



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:19 PM EDT

PDB ID : 3WU2 / pdb_00003wu2
Title : Crystal structure analysis of Photosystem II complex
Authors : Umena, Y.; Kawakami, K.; Shen, J.R.; Kamiya, N.
Deposited on : 2014-04-21
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

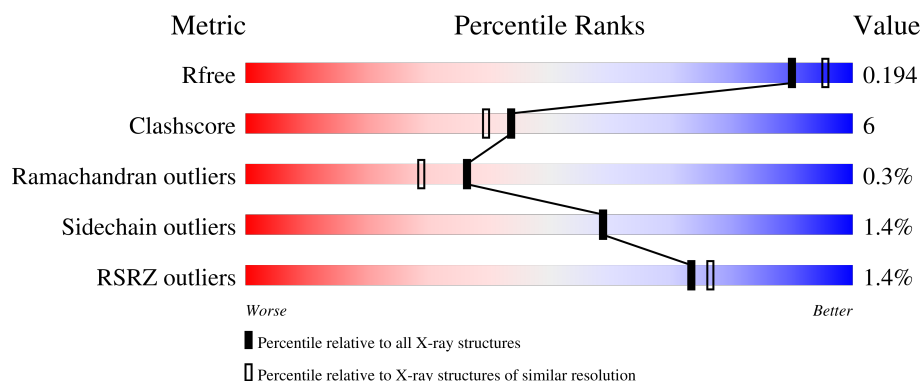
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



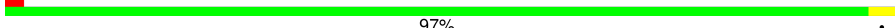
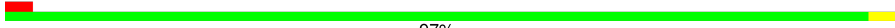
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	344	87% 9% . .
1	a	344	84% 13% .
2	B	504	2% 89% 11%
2	b	504	3% 90% 9% .
3	C	455	90% 9% .

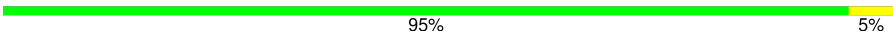
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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

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
29	UNL	D	412	-	-	X	-
29	UNL	b	628	-	-	X	-
31	GOL	C	524	-	-	X	-

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 54036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2633	1729	429	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2625	1722	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4009	2633	668	695	13			
2	b	501	Total	C	N	O	S	0	11	0
			3964	2605	658	688	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3502	2291	588	610	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2315	593	615	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	SEE REMARK 999	UNP D0VWR7
C	20	SER	-	SEE REMARK 999	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	SEE REMARK 999	UNP D0VWR7
C	22	PHE	-	SEE REMARK 999	UNP D0VWR7
c	19	ASN	-	SEE REMARK 999	UNP D0VWR7
c	20	SER	-	SEE REMARK 999	UNP D0VWR7
c	21	ILE	-	SEE REMARK 999	UNP D0VWR7
c	22	PHE	-	SEE REMARK 999	UNP D0VWR7

- 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	2	0
			2726	1809	443	462	12			
4	d	341	Total	C	N	O	S	0	4	0
			2741	1817	449	463	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	79	Total	C	N	O		0	0	0
			639	419	103	117				

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	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
			294	199	45	49	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	1			

- 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
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	48	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	1	0
			290	202	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	SEE REMARK 999	UNP P19054
K	39	TRP	VAL	SEE REMARK 999	UNP P19054
k	33	LEU	PHE	SEE REMARK 999	UNP P19054
k	39	TRP	VAL	SEE REMARK 999	UNP P19054

- 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	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	2	0
			300	204	45	51			

- 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	1	0
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			271	184	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	SEE REMARK 999	UNP P12312
m	8	LEU	PHE	SEE REMARK 999	UNP P12312

- 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	5	0
			1878	1177	314	382	5			
13	o	241	Total	C	N	O	S	0	5	0
			1855	1163	305	381	6			

- 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
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			770	489	129	152				
15	u	97	Total	C	N	O		0	1	0
			772	490	129	153				

- 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	2	0
			1066	677	180	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	130	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

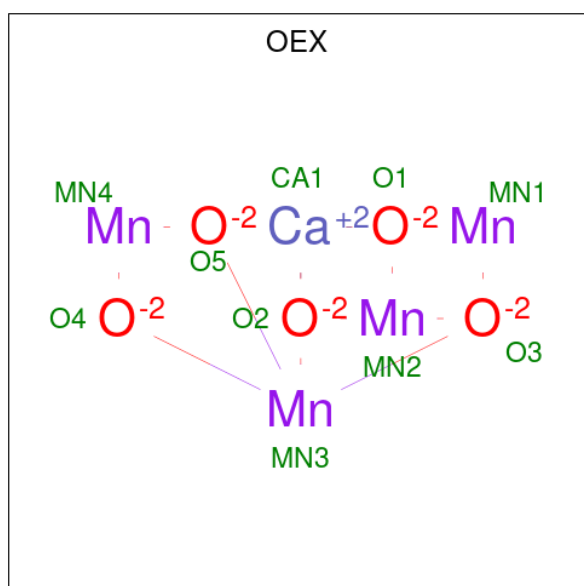
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O		0	1	0
			280	190	44	46				

- 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
			459	318	67	73	1			
19	z	60	Total	C	N	O	S	0	0	0
			431	301	64	65	1			

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

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

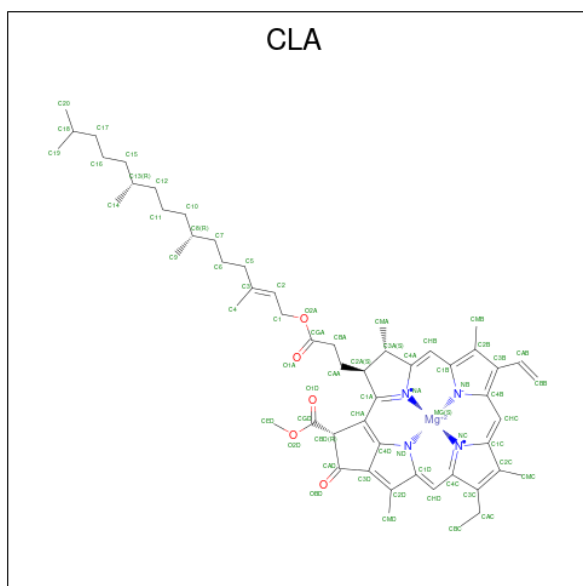
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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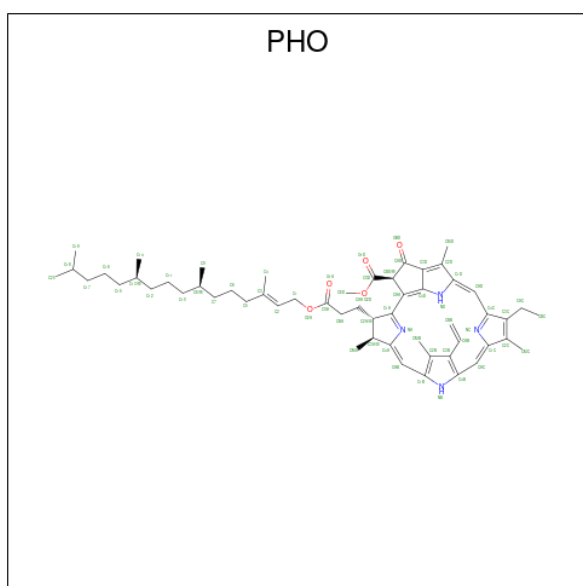
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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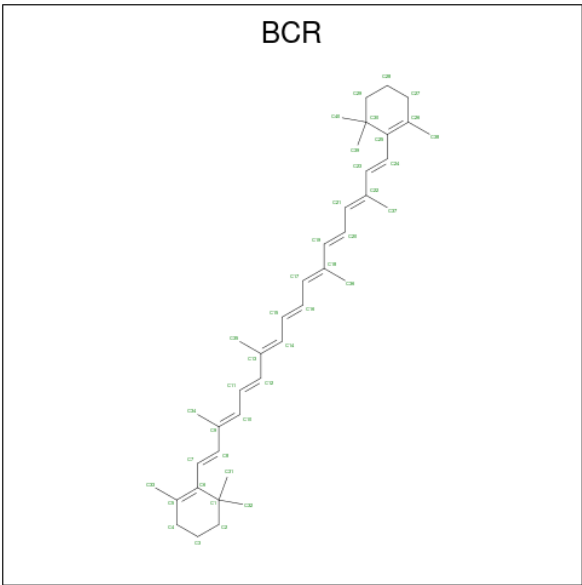
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



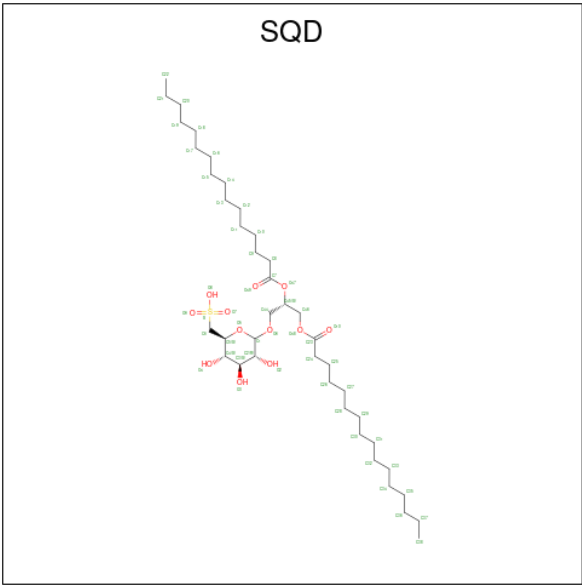
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



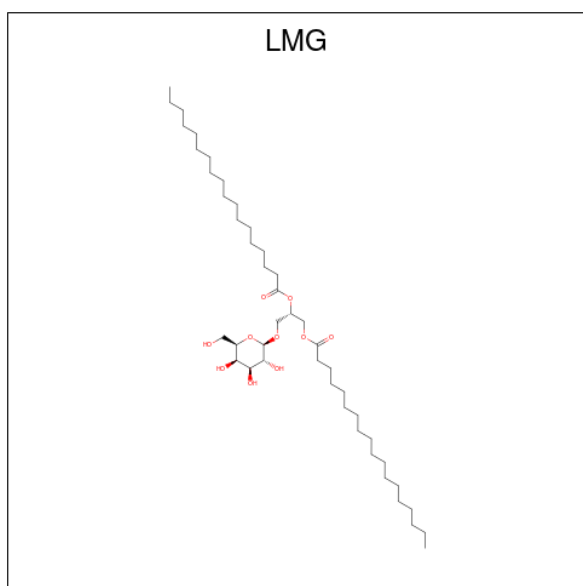
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			33	23	9	1		

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



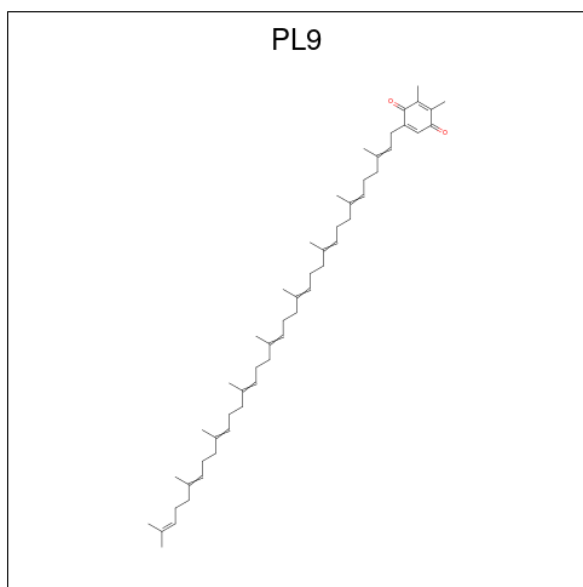
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O		0	0
			51	41	10			
27	B	1	Total	C	O		0	0
			51	41	10			
27	C	1	Total	C	O		0	0
			51	41	10			
27	D	1	Total	C	O		0	0
			51	41	10			
27	Z	1	Total	C	O		0	0
			51	41	10			
27	a	1	Total	C	O		0	0
			51	41	10			
27	b	1	Total	C	O		0	0
			51	41	10			
27	c	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			51	41	10		
27	d	1	Total	C	O	0	0
			51	41	10		

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

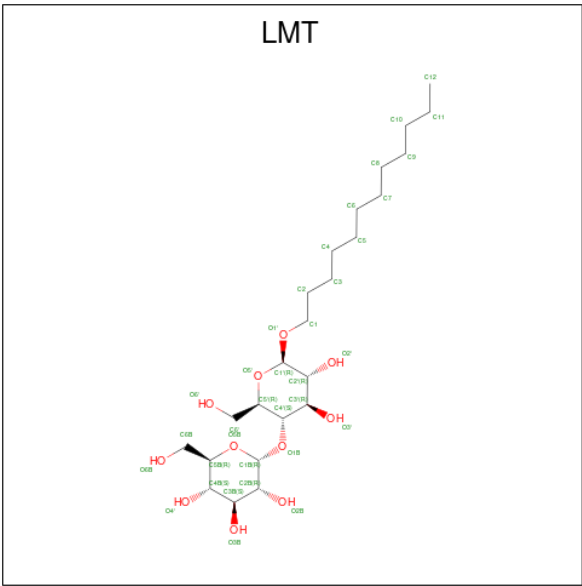
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	4	Total	C	O	0	0
			69	64	5		
29	B	4	Total	C		0	0
			56	56			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	1	Total C O 34 29 5	0	0
29	D	2	Total C O 56 51 5	0	0
29	E	2	Total C 27 27	0	0
29	H	1	Total C 10 10	0	0
29	I	2	Total C 24 24	0	0
29	J	2	Total C 26 26	0	0
29	L	1	Total C 14 14	0	0
29	M	1	Total C 16 16	0	0
29	T	1	Total C 13 13	0	0
29	X	1	Total C 16 16	0	0
29	Z	1	Total C 16 16	0	0
29	a	3	Total C O 56 51 5	0	0
29	b	4	Total C O 84 79 5	0	0
29	c	2	Total C O 40 35 5	0	0
29	d	1	Total C 16 16	0	0
29	e	1	Total C 11 11	0	0
29	i	4	Total C 55 55	0	0
29	j	2	Total C 28 28	0	0
29	t	1	Total C 16 16	0	0
29	x	1	Total C 16 16	0	0
29	z	1	Total C 16 16	0	0

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



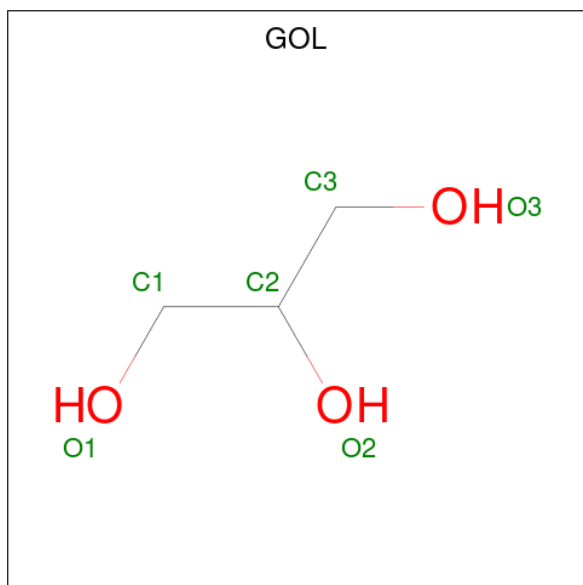
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	C	1	Total	C	O	0	0
			35	24	11		
30	F	1	Total	C	O	0	0
			35	24	11		
30	J	1	Total	C	O	0	0
			24	18	6		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	b	1	Total	C	O	0	0
			24	18	6		
30	c	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	O	0	0
			35	24	11		
30	t	1	Total	C	O	0	0
			24	18	6		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			6	3	3		
31	A	1	Total	C	O	0	0
			6	3	3		
31	A	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	D	1	Total 6	C 3	O 3	0	0
31	L	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0

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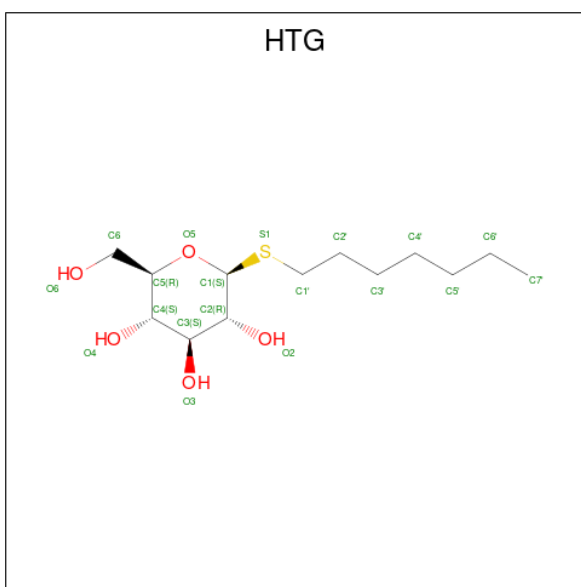
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 6 3 3	0	0
31	f	1	Total C O 6 3 3	0	0
31	h	1	Total C O 6 3 3	0	0
31	l	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0

- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total Ca 1 1	0	0
32	F	1	Total Ca 1 1	0	0
32	O	1	Total Ca 1 1	0	0
32	b	1	Total Ca 1 1	0	0
32	c	1	Total Ca 1 1	0	0
32	f	1	Total Ca 1 1	0	0
32	o	1	Total Ca 1 1	0	0

