



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:36 PM UTC

PDB ID : 5KAF / pdb_00005kaf
Title : RT XFEL structure of Photosystem II in the dark state at 3.0 Å resolution
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2016-06-01
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)

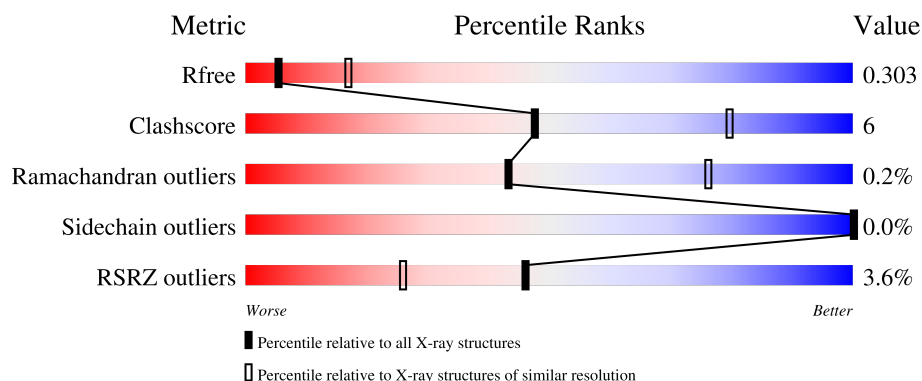
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

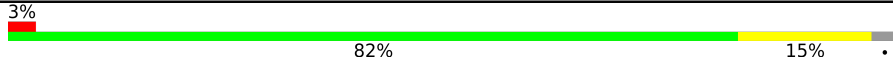
The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	

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

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Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

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Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	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	609	X	-	-	-
25	CLA	A	615	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	b	618	X	-	-	-
25	CLA	b	619	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	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	c	514	X	-	-	-
25	CLA	c	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	d	404	X	-	-	-
32	BCT	A	620	-	X	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 50162 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2618	1715	431	457	15			
1	a	334	Total	C	N	O	S	0	0	0
			2613	1713	428	457	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3953	2596	658	686	13			
2	b	504	Total	C	N	O	S	3	1	0
			3960	2600	658	689	13			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			
4	d	341	Total	C	N	O	S	0	0	0
			2709	1798	441	458	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			657	429	106	122			
5	e	82	Total	C	N	O	0	0	0
			665	434	108	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	0	0
			1845	1154	309	378	4			
13	o	244	Total	C	N	O	S	0	0	0
			1853	1160	312	377	4			

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			774	491	129	154				
15	u	97	Total	C	N	O		0	0	0
			774	491	129	154				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

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

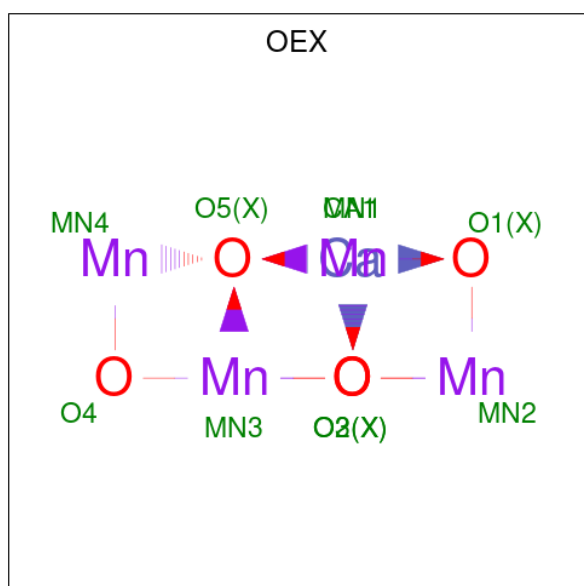
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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	34	Total	C	N	O		0	0	0
			273	186	47	40				

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



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

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

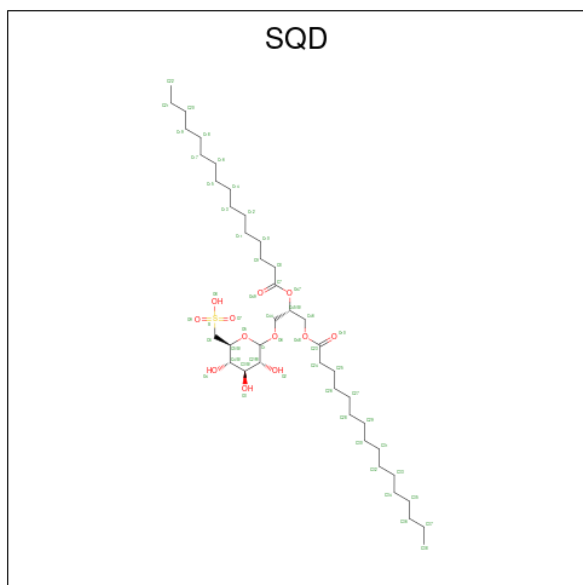
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).

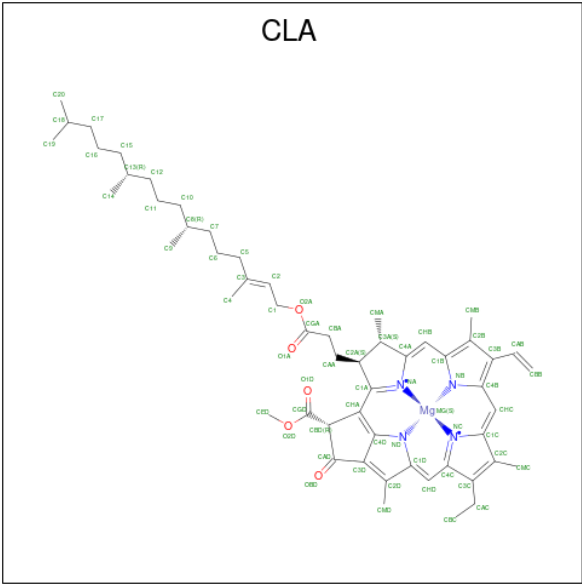


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	S	0	0
			52	39	12	1		
23	A	1	Total	C	O		0	0
			40	35	5			
23	B	1	Total	C	O	S	0	0
			54	41	12	1		
23	D	1	Total	C	O	S	0	0
			47	34	12	1		
23	D	1	Total	C	O	S	0	0
			43	30	12	1		
23	I	1	Total	C	O		0	0
			40	35	5			
23	b	1	Total	C	O	S	0	0
			54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

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

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 57 47 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 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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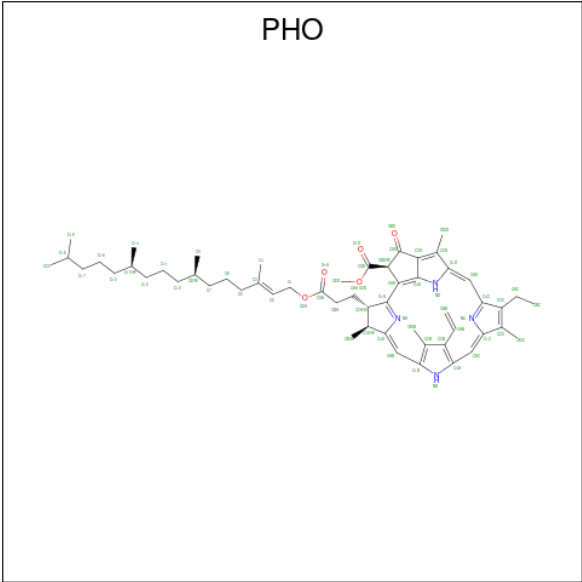
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 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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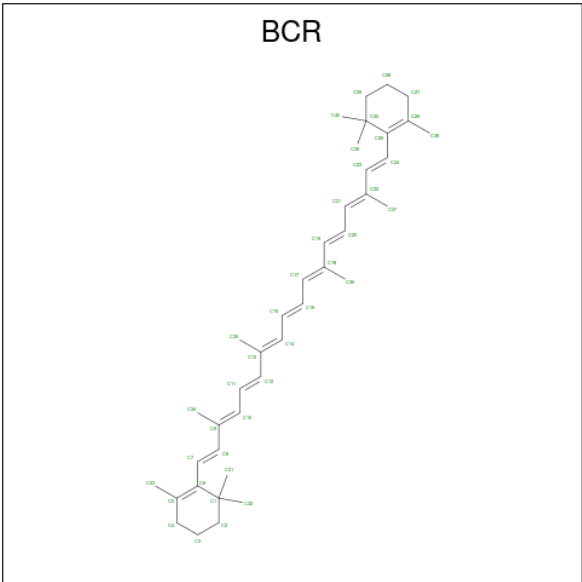
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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
			58	48	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 PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



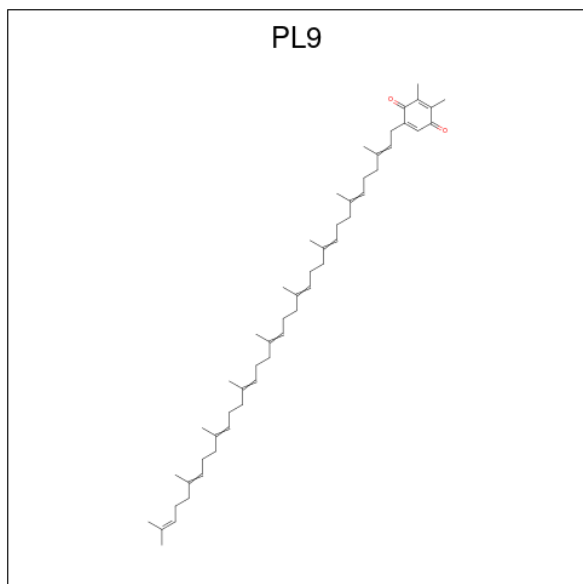
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



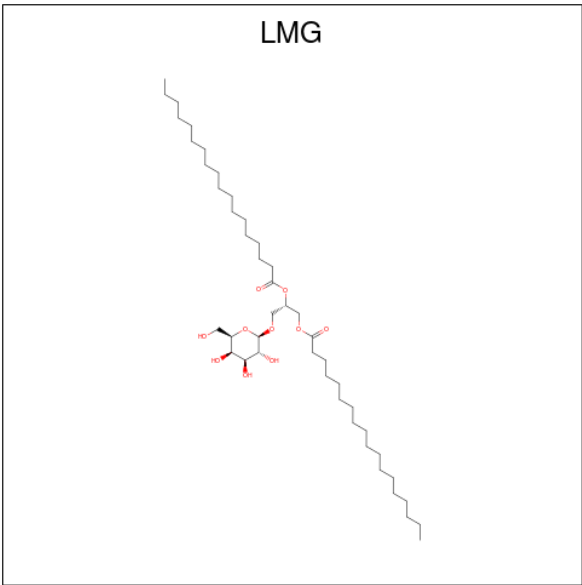
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	y	1	Total C 40 40	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C		0	0
			9	9			
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		

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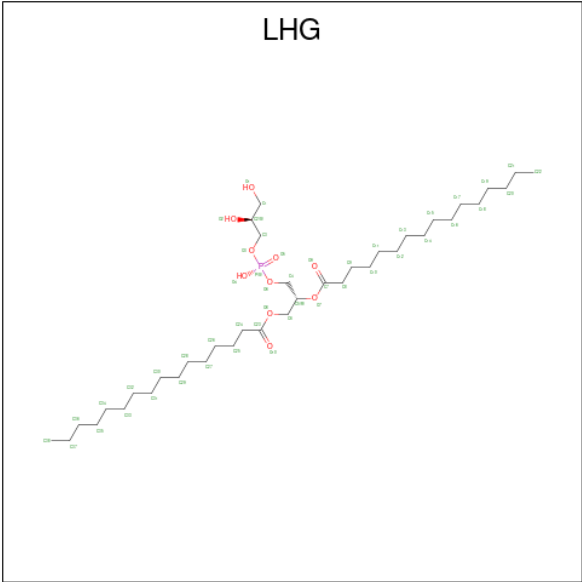
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	d	1	Total	C	O	0	0
			42	32	10		
29	d	1	Total	C	O	0	0
			40	35	5		

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

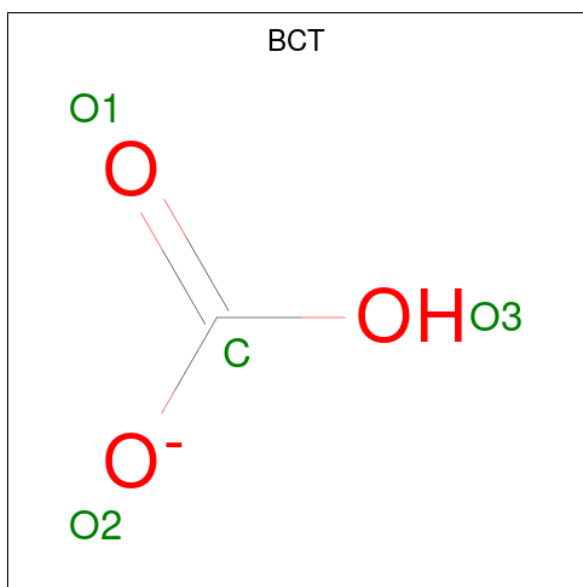
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C		0	0
			7	7			
30	B	3	Total	C		0	0
			28	28			
30	C	1	Total	C		0	0
			9	9			
30	H	1	Total	C		0	0
			8	8			
30	M	2	Total	C		0	0
			23	23			
30	b	2	Total	C		0	0
			26	26			
30	d	1	Total	C		0	0
			22	22			
30	i	1	Total	C		0	0
			12	12			
30	j	1	Total	C		0	0
			9	9			
30	m	2	Total	C		0	0
			21	21			
30	t	1	Total	C		0	0
			10	10			
30	z	1	Total	C		0	0
			11	11			

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



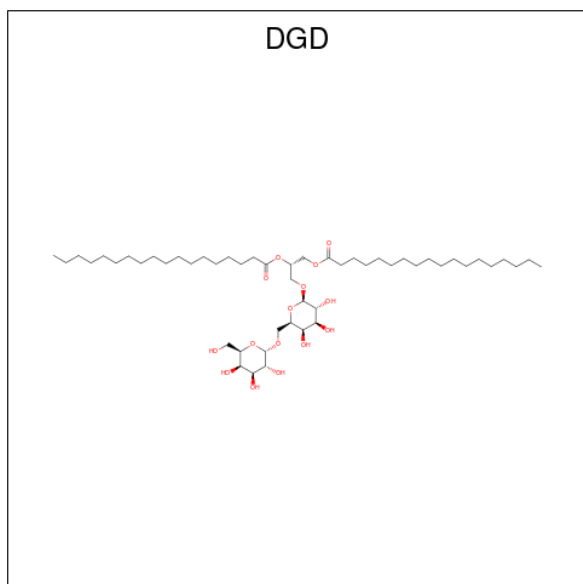
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			35	24	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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



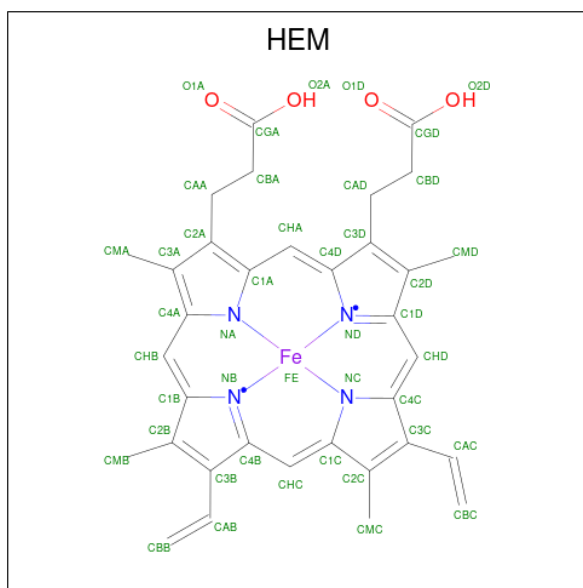
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		

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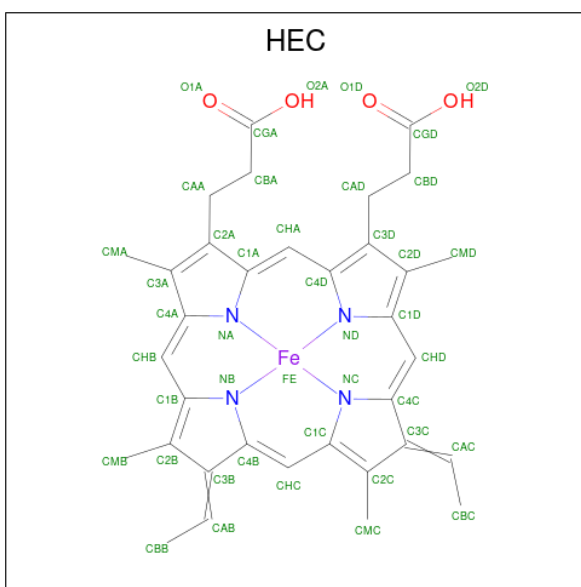
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

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



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	10	Total	O		
			10	10	0	0
36	B	17	Total	O		
			17	17	0	0
36	C	11	Total	O		
			11	11	0	0
36	D	9	Total	O		
			9	9	0	0
36	E	3	Total	O		
			3	3	0	0
36	L	2	Total	O		
			2	2	0	0
36	M	2	Total	O		
			2	2	0	0
36	O	5	Total	O		
			5	5	0	0
36	T	1	Total	O		
			1	1	0	0
36	V	2	Total	O		
			2	2	0	0

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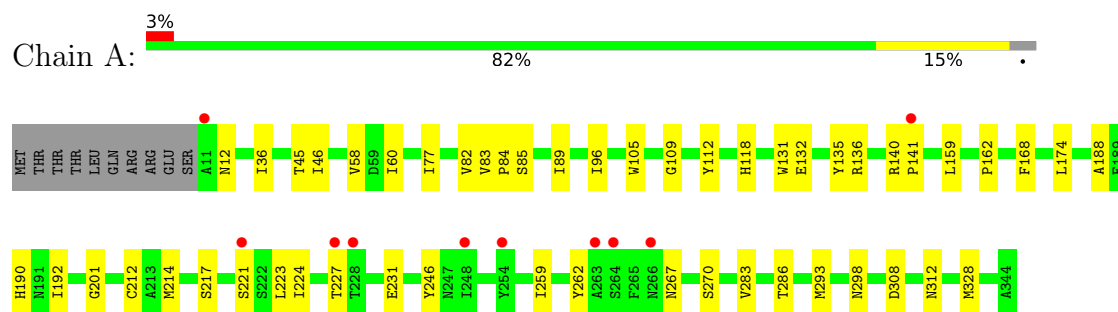
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	X	1	Total 1	O 1	0	0
36	Z	1	Total 1	O 1	0	0
36	a	11	Total 11	O 11	0	0
36	b	12	Total 12	O 12	0	0
36	c	11	Total 11	O 11	0	0
36	d	9	Total 9	O 9	0	0
36	i	1	Total 1	O 1	0	0
36	l	2	Total 2	O 2	0	0
36	o	9	Total 9	O 9	0	0
36	u	2	Total 2	O 2	0	0
36	v	3	Total 3	O 3	0	0

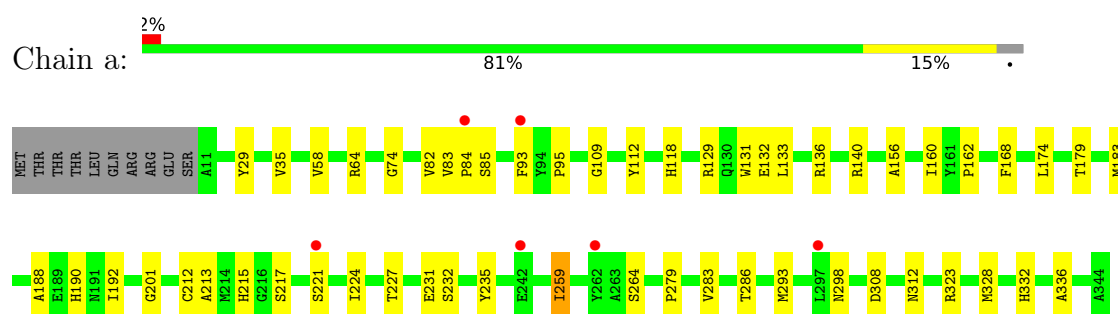
3 Residue-property plots [i](#)

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.

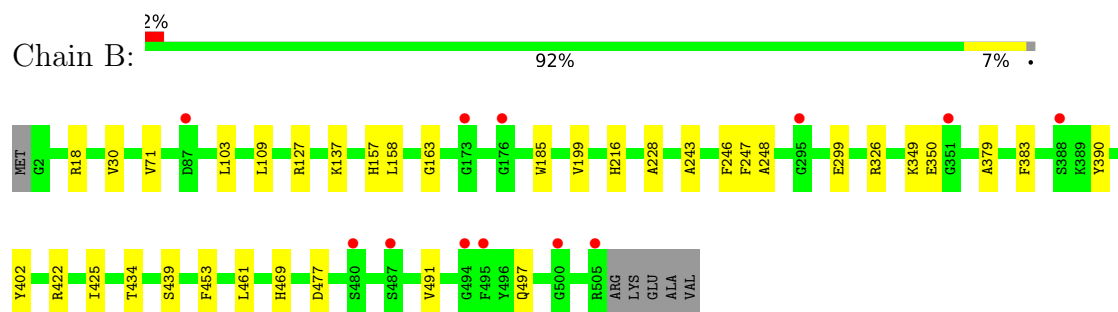
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

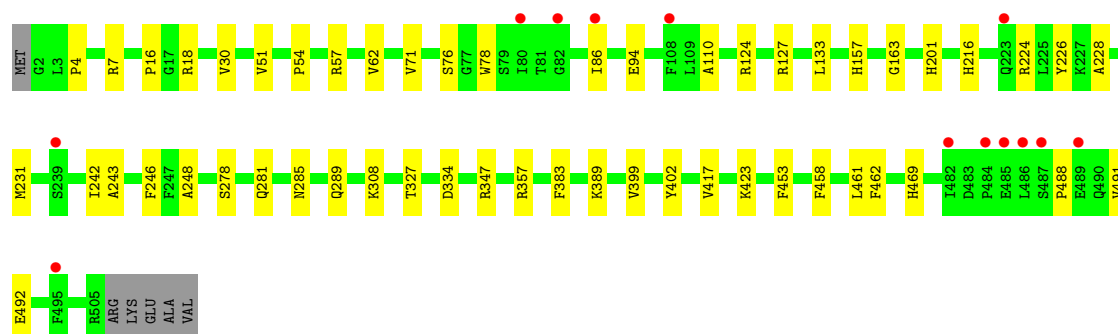


- Molecule 2: Photosystem II CP47 reaction center protein

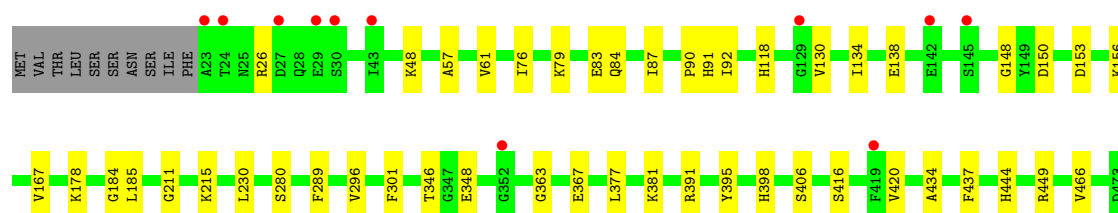
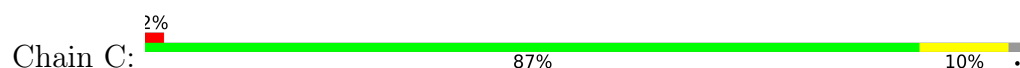


- Molecule 2: Photosystem II CP47 reaction center protein

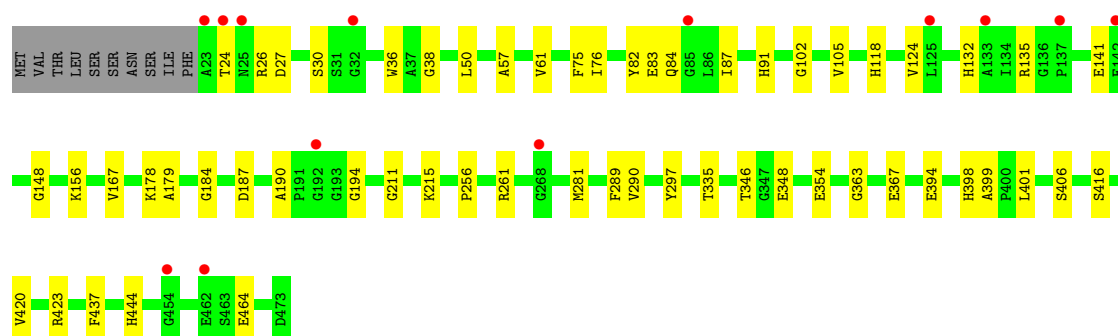
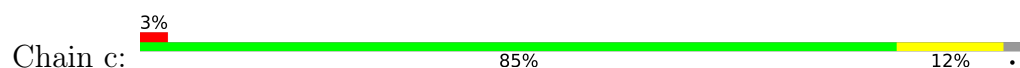




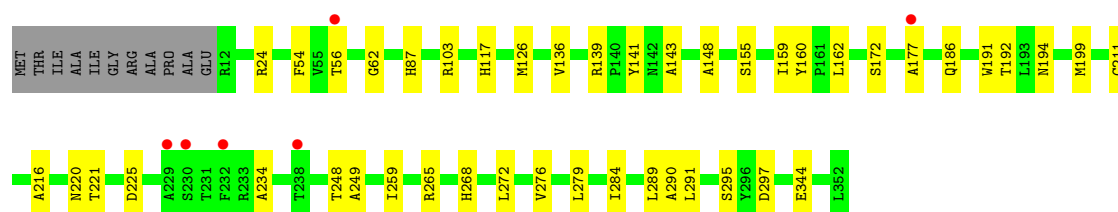
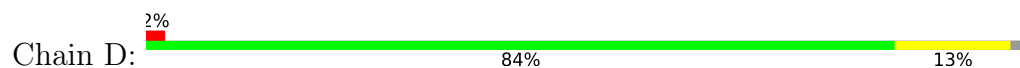
• Molecule 3: Photosystem II CP43 reaction center protein



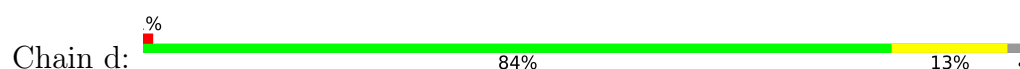
• Molecule 3: Photosystem II CP43 reaction center protein

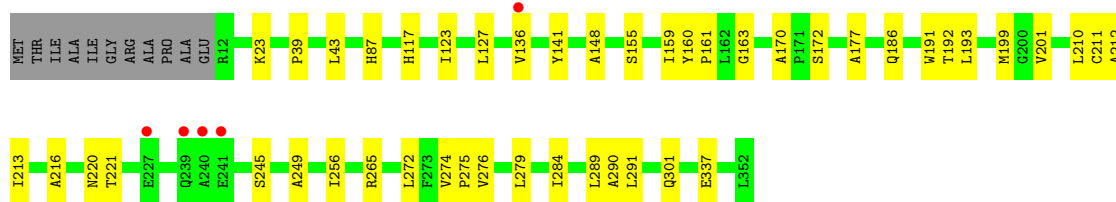


• Molecule 4: Photosystem II D2 protein

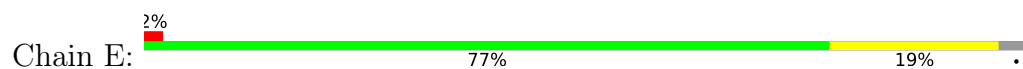


• Molecule 4: Photosystem II D2 protein

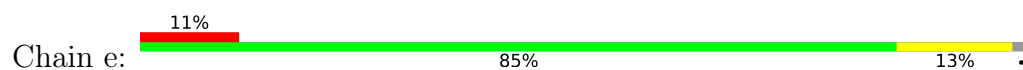




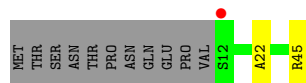
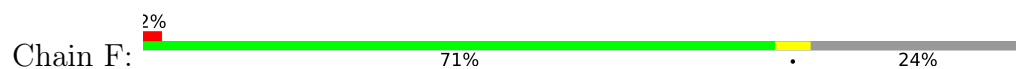
- Molecule 5: Cytochrome b559 subunit alpha



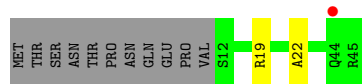
- Molecule 5: Cytochrome b559 subunit alpha



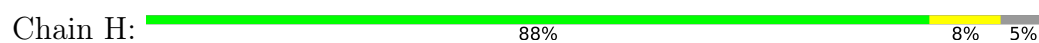
- Molecule 6: Cytochrome b559 subunit beta



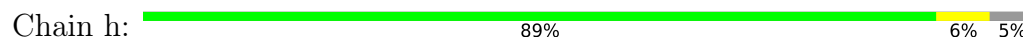
- Molecule 6: Cytochrome b559 subunit beta



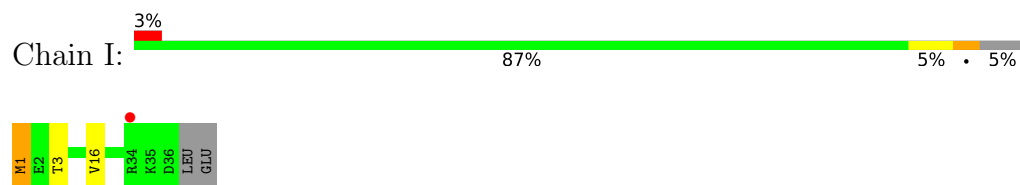
- Molecule 7: Photosystem II reaction center protein H



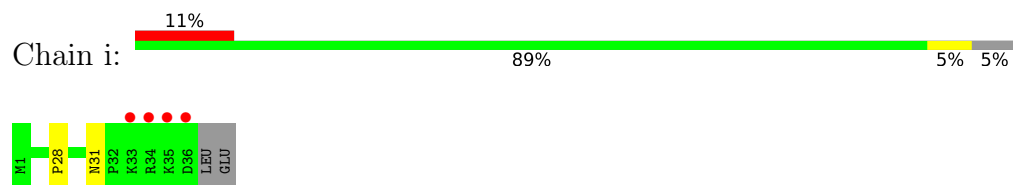
- Molecule 7: Photosystem II reaction center protein H



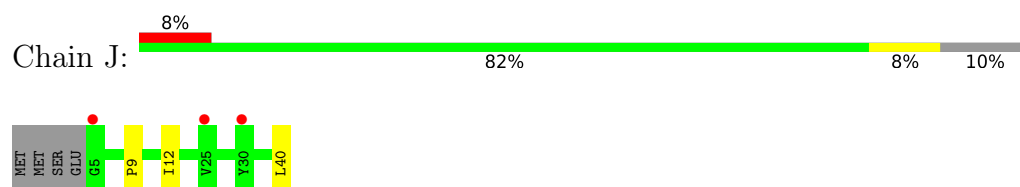
- Molecule 8: Photosystem II reaction center protein I



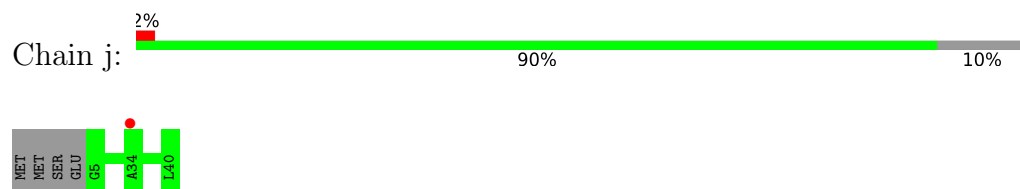
- Molecule 8: Photosystem II reaction center protein I



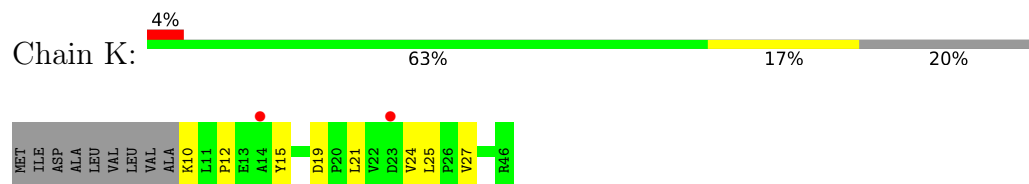
- Molecule 9: Photosystem II reaction center protein J



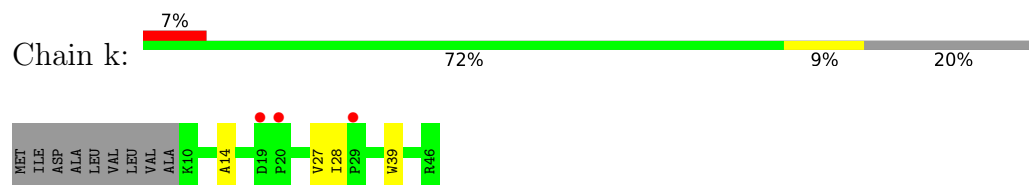
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

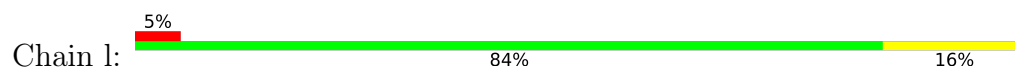


- Molecule 11: Photosystem II reaction center protein L

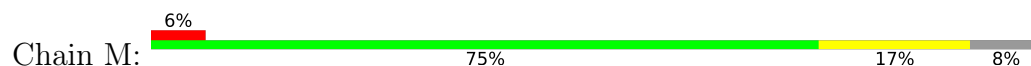




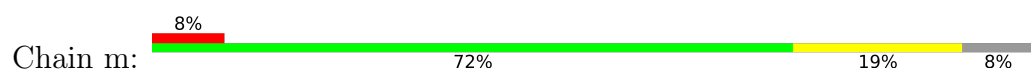
- Molecule 11: Photosystem II reaction center protein L



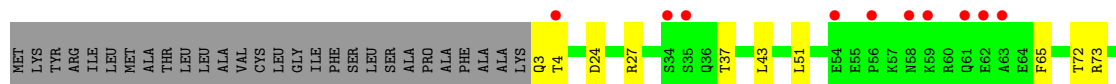
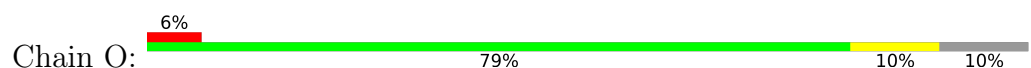
- Molecule 12: Photosystem II reaction center protein M



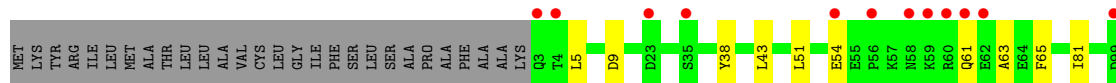
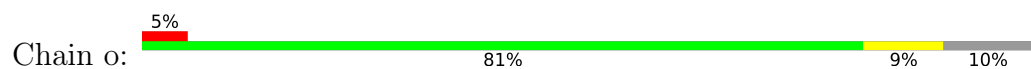
- Molecule 12: Photosystem II reaction center protein M



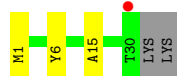
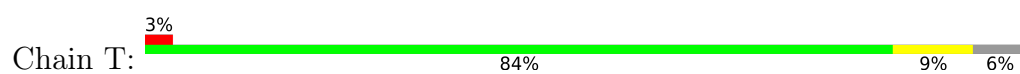
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



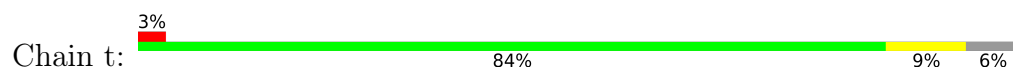
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



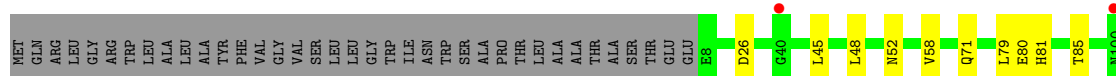
- Molecule 14: Photosystem II reaction center protein T



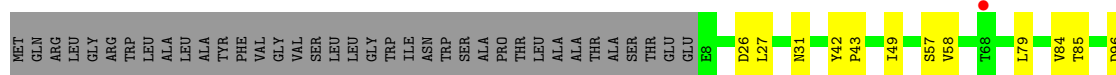
- Molecule 14: Photosystem II reaction center protein T



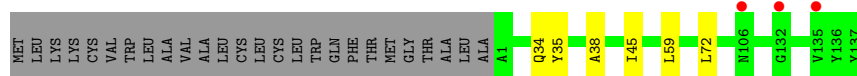
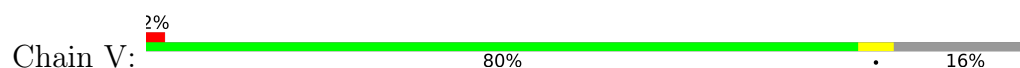
- Molecule 15: Photosystem II 12 kDa extrinsic protein



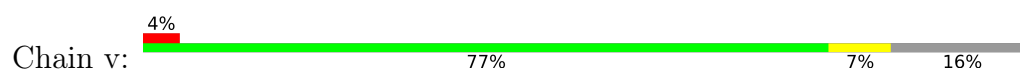
- Molecule 15: Photosystem II 12 kDa extrinsic protein



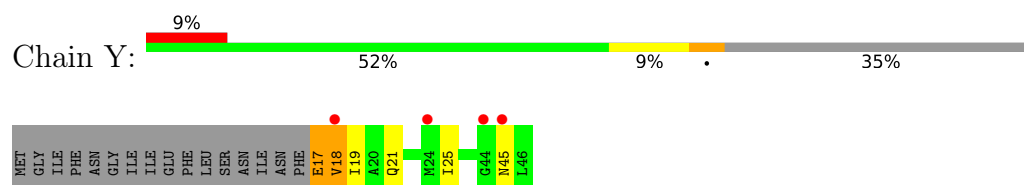
- Molecule 16: Cytochrome c-550



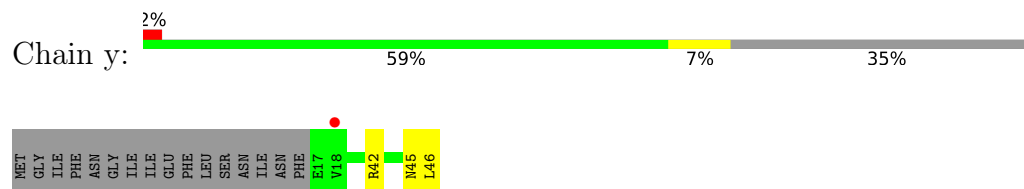
- Molecule 16: Cytochrome c-550



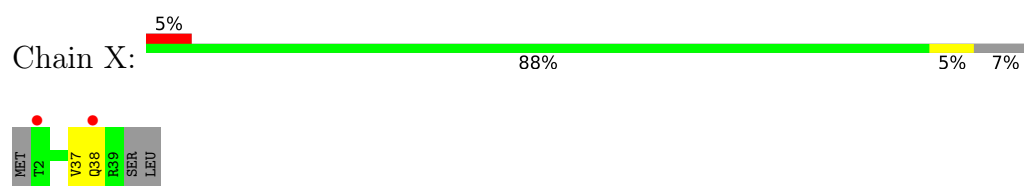
- Molecule 17: Photosystem II reaction center protein Ycf12



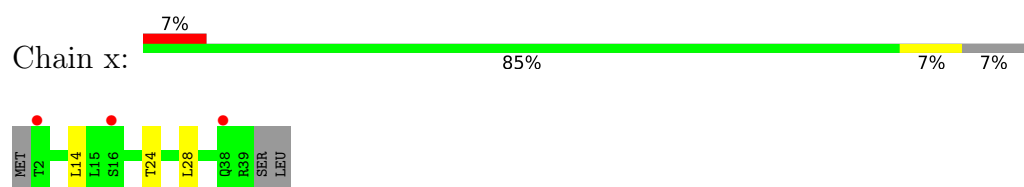
- Molecule 17: Photosystem II reaction center protein Ycf12



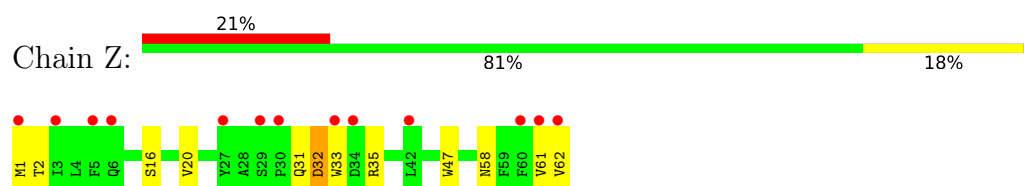
- Molecule 18: Photosystem II reaction center X protein



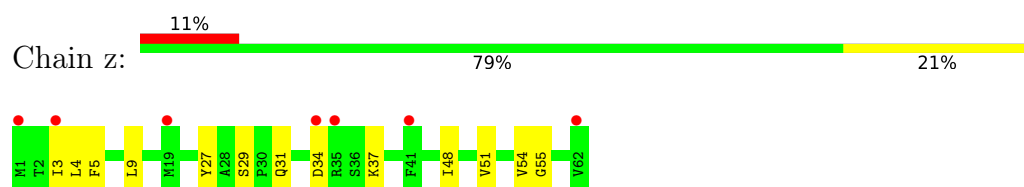
- Molecule 18: Photosystem II reaction center X protein



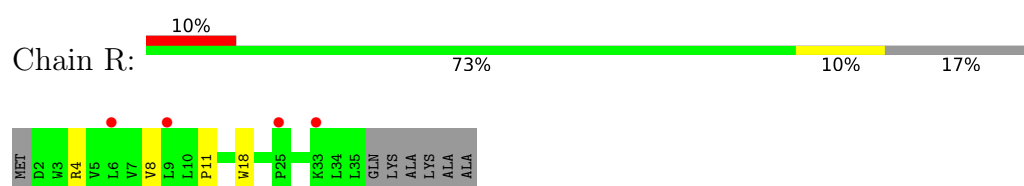
- Molecule 19: Photosystem II reaction center protein Z



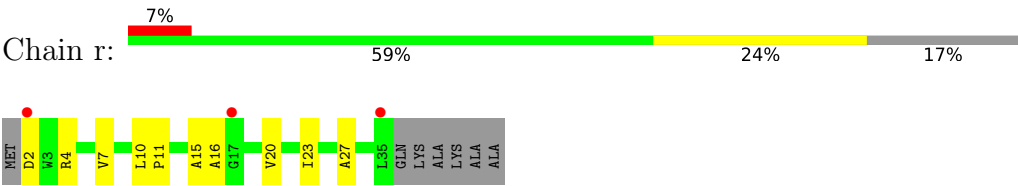
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.73Å 223.81Å 330.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 3.00 43.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.12-3.00) 86.2 (43.12-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_2411	Depositor
R, R_{free}	0.264 , 0.303 0.266 , 0.303	Depositor DCC
R_{free} test set	1446 reflections (0.83%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50162	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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: BCR, UNL, LMG, FME, CL, LHG, BCT, OEX, HEC, HEM, CLA, PL9, FE2, SQD, PHO, DGD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/2703	0.24	0/3687
1	a	0.08	0/2698	0.24	0/3681
2	B	0.09	0/4093	0.24	0/5580
2	b	0.08	0/4103	0.24	0/5593
3	C	0.08	0/3599	0.23	0/4900
3	c	0.09	0/3599	0.24	0/4900
4	D	0.08	0/2811	0.24	0/3830
4	d	0.09	0/2804	0.25	0/3821
5	E	0.17	0/676	0.26	0/924
5	e	0.10	0/684	0.27	0/933
6	F	0.08	0/283	0.23	0/386
6	f	0.08	0/283	0.24	0/386
7	H	0.09	0/511	0.25	0/697
7	h	0.11	0/511	0.25	0/697
8	I	0.09	0/293	0.23	0/396
8	i	0.09	0/293	0.24	0/396
9	J	0.09	0/263	0.28	0/356
9	j	0.07	0/263	0.22	0/356
10	K	0.12	0/303	0.31	0/416
10	k	0.11	0/303	0.30	0/416
11	L	0.09	0/308	0.24	0/419
11	l	0.07	0/308	0.22	0/419
12	M	0.08	0/249	0.21	0/341
12	m	0.08	0/249	0.26	0/341
13	O	0.09	0/1876	0.28	0/2549
13	o	0.08	0/1884	0.27	0/2557
14	T	0.07	0/257	0.24	0/349
14	t	0.08	0/257	0.24	0/349
15	U	0.08	0/785	0.26	0/1064
15	u	0.11	0/785	0.27	0/1064
16	V	0.09	0/1085	0.23	0/1473
16	v	0.11	0/1085	0.24	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.18	0/225	0.61	2/301 (0.7%)
17	y	0.10	0/225	0.29	0/301
18	X	0.06	0/282	0.16	0/381
18	x	0.11	0/284	0.26	0/384
19	Z	0.08	0/490	0.27	0/669
19	z	0.10	0/490	0.28	0/669
20	R	0.09	0/279	0.26	0/383
20	r	0.10	0/279	0.29	0/383
All	All	0.09	0/42758	0.25	2/58220 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	17	GLU	CA-C-N	6.13	132.74	121.70
17	Y	17	GLU	C-N-CA	6.13	132.74	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2618	0	2515	38	0
1	a	2613	0	2506	40	0
2	B	3953	0	3802	33	0
2	b	3960	0	3811	40	0
3	C	3486	0	3407	29	0
3	c	3486	0	3407	39	0
4	D	2716	0	2621	36	0
4	d	2709	0	2612	38	0
5	E	657	0	637	14	0
5	e	665	0	651	9	0
6	F	274	0	279	3	0
6	f	274	0	279	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	498	0	518	3	0
7	h	498	0	518	4	0
8	I	296	0	311	2	0
8	i	296	0	311	1	0
9	J	257	0	268	2	0
9	j	257	0	268	0	0
10	K	293	0	305	7	0
10	k	293	0	305	4	0
11	L	301	0	309	3	0
11	l	301	0	309	6	0
12	M	256	0	269	5	0
12	m	256	0	269	6	0
13	O	1845	0	1793	15	0
13	o	1853	0	1817	15	0
14	T	258	0	261	4	0
14	t	258	0	261	2	0
15	U	774	0	773	5	0
15	u	774	0	773	7	0
16	V	1064	0	1073	4	0
16	v	1064	0	1073	8	0
17	Y	224	0	252	5	0
17	y	224	0	252	4	0
18	X	279	0	307	2	0
18	x	281	0	312	2	0
19	Z	479	0	516	7	0
19	z	479	0	516	9	0
20	R	273	0	305	3	0
20	r	273	0	305	7	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	92	0	138	4	0
23	B	54	0	78	7	0
23	D	90	0	111	1	0
23	I	40	0	67	0	0
23	b	54	0	77	1	0
23	c	54	0	78	1	0
23	f	43	0	53	0	0
24	A	2	0	0	0	0
24	a	2	0	0	1	0
25	A	252	0	269	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	1040	0	1152	35	0
25	C	845	0	936	27	0
25	D	130	0	144	5	0
25	a	254	0	274	9	0
25	b	1040	0	1152	31	0
25	c	838	0	919	23	0
25	d	130	0	144	10	0
26	A	64	0	74	1	0
26	D	64	0	74	3	0
26	a	64	0	74	1	0
26	d	64	0	74	4	0
27	A	40	0	56	3	0
27	B	160	0	224	11	0
27	C	80	0	112	3	0
27	D	40	0	56	3	0
27	H	40	0	56	4	0
27	K	40	0	56	2	0
27	T	40	0	56	7	0
27	Y	40	0	56	1	0
27	a	40	0	56	3	0
27	b	120	0	168	8	0
27	c	80	0	112	7	0
27	d	40	0	56	2	0
27	h	40	0	56	2	0
27	k	40	0	56	2	0
27	y	40	0	56	3	0
28	A	55	0	80	4	0
28	D	55	0	80	2	0
28	a	55	0	80	4	0
28	d	55	0	80	5	0
29	A	102	0	144	2	0
29	B	153	0	216	3	0
29	C	102	0	144	3	0
29	D	51	0	72	2	0
29	b	111	0	158	5	0
29	c	153	0	216	5	0
29	d	82	0	115	3	0
30	A	7	0	0	0	0
30	B	28	0	0	0	0
30	C	9	0	0	0	0
30	H	8	0	0	0	0
30	M	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	26	0	0	0	0
30	d	22	0	0	0	0
30	i	12	0	0	0	0
30	j	9	0	0	0	0
30	m	21	0	0	0	0
30	t	10	0	0	0	0
30	z	11	0	0	0	0
31	A	147	0	222	12	0
31	D	49	0	74	1	0
31	L	49	0	74	3	0
31	a	126	0	171	4	0
31	d	49	0	74	2	0
31	l	49	0	74	5	0
32	A	4	0	0	1	0
32	a	4	0	0	0	0
33	C	186	0	246	5	0
33	H	62	0	82	2	0
33	c	186	0	246	3	0
33	h	62	0	82	3	0
34	E	43	0	30	3	0
34	e	43	0	30	3	0
35	V	43	0	30	1	0
35	v	43	0	29	2	0
36	A	10	0	0	0	0
36	B	17	0	0	0	0
36	C	11	0	0	0	0
36	D	9	0	0	0	0
36	E	3	0	0	0	0
36	L	2	0	0	0	0
36	M	2	0	0	0	0
36	O	5	0	0	0	0
36	T	1	0	0	0	0
36	V	2	0	0	0	0
36	X	1	0	0	0	0
36	Z	1	0	0	0	0
36	a	11	0	0	0	0
36	b	12	0	0	0	0
36	c	11	0	0	0	0
36	d	9	0	0	0	0
36	i	1	0	0	0	0
36	l	2	0	0	0	0
36	o	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	u	2	0	0	0	0
36	v	3	0	0	0	0
All	All	50162	0	51045	563	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 6.

All (563) 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)
31:a:613:LHG:O4	4:d:141:TYR:OH	1.90	0.88
2:B:157:HIS:HE1	25:B:606:CLA:NA	1.76	0.83
31:A:618:LHG:HC31	5:E:9:PRO:HB3	1.61	0.81
31:A:616:LHG:O4	4:D:141:TYR:OH	1.98	0.80
25:a:607:CLA:HAB	25:d:403:CLA:H72	1.69	0.74
29:C:519:LMG:H191	10:K:27:VAL:HG11	1.70	0.74
25:B:607:CLA:HAC2	27:B:627:BCR:H272	1.71	0.72
3:C:48:LYS:HE3	3:C:138:GLU:HG2	1.70	0.72
25:B:612:CLA:H171	25:B:613:CLA:HBB2	1.73	0.70
25:c:505:CLA:H172	25:c:512:CLA:HBB2	1.74	0.69
14:T:15:ALA:HB2	27:T:101:BCR:H14C	1.73	0.69
2:b:124:ARG:O	7:h:12:ARG:NH2	2.26	0.69
4:D:279:LEU:HD22	26:D:401:PHO:HBC3	1.72	0.69
1:a:217:SER:O	1:a:221:SER:OG	2.10	0.69
13:O:27:ARG:NH1	13:O:202:ALA:O	2.25	0.68
4:d:279:LEU:HD22	26:d:401:PHO:HBC3	1.76	0.67
12:M:24:ILE:HG12	12:m:24:ILE:HG12	1.78	0.66
1:a:201:GLY:HA3	1:a:286:THR:HB	1.78	0.66
1:a:227:THR:HB	1:a:231:GLU:HG3	1.76	0.66
5:e:40:THR:HB	20:r:4:ARG:HG2	1.77	0.65
20:r:2:ASP:OD2	20:r:4:ARG:NH1	2.30	0.65
2:B:469:HIS:HE1	25:B:611:CLA:NA	1.94	0.64
19:Z:32:ASP:HB2	19:Z:35:ARG:HE	1.63	0.64
13:O:24:ASP:OD1	13:O:203:LYS:NZ	2.31	0.63
4:d:192:THR:HG23	25:d:403:CLA:HBC2	1.80	0.63
1:A:224:ILE:O	4:D:265:ARG:NH2	2.32	0.63
5:e:26:THR:HA	20:r:15:ALA:HB1	1.79	0.63
23:A:603:SQD:H251	31:A:617:LHG:H131	1.81	0.62
31:A:617:LHG:H192	25:C:504:CLA:H202	1.80	0.62
5:E:45:ASP:OD2	20:R:4:ARG:NH2	2.33	0.62
4:D:192:THR:HG23	25:D:402:CLA:HBC2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:38:GLY:HA3	25:c:513:CLA:HMD2	1.82	0.61
2:B:127:ARG:NH2	7:H:18:TYR:O	2.30	0.61
25:B:604:CLA:H121	25:B:615:CLA:H42	1.82	0.61
3:c:27:ASP:OD1	3:c:30:SER:OG	2.18	0.61
27:c:516:BCR:HC41	19:z:55:GLY:HA2	1.80	0.61
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.82	0.60
4:d:186:GLN:HB2	25:d:403:CLA:HBC1	1.82	0.60
10:K:10:LYS:NZ	10:K:19:ASP:OD2	2.34	0.60
11:L:23:LEU:HD22	31:L:101:LHG:H122	1.82	0.60
25:a:609:CLA:H143	25:c:507:CLA:H192	1.83	0.60
31:A:616:LHG:H223	25:B:613:CLA:H192	1.84	0.60
4:d:127:LEU:HD13	29:d:409:LMG:H371	1.83	0.60
19:z:34:ASP:HA	19:z:37:LYS:HD3	1.84	0.60
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.83	0.60
16:v:66:ARG:NH2	16:v:80:THR:OG1	2.34	0.60
27:T:101:BCR:H272	25:b:610:CLA:HAC2	1.82	0.59
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.84	0.59
3:c:26:ARG:NH2	17:y:45:ASN:OD1	2.35	0.59
5:e:5:THR:OG1	5:e:7:GLU:OE1	2.18	0.59
5:e:30:LEU:HD11	34:e:101:HEM:HAB	1.84	0.59
13:o:51:LEU:HB2	13:o:234:LYS:HB3	1.84	0.59
13:O:158:ASP:OD1	13:O:162:ARG:N	2.27	0.59
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.84	0.59
4:d:87:HIS:HB2	33:h:102:DGD:HG11	1.85	0.59
3:C:26:ARG:NH2	17:Y:45:ASN:OD1	2.36	0.58
25:C:504:CLA:H42	33:C:517:DGD:HB42	1.85	0.58
31:A:617:LHG:H371	25:C:508:CLA:H92	1.84	0.58
27:T:101:BCR:H19C	27:b:621:BCR:H363	1.85	0.58
34:e:101:HEM:HBC2	34:e:101:HEM:HMC2	1.86	0.58
25:a:609:CLA:H171	25:c:508:CLA:H121	1.86	0.57
5:e:36:LEU:HD13	20:r:7:VAL:HG12	1.85	0.57
4:D:259:ILE:HD13	31:D:406:LHG:H262	1.86	0.57
3:c:167:VAL:HG13	25:c:514:CLA:H102	1.87	0.57
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.86	0.57
2:b:18:ARG:NH2	23:b:601:SQD:O8	2.31	0.57
25:C:501:CLA:H71	25:C:501:CLA:HBB1	1.86	0.57
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.86	0.57
2:B:497:GLN:NE2	18:X:38:GLN:O	2.38	0.57
34:E:101:HEM:HBB2	34:E:101:HEM:HMB2	1.87	0.57
3:c:83:GLU:OE2	3:c:398:HIS:NE2	2.34	0.57
8:i:28:PRO:O	8:i:31:ASN:ND2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:444:HIS:CE1	25:c:510:CLA:NA	2.73	0.56
25:C:511:CLA:H171	19:Z:20:VAL:HA	1.86	0.56
4:d:216:ALA:O	4:d:220:ASN:ND2	2.36	0.56
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.88	0.56
25:B:602:CLA:H172	33:H:103:DGD:HAT1	1.87	0.56
1:a:217:SER:HA	4:d:272:LEU:HD12	1.88	0.56
4:d:160:TYR:HA	4:d:290:ALA:HB2	1.87	0.56
23:A:619:SQD:H102	2:b:94:GLU:HG2	1.86	0.55
2:b:469:HIS:CE1	25:b:614:CLA:NA	2.74	0.55
34:E:101:HEM:HMC1	34:E:101:HEM:HBC2	1.88	0.55
25:B:604:CLA:HBB1	25:B:607:CLA:HAB	1.88	0.55
3:c:178:LYS:NZ	3:c:184:GLY:O	2.38	0.55
3:C:87:ILE:O	3:C:91:HIS:ND1	2.37	0.55
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.89	0.55
28:A:611:PL9:H403	6:F:22:ALA:HB2	1.89	0.55
2:B:185:TRP:HB3	25:B:601:CLA:HMA3	1.88	0.55
25:b:618:CLA:H93	25:b:619:CLA:H192	1.89	0.54
29:c:521:LMG:H192	10:k:27:VAL:HG11	1.90	0.54
4:d:221:THR:HG21	4:d:249:ALA:HB2	1.88	0.54
31:d:407:LHG:H131	28:d:408:PL9:H153	1.89	0.54
31:A:617:LHG:H352	31:A:617:LHG:H151	1.87	0.54
16:v:87:GLU:OE1	16:v:96:ARG:NH1	2.35	0.54
5:E:60:GLN:NE2	5:E:62:SER:O	2.40	0.54
3:c:135:ARG:HG2	19:z:27:TYR:CG	2.42	0.54
25:C:503:CLA:H172	25:C:510:CLA:HBB2	1.89	0.54
19:Z:1:MET:SD	19:Z:1:MET:N	2.81	0.54
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.90	0.54
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.33	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.43	0.54
1:A:131:TRP:CH2	25:C:505:CLA:HAA2	2.44	0.53
3:c:124:VAL:HB	27:c:516:BCR:H362	1.89	0.53
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.90	0.53
34:e:101:HEM:HBB2	34:e:101:HEM:HMB2	1.88	0.53
1:a:64:ARG:NH1	13:o:105:PRO:O	2.34	0.53
2:b:327:THR:HG22	25:b:610:CLA:H12	1.91	0.53
13:o:118:LEU:HD22	13:o:233:VAL:HG11	1.89	0.53
1:A:221:SER:OG	4:D:139:ARG:O	2.27	0.53
13:O:103:PHE:HB3	13:O:123:LYS:HE2	1.89	0.53
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.90	0.52
25:B:614:CLA:H121	23:B:626:SQD:H381	1.91	0.52
4:D:54:PHE:O	5:E:49:THR:OG1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:297:TYR:O	3:c:423:ARG:NH2	2.39	0.52
3:C:92:ILE:HD11	25:C:503:CLA:HED2	1.91	0.52
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.91	0.52
4:D:186:GLN:HB2	25:D:402:CLA:HBC1	1.91	0.52
15:U:26:ASP:OD2	15:U:85:THR:OG1	2.24	0.52
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.92	0.52
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.92	0.52
25:b:611:CLA:H162	25:d:404:CLA:HBA1	1.91	0.52
13:O:3:GLN:N	13:O:4:THR:HA	2.25	0.52
2:b:228:ALA:HB1	29:b:625:LMG:H111	1.92	0.52
13:O:189:ARG:NH1	13:O:226:GLY:O	2.43	0.52
3:C:444:HIS:CE1	25:C:508:CLA:NA	2.77	0.52
25:C:501:CLA:H193	25:C:507:CLA:HBB1	1.91	0.52
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.91	0.52
1:a:283:VAL:HA	1:a:286:THR:HG22	1.91	0.52
3:C:167:VAL:HG13	25:C:512:CLA:H102	1.92	0.52
11:L:12:LEU:HD12	31:L:101:LHG:HC11	1.93	0.51
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.91	0.51
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.75	0.51
3:c:281:MET:HG3	29:c:502:LMG:H421	1.91	0.51
4:D:62:GLY:HA3	5:E:63:ILE:HD13	1.92	0.51
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.75	0.51
17:y:42:ARG:HH21	19:z:29:SER:HB3	1.74	0.51
13:o:54:GLU:HG2	13:o:63:ALA:HB1	1.91	0.51
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.91	0.51
1:a:232:SER:OG	31:l:101:LHG:O5	2.28	0.51
3:c:346:THR:OG1	3:c:348:GLU:OE2	2.28	0.51
23:B:626:SQD:H162	23:B:626:SQD:H371	1.93	0.51
1:A:308:ASP:OD1	1:A:312:ASN:N	2.42	0.51
25:C:501:CLA:C3D	25:C:503:CLA:H2	2.40	0.51
25:a:612:CLA:HMA2	28:d:408:PL9:H402	1.93	0.51
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.92	0.51
4:D:221:THR:HG21	4:D:249:ALA:HB2	1.93	0.50
1:a:156:ALA:HA	1:a:160:ILE:HB	1.92	0.50
2:B:216:HIS:HE1	25:B:609:CLA:C1A	2.24	0.50
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.93	0.50
27:B:627:BCR:H14C	14:t:15:ALA:HB2	1.92	0.50
29:b:625:LMG:H112	29:d:409:LMG:H141	1.93	0.50
3:c:148:GLY:O	3:c:156:LYS:NZ	2.35	0.50
19:z:3:ILE:HG23	19:z:4:LEU:HD22	1.94	0.50
1:A:201:GLY:HA3	1:A:286:THR:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:611:PL9:H403	6:f:22:ALA:HB2	1.94	0.50
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.50
19:Z:31:GLN:O	19:Z:33:TRP:N	2.45	0.50
2:b:4:PRO:HD2	2:b:7:ARG:HD2	1.93	0.50
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.50
2:B:248:ALA:HA	25:B:603:CLA:H42	1.94	0.50
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.93	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.46	0.50
17:Y:17:GLU:HB3	17:Y:19:ILE:N	2.26	0.50
31:A:617:LHG:H211	33:C:518:DGD:HBN2	1.93	0.49
1:a:286:THR:OG1	25:a:606:CLA:O1D	2.21	0.49
2:b:285:ASN:O	2:b:289:GLN:HG2	2.12	0.49
3:c:437:PHE:HA	25:c:510:CLA:HMC2	1.93	0.49
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.46	0.49
4:D:117:HIS:CE1	25:D:403:CLA:NA	2.80	0.49
4:D:199:MET:HG2	28:D:407:PL9:H321	1.95	0.49
2:B:71:VAL:HG23	25:B:606:CLA:HMA2	1.94	0.49
25:B:608:CLA:H193	25:D:403:CLA:HAA2	1.93	0.49
25:C:502:CLA:H61	25:C:512:CLA:H42	1.94	0.49
1:A:118:HIS:CE1	25:A:609:CLA:NA	2.80	0.49
23:B:626:SQD:H361	27:B:627:BCR:H362	1.94	0.49
3:C:406:SER:HA	3:C:420:VAL:HG23	1.95	0.49
29:C:520:LMG:H331	29:C:520:LMG:H171	1.95	0.49
4:d:161:PRO:HB3	4:d:170:ALA:HB2	1.94	0.49
26:D:401:PHO:HBA2	25:D:402:CLA:H142	1.95	0.49
25:b:614:CLA:H71	31:l:101:LHG:H322	1.93	0.49
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.95	0.49
16:v:13:ASN:HD21	16:v:17:LYS:HD2	1.77	0.49
3:c:57:ALA:O	3:c:61:VAL:HG23	2.12	0.49
25:c:503:CLA:H71	25:c:503:CLA:HBB1	1.93	0.49
15:u:27:LEU:HD22	15:u:49:ILE:HG21	1.93	0.49
5:E:30:LEU:HD11	34:E:101:HEM:HAB	1.95	0.49
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.95	0.48
19:Z:61:VAL:HG23	19:Z:62:VAL:HG23	1.94	0.48
25:d:404:CLA:H172	18:x:14:LEU:HD23	1.95	0.48
15:u:104:LYS:HE3	16:v:45:ILE:HG22	1.95	0.48
1:A:262:TYR:CD2	31:A:618:LHG:HC42	2.48	0.48
2:B:18:ARG:NH2	23:B:626:SQD:O7	2.36	0.48
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.48
2:b:423:LYS:NZ	13:o:175:PRO:O	2.46	0.48
25:c:511:CLA:H161	25:c:514:CLA:HMD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:36:LEU:O	5:e:40:THR:OG1	2.26	0.48
5:E:60:GLN:HG2	5:E:62:SER:H	1.79	0.48
2:B:185:TRP:HD1	29:B:621:LMG:HC2	1.79	0.48
25:B:614:CLA:H62	25:B:614:CLA:H41	1.59	0.48
3:C:61:VAL:HG13	3:C:118:HIS:HD2	1.78	0.48
3:C:90:PRO:HB3	3:C:301:PHE:HB3	1.95	0.48
9:J:9:PRO:HD2	9:J:12:ILE:HD12	1.95	0.48
2:b:71:VAL:HG23	25:b:609:CLA:HMA2	1.96	0.48
13:o:162:ARG:NH1	13:o:186:ASN:OD1	2.45	0.48
25:B:601:CLA:H92	27:H:102:BCR:H402	1.96	0.48
3:C:148:GLY:O	3:C:156:LYS:NZ	2.45	0.48
29:c:502:LMG:H121	25:c:507:CLA:H202	1.96	0.48
11:L:23:LEU:HD13	31:L:101:LHG:H171	1.96	0.47
4:d:87:HIS:O	7:h:50:ASN:ND2	2.44	0.47
1:A:132:GLU:O	1:A:136:ARG:HG2	2.13	0.47
25:A:609:CLA:H193	25:C:505:CLA:H13	1.96	0.47
2:b:201:HIS:HE2	25:b:606:CLA:C2B	2.27	0.47
3:c:464:GLU:OE2	4:d:245:SER:OG	2.32	0.47
1:A:283:VAL:HA	1:A:286:THR:HG22	1.96	0.47
3:c:76:ILE:O	3:c:84:GLN:NE2	2.42	0.47
5:e:57:ALA:HB3	5:e:60:GLN:HB3	1.96	0.47
29:A:613:LMG:H422	27:T:101:BCR:HC7	1.97	0.47
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.49	0.47
2:B:477:ASP:OD1	2:B:477:ASP:N	2.46	0.47
25:b:616:CLA:OBD	25:b:617:CLA:HHC	2.15	0.47
4:d:155:SER:HA	4:d:159:ILE:HB	1.97	0.47
25:b:605:CLA:H101	25:b:612:CLA:H18	1.95	0.47
25:b:619:CLA:H11	25:b:619:CLA:H52	1.72	0.47
25:B:616:CLA:H141	25:B:616:CLA:H161	1.70	0.47
29:C:520:LMG:O2	29:C:520:LMG:HC71	2.15	0.47
4:D:225:ASP:HB2	4:D:234:ALA:HB1	1.97	0.47
27:D:404:BCR:H383	29:D:405:LMG:H161	1.95	0.47
28:a:611:PL9:H251	28:a:611:PL9:H272	1.53	0.47
20:r:16:ALA:O	20:r:20:VAL:HG23	2.14	0.47
1:A:227:THR:HB	1:A:231:GLU:HG3	1.96	0.47
2:B:109:LEU:HD13	29:B:625:LMG:H311	1.97	0.47
3:C:178:LYS:NZ	3:C:184:GLY:O	2.47	0.47
3:C:363:GLY:O	3:C:367:GLU:HG2	2.15	0.46
25:a:609:CLA:H202	25:c:508:CLA:H102	1.97	0.46
13:O:37:THR:OG1	13:O:246:ALA:OXT	2.31	0.46
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:458:PHE:HB3	25:b:607:CLA:HBC2	1.96	0.46
3:c:187:ASP:HB3	3:c:190:ALA:HB2	1.97	0.46
23:A:619:SQD:H262	23:A:619:SQD:H292	1.65	0.46
3:C:377:LEU:HG	3:C:381:LYS:HE2	1.97	0.46
3:C:466:VAL:HG21	4:D:248:THR:HG23	1.98	0.46
32:A:620:BCT:O3	4:D:268:HIS:CE1	2.67	0.46
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.51	0.46
15:u:57:SER:HA	15:u:84:VAL:HG21	1.98	0.46
1:A:223:LEU:HD23	1:A:246:TYR:HB3	1.98	0.46
25:A:607:CLA:HED1	33:C:518:DGD:HAT1	1.98	0.46
2:b:248:ALA:HA	25:b:606:CLA:H42	1.97	0.46
25:b:615:CLA:H162	25:b:615:CLA:H122	1.72	0.46
4:d:199:MET:HG2	28:d:408:PL9:H321	1.98	0.46
31:d:407:LHG:HC62	11:l:15:THR:HG23	1.97	0.46
27:B:627:BCR:HC8	14:t:18:PHE:HB2	1.97	0.46
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.50	0.46
29:c:502:LMG:H382	33:c:518:DGD:HA81	1.97	0.46
10:K:15:TYR:OH	19:Z:58:ASN:OD1	2.23	0.46
1:A:267:ASN:HB3	1:A:270:SER:HB3	1.98	0.46
27:H:102:BCR:H24C	27:H:102:BCR:H371	1.79	0.46
1:a:259:ILE:HA	31:a:615:LHG:H201	1.98	0.46
26:d:401:PHO:HMB2	25:d:403:CLA:H101	1.97	0.46
1:A:286:THR:OG1	25:A:606:CLA:O1D	2.23	0.46
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.97	0.46
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.97	0.46
1:a:131:TRP:CH2	25:c:507:CLA:HAA2	2.51	0.46
2:b:334:ASP:OD1	2:b:334:ASP:N	2.48	0.46
15:u:31:ASN:ND2	15:u:96:ASP:O	2.46	0.46
25:B:606:CLA:H91	25:B:606:CLA:H112	1.77	0.46
10:K:24:VAL:HG11	17:Y:25:ILE:HB	1.98	0.46
2:b:16:PRO:HB3	2:b:133:LEU:HD11	1.98	0.46
29:b:624:LMG:H331	29:b:624:LMG:H361	1.72	0.46
1:A:217:SER:HA	4:D:272:LEU:HD12	1.98	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
14:T:1:FME:HE3	12:m:6:LEU:HD21	1.99	0.45
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.97	0.45
2:b:278:SER:HB3	2:b:281:GLN:HB3	1.98	0.45
27:H:102:BCR:H20C	27:H:102:BCR:H361	1.80	0.45
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.99	0.45
25:b:619:CLA:H141	25:b:619:CLA:H161	1.72	0.45
4:d:201:VAL:HG22	25:d:403:CLA:C1B	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:r:10:LEU:HB3	20:r:11:PRO:HD3	1.98	0.45
1:A:46:ILE:HD12	27:A:610:BCR:H15C	1.99	0.45
1:A:190:HIS:O	1:A:298:ASN:HB3	2.16	0.45
25:B:602:CLA:H62	25:B:602:CLA:H41	1.79	0.45
3:c:102:GLY:N	3:c:194:GLY:O	2.33	0.45
25:c:503:CLA:H142	25:c:503:CLA:H112	1.77	0.45
4:d:117:HIS:CE1	25:d:404:CLA:NA	2.85	0.45
31:A:617:LHG:H331	31:A:617:LHG:H361	1.69	0.45
25:C:505:CLA:H141	8:I:16:VAL:HG22	1.99	0.45
25:a:609:CLA:H91	25:a:609:CLA:H111	1.84	0.45
31:a:613:LHG:H361	25:b:616:CLA:H51	1.98	0.45
27:y:101:BCR:H20C	27:y:101:BCR:H361	1.84	0.45
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.52	0.45
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.98	0.45
25:C:505:CLA:H93	25:C:505:CLA:H111	1.73	0.45
1:a:279:PRO:HG2	4:d:212:ALA:HB2	1.99	0.45
25:b:613:CLA:H142	25:b:615:CLA:H2	1.98	0.45
1:A:214:MET:HB3	28:A:611:PL9:H103	1.99	0.45
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.98	0.45
4:D:155:SER:HA	4:D:159:ILE:HB	1.98	0.45
10:K:25:LEU:HD22	27:Y:101:BCR:H332	1.99	0.45
25:b:604:CLA:HMA3	29:b:624:LMG:H291	1.99	0.45
3:c:363:GLY:O	3:c:367:GLU:HG2	2.17	0.45
27:h:101:BCR:H15C	27:h:101:BCR:H351	1.85	0.45
25:C:504:CLA:H151	25:C:508:CLA:H143	1.99	0.45
27:D:404:BCR:H361	27:D:404:BCR:H20C	1.81	0.45
27:T:101:BCR:H15C	27:T:101:BCR:H351	1.81	0.45
19:Z:16:SER:OG	19:Z:47:TRP:NE1	2.43	0.45
1:a:132:GLU:O	1:a:136:ARG:HG2	2.17	0.45
2:b:347:ARG:NH2	2:b:402:TYR:OH	2.38	0.45
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.50	0.44
1:a:29:TYR:O	1:a:129:ARG:NH2	2.35	0.44
1:A:131:TRP:HD1	1:A:141:PRO:HB2	1.83	0.44
2:B:228:ALA:HB1	23:D:408:SQD:H262	1.98	0.44
27:B:618:BCR:H20C	27:B:618:BCR:H361	1.85	0.44
1:a:74:GLY:O	4:d:301:GLN:NE2	2.44	0.44
1:a:308:ASP:OD1	1:a:312:ASN:N	2.50	0.44
27:d:405:BCR:H15C	27:d:405:BCR:H351	1.90	0.44
5:E:25:ILE:HD11	20:R:18:TRP:HB3	1.99	0.44
1:a:35:VAL:HG13	27:a:610:BCR:HC31	1.99	0.44
25:d:404:CLA:HBA1	25:d:404:CLA:H3A	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:8:ARG:O	6:f:19:ARG:NH2	2.46	0.44
25:C:505:CLA:H43	27:C:515:BCR:HC7	1.99	0.44
25:b:617:CLA:H41	25:b:617:CLA:H62	1.66	0.44
3:c:50:LEU:HD11	25:c:515:CLA:HBB1	1.99	0.44
26:d:401:PHO:HBA2	26:d:401:PHO:H3A	1.81	0.44
15:u:42:TYR:HA	15:u:43:PRO:HA	1.75	0.44
33:C:516:DGD:HAT2	33:C:516:DGD:HAH1	1.80	0.44
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.52	0.44
2:b:127:ARG:NH2	7:h:18:TYR:O	2.43	0.44
25:b:615:CLA:HBA1	25:b:615:CLA:H3A	1.90	0.44
3:c:256:PRO:O	3:c:261:ARG:NH1	2.51	0.44
1:a:133:LEU:HD23	4:d:256:ILE:HG12	2.00	0.44
1:a:213:ALA:HB2	4:d:275:PRO:HG2	1.97	0.44
25:c:503:CLA:H203	25:c:509:CLA:H111	2.00	0.44
25:c:515:CLA:H141	25:c:515:CLA:H162	1.76	0.44
1:A:45:THR:HG21	29:A:613:LMG:H241	1.98	0.44
1:A:270:SER:OG	23:A:603:SQD:O49	2.30	0.44
31:A:617:LHG:H132	31:A:617:LHG:H372	2.00	0.44
25:B:610:CLA:H202	25:B:610:CLA:H161	1.83	0.44
25:B:616:CLA:H11	25:B:616:CLA:H51	1.74	0.44
25:c:503:CLA:H203	25:c:509:CLA:H13	2.00	0.44
27:c:517:BCR:H20C	27:c:517:BCR:H361	1.87	0.44
13:o:224:ASP:HB3	13:o:227:ALA:HB3	1.99	0.44
20:r:23:ILE:O	20:r:27:ALA:N	2.50	0.44
25:B:614:CLA:H162	25:B:614:CLA:H141	1.63	0.44
27:C:515:BCR:H371	27:C:515:BCR:H24C	1.82	0.44
26:D:401:PHO:H112	26:D:401:PHO:H72	1.86	0.44
25:c:503:CLA:C2D	25:c:505:CLA:H2	2.48	0.44
3:C:57:ALA:O	3:C:61:VAL:HG23	2.17	0.44
29:D:405:LMG:H351	29:D:405:LMG:H382	1.72	0.44
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.00	0.44
26:d:401:PHO:HBA2	25:d:403:CLA:H142	1.99	0.44
28:d:408:PL9:H221	28:d:408:PL9:H201	1.84	0.44
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.99	0.44
18:x:24:THR:O	18:x:28:LEU:HD12	2.17	0.43
3:C:211:GLY:O	3:C:215:LYS:HG3	2.18	0.43
10:K:12:PRO:HB2	10:K:15:TYR:HD1	1.83	0.43
1:a:58:VAL:HB	1:a:83:VAL:HB	2.00	0.43
2:b:399:VAL:HG12	2:b:417:VAL:HG22	2.00	0.43
27:A:610:BCR:H24C	27:A:610:BCR:H371	1.80	0.43
5:E:23:HIS:HA	5:E:26:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:212:CYS:HB2	4:d:211:CYS:HB2	2.00	0.43
3:c:141:GLU:HA	3:c:148:GLY:HA3	2.00	0.43
4:d:39:PRO:O	4:d:43:LEU:HG	2.19	0.43
13:o:38:TYR:HD1	13:o:245:PRO:HA	1.83	0.43
2:B:157:HIS:HA	2:B:163:GLY:HA3	2.01	0.43
1:a:336:ALA:O	3:c:354:GLU:HG3	2.18	0.43
3:c:335:THR:O	13:o:152:ARG:NH2	2.52	0.43
4:d:123:ILE:HD11	33:h:102:DGD:HAW1	2.01	0.43
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.01	0.43
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.54	0.43
2:B:103:LEU:HD21	25:B:605:CLA:HMC3	2.01	0.43
2:B:137:LYS:NZ	7:H:17:GLU:OE2	2.45	0.43
28:D:407:PL9:H351	28:D:407:PL9:H371	1.67	0.43
1:a:264:SER:OG	28:a:611:PL9:O2	2.36	0.43
27:a:610:BCR:H20C	27:a:610:BCR:H361	1.85	0.43
2:b:54:PRO:HD2	2:b:57:ARG:HG3	2.00	0.43
25:b:611:CLA:H141	25:b:611:CLA:H161	1.85	0.43
2:B:30:VAL:HG11	25:B:612:CLA:H112	1.99	0.43
2:B:299:GLU:HG2	2:B:402:TYR:HD2	1.84	0.43
3:C:76:ILE:O	3:C:84:GLN:NE2	2.44	0.43
6:F:45:ARG:NH2	9:J:40:LEU:OXT	2.46	0.43
3:c:132:HIS:CE1	25:c:515:CLA:NA	2.86	0.43
29:c:522:LMG:O2	29:c:522:LMG:HC71	2.18	0.43
17:y:42:ARG:NH2	19:z:31:GLN:HB2	2.34	0.43
26:A:608:PHO:H61	26:A:608:PHO:H2	1.74	0.43
25:C:506:CLA:H93	25:C:506:CLA:H112	1.77	0.43
25:C:513:CLA:H141	25:C:513:CLA:H162	1.80	0.43
13:O:72:THR:HG23	13:O:107:THR:HB	2.01	0.43
15:U:48:LEU:O	15:U:52:ASN:ND2	2.38	0.43
3:C:437:PHE:HA	25:C:508:CLA:HMC2	2.01	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.19	0.43
25:B:608:CLA:H62	25:B:609:CLA:H112	2.01	0.43
27:k:101:BCR:H15C	27:k:101:BCR:H351	1.89	0.43
25:B:610:CLA:H142	25:B:612:CLA:H2	2.01	0.43
25:C:509:CLA:HBA2	25:C:509:CLA:H93	2.01	0.43
7:H:62:TRP:O	7:H:64:ALA:N	2.52	0.43
12:M:28:GLN:HB3	12:m:27:VAL:HG12	2.01	0.43
16:V:45:ILE:H	16:V:45:ILE:HG13	1.71	0.43
2:B:469:HIS:HE1	25:B:611:CLA:C1A	2.32	0.42
25:B:602:CLA:H92	25:B:602:CLA:H61	1.76	0.42
23:B:626:SQD:H111	23:B:626:SQD:H242	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:274:VAL:HG22	28:d:408:PL9:H222	2.01	0.42
25:B:602:CLA:H111	25:B:602:CLA:H151	1.86	0.42
2:b:242:ILE:HG23	2:b:462:PHE:HD2	1.83	0.42
25:b:615:CLA:H13	25:b:616:CLA:HAB	2.01	0.42
27:b:621:BCR:H24C	27:b:621:BCR:H371	1.87	0.42
27:c:516:BCR:H15C	27:c:516:BCR:H351	1.83	0.42
27:c:517:BCR:H15C	27:c:517:BCR:H351	1.84	0.42
12:m:17:VAL:HB	12:m:18:PRO:HD3	2.00	0.42
2:B:383:PHE:N	4:D:344:GLU:O	2.39	0.42
27:B:617:BCR:H15C	27:B:617:BCR:H351	1.84	0.42
8:I:1:FME:O1	8:I:3:THR:N	2.52	0.42
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.55	0.42
2:b:357:ARG:NH2	4:d:337:GLU:O	2.52	0.42
2:b:389:LYS:HE3	2:b:389:LYS:HB2	1.87	0.42
3:c:179:ALA:HA	3:c:184:GLY:HA2	2.01	0.42
25:B:609:CLA:H92	25:B:609:CLA:H62	1.81	0.42
1:a:179:THR:O	1:a:183:MET:HG3	2.20	0.42
27:b:622:BCR:H15C	27:b:622:BCR:H351	1.88	0.42
29:b:623:LMG:H411	31:l:101:LHG:H362	2.00	0.42
1:A:12:ASN:OD1	1:A:12:ASN:N	2.52	0.42
2:B:247:PHE:HB2	25:B:608:CLA:HBC1	2.01	0.42
3:C:79:LYS:HB2	3:C:84:GLN:NE2	2.34	0.42
2:B:349:LYS:HG3	2:B:350:GLU:HG3	2.01	0.42
3:C:79:LYS:HD2	16:V:35:TYR:HE1	1.83	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.02	0.42
4:D:194:ASN:HA	4:D:295:SER:HB2	2.01	0.42
3:c:82:TYR:OH	3:c:394:GLU:OE2	2.31	0.42
3:c:211:GLY:O	3:c:215:LYS:HG3	2.20	0.42
16:v:81:THR:OG1	16:v:83:ASP:OD1	2.37	0.42
19:z:48:ILE:O	19:z:51:VAL:HG12	2.19	0.42
31:A:618:LHG:H141	31:A:618:LHG:H112	1.92	0.42
25:b:619:CLA:H142	27:b:622:BCR:H12C	2.01	0.42
27:b:620:BCR:H11C	27:b:620:BCR:H341	1.93	0.42
3:c:290:VAL:O	3:c:423:ARG:NH1	2.44	0.42
4:d:23:LYS:NZ	29:d:409:LMG:HC91	2.35	0.42
27:B:617:BCR:H383	23:B:626:SQD:H91	2.01	0.42
3:C:296:VAL:HG11	25:C:501:CLA:HMA2	2.02	0.42
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.85	0.42
4:D:126:MET:HE3	4:D:143:ALA:O	2.20	0.42
13:O:99:ASP:OD1	13:O:100:GLY:N	2.53	0.42
1:a:118:HIS:CE1	25:a:609:CLA:NA	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:405:BCR:H11C	27:d:405:BCR:H341	1.92	0.42
28:A:611:PL9:HC8	28:A:611:PL9:HC2	1.81	0.42
15:U:80:GLU:HG3	15:U:81:HIS:CD2	2.55	0.42
16:V:59:LEU:HD13	16:V:72:LEU:HD21	2.02	0.42
25:b:615:CLA:H61	25:b:615:CLA:H102	1.80	0.42
27:c:517:BCR:H11C	27:c:517:BCR:H341	1.95	0.42
11:l:22:LEU:HG	31:l:101:LHG:H181	2.02	0.42
13:o:5:LEU:HD22	13:o:9:ASP:HB3	2.02	0.42
16:v:45:ILE:H	16:v:45:ILE:HG13	1.68	0.42
25:B:614:CLA:H142	23:B:626:SQD:H372	2.01	0.42
12:M:20:VAL:HG11	12:m:20:VAL:HG22	2.01	0.42
10:k:28:ILE:HD13	27:y:101:BCR:HC8	2.01	0.42
25:B:605:CLA:H62	25:B:605:CLA:H41	1.89	0.41
5:E:17:VAL:O	5:E:21:VAL:HG23	2.20	0.41
13:O:214:THR:HA	13:O:238:VAL:HA	2.00	0.41
3:c:61:VAL:HG12	3:c:118:HIS:O	2.20	0.41
27:k:101:BCR:H20C	27:k:101:BCR:H361	1.82	0.41
11:l:7:ARG:HE	11:l:7:ARG:HB3	1.71	0.41
13:o:158:ASP:OD1	13:o:162:ARG:N	2.39	0.41
1:A:58:VAL:HB	1:A:83:VAL:HB	2.01	0.41
27:B:618:BCR:H24C	27:B:618:BCR:H371	1.86	0.41
1:a:332:HIS:HA	24:a:603:CL:CL	2.57	0.41
25:b:607:CLA:H41	25:b:607:CLA:H62	1.74	0.41
27:c:517:BCR:H24C	27:c:517:BCR:H371	1.83	0.41
25:C:501:CLA:H203	25:C:507:CLA:H111	2.02	0.41
27:D:404:BCR:H15C	27:D:404:BCR:H351	1.87	0.41
5:E:25:ILE:HG13	5:E:26:THR:N	2.34	0.41
16:V:34:GLN:HA	16:V:38:ALA:HB2	2.01	0.41
1:a:235:TYR:OH	11:l:11:GLU:OE1	2.27	0.41
2:b:216:HIS:HE1	25:b:612:CLA:CHA	2.33	0.41
25:c:505:CLA:H101	25:c:505:CLA:H62	1.81	0.41
27:B:619:BCR:H15C	27:B:619:BCR:H351	1.87	0.41
2:b:30:VAL:HG12	25:b:608:CLA:HHD	2.02	0.41
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.01	0.41
13:O:188:LYS:HB3	13:O:225:MET:HB3	2.03	0.41
17:Y:18:VAL:O	17:Y:21:GLN:N	2.53	0.41
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.55	0.41
2:b:76:SER:HG	2:b:78:TRP:CD1	2.38	0.41
2:b:216:HIS:HE1	25:b:612:CLA:C1A	2.34	0.41
25:b:612:CLA:HAB	27:h:101:BCR:H323	2.02	0.41
15:u:26:ASP:OD2	15:u:85:THR:OG1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.84	0.41
25:A:615:CLA:H121	25:A:615:CLA:HMA1	2.03	0.41
27:B:619:BCR:H20C	27:B:619:BCR:H361	1.83	0.41
35:V:201:HEC:HHH	35:V:201:HEC:CBC	2.51	0.41
3:c:444:HIS:HE1	25:c:510:CLA:C1A	2.34	0.41
2:B:216:HIS:HE1	25:B:609:CLA:NA	2.12	0.41
27:B:627:BCR:H11C	27:B:627:BCR:H341	1.94	0.41
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.01	0.41
33:C:517:DGD:HBN1	33:C:517:DGD:HBW1	1.81	0.41
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.01	0.41
12:M:27:VAL:HG12	12:m:28:GLN:HB3	2.03	0.41
17:Y:17:GLU:HA	17:Y:18:VAL:HB	2.03	0.41
25:a:609:CLA:H161	25:a:609:CLA:H122	1.93	0.41
2:b:110:ALA:HB2	27:b:622:BCR:H17C	2.02	0.41
2:b:453:PHE:HB2	4:d:291:LEU:HD12	2.02	0.41
4:d:193:LEU:O	11:l:34:TYR:OH	2.26	0.41
33:h:102:DGD:HB62	33:h:102:DGD:HB91	1.64	0.41
1:A:36:ILE:HG23	25:A:609:CLA:HBB1	2.01	0.41
1:a:323:ARG:NH1	16:v:137:TYR:OXT	2.52	0.41
27:a:610:BCR:H11C	27:a:610:BCR:H341	1.94	0.41
2:b:488:PRO:O	2:b:492:GLU:HB2	2.20	0.41
5:e:27:ILE:HB	5:e:28:PRO:HD3	2.02	0.41
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.02	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.46	0.41
3:C:130:VAL:O	3:C:134:ILE:HG12	2.21	0.41
3:C:346:THR:OG1	3:C:348:GLU:OE2	2.32	0.41
4:D:87:HIS:HB2	33:H:103:DGD:HG11	2.03	0.41
4:D:216:ALA:O	4:D:220:ASN:ND2	2.45	0.41
20:R:8:VAL:O	20:R:11:PRO:HD2	2.21	0.41
1:a:174:LEU:HD22	26:a:608:PHO:H151	2.03	0.41
1:a:224:ILE:O	4:d:265:ARG:NH2	2.54	0.41
2:b:86:ILE:H	2:b:86:ILE:HG13	1.77	0.41
3:c:61:VAL:HG13	3:c:118:HIS:HD2	1.85	0.41
3:c:87:ILE:O	3:c:91:HIS:ND1	2.43	0.41
10:k:39:TRP:NE1	17:y:46:LEU:O	2.42	0.41
27:y:101:BCR:H371	27:y:101:BCR:H24C	1.86	0.41
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.03	0.41
1:A:308:ASP:O	6:F:45:ARG:HD2	2.21	0.41
25:A:609:CLA:H51	25:A:609:CLA:H8	1.86	0.41
29:B:620:LMG:H401	12:M:17:VAL:HG21	2.03	0.41
1:a:190:HIS:O	1:a:298:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:62:VAL:HB	25:b:608:CLA:HED3	2.02	0.41
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.56	0.41
27:b:622:BCR:H24C	27:b:622:BCR:H371	1.92	0.41
3:c:135:ARG:HD2	3:c:135:ARG:HA	1.89	0.41
23:c:501:SQD:H332	23:c:501:SQD:H361	1.98	0.41
16:v:64:PRO:HD2	16:v:66:ARG:NH2	2.36	0.41
1:A:135:TYR:CE1	3:C:449:ARG:HB3	2.56	0.40
27:A:610:BCR:H11C	27:A:610:BCR:H341	1.96	0.40
28:A:611:PL9:HC8	28:A:611:PL9:H121	1.67	0.40
25:C:503:CLA:H101	25:C:503:CLA:H62	1.81	0.40
3:c:399:ALA:O	3:c:401:LEU:N	2.52	0.40
33:c:519:DGD:HBE2	33:c:519:DGD:HBF2	1.84	0.40
10:K:21:LEU:O	10:K:25:LEU:HG	2.21	0.40
27:T:101:BCR:H361	27:T:101:BCR:H20C	1.82	0.40
1:a:85:SER:HA	1:a:109:GLY:HA3	2.02	0.40
2:b:461:LEU:HD21	4:d:284:ILE:HD11	2.03	0.40
25:c:511:CLA:O1A	25:c:511:CLA:H2A	2.21	0.40
33:c:519:DGD:HAH2	33:c:519:DGD:HA81	2.02	0.40
25:B:601:CLA:H93	25:B:601:CLA:H111	1.75	0.40
1:a:215:HIS:ND1	28:a:611:PL9:O1	2.40	0.40
25:b:605:CLA:H61	25:b:605:CLA:H92	1.73	0.40
25:c:509:CLA:H162	25:c:509:CLA:H141	1.77	0.40
10:k:14:ALA:HB1	19:z:5:PHE:CE2	2.56	0.40
35:v:201:HEC:HHD	35:v:201:HEC:CBC	2.51	0.40
35:v:201:HEC:HHD	35:v:201:HEC:HBC2	2.03	0.40
2:B:453:PHE:HB2	4:D:291:LEU:HD12	2.03	0.40
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.57	0.40
25:C:506:CLA:H192	25:C:506:CLA:H161	1.83	0.40
27:K:101:BCR:H11C	27:K:101:BCR:H341	1.99	0.40
13:o:103:PHE:HB3	13:o:123:LYS:HE2	2.03	0.40
2:B:434:THR:HG22	2:B:439:SER:HB2	2.02	0.40
3:C:280:SER:OG	3:C:434:ALA:O	2.34	0.40
25:C:508:CLA:H162	25:C:508:CLA:H122	1.86	0.40
27:H:102:BCR:H15C	27:H:102:BCR:H351	1.86	0.40
27:K:101:BCR:H15C	27:K:101:BCR:H351	1.85	0.40
14:T:15:ALA:HA	27:T:101:BCR:H12C	2.03	0.40
31:a:614:LHG:H101	3:c:36:TRP:CE3	2.56	0.40
27:b:620:BCR:H20C	27:b:620:BCR:H361	1.85	0.40
4:d:163:GLY:HA3	4:d:290:ALA:HB1	2.03	0.40
11:l:26:VAL:HG11	31:l:101:LHG:H201	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	36	70
1	a	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	36	70
2	B	502/510 (98%)	483 (96%)	19 (4%)	0	100	100
2	b	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
3	C	449/461 (97%)	436 (97%)	12 (3%)	1 (0%)	43	76
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	30	65
4	D	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
4	d	339/352 (96%)	324 (96%)	15 (4%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	7	34
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	242/272 (89%)	228 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	232 (96%)	9 (4%)	1 (0%)	30	65
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	90 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2	16
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	36/41 (88%)	32 (89%)	4 (11%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	17
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5240/5700 (92%)	5040 (96%)	190 (4%)	10 (0%)	43	76

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Y	18	VAL
19	Z	32	ASP
13	o	61	GLN
3	C	416	SER
7	H	63	LYS
3	c	24	THR
3	c	416	SER
19	Z	2	THR
1	A	259	ILE
1	a	259	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	269/280 (96%)	269 (100%)	0	100	100
1	a	268/280 (96%)	268 (100%)	0	100	100
2	B	398/407 (98%)	398 (100%)	0	100	100
2	b	400/407 (98%)	400 (100%)	0	100	100
3	C	352/362 (97%)	351 (100%)	1 (0%)	86	91
3	c	352/362 (97%)	351 (100%)	1 (0%)	86	91
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	274/283 (97%)	274 (100%)	0	100	100
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
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
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	200/228 (88%)	200 (100%)	0	100	100
13	o	202/228 (89%)	202 (100%)	0	100	100
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	117 (100%)	0	100	100
17	Y	23/37 (62%)	23 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
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%)	52 (100%)	0	100	100
19	z	52/52 (100%)	52 (100%)	0	100	100
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	29/33 (88%)	29 (100%)	0	100	100
All	All	4313/4654 (93%)	4311 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	289	PHE
3	c	289	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	296	ASN
1	A	315	ASN
2	B	216	HIS
2	B	223	GLN
2	B	289	GLN
2	B	331	ASN
3	C	201	ASN
4	D	332	GLN
6	F	44	GLN
11	L	6	ASN
13	O	88	ASN
13	O	231	HIS
17	Y	21	GLN
19	Z	31	GLN
19	Z	38	GLN

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Mol	Chain	Res	Type
1	a	165	GLN
1	a	261	GLN
1	a	296	ASN
1	a	315	ASN
1	a	338	ASN
2	b	216	HIS
2	b	289	GLN
2	b	317	ASN
2	b	374	ASN
3	c	201	ASN
4	d	186	GLN
4	d	322	ASN
4	d	332	GLN
4	d	334	GLN
10	k	40	GLN
12	m	5	GLN
13	o	104	GLN
13	o	124	ASN
13	o	147	ASN
13	o	231	HIS
16	v	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.88	0	8,9,11	1.65	2 (25%)
8	FME	i	1	8	8,9,10	0.96	0	8,9,11	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	1.00	0
12	FME	M	1	12	8,9,10	0.97	0	8,9,11	1.02	1 (12%)
14	FME	t	1	14	8,9,10	0.97	0	8,9,11	1.12	1 (12%)
14	FME	T	1	14	8,9,10	0.96	0	8,9,11	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	C-CA-N	3.42	116.10	109.50
8	I	1	FME	CA-N-CN	2.44	126.57	122.82
14	t	1	FME	CB-CA-N	2.28	114.67	110.52
12	M	1	FME	CB-CA-N	2.03	114.22	110.52

