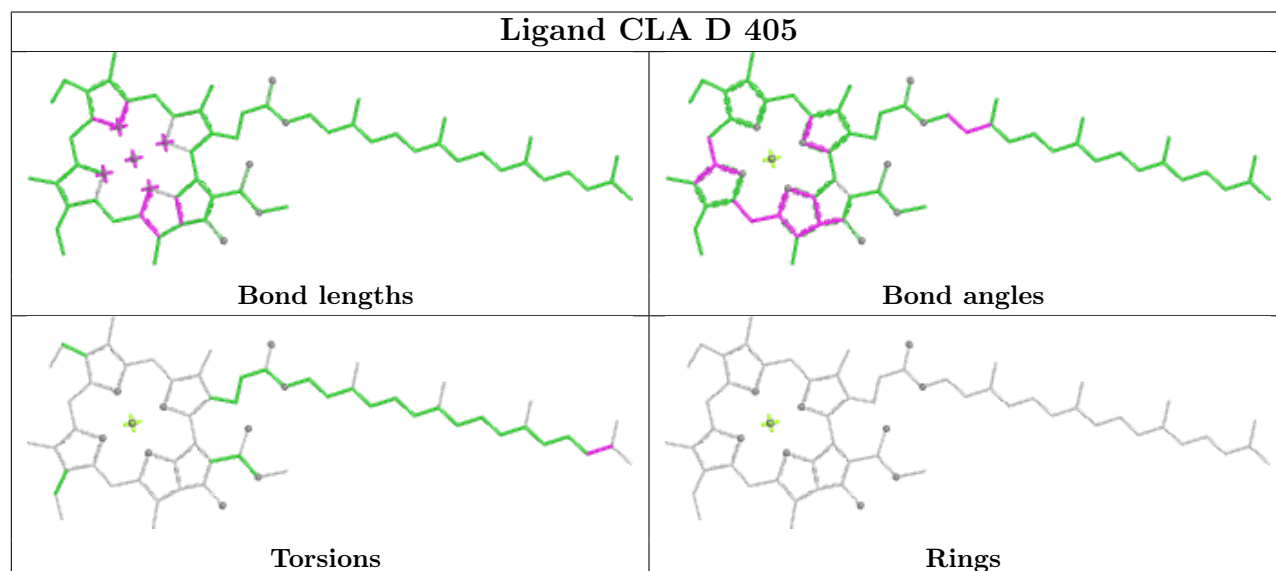
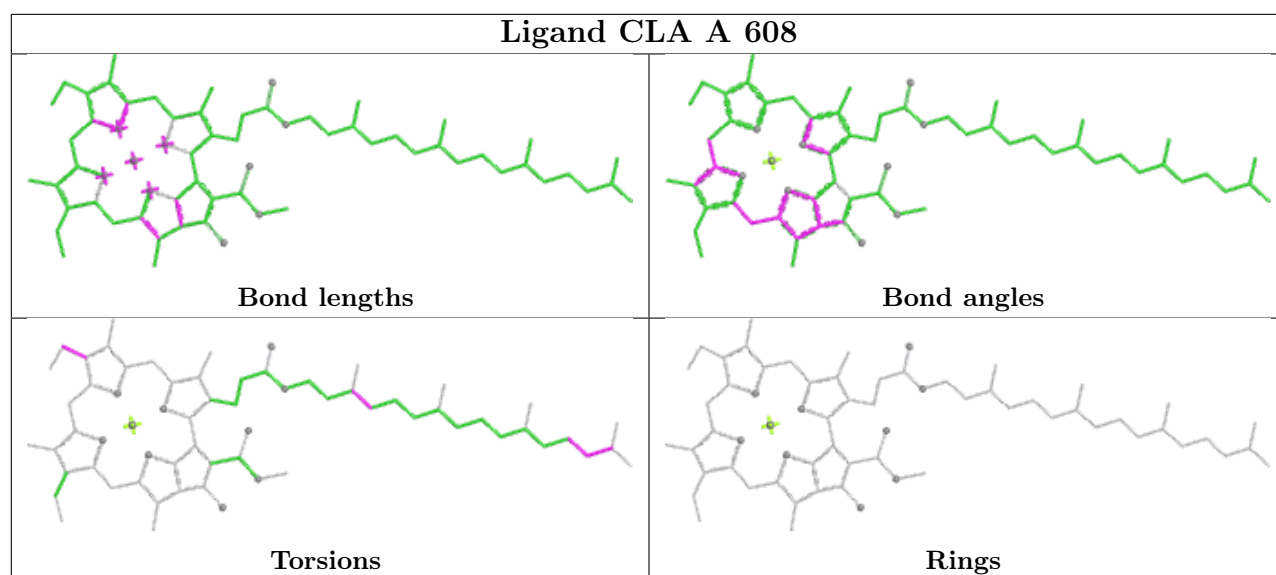


Ligand CLA B 601

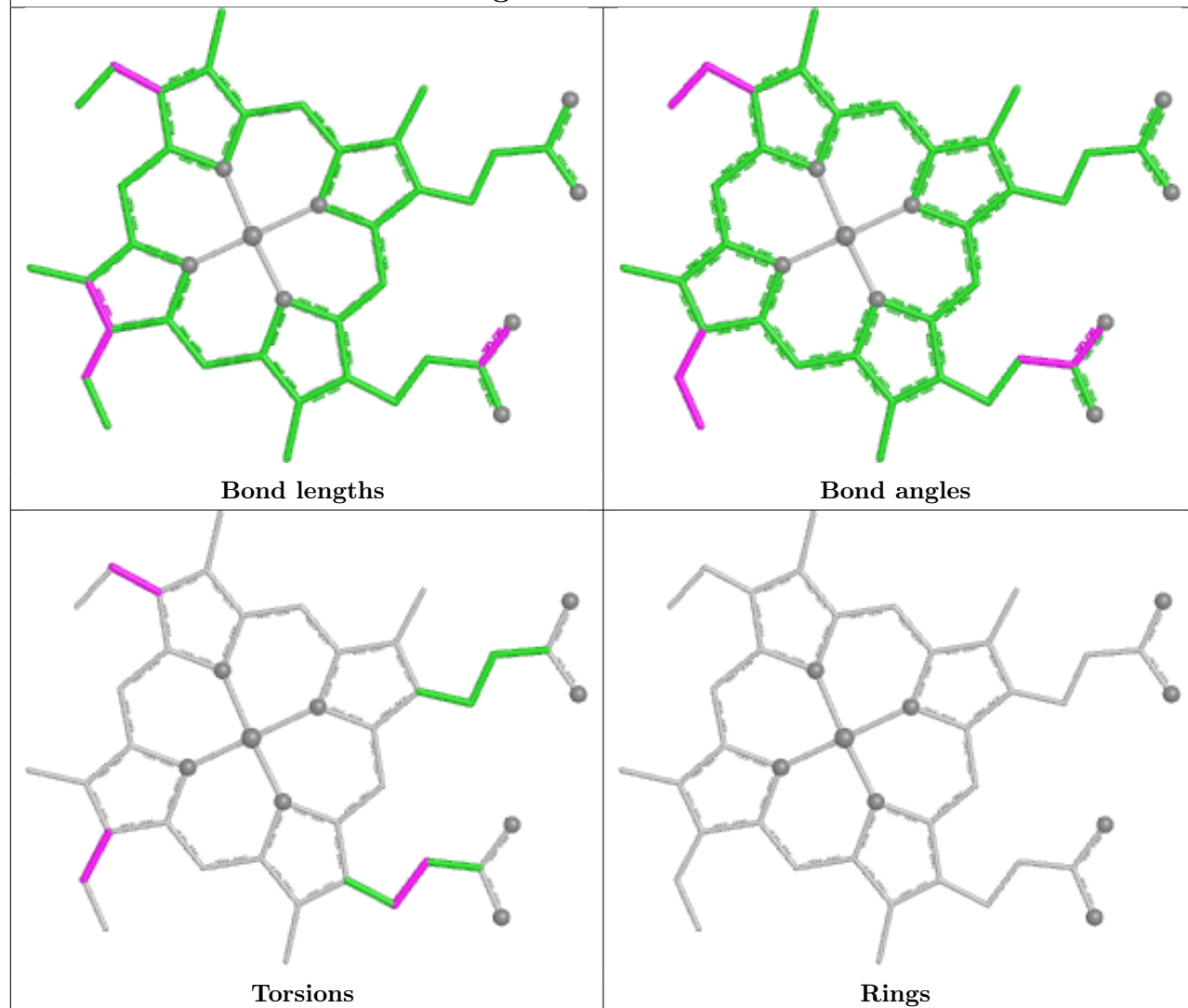


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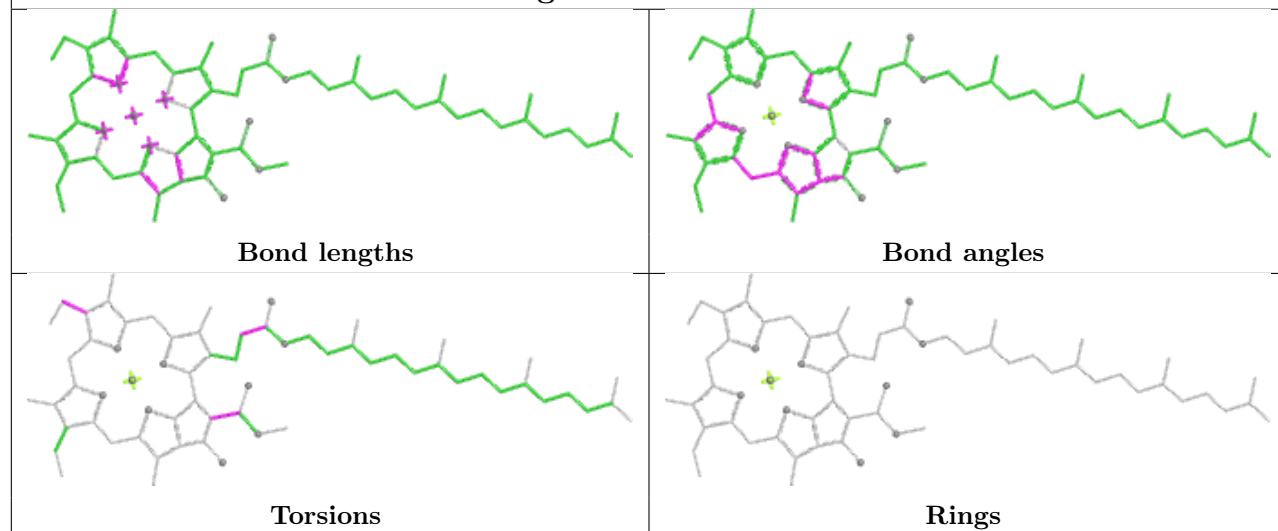


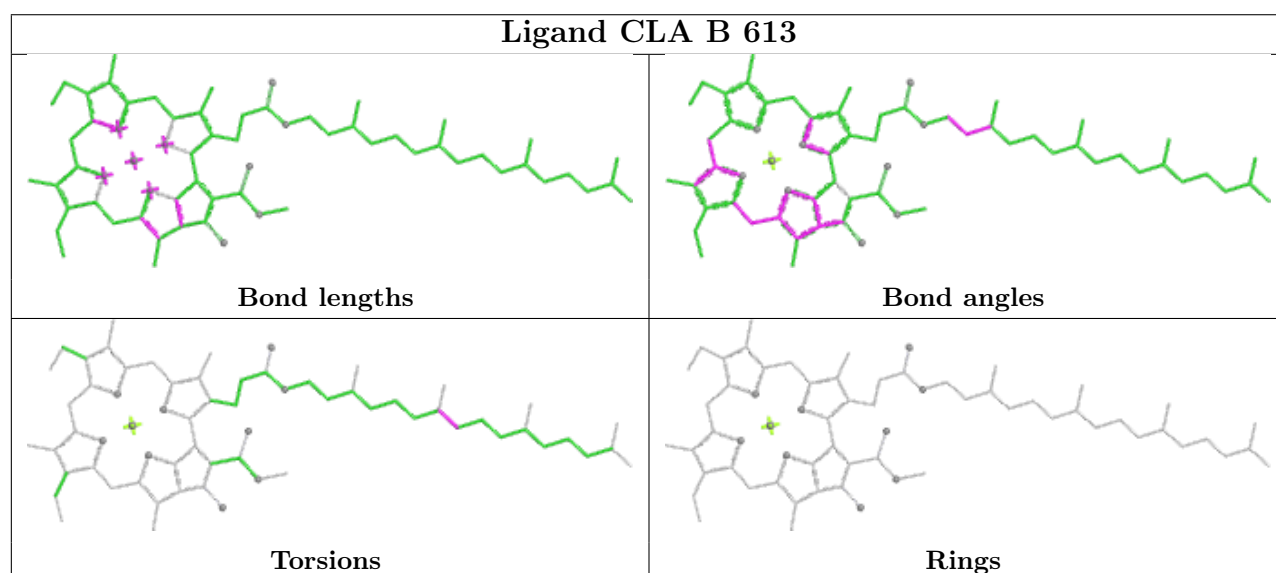
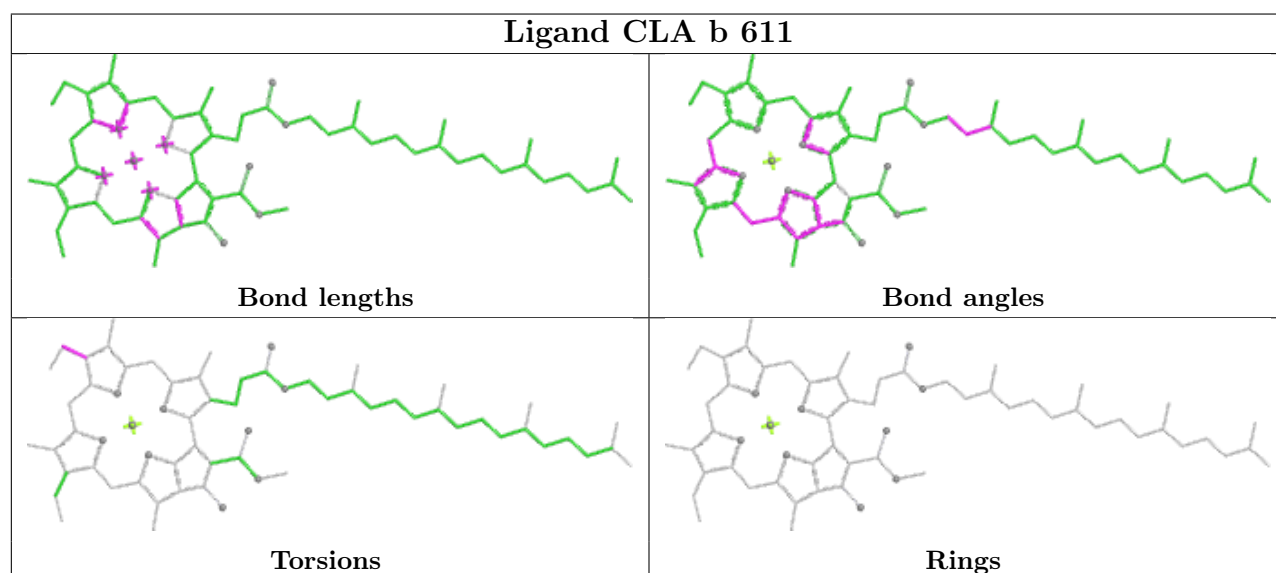
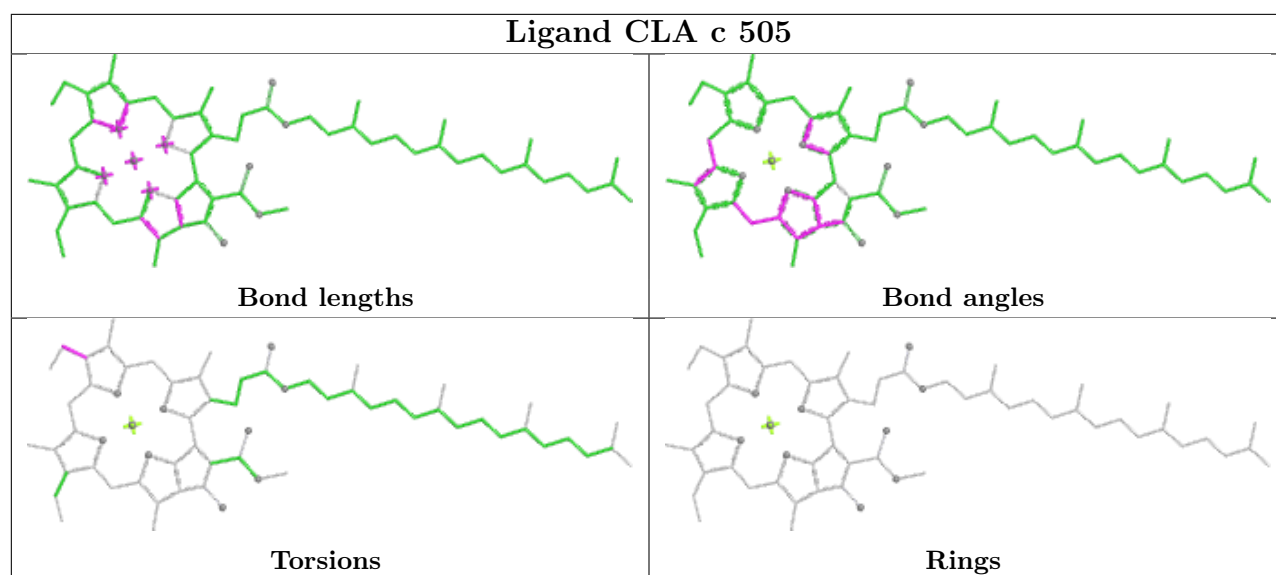


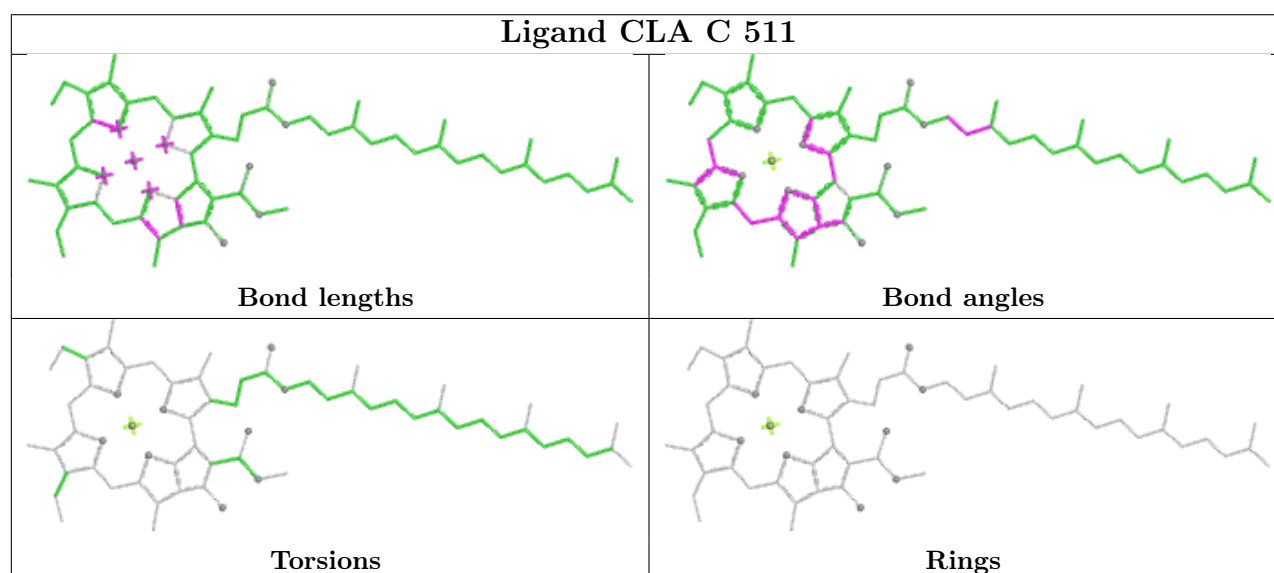
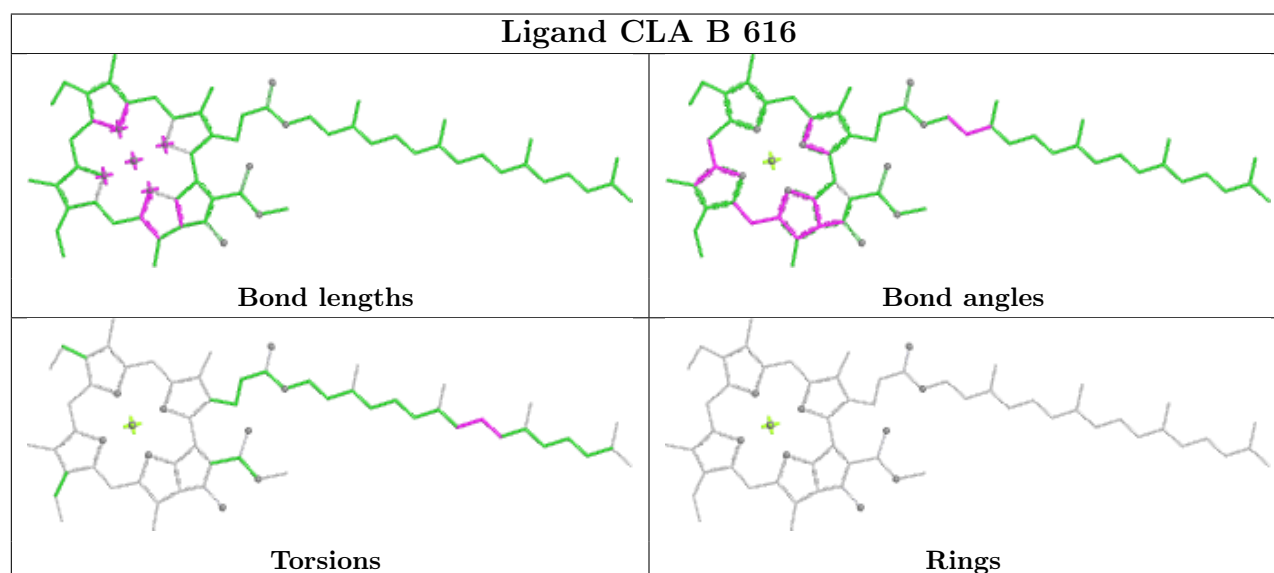
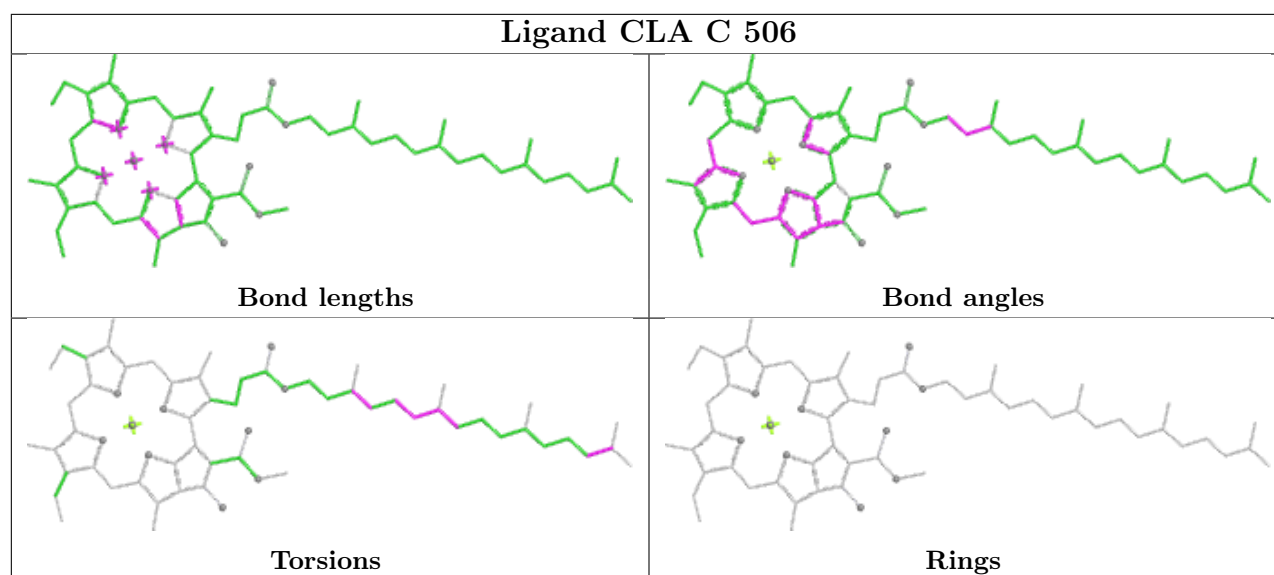
Ligand HEC V 201