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



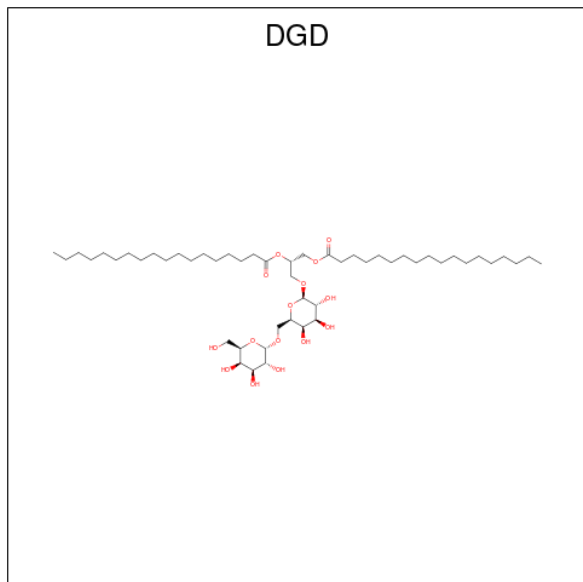
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	C	1	Total 19	C 13	O 5	S 1	0	0
33	C	1	Total 19	C 13	O 5	S 1	0	0
33	D	1	Total 19	C 13	O 5	S 1	0	0
33	O	1	Total 19	C 13	O 5	S 1	0	0
33	U	1	Total 9	C 8	S 1		0	0
33	V	1	Total 13	C 7	O 5	S 1	0	0
33	b	1	Total 19	C 13	O 5	S 1	0	0
33	b	1	Total 19	C 13	O 5	S 1	0	0
33	b	1	Total 19	C 13	O 5	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	d	1	Total	C	O	S	0	0
			19	13	5	1		
33	u	1	Total	C	O	S	0	0
			14	10	3	1		

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



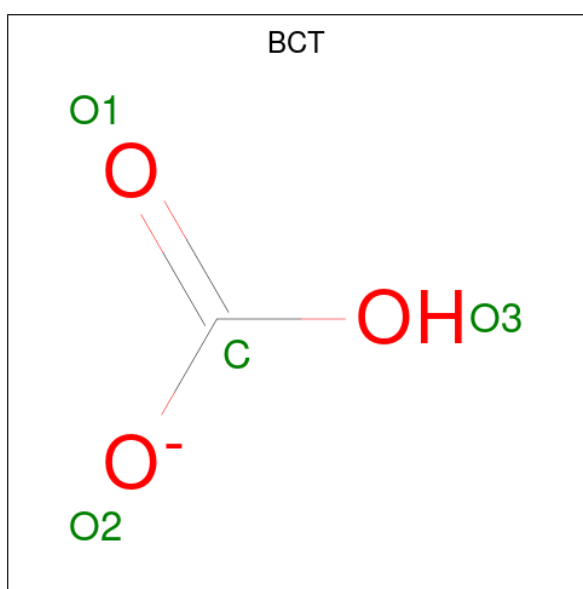
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	C	1	Total	C	O	0	0
			62	47	15		
34	C	1	Total	C	O	0	0
			62	47	15		
34	C	1	Total	C	O	0	0
			62	47	15		
34	D	1	Total	C	O	0	0
			53	42	11		
34	H	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		

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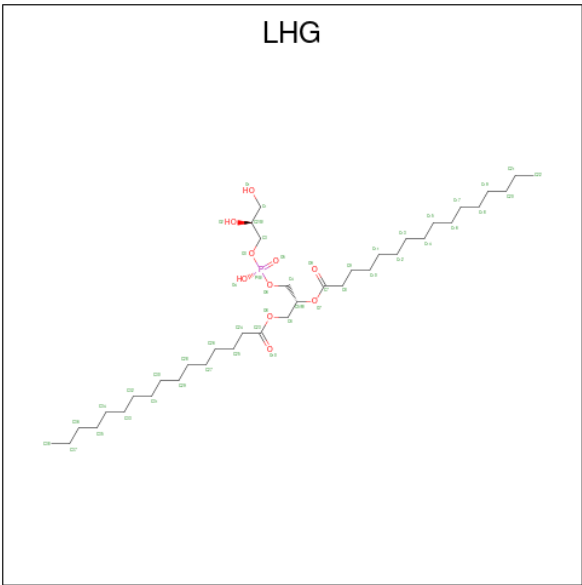
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		
34	d	1	Total	C	O	0	0
			50	41	9		
34	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



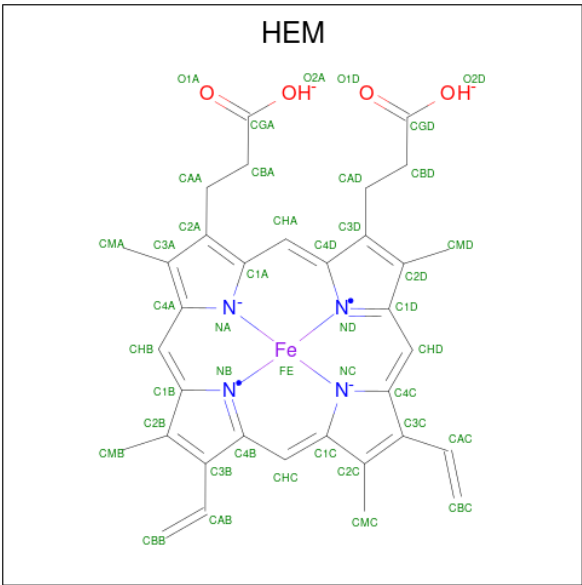
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	D	1	Total	C	O	0	0
			4	1	3		
35	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



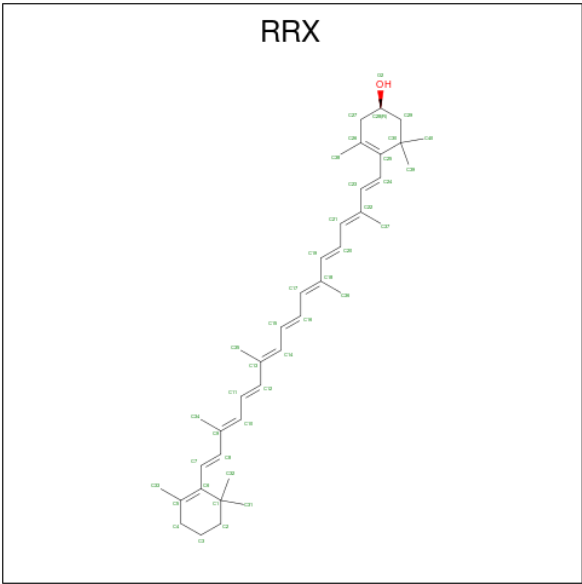
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			46	35	10	1		
36	E	1	Total	C	O	P	0	0
			49	38	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			40	29	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).

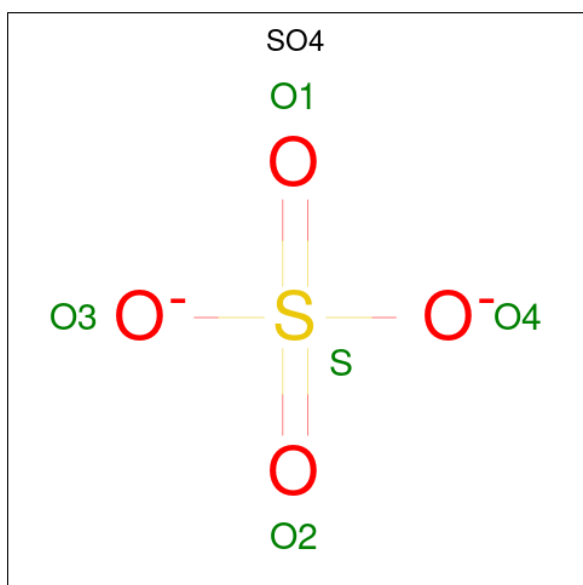


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg	0	0
			1	1		
39	j	1	Total	Mg	0	0
			1	1		

- Molecule 40 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	168	Total	O	0	2
			170	170		
41	B	311	Total	O	0	8
			319	319		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	253	Total O 263 263	0	10
41	D	156	Total O 161 161	0	5
41	E	32	Total O 35 35	0	3
41	F	12	Total O 12 12	0	0
41	H	50	Total O 52 52	0	2
41	I	8	Total O 8 8	0	0
41	J	9	Total O 9 9	0	0
41	K	8	Total O 8 8	0	0
41	L	23	Total O 24 24	0	1
41	M	15	Total O 16 16	0	1
41	O	193	Total O 202 202	0	9
41	T	10	Total O 10 10	0	0
41	U	98	Total O 100 100	0	2
41	V	140	Total O 144 144	0	4
41	Y	6	Total O 6 6	0	0
41	X	13	Total O 14 14	0	1
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 155 155	0	2
41	b	295	Total O 306 306	0	11
41	c	238	Total O 245 245	0	7
41	d	156	Total O 160 160	0	4

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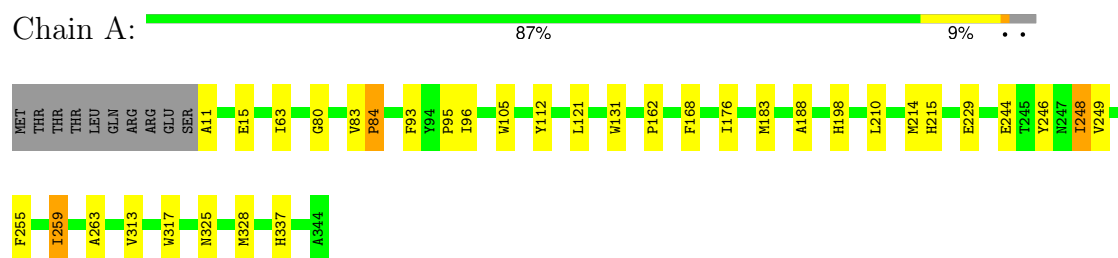
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	e	22	Total 22	O 22	0	0
41	f	13	Total 14	O 14	0	1
41	h	48	Total 53	O 53	0	5
41	i	13	Total 14	O 14	0	1
41	j	9	Total 9	O 9	0	0
41	k	5	Total 5	O 5	0	0
41	l	17	Total 18	O 18	0	1
41	m	15	Total 16	O 16	0	1
41	o	167	Total 175	O 175	0	8
41	t	12	Total 12	O 12	0	0
41	u	102	Total 106	O 106	0	4
41	v	98	Total 104	O 104	0	6
41	y	7	Total 7	O 7	0	0
41	x	6	Total 6	O 6	0	0
41	z	2	Total 2	O 2	0	0

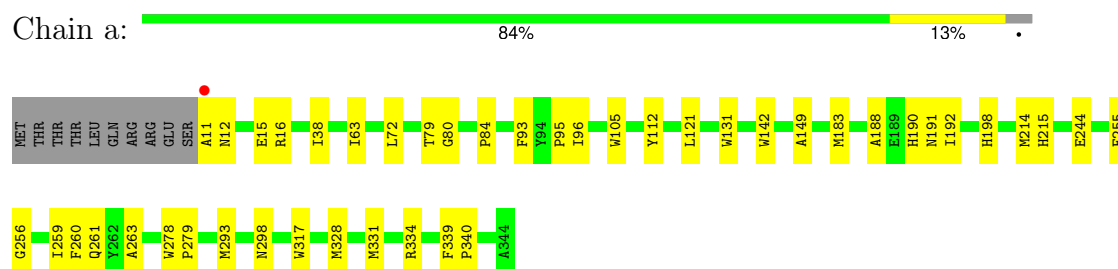
3 Residue-property plots [i](#)

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

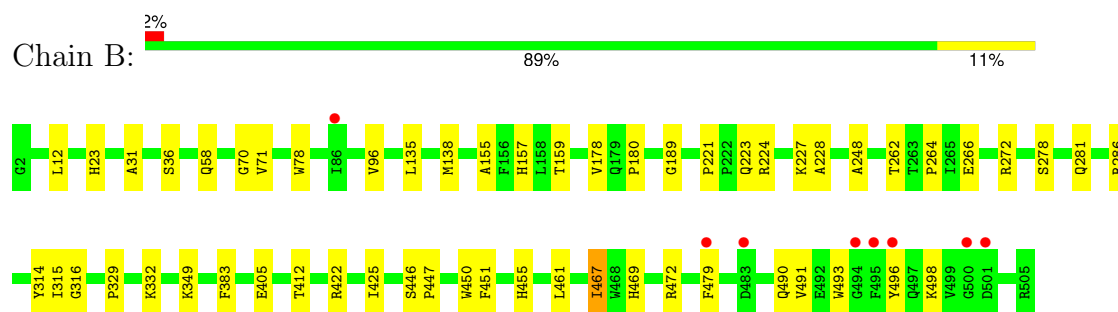
- Molecule 1: Photosystem Q(B) protein



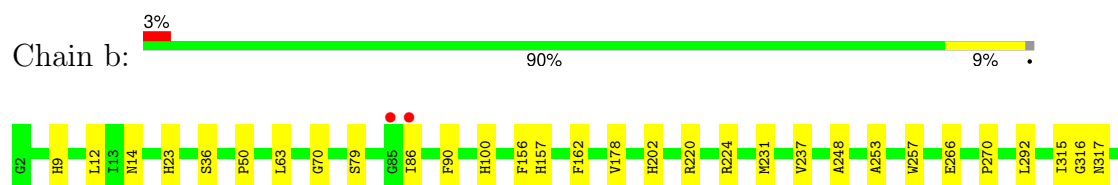
- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

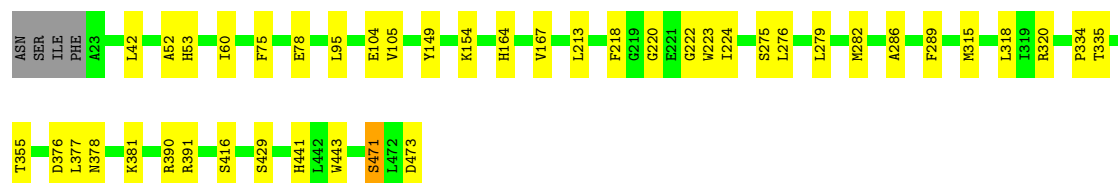
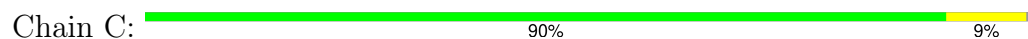


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

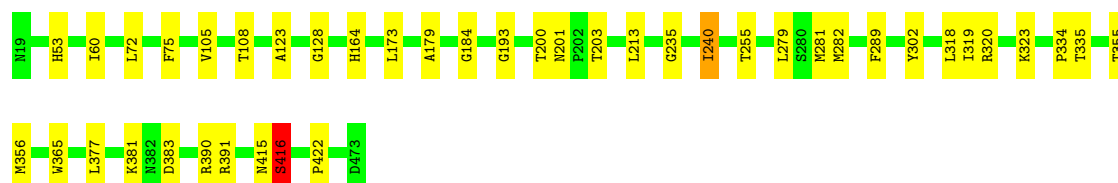




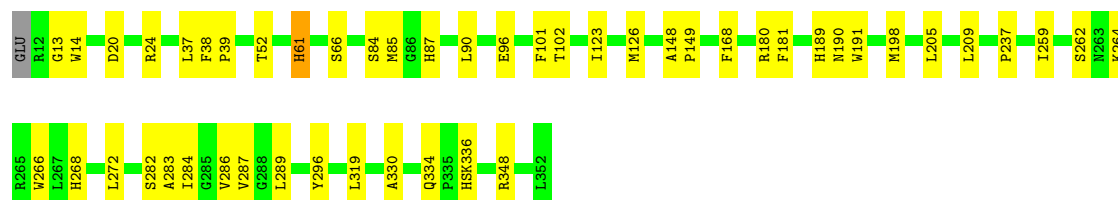
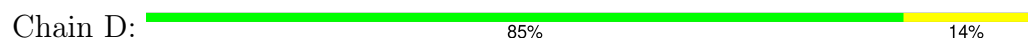
- Molecule 3: Photosystem II 44 kDa reaction center protein



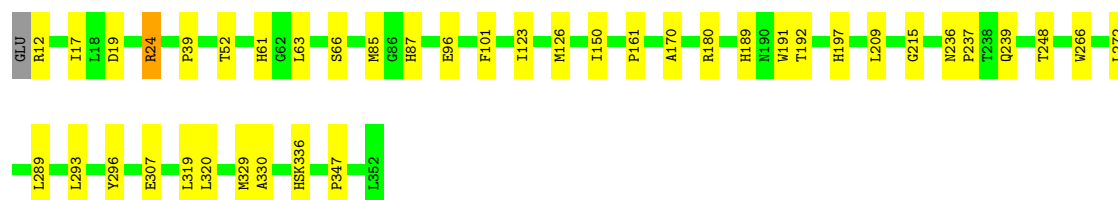
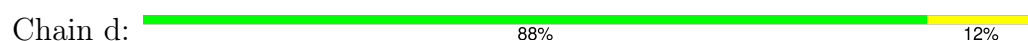
- Molecule 3: Photosystem II 44 kDa reaction center protein



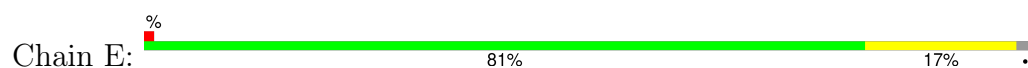
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha





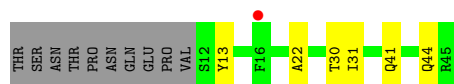
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 80% 14% 5%



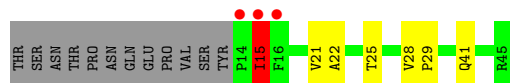
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 2% 64% 14% 23%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 7% 57% 14% 27%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 2% 97% 1%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 2% 86% 14%