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	FME	1	0
14	T	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 6 are monoatomic and 17 are unknown - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	CLA	c	503	-	69,73,73	1.12	6 (8%)	82,113,113	1.19	7 (8%)
25	CLA	b	613	36	69,73,73	1.13	5 (7%)	82,113,113	1.12	6 (7%)
25	CLA	c	507	-	69,73,73	1.13	7 (10%)	82,113,113	1.16	6 (7%)
27	BCR	H	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
29	LMG	A	613	-	51,51,55	0.70	0	59,59,63	1.48	9 (15%)
25	CLA	C	508	-	69,73,73	1.13	6 (8%)	82,113,113	1.19	6 (7%)
33	DGD	h	102	-	63,63,67	0.86	1 (1%)	77,77,81	1.33	8 (10%)
23	SQD	A	603	-	50,52,54	0.97	3 (6%)	60,63,65	1.53	11 (18%)
27	BCR	k	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
25	CLA	c	506	36	69,73,73	1.12	7 (10%)	82,113,113	1.19	6 (7%)
29	LMG	c	502	-	51,51,55	0.76	2 (3%)	59,59,63	1.34	6 (10%)
25	CLA	A	606	-	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
25	CLA	b	617	-	69,73,73	1.13	6 (8%)	82,113,113	1.17	4 (4%)
26	PHO	a	608	-	58,69,69	2.18	9 (15%)	55,99,99	1.43	7 (12%)
25	CLA	B	616	-	69,73,73	1.13	7 (10%)	82,113,113	1.20	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	609	-	69,73,73	1.14	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	a	607	36	63,67,73	1.19	7 (11%)	74,105,113	1.20	7 (9%)
25	CLA	C	504	36	69,73,73	1.12	7 (10%)	82,113,113	1.17	5 (6%)
25	CLA	B	613	-	69,73,73	1.13	6 (8%)	82,113,113	1.22	5 (6%)
23	SQD	D	409	-	41,43,54	1.07	3 (7%)	51,54,65	1.56	10 (19%)
31	LHG	l	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
25	CLA	b	616	-	69,73,73	1.14	7 (10%)	82,113,113	1.21	6 (7%)
25	CLA	b	608	-	69,73,73	1.13	7 (10%)	82,113,113	1.16	6 (7%)
25	CLA	C	506	-	69,73,73	1.14	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	c	511	-	69,73,73	1.13	6 (8%)	82,113,113	1.22	5 (6%)
25	CLA	C	511	3	69,73,73	1.14	5 (7%)	82,113,113	1.23	6 (7%)
25	CLA	C	512	-	69,73,73	1.13	6 (8%)	82,113,113	1.22	5 (6%)
26	PHO	d	401	-	58,69,69	2.18	9 (15%)	55,99,99	1.43	6 (10%)
29	LMG	d	409	-	39,39,55	0.58	1 (2%)	41,41,63	1.30	3 (7%)
25	CLA	B	612	-	69,73,73	1.12	7 (10%)	82,113,113	1.21	6 (7%)
25	CLA	C	509	-	69,73,73	1.13	6 (8%)	82,113,113	1.20	5 (6%)
25	CLA	a	609	-	69,73,73	1.12	7 (10%)	82,113,113	1.14	7 (8%)
27	BCR	b	621	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	4 (7%)
31	LHG	a	613	-	48,48,48	0.63	1 (2%)	51,54,54	1.30	6 (11%)
27	BCR	d	405	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
27	BCR	B	627	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	6 (10%)
31	LHG	D	406	-	48,48,48	0.63	2 (4%)	51,54,54	1.26	6 (11%)
25	CLA	B	605	-	69,73,73	1.13	7 (10%)	82,113,113	1.15	4 (4%)
27	BCR	c	516	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	6 (10%)
25	CLA	C	513	-	69,73,73	1.13	5 (7%)	82,113,113	1.16	6 (7%)
33	DGD	c	520	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	11 (14%)
29	LMG	b	623	-	51,51,55	0.72	0	59,59,63	1.36	7 (11%)
23	SQD	B	626	-	52,54,54	0.95	3 (5%)	62,65,65	1.60	12 (19%)
23	SQD	D	408	-	45,47,54	1.01	2 (4%)	55,58,65	1.72	11 (20%)
25	CLA	b	605	-	69,73,73	1.13	6 (8%)	82,113,113	1.13	5 (6%)
27	BCR	C	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	7 (12%)
25	CLA	C	505	-	69,73,73	1.13	7 (10%)	82,113,113	1.17	6 (7%)
27	BCR	Y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	4 (7%)
27	BCR	B	617	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	8 (14%)
25	CLA	b	609	-	69,73,73	1.12	6 (8%)	82,113,113	1.19	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	e	101	5,6	50,50,50	1.46	10 (20%)	67,82,82	1.09	5 (7%)
25	CLA	B	606	-	69,73,73	1.14	6 (8%)	82,113,113	1.21	6 (7%)
27	BCR	B	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	8 (14%)
27	BCR	D	404	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	7 (12%)
29	LMG	A	612	-	51,51,55	0.72	1 (1%)	59,59,63	1.31	4 (6%)
25	CLA	c	512	-	69,73,73	1.13	6 (8%)	82,113,113	1.18	5 (6%)
25	CLA	b	618	-	69,73,73	1.14	7 (10%)	82,113,113	1.23	7 (8%)
27	BCR	C	515	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	7 (12%)
25	CLA	b	604	36	69,73,73	1.14	6 (8%)	82,113,113	1.22	6 (7%)
25	CLA	B	615	-	69,73,73	1.14	6 (8%)	82,113,113	1.23	5 (6%)
33	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	8 (10%)
35	HEC	V	201	16	46,50,50	1.86	7 (15%)	58,82,82	1.13	3 (5%)
29	LMG	C	519	-	51,51,55	0.72	1 (1%)	59,59,63	1.33	6 (10%)
25	CLA	b	615	-	69,73,73	1.13	8 (11%)	82,113,113	1.20	6 (7%)
28	PL9	d	408	-	55,55,55	0.99	4 (7%)	68,69,69	1.48	11 (16%)
28	PL9	D	407	-	55,55,55	0.98	4 (7%)	68,69,69	1.51	13 (19%)
27	BCR	c	517	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
25	CLA	C	501	-	69,73,73	1.13	5 (7%)	82,113,113	1.20	5 (6%)
25	CLA	c	505	-	69,73,73	1.14	6 (8%)	82,113,113	1.23	5 (6%)
25	CLA	a	606	-	69,73,73	1.13	6 (8%)	82,113,113	1.15	7 (8%)
26	PHO	D	401	-	58,69,69	2.18	9 (15%)	55,99,99	1.44	6 (10%)
31	LHG	A	618	-	48,48,48	0.66	2 (4%)	51,54,54	1.27	7 (13%)
33	DGD	H	103	-	63,63,67	0.87	1 (1%)	77,77,81	1.34	7 (9%)
29	LMG	B	621	-	51,51,55	0.72	0	59,59,63	1.39	6 (10%)
25	CLA	c	514	-	69,73,73	1.13	6 (8%)	82,113,113	1.24	7 (8%)
29	LMG	b	624	-	51,51,55	0.74	0	59,59,63	1.31	6 (10%)
25	CLA	C	502	-	69,73,73	1.13	7 (10%)	82,113,113	1.20	6 (7%)
25	CLA	C	503	-	69,73,73	1.14	6 (8%)	82,113,113	1.23	5 (6%)
31	LHG	A	616	-	48,48,48	0.63	2 (4%)	51,54,54	1.29	6 (11%)
25	CLA	b	611	-	69,73,73	1.12	7 (10%)	82,113,113	1.15	5 (6%)
25	CLA	B	603	-	69,73,73	1.12	7 (10%)	82,113,113	1.13	6 (7%)
25	CLA	d	404	-	69,73,73	1.13	5 (7%)	82,113,113	1.19	6 (7%)
25	CLA	B	602	-	69,73,73	1.12	6 (8%)	82,113,113	1.13	6 (7%)
25	CLA	c	513	3	69,73,73	1.13	5 (7%)	82,113,113	1.25	5 (6%)
25	CLA	c	515	-	69,73,73	1.13	6 (8%)	82,113,113	1.17	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	7 (12%)
29	LMG	B	625	-	51,51,55	0.83	3 (5%)	59,59,63	1.41	8 (13%)
27	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	7 (12%)
23	SQD	I	101	-	39,39,54	0.87	2 (5%)	41,41,65	1.20	2 (4%)
23	SQD	f	101	-	41,43,54	1.07	3 (7%)	51,54,65	1.58	11 (21%)
21	OEX	A	601	36,3,1	0,15,15	-	-	-	-	-
29	LMG	b	625	-	8,8,55	0.14	0	7,7,63	0.94	0
25	CLA	A	607	36	61,65,73	1.20	7 (11%)	72,103,113	1.25	7 (9%)
27	BCR	b	620	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
34	HEM	E	101	5,6	50,50,50	1.47	9 (18%)	67,82,82	1.06	5 (7%)
27	BCR	T	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	6 (10%)
25	CLA	B	610	36	69,73,73	1.14	7 (10%)	82,113,113	1.10	6 (7%)
29	LMG	C	520	-	51,51,55	0.78	1 (1%)	59,59,63	1.35	6 (10%)
25	CLA	D	403	-	69,73,73	1.13	7 (10%)	82,113,113	1.18	6 (7%)
25	CLA	B	608	-	69,73,73	1.14	7 (10%)	82,113,113	1.17	6 (7%)
27	BCR	A	610	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	6 (10%)
29	LMG	d	406	-	42,42,55	0.79	1 (2%)	50,50,63	1.31	6 (12%)
33	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	1.38	8 (10%)
31	LHG	a	614	-	34,34,48	0.73	1 (2%)	37,40,54	1.22	3 (8%)
25	CLA	c	510	-	62,66,73	1.19	7 (11%)	73,104,113	1.25	7 (9%)
25	CLA	B	601	36	69,73,73	1.12	7 (10%)	82,113,113	1.20	6 (7%)
25	CLA	B	611	-	69,73,73	1.13	7 (10%)	82,113,113	1.21	6 (7%)
25	CLA	C	507	36	69,73,73	1.13	6 (8%)	82,113,113	1.24	4 (4%)
26	PHO	A	608	-	58,69,69	2.18	9 (15%)	55,99,99	1.42	6 (10%)
27	BCR	a	610	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	5 (8%)
31	LHG	A	617	-	48,48,48	0.62	0	51,54,54	1.26	6 (11%)
25	CLA	b	614	-	69,73,73	1.13	6 (8%)	82,113,113	1.22	6 (7%)
35	HEC	v	201	16	46,50,50	1.87	6 (13%)	58,82,82	1.15	3 (5%)
25	CLA	b	619	-	69,73,73	1.13	7 (10%)	82,113,113	1.16	6 (7%)
23	SQD	b	601	-	52,54,54	0.96	3 (5%)	62,65,65	1.39	9 (14%)
28	PL9	A	611	-	55,55,55	1.00	3 (5%)	68,69,69	1.51	14 (20%)
25	CLA	a	612	36	69,73,73	1.12	7 (10%)	82,113,113	1.17	6 (7%)
25	CLA	b	610	36	69,73,73	1.13	5 (7%)	82,113,113	1.14	6 (7%)
23	SQD	c	501	-	52,54,54	0.95	3 (5%)	62,65,65	1.45	9 (14%)
31	LHG	a	615	-	41,41,48	0.68	2 (4%)	44,47,54	1.33	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	c	521	-	51,51,55	0.71	0	59,59,63	1.34	6 (10%)
23	SQD	A	619	-	39,39,54	0.89	2 (5%)	41,41,65	1.18	2 (4%)
25	CLA	c	508	-	69,73,73	1.13	6 (8%)	82,113,113	1.16	6 (7%)
25	CLA	b	606	-	69,73,73	1.13	7 (10%)	82,113,113	1.12	5 (6%)
31	LHG	d	407	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
25	CLA	A	609	-	69,73,73	1.12	6 (8%)	82,113,113	1.21	7 (8%)
33	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.42	9 (11%)
25	CLA	b	607	-	69,73,73	1.14	7 (10%)	82,113,113	1.27	7 (8%)
29	LMG	c	522	-	51,51,55	0.79	1 (1%)	59,59,63	1.37	6 (10%)
25	CLA	B	607	36	69,73,73	1.13	6 (8%)	82,113,113	1.10	7 (8%)
25	CLA	c	509	36	69,73,73	1.14	6 (8%)	82,113,113	1.23	4 (4%)
28	PL9	a	611	-	55,55,55	0.93	4 (7%)	68,69,69	1.50	12 (17%)
25	CLA	B	604	-	69,73,73	1.14	7 (10%)	82,113,113	1.27	7 (8%)
29	LMG	D	405	-	51,51,55	0.72	1 (1%)	59,59,63	1.32	6 (10%)
32	BCT	A	620	22	3,3,3	3.24	1 (33%)	2,3,3	2.76	2 (100%)
27	BCR	B	618	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	c	504	-	69,73,73	1.13	8 (11%)	82,113,113	1.20	6 (7%)
32	BCT	a	605	22	3,3,3	3.24	1 (33%)	2,3,3	2.64	1 (50%)
25	CLA	A	615	36	69,73,73	1.12	7 (10%)	82,113,113	1.17	5 (6%)
33	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.42	9 (11%)
25	CLA	B	614	-	69,73,73	1.12	6 (8%)	82,113,113	1.15	4 (4%)
25	CLA	C	510	-	69,73,73	1.13	7 (10%)	82,113,113	1.15	6 (7%)
25	CLA	D	402	-	69,73,73	1.13	7 (10%)	82,113,113	1.14	6 (7%)
25	CLA	b	612	-	69,73,73	1.14	7 (10%)	82,113,113	1.19	6 (7%)
21	OEX	a	601	36,3,1	0,15,15	-	-	-	-	-
29	LMG	B	620	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)
31	LHG	L	101	-	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
33	DGD	C	517	-	63,63,67	0.90	3 (4%)	77,77,81	1.35	9 (11%)
27	BCR	y	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	5 (8%)
25	CLA	d	403	-	69,73,73	1.13	6 (8%)	82,113,113	1.14	4 (4%)
27	BCR	h	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.32	8 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	503	-	1/1/15/20	7/39/115/115	-
25	CLA	b	613	36	1/1/15/20	10/39/115/115	-
25	CLA	c	507	-	-	11/39/115/115	-
27	BCR	H	102	-	-	4/29/63/63	0/2/2/2
29	LMG	A	613	-	-	15/46/66/70	0/1/1/1
25	CLA	C	508	-	1/1/15/20	3/39/115/115	-
33	DGD	h	102	-	-	10/51/91/95	0/2/2/2
23	SQD	A	603	-	-	15/47/67/69	0/1/1/1
27	BCR	k	101	-	-	5/29/63/63	0/2/2/2
25	CLA	c	506	36	1/1/15/20	7/39/115/115	-
29	LMG	c	502	-	-	27/46/66/70	0/1/1/1
25	CLA	A	606	-	1/1/15/20	3/39/115/115	-
25	CLA	b	617	-	1/1/15/20	10/39/115/115	-
26	PHO	a	608	-	-	7/37/103/103	0/5/6/6
25	CLA	B	616	-	1/1/15/20	15/39/115/115	-
25	CLA	a	607	36	1/1/13/20	6/32/108/115	-
25	CLA	B	609	-	-	12/39/115/115	-
25	CLA	C	504	36	1/1/15/20	5/39/115/115	-
25	CLA	B	613	-	1/1/15/20	2/39/115/115	-
23	SQD	D	409	-	-	17/38/58/69	0/1/1/1
31	LHG	l	101	-	-	19/53/53/53	-
25	CLA	b	616	-	1/1/15/20	8/39/115/115	-
25	CLA	b	608	-	-	8/39/115/115	-
25	CLA	C	506	-	-	17/39/115/115	-
25	CLA	c	511	-	1/1/15/20	9/39/115/115	-
25	CLA	C	511	3	-	5/39/115/115	-
25	CLA	C	512	-	1/1/15/20	15/39/115/115	-
26	PHO	d	401	-	-	6/37/103/103	0/5/6/6
29	LMG	d	409	-	-	21/41/41/70	-
25	CLA	B	612	-	1/1/15/20	7/39/115/115	-
25	CLA	C	509	-	1/1/15/20	10/39/115/115	-
25	CLA	a	609	-	1/1/15/20	11/39/115/115	-
27	BCR	b	621	-	-	6/29/63/63	0/2/2/2
31	LHG	a	613	-	-	19/53/53/53	-
27	BCR	d	405	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	B	627	-	-	10/29/63/63	0/2/2/2
31	LHG	D	406	-	-	20/53/53/53	-
25	CLA	B	605	-	-	10/39/115/115	-
27	BCR	c	516	-	-	6/29/63/63	0/2/2/2
25	CLA	C	513	-	1/1/15/20	6/39/115/115	-
33	DGD	c	520	-	-	12/51/91/95	0/2/2/2
29	LMG	b	623	-	-	11/46/66/70	0/1/1/1
25	CLA	b	605	-	1/1/15/20	10/39/115/115	-
23	SQD	B	626	-	-	27/49/69/69	0/1/1/1
23	SQD	D	408	-	-	19/42/62/69	0/1/1/1
27	BCR	C	514	-	-	3/29/63/63	0/2/2/2
25	CLA	C	505	-	-	16/39/115/115	-
27	BCR	Y	101	-	-	7/29/63/63	0/2/2/2
27	BCR	B	617	-	-	3/29/63/63	0/2/2/2
25	CLA	b	609	-	1/1/15/20	6/39/115/115	-
34	HEM	e	101	5,6	-	3/14/54/54	-
25	CLA	B	606	-	1/1/15/20	7/39/115/115	-
27	BCR	B	619	-	-	4/29/63/63	0/2/2/2
27	BCR	D	404	-	-	6/29/63/63	0/2/2/2
29	LMG	A	612	-	-	17/46/66/70	0/1/1/1
25	CLA	c	512	-	1/1/15/20	8/39/115/115	-
25	CLA	b	618	-	1/1/15/20	10/39/115/115	-
27	BCR	C	515	-	-	5/29/63/63	0/2/2/2
25	CLA	b	604	36	1/1/15/20	18/39/115/115	-
25	CLA	B	615	-	1/1/15/20	4/39/115/115	-
33	DGD	C	518	-	-	14/51/91/95	0/2/2/2
35	HEC	V	201	16	-	1/14/54/54	-
29	LMG	C	519	-	-	21/46/66/70	0/1/1/1
25	CLA	b	615	-	1/1/15/20	11/39/115/115	-
28	PL9	d	408	-	-	10/53/73/73	0/1/1/1
28	PL9	D	407	-	-	9/53/73/73	0/1/1/1
27	BCR	c	517	-	-	6/29/63/63	0/2/2/2
25	CLA	C	501	-	1/1/15/20	6/39/115/115	-
25	CLA	c	505	-	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	606	-	1/1/15/20	3/39/115/115	-
26	PHO	D	401	-	-	7/37/103/103	0/5/6/6
31	LHG	A	618	-	-	23/53/53/53	-
33	DGD	H	103	-	-	13/51/91/95	0/2/2/2
29	LMG	B	621	-	-	18/46/66/70	0/1/1/1
25	CLA	c	514	-	1/1/15/20	7/39/115/115	-
29	LMG	b	624	-	-	23/46/66/70	0/1/1/1
25	CLA	C	502	-	-	6/39/115/115	-
25	CLA	C	503	-	1/1/15/20	3/39/115/115	-
31	LHG	A	616	-	-	17/53/53/53	-
25	CLA	b	611	-	1/1/15/20	5/39/115/115	-
25	CLA	B	603	-	1/1/15/20	10/39/115/115	-
25	CLA	d	404	-	1/1/15/20	5/39/115/115	-
25	CLA	B	602	-	1/1/15/20	11/39/115/115	-
25	CLA	c	513	3	1/1/15/20	4/39/115/115	-
25	CLA	c	515	-	1/1/15/20	5/39/115/115	-
27	BCR	b	622	-	-	6/29/63/63	0/2/2/2
29	LMG	B	625	-	-	21/46/66/70	0/1/1/1
27	BCR	K	101	-	-	6/29/63/63	0/2/2/2
23	SQD	I	101	-	-	22/41/41/69	-
23	SQD	f	101	-	-	18/38/58/69	0/1/1/1
29	LMG	b	625	-	-	1/6/6/70	-
25	CLA	A	607	36	1/1/13/20	9/30/106/115	-
27	BCR	b	620	-	-	3/29/63/63	0/2/2/2
34	HEM	E	101	5,6	-	5/14/54/54	-
27	BCR	T	101	-	-	10/29/63/63	0/2/2/2
25	CLA	B	610	36	1/1/15/20	9/39/115/115	-
29	LMG	C	520	-	-	16/46/66/70	0/1/1/1
25	CLA	D	403	-	1/1/15/20	3/39/115/115	-
25	CLA	B	608	-	1/1/15/20	4/39/115/115	-
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
29	LMG	d	406	-	-	5/37/57/70	0/1/1/1
33	DGD	c	519	-	-	19/51/91/95	0/2/2/2
31	LHG	a	614	-	-	16/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	510	-	1/1/13/20	3/31/107/115	-
25	CLA	B	601	36	1/1/15/20	15/39/115/115	-
25	CLA	B	611	-	1/1/15/20	4/39/115/115	-
25	CLA	C	507	36	1/1/15/20	6/39/115/115	-
26	PHO	A	608	-	-	8/37/103/103	0/5/6/6
27	BCR	a	610	-	-	5/29/63/63	0/2/2/2
31	LHG	A	617	-	-	14/53/53/53	-
25	CLA	b	614	-	1/1/15/20	6/39/115/115	-
35	HEC	v	201	16	-	2/14/54/54	-
25	CLA	b	619	-	1/1/15/20	14/39/115/115	-
23	SQD	b	601	-	-	17/49/69/69	0/1/1/1
28	PL9	A	611	-	-	10/53/73/73	0/1/1/1
25	CLA	a	612	36	1/1/15/20	2/39/115/115	-
25	CLA	b	610	36	1/1/15/20	10/39/115/115	-
23	SQD	c	501	-	-	21/49/69/69	0/1/1/1
31	LHG	a	615	-	-	21/46/46/53	-
29	LMG	c	521	-	-	24/46/66/70	0/1/1/1
23	SQD	A	619	-	-	27/41/41/69	-
25	CLA	c	508	-	1/1/15/20	18/39/115/115	-
25	CLA	b	606	-	1/1/15/20	7/39/115/115	-
31	LHG	d	407	-	-	15/53/53/53	-
25	CLA	A	609	-	1/1/15/20	8/39/115/115	-
33	DGD	C	516	-	-	10/51/91/95	0/2/2/2
25	CLA	b	607	-	1/1/15/20	8/39/115/115	-
29	LMG	c	522	-	-	15/46/66/70	0/1/1/1
25	CLA	B	607	36	1/1/15/20	10/39/115/115	-
25	CLA	c	509	36	1/1/15/20	13/39/115/115	-
28	PL9	a	611	-	-	16/53/73/73	0/1/1/1
25	CLA	B	604	-	1/1/15/20	5/39/115/115	-
29	LMG	D	405	-	-	15/46/66/70	0/1/1/1
27	BCR	B	618	-	-	4/29/63/63	0/2/2/2
25	CLA	c	504	-	-	6/39/115/115	-
25	CLA	A	615	36	1/1/15/20	3/39/115/115	-
33	DGD	c	518	-	-	15/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	614	-	1/1/15/20	19/39/115/115	-
25	CLA	C	510	-	1/1/15/20	7/39/115/115	-
25	CLA	D	402	-	-	9/39/115/115	-
25	CLA	b	612	-	-	11/39/115/115	-
29	LMG	B	620	-	-	16/46/66/70	0/1/1/1
31	LHG	L	101	-	-	17/53/53/53	-
33	DGD	C	517	-	-	16/51/91/95	0/2/2/2
27	BCR	y	101	-	-	5/29/63/63	0/2/2/2
25	CLA	d	403	-	-	9/39/115/115	-
27	BCR	h	101	-	-	4/29/63/63	0/2/2/2

All (641) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	401	PHO	C1B-C2B	9.67	1.50	1.39
26	D	401	PHO	C1B-C2B	9.66	1.50	1.39
26	A	608	PHO	C1B-C2B	9.64	1.50	1.39
26	a	608	PHO	C1B-C2B	9.63	1.50	1.39
26	D	401	PHO	C3B-C4B	8.74	1.50	1.41
26	d	401	PHO	C3B-C4B	8.73	1.50	1.41
26	a	608	PHO	C3B-C4B	8.70	1.50	1.41
26	A	608	PHO	C3B-C4B	8.66	1.50	1.41
35	v	201	HEC	CAB-C3B	6.39	1.55	1.35
35	V	201	HEC	CAB-C3B	6.35	1.55	1.35
35	V	201	HEC	CAC-C3C	6.30	1.55	1.35
35	v	201	HEC	CAC-C3C	6.30	1.55	1.35
32	a	605	BCT	O1-C	5.33	1.44	1.25
32	A	620	BCT	O1-C	5.32	1.44	1.25
26	d	401	PHO	C1D-C2D	4.29	1.44	1.39
26	D	401	PHO	C1D-C2D	4.27	1.44	1.39
26	A	608	PHO	C1D-C2D	4.27	1.44	1.39
26	a	608	PHO	C1D-C2D	4.27	1.44	1.39
35	v	201	HEC	CBC-CAC	-4.14	1.34	1.49
35	V	201	HEC	CBB-CAB	-4.11	1.34	1.49
35	v	201	HEC	CBB-CAB	-4.11	1.34	1.49
35	V	201	HEC	CBC-CAC	-4.10	1.34	1.49
27	B	627	BCR	C1-C6	-3.84	1.48	1.53
26	A	608	PHO	C4D-CHA	3.83	1.45	1.39
26	d	401	PHO	C4D-CHA	3.80	1.45	1.39
26	D	401	PHO	C4D-CHA	3.77	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	515	BCR	C1-C6	-3.77	1.49	1.53
34	E	101	HEM	FE-NB	3.75	2.06	1.94
27	C	514	BCR	C1-C6	-3.75	1.49	1.53
27	B	617	BCR	C1-C6	-3.74	1.49	1.53
27	T	101	BCR	C1-C6	-3.73	1.49	1.53
27	D	404	BCR	C1-C6	-3.72	1.49	1.53
26	a	608	PHO	C4D-CHA	3.69	1.45	1.39
27	b	620	BCR	C1-C6	-3.68	1.49	1.53
27	y	101	BCR	C1-C6	-3.68	1.49	1.53
27	c	517	BCR	C1-C6	-3.63	1.49	1.53
25	B	610	CLA	C1D-ND	3.63	1.42	1.37
27	B	618	BCR	C1-C6	-3.63	1.49	1.53
25	b	613	CLA	C1D-ND	3.62	1.42	1.37
25	b	619	CLA	C1D-ND	3.60	1.42	1.37
25	c	509	CLA	C1D-ND	3.59	1.42	1.37
25	b	616	CLA	C1D-ND	3.59	1.42	1.37
27	b	621	BCR	C1-C6	-3.57	1.49	1.53
25	B	616	CLA	C1D-ND	3.57	1.42	1.37
25	b	607	CLA	C1D-ND	3.56	1.42	1.37
34	e	101	HEM	FE-NB	3.56	2.05	1.94
25	C	509	CLA	C1D-ND	3.56	1.42	1.37
34	e	101	HEM	FE-ND	3.55	2.05	1.94
27	a	610	BCR	C1-C6	-3.55	1.49	1.53
27	B	617	BCR	C30-C25	-3.55	1.49	1.53
25	C	507	CLA	C1D-ND	3.55	1.42	1.37
25	b	615	CLA	C1D-ND	3.55	1.42	1.37
25	c	511	CLA	C1D-ND	3.55	1.42	1.37
25	c	514	CLA	C1D-ND	3.55	1.42	1.37
27	A	610	BCR	C1-C6	-3.54	1.49	1.53
27	b	620	BCR	C30-C25	-3.54	1.49	1.53
25	B	615	CLA	C1D-ND	3.53	1.42	1.37
25	C	511	CLA	C1D-ND	3.53	1.42	1.37
25	b	605	CLA	C1D-ND	3.52	1.42	1.37
25	C	502	CLA	C1D-ND	3.52	1.42	1.37
25	C	512	CLA	C1D-ND	3.52	1.42	1.37
27	Y	101	BCR	C1-C6	-3.52	1.49	1.53
25	B	604	CLA	C1D-ND	3.52	1.42	1.37
25	C	506	CLA	C1D-ND	3.51	1.42	1.37
25	b	604	CLA	C1D-ND	3.51	1.42	1.37
25	c	504	CLA	C1D-ND	3.51	1.42	1.37
25	B	613	CLA	C1D-ND	3.51	1.42	1.37
25	b	618	CLA	C1D-ND	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	CLA	C1D-ND	3.50	1.42	1.37
25	b	614	CLA	C1D-ND	3.49	1.42	1.37
25	c	513	CLA	C1D-ND	3.49	1.42	1.37
27	B	619	BCR	C1-C6	-3.49	1.49	1.53
25	c	512	CLA	C1D-ND	3.49	1.42	1.37
34	E	101	HEM	FE-ND	3.49	2.05	1.94
25	B	601	CLA	C1D-ND	3.49	1.42	1.37
27	k	101	BCR	C1-C6	-3.48	1.49	1.53
25	B	606	CLA	C1D-ND	3.48	1.42	1.37
25	b	610	CLA	C1D-ND	3.48	1.42	1.37
25	b	612	CLA	C1D-ND	3.48	1.42	1.37
25	B	609	CLA	C1D-ND	3.48	1.42	1.37
27	B	619	BCR	C30-C25	-3.48	1.49	1.53
25	D	402	CLA	C1D-ND	3.48	1.42	1.37
25	B	602	CLA	C1D-ND	3.47	1.42	1.37
25	C	503	CLA	C1D-ND	3.47	1.42	1.37
25	d	404	CLA	C1D-ND	3.47	1.42	1.37
25	D	403	CLA	C1D-ND	3.46	1.42	1.37
25	B	605	CLA	C1D-ND	3.46	1.42	1.37
25	b	608	CLA	C1D-ND	3.45	1.42	1.37
25	C	508	CLA	C1D-ND	3.45	1.42	1.37
25	c	508	CLA	C1D-ND	3.45	1.42	1.37
25	a	607	CLA	C1D-ND	3.45	1.42	1.37
25	a	612	CLA	C1D-ND	3.45	1.42	1.37
25	C	510	CLA	C1D-ND	3.44	1.42	1.37
25	A	615	CLA	C1D-ND	3.44	1.42	1.37
25	b	617	CLA	C1D-ND	3.43	1.42	1.37
25	c	510	CLA	C1D-ND	3.43	1.42	1.37
25	c	505	CLA	C1D-ND	3.43	1.42	1.37
25	B	608	CLA	C1D-ND	3.43	1.42	1.37
25	d	403	CLA	C1D-ND	3.42	1.42	1.37
25	c	507	CLA	C1D-ND	3.42	1.42	1.37
27	K	101	BCR	C30-C25	-3.42	1.49	1.53
25	B	603	CLA	C1D-ND	3.41	1.42	1.37
25	C	513	CLA	C1D-ND	3.41	1.42	1.37
25	c	515	CLA	C1D-ND	3.41	1.42	1.37
25	a	609	CLA	C1D-ND	3.41	1.42	1.37
25	a	606	CLA	C1D-ND	3.41	1.42	1.37
25	B	611	CLA	C1D-ND	3.40	1.42	1.37
25	A	606	CLA	C1D-ND	3.40	1.42	1.37
25	c	506	CLA	C1D-ND	3.39	1.42	1.37
27	y	101	BCR	C30-C25	-3.39	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	C1D-ND	3.39	1.42	1.37
25	C	505	CLA	C1D-ND	3.39	1.42	1.37
25	A	607	CLA	C1D-ND	3.39	1.42	1.37
25	C	501	CLA	C1D-ND	3.38	1.42	1.37
25	b	611	CLA	C1D-ND	3.38	1.42	1.37
25	b	609	CLA	C1D-ND	3.37	1.42	1.37
27	c	516	BCR	C30-C25	-3.37	1.49	1.53
25	B	612	CLA	C1D-ND	3.37	1.42	1.37
25	B	614	CLA	C1D-ND	3.37	1.42	1.37
27	b	621	BCR	C30-C25	-3.36	1.49	1.53
25	c	503	CLA	C1D-ND	3.36	1.42	1.37
27	b	622	BCR	C30-C25	-3.36	1.49	1.53
27	c	517	BCR	C30-C25	-3.35	1.49	1.53
25	C	504	CLA	C1D-ND	3.35	1.42	1.37
27	Y	101	BCR	C30-C25	-3.32	1.49	1.53
25	b	606	CLA	C1D-ND	3.32	1.42	1.37
27	c	516	BCR	C1-C6	-3.32	1.49	1.53
27	d	405	BCR	C1-C6	-3.31	1.49	1.53
34	E	101	HEM	FE-NA	3.31	2.06	1.95
27	C	514	BCR	C30-C25	-3.31	1.49	1.53
27	h	101	BCR	C30-C25	-3.30	1.49	1.53
27	A	610	BCR	C30-C25	-3.30	1.49	1.53
27	C	515	BCR	C30-C25	-3.29	1.49	1.53
27	K	101	BCR	C1-C6	-3.29	1.49	1.53
27	D	404	BCR	C30-C25	-3.29	1.49	1.53
27	h	101	BCR	C1-C6	-3.29	1.49	1.53
27	d	405	BCR	C30-C25	-3.29	1.49	1.53
25	B	609	CLA	C4B-NB	3.28	1.42	1.37
27	b	622	BCR	C1-C6	-3.28	1.49	1.53
27	B	618	BCR	C30-C25	-3.28	1.49	1.53
23	A	619	SQD	O48-C23	3.27	1.42	1.33
34	e	101	HEM	FE-NA	3.23	2.05	1.95
27	a	610	BCR	C30-C25	-3.22	1.49	1.53
23	I	101	SQD	O48-C23	3.21	1.42	1.33
25	C	512	CLA	C4B-NB	3.21	1.42	1.37
25	D	402	CLA	C4B-NB	3.21	1.42	1.37
25	C	506	CLA	C4B-NB	3.19	1.42	1.37
27	B	627	BCR	C30-C25	-3.19	1.49	1.53
25	d	403	CLA	C4B-NB	3.18	1.42	1.37
23	c	501	SQD	O48-C23	3.17	1.42	1.33
25	B	603	CLA	C4B-NB	3.17	1.42	1.37
25	c	507	CLA	C4B-NB	3.17	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	H	102	BCR	C1-C6	-3.16	1.49	1.53
23	B	626	SQD	O48-C23	3.16	1.42	1.33
25	B	605	CLA	C4B-NB	3.16	1.42	1.37
23	f	101	SQD	O48-C23	3.16	1.42	1.33
27	k	101	BCR	C30-C25	-3.16	1.49	1.53
27	H	102	BCR	C30-C25	-3.15	1.49	1.53
34	E	101	HEM	FE-NC	3.15	2.05	1.95
23	D	409	SQD	O48-C23	3.15	1.42	1.33
25	c	508	CLA	C4B-NB	3.15	1.42	1.37
23	A	603	SQD	O48-C23	3.15	1.42	1.33
25	b	612	CLA	C4B-NB	3.15	1.42	1.37
25	C	505	CLA	C4B-NB	3.14	1.42	1.37
34	e	101	HEM	FE-NC	3.14	2.05	1.95
25	a	609	CLA	C4B-NB	3.14	1.42	1.37
25	b	606	CLA	C4B-NB	3.12	1.42	1.37
34	e	101	HEM	CAB-C3B	3.11	1.55	1.47
25	b	617	CLA	C4B-NB	3.11	1.41	1.37
23	b	601	SQD	O48-C23	3.11	1.42	1.33
23	D	408	SQD	O48-C23	3.10	1.42	1.33
34	E	101	HEM	CAC-C3C	3.10	1.55	1.47
25	b	605	CLA	C4B-NB	3.10	1.41	1.37
25	b	608	CLA	C4B-NB	3.10	1.41	1.37
34	e	101	HEM	CAC-C3C	3.09	1.55	1.47
25	A	609	CLA	C4B-NB	3.09	1.41	1.37
25	B	614	CLA	C4B-NB	3.09	1.41	1.37
25	D	403	CLA	C4B-NB	3.09	1.41	1.37
25	b	611	CLA	C4B-NB	3.09	1.41	1.37
34	E	101	HEM	CAB-C3B	3.08	1.55	1.47
25	B	615	CLA	C4B-NB	3.08	1.41	1.37
25	b	618	CLA	C4B-NB	3.06	1.41	1.37
25	c	509	CLA	C4B-NB	3.06	1.41	1.37
27	T	101	BCR	C30-C25	-3.06	1.49	1.53
25	B	606	CLA	C4B-NB	3.05	1.41	1.37
25	C	508	CLA	C4B-NB	3.04	1.41	1.37
25	B	607	CLA	C4B-NB	3.04	1.41	1.37
25	d	404	CLA	C4B-NB	3.03	1.41	1.37
25	B	608	CLA	C4B-NB	3.03	1.41	1.37
25	b	604	CLA	C4B-NB	3.03	1.41	1.37
25	c	505	CLA	C4B-NB	3.03	1.41	1.37
25	C	507	CLA	C4B-NB	3.03	1.41	1.37
25	B	611	CLA	C4B-NB	3.02	1.41	1.37
25	b	607	CLA	C4B-NB	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	513	CLA	C4B-NB	3.02	1.41	1.37
25	B	610	CLA	C4B-NB	3.02	1.41	1.37
25	C	502	CLA	C4B-NB	3.02	1.41	1.37
25	B	602	CLA	C4B-NB	3.02	1.41	1.37
25	b	615	CLA	C4B-NB	3.01	1.41	1.37
25	B	601	CLA	C4B-NB	3.01	1.41	1.37
25	a	612	CLA	C4B-NB	3.01	1.41	1.37
25	B	616	CLA	C4B-NB	3.00	1.41	1.37
25	a	606	CLA	C4B-NB	3.00	1.41	1.37
25	b	610	CLA	C4B-NB	3.00	1.41	1.37
25	c	512	CLA	C4B-NB	3.00	1.41	1.37
25	C	503	CLA	C4B-NB	2.99	1.41	1.37
25	B	604	CLA	C4B-NB	2.99	1.41	1.37
25	c	510	CLA	C4B-NB	2.99	1.41	1.37
25	A	606	CLA	C4B-NB	2.99	1.41	1.37
25	C	511	CLA	C4B-NB	2.98	1.41	1.37
25	b	616	CLA	C4B-NB	2.98	1.41	1.37
25	b	613	CLA	C4B-NB	2.98	1.41	1.37
25	b	609	CLA	C4B-NB	2.98	1.41	1.37
25	B	613	CLA	C4B-NB	2.97	1.41	1.37
25	c	504	CLA	C4B-NB	2.97	1.41	1.37
23	A	619	SQD	O47-C7	2.97	1.42	1.34
25	C	510	CLA	C4B-NB	2.97	1.41	1.37
25	A	607	CLA	C4B-NB	2.97	1.41	1.37
25	c	514	CLA	C4B-NB	2.96	1.41	1.37
25	c	515	CLA	C4B-NB	2.95	1.41	1.37
25	b	614	CLA	C4B-NB	2.95	1.41	1.37
25	a	607	CLA	C4B-NB	2.95	1.41	1.37
25	c	503	CLA	C4B-NB	2.94	1.41	1.37
25	C	504	CLA	C4B-NB	2.94	1.41	1.37
25	B	612	CLA	C4B-NB	2.92	1.41	1.37
25	C	501	CLA	C4B-NB	2.92	1.41	1.37
25	c	506	CLA	C4B-NB	2.91	1.41	1.37
23	D	408	SQD	O47-C7	2.91	1.42	1.34
23	B	626	SQD	O47-C7	2.91	1.42	1.34
25	c	511	CLA	C4B-NB	2.90	1.41	1.37
25	C	513	CLA	C4B-NB	2.90	1.41	1.37
28	d	408	PL9	C3-C4	-2.89	1.45	1.49
25	A	615	CLA	C4B-NB	2.89	1.41	1.37
23	D	409	SQD	O47-C7	2.89	1.42	1.34
25	b	619	CLA	C4B-NB	2.89	1.41	1.37
28	A	611	PL9	C7-C3	-2.87	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	407	PL9	C3-C4	-2.87	1.45	1.49
25	c	504	CLA	C1B-C2B	2.86	1.49	1.43
28	A	611	PL9	C3-C4	-2.85	1.45	1.49
23	I	101	SQD	O47-C7	2.85	1.42	1.34
23	c	501	SQD	O47-C7	2.85	1.42	1.34
23	A	603	SQD	O47-C7	2.85	1.42	1.34
23	f	101	SQD	O47-C7	2.84	1.42	1.34
25	C	509	CLA	C4B-NB	2.82	1.41	1.37
25	b	616	CLA	C1B-C2B	2.82	1.49	1.43
25	C	502	CLA	C1B-C2B	2.81	1.49	1.43
25	c	513	CLA	C1B-C2B	2.81	1.49	1.43
25	C	501	CLA	C1B-C2B	2.81	1.49	1.43
25	B	616	CLA	C1B-C2B	2.81	1.49	1.43
25	B	604	CLA	C1B-C2B	2.81	1.49	1.43
25	C	509	CLA	C1B-C2B	2.81	1.49	1.43
25	B	613	CLA	C1B-C2B	2.80	1.49	1.43
25	b	612	CLA	C1B-C2B	2.80	1.49	1.43
25	b	619	CLA	C1B-C2B	2.80	1.49	1.43
25	c	505	CLA	C1B-C2B	2.80	1.49	1.43
25	c	514	CLA	C1B-C2B	2.80	1.49	1.43
23	b	601	SQD	O47-C7	2.80	1.42	1.34
25	d	404	CLA	C1B-C2B	2.80	1.49	1.43
25	b	604	CLA	C1B-C2B	2.80	1.49	1.43
25	B	605	CLA	C1B-C2B	2.80	1.49	1.43
25	c	512	CLA	C1B-C2B	2.80	1.49	1.43
25	b	618	CLA	C1B-C2B	2.79	1.49	1.43
25	B	615	CLA	C1B-C2B	2.79	1.49	1.43
25	B	601	CLA	C1B-C2B	2.79	1.49	1.43
25	B	609	CLA	C1B-C2B	2.79	1.49	1.43
25	C	503	CLA	C1B-C2B	2.79	1.49	1.43
25	c	503	CLA	C1B-C2B	2.79	1.49	1.43
25	B	610	CLA	C1B-C2B	2.78	1.49	1.43
25	B	612	CLA	C1B-C2B	2.78	1.49	1.43
25	C	507	CLA	C1B-C2B	2.78	1.49	1.43
25	a	612	CLA	C1B-C2B	2.78	1.49	1.43
25	C	505	CLA	C1B-C2B	2.78	1.49	1.43
25	D	402	CLA	C1B-C2B	2.78	1.49	1.43
25	a	607	CLA	C1B-C2B	2.77	1.49	1.43
25	B	602	CLA	C1B-C2B	2.77	1.49	1.43
25	C	511	CLA	C1B-C2B	2.77	1.49	1.43
25	b	610	CLA	C1B-C2B	2.77	1.49	1.43
25	b	614	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C1B-C2B	2.77	1.49	1.43
25	b	617	CLA	C1B-C2B	2.77	1.49	1.43
25	B	614	CLA	C1B-C2B	2.77	1.49	1.43
25	C	504	CLA	C1B-C2B	2.77	1.49	1.43
25	C	508	CLA	C1B-C2B	2.76	1.49	1.43
25	A	606	CLA	C1B-C2B	2.76	1.49	1.43
25	c	510	CLA	C1B-C2B	2.76	1.49	1.43
25	C	510	CLA	C1B-C2B	2.75	1.49	1.43
25	b	607	CLA	C1B-C2B	2.75	1.49	1.43
25	c	507	CLA	C1B-C2B	2.75	1.49	1.43
25	a	606	CLA	C1B-C2B	2.75	1.49	1.43
25	c	515	CLA	C1B-C2B	2.75	1.49	1.43
25	b	615	CLA	C1B-C2B	2.75	1.49	1.43
25	A	615	CLA	C1B-C2B	2.75	1.49	1.43
25	B	608	CLA	C1B-C2B	2.75	1.49	1.43
25	C	512	CLA	C1B-C2B	2.75	1.49	1.43
25	c	511	CLA	C1B-C2B	2.74	1.49	1.43
25	C	513	CLA	C1B-C2B	2.74	1.49	1.43
25	A	607	CLA	C1B-C2B	2.74	1.49	1.43
25	D	403	CLA	C1B-C2B	2.74	1.49	1.43
25	B	606	CLA	C1B-C2B	2.73	1.49	1.43
25	b	605	CLA	C1B-C2B	2.73	1.49	1.43
25	b	611	CLA	C1B-C2B	2.73	1.49	1.43
25	b	608	CLA	C1B-C2B	2.73	1.49	1.43
25	b	609	CLA	C1B-C2B	2.73	1.49	1.43
25	d	403	CLA	C1B-C2B	2.71	1.49	1.43
25	b	606	CLA	C1B-C2B	2.71	1.49	1.43
25	a	609	CLA	C1B-C2B	2.71	1.49	1.43
25	c	509	CLA	C1B-C2B	2.71	1.49	1.43
25	b	613	CLA	C1B-C2B	2.71	1.49	1.43
25	C	506	CLA	C1B-C2B	2.71	1.49	1.43
25	B	603	CLA	C1B-C2B	2.70	1.49	1.43
25	B	611	CLA	C1B-C2B	2.69	1.49	1.43
25	B	607	CLA	C1B-C2B	2.68	1.49	1.43
25	A	609	CLA	C1B-C2B	2.67	1.49	1.43
28	a	611	PL9	C3-C4	-2.64	1.45	1.49
25	c	508	CLA	C1B-C2B	2.62	1.49	1.43
26	d	401	PHO	C3D-C4D	2.62	1.44	1.41
26	a	608	PHO	C3D-C4D	2.60	1.44	1.41
28	D	407	PL9	C7-C3	-2.59	1.47	1.51
26	A	608	PHO	C3D-C4D	2.59	1.44	1.41
26	A	608	PHO	CMC-C2C	-2.57	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	401	PHO	C3D-C4D	2.54	1.44	1.41
26	d	401	PHO	CMC-C2C	-2.53	1.46	1.50
26	D	401	PHO	CMC-C2C	-2.52	1.46	1.50
26	a	608	PHO	CMC-C2C	-2.50	1.46	1.50
26	a	608	PHO	CMB-C2B	-2.49	1.46	1.51
28	d	408	PL9	C7-C3	-2.47	1.48	1.51
26	A	608	PHO	CMD-C2D	-2.47	1.46	1.51
28	a	611	PL9	C7-C3	-2.45	1.48	1.51
26	d	401	PHO	CMD-C2D	-2.45	1.46	1.51
29	c	522	LMG	C1-C2	2.45	1.59	1.52
26	a	608	PHO	CMD-C2D	-2.44	1.46	1.51
26	A	608	PHO	CMB-C2B	-2.43	1.46	1.51
26	D	401	PHO	CMD-C2D	-2.42	1.46	1.51
25	A	609	CLA	CHC-C1C	2.42	1.43	1.38
25	b	613	CLA	C3B-C4B	2.42	1.49	1.42
25	c	515	CLA	CHC-C1C	2.42	1.43	1.38
25	A	609	CLA	C3B-C4B	2.39	1.49	1.42
25	b	617	CLA	CHC-C1C	2.39	1.43	1.38
25	c	512	CLA	CHC-C1C	2.39	1.43	1.38
25	B	610	CLA	C3B-C4B	2.39	1.49	1.42
25	C	508	CLA	C3B-C4B	2.38	1.49	1.42
25	c	510	CLA	C3B-C4B	2.38	1.49	1.42
25	b	617	CLA	C3B-C4B	2.38	1.49	1.42
25	c	513	CLA	C3B-C4B	2.38	1.49	1.42
29	C	520	LMG	C1-C2	2.38	1.59	1.52
25	d	404	CLA	C3B-C4B	2.38	1.49	1.42
26	D	401	PHO	CMB-C2B	-2.37	1.46	1.51
25	b	606	CLA	C3B-C4B	2.37	1.49	1.42
25	C	510	CLA	C3B-C4B	2.37	1.49	1.42
25	B	613	CLA	C3B-C4B	2.37	1.49	1.42
25	c	515	CLA	C3B-C4B	2.37	1.49	1.42
31	l	101	LHG	O7-C5	-2.36	1.41	1.46
25	C	508	CLA	CHC-C1C	2.36	1.43	1.38
25	A	607	CLA	C3B-C4B	2.36	1.49	1.42
25	C	510	CLA	CHC-C1C	2.36	1.43	1.38
25	a	607	CLA	C3B-C4B	2.36	1.49	1.42
25	C	503	CLA	C3B-C4B	2.36	1.49	1.42
25	C	513	CLA	CHC-C1C	2.36	1.43	1.38
25	c	505	CLA	C3B-C4B	2.36	1.49	1.42
25	a	606	CLA	C3B-C4B	2.36	1.49	1.42
25	a	606	CLA	CHC-C1C	2.36	1.43	1.38
25	d	403	CLA	C3B-C4B	2.36	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	615	CLA	C3B-C4B	2.36	1.49	1.42
33	c	518	DGD	O2G-C2G	-2.36	1.41	1.46
25	D	403	CLA	C3B-C4B	2.36	1.49	1.42
25	c	510	CLA	CHC-C1C	2.36	1.43	1.38
25	C	509	CLA	C3B-C4B	2.36	1.49	1.42
26	a	608	PHO	CAC-C3C	-2.36	1.47	1.51
25	a	607	CLA	CHC-C1C	2.35	1.43	1.38
25	b	607	CLA	C3B-C4B	2.35	1.49	1.42
25	b	615	CLA	CHC-C1C	2.35	1.43	1.38
25	B	612	CLA	C3B-C4B	2.35	1.49	1.42
25	b	619	CLA	C3B-C4B	2.35	1.49	1.42
25	B	601	CLA	C3B-C4B	2.35	1.49	1.42
25	A	615	CLA	C3B-C4B	2.35	1.49	1.42
25	c	511	CLA	C3B-C4B	2.35	1.49	1.42
25	B	612	CLA	CHC-C1C	2.35	1.43	1.38
25	b	605	CLA	C3B-C4B	2.35	1.49	1.42
25	B	615	CLA	CHC-C1C	2.35	1.43	1.38
26	d	401	PHO	CMB-C2B	-2.35	1.46	1.51
25	b	613	CLA	CHC-C1C	2.35	1.43	1.38
25	d	403	CLA	CHC-C1C	2.35	1.43	1.38
25	B	616	CLA	C3B-C4B	2.35	1.49	1.42
25	C	505	CLA	C3B-C4B	2.35	1.49	1.42
25	c	514	CLA	C3B-C4B	2.35	1.49	1.42
25	b	609	CLA	C3B-C4B	2.34	1.49	1.42
25	C	511	CLA	CHC-C1C	2.34	1.43	1.38
25	B	606	CLA	C3B-C4B	2.34	1.49	1.42
25	C	511	CLA	C3B-C4B	2.34	1.49	1.42
25	b	611	CLA	CHC-C1C	2.34	1.43	1.38
25	d	404	CLA	CHC-C1C	2.34	1.43	1.38
25	b	606	CLA	CHC-C1C	2.34	1.43	1.38
25	C	503	CLA	CHC-C1C	2.34	1.43	1.38
25	c	503	CLA	C3B-C4B	2.34	1.49	1.42
25	B	602	CLA	CHC-C1C	2.34	1.43	1.38
25	B	607	CLA	C3B-C4B	2.34	1.49	1.42
25	C	513	CLA	C3B-C4B	2.34	1.49	1.42
25	B	611	CLA	C3B-C4B	2.34	1.49	1.42
25	C	502	CLA	C3B-C4B	2.34	1.49	1.42
25	C	504	CLA	CHC-C1C	2.34	1.43	1.38
25	B	606	CLA	CHC-C1C	2.34	1.43	1.38
25	B	608	CLA	C3B-C4B	2.34	1.49	1.42
25	c	512	CLA	C3B-C4B	2.34	1.49	1.42
25	C	512	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	C3B-C4B	2.33	1.49	1.42
25	c	506	CLA	C3B-C4B	2.33	1.49	1.42
25	c	505	CLA	CHC-C1C	2.33	1.43	1.38
25	c	513	CLA	CHC-C1C	2.33	1.43	1.38
25	b	616	CLA	C3B-C4B	2.33	1.49	1.42
25	c	506	CLA	CHC-C1C	2.33	1.43	1.38
25	b	610	CLA	C3B-C4B	2.33	1.49	1.42
25	D	402	CLA	C3B-C4B	2.33	1.49	1.42
25	B	607	CLA	CHC-C1C	2.33	1.43	1.38
25	b	605	CLA	CHC-C1C	2.33	1.43	1.38
25	A	606	CLA	CHC-C1C	2.33	1.43	1.38
25	B	608	CLA	CHC-C1C	2.33	1.43	1.38
25	b	610	CLA	CHC-C1C	2.33	1.43	1.38
25	B	614	CLA	CHC-C1C	2.33	1.43	1.38
25	b	608	CLA	CHC-C1C	2.33	1.43	1.38
25	c	507	CLA	C3B-C4B	2.33	1.49	1.42
26	D	401	PHO	CAC-C3C	-2.33	1.47	1.51
25	c	511	CLA	CHC-C1C	2.33	1.43	1.38
25	B	605	CLA	CHC-C1C	2.32	1.43	1.38
25	A	606	CLA	C3B-C4B	2.32	1.49	1.42
25	B	605	CLA	C3B-C4B	2.32	1.49	1.42
25	b	611	CLA	C3B-C4B	2.32	1.49	1.42
25	B	603	CLA	CHC-C1C	2.32	1.43	1.38
25	B	604	CLA	C3B-C4B	2.32	1.49	1.42
25	c	509	CLA	C3B-C4B	2.32	1.49	1.42
25	c	503	CLA	CHC-C1C	2.32	1.43	1.38
25	B	614	CLA	C3B-C4B	2.32	1.49	1.42
25	b	614	CLA	C3B-C4B	2.32	1.49	1.42
25	A	607	CLA	CHC-C1C	2.32	1.43	1.38
25	C	502	CLA	CHC-C1C	2.31	1.43	1.38
33	c	519	DGD	O2G-C2G	-2.31	1.41	1.46
25	A	615	CLA	CHC-C1C	2.31	1.43	1.38
25	b	618	CLA	C3B-C4B	2.31	1.49	1.42
25	B	610	CLA	CHC-C1C	2.31	1.43	1.38
25	B	602	CLA	C3B-C4B	2.31	1.49	1.42
25	B	615	CLA	C3B-C4B	2.31	1.49	1.42
25	C	501	CLA	CHC-C1C	2.31	1.43	1.38
25	C	504	CLA	C3B-C4B	2.31	1.49	1.42
25	a	612	CLA	C3B-C4B	2.31	1.49	1.42
29	B	625	LMG	O6-C5	-2.30	1.38	1.44
25	b	609	CLA	CHC-C1C	2.30	1.43	1.38
25	b	608	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	612	CLA	C3B-C4B	2.30	1.49	1.42
25	D	402	CLA	CHC-C1C	2.30	1.43	1.38
25	B	613	CLA	CHC-C1C	2.30	1.43	1.38
25	b	616	CLA	CHC-C1C	2.30	1.43	1.38
25	C	501	CLA	C3B-C4B	2.30	1.49	1.42
25	B	611	CLA	CHC-C1C	2.30	1.43	1.38
25	b	612	CLA	CHC-C1C	2.30	1.43	1.38
25	B	609	CLA	C3B-C4B	2.30	1.49	1.42
25	b	614	CLA	CHC-C1C	2.29	1.43	1.38
25	B	603	CLA	C3B-C4B	2.29	1.49	1.42
25	B	609	CLA	CHC-C1C	2.29	1.43	1.38
25	a	609	CLA	CHC-C1C	2.29	1.43	1.38
25	c	514	CLA	CHC-C1C	2.29	1.43	1.38
25	D	403	CLA	CHC-C1C	2.29	1.43	1.38
25	C	509	CLA	CHC-C1C	2.29	1.43	1.38
25	c	504	CLA	C3B-C4B	2.29	1.49	1.42
26	d	401	PHO	CAC-C3C	-2.29	1.47	1.51
25	c	508	CLA	C3B-C4B	2.29	1.49	1.42
25	a	609	CLA	C3B-C4B	2.29	1.49	1.42
25	C	506	CLA	C3B-C4B	2.28	1.49	1.42
25	B	604	CLA	CHC-C1C	2.28	1.43	1.38
25	B	601	CLA	CHC-C1C	2.28	1.43	1.38
25	c	504	CLA	CHC-C1C	2.28	1.43	1.38
31	L	101	LHG	O7-C5	-2.27	1.41	1.46
25	c	507	CLA	CHC-C1C	2.27	1.43	1.38
31	D	406	LHG	O7-C5	-2.27	1.41	1.46
25	C	505	CLA	CHC-C1C	2.27	1.43	1.38
25	b	604	CLA	CHC-C1C	2.27	1.43	1.38
25	C	506	CLA	CHC-C1C	2.26	1.43	1.38
25	a	612	CLA	CHC-C1C	2.26	1.43	1.38
25	B	616	CLA	CHC-C1C	2.25	1.43	1.38
25	b	618	CLA	CHC-C1C	2.25	1.43	1.38
25	b	607	CLA	CHC-C1C	2.25	1.43	1.38
28	D	407	PL9	C6-C1	-2.25	1.44	1.48
33	H	103	DGD	O2G-C2G	-2.25	1.41	1.46
25	C	505	CLA	CMD-C2D	-2.25	1.46	1.50
31	d	407	LHG	O7-C5	-2.24	1.41	1.46
28	d	408	PL9	C6-C1	-2.24	1.44	1.48
25	c	508	CLA	CHC-C1C	2.24	1.43	1.38
33	c	520	DGD	O2G-C2G	-2.24	1.41	1.46
25	C	507	CLA	C3B-C4B	2.23	1.49	1.42
25	c	507	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	619	CLA	CHC-C1C	2.23	1.43	1.38
25	C	512	CLA	CHC-C1C	2.23	1.42	1.38
25	c	509	CLA	CHC-C1C	2.23	1.42	1.38
26	A	608	PHO	CAC-C3C	-2.22	1.47	1.51
33	C	516	DGD	O1G-C1G	-2.22	1.40	1.45
33	C	517	DGD	O1G-C1G	-2.21	1.40	1.45
33	c	519	DGD	O1G-C1G	-2.21	1.40	1.45
31	A	616	LHG	O7-C5	-2.21	1.41	1.46
25	c	508	CLA	CMB-C2B	-2.21	1.46	1.50
25	C	506	CLA	CMB-C2B	-2.21	1.46	1.50
25	C	507	CLA	CHC-C1C	2.20	1.42	1.38
33	c	518	DGD	O1G-C1G	-2.20	1.40	1.45
31	a	613	LHG	O7-C5	-2.18	1.41	1.46
25	b	619	CLA	CMC-C2C	-2.18	1.46	1.50
33	c	520	DGD	O1G-C1G	-2.17	1.40	1.45
29	C	519	LMG	O7-C8	-2.15	1.41	1.46
33	C	516	DGD	O2G-C2G	-2.15	1.41	1.46
29	B	625	LMG	O7-C8	-2.15	1.41	1.46
29	B	625	LMG	C3-C2	2.15	1.57	1.52
33	h	102	DGD	O2G-C2G	-2.15	1.41	1.46
33	C	518	DGD	O2G-C2G	-2.15	1.41	1.46
28	a	611	PL9	C6-C1	-2.15	1.45	1.48
31	A	618	LHG	P-O6	2.15	1.67	1.59
28	d	408	PL9	C53-C6	-2.14	1.46	1.50
33	C	517	DGD	O2G-C2G	-2.14	1.41	1.46
25	B	616	CLA	CMC-C2C	-2.14	1.46	1.50
25	b	606	CLA	CMD-C2D	-2.14	1.46	1.50
33	C	518	DGD	O1G-C1G	-2.13	1.40	1.45
29	d	406	LMG	O7-C8	-2.12	1.41	1.46
25	b	614	CLA	CMB-C2B	-2.12	1.46	1.50
34	E	101	HEM	CMB-C2B	2.12	1.55	1.50
25	D	402	CLA	CMD-C2D	-2.12	1.46	1.50
28	a	611	PL9	C53-C6	-2.11	1.46	1.50
28	A	611	PL9	C53-C6	-2.11	1.46	1.50
31	a	614	LHG	O7-C5	-2.11	1.41	1.46
35	v	201	HEC	C3C-C2C	-2.11	1.34	1.41
31	a	615	LHG	O7-C5	-2.10	1.41	1.46
34	E	101	HEM	CMD-C2D	2.10	1.55	1.50
34	e	101	HEM	CMB-C2B	2.10	1.55	1.50
25	B	611	CLA	CMB-C2B	-2.09	1.46	1.50
23	c	501	SQD	O2-C2	-2.09	1.37	1.43
34	e	101	HEM	CMC-C2C	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	V	201	HEC	C3C-C2C	-2.09	1.34	1.41
25	B	612	CLA	CMD-C2D	-2.08	1.46	1.50
28	D	407	PL9	C53-C6	-2.08	1.46	1.50
25	B	603	CLA	CMD-C2D	-2.08	1.46	1.50
25	C	503	CLA	CMD-C2D	-2.08	1.46	1.50
35	V	201	HEC	CMD-C2D	2.08	1.55	1.50
25	A	607	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	614	CLA	CMD-C2D	-2.07	1.46	1.50
25	a	607	CLA	CMD-C2D	-2.07	1.46	1.50
25	C	512	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	607	CLA	CMD-C2D	-2.07	1.46	1.50
25	a	606	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	615	CLA	CMC-C2C	-2.07	1.46	1.50
25	c	504	CLA	CMB-C2B	-2.07	1.46	1.50
25	B	605	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	615	CLA	CMD-C2D	-2.07	1.46	1.50
31	A	618	LHG	O7-C5	-2.07	1.41	1.46
25	B	604	CLA	CMB-C2B	-2.07	1.46	1.50
35	v	201	HEC	CMB-C2B	2.07	1.55	1.50
23	A	603	SQD	O2-C2	-2.07	1.37	1.43
25	c	511	CLA	CMB-C2B	-2.06	1.46	1.50
25	b	604	CLA	CMB-C2B	-2.06	1.46	1.50
25	b	617	CLA	CMD-C2D	-2.06	1.46	1.50
23	f	101	SQD	O2-C2	-2.06	1.37	1.43
23	D	409	SQD	O2-C2	-2.06	1.37	1.43
25	C	510	CLA	CMD-C2D	-2.06	1.46	1.50
29	D	405	LMG	O7-C8	-2.06	1.41	1.46
31	a	615	LHG	P-O6	2.06	1.67	1.59
25	b	608	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	611	CLA	CMB-C2B	-2.05	1.46	1.50
25	C	509	CLA	CMD-C2D	-2.05	1.46	1.50
25	B	607	CLA	CMD-C2D	-2.05	1.46	1.50
25	b	619	CLA	CMD-C2D	-2.05	1.46	1.50
29	c	502	LMG	C4-C5	2.05	1.57	1.53
25	A	615	CLA	CMB-C2B	-2.05	1.46	1.50
33	C	517	DGD	O5D-C6D	-2.05	1.40	1.43
35	V	201	HEC	CMB-C2B	2.05	1.55	1.50
25	B	604	CLA	CMD-C2D	-2.05	1.46	1.50
25	C	510	CLA	CMB-C2B	-2.05	1.46	1.50
25	B	606	CLA	CMB-C2B	-2.04	1.46	1.50
31	A	616	LHG	P-O6	2.04	1.67	1.59
25	A	606	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	101	HEM	CMC-C2C	2.04	1.55	1.50
25	c	510	CLA	CMB-C2B	-2.04	1.46	1.50
25	C	504	CLA	CMD-C2D	-2.04	1.46	1.50
25	c	515	CLA	CMD-C2D	-2.04	1.46	1.50
25	C	507	CLA	CMB-C2B	-2.04	1.46	1.50
23	B	626	SQD	O2-C2	-2.04	1.37	1.43
29	A	612	LMG	O7-C8	-2.04	1.41	1.46
25	c	505	CLA	CMD-C2D	-2.04	1.46	1.50
25	a	609	CLA	CMB-C2B	-2.04	1.46	1.50
25	b	618	CLA	CMB-C2B	-2.04	1.46	1.50
25	c	506	CLA	CMB-C2B	-2.03	1.46	1.50
25	B	608	CLA	CMB-C2B	-2.03	1.46	1.50
25	c	504	CLA	CMD-C2D	-2.03	1.46	1.50
25	a	607	CLA	CMB-C2B	-2.03	1.46	1.50
25	B	609	CLA	CMB-C2B	-2.03	1.46	1.50
25	B	610	CLA	CMB-C2B	-2.03	1.46	1.50
25	B	608	CLA	CMD-C2D	-2.03	1.46	1.50
25	b	609	CLA	CMD-C2D	-2.03	1.46	1.50
25	C	504	CLA	CMB-C2B	-2.03	1.46	1.50
29	c	502	LMG	O7-C8	-2.02	1.41	1.46
25	c	514	CLA	CMD-C2D	-2.02	1.46	1.50
25	d	403	CLA	CMD-C2D	-2.02	1.46	1.50
31	D	406	LHG	P-O6	2.02	1.67	1.59
25	B	612	CLA	CMB-C2B	-2.02	1.46	1.50
25	B	611	CLA	CMD-C2D	-2.02	1.46	1.50
25	D	403	CLA	CMD-C2D	-2.02	1.46	1.50
25	A	609	CLA	CMD-C2D	-2.02	1.46	1.50
25	a	612	CLA	CMD-C2D	-2.02	1.46	1.50
25	a	609	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	607	CLA	CMB-C2B	-2.02	1.46	1.50
25	b	616	CLA	CMD-C2D	-2.02	1.46	1.50
25	C	502	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	618	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	601	SQD	O2-C2	-2.02	1.38	1.43
25	b	616	CLA	CMB-C2B	-2.02	1.46	1.50
34	e	101	HEM	CMA-C3A	2.02	1.54	1.50
25	B	603	CLA	CMB-C2B	-2.01	1.46	1.50
25	b	605	CLA	CMD-C2D	-2.01	1.46	1.50
25	B	602	CLA	CMD-C2D	-2.01	1.46	1.50
25	B	613	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	512	CLA	CMD-C2D	-2.01	1.46	1.50
34	e	101	HEM	CMD-C2D	2.01	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	CMB-C2B	-2.01	1.46	1.50
25	B	601	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	608	CLA	CMB-C2B	-2.01	1.46	1.50
25	a	612	CLA	CMB-C2B	-2.01	1.46	1.50
25	B	616	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	508	CLA	CMB-C2B	-2.01	1.46	1.50
25	c	504	CLA	CMC-C2C	-2.01	1.46	1.50
25	B	605	CLA	CMB-C2B	-2.01	1.46	1.50
25	b	606	CLA	CMB-C2B	-2.01	1.46	1.50
25	c	503	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	502	CLA	CMC-C2C	-2.01	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	612	CLA	CMB-C2B	-2.01	1.46	1.50
25	b	612	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	615	CLA	CMB-C2B	-2.01	1.46	1.50
25	c	509	CLA	CMB-C2B	-2.01	1.46	1.50
25	c	507	CLA	CMB-C2B	-2.01	1.46	1.50
29	d	409	LMG	O7-C8	-2.00	1.41	1.46
25	A	615	CLA	CMD-C2D	-2.00	1.46	1.50
25	B	610	CLA	CMD-C2D	-2.00	1.46	1.50
25	C	505	CLA	CMB-C2B	-2.00	1.46	1.50
25	c	510	CLA	CMD-C2D	-2.00	1.46	1.50
25	B	615	CLA	CMD-C2D	-2.00	1.46	1.50
25	A	607	CLA	CMB-C2B	-2.00	1.46	1.50
25	D	403	CLA	CMB-C2B	-2.00	1.46	1.50
25	b	611	CLA	CMD-C2D	-2.00	1.46	1.50
25	D	402	CLA	CMB-C2B	-2.00	1.46	1.50

All (929) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	C4A-NA-C1A	6.35	109.58	106.68
25	C	503	CLA	C4A-NA-C1A	6.25	109.53	106.68
25	B	604	CLA	C4A-NA-C1A	6.25	109.53	106.68
25	b	607	CLA	C4A-NA-C1A	6.23	109.52	106.68
25	c	513	CLA	C4A-NA-C1A	6.21	109.51	106.68
25	C	512	CLA	C4A-NA-C1A	6.16	109.49	106.68
25	C	511	CLA	C4A-NA-C1A	6.05	109.44	106.68
25	c	514	CLA	C4A-NA-C1A	6.05	109.44	106.68
26	D	401	PHO	C4D-CHA-CBD	-6.00	105.58	108.45
25	c	509	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	c	505	CLA	C4A-NA-C1A	5.96	109.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	C4A-NA-C1A	5.96	109.40	106.68
26	d	401	PHO	C4D-CHA-CBD	-5.94	105.61	108.45
25	B	615	CLA	C4A-NA-C1A	5.94	109.39	106.68
25	c	511	CLA	C4A-NA-C1A	5.93	109.39	106.68
25	b	618	CLA	C4A-NA-C1A	5.90	109.37	106.68
26	A	608	PHO	C4D-CHA-CBD	-5.89	105.63	108.45
26	a	608	PHO	C4D-CHA-CBD	-5.88	105.64	108.45
25	b	604	CLA	C4A-NA-C1A	5.87	109.36	106.68
25	b	612	CLA	C4A-NA-C1A	5.83	109.34	106.68
25	b	616	CLA	C4A-NA-C1A	5.83	109.34	106.68
25	B	613	CLA	C4A-NA-C1A	5.81	109.33	106.68
25	B	601	CLA	C4A-NA-C1A	5.79	109.32	106.68
25	C	502	CLA	C4A-NA-C1A	5.76	109.31	106.68
25	C	509	CLA	C4A-NA-C1A	5.74	109.30	106.68
25	B	616	CLA	C4A-NA-C1A	5.62	109.24	106.68
25	C	505	CLA	C4A-NA-C1A	5.62	109.24	106.68
25	B	612	CLA	C4A-NA-C1A	5.60	109.23	106.68
25	C	506	CLA	C4A-NA-C1A	5.56	109.21	106.68
25	B	609	CLA	C4A-NA-C1A	5.54	109.20	106.68
25	c	507	CLA	C4A-NA-C1A	5.53	109.20	106.68
25	B	606	CLA	C4A-NA-C1A	5.49	109.18	106.68
25	C	501	CLA	C4A-NA-C1A	5.46	109.17	106.68
25	b	615	CLA	C4A-NA-C1A	5.42	109.15	106.68
25	c	512	CLA	C4A-NA-C1A	5.39	109.14	106.68
25	B	605	CLA	C4A-NA-C1A	5.37	109.13	106.68
25	b	614	CLA	C4A-NA-C1A	5.35	109.12	106.68
28	a	611	PL9	C7-C3-C4	5.35	121.32	116.91
25	d	403	CLA	C4A-NA-C1A	5.34	109.11	106.68
25	B	611	CLA	C4A-NA-C1A	5.34	109.11	106.68
25	D	403	CLA	C4A-NA-C1A	5.26	109.08	106.68
25	D	402	CLA	C4A-NA-C1A	5.25	109.07	106.68
25	d	404	CLA	C4A-NA-C1A	5.24	109.07	106.68
25	b	608	CLA	C4A-NA-C1A	5.20	109.05	106.68
25	c	503	CLA	C4A-NA-C1A	5.19	109.05	106.68
25	A	607	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	b	609	CLA	C4A-NA-C1A	5.17	109.04	106.68
25	b	617	CLA	C4A-NA-C1A	5.17	109.04	106.68
28	D	407	PL9	C7-C3-C4	5.17	121.17	116.91
25	c	506	CLA	C4A-NA-C1A	5.15	109.03	106.68
25	c	510	CLA	C4A-NA-C1A	5.12	109.02	106.68
25	C	504	CLA	C4A-NA-C1A	5.12	109.01	106.68
25	A	609	CLA	C4A-NA-C1A	5.11	109.01	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	614	CLA	C4A-NA-C1A	5.10	109.01	106.68
25	C	508	CLA	C4A-NA-C1A	5.08	109.00	106.68
28	d	408	PL9	C7-C3-C4	5.07	121.09	116.91
28	A	611	PL9	C7-C3-C4	5.06	121.08	116.91
25	a	612	CLA	C4A-NA-C1A	5.03	108.97	106.68
25	c	508	CLA	C4A-NA-C1A	4.93	108.93	106.68
25	c	515	CLA	C4A-NA-C1A	4.91	108.92	106.68
23	D	408	SQD	O5-C5-C4	4.89	118.52	109.70
25	B	608	CLA	C4A-NA-C1A	4.88	108.91	106.68
25	b	619	CLA	C4A-NA-C1A	4.77	108.86	106.68
25	A	615	CLA	C4A-NA-C1A	4.75	108.85	106.68
23	D	408	SQD	C1-O5-C5	4.71	122.92	113.72
25	b	611	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	B	602	CLA	C4A-NA-C1A	4.61	108.78	106.68
25	b	605	CLA	C4A-NA-C1A	4.55	108.75	106.68
25	C	510	CLA	C4A-NA-C1A	4.54	108.75	106.68
25	C	513	CLA	C4A-NA-C1A	4.51	108.74	106.68
25	b	610	CLA	C4A-NA-C1A	4.47	108.72	106.68
25	a	607	CLA	C4A-NA-C1A	4.46	108.71	106.68
25	a	609	CLA	C4A-NA-C1A	4.46	108.71	106.68
31	a	614	LHG	O4-P-O5	4.45	133.16	112.44
25	b	613	CLA	C4A-NA-C1A	4.44	108.71	106.68
25	a	606	CLA	C4A-NA-C1A	4.43	108.70	106.68
25	B	603	CLA	C4A-NA-C1A	4.43	108.70	106.68
31	L	101	LHG	O4-P-O5	4.42	133.02	112.44
31	A	617	LHG	O4-P-O5	4.42	133.01	112.44
31	a	613	LHG	O4-P-O5	4.41	132.97	112.44
31	A	616	LHG	O4-P-O5	4.41	132.96	112.44
31	l	101	LHG	O4-P-O5	4.41	132.95	112.44
31	D	406	LHG	O4-P-O5	4.40	132.93	112.44
31	d	407	LHG	O4-P-O5	4.40	132.93	112.44
33	c	518	DGD	O3G-C3G-C2G	-4.39	100.14	110.82
31	a	615	LHG	O4-P-O5	4.39	132.86	112.44
33	C	516	DGD	O3G-C3G-C2G	-4.36	100.21	110.82
31	A	618	LHG	O4-P-O5	4.34	132.66	112.44
23	B	626	SQD	O5-C5-C4	4.27	117.39	109.70
33	C	518	DGD	O3G-C3G-C2G	-4.18	100.66	110.82
33	c	520	DGD	O3G-C3G-C2G	-4.16	100.69	110.82
33	c	519	DGD	O3G-C3G-C2G	-4.10	100.85	110.82
28	a	611	PL9	C7-C3-C2	-4.07	118.59	123.39
25	B	610	CLA	C4A-NA-C1A	4.06	108.53	106.68
28	D	407	PL9	C7-C3-C2	-4.02	118.64	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	611	PL9	C7-C3-C2	-4.02	118.65	123.39
23	A	603	SQD	O9-S-O7	-4.01	100.79	113.82
23	B	626	SQD	O47-C7-C8	3.95	120.02	111.48
28	d	408	PL9	C7-C3-C2	-3.94	118.74	123.39
29	A	613	LMG	O1-C1-C2	-3.94	102.28	108.27
23	D	408	SQD	O9-S-O7	-3.92	101.08	113.82
23	B	626	SQD	O9-S-O7	-3.91	101.11	113.82
29	c	522	LMG	O6-C1-O1	-3.88	100.88	110.04
23	f	101	SQD	O9-S-O7	-3.88	101.22	113.82
23	D	409	SQD	O9-S-O7	-3.87	101.24	113.82
29	C	520	LMG	O6-C1-O1	-3.87	100.90	110.04
25	b	606	CLA	C4A-NA-C1A	3.86	108.44	106.68
23	c	501	SQD	O9-S-O7	-3.85	101.31	113.82
23	b	601	SQD	O9-S-O7	-3.82	101.40	113.82
27	c	516	BCR	C2-C1-C6	3.81	115.97	110.44
26	A	608	PHO	C2B-C1B-NB	-3.78	106.70	109.43
33	H	103	DGD	O3G-C3G-C2G	-3.77	101.66	110.82
23	f	101	SQD	O47-C7-C8	3.75	119.60	111.48
23	I	101	SQD	O47-C7-C8	3.70	119.49	111.48
23	A	619	SQD	O47-C7-C8	3.68	119.44	111.48
26	a	608	PHO	C2B-C1B-NB	-3.67	106.78	109.43
23	A	603	SQD	O5-C5-C4	3.67	116.31	109.70
33	C	517	DGD	O3G-C3G-C2G	-3.64	101.95	110.82
33	h	102	DGD	O3G-C3G-C2G	-3.64	101.96	110.82
23	b	601	SQD	O47-C7-C8	3.63	119.33	111.48
26	d	401	PHO	C2B-C1B-NB	-3.62	106.81	109.43
29	B	621	LMG	O6-C1-O1	-3.62	101.48	110.04
23	D	408	SQD	O47-C7-C8	3.61	119.30	111.48
23	A	603	SQD	O47-C7-C8	3.58	119.22	111.48
26	D	401	PHO	C2B-C1B-NB	-3.54	106.87	109.43
23	B	626	SQD	O6-C1-C2	3.49	113.58	108.27
23	D	409	SQD	O47-C7-C8	3.49	119.02	111.48
33	C	517	DGD	O6D-C1D-O3G	-3.48	101.82	110.04
33	c	518	DGD	O6D-C1D-O3G	-3.48	101.83	110.04
23	A	603	SQD	O9-S-C6	3.45	111.91	106.76
33	c	520	DGD	O6D-C1D-O3G	-3.44	101.92	110.04
23	c	501	SQD	O47-C7-C8	3.44	118.92	111.48
33	C	516	DGD	O6D-C1D-O3G	-3.43	101.94	110.04
33	C	518	DGD	O6D-C1D-O3G	-3.42	101.96	110.04
23	c	501	SQD	O5-C5-C4	3.42	115.85	109.70
29	A	613	LMG	O6-C1-O1	-3.41	101.99	110.04
25	A	606	CLA	C4A-NA-C1A	3.40	108.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	607	CLA	C4A-NA-C1A	3.39	108.22	106.68
23	f	101	SQD	O6-C1-C2	3.38	113.41	108.27
33	c	519	DGD	O6D-C1D-O3G	-3.35	102.14	110.04
23	c	501	SQD	O7-S-C6	3.32	111.71	106.76
23	f	101	SQD	O9-S-C6	3.32	111.71	106.76
23	B	626	SQD	O9-S-C6	3.31	111.70	106.76
23	D	409	SQD	O6-C1-C2	3.31	113.29	108.27
23	b	601	SQD	O7-S-C6	3.30	111.68	106.76
23	D	409	SQD	O9-S-C6	3.27	111.64	106.76
32	A	620	BCT	O2-C-O1	-3.26	111.33	119.68
23	D	409	SQD	O5-C5-C4	3.26	115.57	109.70
23	D	409	SQD	O7-S-C6	3.22	111.56	106.76
33	H	103	DGD	O6D-C1D-O3G	-3.20	102.47	110.04
32	a	605	BCT	O2-C-O1	-3.17	111.56	119.68
23	f	101	SQD	O7-S-C6	3.14	111.44	106.76
27	H	102	BCR	C2-C1-C6	3.13	114.99	110.44
23	A	603	SQD	O7-S-C6	3.12	111.42	106.76
25	b	607	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
23	B	626	SQD	C3-C4-C5	3.11	115.86	110.23
23	c	501	SQD	O9-S-C6	3.10	111.39	106.76
33	h	102	DGD	O6D-C1D-O3G	-3.08	102.77	110.04
23	f	101	SQD	O5-C5-C4	3.07	115.23	109.70
25	b	610	CLA	CHB-C4A-NA	3.07	128.83	124.40
23	c	501	SQD	O6-C1-C2	3.07	112.93	108.27
26	A	608	PHO	O1D-CGD-CBD	3.07	129.38	124.72
25	b	617	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	D	408	SQD	O9-S-C6	3.06	111.33	106.76
27	b	622	BCR	C2-C1-C6	3.06	114.89	110.44
26	a	608	PHO	O1D-CGD-CBD	3.06	129.36	124.72
26	d	401	PHO	O1D-CGD-CBD	3.06	129.36	124.72
26	D	401	PHO	O1D-CGD-CBD	3.05	129.35	124.72
23	A	603	SQD	O6-C1-C2	3.04	112.90	108.27
25	b	609	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
27	c	516	BCR	C15-C16-C17	-3.04	117.30	123.52
25	B	606	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
29	A	613	LMG	O1-C7-C8	-3.03	103.45	110.82
29	B	625	LMG	O6-C1-O1	-3.02	102.90	110.04
25	A	615	CLA	CHB-C4A-NA	3.02	128.76	124.40
25	c	510	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
27	D	404	BCR	C27-C26-C25	3.01	126.77	122.70
25	a	612	CLA	CHB-C4A-NA	3.01	128.74	124.40
25	b	604	CLA	O2D-CGD-O1D	-3.00	118.01	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	405	BCR	C27-C26-C25	2.99	126.75	122.70
25	d	404	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
29	b	624	LMG	O6-C1-O1	-2.99	102.98	110.04
28	d	408	PL9	C22-C23-C24	-2.99	120.78	127.62
25	b	606	CLA	CHB-C4A-NA	2.99	128.71	124.40
25	B	601	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	b	621	BCR	C27-C26-C25	2.98	126.73	122.70
25	c	509	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	B	607	CLA	CHB-C4A-NA	2.97	128.69	124.40
27	B	619	BCR	C27-C26-C25	2.97	126.72	122.70
25	B	603	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
25	b	619	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
27	B	618	BCR	C27-C26-C25	2.96	126.70	122.70
25	c	515	CLA	C3B-C4B-NB	-2.96	107.89	110.53
28	D	407	PL9	C40-C39-C41	2.96	120.36	115.23
25	B	604	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
26	d	401	PHO	CMB-C2B-C3B	2.95	130.58	124.68
25	C	507	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
25	b	606	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
27	B	627	BCR	C15-C14-C13	-2.95	123.14	127.28
25	B	614	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
27	h	101	BCR	C29-C30-C25	2.95	114.72	110.44
23	b	601	SQD	O9-S-C6	2.94	111.15	106.76
27	C	515	BCR	C15-C16-C17	-2.94	117.50	123.52
25	C	505	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
27	h	101	BCR	C24-C23-C22	-2.94	121.89	126.23
25	A	606	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	c	509	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	b	618	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	c	506	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	C	508	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	c	503	CLA	C3B-C4B-NB	-2.93	107.92	110.53
25	C	504	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
25	c	503	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
27	T	101	BCR	C33-C5-C6	-2.92	121.30	124.48
25	C	501	CLA	C3B-C4B-NB	-2.92	107.92	110.53
26	D	401	PHO	CMB-C2B-C3B	2.92	130.51	124.68
25	c	505	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
25	C	507	CLA	CHB-C4A-NA	2.91	128.60	124.40
25	B	602	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
25	A	607	CLA	C3B-C4B-NB	-2.91	107.93	110.53
27	b	622	BCR	C27-C26-C25	2.91	126.63	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	607	CLA	CHB-C4A-NA	2.91	128.60	124.40
25	A	609	CLA	CHB-C4A-NA	2.91	128.59	124.40
25	b	605	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
25	B	613	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
25	B	603	CLA	CHB-C4A-NA	2.90	128.59	124.40
23	D	408	SQD	O7-S-C6	2.90	111.09	106.76
25	C	513	CLA	C3B-C4B-NB	-2.90	107.94	110.53
27	B	627	BCR	C33-C5-C6	-2.89	121.33	124.48
25	B	610	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	c	507	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
31	A	616	LHG	O8-C23-C24	2.89	120.66	111.83
25	a	607	CLA	C3B-C4B-NB	-2.89	107.95	110.53
31	a	614	LHG	O8-C23-C24	2.89	120.65	111.83
25	B	615	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
25	b	610	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
25	a	612	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	C	510	CLA	C3B-C4B-NB	-2.88	107.96	110.53
25	c	506	CLA	CHB-C4A-NA	2.88	128.55	124.40
27	K	101	BCR	C27-C26-C25	2.87	126.59	122.70
31	A	618	LHG	O8-C23-C24	2.87	120.60	111.83
25	C	513	CLA	CHB-C4A-NA	2.87	128.55	124.40
27	d	405	BCR	C2-C1-C6	2.87	114.61	110.44
27	B	617	BCR	C15-C16-C17	-2.87	117.64	123.52
25	b	615	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
25	A	607	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
27	H	102	BCR	C27-C26-C25	2.87	126.58	122.70
25	B	616	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	b	607	CLA	CHB-C4A-NA	2.86	128.53	124.40
25	c	515	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
25	b	616	CLA	C3B-C4B-NB	-2.86	107.97	110.53
27	C	514	BCR	C15-C16-C17	-2.86	117.66	123.52
25	b	614	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	B	612	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	A	609	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
25	b	616	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
25	C	502	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
29	b	623	LMG	O6-C1-O1	-2.85	103.30	110.04
25	c	505	CLA	C3B-C4B-NB	-2.85	107.98	110.53
25	C	501	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	a	606	CLA	CHB-C4A-NA	2.85	128.52	124.40
25	b	609	CLA	CHB-C4A-NA	2.85	128.51	124.40
25	C	503	CLA	C3B-C4B-NB	-2.85	107.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
25	C	506	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
25	C	510	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
23	A	603	SQD	C3-C4-C5	2.84	115.38	110.23
27	T	101	BCR	C15-C14-C13	-2.84	123.29	127.28
25	C	504	CLA	CHB-C4A-NA	2.84	128.50	124.40
25	c	508	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
25	A	609	CLA	C1-C2-C3	-2.84	121.55	126.20
25	b	615	CLA	CHB-C4A-NA	2.84	128.49	124.40
27	c	517	BCR	C15-C16-C17	-2.83	117.72	123.52
25	a	609	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	a	609	CLA	CHB-C4A-NA	2.83	128.49	124.40
25	c	515	CLA	CHB-C4A-NA	2.83	128.49	124.40
26	D	401	PHO	O2D-CGD-O1D	-2.83	118.34	123.85
23	D	408	SQD	C3-C4-C5	2.83	115.36	110.23
25	B	607	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	D	403	CLA	CHB-C4A-NA	2.83	128.48	124.40
31	d	407	LHG	O8-C23-C24	2.83	120.45	111.83
25	C	509	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
25	c	512	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
25	C	504	CLA	C3B-C4B-NB	-2.82	108.01	110.53
25	c	514	CLA	CHB-C4A-NA	2.82	128.47	124.40
25	B	611	CLA	C1-C2-C3	-2.82	121.58	126.20
25	C	512	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
25	B	611	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
25	c	513	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	B	602	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	c	506	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	A	615	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	a	607	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
27	K	101	BCR	C15-C16-C17	-2.81	117.77	123.52
25	B	601	CLA	CHB-C4A-NA	2.81	128.45	124.40
25	C	513	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	b	609	CLA	C3B-C4B-NB	-2.81	108.03	110.53
25	c	514	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
25	C	509	CLA	CHB-C4A-NA	2.80	128.45	124.40
26	A	608	PHO	O2D-CGD-O1D	-2.80	118.39	123.85
25	b	615	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	B	604	CLA	CHB-C4A-NA	2.80	128.44	124.40
25	D	403	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
31	A	617	LHG	O8-C23-C24	2.80	120.37	111.83
25	b	612	CLA	O2D-CGD-O1D	-2.80	118.40	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	401	PHO	O2D-CGD-O1D	-2.80	118.40	123.85
25	c	513	CLA	CHB-C4A-NA	2.80	128.44	124.40
25	A	607	CLA	CHB-C4A-NA	2.80	128.43	124.40
25	A	615	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
27	B	617	BCR	C27-C26-C25	2.79	126.48	122.70
33	h	102	DGD	CDB-CCB-CBB	-2.79	100.25	114.37
27	K	101	BCR	C24-C23-C22	-2.79	122.10	126.23
25	C	508	CLA	CHB-C4A-NA	2.79	128.43	124.40
27	B	627	BCR	C15-C16-C17	-2.79	117.81	123.52
25	b	611	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
25	C	503	CLA	CHB-C4A-NA	2.79	128.42	124.40
25	c	513	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
27	c	516	BCR	C15-C14-C13	-2.79	123.37	127.28
25	B	609	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
25	b	613	CLA	C3B-C4B-NB	-2.78	108.05	110.53
25	b	617	CLA	C3B-C4B-NB	-2.78	108.05	110.53
25	B	608	CLA	C3B-C4B-NB	-2.78	108.05	110.53
25	c	511	CLA	CHB-C4A-NA	2.78	128.41	124.40
25	c	510	CLA	C3B-C4B-NB	-2.78	108.05	110.53
27	b	620	BCR	C33-C5-C6	-2.78	121.45	124.48
27	b	620	BCR	C15-C16-C17	-2.78	117.84	123.52
27	b	620	BCR	C27-C26-C25	2.78	126.46	122.70
25	c	510	CLA	CHB-C4A-NA	2.78	128.41	124.40
33	C	518	DGD	CDB-CCB-CBB	-2.77	100.34	114.37
25	B	612	CLA	CHB-C4A-NA	2.77	128.40	124.40
33	c	518	DGD	CDB-CCB-CBB	-2.77	100.36	114.37
25	b	614	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	c	511	CLA	C3B-C4B-NB	-2.77	108.06	110.53
29	B	621	LMG	O1-C7-C8	-2.77	104.09	110.82
25	c	511	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
28	A	611	PL9	C22-C23-C24	-2.76	121.30	127.62
25	b	604	CLA	C3B-C4B-NB	-2.76	108.06	110.53
25	b	605	CLA	CHB-C4A-NA	2.76	128.38	124.40
27	B	617	BCR	C33-C5-C6	-2.76	121.47	124.48
25	B	612	CLA	C3B-C4B-NB	-2.75	108.07	110.53
25	B	613	CLA	C3B-C4B-NB	-2.75	108.07	110.53
29	C	519	LMG	O6-C1-O1	-2.75	103.55	110.04
27	C	514	BCR	C33-C5-C6	-2.75	121.48	124.48
25	B	608	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	B	615	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	b	604	CLA	CHB-C4A-NA	2.75	128.37	124.40
33	c	519	DGD	CDB-CCB-CBB	-2.75	100.48	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	SQD	C44-O6-C1	2.74	119.68	113.80
25	B	604	CLA	C3B-C4B-NB	-2.74	108.08	110.53
31	D	406	LHG	O8-C23-C24	2.74	120.19	111.83
25	C	503	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
25	B	613	CLA	CHB-C4A-NA	2.74	128.35	124.40
26	a	608	PHO	CMB-C2B-C3B	2.74	130.15	124.68
25	C	511	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
31	L	101	LHG	O8-C23-C24	2.73	120.17	111.83
25	C	512	CLA	CHB-C4A-NA	2.73	128.34	124.40
25	d	404	CLA	CHB-C4A-NA	2.73	128.34	124.40
25	b	611	CLA	CHB-C4A-NA	2.73	128.34	124.40
33	H	103	DGD	CDB-CCB-CBB	-2.73	100.57	114.37
33	c	520	DGD	CDB-CCB-CBB	-2.73	100.59	114.37
25	b	613	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
27	C	514	BCR	C15-C14-C13	-2.73	123.46	127.28
25	b	617	CLA	CHB-C4A-NA	2.72	128.33	124.40
25	b	618	CLA	CHB-C4A-NA	2.72	128.33	124.40
31	a	613	LHG	O8-C23-C24	2.72	120.13	111.83
28	A	611	PL9	C7-C8-C9	-2.72	122.15	126.83
25	A	606	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
25	C	501	CLA	CHB-C4A-NA	2.71	128.32	124.40
25	B	601	CLA	C3B-C4B-NB	-2.71	108.11	110.53
25	b	614	CLA	C1-C2-C3	-2.71	121.76	126.20
25	D	403	CLA	C3B-C4B-NB	-2.71	108.11	110.53
25	B	616	CLA	CHB-C4A-NA	2.71	128.31	124.40
25	B	606	CLA	CHB-C4A-NA	2.71	128.31	124.40
25	B	611	CLA	CHB-C4A-NA	2.71	128.31	124.40
25	B	606	CLA	C3B-C4B-NB	-2.71	108.11	110.53
25	B	610	CLA	C3B-C4B-NB	-2.71	108.11	110.53
27	B	619	BCR	C24-C23-C22	-2.71	122.23	126.23
35	V	201	HEC	C2A-C1A-NA	-2.71	107.71	110.32
25	d	403	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
25	b	613	CLA	CHB-C4A-NA	2.71	128.31	124.40
35	v	201	HEC	C2A-C1A-NA	-2.70	107.71	110.32
25	c	512	CLA	C3B-C4B-NB	-2.70	108.12	110.53
27	y	101	BCR	C27-C26-C25	2.70	126.36	122.70
28	A	611	PL9	C40-C39-C41	2.70	119.92	115.23
25	c	503	CLA	CHB-C4A-NA	2.70	128.30	124.40
25	a	606	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
25	b	619	CLA	CHB-C4A-NA	2.69	128.29	124.40
25	b	607	CLA	C3B-C4B-NB	-2.69	108.13	110.53
25	c	505	CLA	CHB-C4A-NA	2.69	128.28	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	608	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
31	a	615	LHG	O8-C23-C24	2.69	120.02	111.83
25	C	511	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	D	402	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
25	B	608	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
26	a	608	PHO	O2D-CGD-O1D	-2.68	118.64	123.85
27	C	515	BCR	C15-C14-C13	-2.68	123.53	127.28
23	B	626	SQD	O7-S-C6	2.67	110.75	106.76
25	B	610	CLA	CHB-C4A-NA	2.67	128.25	124.40
23	I	101	SQD	O48-C23-C24	2.67	119.96	111.83
25	C	510	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	B	605	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
25	B	615	CLA	C3B-C4B-NB	-2.65	108.16	110.53
25	C	502	CLA	CHB-C4A-NA	2.65	128.23	124.40
25	c	504	CLA	CHB-C4A-NA	2.65	128.22	124.40
33	C	517	DGD	CDB-CCB-CBB	-2.65	100.99	114.37
25	b	608	CLA	CHB-C4A-NA	2.64	128.22	124.40
28	a	611	PL9	C40-C39-C41	2.64	119.82	115.23
28	a	611	PL9	C22-C23-C24	-2.64	121.57	127.62
25	b	612	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	B	614	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	C	511	CLA	C3B-C4B-NB	-2.64	108.17	110.53
25	b	614	CLA	CHB-C4A-NA	2.64	128.21	124.40
29	B	620	LMG	O6-C1-O1	-2.64	103.81	110.04
25	A	609	CLA	C3B-C4B-NB	-2.63	108.18	110.53
25	B	611	CLA	C3B-C4B-NB	-2.63	108.18	110.53
25	C	502	CLA	C3B-C4B-NB	-2.63	108.18	110.53
27	D	404	BCR	C33-C5-C6	-2.63	121.61	124.48
27	B	617	BCR	C24-C23-C22	-2.63	122.35	126.23
27	B	627	BCR	C24-C23-C22	-2.63	122.35	126.23
27	a	610	BCR	C27-C26-C25	2.63	126.25	122.70
28	A	611	PL9	C27-C28-C29	-2.62	121.62	127.62
29	A	612	LMG	O6-C1-O1	-2.62	103.84	110.04
25	c	512	CLA	CHB-C4A-NA	2.62	128.19	124.40
27	c	516	BCR	C27-C26-C25	2.62	126.25	122.70
25	B	605	CLA	CHB-C4A-NA	2.62	128.19	124.40
25	b	616	CLA	CHB-C4A-NA	2.62	128.18	124.40
27	c	517	BCR	C15-C14-C13	-2.62	123.60	127.28
33	C	518	DGD	C3G-C2G-C1G	-2.62	105.68	111.78
27	C	515	BCR	C27-C26-C25	2.61	126.24	122.70
29	c	521	LMG	O6-C1-O1	-2.61	103.87	110.04
23	B	626	SQD	O48-C23-C24	2.61	119.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	408	SQD	C44-O6-C1	2.61	119.40	113.80
29	d	406	LMG	O6-C1-O1	-2.61	103.87	110.04
25	C	508	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	B	619	BCR	C33-C5-C6	-2.61	121.64	124.48
28	D	407	PL9	C22-C23-C24	-2.61	121.66	127.62
27	C	514	BCR	C27-C26-C25	2.60	126.22	122.70
33	C	516	DGD	CDB-CCB-CBB	-2.60	101.23	114.37
27	c	517	BCR	C27-C26-C25	2.59	126.21	122.70
27	b	620	BCR	C15-C14-C13	-2.59	123.64	127.28
25	c	508	CLA	CHB-C4A-NA	2.59	128.14	124.40
25	c	504	CLA	C3B-C4B-NB	-2.59	108.22	110.53
27	y	101	BCR	C33-C5-C6	-2.59	121.66	124.48
29	A	613	LMG	C40-C39-C38	-2.59	101.27	114.37
25	B	614	CLA	C3B-C4B-NB	-2.59	108.22	110.53
23	B	626	SQD	C44-O6-C1	2.59	119.34	113.80
27	B	619	BCR	C15-C16-C17	-2.58	118.23	123.52
23	B	626	SQD	C1-O5-C5	2.58	118.76	113.72
29	B	625	LMG	O1-C1-C2	-2.58	104.35	108.27
28	d	408	PL9	C27-C28-C29	-2.58	121.72	127.62
27	A	610	BCR	C27-C26-C25	2.58	126.19	122.70
31	A	616	LHG	C11-C10-C9	-2.58	101.34	114.37
27	B	617	BCR	C15-C14-C13	-2.57	123.67	127.28
25	d	404	CLA	C3B-C4B-NB	-2.57	108.23	110.53
27	T	101	BCR	C24-C23-C22	-2.57	122.43	126.23
25	a	606	CLA	C3B-C4B-NB	-2.57	108.24	110.53
27	T	101	BCR	C15-C16-C17	-2.57	118.27	123.52
29	B	625	LMG	O1-C7-C8	-2.57	104.58	110.82
23	B	626	SQD	O8-S-C6	2.56	110.91	105.97
25	b	606	CLA	C3B-C4B-NB	-2.56	108.25	110.53
27	k	101	BCR	C29-C30-C25	2.55	114.15	110.44
23	b	601	SQD	O48-C23-C24	2.55	119.62	111.83
29	B	625	LMG	O2-C2-C1	-2.55	103.99	110.08
25	B	609	CLA	CHB-C4A-NA	2.55	128.08	124.40
31	a	613	LHG	C11-C10-C9	-2.55	101.48	114.37
25	d	403	CLA	CHB-C4A-NA	2.55	128.08	124.40
27	B	617	BCR	C11-C10-C9	-2.55	123.70	127.28
28	a	611	PL9	C27-C28-C29	-2.55	121.80	127.62
27	k	101	BCR	C24-C23-C22	-2.55	122.47	126.23
25	B	605	CLA	C3B-C4B-NB	-2.54	108.26	110.53
25	C	509	CLA	C3B-C4B-NB	-2.54	108.26	110.53
27	Y	101	BCR	C27-C26-C25	2.54	126.13	122.70
25	C	506	CLA	CHB-C4A-NA	2.54	128.06	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	C3B-C4B-NB	-2.53	108.27	110.53
25	B	602	CLA	C3B-C4B-NB	-2.53	108.27	110.53
25	c	510	CLA	C1-C2-C3	-2.52	122.06	126.20
25	D	402	CLA	CHB-C4A-NA	2.52	128.04	124.40
31	l	101	LHG	O8-C23-C24	2.52	119.52	111.83
27	A	610	BCR	C15-C16-C17	-2.52	118.36	123.52
26	A	608	PHO	CMB-C2B-C3B	2.52	129.72	124.68
25	a	612	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	b	618	CLA	C3B-C4B-NB	-2.51	108.28	110.53
27	k	101	BCR	C27-C26-C25	2.51	126.10	122.70
29	c	502	LMG	O6-C1-O1	-2.51	104.11	110.04
28	D	407	PL9	C27-C28-C29	-2.51	121.87	127.62
31	a	613	LHG	C20-C19-C18	-2.51	101.67	114.37
23	A	619	SQD	O48-C23-C24	2.51	119.49	111.83
29	B	625	LMG	C40-C39-C38	-2.51	101.68	114.37
27	B	618	BCR	C15-C16-C17	-2.51	118.38	123.52
23	A	603	SQD	O48-C23-C24	2.51	119.49	111.83
29	B	620	LMG	C40-C39-C38	-2.51	101.69	114.37
25	c	514	CLA	C3B-C4B-NB	-2.51	108.29	110.53
31	l	101	LHG	C11-C10-C9	-2.50	101.73	114.37
31	a	615	LHG	C11-C10-C9	-2.50	101.74	114.37
28	d	408	PL9	C7-C8-C9	-2.49	122.54	126.83
29	B	625	LMG	O3-C3-C2	-2.49	104.50	110.38
27	K	101	BCR	C15-C14-C13	-2.49	123.79	127.28
27	C	514	BCR	C11-C10-C9	-2.48	123.79	127.28
27	C	515	BCR	C33-C5-C6	-2.48	121.77	124.48
29	A	613	LMG	C3-C4-C5	-2.48	105.73	110.23
25	b	608	CLA	C3B-C4B-NB	-2.47	108.32	110.53
27	c	517	BCR	C33-C5-C6	-2.47	121.79	124.48
33	C	516	DGD	C3G-C2G-C1G	-2.47	106.03	111.78
23	D	409	SQD	O48-C23-C24	2.47	119.36	111.83
27	B	627	BCR	C27-C26-C25	2.47	126.04	122.70
31	D	406	LHG	C20-C19-C18	-2.46	101.92	114.37
28	A	611	PL9	O2-C1-C6	2.46	124.40	120.48
31	L	101	LHG	C11-C10-C9	-2.46	101.93	114.37
27	B	618	BCR	C15-C14-C13	-2.46	123.83	127.28
25	B	607	CLA	C3B-C4B-NB	-2.46	108.34	110.53
23	c	501	SQD	O48-C23-C24	2.45	119.32	111.83
27	B	618	BCR	C33-C5-C6	-2.45	121.81	124.48
25	C	508	CLA	C1-C2-C3	-2.45	122.18	126.20
34	e	101	HEM	C4D-ND-C1D	2.45	108.11	105.21
27	a	610	BCR	C15-C16-C17	-2.45	118.52	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	408	SQD	O8-S-C6	2.44	110.69	105.97
29	D	405	LMG	C40-C39-C38	-2.44	102.02	114.37
27	a	610	BCR	C33-C5-C6	-2.44	121.82	124.48
29	c	521	LMG	C40-C39-C38	-2.44	102.03	114.37
25	a	609	CLA	C1-C2-C3	-2.44	122.20	126.20
29	D	405	LMG	O6-C1-O1	-2.44	104.28	110.04
23	c	501	SQD	C44-O6-C1	2.44	119.03	113.80
29	b	623	LMG	C40-C39-C38	-2.44	102.04	114.37
27	A	610	BCR	C15-C14-C13	-2.44	123.86	127.28
27	k	101	BCR	C33-C5-C6	-2.44	121.83	124.48
27	h	101	BCR	C2-C1-C6	2.43	113.97	110.44
29	b	624	LMG	C38-C37-C36	-2.43	102.09	114.37
29	b	623	LMG	C38-C37-C36	-2.43	102.09	114.37
31	A	617	LHG	C11-C10-C9	-2.43	102.10	114.37
25	b	611	CLA	C3B-C4B-NB	-2.43	108.36	110.53
29	c	521	LMG	C38-C37-C36	-2.42	102.12	114.37
27	b	621	BCR	C33-C5-C6	-2.42	121.84	124.48
25	B	609	CLA	C3B-C4B-NB	-2.42	108.37	110.53
29	B	620	LMG	C38-C37-C36	-2.42	102.13	114.37
33	c	520	DGD	C3G-C2G-C1G	-2.42	106.14	111.78
31	d	407	LHG	C20-C19-C18	-2.42	102.13	114.37
33	h	102	DGD	C3G-C2G-C1G	-2.42	106.15	111.78
28	D	407	PL9	C7-C8-C9	-2.42	122.67	126.83
31	a	615	LHG	C20-C19-C18	-2.42	102.15	114.37
27	a	610	BCR	C15-C14-C13	-2.42	123.89	127.28
33	c	518	DGD	C3G-C2G-C1G	-2.42	106.15	111.78
27	Y	101	BCR	C33-C5-C6	-2.41	121.85	124.48
29	C	520	LMG	C40-C39-C38	-2.41	102.17	114.37
25	b	605	CLA	C3B-C4B-NB	-2.41	108.38	110.53
29	C	519	LMG	C38-C37-C36	-2.41	102.17	114.37
28	a	611	PL9	C7-C8-C9	-2.41	122.68	126.83
29	A	612	LMG	C40-C39-C38	-2.41	102.19	114.37
23	A	603	SQD	C4-C3-C2	2.41	115.05	110.83
23	f	101	SQD	C44-O6-C1	2.40	118.95	113.80
25	C	505	CLA	CHB-C4A-NA	2.40	127.87	124.40
27	y	101	BCR	C24-C23-C22	-2.40	122.68	126.23
25	C	510	CLA	C1-C2-C3	-2.40	122.27	126.20
31	d	407	LHG	C11-C10-C9	-2.40	102.24	114.37
29	c	502	LMG	C40-C39-C38	-2.40	102.24	114.37
29	C	519	LMG	C40-C39-C38	-2.39	102.26	114.37
27	B	619	BCR	C2-C1-C6	2.39	113.92	110.44
27	A	610	BCR	C33-C5-C6	-2.39	121.87	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	611	PL9	O2-C1-C6	2.39	124.29	120.48
28	A	611	PL9	C37-C38-C39	-2.39	122.16	127.62
27	C	515	BCR	C11-C10-C9	-2.39	123.93	127.28
27	H	102	BCR	C15-C14-C13	-2.39	123.93	127.28
31	l	101	LHG	C20-C19-C18	-2.39	102.31	114.37
25	c	507	CLA	CHB-C4A-NA	2.38	127.84	124.40
25	c	503	CLA	C1-C2-C3	-2.38	122.30	126.20
29	B	625	LMG	C38-C37-C36	-2.38	102.34	114.37
29	c	502	LMG	C38-C37-C36	-2.38	102.34	114.37
29	c	522	LMG	C40-C39-C38	-2.38	102.35	114.37
29	A	612	LMG	C38-C37-C36	-2.38	102.36	114.37
27	h	101	BCR	C15-C14-C13	-2.38	123.95	127.28
31	L	101	LHG	C20-C19-C18	-2.37	102.38	114.37
27	c	516	BCR	C11-C10-C9	-2.37	123.95	127.28
29	B	621	LMG	C40-C39-C38	-2.37	102.40	114.37
31	A	617	LHG	C20-C19-C18	-2.36	102.42	114.37
25	b	607	CLA	O2D-CGD-CBD	2.36	115.36	111.23
27	b	620	BCR	C24-C23-C22	-2.36	122.74	126.23
34	E	101	HEM	C4D-ND-C1D	2.36	108.00	105.21
25	c	508	CLA	C3B-C4B-NB	-2.36	108.42	110.53
29	d	406	LMG	C40-C39-C38	-2.36	102.44	114.37
27	h	101	BCR	C11-C10-C9	-2.36	123.97	127.28
33	H	103	DGD	C3G-C2G-C1G	-2.36	106.29	111.78
28	D	407	PL9	O2-C1-C6	2.36	124.23	120.48
31	A	616	LHG	C20-C19-C18	-2.36	102.45	114.37
25	B	606	CLA	C1-C2-C3	-2.36	122.34	126.20
29	b	624	LMG	C40-C39-C38	-2.35	102.46	114.37
31	A	618	LHG	C11-C10-C9	-2.35	102.47	114.37
29	C	520	LMG	C38-C37-C36	-2.35	102.51	114.37
28	d	408	PL9	O2-C1-C6	2.34	124.20	120.48
27	T	101	BCR	C27-C26-C25	2.34	125.86	122.70
27	d	405	BCR	C33-C5-C6	-2.34	121.93	124.48
27	b	621	BCR	C15-C16-C17	-2.34	118.74	123.52
28	D	407	PL9	C20-C19-C21	2.34	119.28	115.23
28	d	408	PL9	C40-C39-C41	2.34	119.28	115.23
31	a	613	LHG	C18-C17-C16	-2.34	102.56	114.37
33	c	519	DGD	C3G-C2G-C1G	-2.33	106.35	111.78
25	B	612	CLA	C1-C2-C3	-2.33	122.38	126.20
27	H	102	BCR	C24-C23-C22	-2.33	122.79	126.23
27	H	102	BCR	C11-C10-C9	-2.33	124.01	127.28
31	D	406	LHG	C11-C10-C9	-2.33	102.61	114.37
29	c	522	LMG	C38-C37-C36	-2.32	102.63	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	625	LMG	C1-O6-C5	-2.32	109.19	113.72
27	D	404	BCR	C11-C10-C9	-2.32	124.03	127.28
28	a	611	PL9	C37-C38-C39	-2.31	122.33	127.62
33	C	517	DGD	O5D-C6D-C5D	-2.31	104.21	109.42
29	b	623	LMG	O1-C7-C8	-2.31	105.20	110.82
25	C	507	CLA	C3B-C4B-NB	-2.31	108.47	110.53
29	d	409	LMG	C40-C39-C38	-2.30	102.75	114.37
35	v	201	HEC	CBC-CAC-C3C	-2.30	122.85	127.43
31	A	618	LHG	C20-C19-C18	-2.29	102.77	114.37
27	A	610	BCR	C24-C23-C22	-2.29	122.84	126.23
25	C	511	CLA	C1-C2-C3	-2.29	122.44	126.20
29	d	409	LMG	O1-C7-C8	-2.29	105.88	111.77
27	K	101	BCR	C2-C1-C6	2.29	113.76	110.44
27	C	514	BCR	C24-C23-C22	-2.29	122.85	126.23
25	C	505	CLA	C1-C2-C3	-2.29	122.45	126.20
25	c	509	CLA	C3B-C4B-NB	-2.29	108.49	110.53
29	d	406	LMG	C38-C37-C36	-2.28	102.83	114.37
25	b	612	CLA	C3B-C4B-NB	-2.28	108.49	110.53
25	C	506	CLA	C1-C2-C3	-2.28	122.46	126.20
25	A	606	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
28	A	611	PL9	C20-C19-C21	2.28	119.19	115.23
29	D	405	LMG	C38-C37-C36	-2.28	102.85	114.37
25	b	612	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
28	D	407	PL9	O1-C4-C3	-2.27	118.33	120.73
28	D	407	PL9	C37-C38-C39	-2.27	122.43	127.62
33	c	519	DGD	O5D-C6D-C5D	-2.27	104.30	109.42
25	c	514	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
25	B	616	CLA	C3B-C4B-NB	-2.27	108.51	110.53
27	D	404	BCR	C24-C23-C22	-2.27	122.88	126.23
33	c	519	DGD	CBB-CAB-C9B	-2.27	102.92	114.37
27	K	101	BCR	C33-C5-C6	-2.26	122.01	124.48
35	v	201	HEC	C3D-C4D-ND	-2.26	107.64	110.15
28	d	408	PL9	O1-C4-C3	-2.26	118.34	120.73
27	y	101	BCR	C15-C16-C17	-2.26	118.89	123.52
25	a	609	CLA	C3B-C4B-NB	-2.26	108.52	110.53
23	D	408	SQD	O5-C1-C2	2.26	115.01	110.37
25	B	603	CLA	C3B-C4B-NB	-2.26	108.52	110.53
34	E	101	HEM	C2A-C1A-NA	-2.26	107.65	110.15
27	c	516	BCR	C3-C4-C5	-2.26	110.03	114.06
25	B	609	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
23	b	601	SQD	O6-C1-C2	2.25	111.70	108.27
29	B	621	LMG	O3-C3-C2	-2.25	105.06	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	610	BCR	C24-C23-C22	-2.25	122.90	126.23
33	C	516	DGD	O5D-C6D-C5D	-2.25	104.35	109.42
31	A	617	LHG	C27-C26-C25	-2.25	103.00	114.37
27	b	622	BCR	C33-C5-C6	-2.25	122.03	124.48
34	e	101	HEM	C1B-NB-C4B	2.25	107.87	105.21
29	d	409	LMG	C38-C37-C36	-2.25	103.01	114.37
33	c	520	DGD	O5D-C6D-C5D	-2.25	104.36	109.42
35	V	201	HEC	CBC-CAC-C3C	-2.24	122.95	127.43
25	A	606	CLA	C3B-C4B-NB	-2.24	108.53	110.53
29	B	621	LMG	C38-C37-C36	-2.24	103.07	114.37
25	c	508	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
28	d	408	PL9	C36-C34-C33	-2.23	116.15	121.17
25	A	607	CLA	C1-C2-C3	-2.23	122.54	126.20
23	A	603	SQD	C44-O6-C1	2.23	118.57	113.80
25	c	515	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
28	a	611	PL9	C20-C19-C21	2.22	119.09	115.23
27	h	101	BCR	C15-C16-C17	-2.22	118.97	123.52
29	A	613	LMG	O3-C3-C2	-2.22	105.14	110.38
27	d	405	BCR	C15-C16-C17	-2.22	118.97	123.52
27	K	101	BCR	C8-C7-C6	-2.22	121.07	127.00
29	b	623	LMG	O2-C2-C1	-2.22	104.79	110.08
29	c	502	LMG	C1-C2-C3	-2.22	105.35	110.01
27	Y	101	BCR	C15-C16-C17	-2.21	118.99	123.52
29	c	502	LMG	O3-C3-C2	-2.21	105.17	110.38
25	B	603	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
27	B	619	BCR	C15-C14-C13	-2.21	124.18	127.28
29	C	520	LMG	O3-C3-C2	-2.21	105.17	110.38
25	C	513	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
28	d	408	PL9	C42-C43-C44	-2.21	122.57	127.62
23	b	601	SQD	O5-C5-C4	2.21	113.67	109.70
31	d	407	LHG	C27-C26-C25	-2.21	103.22	114.37
34	E	101	HEM	C1B-NB-C4B	2.20	107.82	105.21
26	A	608	PHO	C1-C2-C3	-2.20	122.59	126.20
31	a	614	LHG	C27-C26-C25	-2.20	103.24	114.37
29	c	521	LMG	O2-C2-C1	-2.20	104.83	110.08
23	b	601	SQD	O8-S-C6	2.20	110.22	105.97
31	l	101	LHG	C18-C17-C16	-2.20	103.25	114.37
25	c	507	CLA	C3B-C4B-NB	-2.20	108.57	110.53
31	A	616	LHG	C27-C26-C25	-2.20	103.25	114.37
33	C	516	DGD	CAB-C9B-C8B	-2.20	103.26	114.37
25	D	402	CLA	C3B-C4B-NB	-2.20	108.57	110.53
28	A	611	PL9	O1-C4-C3	-2.20	118.42	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	C1-C2-C3	-2.20	122.60	126.20
29	B	620	LMG	O3-C3-C2	-2.19	105.20	110.38
27	B	617	BCR	C7-C8-C9	-2.19	122.99	126.23
27	b	622	BCR	C24-C23-C22	-2.19	122.99	126.23
25	a	607	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
25	c	511	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
25	c	510	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
31	a	613	LHG	C27-C26-C25	-2.19	103.30	114.37
29	B	621	LMG	C3-C4-C5	-2.19	106.26	110.23
27	C	515	BCR	C24-C23-C22	-2.19	123.00	126.23
27	d	405	BCR	C11-C10-C9	-2.19	124.21	127.28
25	B	604	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
27	D	404	BCR	C15-C16-C17	-2.18	119.05	123.52
29	b	624	LMG	O3-C3-C2	-2.18	105.23	110.38
31	a	615	LHG	C18-C17-C16	-2.18	103.34	114.37
33	C	517	DGD	C1D-C2D-C3D	-2.18	105.42	110.01
29	c	522	LMG	O3-C3-C2	-2.18	105.23	110.38
29	A	613	LMG	C38-C37-C36	-2.18	103.34	114.37
23	D	408	SQD	O48-C23-C24	2.18	118.48	111.83
33	c	518	DGD	CBB-CAB-C9B	-2.18	103.36	114.37
25	a	609	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
27	b	622	BCR	C15-C16-C17	-2.17	119.07	123.52
31	d	407	LHG	C18-C17-C16	-2.17	103.38	114.37
33	c	518	DGD	O5D-C6D-C5D	-2.17	104.52	109.42
25	b	614	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
27	h	101	BCR	C27-C26-C25	2.17	125.64	122.70
33	C	518	DGD	CAB-C9B-C8B	-2.17	103.40	114.37
29	b	623	LMG	O3-C3-C2	-2.17	105.26	110.38
31	A	618	LHG	C27-C26-C25	-2.17	103.41	114.37
29	c	502	LMG	O2-C2-C1	-2.17	104.91	110.08
27	B	618	BCR	C11-C10-C9	-2.17	124.24	127.28
29	A	612	LMG	O3-C3-C2	-2.17	105.27	110.38
25	a	607	CLA	C1-C2-C3	-2.17	122.65	126.20
34	e	101	HEM	C2A-C1A-NA	-2.16	107.75	110.15
23	B	626	SQD	C4-C3-C2	2.16	114.63	110.83
23	f	101	SQD	C4-C3-C2	2.16	114.63	110.83
31	A	618	LHG	C5-O7-C7	-2.16	112.62	117.80
29	c	522	LMG	C3-C4-C5	-2.16	106.31	110.23
31	L	101	LHG	C18-C17-C16	-2.16	103.44	114.37
34	e	101	HEM	C3D-C4D-ND	-2.16	107.80	110.17
28	a	611	PL9	O1-C4-C3	-2.16	118.45	120.73
27	D	404	BCR	C7-C8-C9	-2.16	123.04	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	514	BCR	C7-C8-C9	-2.15	123.05	126.23
25	b	619	CLA	C1-C2-C3	-2.15	122.67	126.20
25	C	506	CLA	C3B-C4B-NB	-2.15	108.61	110.53
28	a	611	PL9	O2-C1-C2	-2.15	116.93	121.83
23	D	409	SQD	C3-C4-C5	2.15	114.14	110.23
25	B	611	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
25	b	611	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
27	D	404	BCR	C15-C14-C13	-2.15	124.26	127.28
27	h	101	BCR	C33-C5-C6	-2.15	122.14	124.48
33	H	103	DGD	CBB-CAB-C9B	-2.15	103.50	114.37
29	C	519	LMG	O2-C2-C1	-2.15	104.95	110.08
25	d	403	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	Y	101	BCR	C8-C7-C6	-2.15	121.26	127.00
25	b	618	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
32	A	620	BCT	O3-C-O1	-2.15	114.18	119.68
28	D	407	PL9	O2-C1-C2	-2.15	116.95	121.83
25	C	505	CLA	C3B-C4B-NB	-2.15	108.61	110.53
25	B	608	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
23	f	101	SQD	C3-C4-C5	2.15	114.12	110.23
31	a	615	LHG	C27-C26-C25	-2.15	103.52	114.37
23	f	101	SQD	O48-C23-C24	2.14	118.37	111.83
25	b	607	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
28	D	407	PL9	C32-C33-C34	-2.14	122.72	127.62
25	b	606	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
27	T	101	BCR	C11-C10-C9	-2.14	124.28	127.28
25	A	609	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
27	B	627	BCR	C11-C10-C9	-2.14	124.28	127.28
25	a	612	CLA	C1-C2-C3	-2.14	122.69	126.20
27	k	101	BCR	C15-C16-C17	-2.14	119.14	123.52
29	b	623	LMG	O1-C1-C2	-2.14	105.03	108.27
25	B	602	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
29	C	519	LMG	O3-C3-C2	-2.14	105.34	110.38
31	D	406	LHG	C18-C17-C16	-2.14	103.57	114.37
29	c	521	LMG	O3-C3-C2	-2.13	105.34	110.38
25	c	504	CLA	C1-C2-C3	-2.13	122.70	126.20
33	C	518	DGD	O5D-C6D-C5D	-2.13	104.61	109.42
33	c	520	DGD	CBB-CAB-C9B	-2.13	103.59	114.37
28	A	611	PL9	O2-C1-C2	-2.13	116.98	121.83
29	d	406	LMG	O1-C7-C8	-2.13	105.64	110.82
26	a	608	PHO	C1-C2-C3	-2.13	122.71	126.20
29	B	620	LMG	O2-C2-C1	-2.13	105.00	110.08
25	C	508	CLA	O2A-CGA-O1A	-2.13	118.30	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	613	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
23	f	101	SQD	O8-S-C6	2.13	110.08	105.97
31	A	616	LHG	C18-C17-C16	-2.12	103.63	114.37
25	a	612	CLA	CHD-C1D-ND	-2.12	121.82	124.80
33	h	102	DGD	CBB-CAB-C9B	-2.12	103.65	114.37
29	A	613	LMG	O2-C2-C1	-2.12	105.02	110.08
25	b	616	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
33	c	518	DGD	CAB-C9B-C8B	-2.12	103.67	114.37
29	C	520	LMG	O2-C2-C3	-2.12	105.39	110.38
27	B	619	BCR	C38-C26-C25	-2.12	122.18	124.48
27	c	517	BCR	C11-C10-C9	-2.11	124.31	127.28
25	A	607	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
25	B	601	CLA	C1-C2-C3	-2.11	122.74	126.20
27	b	621	BCR	C15-C14-C13	-2.11	124.32	127.28
25	c	503	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
33	c	520	DGD	CAB-C9B-C8B	-2.11	103.72	114.37
25	A	615	CLA	CHD-C1D-ND	-2.11	121.84	124.80
31	l	101	LHG	C27-C26-C25	-2.11	103.72	114.37
29	D	405	LMG	O2-C2-C1	-2.10	105.06	110.08
31	A	617	LHG	C18-C17-C16	-2.10	103.74	114.37
25	B	608	CLA	C1-C2-C3	-2.10	122.75	126.20
31	D	406	LHG	C27-C26-C25	-2.10	103.75	114.37
31	L	101	LHG	C27-C26-C25	-2.10	103.76	114.37
25	b	604	CLA	C1-C2-C3	-2.09	122.77	126.20
25	B	615	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
23	D	409	SQD	C4-C3-C2	2.09	114.50	110.83
25	A	606	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	d	404	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
31	A	618	LHG	C18-C17-C16	-2.09	103.80	114.37
28	d	408	PL9	O2-C1-C2	-2.09	117.07	121.83
25	b	619	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
27	H	102	BCR	C15-C16-C17	-2.09	119.24	123.52
23	A	603	SQD	O8-S-C6	2.09	110.01	105.97
25	c	512	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
27	C	515	BCR	C7-C8-C9	-2.09	123.15	126.23
27	B	619	BCR	C8-C7-C6	-2.09	121.42	127.00
25	C	502	CLA	C1-C2-C3	-2.09	122.78	126.20
29	d	406	LMG	O2-C2-C1	-2.09	105.10	110.08
29	b	624	LMG	O1-C7-C8	-2.09	105.74	110.82
29	b	624	LMG	O1-C1-C2	-2.08	105.11	108.27
26	d	401	PHO	C1-C2-C3	-2.08	122.78	126.20
25	A	609	CLA	CHD-C1D-ND	-2.08	121.88	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	610	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	B	612	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	b	613	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
33	C	518	DGD	C5B-C4B-C3B	-2.08	103.86	114.37
23	D	409	SQD	O8-S-C6	2.08	109.98	105.97
33	C	517	DGD	CBB-CAB-C9B	-2.08	103.86	114.37
28	A	611	PL9	C32-C33-C34	-2.08	122.87	127.62
25	B	607	CLA	C1-C2-C3	-2.08	122.79	126.20
25	C	501	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
25	C	512	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
25	B	616	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
25	a	606	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
25	C	503	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
29	D	405	LMG	C1-C2-C3	-2.07	105.65	110.01
27	b	620	BCR	C11-C10-C9	-2.07	124.38	127.28
25	b	604	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
33	c	520	DGD	O2D-C2D-C1D	-2.07	105.15	110.08
33	C	518	DGD	CBB-CAB-C9B	-2.07	103.92	114.37
33	h	102	DGD	C5B-C4B-C3B	-2.07	103.92	114.37
25	C	506	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
33	c	520	DGD	C3D-C4D-C5D	-2.07	106.48	110.23
25	c	506	CLA	CHD-C1D-ND	-2.07	121.89	124.80
29	d	406	LMG	O3-C3-C2	-2.07	105.51	110.38
25	a	607	CLA	CHD-C1D-ND	-2.07	121.90	124.80
25	D	402	CLA	C1-C2-C3	-2.06	122.81	126.20
25	D	403	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
27	c	517	BCR	C24-C23-C22	-2.06	123.18	126.23
35	V	201	HEC	C3D-C4D-ND	-2.06	107.86	110.15
25	b	618	CLA	C1-C2-C3	-2.06	122.82	126.20
25	c	504	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	B	606	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	c	503	CLA	CHD-C1D-ND	-2.06	121.90	124.80
33	c	520	DGD	C5B-C4B-C3B	-2.06	103.96	114.37
25	C	512	CLA	C3B-C4B-NB	-2.06	108.69	110.53
23	c	501	SQD	O8-S-C6	2.06	109.94	105.97
27	k	101	BCR	C8-C7-C6	-2.06	121.51	127.00
25	b	605	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
25	B	609	CLA	C1-C2-C3	-2.06	122.83	126.20
25	B	607	CLA	CHD-C1D-ND	-2.05	121.91	124.80
25	d	404	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
25	b	608	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	c	505	CLA	O2A-CGA-O1A	-2.05	118.50	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	613	CLA	C1-C2-C3	-2.05	122.84	126.20
25	c	513	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
33	c	518	DGD	C5B-C4B-C3B	-2.05	104.02	114.37
25	B	601	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	b	618	CLA	O2D-CGD-CBD	2.05	114.81	111.23
33	h	102	DGD	C1D-C2D-C3D	-2.05	105.70	110.01
25	C	504	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	B	607	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
33	C	516	DGD	C4E-C3E-C2E	-2.05	107.24	110.83
25	c	507	CLA	C1-C2-C3	-2.05	122.85	126.20
26	D	401	PHO	C1-C2-C3	-2.04	122.85	126.20
27	b	622	BCR	C38-C26-C25	-2.04	122.25	124.48
25	b	615	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
25	D	403	CLA	CHD-C1D-ND	-2.04	121.93	124.80
33	c	518	DGD	O2D-C2D-C1D	-2.04	105.21	110.08
25	B	604	CLA	O2D-CGD-CBD	2.04	114.80	111.23
25	C	502	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
33	H	103	DGD	CAB-C9B-C8B	-2.04	104.05	114.37
34	E	101	HEM	C3D-C4D-ND	-2.04	107.94	110.17
27	y	101	BCR	C8-C7-C6	-2.04	121.55	127.00
33	c	519	DGD	O3E-C3E-C2E	-2.04	105.57	110.38
28	a	611	PL9	C32-C33-C34	-2.04	122.96	127.62
25	c	510	CLA	O2D-CGD-CBD	2.04	114.79	111.23
25	C	513	CLA	CHD-C1D-ND	-2.04	121.94	124.80
25	c	514	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
27	b	622	BCR	C15-C14-C13	-2.04	124.42	127.28
25	a	606	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
29	c	522	LMG	O2-C2-C3	-2.03	105.58	110.38
27	A	610	BCR	C8-C7-C6	-2.03	121.56	127.00
25	B	603	CLA	C1-C2-C3	-2.03	122.86	126.20
29	c	521	LMG	O1-C7-C8	-2.03	105.87	110.82
25	c	514	CLA	CMB-C2B-C3B	2.03	131.33	126.55
25	C	509	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
28	A	611	PL9	C36-C34-C33	-2.03	116.61	121.17
29	D	405	LMG	O3-C3-C2	-2.03	105.59	110.38
29	B	620	LMG	O1-C7-C8	-2.03	105.88	110.82
33	h	102	DGD	CAB-C9B-C8B	-2.03	104.11	114.37
25	b	619	CLA	O1D-CGD-CBD	2.03	128.52	124.52
25	c	506	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	a	606	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	c	507	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
33	H	103	DGD	O2D-C2D-C1D	-2.03	105.25	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	517	DGD	C3G-C2G-C1G	-2.03	107.06	111.78
33	c	520	DGD	O6E-C1E-O5D	-2.02	105.26	110.04
33	c	519	DGD	CAB-C9B-C8B	-2.02	104.13	114.37
27	H	102	BCR	C33-C5-C6	-2.02	122.28	124.48
34	e	101	HEM	C3B-C2B-C1B	2.02	107.93	106.41
25	B	604	CLA	C1-C2-C3	-2.02	122.88	126.20
25	C	505	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	c	515	CLA	CHD-C1D-ND	-2.02	121.96	124.80
25	A	606	CLA	CMB-C2B-C3B	2.02	131.30	126.55
25	B	610	CLA	C1-C2-C3	-2.02	122.89	126.20
29	C	520	LMG	C3-C4-C5	-2.02	106.57	110.23
33	C	516	DGD	C5B-C4B-C3B	-2.02	104.15	114.37
28	A	611	PL9	C12-C13-C14	-2.02	123.00	127.62
28	D	407	PL9	C42-C43-C44	-2.02	123.00	127.62
27	B	617	BCR	C2-C1-C6	2.02	113.37	110.44
25	D	402	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
33	C	517	DGD	O3E-C3E-C2E	-2.02	105.62	110.38
27	d	405	BCR	C7-C8-C9	-2.02	123.25	126.23
25	b	612	CLA	C1-C2-C3	-2.02	122.89	126.20
33	C	517	DGD	CAB-C9B-C8B	-2.02	104.18	114.37
29	C	519	LMG	O1-C7-C8	-2.01	105.92	110.82
25	c	508	CLA	C1-C2-C3	-2.01	122.90	126.20
25	C	510	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
29	A	613	LMG	C6-C5-C4	-2.01	108.08	113.02
25	b	610	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
25	b	610	CLA	CHD-C1D-ND	-2.01	121.97	124.80
25	b	608	CLA	CHD-C1D-ND	-2.01	121.98	124.80
33	C	516	DGD	CBB-CAB-C9B	-2.01	104.23	114.37
25	b	607	CLA	C1-C2-C3	-2.01	122.91	126.20
25	A	607	CLA	CHD-C1D-ND	-2.00	121.98	124.80
25	b	616	CLA	C1-C2-C3	-2.00	122.92	126.20
26	a	608	PHO	O2A-CGA-O1A	-2.00	118.62	123.63
25	a	609	CLA	CHD-C1D-ND	-2.00	121.98	124.80
25	C	511	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
25	B	602	CLA	CHD-C1D-ND	-2.00	121.99	124.80
34	E	101	HEM	C3B-C2B-C1B	2.00	107.91	106.41