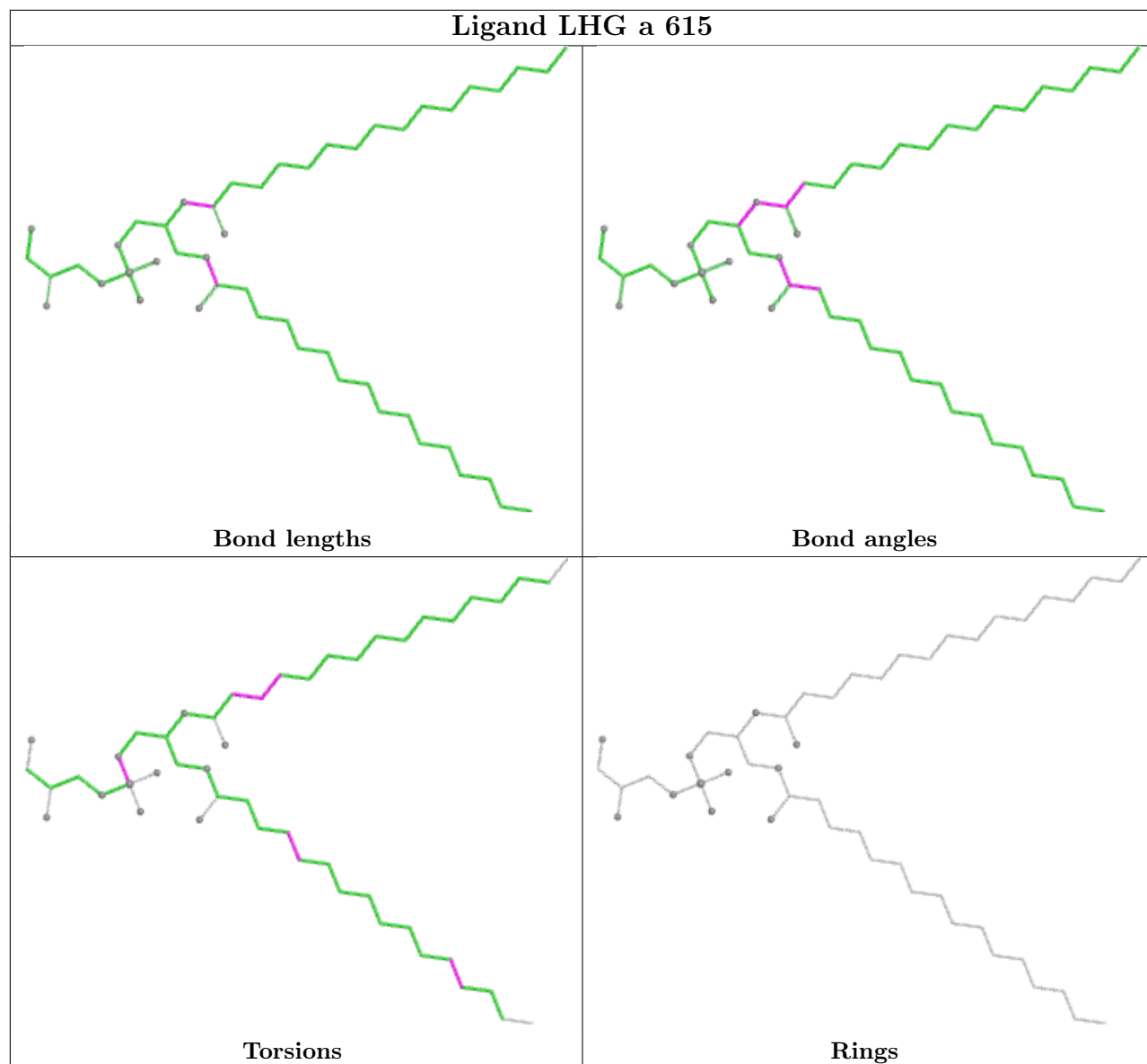
Ligand CLA c 512



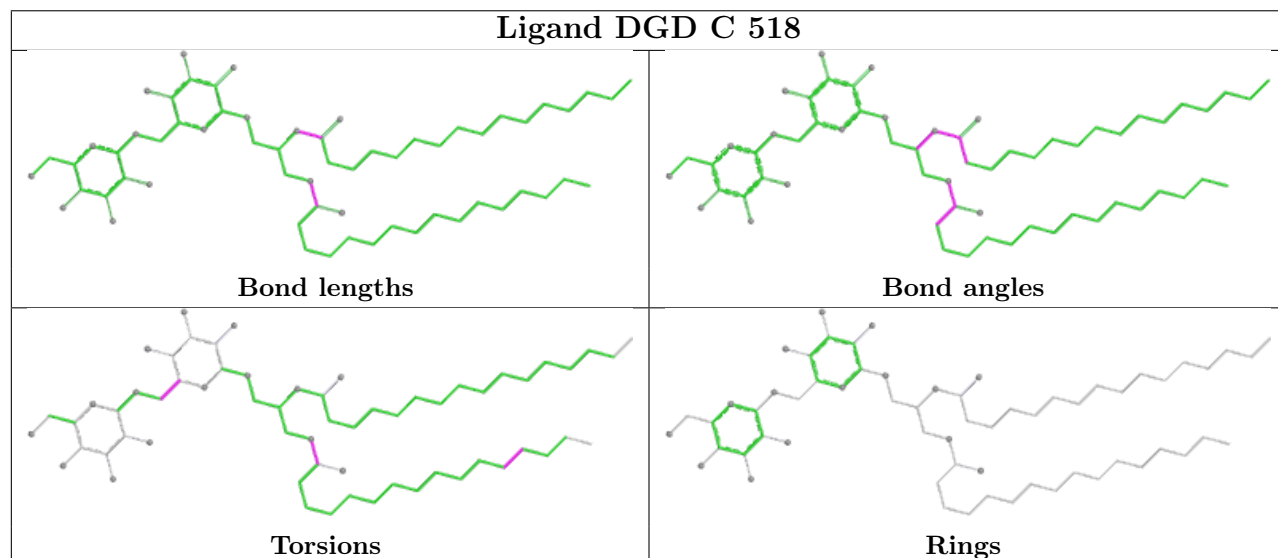




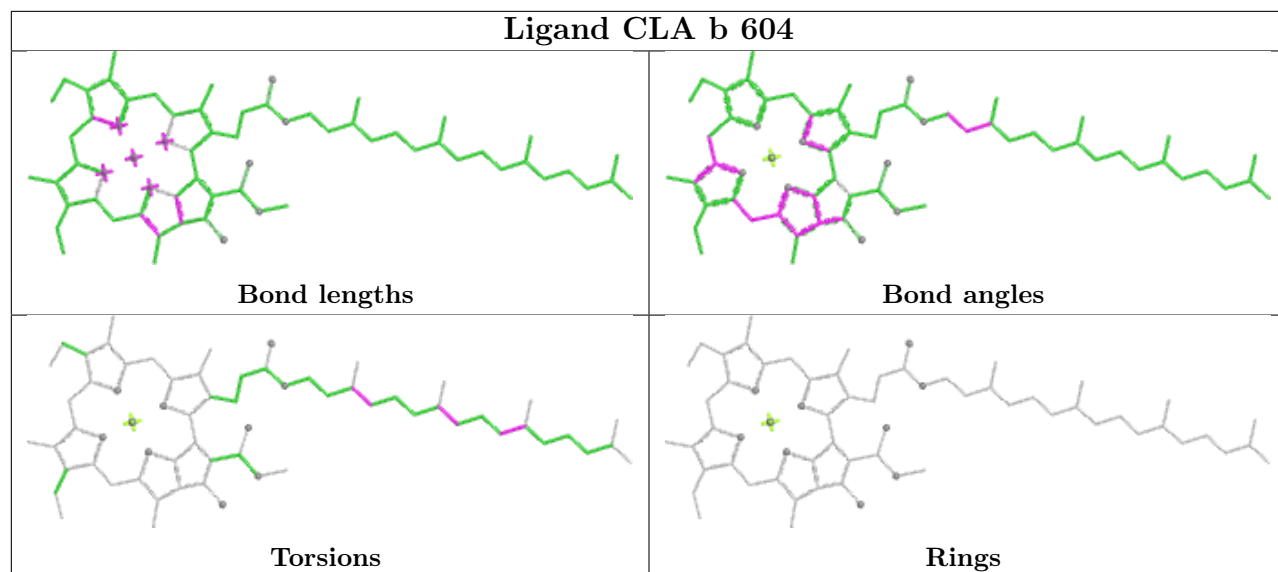
Ligand LHG a 615



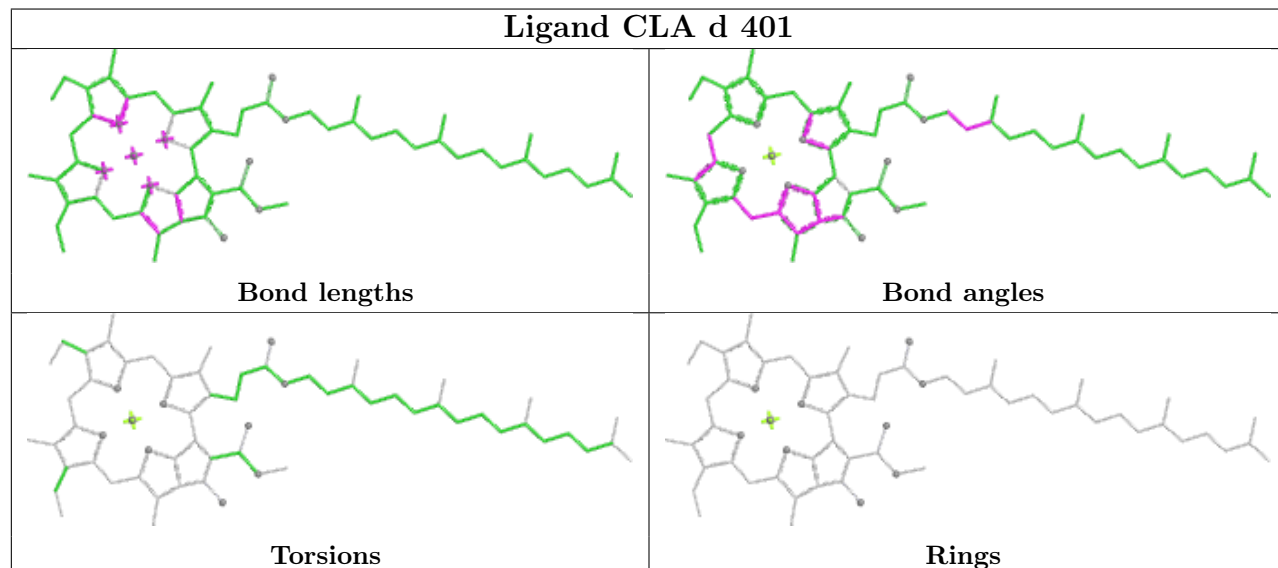
Ligand DGD C 518



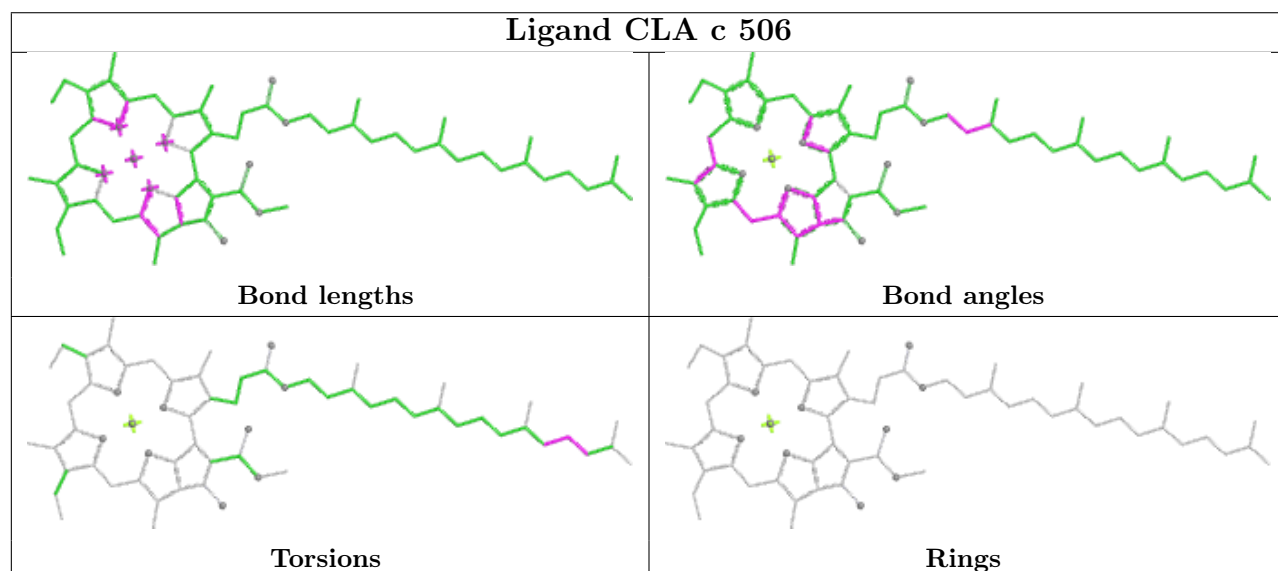
Ligand CLA b 604

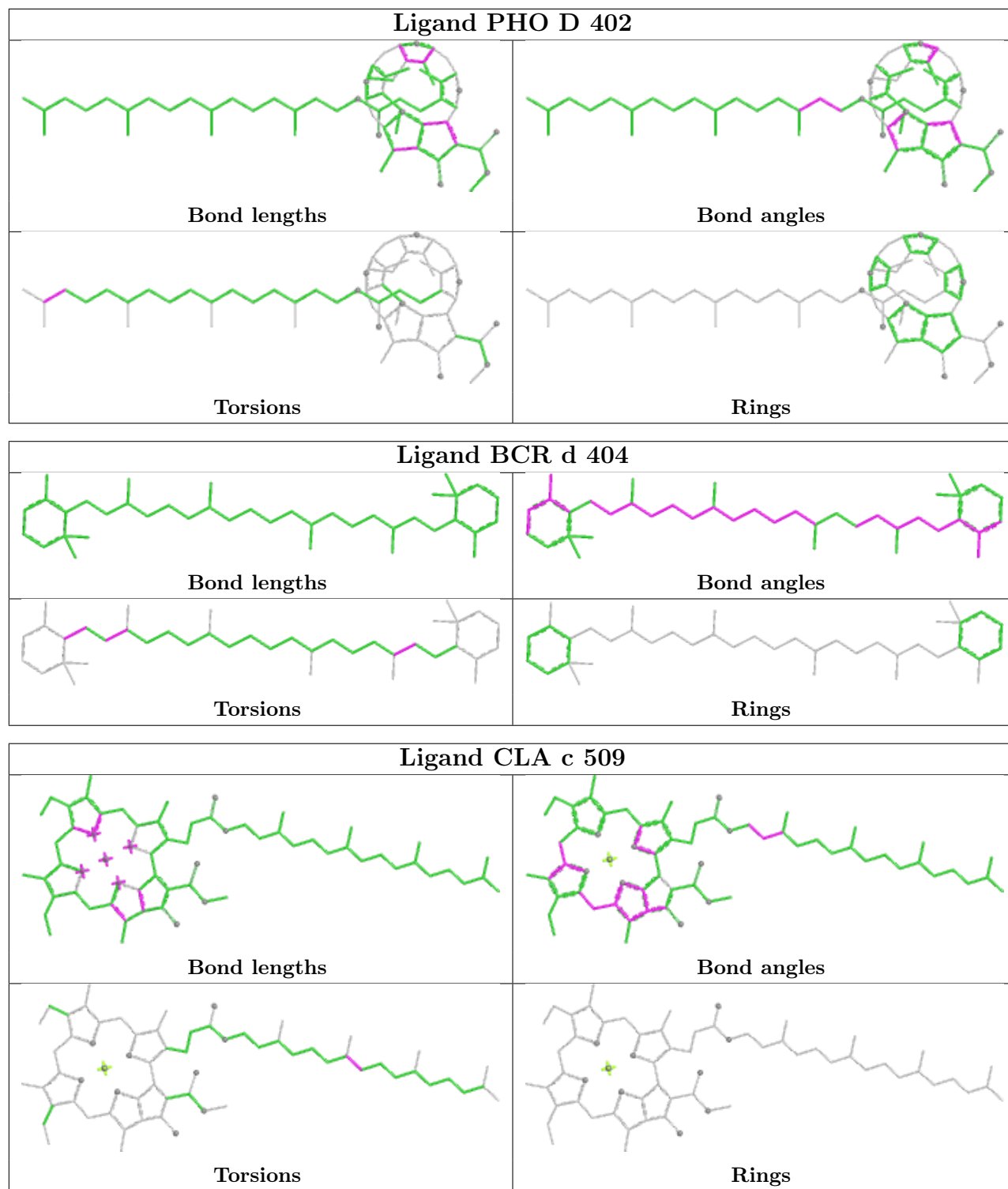


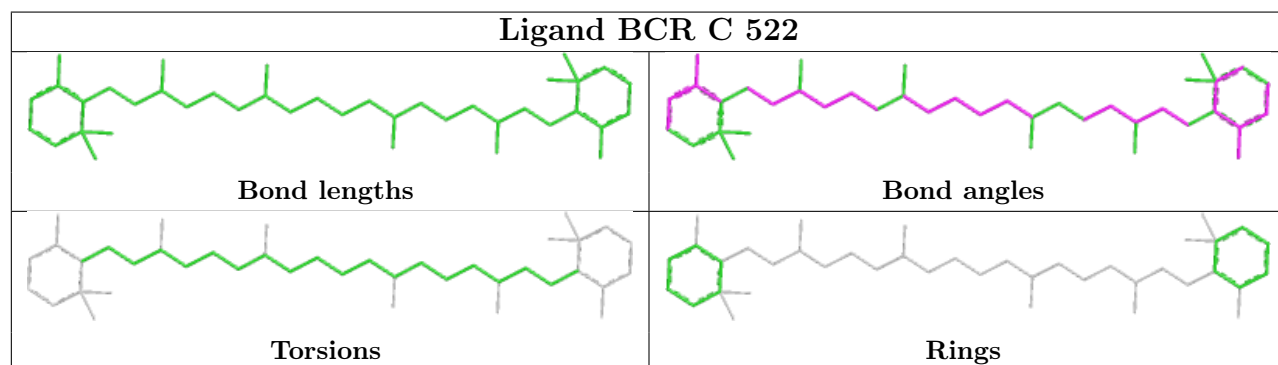
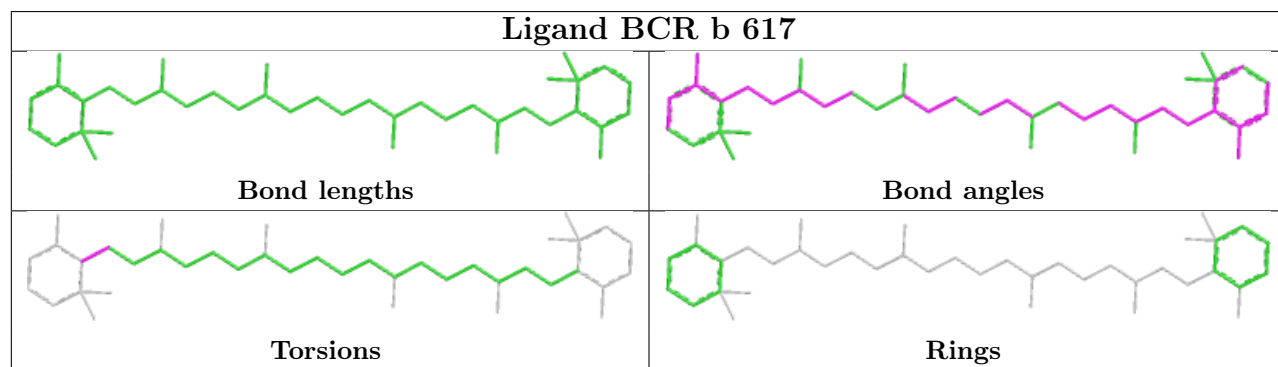
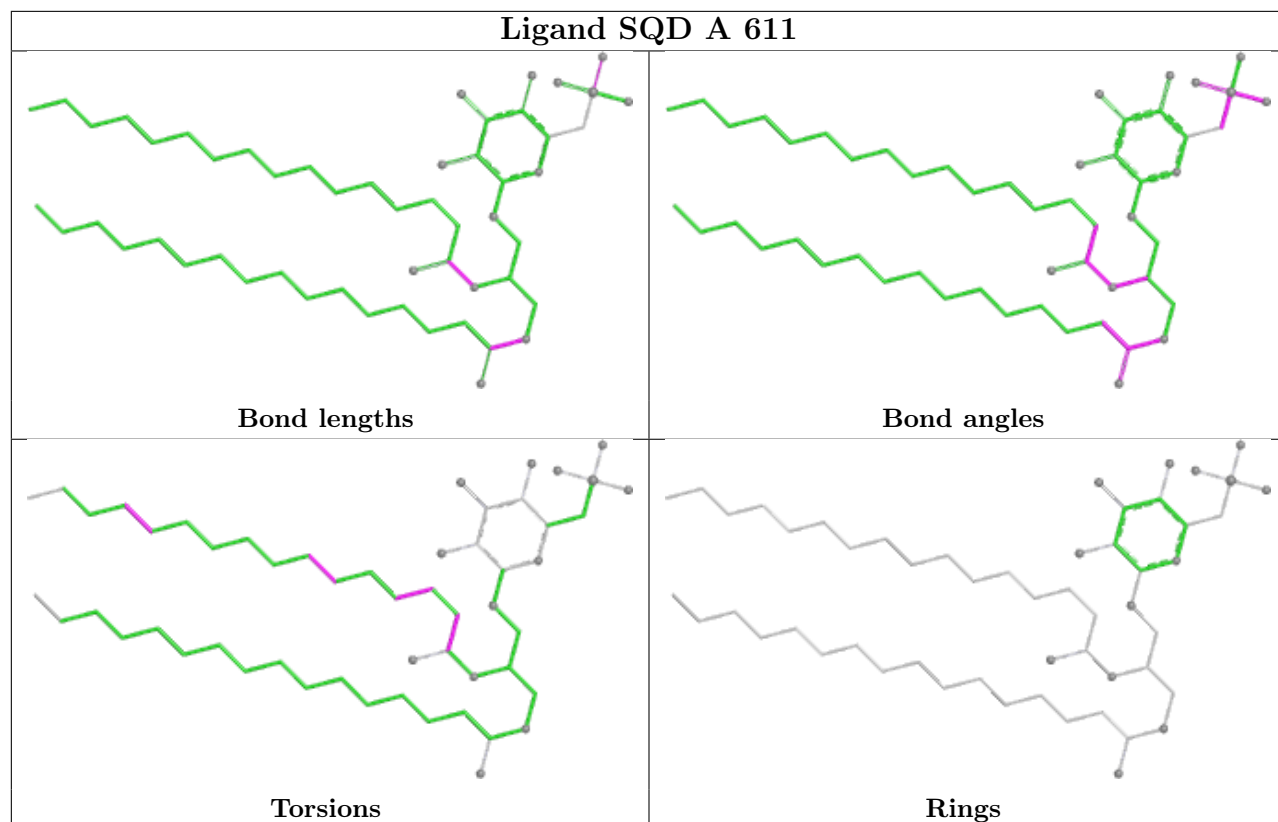
Ligand CLA d 401



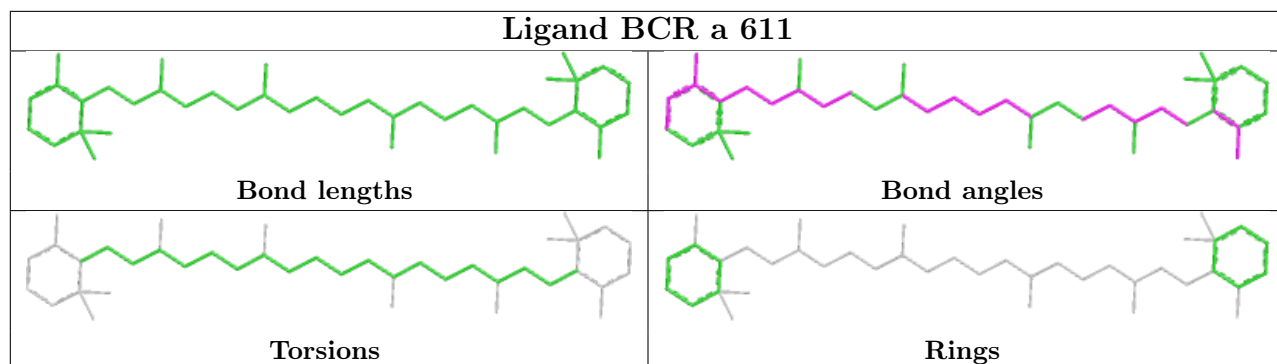
Ligand CLA c 506



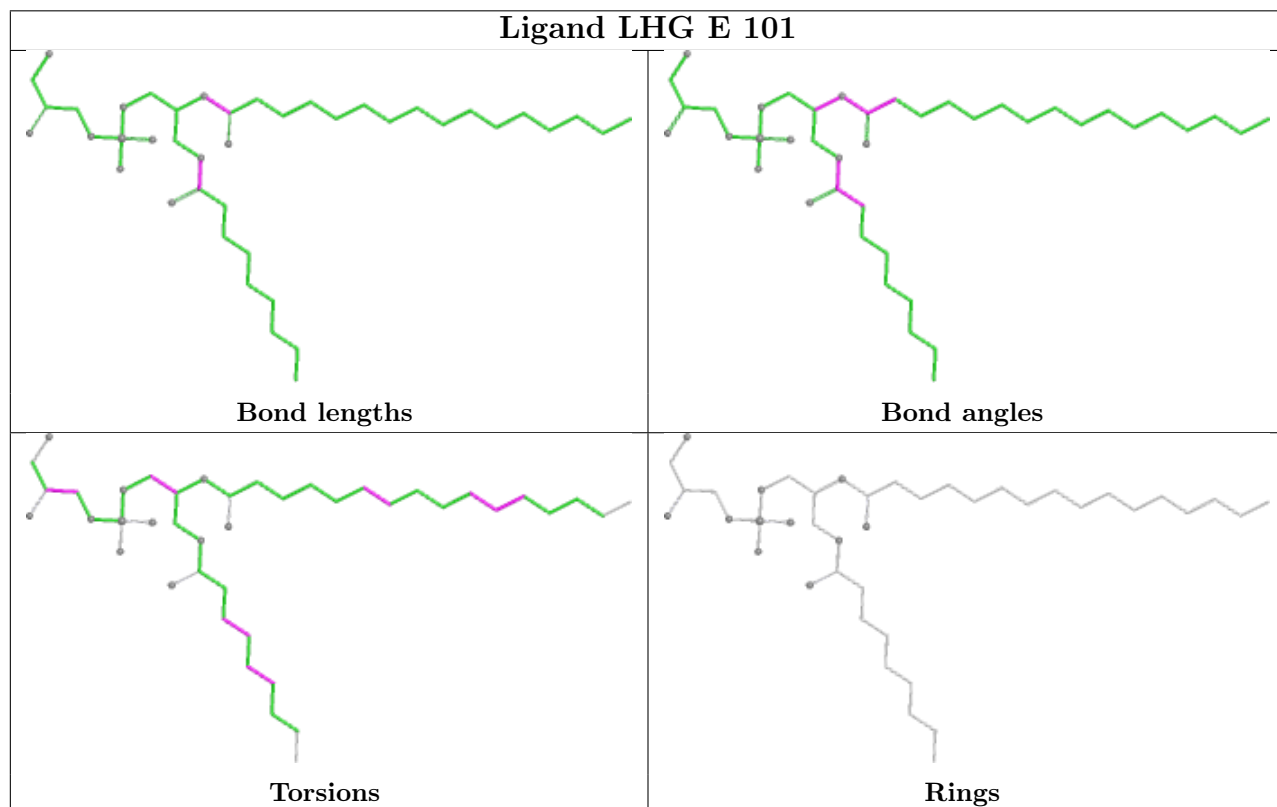




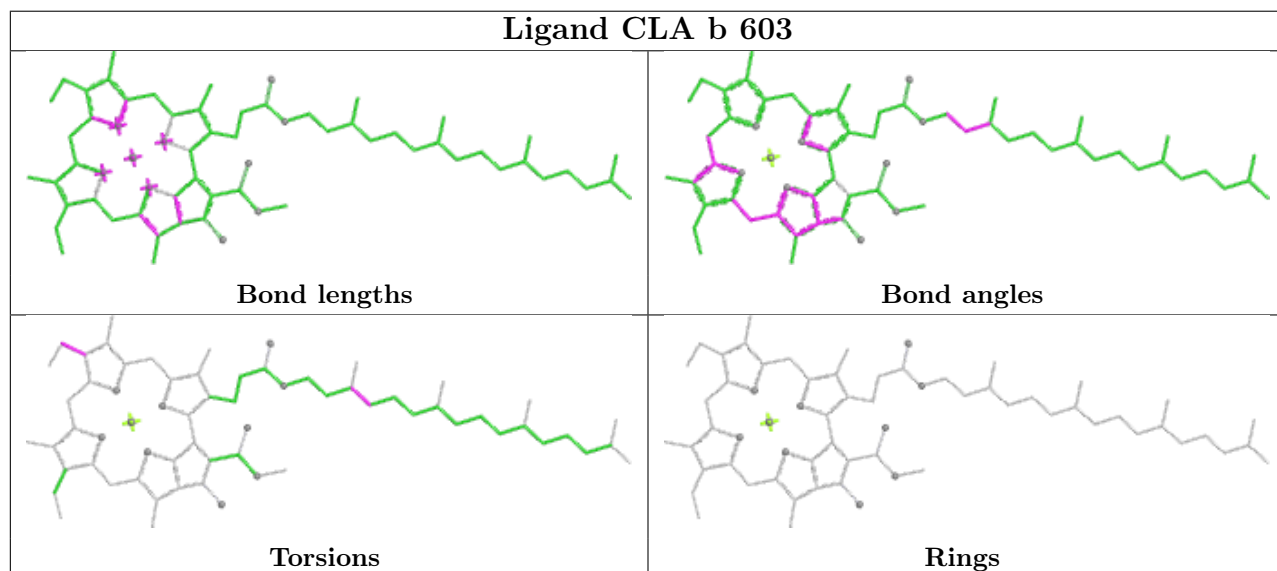
Ligand BCR a 611



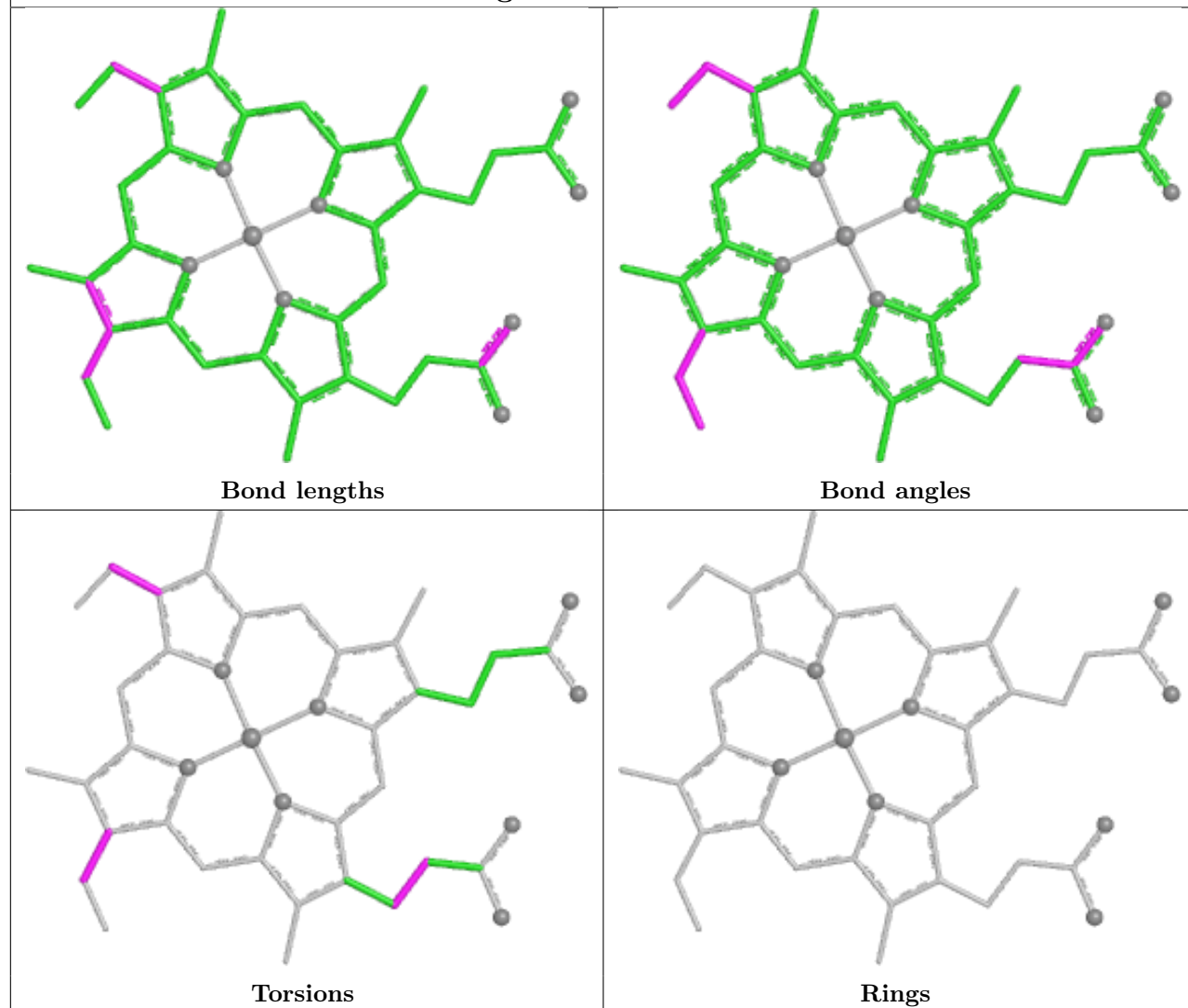
Ligand LHG E 101



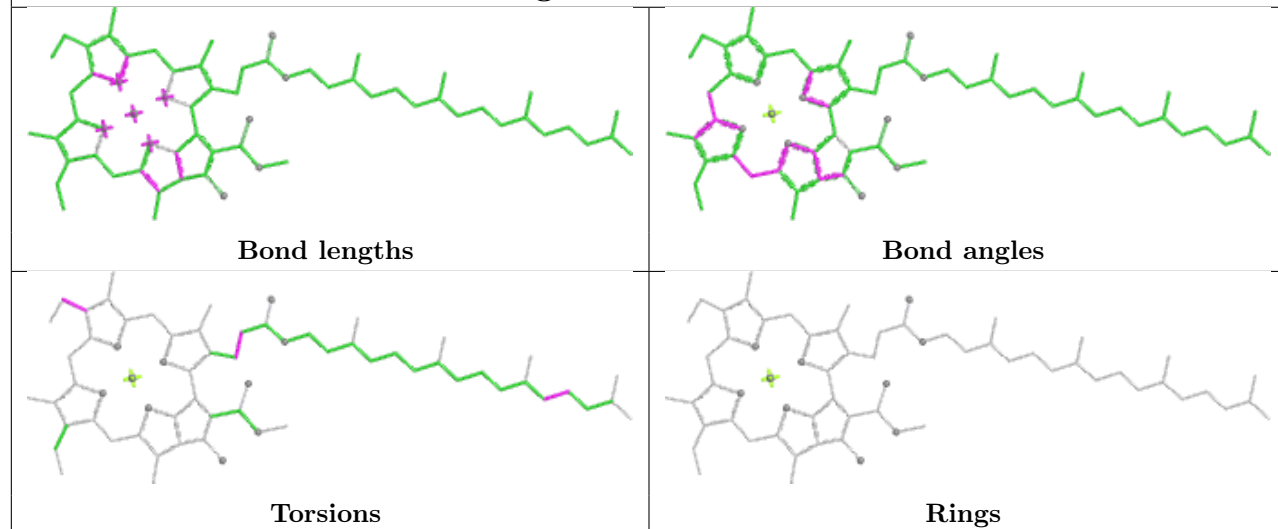
Ligand CLA b 603

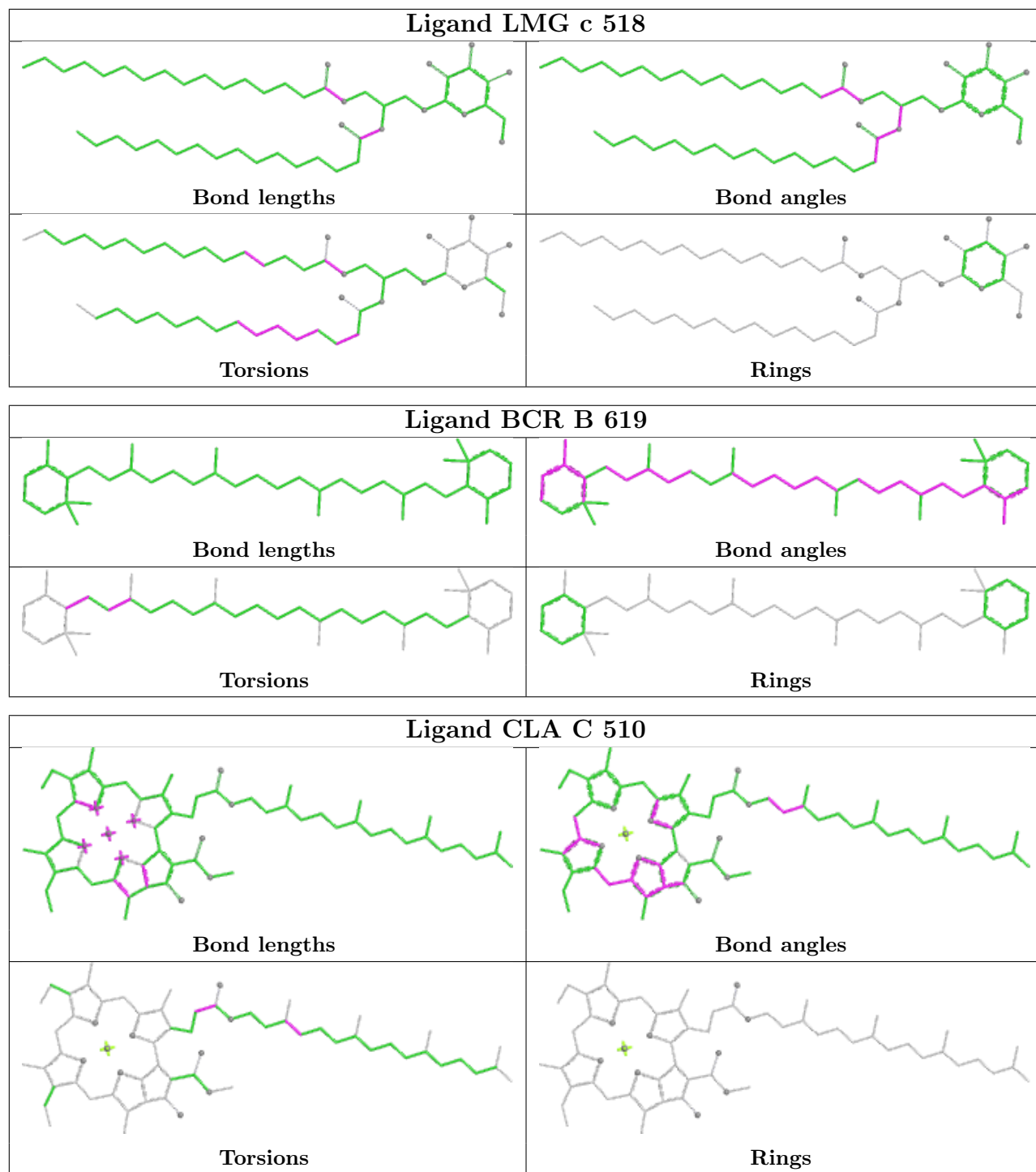


Ligand HEC v 201

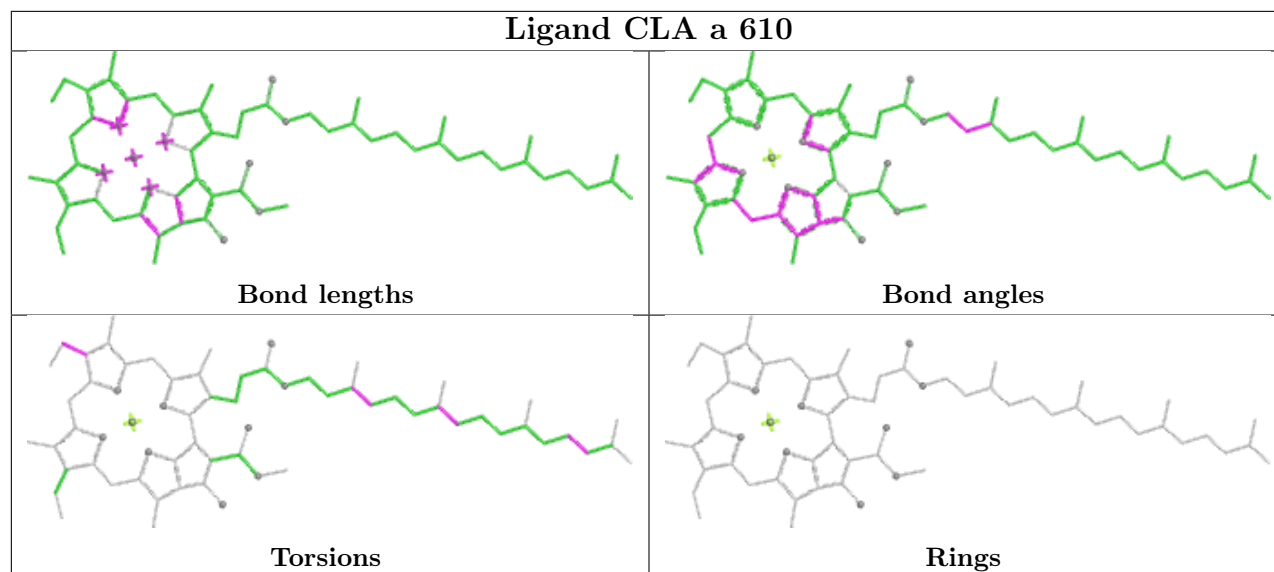


Ligand CLA b 606

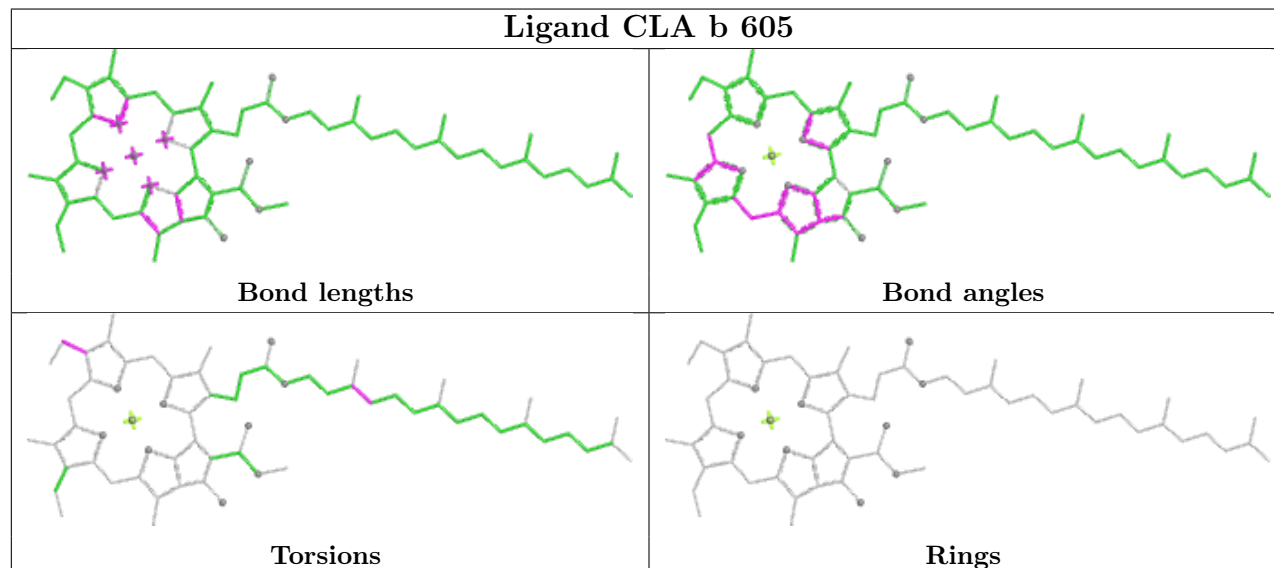




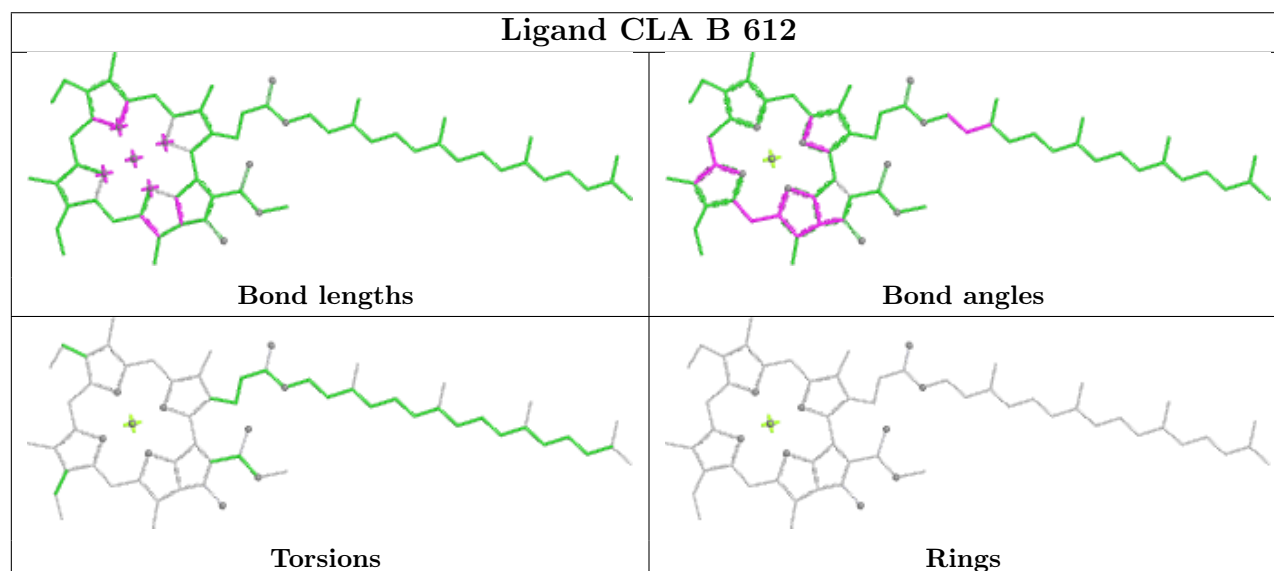
Ligand CLA a 610

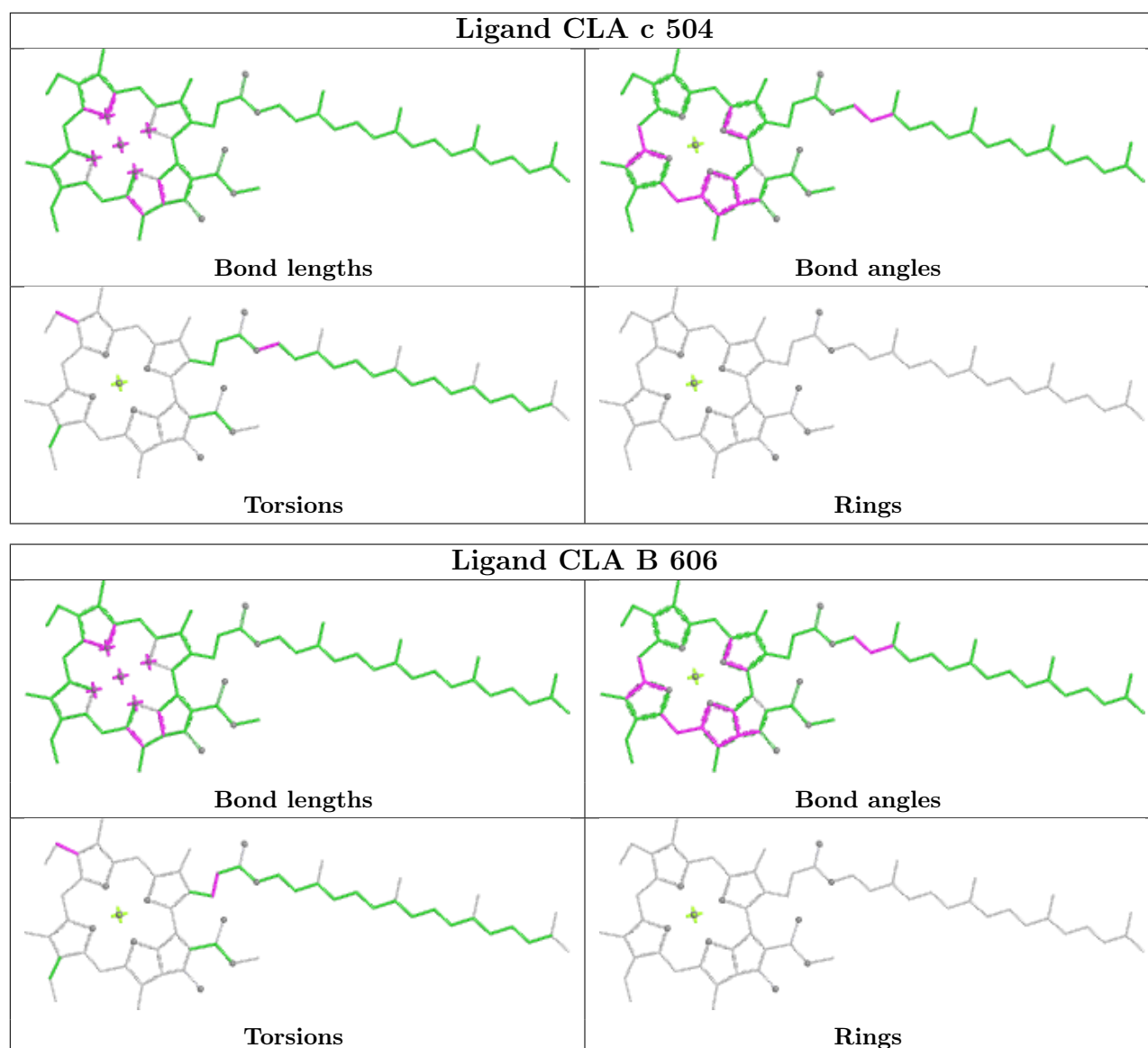


Ligand CLA b 605



Ligand CLA B 612





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	333/344 (96%)	-0.01	5 (1%) 72 73	24, 32, 54, 72	0
1	a	333/344 (96%)	0.06	7 (2%) 63 64	24, 34, 62, 76	0
2	B	505/510 (99%)	0.07	19 (3%) 44 42	24, 35, 61, 84	0
2	b	503/510 (98%)	0.15	14 (2%) 55 54	26, 38, 67, 87	0
3	C	448/461 (97%)	0.17	10 (2%) 62 63	24, 40, 59, 77	0
3	c	448/461 (97%)	0.22	8 (1%) 67 68	29, 42, 60, 80	0
4	D	340/352 (96%)	-0.01	5 (1%) 72 73	25, 34, 52, 70	0
4	d	340/352 (96%)	0.06	2 (0%) 85 87	26, 37, 59, 74	0
5	E	82/84 (97%)	0.94	11 (13%) 7 5	39, 57, 71, 75	0
5	e	79/84 (94%)	0.95	5 (6%) 26 23	43, 58, 71, 81	0
6	F	33/45 (73%)	0.43	0 100 100	42, 49, 63, 71	0
6	f	33/45 (73%)	0.74	1 (3%) 52 52	46, 52, 73, 82	0
7	H	63/66 (95%)	0.33	1 (1%) 70 72	34, 41, 48, 60	0
7	h	63/66 (95%)	0.58	3 (4%) 35 33	39, 48, 59, 69	0
8	I	33/38 (86%)	-0.05	1 (3%) 52 52	30, 36, 44, 55	0
8	i	35/38 (92%)	0.17	0 100 100	31, 39, 56, 66	0
9	J	34/40 (85%)	0.58	1 (2%) 53 53	40, 53, 64, 78	0
9	j	33/40 (82%)	0.66	0 100 100	43, 52, 61, 65	0
10	K	36/46 (78%)	1.09	6 (16%) 4 3	52, 61, 75, 77	0
10	k	36/46 (78%)	0.83	1 (2%) 55 54	48, 60, 76, 78	0
11	L	36/37 (97%)	-0.09	0 100 100	26, 33, 53, 59	0
11	l	36/37 (97%)	-0.09	0 100 100	28, 35, 50, 62	0
12	M	32/36 (88%)	0.07	0 100 100	30, 36, 56, 58	0
12	m	32/36 (88%)	0.14	0 100 100	30, 38, 57, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/272 (88%)	0.33	11 (4%) 38 35	30, 44, 70, 104	0
13	o	243/272 (89%)	0.42	12 (4%) 35 32	28, 45, 72, 108	0
14	T	29/32 (90%)	0.02	2 (6%) 23 19	26, 35, 56, 62	0
14	t	29/32 (90%)	0.10	3 (10%) 12 9	31, 36, 55, 67	0
15	U	96/134 (71%)	0.35	1 (1%) 79 81	34, 43, 64, 72	0
15	u	96/134 (71%)	0.33	0 100 100	35, 45, 58, 65	0
16	V	137/163 (84%)	0.39	2 (1%) 72 73	33, 44, 56, 64	0
16	v	137/163 (84%)	0.51	1 (0%) 84 85	37, 50, 67, 82	0
17	Y	29/46 (63%)	1.87	12 (41%) 0 0	63, 76, 95, 96	0
17	y	29/46 (63%)	1.43	4 (13%) 6 5	61, 71, 90, 91	0
18	X	37/41 (90%)	0.32	1 (2%) 56 55	42, 50, 65, 79	0
18	x	38/41 (92%)	0.57	4 (10%) 11 9	41, 52, 74, 84	0
19	Z	62/62 (100%)	1.47	16 (25%) 1 1	57, 73, 104, 111	0
19	z	62/62 (100%)	1.44	9 (14%) 6 4	62, 74, 100, 107	0
20	R	34/41 (82%)	1.56	8 (23%) 2 1	61, 74, 88, 92	0
20	r	33/41 (80%)	1.70	14 (42%) 0 0	64, 73, 86, 91	0
All	All	5279/5700 (92%)	0.28	200 (3%) 44 42	24, 41, 72, 111	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	49	TYR	5.8
13	O	56	PRO	5.3
17	y	18	VAL	5.1
19	Z	33	TRP	4.9
17	Y	19	ILE	4.5
13	O	58	ASN	4.3
19	Z	30	PRO	4.2
17	Y	18	VAL	4.1
19	Z	37	LYS	3.9
13	o	57	LYS	3.9
13	O	63	ALA	3.8
2	b	495	PHE	3.6
2	b	128	THR	3.6
20	R	2	ASP	3.6
19	Z	41	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	339	ALA	3.5
2	B	484	PRO	3.5
20	r	26	TYR	3.4
7	H	64	ALA	3.4
19	Z	34	ASP	3.4
6	f	13	TYR	3.3
2	b	499	VAL	3.3
2	B	485	GLU	3.3
2	b	85	GLY	3.3
19	z	3	ILE	3.3
5	e	74	GLN	3.2
2	B	496	TYR	3.2
17	y	19	ILE	3.2
3	c	149	TYR	3.2
20	R	6	LEU	3.2
19	Z	31	GLN	3.2
2	B	479	PHE	3.1
17	Y	20	ALA	3.1
17	y	20	ALA	3.1
13	o	61	GLN	3.1
2	b	126	PRO	3.1
17	Y	25	ILE	3.1
19	z	39	LEU	3.0
4	D	236	ASN	3.0
19	z	37	LYS	3.0
19	z	33	TRP	3.0
10	K	11	LEU	3.0
1	a	230	THR	3.0
16	V	1	ALA	3.0
13	O	61	GLN	3.0
13	o	56	PRO	2.9
19	z	32	ASP	2.9
13	o	89	SER	2.9
3	C	148	GLY	2.9
3	c	142	GLU	2.9
10	K	46	ARG	2.9
2	b	484	PRO	2.9
14	T	29	ILE	2.9
14	t	28	ARG	2.9
13	o	63	ALA	2.9
20	R	27	ALA	2.9
19	z	36	SER	2.8