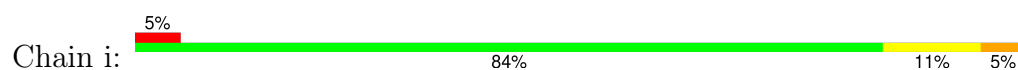


- Molecule 8: Photosystem II reaction center protein I

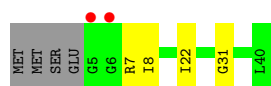
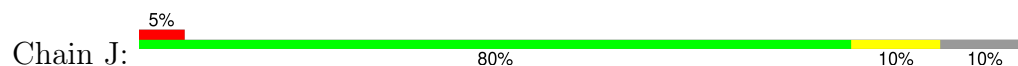
Chain I: 84% 11% 5%



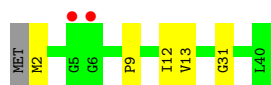
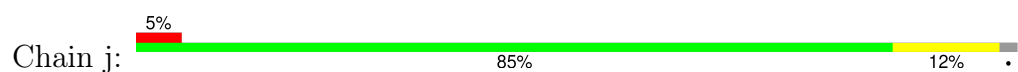
- Molecule 8: Photosystem II reaction center protein I



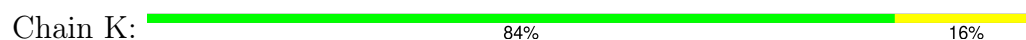
- Molecule 9: Photosystem II reaction center protein J



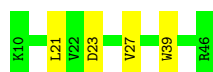
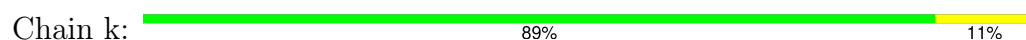
- Molecule 9: Photosystem II reaction center protein J



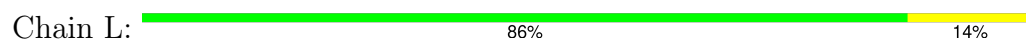
- Molecule 10: Photosystem II reaction center protein K



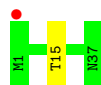
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  72% 17% 8%



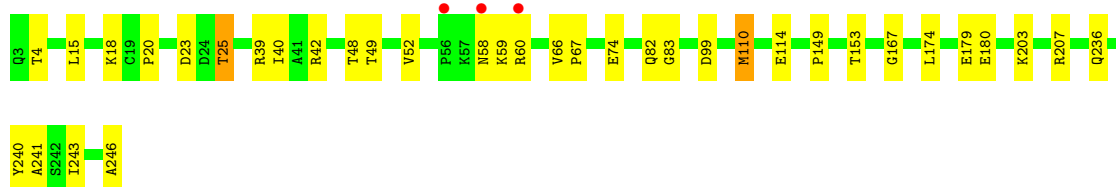
- Molecule 12: Photosystem II reaction center protein M

Chain m:  3% 81% 11% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  0% 85% 14%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  2% 87% 11%



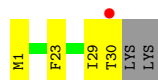
- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 84% 9% 6%



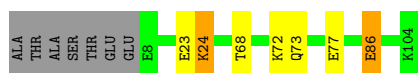
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 81% 12% 6%

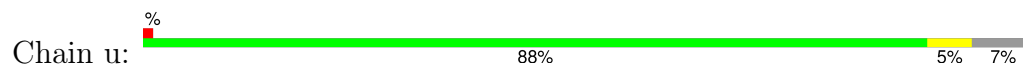


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  87% 5% 7%



- Molecule 15: Photosystem II 12 kDa extrinsic protein



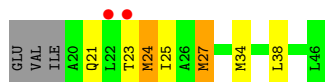
- Molecule 16: Cytochrome c-550



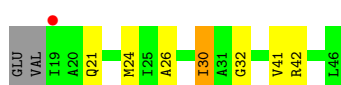
- Molecule 16: Cytochrome c-550



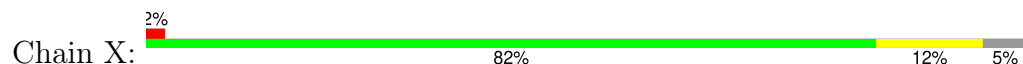
- Molecule 17: Photosystem II reaction center protein Ycf12



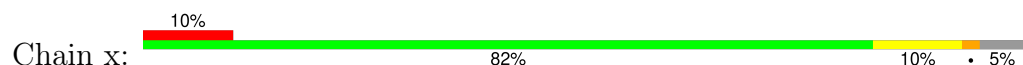
- Molecule 17: Photosystem II reaction center protein Ycf12

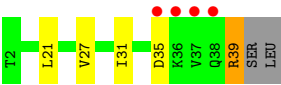


- Molecule 18: Photosystem II reaction center protein X

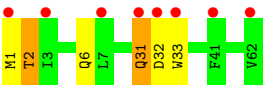
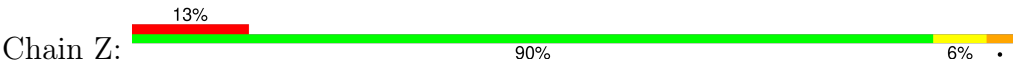


- Molecule 18: Photosystem II reaction center protein X

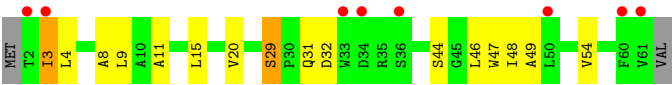




● Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (20.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.194 0.157 , 0.194	Depositor DCC
R_{free} test set	31215 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54036	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: MG, LHG, HEM, OEX, CL, DGD, SQD, FE2, BCR, BCT, LMT, GOL, LMG, PHO, PL9, CA, SO4, HSK, CLA, UNL, HTG, RRX, FME

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	1.33	5/2730 (0.2%)	1.14	2/3723 (0.1%)
1	a	1.32	8/2721 (0.3%)	1.10	3/3711 (0.1%)
2	B	1.29	9/4179 (0.2%)	1.10	8/5693 (0.1%)
2	b	1.25	9/4134 (0.2%)	1.06	7/5633 (0.1%)
3	C	1.23	3/3624 (0.1%)	1.04	1/4933 (0.0%)
3	c	1.19	3/3662 (0.1%)	1.05	2/4986 (0.0%)
4	D	1.38	17/2804 (0.6%)	1.15	8/3820 (0.2%)
4	d	1.26	6/2825 (0.2%)	1.07	1/3847 (0.0%)
5	E	1.03	0/676	1.03	0/924
5	e	1.05	1/658 (0.2%)	1.09	1/899 (0.1%)
6	F	1.11	0/283	1.04	2/386 (0.5%)
6	f	1.12	0/265	0.93	1/360 (0.3%)
7	H	1.13	0/511	1.04	0/697
7	h	1.13	0/511	1.02	0/697
8	I	1.06	0/291	1.05	1/394 (0.3%)
8	i	1.03	1/308 (0.3%)	1.01	0/415
9	J	1.11	0/257	1.02	1/349 (0.3%)
9	j	0.96	0/277	1.04	0/376
10	K	0.94	0/303	1.11	0/418
10	k	0.99	0/296	1.09	0/408
11	L	1.17	1/312 (0.3%)	1.09	0/425
11	l	1.16	0/313	1.01	0/428
12	M	1.11	0/257	1.26	2/352 (0.6%)
12	m	1.08	0/270	1.03	0/370
13	O	1.09	0/1924	1.08	3/2610 (0.1%)
13	o	1.03	1/1900 (0.1%)	1.09	6/2577 (0.2%)
14	T	1.13	0/255	1.05	0/346
14	t	1.21	0/255	1.13	0/346
15	U	1.15	0/781	1.07	0/1059
15	u	1.18	0/786	1.07	1/1067 (0.1%)
16	V	1.28	3/1093 (0.3%)	1.13	2/1485 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	1.17	1/1084 (0.1%)	1.10	4/1475 (0.3%)
17	Y	0.79	0/197	0.98	0/263
17	y	0.76	0/197	1.27	2/264 (0.8%)
18	X	0.95	0/286	1.10	2/387 (0.5%)
18	x	0.95	0/286	1.06	0/387
19	Z	0.88	0/470	1.05	0/645
19	z	0.82	0/442	1.15	1/608 (0.2%)
All	All	1.21	68/42423 (0.2%)	1.08	61/57763 (0.1%)

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	33	LYS	N-CA	7.62	1.51	1.46
4	D	87	HIS	CE1-NE2	7.31	1.39	1.32
4	D	87	HIS	CG-CD2	7.20	1.43	1.35
4	D	319	LEU	N-CA	7.07	1.55	1.46
1	a	149	ALA	N-CA	-6.90	1.42	1.46
4	d	248	THR	CA-C	6.52	1.61	1.52
1	A	80	GLY	N-CA	6.48	1.53	1.45
1	a	198	HIS	ND1-CE1	6.35	1.39	1.32
4	d	87	HIS	CG-CD2	6.35	1.42	1.35
4	D	189	HIS	CG-CD2	6.24	1.42	1.35
2	b	9	HIS	CG-CD2	6.19	1.42	1.35
3	c	356	MET	C-O	-6.05	1.16	1.24
16	V	118	HIS	CG-CD2	5.95	1.42	1.35
16	v	92	HIS	CE1-NE2	5.93	1.38	1.32
1	A	325	ASN	N-CA	5.90	1.53	1.46
1	A	198	HIS	ND1-CE1	5.85	1.38	1.32
4	d	189	HIS	CG-CD2	5.83	1.42	1.35
4	D	198	MET	N-CA	5.79	1.53	1.46
1	a	149	ALA	CA-C	5.79	1.58	1.52
4	D	181	PHE	C-O	-5.78	1.17	1.24
4	d	330	ALA	CA-C	5.78	1.59	1.52
2	B	221	PRO	CA-C	5.77	1.55	1.51
2	b	63	LEU	CA-C	5.75	1.59	1.52
4	D	189	HIS	ND1-CE1	5.74	1.38	1.32
2	B	469	HIS	ND1-CE1	5.73	1.38	1.32
3	C	164	HIS	ND1-CE1	5.73	1.38	1.32
2	B	23	HIS	ND1-CE1	5.71	1.38	1.32
2	b	384	ARG	N-CA	5.70	1.53	1.46
1	a	80	GLY	N-CA	5.68	1.53	1.45
4	D	259	ILE	N-CA	-5.62	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	286	VAL	C-O	-5.54	1.17	1.24
4	D	87	HIS	ND1-CE1	5.54	1.38	1.32
2	B	23	HIS	CG-CD2	5.54	1.42	1.35
11	L	34	TYR	C-O	5.54	1.31	1.24
4	D	38	PHE	C-O	-5.50	1.19	1.24
4	D	334	GLN	CA-C	5.49	1.59	1.52
1	a	190	HIS	CE1-NE2	5.46	1.38	1.32
1	a	38	ILE	CA-CB	5.46	1.57	1.54
2	B	155	ALA	N-CA	5.44	1.53	1.46
2	b	100	HIS	CG-CD2	5.43	1.41	1.35
16	V	69	ILE	C-O	5.42	1.30	1.24
2	b	23	HIS	ND1-CE1	5.41	1.38	1.32
13	o	158	ASP	CA-C	5.36	1.59	1.52
3	C	441	HIS	CG-CD2	5.36	1.41	1.35
4	D	84	SER	N-CA	5.34	1.53	1.46
16	V	41	HIS	ND1-CE1	5.33	1.37	1.32
5	e	58	GLN	C-O	5.31	1.30	1.24
2	b	469	HIS	CG-CD2	5.26	1.41	1.35
4	D	190	ASN	N-CA	5.26	1.54	1.46
2	b	9	HIS	ND1-CE1	5.25	1.37	1.32
4	D	268	HIS	ND1-CE1	5.24	1.37	1.32
4	d	87	HIS	ND1-CE1	5.21	1.37	1.32
3	C	53	HIS	CG-CD2	5.20	1.41	1.35
3	c	164	HIS	CG-CD2	5.19	1.41	1.35
2	B	78	TRP	CD2-CE2	5.18	1.50	1.41
2	b	202	HIS	CG-CD2	5.13	1.41	1.35
3	c	193	GLY	N-CA	5.12	1.50	1.45
1	a	190	HIS	ND1-CE1	5.11	1.37	1.32
4	d	197	HIS	ND1-CE1	5.09	1.37	1.32
4	D	330	ALA	N-CA	5.08	1.51	1.46
2	B	455	HIS	ND1-CE1	5.08	1.37	1.32
2	b	220	ARG	C-N	5.07	1.38	1.33
1	A	337	HIS	ND1-CE1	5.06	1.37	1.32
1	a	191	ASN	N-CA	5.06	1.54	1.46
1	A	176	ILE	N-CA	5.04	1.52	1.46
2	B	450	TRP	NE1-CE2	-5.04	1.31	1.37
2	B	332	LYS	C-O	5.02	1.30	1.24
4	D	61	HIS	ND1-CE1	5.01	1.37	1.32