All (58) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND

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Mol	Chain	Res	Type	Atom
25	A	609	CLA	ND
25	A	615	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	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	503	CLA	ND
25	C	504	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	403	CLA	ND
25	a	606	CLA	ND
25	a	607	CLA	ND
25	a	609	CLA	ND
25	a	612	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	b	617	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	618	CLA	ND
25	b	619	CLA	ND
25	c	503	CLA	ND
25	c	505	CLA	ND
25	c	506	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	c	514	CLA	ND
25	c	515	CLA	ND
25	d	404	CLA	ND

All (1518) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	603	SQD	C5-C6-S-O7
23	A	603	SQD	C5-C6-S-O8
23	A	603	SQD	C5-C6-S-O9
23	A	619	SQD	O6-C44-C45-C46
23	B	626	SQD	C2-C1-O6-C44
23	B	626	SQD	O5-C1-O6-C44
23	B	626	SQD	O6-C44-C45-O47
23	B	626	SQD	O49-C7-O47-C45
23	B	626	SQD	C8-C7-O47-C45
23	D	408	SQD	C2-C1-O6-C44
23	D	408	SQD	O49-C7-O47-C45
23	D	408	SQD	C5-C6-S-O7
23	D	408	SQD	C5-C6-S-O8
23	D	408	SQD	C5-C6-S-O9
23	I	101	SQD	O6-C44-C45-O47
23	I	101	SQD	C8-C7-O47-C45
23	b	601	SQD	O5-C1-O6-C44
23	b	601	SQD	C8-C7-O47-C45
23	b	601	SQD	O5-C5-C6-S
23	c	501	SQD	C5-C6-S-O7
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	A	615	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	607	CLA	CBD-CGD-O2D-CED
25	B	609	CLA	C2B-C3B-CAB-CBB
25	B	609	CLA	C4B-C3B-CAB-CBB
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C2-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	B	615	CLA	C2B-C3B-CAB-CBB
25	B	615	CLA	C4B-C3B-CAB-CBB
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	C2B-C3B-CAB-CBB
25	C	506	CLA	C4B-C3B-CAB-CBB
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C6-C7-C8-C9
25	D	402	CLA	C1A-C2A-CAA-CBA
25	a	606	CLA	CBD-CGD-O2D-CED
25	a	607	CLA	C2B-C3B-CAB-CBB
25	a	607	CLA	C4B-C3B-CAB-CBB
25	a	609	CLA	C2B-C3B-CAB-CBB
25	a	609	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	CAD-CBD-CGD-O1D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CBD-CGD-O2D-CED
25	b	604	CLA	C14-C13-C15-C16
25	b	608	CLA	C2B-C3B-CAB-CBB
25	b	608	CLA	C4B-C3B-CAB-CBB
25	b	608	CLA	C14-C13-C15-C16
25	b	609	CLA	C2B-C3B-CAB-CBB
25	b	609	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	CAD-CBD-CGD-O1D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	b	612	CLA	C2B-C3B-CAB-CBB
25	b	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C1A-C2A-CAA-CBA
25	b	615	CLA	C3A-C2A-CAA-CBA
25	b	617	CLA	CAD-CBD-CGD-O1D
25	b	617	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	c	507	CLA	C4B-C3B-CAB-CBB
25	c	508	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C3A-C2A-CAA-CBA
27	B	627	BCR	C7-C8-C9-C10
27	B	627	BCR	C21-C22-C23-C24
27	D	404	BCR	C7-C8-C9-C10
27	D	404	BCR	C21-C22-C23-C24
27	H	102	BCR	C7-C8-C9-C10
27	H	102	BCR	C7-C8-C9-C34
27	T	101	BCR	C21-C22-C23-C24
27	d	405	BCR	C7-C8-C9-C10
27	h	101	BCR	C7-C8-C9-C10
27	h	101	BCR	C7-C8-C9-C34
27	y	101	BCR	C7-C8-C9-C10
27	y	101	BCR	C7-C8-C9-C34
28	A	611	PL9	C42-C43-C44-C46
28	D	407	PL9	C35-C34-C36-C37
28	a	611	PL9	C35-C34-C36-C37
28	d	408	PL9	C33-C34-C36-C37
28	d	408	PL9	C37-C38-C39-C41
29	A	613	LMG	O1-C7-C8-O7
29	B	621	LMG	O6-C1-O1-C7
29	C	520	LMG	O6-C1-O1-C7
29	b	624	LMG	O6-C1-O1-C7
29	c	522	LMG	O6-C1-O1-C7
29	d	409	LMG	O9-C10-O7-C8
31	A	616	LHG	O1-C1-C2-C3
31	A	616	LHG	C3-O3-P-O6
31	A	618	LHG	C1-C2-C3-O3
31	A	618	LHG	C4-O6-P-O5
31	A	618	LHG	O6-C4-C5-O7
31	D	406	LHG	O1-C1-C2-C3
31	D	406	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
31	D	406	LHG	C3-O3-P-O6
31	D	406	LHG	C4-O6-P-O3
31	D	406	LHG	C4-O6-P-O4
31	D	406	LHG	C4-O6-P-O5
31	L	101	LHG	C4-O6-P-O5
31	a	613	LHG	C3-O3-P-O5
31	a	613	LHG	C3-O3-P-O6
31	a	613	LHG	C4-O6-P-O5
31	a	614	LHG	C4-O6-P-O3
31	a	614	LHG	C4-O6-P-O4
31	a	615	LHG	O1-C1-C2-C3
31	a	615	LHG	C3-O3-P-O4
31	a	615	LHG	C3-O3-P-O6
31	a	615	LHG	O7-C5-C6-O8
31	d	407	LHG	C3-O3-P-O4
31	d	407	LHG	C3-O3-P-O6
31	d	407	LHG	C4-O6-P-O3
31	l	101	LHG	C3-O3-P-O4
31	l	101	LHG	C4-O6-P-O5
33	C	517	DGD	C2E-C1E-O5D-C6D
33	c	519	DGD	C2E-C1E-O5D-C6D
25	b	610	CLA	O1D-CGD-O2D-CED
25	A	606	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	b	619	CLA	CBD-CGD-O2D-CED
23	A	619	SQD	O10-C23-O48-C46
23	B	626	SQD	O10-C23-O48-C46
25	B	610	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
25	B	607	CLA	O1D-CGD-O2D-CED
25	a	606	CLA	O1D-CGD-O2D-CED
25	c	508	CLA	O1D-CGD-O2D-CED
23	A	619	SQD	O49-C7-O47-C45
23	I	101	SQD	O49-C7-O47-C45
23	b	601	SQD	O49-C7-O47-C45
33	h	102	DGD	C4E-C5E-C6E-O5E
25	B	601	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	C	506	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	b	619	CLA	C3-C5-C6-C7
23	A	619	SQD	C24-C23-O48-C46
23	B	626	SQD	C24-C23-O48-C46
25	B	603	CLA	CBD-CGD-O2D-CED
25	B	604	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	c	514	CLA	CBD-CGD-O2D-CED
26	D	401	PHO	CBD-CGD-O2D-CED
23	D	408	SQD	C8-C7-O47-C45
29	d	409	LMG	C11-C10-O7-C8
25	B	601	CLA	O1D-CGD-O2D-CED
25	B	609	CLA	O1D-CGD-O2D-CED
25	b	604	CLA	O1D-CGD-O2D-CED
25	b	619	CLA	O1D-CGD-O2D-CED
25	a	609	CLA	C4-C3-C5-C6
25	b	617	CLA	C4-C3-C5-C6
28	a	611	PL9	C25-C24-C26-C27
25	a	609	CLA	C2-C3-C5-C6
25	b	617	CLA	C2-C3-C5-C6
28	D	407	PL9	C33-C34-C36-C37
28	d	408	PL9	C18-C19-C21-C22
25	B	605	CLA	CBD-CGD-O2D-CED
23	b	601	SQD	C24-C23-O48-C46
25	b	619	CLA	CBA-CGA-O2A-C1
29	B	625	LMG	C4-C5-C6-O5
29	c	521	LMG	O6-C5-C6-O5
23	b	601	SQD	O10-C23-O48-C46
29	c	502	LMG	O6-C5-C6-O5
33	h	102	DGD	O6E-C5E-C6E-O5E
25	b	613	CLA	CBD-CGD-O2D-CED
25	c	515	CLA	CBD-CGD-O2D-CED
31	A	618	LHG	O2-C2-C3-O3
31	a	615	LHG	O2-C2-C3-O3
31	d	407	LHG	O2-C2-C3-O3
23	D	408	SQD	C24-C23-O48-C46
25	B	616	CLA	CBA-CGA-O2A-C1
33	c	519	DGD	O6E-C5E-C6E-O5E
25	b	619	CLA	O1A-CGA-O2A-C1
33	C	517	DGD	O6E-C5E-C6E-O5E
29	c	521	LMG	C4-C5-C6-O5
25	A	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	O1D-CGD-O2D-CED
25	b	604	CLA	C3-C5-C6-C7
25	c	508	CLA	C3-C5-C6-C7
33	H	103	DGD	C4D-C5D-C6D-O5D
25	B	616	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	b	608	CLA	C4-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	b	608	CLA	C2-C3-C5-C6
28	a	611	PL9	C23-C24-C26-C27
28	A	611	PL9	C9-C11-C12-C13
28	a	611	PL9	C9-C11-C12-C13
28	d	408	PL9	C9-C11-C12-C13
28	d	408	PL9	C39-C41-C42-C43
29	C	519	LMG	O6-C5-C6-O5
34	E	101	HEM	C3D-CAD-CBD-CGD
34	e	101	HEM	C3D-CAD-CBD-CGD
25	B	616	CLA	O1A-CGA-O2A-C1
23	D	408	SQD	O5-C1-O6-C44
23	f	101	SQD	O5-C1-O6-C44
29	A	612	LMG	O6-C1-O1-C7
29	c	521	LMG	O6-C1-O1-C7
33	C	517	DGD	O6E-C1E-O5D-C6D
33	c	519	DGD	O6E-C1E-O5D-C6D
25	A	606	CLA	O1D-CGD-O2D-CED
23	I	101	SQD	C24-C23-O48-C46
25	C	511	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	612	CLA	CBD-CGD-O2D-CED
29	B	625	LMG	O6-C5-C6-O5
29	b	624	LMG	O6-C5-C6-O5
25	b	607	CLA	CBD-CGD-O2D-CED
29	c	502	LMG	C4-C5-C6-O5
31	a	615	LHG	C1-C2-C3-O3
29	b	624	LMG	C4-C5-C6-O5
26	D	401	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C4-C3-C5-C6
25	B	602	CLA	C2-C3-C5-C6
25	B	601	CLA	C14-C13-C15-C16
25	B	602	CLA	C6-C7-C8-C9
25	B	602	CLA	C14-C13-C15-C16
25	B	605	CLA	C14-C13-C15-C16
25	B	609	CLA	C14-C13-C15-C16
25	B	610	CLA	C11-C12-C13-C14
25	B	614	CLA	C6-C7-C8-C9
25	C	506	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C12-C13-C14
25	b	604	CLA	C11-C10-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	b	612	CLA	C14-C13-C15-C16
25	b	613	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
25	c	511	CLA	C11-C10-C8-C9
25	b	606	CLA	O1D-CGD-O2D-CED
23	D	409	SQD	C2-C1-O6-C44
23	f	101	SQD	C2-C1-O6-C44
29	A	612	LMG	C2-C1-O1-C7
29	B	621	LMG	C2-C1-O1-C7
29	b	624	LMG	C2-C1-O1-C7
31	a	614	LHG	O2-C2-C3-O3
29	C	519	LMG	C4-C5-C6-O5
27	B	627	BCR	C7-C8-C9-C34
27	T	101	BCR	C7-C8-C9-C34
27	Y	101	BCR	C7-C8-C9-C34
27	c	516	BCR	C7-C8-C9-C34
27	d	405	BCR	C7-C8-C9-C34
27	d	405	BCR	C37-C22-C23-C24
27	T	101	BCR	C7-C8-C9-C10
27	c	516	BCR	C7-C8-C9-C10
33	c	519	DGD	C4E-C5E-C6E-O5E
33	C	517	DGD	C4E-C5E-C6E-O5E
23	A	619	SQD	C8-C7-O47-C45
25	B	601	CLA	CBA-CGA-O2A-C1
29	A	612	LMG	C28-C29-C30-C31
29	B	621	LMG	C10-C11-C12-C13
25	B	614	CLA	O1D-CGD-O2D-CED
25	c	514	CLA	O1D-CGD-O2D-CED
31	D	406	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
31	A	616	LHG	O1-C1-C2-O2
33	c	520	DGD	O6E-C5E-C6E-O5E
25	B	610	CLA	C13-C15-C16-C17
28	A	611	PL9	C24-C26-C27-C28
28	D	407	PL9	C39-C41-C42-C43
28	d	408	PL9	C34-C36-C37-C38
25	A	609	CLA	C13-C15-C16-C17
31	d	407	LHG	C32-C33-C34-C35
29	c	522	LMG	O6-C5-C6-O5
29	c	502	LMG	C10-C11-C12-C13
31	A	618	LHG	C7-C8-C9-C10
31	a	615	LHG	C23-C24-C25-C26
33	c	519	DGD	C1B-C2B-C3B-C4B
23	D	409	SQD	C8-C7-O47-C45
25	B	604	CLA	O1D-CGD-O2D-CED
25	C	505	CLA	C5-C6-C7-C8
25	b	619	CLA	C10-C11-C12-C13
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	609	CLA	C2A-CAA-CBA-CGA
25	A	609	CLA	C10-C11-C12-C13
23	D	409	SQD	C23-C24-C25-C26
23	I	101	SQD	C23-C24-C25-C26
23	b	601	SQD	C7-C8-C9-C10
29	b	623	LMG	C28-C29-C30-C31
31	l	101	LHG	C23-C24-C25-C26
33	C	517	DGD	C1B-C2B-C3B-C4B
29	c	502	LMG	O6-C1-O1-C7
25	B	603	CLA	O1D-CGD-O2D-CED
25	B	613	CLA	C5-C6-C7-C8
25	B	614	CLA	C13-C15-C16-C17
25	b	604	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
23	A	619	SQD	C23-C24-C25-C26
31	A	618	LHG	C23-C24-C25-C26
25	b	619	CLA	C8-C10-C11-C12
25	b	613	CLA	O1D-CGD-O2D-CED
29	d	409	LMG	C10-C11-C12-C13
31	a	613	LHG	C7-C8-C9-C10
25	B	605	CLA	O1D-CGD-O2D-CED
25	C	506	CLA	C8-C10-C11-C12
25	b	604	CLA	C10-C11-C12-C13
25	b	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	c	515	CLA	O1D-CGD-O2D-CED
31	d	407	LHG	C23-C24-C25-C26
23	f	101	SQD	O49-C7-O47-C45
31	d	407	LHG	C1-C2-C3-O3
23	f	101	SQD	C24-C23-O48-C46
29	C	519	LMG	C29-C28-O8-C9
25	a	609	CLA	C8-C10-C11-C12
25	c	503	CLA	CBD-CGD-O2D-CED
25	A	609	CLA	O1D-CGD-O2D-CED
31	L	101	LHG	C23-C24-C25-C26
25	b	615	CLA	C13-C15-C16-C17
29	B	621	LMG	O6-C5-C6-O5
25	B	601	CLA	C10-C11-C12-C13
25	B	616	CLA	C10-C11-C12-C13
29	B	625	LMG	C10-C11-C12-C13
25	C	510	CLA	C5-C6-C7-C8
25	b	608	CLA	C13-C15-C16-C17
23	f	101	SQD	C8-C7-O47-C45
29	A	613	LMG	C11-C10-O7-C8
25	B	606	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	O1D-CGD-O2D-CED
29	c	502	LMG	C2-C1-O1-C7
29	c	521	LMG	C2-C1-O1-C7
31	A	616	LHG	C23-C24-C25-C26
25	b	615	CLA	O1D-CGD-O2D-CED
25	b	610	CLA	CBA-CGA-O2A-C1
25	d	404	CLA	C16-C17-C18-C20
25	C	502	CLA	O1D-CGD-O2D-CED
25	c	508	CLA	C10-C11-C12-C13
27	A	610	BCR	C7-C8-C9-C34
27	B	627	BCR	C37-C22-C23-C24
27	D	404	BCR	C7-C8-C9-C34
27	T	101	BCR	C37-C22-C23-C24
27	Y	101	BCR	C37-C22-C23-C24
27	a	610	BCR	C7-C8-C9-C34
27	b	622	BCR	C37-C22-C23-C24
27	c	517	BCR	C7-C8-C9-C34
27	d	405	BCR	C21-C22-C23-C24
31	a	613	LHG	O1-C1-C2-C3
25	B	601	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
23	D	409	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
29	B	620	LMG	C28-C29-C30-C31
25	a	609	CLA	C16-C17-C18-C19
25	B	614	CLA	C8-C10-C11-C12
23	B	626	SQD	C31-C32-C33-C34
23	f	101	SQD	C27-C28-C29-C30
29	A	612	LMG	C14-C15-C16-C17
29	B	625	LMG	C14-C15-C16-C17
33	C	517	DGD	C5A-C6A-C7A-C8A
23	A	619	SQD	C12-C13-C14-C15
23	B	626	SQD	C14-C15-C16-C17
23	b	601	SQD	C9-C10-C11-C12
23	b	601	SQD	C27-C28-C29-C30
29	B	625	LMG	C19-C20-C21-C22
29	B	625	LMG	C20-C21-C22-C23
29	C	519	LMG	C31-C32-C33-C34
29	D	405	LMG	C17-C18-C19-C20
29	b	624	LMG	C19-C20-C21-C22
29	c	521	LMG	C31-C32-C33-C34
31	A	617	LHG	C12-C13-C14-C15
31	a	615	LHG	C11-C12-C13-C14
31	l	101	LHG	C34-C35-C36-C37
33	C	517	DGD	C4A-C5A-C6A-C7A
33	C	518	DGD	C6B-C7B-C8B-C9B
33	C	518	DGD	C7B-C8B-C9B-CAB
29	c	502	LMG	C28-C29-C30-C31
23	B	626	SQD	C9-C10-C11-C12
23	I	101	SQD	C13-C14-C15-C16
29	C	519	LMG	C15-C16-C17-C18
23	B	626	SQD	C10-C11-C12-C13
23	f	101	SQD	C33-C34-C35-C36
29	A	613	LMG	C17-C18-C19-C20
29	b	624	LMG	C29-C30-C31-C32
31	d	407	LHG	C25-C26-C27-C28
31	l	101	LHG	C10-C11-C12-C13
33	C	517	DGD	C7B-C8B-C9B-CAB
33	c	519	DGD	C6B-C7B-C8B-C9B
33	h	102	DGD	C3B-C4B-C5B-C6B
31	a	615	LHG	O1-C1-C2-O2
23	A	619	SQD	C28-C29-C30-C31
23	I	101	SQD	C10-C11-C12-C13
29	A	613	LMG	C14-C15-C16-C17
29	C	520	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	C	520	LMG	C30-C31-C32-C33
25	B	601	CLA	C4B-C3B-CAB-CBB
25	B	602	CLA	C4B-C3B-CAB-CBB
25	C	502	CLA	C4B-C3B-CAB-CBB
25	C	503	CLA	C4B-C3B-CAB-CBB
29	D	405	LMG	C10-C11-C12-C13
23	A	619	SQD	C17-C18-C19-C20
23	b	601	SQD	C11-C10-C9-C8
25	D	403	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C20
25	a	609	CLA	C16-C17-C18-C20
25	C	511	CLA	O1D-CGD-O2D-CED
25	b	604	CLA	O1A-CGA-O2A-C1
25	c	503	CLA	C2A-CAA-CBA-CGA
25	B	602	CLA	C5-C6-C7-C8
29	A	612	LMG	C11-C10-O7-C8
23	A	603	SQD	C30-C31-C32-C33
23	I	101	SQD	C9-C10-C11-C12
29	C	519	LMG	C32-C33-C34-C35
29	c	502	LMG	C13-C14-C15-C16
25	B	602	CLA	C12-C13-C15-C16
25	b	619	CLA	C11-C12-C13-C15
25	c	514	CLA	C12-C13-C15-C16
29	B	625	LMG	C30-C31-C32-C33
29	c	521	LMG	C29-C28-O8-C9
25	B	616	CLA	C13-C15-C16-C17
25	D	402	CLA	C3A-C2A-CAA-CBA
26	a	608	PHO	C3A-C2A-CAA-CBA
23	A	603	SQD	C29-C30-C31-C32
29	B	621	LMG	C29-C30-C31-C32
25	B	605	CLA	C13-C15-C16-C17
25	d	404	CLA	C16-C17-C18-C19
23	I	101	SQD	C14-C15-C16-C17
29	A	612	LMG	C13-C14-C15-C16
23	c	501	SQD	C10-C11-C12-C13
29	C	519	LMG	C11-C12-C13-C14
29	D	405	LMG	C30-C31-C32-C33
33	C	518	DGD	C2A-C1A-O1G-C1G
31	L	101	LHG	C34-C35-C36-C37
31	a	613	LHG	C25-C26-C27-C28
31	a	614	LHG	C29-C30-C31-C32
31	d	407	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
33	c	519	DGD	C9A-CAA-CBA-CCA
25	b	609	CLA	O1D-CGD-O2D-CED
23	I	101	SQD	C11-C12-C13-C14
29	B	625	LMG	C13-C14-C15-C16
29	C	520	LMG	C12-C13-C14-C15
29	c	521	LMG	C32-C33-C34-C35
31	D	406	LHG	C11-C10-C9-C8
31	a	615	LHG	C9-C10-C11-C12
31	l	101	LHG	C14-C15-C16-C17
33	C	516	DGD	C4B-C5B-C6B-C7B
33	H	103	DGD	CBA-CCA-CDA-CEA
33	c	519	DGD	CAA-CBA-CCA-CDA
33	c	519	DGD	C4B-C5B-C6B-C7B
23	D	408	SQD	O10-C23-O48-C46
25	b	610	CLA	O1A-CGA-O2A-C1
23	B	626	SQD	C15-C16-C17-C18
23	I	101	SQD	C25-C26-C27-C28
29	B	620	LMG	C30-C31-C32-C33
29	B	625	LMG	C18-C19-C20-C21
29	C	519	LMG	C18-C19-C20-C21
33	H	103	DGD	CCA-CDA-CEA-CFA
33	c	518	DGD	C4B-C5B-C6B-C7B
25	b	612	CLA	O1D-CGD-O2D-CED
23	c	501	SQD	C9-C10-C11-C12
23	f	101	SQD	C34-C35-C36-C37
31	l	101	LHG	C16-C17-C18-C19
23	B	626	SQD	C12-C13-C14-C15
23	I	101	SQD	C26-C27-C28-C29
23	c	501	SQD	C17-C18-C19-C20
29	D	405	LMG	C20-C21-C22-C23
33	c	518	DGD	C4A-C5A-C6A-C7A
33	c	518	DGD	C5B-C6B-C7B-C8B
25	A	609	CLA	C16-C17-C18-C20
23	I	101	SQD	C7-C8-C9-C10
23	I	101	SQD	O10-C23-O48-C46
25	A	615	CLA	C2B-C3B-CAB-CBB
25	B	601	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C2B-C3B-CAB-CBB
25	b	604	CLA	C2B-C3B-CAB-CBB
25	c	507	CLA	C2B-C3B-CAB-CBB
27	B	627	BCR	C1-C6-C7-C8
27	B	627	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	b	620	BCR	C1-C6-C7-C8
27	y	101	BCR	C1-C6-C7-C8
29	C	520	LMG	C20-C21-C22-C23
29	c	522	LMG	C19-C20-C21-C22
26	d	401	PHO	CBD-CGD-O2D-CED
25	C	505	CLA	C8-C10-C11-C12
25	c	511	CLA	C3-C5-C6-C7
29	C	519	LMG	C16-C17-C18-C19
29	b	623	LMG	C30-C31-C32-C33
31	L	101	LHG	C10-C11-C12-C13
31	a	614	LHG	C30-C31-C32-C33
33	C	517	DGD	C6B-C7B-C8B-C9B
35	V	201	HEC	C3D-CAD-CBD-CGD
23	A	603	SQD	C13-C14-C15-C16
31	L	101	LHG	C29-C30-C31-C32
31	l	101	LHG	C27-C28-C29-C30
29	d	409	LMG	C33-C34-C35-C36
31	A	617	LHG	C27-C28-C29-C30
29	A	612	LMG	C18-C19-C20-C21
27	B	627	BCR	C10-C11-C12-C13
27	T	101	BCR	C10-C11-C12-C13
29	b	624	LMG	C37-C38-C39-C40
31	a	615	LHG	C14-C15-C16-C17
31	a	615	LHG	C27-C28-C29-C30
25	B	607	CLA	CBA-CGA-O2A-C1
25	b	619	CLA	C6-C7-C8-C9
25	C	505	CLA	C13-C15-C16-C17
29	C	519	LMG	C19-C20-C21-C22
29	C	519	LMG	C29-C30-C31-C32
29	c	522	LMG	C17-C18-C19-C20
29	B	621	LMG	C16-C17-C18-C19
29	C	519	LMG	C14-C15-C16-C17
33	H	103	DGD	O6E-C5E-C6E-O5E
25	a	609	CLA	C15-C16-C17-C18
29	B	621	LMG	C20-C21-C22-C23
29	D	405	LMG	C15-C16-C17-C18
29	c	502	LMG	C32-C33-C34-C35
31	A	616	LHG	C32-C33-C34-C35
33	C	518	DGD	CBA-CCA-CDA-CEA
23	f	101	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
29	b	623	LMG	C36-C37-C38-C39
29	d	409	LMG	C31-C32-C33-C34
29	c	502	LMG	C36-C37-C38-C39
25	b	605	CLA	C5-C6-C7-C8
33	c	520	DGD	C2A-C1A-O1G-C1G
23	D	408	SQD	C7-C8-C9-C10
31	a	614	LHG	C7-C8-C9-C10
31	A	617	LHG	C32-C33-C34-C35
29	A	612	LMG	C17-C18-C19-C20
25	B	614	CLA	C3-C5-C6-C7
25	C	506	CLA	C16-C17-C18-C20
25	b	619	CLA	C16-C17-C18-C19
25	b	619	CLA	C16-C17-C18-C20
25	C	513	CLA	CBD-CGD-O2D-CED
23	B	626	SQD	C32-C33-C34-C35
23	c	501	SQD	C12-C13-C14-C15
29	B	621	LMG	C31-C32-C33-C34
31	l	101	LHG	C30-C31-C32-C33
25	C	505	CLA	C4-C3-C5-C6
25	C	505	CLA	C2-C3-C5-C6
29	A	613	LMG	C11-C12-C13-C14
29	B	625	LMG	C31-C32-C33-C34
29	c	522	LMG	C20-C21-C22-C23
23	B	626	SQD	C13-C14-C15-C16
29	c	502	LMG	C31-C32-C33-C34
23	A	619	SQD	C11-C10-C9-C8
29	b	623	LMG	C31-C32-C33-C34
29	A	613	LMG	O9-C10-O7-C8
31	A	617	LHG	O6-C4-C5-O7
29	D	405	LMG	O6-C5-C6-O5
29	B	620	LMG	C32-C33-C34-C35
29	C	520	LMG	C19-C20-C21-C22
29	d	409	LMG	C11-C12-C13-C14
25	B	608	CLA	C15-C16-C17-C18
25	c	511	CLA	C8-C10-C11-C12
29	c	522	LMG	C14-C15-C16-C17
33	C	516	DGD	C4A-C5A-C6A-C7A
29	C	520	LMG	O6-C5-C6-O5
23	I	101	SQD	C17-C18-C19-C20
29	A	613	LMG	C37-C38-C39-C40
25	b	613	CLA	C13-C15-C16-C17
29	b	623	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
31	a	613	LHG	C32-C33-C34-C35
33	C	517	DGD	C6A-C7A-C8A-C9A
23	A	619	SQD	C32-C33-C34-C35
31	A	616	LHG	C11-C10-C9-C8
33	H	103	DGD	C5B-C6B-C7B-C8B
23	D	408	SQD	C12-C13-C14-C15
29	c	502	LMG	C20-C21-C22-C23
23	A	619	SQD	C18-C19-C20-C21
29	C	520	LMG	C34-C35-C36-C37
29	c	502	LMG	C29-C30-C31-C32
23	I	101	SQD	C27-C28-C29-C30
31	l	101	LHG	C9-C10-C11-C12
23	D	409	SQD	O49-C7-O47-C45
29	C	519	LMG	C30-C31-C32-C33
31	A	616	LHG	C25-C26-C27-C28
25	B	603	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	C	505	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CBD-CGD-O2D-CED
29	A	613	LMG	C31-C32-C33-C34
29	C	519	LMG	C20-C21-C22-C23
31	A	618	LHG	C8-C7-O7-C5
23	D	408	SQD	C24-C25-C26-C27
29	B	621	LMG	C14-C15-C16-C17
31	l	101	LHG	C33-C34-C35-C36
31	a	613	LHG	O1-C1-C2-O2
23	I	101	SQD	C31-C32-C33-C34
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
29	A	612	LMG	C15-C16-C17-C18
25	B	607	CLA	O1A-CGA-O2A-C1
23	B	626	SQD	C29-C30-C31-C32
29	c	502	LMG	C21-C22-C23-C24
31	A	618	LHG	C32-C33-C34-C35
31	A	618	LHG	O6-C4-C5-C6
31	A	618	LHG	C30-C31-C32-C33
25	A	607	CLA	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	C	510	CLA	C6-C7-C8-C10
25	C	512	CLA	C6-C7-C8-C10
25	C	512	CLA	C11-C10-C8-C7
25	C	512	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	a	607	CLA	C6-C7-C8-C10
25	b	604	CLA	C11-C10-C8-C7
25	b	607	CLA	C6-C7-C8-C10
25	c	508	CLA	C11-C12-C13-C15
25	d	403	CLA	C12-C13-C15-C16
23	b	601	SQD	C28-C29-C30-C31
23	c	501	SQD	C16-C17-C18-C19
29	C	519	LMG	C38-C39-C40-C41
25	b	607	CLA	O1D-CGD-O2D-CED
23	I	101	SQD	C30-C31-C32-C33
29	B	625	LMG	C34-C35-C36-C37
25	D	403	CLA	C13-C15-C16-C17
25	C	501	CLA	C2A-CAA-CBA-CGA
25	B	616	CLA	C6-C7-C8-C9
25	C	510	CLA	C6-C7-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	614	CLA	C14-C13-C15-C16
25	b	619	CLA	C14-C13-C15-C16
25	c	508	CLA	C11-C12-C13-C14
29	c	522	LMG	C30-C31-C32-C33
25	b	615	CLA	CBA-CGA-O2A-C1
29	b	624	LMG	C29-C28-O8-C9
25	c	512	CLA	CBD-CGD-O2D-CED
23	A	619	SQD	C44-C45-C46-O48
23	D	409	SQD	C44-C45-C46-O48
29	B	625	LMG	O1-C7-C8-C9
29	c	502	LMG	C7-C8-C9-O8
31	A	618	LHG	C4-C5-C6-O8
29	A	612	LMG	C29-C30-C31-C32
33	C	518	DGD	C8A-C9A-CAA-CBA
33	c	519	DGD	CCB-CDB-CEB-CFB
29	B	620	LMG	C18-C19-C20-C21
33	H	103	DGD	C7A-C8A-C9A-CAA
33	c	520	DGD	CBA-CCA-CDA-CEA
25	C	505	CLA	CBA-CGA-O2A-C1
29	B	625	LMG	C29-C28-O8-C9
33	C	516	DGD	O6E-C5E-C6E-O5E
23	c	501	SQD	C28-C29-C30-C31
31	A	618	LHG	C28-C29-C30-C31
31	a	614	LHG	C11-C10-C9-C8
33	c	518	DGD	O6E-C5E-C6E-O5E
23	A	603	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	b	623	LMG	C17-C18-C19-C20
27	T	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C20-C21-C22-C37
25	b	616	CLA	C5-C6-C7-C8
33	C	518	DGD	C4B-C5B-C6B-C7B
28	a	611	PL9	C12-C11-C9-C10
29	d	406	LMG	O6-C5-C6-O5
25	C	506	CLA	C15-C16-C17-C18
23	A	619	SQD	C24-C25-C26-C27
29	D	405	LMG	C16-C17-C18-C19
31	A	616	LHG	C30-C31-C32-C33
29	D	405	LMG	C19-C20-C21-C22
33	C	516	DGD	C4D-C5D-C6D-O5D
33	c	518	DGD	C4D-C5D-C6D-O5D
29	B	621	LMG	C18-C19-C20-C21
23	D	409	SQD	C24-C23-O48-C46
29	B	625	LMG	C37-C38-C39-C40
31	A	616	LHG	C11-C12-C13-C14
33	C	516	DGD	O6D-C5D-C6D-O5D
33	c	518	DGD	O6D-C5D-C6D-O5D
29	c	521	LMG	C20-C21-C22-C23
31	A	618	LHG	C17-C18-C19-C20
31	L	101	LHG	C30-C31-C32-C33
33	h	102	DGD	C8A-C9A-CAA-CBA
27	c	516	BCR	C9-C10-C11-C12
29	B	620	LMG	C17-C18-C19-C20
29	d	409	LMG	C17-C18-C19-C20
27	c	516	BCR	C11-C10-C9-C8
29	c	502	LMG	C37-C38-C39-C40
31	a	614	LHG	C1-C2-C3-O3
29	c	521	LMG	C19-C20-C21-C22
23	B	626	SQD	C11-C12-C13-C14
33	C	516	DGD	C6A-C7A-C8A-C9A
31	A	616	LHG	C29-C30-C31-C32
23	f	101	SQD	C25-C26-C27-C28
33	h	102	DGD	CAA-CBA-CCA-CDA
29	b	624	LMG	C40-C41-C42-C43
31	L	101	LHG	O2-C2-C3-O3
31	a	613	LHG	O2-C2-C3-O3
23	B	626	SQD	C11-C10-C9-C8
33	C	516	DGD	C5B-C6B-C7B-C8B
33	c	520	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
33	h	102	DGD	C9A-CAA-CBA-CCA
33	c	520	DGD	C4E-C5E-C6E-O5E
23	D	408	SQD	C10-C11-C12-C13
29	c	521	LMG	C29-C30-C31-C32
33	C	517	DGD	CBB-CCB-CDB-CEB
31	L	101	LHG	C27-C28-C29-C30
23	D	408	SQD	C14-C15-C16-C17
25	c	508	CLA	C8-C10-C11-C12
29	A	612	LMG	C22-C23-C24-C25
29	C	519	LMG	C17-C18-C19-C20
29	b	624	LMG	C14-C15-C16-C17
31	a	613	LHG	C10-C11-C12-C13
33	C	518	DGD	CAA-CBA-CCA-CDA
25	b	612	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
31	A	618	LHG	C19-C20-C21-C22
28	d	408	PL9	C37-C38-C39-C40
25	c	508	CLA	C15-C16-C17-C18
25	C	509	CLA	C10-C11-C12-C13
29	b	624	LMG	O10-C28-O8-C9
28	D	407	PL9	C2-C3-C7-C8
29	B	621	LMG	C12-C13-C14-C15
25	b	614	CLA	O1D-CGD-O2D-CED
29	d	409	LMG	C13-C14-C15-C16
29	A	612	LMG	O9-C10-O7-C8
25	A	607	CLA	C6-C7-C8-C9
25	B	611	CLA	C11-C12-C13-C14
25	B	614	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C10-C8-C9
25	C	512	CLA	C14-C13-C15-C16
25	a	609	CLA	C11-C12-C13-C14
25	b	617	CLA	C11-C12-C13-C14
25	c	508	CLA	C11-C10-C8-C9
25	c	512	CLA	C6-C7-C8-C9
25	c	514	CLA	C14-C13-C15-C16
29	C	519	LMG	C34-C35-C36-C37
25	b	605	CLA	C8-C10-C11-C12
25	B	610	CLA	C4B-C3B-CAB-CBB
25	C	501	CLA	C4B-C3B-CAB-CBB
25	C	513	CLA	C4B-C3B-CAB-CBB
25	D	402	CLA	C4B-C3B-CAB-CBB
25	a	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	C4B-C3B-CAB-CBB
25	b	606	CLA	C4B-C3B-CAB-CBB
25	b	618	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
25	c	504	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
31	A	618	LHG	C29-C30-C31-C32
33	C	518	DGD	C2B-C3B-C4B-C5B
25	b	617	CLA	C10-C11-C12-C13
29	B	620	LMG	C31-C32-C33-C34
29	B	625	LMG	C17-C18-C19-C20
29	C	520	LMG	C2-C1-O1-C7
29	c	522	LMG	C2-C1-O1-C7
29	C	520	LMG	C40-C41-C42-C43
31	A	617	LHG	O6-C4-C5-C6
31	L	101	LHG	O6-C4-C5-C6
31	l	101	LHG	O6-C4-C5-C6
23	D	409	SQD	C32-C33-C34-C35
25	B	605	CLA	C12-C13-C15-C16
25	B	614	CLA	C11-C12-C13-C15
25	B	616	CLA	C6-C7-C8-C10
25	C	509	CLA	C12-C13-C15-C16
25	a	609	CLA	C11-C12-C13-C15
25	b	604	CLA	C11-C12-C13-C15
25	b	608	CLA	C12-C13-C15-C16
25	b	612	CLA	C12-C13-C15-C16
25	b	614	CLA	C12-C13-C15-C16
25	b	617	CLA	C11-C12-C13-C15
25	c	508	CLA	C11-C10-C8-C7
25	c	509	CLA	C11-C10-C8-C7
25	c	511	CLA	C11-C10-C8-C7
25	c	512	CLA	C6-C7-C8-C10
29	c	521	LMG	C38-C39-C40-C41
29	c	522	LMG	C32-C33-C34-C35
25	b	615	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	C3A-C2A-CAA-CBA
28	a	611	PL9	C20-C19-C21-C22
25	C	506	CLA	C13-C15-C16-C17
25	c	503	CLA	O1D-CGD-O2D-CED
28	a	611	PL9	C13-C14-C16-C17
29	b	624	LMG	C32-C33-C34-C35
23	c	501	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	O1A-CGA-O2A-C1
29	c	502	LMG	O10-C28-O8-C9
33	c	518	DGD	C6A-C7A-C8A-C9A
31	A	618	LHG	C33-C34-C35-C36
27	b	621	BCR	C7-C8-C9-C34
29	A	612	LMG	C38-C39-C40-C41
29	A	613	LMG	C33-C34-C35-C36
29	b	623	LMG	C18-C19-C20-C21
23	B	626	SQD	O6-C44-C45-C46
29	B	621	LMG	O1-C7-C8-C9
29	b	624	LMG	O1-C7-C8-C9
29	b	624	LMG	C7-C8-C9-O8
29	c	502	LMG	O1-C7-C8-C9
29	c	521	LMG	O1-C7-C8-C9
29	d	409	LMG	C7-C8-C9-O8
31	a	615	LHG	C4-C5-C6-O8
29	d	409	LMG	C21-C22-C23-C24
31	a	615	LHG	C13-C14-C15-C16
33	h	102	DGD	CDA-CEA-CFA-CGA
29	b	624	LMG	C16-C17-C18-C19
25	A	609	CLA	C16-C17-C18-C19
25	b	615	CLA	C10-C11-C12-C13
29	b	624	LMG	C15-C16-C17-C18
31	A	616	LHG	C9-C10-C11-C12
23	I	101	SQD	O6-C44-C45-C46
26	a	608	PHO	C1A-C2A-CAA-CBA
26	A	608	PHO	C13-C15-C16-C17
29	b	624	LMG	C30-C31-C32-C33
25	b	607	CLA	C4-C3-C5-C6
23	A	603	SQD	C25-C26-C27-C28
31	d	407	LHG	O6-C4-C5-O7
33	H	103	DGD	O6D-C5D-C6D-O5D
33	c	518	DGD	C8A-C9A-CAA-CBA
27	B	617	BCR	C1-C6-C7-C8
27	B	619	BCR	C1-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C30
27	C	514	BCR	C1-C6-C7-C8
27	b	622	BCR	C23-C24-C25-C30
29	c	502	LMG	C33-C34-C35-C36
29	c	521	LMG	C30-C31-C32-C33
25	d	404	CLA	C13-C15-C16-C17
23	I	101	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	b	625	LMG	C12-C13-C14-C15
29	c	521	LMG	C14-C15-C16-C17
23	D	409	SQD	O6-C44-C45-O47
29	A	612	LMG	O1-C7-C8-O7
29	C	520	LMG	O7-C8-C9-O8
29	b	624	LMG	O7-C8-C9-O8
29	c	502	LMG	O7-C8-C9-O8
29	c	521	LMG	O1-C7-C8-O7
29	c	522	LMG	O7-C8-C9-O8
29	c	522	LMG	C4-C5-C6-O5
28	D	407	PL9	C4-C3-C7-C8
28	a	611	PL9	C4-C3-C7-C8
25	B	609	CLA	C4-C3-C5-C6
28	D	407	PL9	C45-C44-C46-C47
28	a	611	PL9	C15-C14-C16-C17
29	c	521	LMG	C34-C35-C36-C37
29	d	409	LMG	C35-C36-C37-C38
31	L	101	LHG	C33-C34-C35-C36
25	a	609	CLA	C10-C11-C12-C13
25	b	616	CLA	C13-C15-C16-C17
25	B	609	CLA	C2-C3-C5-C6
29	B	621	LMG	C19-C20-C21-C22
31	A	616	LHG	C10-C11-C12-C13
33	C	518	DGD	CBB-CCB-CDB-CEB
23	A	619	SQD	C35-C36-C37-C38
25	B	614	CLA	C11-C12-C13-C14
25	a	607	CLA	C6-C7-C8-C9
27	T	101	BCR	C6-C7-C8-C9
27	b	620	BCR	C22-C23-C24-C25
33	c	519	DGD	O1A-C1A-O1G-C1G
33	C	517	DGD	C4B-C5B-C6B-C7B
26	d	401	PHO	O1D-CGD-O2D-CED
26	A	608	PHO	C3-C5-C6-C7
33	c	518	DGD	C5A-C6A-C7A-C8A
25	B	601	CLA	C8-C10-C11-C12
29	c	502	LMG	C22-C23-C24-C25
29	D	405	LMG	C32-C33-C34-C35
23	c	501	SQD	C11-C12-C13-C14
31	D	406	LHG	O1-C1-C2-O2
31	l	101	LHG	O1-C1-C2-O2
29	c	502	LMG	C29-C28-O8-C9
29	c	502	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	A	611	PL9	C12-C11-C9-C8
28	a	611	PL9	C12-C11-C9-C8
29	C	519	LMG	C11-C10-O7-C8
25	C	513	CLA	O1D-CGD-O2D-CED
23	c	501	SQD	C34-C35-C36-C37
33	C	516	DGD	C3B-C4B-C5B-C6B
27	B	627	BCR	C20-C21-C22-C37
27	b	622	BCR	C20-C21-C22-C37
31	d	407	LHG	O6-C4-C5-C6
25	C	506	CLA	C16-C17-C18-C19
31	A	617	LHG	C30-C31-C32-C33
25	B	607	CLA	C12-C13-C15-C16
25	B	616	CLA	C11-C10-C8-C7
23	D	409	SQD	C34-C35-C36-C37
33	C	516	DGD	C7A-C8A-C9A-CAA
33	H	103	DGD	C5A-C6A-C7A-C8A
25	A	609	CLA	C15-C16-C17-C18
25	b	611	CLA	C15-C16-C17-C18
25	b	619	CLA	C13-C15-C16-C17
27	Y	101	BCR	C21-C22-C23-C24
23	c	501	SQD	C5-C6-S-O8
33	c	519	DGD	C5D-C6D-O5D-C1E
29	d	409	LMG	C16-C17-C18-C19
31	a	615	LHG	C28-C29-C30-C31
29	D	405	LMG	C11-C10-O7-C8
28	d	408	PL9	C20-C19-C21-C22
33	H	103	DGD	O2G-C1B-C2B-C3B
29	C	519	LMG	O10-C28-O8-C9
29	B	620	LMG	C34-C35-C36-C37
29	c	521	LMG	C10-C11-C12-C13
23	f	101	SQD	C44-C45-O47-C7
33	H	103	DGD	O1A-C1A-O1G-C1G
33	c	520	DGD	C5B-C6B-C7B-C8B
23	A	619	SQD	C16-C17-C18-C19
33	c	519	DGD	CCA-CDA-CEA-CFA
25	b	612	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
25	B	605	CLA	C15-C16-C17-C18
33	C	518	DGD	O1B-C1B-O2G-C2G
31	D	406	LHG	O6-C4-C5-O7
31	L	101	LHG	O6-C4-C5-O7
31	l	101	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
29	b	623	LMG	C15-C16-C17-C18
29	A	613	LMG	O1-C7-C8-C9
29	A	613	LMG	C7-C8-C9-O8
25	b	613	CLA	C16-C17-C18-C20
26	a	608	PHO	C4-C3-C5-C6
28	a	611	PL9	C18-C19-C21-C22
29	c	521	LMG	C16-C17-C18-C19
31	A	616	LHG	C33-C34-C35-C36
23	A	619	SQD	O47-C45-C46-O48
23	D	408	SQD	O47-C45-C46-O48
23	b	601	SQD	O6-C44-C45-O47
23	f	101	SQD	O6-C44-C45-O47
29	B	621	LMG	O1-C7-C8-O7
29	b	624	LMG	O1-C7-C8-O7
29	d	409	LMG	O7-C8-C9-O8
31	a	614	LHG	O7-C5-C6-O8
25	B	616	CLA	C11-C10-C8-C9
25	b	614	CLA	C11-C12-C13-C14
31	D	406	LHG	C25-C26-C27-C28
33	C	517	DGD	O1B-C1B-O2G-C2G
23	f	101	SQD	C28-C29-C30-C31
23	B	626	SQD	C24-C25-C26-C27
25	C	504	CLA	C13-C15-C16-C17
23	c	501	SQD	C11-C10-C9-C8
29	A	612	LMG	C32-C33-C34-C35
29	b	624	LMG	C17-C18-C19-C20
29	B	621	LMG	C28-C29-C30-C31
25	B	604	CLA	C3-C5-C6-C7
31	L	101	LHG	C1-C2-C3-O3
31	a	613	LHG	C1-C2-C3-O3
25	B	616	CLA	C16-C17-C18-C20
23	c	501	SQD	C24-C25-C26-C27
25	c	512	CLA	O1D-CGD-O2D-CED
27	b	621	BCR	C11-C12-C13-C35
28	a	611	PL9	C24-C26-C27-C28
25	A	615	CLA	C1A-C2A-CAA-CBA
25	a	607	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C1A-C2A-CAA-CBA
25	C	505	CLA	O1D-CGD-O2D-CED
25	c	507	CLA	O1D-CGD-O2D-CED
27	T	101	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
23	D	409	SQD	C24-C25-C26-C27
23	D	408	SQD	C11-C12-C13-C14
29	A	613	LMG	C22-C23-C24-C25
31	l	101	LHG	C32-C33-C34-C35
31	D	406	LHG	O6-C4-C5-C6
23	b	601	SQD	C5-C6-S-O9
26	D	401	PHO	C3-C5-C6-C7
25	A	607	CLA	C11-C10-C8-C7
25	B	615	CLA	C12-C13-C15-C16
25	C	504	CLA	C12-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C12-C13-C15
25	C	510	CLA	C11-C10-C8-C7
25	D	402	CLA	C11-C12-C13-C15
25	b	610	CLA	C12-C13-C15-C16
25	c	506	CLA	C12-C13-C15-C16
25	c	508	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C7
25	c	514	CLA	C11-C10-C8-C7
31	a	613	LHG	C12-C13-C14-C15
26	a	608	PHO	C16-C17-C18-C19
25	b	613	CLA	C15-C16-C17-C18
31	a	613	LHG	C18-C19-C20-C21
33	C	518	DGD	CCB-CDB-CEB-CFB
25	B	612	CLA	CBA-CGA-O2A-C1
25	C	508	CLA	CBA-CGA-O2A-C1
23	A	619	SQD	C29-C30-C31-C32
29	C	520	LMG	O10-C28-O8-C9
29	C	519	LMG	C40-C41-C42-C43
25	B	611	CLA	C16-C17-C18-C19
25	C	509	CLA	C16-C17-C18-C20
31	D	406	LHG	C27-C28-C29-C30
25	B	607	CLA	C14-C13-C15-C16
25	B	615	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C9
26	A	608	PHO	C14-C13-C15-C16
29	c	521	LMG	O10-C28-O8-C9
29	B	620	LMG	C35-C36-C37-C38
23	A	603	SQD	C9-C10-C11-C12
25	B	603	CLA	C5-C6-C7-C8
33	H	103	DGD	C7B-C8B-C9B-CAB
23	D	409	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
29	B	625	LMG	O1-C7-C8-O7
29	c	502	LMG	O1-C7-C8-O7
31	A	618	LHG	O7-C5-C6-O8
33	c	518	DGD	O2G-C2G-C3G-O3G
25	b	615	CLA	C15-C16-C17-C18
31	a	613	LHG	C24-C23-O8-C6
29	B	621	LMG	C15-C16-C17-C18
23	D	409	SQD	O6-C44-C45-C46
23	b	601	SQD	O6-C44-C45-C46
23	f	101	SQD	O6-C44-C45-C46
29	A	612	LMG	O1-C7-C8-C9
31	a	614	LHG	C4-C5-C6-O8
33	c	518	DGD	C1G-C2G-C3G-O3G
33	c	519	DGD	C5A-C6A-C7A-C8A
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	CAD-CBD-CGD-O2D
25	B	609	CLA	CAD-CBD-CGD-O2D
31	a	615	LHG	C17-C18-C19-C20
25	C	508	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	CBA-CGA-O2A-C1
29	b	623	LMG	C10-C11-C12-C13
26	A	608	PHO	C16-C17-C18-C19
25	C	507	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C5-C6-C7-C8
25	C	501	CLA	O1A-CGA-O2A-C1
29	B	625	LMG	C16-C17-C18-C19
25	B	612	CLA	O1A-CGA-O2A-C1
29	c	502	LMG	C17-C18-C19-C20
29	c	521	LMG	C37-C38-C39-C40
29	d	409	LMG	C38-C39-C40-C41
33	C	518	DGD	C3B-C4B-C5B-C6B
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	607	CLA	CAD-CBD-CGD-O1D
25	B	609	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O2D
25	c	511	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CHA-CBD-CGD-O2D
26	D	401	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	D	401	PHO	CHA-CBD-CGD-O2D
31	A	616	LHG	C3-O3-P-O5
31	A	617	LHG	C4-O6-P-O5
31	A	618	LHG	C3-O3-P-O5
31	a	614	LHG	C3-O3-P-O4
31	a	614	LHG	C3-O3-P-O5
31	a	614	LHG	C3-O3-P-O6
31	a	614	LHG	C4-O6-P-O5
31	d	407	LHG	C4-O6-P-O5
31	a	615	LHG	C11-C10-C9-C8
25	B	602	CLA	C2B-C3B-CAB-CBB
25	B	610	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
25	C	503	CLA	C2B-C3B-CAB-CBB
25	D	402	CLA	C2B-C3B-CAB-CBB
25	a	612	CLA	C2B-C3B-CAB-CBB
31	D	406	LHG	C18-C19-C20-C21
26	a	608	PHO	C2-C3-C5-C6
27	c	516	BCR	C37-C22-C23-C24
31	A	618	LHG	C2-C3-O3-P
29	B	625	LMG	C15-C16-C17-C18
33	C	517	DGD	CCA-CDA-CEA-CFA
25	C	506	CLA	C5-C6-C7-C8
29	A	613	LMG	C35-C36-C37-C38
28	A	611	PL9	C4-C3-C7-C8
26	a	608	PHO	C13-C15-C16-C17
23	A	619	SQD	C46-C45-O47-C7
23	D	408	SQD	C46-C45-O47-C7
29	b	624	LMG	C7-C8-O7-C10
28	A	611	PL9	C12-C11-C9-C10
29	b	623	LMG	C34-C35-C36-C37
31	L	101	LHG	C9-C10-C11-C12
23	D	409	SQD	C7-C8-C9-C10
29	C	520	LMG	C36-C37-C38-C39
27	k	101	BCR	C19-C20-C21-C22
25	B	616	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C19
29	c	522	LMG	C29-C28-O8-C9
33	C	517	DGD	CDA-CEA-CFA-CGA
25	B	609	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	c	514	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C11-C12-C13-C15
25	c	511	CLA	C11-C12-C13-C15
29	d	409	LMG	C28-C29-C30-C31
25	c	509	CLA	C2A-CAA-CBA-CGA
33	h	102	DGD	O2G-C1B-C2B-C3B
31	a	613	LHG	C23-C24-C25-C26
25	b	612	CLA	C4-C3-C5-C6
23	c	501	SQD	C27-C28-C29-C30
29	d	406	LMG	C38-C39-C40-C41
31	a	615	LHG	C10-C11-C12-C13
29	B	620	LMG	C38-C39-C40-C41
31	A	618	LHG	C31-C32-C33-C34
27	K	101	BCR	C19-C20-C21-C22
31	a	613	LHG	C11-C12-C13-C14
31	D	406	LHG	C12-C13-C14-C15
25	c	506	CLA	C13-C15-C16-C17
31	d	407	LHG	C16-C17-C18-C19
29	D	405	LMG	C31-C32-C33-C34
29	A	612	LMG	C33-C34-C35-C36
31	D	406	LHG	C14-C15-C16-C17
25	c	507	CLA	CBA-CGA-O2A-C1
25	c	508	CLA	CBA-CGA-O2A-C1
23	A	603	SQD	C45-C44-O6-C1
23	f	101	SQD	C45-C44-O6-C1
25	C	509	CLA	C16-C17-C18-C19
23	A	619	SQD	C10-C11-C12-C13
29	d	406	LMG	C30-C31-C32-C33
25	b	618	CLA	C4-C3-C5-C6
25	b	613	CLA	C16-C17-C18-C19
28	A	611	PL9	C47-C48-C49-C51
25	C	504	CLA	C14-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	b	618	CLA	C14-C13-C15-C16
25	c	508	CLA	O1A-CGA-O2A-C1
25	B	608	CLA	C4B-C3B-CAB-CBB
25	C	511	CLA	C4B-C3B-CAB-CBB
25	C	512	CLA	C4B-C3B-CAB-CBB
25	b	617	CLA	C4B-C3B-CAB-CBB
25	c	509	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	c	522	LMG	C40-C41-C42-C43
26	D	401	PHO	C16-C17-C18-C20
23	A	619	SQD	C34-C35-C36-C37
29	C	520	LMG	C15-C16-C17-C18
25	b	604	CLA	C8-C10-C11-C12
31	a	613	LHG	C9-C10-C11-C12
25	B	614	CLA	C11-C10-C8-C7
25	C	506	CLA	C11-C10-C8-C7
25	D	402	CLA	C12-C13-C15-C16
25	b	605	CLA	C11-C12-C13-C15
23	A	619	SQD	C33-C34-C35-C36
25	c	509	CLA	C16-C17-C18-C20
31	a	615	LHG	O10-C23-O8-C6
26	D	401	PHO	C3A-C2A-CAA-CBA
28	D	407	PL9	C13-C14-C16-C17
27	B	627	BCR	C6-C7-C8-C9
31	L	101	LHG	C16-C17-C18-C19
25	B	603	CLA	C15-C16-C17-C18
25	B	613	CLA	C13-C15-C16-C17
25	b	606	CLA	C15-C16-C17-C18
25	b	619	CLA	C5-C6-C7-C8
27	D	404	BCR	C37-C22-C23-C24
26	d	401	PHO	C13-C15-C16-C17
33	H	103	DGD	C9B-CAB-CBB-CCB
23	B	626	SQD	C19-C20-C21-C22
28	d	408	PL9	C35-C34-C36-C37
23	b	601	SQD	C12-C13-C14-C15
29	b	624	LMG	C31-C32-C33-C34
33	c	520	DGD	C8A-C9A-CAA-CBA
28	a	611	PL9	C39-C41-C42-C43
29	B	625	LMG	C38-C39-C40-C41
25	B	607	CLA	C11-C12-C13-C14
25	B	611	CLA	C14-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	b	605	CLA	C6-C7-C8-C9
25	b	612	CLA	C11-C10-C8-C9
25	b	618	CLA	C11-C12-C13-C14
25	c	504	CLA	C6-C7-C8-C9
25	c	504	CLA	C14-C13-C15-C16
25	c	508	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	A	617	LHG	O1-C1-C2-C3
31	l	101	LHG	O1-C1-C2-C3
29	B	620	LMG	C10-C11-C12-C13
23	B	626	SQD	C18-C19-C20-C21
23	I	101	SQD	C12-C13-C14-C15
29	c	502	LMG	C39-C40-C41-C42
33	c	519	DGD	C8A-C9A-CAA-CBA
35	v	201	HEC	CAD-CBD-CGD-O2D
25	B	601	CLA	CAA-CBA-CGA-O2A
25	B	610	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18
25	b	607	CLA	C3-C5-C6-C7
26	A	608	PHO	C1A-C2A-CAA-CBA
28	D	407	PL9	C15-C14-C16-C17
29	B	625	LMG	C28-C29-C30-C31
25	b	618	CLA	C2-C3-C5-C6
29	C	519	LMG	C37-C38-C39-C40
29	d	406	LMG	C34-C35-C36-C37
31	d	407	LHG	C26-C27-C28-C29
35	v	201	HEC	CAD-CBD-CGD-O1D
25	b	613	CLA	C2A-CAA-CBA-CGA
31	D	406	LHG	C26-C27-C28-C29
25	B	607	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
27	Y	101	BCR	C20-C21-C22-C23
25	B	616	CLA	C8-C10-C11-C12
33	c	520	DGD	C2B-C3B-C4B-C5B
25	B	603	CLA	C2B-C3B-CAB-CBB
25	B	604	CLA	C2B-C3B-CAB-CBB
25	C	501	CLA	C2B-C3B-CAB-CBB
25	C	505	CLA	C2B-C3B-CAB-CBB
25	C	513	CLA	C2B-C3B-CAB-CBB
25	b	606	CLA	C2B-C3B-CAB-CBB
25	b	610	CLA	C2B-C3B-CAB-CBB
25	b	611	CLA	C2B-C3B-CAB-CBB
25	b	613	CLA	C2B-C3B-CAB-CBB
25	b	617	CLA	C2B-C3B-CAB-CBB
25	b	618	CLA	C2B-C3B-CAB-CBB
25	c	504	CLA	C2B-C3B-CAB-CBB
25	c	506	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	c	515	CLA	C2B-C3B-CAB-CBB
27	A	610	BCR	C1-C6-C7-C8
27	A	610	BCR	C23-C24-C25-C30
27	B	617	BCR	C5-C6-C7-C8
27	B	618	BCR	C1-C6-C7-C8
27	B	619	BCR	C5-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C26
27	C	514	BCR	C5-C6-C7-C8
27	C	515	BCR	C1-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C30
27	D	404	BCR	C1-C6-C7-C8
27	H	102	BCR	C23-C24-C25-C30
27	K	101	BCR	C1-C6-C7-C8
27	K	101	BCR	C23-C24-C25-C30
27	Y	101	BCR	C1-C6-C7-C8
27	a	610	BCR	C1-C6-C7-C8
27	a	610	BCR	C23-C24-C25-C30
27	b	620	BCR	C5-C6-C7-C8
27	b	621	BCR	C1-C6-C7-C8
27	b	621	BCR	C23-C24-C25-C30
27	b	622	BCR	C1-C6-C7-C8
27	b	622	BCR	C23-C24-C25-C26
27	c	517	BCR	C1-C6-C7-C8
27	c	517	BCR	C23-C24-C25-C30
27	d	405	BCR	C1-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C23-C24-C25-C30
27	y	101	BCR	C5-C6-C7-C8
23	B	626	SQD	C30-C31-C32-C33
31	a	615	LHG	C5-C4-O6-P
29	d	409	LMG	C36-C37-C38-C39
31	A	616	LHG	C27-C28-C29-C30
29	c	521	LMG	C17-C18-C19-C20
29	d	409	LMG	C22-C23-C24-C25
23	D	409	SQD	C30-C31-C32-C33
25	b	618	CLA	C12-C13-C15-C16
25	c	507	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C12-C13-C15
25	C	505	CLA	C2A-CAA-CBA-CGA
33	c	519	DGD	O1G-C1G-C2G-O2G
29	D	405	LMG	O9-C10-O7-C8
23	c	501	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
28	d	408	PL9	C15-C14-C16-C17
33	c	518	DGD	CAA-CBA-CCA-CDA
25	C	509	CLA	C5-C6-C7-C8
25	b	607	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
29	B	620	LMG	C33-C34-C35-C36
23	c	501	SQD	C15-C16-C17-C18
29	d	409	LMG	C12-C13-C14-C15
31	A	617	LHG	C11-C12-C13-C14
23	I	101	SQD	C18-C19-C20-C21
26	A	608	PHO	C15-C16-C17-C18
23	f	101	SQD	C35-C36-C37-C38
27	B	617	BCR	C22-C23-C24-C25
28	A	611	PL9	C40-C39-C41-C42
34	E	101	HEM	CAD-CBD-CGD-O2D
31	a	614	LHG	C2-C3-O3-P
23	f	101	SQD	C31-C32-C33-C34
28	a	611	PL9	C33-C34-C36-C37
23	A	619	SQD	O6-C44-C45-O47
31	A	617	LHG	C15-C16-C17-C18
31	D	406	LHG	C30-C31-C32-C33
23	B	626	SQD	C17-C18-C19-C20
28	a	611	PL9	C30-C29-C31-C32
31	A	617	LHG	C13-C14-C15-C16
25	B	604	CLA	C4B-C3B-CAB-CBB
25	C	505	CLA	C4B-C3B-CAB-CBB
25	C	507	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	C4B-C3B-CAB-CBB
25	b	616	CLA	C4B-C3B-CAB-CBB
25	c	506	CLA	C4B-C3B-CAB-CBB
25	c	515	CLA	C4B-C3B-CAB-CBB
25	B	614	CLA	C5-C6-C7-C8
25	b	604	CLA	CAA-CBA-CGA-O2A
25	B	614	CLA	C16-C17-C18-C19
26	a	608	PHO	CHA-CBD-CGD-O1D
27	C	515	BCR	C20-C21-C22-C37
25	b	615	CLA	C8-C10-C11-C12
29	D	405	LMG	C13-C14-C15-C16
31	A	618	LHG	C13-C14-C15-C16
29	A	613	LMG	O7-C8-C9-O8
31	A	616	LHG	C7-C8-C9-C10
33	C	518	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C6-C7-C8-C10
23	A	603	SQD	C33-C34-C35-C36
23	A	619	SQD	C11-C12-C13-C14
29	d	409	LMG	C39-C40-C41-C42
23	D	409	SQD	O48-C23-C24-C25
29	c	522	LMG	C21-C22-C23-C24
34	E	101	HEM	CAD-CBD-CGD-O1D
25	c	505	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	C6-C7-C8-C9
25	B	606	CLA	C14-C13-C15-C16
25	C	505	CLA	C11-C12-C13-C14
25	C	506	CLA	C11-C12-C13-C14
25	C	510	CLA	C11-C10-C8-C9
25	D	402	CLA	C11-C12-C13-C14
25	c	506	CLA	C14-C13-C15-C16
25	c	514	CLA	C11-C10-C8-C9
31	A	617	LHG	C34-C35-C36-C37
29	D	405	LMG	C8-C7-O1-C1
29	d	406	LMG	C8-C7-O1-C1
33	C	517	DGD	C5D-C6D-O5D-C1E
31	A	617	LHG	C26-C27-C28-C29
25	b	611	CLA	C2A-CAA-CBA-CGA
25	b	617	CLA	C2A-CAA-CBA-CGA
25	b	616	CLA	C2-C1-O2A-CGA
26	A	608	PHO	C3A-C2A-CAA-CBA
26	d	401	PHO	C3A-C2A-CAA-CBA
25	c	505	CLA	CBD-CGD-O2D-CED
29	B	620	LMG	C40-C41-C42-C43
31	a	613	LHG	C28-C29-C30-C31
25	c	511	CLA	C13-C15-C16-C17
31	A	616	LHG	C24-C25-C26-C27
26	d	401	PHO	C16-C17-C18-C20
29	B	625	LMG	C32-C33-C34-C35
31	d	407	LHG	C28-C29-C30-C31
33	c	520	DGD	C4B-C5B-C6B-C7B
23	A	603	SQD	C24-C23-O48-C46
23	D	408	SQD	C13-C14-C15-C16
23	D	408	SQD	C44-C45-C46-O48
28	A	611	PL9	C39-C41-C42-C43
33	h	102	DGD	C1G-C2G-C3G-O3G
33	C	518	DGD	O1A-C1A-O1G-C1G
34	E	101	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	c	502	LMG	O8-C28-C29-C30
23	A	603	SQD	C10-C11-C12-C13
29	B	620	LMG	C19-C20-C21-C22
25	A	607	CLA	C11-C10-C8-C9
25	b	610	CLA	C14-C13-C15-C16
25	b	616	CLA	C14-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C9
25	b	616	CLA	CAA-CBA-CGA-O2A
31	l	101	LHG	O7-C7-C8-C9
31	L	101	LHG	C17-C18-C19-C20
25	B	603	CLA	C6-C7-C8-C10
25	B	606	CLA	C12-C13-C15-C16
25	B	610	CLA	C11-C10-C8-C7
25	B	611	CLA	C12-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C15
25	C	505	CLA	C11-C12-C13-C15
25	C	506	CLA	C11-C12-C13-C15
25	C	506	CLA	C12-C13-C15-C16
25	a	607	CLA	C11-C10-C8-C7
25	b	604	CLA	C12-C13-C15-C16
25	b	616	CLA	C11-C10-C8-C7
25	b	618	CLA	C11-C12-C13-C15
31	A	618	LHG	C26-C27-C28-C29
33	h	102	DGD	O1A-C1A-O1G-C1G
25	B	608	CLA	C2B-C3B-CAB-CBB
25	B	614	CLA	C2B-C3B-CAB-CBB
25	C	511	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C2B-C3B-CAB-CBB
25	b	605	CLA	C2B-C3B-CAB-CBB
25	b	607	CLA	C2B-C3B-CAB-CBB
25	b	614	CLA	C2B-C3B-CAB-CBB
25	c	503	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C2B-C3B-CAB-CBB
25	c	508	CLA	C2B-C3B-CAB-CBB
25	c	509	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
27	A	610	BCR	C5-C6-C7-C8
27	A	610	BCR	C23-C24-C25-C26
27	B	618	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
27	C	515	BCR	C5-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C26
27	D	404	BCR	C5-C6-C7-C8
27	H	102	BCR	C23-C24-C25-C26
27	K	101	BCR	C5-C6-C7-C8
27	K	101	BCR	C23-C24-C25-C26
27	Y	101	BCR	C5-C6-C7-C8
27	a	610	BCR	C5-C6-C7-C8
27	a	610	BCR	C23-C24-C25-C26
27	b	621	BCR	C5-C6-C7-C8
27	b	621	BCR	C23-C24-C25-C26
27	b	622	BCR	C5-C6-C7-C8
27	c	517	BCR	C5-C6-C7-C8
27	c	517	BCR	C23-C24-C25-C26
27	d	405	BCR	C5-C6-C7-C8
27	h	101	BCR	C23-C24-C25-C26
27	h	101	BCR	C23-C24-C25-C30
27	k	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C23-C24-C25-C26
27	y	101	BCR	C23-C24-C25-C30
25	c	508	CLA	C5-C6-C7-C8
25	C	510	CLA	CAA-CBA-CGA-O2A
25	a	606	CLA	C2-C1-O2A-CGA
25	b	618	CLA	C13-C15-C16-C17
29	d	409	LMG	O7-C10-C11-C12
25	B	608	CLA	C2A-CAA-CBA-CGA
23	D	409	SQD	C35-C36-C37-C38
29	c	521	LMG	O7-C10-C11-C12
33	c	518	DGD	C2A-C3A-C4A-C5A
25	b	609	CLA	C8-C10-C11-C12
23	A	619	SQD	O47-C7-C8-C9
29	B	620	LMG	O8-C28-C29-C30
23	b	601	SQD	C4-C5-C6-S
25	c	512	CLA	CAA-CBA-CGA-O2A
29	B	621	LMG	C36-C37-C38-C39
31	D	406	LHG	C34-C35-C36-C37
25	C	512	CLA	CAA-CBA-CGA-O2A
23	A	619	SQD	C15-C16-C17-C18
34	e	101	HEM	CAA-CBA-CGA-O2A
25	B	601	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C12-C13-C14
25	c	515	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	a	613	LHG	C29-C30-C31-C32
33	H	103	DGD	C6A-C7A-C8A-C9A
25	d	403	CLA	CAA-CBA-CGA-O2A
29	C	520	LMG	C7-C8-C9-O8
33	C	516	DGD	C1G-C2G-C3G-O3G
29	B	620	LMG	C29-C30-C31-C32
31	A	618	LHG	C27-C28-C29-C30
25	c	505	CLA	C15-C16-C17-C18
25	B	603	CLA	C4B-C3B-CAB-CBB
25	b	611	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C1A-C2A-CAA-CBA
31	l	101	LHG	C11-C12-C13-C14
25	B	603	CLA	C13-C15-C16-C17
33	c	520	DGD	O6D-C1D-O3G-C3G
25	B	612	CLA	CAA-CBA-CGA-O2A
31	L	101	LHG	O7-C7-C8-C9
28	D	407	PL9	C43-C44-C46-C47
29	c	521	LMG	O7-C8-C9-O8
31	L	101	LHG	O7-C5-C6-O8
34	E	101	HEM	CAA-CBA-CGA-O1A
27	K	101	BCR	C21-C22-C23-C24
27	c	517	BCR	C7-C8-C9-C10
23	c	501	SQD	C31-C32-C33-C34
25	D	402	CLA	CAA-CBA-CGA-O2A
31	a	614	LHG	O8-C23-C24-C25
25	b	618	CLA	C16-C17-C18-C19
29	c	502	LMG	C15-C16-C17-C18
23	c	501	SQD	C5-C6-S-O9
33	c	519	DGD	C4A-C5A-C6A-C7A
25	A	606	CLA	C2-C1-O2A-CGA
25	A	607	CLA	C2-C1-O2A-CGA
33	c	518	DGD	O2G-C1B-C2B-C3B
25	A	609	CLA	C12-C13-C15-C16
25	B	602	CLA	C6-C7-C8-C10
25	B	609	CLA	C12-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C10
25	C	513	CLA	C11-C10-C8-C7
25	b	605	CLA	C12-C13-C15-C16
25	B	614	CLA	C15-C16-C17-C18
31	a	615	LHG	C25-C26-C27-C28
25	c	507	CLA	C16-C17-C18-C19
29	D	405	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	b	624	LMG	C9-C8-O7-C10
29	C	520	LMG	C21-C22-C23-C24
25	b	611	CLA	C13-C15-C16-C17
25	c	507	CLA	C2A-CAA-CBA-CGA
26	d	401	PHO	C15-C16-C17-C18
23	B	626	SQD	C27-C28-C29-C30
23	f	101	SQD	O10-C23-O48-C46
33	c	520	DGD	C9B-CAB-CBB-CCB
25	C	512	CLA	C3A-C2A-CAA-CBA
25	A	607	CLA	O1A-CGA-O2A-C1
25	B	612	CLA	C13-C15-C16-C17
25	B	602	CLA	C16-C17-C18-C20
25	B	610	CLA	C16-C17-C18-C20
33	c	520	DGD	C2A-C3A-C4A-C5A
25	d	403	CLA	O1A-CGA-O2A-C1
25	A	607	CLA	CBA-CGA-O2A-C1
28	A	611	PL9	C36-C37-C38-C39
25	c	509	CLA	CBA-CGA-O2A-C1
25	d	403	CLA	CBA-CGA-O2A-C1
34	e	101	HEM	CAA-CBA-CGA-O1A
25	C	508	CLA	C11-C10-C8-C9
25	C	511	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	510	CLA	C11-C10-C8-C9
25	c	511	CLA	C11-C12-C13-C14
25	d	403	CLA	C14-C13-C15-C16
29	B	621	LMG	O7-C10-C11-C12
23	A	603	SQD	O49-C7-C8-C9
23	c	501	SQD	O49-C7-C8-C9
23	A	619	SQD	C26-C27-C28-C29
31	D	406	LHG	O2-C2-C3-O3
25	d	403	CLA	CAA-CBA-CGA-O1A
23	B	626	SQD	O5-C5-C6-S
28	a	611	PL9	C42-C43-C44-C45
25	B	612	CLA	CAA-CBA-CGA-O1A
29	d	409	LMG	O9-C10-C11-C12
25	C	510	CLA	CAA-CBA-CGA-O1A
23	B	626	SQD	C45-C44-O6-C1
23	c	501	SQD	C45-C44-O6-C1
29	A	613	LMG	C8-C7-O1-C1
33	c	518	DGD	C5D-C6D-O5D-C1E
25	c	509	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	b	616	CLA	CAA-CBA-CGA-O1A
29	b	623	LMG	O10-C28-C29-C30
33	c	519	DGD	O1B-C1B-C2B-C3B
23	b	601	SQD	O47-C7-C8-C9
29	c	522	LMG	C37-C38-C39-C40
25	B	609	CLA	C5-C6-C7-C8
25	C	512	CLA	CAA-CBA-CGA-O1A
29	c	521	LMG	O9-C10-C11-C12
25	B	612	CLA	CAD-CBD-CGD-O2D
25	B	616	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
25	D	402	CLA	CAA-CBA-CGA-O1A
25	c	512	CLA	CAA-CBA-CGA-O1A
31	l	101	LHG	O9-C7-C8-C9
27	B	627	BCR	C22-C23-C24-C25
27	c	516	BCR	C6-C7-C8-C9
23	A	603	SQD	O47-C7-C8-C9
23	c	501	SQD	O47-C7-C8-C9
25	C	501	CLA	CAA-CBA-CGA-O2A
25	c	503	CLA	CAA-CBA-CGA-O1A
29	B	620	LMG	O10-C28-C29-C30
25	b	615	CLA	CAA-CBA-CGA-O2A
31	A	617	LHG	O8-C23-C24-C25
33	c	519	DGD	C3B-C4B-C5B-C6B

There are no ring outliers.

139 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	503	CLA	5	0
25	b	613	CLA	1	0
25	c	507	CLA	3	0
27	H	102	BCR	4	0
29	A	613	LMG	2	0
25	C	508	CLA	5	0
33	h	102	DGD	3	0
23	A	603	SQD	2	0
27	k	101	BCR	2	0
29	c	502	LMG	3	0
25	A	606	CLA	1	0
25	b	617	CLA	2	0
26	a	608	PHO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	616	CLA	2	0
25	B	609	CLA	4	0
25	a	607	CLA	1	0
25	C	504	CLA	3	0
25	B	613	CLA	2	0
31	l	101	LHG	5	0
25	b	616	CLA	3	0
25	b	608	CLA	2	0
25	C	506	CLA	2	0
25	c	511	CLA	2	0
25	C	511	CLA	1	0
25	C	512	CLA	2	0
26	d	401	PHO	4	0
29	d	409	LMG	3	0
25	B	612	CLA	3	0
25	C	509	CLA	1	0
25	a	609	CLA	6	0
27	b	621	BCR	2	0
31	a	613	LHG	2	0
27	d	405	BCR	2	0
27	B	627	BCR	5	0
31	D	406	LHG	1	0
25	B	605	CLA	2	0
27	c	516	BCR	3	0
25	C	513	CLA	1	0
29	b	623	LMG	1	0
23	B	626	SQD	7	0
23	D	408	SQD	1	0
25	b	605	CLA	2	0
25	C	505	CLA	5	0
27	Y	101	BCR	1	0
27	B	617	BCR	2	0
25	b	609	CLA	1	0
34	e	101	HEM	3	0
25	B	606	CLA	3	0
27	B	619	BCR	2	0
27	D	404	BCR	3	0
25	c	512	CLA	1	0
25	b	618	CLA	1	0
27	C	515	BCR	3	0
25	b	604	CLA	1	0
25	B	615	CLA	1	0

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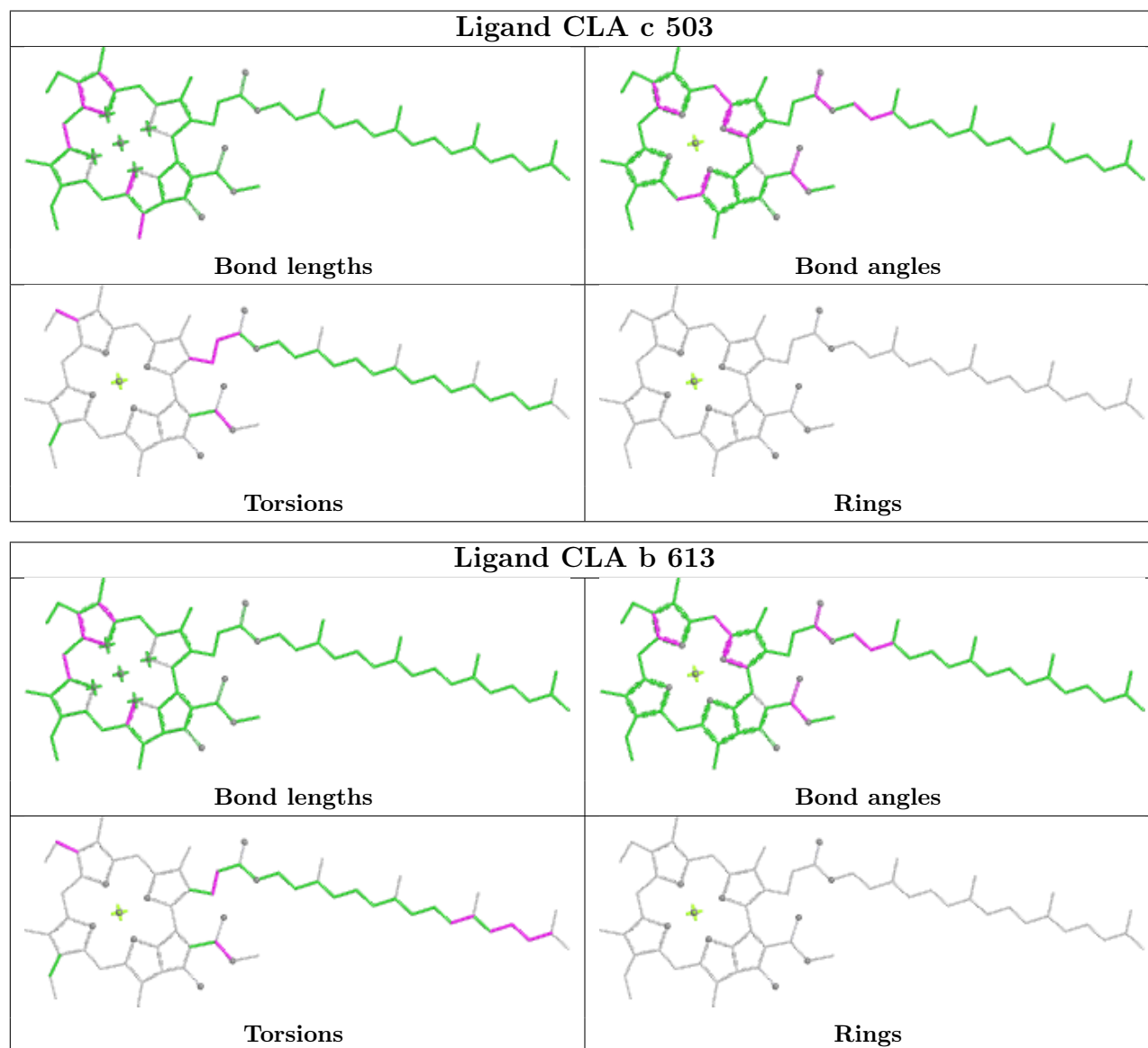
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33	C	518	DGD	2	0
35	V	201	HEC	1	0
29	C	519	LMG	1	0
25	b	615	CLA	5	0
28	d	408	PL9	5	0
28	D	407	PL9	2	0
27	c	517	BCR	4	0
25	C	501	CLA	5	0
25	c	505	CLA	3	0
25	a	606	CLA	1	0
26	D	401	PHO	3	0
31	A	618	LHG	3	0
33	H	103	DGD	2	0
29	B	621	LMG	1	0
25	c	514	CLA	2	0
29	b	624	LMG	2	0
25	C	502	CLA	1	0
25	C	503	CLA	4	0
31	A	616	LHG	2	0
25	b	611	CLA	2	0
25	B	603	CLA	1	0
25	d	404	CLA	4	0
25	B	602	CLA	4	0
25	c	513	CLA	1	0
25	c	515	CLA	3	0
27	b	622	BCR	4	0
29	B	625	LMG	1	0
27	K	101	BCR	2	0
29	b	625	LMG	2	0
25	A	607	CLA	1	0
27	b	620	BCR	2	0
34	E	101	HEM	3	0
27	T	101	BCR	7	0
25	B	610	CLA	2	0
29	C	520	LMG	2	0
25	D	403	CLA	2	0
25	B	608	CLA	3	0
27	A	610	BCR	3	0
33	c	519	DGD	2	0
31	a	614	LHG	1	0
25	c	510	CLA	3	0
25	B	601	CLA	3	0

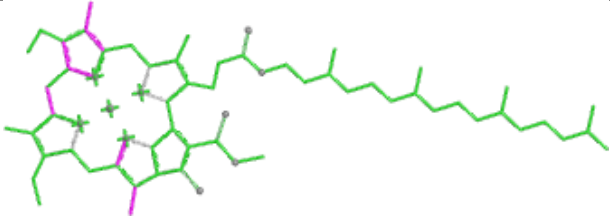
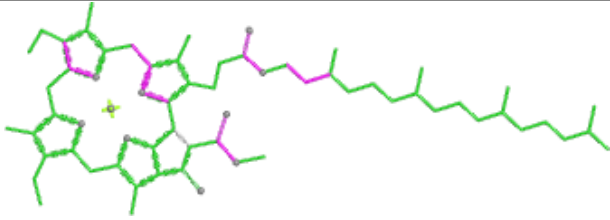
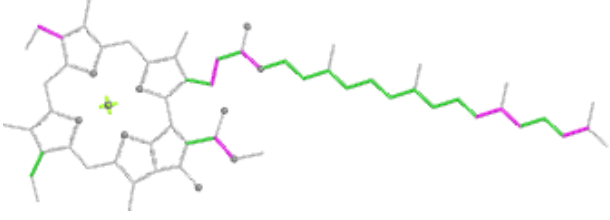
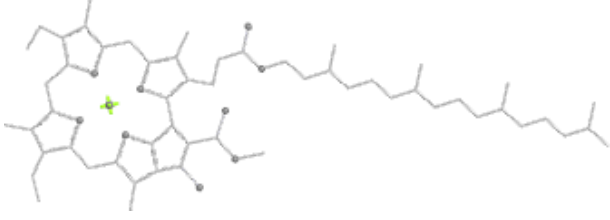
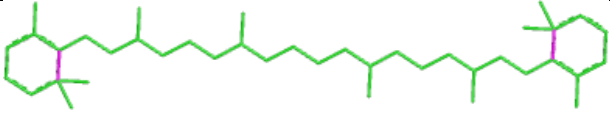
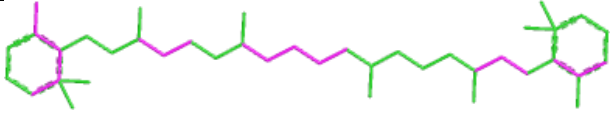
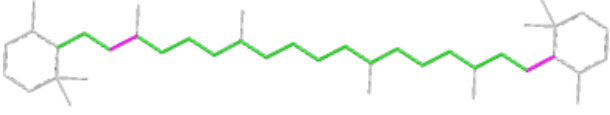
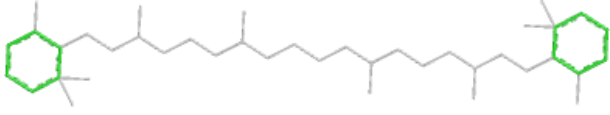
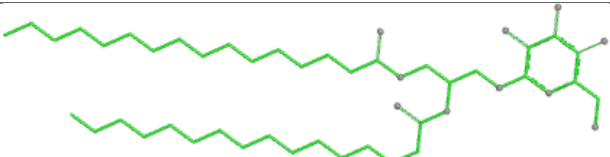
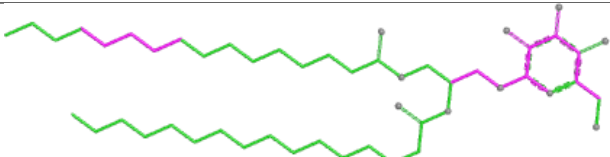
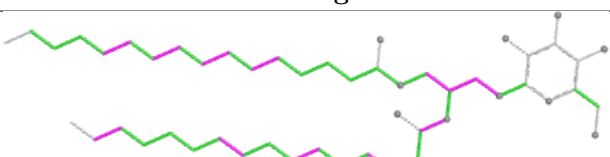
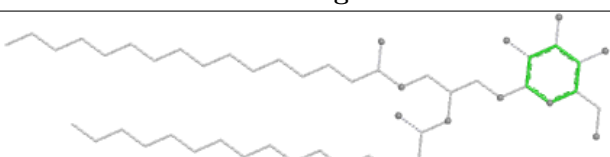
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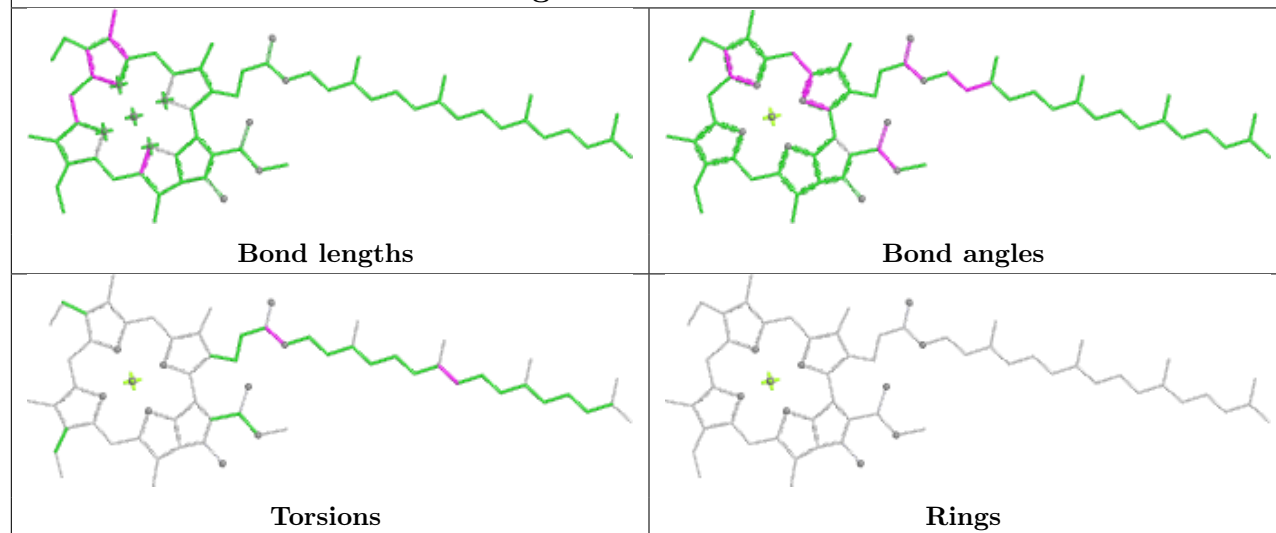
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	611	CLA	2	0
25	C	507	CLA	2	0
26	A	608	PHO	1	0
27	a	610	BCR	3	0
31	A	617	LHG	7	0
25	b	614	CLA	2	0
35	v	201	HEC	2	0
25	b	619	CLA	4	0
23	b	601	SQD	1	0
28	A	611	PL9	4	0
25	a	612	CLA	1	0
25	b	610	CLA	2	0
23	c	501	SQD	1	0
31	a	615	LHG	1	0
29	c	521	LMG	1	0
23	A	619	SQD	2	0
25	c	508	CLA	2	0
25	b	606	CLA	2	0
31	d	407	LHG	2	0
25	A	609	CLA	4	0
33	C	516	DGD	1	0
25	b	607	CLA	2	0
29	c	522	LMG	1	0
25	B	607	CLA	2	0
25	c	509	CLA	3	0
28	a	611	PL9	4	0
25	B	604	CLA	2	0
29	D	405	LMG	2	0
32	A	620	BCT	1	0
27	B	618	BCR	2	0
25	A	615	CLA	1	0
33	c	518	DGD	1	0
25	B	614	CLA	4	0
25	C	510	CLA	1	0
25	D	402	CLA	3	0
25	b	612	CLA	4	0
29	B	620	LMG	1	0
31	L	101	LHG	3	0
33	C	517	DGD	2	0
27	y	101	BCR	3	0
25	d	403	CLA	6	0
27	h	101	BCR	2	0

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

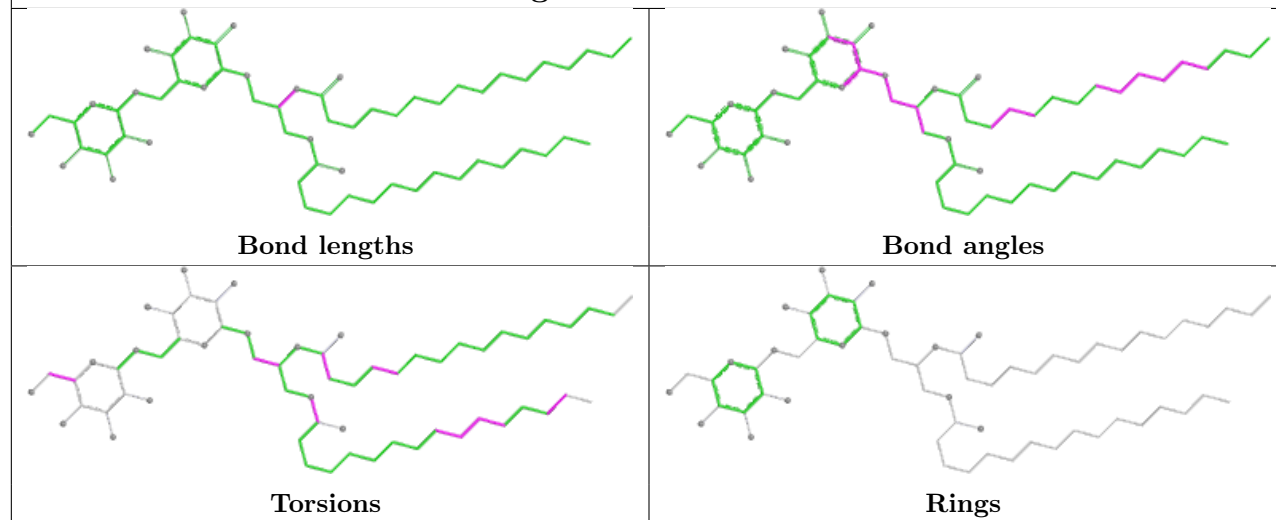


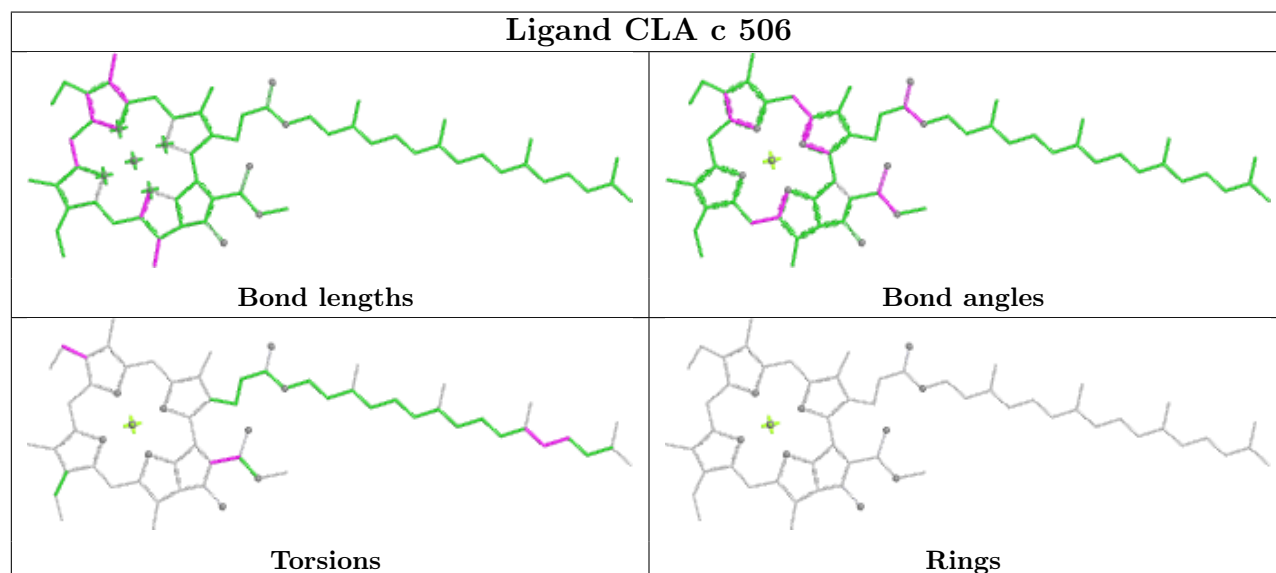
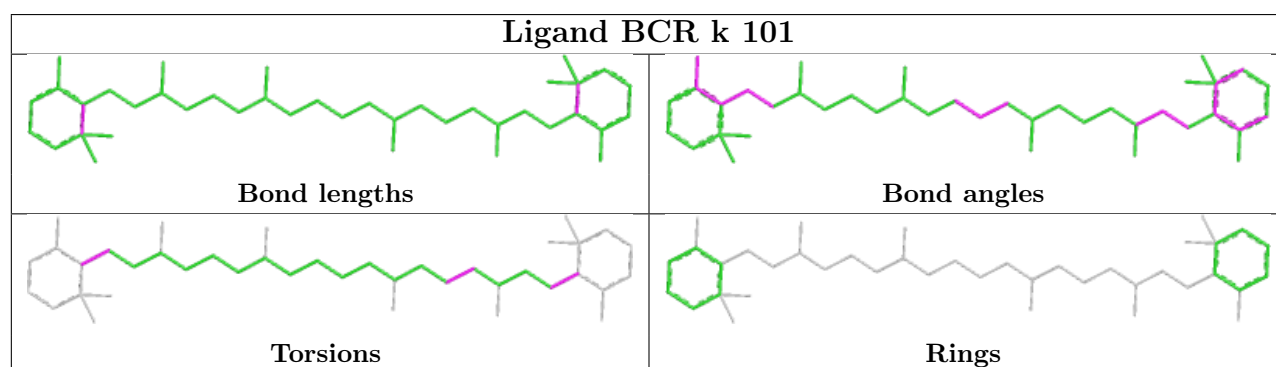
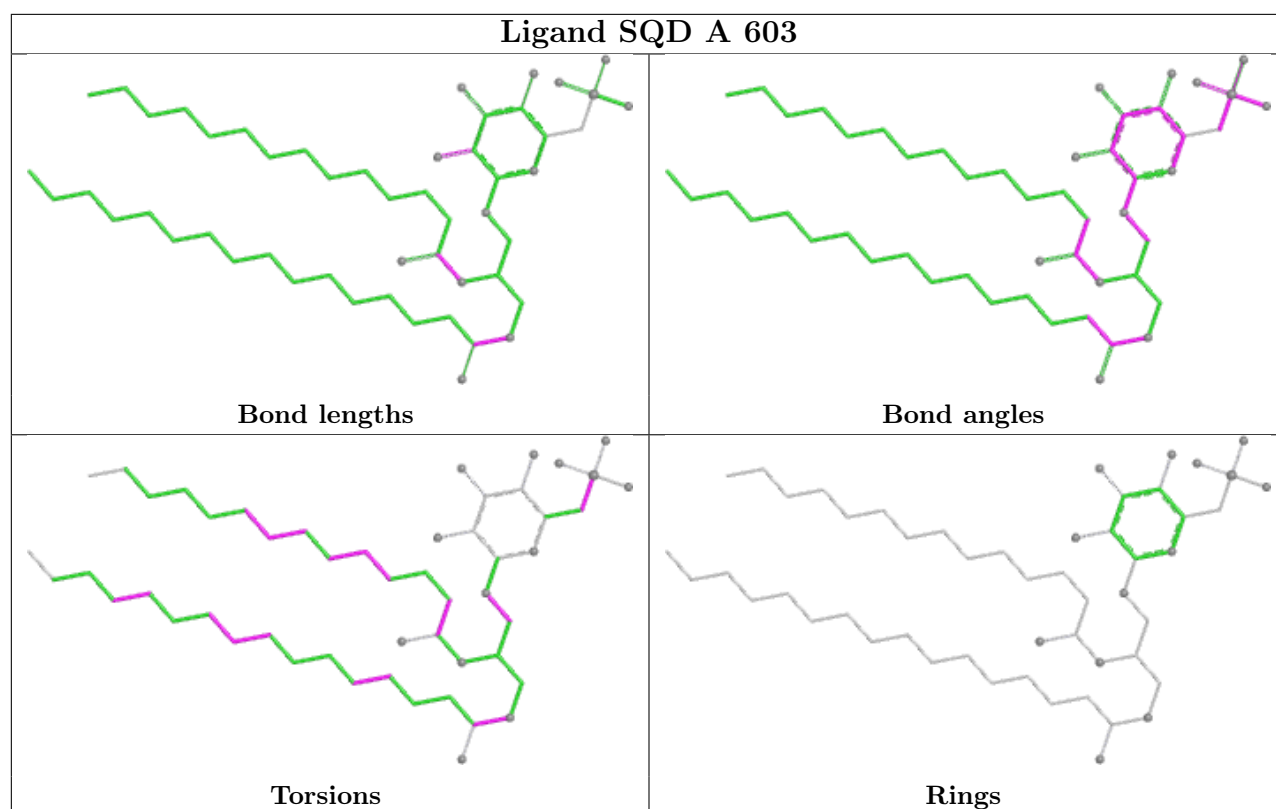
Ligand CLA c 507	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