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Mol	Chain	Res	Type	RSRZ
19	z	1	MET	2.8
13	o	54	GLU	2.8
16	V	42	VAL	2.8
5	E	60	GLN	2.8
19	Z	62	VAL	2.8
3	c	146	PHE	2.8
19	Z	60	PHE	2.8
2	b	487	SER	2.7
1	A	249	VAL	2.7
20	r	5	VAL	2.7
1	a	13	LEU	2.7
20	r	12	VAL	2.7
2	B	490	GLN	2.7
3	c	143	TYR	2.7
2	b	479	PHE	2.6
2	B	503	THR	2.6
10	K	18	PHE	2.6
20	r	9	LEU	2.6
18	x	4	THR	2.6
3	c	462	GLU	2.6
20	r	24	LEU	2.6
14	t	29	ILE	2.5
19	Z	39	LEU	2.5
3	C	28	GLN	2.5
19	z	30	PRO	2.5
10	K	39	TRP	2.5
5	E	79	PHE	2.5
19	Z	61	VAL	2.5
18	x	2	THR	2.5
14	T	28	ARG	2.5
20	r	35	LEU	2.5
13	O	57	LYS	2.5
17	Y	23	THR	2.5
13	o	5	LEU	2.5
20	r	6	LEU	2.5
5	E	61	ARG	2.5
13	O	60	ARG	2.5
5	E	62	SER	2.5
13	o	25	THR	2.5
2	B	495	PHE	2.4
5	E	2	ALA	2.4
2	B	130	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
17	Y	44	GLY	2.4
1	a	224	ILE	2.4
1	A	13	LEU	2.4
16	v	12	LEU	2.4
20	R	12	VAL	2.4
3	C	29	GLU	2.4
3	C	144	SER	2.4
5	E	64	PRO	2.4
13	O	54	GLU	2.4
13	O	59	LYS	2.4
5	E	68	ASP	2.4
17	Y	46	LEU	2.4
18	X	2	THR	2.4
2	b	488	PRO	2.4
8	I	33	LYS	2.4
1	A	225	ARG	2.4
17	Y	45	ASN	2.4
2	B	481	GLY	2.3
13	o	59	LYS	2.3
5	E	4	THR	2.3
5	E	5	THR	2.3
20	R	32	GLN	2.3
2	b	125	ASP	2.3
5	e	81	GLU	2.3
3	c	463	SER	2.3
17	Y	22	LEU	2.3
5	e	17	VAL	2.3
13	o	84	GLU	2.3
2	B	85	GLY	2.3
5	E	3	GLY	2.3
20	R	35	LEU	2.3
20	r	3	TRP	2.3
18	x	39	ARG	2.3
19	Z	35	ARG	2.3
7	h	64	ALA	2.2
13	O	35	SER	2.2
17	Y	41	VAL	2.2
20	r	20	VAL	2.2
2	b	496	TYR	2.2
3	C	143	TYR	2.2
13	o	4	THR	2.2
4	D	352	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
20	r	13	LEU	2.2
3	C	134	ILE	2.2
10	k	14	ALA	2.2
1	A	227	THR	2.2
20	r	34	LEU	2.2
2	B	501	ASP	2.2
1	a	244	GLU	2.2
2	B	493	TRP	2.2
13	o	60	ARG	2.2
4	d	27	PHE	2.2
1	a	250	ALA	2.2
2	B	486	LEU	2.2
3	c	135	ARG	2.2
1	a	238	LYS	2.2
5	E	82	GLN	2.1
17	Y	26	ALA	2.1
20	R	34	LEU	2.1
7	h	54	ILE	2.1
2	b	419	SER	2.1
4	D	237	PRO	2.1
10	K	38	VAL	2.1
17	Y	24	MET	2.1
20	r	30	GLN	2.1
9	J	14	ALA	2.1
1	a	228	THR	2.1
2	B	494	GLY	2.1
4	D	238	THR	2.1
2	B	482	ILE	2.1
20	r	33	LYS	2.1
20	r	25	PRO	2.1
19	Z	59	PHE	2.1
2	B	491	VAL	2.1
4	D	229	ALA	2.1
19	Z	4	LEU	2.1
5	e	61	ARG	2.1
2	b	130	GLU	2.1
13	O	55	GLU	2.1
2	B	499	VAL	2.1
19	z	62	VAL	2.1
3	C	140	LEU	2.1
2	B	500	GLY	2.1
3	c	26	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
10	K	17	ILE	2.1
17	y	30	ILE	2.1
19	Z	3	ILE	2.1
15	U	65	PRO	2.1
14	t	1	MET	2.1
4	d	240	ALA	2.0
20	R	24	LEU	2.0
19	Z	40	ILE	2.0
3	C	27	ASP	2.0
3	C	31	SER	2.0
2	b	490	GLN	2.0
5	e	79	PHE	2.0
18	x	37	VAL	2.0
13	O	64	GLU	2.0
1	A	245	THR	2.0
19	Z	1	MET	2.0
3	C	30	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	SO4	u	202	5/5	0.67	0.17	64,73,90,96	0
32	UNL	D	410	15/-	0.72	0.25	36,44,67,68	0
30	SO4	V	202	5/5	0.74	0.25	71,72,81,81	0
32	UNL	i	101	16/-	0.74	0.20	33,42,48,48	0
28	SQD	L	103	54/54	0.77	0.17	34,53,92,102	0
32	UNL	b	621	10/-	0.77	0.18	32,41,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	UNL	B	626	9/-	0.77	0.19	35,40,44,47	0
27	PL9	a	612	55/55	0.78	0.20	48,64,76,81	0
32	UNL	b	625	16/-	0.80	0.16	37,43,48,49	0
32	UNL	B	622	8/-	0.80	0.20	38,42,45,46	0
32	UNL	m	101	10/-	0.80	0.16	44,53,58,59	0
28	SQD	L	101	54/54	0.81	0.15	34,54,89,94	0
32	UNL	M	101	10/-	0.81	0.17	45,49,60,62	0
32	UNL	T	102	15/-	0.82	0.18	36,46,51,51	0
28	SQD	f	101	43/54	0.82	0.19	55,77,85,88	0
32	UNL	b	622	12/-	0.82	0.18	37,47,51,51	0
29	LHG	E	101	42/49	0.82	0.15	44,67,78,83	0
27	PL9	A	610	55/55	0.82	0.16	34,52,63,70	0
23	LMG	a	603	51/55	0.82	0.16	37,52,70,80	0
32	UNL	J	101	11/-	0.83	0.22	48,58,64,67	0
32	UNL	j	101	15/-	0.83	0.18	43,53,57,59	0
23	LMG	C	519	51/55	0.83	0.17	48,64,79,84	0
23	LMG	B	624	51/55	0.84	0.14	41,50,60,66	0
32	UNL	B	627	12/-	0.84	0.15	33,39,45,50	0
23	LMG	b	624	51/55	0.84	0.15	43,59,69,72	0
30	SO4	a	617	5/5	0.84	0.18	52,57,70,79	0
26	BCR	K	101	40/40	0.84	0.16	51,61,70,73	0
23	LMG	A	603	51/55	0.84	0.14	36,49,64,72	0
23	LMG	c	520	51/55	0.85	0.15	41,54,74,79	0
23	LMG	B	620	51/55	0.85	0.14	27,50,57,64	0
28	SQD	a	613	54/54	0.85	0.16	37,65,73,77	0
26	BCR	c	521	40/40	0.85	0.16	43,53,62,66	0
23	LMG	a	614	51/55	0.85	0.15	34,50,68,75	0
32	UNL	d	409	15/-	0.85	0.16	39,45,52,53	0
29	LHG	a	616	42/49	0.85	0.16	53,71,80,87	0
32	UNL	I	101	14/-	0.85	0.15	32,41,48,49	0
23	LMG	C	521	51/55	0.85	0.15	38,51,63,67	0
25	CLA	C	513	65/65	0.86	0.14	51,62,77,82	0
30	SO4	O	302	5/5	0.86	0.18	65,66,78,80	0
25	CLA	b	601	65/65	0.86	0.14	39,59,77,84	0
28	SQD	F	101	43/54	0.86	0.17	46,63,76,85	0
30	SO4	u	201	5/5	0.86	0.14	63,66,73,73	0
26	BCR	C	514	40/40	0.86	0.15	50,58,65,66	0
32	UNL	B	621	10/-	0.86	0.15	34,41,45,46	0
32	UNL	b	626	9/-	0.86	0.18	32,45,53,56	0
23	LMG	A	612	51/55	0.86	0.15	38,52,61,63	0
23	LMG	b	620	51/55	0.86	0.14	31,44,58,60	0
26	BCR	d	404	40/40	0.86	0.14	38,50,62,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	z	101	40/40	0.86	0.14	49,59,63,67	0
32	UNL	m	102	15/-	0.86	0.14	34,43,51,52	0
32	UNL	B	623	13/-	0.87	0.15	36,40,48,51	0
23	LMG	c	518	51/55	0.87	0.15	38,58,76,80	0
32	UNL	c	519	15/-	0.87	0.15	40,46,51,53	0
32	UNL	M	102	16/-	0.87	0.13	28,43,53,56	0
31	BCT	a	618	4/4	0.87	0.12	36,38,43,44	0
32	UNL	T	103	12/-	0.87	0.13	35,42,49,49	0
30	SO4	o	301	5/5	0.87	0.20	62,68,71,91	0
26	BCR	k	102	40/40	0.87	0.15	48,59,65,65	0
32	UNL	t	101	15/-	0.87	0.13	31,49,57,57	0
26	BCR	h	101	40/40	0.88	0.12	34,44,52,53	0
25	CLA	C	511	65/65	0.88	0.13	42,58,67,70	0
25	CLA	C	512	65/65	0.88	0.13	45,56,66,71	0
32	UNL	x	101	16/-	0.88	0.12	31,42,52,54	0
28	SQD	A	611	54/54	0.89	0.14	32,57,74,79	0
30	SO4	d	410	5/5	0.89	0.10	73,73,83,84	0
25	CLA	c	513	65/65	0.89	0.14	45,60,76,79	0
26	BCR	B	619	40/40	0.89	0.12	33,39,46,50	0
25	CLA	B	601	65/65	0.89	0.12	36,49,72,80	0
32	UNL	b	623	13/-	0.89	0.15	37,44,53,54	0
26	BCR	C	522	40/40	0.89	0.14	45,55,63,64	0
26	BCR	t	102	40/40	0.89	0.12	28,39,45,49	0
29	LHG	A	614	49/49	0.89	0.15	29,48,70,78	0
26	BCR	D	406	40/40	0.89	0.14	28,45,64,66	0
26	BCR	H	101	40/40	0.89	0.12	32,37,53,54	0
29	LHG	d	407	49/49	0.89	0.16	38,50,68,76	0
30	SO4	A	615	5/5	0.89	0.21	49,50,62,64	0
30	SO4	O	301	5/5	0.89	0.15	51,67,76,82	0
25	CLA	C	503	65/65	0.89	0.11	32,44,49,50	0
27	PL9	d	405	55/55	0.89	0.13	29,37,50,55	0
33	DGD	C	517	62/66	0.89	0.13	36,50,69,82	0
25	CLA	c	511	65/65	0.90	0.12	39,54,62,66	0
25	CLA	c	512	65/65	0.90	0.13	44,57,65,68	0
32	UNL	B	625	16/-	0.90	0.12	37,42,49,50	0
23	LMG	d	408	51/55	0.90	0.14	35,49,72,80	0
32	UNL	k	101	9/-	0.90	0.13	44,52,56,56	0
25	CLA	C	510	65/65	0.90	0.11	36,46,58,68	0
32	UNL	C	520	15/-	0.90	0.12	31,42,47,47	0
27	PL9	D	407	55/55	0.90	0.13	21,37,44,47	0
30	SO4	U	201	5/5	0.90	0.10	47,60,63,71	5
29	LHG	a	615	49/49	0.90	0.12	32,42,53,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	DGD	c	516	62/66	0.90	0.14	32,46,78,87	0
25	CLA	C	502	65/65	0.91	0.10	35,43,48,50	0
26	BCR	A	609	40/40	0.91	0.10	24,34,39,40	0
26	BCR	B	618	40/40	0.91	0.10	23,35,48,50	0
23	LMG	D	409	51/55	0.91	0.14	31,48,74,83	0
29	LHG	L	102	49/49	0.91	0.11	27,39,46,50	0
25	CLA	C	508	65/65	0.91	0.12	36,43,79,88	0
26	BCR	C	515	40/40	0.91	0.12	30,40,50,54	0
29	LHG	d	406	49/49	0.91	0.11	25,41,48,53	0
25	CLA	b	614	65/65	0.91	0.11	25,38,57,65	0
29	LHG	l	101	49/49	0.91	0.11	28,39,50,53	0
25	CLA	c	503	65/65	0.91	0.10	33,43,50,57	0
25	CLA	B	614	65/65	0.91	0.11	27,36,57,61	0
25	CLA	B	616	65/65	0.91	0.13	26,36,78,87	0
26	BCR	T	101	40/40	0.91	0.12	30,41,48,50	0
26	BCR	a	611	40/40	0.91	0.10	26,35,41,44	0
26	BCR	b	617	40/40	0.91	0.11	31,41,48,51	0
33	DGD	C	518	62/66	0.91	0.13	30,46,63,70	0
26	BCR	b	619	40/40	0.91	0.12	35,44,50,54	0
33	DGD	h	102	62/66	0.91	0.12	35,44,51,56	0
25	CLA	c	508	65/65	0.92	0.12	35,44,73,77	0
25	CLA	c	509	65/65	0.92	0.11	32,45,56,61	0
25	CLA	c	510	65/65	0.92	0.11	41,46,53,57	0
25	CLA	a	608	65/65	0.92	0.12	28,36,75,85	0
25	CLA	C	504	65/65	0.92	0.11	35,49,67,75	0
25	CLA	b	606	65/65	0.92	0.10	24,35,55,62	0
26	BCR	b	618	40/40	0.92	0.10	27,36,41,48	0
25	CLA	d	403	65/65	0.92	0.12	28,39,77,85	0
25	CLA	C	509	65/65	0.92	0.10	35,43,55,60	0
25	CLA	b	615	65/65	0.92	0.10	31,39,49,52	0
29	LHG	A	613	49/49	0.92	0.12	21,37,47,56	0
25	CLA	b	616	65/65	0.92	0.11	28,42,62,69	0
25	CLA	C	505	65/65	0.92	0.11	29,39,49,57	0
25	CLA	c	504	65/65	0.92	0.12	35,42,61,74	0
33	DGD	H	102	62/66	0.92	0.10	27,36,47,58	0
31	BCT	A	616	4/4	0.92	0.11	28,33,33,38	0
33	DGD	c	517	62/66	0.92	0.12	33,45,66,77	0
25	CLA	c	507	65/65	0.92	0.11	31,41,50,52	0
34	PHO	d	402	64/64	0.92	0.10	29,40,48,54	0
25	CLA	c	501	65/65	0.93	0.09	27,39,45,54	0
25	CLA	c	502	65/65	0.93	0.09	31,41,49,55	0
25	CLA	a	607	65/65	0.93	0.10	22,30,37,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	609	65/65	0.93	0.10	28,36,43,52	0
25	CLA	c	505	65/65	0.93	0.10	32,40,48,51	0
25	CLA	c	506	65/65	0.93	0.11	35,44,66,73	0
25	CLA	B	606	65/65	0.93	0.10	25,33,57,62	0
25	CLA	b	604	65/65	0.93	0.10	23,34,50,58	0
25	CLA	B	615	65/65	0.93	0.10	28,36,47,55	0
25	CLA	b	610	65/65	0.93	0.10	23,35,45,48	0
25	CLA	b	611	65/65	0.93	0.10	23,36,45,48	0
25	CLA	b	612	65/65	0.93	0.10	24,34,43,48	0
25	CLA	B	608	65/65	0.93	0.09	21,32,41,47	0
26	BCR	c	514	40/40	0.93	0.11	26,42,50,53	0
32	UNL	X	101	10/-	0.93	0.14	36,38,40,40	0
25	CLA	C	506	65/65	0.93	0.10	32,41,67,71	0
25	CLA	C	507	65/65	0.93	0.11	26,41,51,57	0
34	PHO	D	402	64/64	0.93	0.09	24,33,41,49	0
34	PHO	a	609	64/64	0.93	0.09	24,30,39,42	0
26	BCR	B	617	40/40	0.93	0.09	32,38,44,47	0
25	CLA	A	607	65/65	0.94	0.11	23,36,71,74	0
25	CLA	b	608	65/65	0.94	0.10	28,40,49,56	0
25	CLA	b	609	65/65	0.94	0.10	28,41,55,60	0
25	CLA	A	606	65/65	0.94	0.09	19,29,35,47	0
25	CLA	B	602	65/65	0.94	0.10	21,34,47,50	0
25	CLA	B	610	65/65	0.94	0.09	20,29,37,40	0
25	CLA	b	613	65/65	0.94	0.09	21,29,52,58	0
25	CLA	D	403	65/65	0.94	0.09	23,30,39,49	0
33	DGD	C	516	62/66	0.94	0.11	25,35,67,72	0
25	CLA	D	405	65/65	0.94	0.11	24,35,63,68	0
25	CLA	a	606	65/65	0.94	0.08	19,30,40,48	0
29	LHG	D	408	49/49	0.94	0.10	20,36,45,51	0
33	DGD	c	515	62/66	0.94	0.12	26,37,70,73	0
25	CLA	B	612	65/65	0.94	0.08	25,31,40,44	0
25	CLA	B	603	65/65	0.94	0.09	21,31,48,53	0
25	CLA	B	604	65/65	0.94	0.09	20,32,50,65	0
25	CLA	b	602	65/65	0.94	0.09	29,41,55,60	0
25	CLA	b	603	65/65	0.94	0.10	24,36,50,60	0
25	CLA	B	605	65/65	0.94	0.08	21,30,37,42	0
35	HEM	E	102	43/43	0.94	0.13	42,53,68,74	0
35	HEM	e	101	43/43	0.94	0.12	49,57,69,72	0
25	CLA	C	501	65/65	0.95	0.08	21,34,46,51	0
25	CLA	B	611	65/65	0.95	0.08	19,27,39,42	0
25	CLA	b	605	65/65	0.95	0.09	24,33,42,47	0
34	PHO	D	401	64/64	0.95	0.08	24,30,36,39	0

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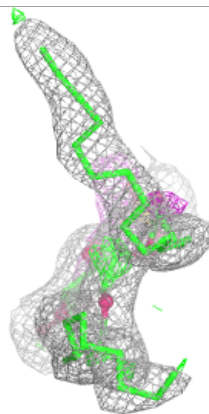
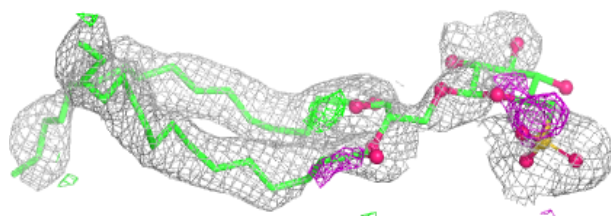
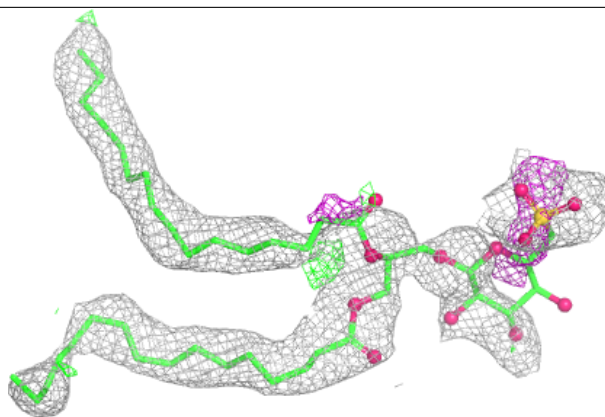
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	a	610	65/65	0.95	0.10	23,30,65,76	0
25	CLA	b	607	65/65	0.95	0.09	22,29,42,44	0
24	CL	a	604	1/1	0.95	0.09	40,40,40,40	0
25	CLA	d	401	65/65	0.95	0.08	20,30,45,53	0
25	CLA	B	613	65/65	0.95	0.08	21,30,50,60	0
36	HEC	v	201	43/43	0.95	0.10	29,39,47,55	0
25	CLA	D	404	65/65	0.96	0.08	18,28,40,43	0
25	CLA	B	607	65/65	0.96	0.09	19,28,53,54	0
24	CL	A	604	1/1	0.96	0.07	35,35,35,35	0
22	FE	a	602	1/1	0.96	0.06	37,37,37,37	0
36	HEC	V	201	43/43	0.96	0.10	31,38,46,48	0
25	CLA	A	608	65/65	0.96	0.10	14,27,68,74	0
21	OEX	A	601	10/10	0.98	0.06	34,40,52,57	0
24	CL	a	605	1/1	0.98	0.05	38,38,38,38	1
21	OEX	a	601	10/10	0.98	0.06	33,37,46,51	0
24	CL	A	605	1/1	0.99	0.02	26,26,26,26	0
22	FE	A	602	1/1	0.99	0.03	34,34,34,34	0

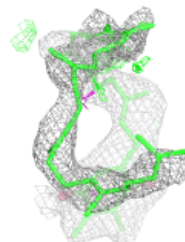
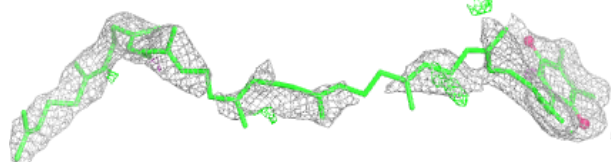
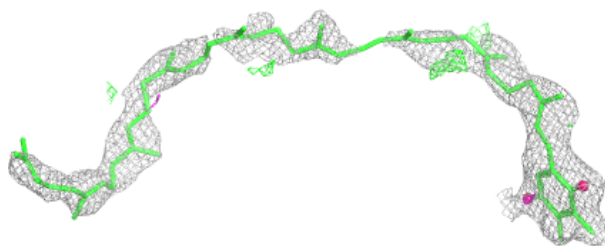
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SQD L 103:

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

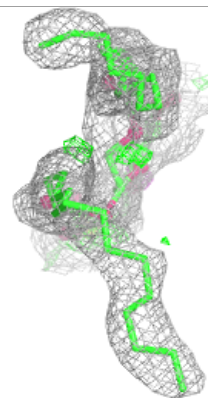
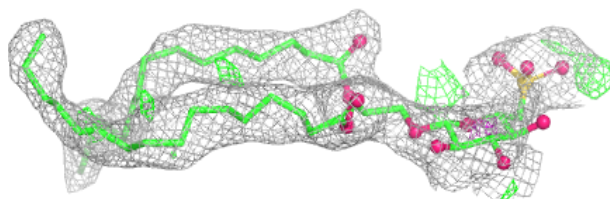
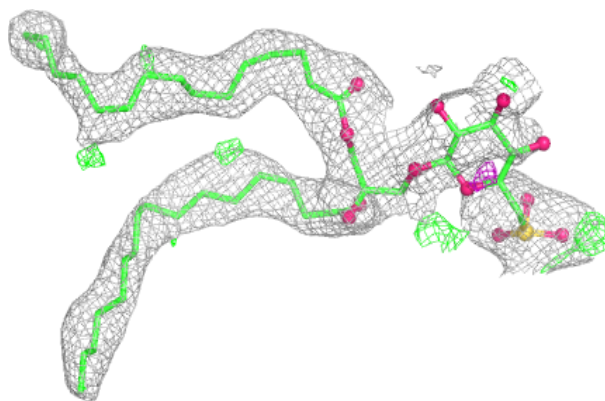
**Electron density around PL9 a 612:**

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

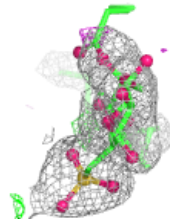
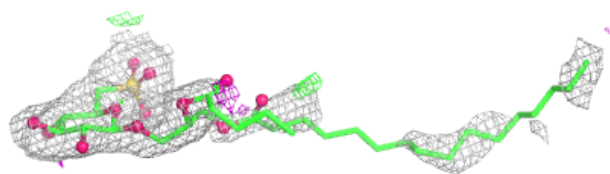
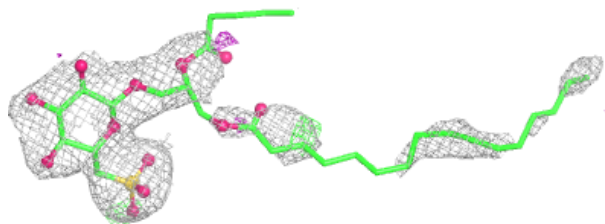


Electron density around SQD L 101:

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

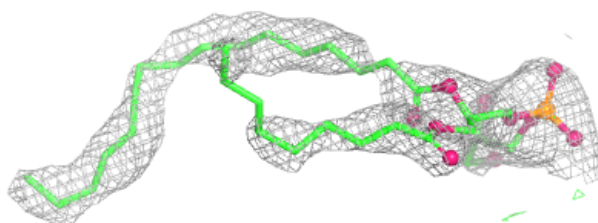
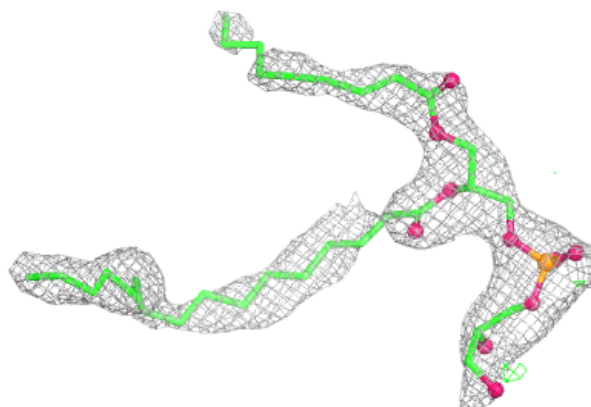
**Electron density around SQD f 101:**

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

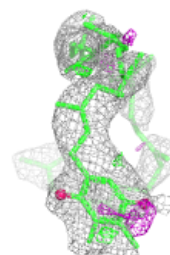
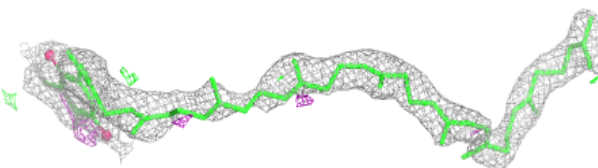
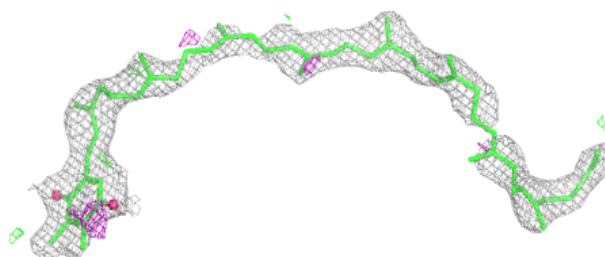


Electron density around LHG E 101:

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

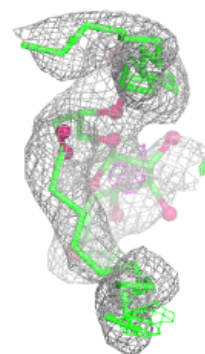
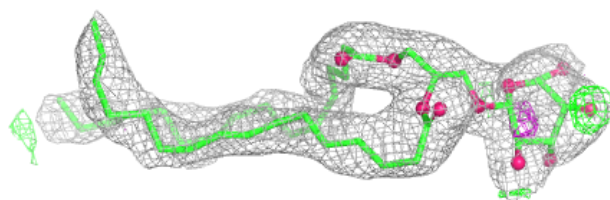
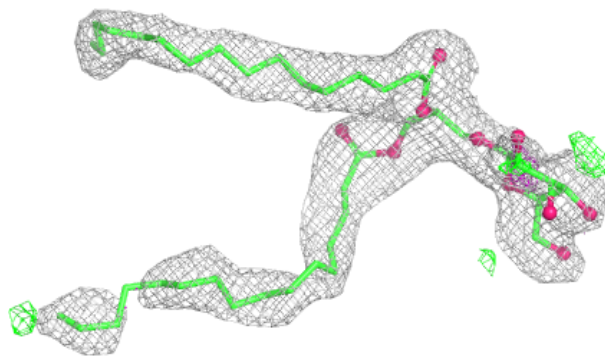
**Electron density around PL9 A 610:**

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

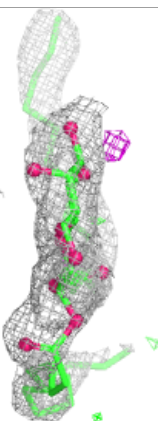
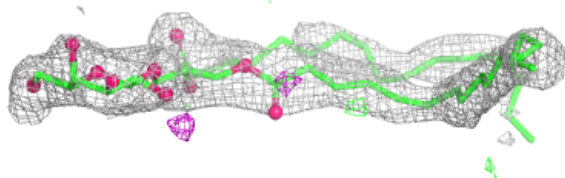
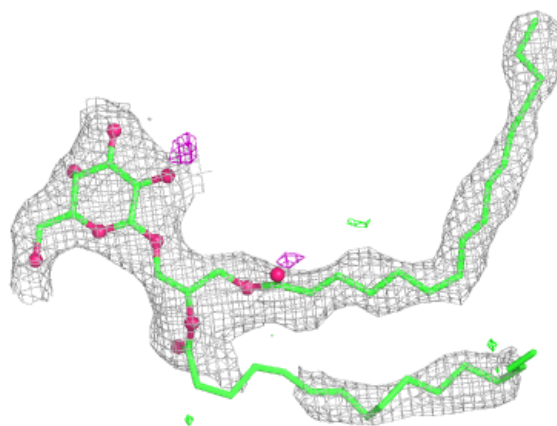


Electron density around LMG a 603:

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

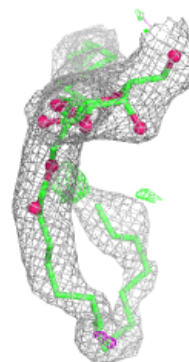
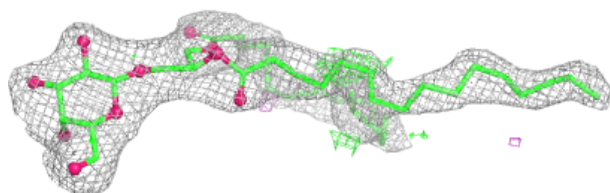
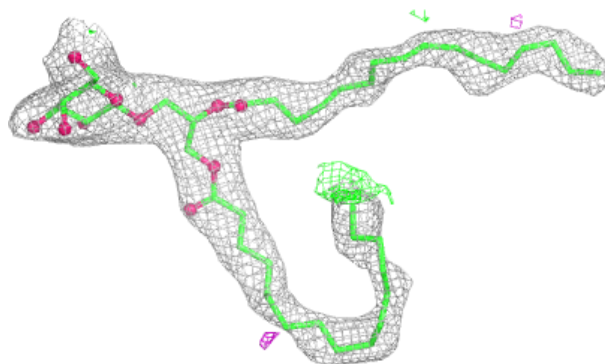
**Electron density around LMG C 519:**

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

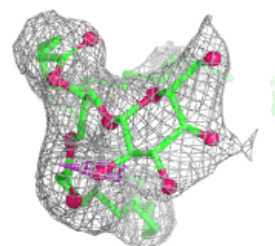
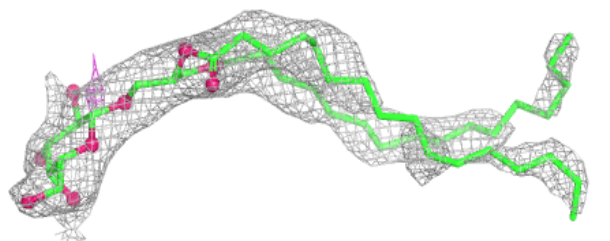
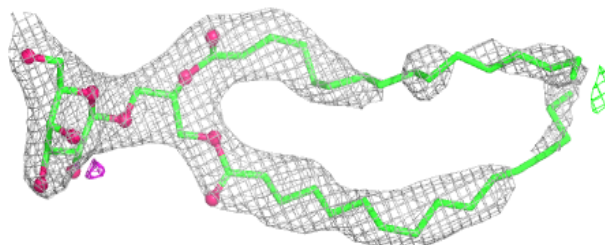


Electron density around LMG B 624:

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

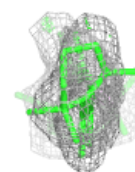
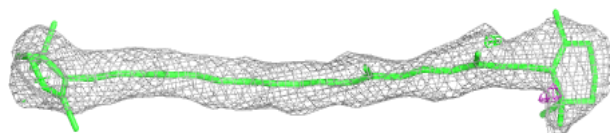
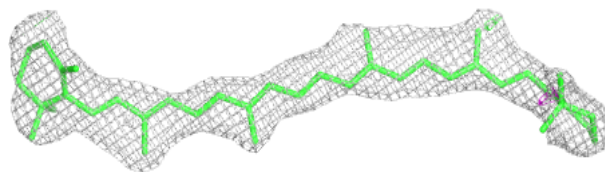
**Electron density around LMG b 624:**

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

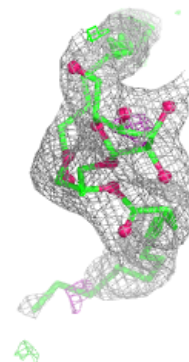
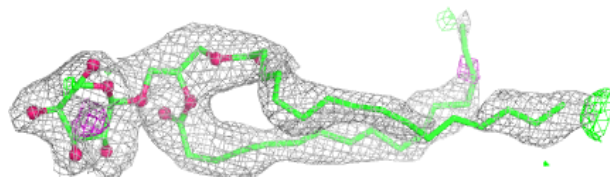
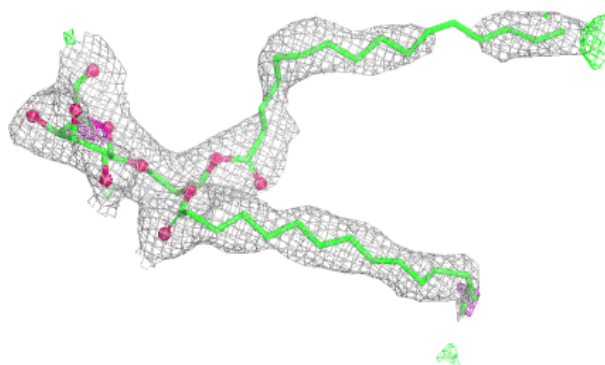


Electron density around BCR K 101:

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and green (positive)

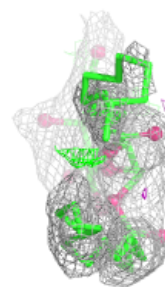
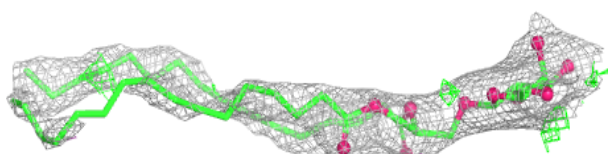
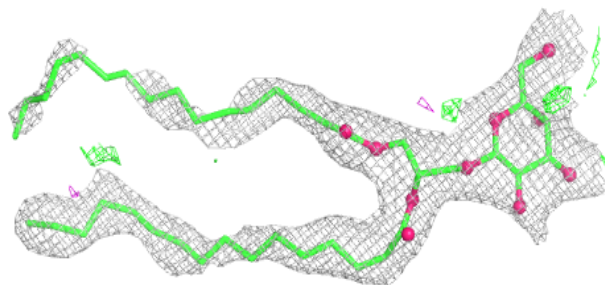
**Electron density around LMG A 603:**