All (61) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	58	GLN	N-CA-C	8.24	121.30	111.33
16	V	85	GLU	N-CA-C	7.08	119.07	111.36
1	a	142	TRP	N-CA-C	6.95	121.46	112.92
16	v	105	ARG	N-CA-C	6.72	119.46	111.33
2	b	316	GLY	N-CA-C	-6.68	106.57	115.32
2	B	479	PHE	N-CA-C	6.64	120.48	112.38
13	o	58	ASN	N-CA-C	6.63	120.42	108.48
2	B	31	ALA	N-CA-C	-6.26	104.54	111.36
18	X	4	THR	CA-C-N	-6.18	112.64	119.19
18	X	4	THR	C-N-CA	-6.18	112.64	119.19
16	v	85	GLU	N-CA-C	6.12	119.94	112.23
12	M	4	ASN	CA-C-N	6.08	129.03	120.28
12	M	4	ASN	C-N-CA	6.08	129.03	120.28
2	B	221	PRO	CB-CA-C	-5.96	105.79	111.39
4	D	37	LEU	N-CA-C	5.90	117.39	111.07
13	O	4	THR	N-CA-C	5.89	118.84	109.24
13	o	104	GLN	CA-C-N	-5.89	113.63	119.99
13	o	104	GLN	C-N-CA	-5.89	113.63	119.99
6	F	13	TYR	CA-C-N	-5.80	114.64	120.21
6	F	13	TYR	C-N-CA	-5.80	114.64	120.21
2	B	412	THR	N-CA-C	-5.74	106.07	114.39
2	b	36	SER	CB-CA-C	-5.73	101.84	110.90
13	o	121	THR	N-CA-C	5.71	117.75	109.07
16	V	7	VAL	N-CA-C	-5.61	104.89	110.62
16	v	105	ARG	CA-C-N	-5.60	113.82	122.49
16	v	105	ARG	C-N-CA	-5.60	113.82	122.49
2	b	479	PHE	N-CA-C	5.59	119.71	113.01
1	a	79	THR	N-CA-C	-5.56	106.66	113.50
2	B	189	GLY	N-CA-C	-5.55	107.44	114.16
15	u	32	ILE	N-CA-C	5.52	117.95	111.05
6	f	15	ILE	N-CA-C	5.49	115.69	107.51
2	b	257	TRP	N-CA-C	5.44	117.29	111.36
3	C	220	GLY	N-CA-C	-5.43	107.82	115.32
4	D	262	SER	N-CA-C	-5.43	106.51	114.39
9	J	7	ARG	N-CA-C	5.43	117.19	111.28
4	D	348	ARG	CA-C-N	-5.42	116.90	122.27
4	D	348	ARG	C-N-CA	-5.42	116.90	122.27
3	c	53	HIS	N-CA-C	5.41	116.86	111.07
2	b	446	SER	CA-C-N	-5.38	114.12	119.56
2	b	446	SER	C-N-CA	-5.38	114.12	119.56
1	a	131	TRP	CA-CB-CG	-5.37	103.40	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	34	ARG	N-CA-C	5.36	116.87	109.15
17	y	32	GLY	CA-C-N	5.32	125.14	119.28
17	y	32	GLY	C-N-CA	5.32	125.14	119.28
13	O	48	THR	N-CA-C	-5.30	107.48	114.31
3	c	383	ASP	N-CA-C	5.29	119.71	112.88
4	D	205	LEU	CA-C-N	5.27	125.83	119.98
4	D	205	LEU	C-N-CA	5.27	125.83	119.98
13	o	229	GLU	CA-C-N	-5.26	115.16	120.21
13	o	229	GLU	C-N-CA	-5.26	115.16	120.21
13	O	174	LEU	N-CA-C	-5.26	101.37	109.79
2	B	135	LEU	CA-C-N	-5.25	113.22	119.05
2	B	135	LEU	C-N-CA	-5.25	113.22	119.05
1	A	83	VAL	N-CA-C	5.25	113.14	108.63
4	D	296	TYR	N-CA-C	-5.24	106.56	113.12
4	d	215	GLY	N-CA-C	-5.22	106.45	112.50
1	A	131	TRP	CA-CB-CG	-5.21	103.71	113.60
2	B	272	ARG	NE-CZ-NH1	-5.14	116.36	121.50
4	D	282	SER	N-CA-C	-5.13	105.87	111.82
2	b	253	ALA	N-CA-C	-5.12	105.78	111.36
19	z	4	LEU	N-CA-C	-5.00	106.02	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2633	0	2544	28	0
1	a	2625	0	2538	31	0
2	B	4009	0	3879	37	0
2	b	3964	0	3817	31	0
3	C	3502	0	3431	35	0
3	c	3536	0	3460	29	0
4	D	2726	0	2629	27	0
4	d	2741	0	2654	28	0
5	E	657	0	637	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	639	0	617	10	0
6	F	274	0	279	4	0
6	f	257	0	269	5	0
7	H	498	0	518	2	0
7	h	498	0	518	9	0
8	I	294	0	304	4	0
8	i	311	0	326	4	0
9	J	251	0	257	3	0
9	j	271	0	270	4	0
10	K	290	0	294	6	0
10	k	286	0	285	3	0
11	L	302	0	316	7	0
11	l	300	0	314	0	0
12	M	261	0	280	18	0
12	m	271	0	293	17	0
13	O	1878	0	1853	25	0
13	o	1855	0	1823	18	0
14	T	256	0	256	2	0
14	t	256	0	256	2	0
15	U	770	0	769	5	0
15	u	772	0	766	3	0
16	V	1066	0	1075	4	0
16	v	1060	0	1053	10	0
17	Y	196	0	219	8	0
17	y	196	0	208	4	0
18	X	280	0	312	5	0
18	x	280	0	312	5	0
19	Z	459	0	484	2	0
19	z	431	0	438	9	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	7	0
23	B	1040	0	1152	31	0
23	C	845	0	936	28	0
23	D	130	0	144	1	0
23	a	260	0	288	6	0
23	b	1040	0	1152	25	0
23	c	845	0	936	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	d	130	0	144	5	0
24	A	128	0	148	3	0
24	a	128	0	148	3	0
25	A	40	0	56	2	0
25	B	120	0	168	5	0
25	C	80	0	112	4	0
25	D	40	0	56	2	0
25	K	80	0	112	6	0
25	T	40	0	56	5	0
25	a	40	0	56	2	0
25	b	120	0	168	3	0
25	c	80	0	112	6	0
25	d	40	0	56	5	0
25	k	80	0	112	5	0
25	t	40	0	56	7	0
26	A	108	0	155	5	0
26	B	54	0	78	5	0
26	D	45	0	57	3	0
26	L	54	0	78	5	0
26	a	108	0	156	10	0
26	f	33	0	39	2	0
27	A	51	0	72	3	0
27	B	51	0	72	4	0
27	C	51	0	72	2	0
27	D	51	0	72	2	0
27	Z	51	0	72	0	0
27	a	51	0	72	7	0
27	b	51	0	72	3	0
27	c	102	0	144	2	0
27	d	51	0	72	1	0
28	A	55	0	80	10	0
28	D	55	0	80	0	0
28	a	55	0	80	9	0
28	d	55	0	80	0	0
29	A	69	0	0	0	0
29	B	56	0	0	3	0
29	C	34	0	0	0	0
29	D	56	0	0	2	0
29	E	27	0	0	0	0
29	H	10	0	0	0	0
29	I	24	0	0	0	0
29	J	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	L	14	0	0	1	0
29	M	16	0	0	1	0
29	T	13	0	0	0	0
29	X	16	0	0	0	0
29	Z	16	0	0	0	0
29	a	56	0	0	1	0
29	b	84	0	0	2	0
29	c	40	0	0	1	0
29	d	16	0	0	0	0
29	e	11	0	0	0	0
29	i	55	0	0	0	0
29	j	28	0	0	0	0
29	t	16	0	0	0	0
29	x	16	0	0	1	0
29	z	16	0	0	0	0
30	A	35	0	46	0	0
30	B	35	0	46	4	0
30	C	35	0	46	4	0
30	F	35	0	46	0	0
30	J	24	0	35	1	0
30	M	70	0	92	2	0
30	Z	35	0	46	2	0
30	a	35	0	46	1	0
30	b	49	0	70	2	0
30	c	35	0	46	1	0
30	m	70	0	92	1	0
30	t	24	0	35	0	0
30	z	32	0	33	5	0
31	A	18	0	22	1	0
31	B	36	0	48	1	0
31	C	18	0	24	4	0
31	D	6	0	8	3	0
31	L	6	0	8	1	0
31	O	6	0	8	0	0
31	V	18	0	24	0	0
31	a	18	0	24	3	0
31	b	30	0	40	3	0
31	c	24	0	32	5	0
31	f	6	0	6	0	0
31	h	6	0	8	0	0
31	l	6	0	8	0	0
31	v	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B	1	0	0	0	0
32	F	1	0	0	0	0
32	O	1	0	0	0	0
32	b	1	0	0	0	0
32	c	1	0	0	0	0
32	f	1	0	0	0	0
32	o	1	0	0	0	0
33	B	95	0	130	1	0
33	C	38	0	52	1	0
33	D	19	0	26	2	0
33	O	19	0	26	0	0
33	U	9	0	15	1	0
33	V	13	0	11	0	0
33	b	76	0	104	3	0
33	c	38	0	52	1	0
33	d	19	0	26	1	0
33	u	14	0	19	0	0
34	C	186	0	246	2	0
34	D	53	0	71	6	0
34	H	62	0	82	1	0
34	c	186	0	246	5	0
34	d	50	0	69	3	0
34	h	62	0	82	1	0
35	D	4	0	0	0	0
35	a	4	0	0	0	0
36	D	144	0	213	15	0
36	E	49	0	74	3	0
36	L	49	0	74	2	0
36	a	40	0	53	1	0
36	d	147	0	222	19	0
36	l	49	0	74	2	0
37	F	43	0	30	2	0
37	V	43	0	30	1	0
37	f	43	0	30	3	0
37	v	43	0	30	0	0
38	H	41	0	56	2	0
38	h	41	0	56	3	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	O	5	0	0	0	0
41	A	170	0	0	0	0
41	B	319	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	C	263	0	0	5	0
41	D	161	0	0	2	0
41	E	35	0	0	4	0
41	F	12	0	0	0	0
41	H	52	0	0	0	0
41	I	8	0	0	0	0
41	J	9	0	0	0	0
41	K	8	0	0	1	0
41	L	24	0	0	0	0
41	M	16	0	0	1	0
41	O	202	0	0	4	0
41	T	10	0	0	0	0
41	U	100	0	0	1	0
41	V	144	0	0	1	0
41	X	14	0	0	0	0
41	Y	6	0	0	0	0
41	Z	1	0	0	0	0
41	a	155	0	0	2	0
41	b	306	0	0	6	0
41	c	245	0	0	4	0
41	d	160	0	0	1	0
41	e	22	0	0	1	0
41	f	14	0	0	0	0
41	h	53	0	0	0	0
41	i	14	0	0	1	0
41	j	9	0	0	1	0
41	k	5	0	0	0	0
41	l	18	0	0	0	0
41	m	16	0	0	2	0
41	o	175	0	0	1	0
41	t	12	0	0	0	0
41	u	106	0	0	3	0
41	v	104	0	0	2	0
41	x	6	0	0	0	0
41	y	7	0	0	0	0
41	z	2	0	0	0	0
All	All	54036	0	51774	623	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 (623) 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)
12:M:16[A]:LEU:HD23	12:m:16[A]:LEU:CD2	1.41	1.49
12:M:16[A]:LEU:CD2	12:m:16[A]:LEU:HD23	1.63	1.27
12:M:16[A]:LEU:CD2	12:m:16[A]:LEU:CD2	2.16	1.21
36:d:409:LHG:C38	36:d:409:LHG:H112	1.72	1.17
26:L:103:SQD:H462	26:L:103:SQD:H1	1.28	1.12
36:d:409:LHG:H131	36:d:409:LHG:H372	1.32	1.10
27:a:418:LMG:C25	27:a:418:LMG:H422	1.80	1.10
1:A:214:MET:CG	28:A:414:PL9:H102	1.84	1.07
5:E:9:PRO:HA	36:E:101:LHG:HC32	1.32	1.07
1:A:214:MET:HG2	28:A:414:PL9:C10	1.84	1.06
2:b:431[B]:GLU:OE2	41:b:905[B]:HOH:O	1.75	1.05
36:d:409:LHG:H112	36:d:409:LHG:H381	1.05	1.04
15:U:86:GLU:H	15:U:86:GLU:CD	1.66	1.01
13:o:33:ASP:OD1	13:o:35:SER:HB3	1.60	1.01
30:C:520:LMT:H6'1	8:I:26:GLY:HA3	1.42	0.99
26:B:621:SQD:H462	26:B:621:SQD:H1	1.44	0.99
12:M:16[A]:LEU:HD23	12:m:16[A]:LEU:HD21	1.44	0.99
31:C:524:GOL:H11	41:C:706:HOH:O	1.63	0.98
36:D:410:LHG:C33	36:D:410:LHG:H152	1.94	0.98
23:B:615:CLA:H18	27:B:622:LMG:H421	1.46	0.96
1:A:214:MET:HG2	28:A:414:PL9:H102	0.98	0.96
23:B:617:CLA:C19	29:B:627:UNL:C16	2.43	0.96
31:a:423:GOL:H11	12:m:1:FME:HG2	1.49	0.90
36:D:410:LHG:H152	36:D:410:LHG:H332	1.54	0.89
12:M:16[A]:LEU:HD23	12:m:16[A]:LEU:HD23	0.91	0.88
5:E:68:ASP:OD1	5:E:71:GLU:HB2	1.75	0.87
12:M:16[A]:LEU:HD21	12:m:16[A]:LEU:HG	1.55	0.86
4:d:236:ASN:O	4:d:239:GLN:HG2	1.75	0.86
23:B:617:CLA:H191	29:B:627:UNL:C16	2.05	0.86
5:E:9:PRO:HA	36:E:101:LHG:C3	2.06	0.85
26:L:103:SQD:H462	26:L:103:SQD:C1	2.06	0.84
23:c:909:CLA:H192	34:c:918:DGD:HAT1	1.59	0.84
27:b:623:LMG:C43	36:l:101:LHG:H383	2.08	0.84
23:C:504:CLA:H201	36:D:410:LHG:C35	2.08	0.82
10:k:21:LEU:HD13	17:y:24:MET:HE3	1.61	0.81
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.61	0.80
13:O:179:GLU:HG2	41:O:569:HOH:O	1.82	0.80
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.16	0.80
36:D:410:LHG:H152	36:D:410:LHG:H331	1.62	0.79
5:E:45:ASP:OD1	41:E:228[A]:HOH:O	1.99	0.79
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.65	0.78
4:D:102:THR:OG1	34:D:406:DGD:HG31	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:279:LEU:HD12	3:c:282:MET:CE	2.13	0.78
12:M:16[A]:LEU:HD21	12:m:16[A]:LEU:CG	2.13	0.78
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.66	0.76
13:O:58:ASN:HA	41:b:799:HOH:O	1.86	0.76
13:O:58:ASN:C	13:O:60:ARG:H	1.94	0.76
31:D:415:GOL:H11	12:M:1:FME:HG2	1.67	0.75
36:d:409:LHG:H372	36:d:409:LHG:C13	2.15	0.75
36:d:409:LHG:H322	36:d:409:LHG:H151	1.67	0.75
26:L:103:SQD:H371	29:M:103:UNL:C16	2.17	0.75
2:b:503:THR:O	18:x:39:ARG:HG2	1.87	0.75
26:a:401:SQD:H383	29:a:403:UNL:C16	2.18	0.74
3:c:279:LEU:HD12	3:c:282:MET:HE3	1.67	0.74
23:C:504:CLA:H191	36:D:410:LHG:C35	2.17	0.73
4:D:13:GLY:HA3	33:D:414:HTG:H62	1.69	0.73
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.71	0.72
31:c:927:GOL:H11	41:c:1139:HOH:O	1.90	0.71
15:u:23:GLU:OE2	41:u:342[A]:HOH:O	2.08	0.71
12:M:16[A]:LEU:HD21	12:m:16[A]:LEU:CD2	2.20	0.71
1:a:72:LEU:HD11	30:a:402:LMT:H52	1.72	0.71
23:B:617:CLA:HED2	23:B:617:CLA:H43	1.73	0.70
26:B:621:SQD:H1	26:B:621:SQD:C46	2.21	0.70
15:U:86:GLU:CD	15:U:86:GLU:N	2.46	0.70
36:d:409:LHG:C38	36:d:409:LHG:C11	2.64	0.70
23:B:617:CLA:H193	29:B:627:UNL:C16	2.22	0.70
23:B:606:CLA:C14	23:B:611:CLA:HED2	2.22	0.69
23:c:911:CLA:H41	36:d:409:LHG:H361	1.74	0.69
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.75	0.69
12:M:16[A]:LEU:CD2	12:m:16[A]:LEU:CG	2.71	0.69
26:a:416:SQD:O10	36:d:409:LHG:H121	1.92	0.69
34:D:406:DGD:HD4	5:E:45:ASP:HB3	1.73	0.69
16:v:2:GLU:HB2	41:v:384:HOH:O	1.93	0.69
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.75	0.68
3:C:320:ARG:HG3	31:C:524:GOL:H2	1.75	0.68
3:c:72:LEU:HD11	3:c:108:THR:HB	1.74	0.68
34:d:406:DGD:HD3	5:e:45:ASP:HB3	1.74	0.68
13:O:74[A]:GLU:OE1	41:O:550:HOH:O	2.11	0.68
31:c:928:GOL:H2	41:c:1155:HOH:O	1.93	0.68
5:E:61:ARG:O	41:E:214[A]:HOH:O	2.10	0.67
1:a:214:MET:HG2	28:a:419:PL9:C10	2.24	0.67
34:D:406:DGD:O1B	34:D:406:DGD:O2D	2.13	0.67
5:E:60:GLN:O	41:E:214[B]:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248[A]:ILE:HD11	4:D:237:PRO:O	1.96	0.66
1:A:248[A]:ILE:HD13	1:A:249:VAL:H	1.59	0.66
25:d:404:BCR:H313	34:d:406:DGD:HAW1	1.77	0.66
30:z:101:LMT:O3'	30:z:101:LMT:H2B	1.96	0.66
28:A:414:PL9:H403	6:F:22:ALA:HB2	1.78	0.65
23:B:611:CLA:HHC	23:B:611:CLA:HBB1	1.77	0.65
23:C:506:CLA:H122	23:C:506:CLA:H18	1.76	0.65
25:K:102:BCR:C8	25:K:102:BCR:H331	2.25	0.65
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.79	0.65
23:c:903:CLA:H61	23:c:913:CLA:H42	1.77	0.65
41:u:374[B]:HOH:O	16:v:85:GLU:OE2	2.13	0.65
4:D:14:TRP:CD1	33:D:414:HTG:H61	2.32	0.65
13:O:82:GLN:NE2	41:O:563:HOH:O	2.29	0.65
13:o:33:ASP:C	13:o:35:SER:H	2.04	0.65
25:C:515:BCR:H331	25:C:515:BCR:C8	2.25	0.64
1:a:259[B]:ILE:HG13	1:a:260:PHE:H	1.62	0.64
4:d:272:LEU:C	4:d:272:LEU:HD23	2.22	0.64
8:i:35:LYS:HB2	8:i:35:LYS:NZ	2.12	0.64
23:c:905:CLA:H193	36:d:409:LHG:H341	1.79	0.64
30:M:101:LMT:O6'	41:M:211[B]:HOH:O	2.15	0.64
3:C:154:LYS:NZ	41:C:824:HOH:O	2.28	0.63
23:c:905:CLA:C19	36:d:409:LHG:H341	2.28	0.63
3:c:318:LEU:C	3:c:318:LEU:HD23	2.24	0.63
10:K:24[A]:VAL:HG13	17:Y:25:ILE:HD13	1.81	0.62
23:b:618:CLA:H2	23:b:619:CLA:HBB2	1.81	0.62
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.33	0.62
13:O:203:LYS:HE3	41:O:584:HOH:O	2.00	0.62
36:a:417:LHG:H222	28:a:419:PL9:H28	1.81	0.62
26:B:621:SQD:H45	14:t:23:PHE:CD1	2.35	0.62
8:i:35:LYS:HB2	8:i:35:LYS:HZ2	1.63	0.62
19:z:15:LEU:HD22	19:z:46:LEU:HD23	1.81	0.62
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.00	0.62
26:a:416:SQD:H251	36:d:409:LHG:H122	1.82	0.61
11:L:24[A]:ILE:CD1	12:M:18:PRO:HB2	2.30	0.61
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.35	0.61
3:C:381:LYS:NZ	13:O:99[A]:ASP:OD2	2.32	0.61
23:C:506:CLA:HMC2	23:C:507:CLA:H102	1.83	0.61
4:d:85:MET:CE	4:d:96:GLU:HG2	2.29	0.61
10:K:24[A]:VAL:CG1	17:Y:25:ILE:HD13	2.31	0.61
23:A:405:CLA:HMB3	23:A:405:CLA:HBB1	1.83	0.60
9:j:9:PRO:HD2	9:j:12:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:423:GOL:H11	12:m:1:FME:CG	2.26	0.60
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.34	0.60
3:C:318:LEU:C	3:C:318:LEU:HD23	2.27	0.60
17:Y:23:THR:HB	17:Y:24:MET:HE2	1.83	0.60
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.35	0.60
34:c:918:DGD:HAE2	34:c:919:DGD:HBN2	1.83	0.59
25:d:404:BCR:H331	25:d:404:BCR:C8	2.31	0.59
13:o:66:VAL:HB	13:o:67:PRO:HD2	1.84	0.59
1:a:259[B]:ILE:HD12	1:a:263:ALA:HB3	1.83	0.59
1:a:214:MET:HG2	28:a:419:PL9:H102	1.83	0.59
3:c:200:THR:OG1	3:c:201[B]:ASN:ND2	2.36	0.59
13:o:42:ARG:O	13:o:241:ALA:HA	2.02	0.59
23:b:607:CLA:H43	23:b:608:CLA:H2	1.83	0.59
30:B:623:LMT:H122	29:D:412:UNL:C22	2.33	0.59
2:b:431[B]:GLU:CD	41:b:905[B]:HOH:O	2.37	0.59
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.84	0.59
23:a:411:CLA:H152	28:a:419:PL9:H262	1.85	0.58
3:C:279:LEU:HD12	3:C:282:MET:CE	2.33	0.58
3:c:320:ARG:HB2	31:c:928:GOL:H32	1.86	0.58
26:A:412:SQD:H383	9:J:22:ILE:HD11	1.86	0.58
25:k:101:BCR:H321	25:k:101:BCR:HC8	1.86	0.58
13:o:181:GLU:CD	13:o:181:GLU:H	2.10	0.58
23:B:612:CLA:HBB1	23:B:612:CLA:HMB3	1.84	0.58
30:C:520:LMT:C6B	8:I:26:GLY:HA3	2.28	0.58
5:E:61:ARG:HG3	41:E:214[B]:HOH:O	2.04	0.58
25:K:102:BCR:H331	25:K:102:BCR:HC8	1.86	0.58
1:A:259:ILE:HD12	28:A:414:PL9:C25	2.34	0.57
23:c:903:CLA:H193	33:c:923:HTG:H3'1	1.86	0.57
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.37	0.57
5:E:15:THR:HB	9:J:8:ILE:O	2.04	0.57
24:a:413:PHO:HHD	24:a:413:PHO:HBC2	1.86	0.57
2:B:467:ILE:HG13	4:D:126:MET:CE	2.33	0.57
23:C:512:CLA:HMB3	23:C:512:CLA:HBB1	1.86	0.57
23:c:910:CLA:HMB1	23:c:910:CLA:HBB1	1.86	0.57
25:T:101:BCR:H382	25:T:101:BCR:H23C	1.87	0.57
23:d:403:CLA:HMB1	23:d:403:CLA:HBB1	1.87	0.57
30:C:520:LMT:H6'1	8:I:26:GLY:CA	2.27	0.56
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.87	0.56
4:d:12:ARG:HG3	4:d:17:ILE:HD11	1.87	0.56
23:A:410:CLA:H91	30:C:520:LMT:H123	1.88	0.56
1:a:183:MET:HA	23:a:409:CLA:HMD1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:102:LMT:O3'	30:Z:102:LMT:H2B	2.05	0.56
13:O:52:VAL:HB	13:O:110:MET:HE1	1.86	0.56
1:a:259[B]:ILE:HD12	1:a:263:ALA:CB	2.36	0.56
23:c:909:CLA:C19	34:c:918:DGD:HAT1	2.34	0.56
34:D:406:DGD:HB21	34:D:406:DGD:HA22	1.86	0.56
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.41	0.56
19:z:44:SER:O	19:z:48:ILE:HG13	2.06	0.56
33:d:401:HTG:H1	7:h:25:TRP:CD1	2.41	0.56
15:u:86:GLU:HG2	41:u:328:HOH:O	2.07	0.55
3:c:319:ILE:HG22	31:c:928:GOL:O3	2.06	0.55
13:o:207:ARG:NH1	41:o:536:HOH:O	2.39	0.55
23:c:905:CLA:H142	27:c:920:LMG:H421	1.88	0.55
23:C:502:CLA:H193	33:C:521:HTG:H3'1	1.87	0.55
23:C:509:CLA:HBB1	23:C:509:CLA:CMB	2.34	0.55
27:a:418:LMG:H232	23:c:906:CLA:H92	1.88	0.55
23:b:610:CLA:H2	27:b:623:LMG:H151	1.89	0.55
3:c:203:THR:O	3:c:235:GLY:HA3	2.07	0.55
3:C:279:LEU:HD22	23:C:509:CLA:HED2	1.89	0.55
2:b:50:PRO:HB2	31:b:633:GOL:H12	1.88	0.55
1:A:214:MET:HE2	1:A:255:PHE:CE2	2.42	0.54
1:a:214:MET:HG2	28:a:419:PL9:H103	1.89	0.54
23:B:614:CLA:HBB1	23:B:614:CLA:HMB1	1.89	0.54
3:C:391[A]:ARG:HD3	41:C:825[A]:HOH:O	2.05	0.54
36:D:410:LHG:H342	36:D:410:LHG:H302	1.89	0.54
23:B:612:CLA:H142	36:L:101:LHG:H361	1.90	0.54
3:c:279:LEU:HA	3:c:282:MET:HE3	1.90	0.54
31:a:423:GOL:C1	12:m:1:FME:HG2	2.29	0.54
2:B:446:SER:HB2	2:B:447:PRO:CD	2.35	0.54
41:b:956:HOH:O	12:m:6:LEU:HD12	2.06	0.54
6:f:15:ILE:HD12	6:f:15:ILE:H	1.73	0.54
25:K:101:BCR:C8	25:K:101:BCR:H311	2.37	0.54
15:U:73:GLN:O	15:U:77:GLU:HG3	2.07	0.54
33:U:201:HTG:H1'1	41:U:372:HOH:O	2.07	0.54
23:b:616:CLA:HMB1	23:b:616:CLA:HBB1	1.90	0.53
3:c:213:LEU:HD11	25:c:916:BCR:H373	1.90	0.53
3:C:376:ASP:OD1	3:C:378[A]:ASN:HB3	2.08	0.53
4:D:123:ILE:HD11	34:H:102:DGD:HAE1	1.89	0.53
3:C:167:VAL:HG21	23:C:512:CLA:HHB	1.91	0.53
13:o:141[B]:ASP:OD2	13:o:143:LYS:HE3	2.08	0.53
5:e:79:PHE:HB3	41:e:922:HOH:O	2.08	0.53
4:d:307:GLU:HG3	41:d:611:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:60:ILE:HG22	23:c:904:CLA:HHD	1.91	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
5:E:28:PRO:O	5:E:32:ILE:HG12	2.09	0.52
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.44	0.52
23:D:403:CLA:H192	18:X:15[A]:LEU:HD11	1.92	0.52
25:K:101:BCR:H321	25:K:101:BCR:HC8	1.90	0.52
23:b:613:CLA:H203	23:b:613:CLA:H152	1.92	0.52
2:b:341:LYS:HZ1	33:b:626:HTG:C2	2.20	0.52
28:A:414:PL9:H502	4:D:39:PRO:HG3	1.91	0.52
3:C:429:SER:HB3	34:C:517:DGD:HBT2	1.92	0.52
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.91	0.52
7:h:39:LEU:C	7:h:39:LEU:HD23	2.34	0.52
26:A:412:SQD:H141	36:D:410:LHG:H172	1.91	0.52
2:b:341:LYS:NZ	33:b:626:HTG:O2	2.29	0.52
23:d:403:CLA:HBB1	23:d:403:CLA:CMB	2.40	0.52
23:B:612:CLA:HBB1	23:B:612:CLA:CMB	2.39	0.52
23:c:914:CLA:HMB3	23:c:914:CLA:HBB1	1.92	0.52
2:b:462:PHE:CZ	23:b:616:CLA:HMB3	2.45	0.52
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.45	0.52
31:D:415:GOL:C1	12:M:1:FME:HG2	2.38	0.51
23:b:618:CLA:H161	7:h:7:LEU:HD21	1.92	0.51
2:B:223[A]:GLN:NE2	2:B:227:LYS:HD2	2.24	0.51
25:B:619:BCR:H331	25:B:619:BCR:C8	2.39	0.51
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.93	0.51
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.44	0.51
16:v:55[B]:ARG:NH1	41:v:357:HOH:O	2.44	0.51
2:B:266:GLU:HB3	31:B:635:GOL:H31	1.92	0.51
2:B:286:ARG:HG2	2:B:286:ARG:HH11	1.76	0.51
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.91	0.51
26:a:416:SQD:H132	36:d:409:LHG:H152	1.91	0.51
4:d:266:TRP:CD1	36:d:408:LHG:HC31	2.46	0.51
31:C:524:GOL:H12	37:V:201:HEM:HMD1	1.93	0.51
13:O:49[B]:THR:OG1	13:O:236:GLN:HB2	2.11	0.51
23:B:607:CLA:H202	33:B:631:HTG:H61	1.92	0.51
23:C:510:CLA:HBC3	23:C:510:CLA:H192	1.93	0.51
5:E:8:ARG:HB3	5:E:13:ILE:HD11	1.92	0.51
27:a:418:LMG:C25	27:a:418:LMG:C42	2.72	0.51
3:C:334:PRO:HA	13:O:153:THR:OG1	2.11	0.51
25:b:622:BCR:H331	25:b:622:BCR:C8	2.41	0.51
23:B:611:CLA:H151	23:B:611:CLA:H203	1.93	0.51