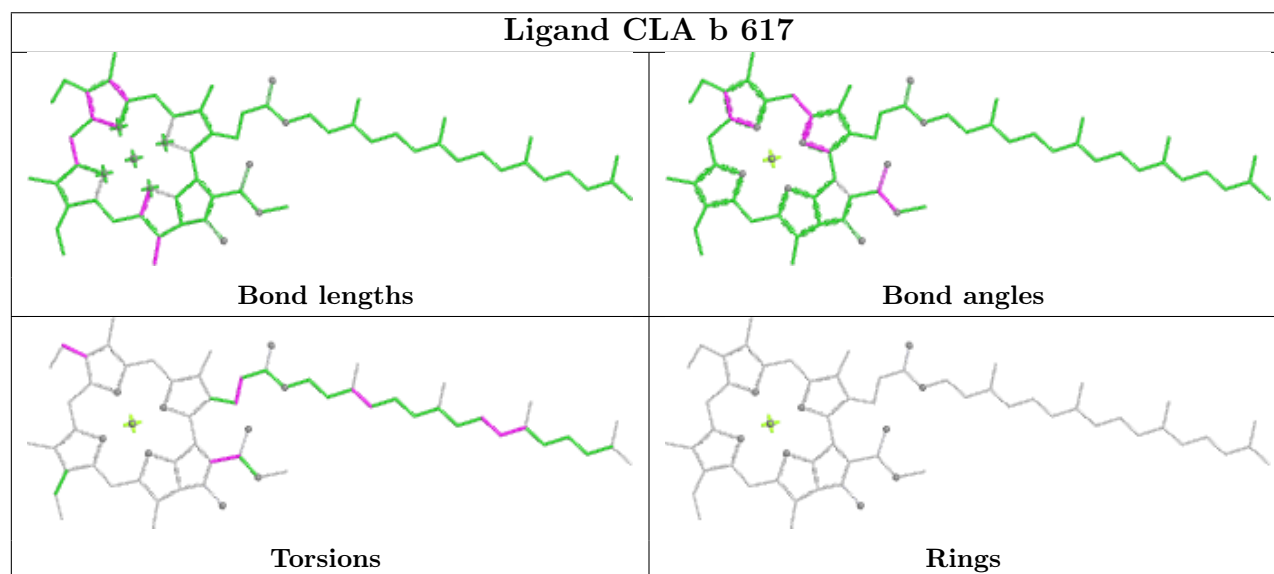
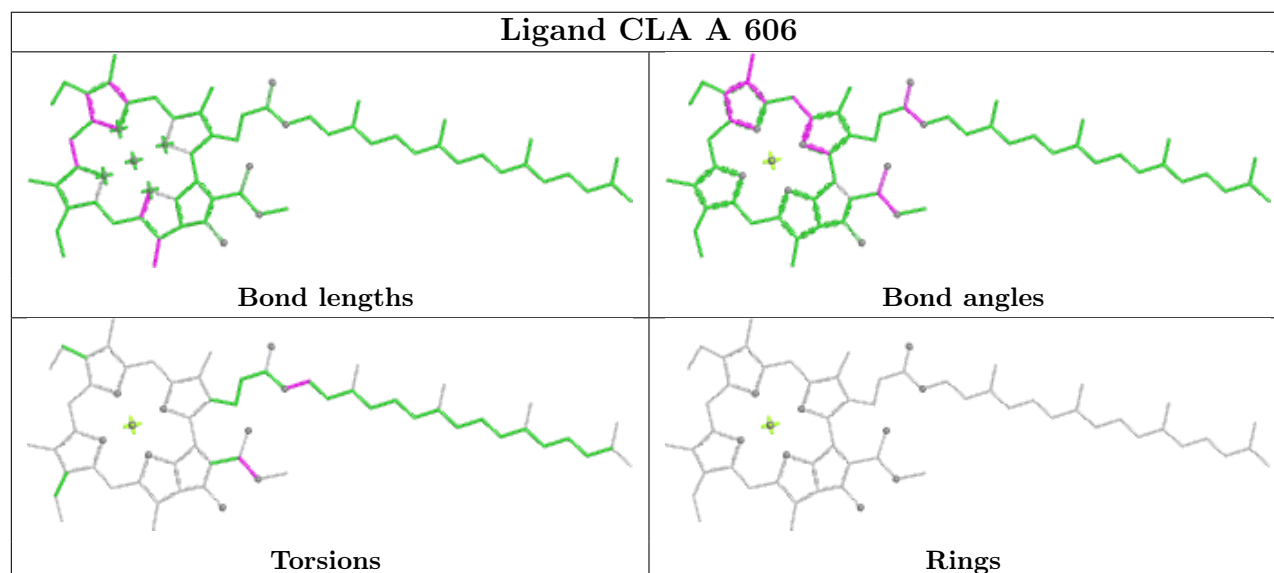
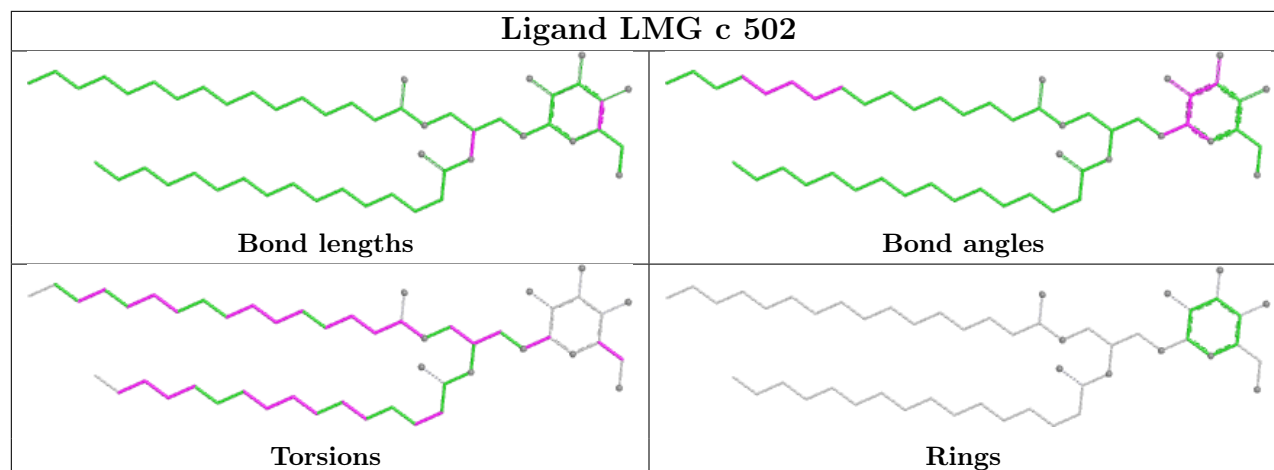
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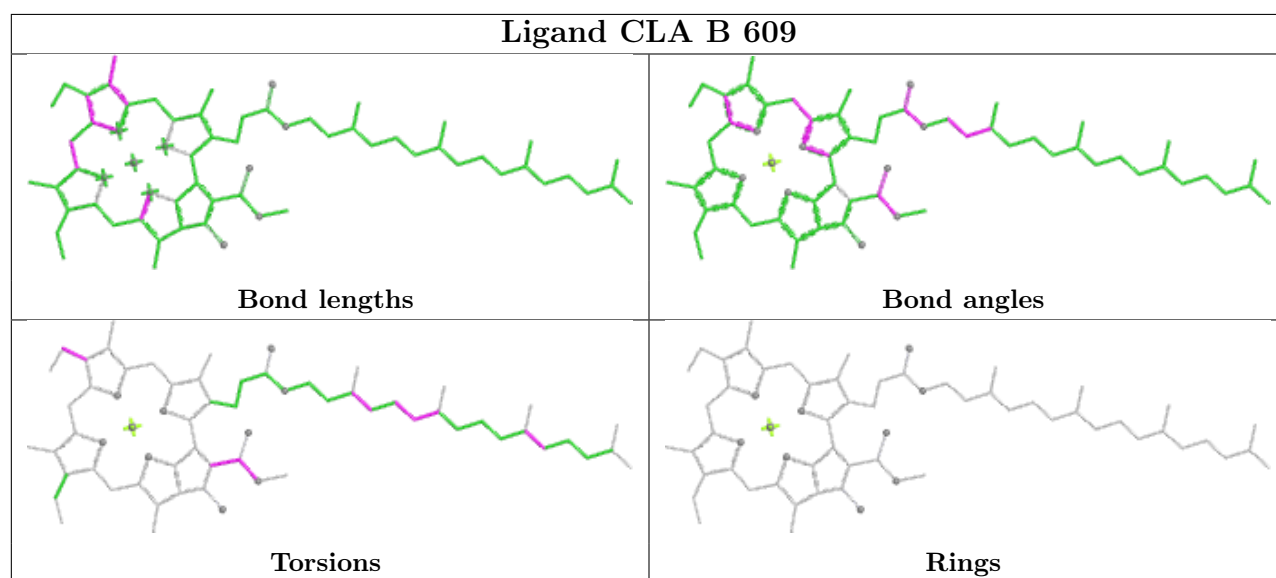
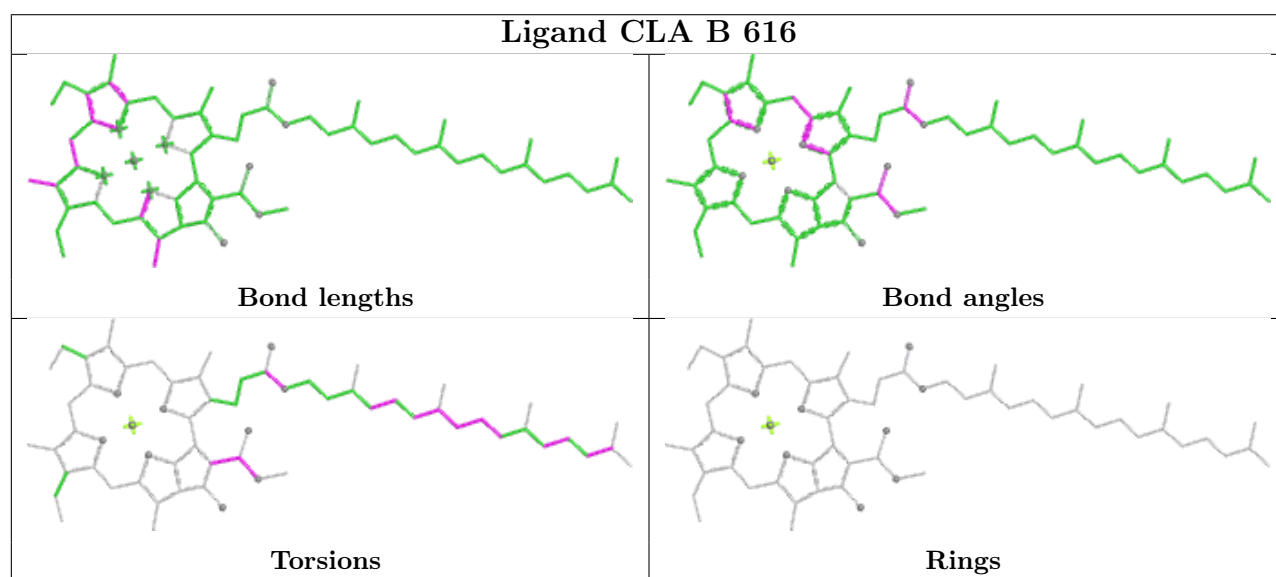
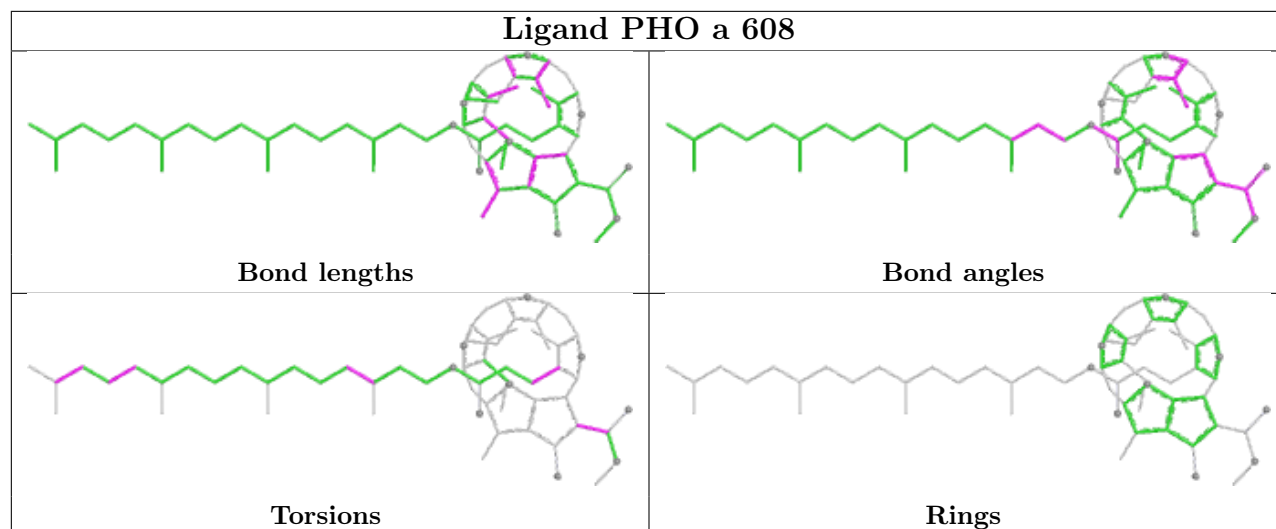


Ligand DGD h 102

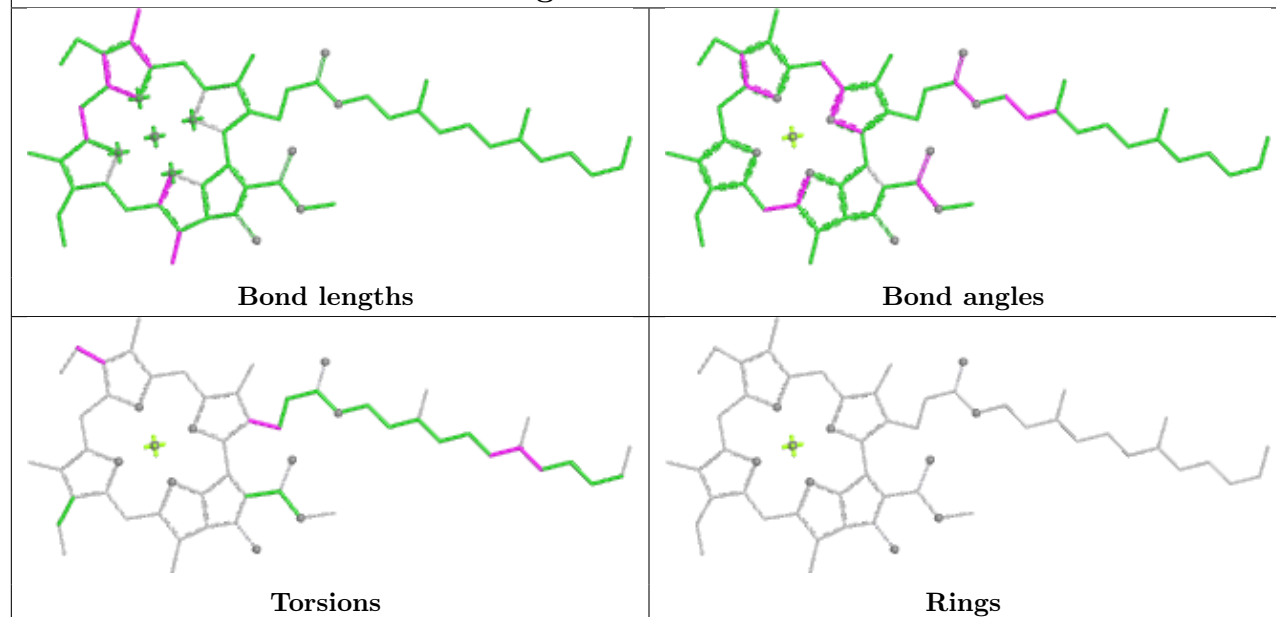




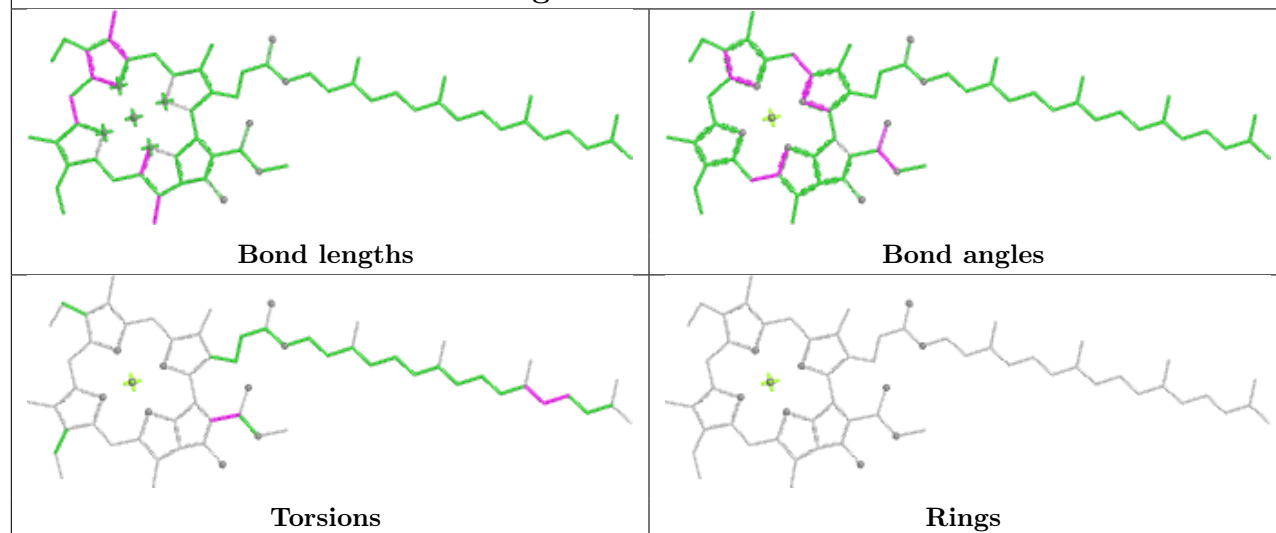


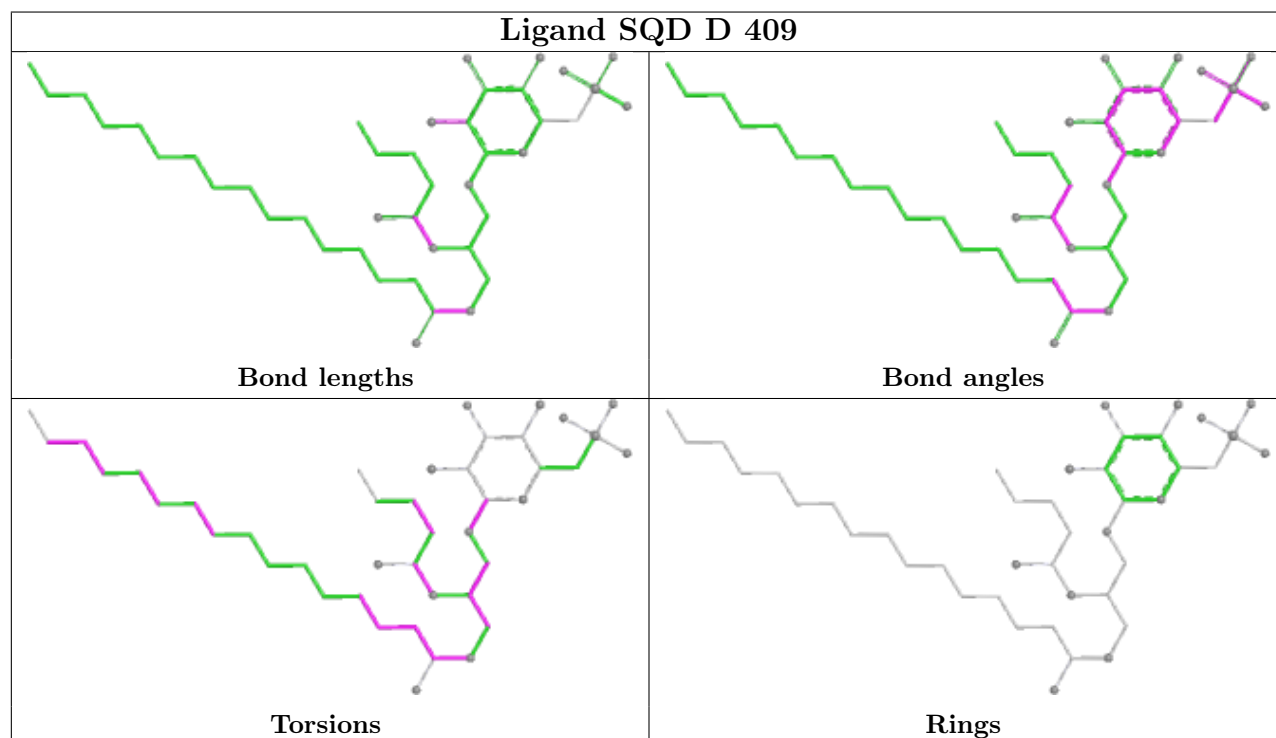
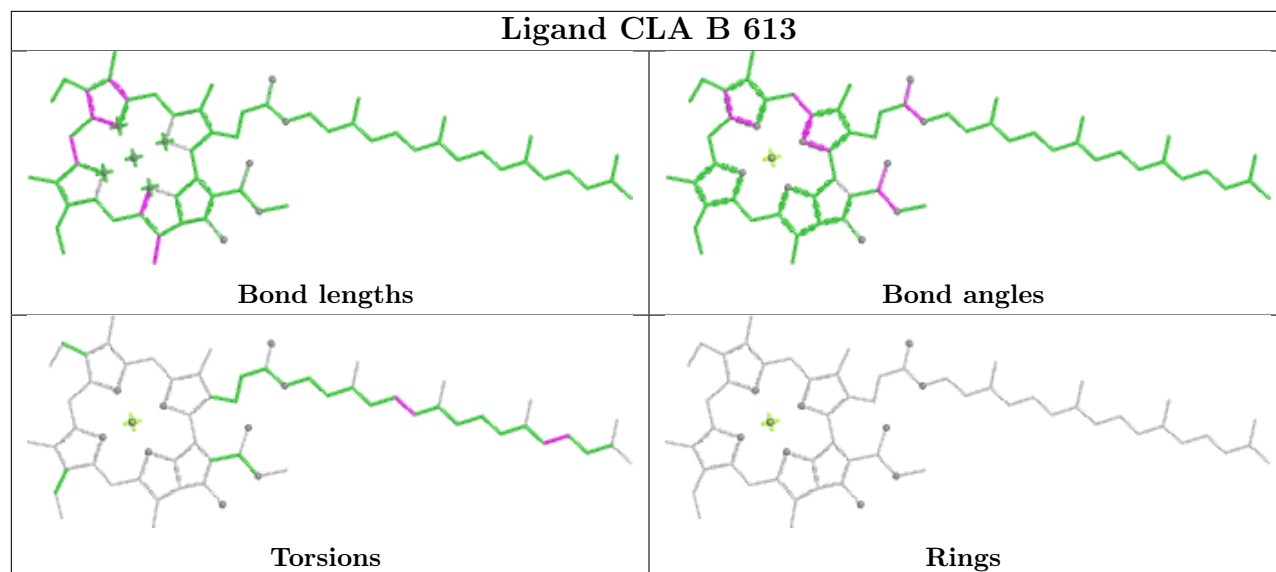


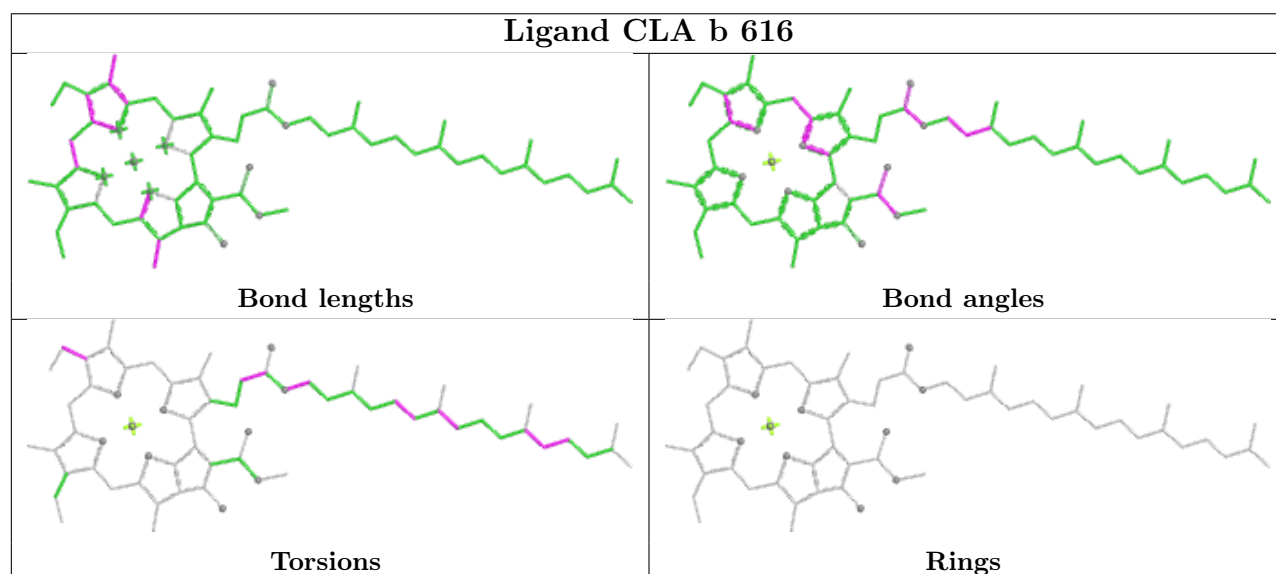
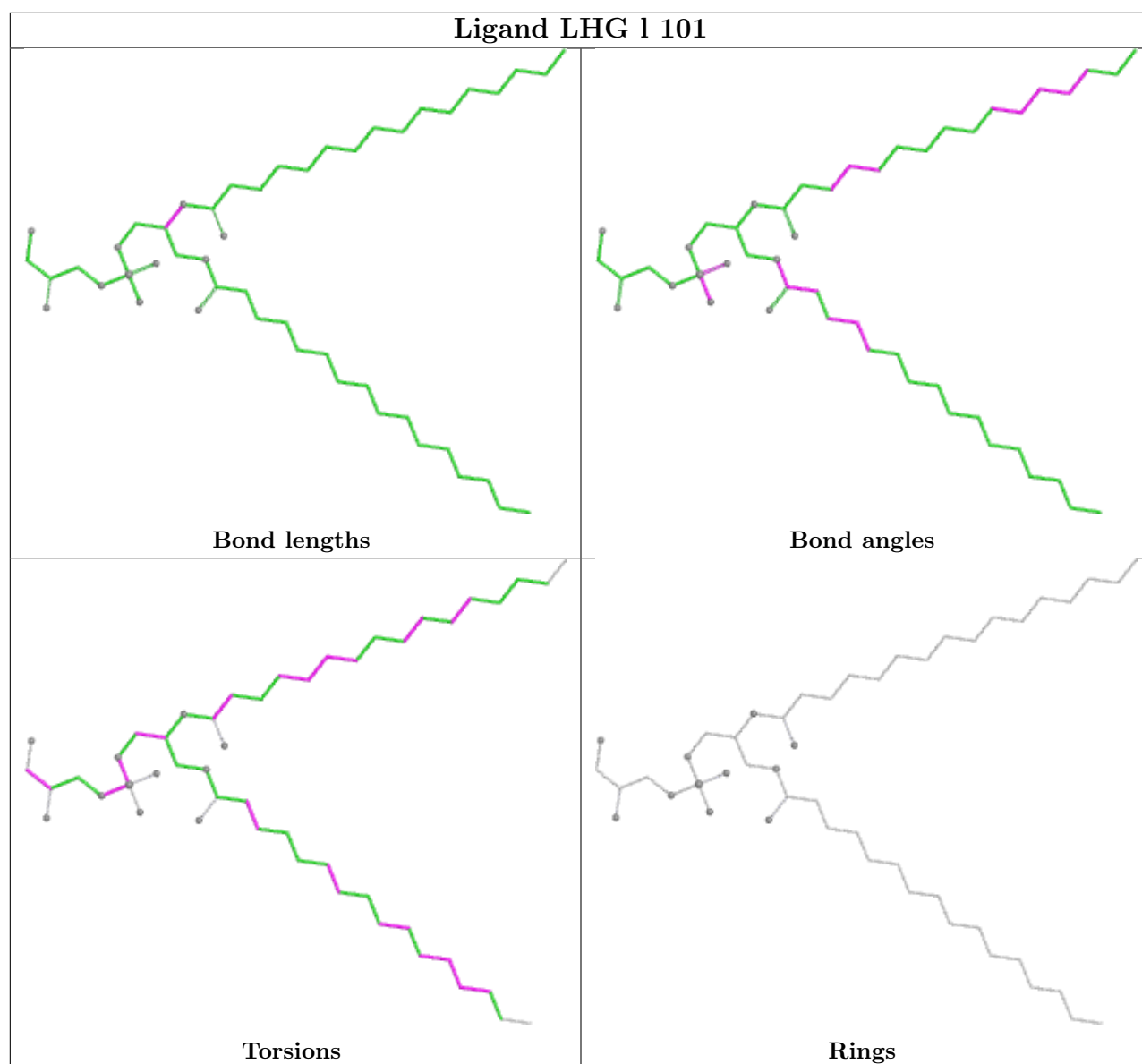
Ligand CLA a 607



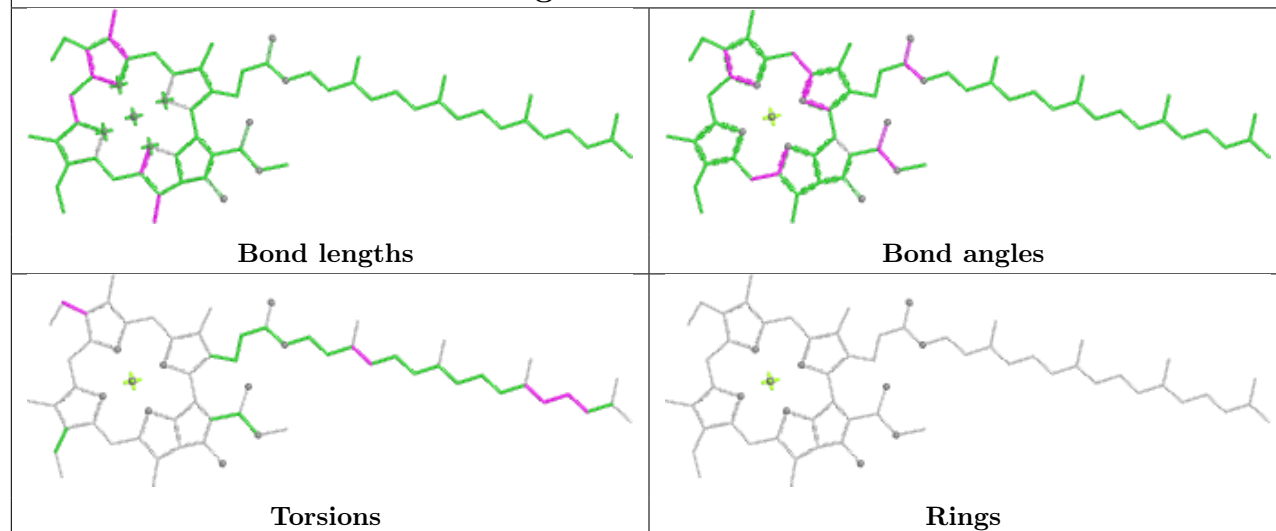
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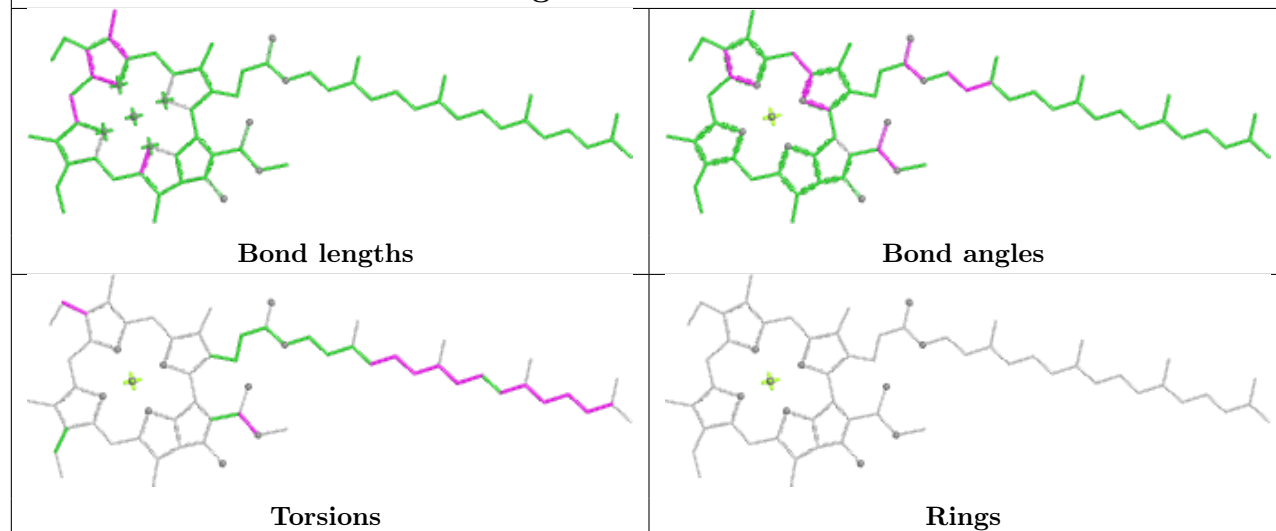




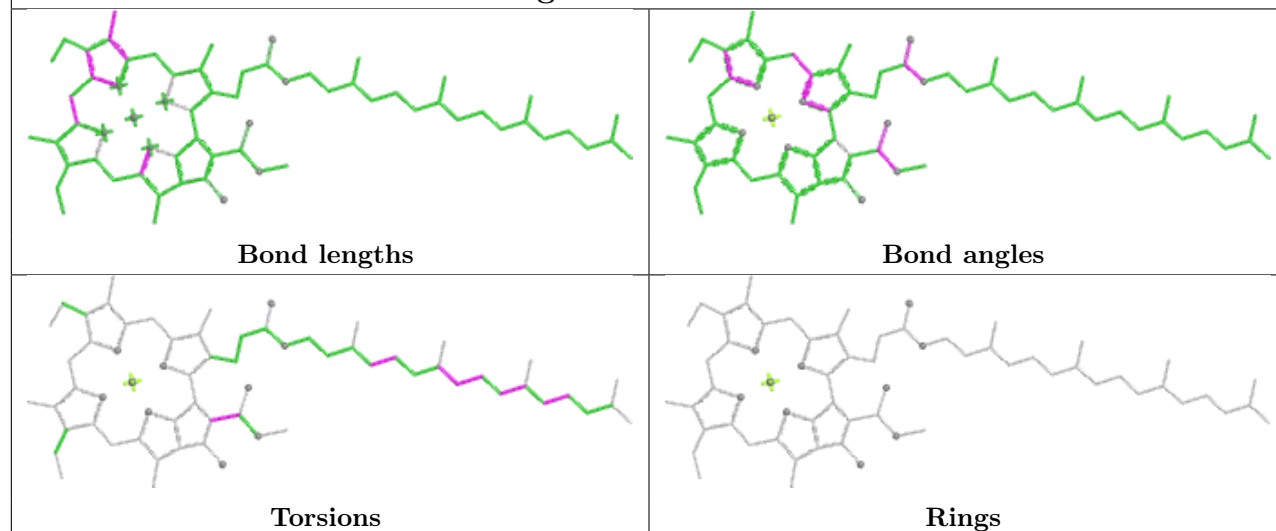
Ligand CLA b 608

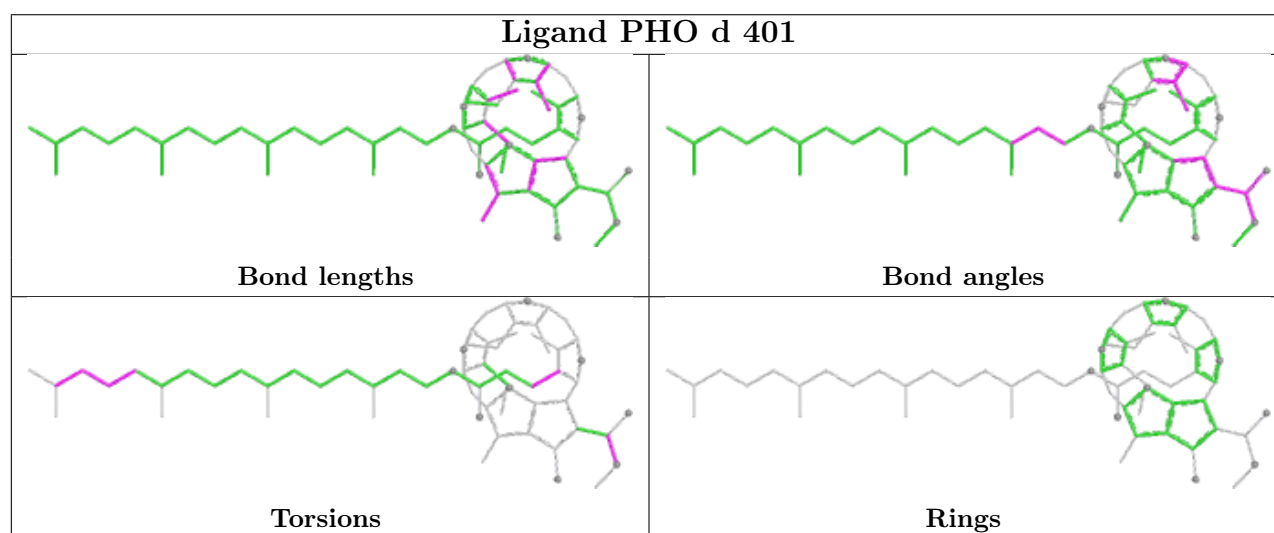
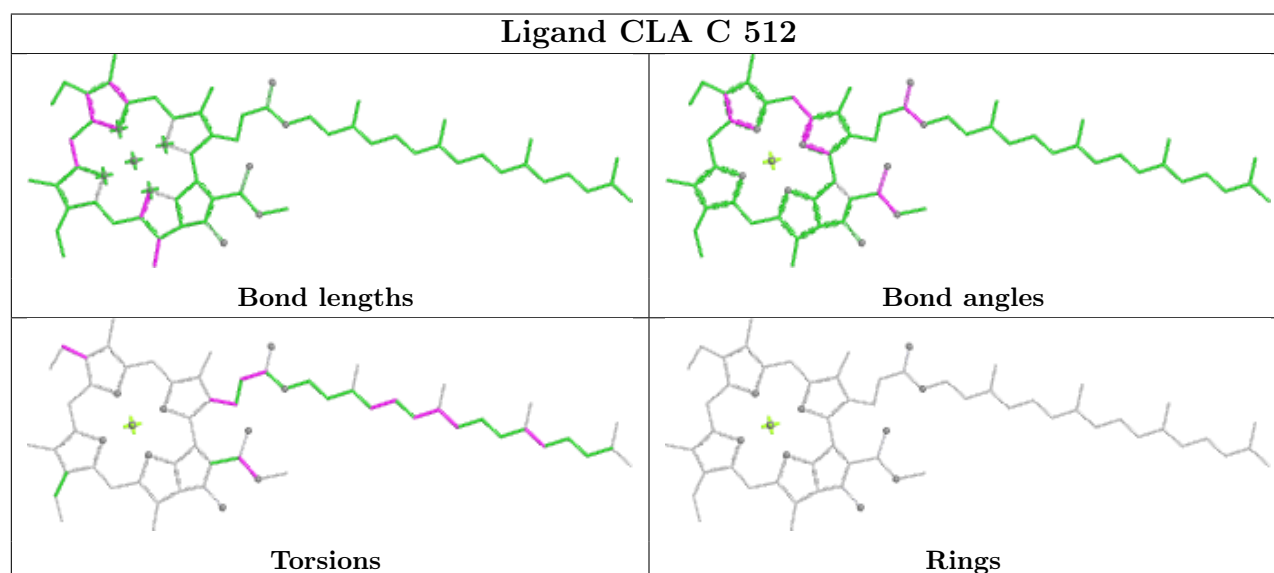
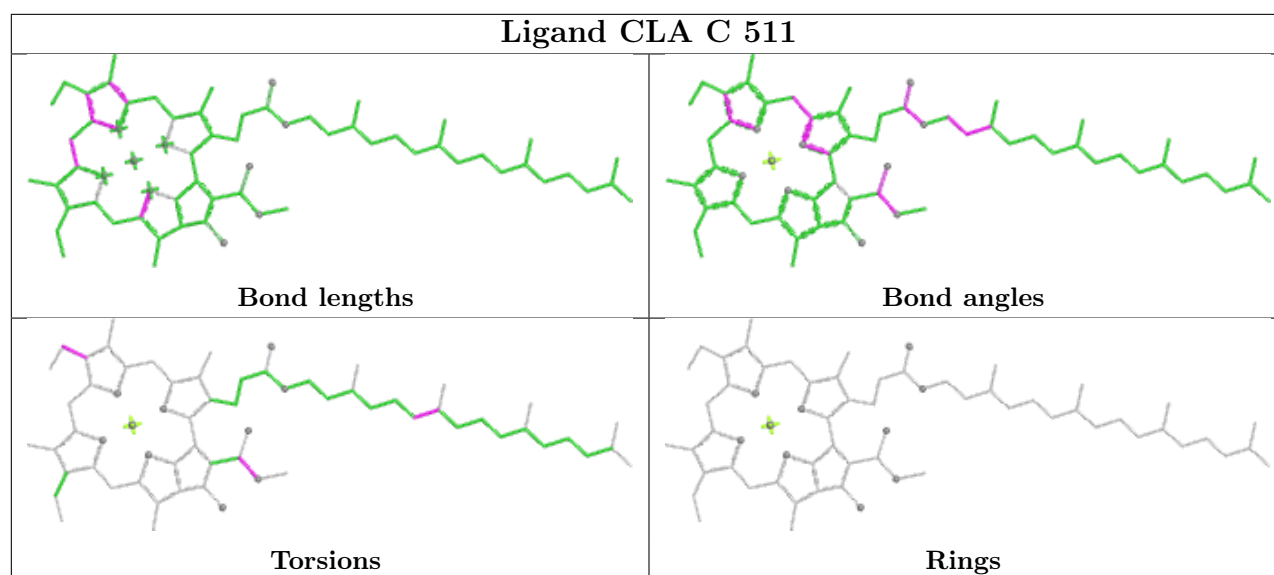


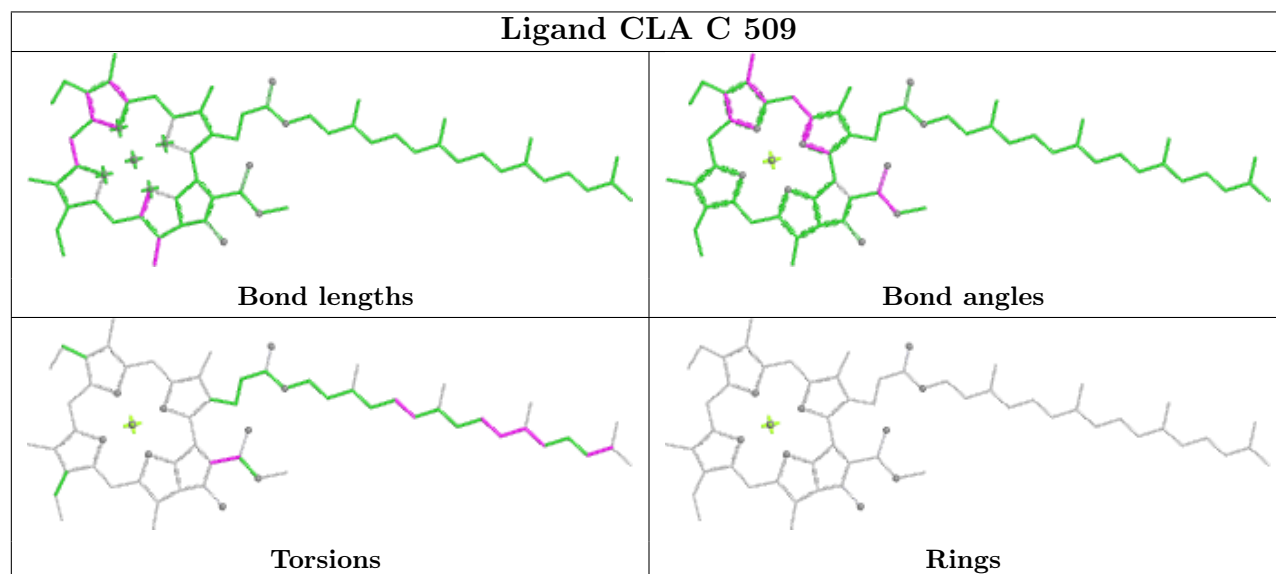
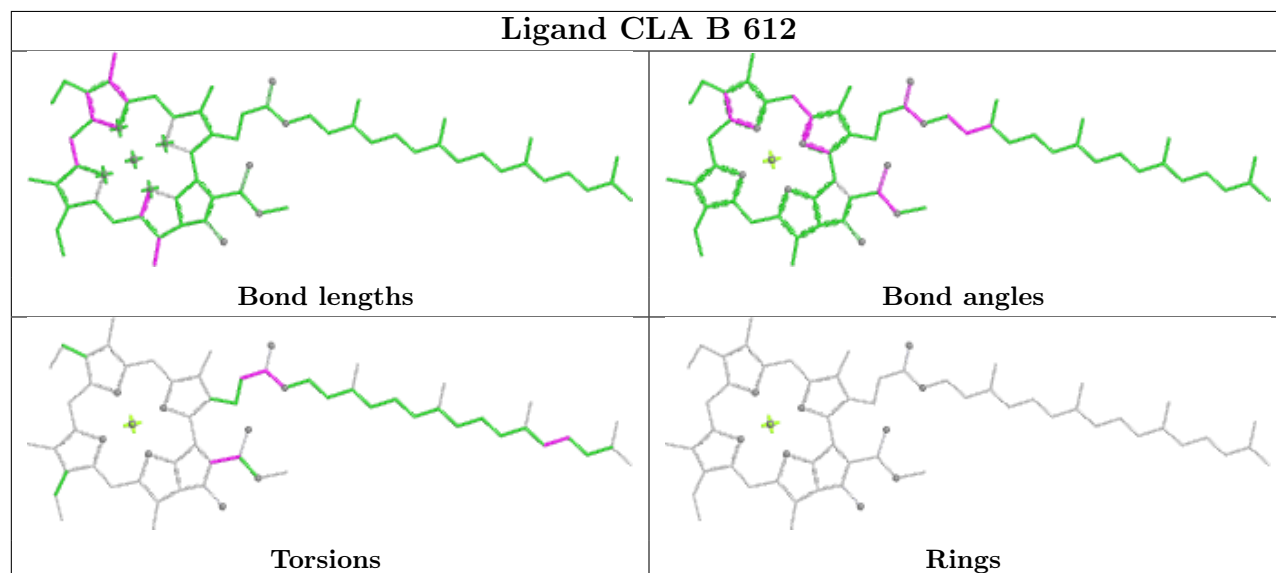
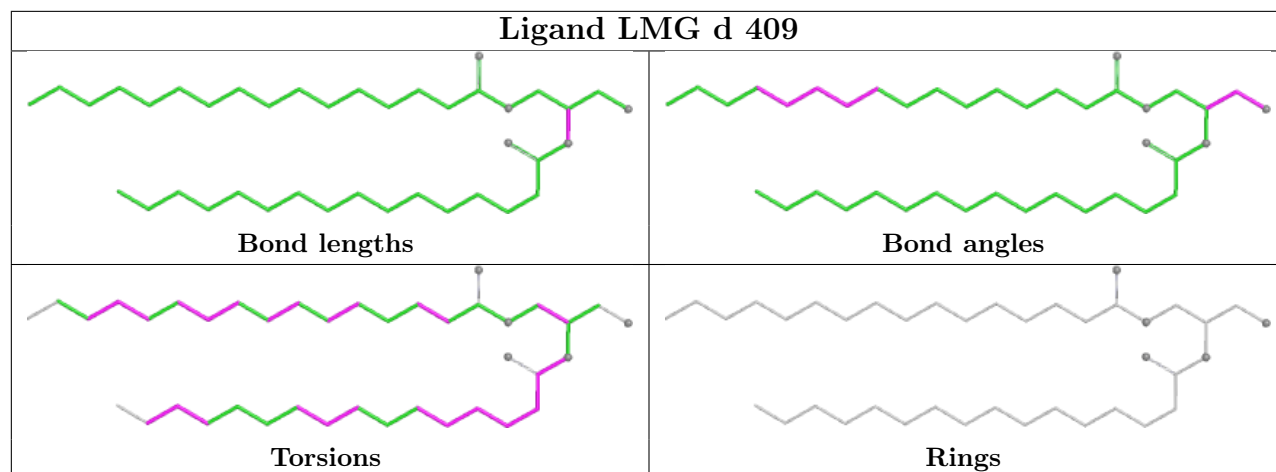
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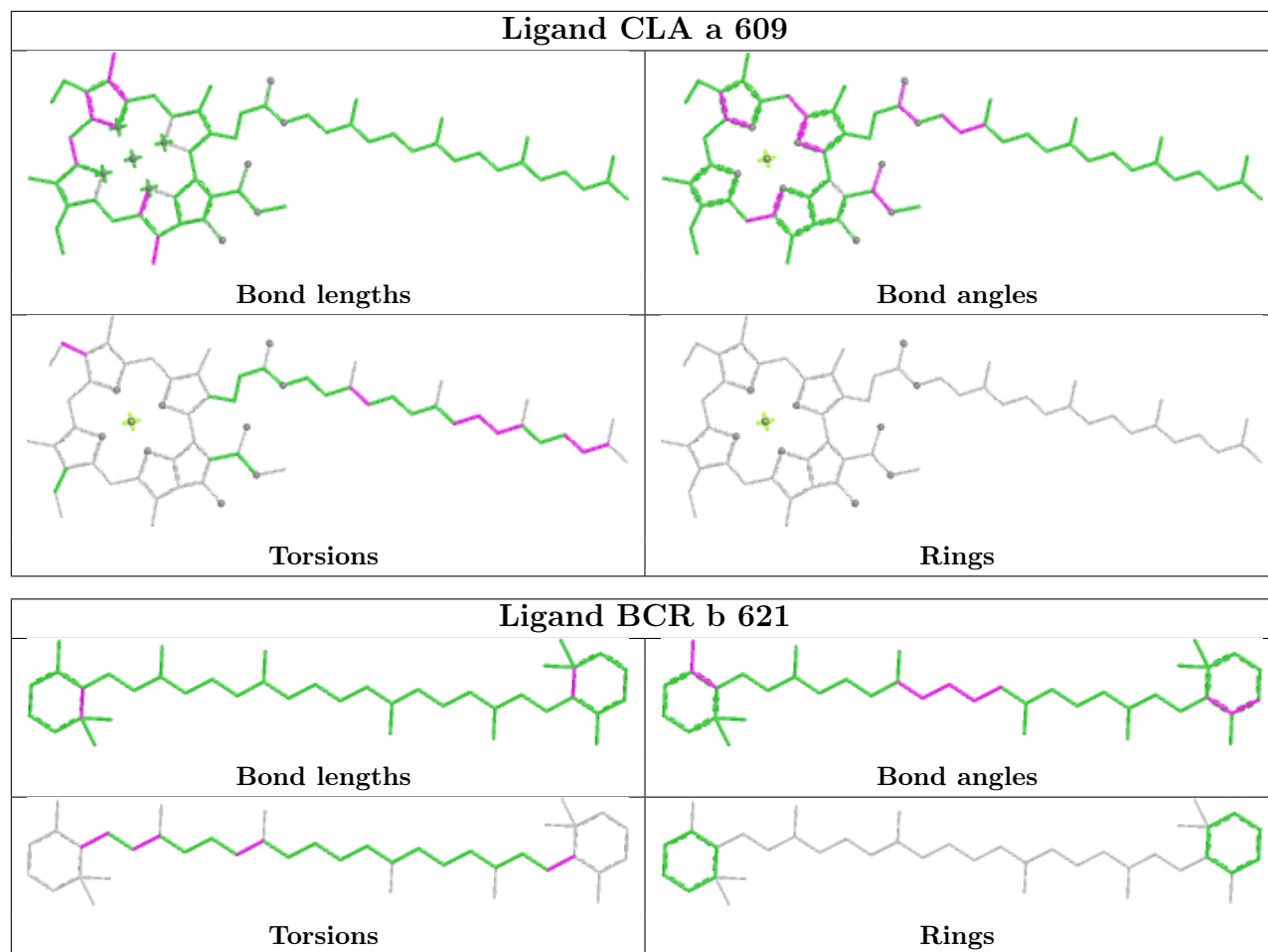


Ligand CLA c 511

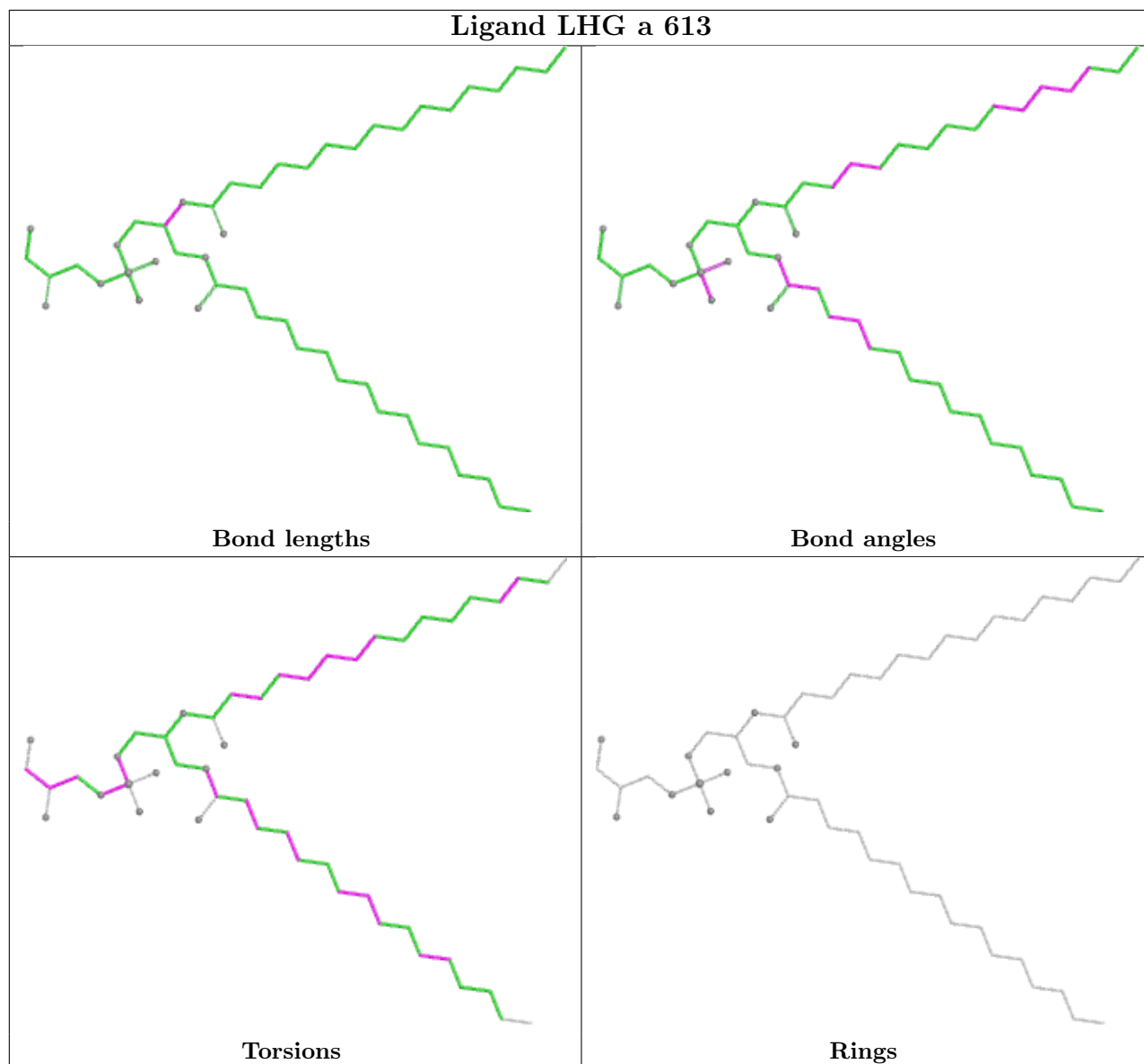




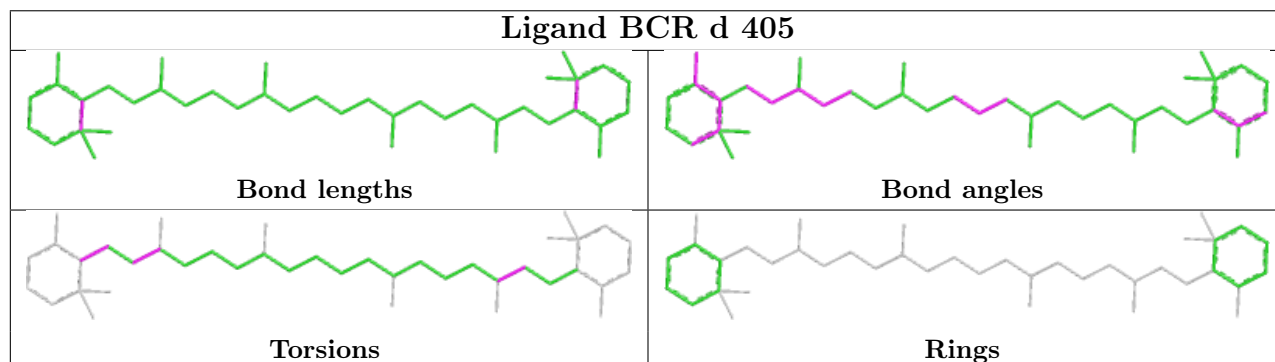


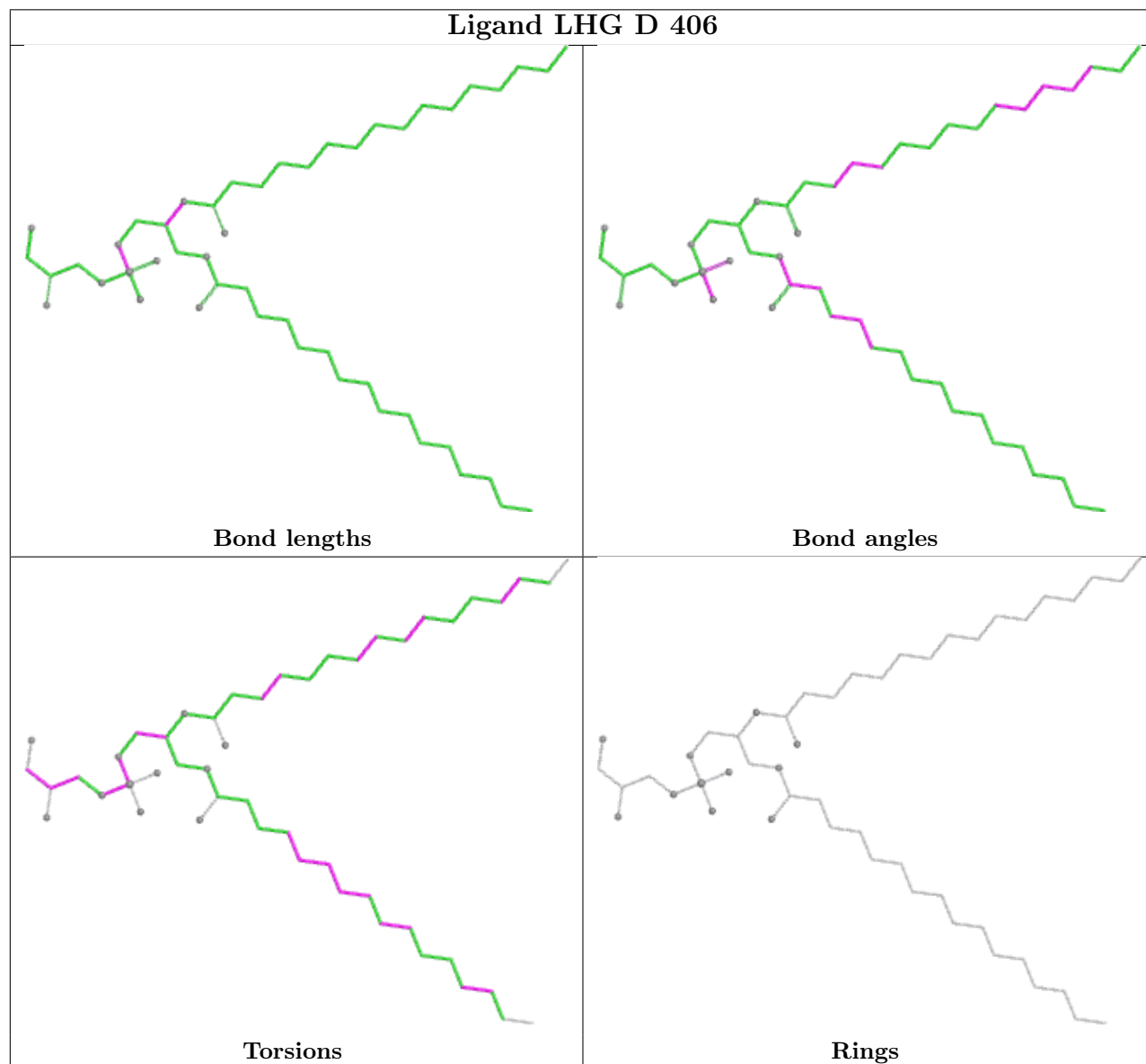
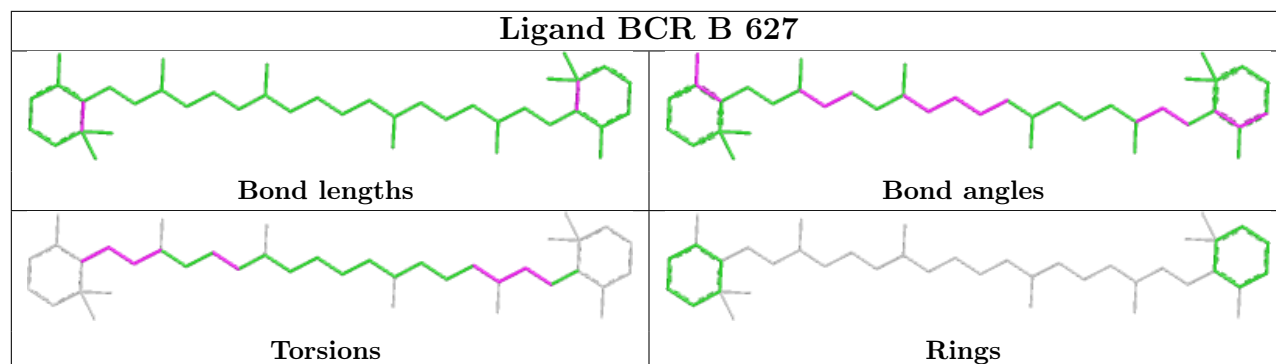


Ligand LHG a 613

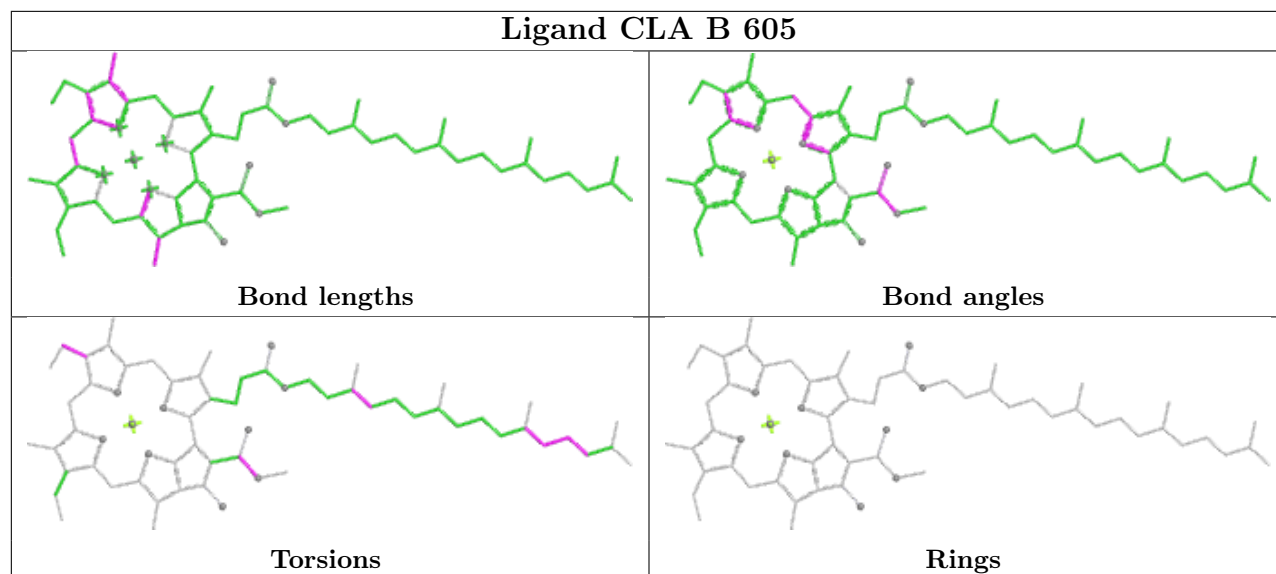


Ligand BCR d 405

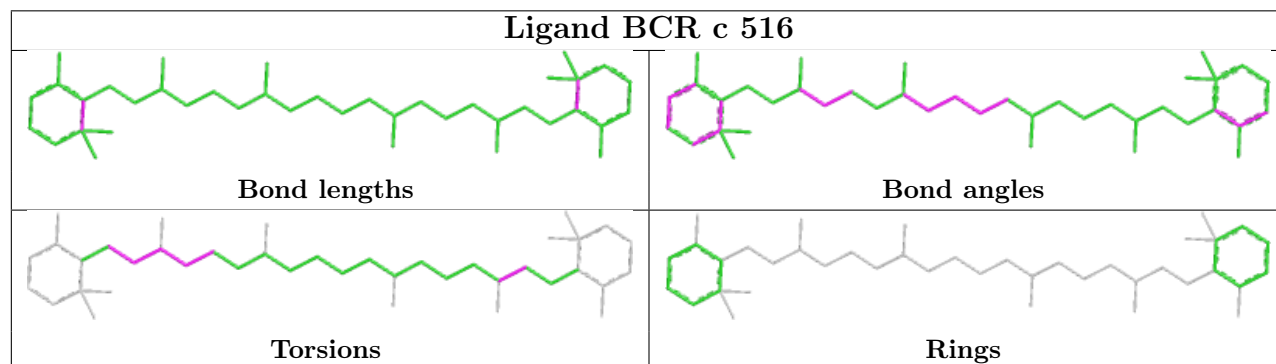




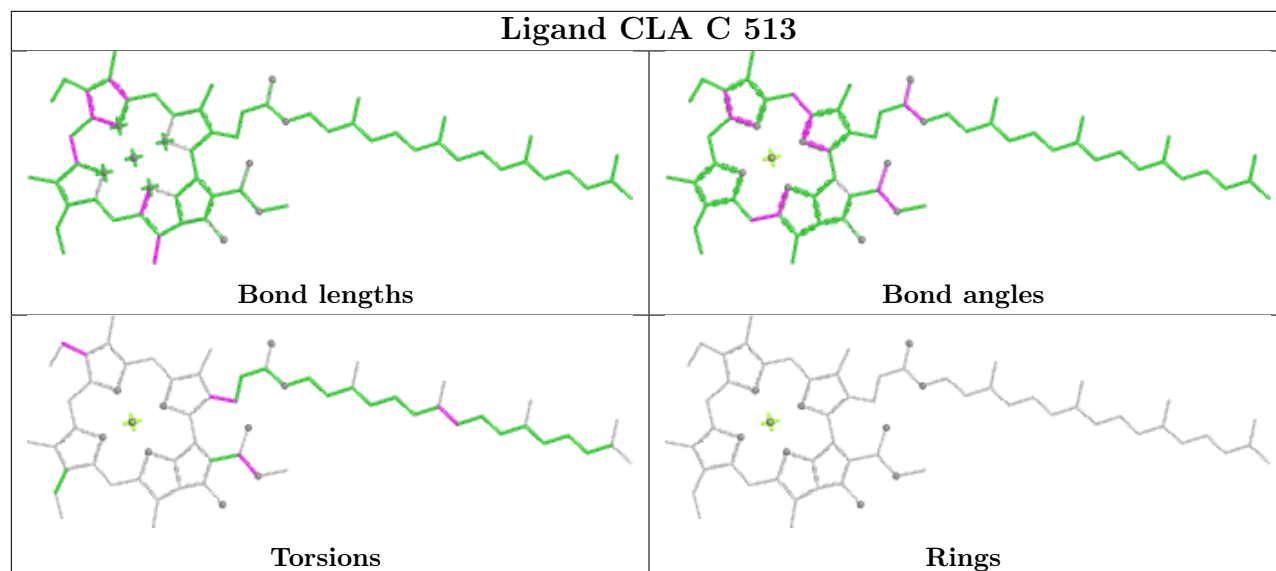
Ligand CLA B 605

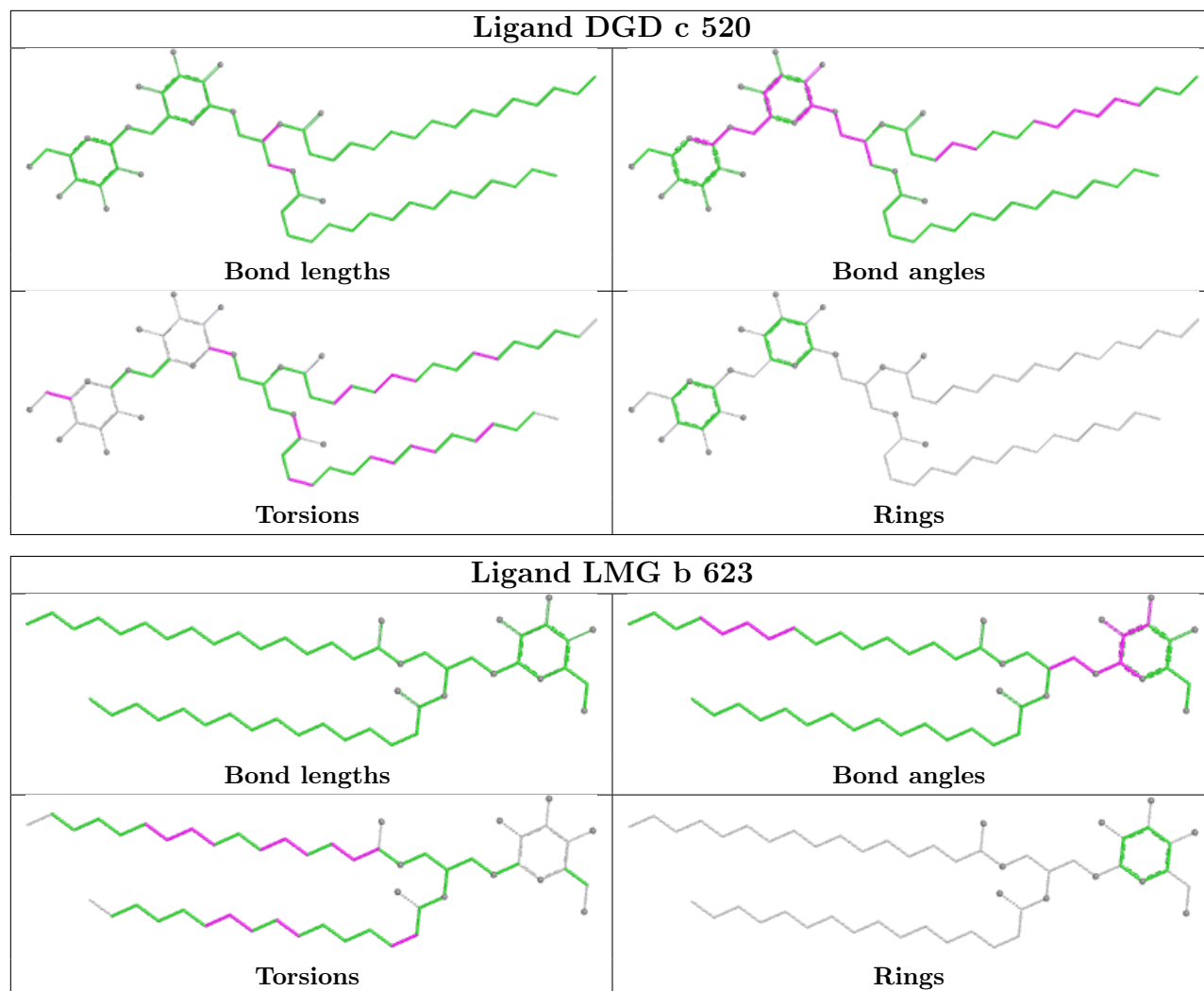


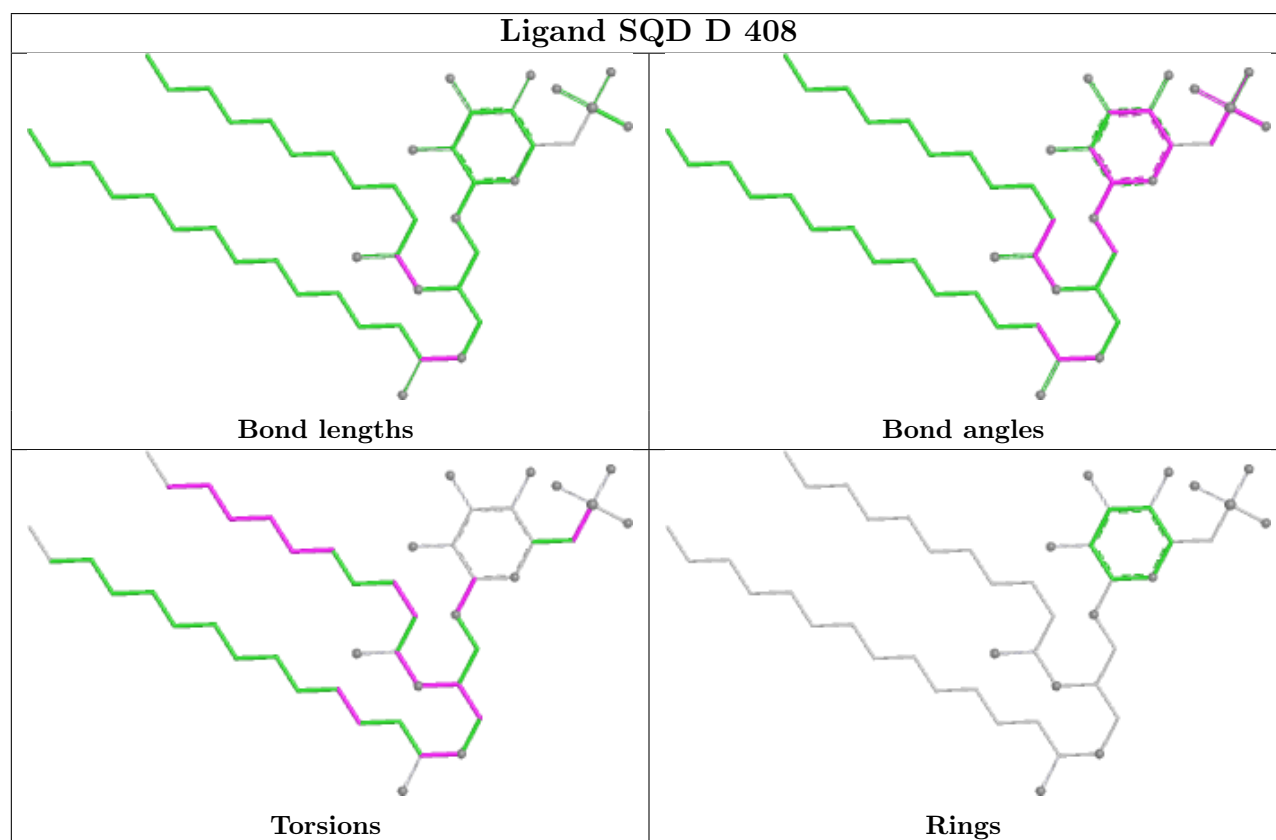
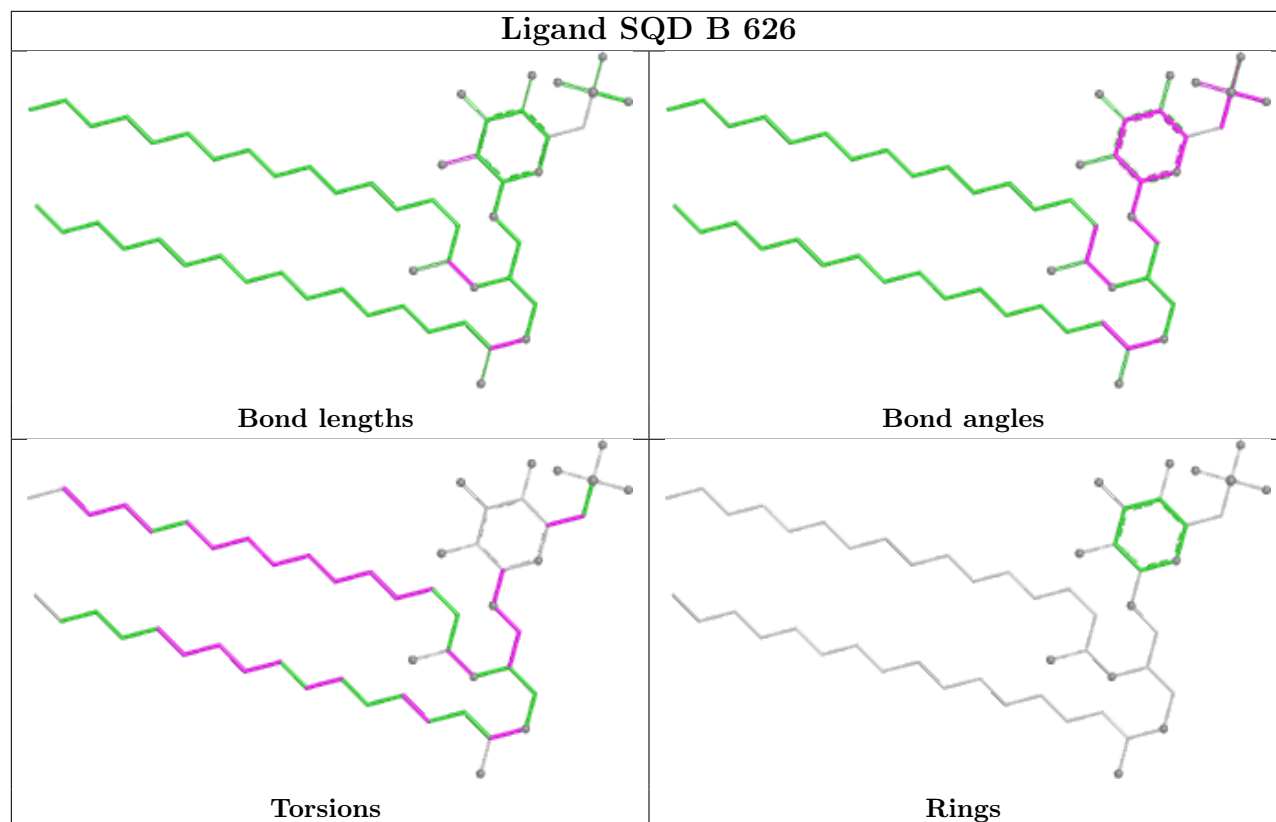
Ligand BCR c 516

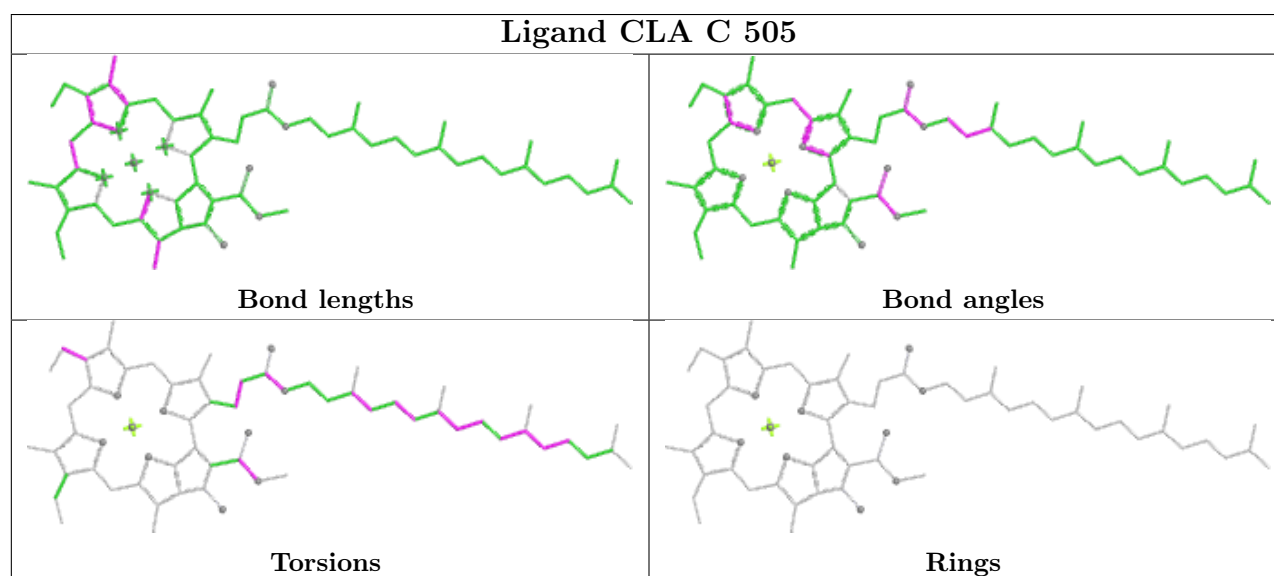
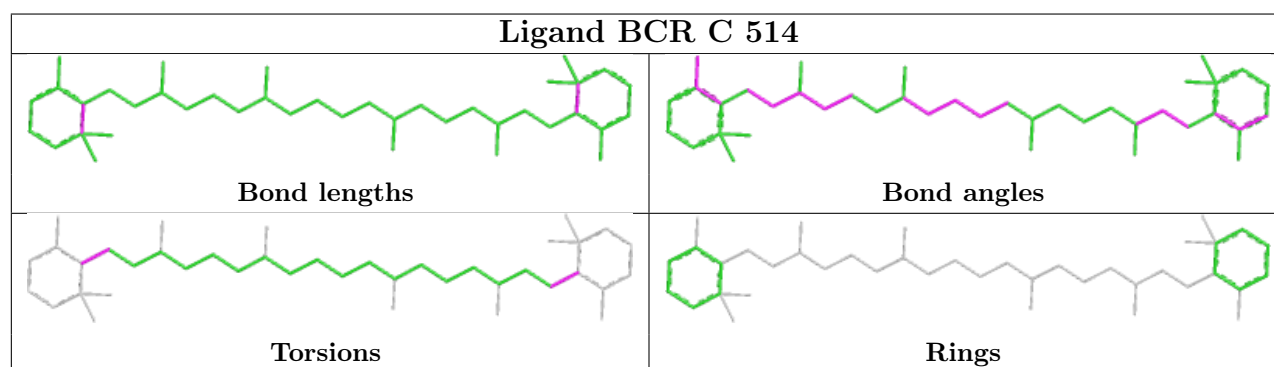
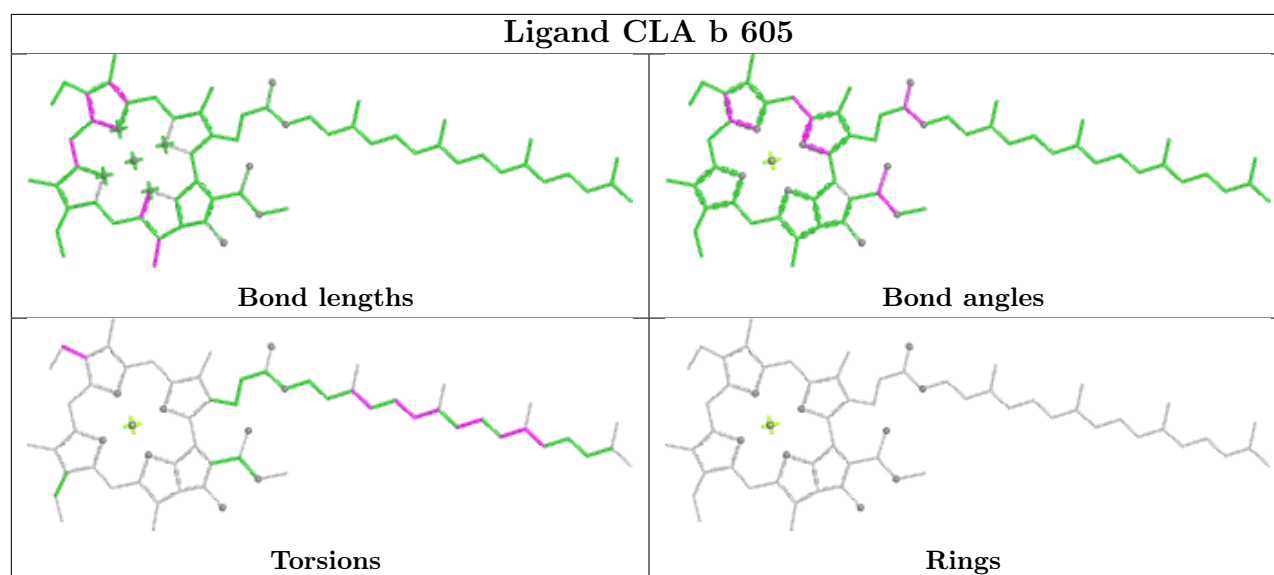


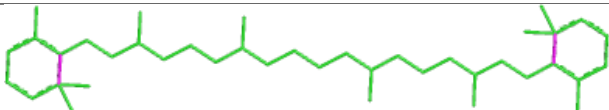
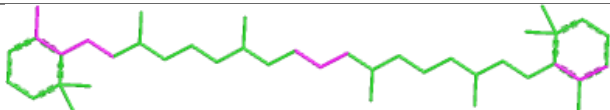
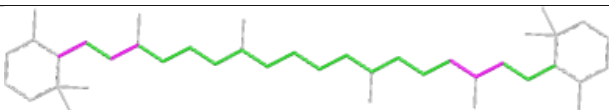
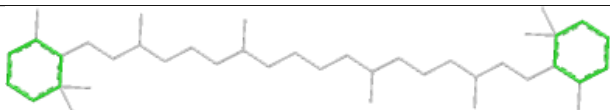
Ligand CLA C 513

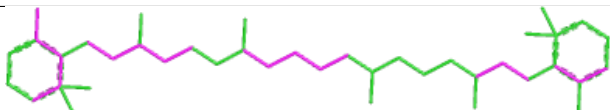
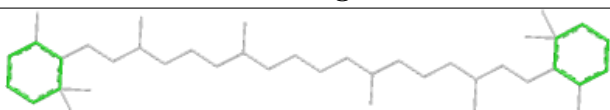


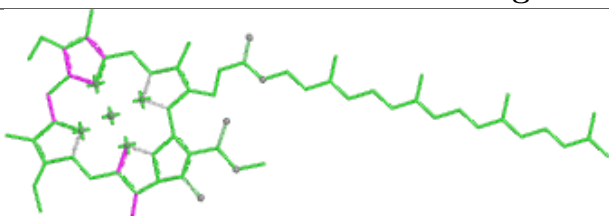
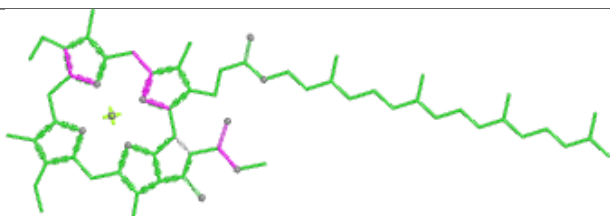
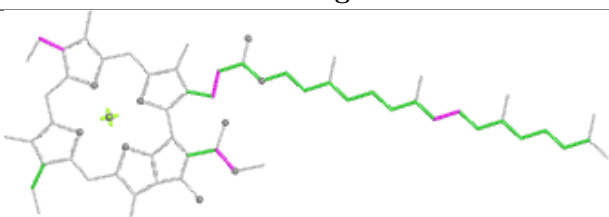
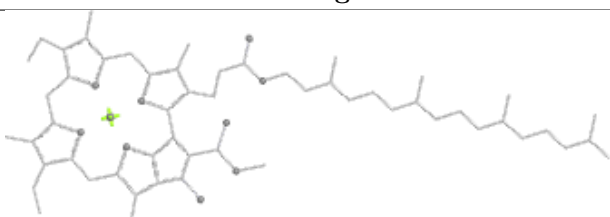




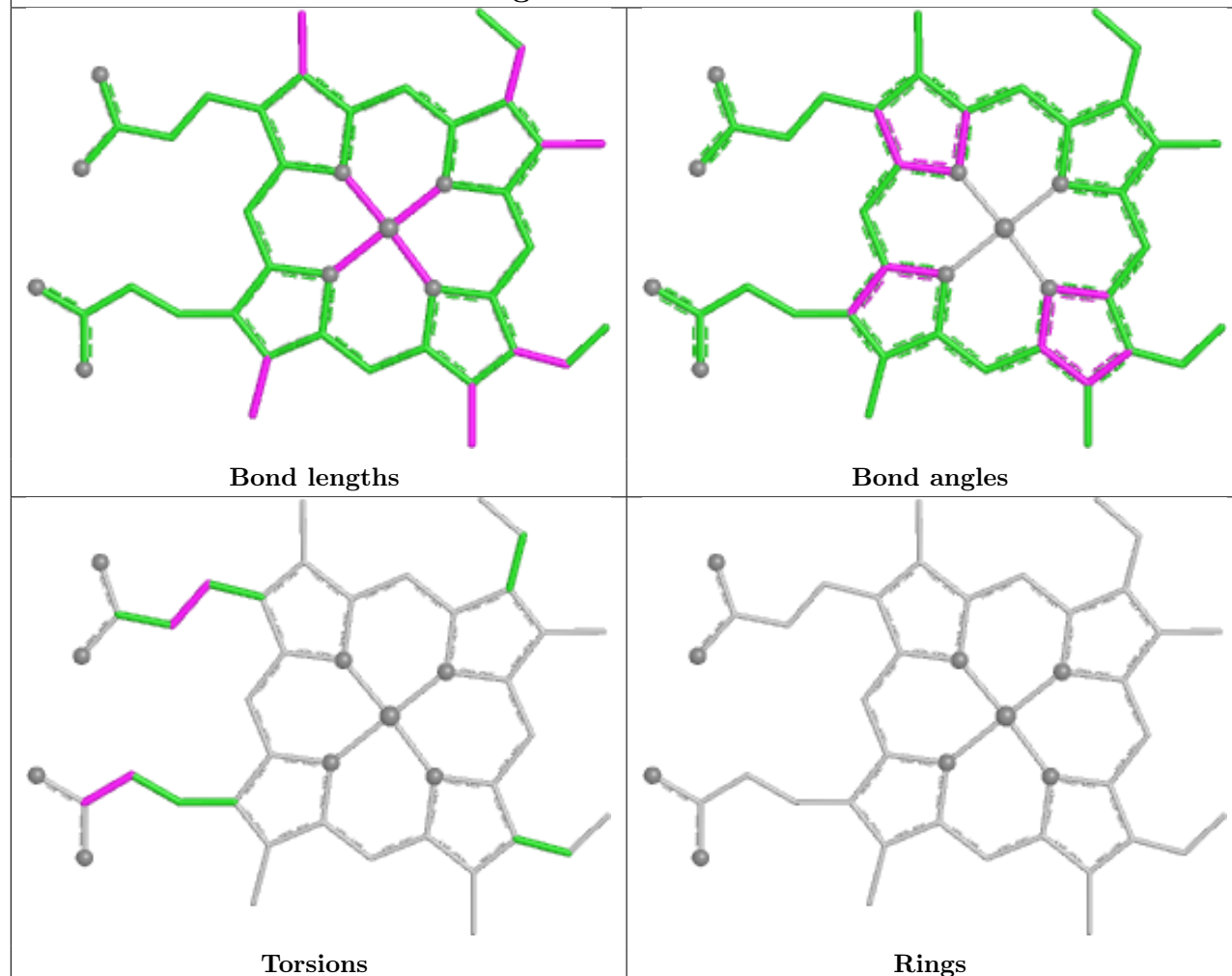


Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

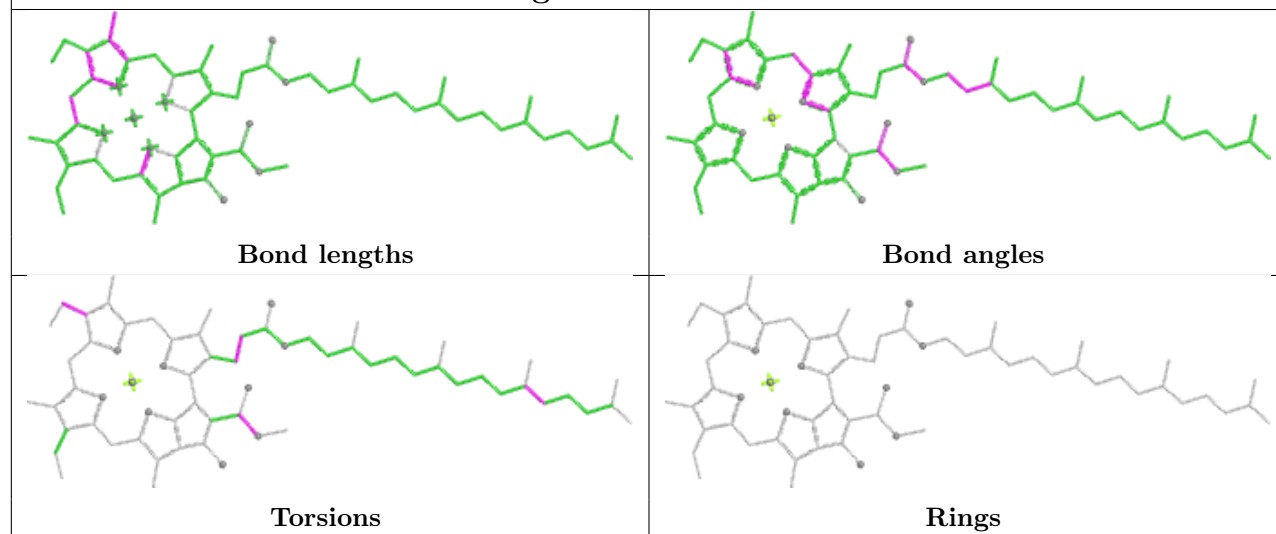
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

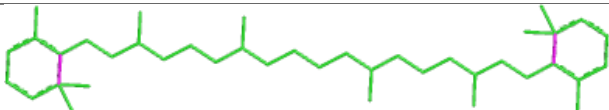
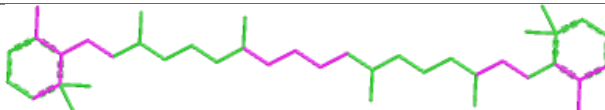
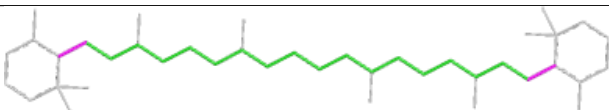
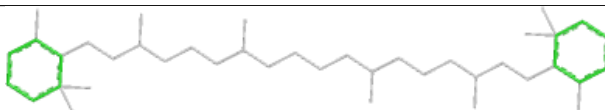
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

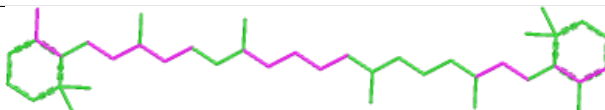
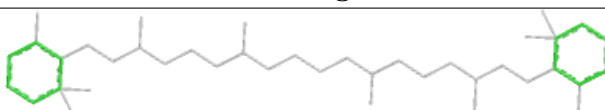
Ligand HEM e 101

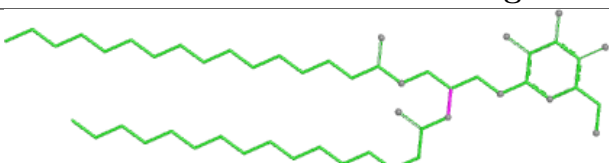
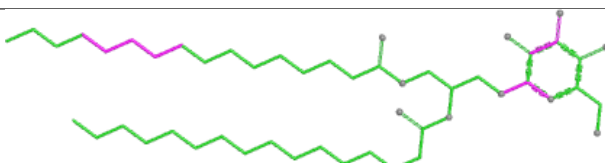
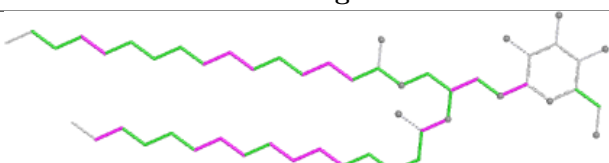
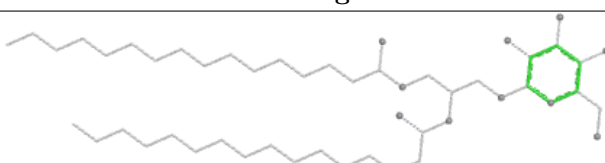


Ligand CLA B 606

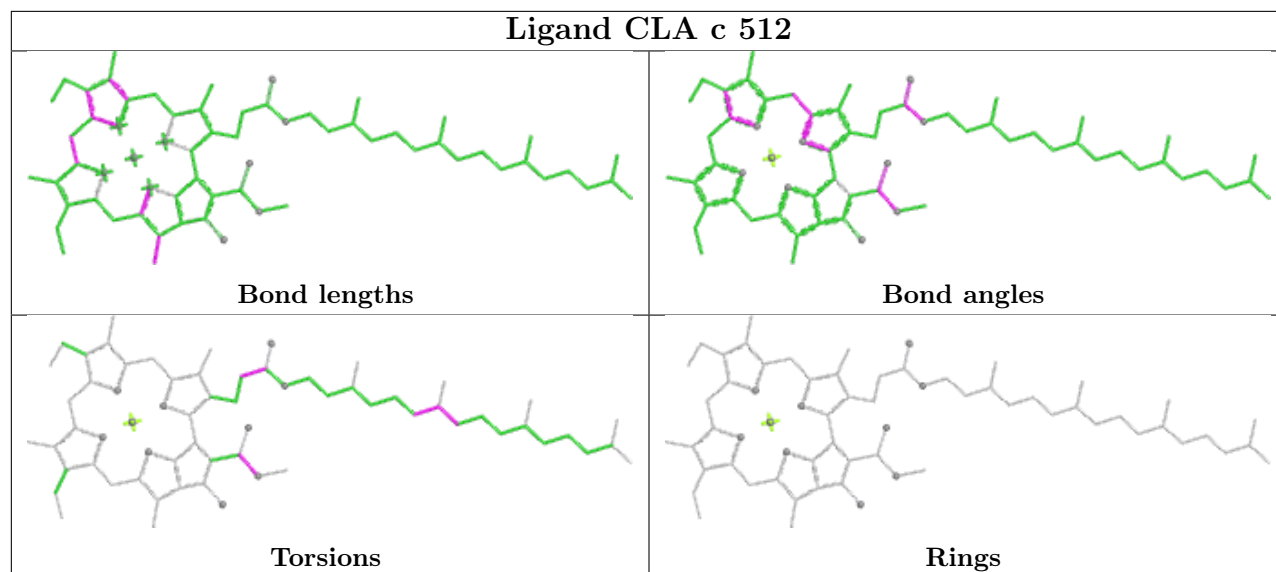


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

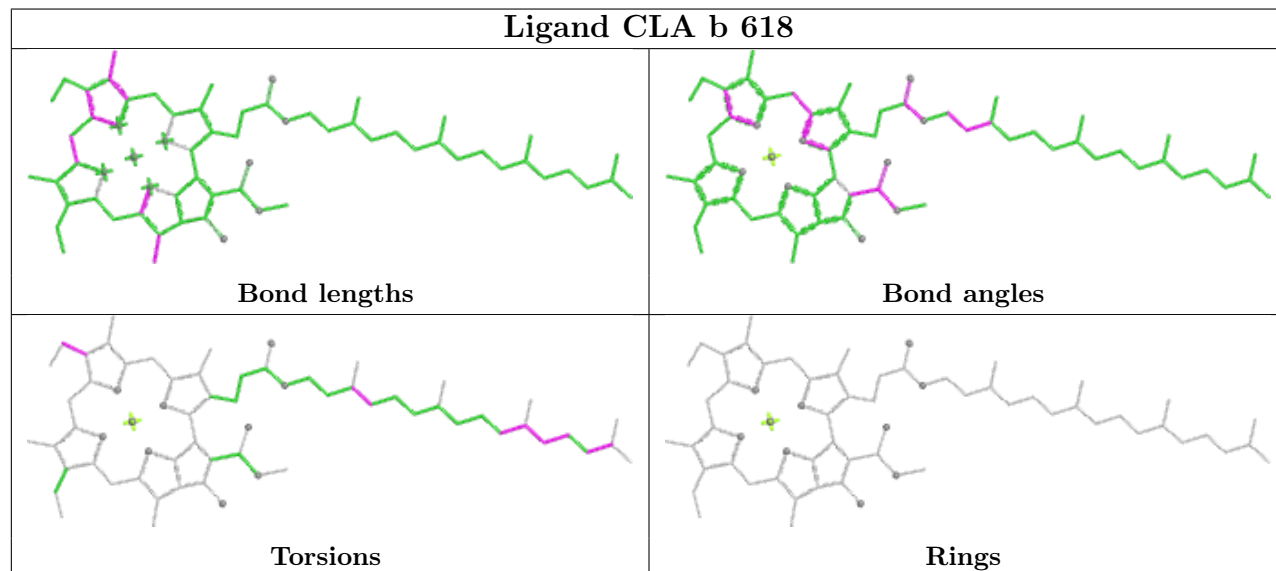
Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