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

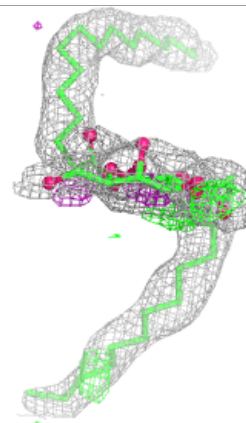
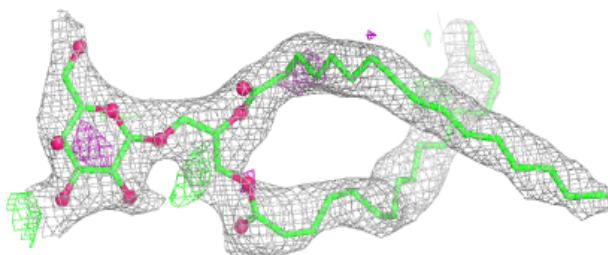
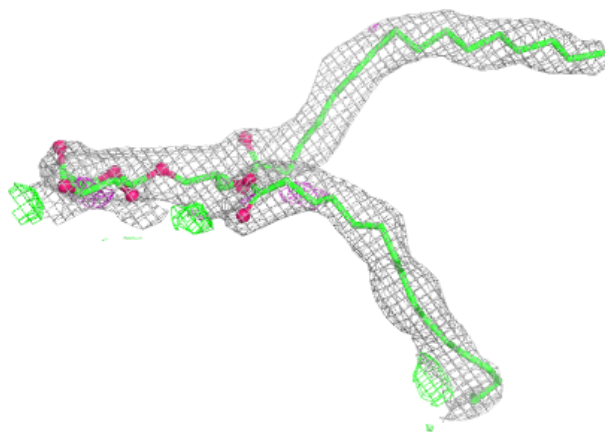


Electron density around LMG c 520:

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

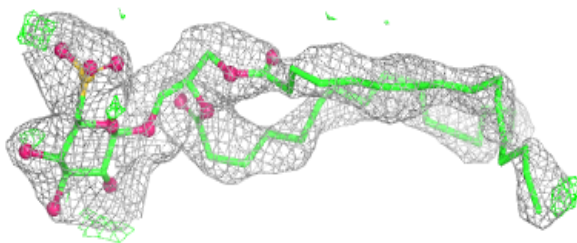
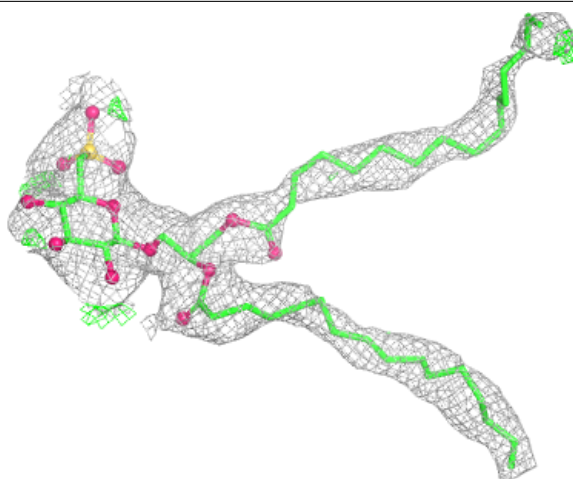
**Electron density around LMG B 620:**

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



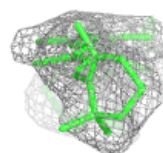
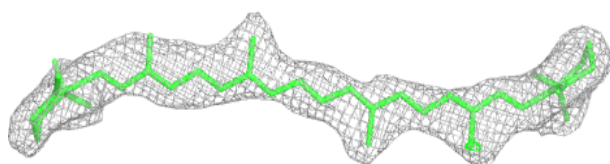
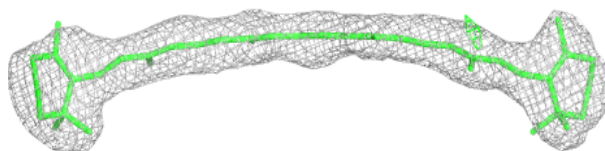
Electron density around SQD a 613:

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

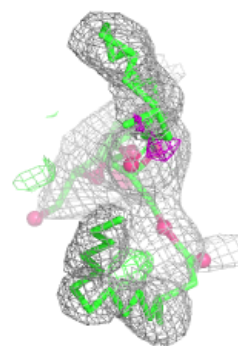
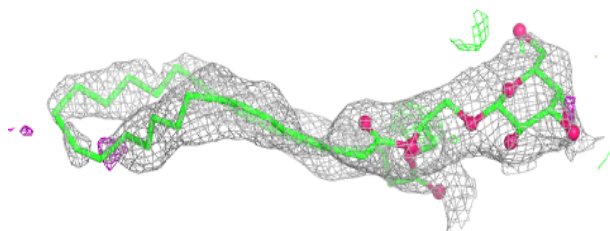
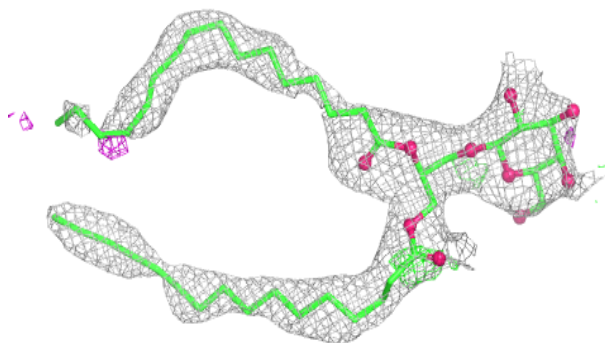


Electron density around BCR c 521:

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

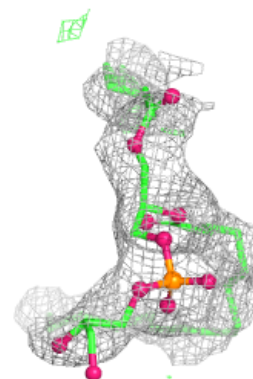
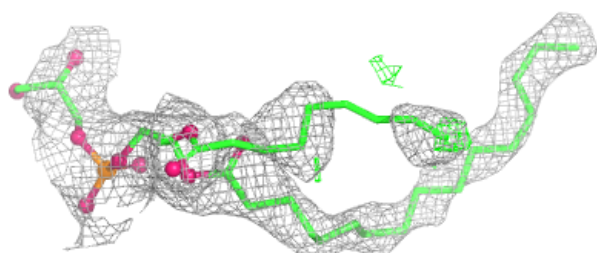
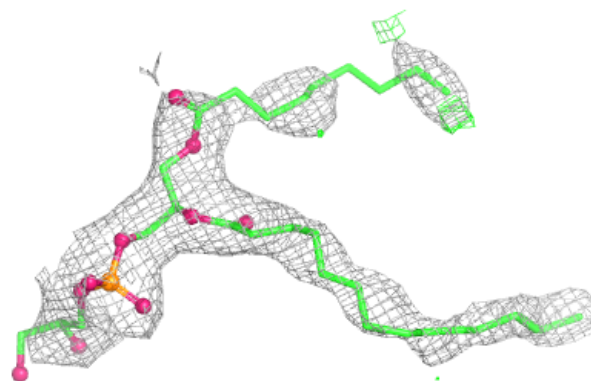
**Electron density around LMG a 614:**

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

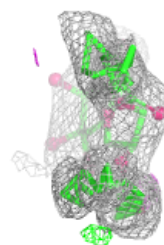
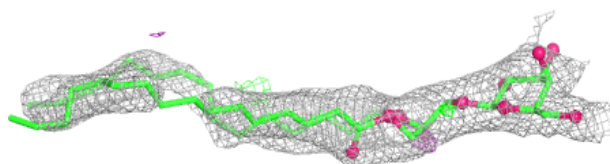
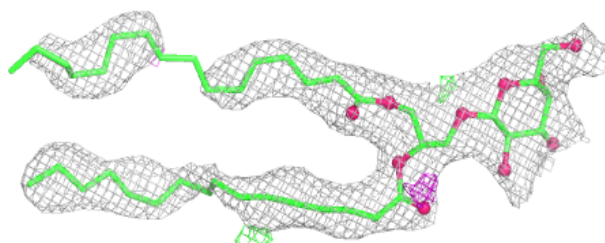


Electron density around LHG a 616:

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

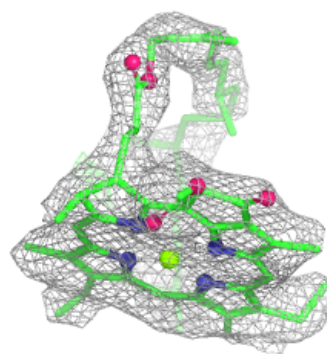
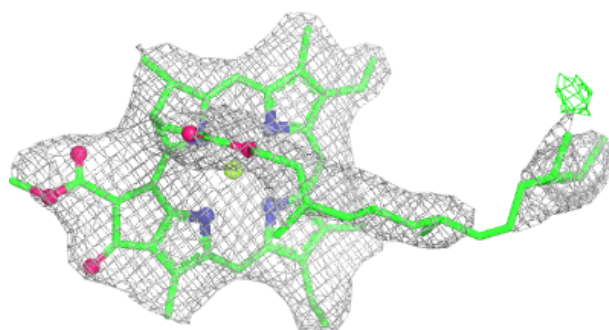
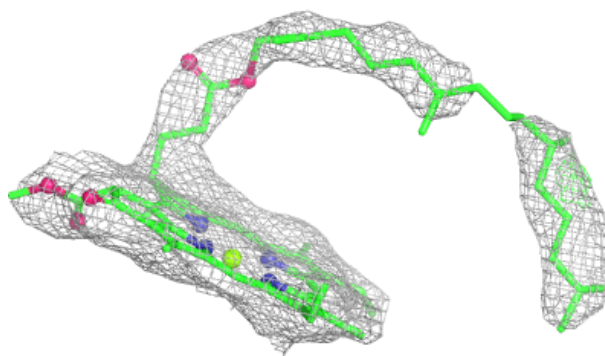
**Electron density around LMG C 521:**

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

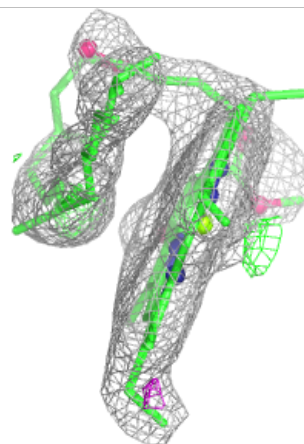
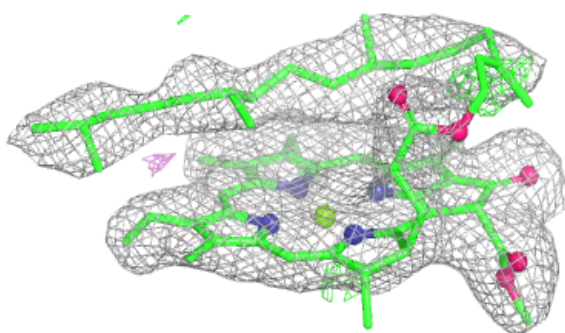
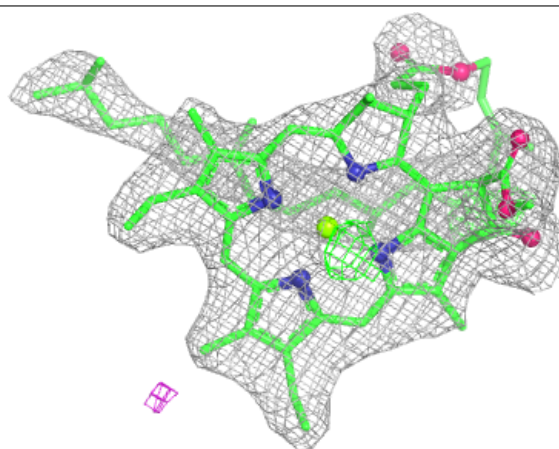


Electron density around CLA C 513:

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

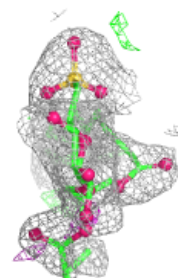
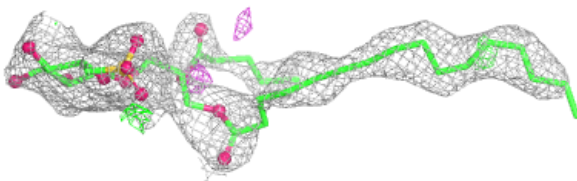
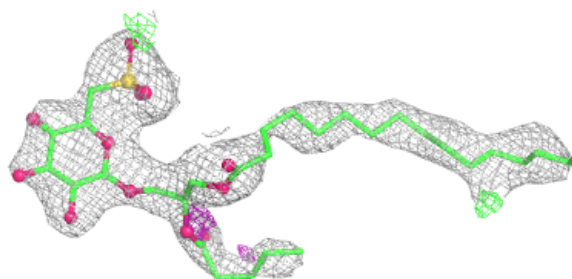
**Electron density around CLA b 601:**

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

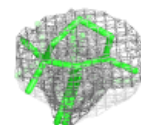
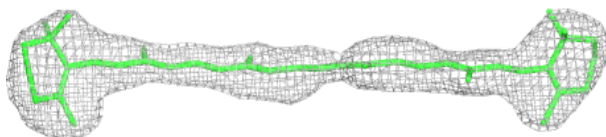
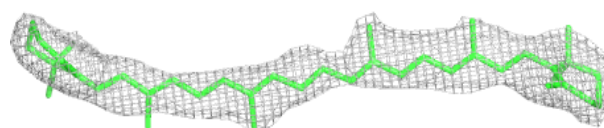


Electron density around SQD F 101:

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

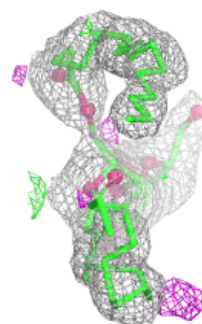
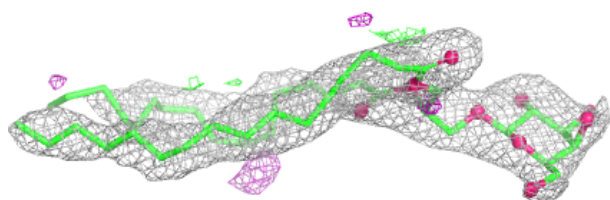
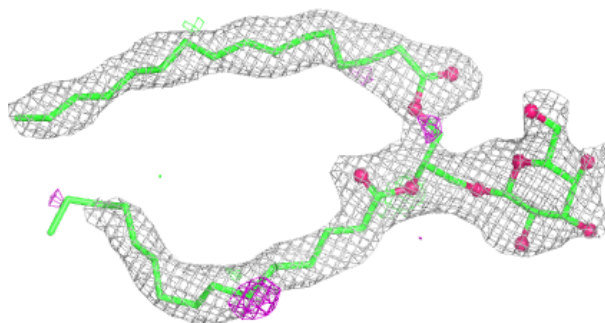
**Electron density around BCR C 514:**

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

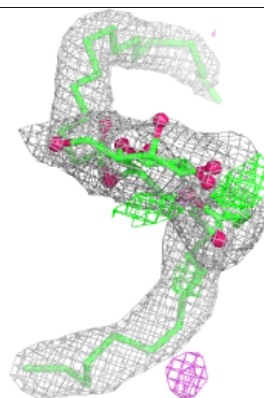
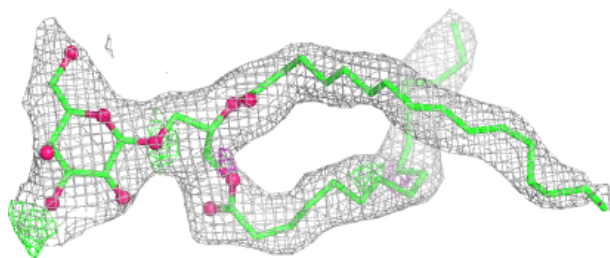
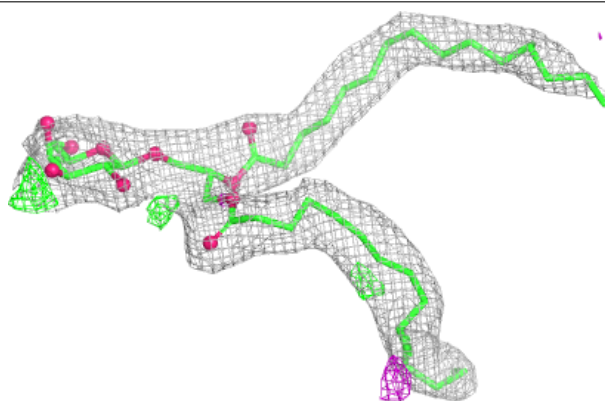


Electron density around LMG A 612:

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

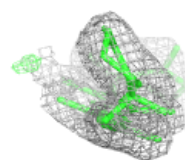
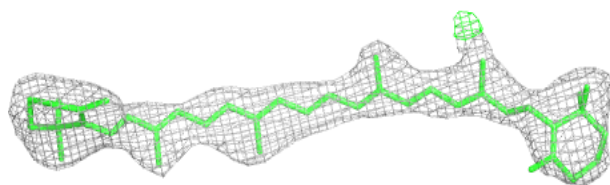
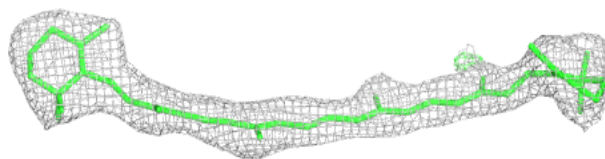
**Electron density around LMG b 620:**

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

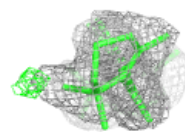
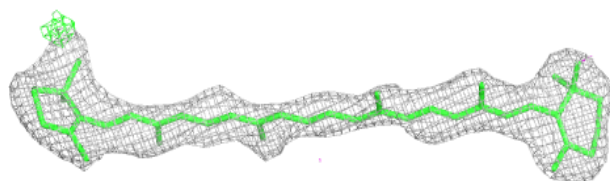
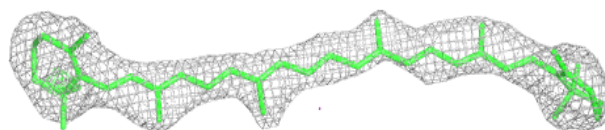


Electron density around BCR d 404:

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

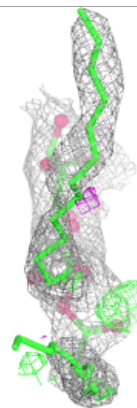
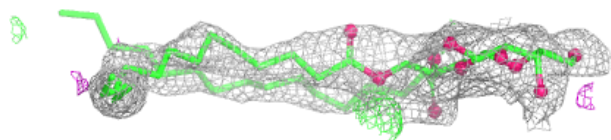
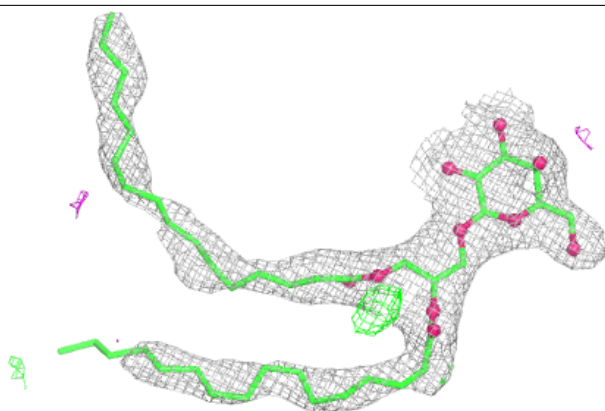
**Electron density around BCR z 101:**

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

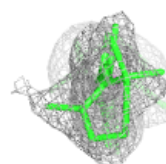
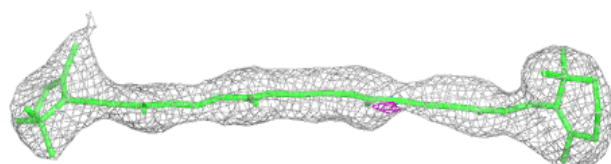


Electron density around LMG c 518:

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

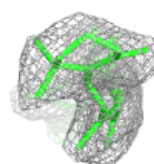
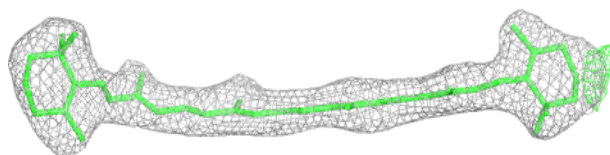
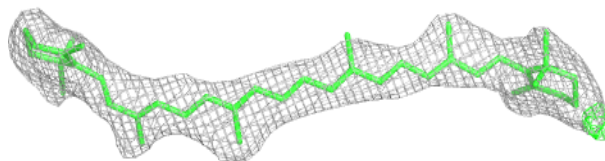
**Electron density around BCR k 102:**

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

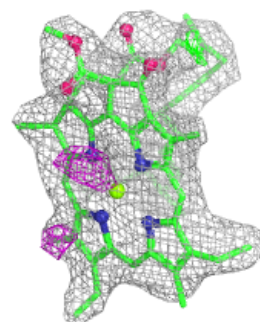
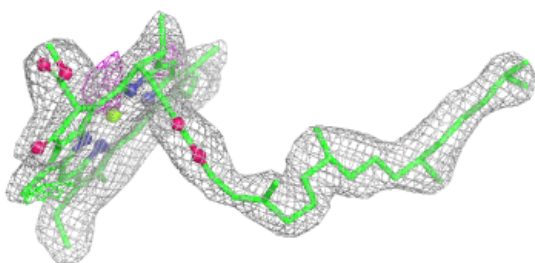
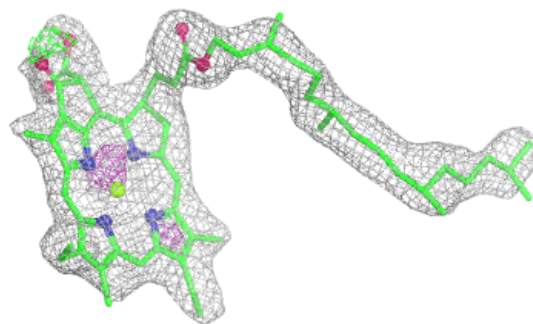


Electron density around BCR h 101:

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

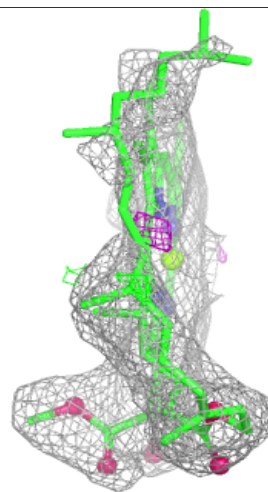
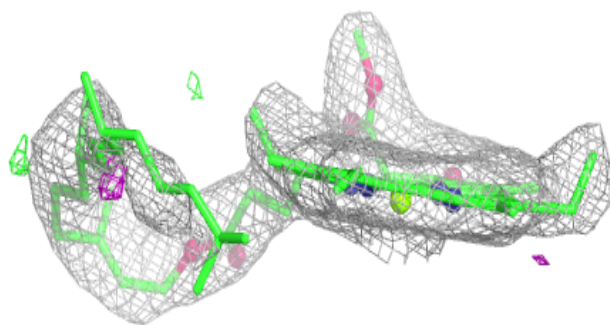
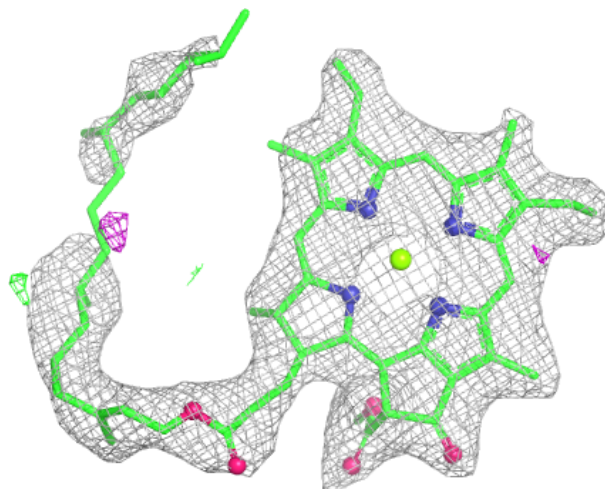
**Electron density around CLA C 511:**

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



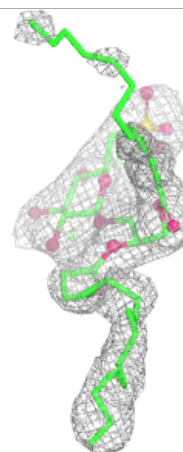
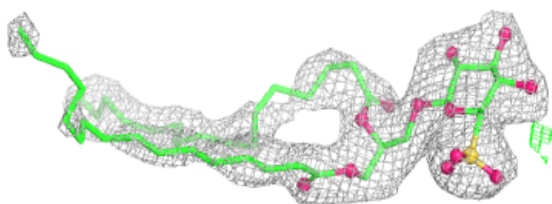
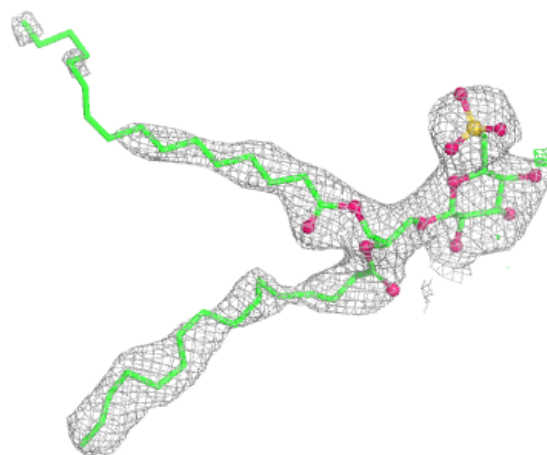
Electron density around CLA C 512:

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



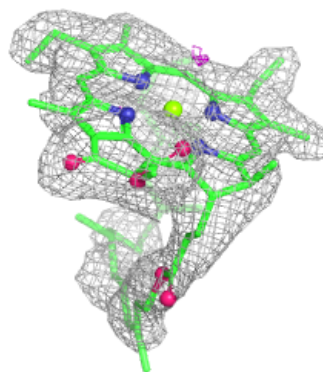
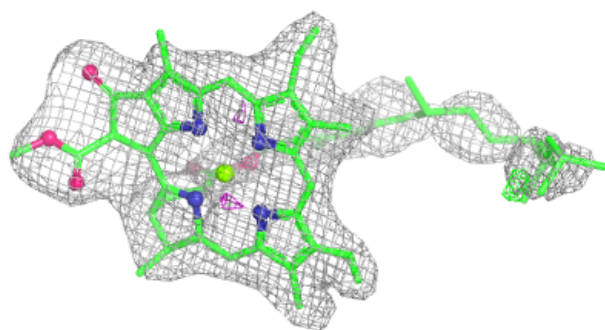
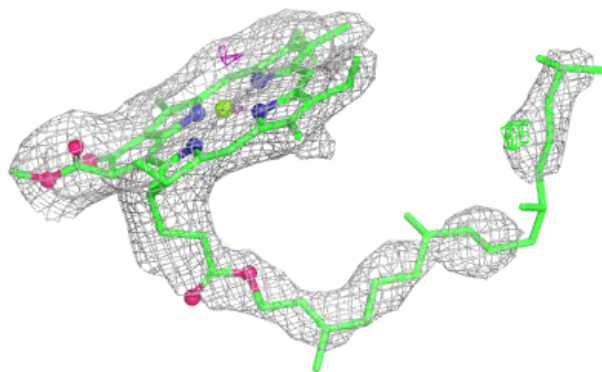
Electron density around SQD A 611:

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

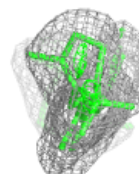
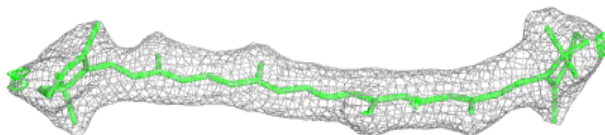
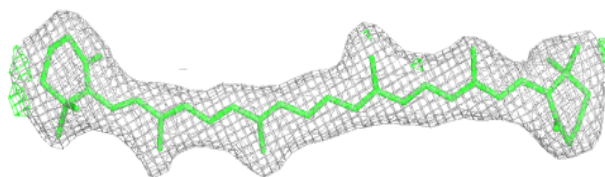


Electron density around CLA c 513:

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

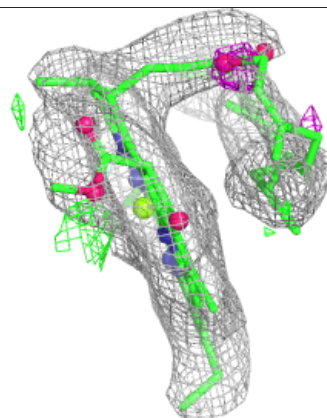
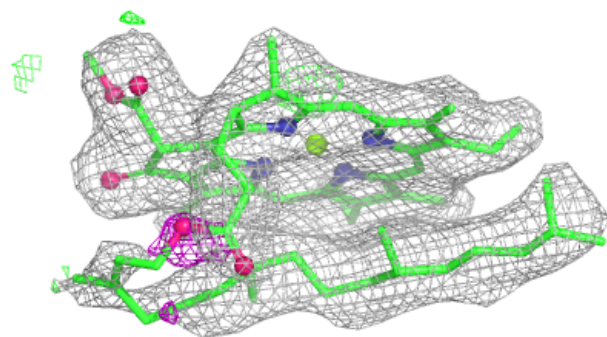
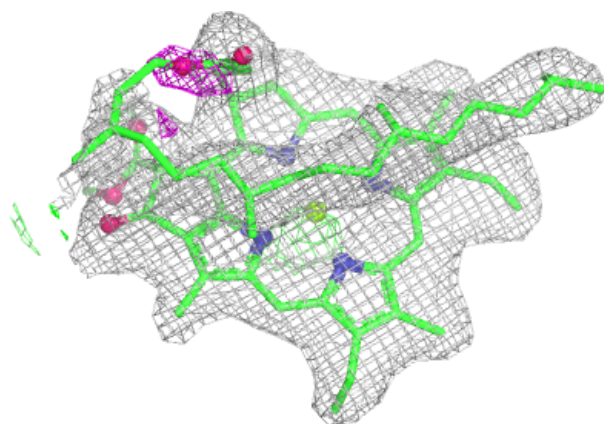
**Electron density around BCR B 619:**

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

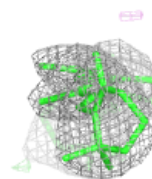
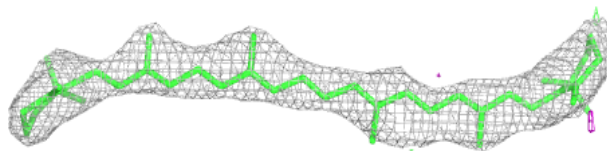
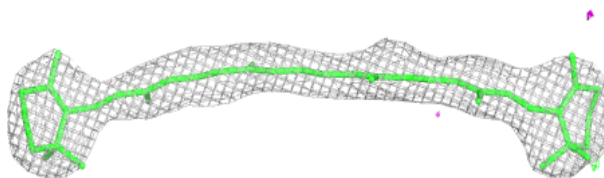


Electron density around CLA B 601:

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

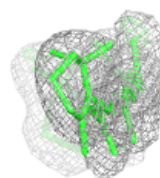
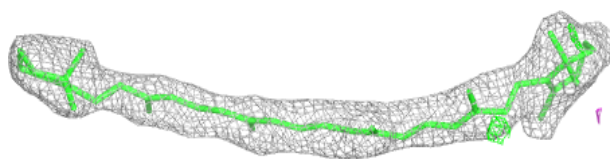
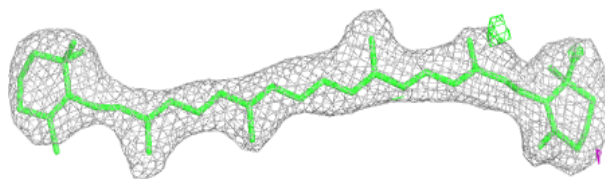
**Electron density around BCR C 522:**

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

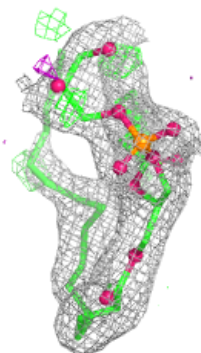
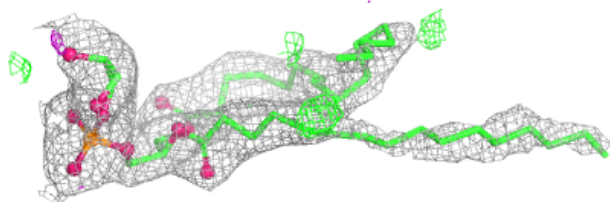
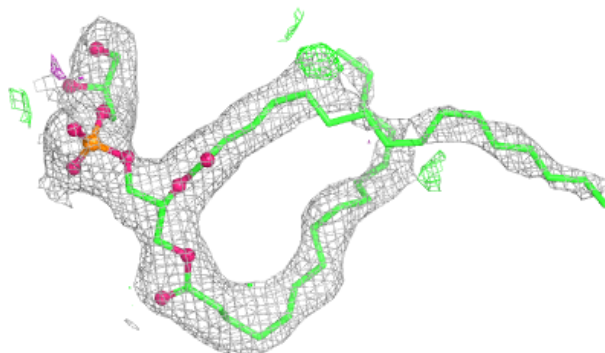


Electron density around BCR t 102:

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

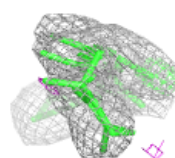
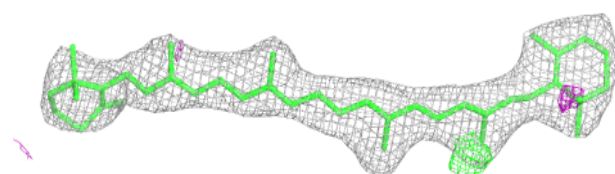
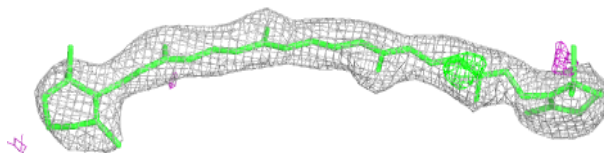
**Electron density around LHG A 614:**

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

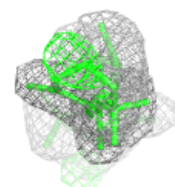
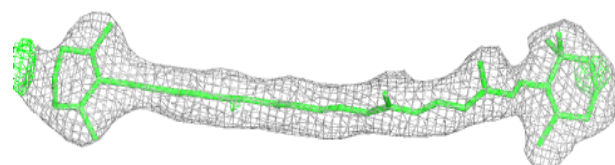
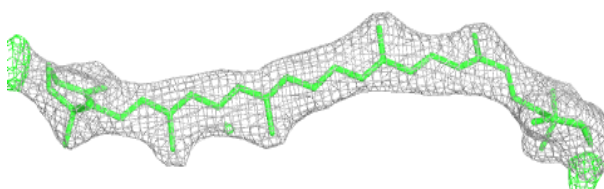


Electron density around BCR D 406:

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

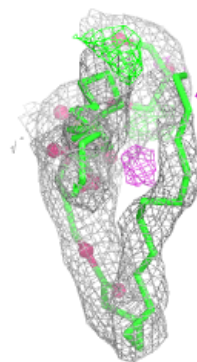
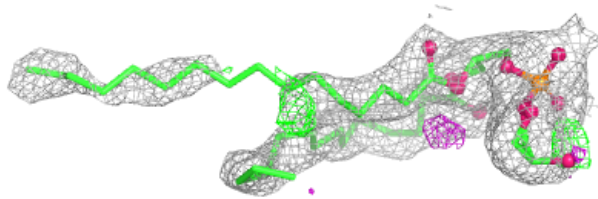
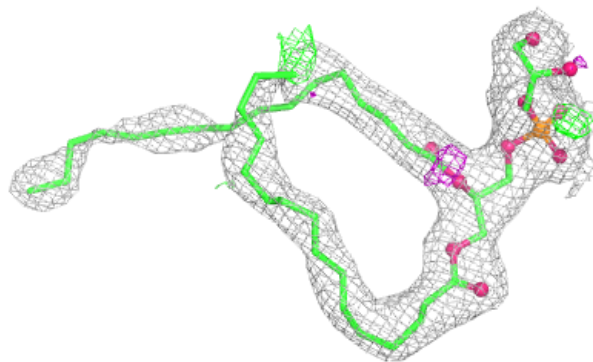
**Electron density around BCR H 101:**

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



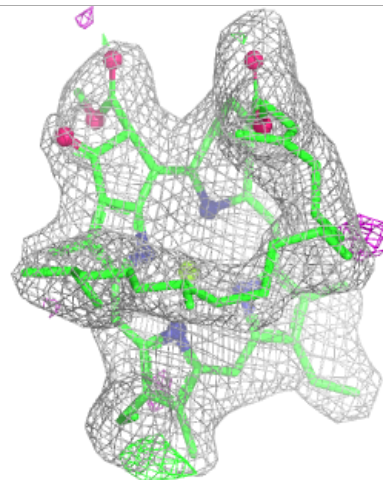
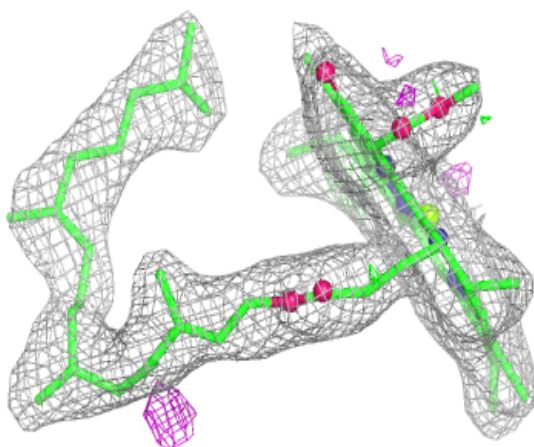
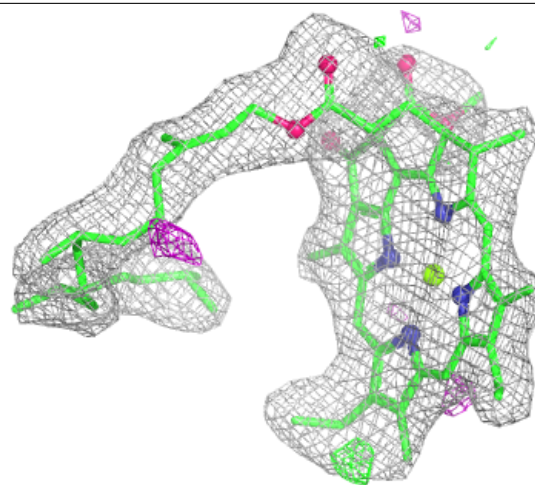
Electron density around LHG d 407:

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



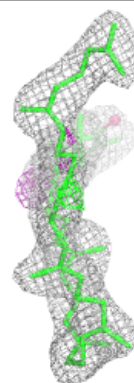
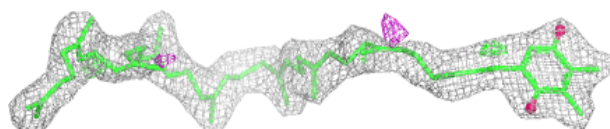
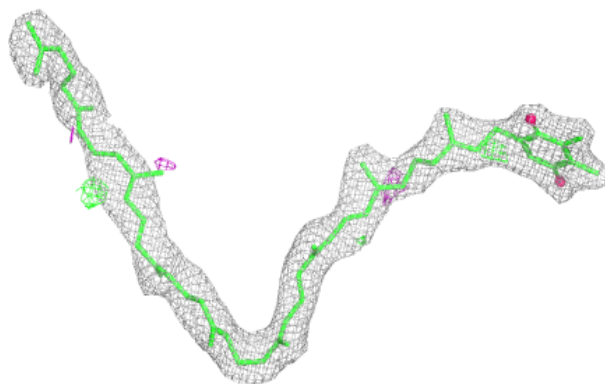
Electron density around CLA C 503:

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

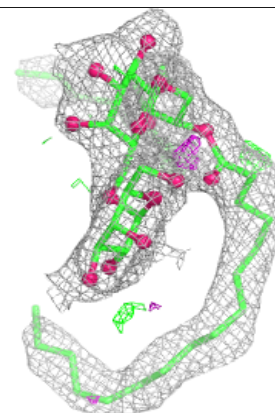
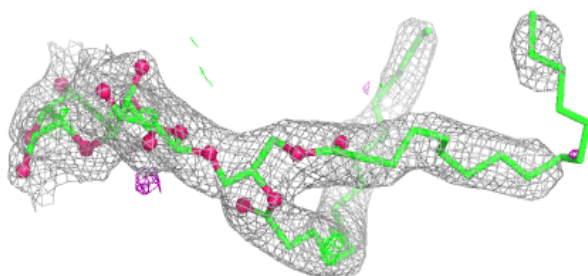
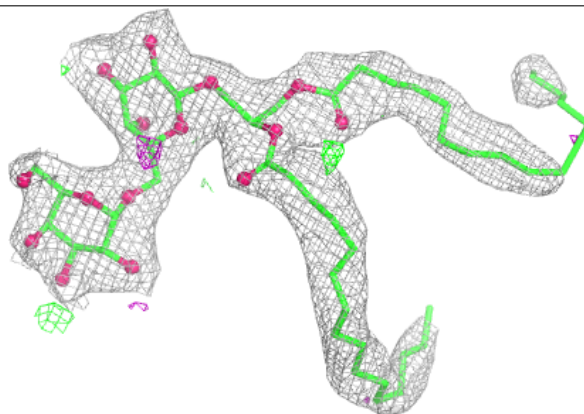


Electron density around PL9 d 405:

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

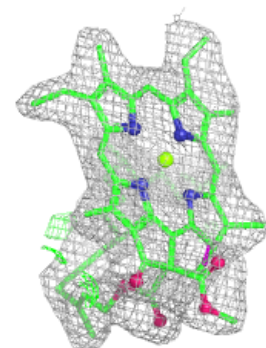
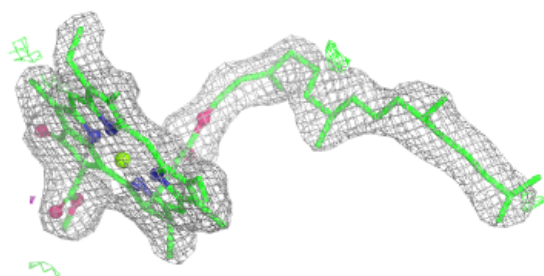
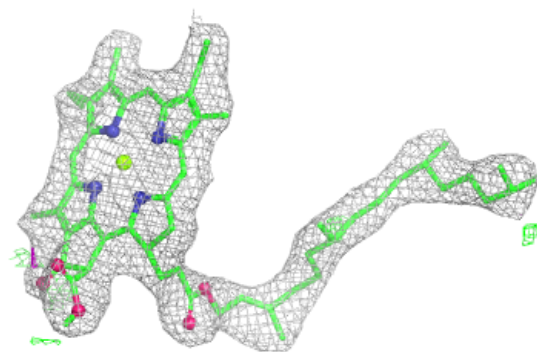
**Electron density around DGD C 517:**

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



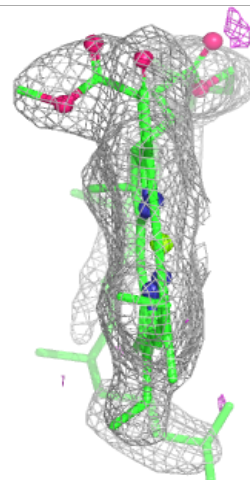
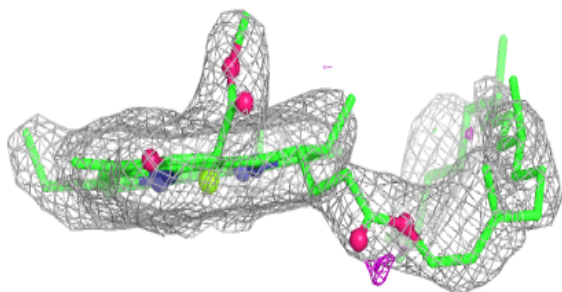
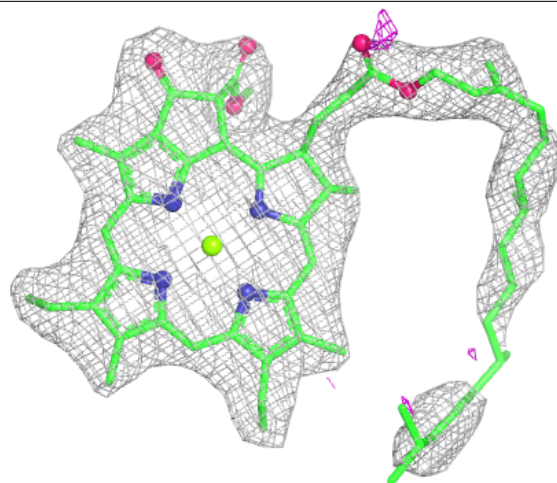
Electron density around CLA c 511:

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



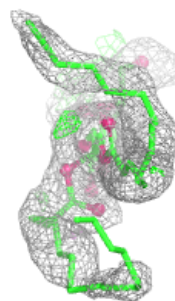
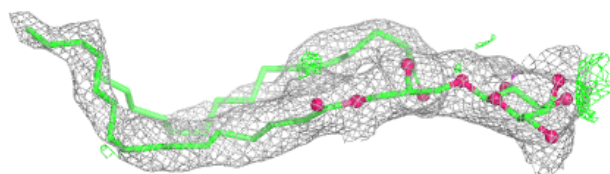
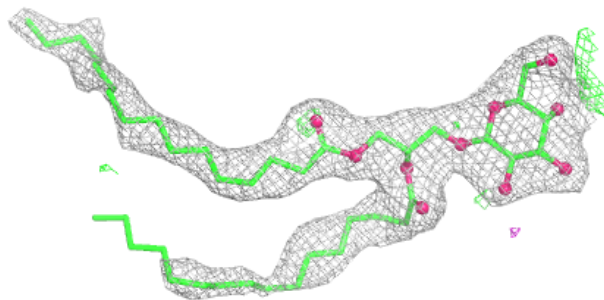
Electron density around CLA c 512:

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



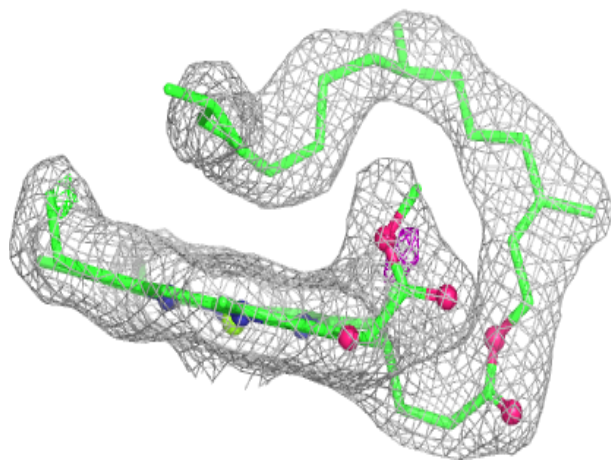
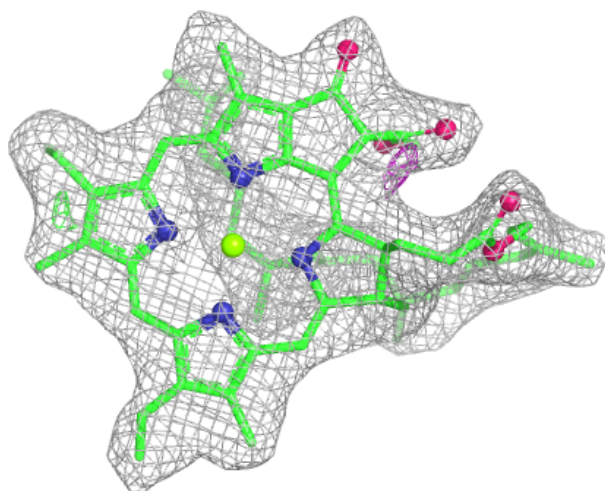
Electron density around LMG d 408:

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



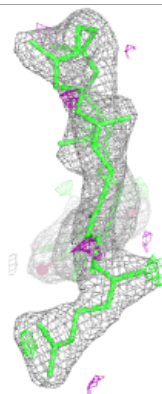
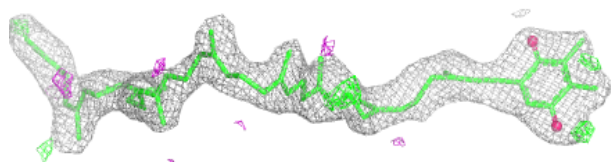
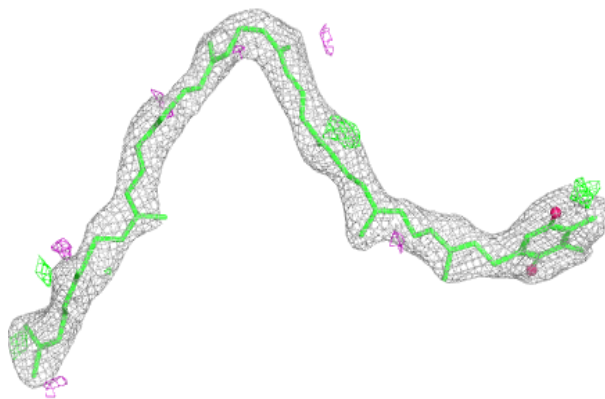
Electron density around CLA C 510:

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

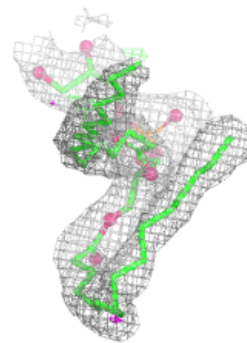
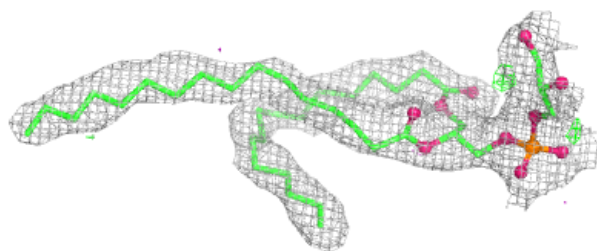
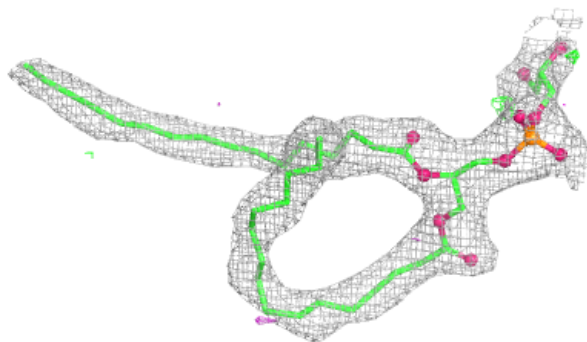


Electron density around PL9 D 407:

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

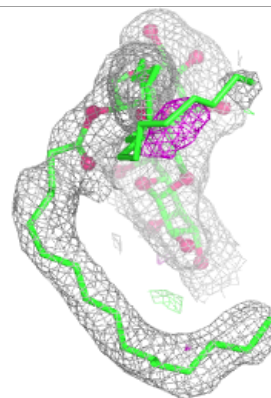
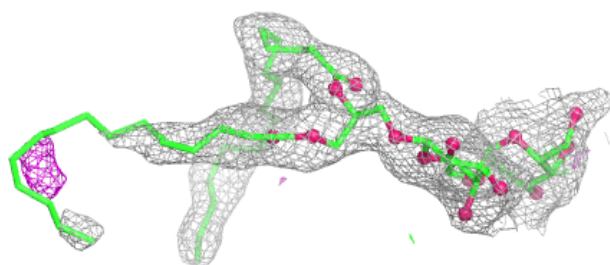
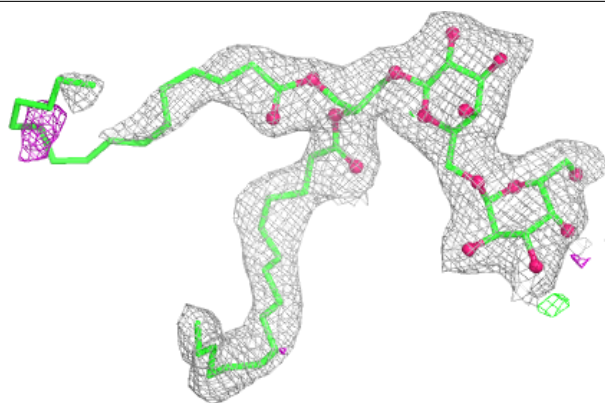
**Electron density around LHG a 615:**

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

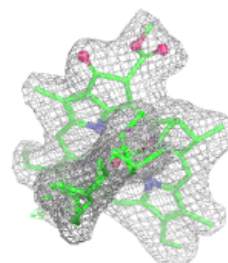
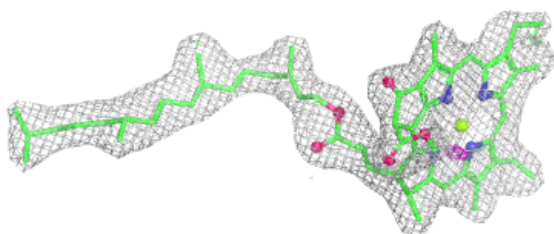
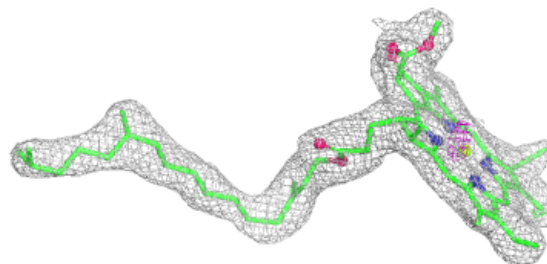


Electron density around DGD c 516:

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

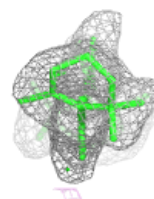
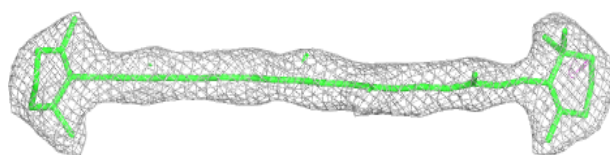
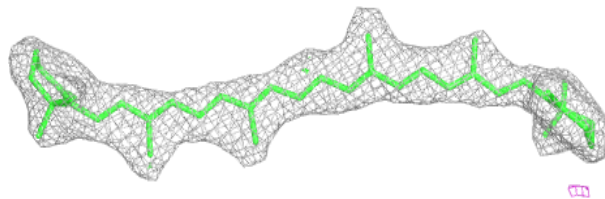
**Electron density around CLA C 502:**

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

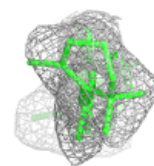
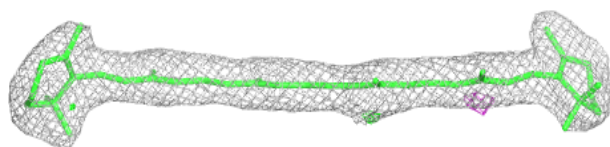
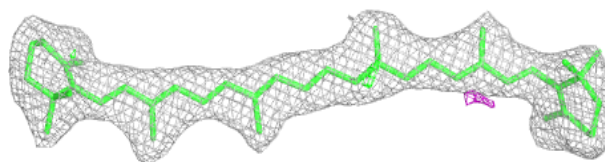


Electron density around BCR A 609:

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

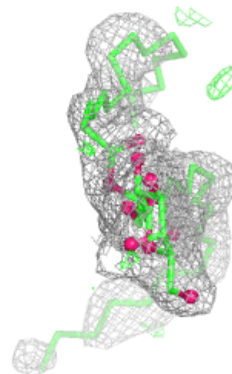
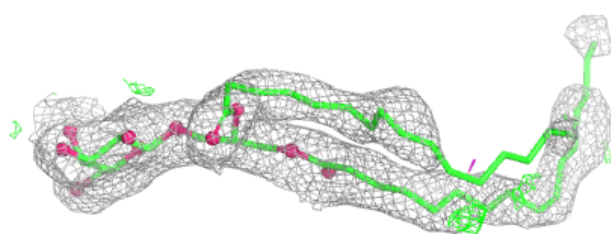
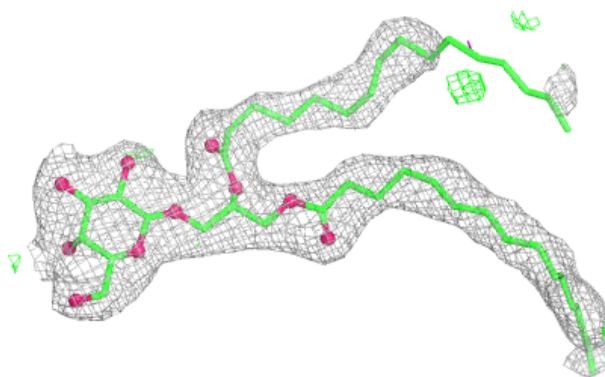
**Electron density around BCR B 618:**

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



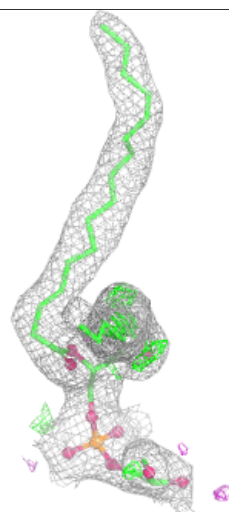
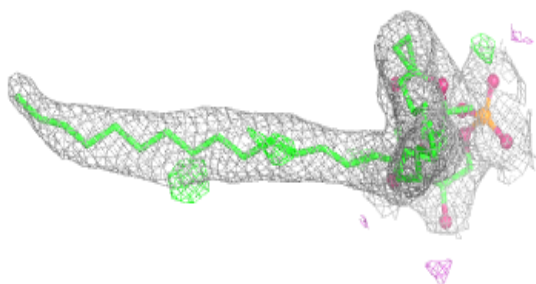
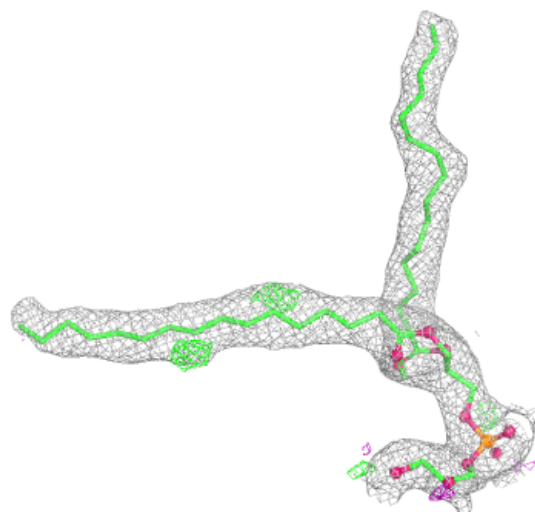
Electron density around LMG D 409:

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



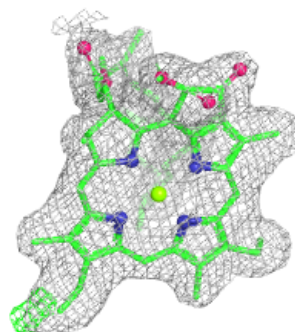
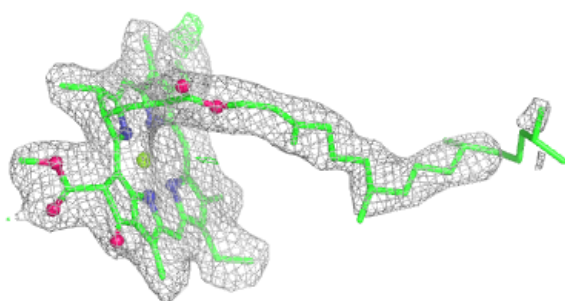
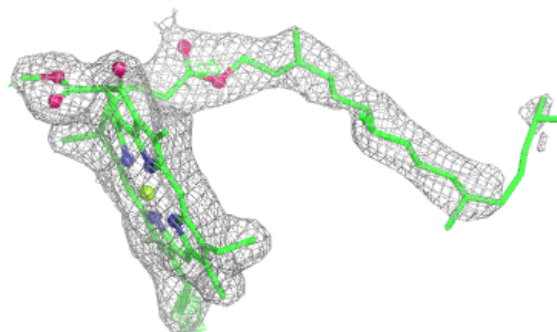
Electron density around LHG L 102:

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

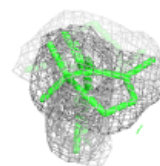
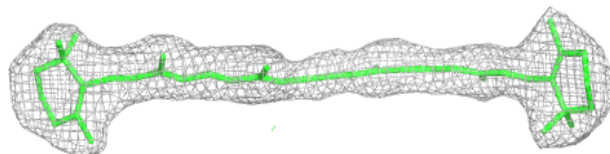
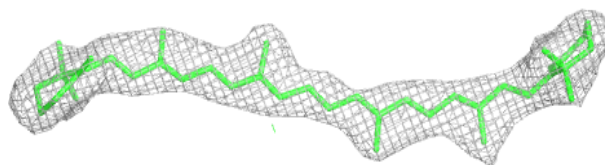


Electron density around CLA C 508:

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

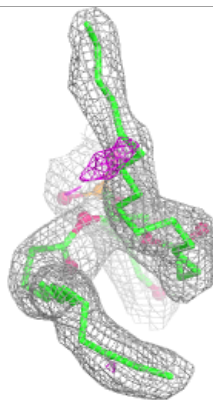
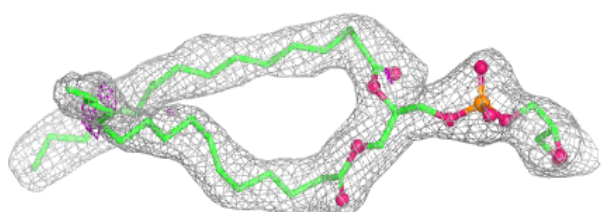
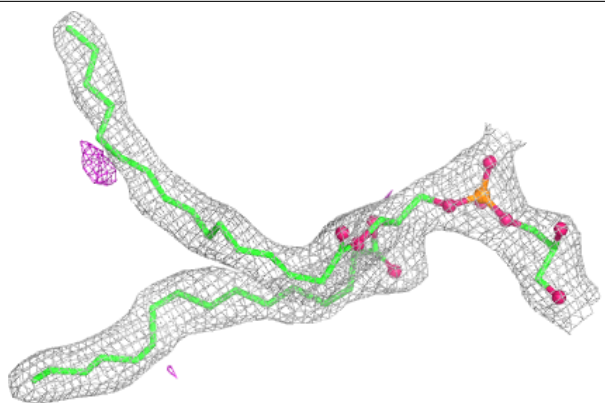
**Electron density around BCR C 515:**

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

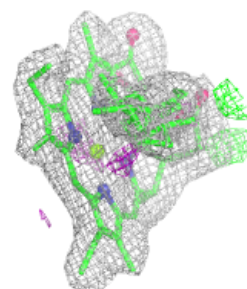
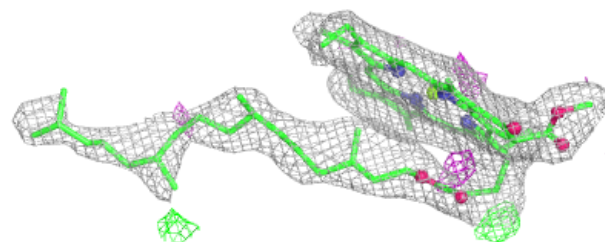
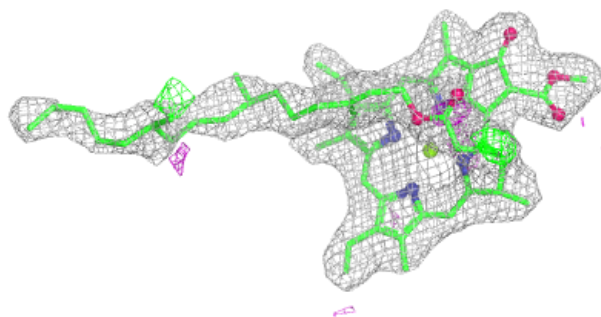


Electron density around LHG d 406:

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

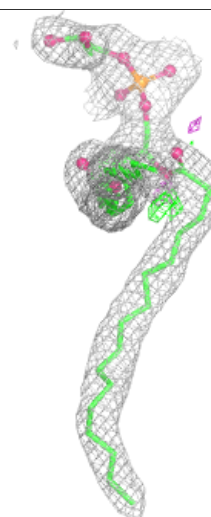
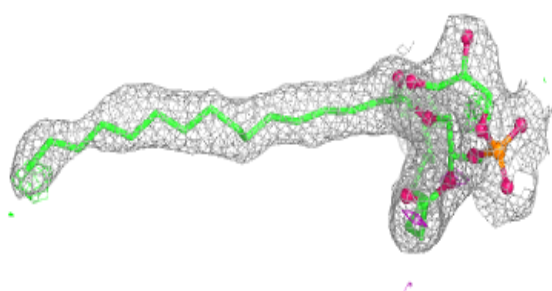
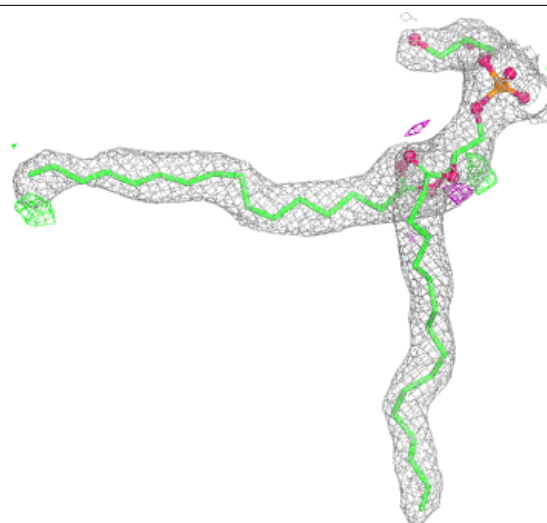
**Electron density around CLA b 614:**

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



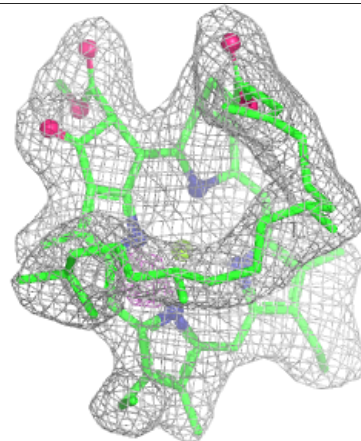
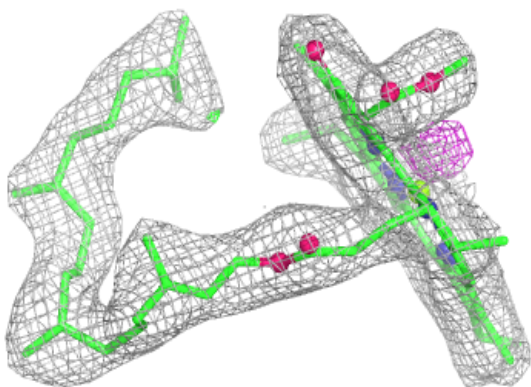
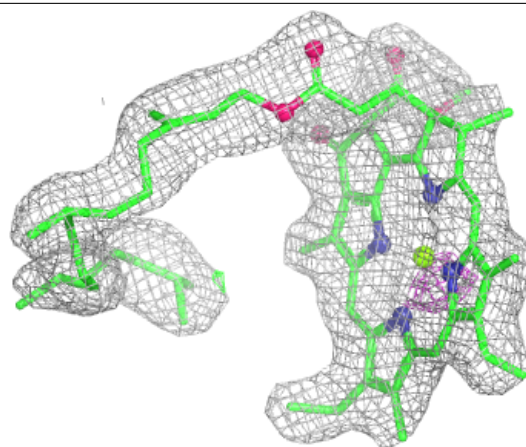
Electron density around LHG 1 101:

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

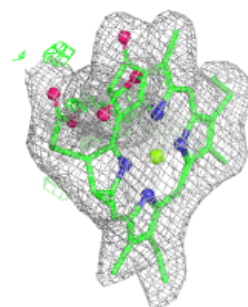
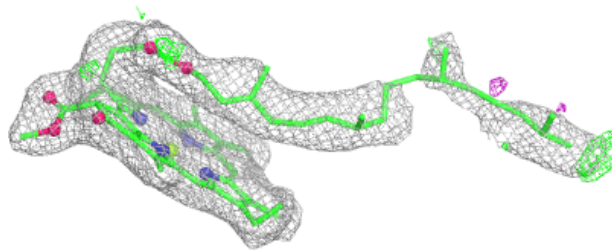
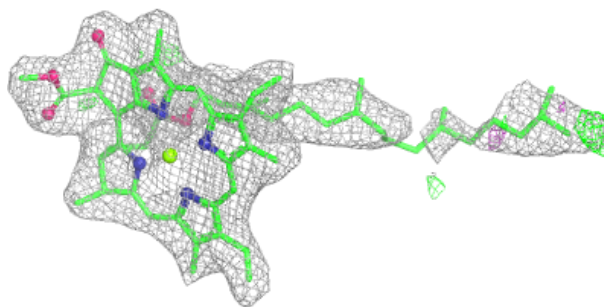


Electron density around CLA c 503:

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

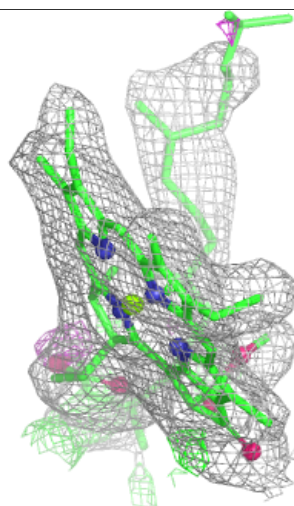
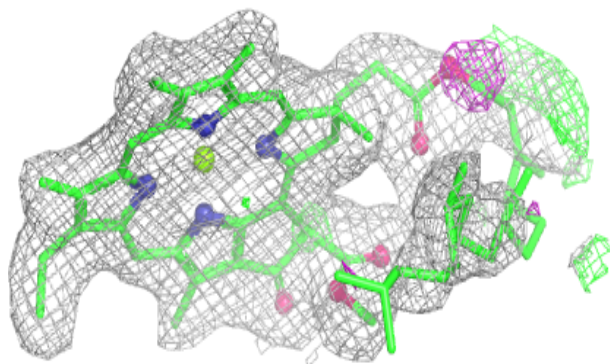
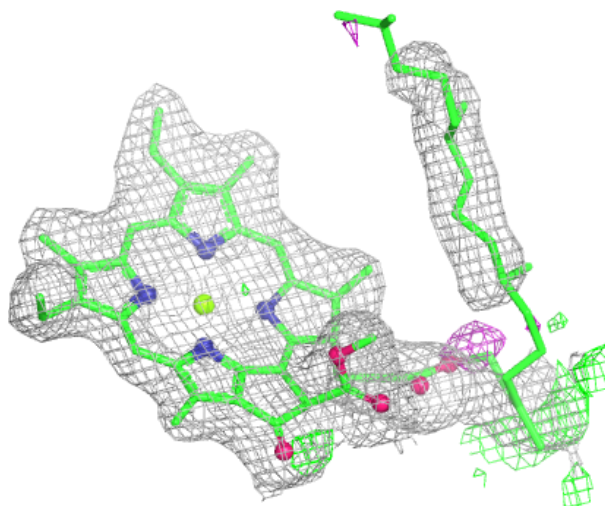
**Electron density around CLA B 614:**

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



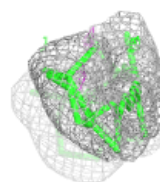
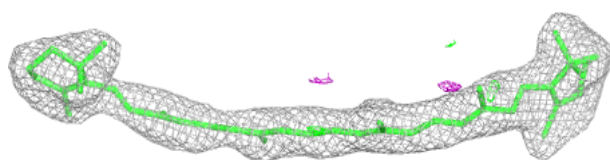
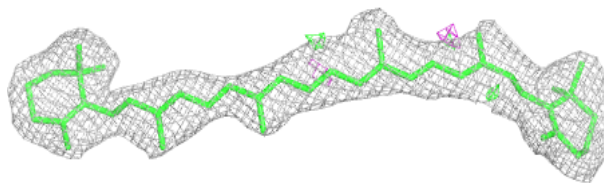
Electron density around CLA B 616:

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

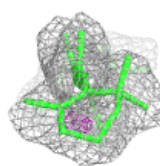
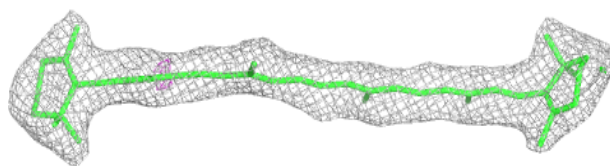
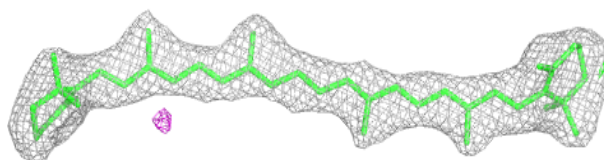


Electron density around BCR T 101:

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

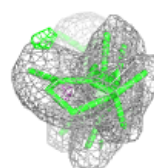
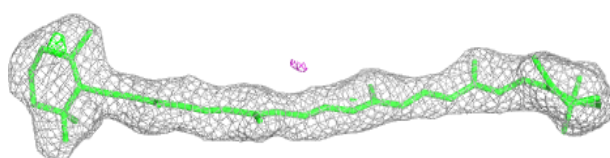
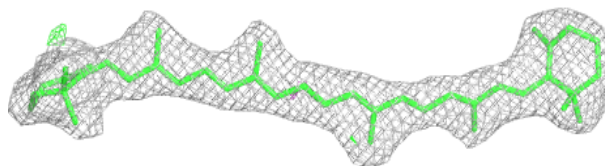
**Electron density around BCR a 611:**

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

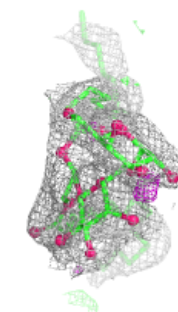
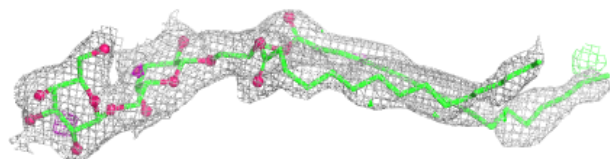
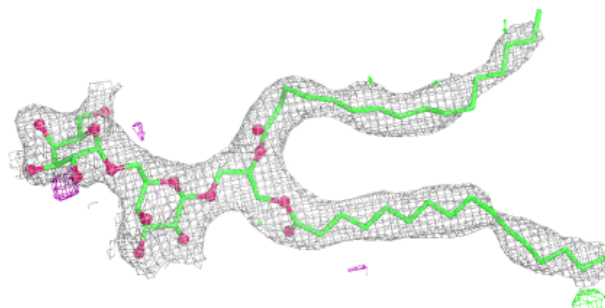


Electron density around BCR b 617:

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

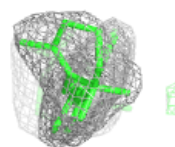
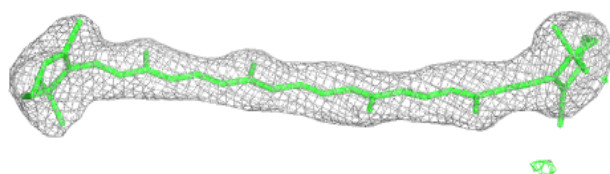
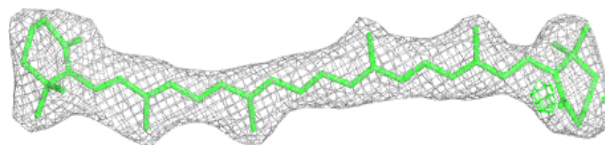
**Electron density around DGD C 518:**

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

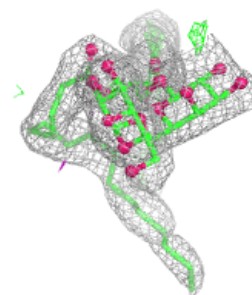
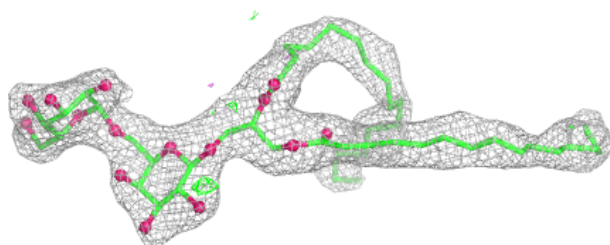
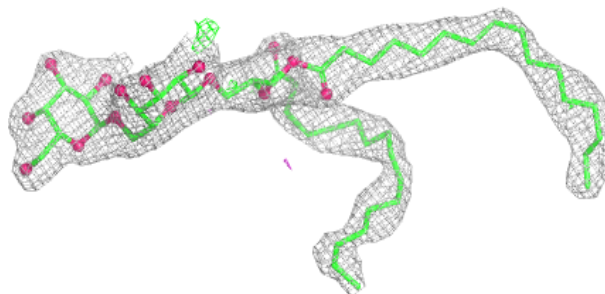