4:D:272:LEU:C	4:D:272:LEU:HD23	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:404:BCR:H331	25:D:404:BCR:C8	2.41	0.51
2:b:79:SER:HB3	2:b:86:ILE:HG12	1.91	0.51
25:t:101:BCR:H321	25:t:101:BCR:HC8	1.92	0.51
3:C:286:ALA:HB2	23:C:502:CLA:HMD2	1.92	0.51
2:B:248:ALA:HA	23:B:604:CLA:H42	1.93	0.50
23:C:512:CLA:H121	23:C:513:CLA:H142	1.93	0.50
27:C:519:LMG:O10	30:J:102:LMT:H42	2.10	0.50
4:D:102:THR:OG1	34:D:406:DGD:HD1	2.11	0.50
17:Y:34:MET:HE3	17:Y:34:MET:HA	1.93	0.50
5:E:27:ILE:HG12	37:F:101:HEM:HMC3	1.92	0.50
7:h:12:ARG:HB3	7:h:13:PRO:HD3	1.92	0.50
27:D:411:LMG:H412	6:F:30:THR:HG21	1.93	0.50
1:a:278:TRP:CE2	26:a:416:SQD:H223	2.46	0.50
30:b:624:LMT:H123	29:b:628:UNL:C37	2.42	0.50
30:b:624:LMT:H6E	4:d:19:ASP:OD1	2.11	0.50
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.93	0.50
2:b:231:MET:HE2	23:b:613:CLA:HMC2	1.93	0.50
23:b:618:CLA:H2	23:b:619:CLA:CBB	2.41	0.50
3:C:78:GLU:OE2	16:V:106[A]:ASN:ND2	2.34	0.50
16:V:106[B]:ASN:ND2	41:V:432:HOH:O	2.42	0.50
25:t:101:BCR:H23C	25:t:101:BCR:H382	1.94	0.49
4:D:101:PHE:HB3	34:D:406:DGD:HG2	1.94	0.49
8:I:29:ALA:O	8:I:35:LYS:HG2	2.12	0.49
4:d:236:ASN:OD1	4:d:237:PRO:HD2	2.12	0.49
1:A:11:ALA:HB1	1:A:15:GLU:HB3	1.94	0.49
13:O:23:ASP:HB3	13:O:25:THR:HG23	1.94	0.49
2:b:162:PHE:O	23:b:609:CLA:HHD	2.12	0.49
23:A:405:CLA:CBD	23:A:406:CLA:HAC2	2.42	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.49
2:B:405[B]:GLU:OE2	13:o:58:ASN:HB2	2.12	0.49
17:y:42:ARG:HD2	19:z:29:SER:OG	2.12	0.49
23:A:406:CLA:HBB1	23:A:406:CLA:HMB1	1.95	0.49
27:A:413:LMG:H111	3:C:218:PHE:HE2	1.77	0.49
25:C:514:BCR:C8	25:C:514:BCR:H331	2.43	0.49
13:O:58:ASN:C	13:O:60:ARG:N	2.63	0.49
2:b:237:VAL:HG11	23:b:613:CLA:H201	1.95	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.49
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49
7:h:38:PHE:HB2	38:h:101:RRX:C10	2.43	0.49
3:C:223:TRP:CG	3:C:224:ILE:H	2.31	0.49
25:K:101:BCR:H311	25:K:101:BCR:HC8	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.95	0.49
4:d:101:PHE:H	34:d:406:DGD:HA22	1.78	0.49
11:L:24[A]:ILE:HD13	12:M:18:PRO:HB2	1.93	0.49
36:d:409:LHG:H112	36:d:409:LHG:C37	2.40	0.49
16:v:102:PRO:HA	16:v:105:ARG:HG3	1.95	0.49
2:b:324:LEU:HA	4:d:293[A]:LEU:HG	1.95	0.48
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.95	0.48
13:o:33:ASP:O	13:o:35:SER:N	2.46	0.48
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.48	0.48
3:c:279:LEU:HD12	3:c:282:MET:HE1	1.94	0.48
3:c:365:TRP:HB3	3:c:391[B]:ARG:HG2	1.94	0.48
1:A:183:MET:HA	23:A:405:CLA:HMD1	1.95	0.48
1:A:263:ALA:HA	36:E:101:LHG:H291	1.95	0.48
31:c:927:GOL:C1	41:c:1139:HOH:O	2.57	0.48
18:x:21:LEU:HD11	29:x:101:UNL:C16	2.44	0.48
1:A:63:ILE:HB	3:C:335:THR:HG21	1.94	0.48
1:a:215:HIS:HA	28:a:419:PL9:O1	2.12	0.48
26:f:102:SQD:H242	18:x:31:ILE:HD13	1.94	0.48
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.48	0.48
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.96	0.48
26:B:621:SQD:O7	11:L:7:ARG:NH1	2.47	0.48
13:O:180:GLU:CD	13:O:180:GLU:H	2.22	0.48
23:B:614:CLA:H112	23:B:614:CLA:H72	1.64	0.47
34:C:517:DGD:HB22	27:C:519:LMG:H302	1.96	0.47
23:B:617:CLA:H171	25:B:620:BCR:H331	1.96	0.47
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.95	0.47
23:c:902:CLA:H192	23:c:907:CLA:C1B	2.44	0.47
23:c:902:CLA:HBB1	25:c:916:BCR:H21C	1.96	0.47
9:j:2:MET:N	41:j:208:HOH:O	2.47	0.47
24:A:408:PHO:NC	24:A:408:PHO:ND	2.62	0.47
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.78	0.47
26:L:103:SQD:H341	26:L:103:SQD:H311	1.56	0.47
13:O:110:MET:HG3	13:O:114:GLU:HB3	1.95	0.47
13:O:15:LEU:HD23	13:O:18:LYS:HD2	1.95	0.47
23:a:414:CLA:C19	23:c:906:CLA:H142	2.44	0.47
3:c:415:ASN:O	3:c:416[B]:SER:HB2	2.15	0.47
1:a:11:ALA:HA	1:a:15:GLU:OE1	2.13	0.47
23:c:911:CLA:H161	23:c:911:CLA:H121	1.76	0.47
36:d:407:LHG:O9	36:l:101:LHG:HC81	2.14	0.47
1:A:248[A]:ILE:HD13	1:A:249:VAL:N	2.26	0.47
23:A:406:CLA:H162	23:A:406:CLA:H203	1.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:415:GOL:H11	12:M:1:FME:CG	2.39	0.47
30:M:101:LMT:O6B	12:m:1:FME:HCN	2.13	0.47
28:a:419:PL9:H502	4:d:39:PRO:HG3	1.95	0.47
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.96	0.47
1:A:313:VAL:O	31:A:422:GOL:H31	2.15	0.47
23:C:511:CLA:H191	30:Z:102:LMT:H122	1.97	0.47
26:a:401:SQD:H442	41:a:633[A]:HOH:O	2.13	0.47
3:C:60:ILE:HG22	23:C:503:CLA:HHD	1.97	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
23:b:612:CLA:NC	38:h:101:RRX:H56	2.30	0.47
23:c:912:CLA:HBA2	10:k:39:TRP:CH2	2.50	0.47
23:B:617:CLA:H91	23:B:617:CLA:H112	1.72	0.46
25:a:415:BCR:H20C	25:a:415:BCR:H361	1.78	0.46
26:a:416:SQD:H182	36:d:409:LHG:H192	1.97	0.46
26:A:418:SQD:H212	25:T:101:BCR:H323	1.96	0.46
4:D:209:LEU:HD23	4:D:209:LEU:C	2.40	0.46
2:b:231:MET:HE2	23:b:613:CLA:CMC	2.45	0.46
23:c:914:CLA:H152	27:c:921:LMG:H422	1.97	0.46
23:b:604:CLA:HAA2	33:b:627:HTG:H62	1.98	0.46
25:b:621:BCR:H331	25:b:621:BCR:C8	2.46	0.46
2:B:451:PHE:CZ	23:B:605:CLA:HED1	2.51	0.46
31:C:524:GOL:C1	41:C:706:HOH:O	2.38	0.46
1:A:246:TYR:CZ	1:A:248[A]:ILE:HG22	2.50	0.46
2:B:493:TRP:HB3	5:E:5:THR:HG23	1.97	0.46
11:L:14:ARG:HH12	26:L:103:SQD:H3	1.80	0.46
23:B:602:CLA:CBB	23:B:602:CLA:HHC	2.46	0.46
23:C:504:CLA:C20	36:D:410:LHG:C35	2.87	0.46
12:M:16[A]:LEU:CD2	12:m:16[A]:LEU:HD21	2.16	0.46
25:T:101:BCR:H321	25:T:101:BCR:C8	2.42	0.46
2:b:12:LEU:HB2	23:b:615:CLA:HMC2	1.97	0.46
2:b:292:LEU:O	41:b:878[B]:HOH:O	2.20	0.46
23:b:613:CLA:H203	23:b:613:CLA:C15	2.46	0.46
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.51	0.46
5:e:61:ARG:HH12	16:v:127:GLY:HA3	1.79	0.46
5:e:60:GLN:HE21	5:e:60:GLN:HB2	1.49	0.46
8:i:35:LYS:HE3	41:i:213[B]:HOH:O	2.16	0.46
25:t:101:BCR:HC8	25:t:101:BCR:H311	1.97	0.46
23:B:605:CLA:H43	23:B:606:CLA:H2	1.98	0.45
27:B:622:LMG:H242	4:D:284:ILE:HD13	1.97	0.45
25:K:102:BCR:H11C	25:K:102:BCR:H341	1.77	0.45
6:f:21:VAL:O	6:f:25:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:47:TRP:CE2	30:z:101:LMT:H92	2.51	0.45
4:D:283:ALA:O	4:D:287:VAL:HG23	2.16	0.45
4:d:24:ARG:NH2	18:x:35:ASP:O	2.49	0.45
23:A:405:CLA:HBD	23:A:406:CLA:HAC2	1.98	0.45
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.99	0.45
1:a:298:ASN:ND2	41:a:636:HOH:O	2.35	0.45
3:c:123:ALA:HB1	30:z:101:LMT:H91	1.97	0.45
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.98	0.45
24:A:409:PHO:HBC2	24:A:409:PHO:HHD	1.98	0.45
36:D:410:LHG:H342	36:D:410:LHG:C30	2.47	0.45
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.17	0.45
23:c:906:CLA:HAA1	23:c:906:CLA:CBD	2.47	0.45
25:c:916:BCR:H11C	25:c:916:BCR:H341	1.87	0.45
26:A:412:SQD:H181	26:A:412:SQD:H211	1.61	0.45
1:a:259[B]:ILE:CD1	1:a:263:ALA:HB3	2.47	0.45
23:c:906:CLA:HAA1	23:c:906:CLA:HBD	1.98	0.45
3:C:78:GLU:CD	16:V:106[A]:ASN:HD21	2.21	0.45
3:C:149:TYR:CZ	23:C:509:CLA:H191	2.52	0.45
23:C:513:CLA:HBB1	23:C:513:CLA:HMB3	1.99	0.45
13:O:58:ASN:O	13:O:60:ARG:N	2.46	0.45
23:b:606:CLA:HAB	23:b:608:CLA:H171	1.98	0.45
3:c:318:LEU:HD23	3:c:318:LEU:O	2.16	0.45
2:B:262:THR:C	2:B:264:PRO:HD3	2.42	0.45
17:Y:27:MET:HE2	17:Y:27:MET:HB3	1.62	0.45
24:a:413:PHO:NC	24:a:413:PHO:ND	2.63	0.45
28:a:419:PL9:H403	6:f:22:ALA:HB2	1.97	0.45
23:B:611:CLA:HHC	23:B:611:CLA:CBB	2.45	0.45
25:B:620:BCR:H331	25:B:620:BCR:C8	2.47	0.45
23:C:511:CLA:HAA1	23:C:511:CLA:HBD	1.98	0.45
36:D:410:LHG:H331	36:D:410:LHG:C15	2.40	0.45
2:b:266:GLU:HB3	31:b:633:GOL:H31	1.97	0.45
2:B:224:ARG:HH21	30:B:623:LMT:H2'	1.82	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.45
2:b:248:ALA:HA	23:b:606:CLA:H42	1.99	0.45
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.97	0.45
4:d:123:ILE:HD11	34:h:102:DGD:HAE1	1.99	0.45
23:d:403:CLA:H161	7:h:37:LEU:HD21	1.99	0.45
18:x:27:VAL:O	18:x:31:ILE:HG13	2.16	0.45
24:A:409:PHO:ND	24:A:409:PHO:NC	2.65	0.45
3:C:52:ALA:HB2	23:C:511:CLA:HMA2	1.99	0.45
4:D:52:THR:O	4:D:66:SER:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:334:PRO:HA	13:o:153:THR:OG1	2.17	0.45
13:o:39:ARG:HG3	13:o:246:ALA:HB2	1.99	0.45
2:B:461:LEU:HD22	36:D:408:LHG:H301	1.99	0.44
41:C:822:HOH:O	13:O:149:PRO:HB2	2.17	0.44
4:D:264:LYS:NZ	41:D:617:HOH:O	2.46	0.44
23:b:617:CLA:H41	23:b:617:CLA:H62	1.35	0.44
25:t:101:BCR:H382	25:t:101:BCR:C23	2.47	0.44
23:B:610:CLA:HMB1	23:B:611:CLA:C1B	2.47	0.44
4:d:293[B]:LEU:HD23	4:d:293[B]:LEU:HA	1.74	0.44
19:z:47:TRP:CD2	30:z:101:LMT:H92	2.52	0.44
28:A:414:PL9:H202	28:A:414:PL9:H162	1.98	0.44
23:B:615:CLA:C9	30:m:101:LMT:H112	2.47	0.44
31:L:104:GOL:H2	14:T:25:GLU:HB3	1.98	0.44
13:O:39:ARG:HB2	13:O:83:GLY:O	2.17	0.44
13:o:93:LEU:O	13:o:128:SER:HA	2.17	0.44
2:B:36[A]:SER:OG	25:B:619:BCR:H362	2.18	0.44
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.99	0.44
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.53	0.44
1:a:12:ASN:HB3	1:a:15:GLU:HB3	1.98	0.44
2:b:157:HIS:C	2:b:157:HIS:CD2	2.95	0.44
2:b:462:PHE:CE1	23:b:616:CLA:HMB3	2.52	0.44
30:B:623:LMT:C12	29:D:412:UNL:C22	2.95	0.44
3:C:222:GLY:O	3:C:223:TRP:C	2.61	0.44
3:C:377:LEU:O	3:C:381:LYS:HG3	2.18	0.44
23:c:912:CLA:HBB1	23:c:912:CLA:HMB3	1.98	0.44
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.52	0.44
26:a:416:SQD:H251	36:d:409:LHG:C12	2.48	0.44
2:b:14[B]:ASN:OD1	31:b:636:GOL:H12	2.18	0.44
2:B:224:ARG:HD2	41:B:894:HOH:O	2.16	0.44
26:B:621:SQD:O9	26:B:621:SQD:H442	2.18	0.44
4:D:266:TRP:CD1	36:D:409:LHG:HC31	2.53	0.44
6:F:31:ILE:HG13	37:F:101:HEM:HMC1	2.00	0.44
3:c:128:GLY:HA3	23:c:914:CLA:C3C	2.48	0.44
29:b:628:UNL:C6	41:b:913:HOH:O	2.65	0.44
23:c:907:CLA:H18	23:c:907:CLA:H122	1.99	0.44
23:c:912:CLA:HBB1	23:c:912:CLA:CMB	2.48	0.44
12:m:9[B]:ILE:HG22	41:m:210:HOH:O	2.18	0.44
27:A:413:LMG:H111	3:C:218:PHE:CE2	2.53	0.43
2:B:228:ALA:HB2	30:B:623:LMT:H21	2.00	0.43
23:C:504:CLA:C19	36:D:410:LHG:C35	2.94	0.43
4:D:24:ARG:NH1	41:D:643:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:D:410:LHG:H332	36:D:410:LHG:H132	2.01	0.43
10:K:46:ARG:NH1	41:K:207:HOH:O	2.50	0.43
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.54	0.43
13:o:33:ASP:C	13:o:35:SER:N	2.68	0.43
19:z:46:LEU:O	19:z:49:ALA:HB3	2.19	0.43
28:A:414:PL9:H512	26:D:407:SQD:H301	1.98	0.43
27:B:622:LMG:H332	11:L:35:PHE:CE2	2.53	0.43
11:L:24[A]:ILE:HD11	12:M:18:PRO:HB2	1.98	0.43
17:Y:34:MET:HE2	17:Y:38:LEU:HG	2.00	0.43
27:a:418:LMG:H382	34:c:917:DGD:HB51	1.99	0.43
5:e:8:ARG:HA	5:e:9:PRO:HD3	1.88	0.43
23:C:501:CLA:C4D	23:C:503:CLA:H2	2.48	0.43
26:a:401:SQD:H211	26:a:401:SQD:H182	1.84	0.43
19:z:47:TRP:CE3	30:z:101:LMT:H71	2.54	0.43
3:C:275:SER:HB3	23:C:509:CLA:HED3	1.99	0.43
13:O:39:ARG:HG2	13:O:246:ALA:HB2	2.01	0.43
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.84	0.43
1:A:121[B]:LEU:HG	27:A:413:LMG:H181	2.00	0.43
23:B:609:CLA:H141	23:B:609:CLA:H161	1.91	0.43
19:Z:31:GLN:O	19:Z:33:TRP:N	2.52	0.43
23:b:616:CLA:OBD	23:b:617:CLA:HHC	2.18	0.43
23:c:902:CLA:C4D	23:c:904:CLA:H2	2.48	0.43
19:z:9:LEU:HD13	19:z:54:VAL:HG11	2.00	0.43
2:B:157:HIS:C	2:B:157:HIS:CD2	2.97	0.43
11:L:7:ARG:HH12	29:L:102:UNL:C4	2.32	0.43
1:a:121[A]:LEU:CD2	27:a:418:LMG:H192	2.48	0.43
25:t:101:BCR:C23	25:t:101:BCR:C38	2.96	0.43
17:y:26:ALA:O	17:y:30:ILE:HB	2.19	0.43
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.01	0.43
2:B:58:GLN:C	2:B:329:PRO:HB3	2.44	0.43
13:O:42:ARG:O	13:O:241:ALA:HA	2.19	0.43
13:O:110:MET:HB3	13:O:110:MET:HE2	1.19	0.43
2:b:156:PHE:HB3	2:b:162:PHE:HB3	2.01	0.43
23:d:403:CLA:H162	7:h:33:VAL:HG13	2.00	0.43
38:h:101:RRX:H55	38:h:101:RRX:H46	1.99	0.43
25:k:101:BCR:C23	25:k:101:BCR:H382	2.48	0.43
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.43
4:d:209:LEU:HD23	4:d:209:LEU:C	2.43	0.43
19:z:8:ALA:O	19:z:11:ALA:HB3	2.19	0.43
1:A:259:ILE:HD12	28:A:414:PL9:H251	2.00	0.42
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:84:PRO:HA	1:a:112:TYR:CG	2.54	0.42
23:c:906:CLA:H112	23:c:906:CLA:H72	1.77	0.42
34:c:919:DGD:HAE2	34:c:919:DGD:HA81	1.84	0.42
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.00	0.42
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.49	0.42
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.54	0.42
1:a:331:MET:SD	4:d:347:PRO:HB2	2.59	0.42
4:d:272:LEU:C	4:d:272:LEU:CD2	2.92	0.42
12:m:5:GLN:C	41:m:206:HOH:O	2.62	0.42
1:A:248[A]:ILE:CD1	4:D:237:PRO:O	2.67	0.42
2:B:12:LEU:HB2	23:B:613:CLA:HMC2	2.01	0.42
1:a:63:ILE:HB	3:c:335:THR:HG21	2.01	0.42
23:c:909:CLA:H92	36:d:409:LHG:H362	2.00	0.42
1:A:215:HIS:ND1	28:A:414:PL9:O1	2.42	0.42
25:B:619:BCR:H363	25:t:101:BCR:H19C	2.01	0.42
23:C:501:CLA:H192	23:C:506:CLA:C1B	2.49	0.42
1:a:256:GLY:O	1:a:260:PHE:C	2.62	0.42
23:b:616:CLA:H121	27:b:623:LMG:H242	2.01	0.42
25:t:101:BCR:H331	25:t:101:BCR:HC7	1.56	0.42
2:B:451:PHE:C	2:B:451:PHE:CD2	2.97	0.42
26:D:407:SQD:H241	18:X:31:ILE:HD13	2.01	0.42
25:a:415:BCR:H24C	25:a:415:BCR:H371	1.88	0.42
23:c:904:CLA:CMB	23:c:904:CLA:HBB1	2.49	0.42
3:C:390:ARG:HD3	16:V:90:GLU:O	2.19	0.42
12:M:28:GLN:O	12:M:32:GLN:HG3	2.19	0.42
3:c:179:ALA:O	3:c:184:GLY:HA2	2.20	0.42
3:c:302:TYR:O	3:c:422:PRO:HD2	2.19	0.42
23:c:907:CLA:H102	25:c:916:BCR:H12C	2.00	0.42
25:c:916:BCR:H20C	25:c:916:BCR:H361	1.84	0.42
5:e:8:ARG:HH21	5:e:12:ASP:HB3	1.83	0.42
25:D:404:BCR:C38	27:D:411:LMG:H231	2.50	0.42
38:H:101:RRX:H40	38:H:101:RRX:H36	1.86	0.42
25:d:404:BCR:C38	27:d:410:LMG:H241	2.50	0.42
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.42
25:A:411:BCR:C8	25:A:411:BCR:H331	2.48	0.42
26:A:412:SQD:H271	36:D:410:LHG:H162	2.01	0.42
2:B:493:TRP:HD1	5:E:5:THR:CG2	2.32	0.42
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.02	0.42
23:c:907:CLA:HMB1	23:c:908:CLA:NB	2.34	0.42
29:c:925:UNL:O10	29:c:925:UNL:C5	2.68	0.42
4:d:61:HIS:HB3	4:d:63:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.55	0.42
3:C:279:LEU:HA	3:C:282:MET:HE3	2.01	0.42
3:C:443:TRP:CZ2	23:C:508:CLA:HMD1	2.55	0.42
38:H:101:RRX:H55	38:H:101:RRX:H46	2.02	0.42
1:a:12:ASN:O	1:a:16:ARG:HG3	2.20	0.42
1:a:15:GLU:HB2	30:c:922:LMT:O6B	2.20	0.42
1:a:278:TRP:HB3	1:a:279:PRO:CD	2.50	0.42
1:a:334:ARG:HD3	4:d:320:LEU:HD13	2.02	0.42
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.01	0.41
4:D:61:HIS:CE1	4:D:168:PHE:CE2	3.08	0.41
2:b:270:PRO:HG2	2:b:317:ASN:O	2.20	0.41
25:d:404:BCR:H11C	25:d:404:BCR:H341	1.92	0.41
5:e:14:ILE:HD12	9:j:13:VAL:HG11	2.02	0.41
3:C:471:SER:HB3	3:C:473:ASP:OXT	2.19	0.41
23:c:904:CLA:HBB1	23:c:904:CLA:HMB1	2.03	0.41
23:c:914:CLA:HBB1	23:c:914:CLA:CMB	2.50	0.41
13:o:180:GLU:CD	13:o:180:GLU:H	2.28	0.41
13:O:20:PRO:HB2	13:O:240:TYR:CD1	2.56	0.41
2:b:90:PHE:CE1	23:b:609:CLA:H162	2.55	0.41
4:d:52:THR:O	4:d:66:SER:HA	2.20	0.41
4:d:192:THR:HG23	23:d:402:CLA:HBC2	2.02	0.41
5:e:13:ILE:HG21	37:f:101:HEM:HAD2	2.01	0.41
25:k:102:BCR:C8	25:k:102:BCR:H331	2.49	0.41
23:B:606:CLA:H62	23:B:606:CLA:H41	1.80	0.41
23:B:617:CLA:H61	23:B:617:CLA:H41	1.76	0.41
3:C:95:LEU:HD21	23:C:501:CLA:OBD	2.21	0.41
23:a:409:CLA:HMB1	23:a:409:CLA:HBB1	2.02	0.41
26:a:416:SQD:H201	26:a:416:SQD:H171	1.85	0.41
2:b:498:LYS:HA	4:d:24:ARG:HA	2.01	0.41
5:e:27:ILE:HG12	37:f:101:HEM:HMC3	2.01	0.41
24:a:412:PHO:NC	24:a:412:PHO:ND	2.69	0.41
23:c:907:CLA:HMB1	23:c:908:CLA:C4B	2.51	0.41
36:d:409:LHG:H272	36:d:409:LHG:H242	1.88	0.41
5:e:35:TRP:CD1	5:e:35:TRP:C	2.98	0.41
16:v:122:GLU:HG3	16:v:126:LEU:HD12	2.02	0.41
2:B:349:LYS:HB3	2:B:349:LYS:HE2	1.91	0.41
23:B:615:CLA:H161	27:B:622:LMG:C43	2.51	0.41
3:C:377:LEU:HG	3:C:381:LYS:HE2	2.02	0.41
25:b:622:BCR:H361	25:b:622:BCR:H20C	1.80	0.41
23:c:910:CLA:H192	23:c:913:CLA:HMD1	2.01	0.41
2:B:138:MET:HE3	23:B:616:CLA:CHD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:LEU:HD21	23:C:508:CLA:CAB	2.51	0.41
15:U:23:GLU:C	15:U:24:LYS:HG2	2.44	0.41
23:b:617:CLA:H43	23:b:617:CLA:H11	1.91	0.41
3:c:390:ARG:HD3	16:v:100:ILE:HD12	2.02	0.41
25:d:404:BCR:H20C	25:d:404:BCR:H361	1.88	0.41
25:A:411:BCR:H15C	25:A:411:BCR:H351	1.93	0.41
2:B:278:SER:HB3	2:B:281:GLN:HE21	1.86	0.41
25:T:101:BCR:C23	25:T:101:BCR:C38	2.99	0.41
23:a:414:CLA:H102	23:a:414:CLA:H61	1.86	0.41
25:k:101:BCR:C23	25:k:101:BCR:C38	2.99	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.56	0.41
23:B:605:CLA:H161	23:B:605:CLA:H141	1.89	0.41
3:c:173:LEU:HD23	3:c:173:LEU:HA	1.89	0.41
25:c:916:BCR:H15C	25:c:916:BCR:H351	1.91	0.41
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.03	0.41
37:f:101:HEM:HBB2	37:f:101:HEM:CMB	2.50	0.41
8:i:33:LYS:HA	8:i:33:LYS:HD3	1.73	0.41
4:d:296:TYR:CE2	4:d:319:LEU:HD22	2.56	0.41
14:t:29:ILE:O	14:t:30:THR:CB	2.69	0.41
18:X:15[A]:LEU:HD23	18:X:15[A]:LEU:HA	1.85	0.40
1:a:121[A]:LEU:HD23	27:a:418:LMG:H192	2.03	0.40
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.82	0.40
13:o:33:ASP:OD1	13:o:35:SER:CB	2.50	0.40
16:v:41:HIS:O	16:v:42:VAL:C	2.63	0.40
3:C:213:LEU:HD11	25:C:515:BCR:C20	2.52	0.40
4:D:85:MET:HE1	4:D:96:GLU:HG2	2.03	0.40
23:a:414:CLA:H191	23:c:906:CLA:H142	2.02	0.40
28:a:419:PL9:H172	28:a:419:PL9:H13	1.45	0.40
23:b:618:CLA:H92	23:b:618:CLA:H61	1.81	0.40
26:D:407:SQD:H321	18:X:24:THR:HA	2.03	0.40
27:a:418:LMG:H132	23:c:906:CLA:H203	2.03	0.40
3:c:281:MET:HE3	3:c:281:MET:HB2	1.90	0.40
2:B:159:THR:O	2:B:180:PRO:HB3	2.22	0.40
36:L:101:LHG:H142	36:L:101:LHG:H171	1.93	0.40
19:Z:1:MET:O	19:Z:2:THR:OG1	2.37	0.40
1:a:339:PHE:HB3	1:a:340:PRO:HD2	2.03	0.40
23:c:913:CLA:H143	23:c:914:CLA:H142	2.04	0.40
26:f:102:SQD:C46	26:f:102:SQD:O9	2.70	0.40
16:v:123:PRO:HD3	16:v:130:TRP:CD1	2.57	0.40
1:A:246:TYR:CE2	1:A:248[A]:ILE:HG22	2.56	0.40
2:B:71:VAL:HG21	2:B:96:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:515:BCR:C8	25:C:515:BCR:C33	2.97	0.40
15:U:68:THR:O	15:U:72:LYS:HG3	2.21	0.40
3:c:323:LYS:NZ	41:c:1042:HOH:O	2.54	0.40
25:k:102:BCR:H371	25:k:102:BCR:H24C	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	36	29
1	a	336/344 (98%)	329 (98%)	7 (2%)	0	100	100
2	B	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
2	b	508/504 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	452/455 (99%)	442 (98%)	9 (2%)	1 (0%)	43	36
3	c	457/455 (100%)	442 (97%)	13 (3%)	2 (0%)	30	22
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
7	h	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	7	2
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	238 (96%)	8 (3%)	1 (0%)	30	22
13	o	242/244 (99%)	232 (96%)	9 (4%)	1 (0%)	30	22
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	129 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	1	0
19	z	58/62 (94%)	50 (86%)	5 (9%)	3 (5%)	1	0
All	All	5224/5344 (98%)	5075 (97%)	134 (3%)	15 (0%)	36	29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
19	Z	31	GLN
19	Z	32	ASP
8	i	36	ASP
19	z	31	GLN
3	C	416	SER
19	Z	2	THR