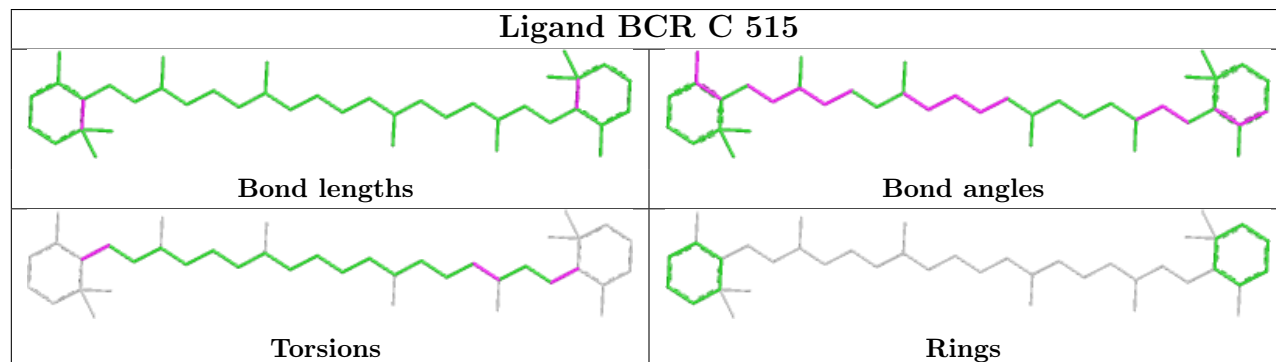
Ligand CLA c 512



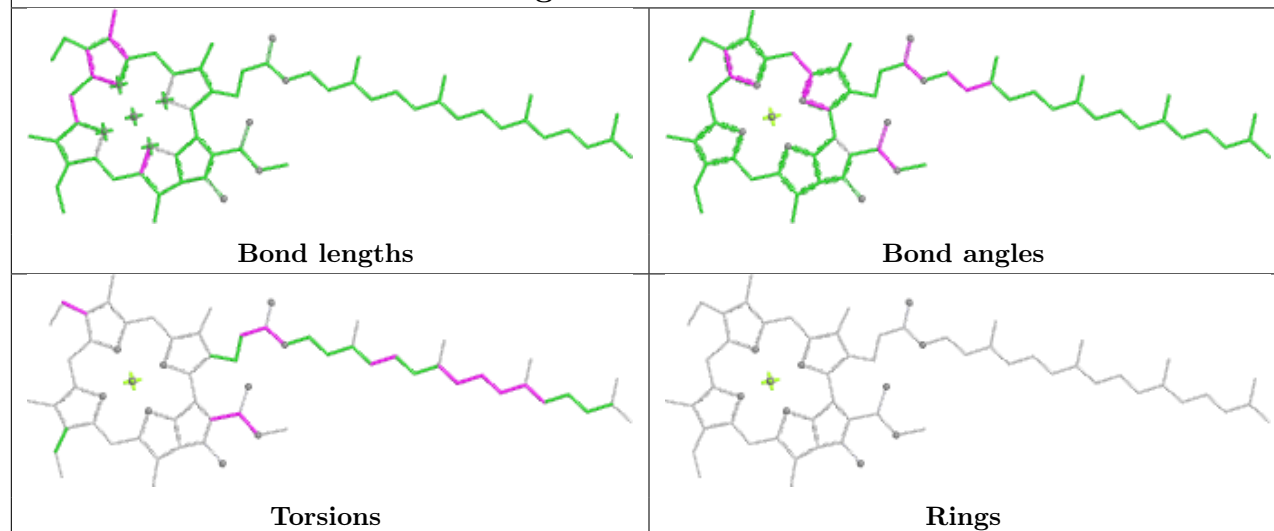
Ligand CLA b 618



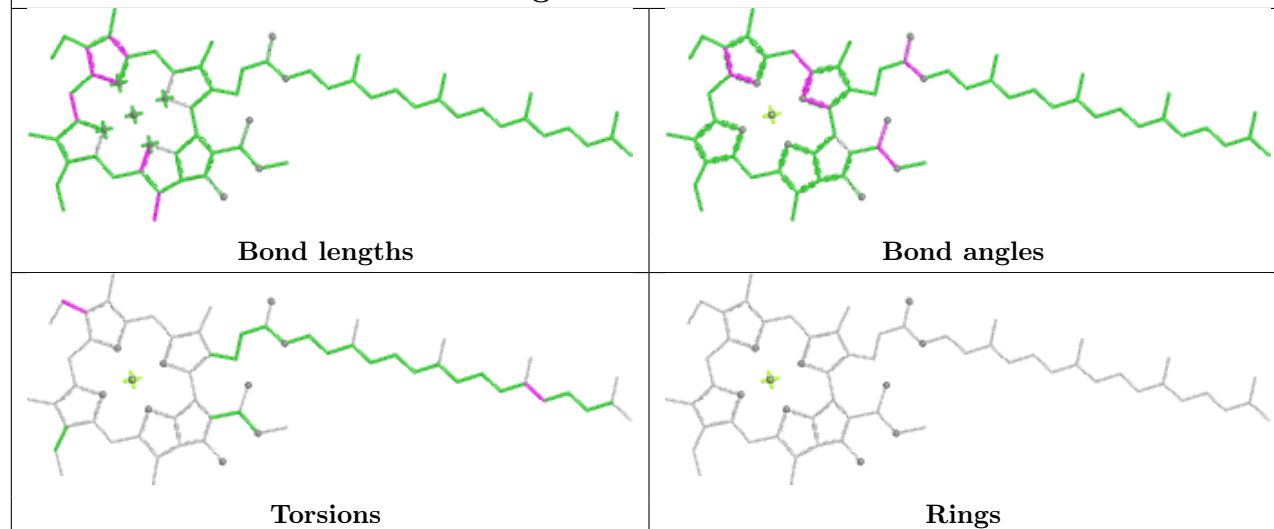
Ligand BCR C 515



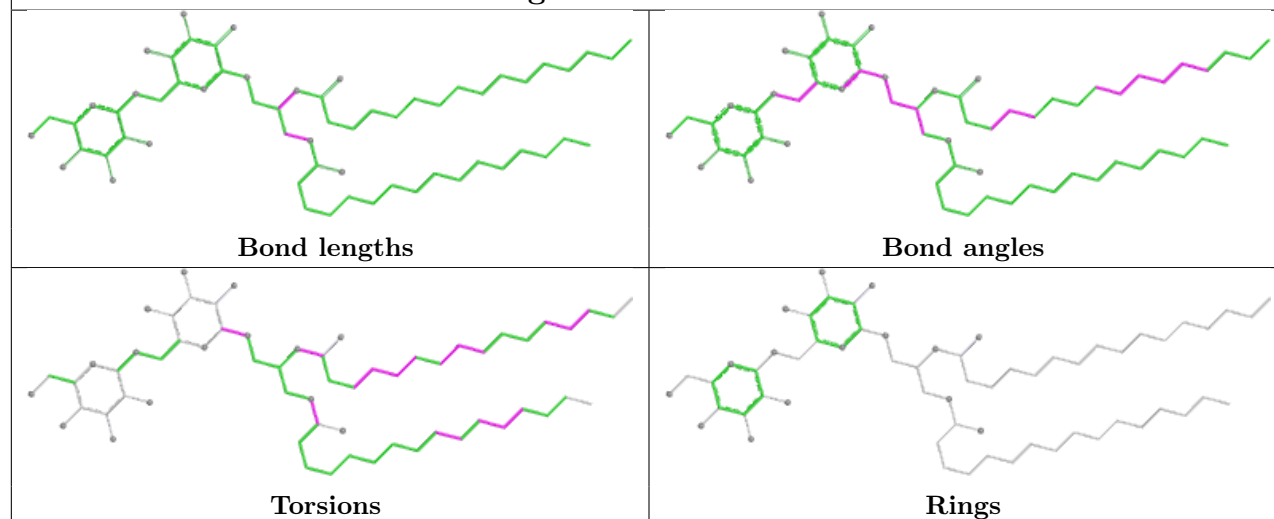
Ligand CLA b 604



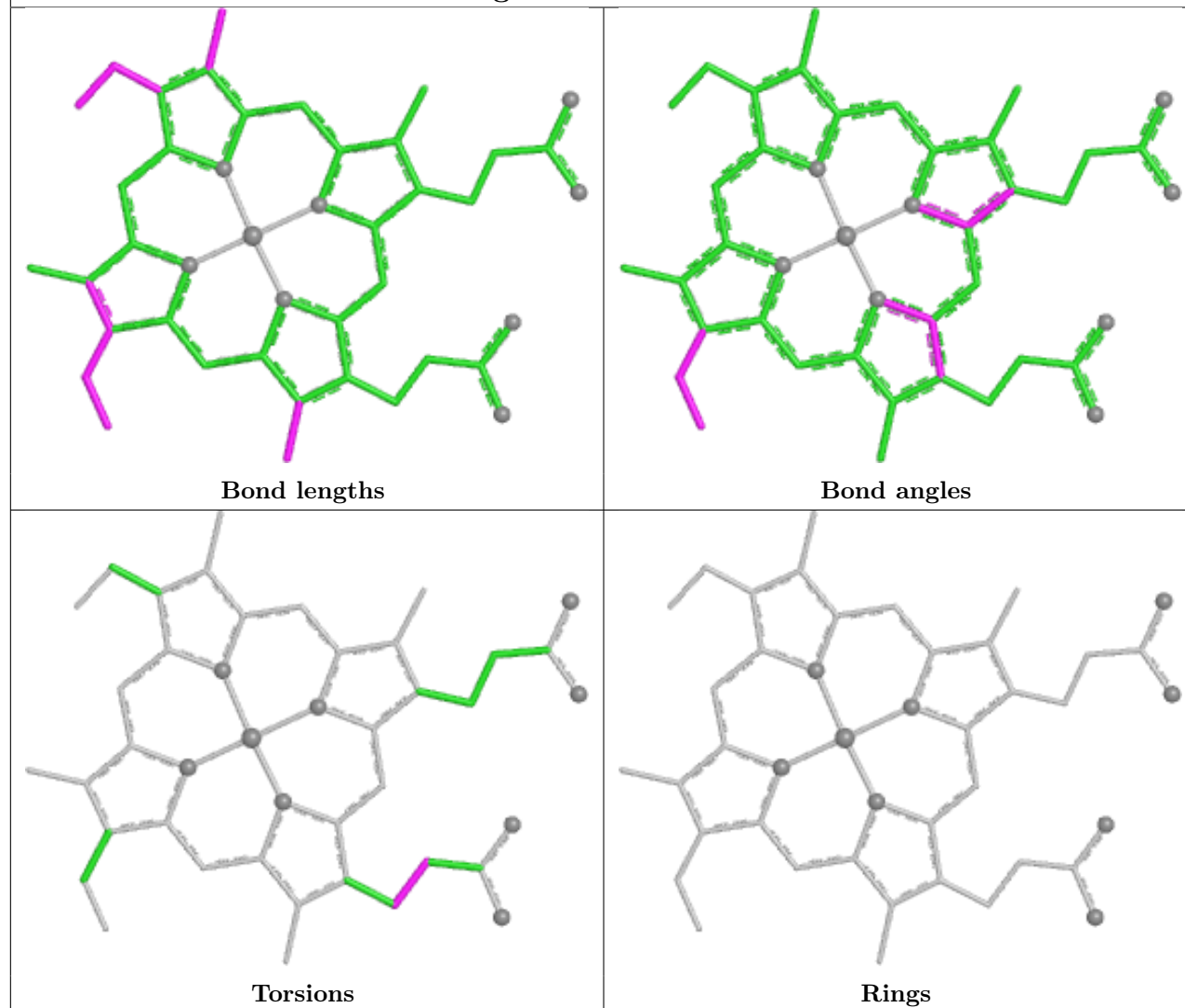
Ligand CLA B 615



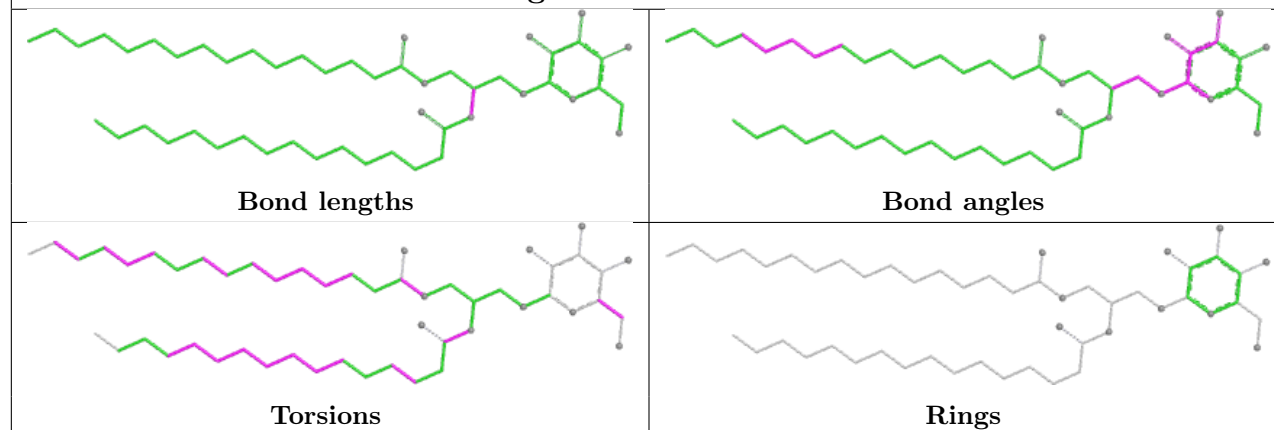
Ligand DGD C 518

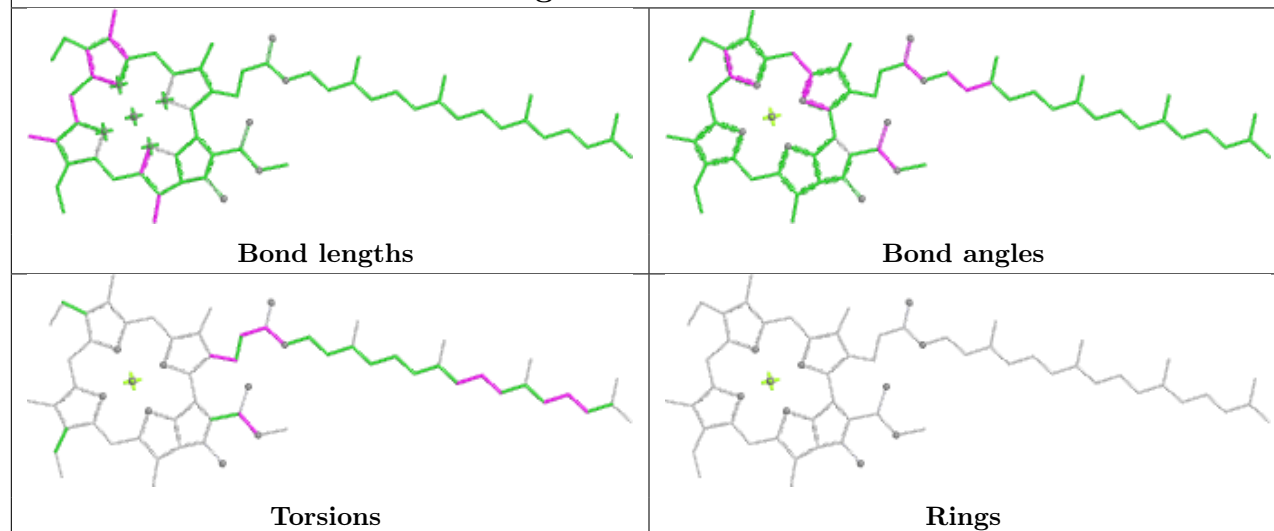
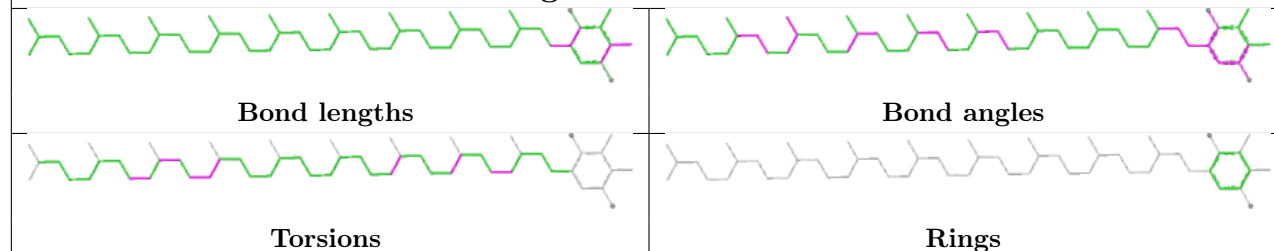
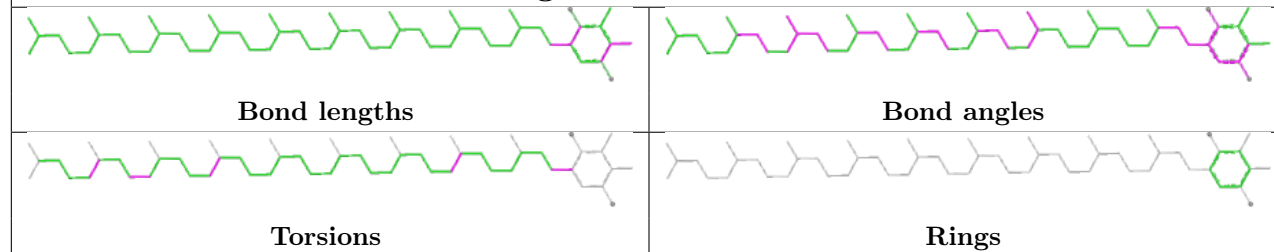
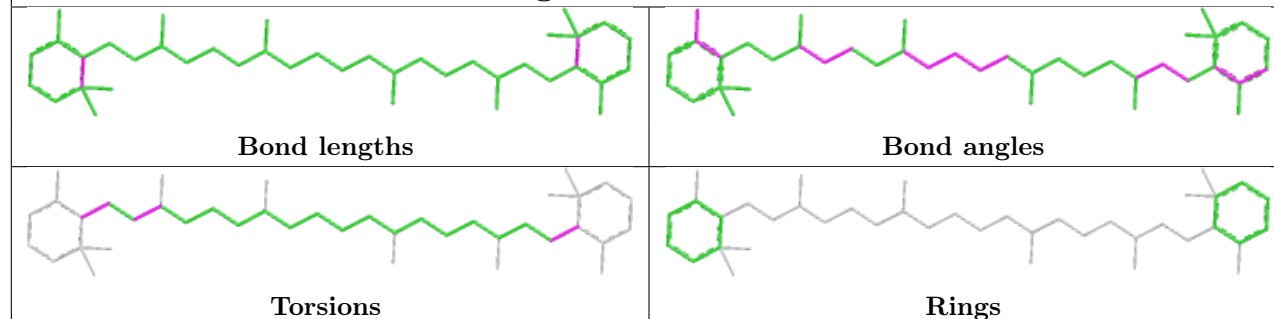


Ligand HEC V 201

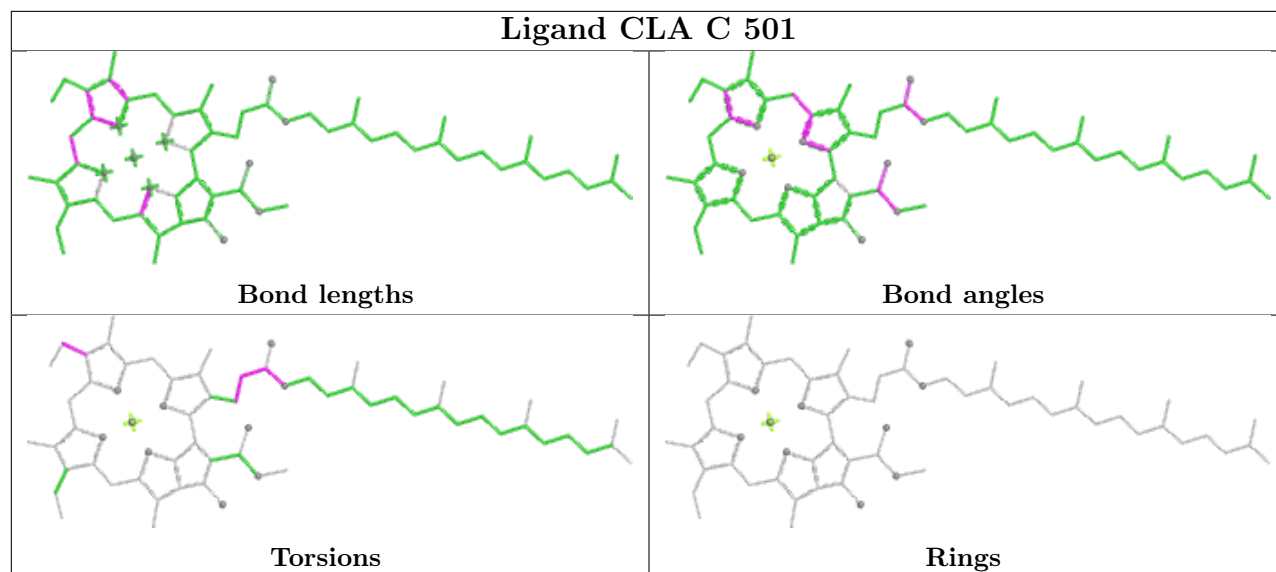


Ligand LMG C 519

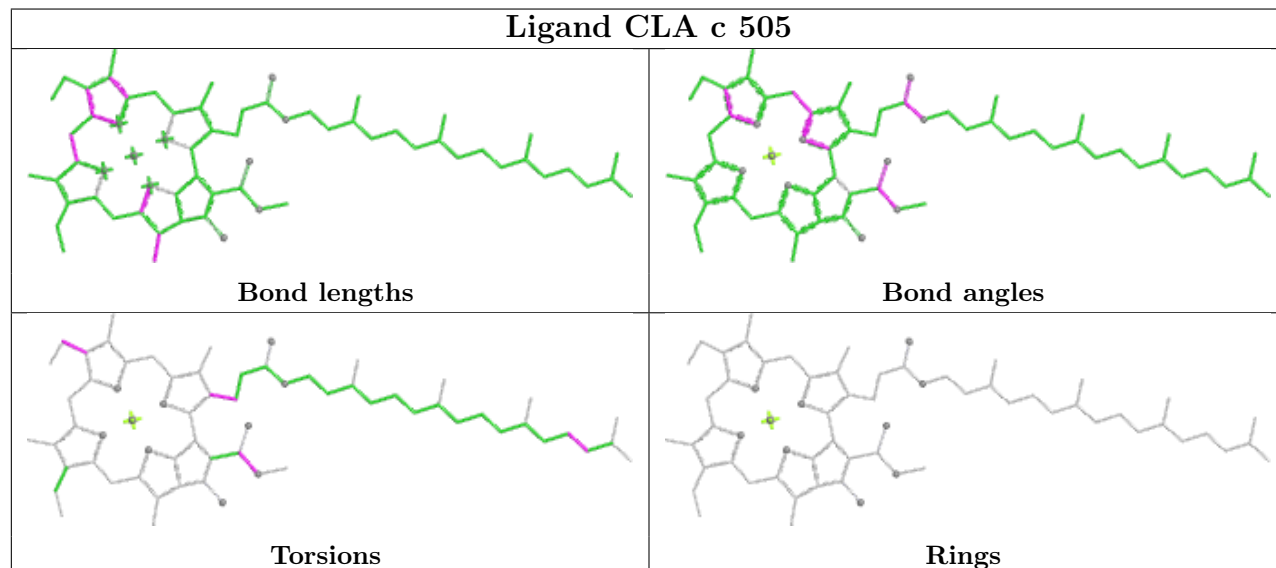


Ligand CLA b 615**Ligand PL9 d 408****Ligand PL9 D 407****Ligand BCR c 517**

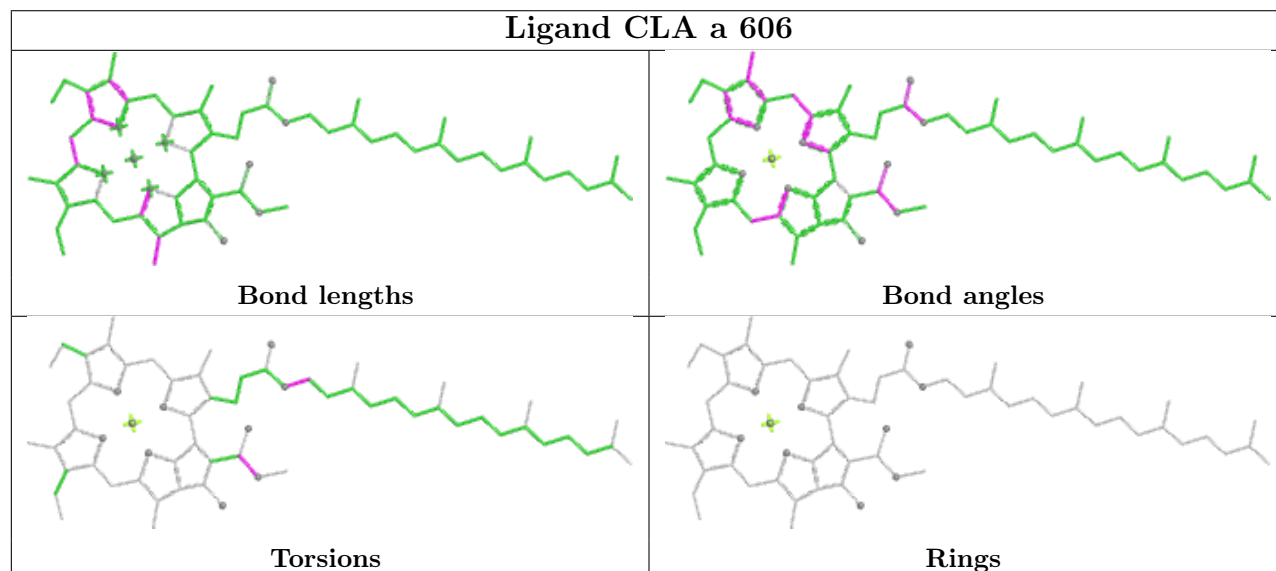
Ligand CLA C 501

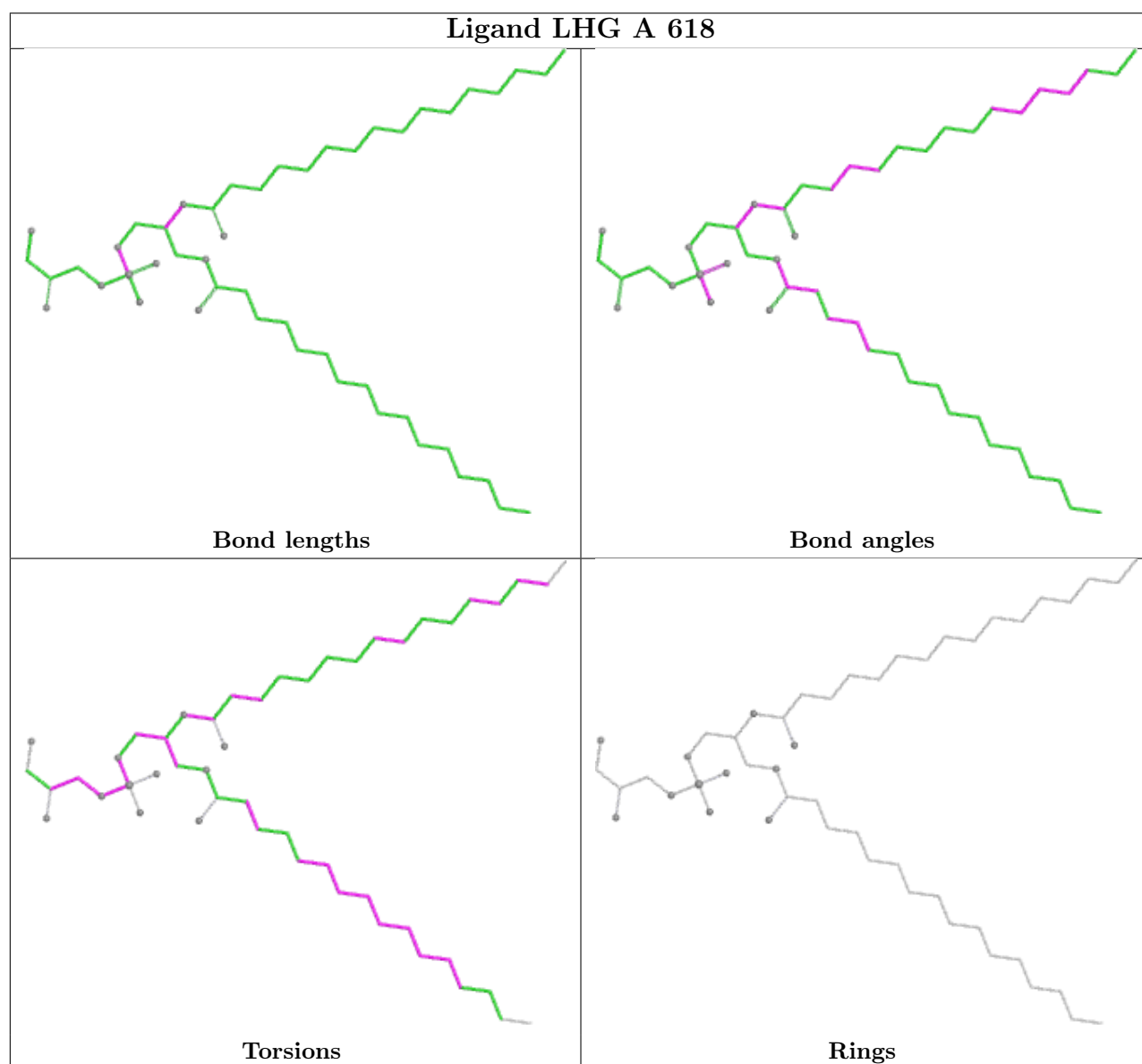
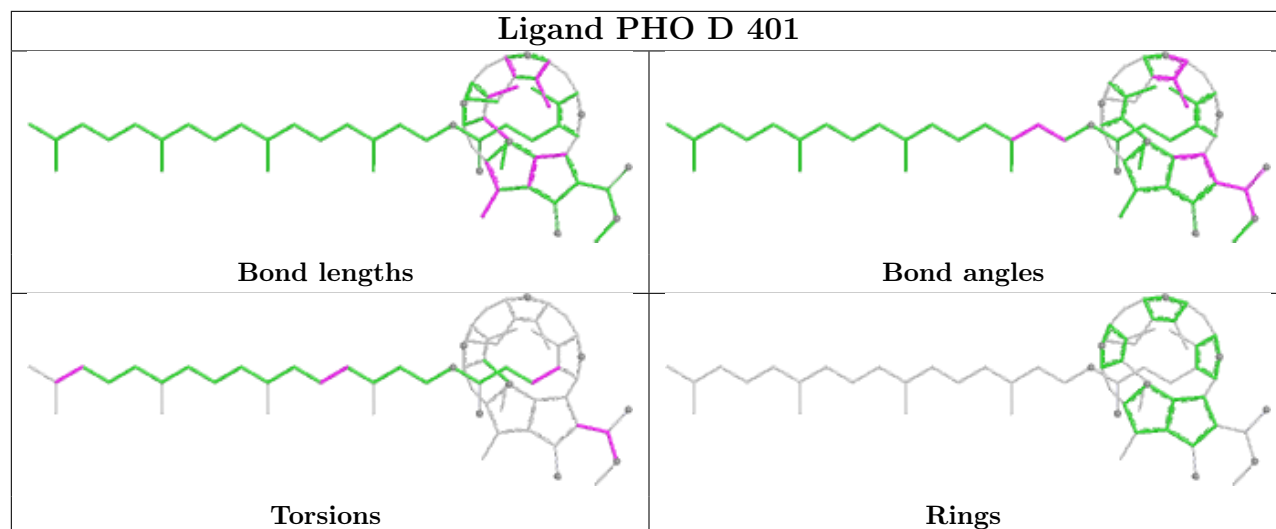


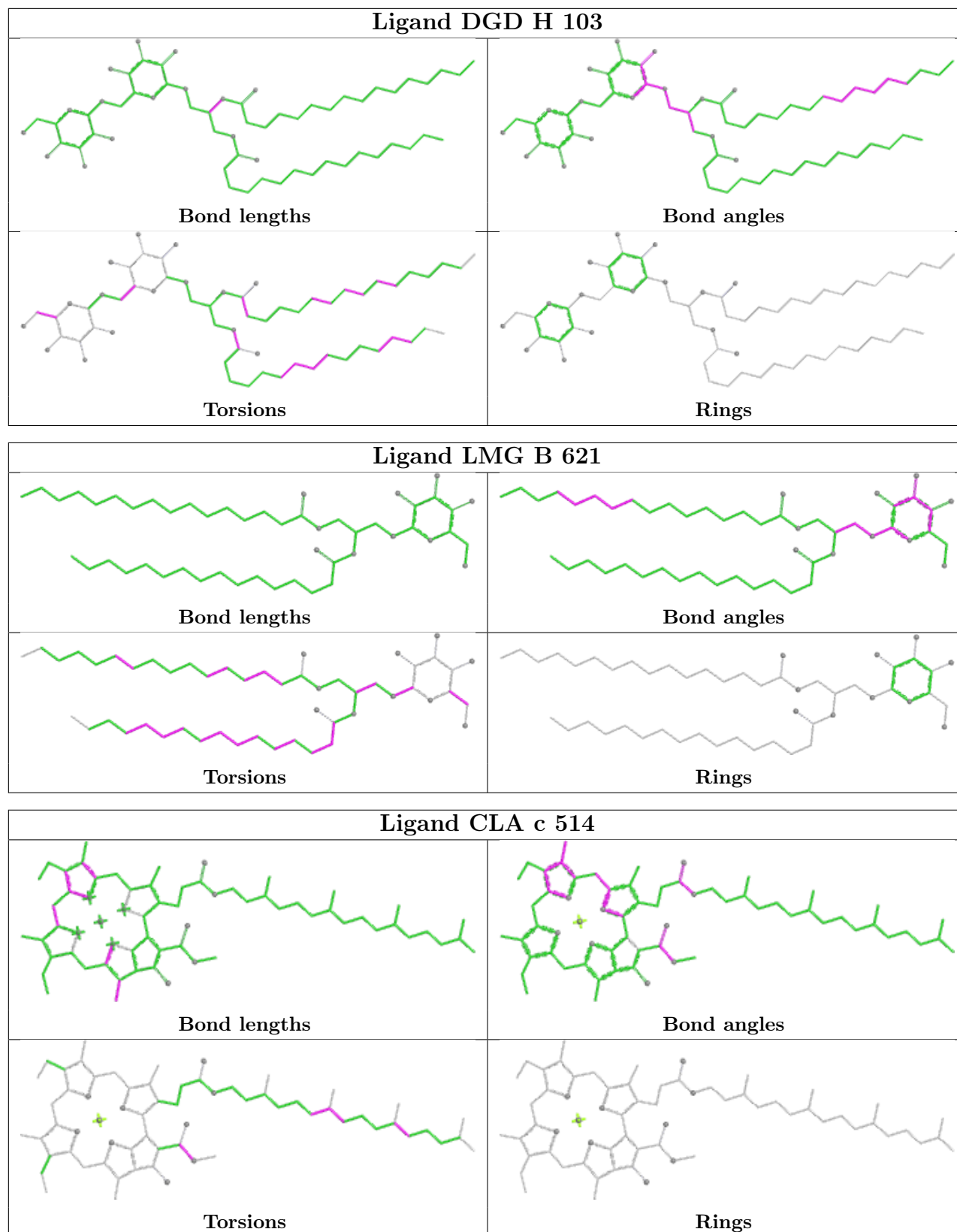
Ligand CLA c 505

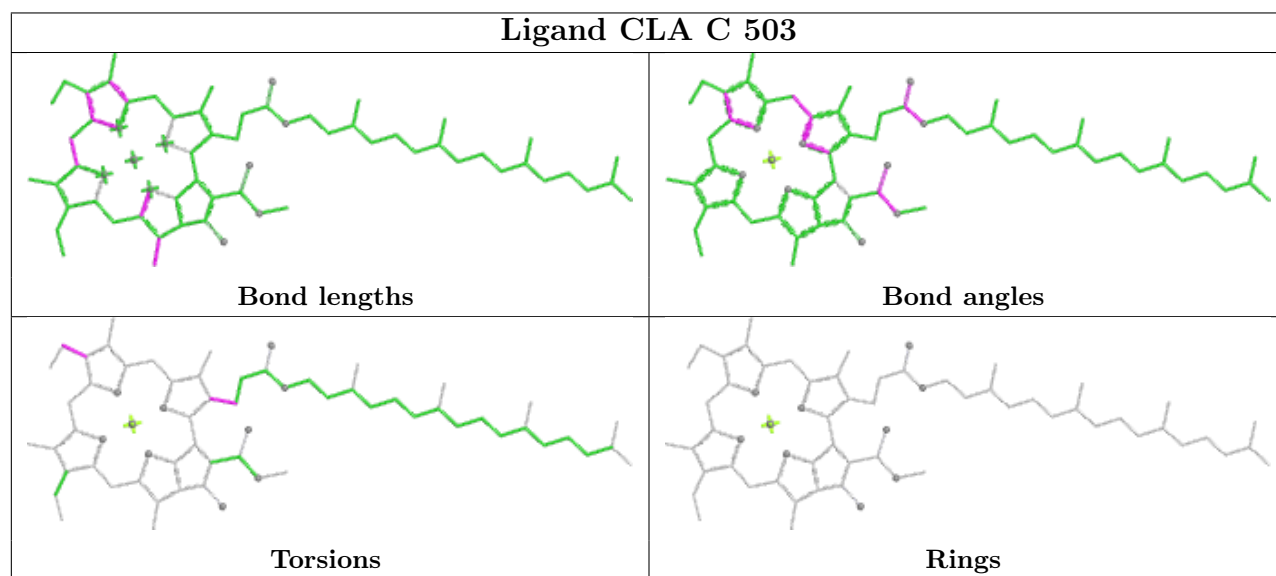
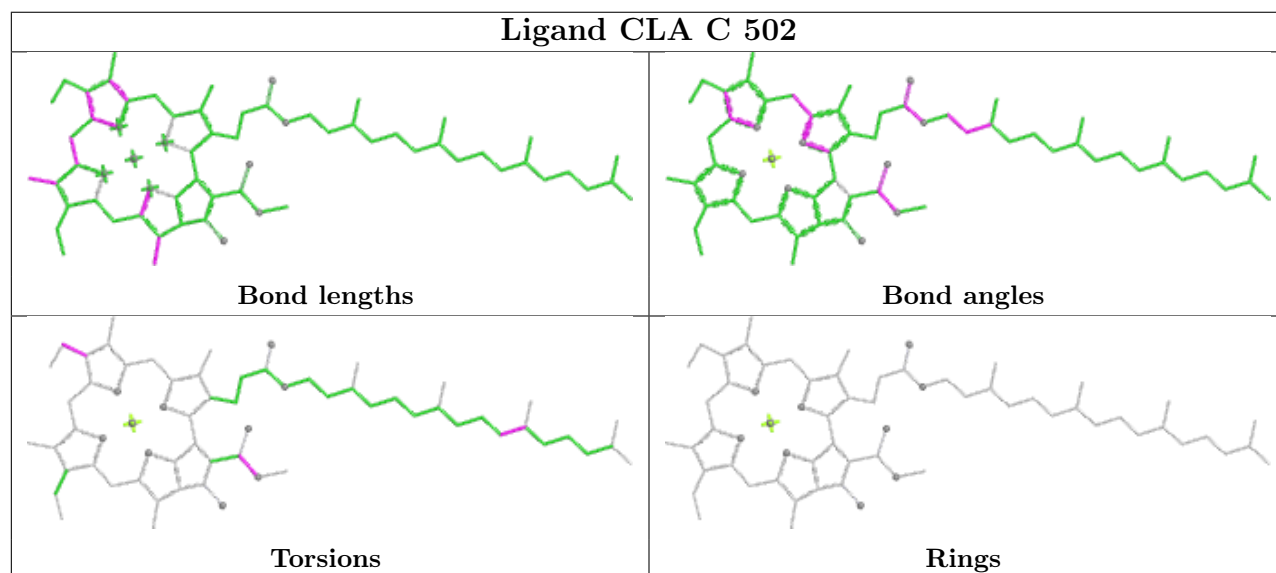
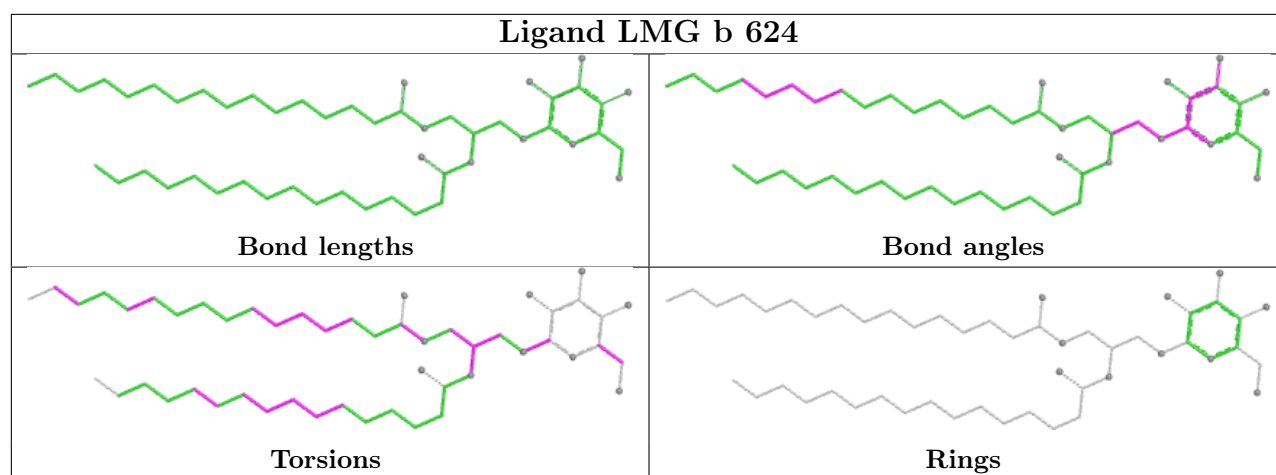


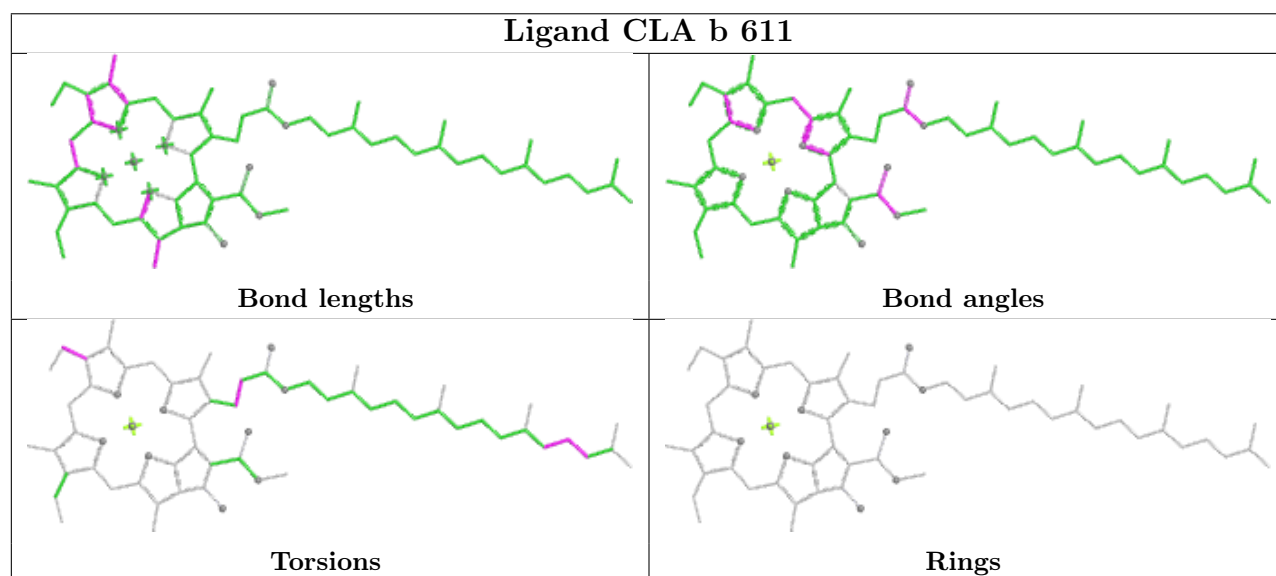
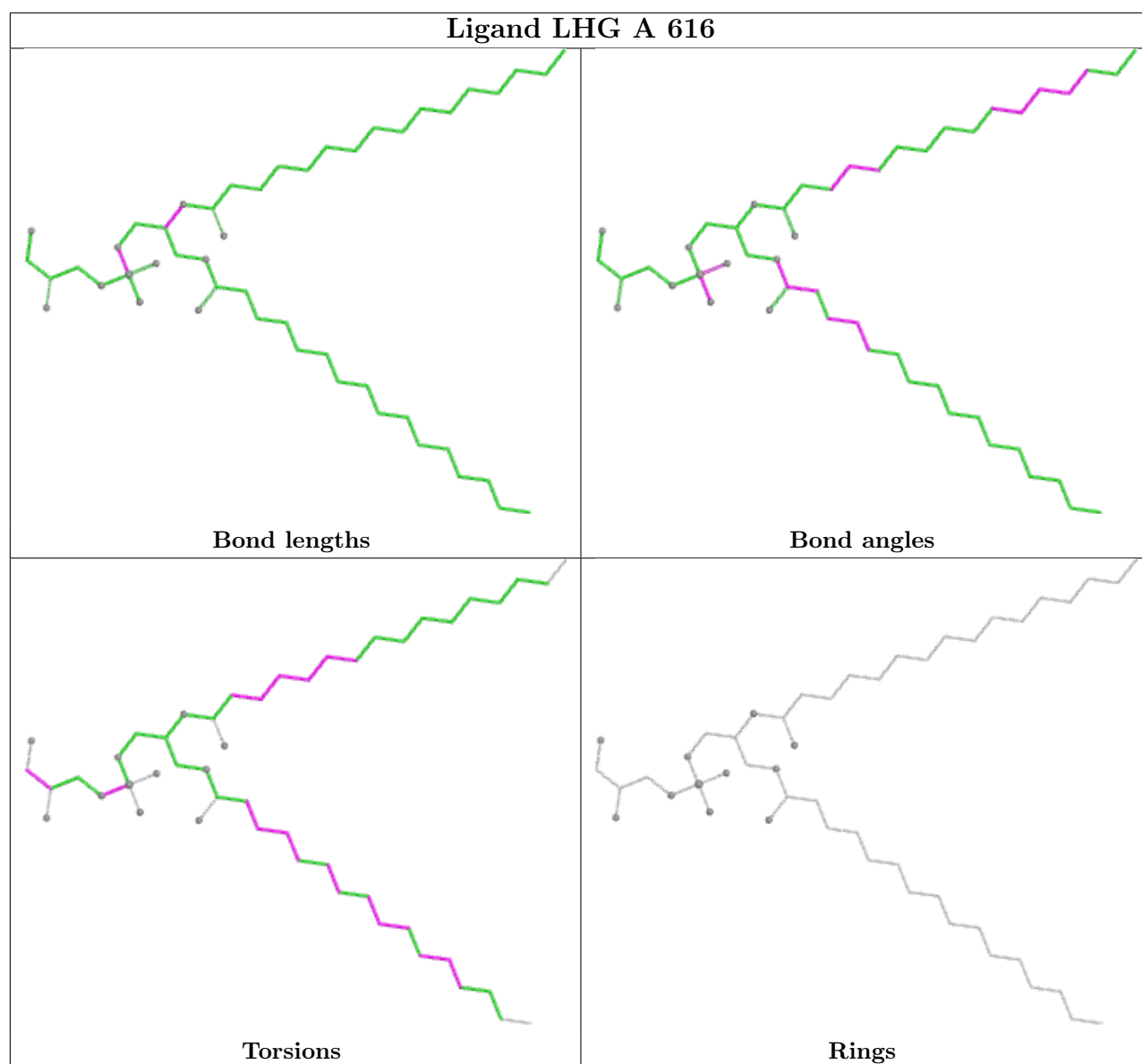
Ligand CLA a 606

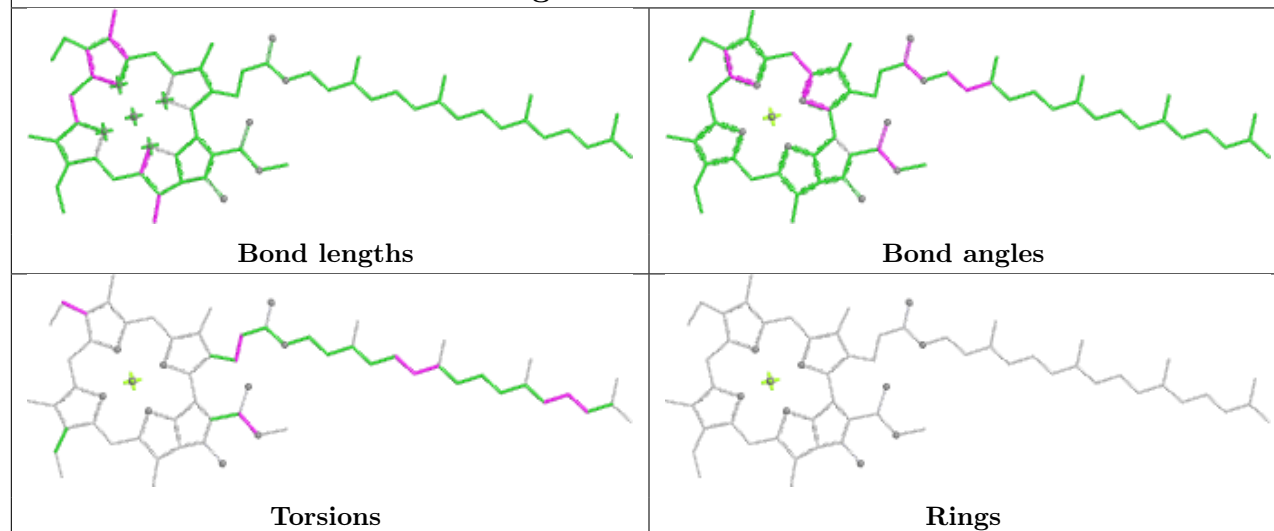
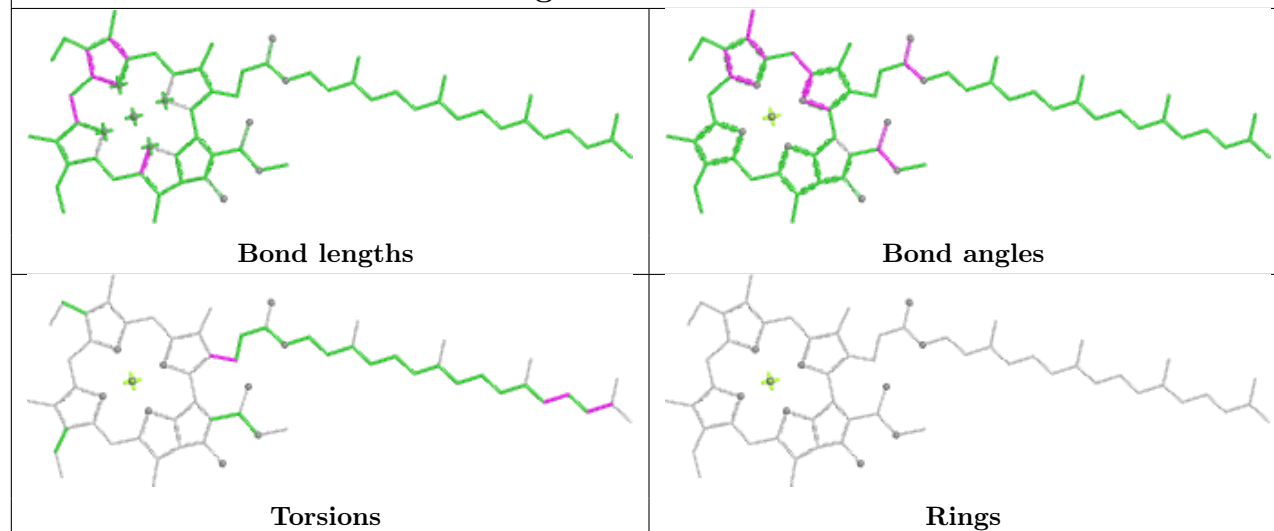
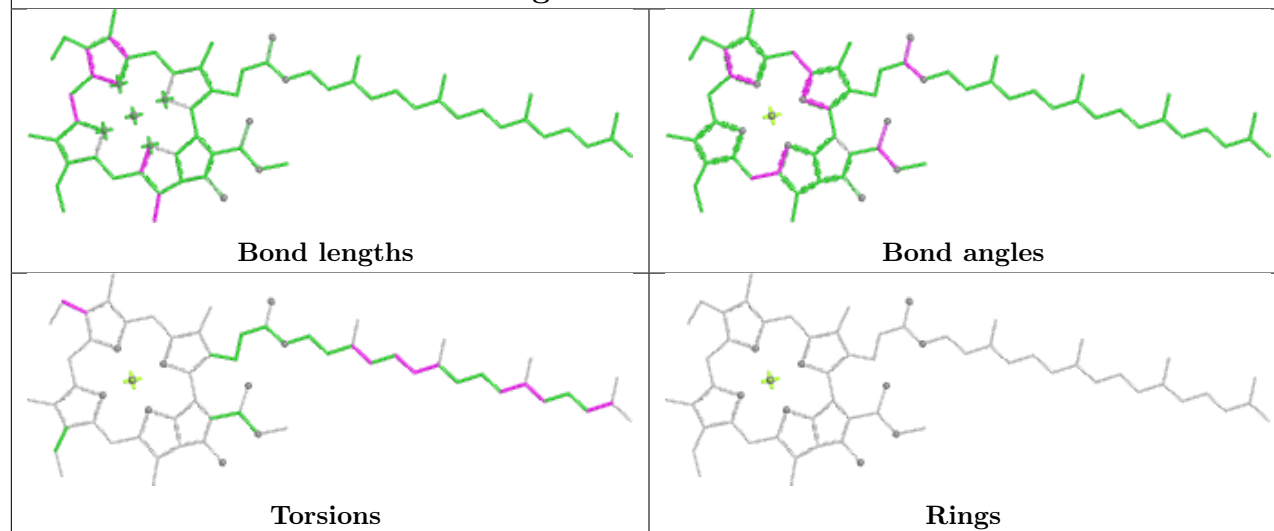




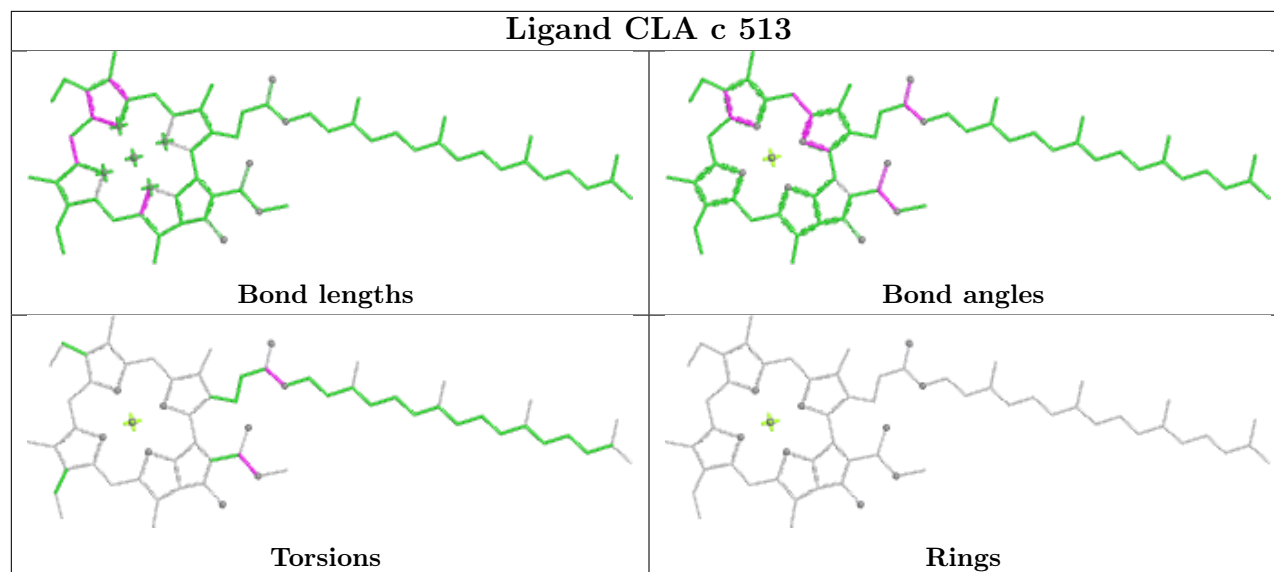




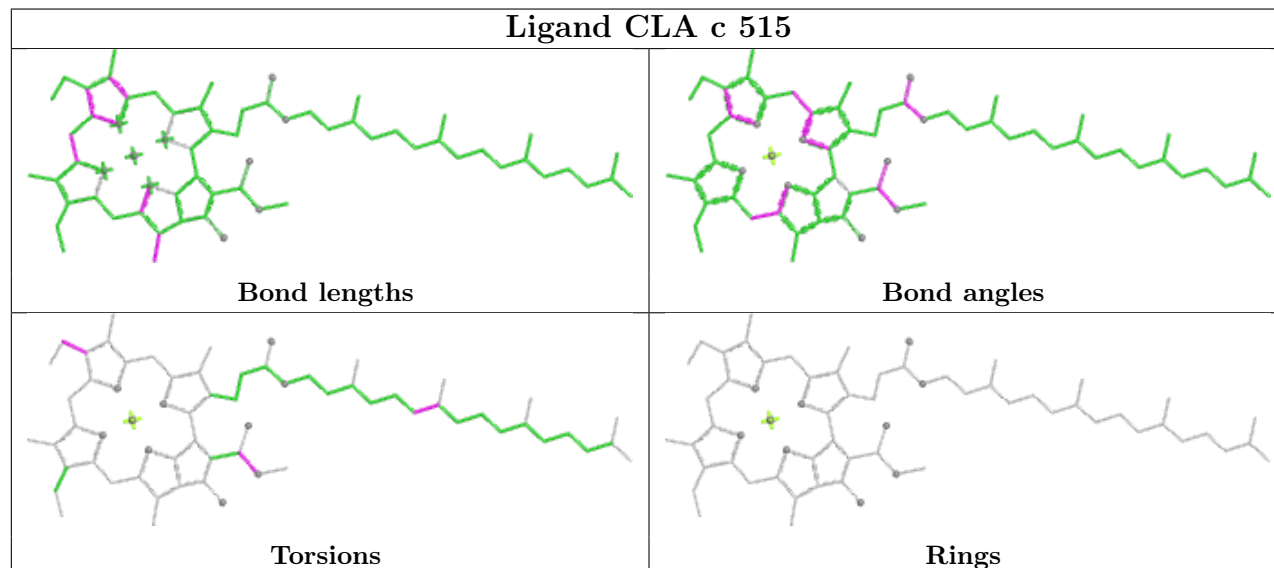


Ligand CLA B 603**Ligand CLA d 404****Ligand CLA B 602**

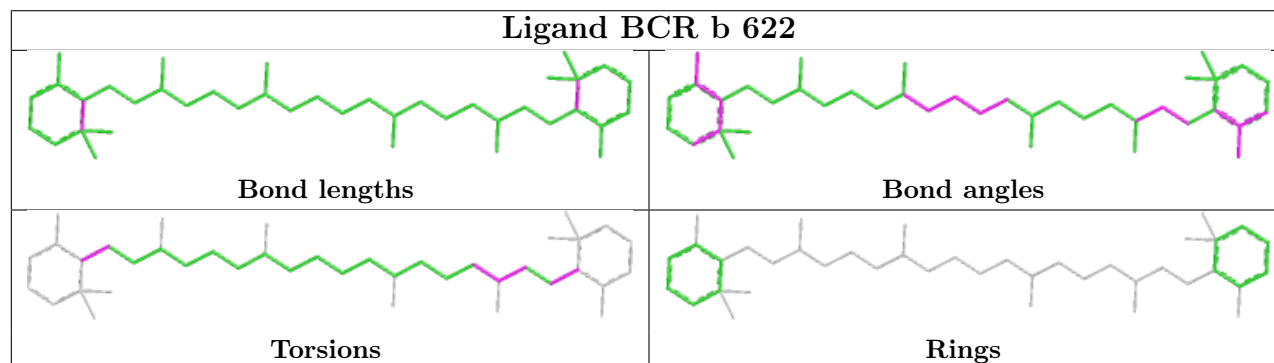
Ligand CLA c 513

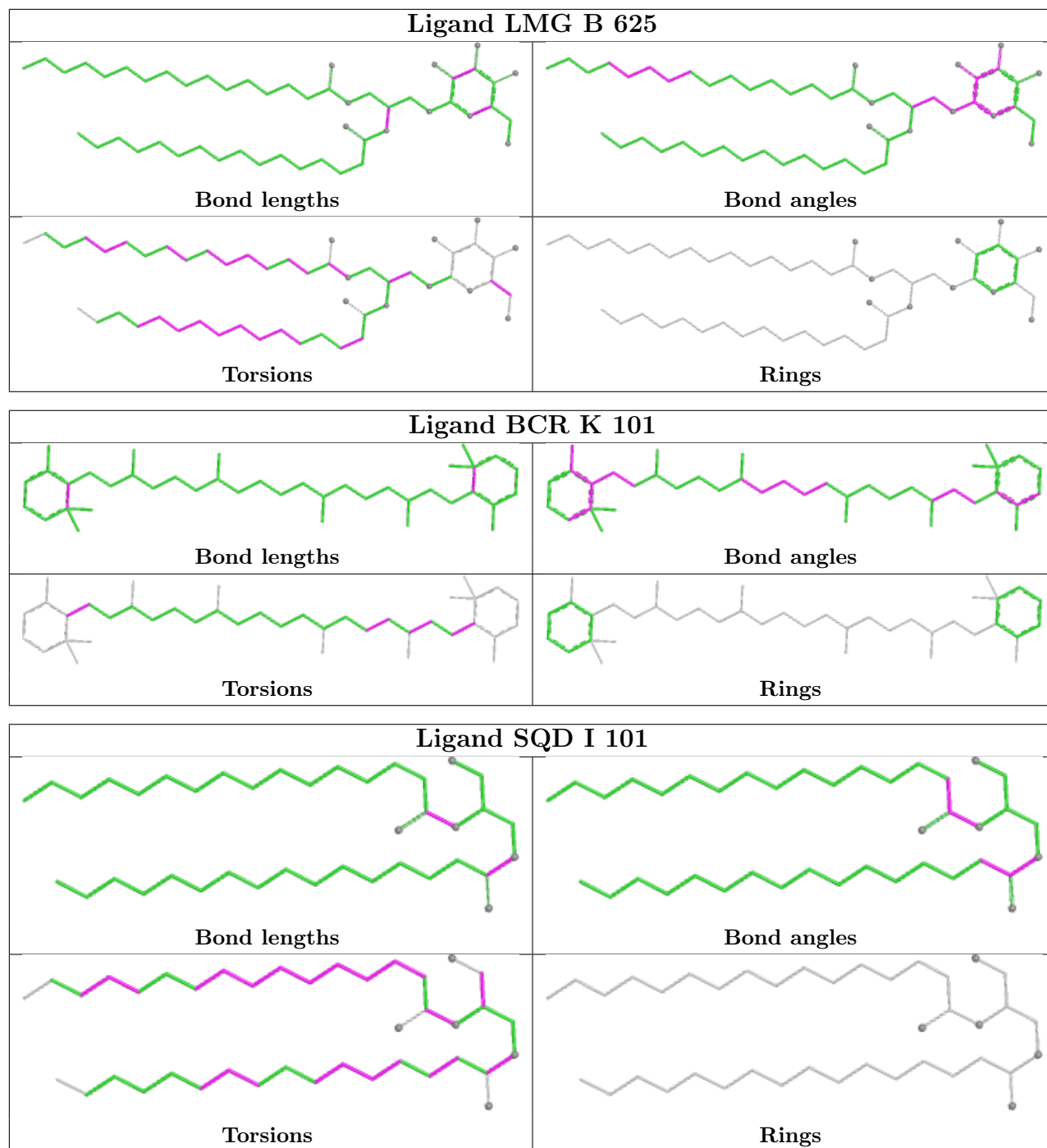


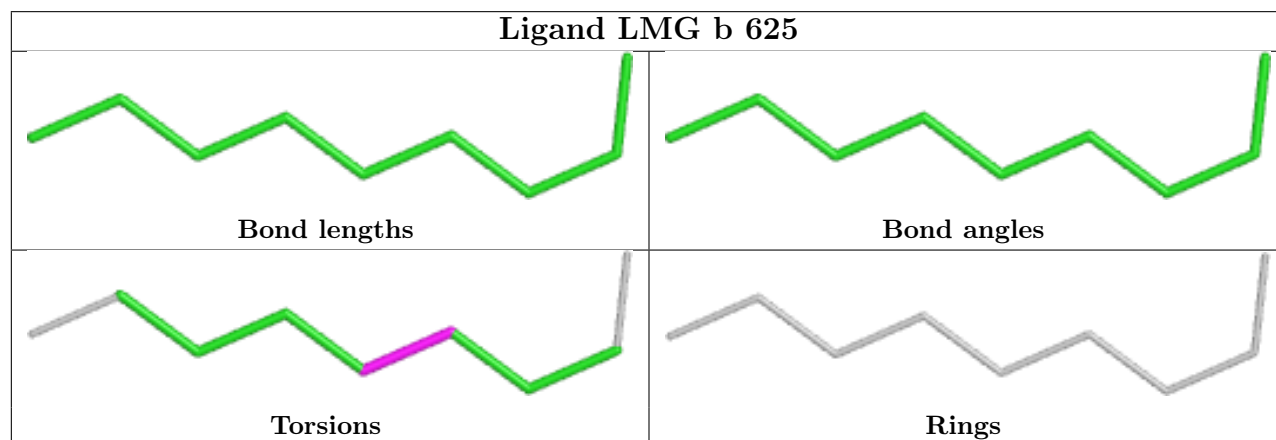
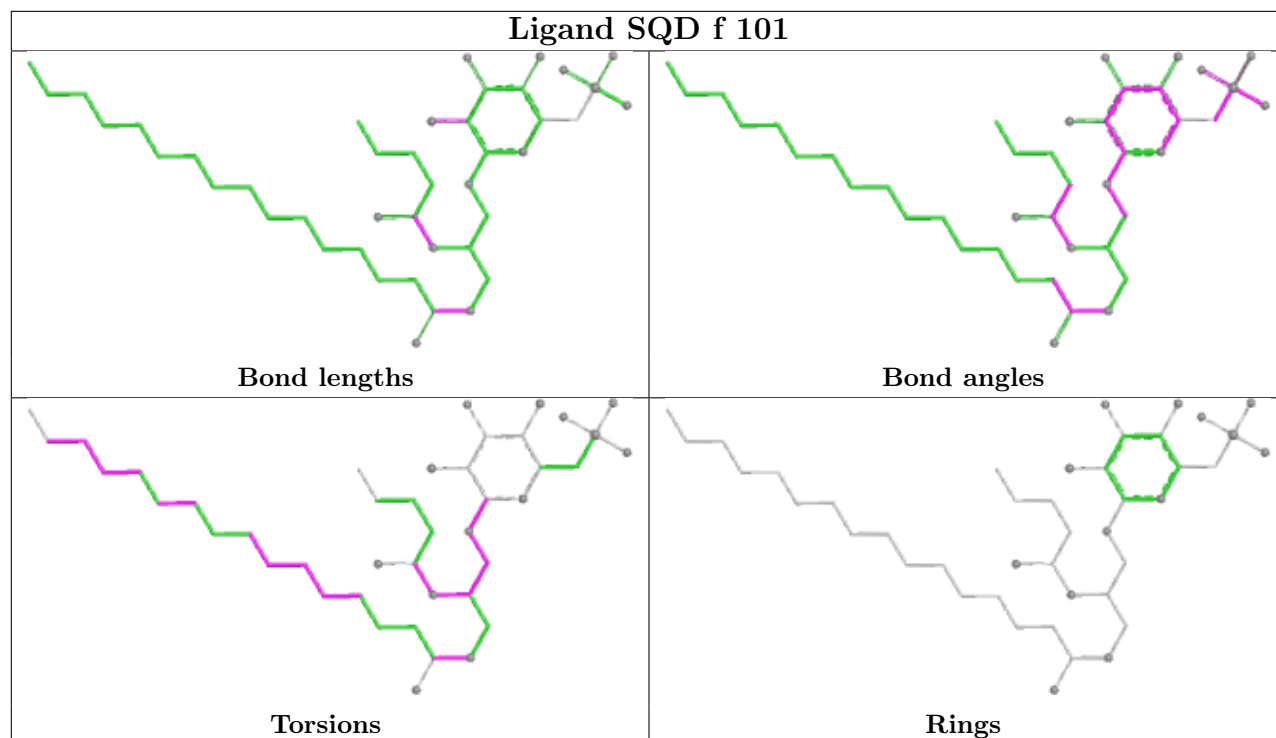
Ligand CLA c 515



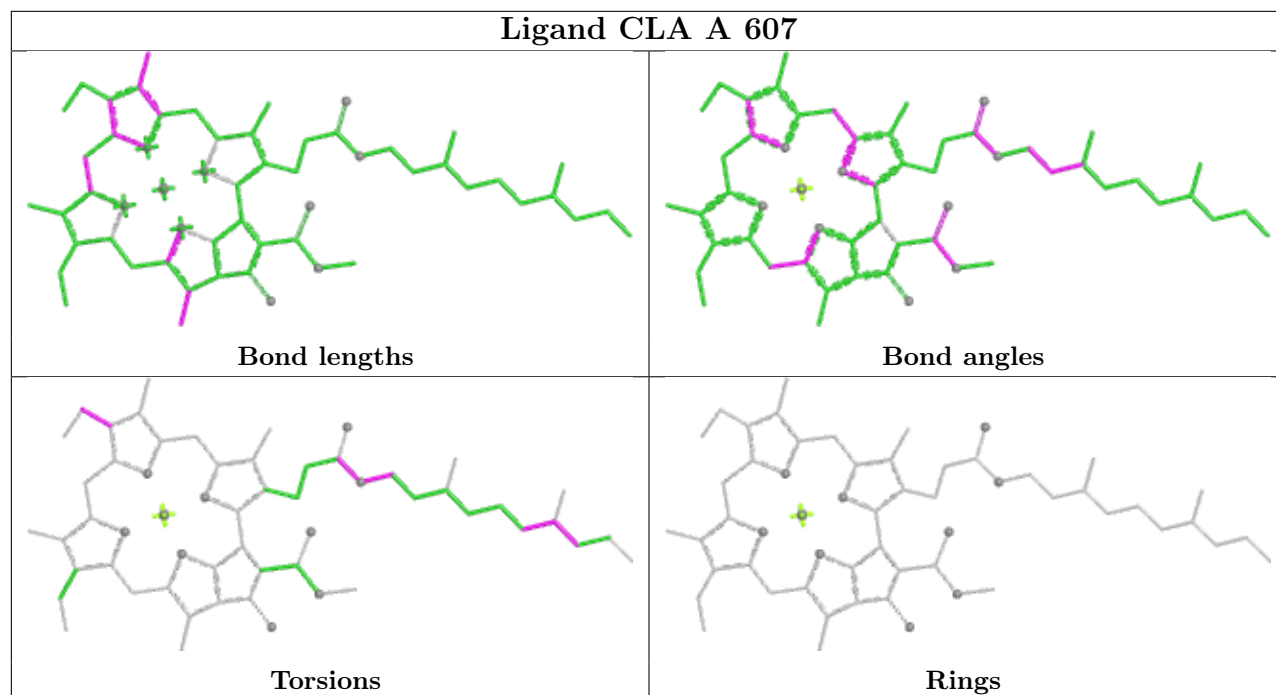
Ligand BCR b 622



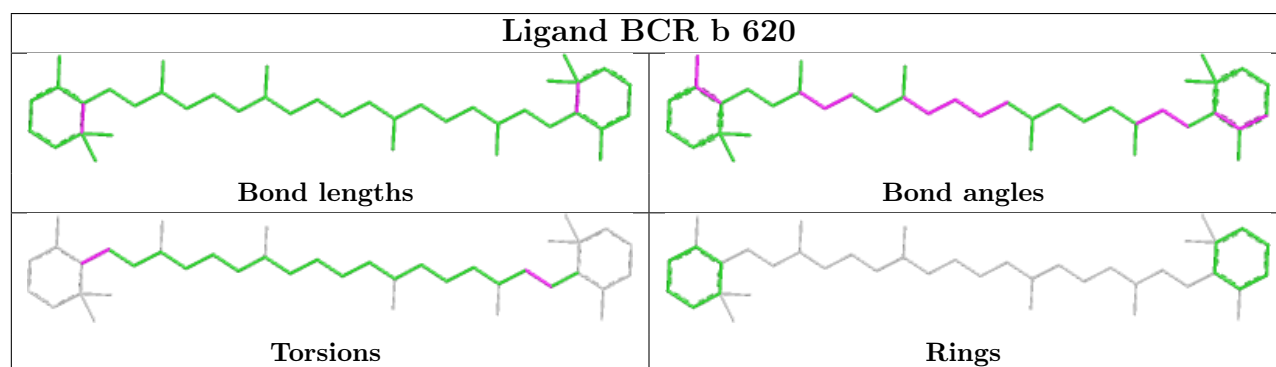


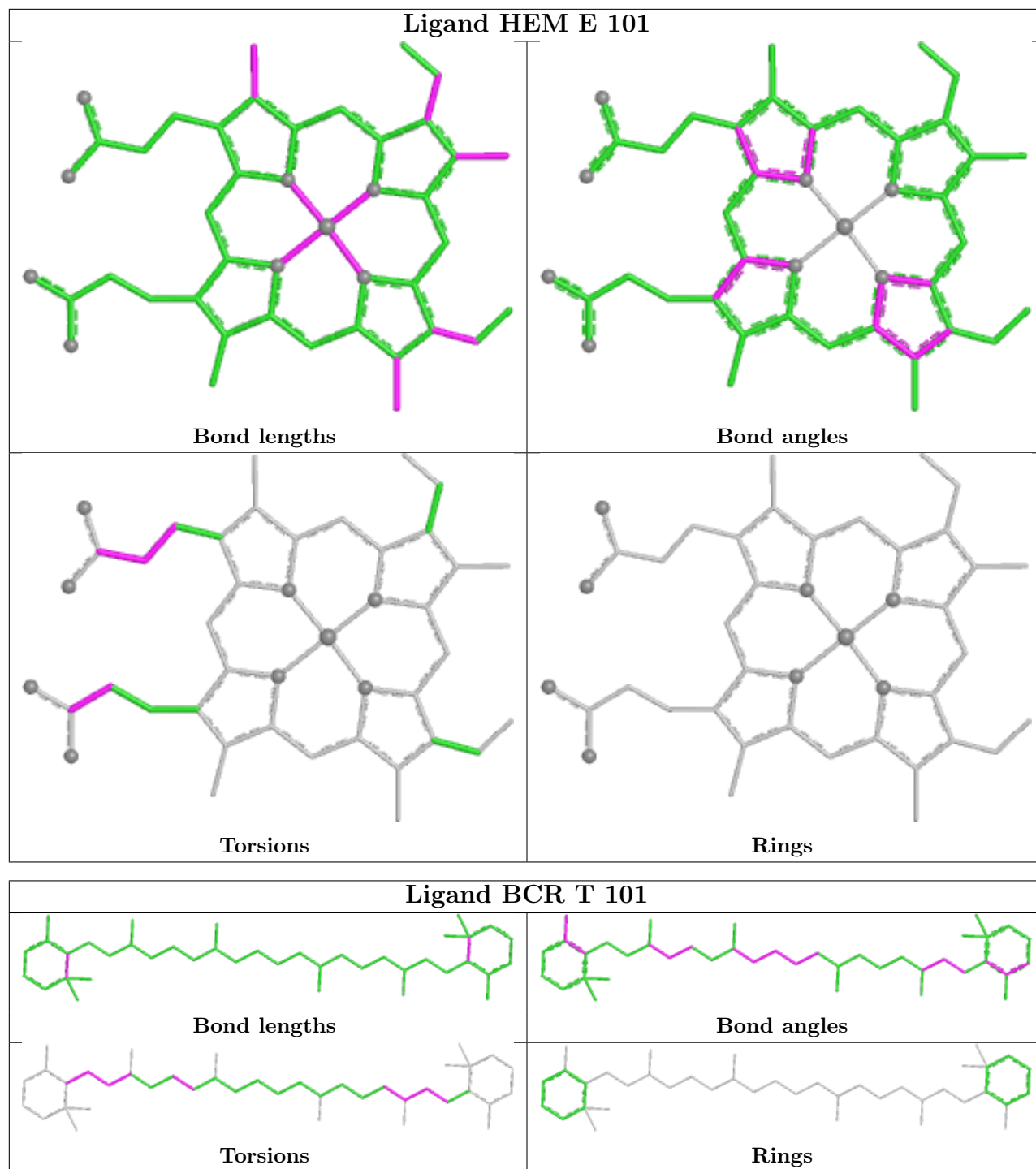


Ligand CLA A 607

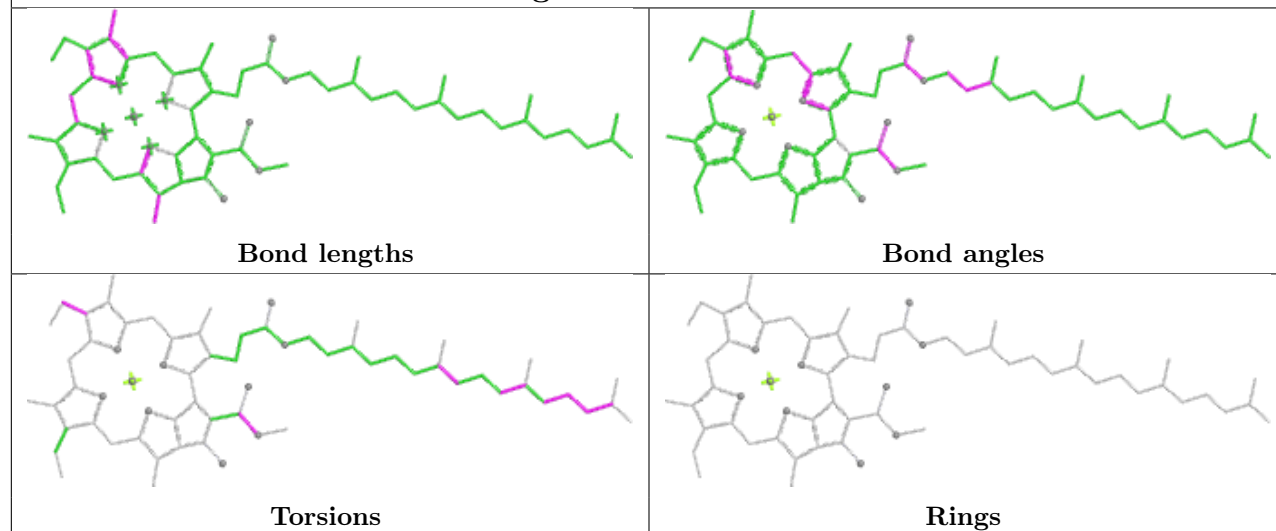


Ligand BCR b 620

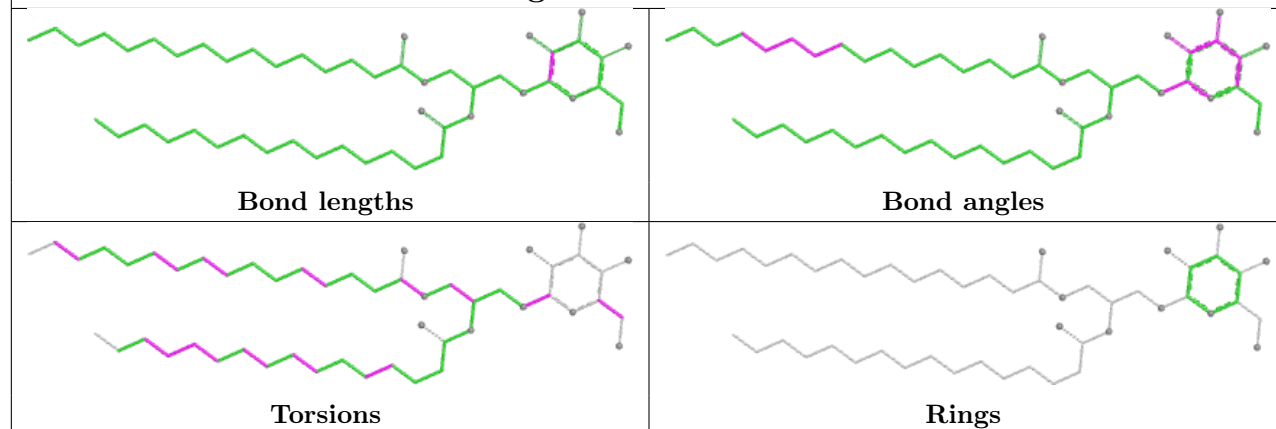




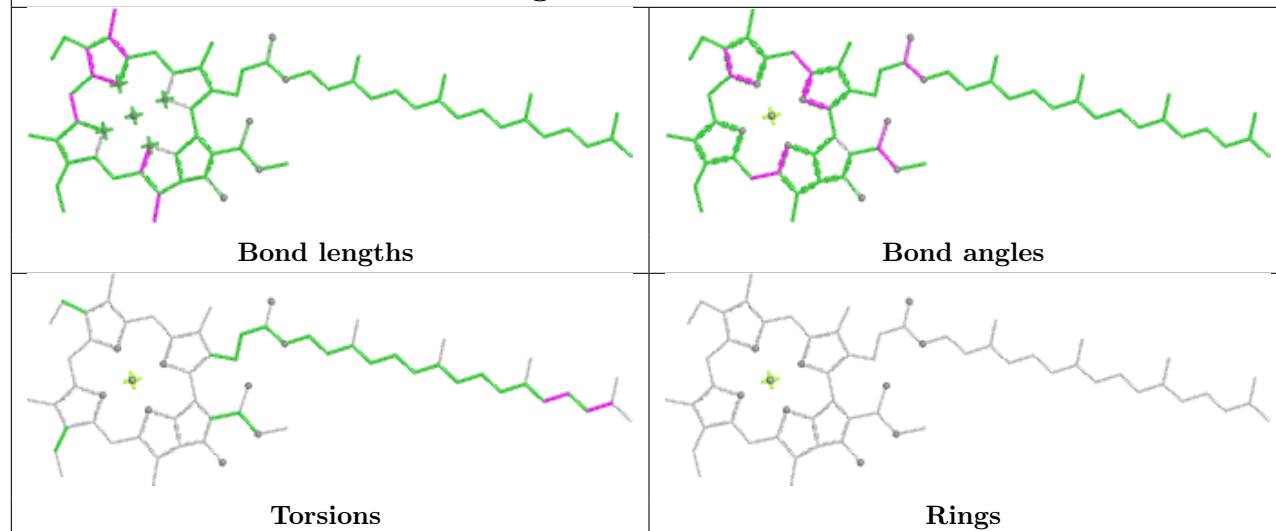
Ligand CLA B 610

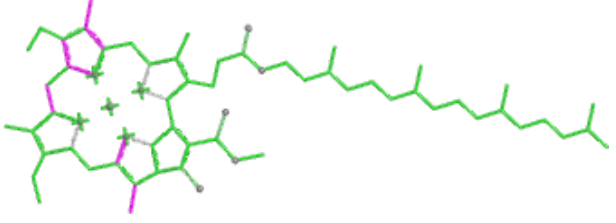
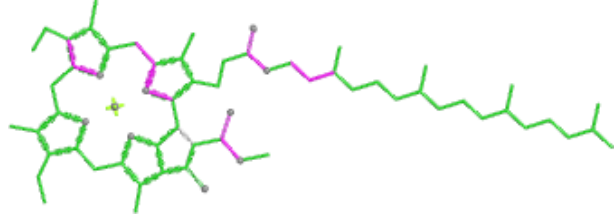
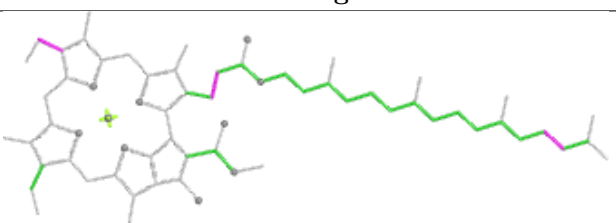
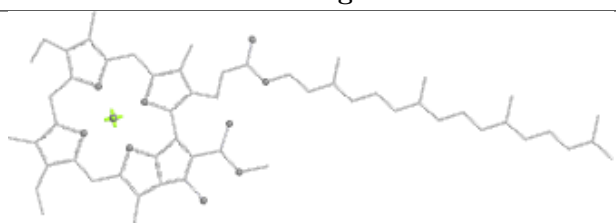
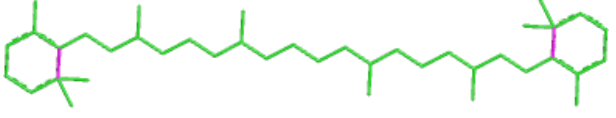
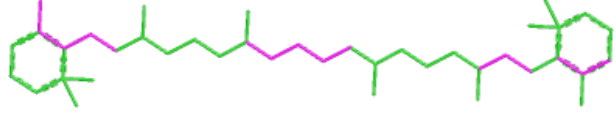
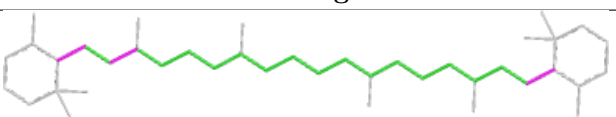
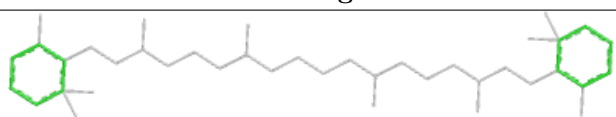
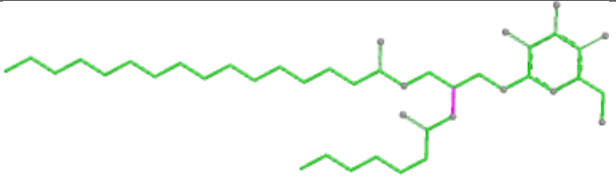
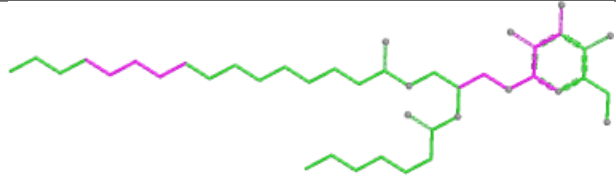
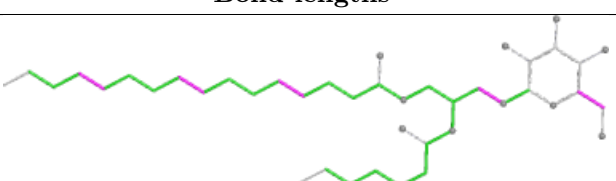
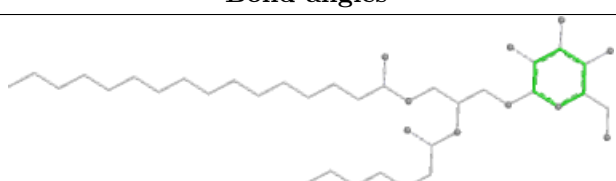


Ligand LMG C 520

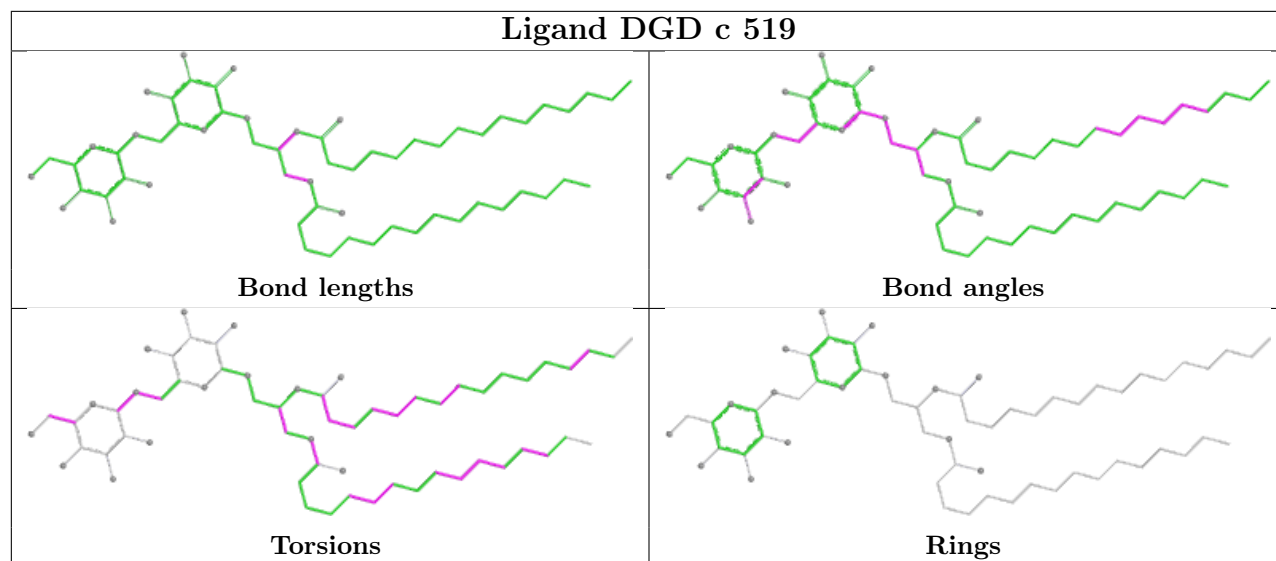


Ligand CLA D 403

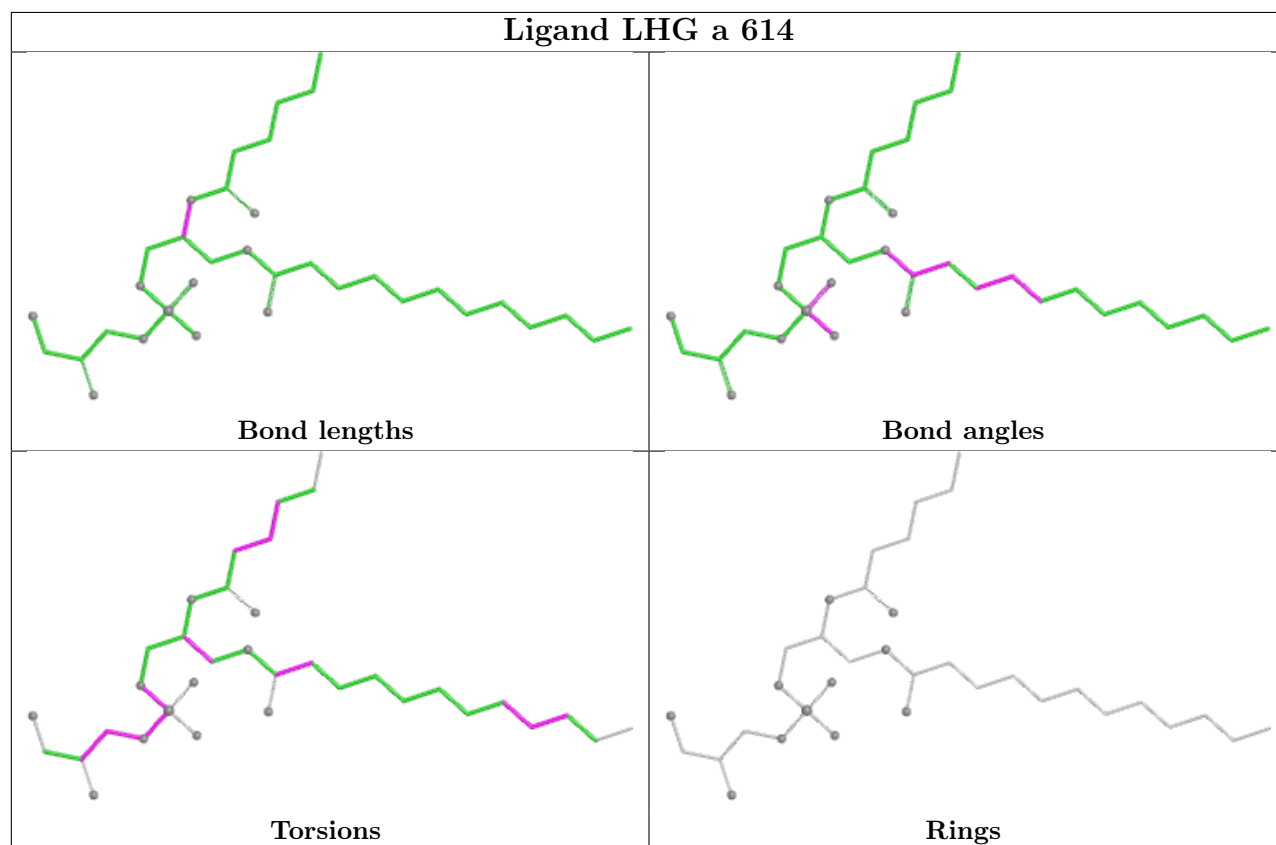


Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

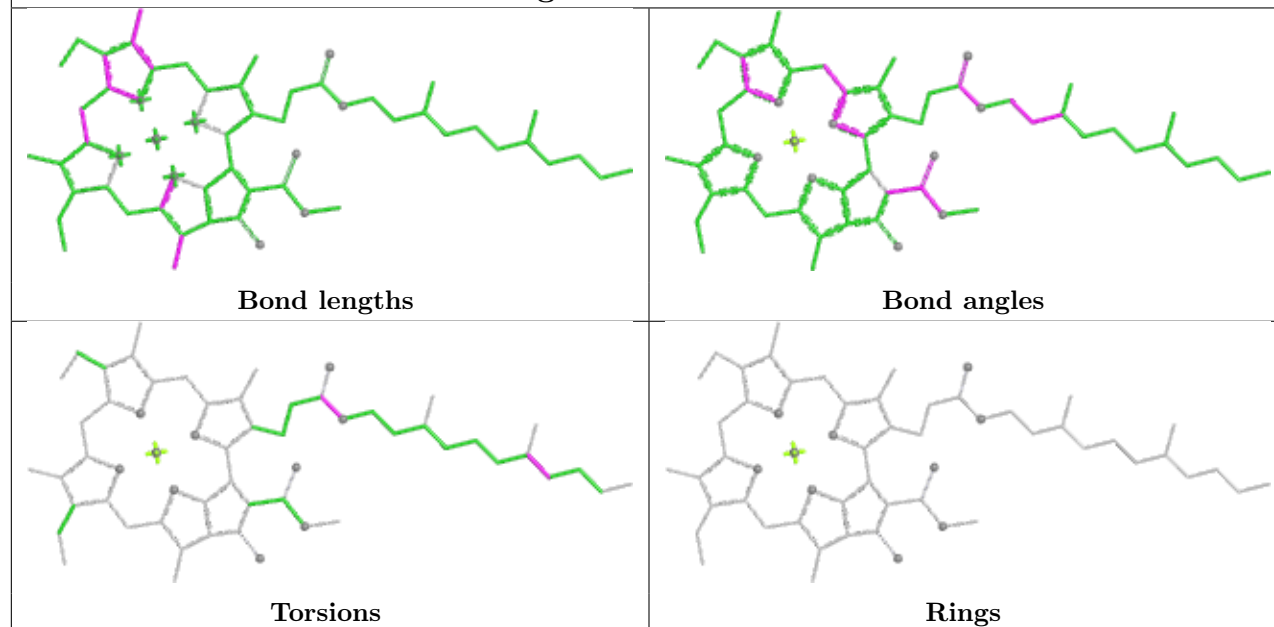
Ligand DGD c 519



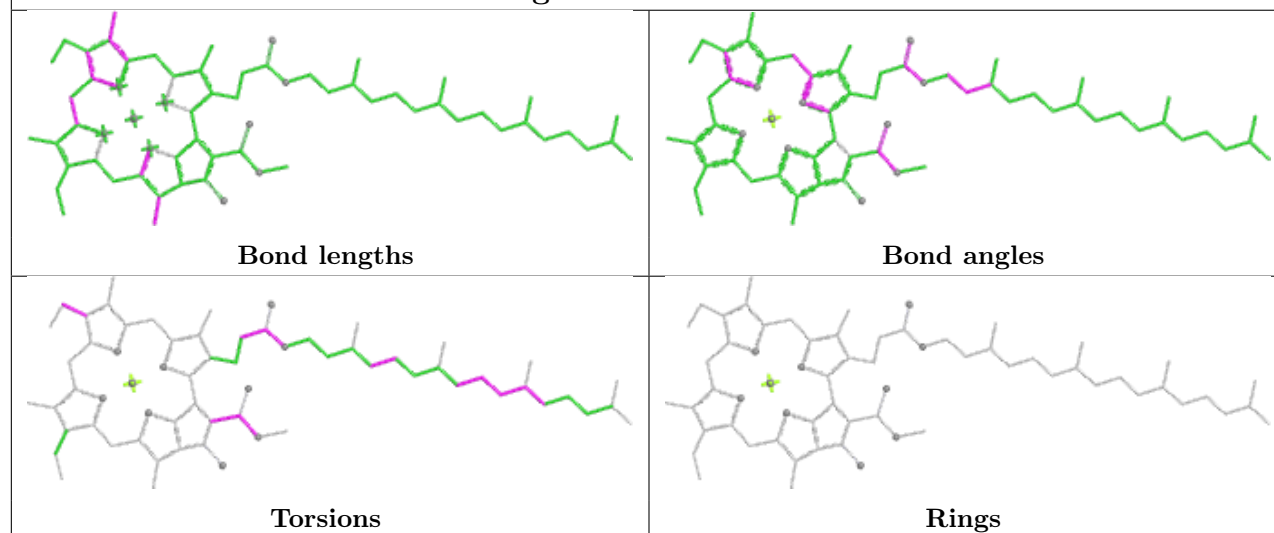
Ligand LHG a 614



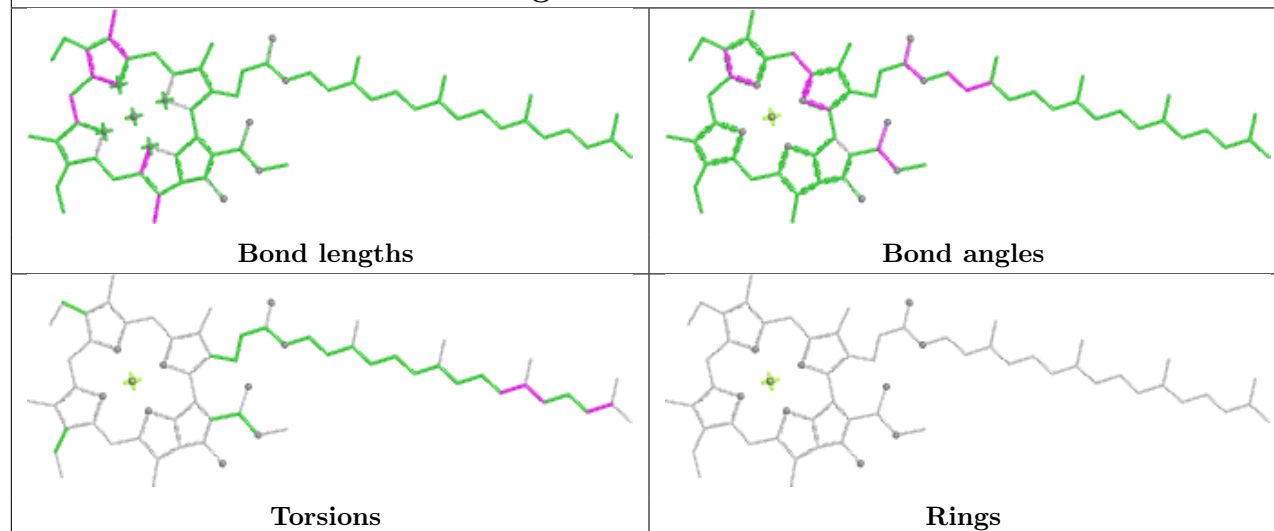
Ligand CLA c 510



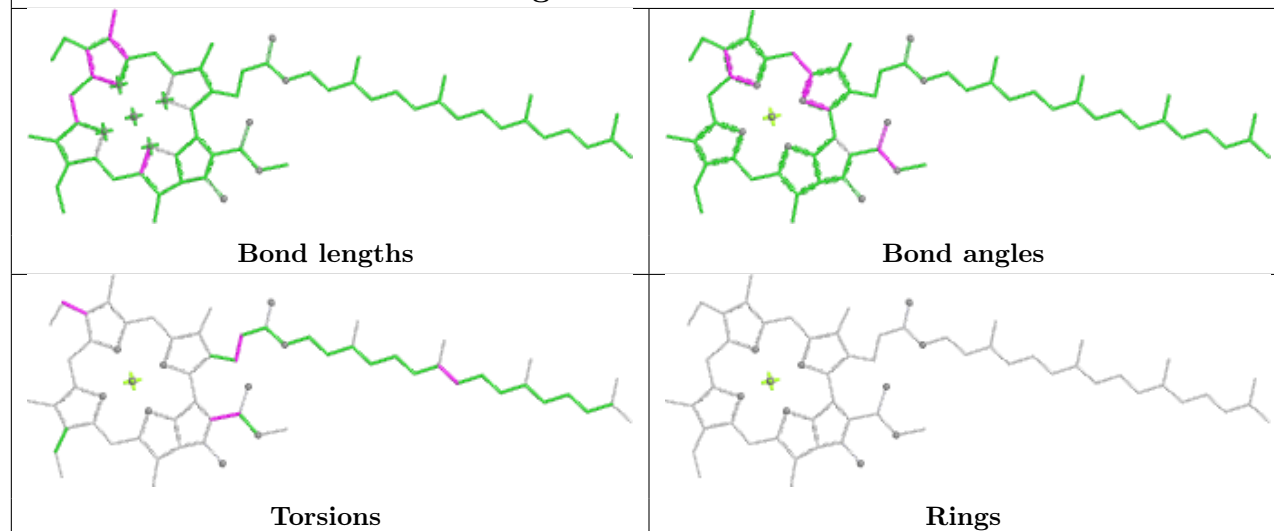
Ligand CLA B 601



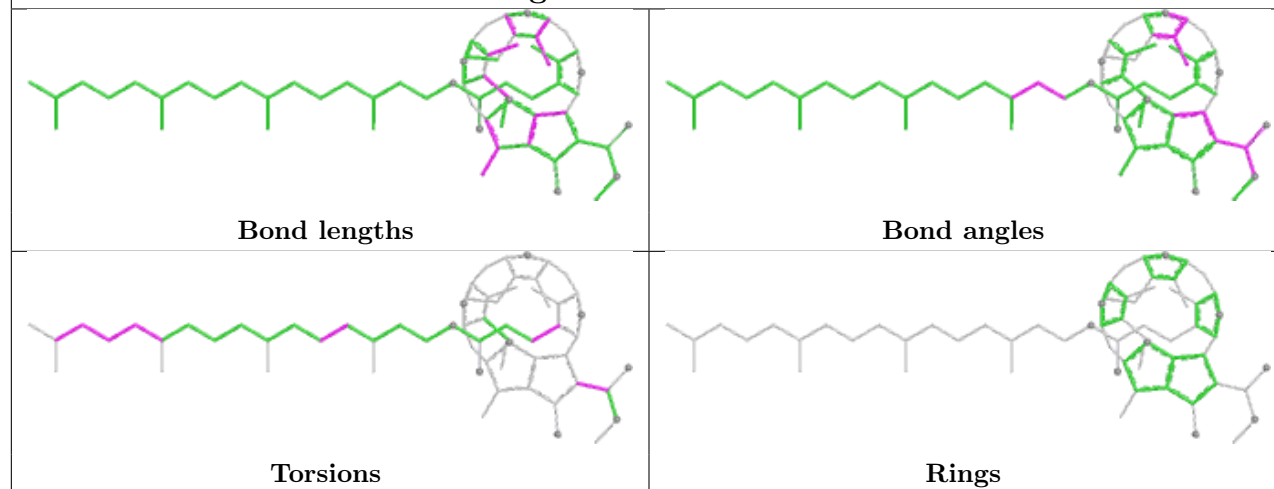
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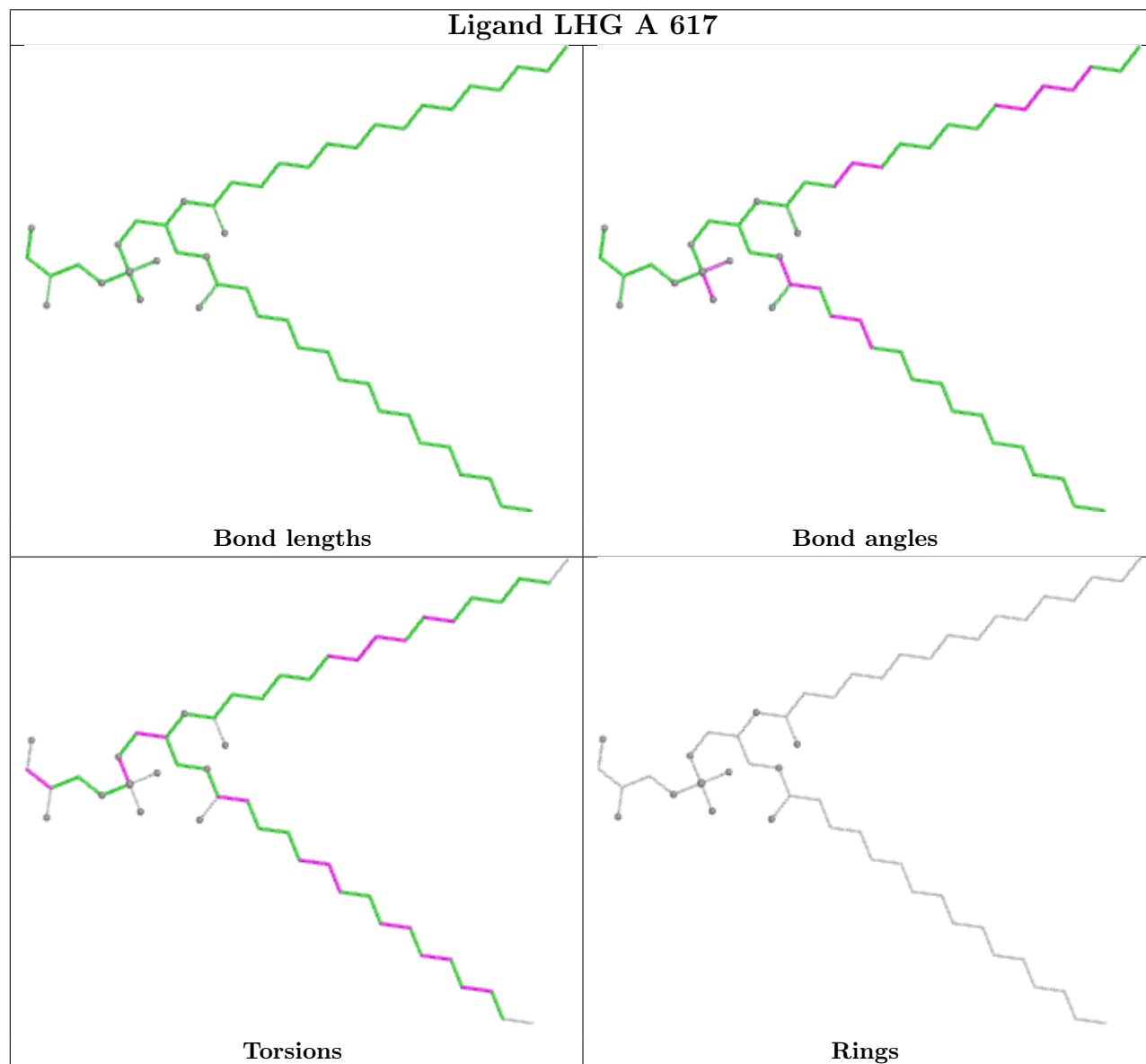
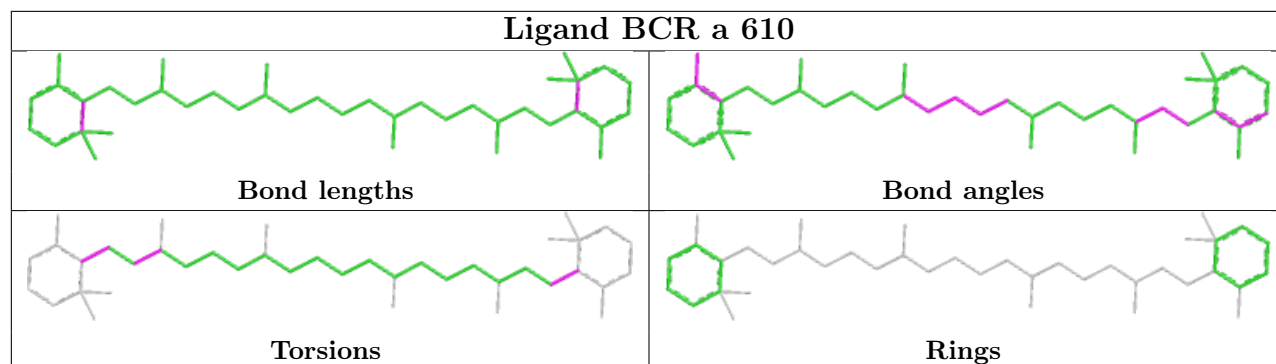