Electron density around BCR b 619:

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

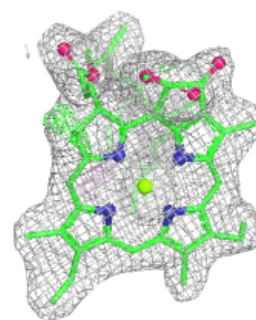
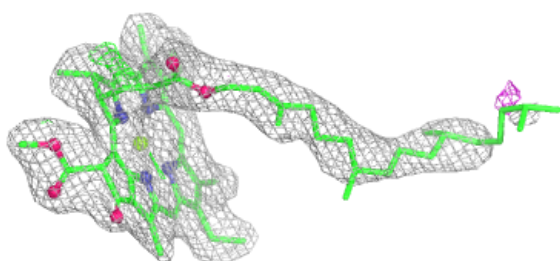
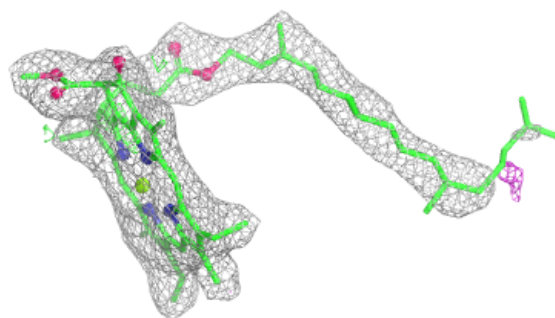
**Electron density around DGD h 102:**

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



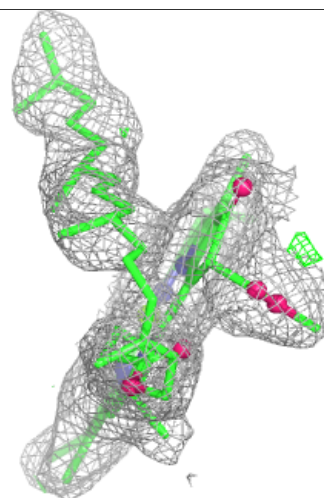
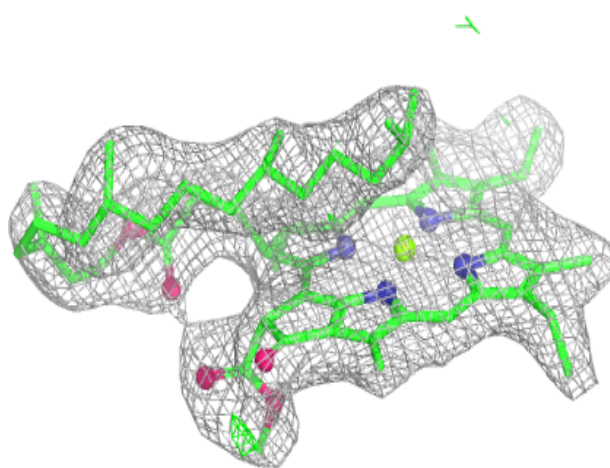
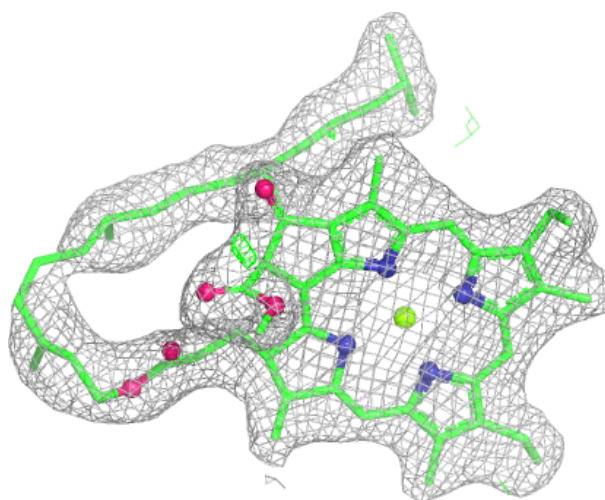
Electron density around CLA c 508:

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



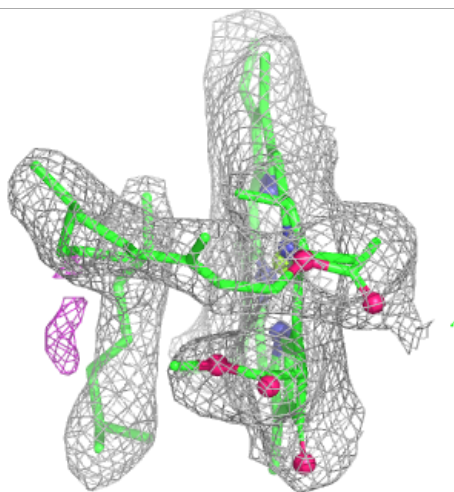
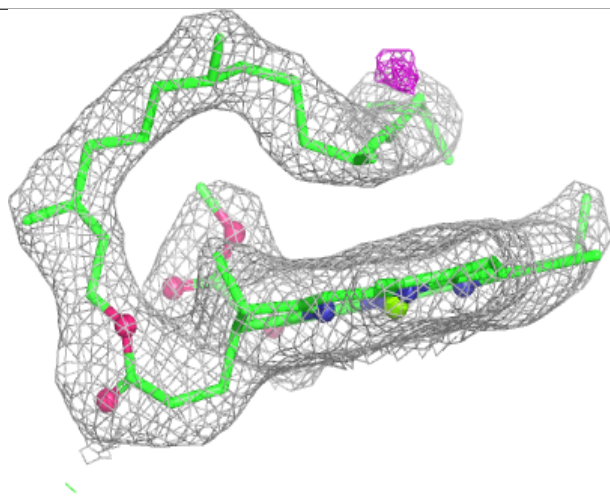
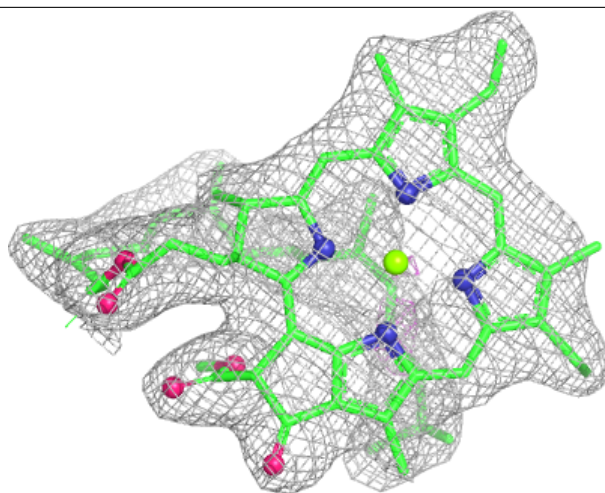
Electron density around CLA c 509:

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



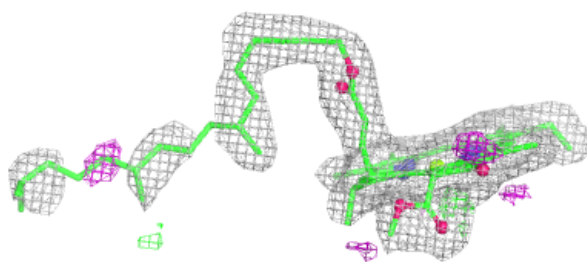
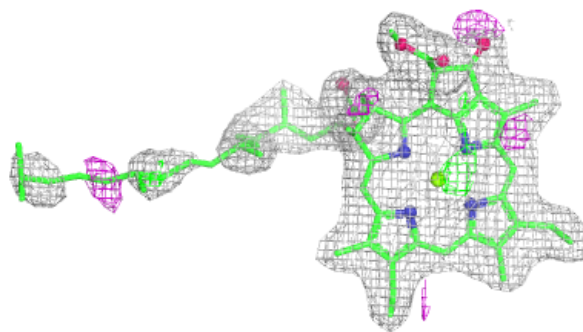
Electron density around CLA c 510:

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

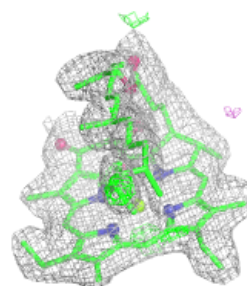
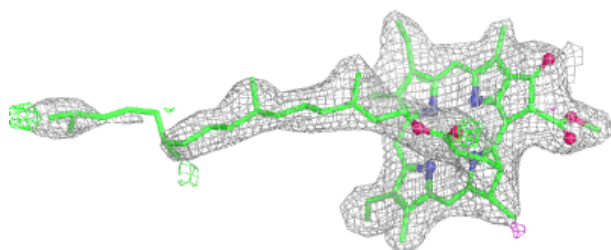
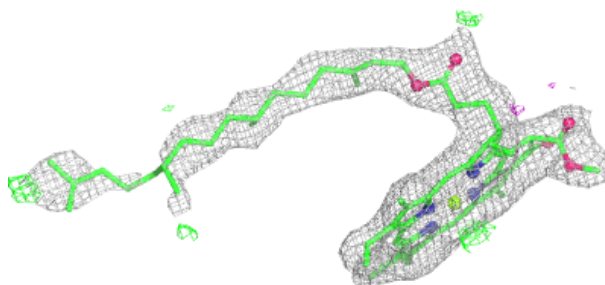


Electron density around CLA a 608:

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

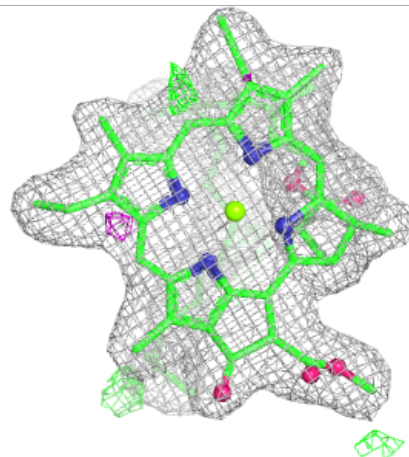
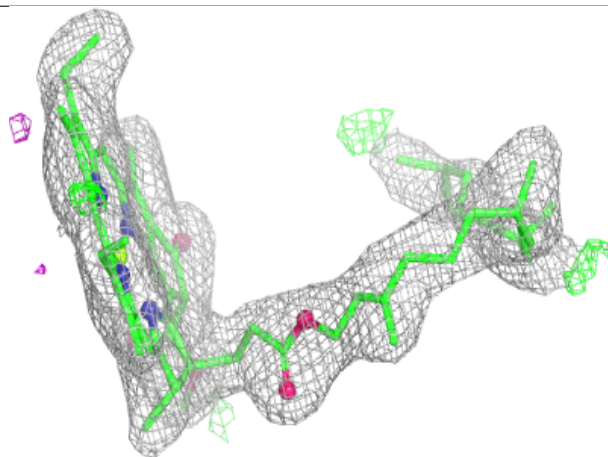
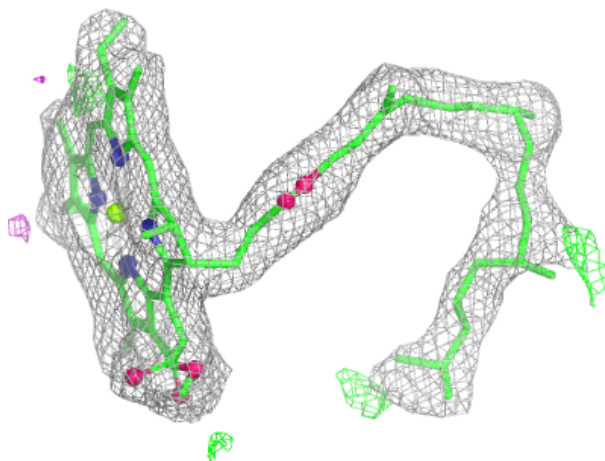
**Electron density around CLA C 504:**

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



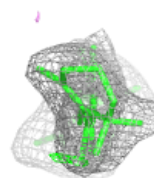
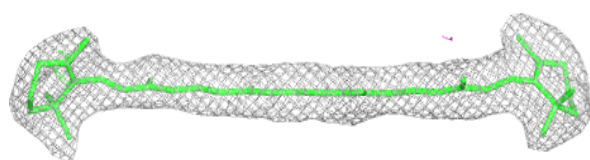
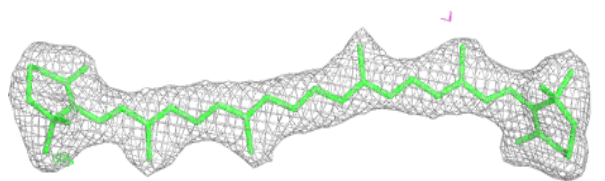
Electron density around CLA b 606:

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

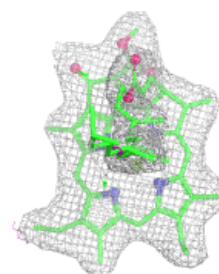
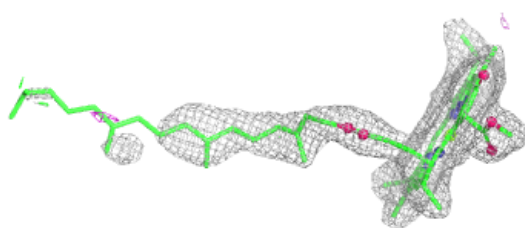
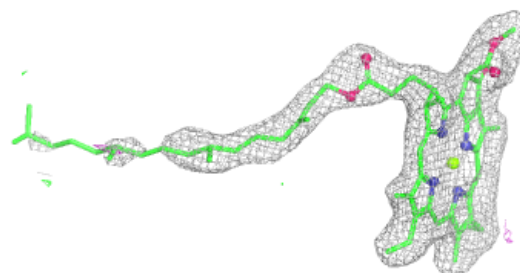


Electron density around BCR b 618:

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

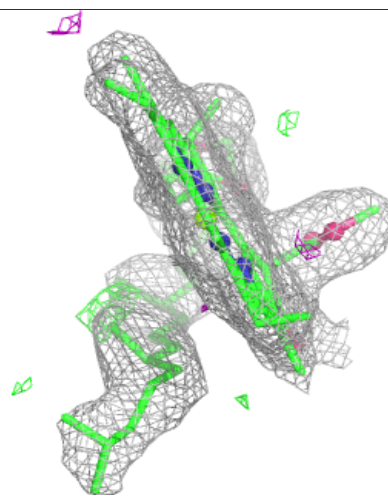
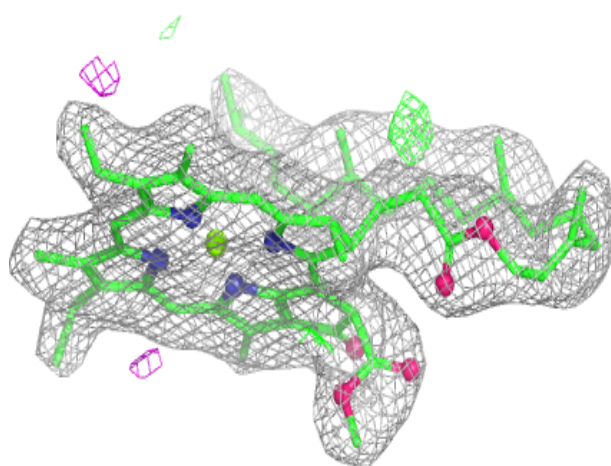
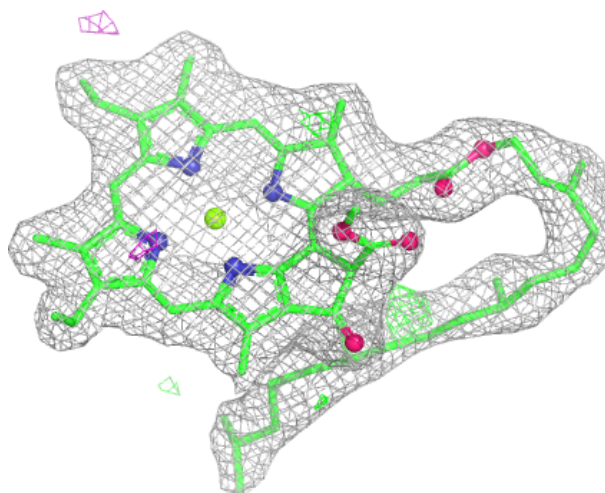
**Electron density around CLA d 403:**

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



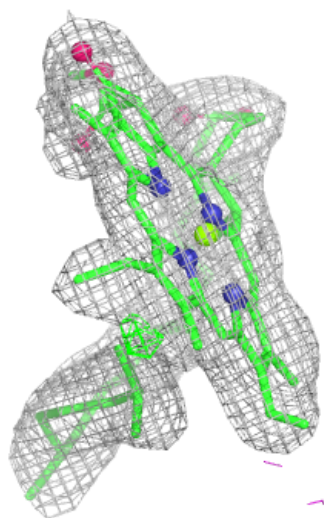
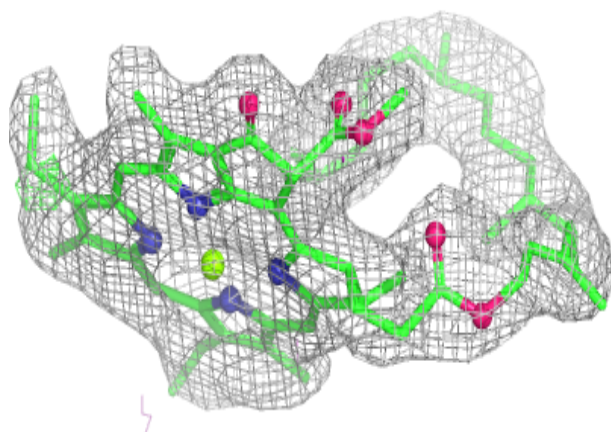
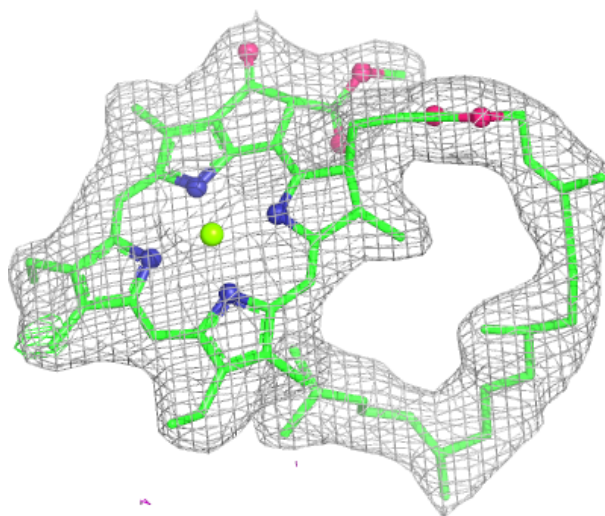
Electron density around CLA C 509:

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



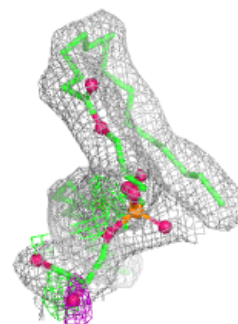
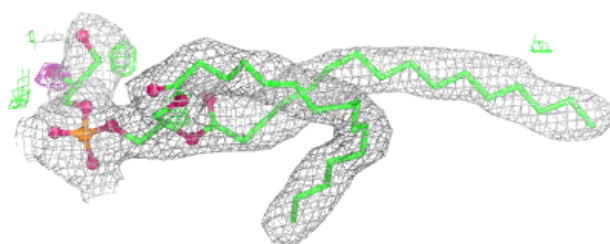
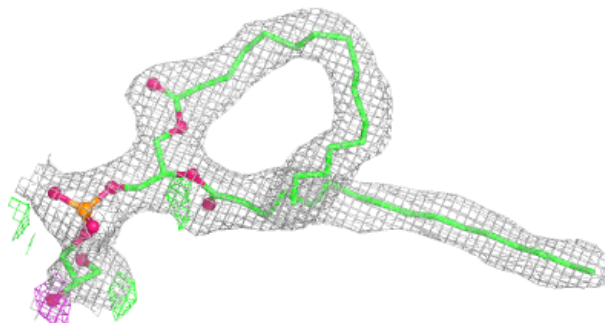
Electron density around CLA b 615:

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



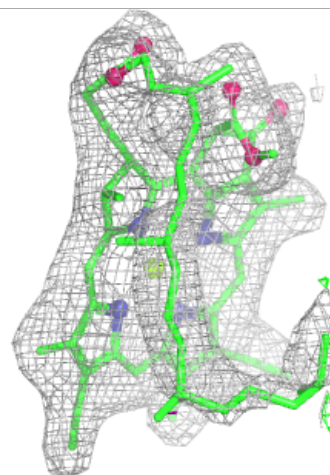
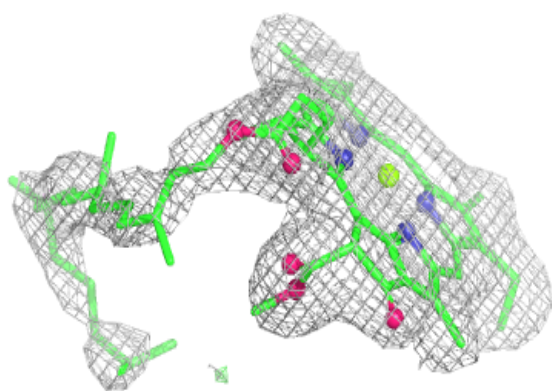
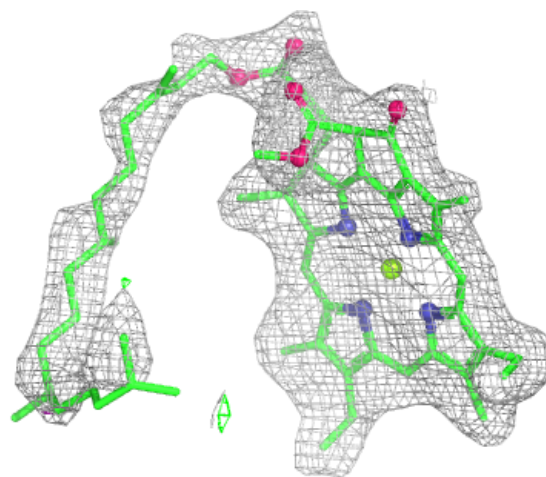
Electron density around LHG A 613:

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



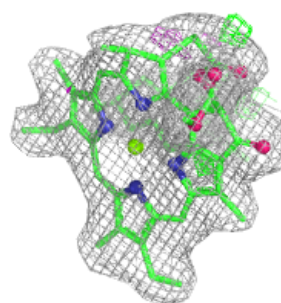
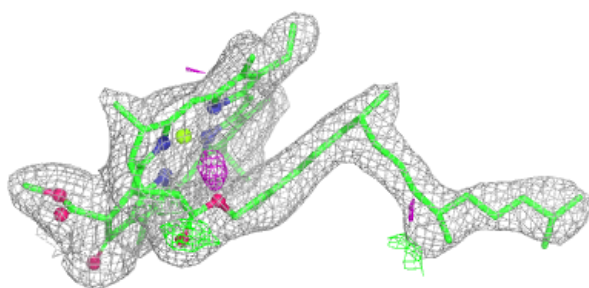
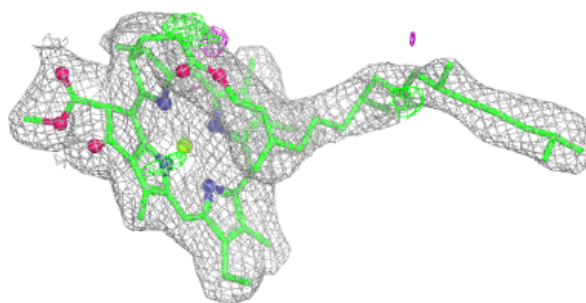
Electron density around CLA b 616:

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

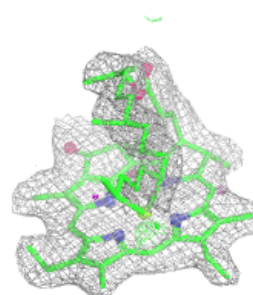
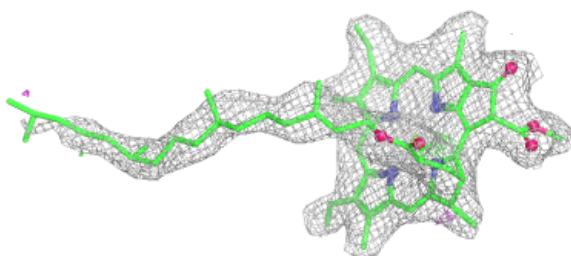
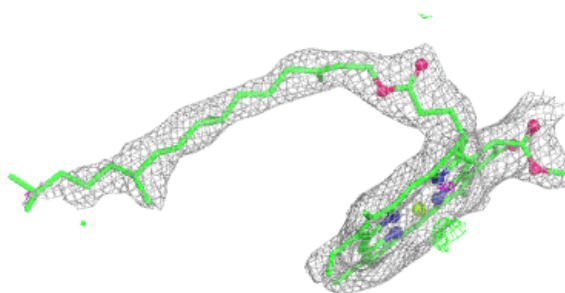


Electron density around CLA C 505:

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

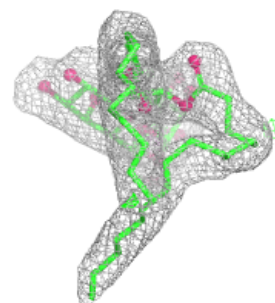
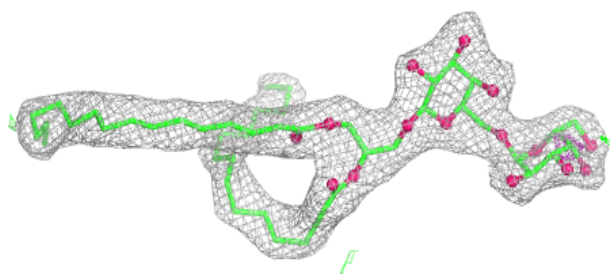
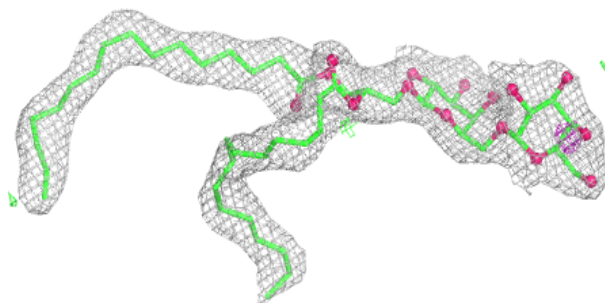
**Electron density around CLA c 504:**

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

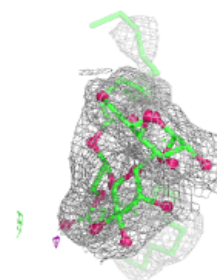
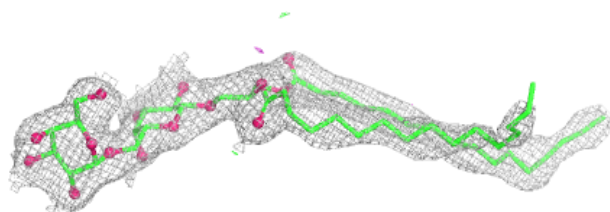
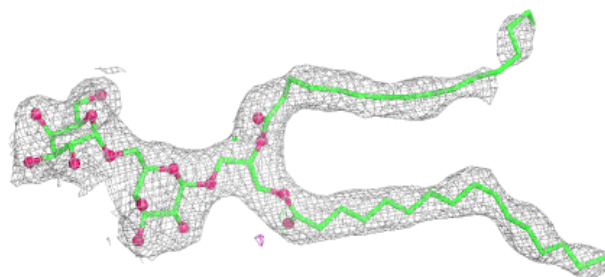


Electron density around DGD H 102:

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

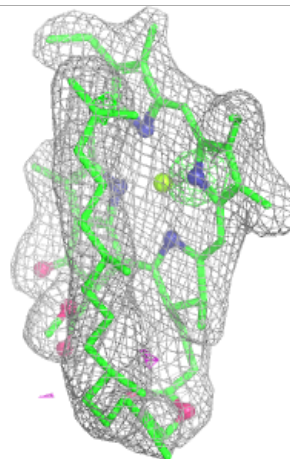
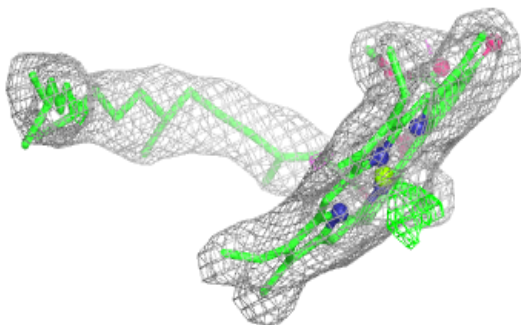
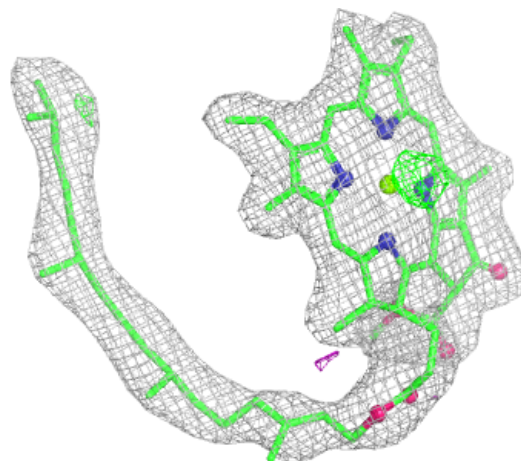
**Electron density around DGD c 517:**

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



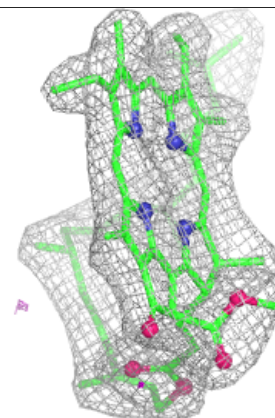
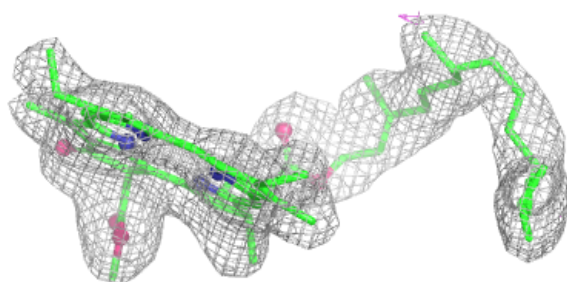
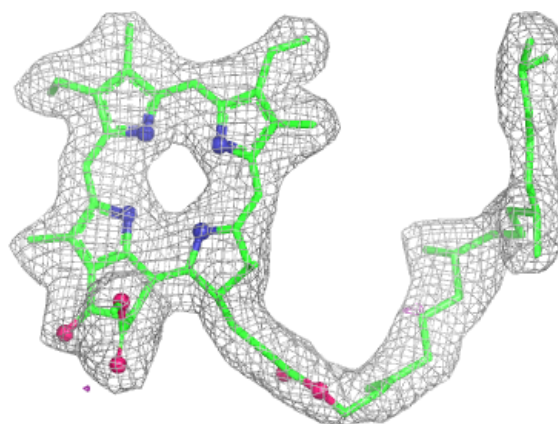
Electron density around CLA c 507:

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

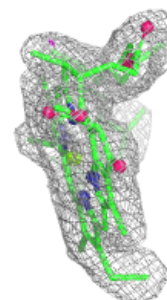
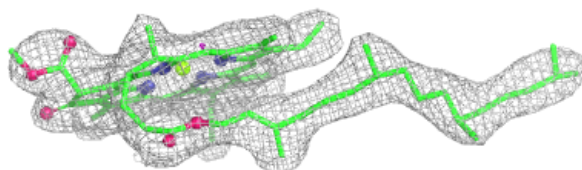
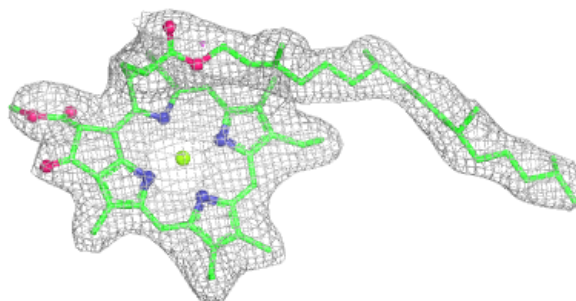


Electron density around PHO d 402:

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

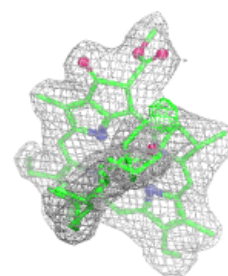
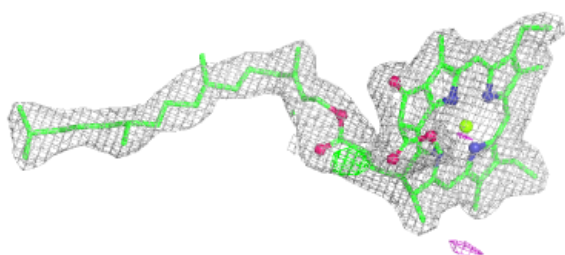
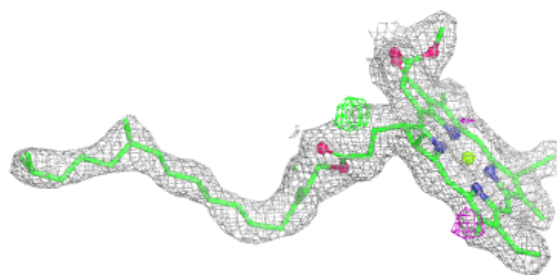
**Electron density around CLA c 501:**

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

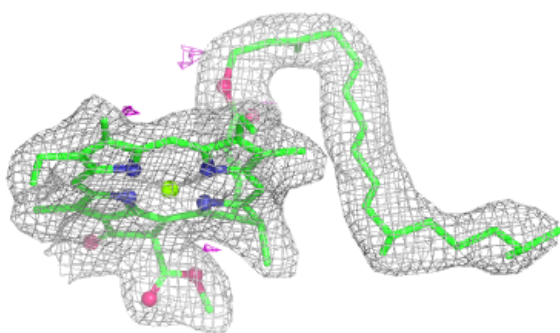
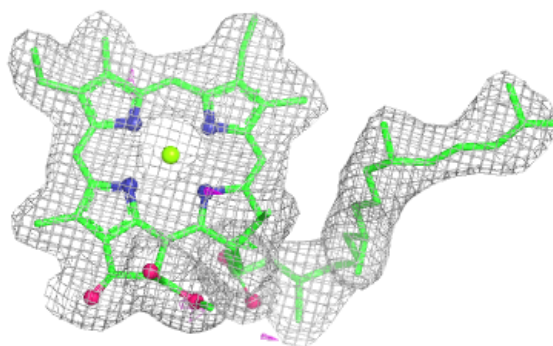


Electron density around CLA c 502:

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

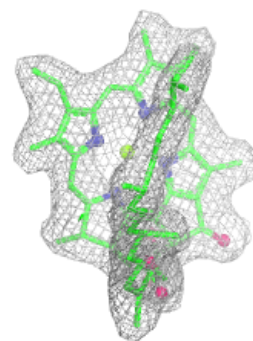
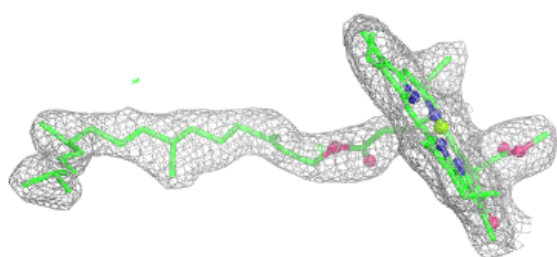
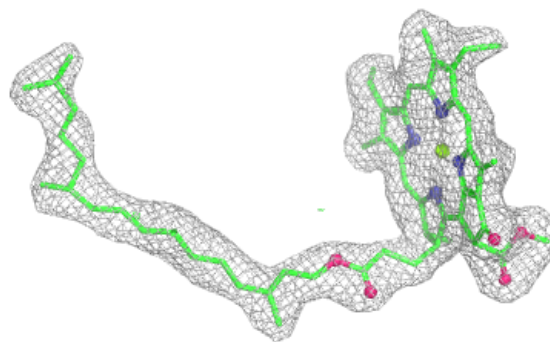
**Electron density around CLA a 607:**

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

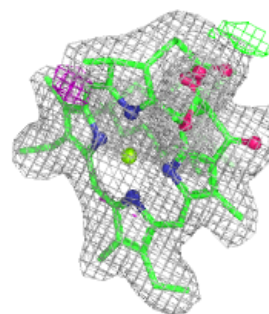
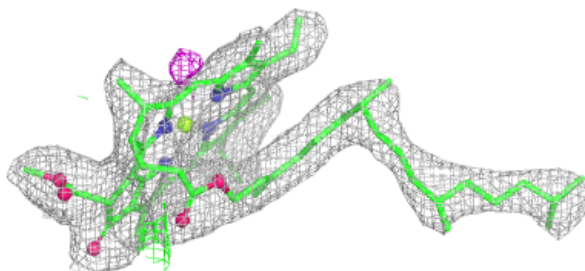
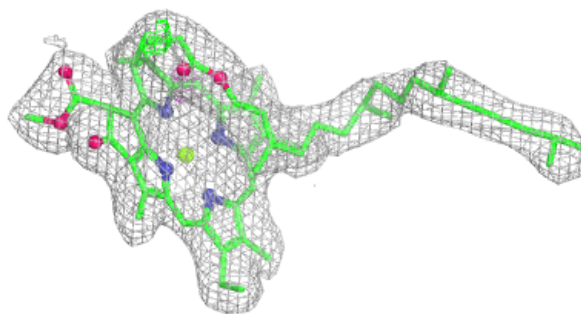


Electron density around CLA B 609:

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

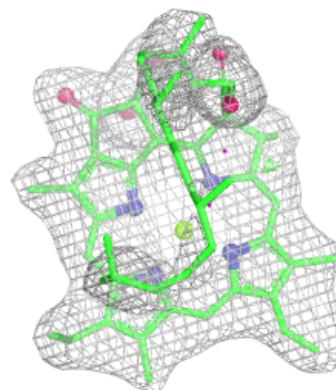
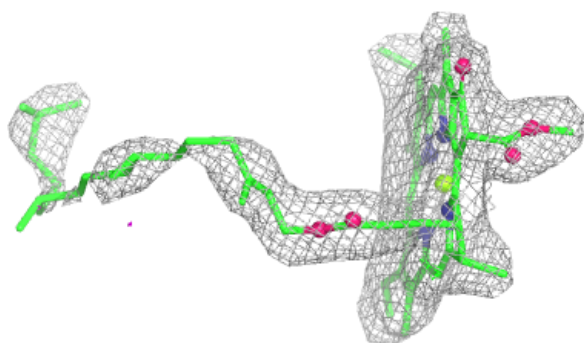
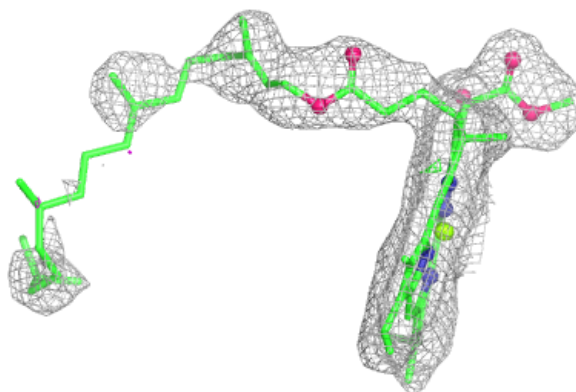
**Electron density around CLA c 505:**

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



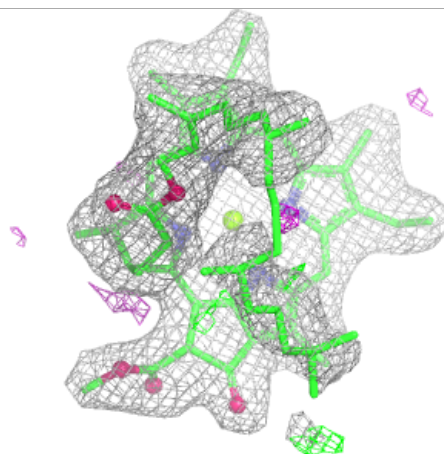
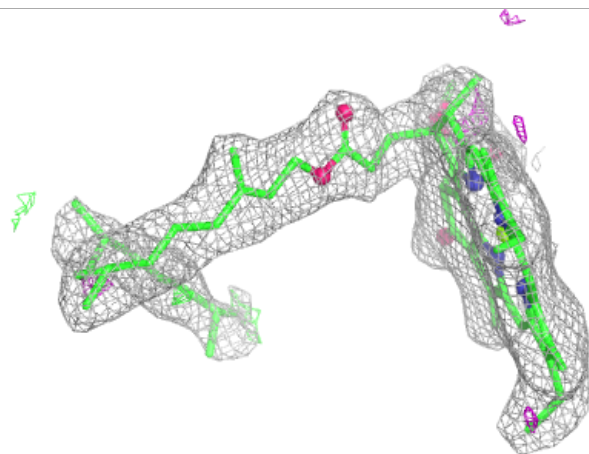
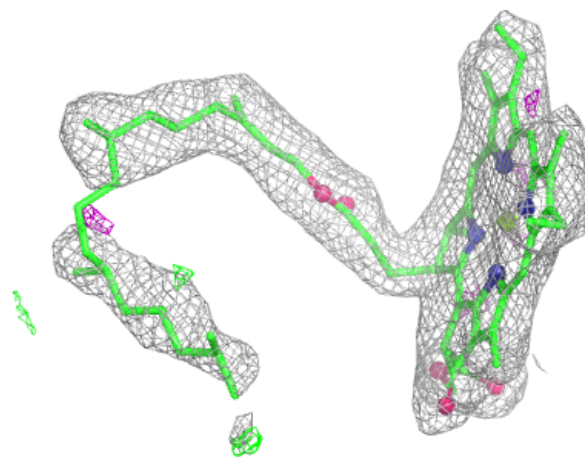
Electron density around CLA c 506:

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



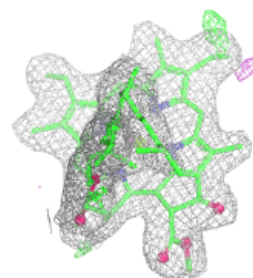
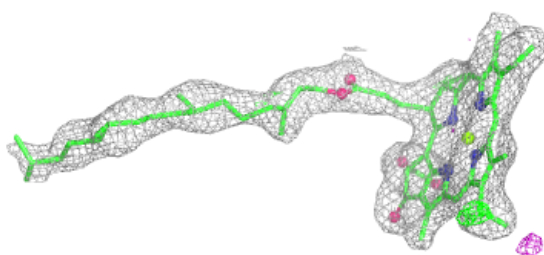
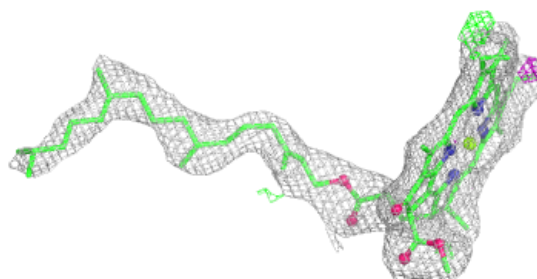
Electron density around CLA B 606:

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



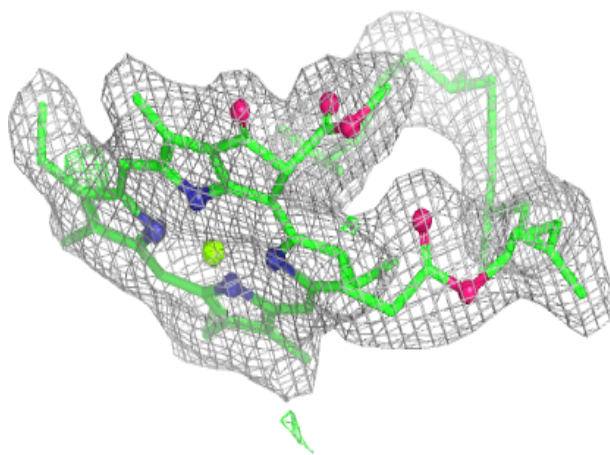
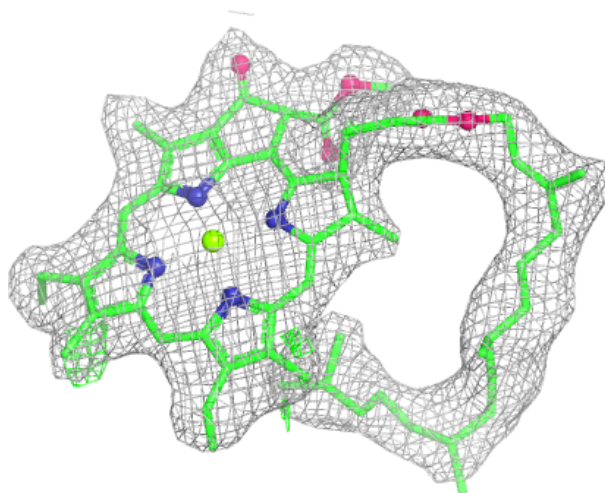
Electron density around CLA b 604:

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



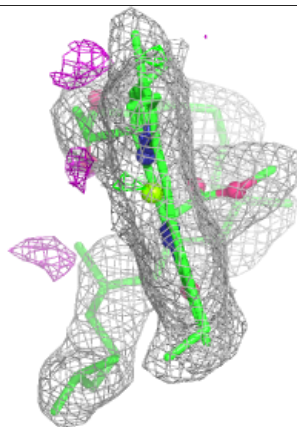
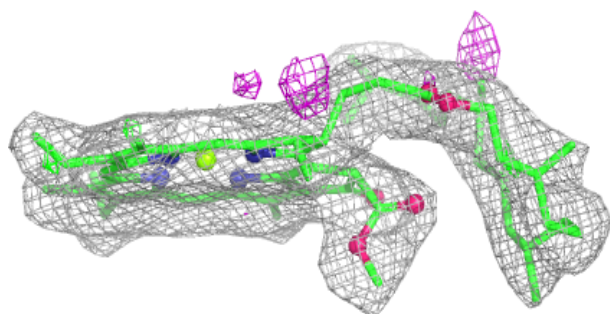
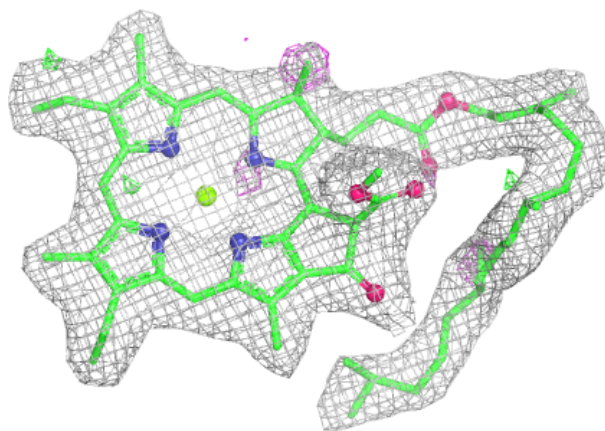
Electron density around CLA B 615:

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



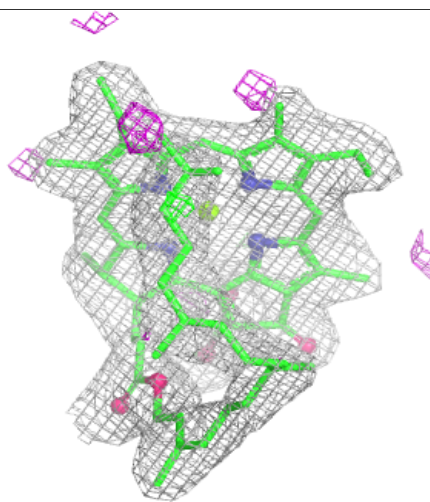
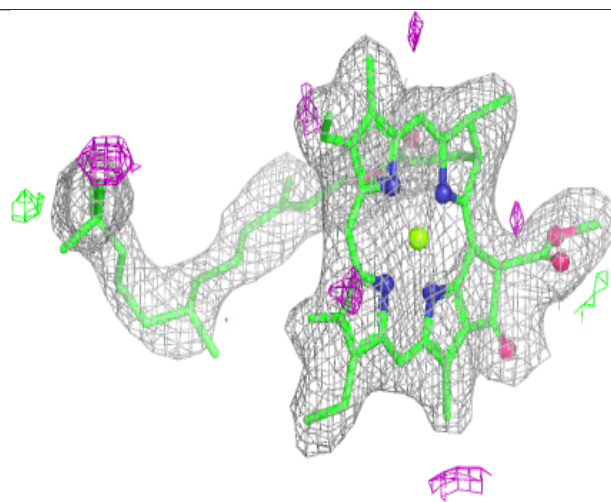
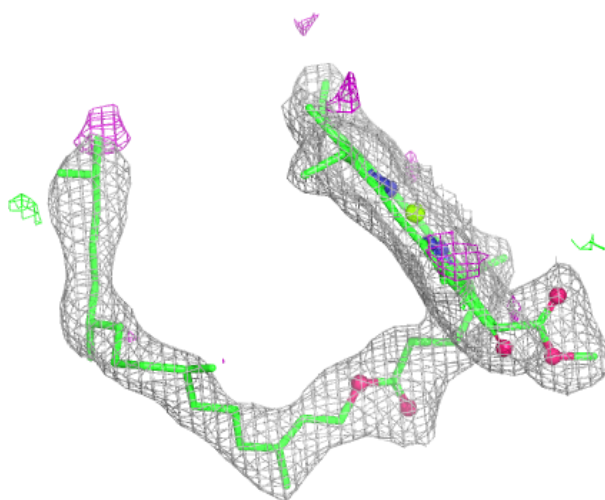
Electron density around CLA b 610:

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



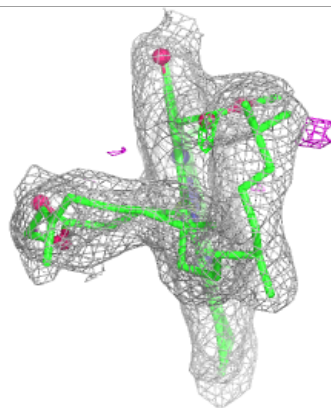
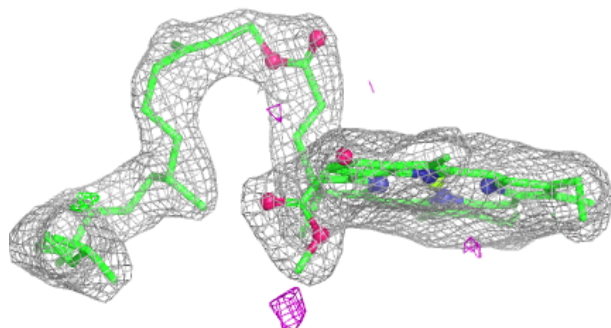
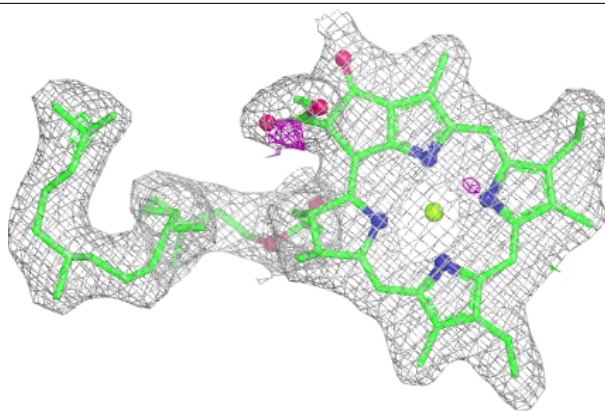
Electron density around CLA b 611:

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

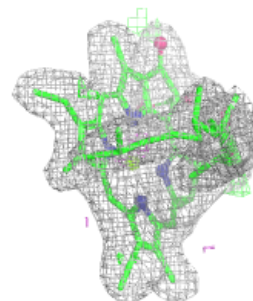
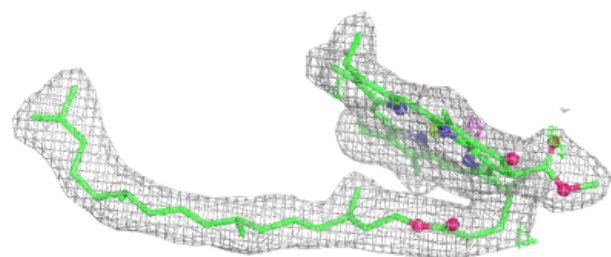
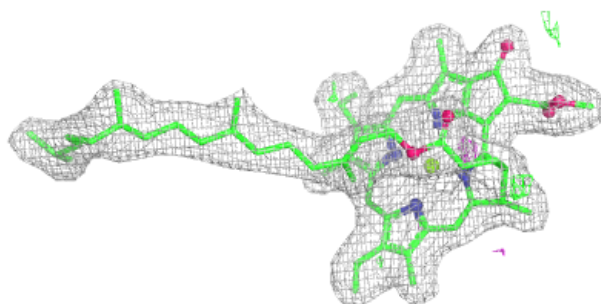


Electron density around CLA b 612:

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

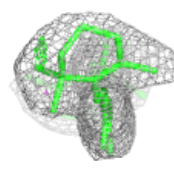
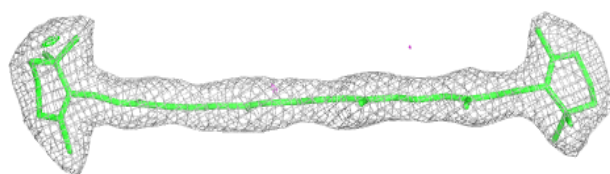
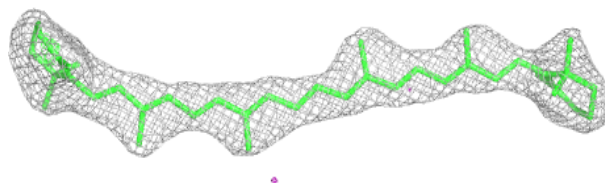
**Electron density around CLA B 608:**

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

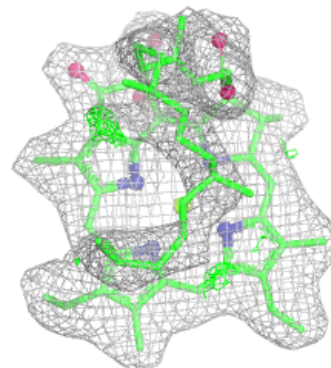
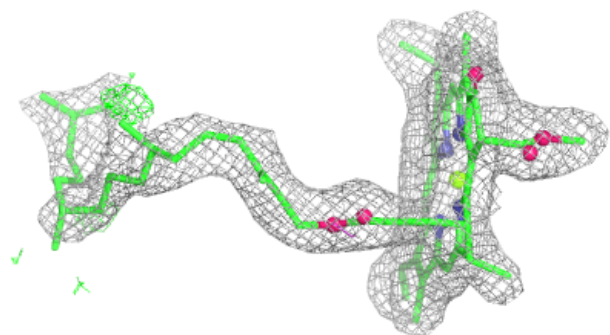
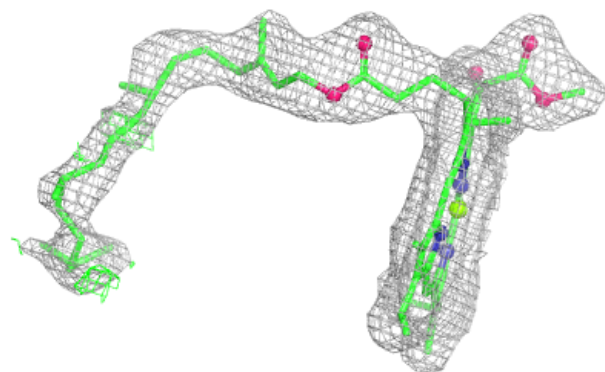


Electron density around BCR c 514:

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

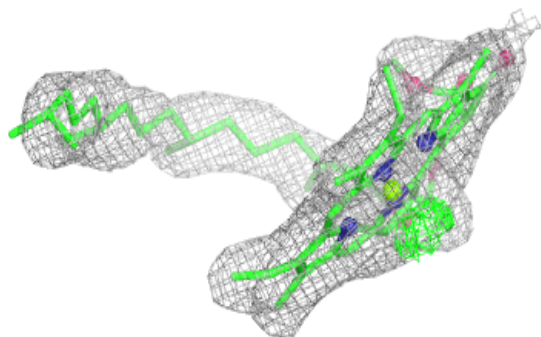
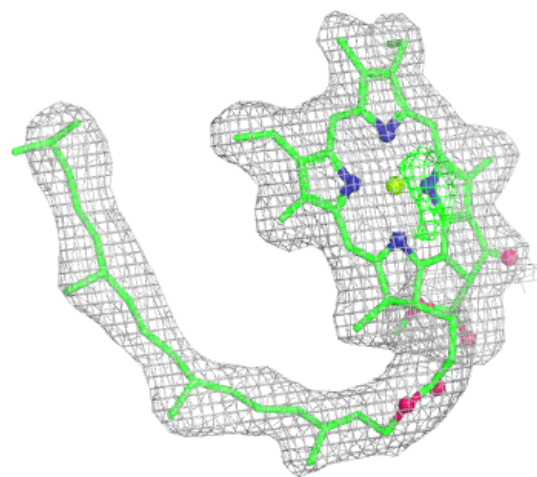
**Electron density around CLA C 506:**

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



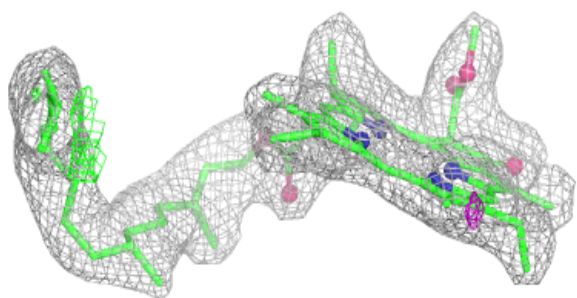
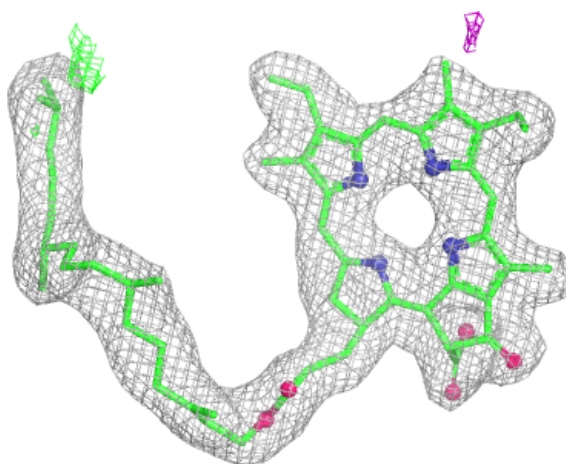
Electron density around CLA C 507:

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



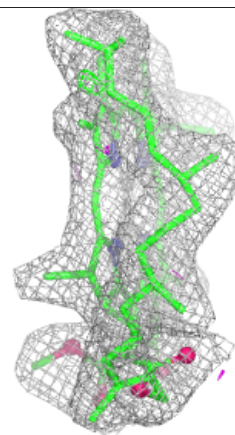
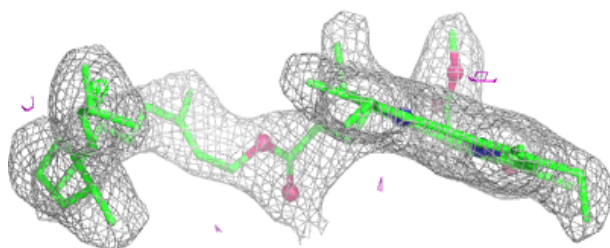
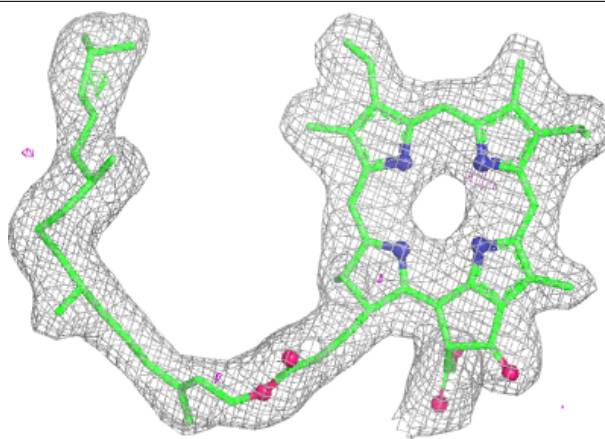
Electron density around PHO D 402:

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

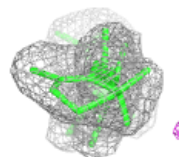
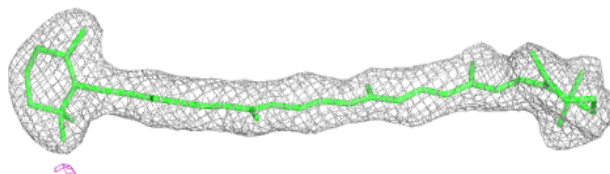
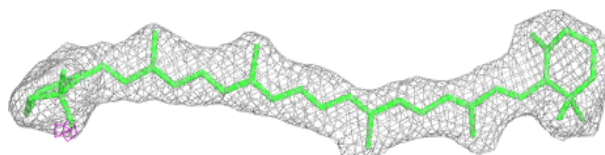


Electron density around PHO a 609:

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

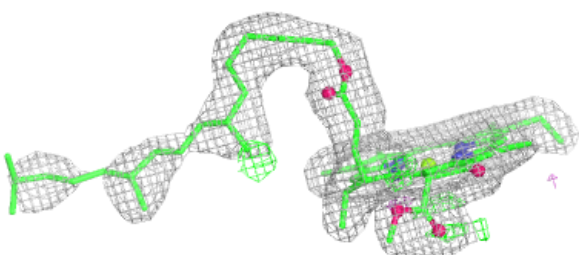
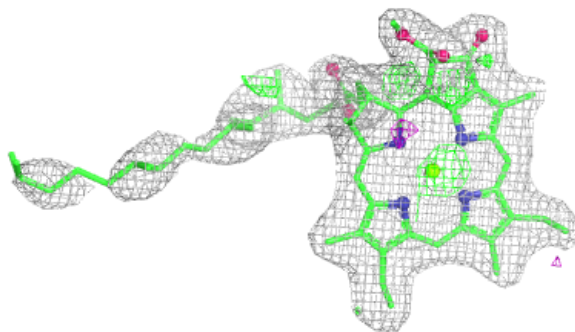
**Electron density around BCR B 617:**

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

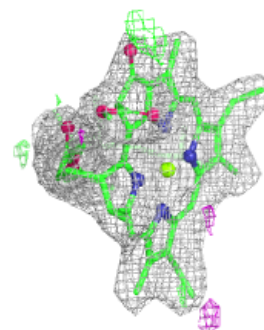
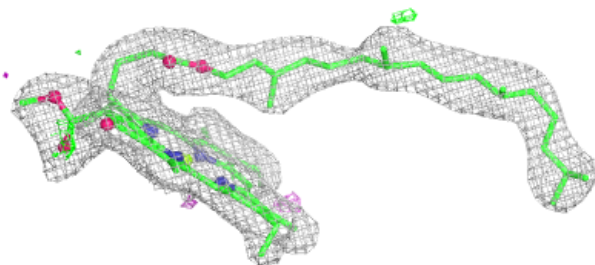
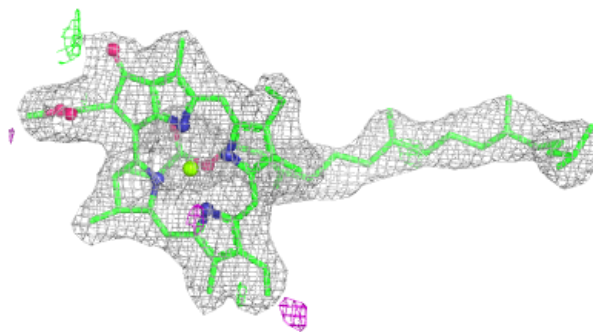


Electron density around CLA A 607:

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

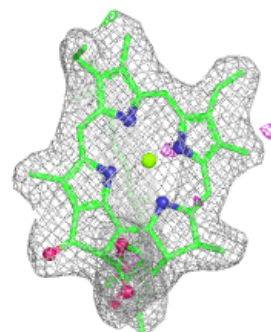
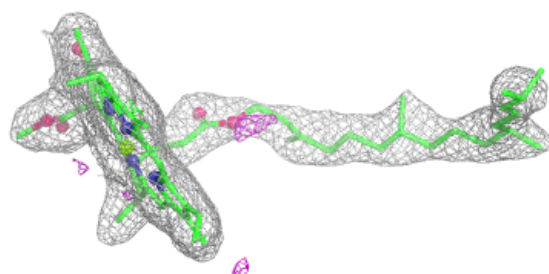
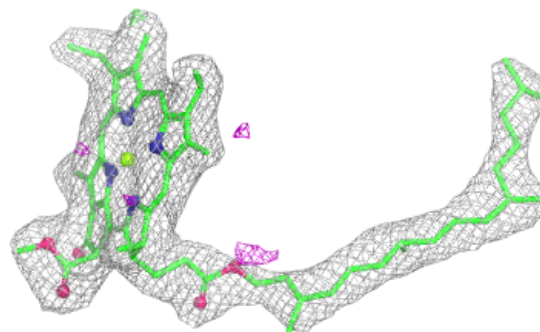
**Electron density around CLA b 608:**

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

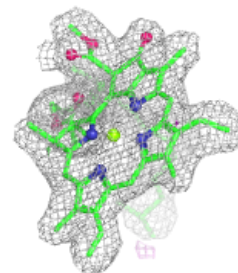
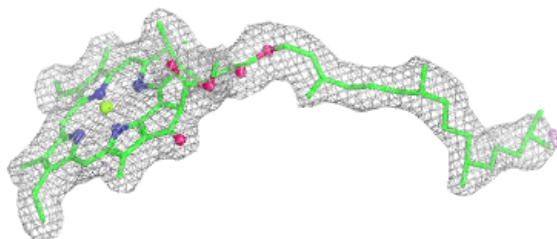
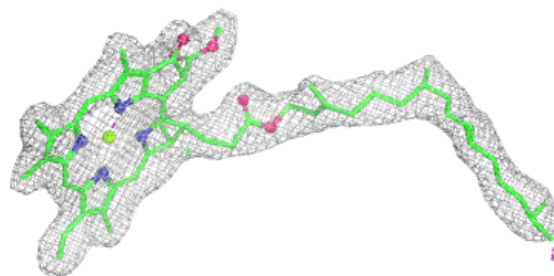


Electron density around CLA b 609:

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

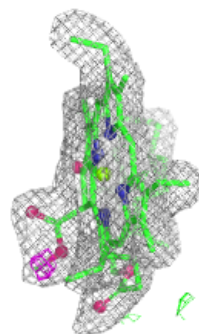
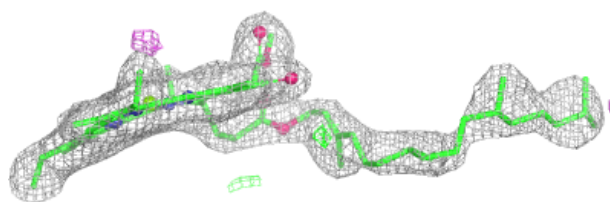
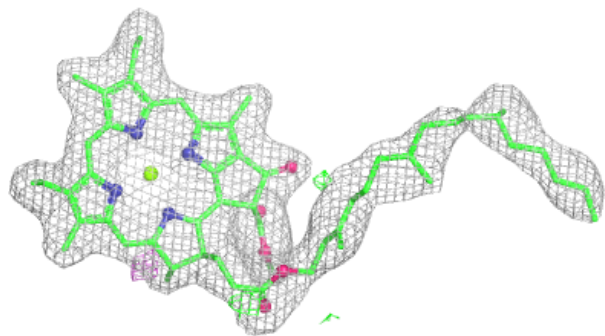
**Electron density around CLA A 606:**

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

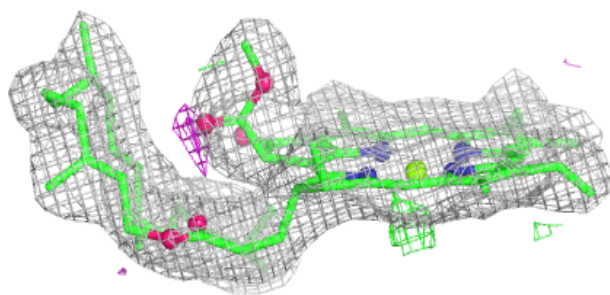
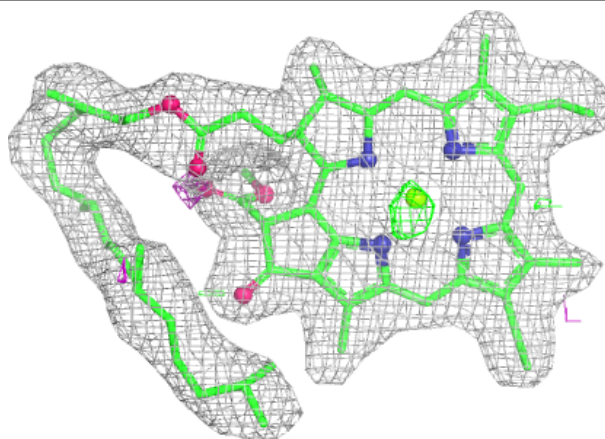


Electron density around CLA B 602:

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

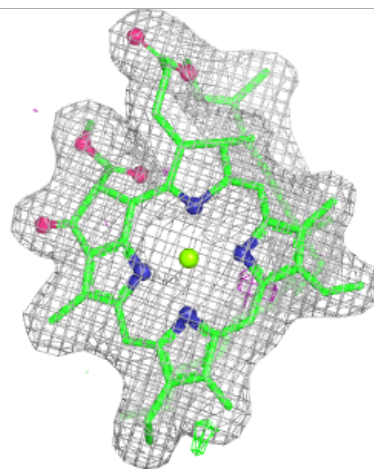
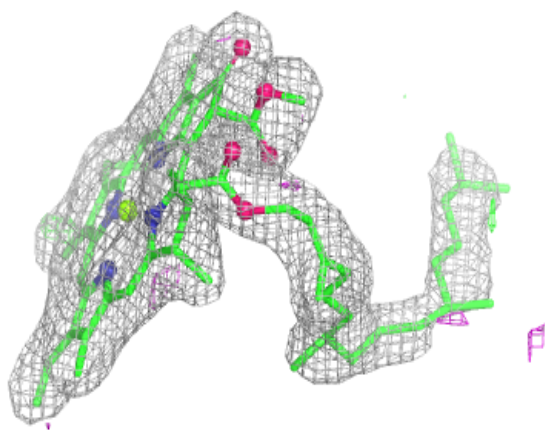
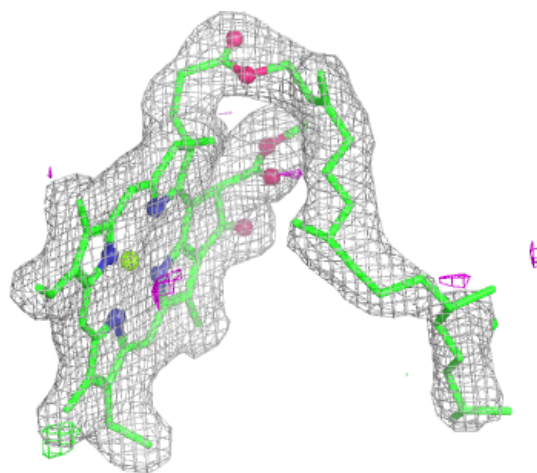
**Electron density around CLA B 610:**

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



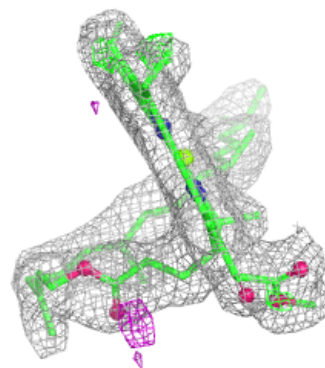
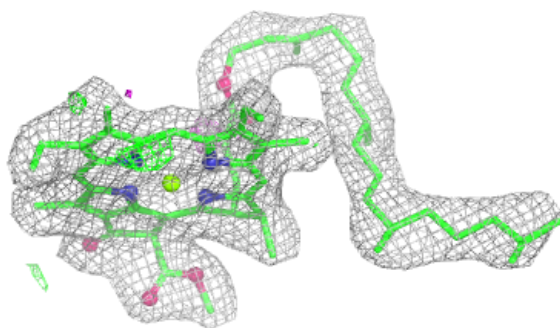
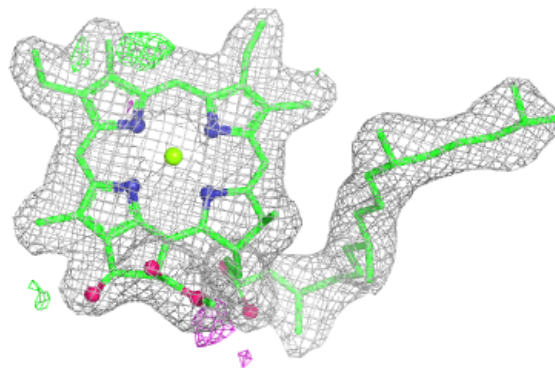
Electron density around CLA b 613:

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

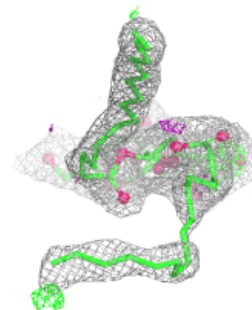
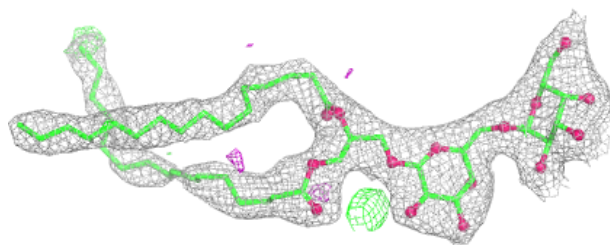
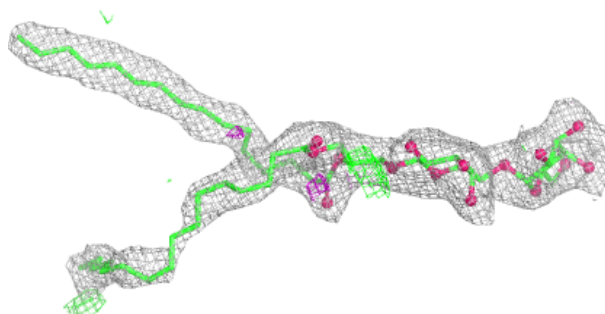


Electron density around CLA D 403:

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

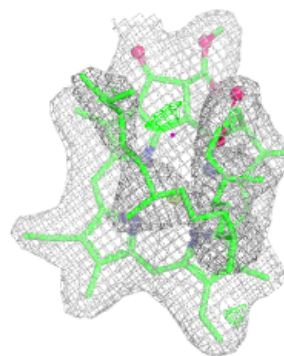
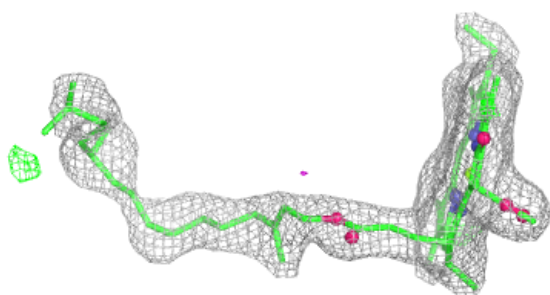
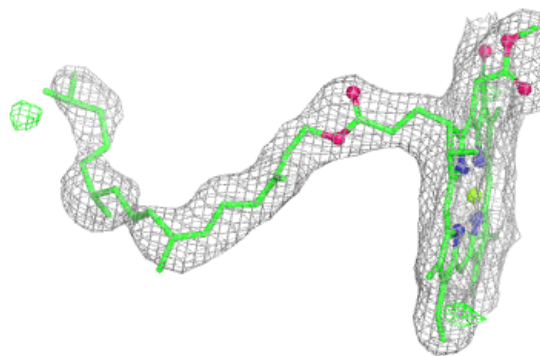
**Electron density around DGD C 516:**

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

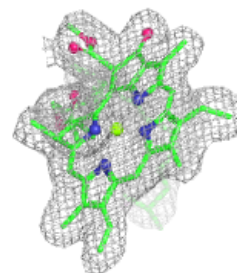
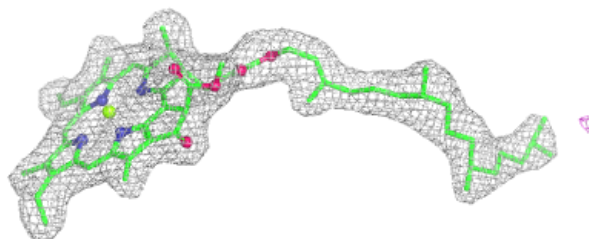
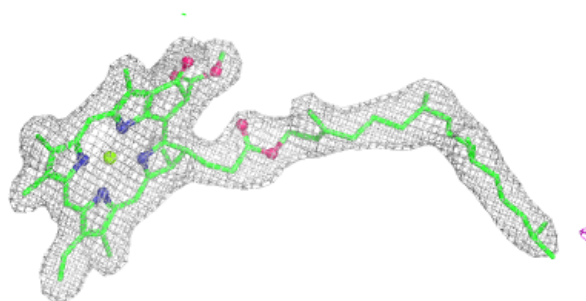