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Mol	Chain	Res	Type
3	c	416[A]	SER
3	c	416[B]	SER
19	z	3	ILE
19	z	32	ASP
8	i	34	ARG
13	o	34	SER
7	h	63	LYS
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	272/279 (98%)	266 (98%)	6 (2%)	45	42
1	a	271/279 (97%)	269 (99%)	2 (1%)	76	78
2	B	407/402 (101%)	404 (99%)	3 (1%)	76	78
2	b	399/402 (99%)	395 (99%)	4 (1%)	68	70
3	C	355/356 (100%)	350 (99%)	5 (1%)	59	59
3	c	358/356 (101%)	352 (98%)	6 (2%)	53	52
4	D	275/276 (100%)	274 (100%)	1 (0%)	84	87
4	d	278/276 (101%)	275 (99%)	3 (1%)	65	67
5	E	71/72 (99%)	70 (99%)	1 (1%)	59	59
5	e	68/72 (94%)	66 (97%)	2 (3%)	37	31
6	F	27/38 (71%)	26 (96%)	1 (4%)	30	22
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	21
7	H	53/53 (100%)	52 (98%)	1 (2%)	50	47
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	33/34 (97%)	31 (94%)	2 (6%)	17	9
9	J	23/28 (82%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/30 (97%)	29 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	31	23
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	33 (97%)	1 (3%)	37	31
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	207/207 (100%)	204 (99%)	3 (1%)	59	59
13	o	206/207 (100%)	201 (98%)	5 (2%)	43	38
14	T	25/28 (89%)	25 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	83/89 (93%)	81 (98%)	2 (2%)	43	38
15	u	83/89 (93%)	83 (100%)	0	100	100
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	114 (99%)	1 (1%)	70	73
17	Y	19/23 (83%)	17 (90%)	2 (10%)	6	2
17	y	18/23 (78%)	16 (89%)	2 (11%)	6	2
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	29 (97%)	1 (3%)	33	26
19	Z	47/52 (90%)	46 (98%)	1 (2%)	47	44
19	z	40/52 (77%)	37 (92%)	3 (8%)	12	6
All	All	4253/4368 (97%)	4193 (99%)	60 (1%)	59	59