Ligand CLA C 507

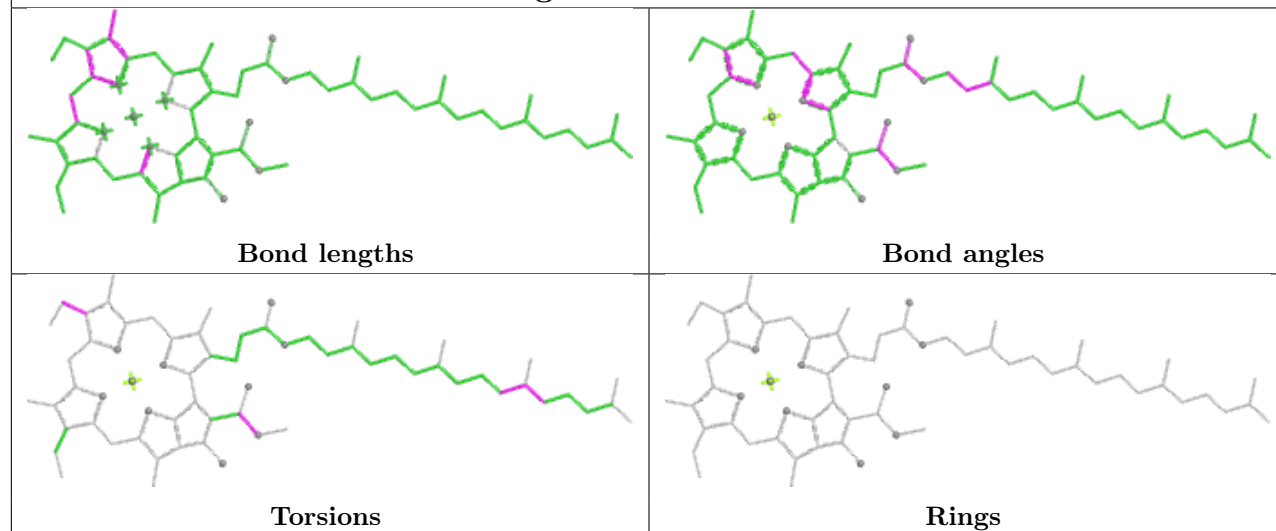


Ligand PHO A 608

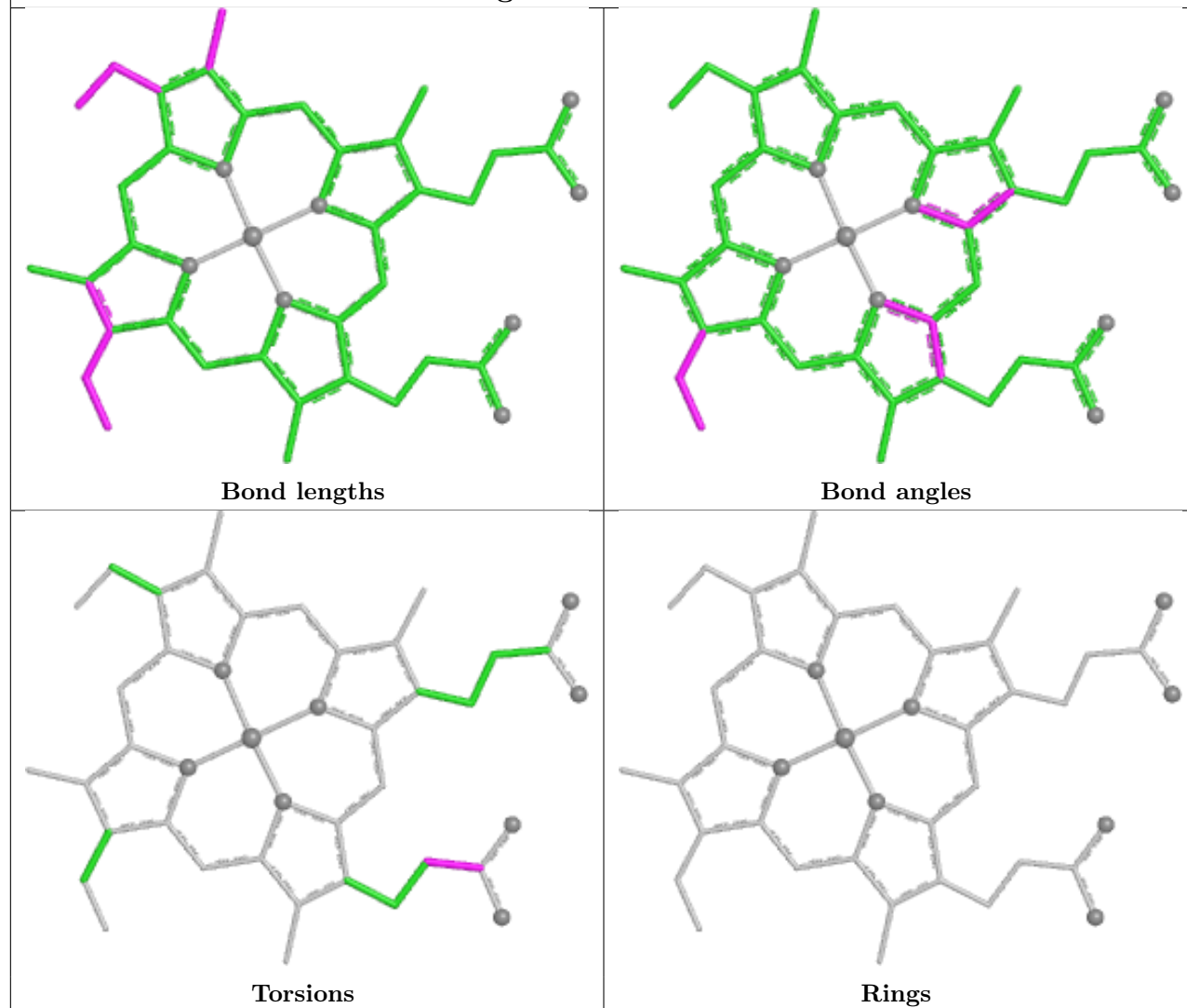


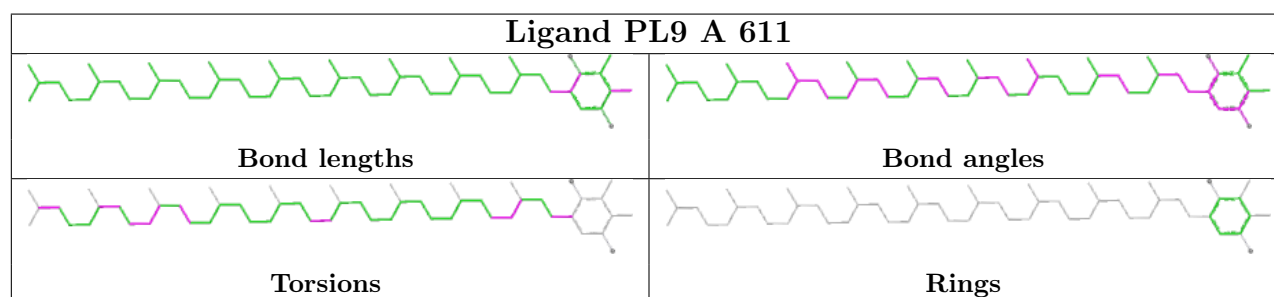
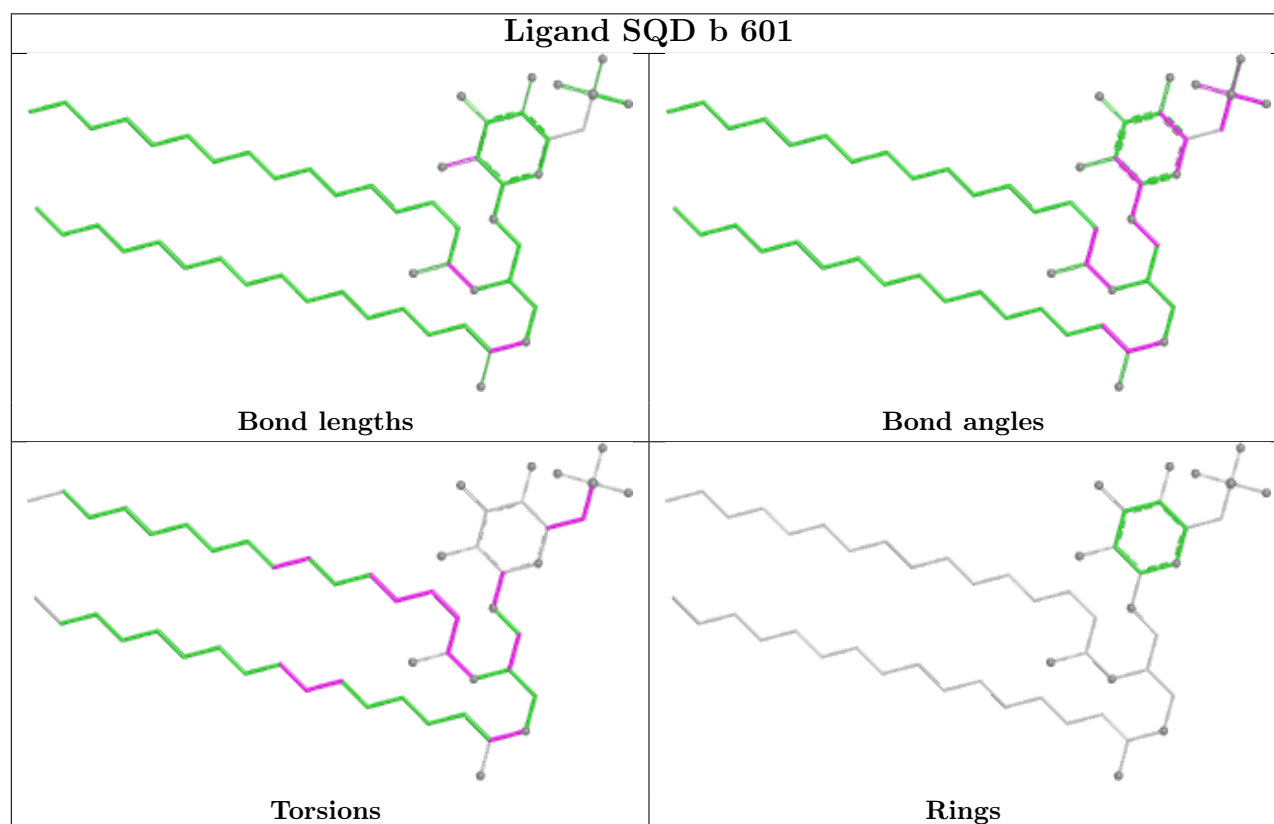
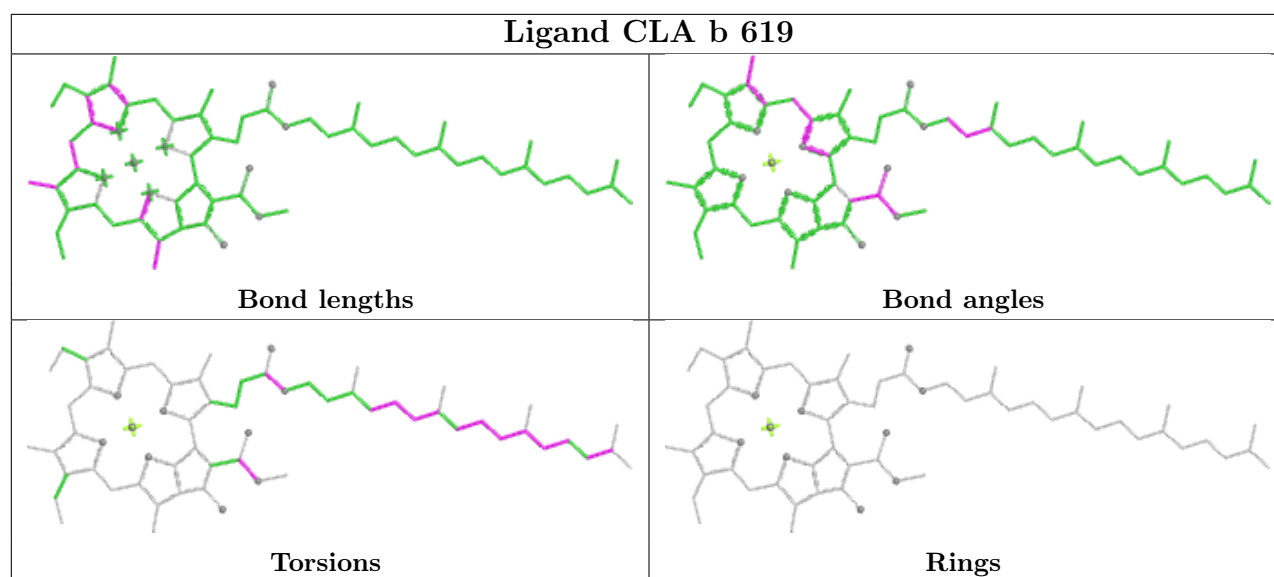


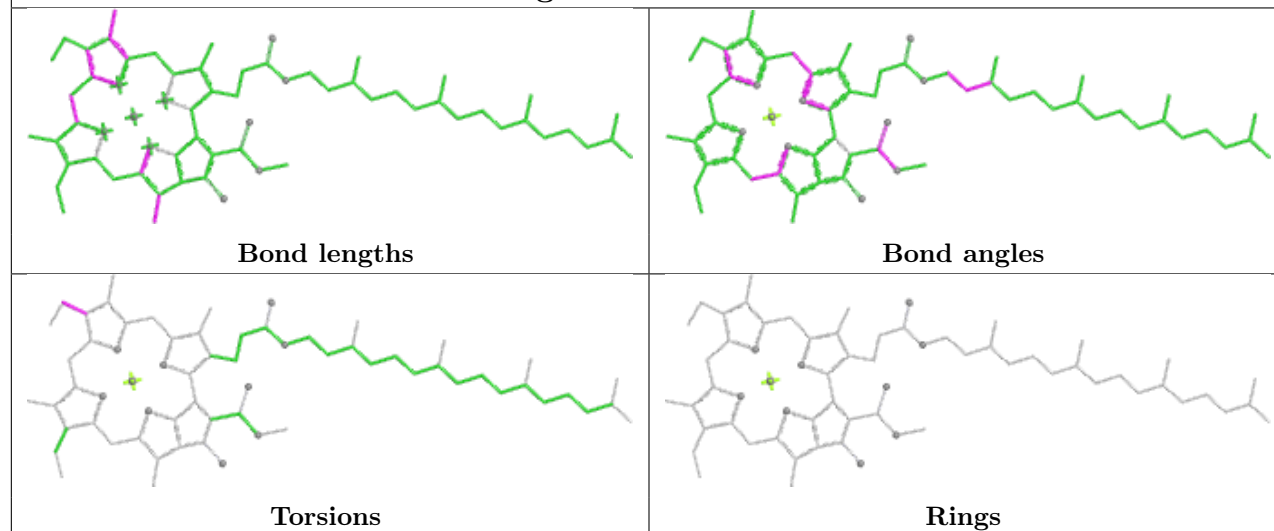
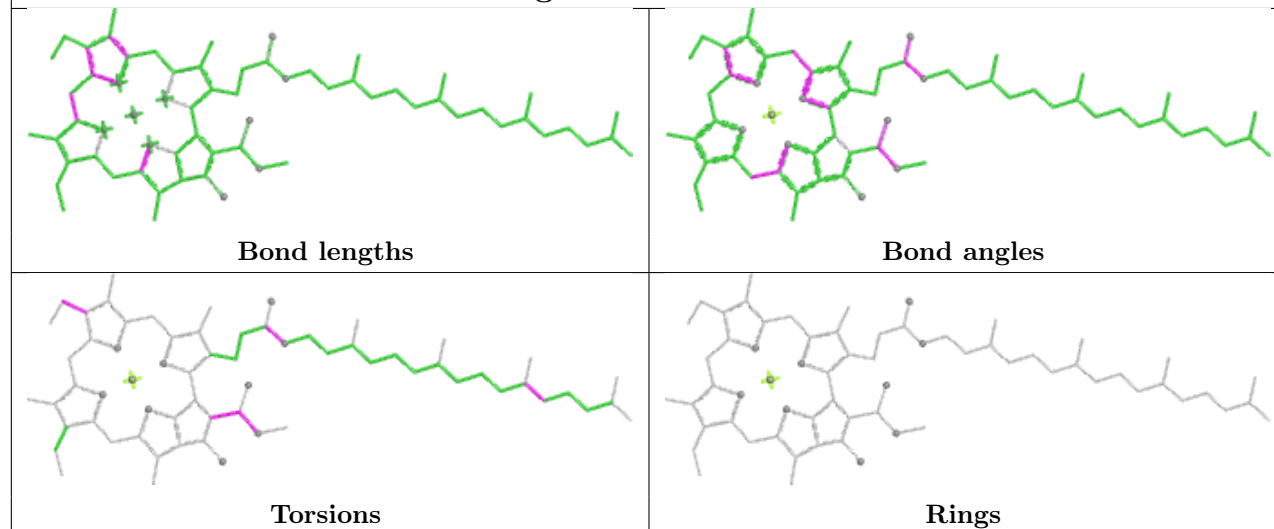
Ligand CLA b 614

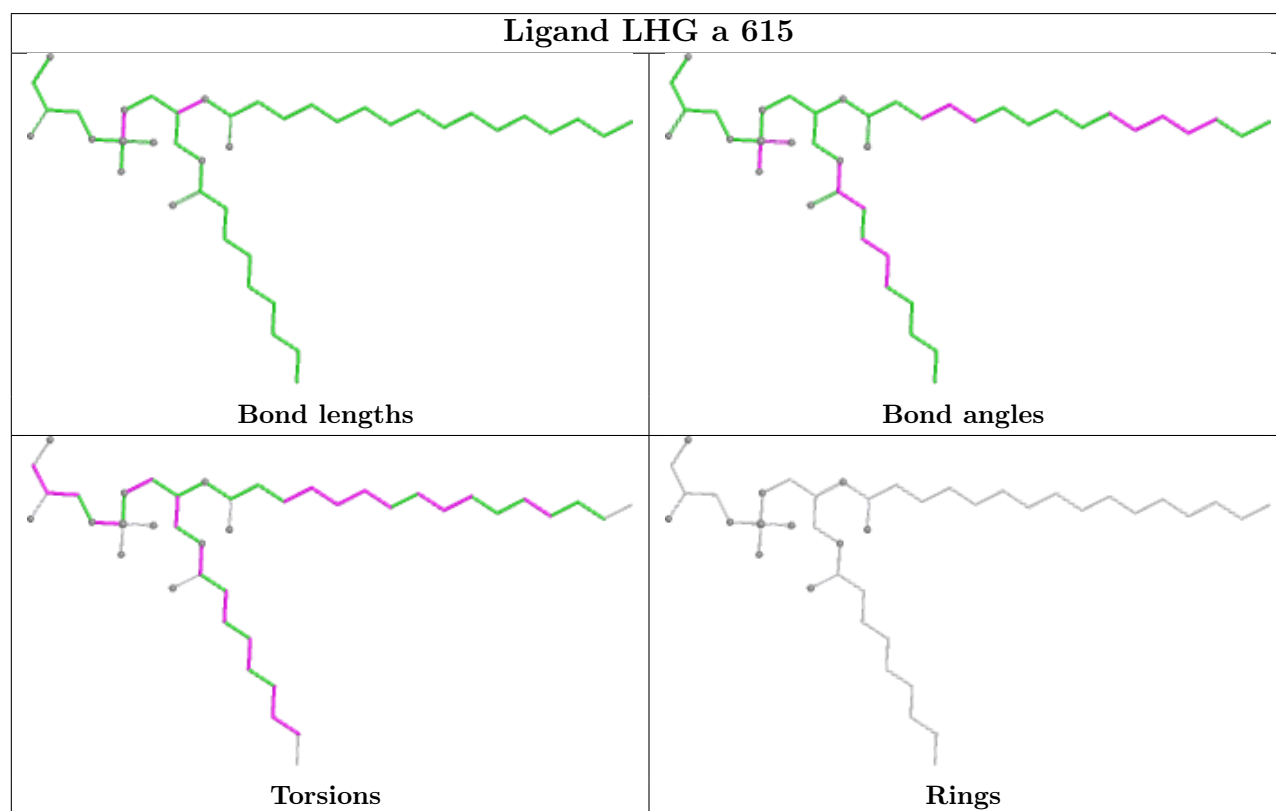
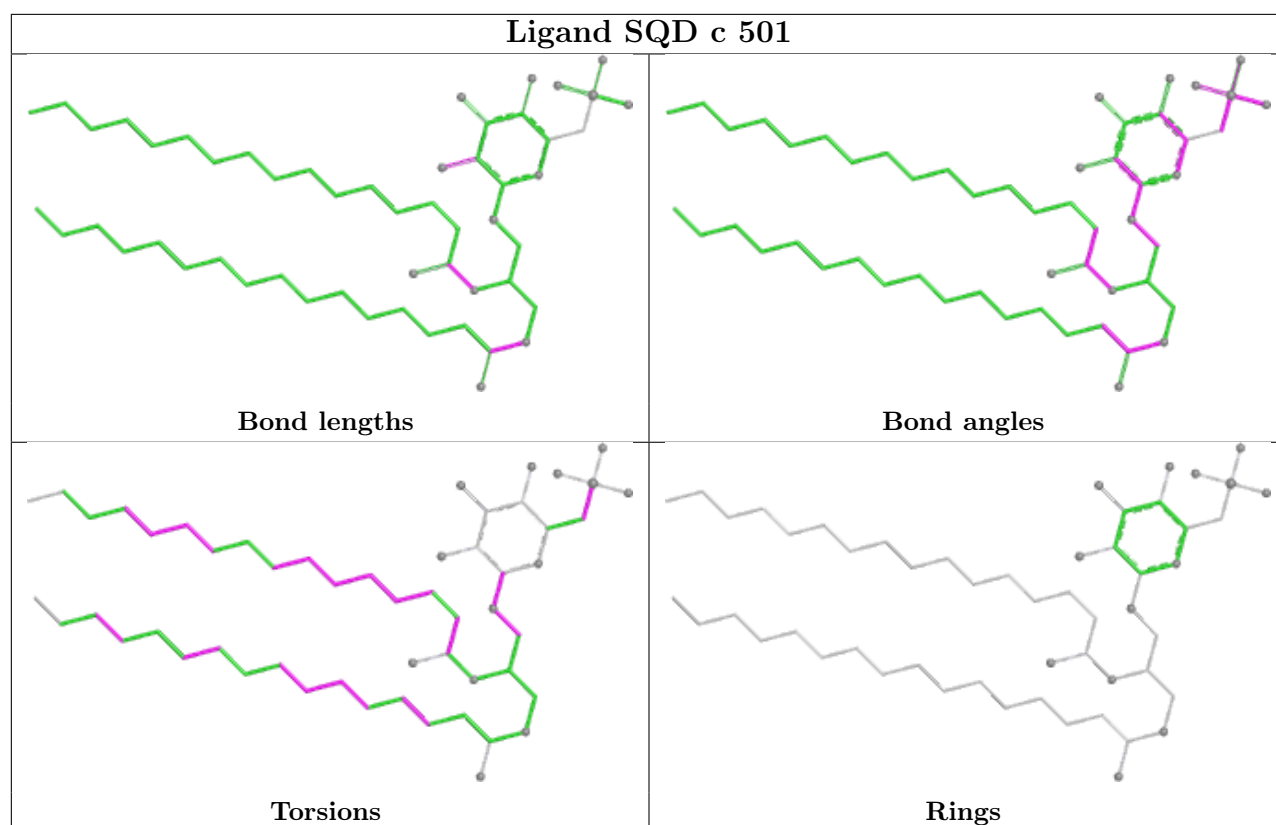


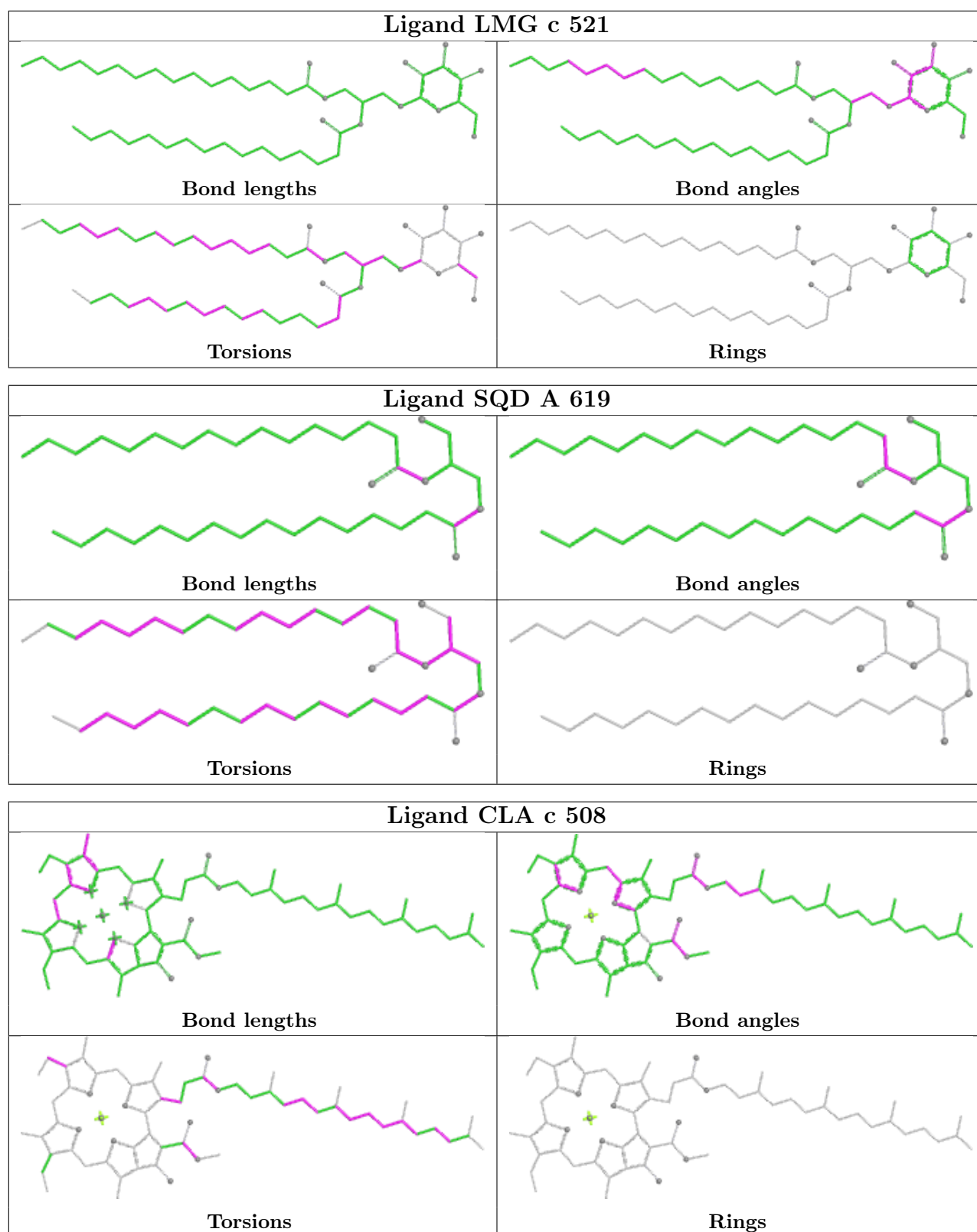
Ligand HEC v 201



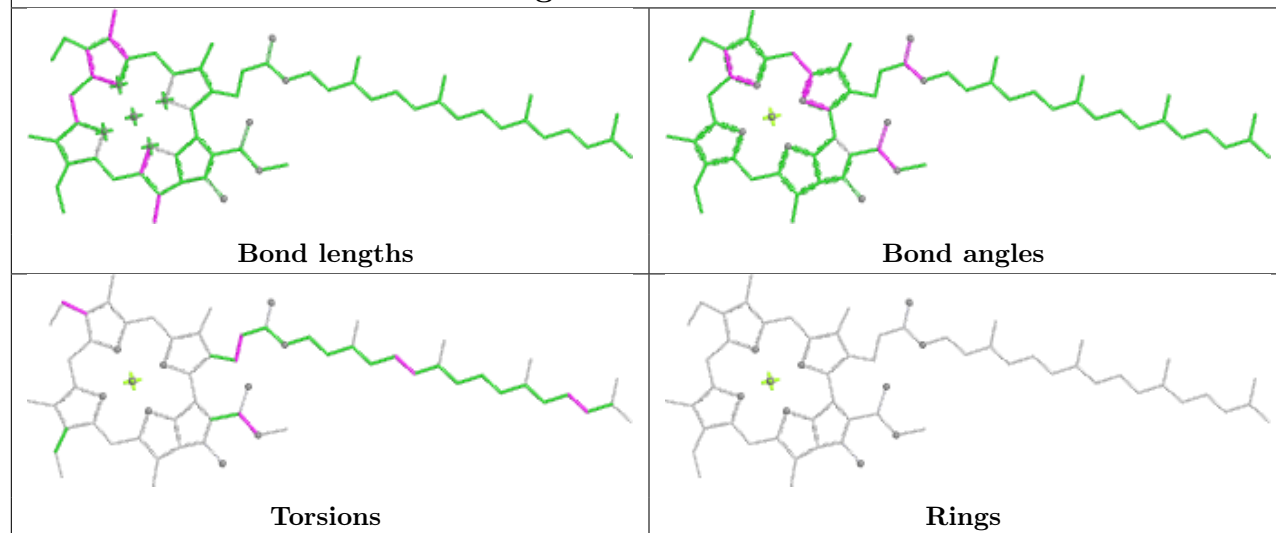


Ligand CLA a 612**Ligand CLA b 610**

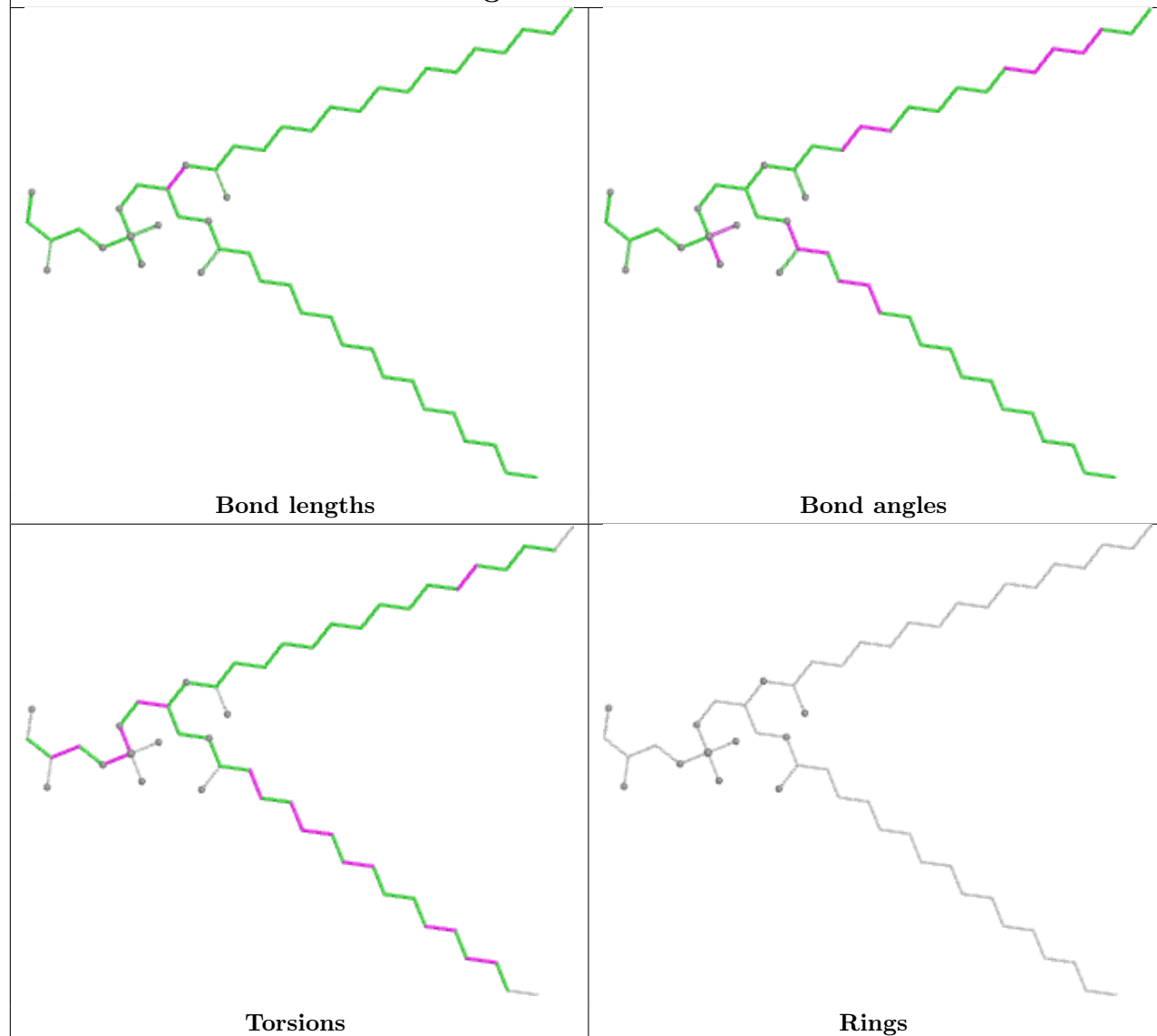




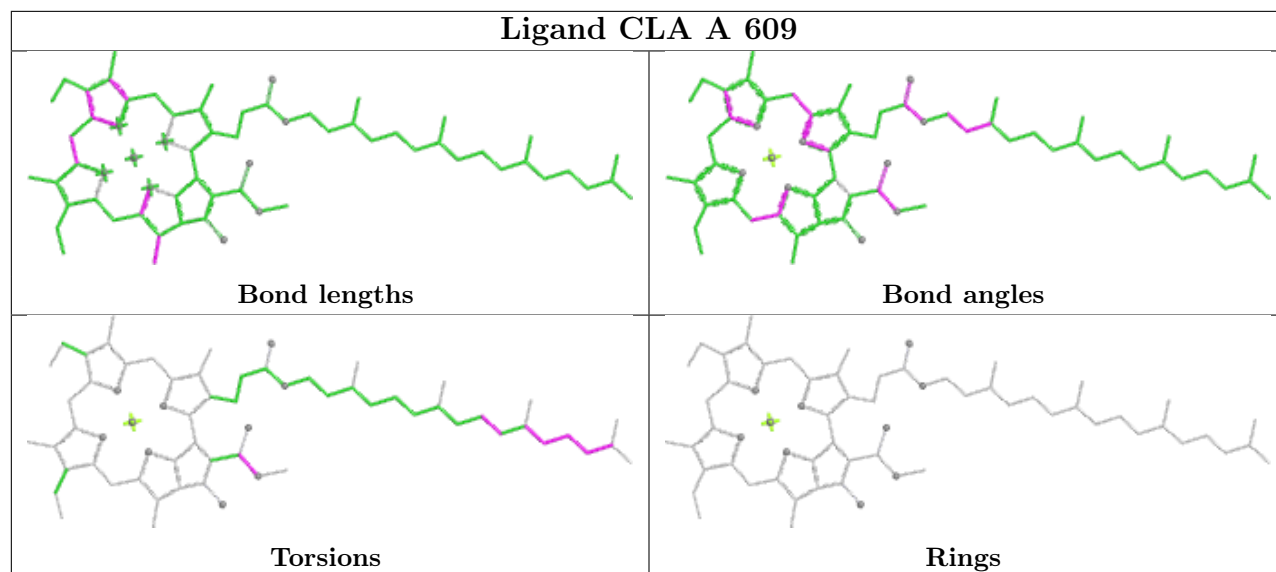
Ligand CLA b 606



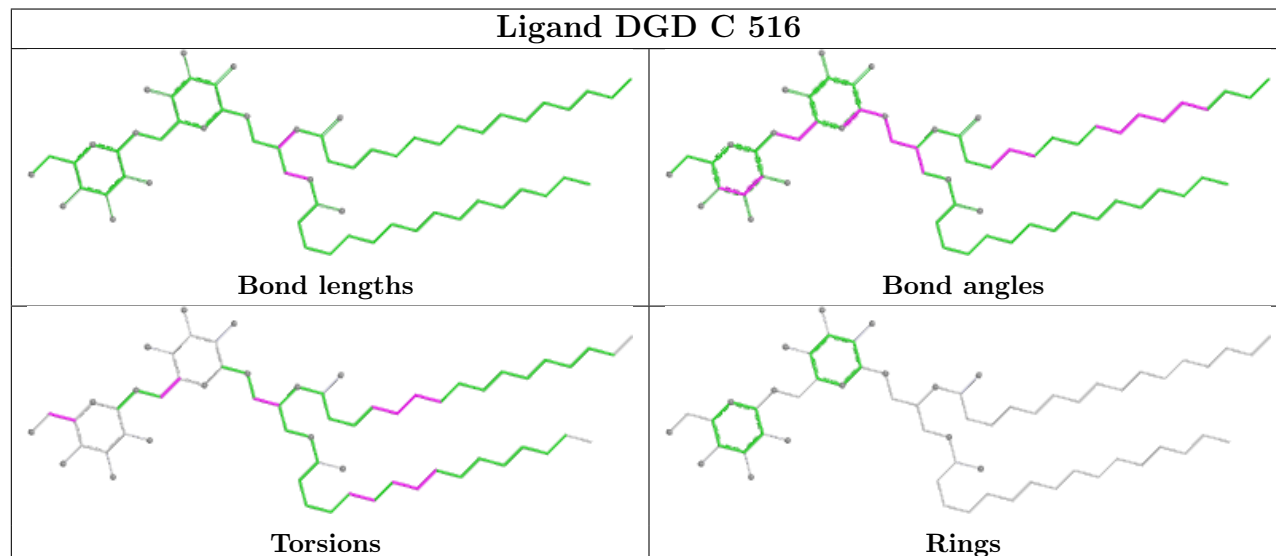
Ligand LHG d 407



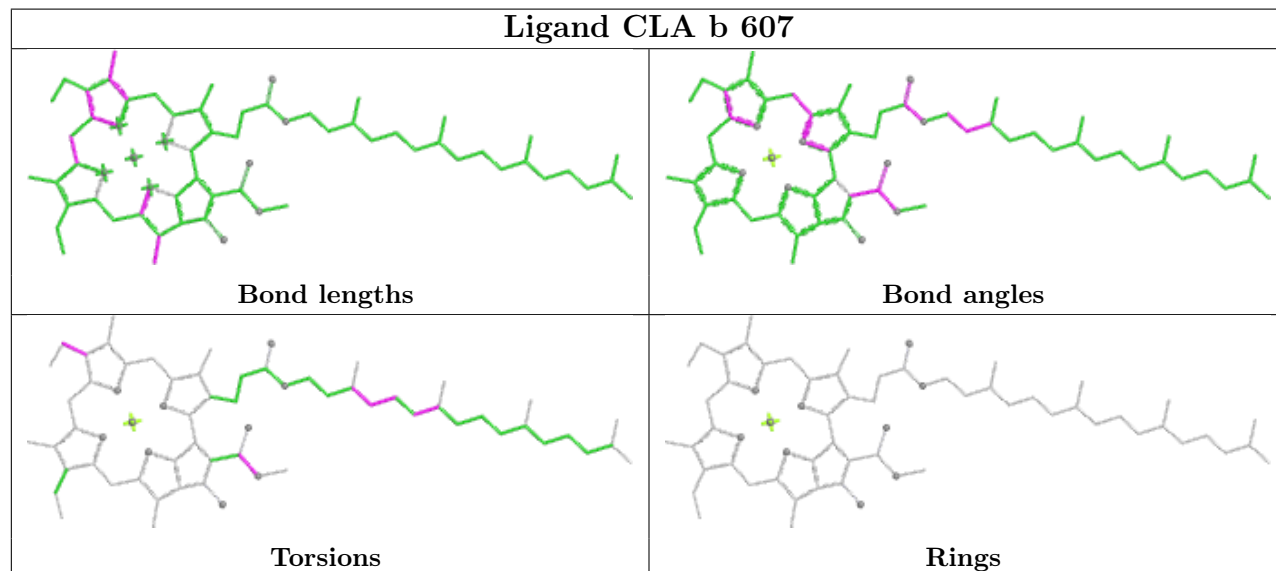
Ligand CLA A 609

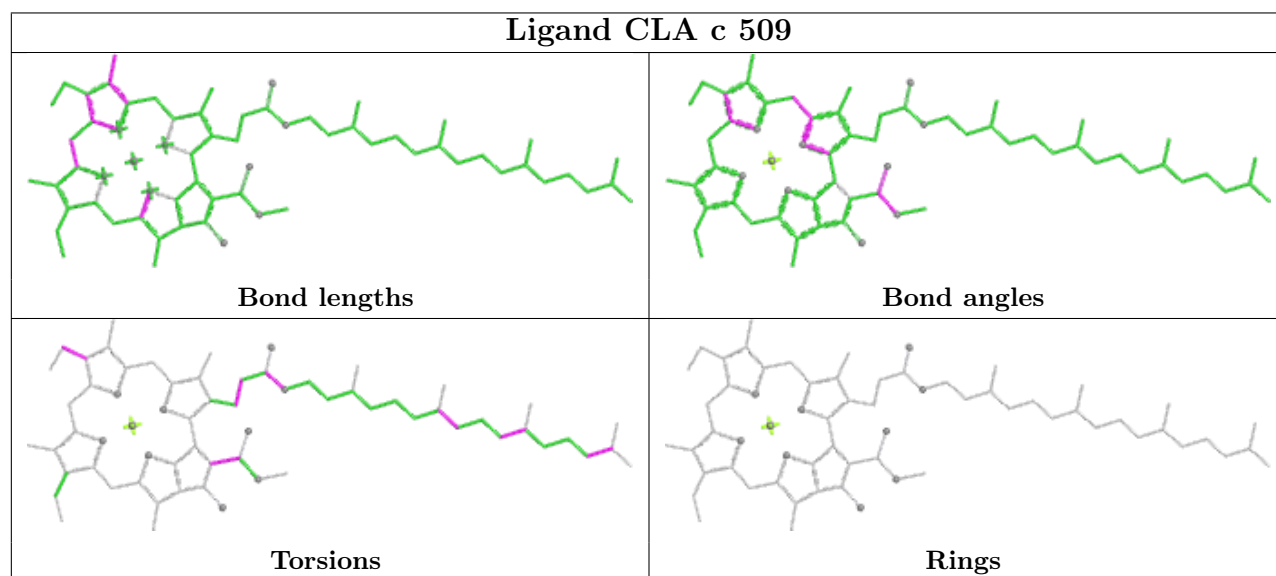
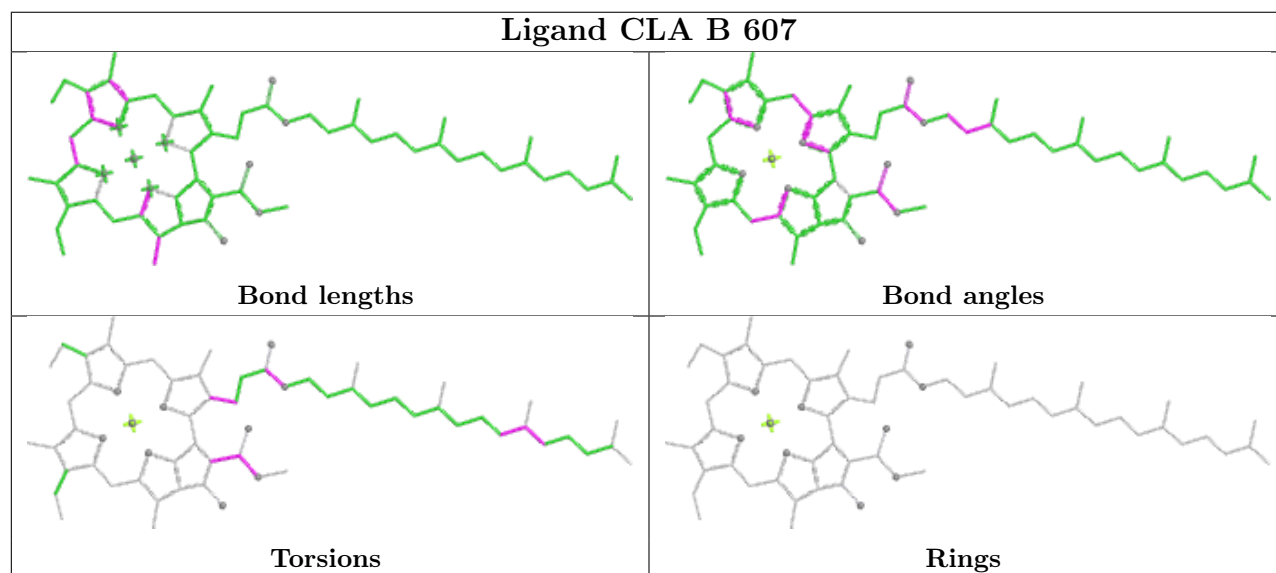
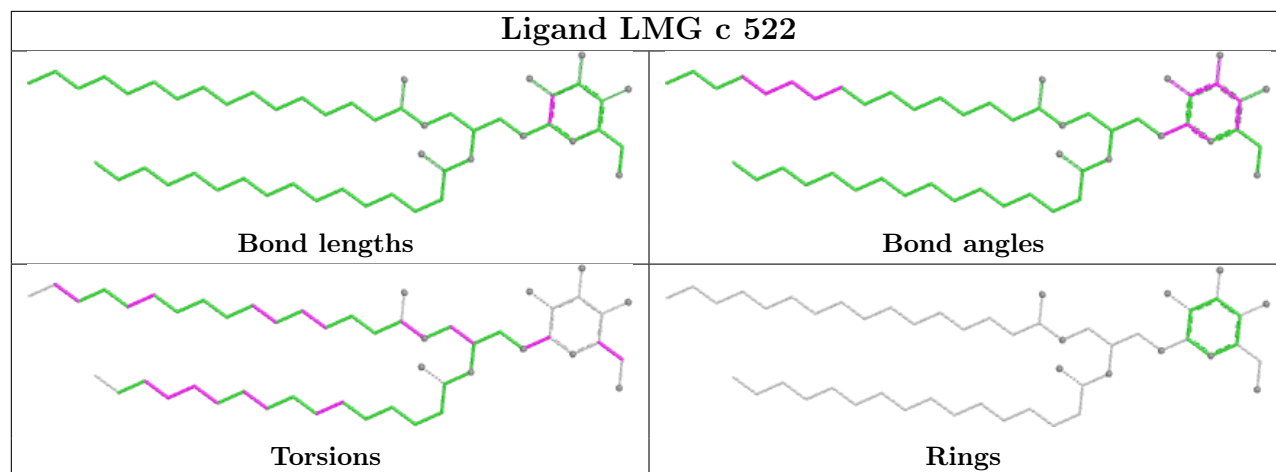


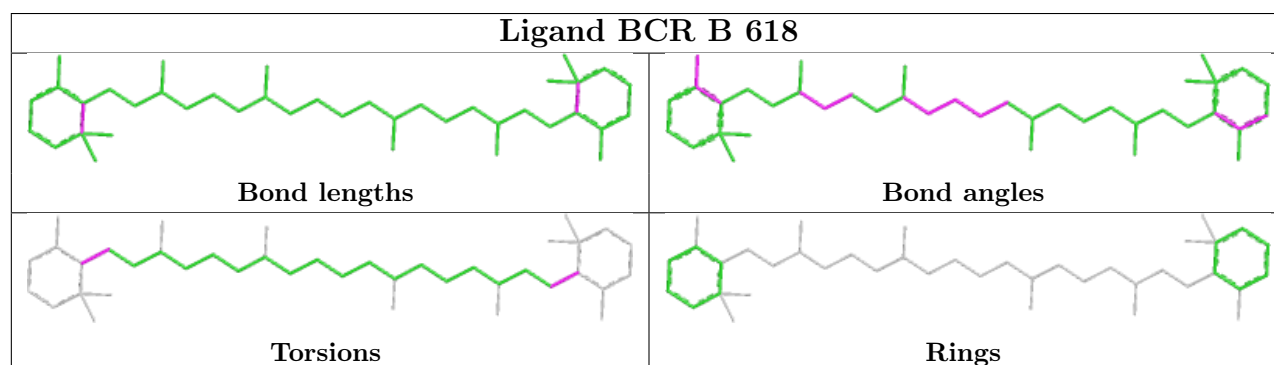
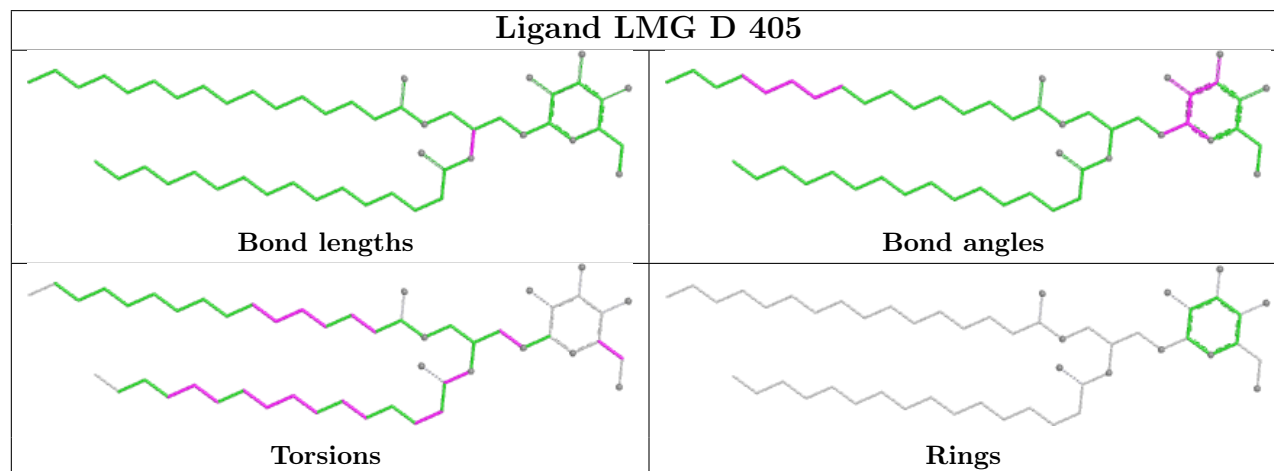
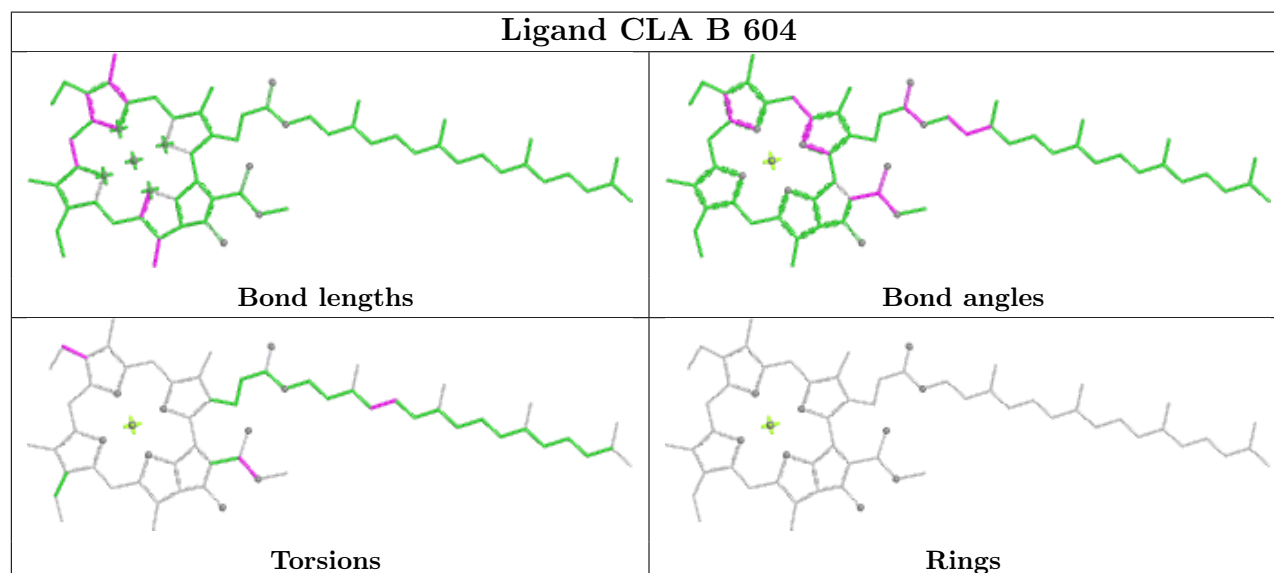
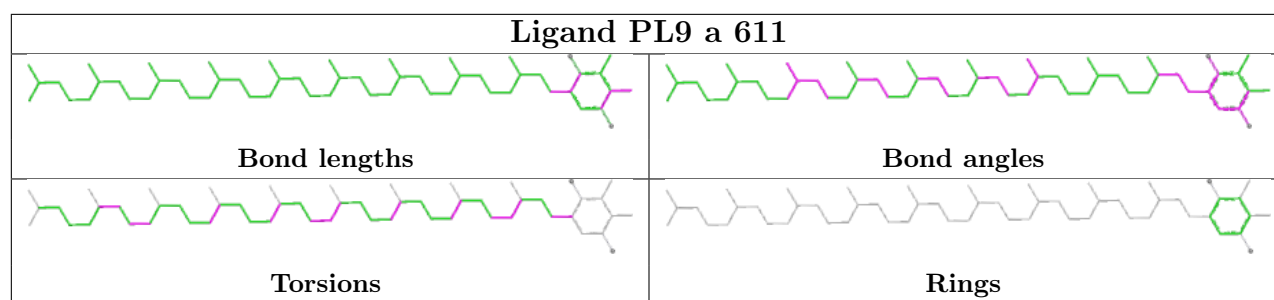
Ligand DGD C 516



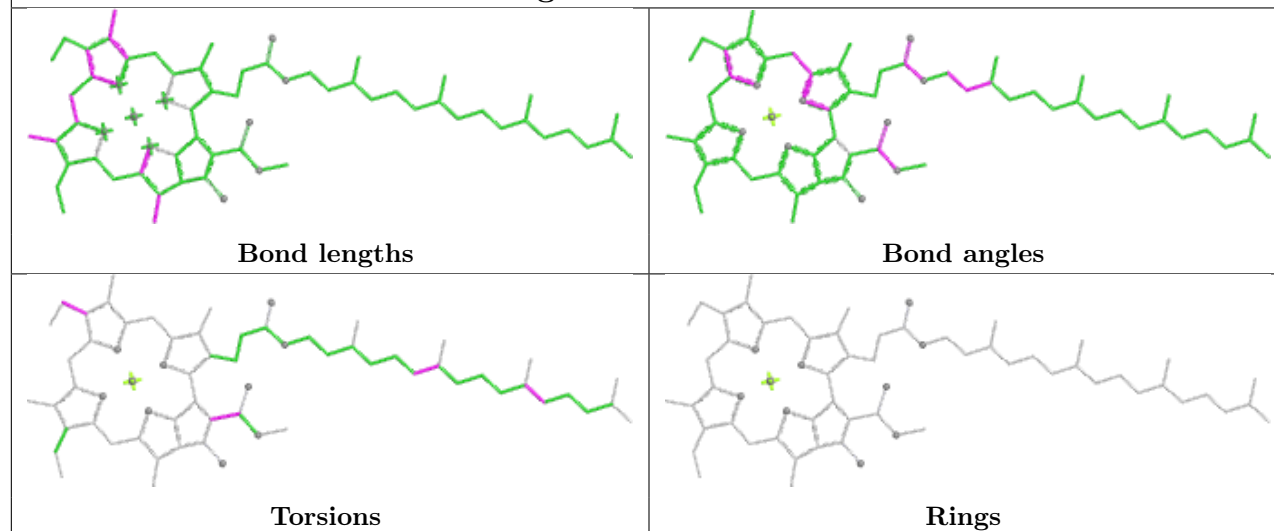
Ligand CLA b 607



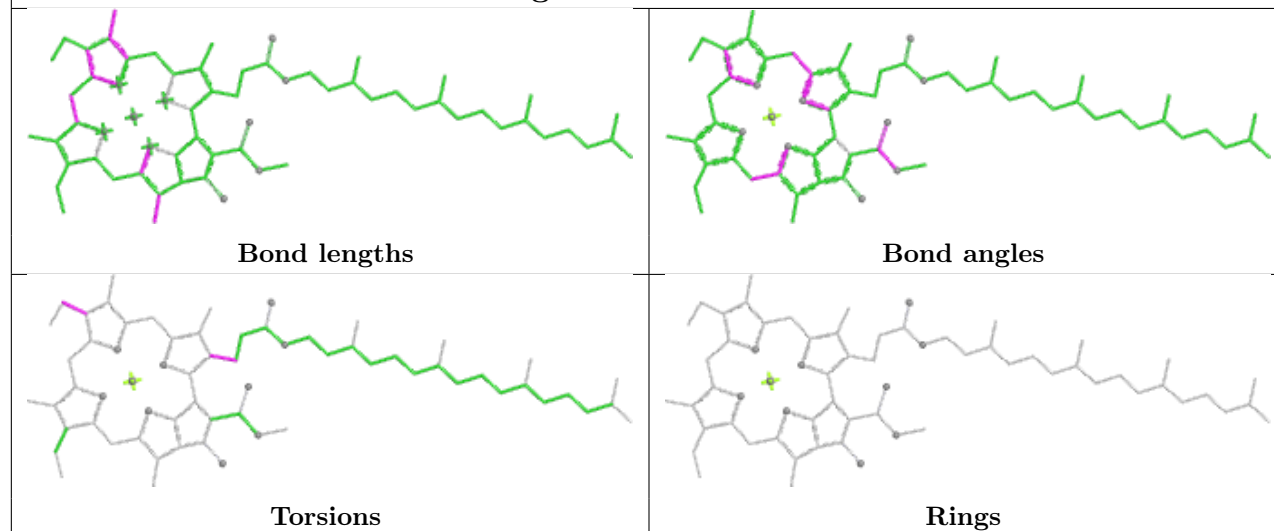




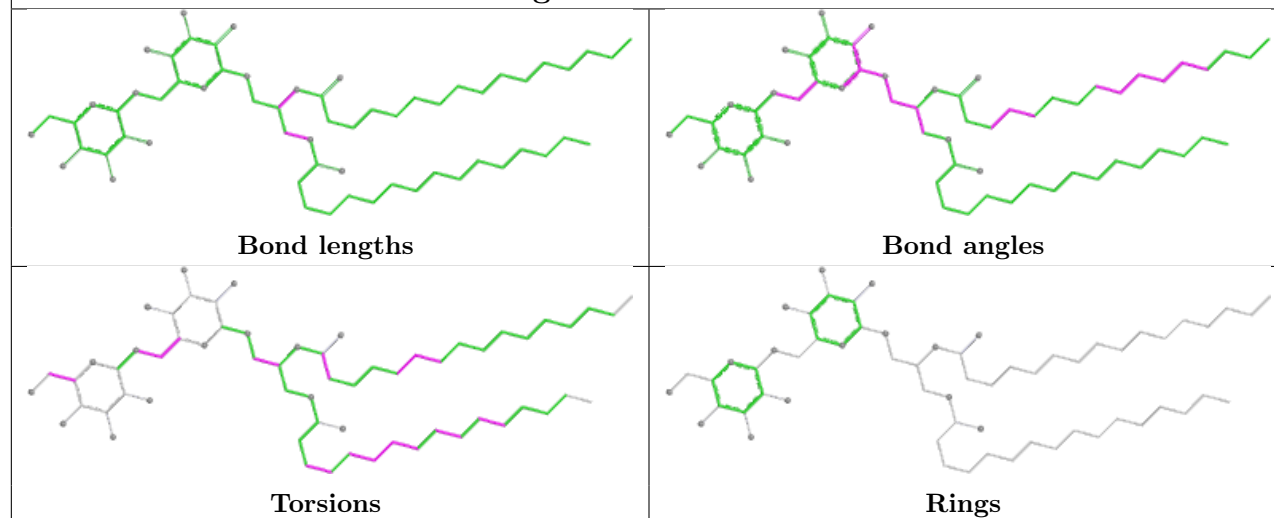
Ligand CLA c 504



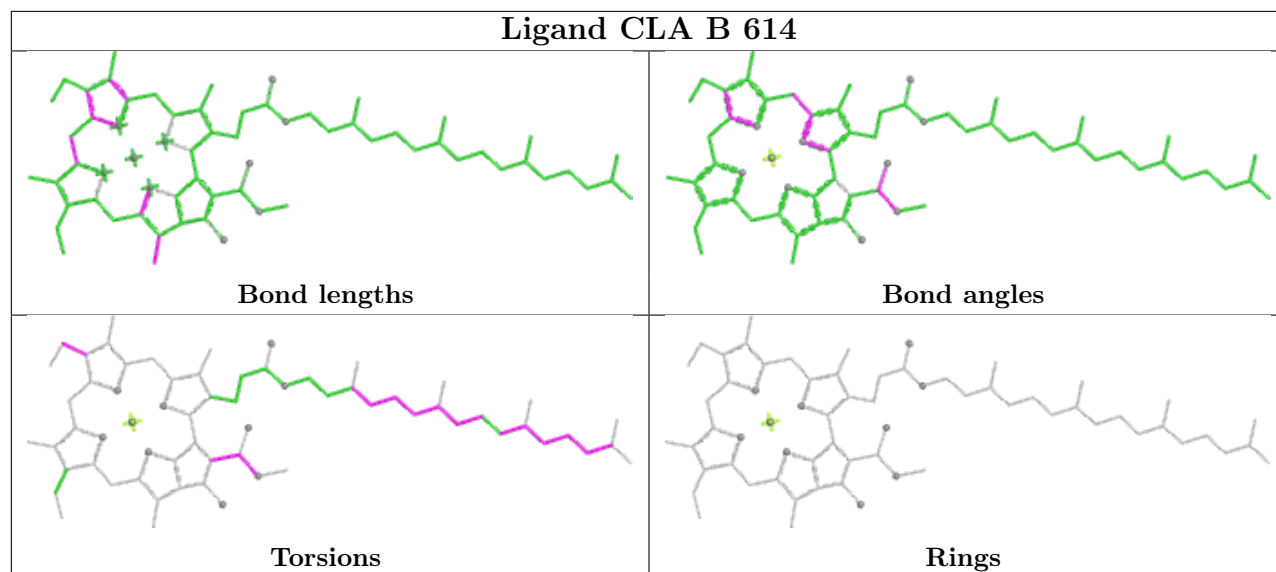
Ligand CLA A 615



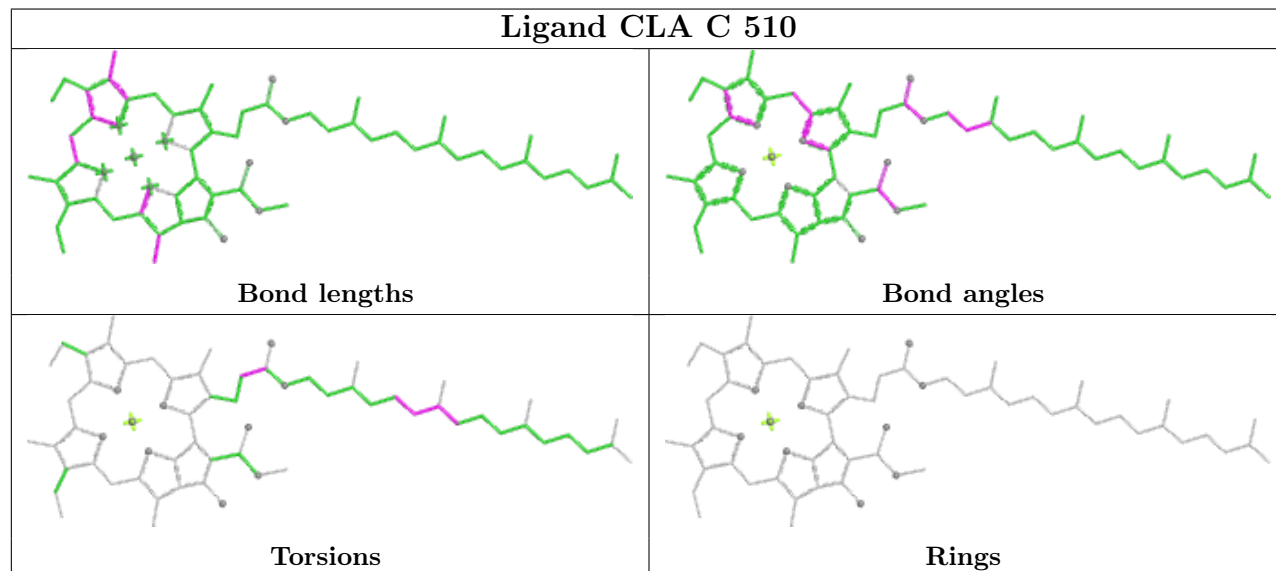
Ligand DGD c 518



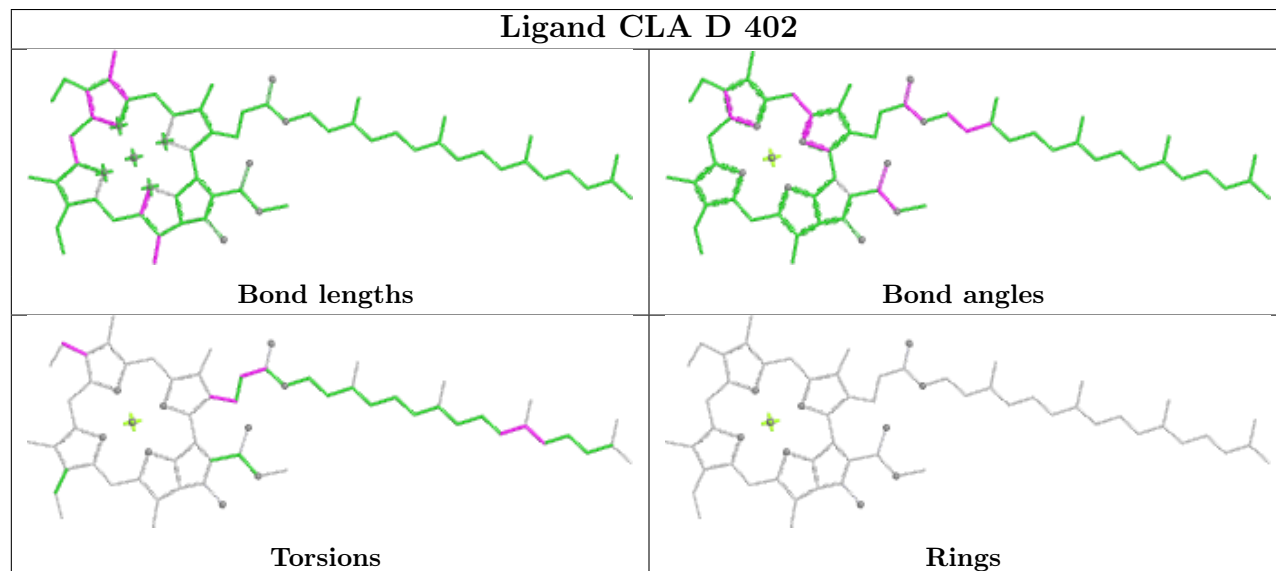
Ligand CLA B 614

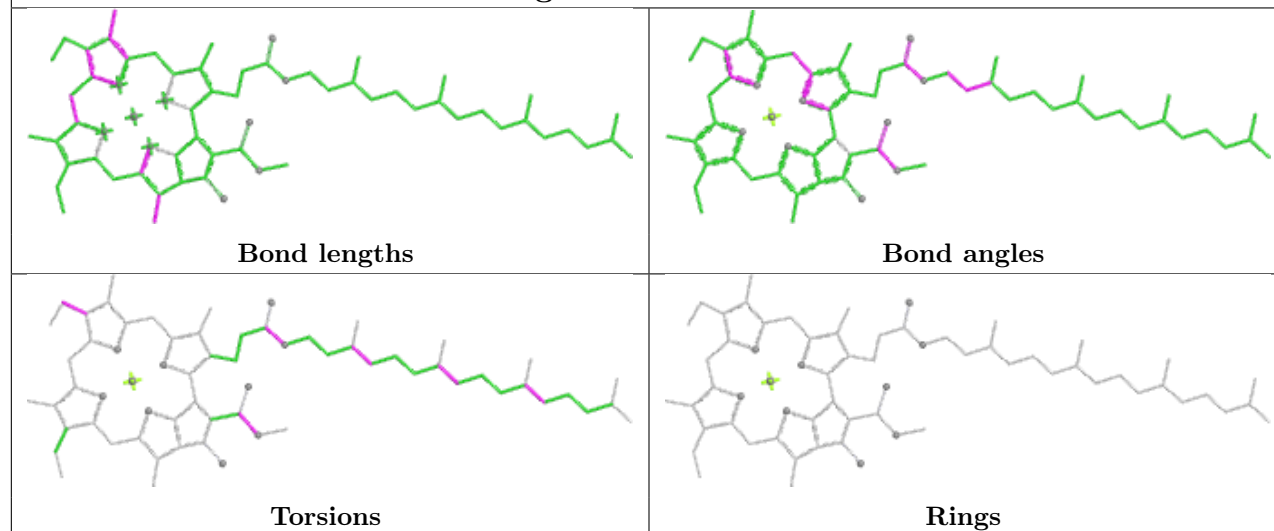
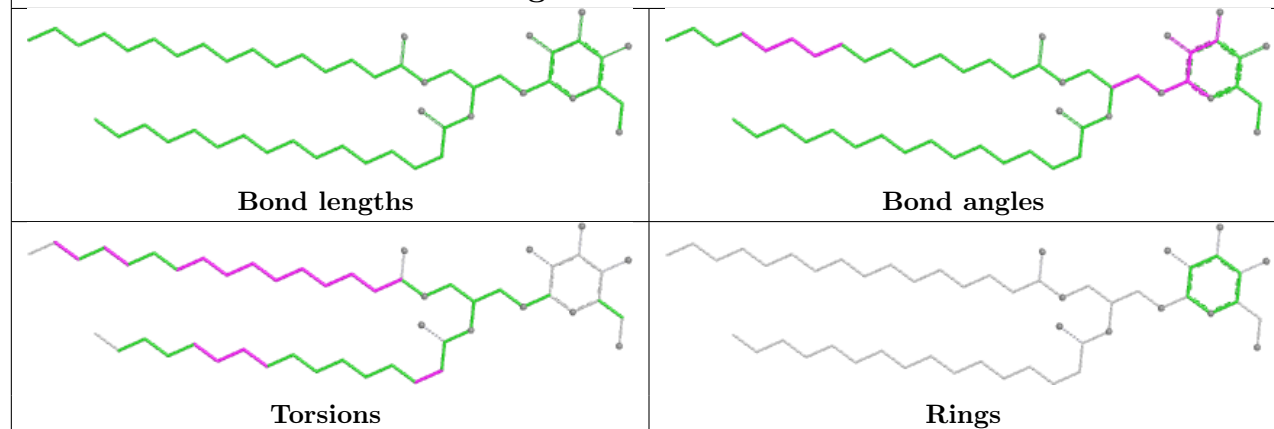


Ligand CLA C 510

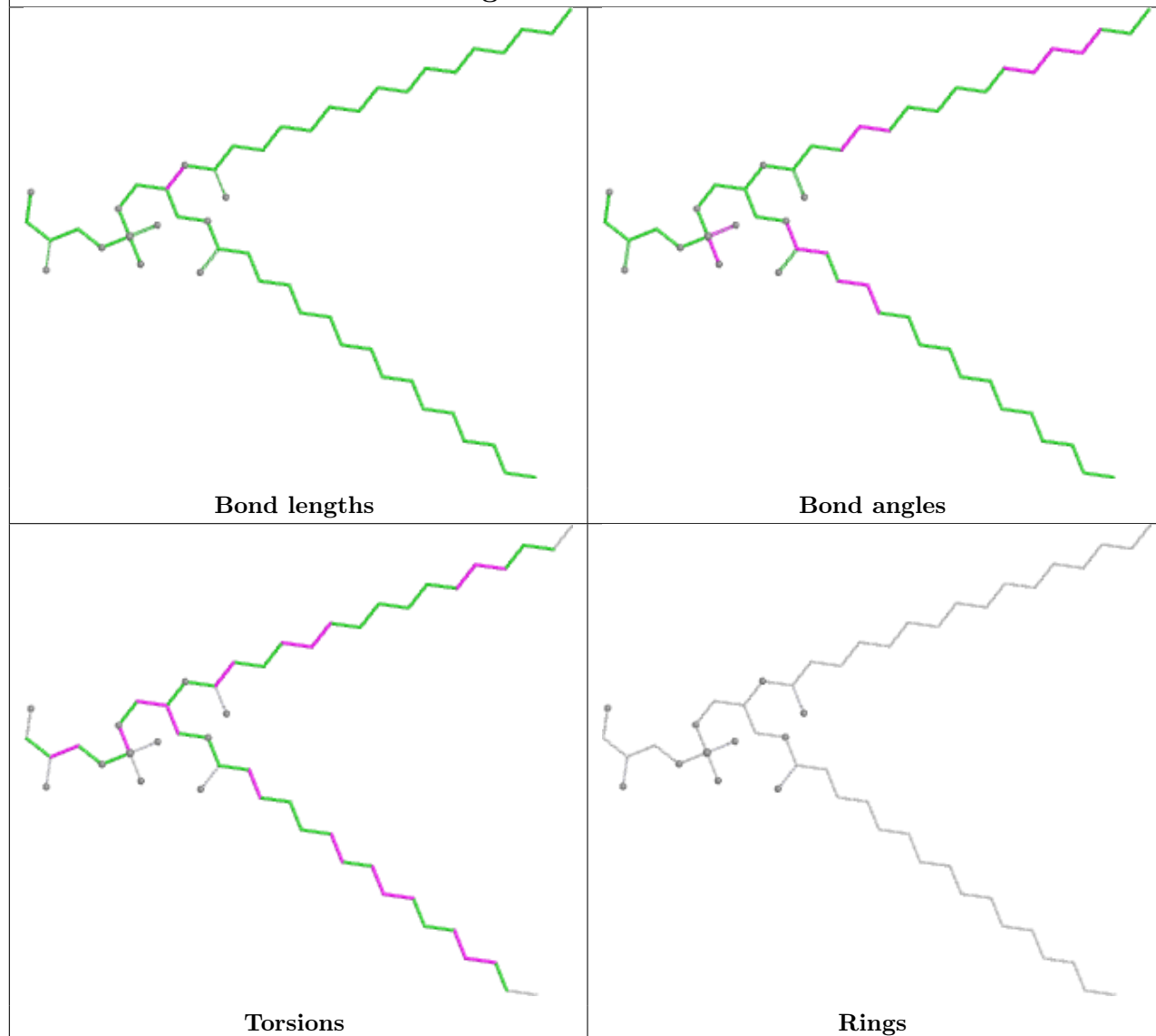


Ligand CLA D 402

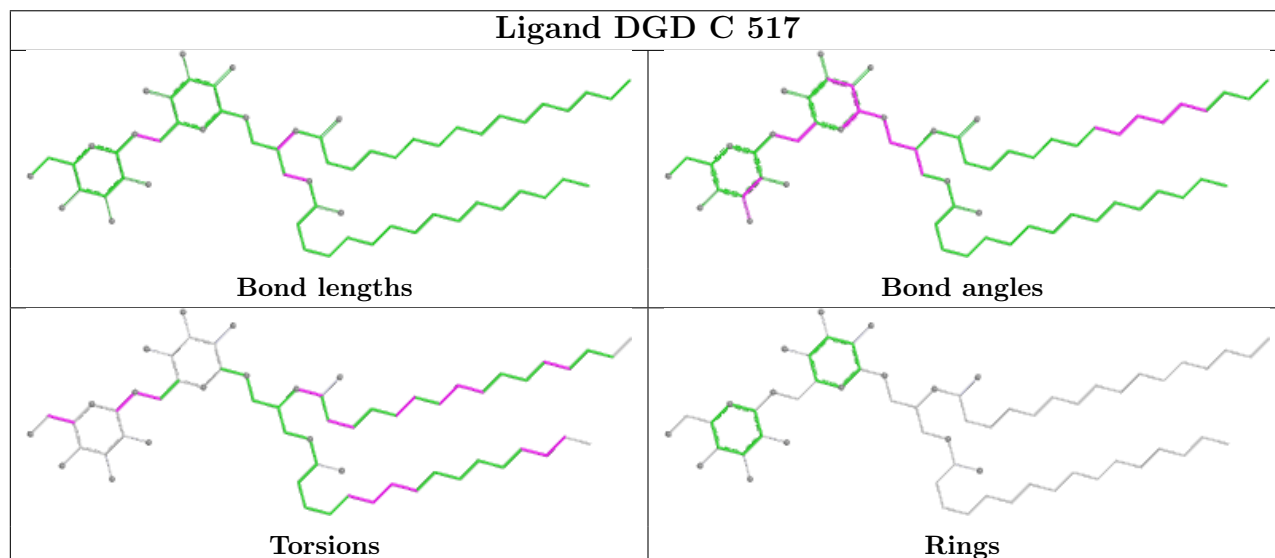


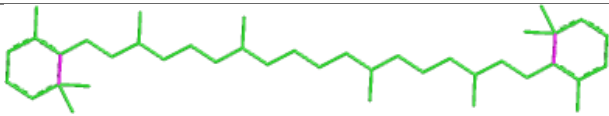
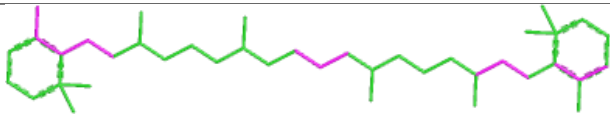
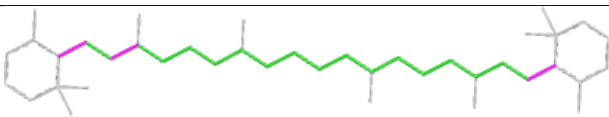
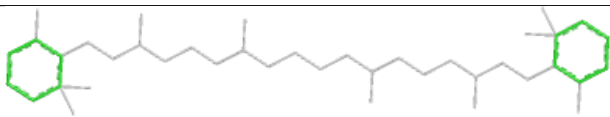
Ligand CLA b 612**Ligand LMG B 620**

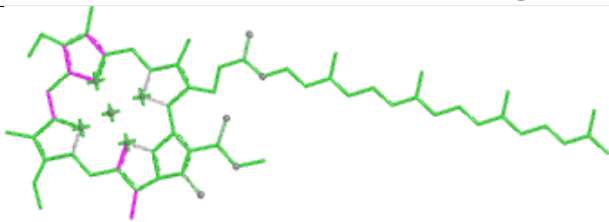
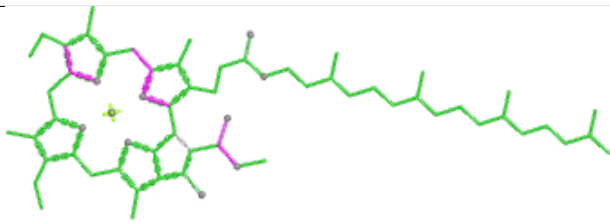
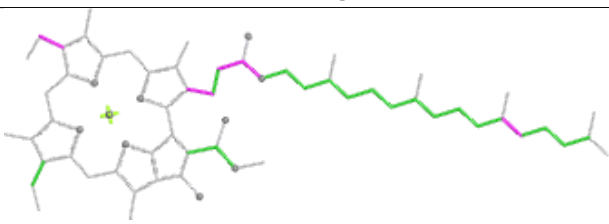
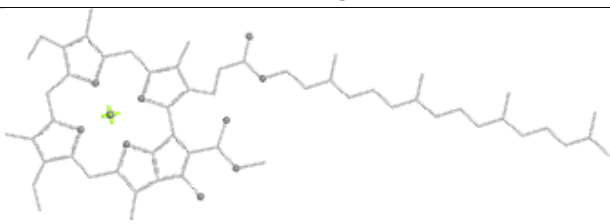
Ligand LHG L 101

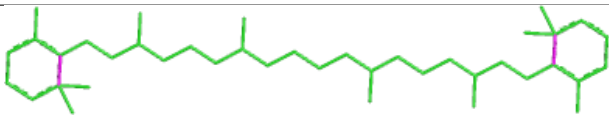
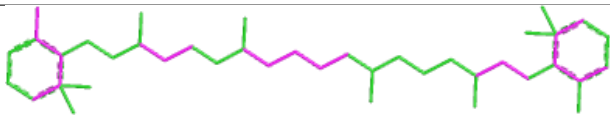
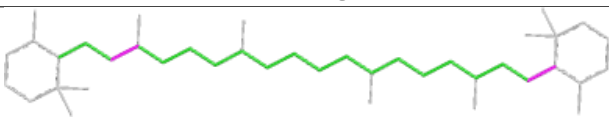
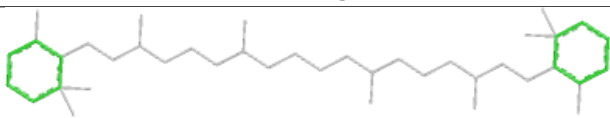


Ligand DGD C 517



Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	0.52	10 (2%) 52 30	28, 38, 60, 76	0
1	a	334/344 (97%)	0.48	6 (1%) 67 44	28, 38, 60, 76	0
2	B	504/510 (98%)	0.50	12 (2%) 59 36	27, 41, 66, 86	0
2	b	504/510 (98%)	0.53	13 (2%) 57 34	29, 42, 67, 85	1 (0%)
3	C	451/461 (97%)	0.58	11 (2%) 59 36	30, 45, 61, 75	0
3	c	451/461 (97%)	0.62	13 (2%) 53 31	31, 46, 63, 93	0
4	D	341/352 (96%)	0.45	6 (1%) 67 44	28, 39, 56, 67	0
4	d	341/352 (96%)	0.49	5 (1%) 72 49	29, 40, 55, 78	0
5	E	81/84 (96%)	0.75	2 (2%) 58 35	39, 54, 72, 89	0
5	e	82/84 (97%)	0.95	9 (10%) 10 6	43, 61, 75, 80	0
6	F	34/45 (75%)	0.67	1 (2%) 53 31	40, 50, 63, 77	0
6	f	34/45 (75%)	0.64	1 (2%) 53 31	39, 51, 69, 72	0
7	H	63/66 (95%)	0.60	0 100 100	39, 47, 57, 63	0
7	h	63/66 (95%)	0.43	0 100 100	35, 47, 58, 68	0
8	I	35/38 (92%)	0.48	1 (2%) 53 31	29, 44, 71, 73	0
8	i	35/38 (92%)	0.63	4 (11%) 10 6	33, 43, 74, 94	0
9	J	36/40 (90%)	0.86	3 (8%) 17 9	44, 58, 68, 75	0
9	j	36/40 (90%)	0.79	1 (2%) 55 32	49, 57, 72, 79	0
10	K	37/46 (80%)	0.95	2 (5%) 31 16	45, 59, 75, 89	0
10	k	37/46 (80%)	0.96	3 (8%) 18 9	47, 56, 72, 79	0
11	L	37/37 (100%)	0.25	1 (2%) 56 33	32, 38, 62, 84	0
11	l	37/37 (100%)	0.35	2 (5%) 31 16	29, 38, 69, 81	0
12	M	32/36 (88%)	0.35	2 (6%) 26 13	33, 38, 56, 74	0
12	m	32/36 (88%)	0.59	3 (9%) 14 7	31, 41, 59, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.69	16 (6%) 24 12	30, 47, 81, 111	0
13	o	244/272 (89%)	0.75	14 (5%) 29 15	31, 46, 80, 127	0
14	T	29/32 (90%)	0.33	1 (3%) 48 27	30, 39, 60, 74	0
14	t	29/32 (90%)	0.26	1 (3%) 48 27	31, 36, 63, 66	0
15	U	97/134 (72%)	0.56	2 (2%) 63 40	36, 49, 69, 75	0
15	u	97/134 (72%)	0.54	1 (1%) 79 59	32, 44, 58, 76	0
16	V	137/163 (84%)	0.65	3 (2%) 62 39	34, 47, 59, 74	0
16	v	137/163 (84%)	0.80	7 (5%) 33 17	34, 54, 67, 81	0
17	Y	30/46 (65%)	1.25	4 (13%) 7 4	60, 73, 84, 87	0
17	y	30/46 (65%)	0.96	1 (3%) 49 28	49, 65, 78, 83	0
18	X	38/41 (92%)	0.56	2 (5%) 32 16	41, 50, 65, 79	0
18	x	38/41 (92%)	0.79	3 (7%) 18 10	46, 55, 74, 76	0
19	Z	62/62 (100%)	1.37	13 (20%) 2 1	52, 69, 88, 98	0
19	z	62/62 (100%)	1.20	7 (11%) 10 6	51, 72, 97, 105	0
20	R	34/41 (82%)	1.27	4 (11%) 9 5	65, 73, 83, 86	0
20	r	34/41 (82%)	1.29	3 (8%) 15 8	65, 78, 86, 90	0
All	All	5313/5700 (93%)	0.61	193 (3%) 46 26	27, 44, 72, 127	1 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	m	31	SER	4.8
13	O	35	SER	4.7
16	v	18	THR	4.7
13	o	60	ARG	4.5
3	C	29	GLU	4.4
13	O	62	GLU	4.4
13	o	61	GLN	4.4
11	l	1	MET	4.3
13	O	58	ASN	3.9
13	o	99	ASP	3.9
12	M	33	GLN	3.7
13	o	3	GLN	3.6
2	B	487	SER	3.5
2	B	351	GLY	3.5
19	Z	3	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
19	z	3	ILE	3.4
20	r	35	LEU	3.4
3	C	142	GLU	3.4
4	D	238	THR	3.3
4	d	227	GLU	3.3
2	B	500	GLY	3.3
3	C	129	GLY	3.3
6	F	12	SER	3.2
13	o	4	THR	3.2
20	R	6	LEU	3.2
12	M	31	SER	3.0
3	c	454	GLY	3.0
13	o	58	ASN	3.0
9	J	25	VAL	3.0
3	c	24	THR	3.0
8	I	34	ARG	3.0
3	c	192	GLY	3.0
8	i	35	LYS	2.9
2	b	82	GLY	2.9
19	z	34	ASP	2.9
19	Z	1	MET	2.9
3	c	23	ALA	2.9
13	o	35	SER	2.9
19	Z	29	SER	2.9
13	O	56	PRO	2.9
19	Z	33	TRP	2.9
19	z	41	PHE	2.9
2	b	239[A]	SER	2.8
19	z	62	VAL	2.8
4	d	239	GLN	2.8
3	C	27	ASP	2.8
13	O	4	THR	2.8
3	C	23	ALA	2.8
2	B	505	ARG	2.8
1	A	264	SER	2.8
2	B	495	PHE	2.8
11	L	1	MET	2.8
8	i	34	ARG	2.8
5	e	12	ASP	2.7
2	B	480	SER	2.7
13	o	54	GLU	2.7
3	C	30	SER	2.7

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Mol	Chain	Res	Type	RSRZ
13	o	59	LYS	2.7
8	i	36	ASP	2.7
15	U	40	GLY	2.7
1	A	248	ILE	2.6
13	O	59	LYS	2.6
3	c	142	GLU	2.6
4	D	229	ALA	2.6
4	D	230	SER	2.6
13	o	23	ASP	2.6
13	o	56	PRO	2.6
2	B	388	SER	2.6
13	O	34	SER	2.6
9	j	34	ALA	2.6
19	Z	60	PHE	2.5
2	b	223	GLN	2.5
12	m	32	GLN	2.5
1	A	266	ASN	2.5
18	X	2	THR	2.5
4	d	136	VAL	2.5
3	C	145	SER	2.5
13	O	139	SER	2.5
17	y	18	VAL	2.5
13	o	135	SER	2.4
17	Y	45	ASN	2.4
18	x	2	THR	2.4
5	e	57	ALA	2.4
3	c	25	ASN	2.4
16	v	10	VAL	2.4
2	b	482	ILE	2.4
5	E	59	GLU	2.4
10	k	19	ASP	2.4
5	e	3	GLY	2.4
13	O	207	ARG	2.4
2	b	487	SER	2.4
13	O	245	PRO	2.4
19	Z	62	VAL	2.4
18	X	38	GLN	2.4
19	Z	5	PHE	2.4
2	b	489	GLU	2.4
3	c	137	PRO	2.4
3	c	32	GLY	2.3
4	D	177	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	221	SER	2.3
1	A	228	THR	2.3
13	O	63	ALA	2.3
1	a	262	TYR	2.3
16	v	78	ASN	2.3
3	c	268	GLY	2.3
1	A	227	THR	2.3
1	a	221	SER	2.3
2	b	486	LEU	2.3
19	Z	6	GLN	2.3
5	e	71	GLU	2.3
19	Z	30	PRO	2.3
19	Z	42	LEU	2.3
2	b	108	PHE	2.3
3	C	419	PHE	2.3
20	R	33	LYS	2.3
1	a	242	GLU	2.3
3	c	462	GLU	2.3
4	d	241	GLU	2.3
17	Y	18	VAL	2.3
2	B	173	GLY	2.3
2	B	494	GLY	2.3
18	x	16	SER	2.3
2	b	485	GLU	2.2
10	k	20	PRO	2.2
1	A	263	ALA	2.2
3	c	133	ALA	2.2
13	o	100	GLY	2.2
8	i	33	LYS	2.2
2	B	295	GLY	2.2
3	c	85	GLY	2.2
3	C	24	THR	2.2
5	E	68	ASP	2.2
19	Z	34	ASP	2.2
14	T	30	THR	2.2
3	C	43	ILE	2.2
13	o	62	GLU	2.2
15	U	100	ASN	2.2
16	v	106	ASN	2.2
1	A	141	PRO	2.2
1	a	84	PRO	2.2
4	D	56	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	11	ALA	2.2
13	O	131	PRO	2.2
19	Z	27	TYR	2.1
2	b	80	ILE	2.1
6	f	44	GLN	2.1
16	v	1	ALA	2.1
20	r	17	GLY	2.1
15	u	68	THR	2.1
13	O	61	GLN	2.1
17	Y	24	MET	2.1
3	C	352	GLY	2.1
20	R	25	PRO	2.1
3	c	125	LEU	2.1
16	v	119	ILE	2.1
19	z	1	MET	2.1
18	x	38	GLN	2.1
5	e	48	GLY	2.1
1	a	93	PHE	2.1
4	D	232	PHE	2.1
20	R	9	LEU	2.1
13	O	202	ALA	2.1
2	b	484	PRO	2.1
2	b	495	PHE	2.1
1	a	297	LEU	2.1
5	e	13	ILE	2.1
19	z	35	ARG	2.1
20	r	2	ASP	2.1
14	t	30	THR	2.1
10	K	14	ALA	2.1
16	v	38	ALA	2.1
11	l	2	GLU	2.1
16	V	106	ASN	2.0
2	B	87	ASP	2.0
4	d	240	ALA	2.0
9	J	30	TYR	2.0
10	K	23	ASP	2.0
13	O	99	ASP	2.0
9	J	5	GLY	2.0
16	V	132	GLY	2.0
10	k	29	PRO	2.0
13	O	54	GLU	2.0
16	V	135	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
19	z	19	MET	2.0
1	A	254	TYR	2.0
2	B	176	GLY	2.0
5	e	6	GLY	2.0
17	Y	44	GLY	2.0
5	e	60	GLN	2.0
12	m	33	GLN	2.0
19	Z	61	VAL	2.0
2	b	86	ILE	2.0
5	e	22	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.87	0.14	43,56,63,71	0
12	FME	m	1	10/11	0.88	0.16	26,45,55,64	0
14	FME	t	1	10/11	0.88	0.13	39,42,63,72	0
12	FME	M	1	10/11	0.89	0.14	30,43,53,54	0
8	FME	i	1	10/11	0.89	0.11	35,50,56,61	0
14	FME	T	1	10/11	0.90	0.10	44,47,53,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UNL	H	101	8/-	0.52	0.24	29,35,43,47	0
29	LMG	b	625	9/55	0.63	0.25	40,46,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMG	b	624	51/55	0.64	0.23	45,64,76,86	0
30	UNL	j	101	9/-	0.67	0.23	40,49,60,63	0
31	LHG	a	615	42/49	0.67	0.21	54,78,89,100	0
31	LHG	A	618	49/49	0.68	0.22	41,72,85,94	0
30	UNL	b	603	13/-	0.69	0.20	39,48,61,62	0
30	UNL	A	614	7/-	0.69	0.24	32,38,42,42	0
30	UNL	B	622	6/-	0.71	0.22	26,42,50,56	0
29	LMG	B	621	51/55	0.71	0.20	32,56,71,74	0
29	LMG	C	520	51/55	0.72	0.22	49,62,82,100	0
30	UNL	t	101	10/-	0.72	0.19	26,41,47,47	0
28	PL9	A	611	55/55	0.73	0.24	39,58,75,79	0
30	UNL	B	623	11/-	0.73	0.19	35,40,47,48	0
29	LMG	c	522	51/55	0.75	0.21	36,68,83,90	0
30	UNL	z	101	11/-	0.75	0.23	31,53,58,60	0
30	UNL	i	101	12/-	0.75	0.20	24,39,51,51	0
29	LMG	d	409	40/55	0.75	0.20	40,55,76,77	0
29	LMG	A	613	51/55	0.76	0.19	31,53,78,84	0
23	SQD	I	101	40/54	0.76	0.18	31,52,84,89	0
23	SQD	D	409	43/54	0.77	0.19	37,68,89,98	0
30	UNL	B	624	11/-	0.77	0.18	26,31,38,41	0
23	SQD	A	619	40/54	0.77	0.20	25,48,67,69	0
30	UNL	m	102	16/-	0.77	0.18	37,45,51,54	0
27	BCR	y	101	40/40	0.78	0.20	50,63,70,74	0
25	CLA	b	604	65/65	0.78	0.17	44,59,76,88	0
23	SQD	D	408	47/54	0.79	0.16	17,53,103,121	0
29	LMG	B	625	51/55	0.79	0.17	28,52,74,78	0
29	LMG	C	519	51/55	0.79	0.19	42,61,73,85	0
23	SQD	B	626	54/54	0.80	0.15	33,52,85,90	0
30	UNL	b	602	13/-	0.80	0.18	30,36,41,45	0
29	LMG	c	521	51/55	0.80	0.21	33,65,83,88	0
27	BCR	Y	101	40/40	0.80	0.19	46,60,72,76	0
23	SQD	b	601	54/54	0.80	0.16	39,60,90,97	0
23	SQD	c	501	54/54	0.80	0.19	38,58,76,77	0
28	PL9	a	611	55/55	0.80	0.20	40,59,72,73	0
29	LMG	b	623	51/55	0.80	0.18	29,48,71,74	0
29	LMG	A	612	51/55	0.80	0.17	34,59,76,85	0
30	UNL	C	521	9/-	0.80	0.20	36,42,46,49	0
29	LMG	c	502	51/55	0.81	0.19	34,57,80,83	0
27	BCR	D	404	40/40	0.81	0.18	28,46,63,67	0
30	UNL	m	101	5/-	0.81	0.16	26,32,37,41	0
25	CLA	C	512	65/65	0.81	0.17	42,58,68,79	0
27	BCR	k	101	40/40	0.81	0.18	37,53,59,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	601	65/65	0.81	0.17	41,59,84,96	0
27	BCR	C	514	40/40	0.81	0.19	45,56,64,66	0
30	UNL	d	402	22/-	0.81	0.19	26,43,60,78	0
33	DGD	c	519	62/66	0.81	0.19	37,57,86,95	0
33	DGD	h	102	62/66	0.81	0.18	35,47,63,73	0
23	SQD	f	101	43/54	0.82	0.17	51,70,77,84	0
25	CLA	C	504	65/65	0.82	0.19	33,51,70,78	0
25	CLA	c	515	65/65	0.82	0.18	45,60,78,81	0
27	BCR	h	101	40/40	0.82	0.17	31,45,55,62	0
32	BCT	a	605	4/4	0.82	0.11	44,47,49,50	0
27	BCR	B	627	40/40	0.82	0.17	30,41,49,53	0
29	LMG	B	620	51/55	0.82	0.16	27,46,67,75	0
27	BCR	b	622	40/40	0.83	0.18	33,43,52,54	0
24	CL	a	603	1/1	0.83	0.13	59,59,59,59	0
25	CLA	C	511	65/65	0.83	0.17	45,57,66,70	0
27	BCR	H	102	40/40	0.83	0.17	34,51,59,65	0
23	SQD	A	603	52/54	0.83	0.17	38,60,78,82	0
27	BCR	B	618	40/40	0.84	0.16	28,40,48,52	0
25	CLA	B	606	65/65	0.84	0.16	29,44,65,84	0
25	CLA	C	510	65/65	0.84	0.15	41,51,58,60	0
25	CLA	b	617	65/65	0.84	0.15	34,45,63,73	0
25	CLA	c	505	65/65	0.84	0.16	32,51,62,68	0
27	BCR	K	101	40/40	0.84	0.18	45,53,60,66	0
27	BCR	T	101	40/40	0.84	0.18	31,43,58,62	0
25	CLA	c	506	65/65	0.84	0.16	36,49,70,74	0
31	LHG	A	617	49/49	0.84	0.20	33,55,78,82	0
25	CLA	c	514	65/65	0.84	0.17	45,59,78,83	0
27	BCR	c	516	40/40	0.84	0.19	33,63,70,72	0
27	BCR	d	405	40/40	0.84	0.17	29,43,56,62	0
33	DGD	C	518	62/66	0.84	0.16	33,48,65,74	0
29	LMG	D	405	51/55	0.84	0.19	34,53,88,92	0
25	CLA	C	503	65/65	0.84	0.16	37,49,58,65	0
25	CLA	C	513	65/65	0.85	0.15	41,62,74,83	0
25	CLA	d	404	65/65	0.85	0.16	32,46,73,91	0
25	CLA	c	508	65/65	0.85	0.16	34,49,72,78	0
27	BCR	B	619	40/40	0.85	0.15	33,44,58,60	0
30	UNL	M	101	6/-	0.85	0.20	41,46,52,65	0
33	DGD	H	103	62/66	0.85	0.16	26,41,53,61	0
25	CLA	c	510	58/65	0.85	0.17	34,46,59,67	0
33	DGD	c	520	62/66	0.85	0.17	36,47,72,80	0
25	CLA	C	502	65/65	0.85	0.16	35,51,62,69	0
30	UNL	M	102	17/-	0.86	0.15	31,37,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	614	65/65	0.86	0.14	32,42,63,82	0
29	LMG	d	406	42/55	0.86	0.16	38,48,63,73	0
25	CLA	C	508	65/65	0.86	0.16	38,49,82,90	0
27	BCR	b	621	40/40	0.86	0.15	31,42,57,59	0
25	CLA	c	507	65/65	0.86	0.15	32,44,61,64	0
31	LHG	a	614	35/49	0.86	0.15	36,47,56,58	0
25	CLA	B	608	65/65	0.87	0.14	29,37,47,52	0
25	CLA	C	509	65/65	0.87	0.15	33,46,59,67	0
25	CLA	B	609	65/65	0.87	0.14	24,44,52,58	0
25	CLA	b	611	65/65	0.87	0.14	27,41,54,57	0
25	CLA	c	509	65/65	0.87	0.14	30,39,51,55	0
31	LHG	l	101	49/49	0.87	0.15	30,45,54,56	0
25	CLA	C	505	65/65	0.87	0.14	33,41,55,62	0
27	BCR	C	515	40/40	0.87	0.17	32,42,52,53	0
25	CLA	c	511	65/65	0.87	0.15	38,46,55,57	0
33	DGD	c	518	62/66	0.87	0.15	28,46,63,79	0
25	CLA	c	513	65/65	0.87	0.16	42,52,58,60	0
25	CLA	c	504	65/65	0.87	0.15	32,46,59,65	0
28	PL9	D	407	55/55	0.87	0.15	26,35,45,50	0
25	CLA	B	615	65/65	0.88	0.13	27,41,51,57	0
25	CLA	D	402	65/65	0.88	0.15	24,36,48,59	0
25	CLA	D	403	65/65	0.88	0.13	21,37,63,69	0
27	BCR	b	620	40/40	0.88	0.15	33,45,53,54	0
25	CLA	C	506	65/65	0.88	0.14	32,47,64,68	0
25	CLA	b	605	65/65	0.88	0.14	31,43,56,58	0
33	DGD	C	516	62/66	0.88	0.15	21,39,63,71	0
33	DGD	C	517	62/66	0.88	0.14	39,51,74,83	0
25	CLA	b	609	65/65	0.88	0.15	21,35,59,81	0
27	BCR	c	517	40/40	0.88	0.14	19,39,50,52	0
25	CLA	C	507	65/65	0.88	0.14	32,42,52,67	0
25	CLA	B	604	65/65	0.88	0.14	28,37,57,65	0
25	CLA	c	512	65/65	0.88	0.14	31,47,56,64	0
25	CLA	b	619	65/65	0.88	0.14	30,44,72,80	0
34	HEM	e	101	43/43	0.88	0.16	50,62,69,70	0
31	LHG	D	406	49/49	0.89	0.13	25,40,50,59	0
31	LHG	L	101	49/49	0.89	0.14	29,41,51,57	0
31	LHG	a	613	49/49	0.89	0.14	26,43,56,60	0
28	PL9	d	408	55/55	0.89	0.14	21,33,43,45	0
25	CLA	b	612	65/65	0.89	0.14	28,41,55,61	0
25	CLA	b	614	65/65	0.89	0.12	25,35,41,50	0
25	CLA	B	616	65/65	0.89	0.13	32,44,70,76	0
25	CLA	b	618	65/65	0.89	0.14	28,40,47,56	0

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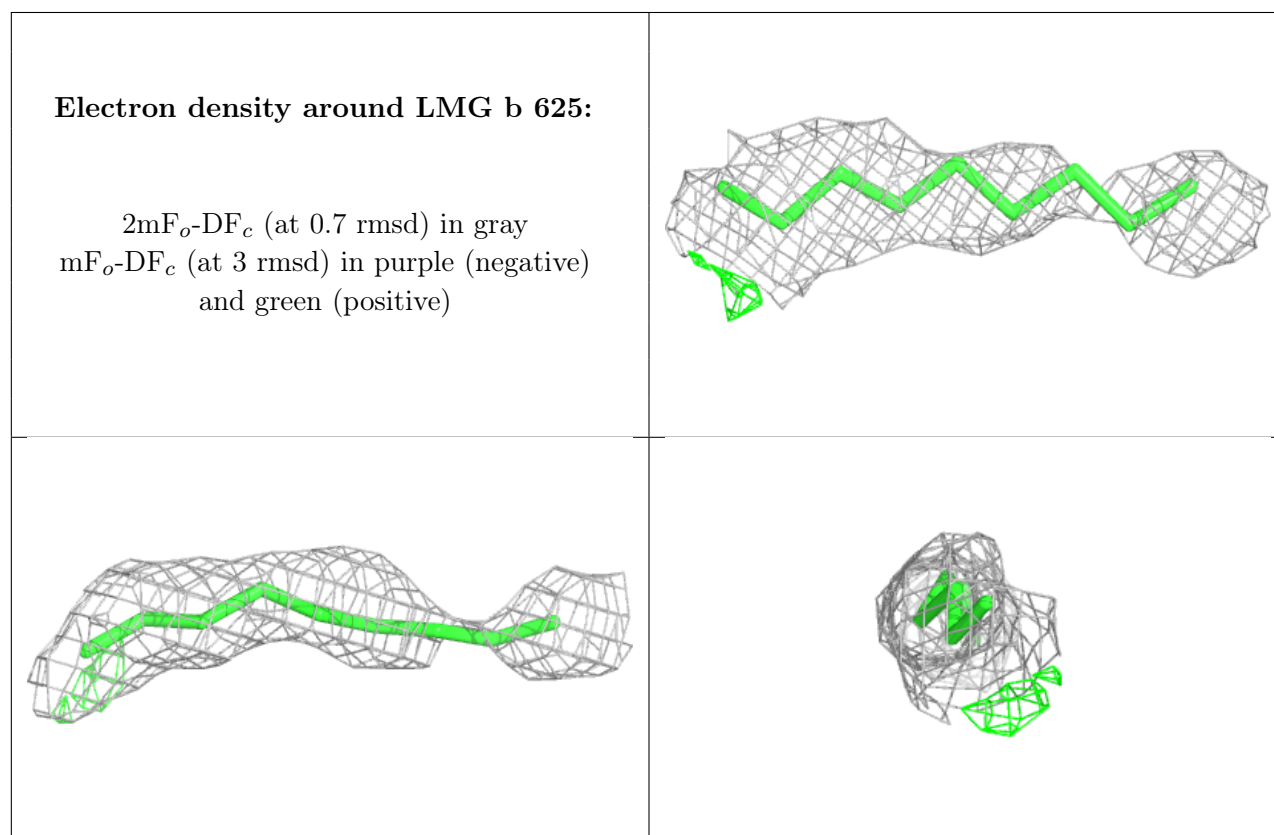
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	603	65/65	0.89	0.14	28,37,45,47	0
25	CLA	b	607	65/65	0.89	0.12	24,34,48,53	0
25	CLA	b	608	65/65	0.89	0.13	30,40,46,51	0
25	CLA	B	607	65/65	0.89	0.13	26,36,44,54	0
25	CLA	a	609	65/65	0.89	0.15	19,34,71,81	0
31	LHG	A	616	49/49	0.89	0.13	24,41,54,58	0
26	PHO	D	401	64/64	0.89	0.13	27,37,47,54	0
26	PHO	d	401	64/64	0.89	0.14	24,39,45,49	0
25	CLA	b	616	65/65	0.90	0.13	25,33,51,62	0
25	CLA	A	606	65/65	0.90	0.14	26,34,45,48	0
25	CLA	A	607	57/65	0.90	0.13	29,37,49,67	0
27	BCR	A	610	40/40	0.90	0.13	22,34,44,47	0
27	BCR	B	617	40/40	0.90	0.13	32,41,49,50	0
24	CL	a	604	1/1	0.90	0.13	42,42,42,42	0
25	CLA	B	610	65/65	0.90	0.12	25,33,39,45	0
25	CLA	B	613	65/65	0.90	0.14	19,33,48,69	0
25	CLA	b	613	65/65	0.90	0.13	24,35,43,45	0
34	HEM	E	101	43/43	0.90	0.14	42,54,67,69	0
25	CLA	b	606	65/65	0.90	0.13	24,36,50,58	0
31	LHG	d	407	49/49	0.91	0.12	20,37,47,51	0
25	CLA	A	609	65/65	0.91	0.15	17,29,79,89	0
26	PHO	A	608	64/64	0.91	0.12	23,32,37,43	0
25	CLA	b	615	65/65	0.91	0.12	22,32,41,50	0
25	CLA	B	611	65/65	0.91	0.12	21,31,38,44	0
25	CLA	a	606	65/65	0.91	0.12	23,31,38,39	0
27	BCR	a	610	40/40	0.91	0.12	19,32,45,47	0
25	CLA	C	501	65/65	0.91	0.12	34,42,49,54	0
25	CLA	b	610	65/65	0.91	0.12	23,37,51,54	0
25	CLA	a	612	65/65	0.91	0.12	17,29,37,39	0
25	CLA	B	605	65/65	0.91	0.12	24,34,40,42	0
25	CLA	A	615	65/65	0.91	0.12	22,34,43,47	0
25	CLA	d	403	65/65	0.91	0.13	24,36,45,50	0
35	HEC	V	201	43/43	0.91	0.13	31,44,52,56	0
25	CLA	c	503	65/65	0.92	0.12	27,40,46,52	0
26	PHO	a	608	64/64	0.92	0.12	19,28,38,42	0
25	CLA	B	612	65/65	0.92	0.12	26,35,42,46	0
25	CLA	B	602	65/65	0.93	0.12	29,39,47,52	0
25	CLA	a	607	59/65	0.93	0.11	27,37,55,72	0
24	CL	A	605	1/1	0.93	0.11	44,44,44,44	0
22	FE2	a	602	1/1	0.93	0.07	62,62,62,62	0
35	HEC	v	201	43/43	0.93	0.11	32,41,48,52	0
32	BCT	A	620	4/4	0.94	0.10	26,36,37,44	0

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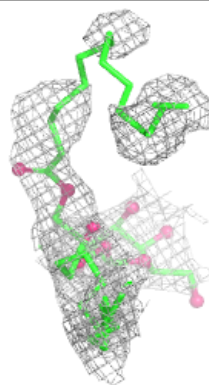
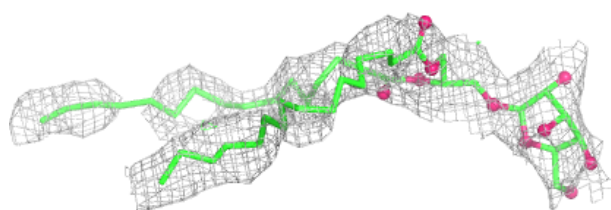
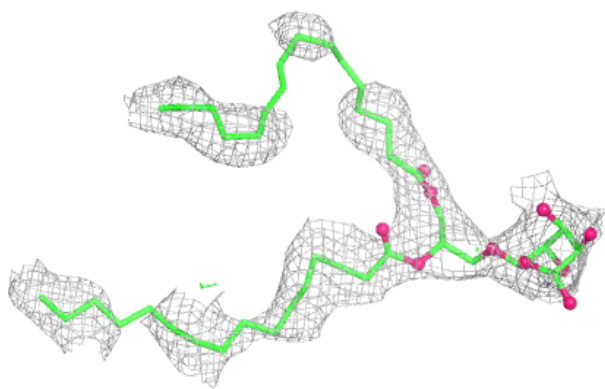
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	FE2	A	602	1/1	0.95	0.08	46,46,46,46	0
24	CL	A	604	1/1	0.97	0.08	43,43,43,43	0
21	OEX	a	601	10/10	0.98	0.05	40,44,48,51	0
21	OEX	A	601	10/10	0.99	0.06	33,40,45,46	0

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.