Electron density around CLA D 405:

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

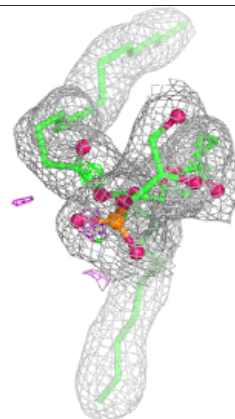
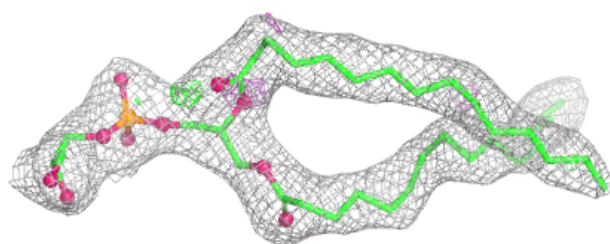
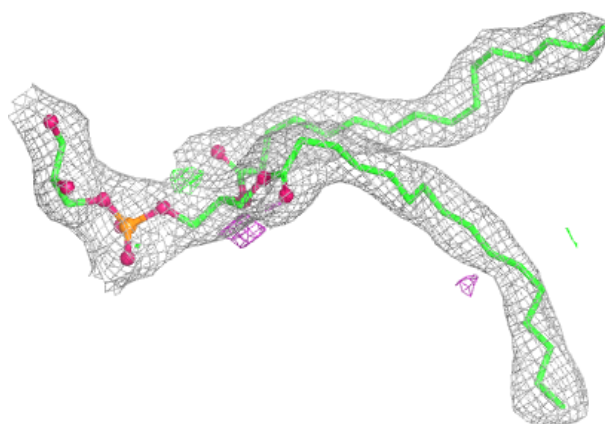
**Electron density around CLA a 606:**

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

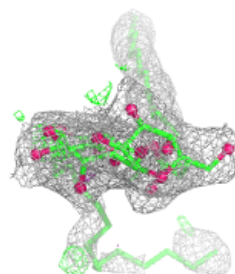
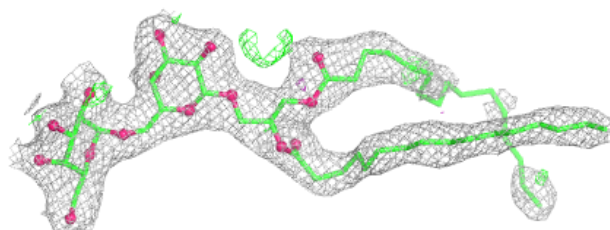
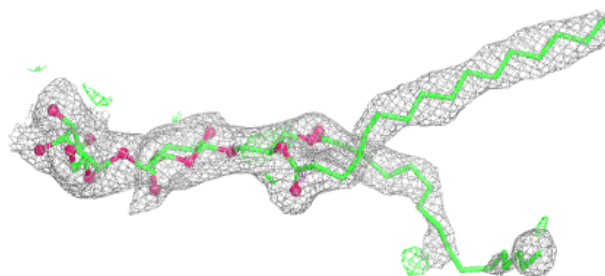


Electron density around LHG D 408:

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

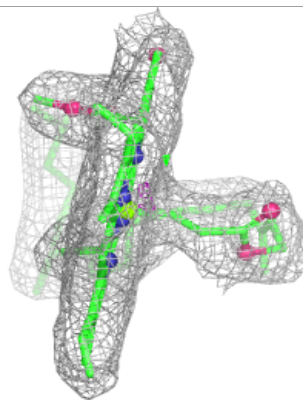
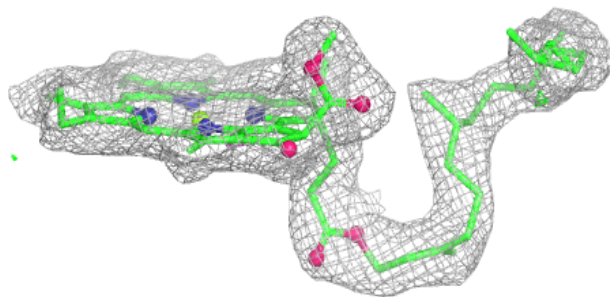
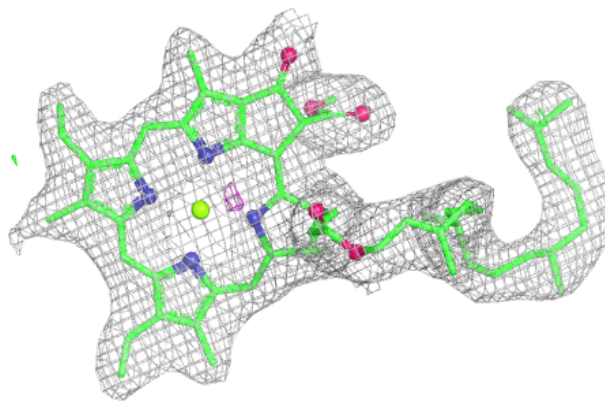
**Electron density around DGD c 515:**

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

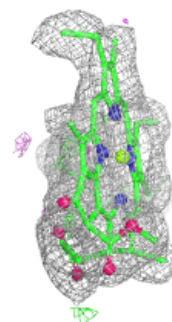
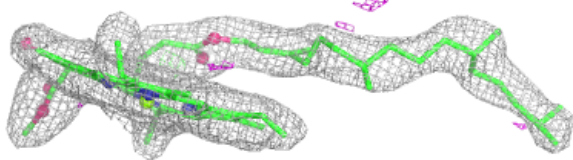
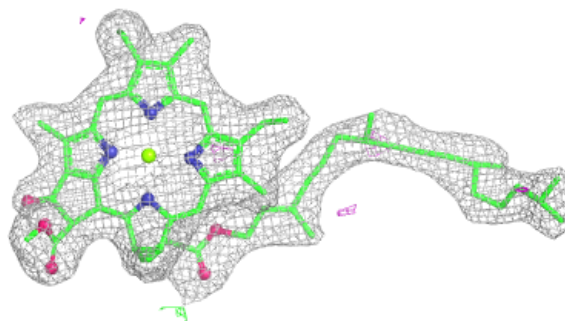


Electron density around CLA B 612:

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

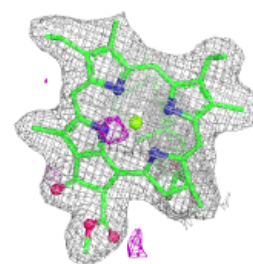
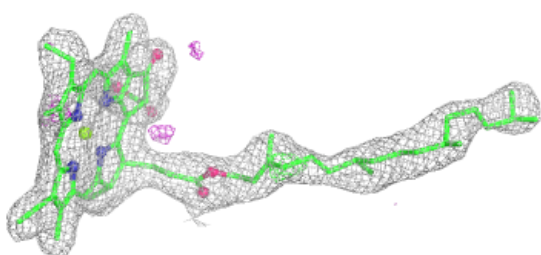
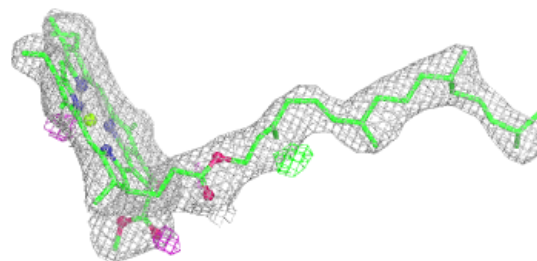
**Electron density around CLA B 603:**

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

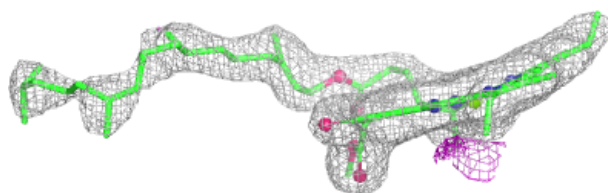
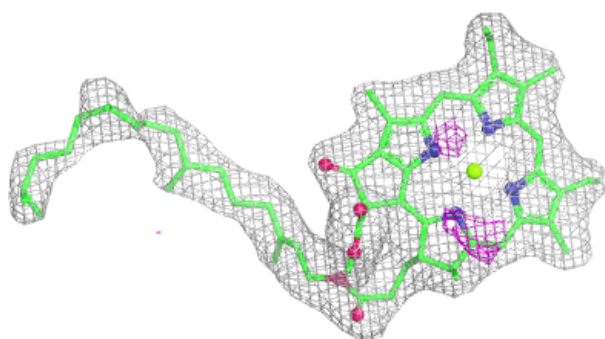


Electron density around CLA B 604:

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

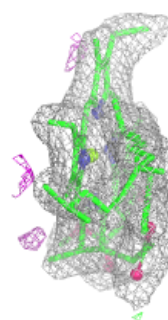
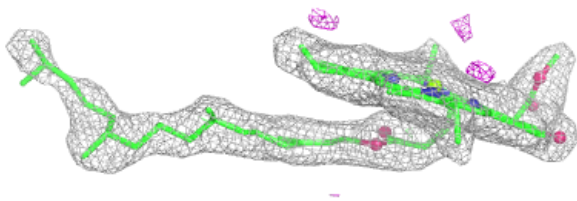
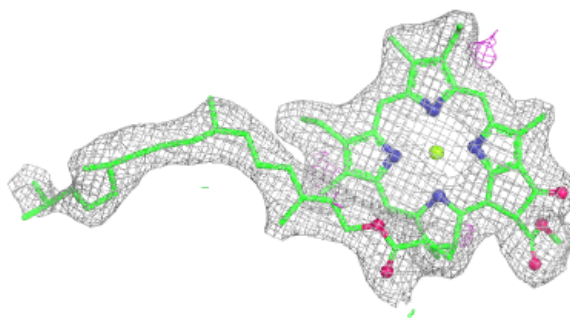
**Electron density around CLA b 602:**

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

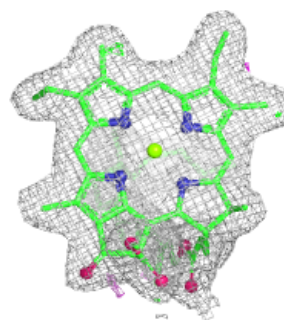
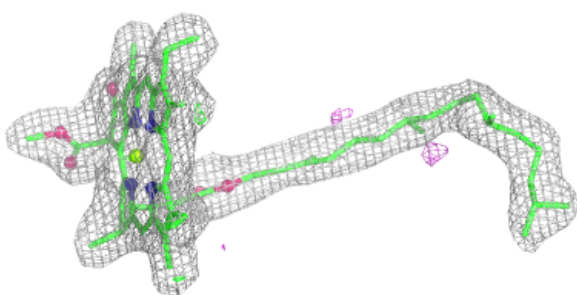
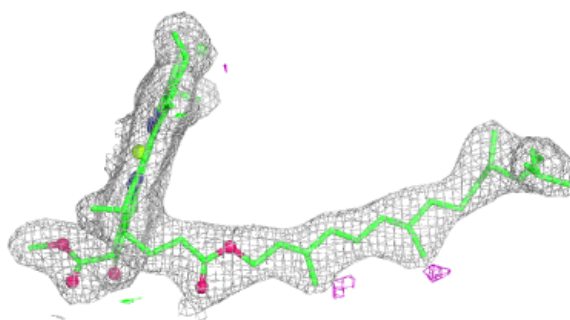


Electron density around CLA b 603:

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

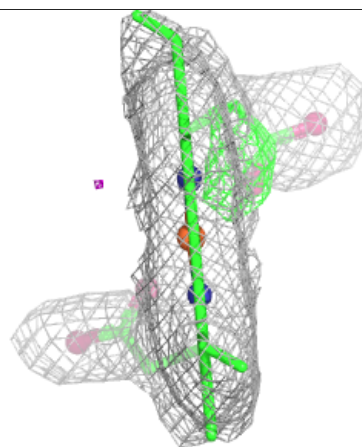
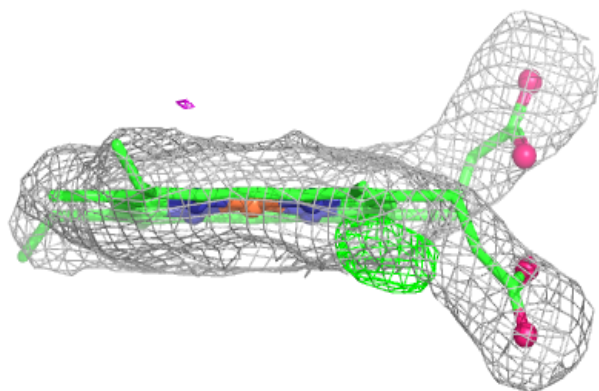
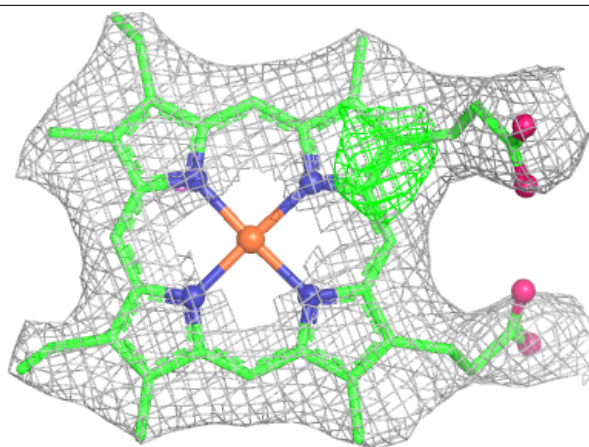
**Electron density around CLA B 605:**

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



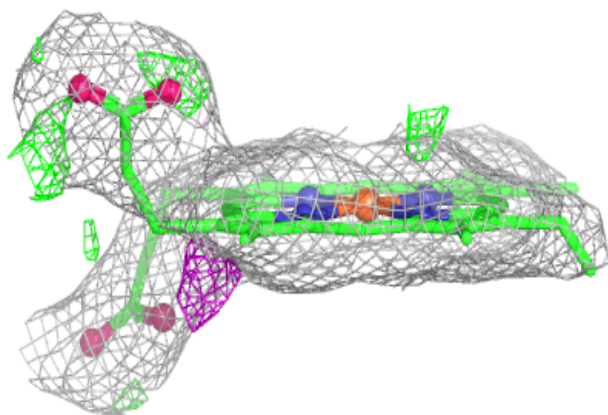
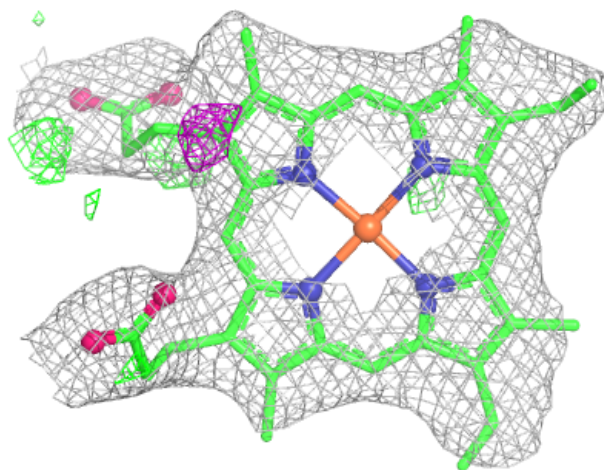
Electron density around HEM E 102:

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



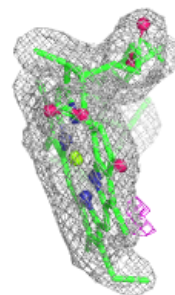
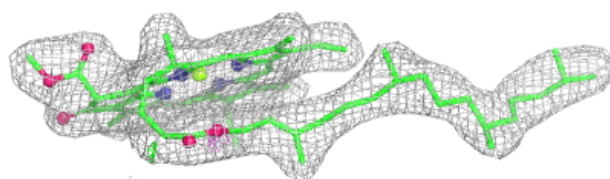
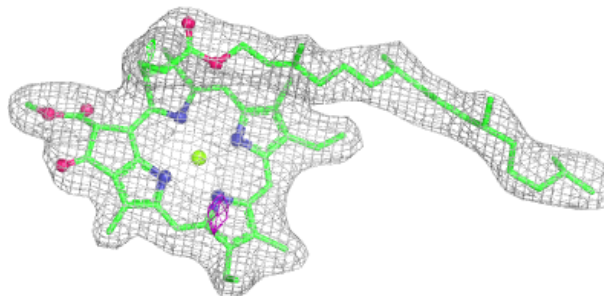
Electron density around HEM e 101:

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



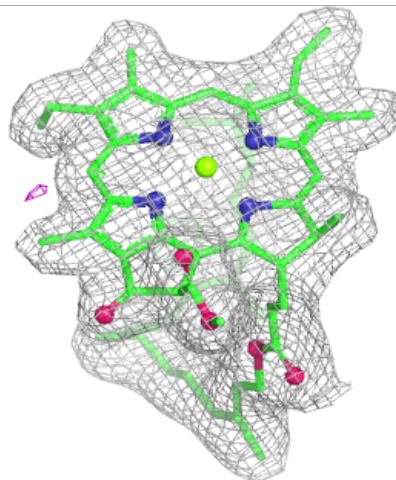
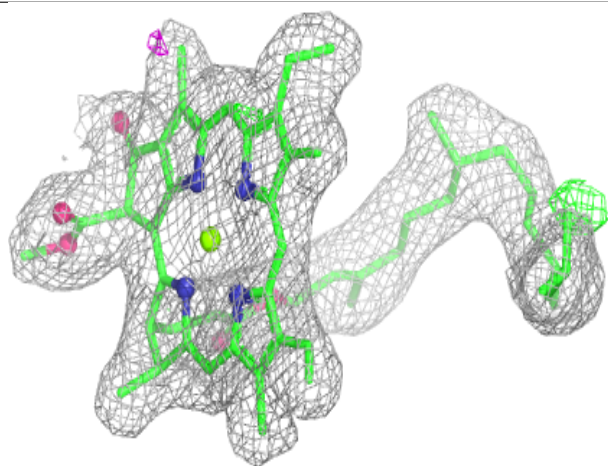
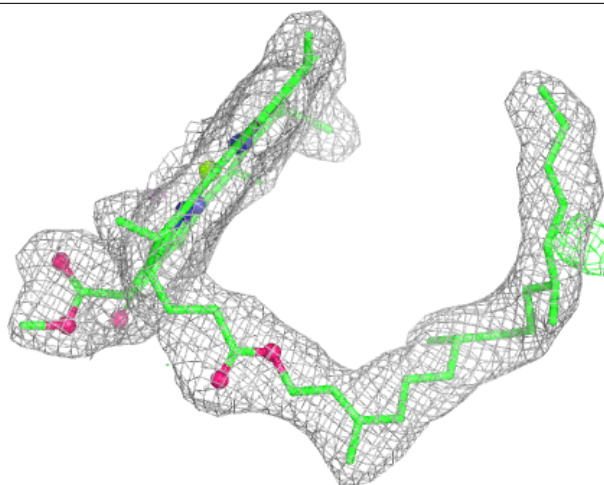
Electron density around CLA C 501:

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



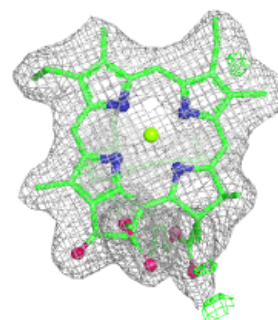
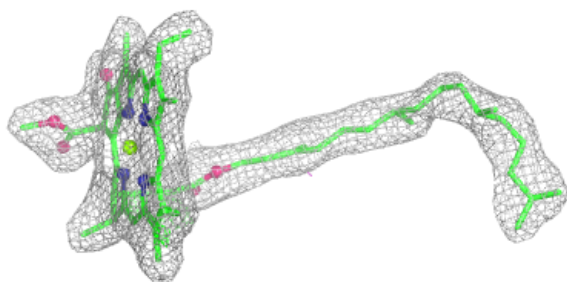
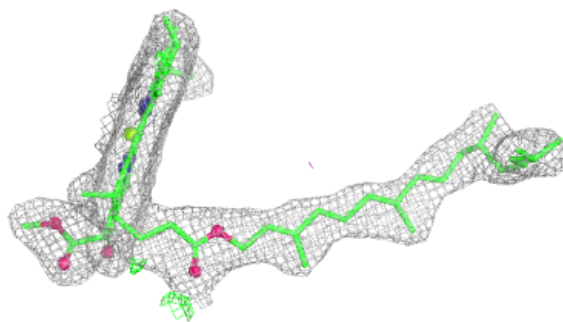
Electron density around CLA B 611:

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



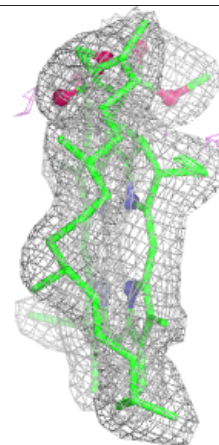
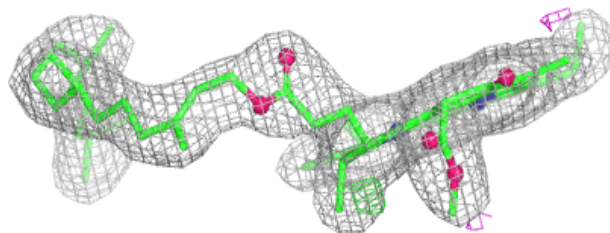
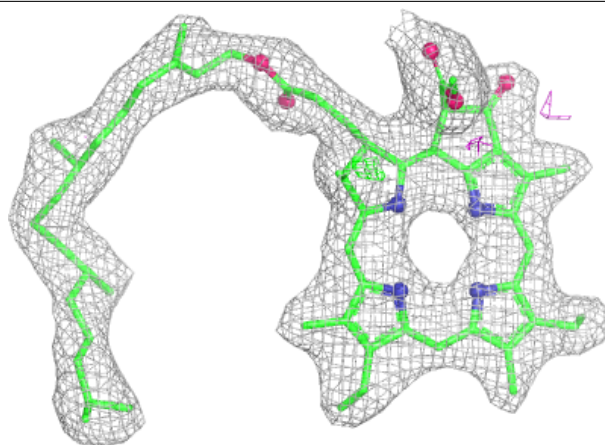
Electron density around CLA b 605:

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



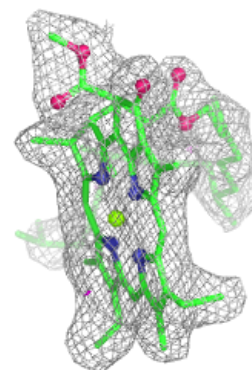
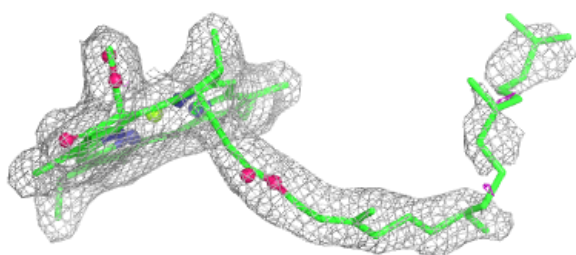
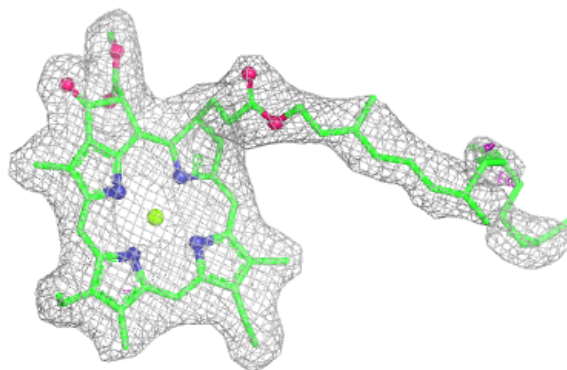
Electron density around PHO D 401:

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

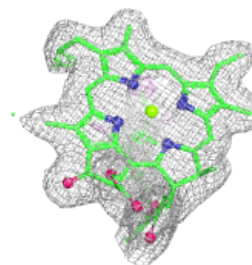
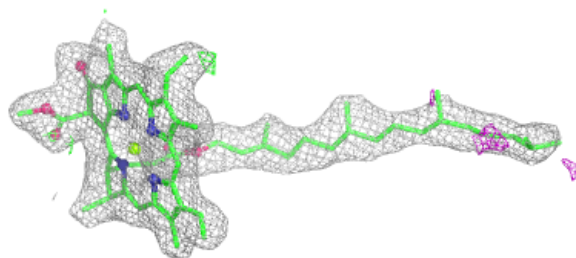
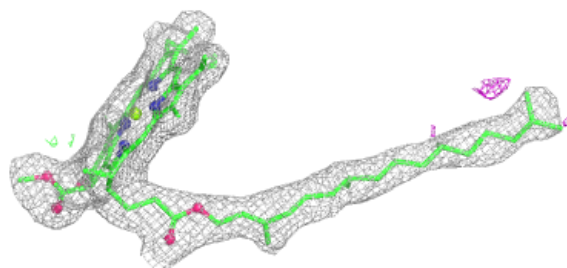


Electron density around CLA a 610:

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

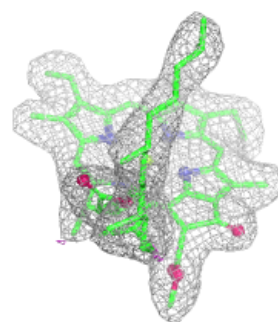
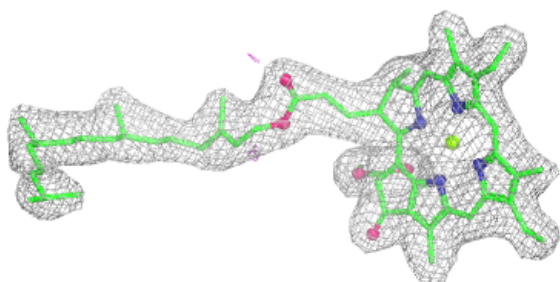
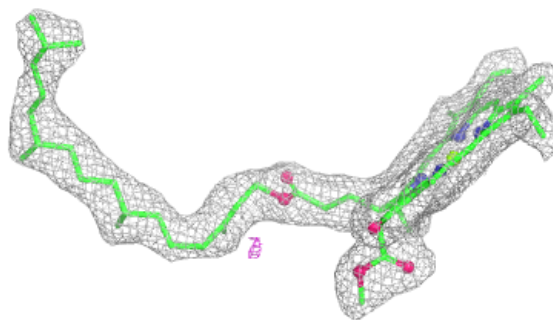
**Electron density around CLA b 607:**

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



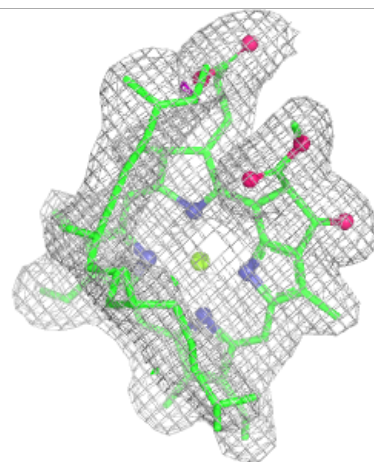
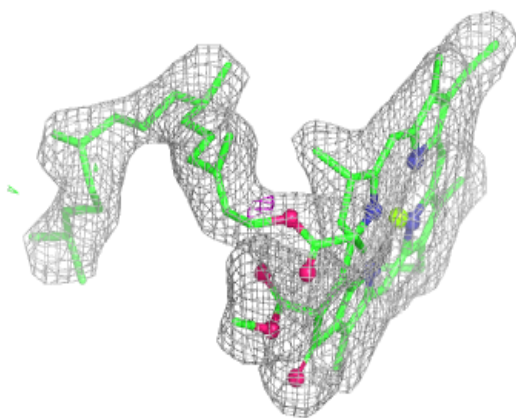
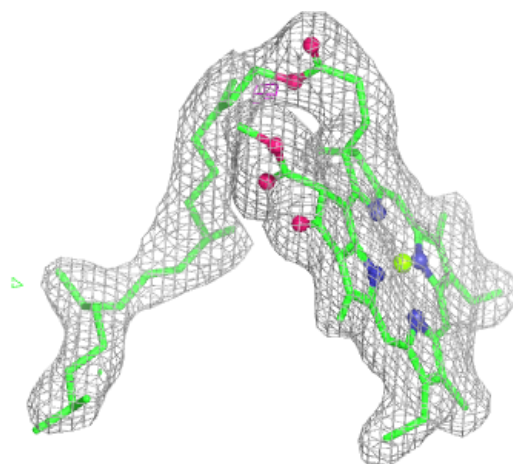
Electron density around CLA d 401:

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



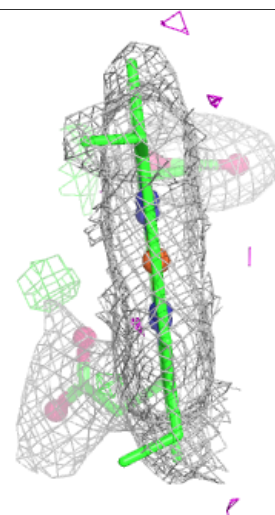
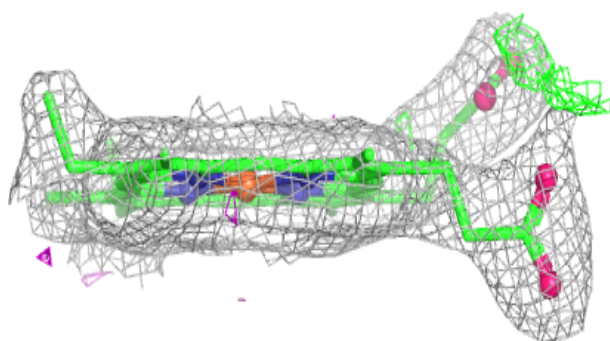
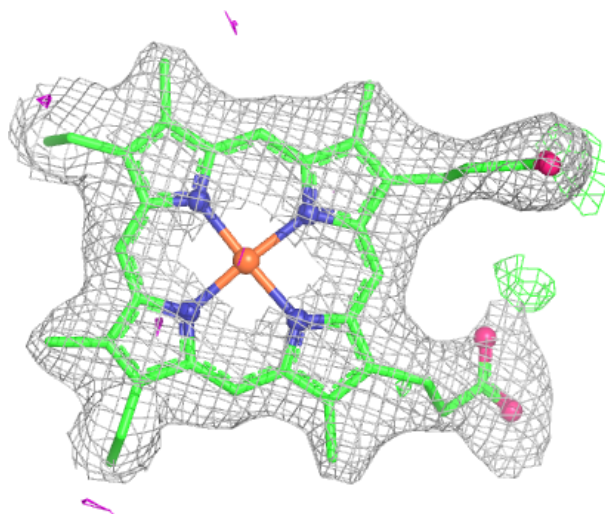
Electron density around CLA B 613:

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



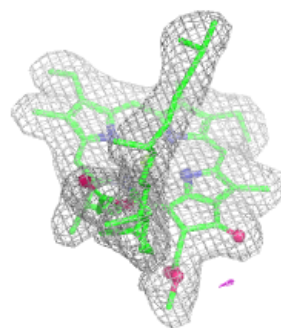
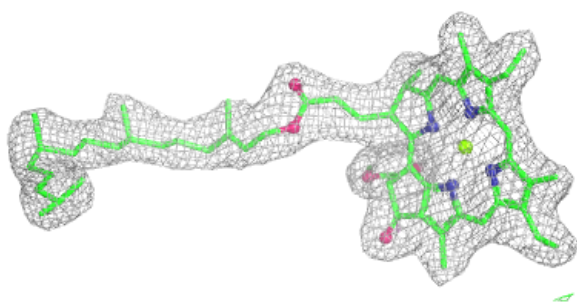
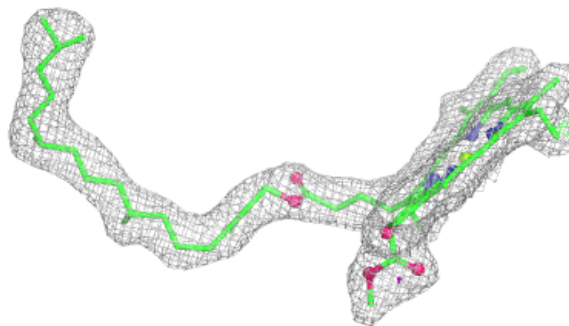
Electron density around HEC v 201:

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

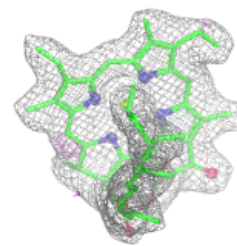
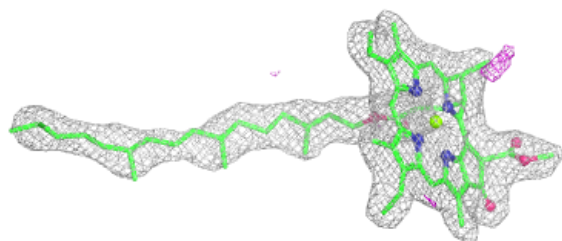
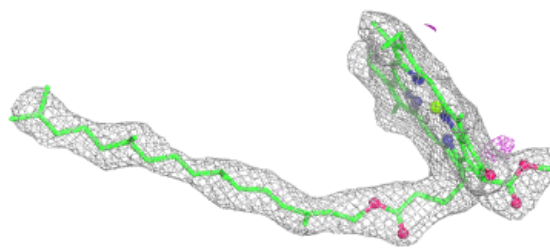


Electron density around CLA D 404:

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

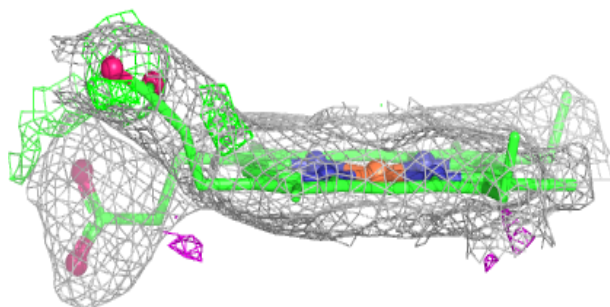
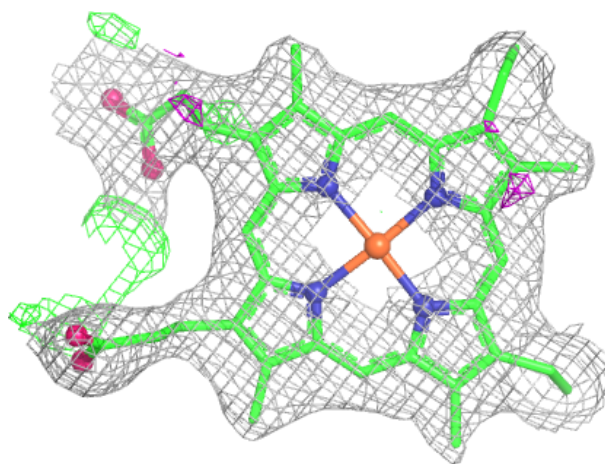
**Electron density around CLA B 607:**

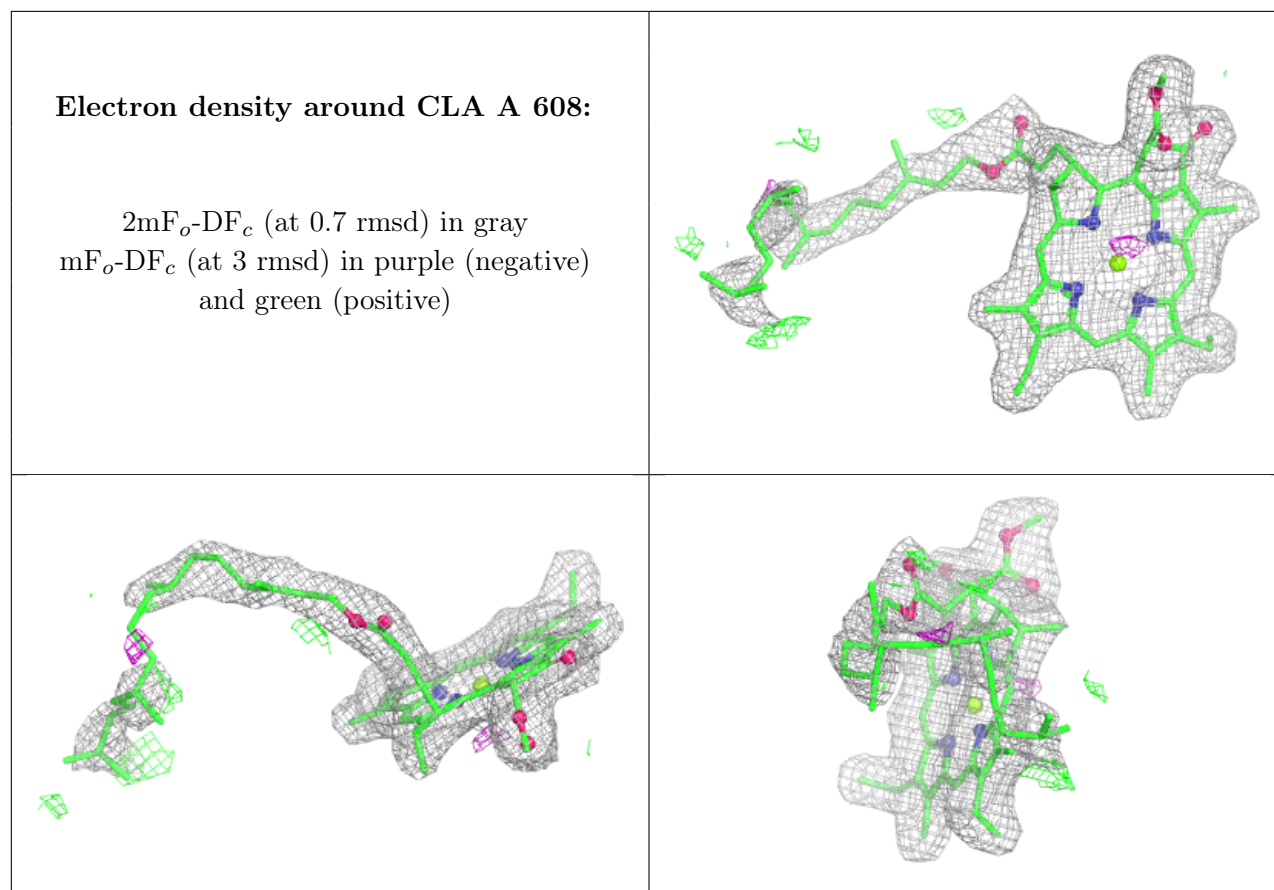
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 ⓘ

There are no such residues in this entry.