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	210	LEU
1	A	229	GLU
1	A	244	GLU
1	A	248[A]	ILE
1	A	248[B]	ILE
2	B	315	ILE
2	B	467	ILE
2	B	472	ARG

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Mol	Chain	Res	Type
3	C	104	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	471	SER
4	D	90	LEU
5	E	4	THR
6	F	44	GLN
7	H	52	THR
13	O	25	THR
13	O	110	MET
13	O	207	ARG
15	U	24	LYS
15	U	86	GLU
17	Y	24	MET
17	Y	27	MET
19	Z	6	GLN
1	a	244	GLU
1	a	261	GLN
2	b	315	ILE
2	b	362	PHE
2	b	373	LYS
2	b	472	ARG
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	355	THR
3	c	416[A]	SER
3	c	416[B]	SER
4	d	24	ARG
4	d	150	ILE
4	d	329	MET
5	e	60	GLN
5	e	62	SER
6	f	15	ILE
8	i	35	LYS
8	i	38	GLU
10	k	27	VAL
11	l	15	THR
13	o	54	GLU
13	o	64	GLU
13	o	143	LYS

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Mol	Chain	Res	Type
13	o	181	GLU
13	o	234	LYS
16	v	23	GLU
17	y	30	ILE
17	y	41	VAL
18	x	39	ARG
19	z	3	ILE
19	z	20	VAL
19	z	29	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	261	GLN
1	A	315	ASN
2	B	53	ASN
2	B	179	GLN
2	B	281	GLN
2	B	331	ASN
2	B	497	GLN
3	C	155	ASN
4	D	186	GLN
4	D	255	GLN
4	D	332	GLN
5	E	74	GLN
13	O	82	GLN
13	O	104	GLN
13	O	231	HIS
16	V	34	GLN
1	a	165	GLN
1	a	315	ASN
2	b	53	ASN
2	b	281	GLN
2	b	289	GLN
2	b	331	ASN
2	b	374	ASN
3	c	44	ASN
3	c	311	GLN
4	d	186	GLN
4	d	255	GLN
4	d	332	GLN

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Mol	Chain	Res	Type
6	f	44	GLN
13	o	36	GLN
13	o	82	GLN
13	o	104	GLN
13	o	155	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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
4	HSK	D	336[A]	-	10,10,12	4.08	3 (30%)	5,12,16	2.44	2 (40%)
4	HSK	d	336[B]	-	10,11,12	2.28	3 (30%)	5,14,16	3.26	3 (60%)
14	FME	T	1	14	8,9,10	0.48	0	8,9,11	1.26	1 (12%)
14	FME	t	1	14	8,9,10	0.83	0	8,9,11	1.38	2 (25%)
12	FME	m	1	12	8,9,10	0.89	0	8,9,11	1.53	1 (12%)
8	FME	i	1	8	8,9,10	0.42	0	8,9,11	1.38	1 (12%)
12	FME	M	1	12	8,9,10	0.83	0	8,9,11	1.55	2 (25%)
4	HSK	D	336[B]	-	10,11,12	2.43	3 (30%)	5,14,16	3.23	3 (60%)
8	FME	I	1	8	8,9,10	0.62	0	8,9,11	1.05	0
4	HSK	d	336[A]	-	10,10,12	3.67	2 (20%)	5,12,16	1.85	2 (40%)