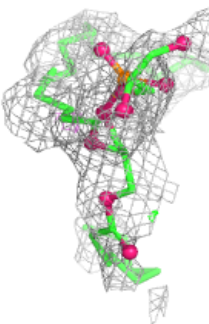
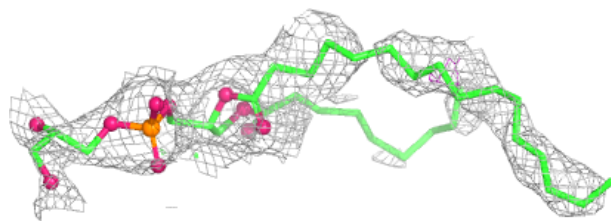
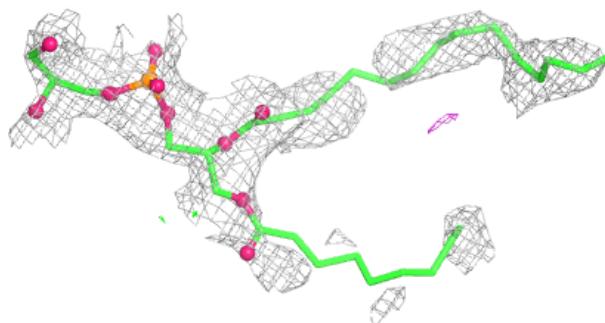


Electron density around LMG b 624:

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

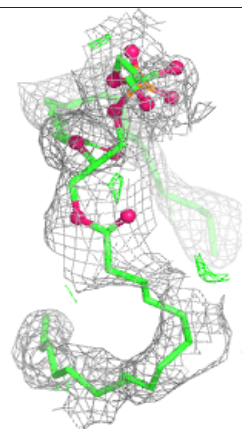
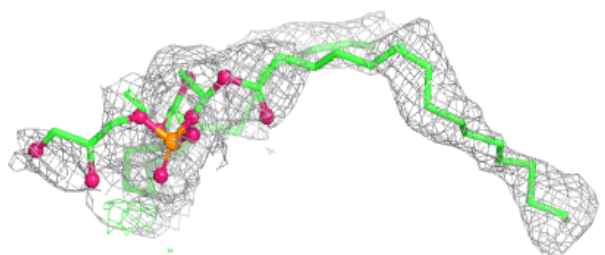
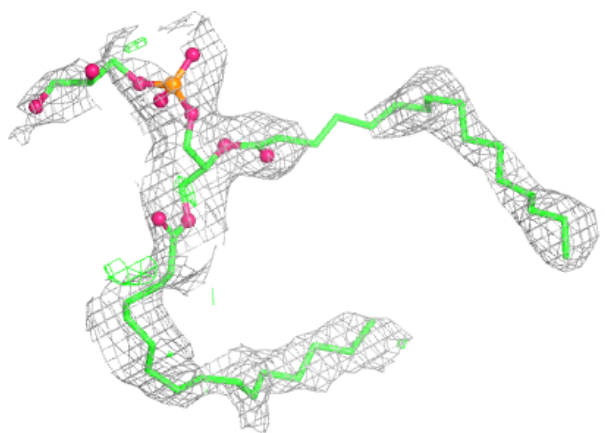
**Electron density around LHG a 615:**

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



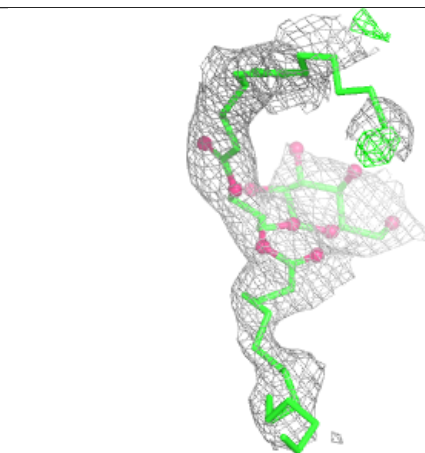
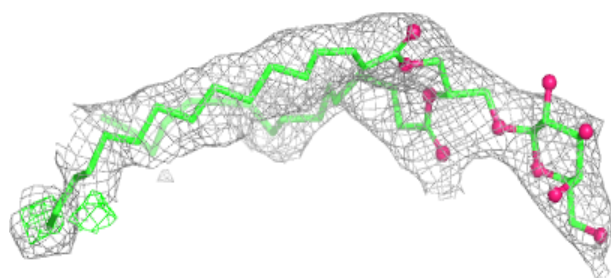
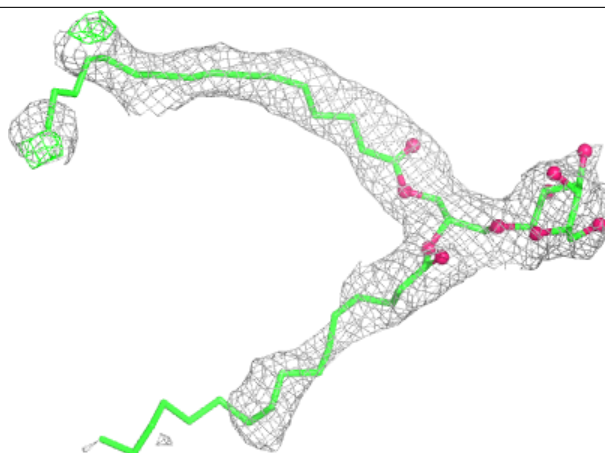
Electron density around LHG A 618:

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

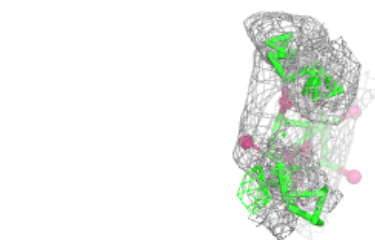
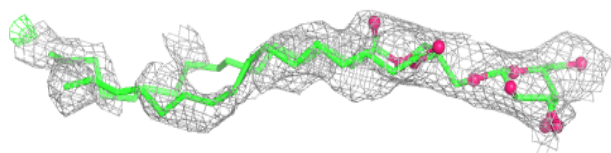
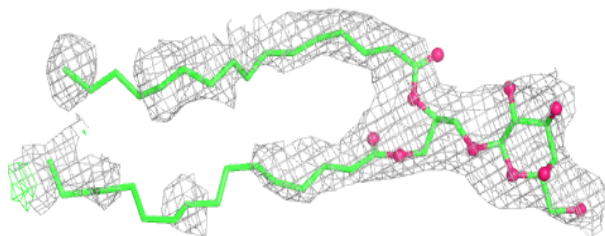


Electron density around LMG B 621:

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

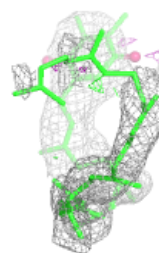
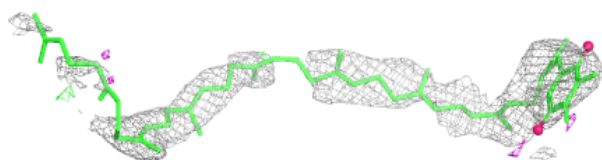
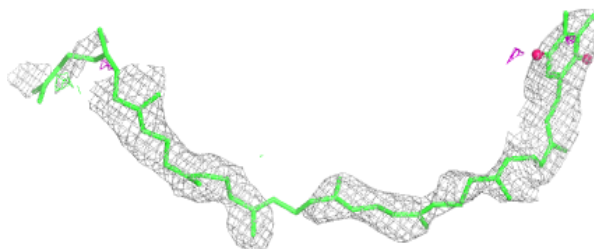
**Electron density around LMG C 520:**

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

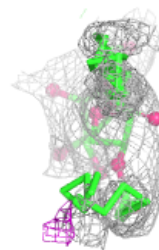
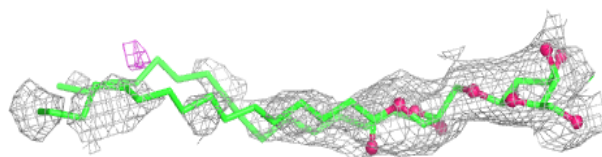
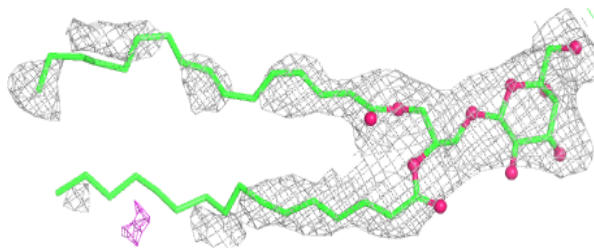


Electron density around PL9 A 611:

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

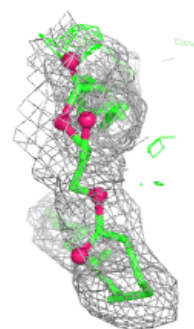
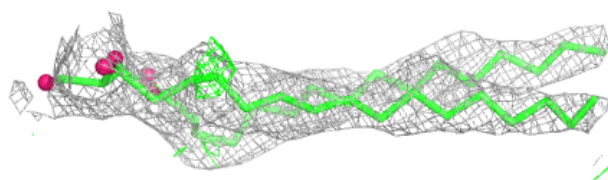
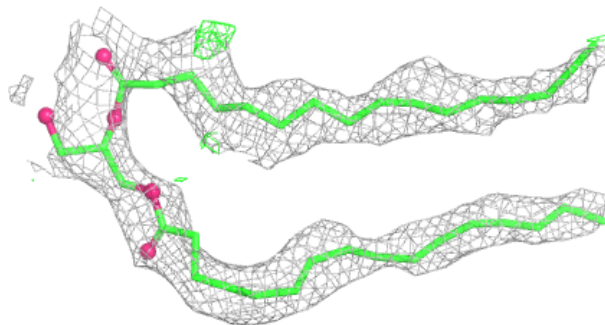
**Electron density around LMG c 522:**

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

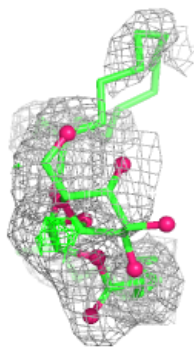
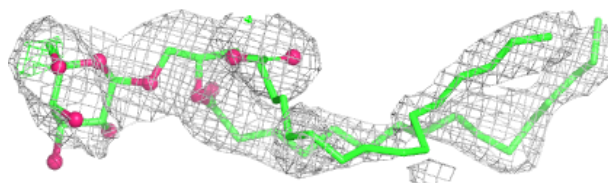
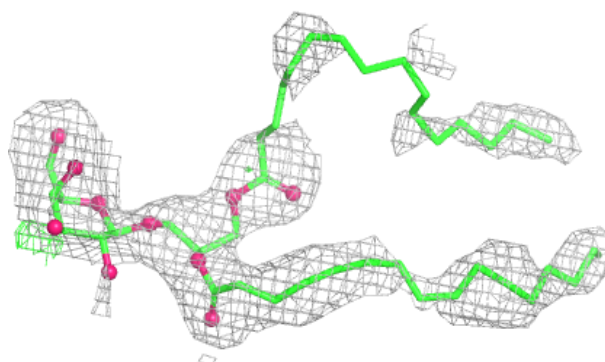


Electron density around LMG d 409:

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

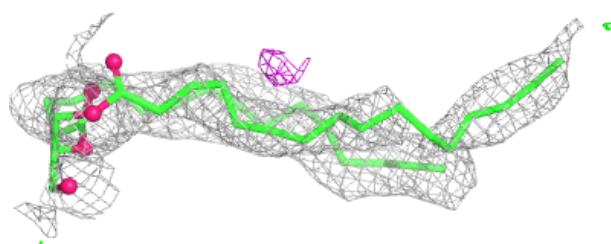
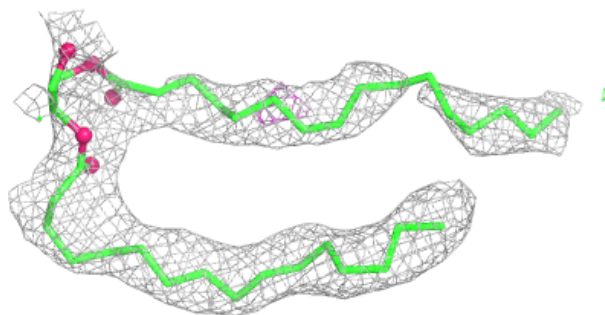
**Electron density around LMG A 613:**

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

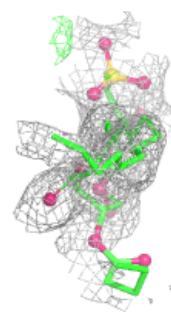
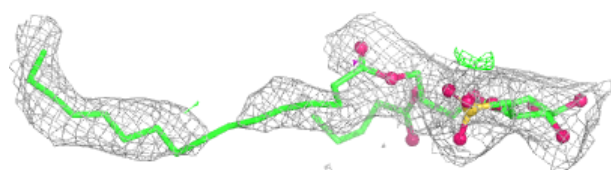
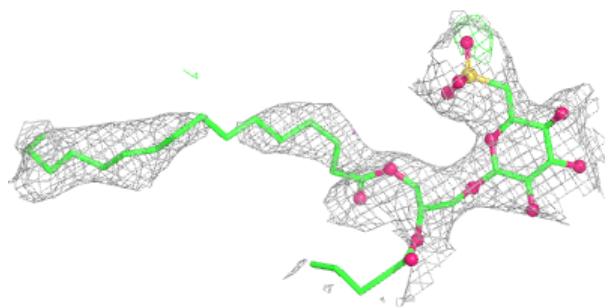


Electron density around SQD I 101:

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

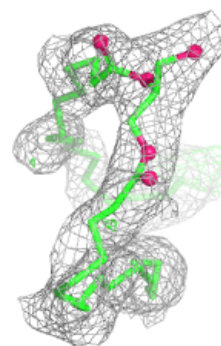
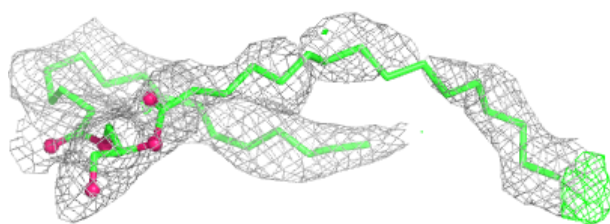
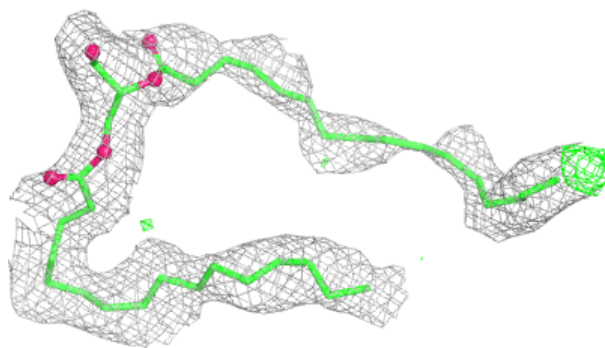
**Electron density around SQD D 409:**

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

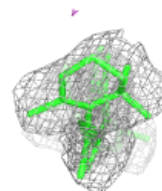
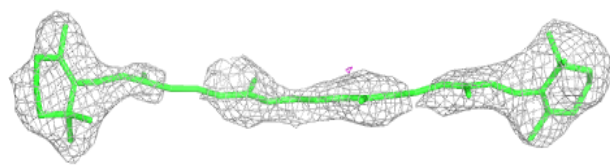
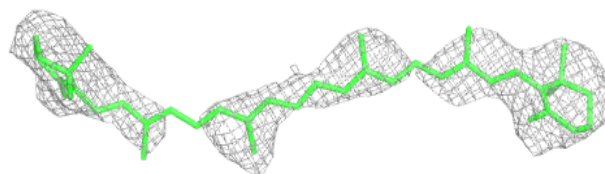


Electron density around SQD A 619:

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

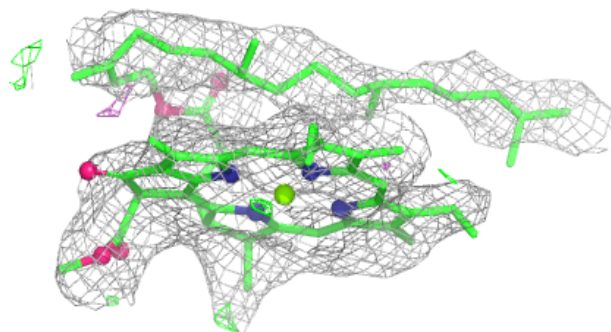
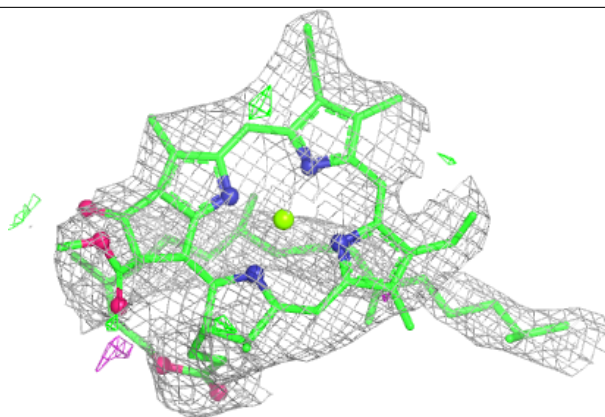
**Electron density around BCR y 101:**

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

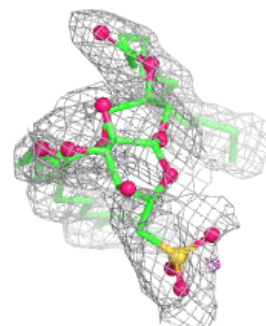
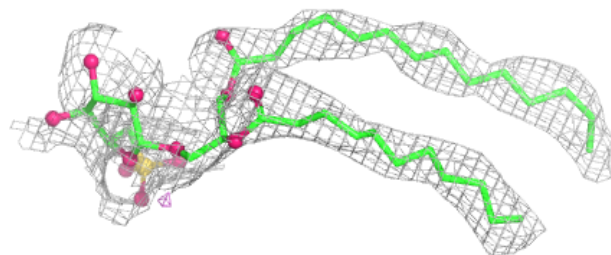
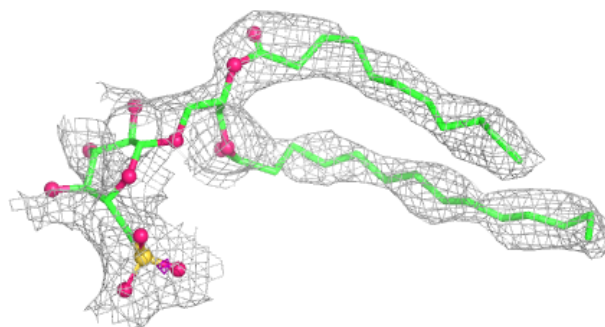


Electron density around CLA b 604:

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

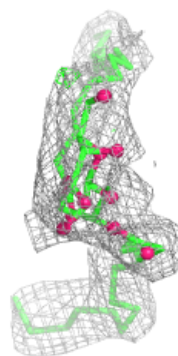
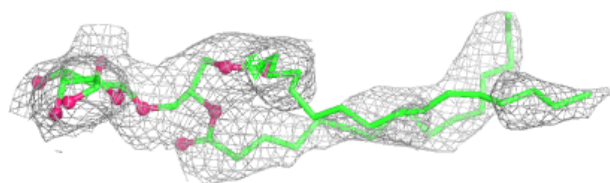
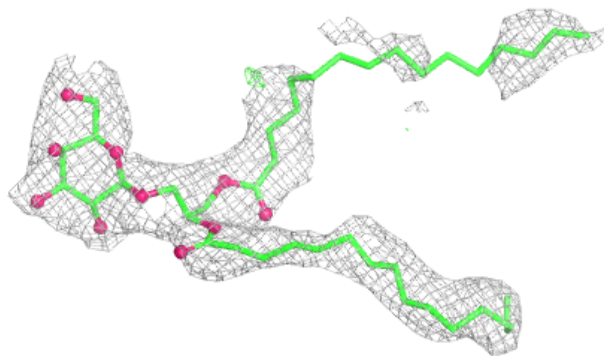
**Electron density around SQD D 408:**

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

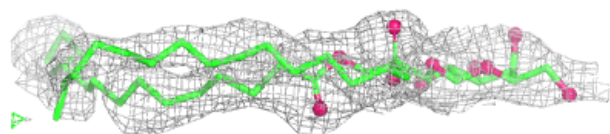
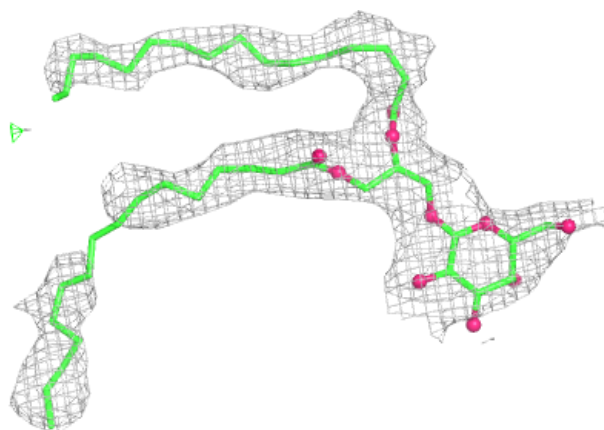


Electron density around LMG B 625:

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

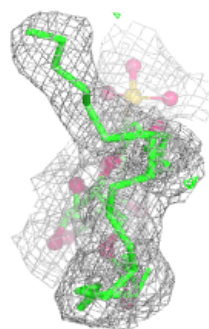
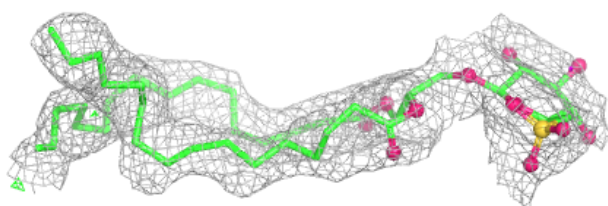
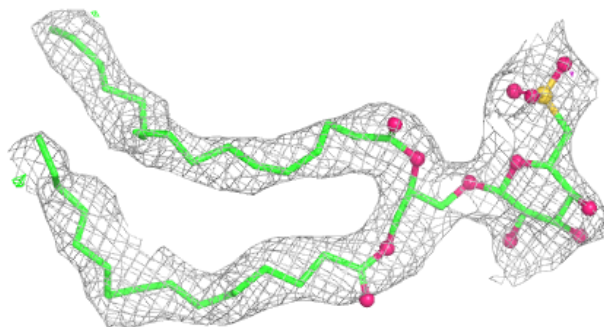
**Electron density around LMG C 519:**

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

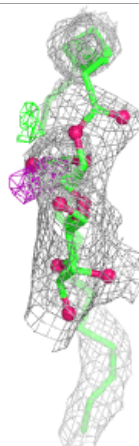
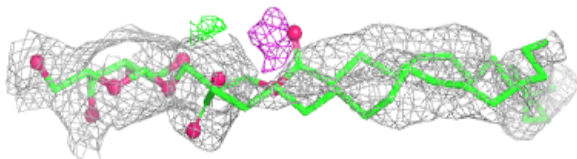
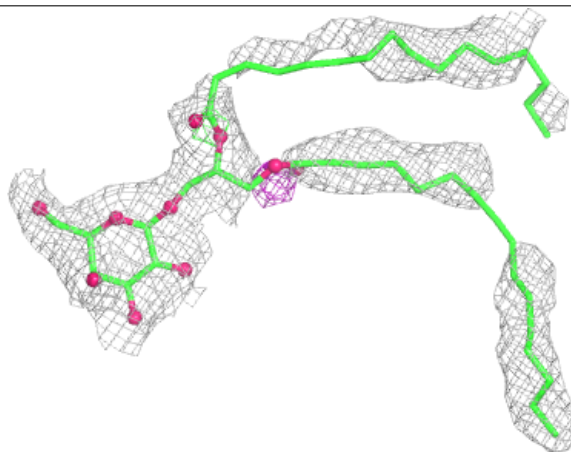


Electron density around SQD B 626:

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

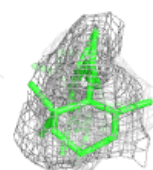
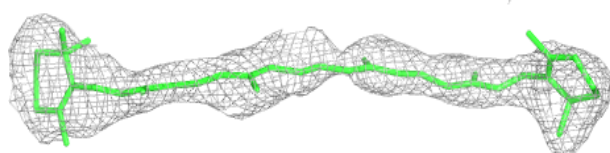
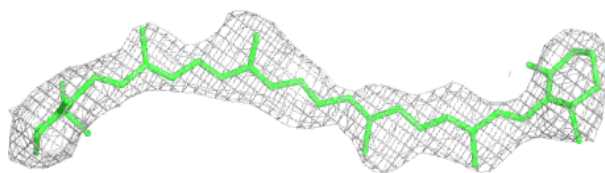
**Electron density around LMG c 521:**

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

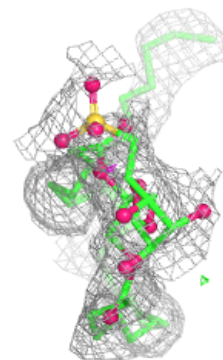
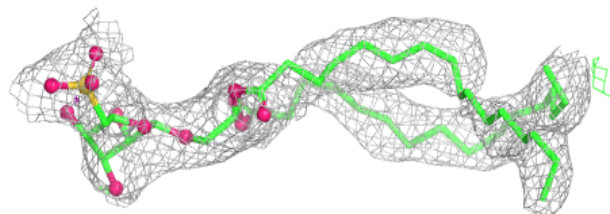
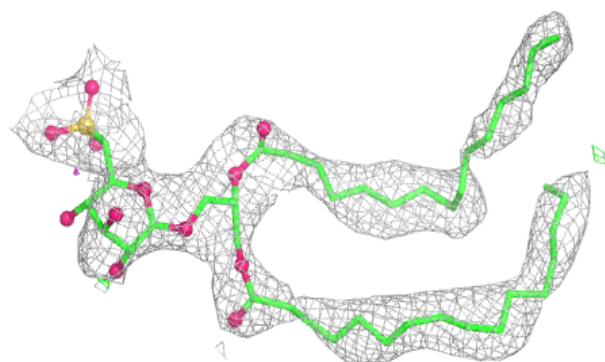


Electron density around BCR Y 101:

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

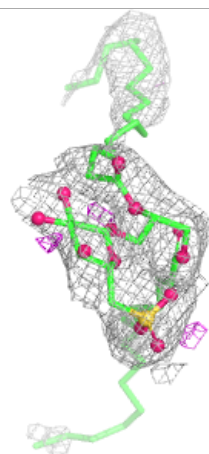
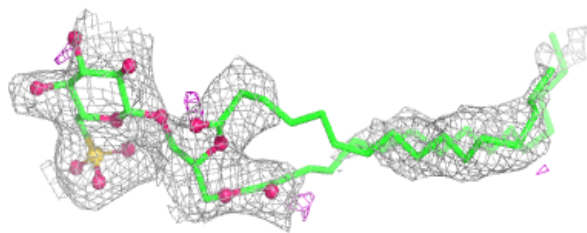
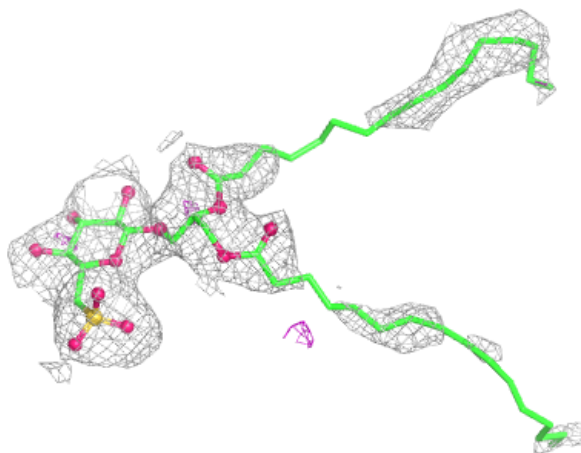
**Electron density around SQD b 601:**

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



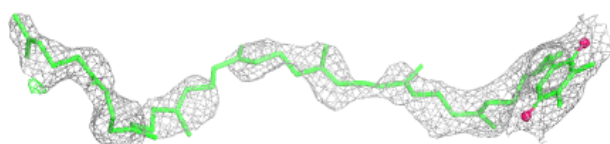
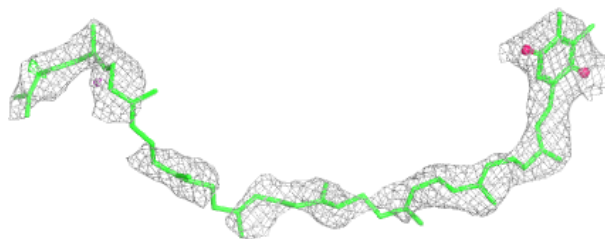
Electron density around SQD c 501:

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

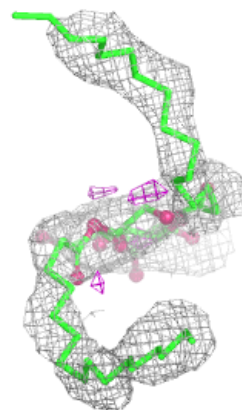
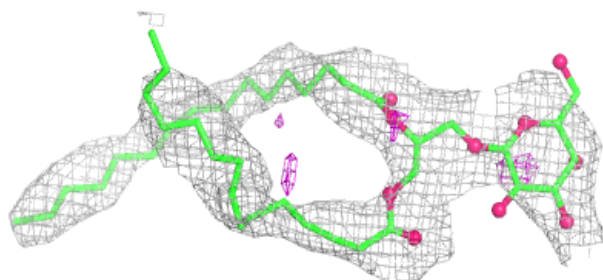


Electron density around PL9 a 611:

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

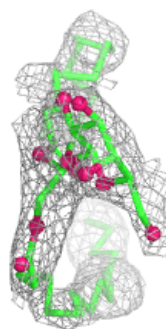
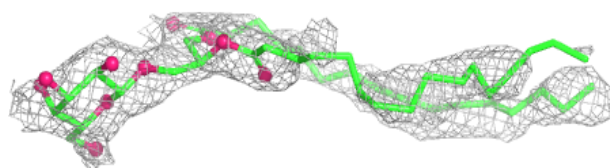
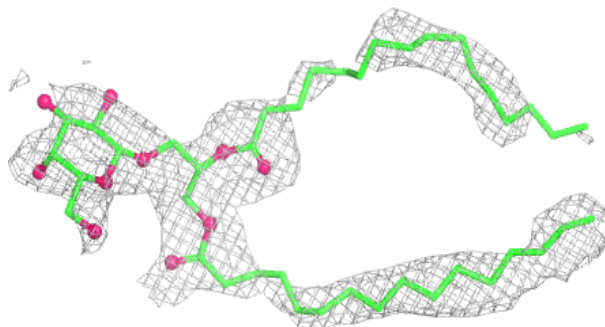
**Electron density around LMG b 623:**

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

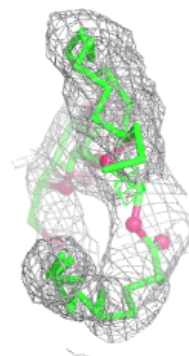
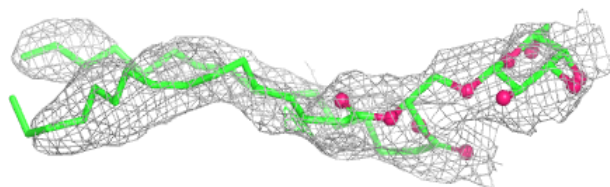
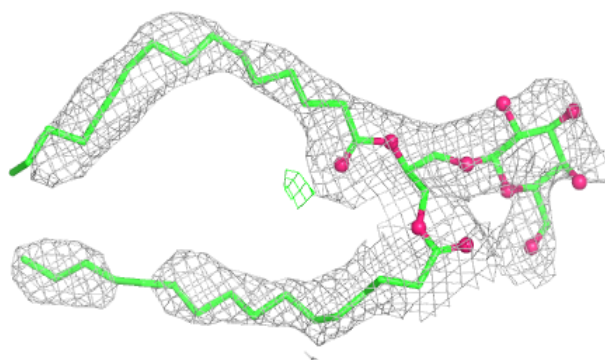


Electron density around LMG A 612:

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

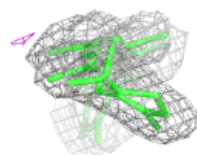
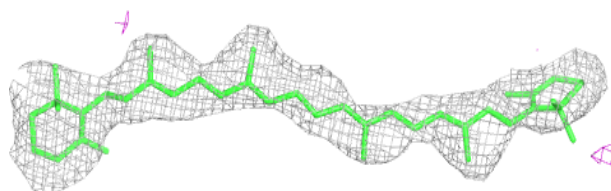
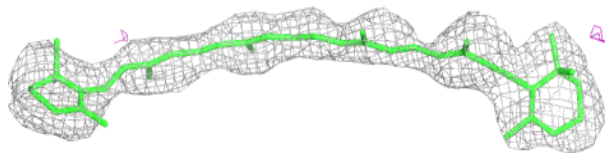
**Electron density around LMG c 502:**

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



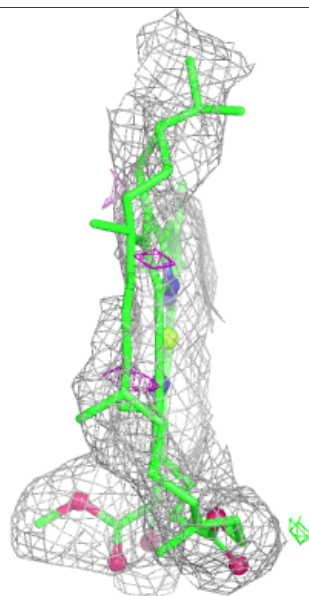
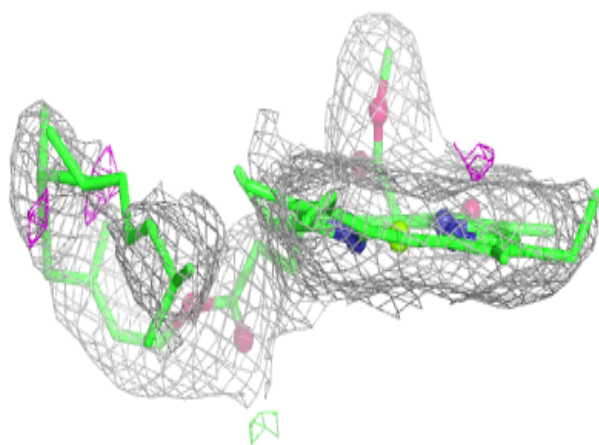
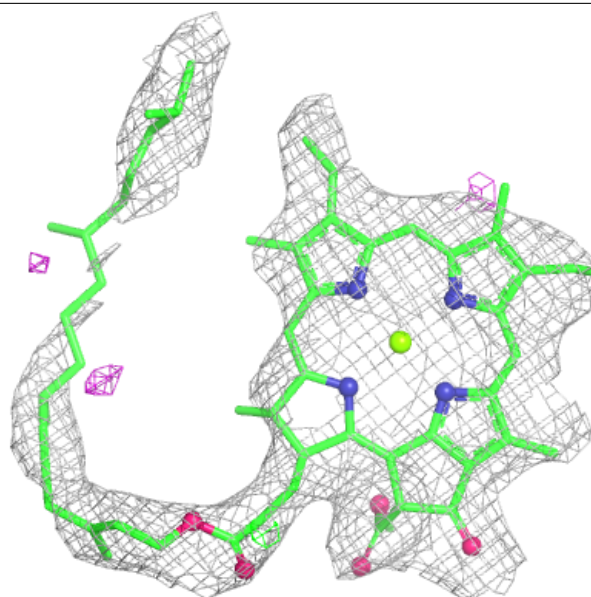
Electron density around BCR D 404:

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



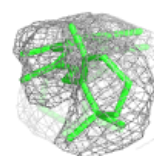
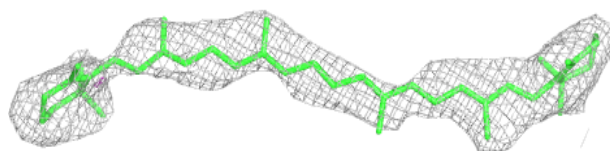
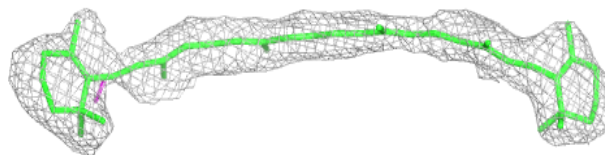
Electron density around CLA C 512:

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

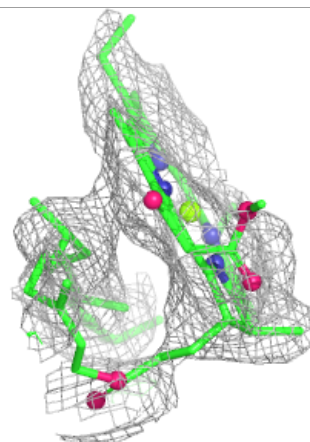
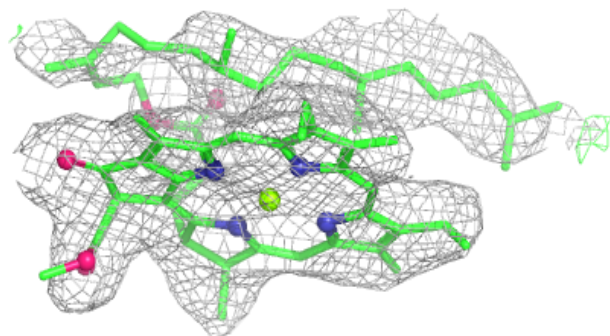
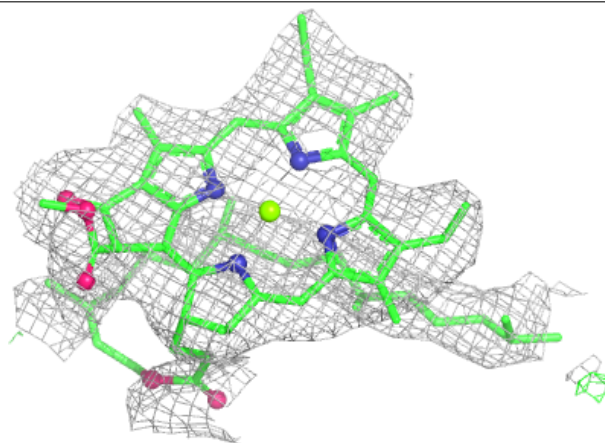


Electron density around BCR k 101:

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

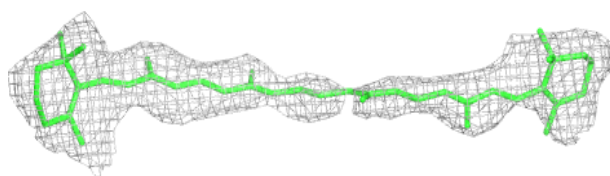
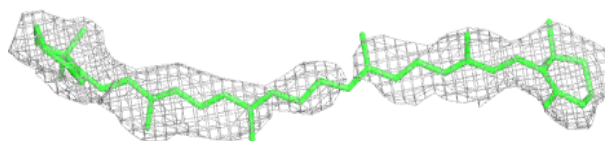
**Electron density around CLA B 601:**

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

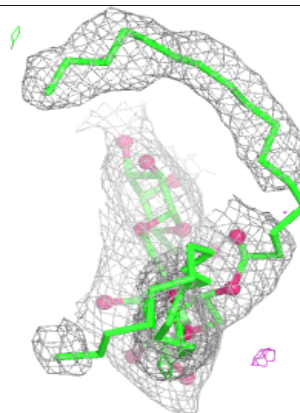
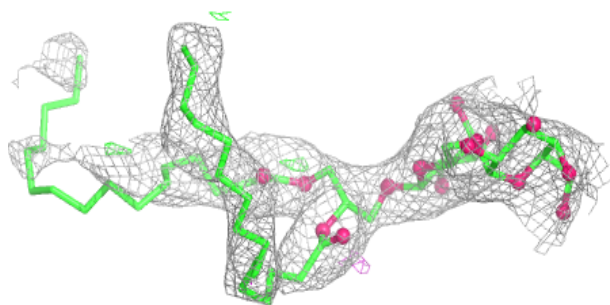
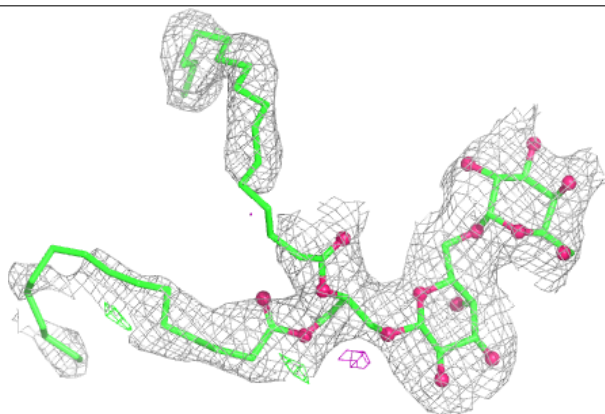


Electron density around BCR C 514:

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

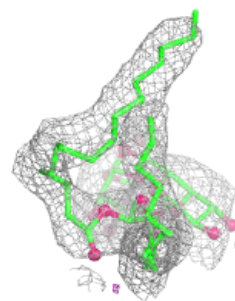
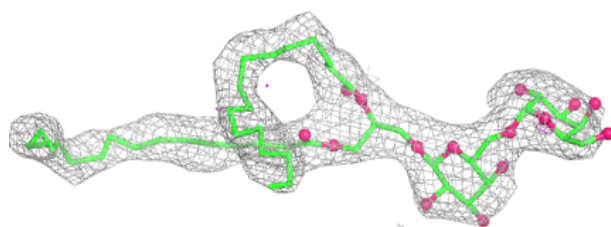
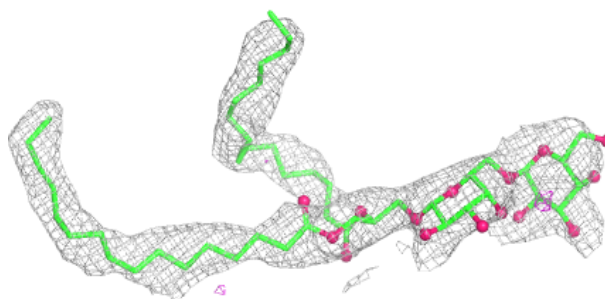
**Electron density around DGD c 519:**

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

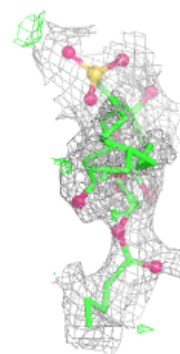
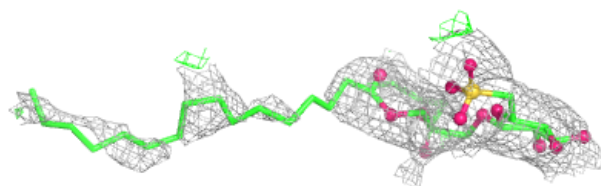
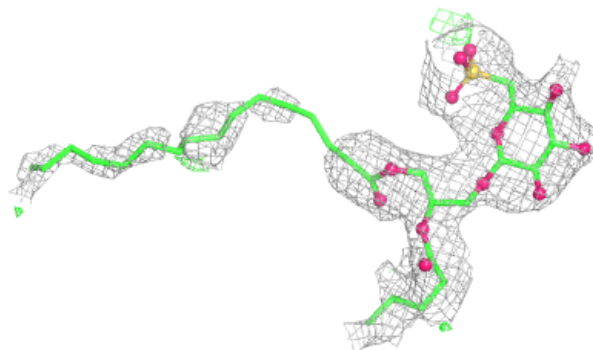


Electron density around DGD h 102:

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

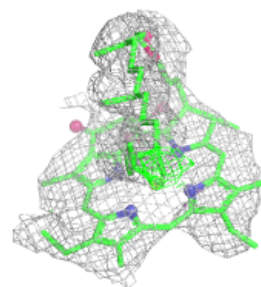
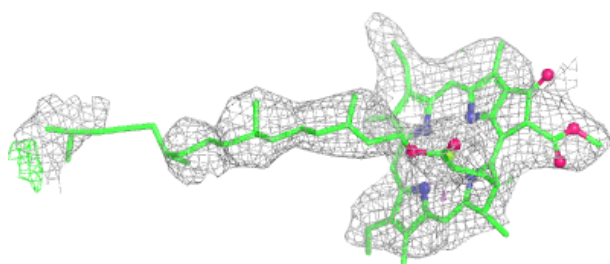
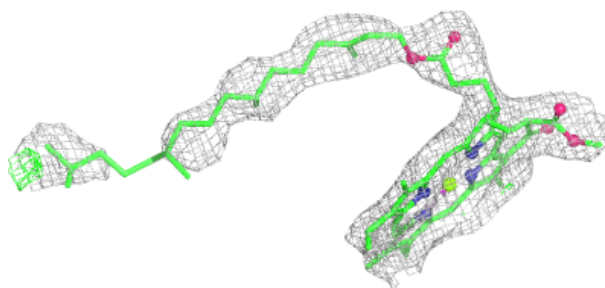
**Electron density around SQD f 101:**

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

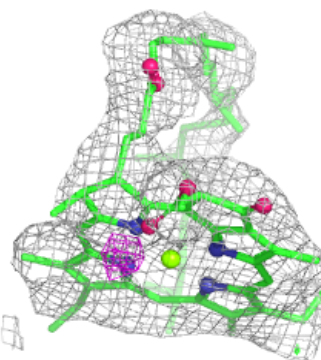
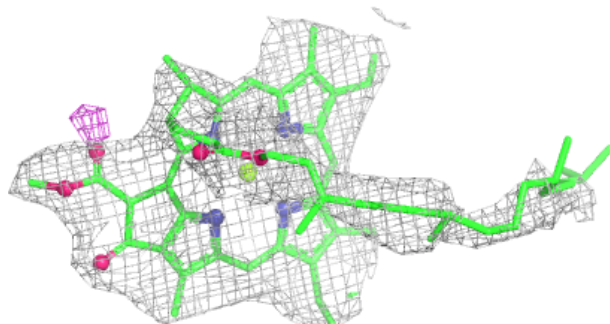
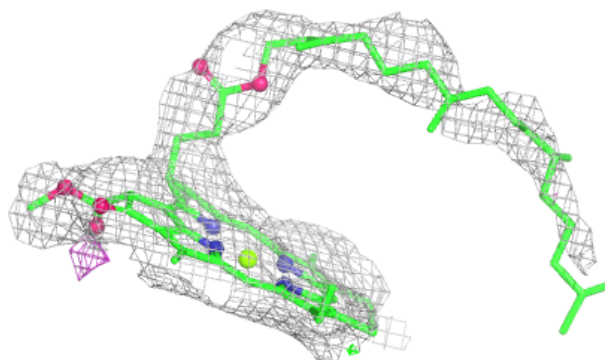


Electron density around CLA C 504:

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

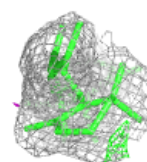
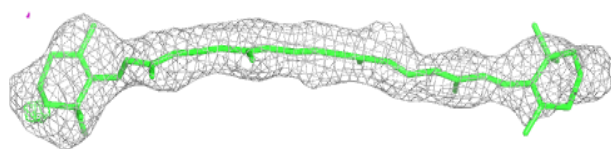
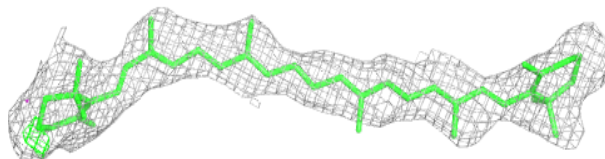
**Electron density around CLA c 515:**

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

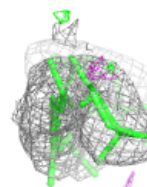
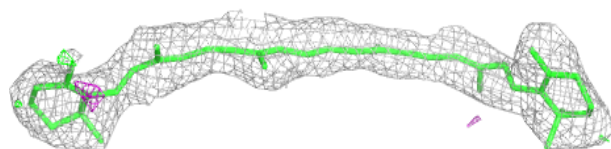
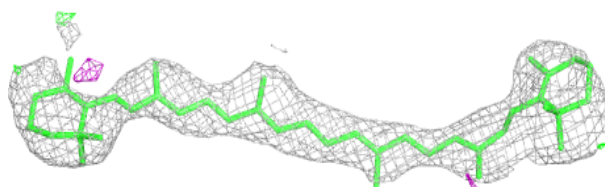


Electron density around BCR h 101:

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

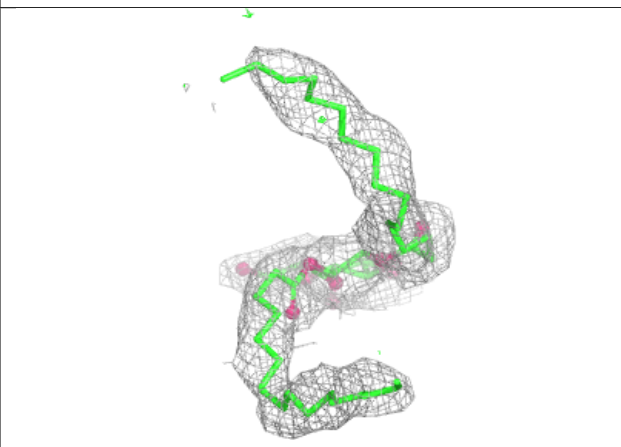
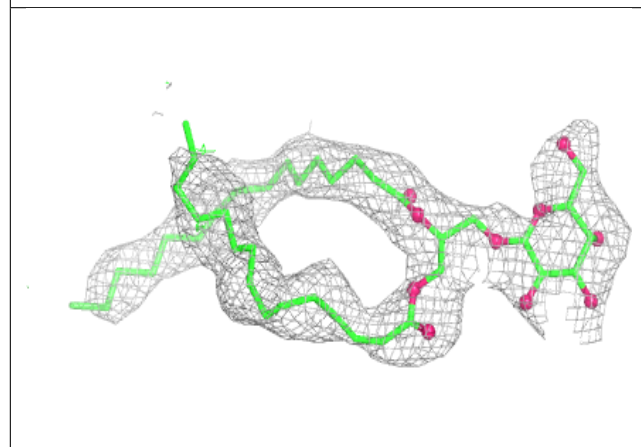
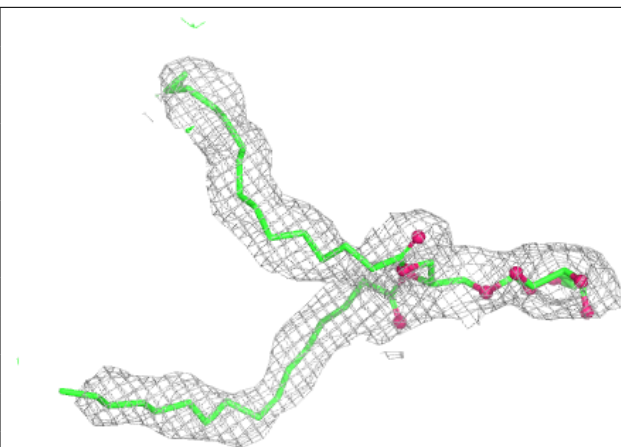
**Electron density around BCR B 627:**

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

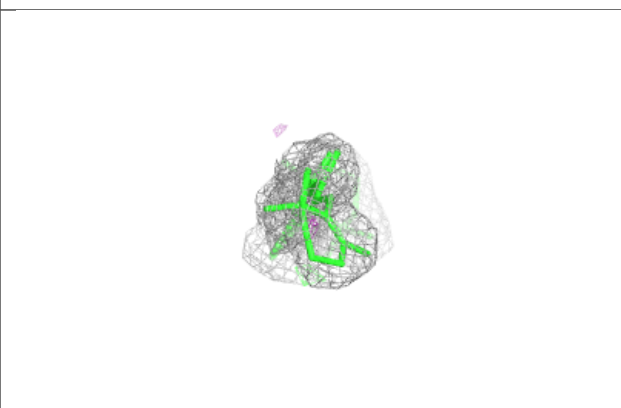
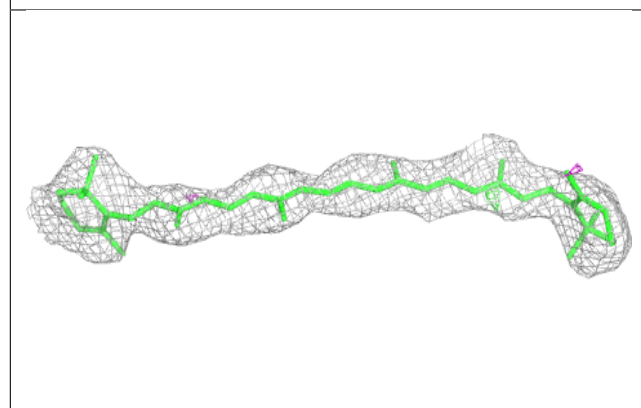
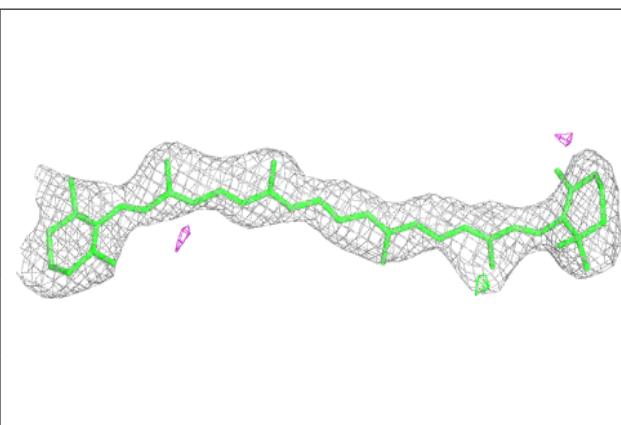


Electron density around LMG B 620:

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

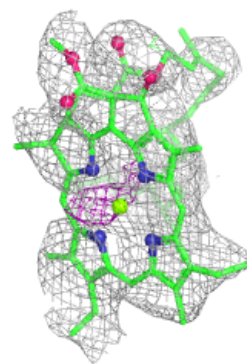
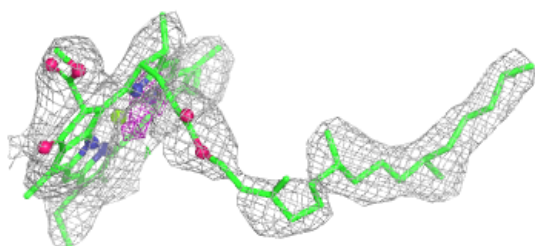
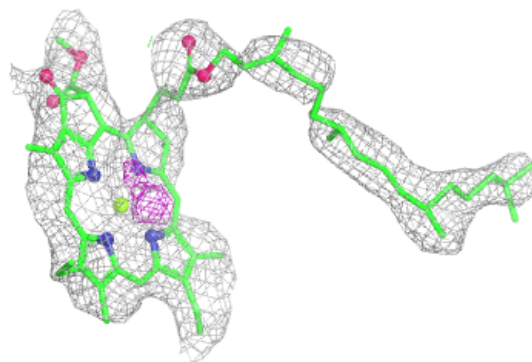
**Electron density around BCR b 622:**

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

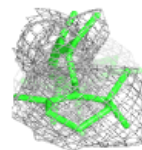
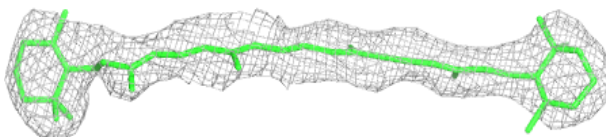
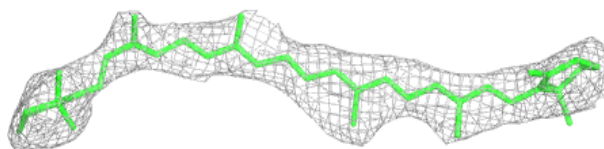


Electron density around CLA C 511:

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

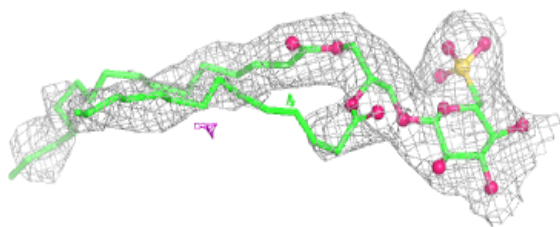
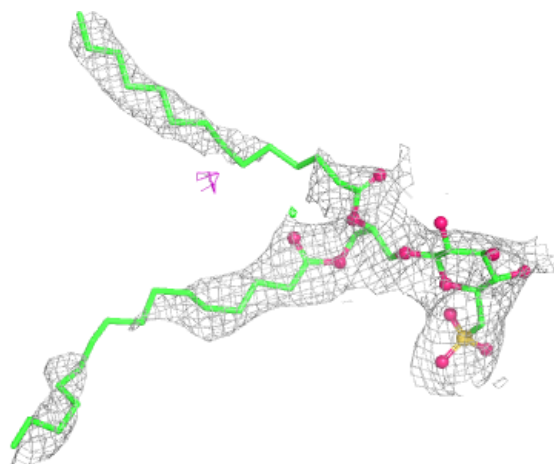
**Electron density around BCR H 102:**

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



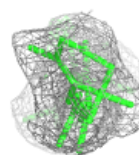
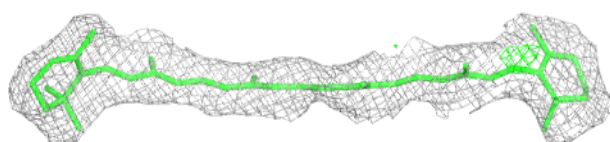
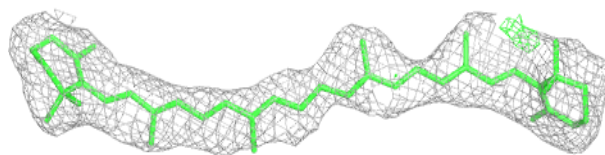
Electron density around SQD A 603:

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

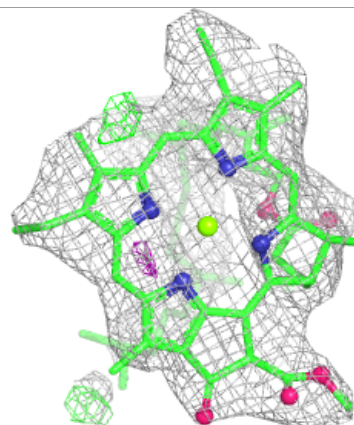
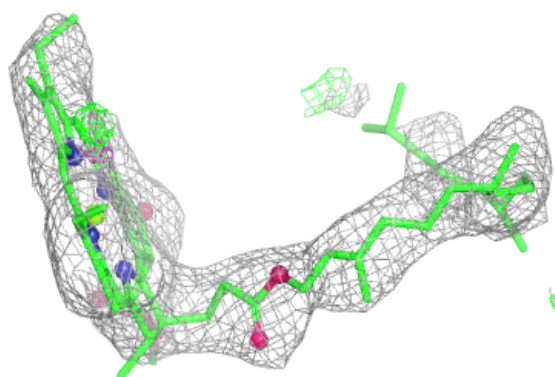
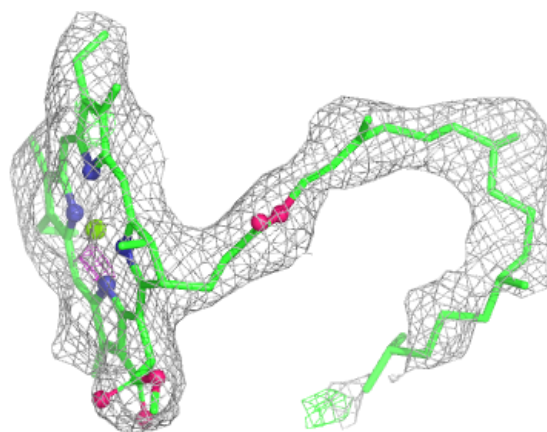


Electron density around BCR B 618:

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

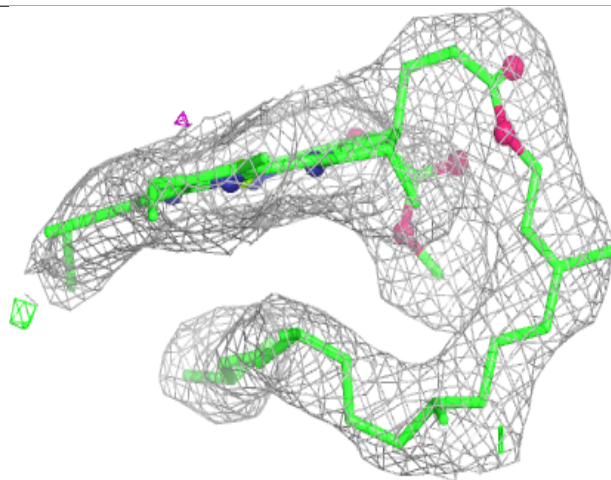
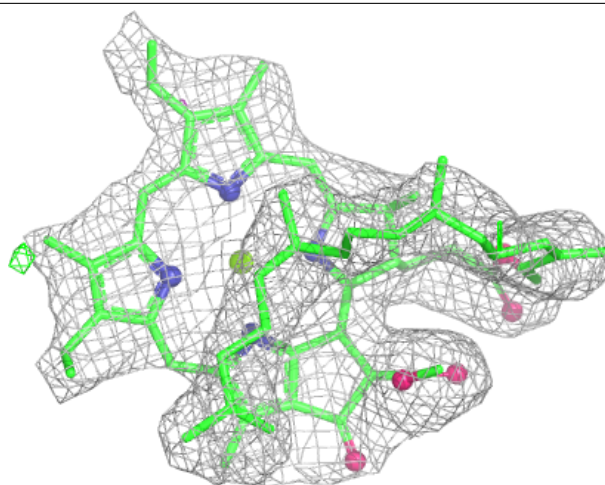
**Electron density around CLA B 606:**

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



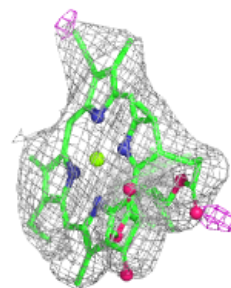
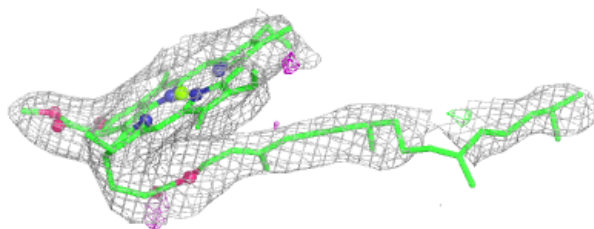
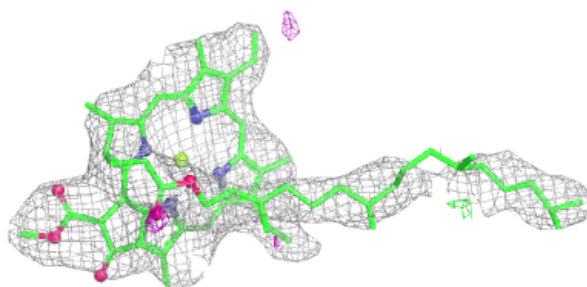
Electron density around CLA C 510:

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



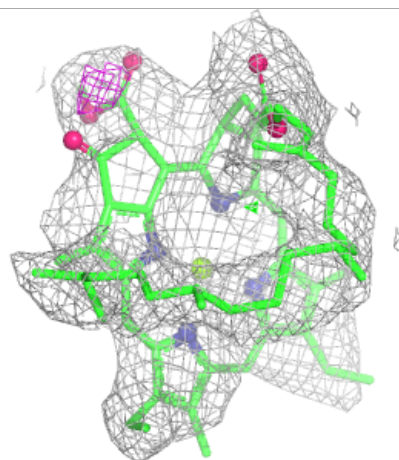
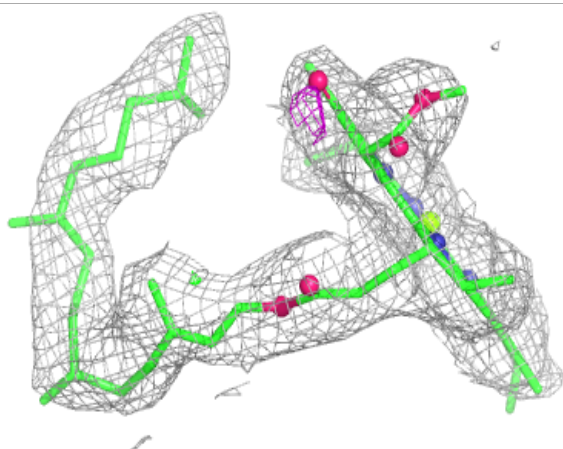
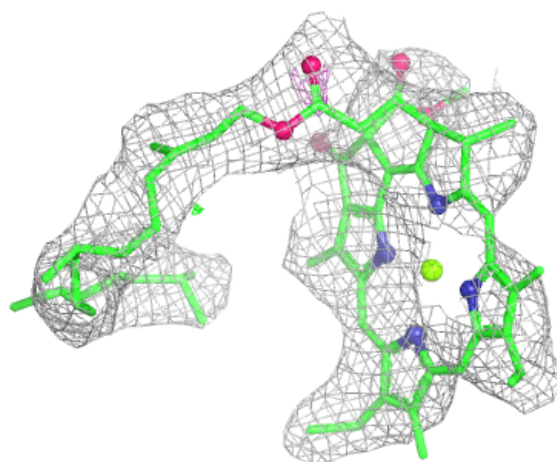
Electron density around CLA b 617:

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



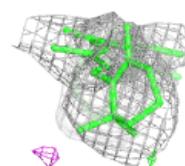
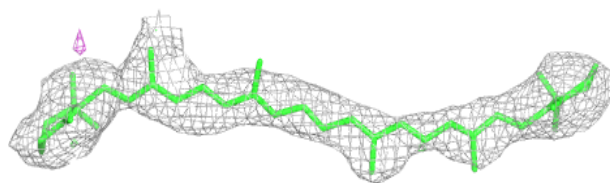
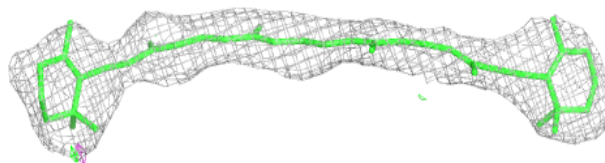
Electron density around CLA c 505:

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

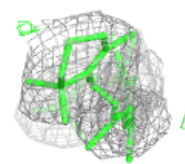
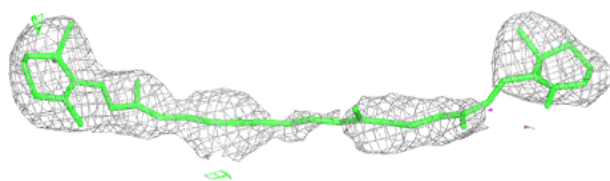
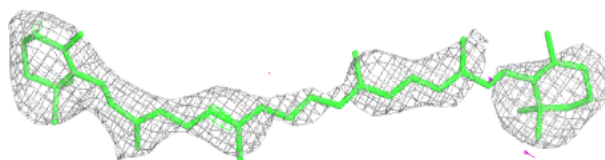


Electron density around BCR K 101:

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

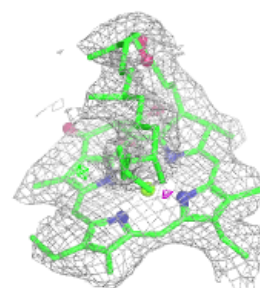
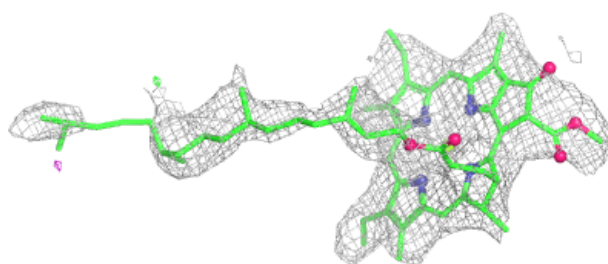
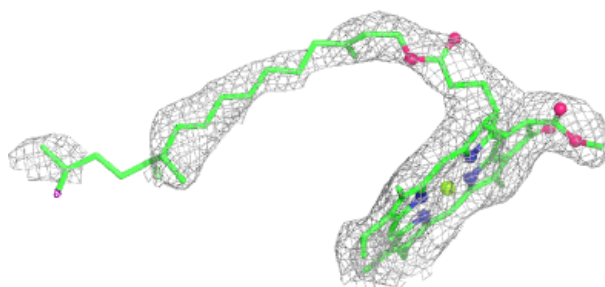
**Electron density around BCR T 101:**

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

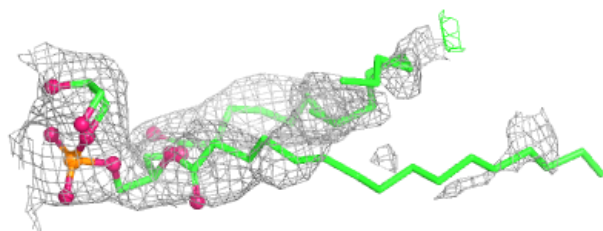
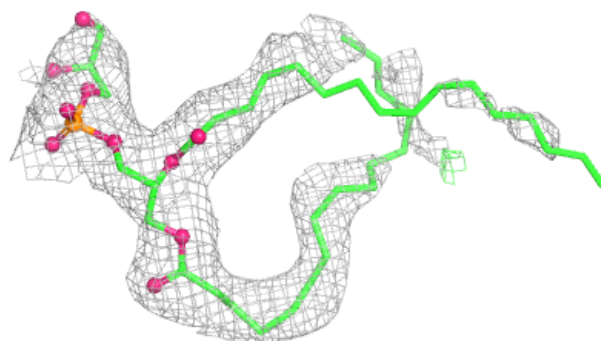


Electron density around CLA c 506:

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

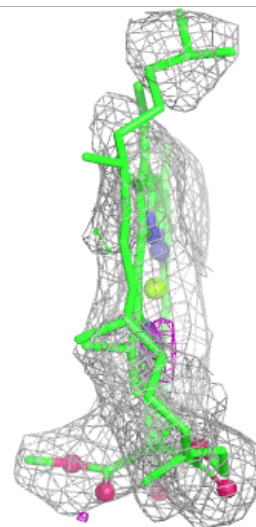
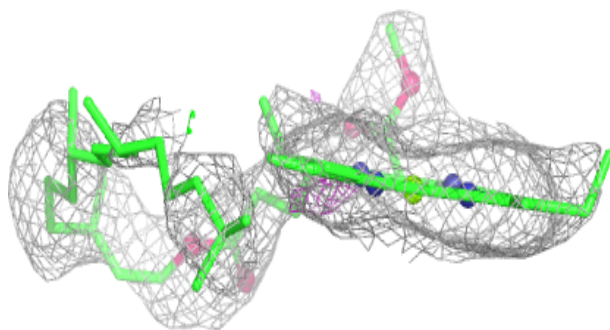
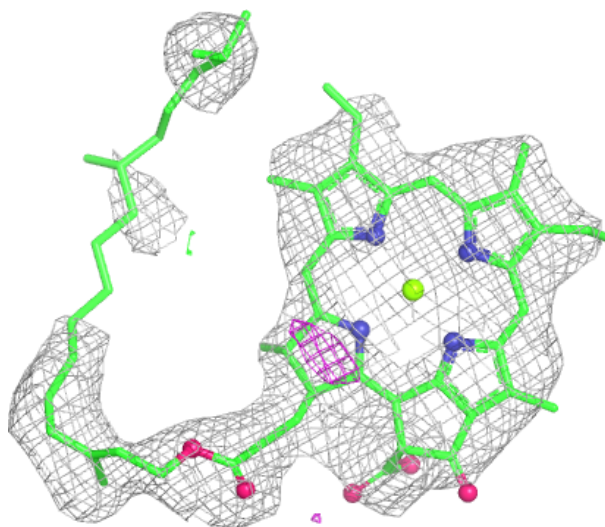
**Electron density around LHG A 617:**

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



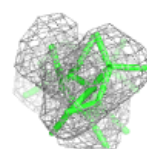
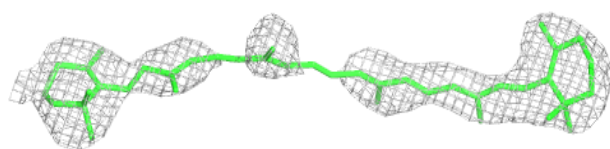
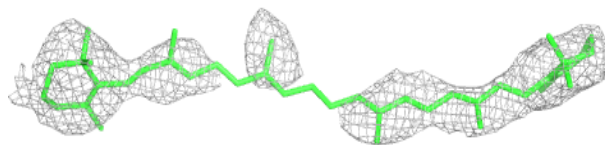
Electron density around CLA c 514:

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

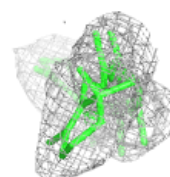
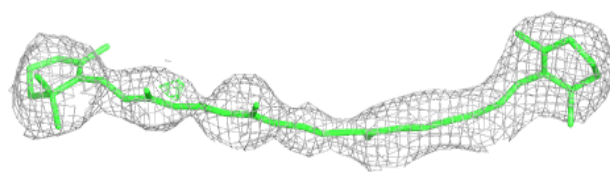
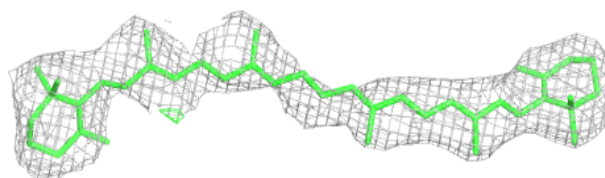


Electron density around BCR c 516:

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

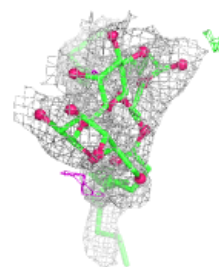
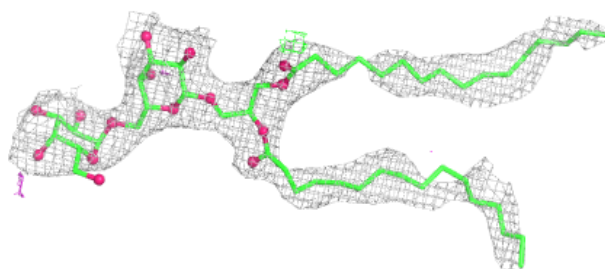
**Electron density around BCR d 405:**

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

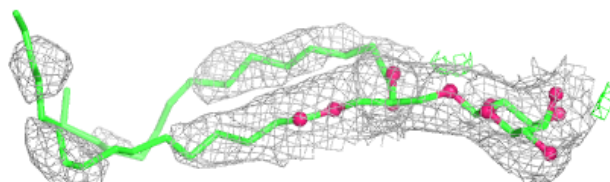
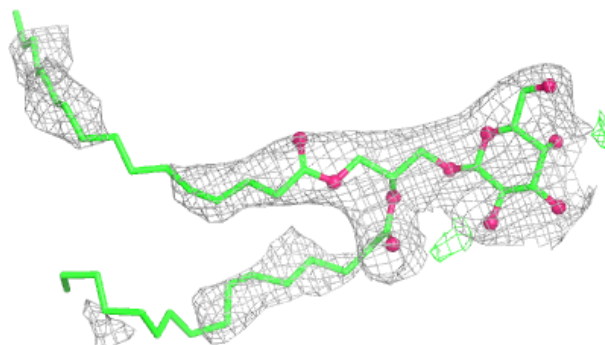


Electron density around DGD C 518:

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

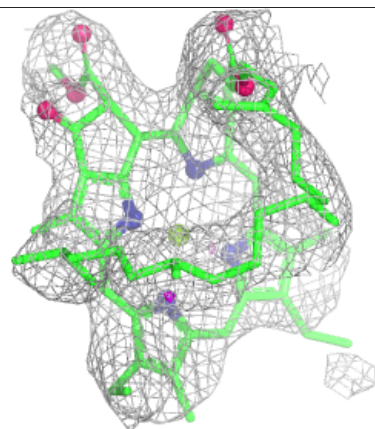
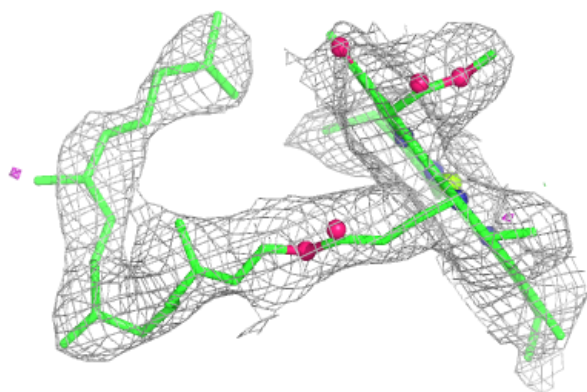
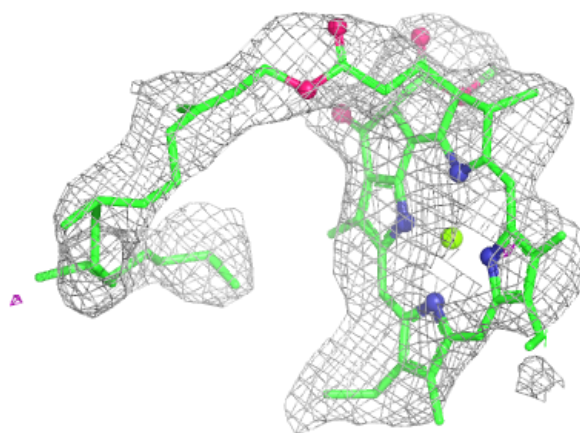
**Electron density around LMG D 405:**

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

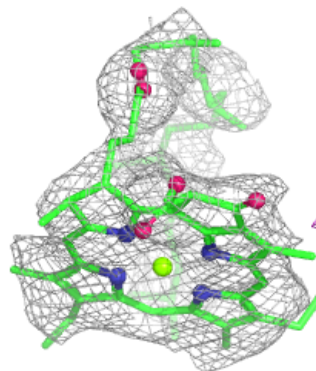
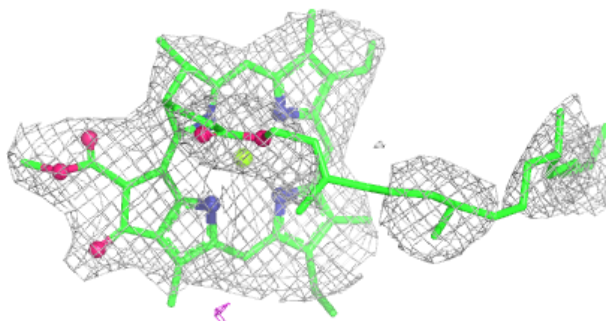
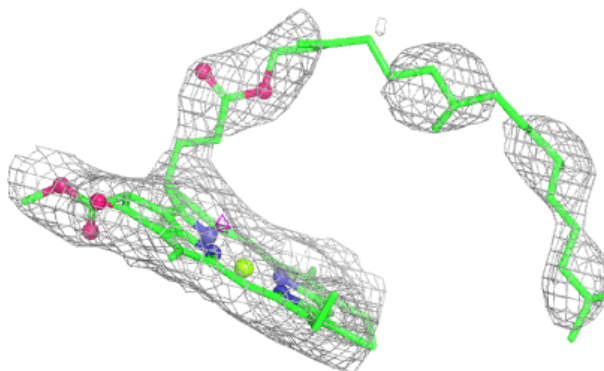


Electron density around CLA C 503:

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

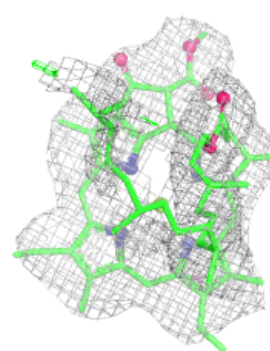
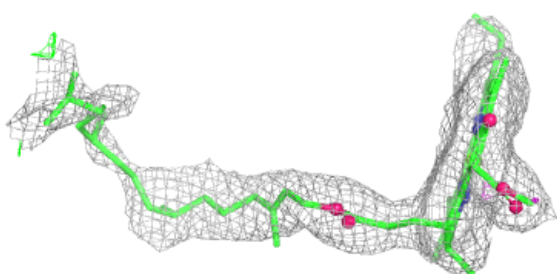
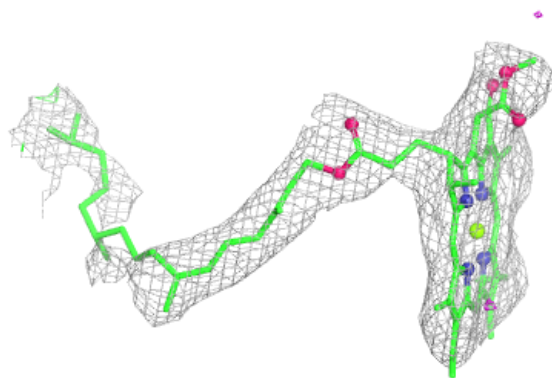
**Electron density around CLA C 513:**

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

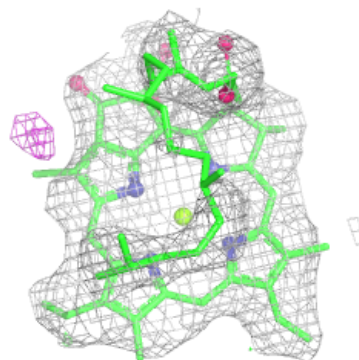
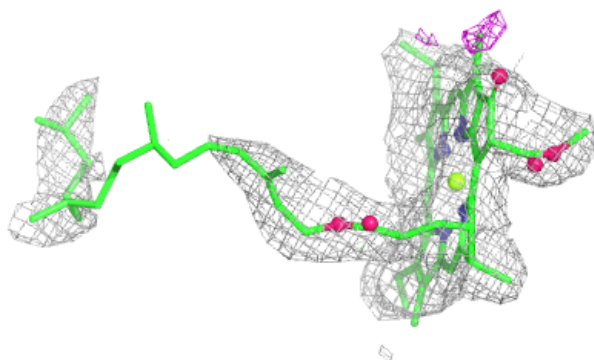
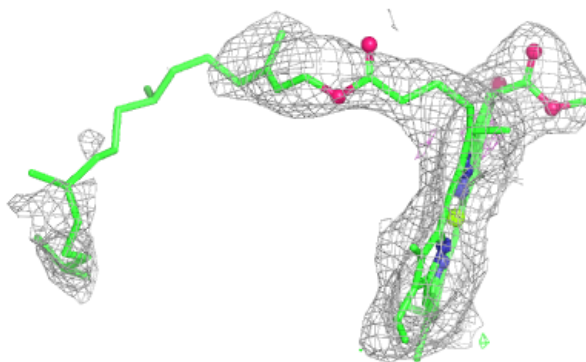


Electron density around CLA d 404:

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

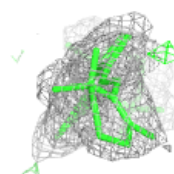
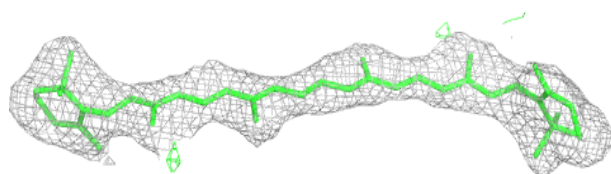
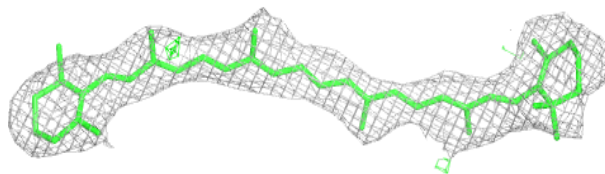
**Electron density around CLA c 508:**

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

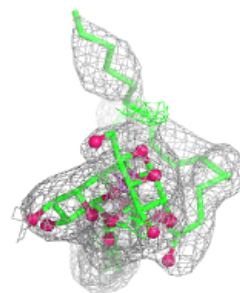
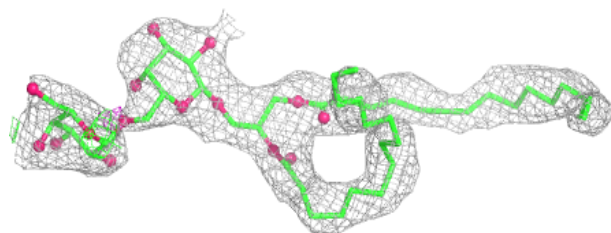
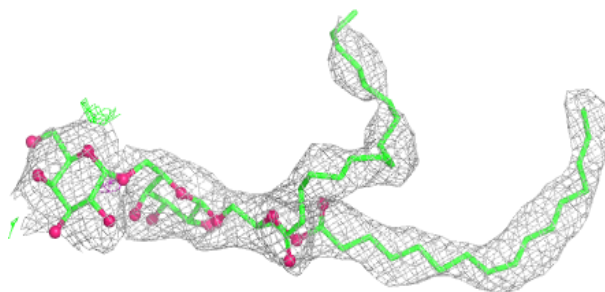


Electron density around BCR B 619:

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

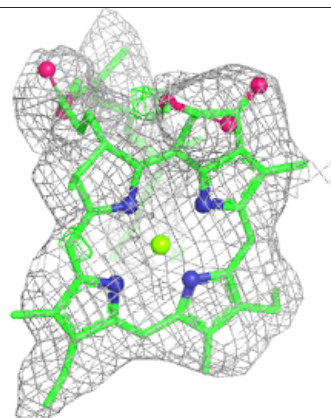
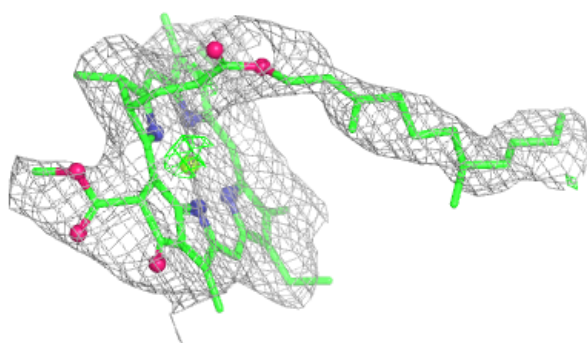
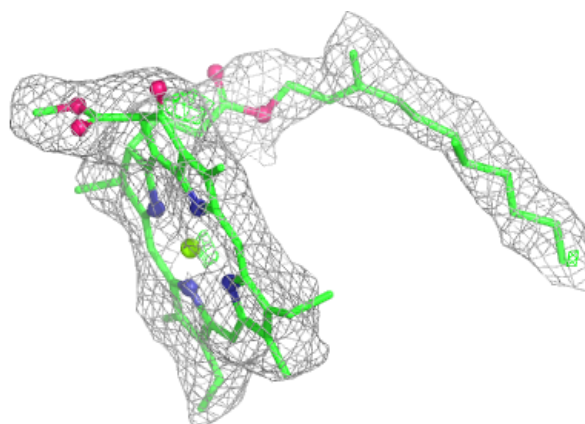
**Electron density around DGD H 103:**

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

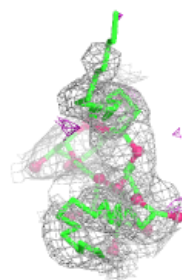
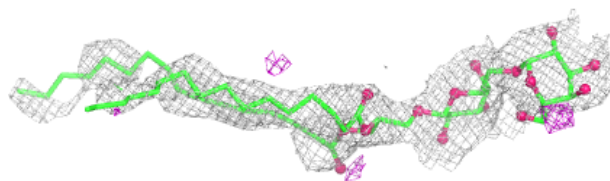
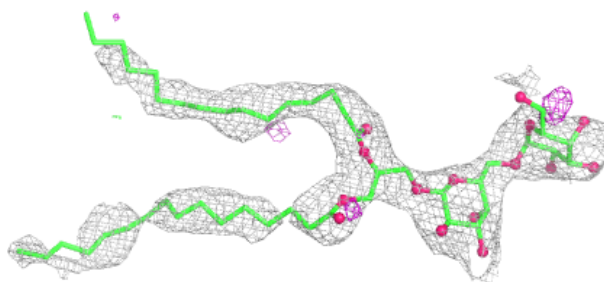


Electron density around CLA c 510:

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

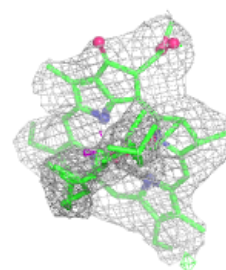
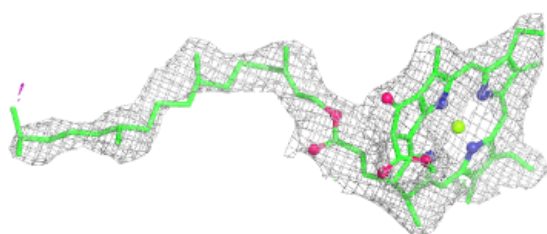
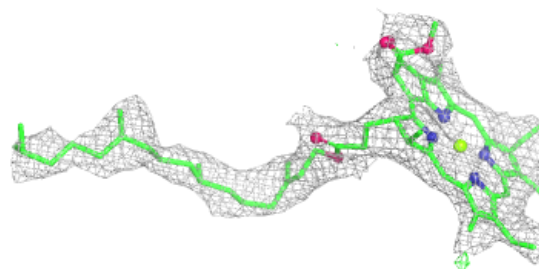
**Electron density around DGD c 520:**

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

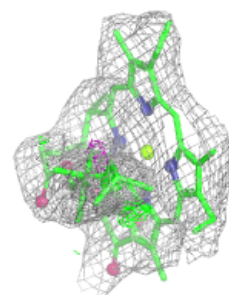
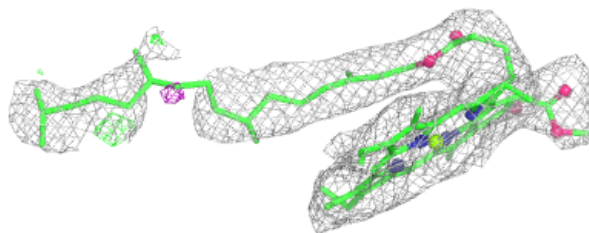
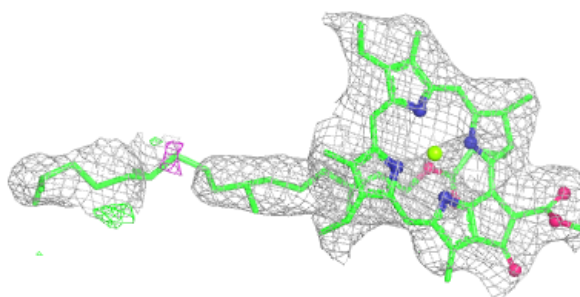


Electron density around CLA C 502:

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

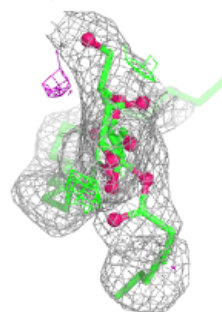
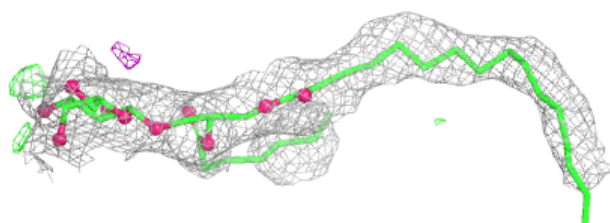
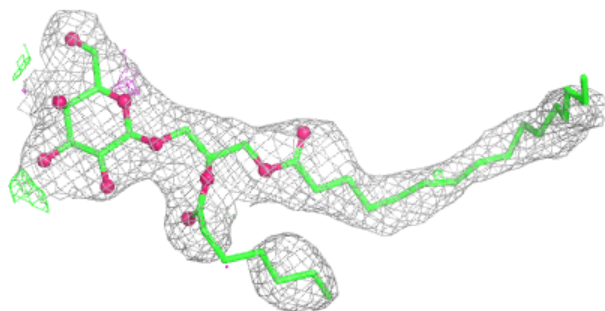
**Electron density around CLA B 614:**

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

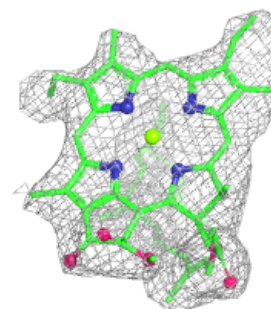
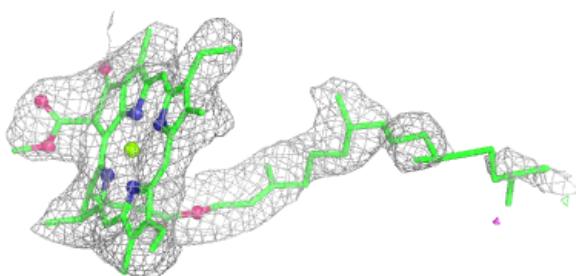
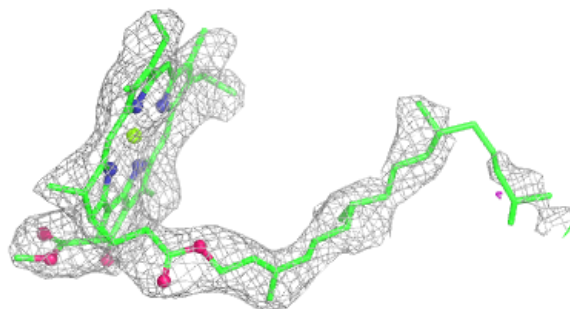


Electron density around LMG d 406:

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

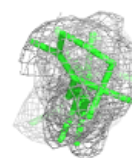
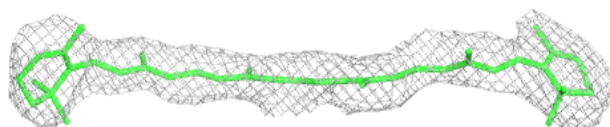
**Electron density around CLA C 508:**

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

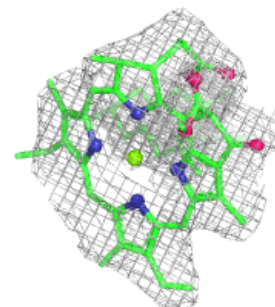
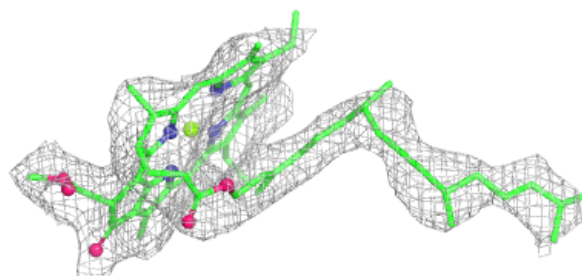
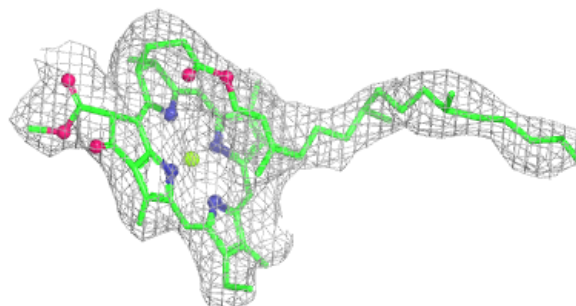


Electron density around BCR b 621:

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

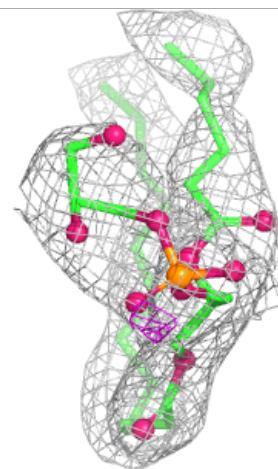
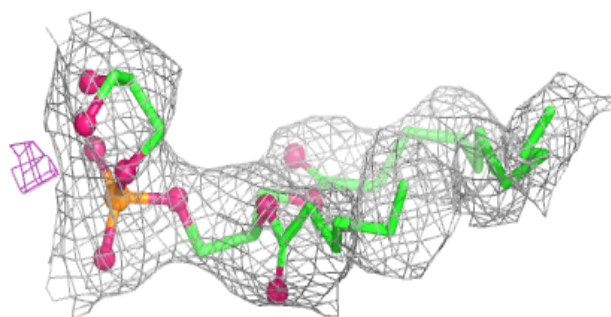
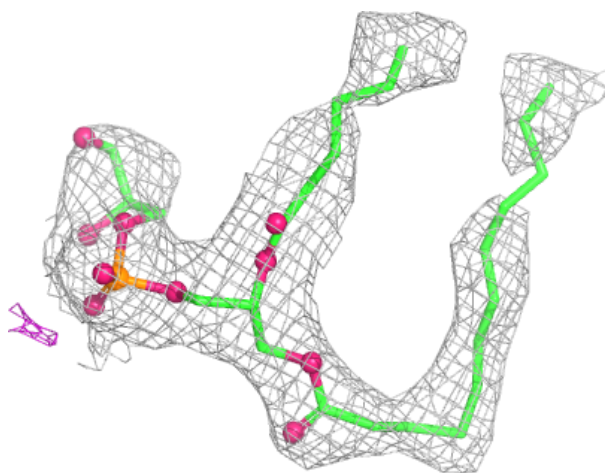
**Electron density around CLA c 507:**

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



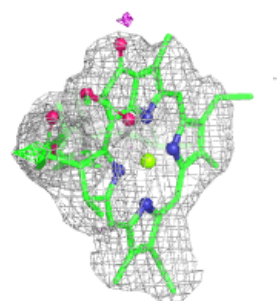
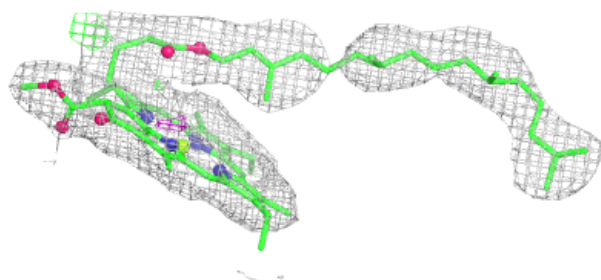
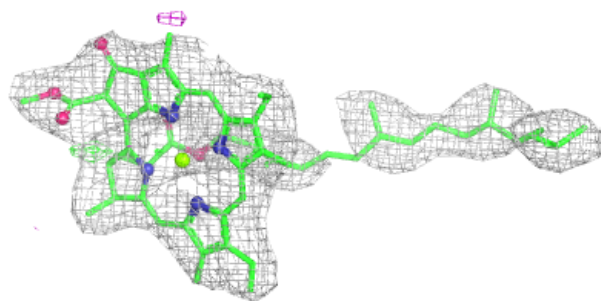
Electron density around LHG a 614:

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



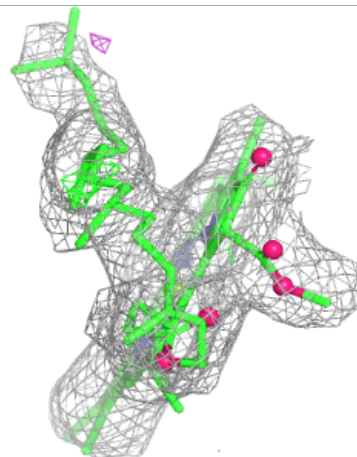
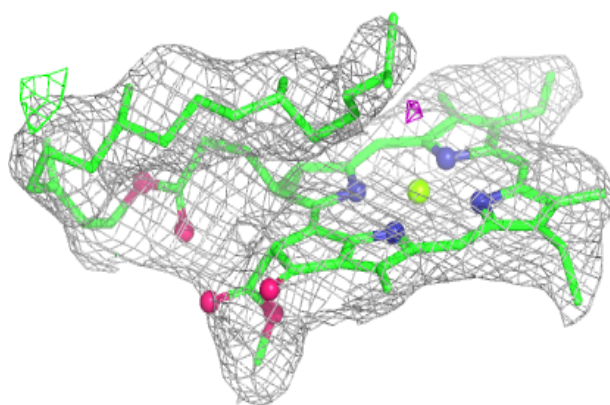
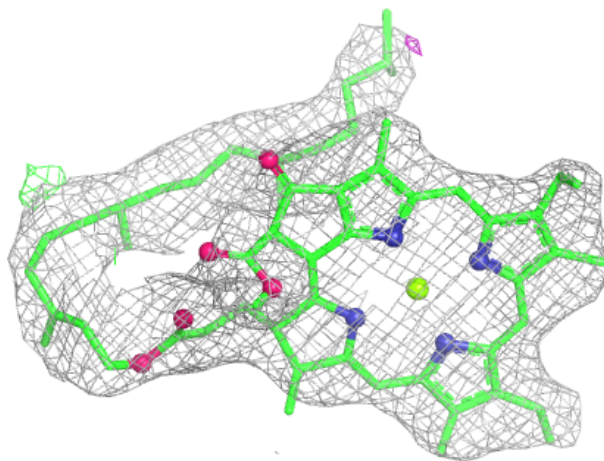
Electron density around CLA B 608:

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



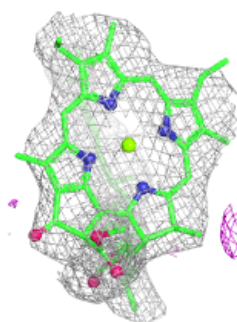
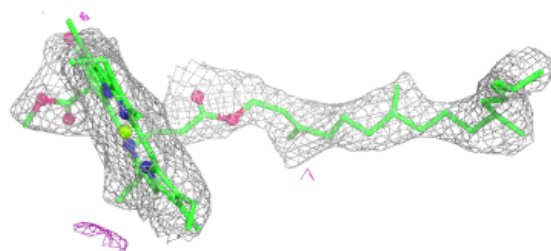
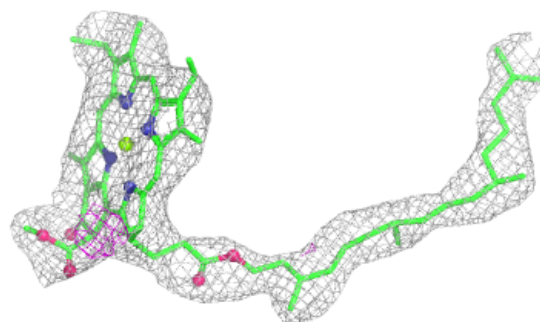
Electron density around CLA C 509:

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

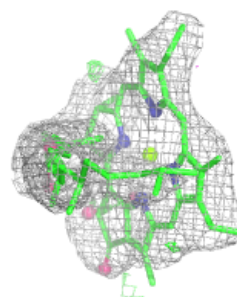
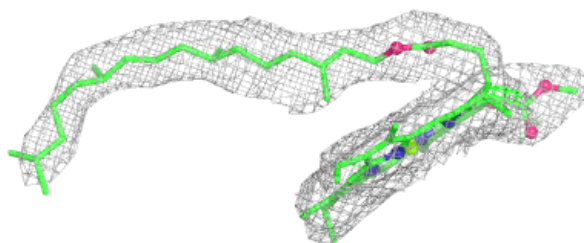
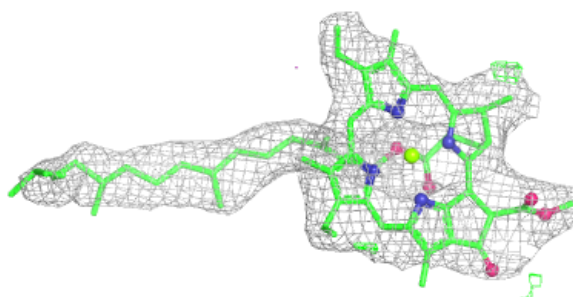


Electron density around CLA B 609:

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

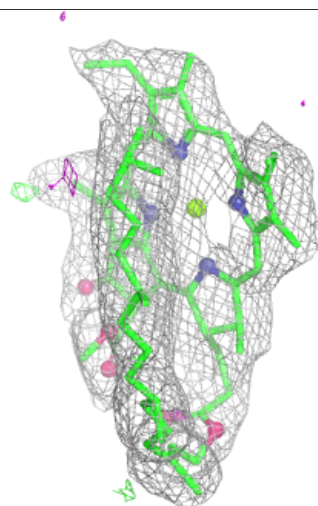
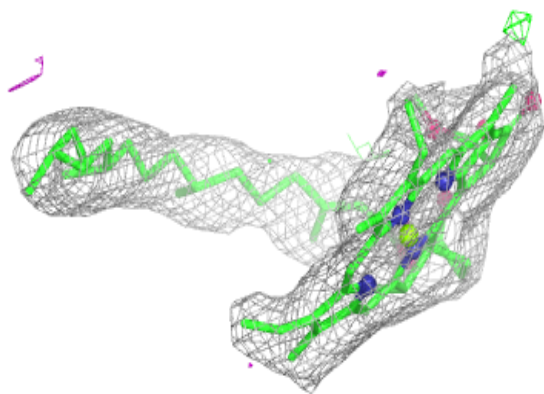
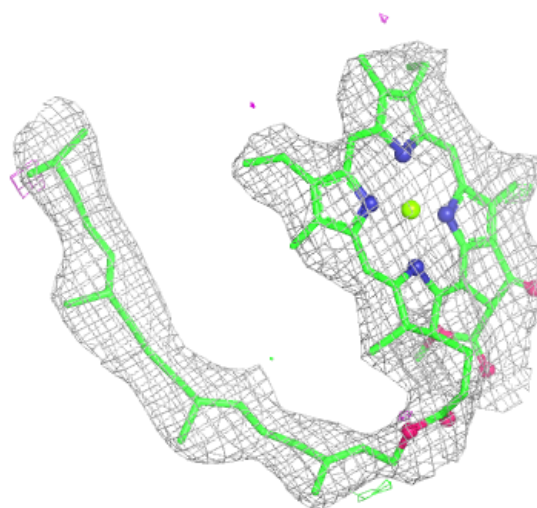
**Electron density around CLA b 611:**

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



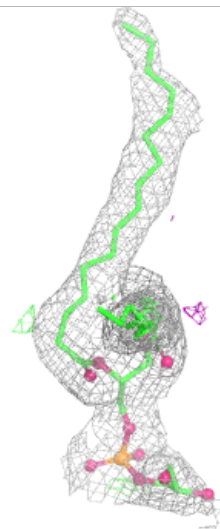
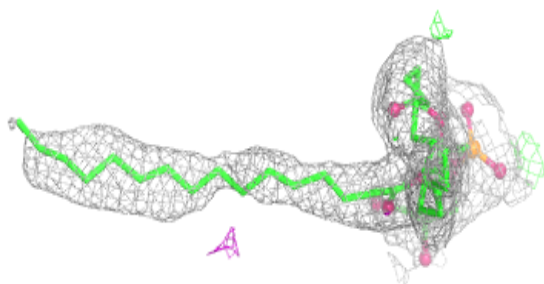
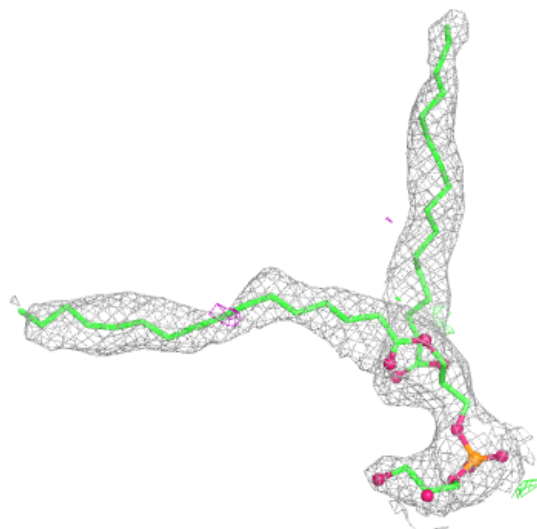
Electron density around CLA c 509:

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



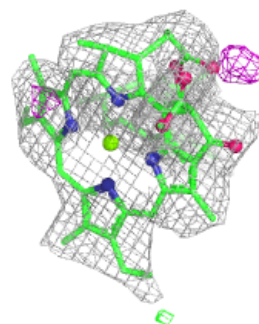
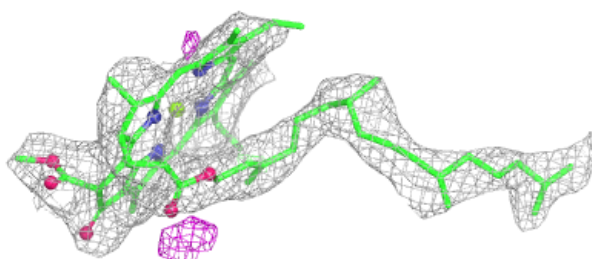
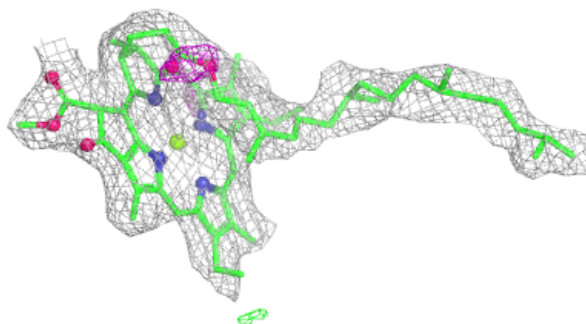
Electron density around LHG 1 101:

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

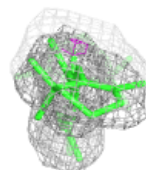
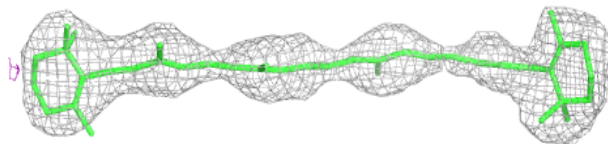
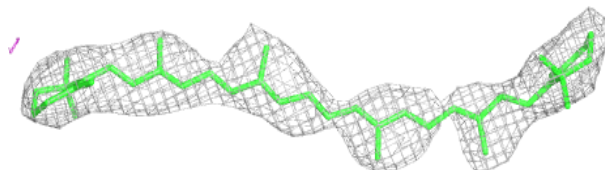


Electron density around CLA C 505:

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

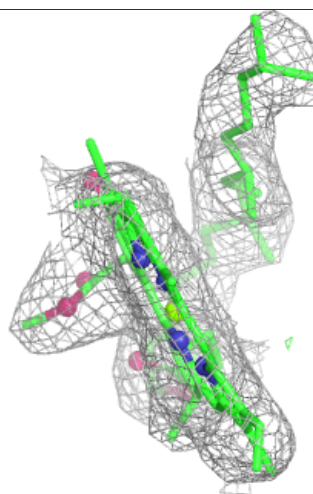
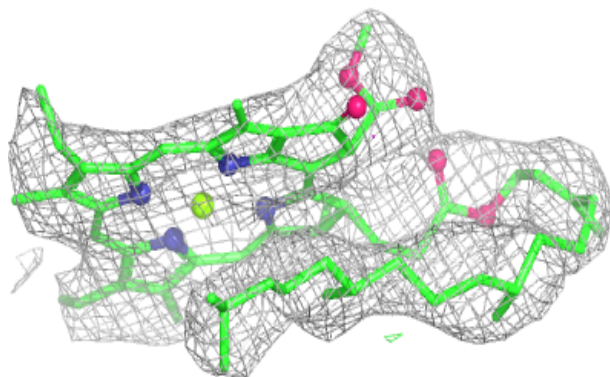
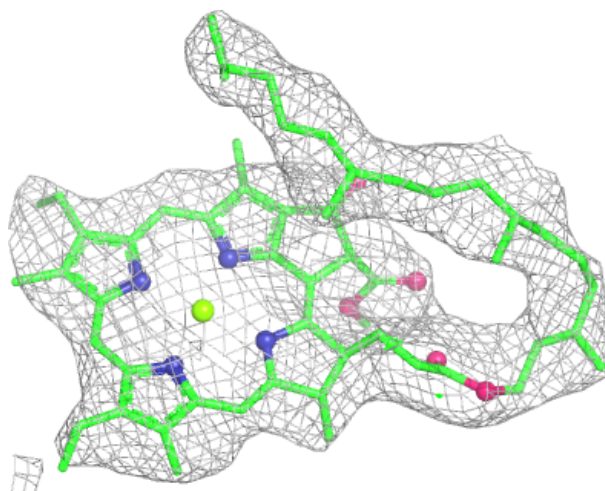
**Electron density around BCR C 515:**

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



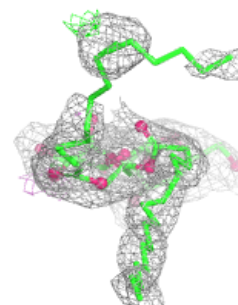
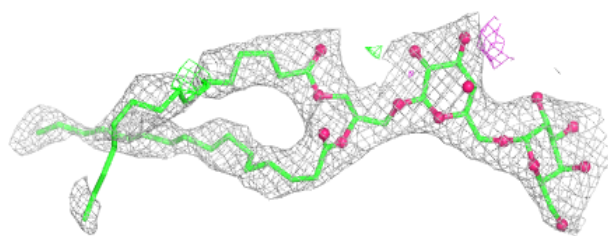
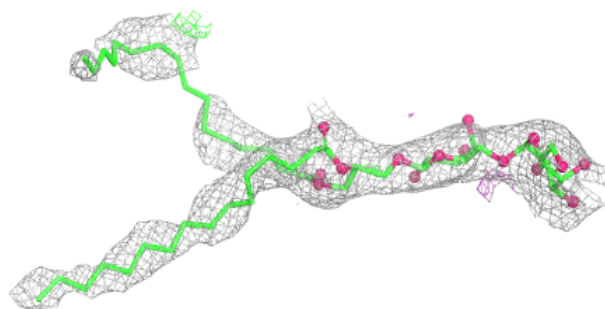
Electron density around CLA c 511:

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

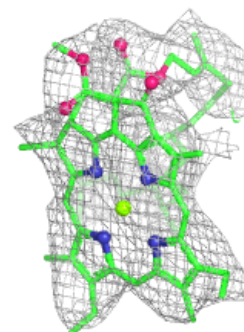
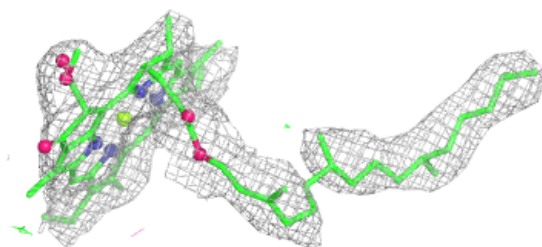
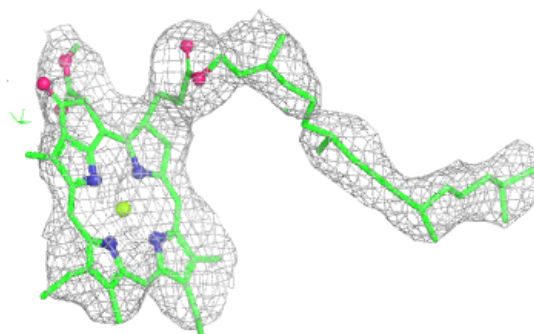


Electron density around DGD c 518:

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

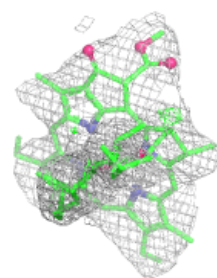
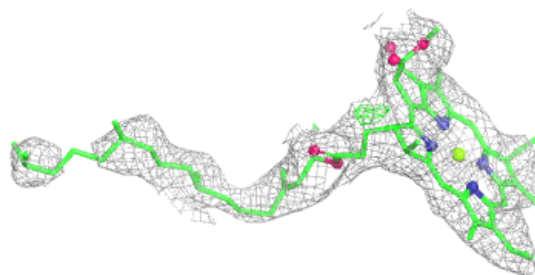
**Electron density around CLA c 513:**

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

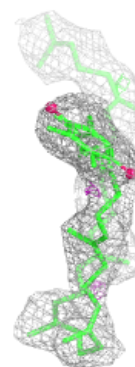
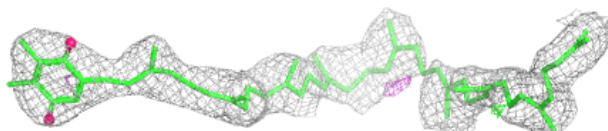
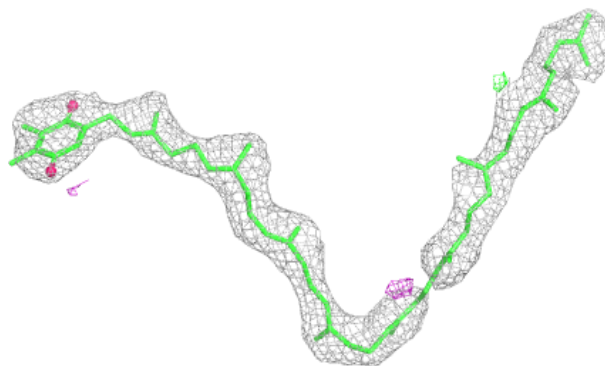


Electron density around CLA c 504:

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

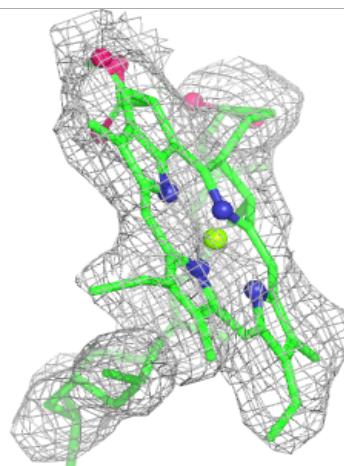
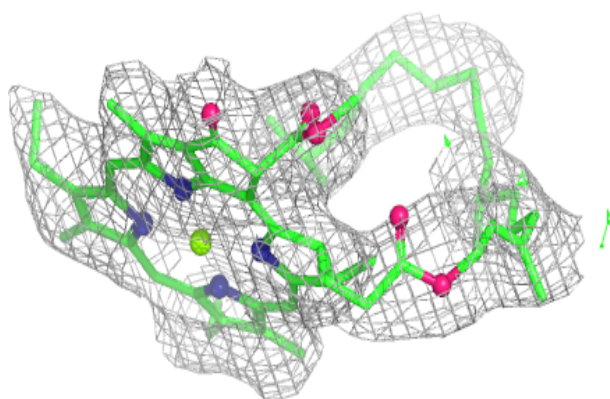
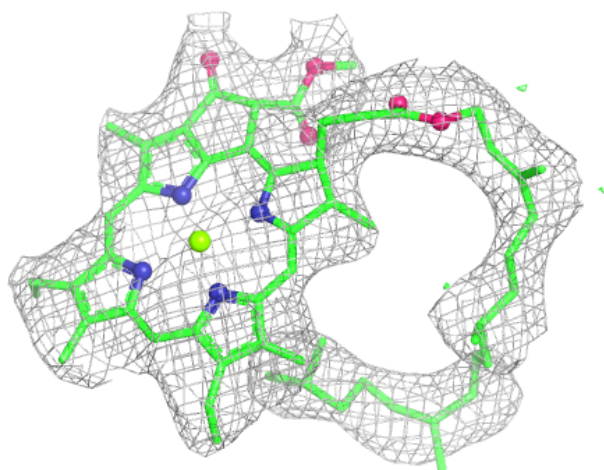
**Electron density around PL9 D 407:**

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



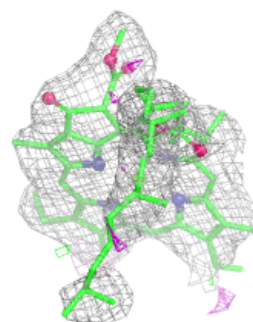
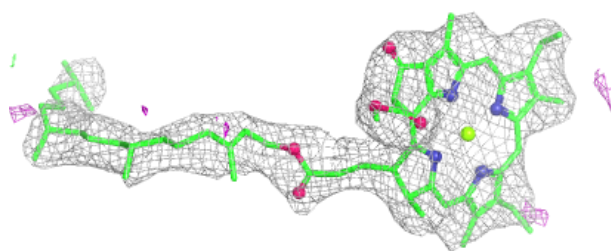
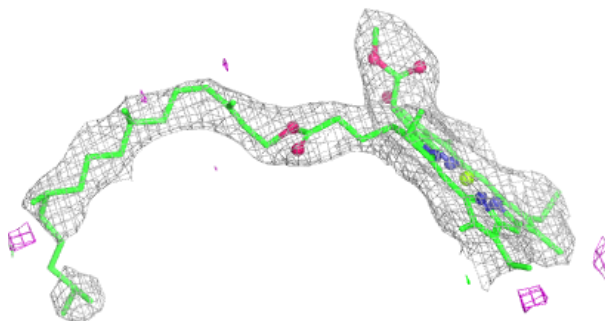
Electron density around CLA B 615:

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

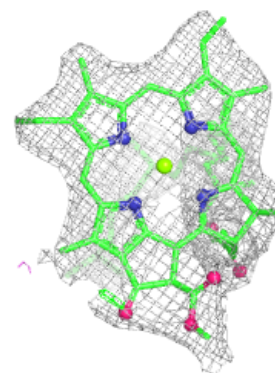
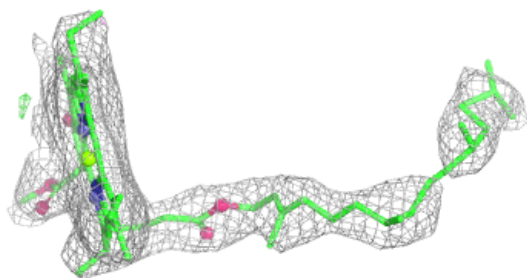
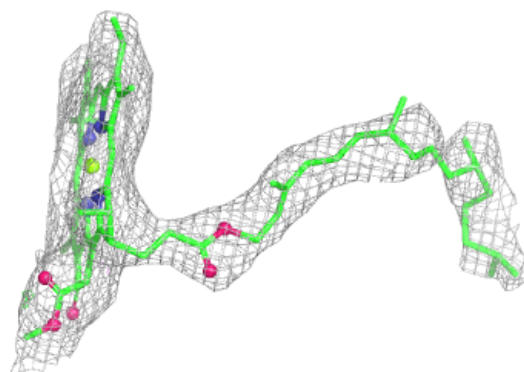


Electron density around CLA D 402:

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

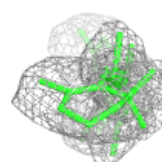
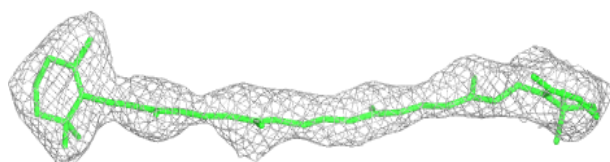
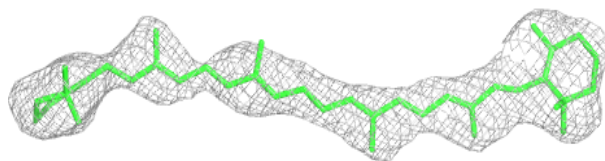
**Electron density around CLA D 403:**

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

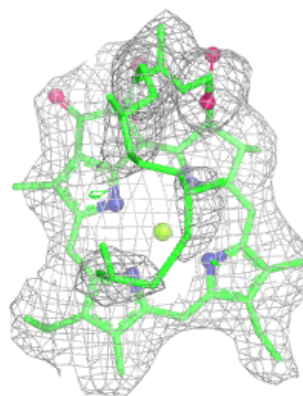
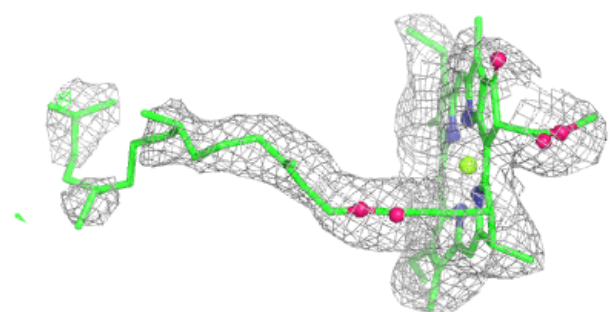
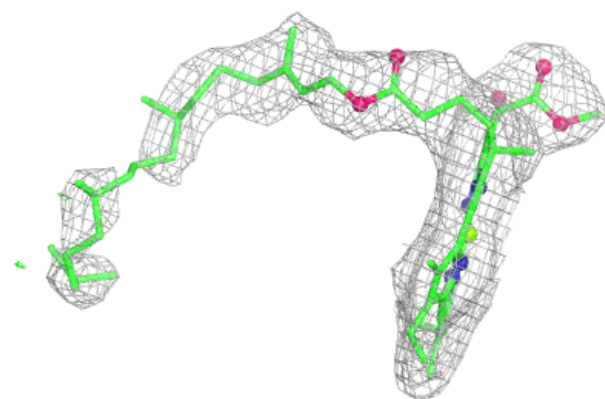


Electron density around BCR b 620:

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

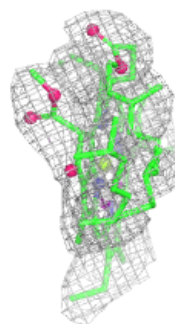
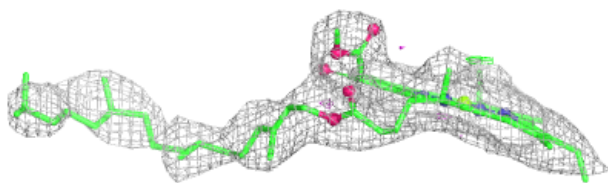
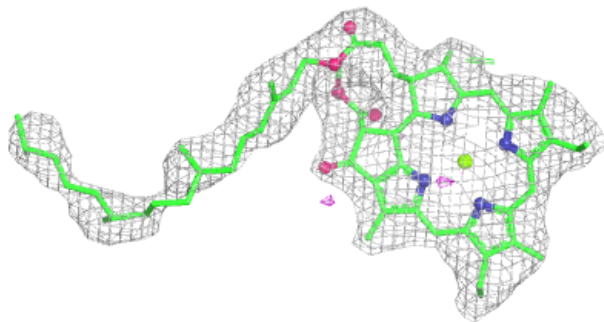
**Electron density around CLA C 506:**

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

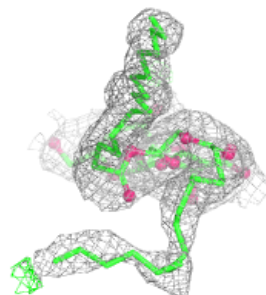
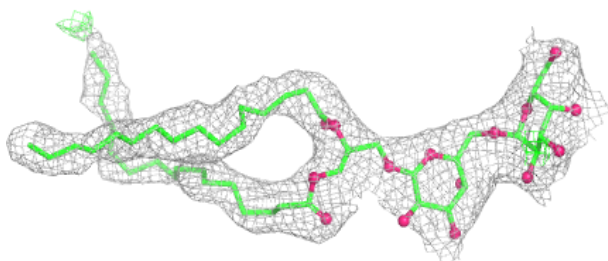
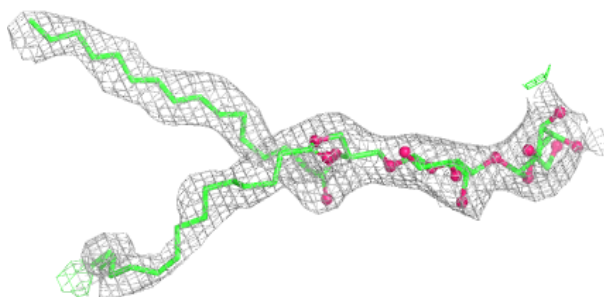


Electron density around CLA b 605:

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

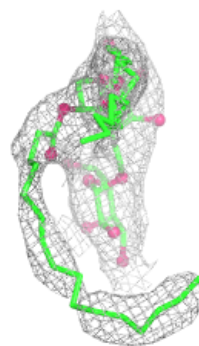
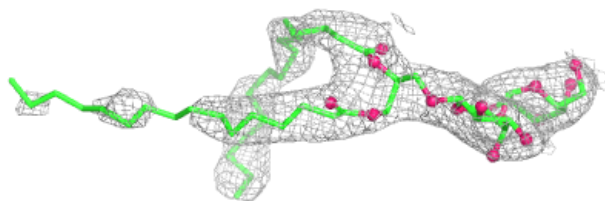
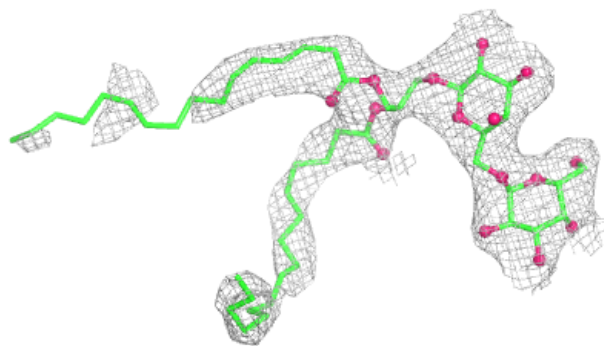
**Electron density around DGD C 516:**

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



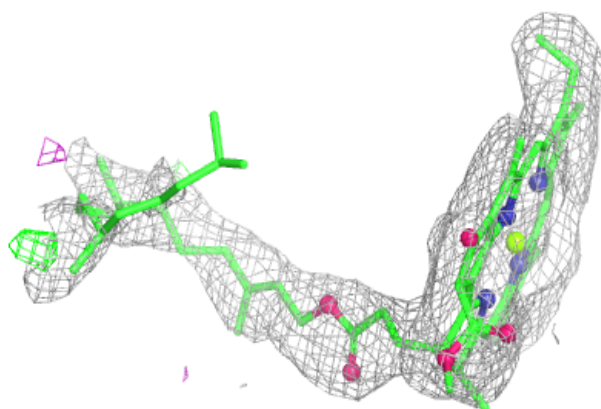
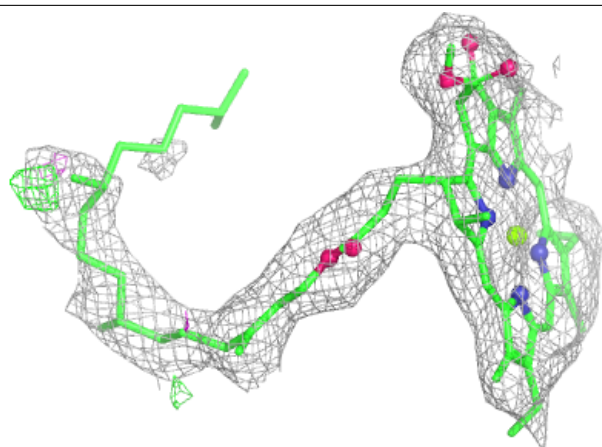
Electron density around DGD C 517:

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

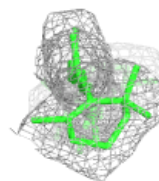
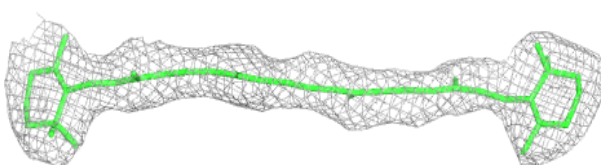
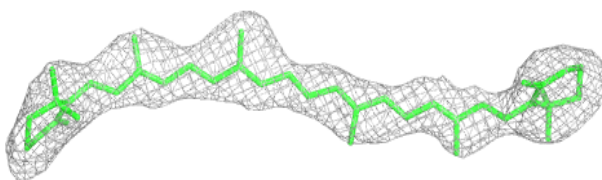


Electron density around CLA b 609:

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

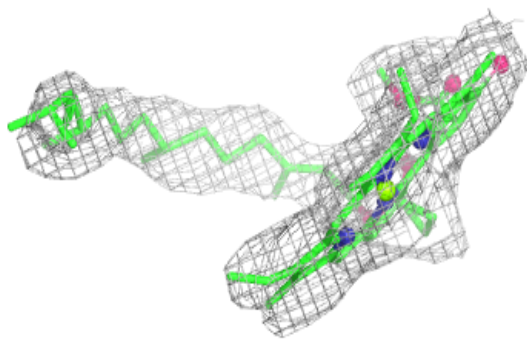
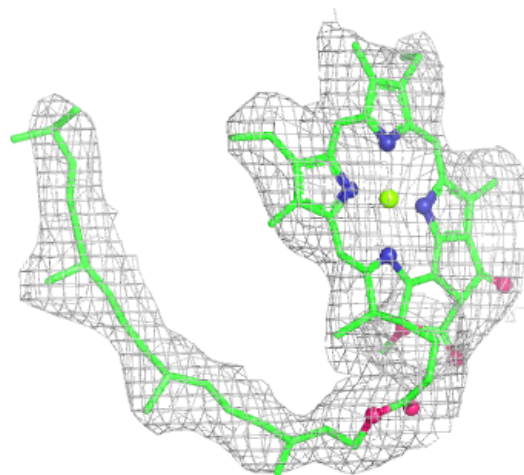
**Electron density around BCR c 517:**

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



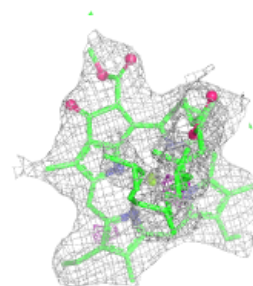
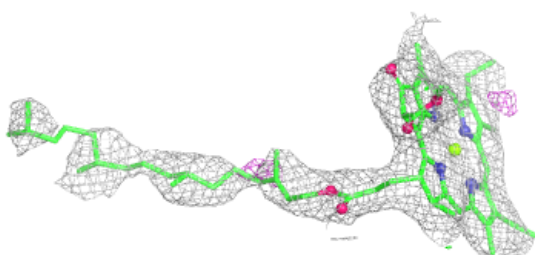
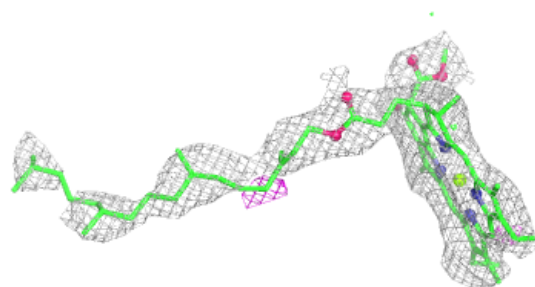
Electron density around CLA C 507:

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



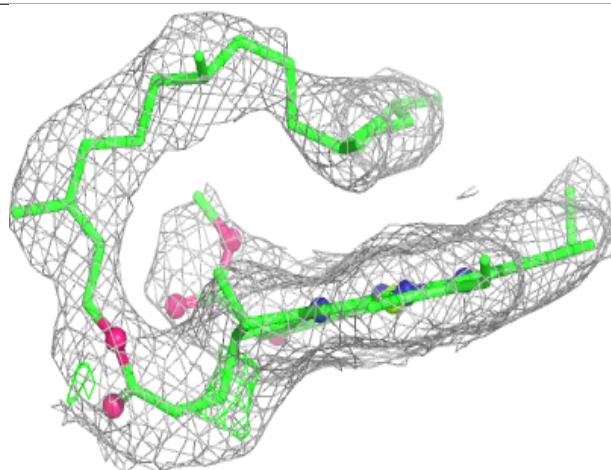
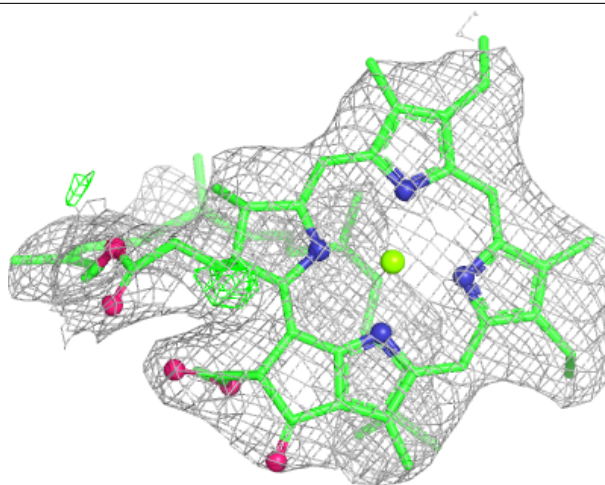
Electron density around CLA B 604:

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



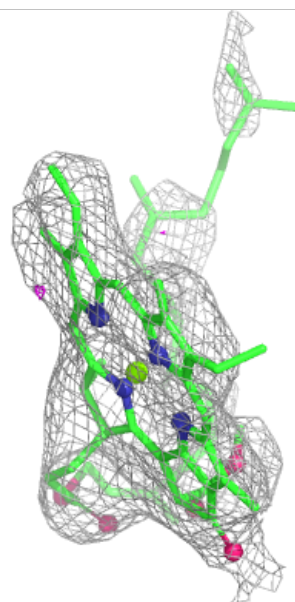
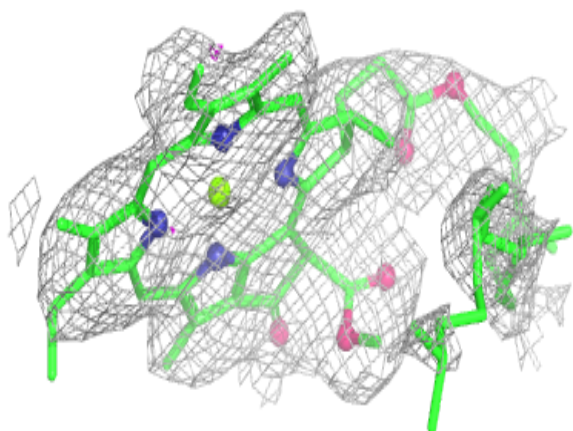
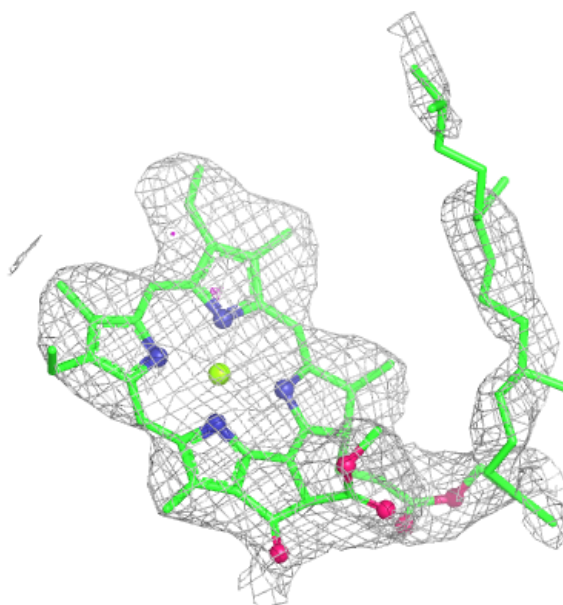
Electron density around CLA c 512:

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



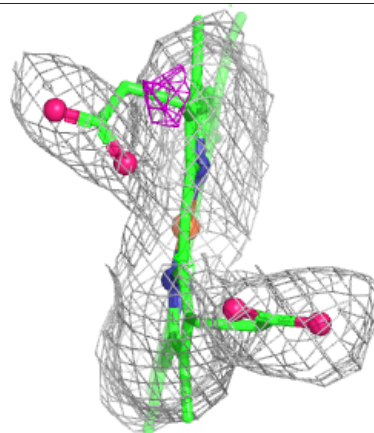
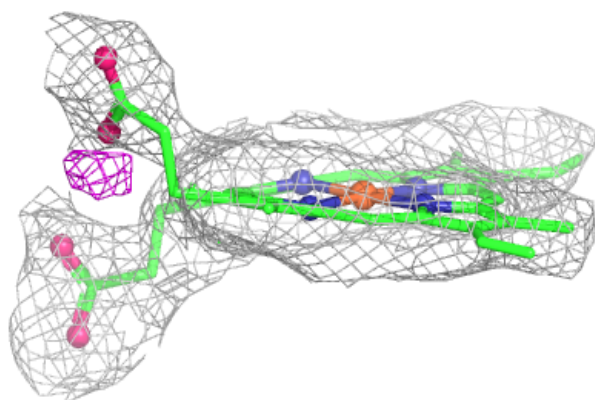
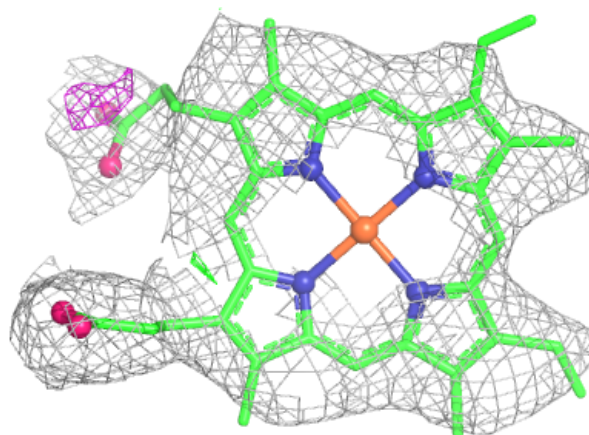
Electron density around CLA b 619:

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



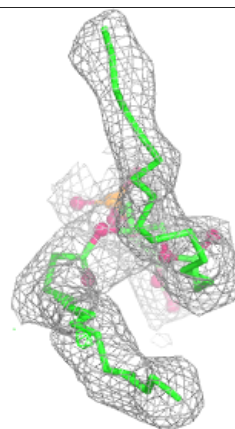
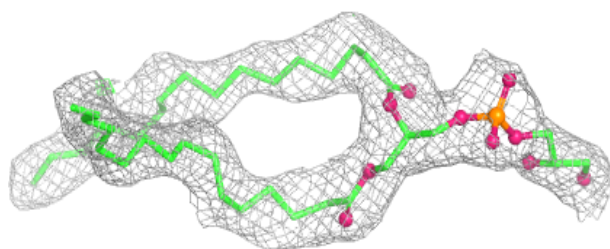
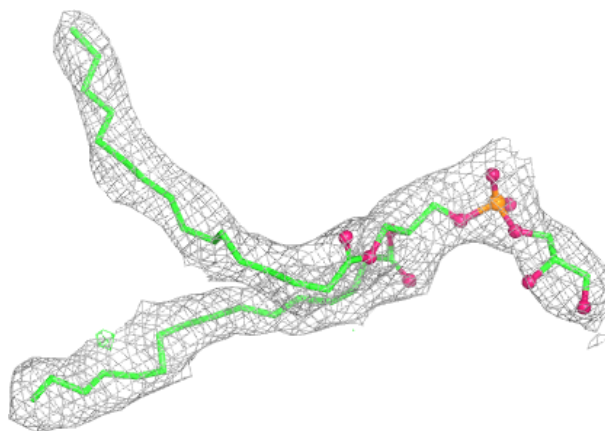
Electron density around HEM e 101:

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



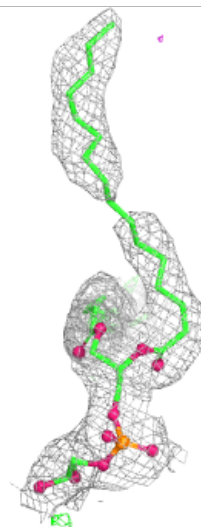
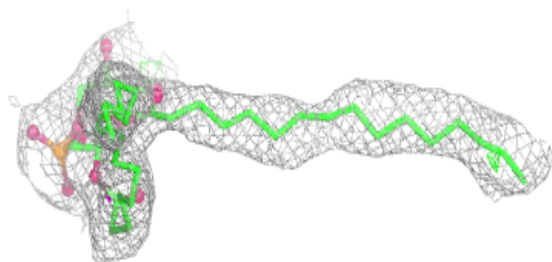
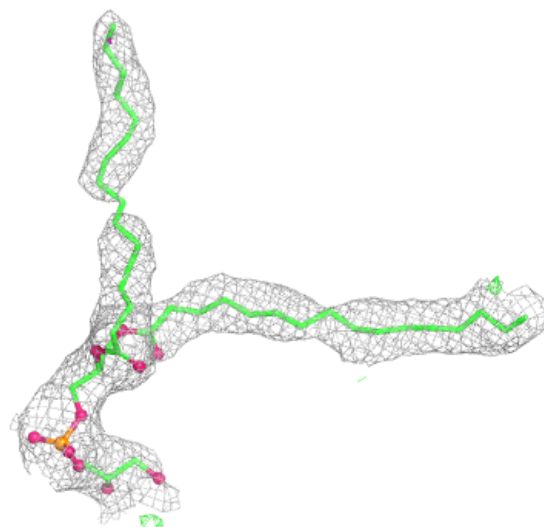
Electron density around LHG D 406:

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



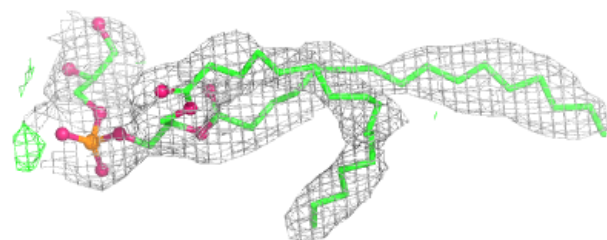
Electron density around LHG L 101:

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

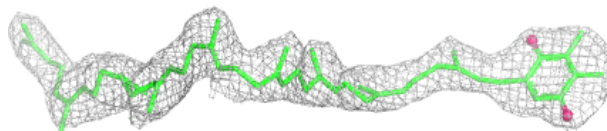
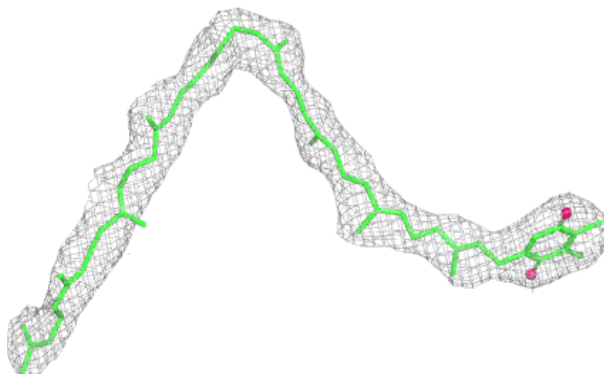


Electron density around LHG a 613:

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

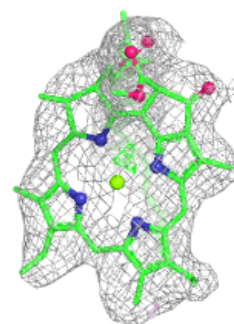
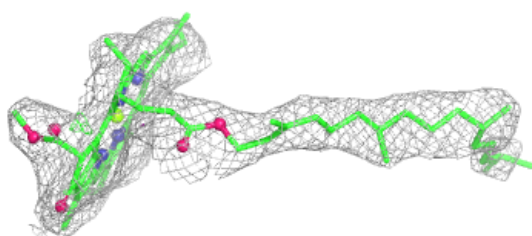
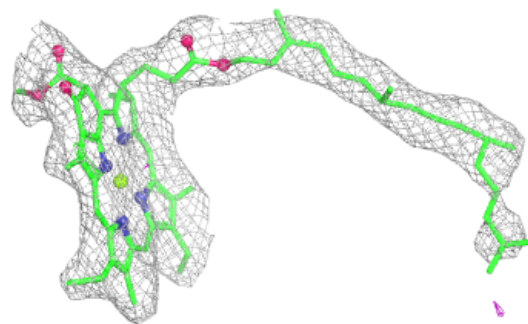
**Electron density around PL9 d 408:**

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



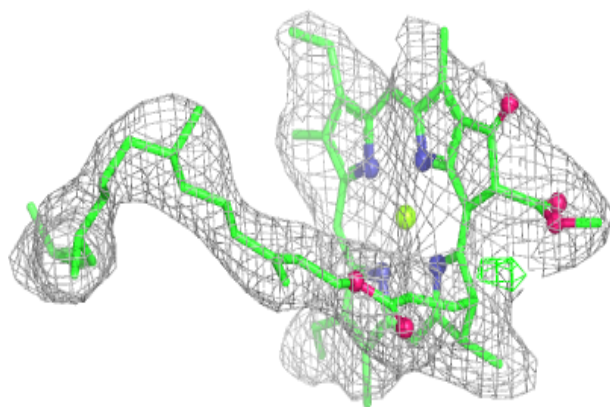
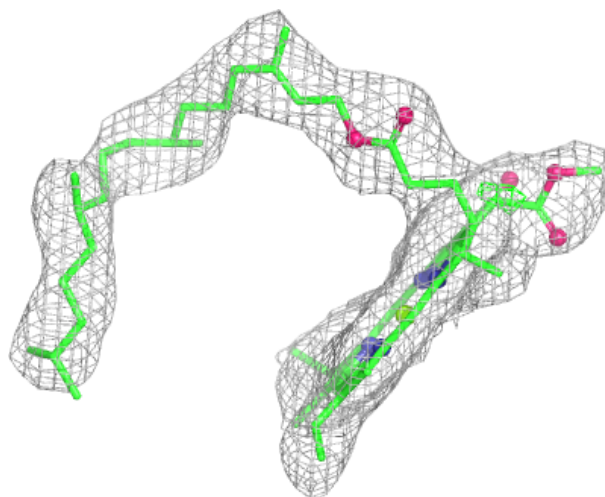
Electron density around CLA b 612:

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



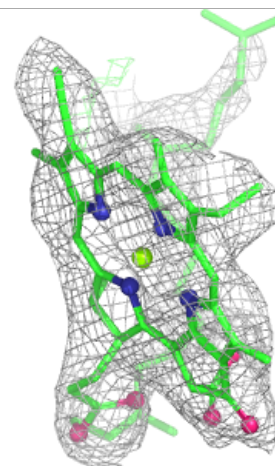
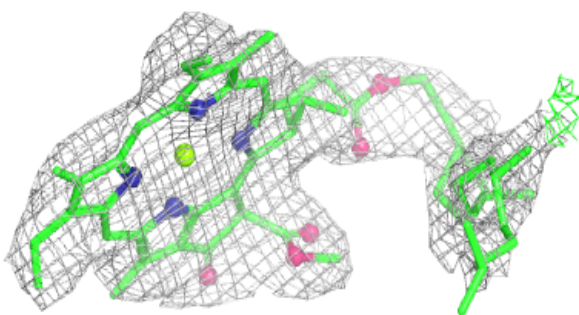
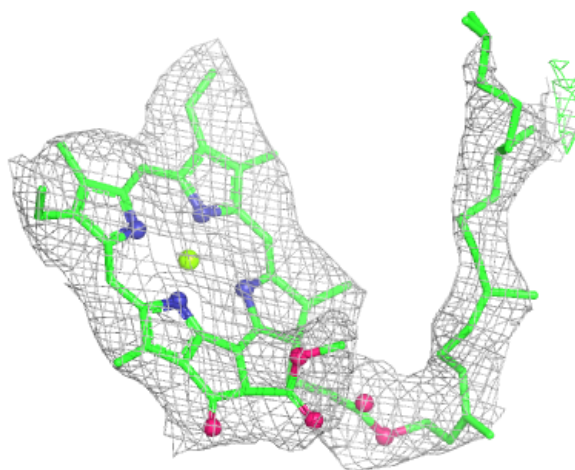
Electron density around CLA b 614:

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



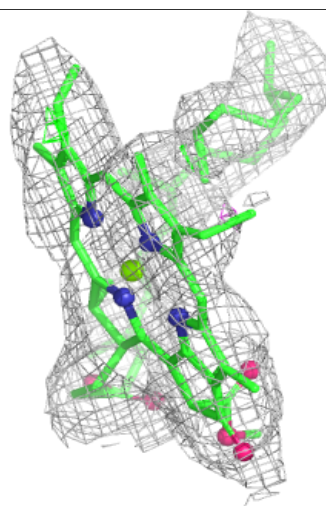
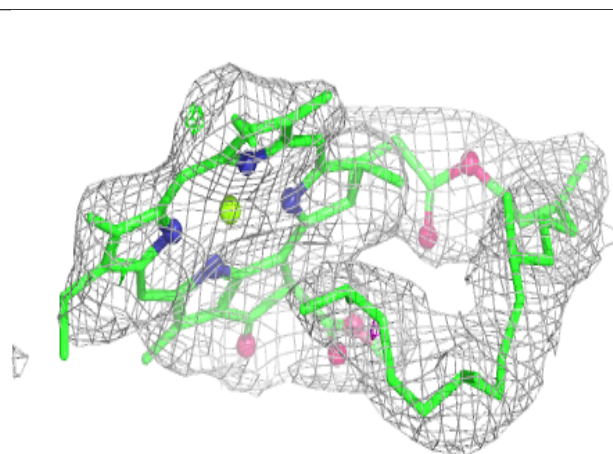
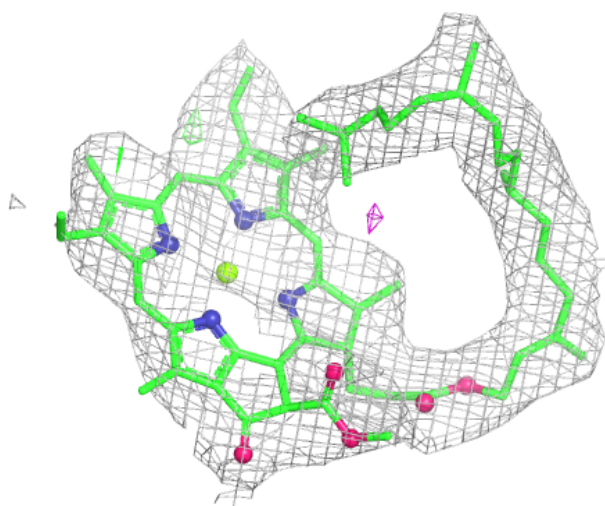
Electron density around CLA B 616:

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



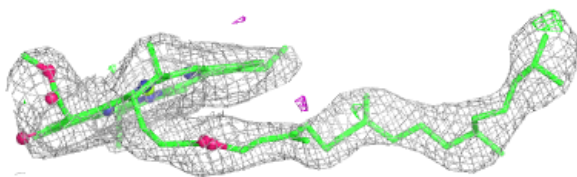
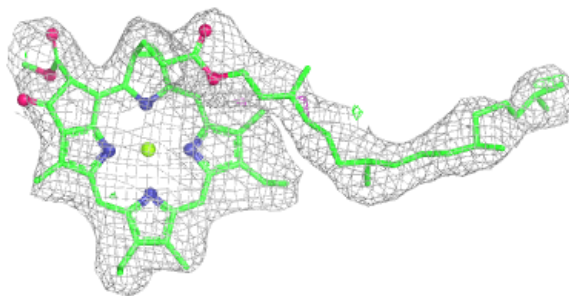
Electron density around CLA b 618:

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

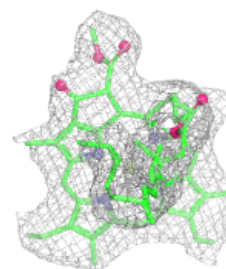
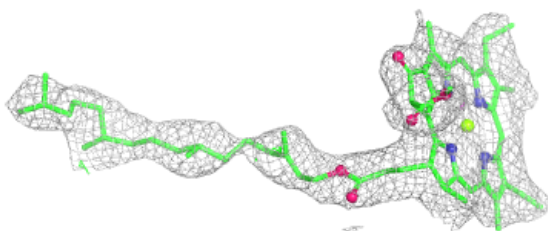
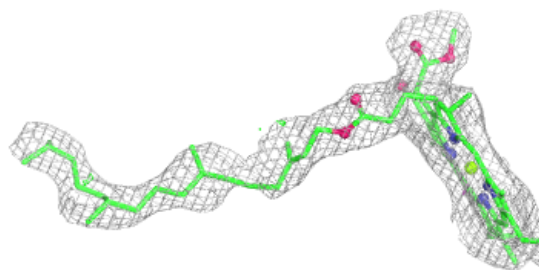


Electron density around CLA B 603:

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

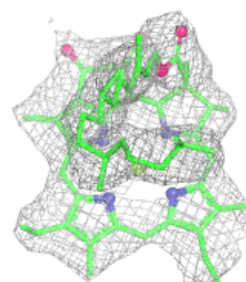
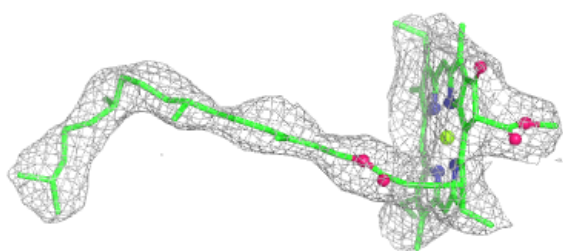
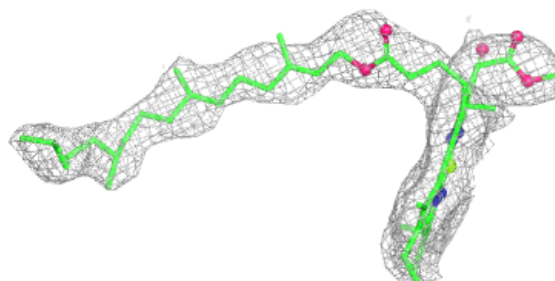
**Electron density around CLA b 607:**

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

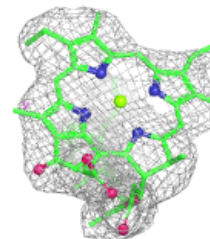
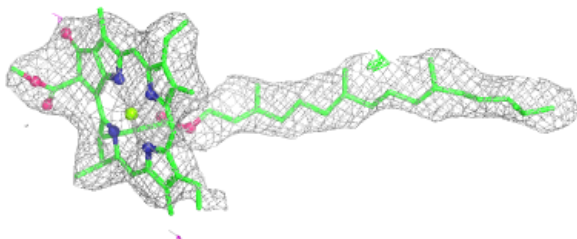
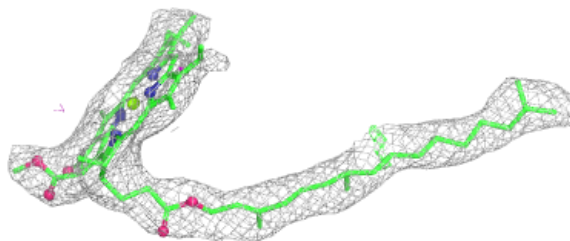


Electron density around CLA b 608:

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

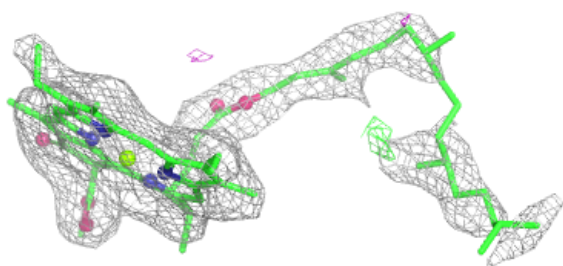
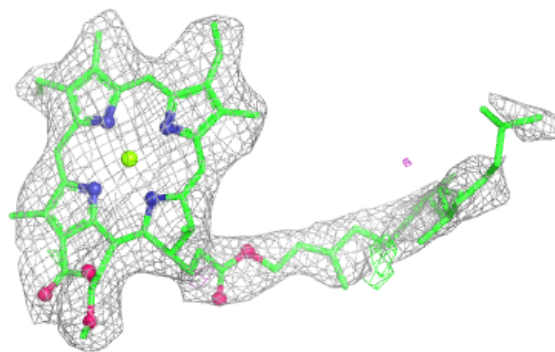
**Electron density around CLA B 607:**

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

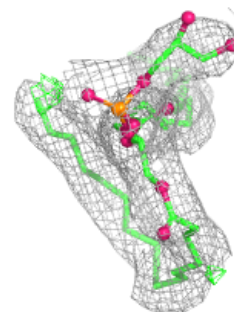
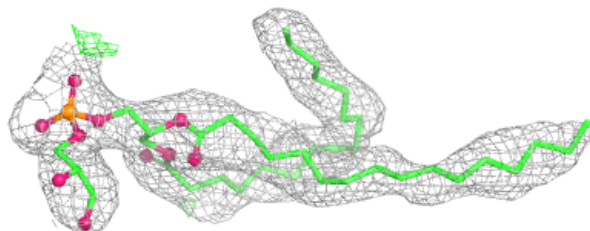
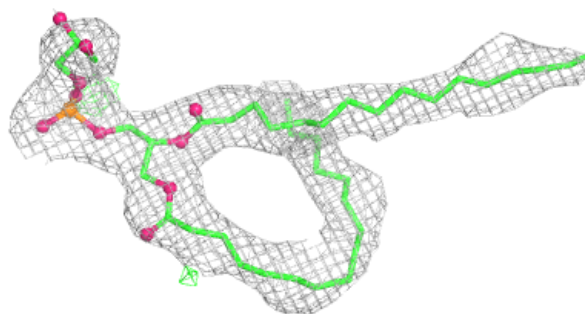


Electron density around CLA a 609:

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

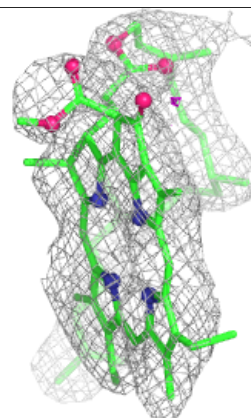
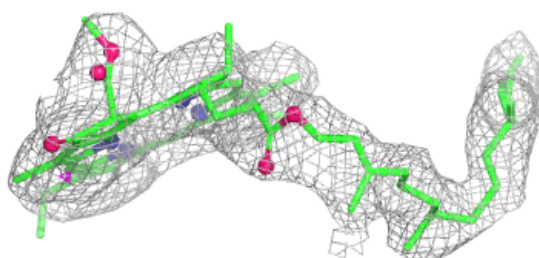
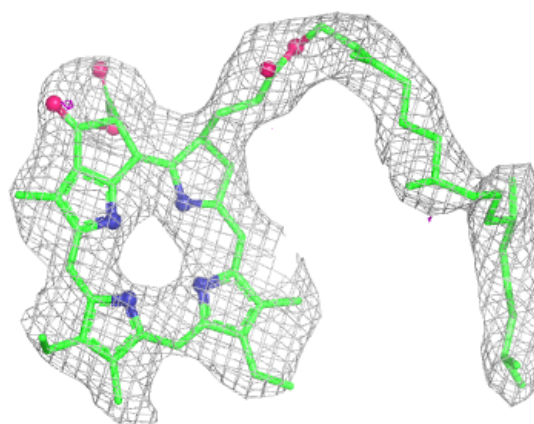
**Electron density around LHG A 616:**

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

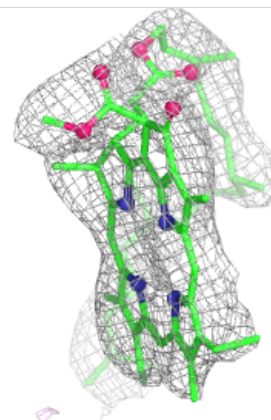
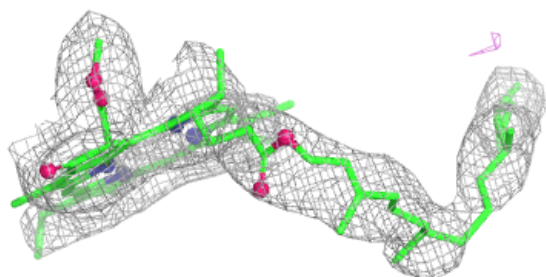
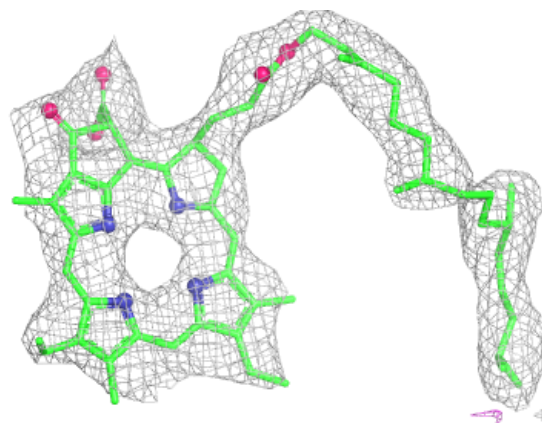


Electron density around PHO D 401:

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

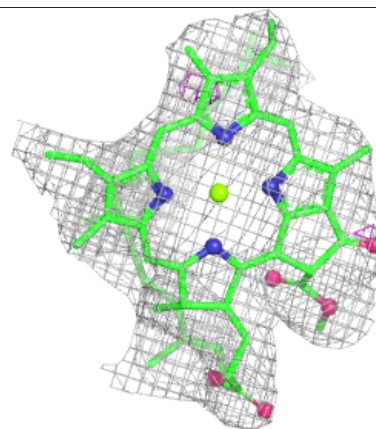
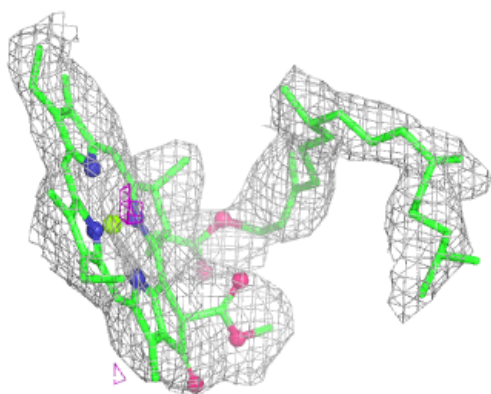
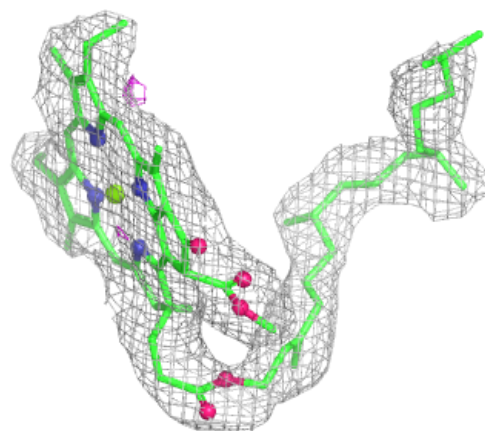
**Electron density around PHO d 401:**

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

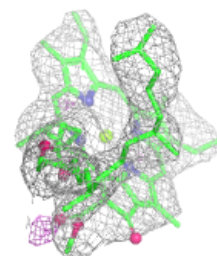
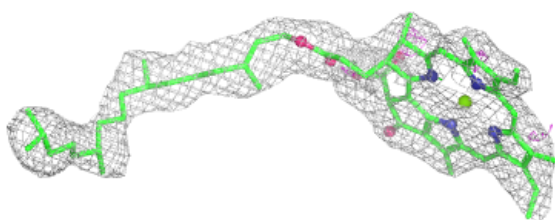
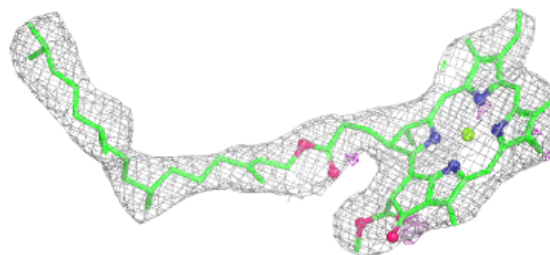


Electron density around CLA b 616:

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

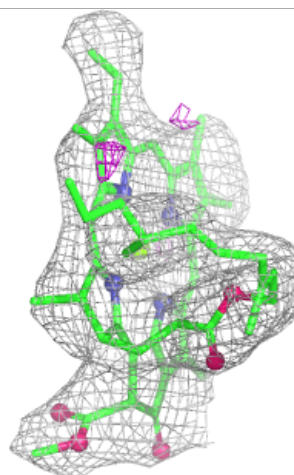
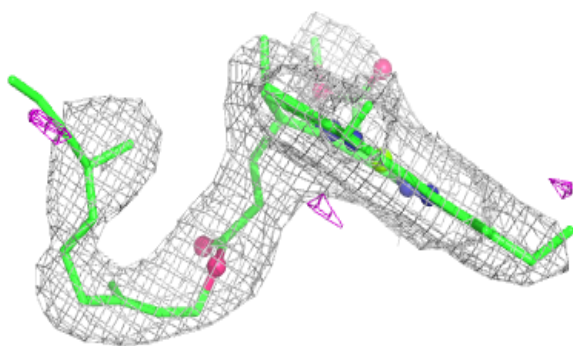
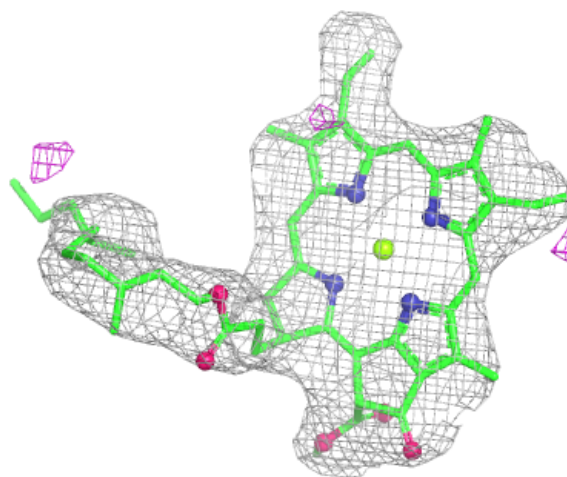
**Electron density around CLA A 606:**

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



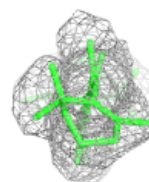
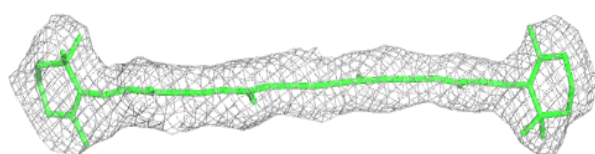
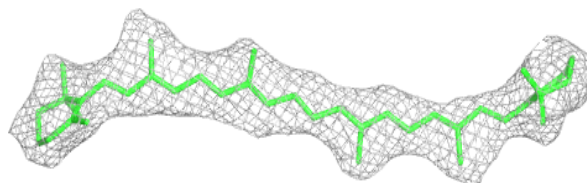
Electron density around CLA A 607:

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

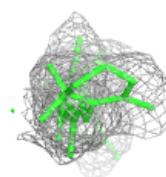
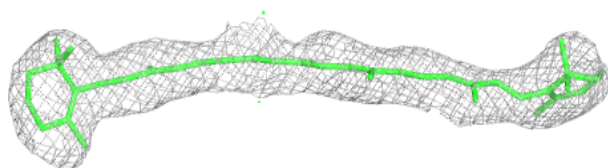
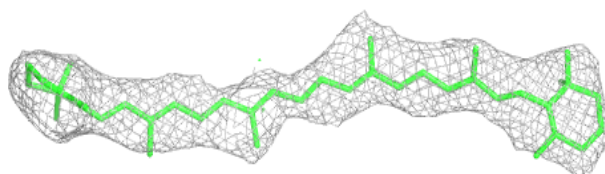


Electron density around BCR A 610:

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

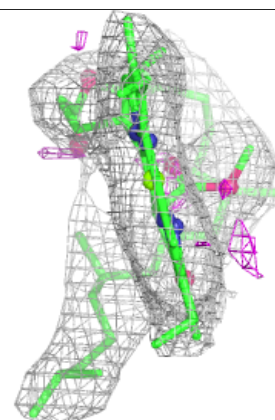
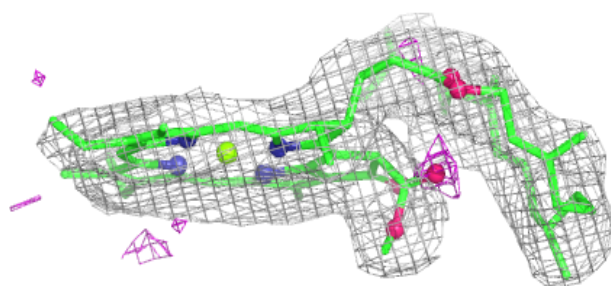
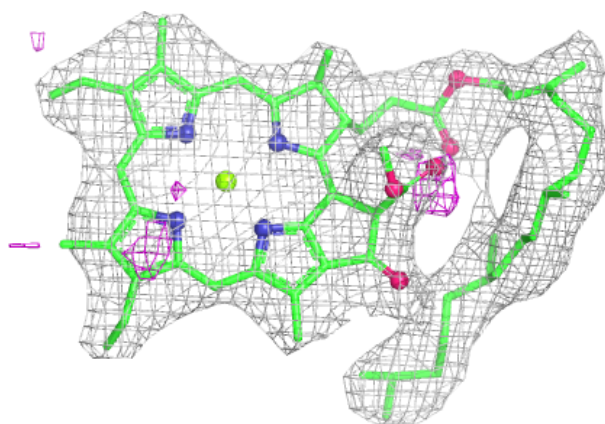
**Electron density around BCR B 617:**

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



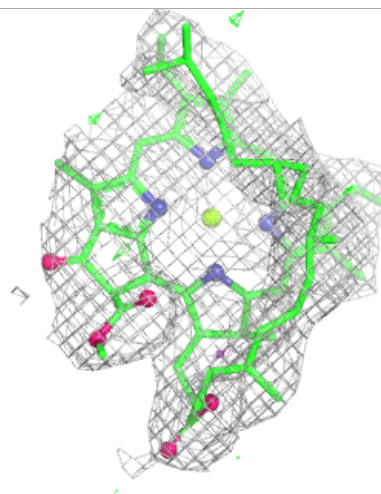
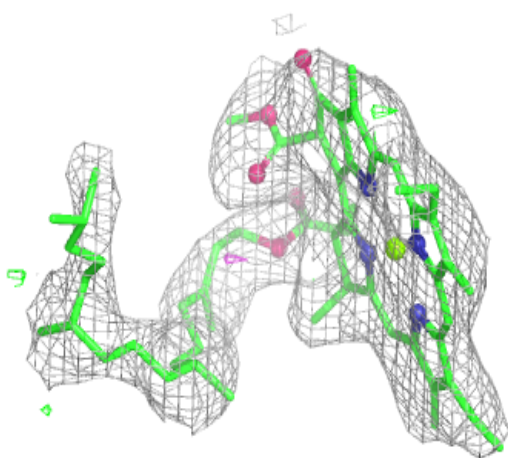
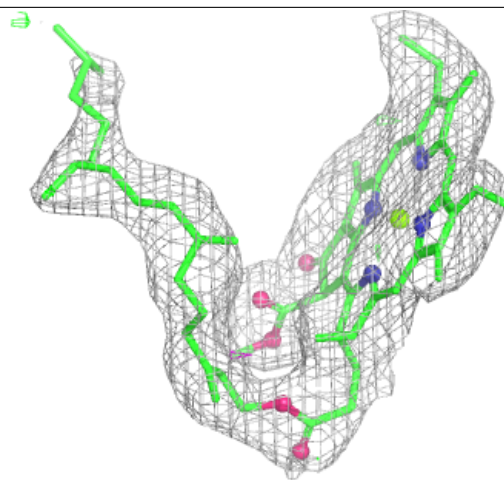
Electron density around CLA B 610:

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



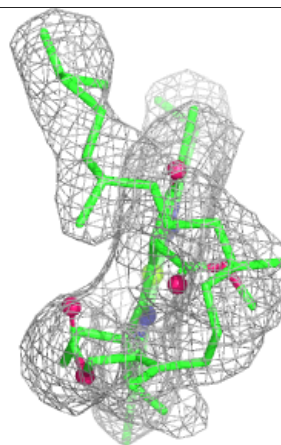
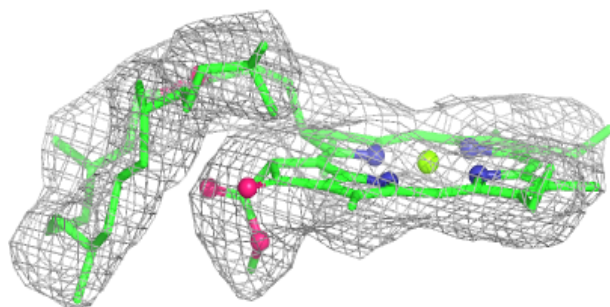
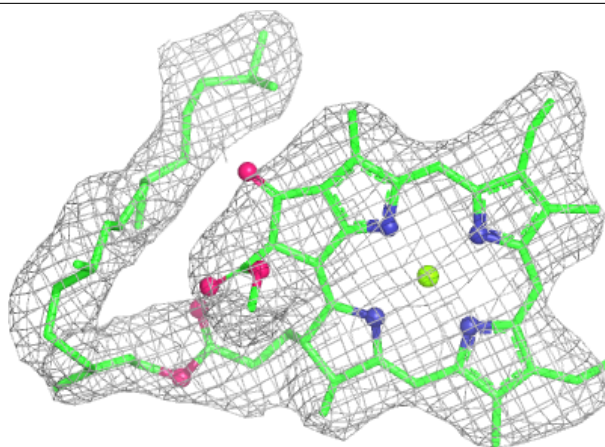
Electron density around CLA B 613:

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



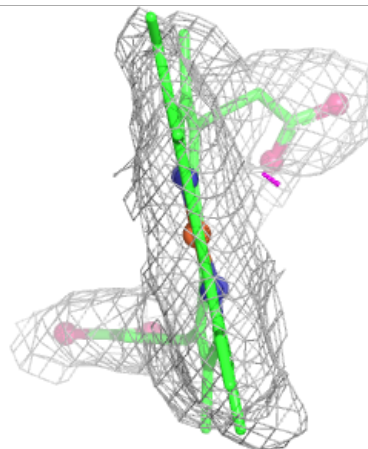
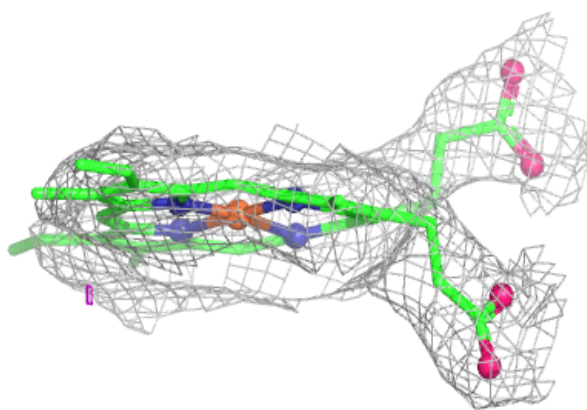
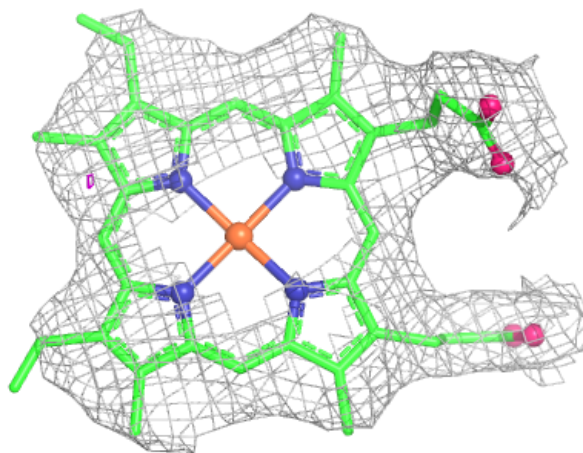
Electron density around CLA b 613:

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



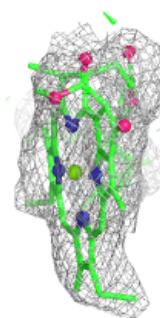
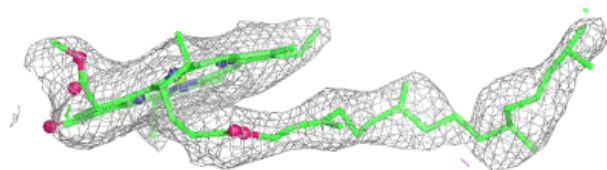
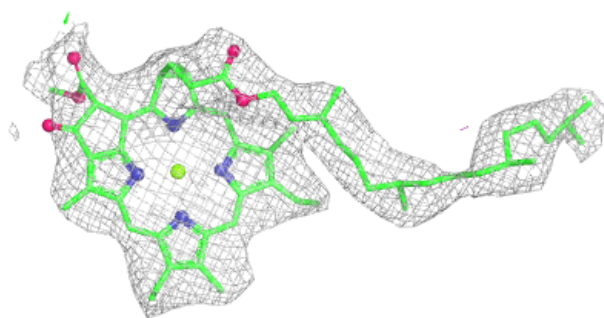
Electron density around HEM E 101:

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

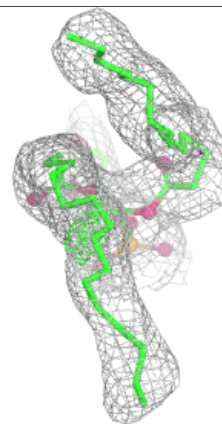
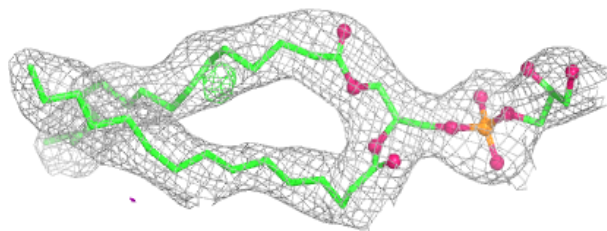
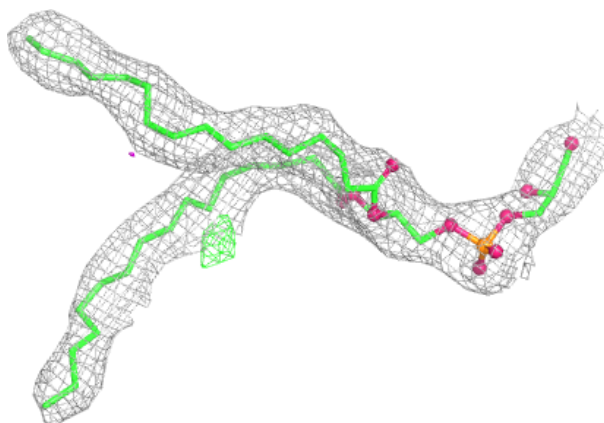


Electron density around CLA b 606:

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

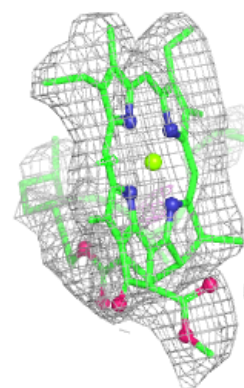
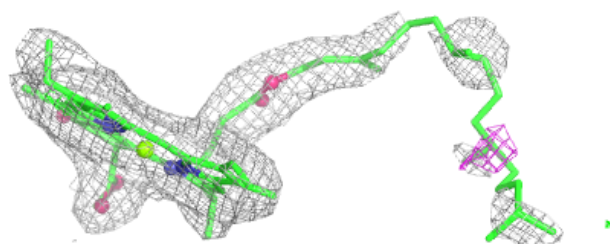
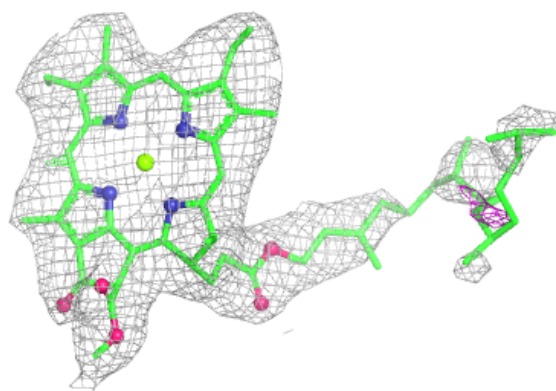
**Electron density around LHG d 407:**

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



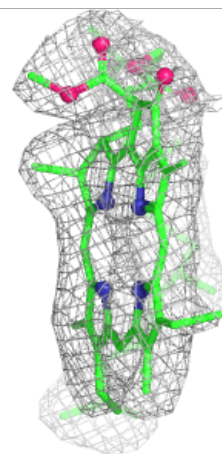
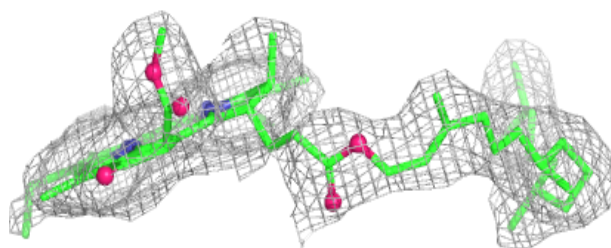
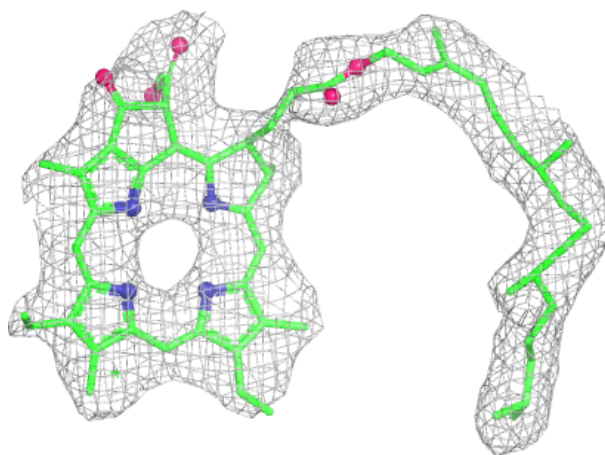
Electron density around CLA A 609:

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



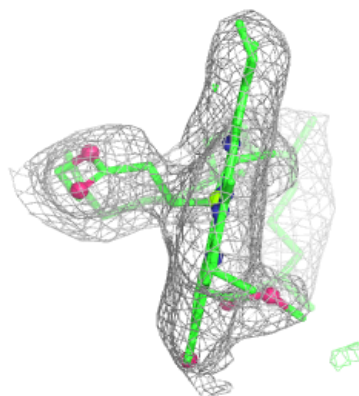
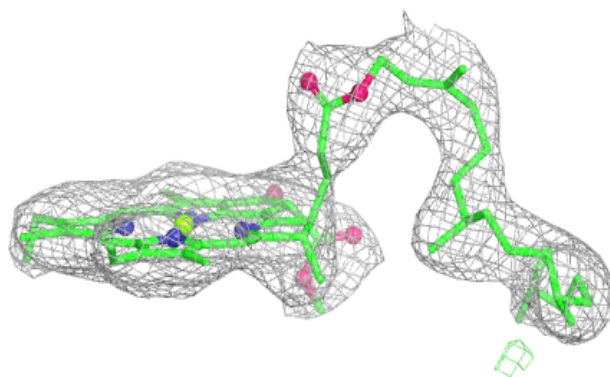
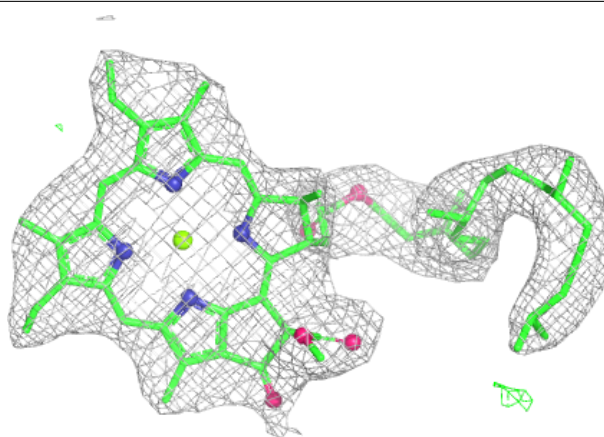
Electron density around PHO A 608:

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



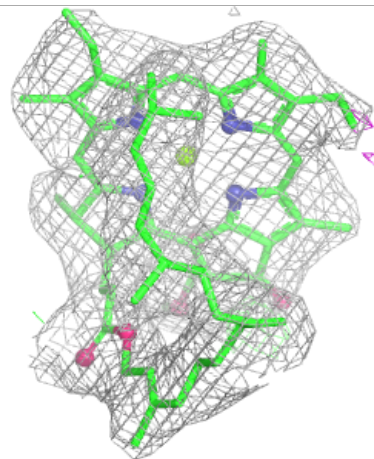
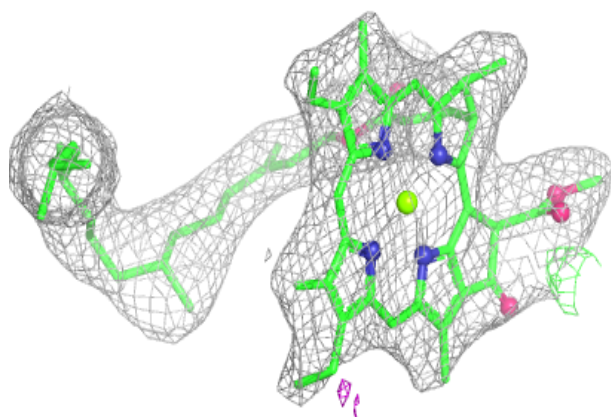
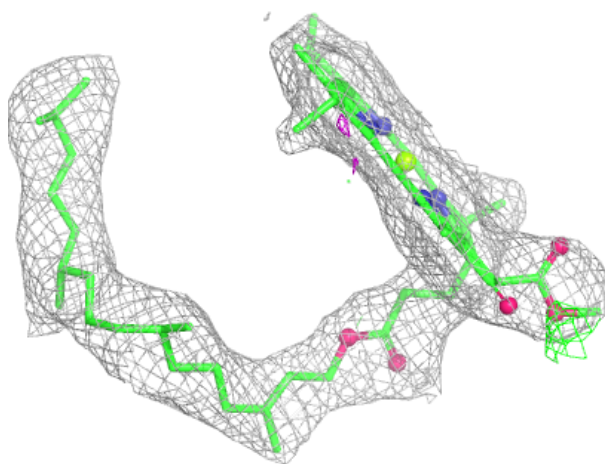
Electron density around CLA b 615:

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



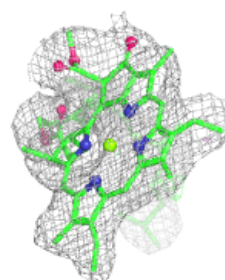
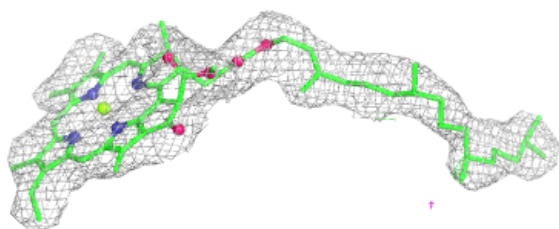
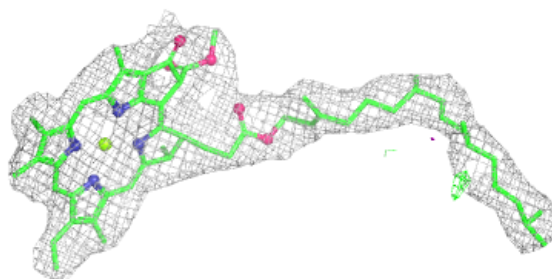
Electron density around CLA B 611:

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

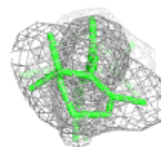
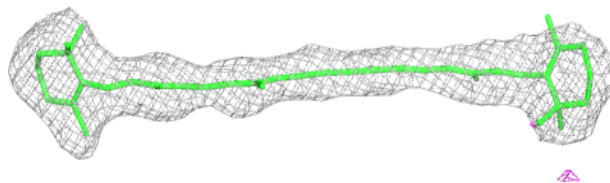
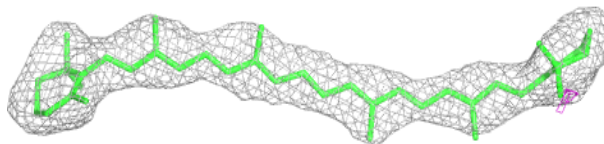


Electron density around CLA a 606:

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

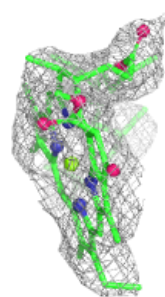
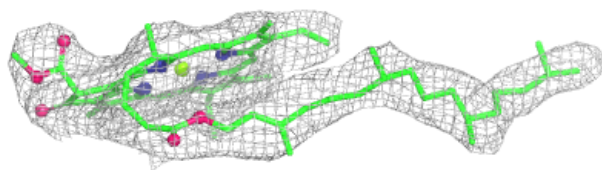
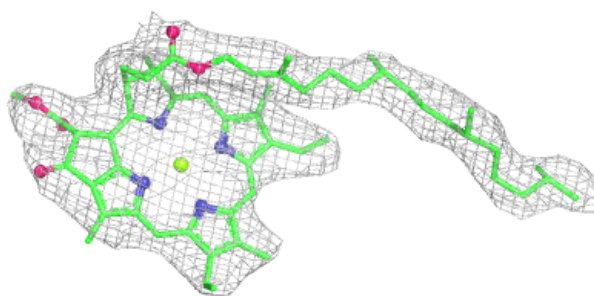
**Electron density around BCR a 610:**

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

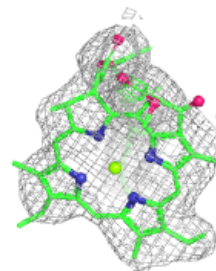
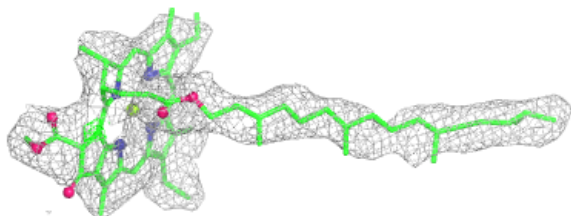
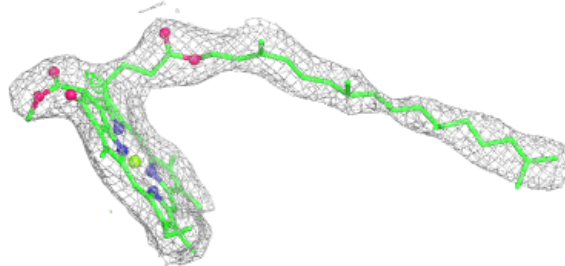


Electron density around CLA C 501:

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

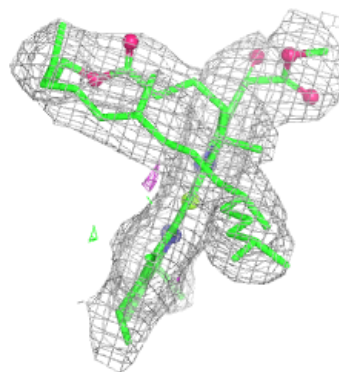
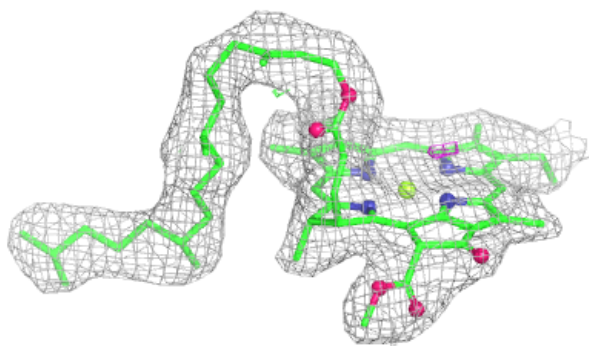
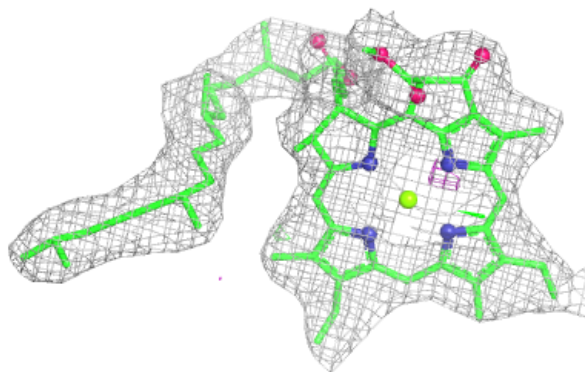
**Electron density around CLA b 610:**

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

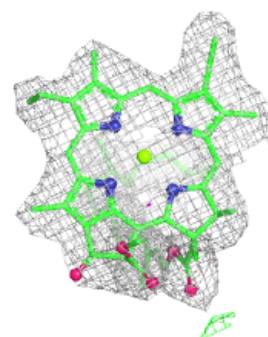
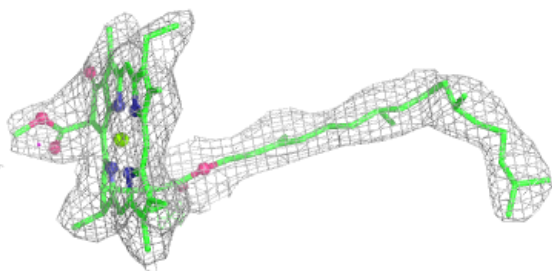
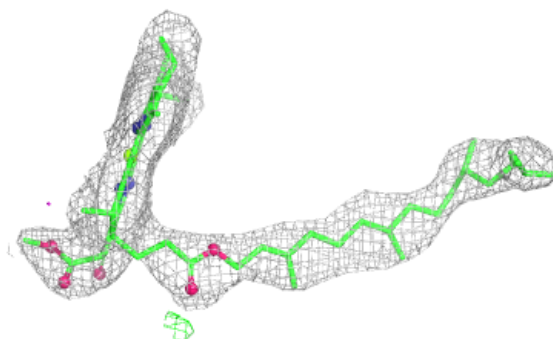


Electron density around CLA a 612:

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

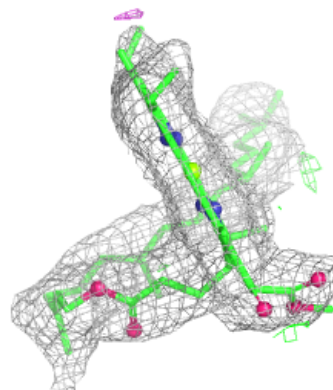
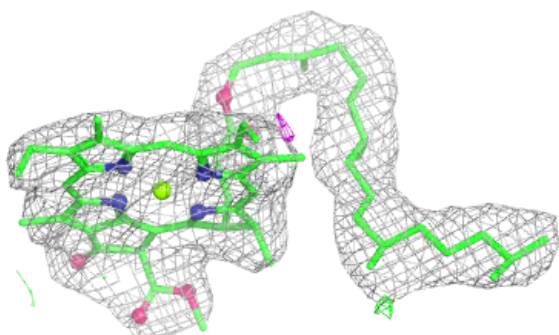
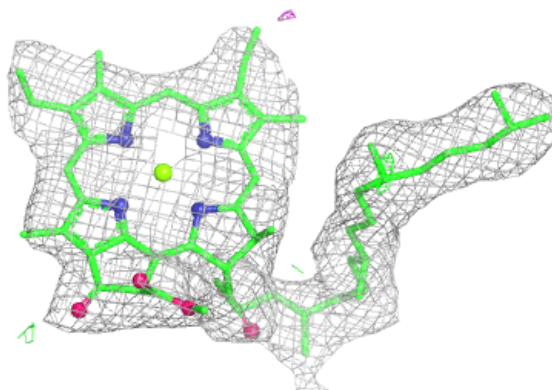
**Electron density around CLA B 605:**

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

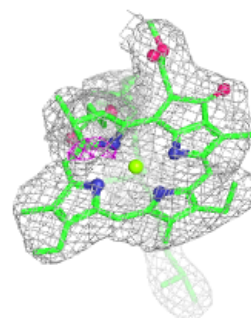
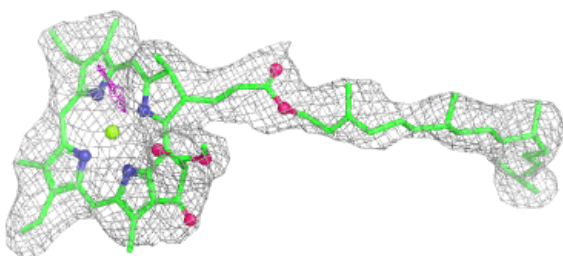
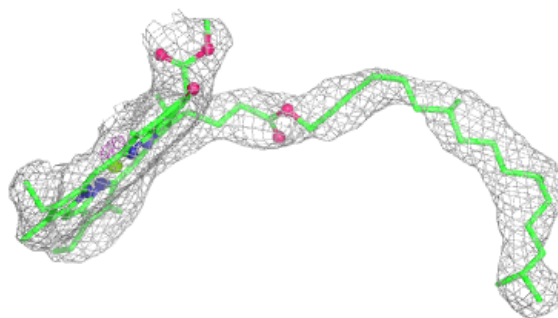


Electron density around CLA A 615:

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

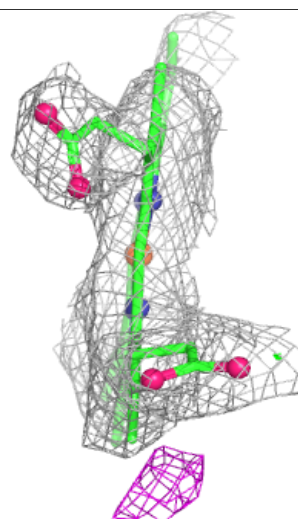
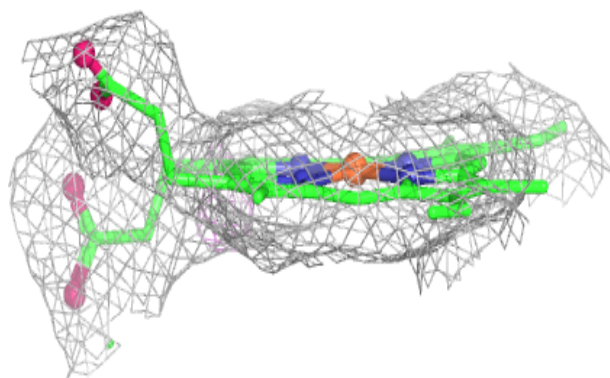
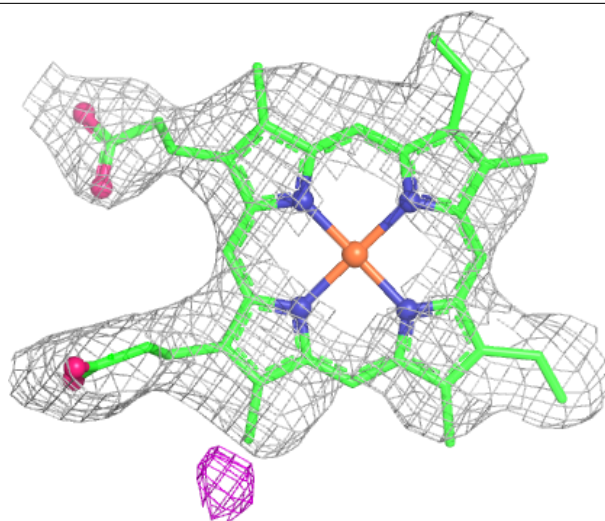
**Electron density around CLA d 403:**

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



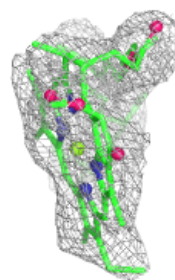
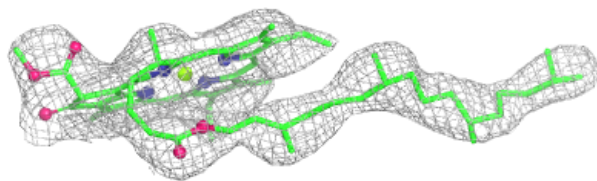
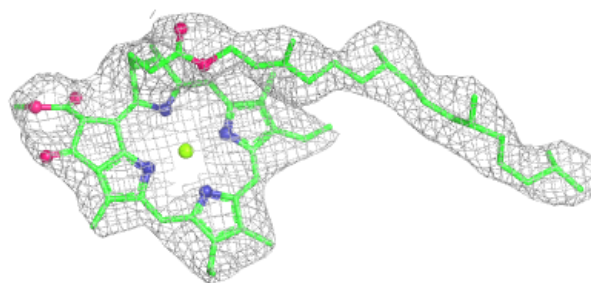
Electron density around HEC V 201:

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



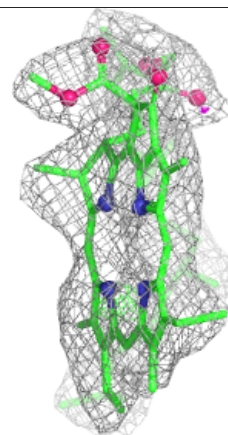
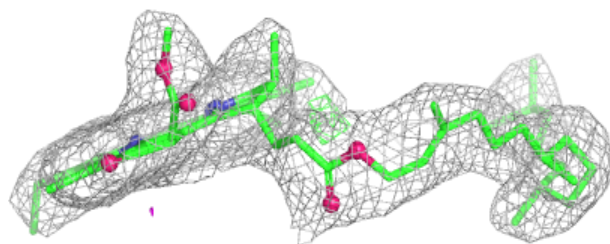
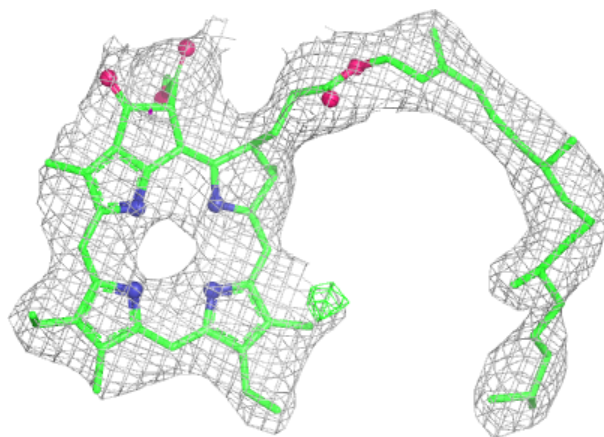
Electron density around CLA c 503:

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

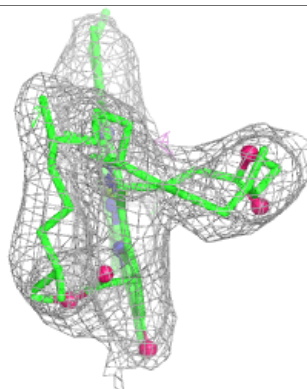
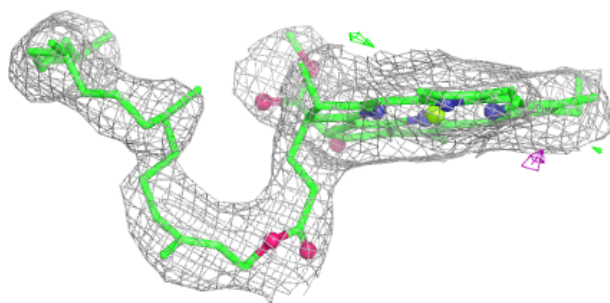
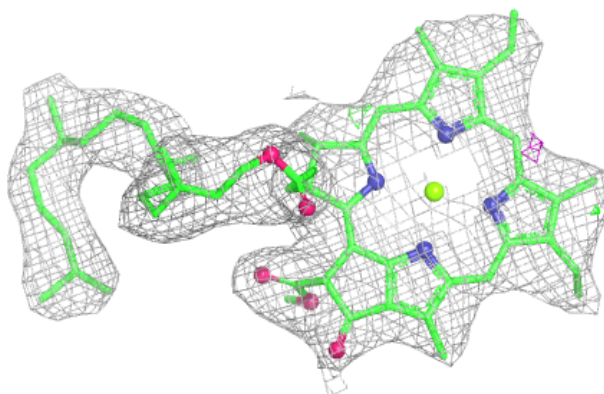


Electron density around PHO a 608:

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

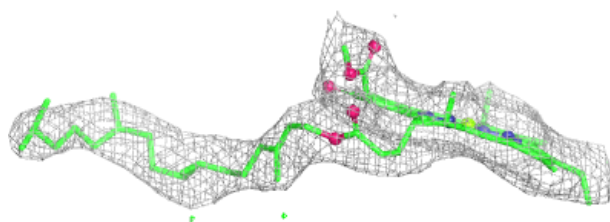
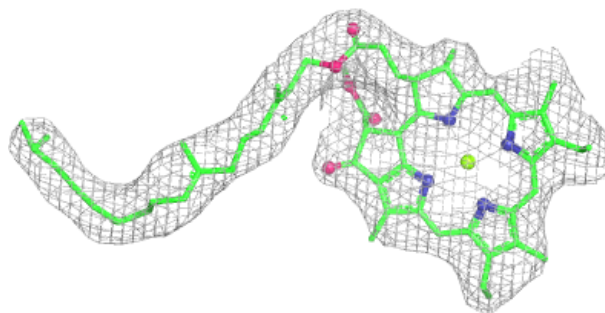
**Electron density around CLA B 612:**

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

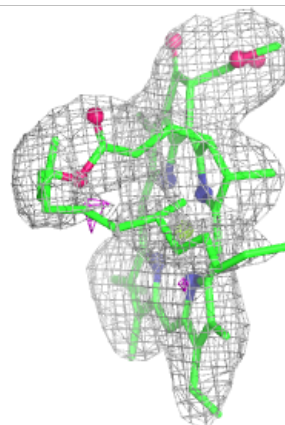
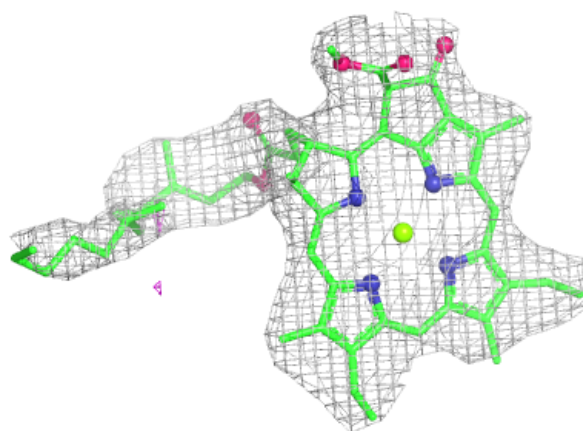


Electron density around CLA B 602:

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

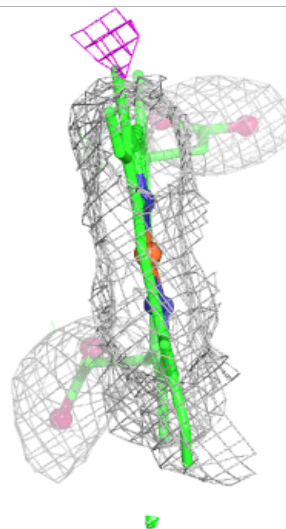
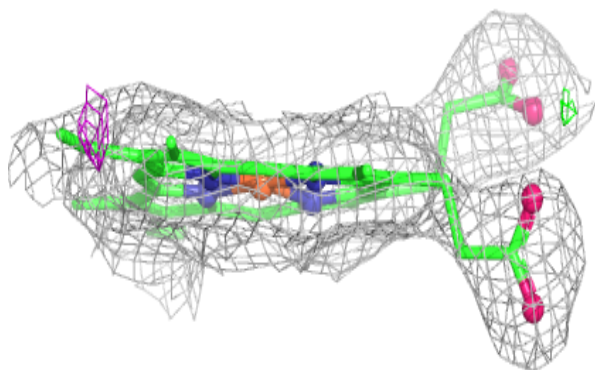
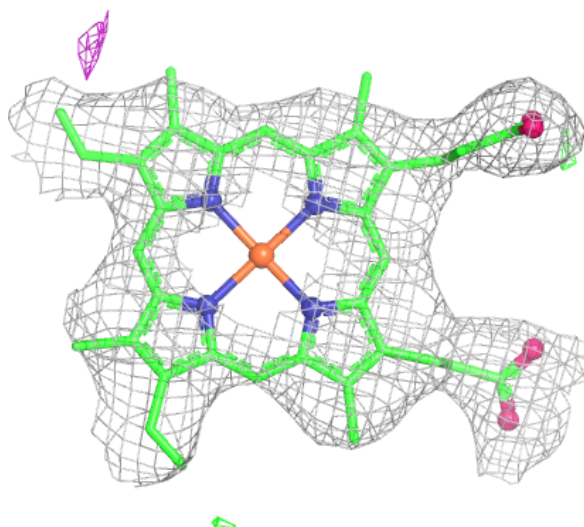
**Electron density around CLA a 607:**

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.