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
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
14	FME	T	1	14	-	2/7/9/11	-
14	FME	t	1	14	-	5/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	1/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-11.73	1.16	1.38
4	d	336[A]	HSK	OM-ND1	-10.19	1.19	1.38
4	D	336[B]	HSK	OM-ND1	4.90	1.47	1.38
4	d	336[B]	HSK	CG-ND1	-4.63	1.34	1.40
4	D	336[B]	HSK	CG-ND1	-4.45	1.34	1.40
4	D	336[A]	HSK	CG-ND1	-4.38	1.34	1.40
4	d	336[A]	HSK	CG-ND1	-4.32	1.34	1.40
4	d	336[B]	HSK	OM-ND1	3.98	1.45	1.38
4	D	336[B]	HSK	CE1-ND1	-2.56	1.32	1.37
4	d	336[B]	HSK	CE1-ND1	-2.39	1.33	1.37
4	D	336[A]	HSK	CE1-ND1	-2.06	1.33	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336[B]	HSK	ND1-CE1-NE2	-5.23	105.50	111.54
4	d	336[B]	HSK	ND1-CE1-NE2	-5.21	105.53	111.54
4	D	336[A]	HSK	ND1-CE1-NE2	-3.56	107.44	111.54
4	D	336[B]	HSK	CD2-NE2-CE1	3.35	109.62	105.24
4	d	336[B]	HSK	CD2-NE2-CE1	3.32	109.58	105.24
4	D	336[A]	HSK	CD2-NE2-CE1	3.32	109.58	105.24
4	d	336[B]	HSK	CB-CG-ND1	3.19	128.26	122.89
4	D	336[B]	HSK	CB-CG-ND1	2.93	127.83	122.89
4	d	336[A]	HSK	CD2-NE2-CE1	2.63	108.69	105.24
12	M	1	FME	CG-CB-CA	2.59	120.80	112.87
12	m	1	FME	CG-CB-CA	2.56	120.69	112.87
12	M	1	FME	C-CA-N	-2.35	104.97	109.50
14	t	1	FME	O1-CN-N	-2.28	119.43	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	O-C-CA	-2.23	119.04	124.77
4	d	336[A]	HSK	ND1-CE1-NE2	-2.18	109.03	111.54
14	t	1	FME	O-C-CA	-2.11	119.35	124.77
14	T	1	FME	O-C-CA	-2.08	119.41	124.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA
14	t	1	FME	O-C-CA-CB
14	t	1	FME	CB-CG-SD-CE
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	C-CA-CB-CG
14	t	1	FME	O1-CN-N-CA
14	t	1	FME	N-CA-CB-CG
12	m	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	4	0
12	M	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 15 are monoatomic and 43 are unknown - leaving 218 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	$\# Z > 2$
31	GOL	V	205	-	5,5,5	0.67	0	5,5,5	0.34	0
31	GOL	C	526	-	5,5,5	0.68	0	5,5,5	0.50	0
23	CLA	B	617	2	69,73,73	1.88	20 (28%)	82,113,113	2.33	25 (30%)
31	GOL	c	927	-	5,5,5	0.64	0	5,5,5	0.43	0
31	GOL	b	634	-	5,5,5	0.51	0	5,5,5	0.25	0
31	GOL	D	415	-	5,5,5	0.73	0	5,5,5	1.33	1 (20%)
31	GOL	f	104	32	5,5,5	0.55	0	5,5,5	0.45	0
34	DGD	d	406	-	50,50,67	1.20	3 (6%)	58,58,81	1.38	9 (15%)
26	SQD	D	407	-	43,45,54	1.26	3 (6%)	53,56,65	2.12	15 (28%)
23	CLA	B	613	2	69,73,73	2.25	20 (28%)	82,113,113	2.15	26 (31%)
23	CLA	C	505	3	69,73,73	2.19	20 (28%)	82,113,113	2.04	26 (31%)
27	LMG	D	411	39	51,51,55	0.87	2 (3%)	59,59,63	1.04	2 (3%)
33	HTG	c	924	-	19,19,19	0.94	1 (5%)	23,24,24	2.17	4 (17%)
25	BCR	C	514	-	41,41,41	0.91	0	56,56,56	1.33	9 (16%)
23	CLA	c	905	41	69,73,73	2.47	21 (30%)	82,113,113	2.48	27 (32%)
23	CLA	c	909	3	69,73,73	2.36	20 (28%)	82,113,113	2.33	29 (35%)
23	CLA	b	605	2	69,73,73	2.14	18 (26%)	82,113,113	2.17	29 (35%)
23	CLA	C	506	3	69,73,73	2.24	18 (26%)	82,113,113	2.31	27 (32%)
23	CLA	B	604	2	69,73,73	2.03	18 (26%)	82,113,113	2.59	30 (36%)
23	CLA	d	403	4	69,73,73	2.16	21 (30%)	82,113,113	2.41	33 (40%)
25	BCR	k	101	-	41,41,41	0.86	0	56,56,56	1.49	12 (21%)
31	GOL	L	104	-	5,5,5	0.52	0	5,5,5	0.64	0
23	CLA	B	609	2	69,73,73	1.84	17 (24%)	82,113,113	2.53	29 (35%)
31	GOL	B	635	-	5,5,5	0.54	0	5,5,5	1.11	0
33	HTG	U	201	-	8,8,19	0.30	0	7,7,24	0.97	0
36	LHG	l	101	-	48,48,48	0.84	2 (4%)	51,54,54	1.12	5 (9%)
30	LMT	Z	102	-	36,36,36	0.68	1 (2%)	47,47,47	0.90	0
23	CLA	a	411	41	69,73,73	1.79	18 (26%)	82,113,113	2.38	36 (43%)
30	LMT	m	102	-	36,36,36	0.73	1 (2%)	47,47,47	1.09	3 (6%)
31	GOL	B	636	-	5,5,5	0.48	0	5,5,5	0.79	0
33	HTG	B	630	-	19,19,19	0.99	2 (10%)	23,24,24	1.42	3 (13%)
25	BCR	K	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.69	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GOL	c	930	-	5,5,5	0.47	0	5,5,5	0.71	0
23	CLA	B	606	2	69,73,73	2.08	19 (27%)	82,113,113	2.20	26 (31%)
23	CLA	b	614	2	69,73,73	2.06	16 (23%)	82,113,113	2.29	29 (35%)
36	LHG	L	101	-	48,48,48	0.83	2 (4%)	51,54,54	1.56	7 (13%)
31	GOL	C	524	-	5,5,5	0.36	0	5,5,5	1.69	1 (20%)
27	LMG	A	413	-	51,51,55	1.00	2 (3%)	59,59,63	1.22	4 (6%)
33	HTG	d	401	-	19,19,19	1.01	1 (5%)	23,24,24	1.25	1 (4%)
31	GOL	B	637	-	5,5,5	0.48	0	5,5,5	1.18	1 (20%)
27	LMG	Z	101	-	51,51,55	1.11	3 (5%)	59,59,63	1.37	7 (11%)
23	CLA	c	908	41	69,73,73	2.36	22 (31%)	82,113,113	2.44	30 (36%)
31	GOL	O	304	-	5,5,5	0.56	0	5,5,5	0.64	0
23	CLA	b	612	2	69,73,73	2.37	22 (31%)	82,113,113	1.98	25 (30%)
25	BCR	T	101	-	41,41,41	0.92	0	56,56,56	1.69	15 (26%)
23	CLA	c	913	3	69,73,73	2.55	21 (30%)	82,113,113	2.27	28 (34%)
31	GOL	B	638	-	5,5,5	0.53	0	5,5,5	0.92	0
33	HTG	C	521	-	19,19,19	0.85	1 (5%)	23,24,24	1.21	1 (4%)
23	CLA	A	405	1	69,73,73	2.00	17 (24%)	82,113,113	2.13	27 (32%)
25	BCR	K	101	-	41,41,41	0.91	0	56,56,56	1.70	12 (21%)
25	BCR	D	404	-	41,41,41	1.17	4 (9%)	56,56,56	2.10	18 (32%)
36	LHG	D	409	-	48,48,48	0.84	2 (4%)	51,54,54	1.14	5 (9%)
27	LMG	d	410	39	51,51,55	1.02	3 (5%)	59,59,63	1.15	7 (11%)
34	DGD	c	918	-	63,63,67	1.01	4 (6%)	77,77,81	1.23	10 (12%)
23	CLA	B	610	2	69,73,73	2.02	20 (28%)	82,113,113	2.19	27 (32%)
25	BCR	c	916	-	41,41,41	0.99	1 (2%)	56,56,56	1.40	7 (12%)
23	CLA	b	610	41	69,73,73	2.32	18 (26%)	82,113,113	2.04	27 (32%)
23	CLA	b	613	41	69,73,73	2.15	18 (26%)	82,113,113	2.44	26 (31%)
26	SQD	a	416	-	52,54,54	0.89	2 (3%)	62,65,65	2.19	14 (22%)
31	GOL	A	423	32	5,5,5	0.33	0	5,5,5	0.83	0
33	HTG	u	201	-	10,13,19	0.76	0	13,14,24	1.69	2 (15%)
23	CLA	d	402	4	69,73,73	1.96	16 (23%)	82,113,113	2.32	29 (35%)
23	CLA	b	611	2	69,73,73	2.10	18 (26%)	82,113,113	2.10	24 (29%)
23	CLA	A	407	41	69,73,73	2.13	18 (26%)	82,113,113	2.33	30 (36%)
23	CLA	c	904	3	69,73,73	2.48	19 (27%)	82,113,113	2.26	26 (31%)
23	CLA	C	509	3	69,73,73	2.31	18 (26%)	82,113,113	2.33	28 (34%)
31	GOL	a	422	-	5,5,5	0.69	0	5,5,5	0.82	0
23	CLA	b	619	2	69,73,73	2.17	19 (27%)	82,113,113	2.33	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	604	41	69,73,73	2.38	19 (27%)	82,113,113	2.32	26 (31%)
33	HTG	O	303	-	19,19,19	1.13	2 (10%)	23,24,24	1.22	1 (4%)
34	DGD	C	516	-	63,63,67	0.92	3 (4%)	77,77,81	1.36	12 (15%)
23	CLA	b	609	2	69,73,73	2.31	20 (28%)	82,113,113	2.43	30 (36%)
35	BCT	D	401	21	3,3,3	1.13	0	2,3,3	1.11	0
25	BCR	k	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.33	7 (12%)
23	CLA	c	911	3	69,73,73	2.13	20 (28%)	82,113,113	2.07	28 (34%)
25	BCR	d	404	-	41,41,41	1.03	3 (7%)	56,56,56	1.83	15 (26%)
24	PHO	A	409	-	58,69,69	2.57	11 (18%)	55,99,99	3.17	18 (32%)
33	HTG	C	522	-	19,19,19	0.95	2 (10%)	23,24,24	2.00	3 (13%)
23	CLA	a	410	41	69,73,73	1.99	21 (30%)	82,113,113	2.20	24 (29%)
25	BCR	B	620	-	41,41,41	1.03	1 (2%)	56,56,56	1.67	12 (21%)
23	CLA	B	615	2	69,73,73	2.19	20 (28%)	82,113,113	2.38	30 (36%)
23	CLA	c	907	3	69,73,73	2.24	18 (26%)	82,113,113	2.57	31 (37%)
31	GOL	C	525	-	5,5,5	0.82	0	5,5,5	0.93	0
31	GOL	b	636	-	5,5,5	0.59	0	5,5,5	1.05	0
31	GOL	A	421	-	5,5,5	0.91	0	5,5,5	0.53	0
37	HEM	F	101	6,5	50,50,50	2.01	9 (18%)	67,82,82	1.68	12 (17%)
34	DGD	h	102	-	63,63,67	1.00	3 (4%)	77,77,81	1.27	11 (14%)
34	DGD	H	102	-	63,63,67	1.13	3 (4%)	77,77,81	1.36	12 (15%)
25	BCR	b	622	-	41,41,41	0.96	2 (4%)	56,56,56	1.28	6 (10%)
38	RRX	H	101	-	42,42,42	1.10	3 (7%)	56,58,58	1.62	10 (17%)
25	BCR	c	915	-	41,41,41	0.87	1 (2%)	56,56,56	1.26	6 (10%)
30	LMT	a	402	-	36,36,36	0.77	1 (2%)	47,47,47	1.60	10 (21%)
31	GOL	B	633	-	5,5,5	0.34	0	5,5,5	1.46	1 (20%)
23	CLA	B	607	2	69,73,73	2.16	14 (20%)	82,113,113	2.61	35 (42%)
23	CLA	B	603	2	69,73,73	2.36	21 (30%)	82,113,113	1.96	27 (32%)
26	SQD	A	412	-	52,54,54	0.86	2 (3%)	62,65,65	2.15	17 (27%)
34	DGD	C	518	-	63,63,67	0.79	3 (4%)	77,77,81	1.31	9 (11%)
25	BCR	b	621	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	7 (12%)
23	CLA	A	406	41	69,73,73	1.93	19 (27%)	82,113,113	2.50	34 (41%)
33	HTG	b	601	-	19,19,19	0.92	2 (10%)	23,24,24	1.24	3 (13%)
23	CLA	C	502	3	69,73,73	1.93	17 (24%)	82,113,113	2.33	29 (35%)
30	LMT	b	624	-	25,25,36	0.75	1 (4%)	30,30,47	1.39	5 (16%)
23	CLA	B	611	41	69,73,73	2.06	19 (27%)	82,113,113	2.50	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	B	625	-	19,19,19	0.93	1 (5%)	23,24,24	1.38	4 (17%)
31	GOL	v	204	-	5,5,5	0.30	0	5,5,5	0.73	0
36	LHG	d	409	-	48,48,48	0.93	3 (6%)	51,54,54	1.09	4 (7%)
30	LMT	z	101	-	32,32,36	0.70	1 (3%)	42,42,47	1.01	4 (9%)
30	LMT	J	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.13	2 (6%)
25	BCR	t	101	-	41,41,41	1.04	3 (7%)	56,56,56	1.86	15 (26%)
23	CLA	B	616	2	69,73,73	2.32	16 (23%)	82,113,113	2.31	28 (34%)
30	LMT	F	102	-	36,36,36	0.75	1 (2%)	47,47,47	1.19	3 (6%)
33	HTG	B	626	-	19,19,19	0.87	1 (5%)	23,24,24	1.59	2 (8%)
31	GOL	h	103	-	5,5,5	0.37	0	5,5,5	0.29	0
23	CLA	C	508	3	69,73,73	2.52	19 (27%)	82,113,113	2.03	23 (28%)
23	CLA	b	617	2	69,73,73	1.91	16 (23%)	82,113,113	2.78	37 (45%)
31	GOL	A	422	-	5,5,5	0.44	0	5,5,5	0.52	0
28	PL9	d	405	-	55,55,55	1.27	9 (16%)	68,69,69	1.53	13 (19%)
31	GOL	c	928	-	5,5,5	0.23	0	5,5,5	0.86	0
38	RRX	h	101	-	42,42,42	0.96	1 (2%)	56,58,58	1.34	8 (14%)
23	CLA	c	903	3	69,73,73	2.20	18 (26%)	82,113,113	2.57	28 (34%)
23	CLA	c	912	3	69,73,73	2.26	19 (27%)	82,113,113	2.38	29 (35%)
36	LHG	D	408	-	48,48,48	0.80	1 (2%)	51,54,54	1.50	6 (11%)
30	LMT	M	101	-	36,36,36	0.87	1 (2%)	47,47,47	1.23	6 (12%)
23	CLA	c	902	3	69,73,73	2.08	19 (27%)	82,113,113	2.68	29 (35%)
31	GOL	a	424	-	5,5,5	0.68	0	5,5,5	0.79	0
23	CLA	b	607	2	69,73,73	2.12	18 (26%)	82,113,113	2.46	28 (34%)
31	GOL	c	929	-	5,5,5	0.56	0	5,5,5	0.90	0
23	CLA	C	501	3	69,73,73	1.99	19 (27%)	82,113,113	2.62	28 (34%)
23	CLA	c	906	3	69,73,73	2.10	20 (28%)	82,113,113	2.19	29 (35%)
31	GOL	b	632	-	5,5,5	0.54	0	5,5,5	1.38	0
23	CLA	D	402	4	69,73,73	1.97	19 (27%)	82,113,113	2.44	31 (37%)
34	DGD	c	919	-	63,63,67	1.06	5 (7%)	77,77,81	1.37	10 (12%)
34	DGD	D	406	-	53,53,67	1.20	3 (5%)	61,61,81	1.38	8 (13%)
40	SO4	O	302	-	4,4,4	0.60	0	6,6,6	0.40	0
36	LHG	d	407	-	48,48,48	0.81	2 (4%)	51,54,54	1.41	6 (11%)
31	GOL	V	203	-	5,5,5	1.03	0	5,5,5	0.84	0
31	GOL	v	203	-	5,5,5	0.75	0	5,5,5	0.51	0
25	BCR	C	515	-	41,41,41	0.95	1 (2%)	56,56,56	1.47	7 (12%)
27	LMG	a	418	-	51,51,55	0.94	2 (3%)	59,59,63	1.34	5 (8%)
34	DGD	c	917	-	63,63,67	0.91	4 (6%)	77,77,81	1.27	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	A	408	-	58,69,69	2.26	11 (18%)	55,99,99	3.25	16 (29%)
25	BCR	b	620	-	41,41,41	1.08	1 (2%)	56,56,56	1.76	15 (26%)
31	GOL	a	423	-	5,5,5	0.60	0	5,5,5	0.63	0
23	CLA	B	602	41	69,73,73	2.34	20 (28%)	82,113,113	2.62	30 (36%)
25	BCR	B	619	-	41,41,41	1.20	4 (9%)	56,56,56	1.25	8 (14%)
30	LMT	m	101	-	36,36,36	0.74	0	47,47,47	1.39	8 (17%)
30	LMT	c	922	-	36,36,36	0.75	1 (2%)	47,47,47	0.96	3 (6%)
31	GOL	B	634	-	5,5,5	0.85	0	5,5,5	0.71	0
37	HEM	v	201	16	50,50,50	1.98	9 (18%)	67,82,82	1.51	8 (11%)
23	CLA	B	605	2	69,73,73	2.00	16 (23%)	82,113,113	2.22	31 (37%)
30	LMT	b	625	-	24,24,36	0.54	0	29,29,47	1.25	4 (13%)
23	CLA	C	503	3	69,73,73	2.18	20 (28%)	82,113,113	2.13	24 (29%)
23	CLA	B	608	41	69,73,73	2.13	19 (27%)	82,113,113	2.19	27 (32%)
31	GOL	b	633	-	5,5,5	0.40	0	5,5,5	0.94	0
23	CLA	a	414	1	69,73,73	1.94	19 (27%)	82,113,113	2.45	33 (40%)
23	CLA	c	914	3	69,73,73	2.67	21 (30%)	82,113,113	2.01	26 (31%)
24	PHO	a	412	-	58,69,69	2.26	12 (20%)	55,99,99	2.74	14 (25%)
34	DGD	C	517	-	63,63,67	0.91	2 (3%)	77,77,81	1.06	3 (3%)
23	CLA	b	606	2	69,73,73	2.06	19 (27%)	82,113,113	2.45	30 (36%)
23	CLA	b	618	2	69,73,73	2.04	17 (24%)	82,113,113	2.39	28 (34%)
30	LMT	B	623	-	36,36,36	1.00	2 (5%)	47,47,47	1.39	8 (17%)
33	HTG	c	923	-	19,19,19	0.93	2 (10%)	23,24,24	1.37	2 (8%)
26	SQD	a	401	-	52,54,54	1.13	2 (3%)	62,65,65	1.59	9 (14%)
25	BCR	a	415	-	41,41,41	1.22	5 (12%)	56,56,56	1.46	8 (14%)
23	CLA	b	616	2	69,73,73	1.93	18 (26%)	82,113,113	2.33	28 (34%)
30	LMT	C	520	-	36,36,36	0.62	1 (2%)	47,47,47	1.49	7 (14%)
33	HTG	b	626	-	19,19,19	0.97	1 (5%)	23,24,24	1.37	3 (13%)
26	SQD	A	418	-	52,54,54	1.09	2 (3%)	62,65,65	1.62	12 (19%)
30	LMT	M	102	-	36,36,36	0.62	0	47,47,47	1.35	7 (14%)
37	HEM	V	201	16	50,50,50	1.94	12 (24%)	67,82,82	1.30	7 (10%)
23	CLA	A	410	1	69,73,73	2.04	18 (26%)	82,113,113	2.52	31 (37%)
23	CLA	D	403	4	69,73,73	2.24	19 (27%)	82,113,113	2.28	29 (35%)
23	CLA	C	510	3	69,73,73	2.18	20 (28%)	82,113,113	2.32	26 (31%)
23	CLA	B	614	2	69,73,73	1.97	15 (21%)	82,113,113	2.10	27 (32%)
37	HEM	f	101	6,5	50,50,50	1.95	12 (24%)	67,82,82	1.43	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	504	41	69,73,73	2.11	20 (28%)	82,113,113	2.19	26 (31%)
23	CLA	C	513	3	69,73,73	2.56	19 (27%)	82,113,113	2.21	24 (29%)
33	HTG	b	627	-	19,19,19	1.05	2 (10%)	23,24,24	1.42	1 (4%)
24	PHO	a	413	-	58,69,69	2.61	12 (20%)	55,99,99	3.10	18 (32%)
31	GOL	b	635	-	5,5,5	0.81	0	5,5,5	0.96	0
27	LMG	c	920	-	51,51,55	1.12	4 (7%)	59,59,63	1.28	9 (15%)
28	PL9	D	405	-	55,55,55	1.38	9 (16%)	68,69,69	1.53	12 (17%)
35	BCT	a	408	21	3,3,3	1.14	0	2,3,3	2.98	1 (50%)
36	LHG	d	408	-	48,48,48	0.79	2 (4%)	51,54,54	1.34	9 (17%)
36	LHG	a	417	-	39,39,48	1.17	2 (5%)	42,45,54	1.00	2 (4%)
20	OEX	A	401	1,41,3	0,14,14	-	-	-	-	-
30	LMT	A	419	-	36,36,36	0.84	1 (2%)	47,47,47	1.35	5 (10%)
33	HTG	V	202	-	12,13,19	0.73	0	17,18,24	3.30	7 (41%)
36	LHG	D	410	-	45,45,48	1.04	2 (4%)	48,51,54	1.06	3 (6%)
25	BCR	B	618	-	41,41,41	1.13	5 (12%)	56,56,56	1.60	9 (16%)
23	CLA	C	507	41	69,73,73	2.31	19 (27%)	82,113,113	2.29	24 (29%)
30	LMT	t	102	-	24,24,36	0.69	0	29,29,47	1.32	3 (10%)
33	HTG	b	602	-	19,19,19	0.74	0	23,24,24	1.09	2 (8%)
27	LMG	c	921	-	51,51,55	1.10	3 (5%)	59,59,63	1.23	6 (10%)
28	PL9	A	414	-	55,55,55	0.93	3 (5%)	68,69,69	1.51	11 (16%)
31	GOL	l	102	-	5,5,5	0.49	0	5,5,5	1.08	0
36	LHG	E	101	-	48,48,48	1.02	2 (4%)	51,54,54	0.94	2 (3%)
25	BCR	A	411	-	41,41,41	1.05	0	56,56,56	1.50	11 (19%)
33	HTG	B	624	-	19,19,19	1.07	1 (5%)	23,24,24	1.40	6 (26%)
23	CLA	b	608	2	69,73,73	1.96	18 (26%)	82,113,113	2.43	28 (34%)
26	SQD	B	621	-	52,54,54	1.10	4 (7%)	62,65,65	1.84	12 (19%)
33	HTG	D	414	-	19,19,19	0.99	1 (5%)	23,24,24	1.04	1 (4%)
31	GOL	V	204	-	5,5,5	0.31	0	5,5,5	0.47	0
20	OEX	a	404	1,41,3	0,14,14	-	-	-	-	-
26	SQD	f	102	-	31,32,54	2.00	3 (9%)	33,36,65	1.61	5 (15%)
26	SQD	L	103	-	52,54,54	1.09	2 (3%)	62,65,65	1.66	12 (19%)
28	PL9	a	419	-	55,55,55	0.86	3 (5%)	68,69,69	1.76	18 (26%)
27	LMG	b	623	-	51,51,55	0.87	2 (3%)	59,59,63	1.47	7 (11%)
33	HTG	B	631	-	19,19,19	0.80	1 (5%)	23,24,24	1.68	3 (13%)
31	GOL	v	202	-	5,5,5	0.59	0	5,5,5	0.55	0
23	CLA	C	511	3	69,73,73	2.36	22 (31%)	82,113,113	2.58	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	409	1	69,73,73	1.91	16 (23%)	82,113,113	2.28	28 (34%)
23	CLA	c	910	3	69,73,73	2.33	21 (30%)	82,113,113	2.47	35 (42%)
27	LMG	B	622	-	51,51,55	0.95	2 (3%)	59,59,63	1.63	9 (15%)
23	CLA	C	512	3	69,73,73	2.40	20 (28%)	82,113,113	2.24	27 (32%)
27	LMG	C	519	-	51,51,55	1.03	3 (5%)	59,59,63	1.48	9 (15%)
23	CLA	B	612	2	69,73,73	1.79	16 (23%)	82,113,113	2.46	30 (36%)
23	CLA	b	615	2	69,73,73	2.21	18 (26%)	82,113,113	2.50	28 (34%)

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
31	GOL	V	205	-	-	0/4/4/4	-
31	GOL	C	526	-	-	0/4/4/4	-
23	CLA	B	617	2	-	15/39/115/115	-
31	GOL	c	927	-	-	2/4/4/4	-
31	GOL	b	634	-	-	0/4/4/4	-
31	GOL	D	415	-	-	2/4/4/4	-
31	GOL	f	104	32	-	2/4/4/4	-
34	DGD	d	406	-	-	26/44/64/95	0/1/1/2
26	SQD	D	407	-	-	13/40/60/69	0/1/1/1
23	CLA	B	613	2	-	2/39/115/115	-
23	CLA	C	505	3	-	2/39/115/115	-
27	LMG	D	411	39	-	9/46/66/70	0/1/1/1
33	HTG	c	924	-	-	1/10/30/30	0/1/1/1
25	BCR	C	514	-	-	2/29/63/63	0/2/2/2
23	CLA	c	905	41	-	10/39/115/115	-
23	CLA	c	909	3	-	1/39/115/115	-
23	CLA	b	605	2	-	2/39/115/115	-
23	CLA	C	506	3	-	11/39/115/115	-
23	CLA	B	604	2	-	4/39/115/115	-
23	CLA	d	403	4	-	8/39/115/115	-
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
31	GOL	L	104	-	-	1/4/4/4	-
23	CLA	B	609	2	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	B	635	-	-	4/4/4/4	-
33	HTG	U	201	-	-	4/6/6/30	-
36	LHG	l	101	-	-	17/53/53/53	-
30	LMT	Z	102	-	-	13/21/61/61	0/2/2/2
23	CLA	a	411	41	-	8/39/115/115	-
30	LMT	m	102	-	-	6/21/61/61	0/2/2/2
31	GOL	B	636	-	-	0/4/4/4	-
33	HTG	B	630	-	-	4/10/30/30	0/1/1/1
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
31	GOL	c	930	-	-	4/4/4/4	-
23	CLA	B	606	2	-	6/39/115/115	-
23	CLA	b	614	2	-	5/39/115/115	-
36	LHG	L	101	-	-	10/53/53/53	-
31	GOL	C	524	-	-	2/4/4/4	-
27	LMG	A	413	-	-	25/46/66/70	0/1/1/1
33	HTG	d	401	-	-	5/10/30/30	0/1/1/1
31	GOL	B	637	-	-	0/4/4/4	-
27	LMG	Z	101	-	-	25/46/66/70	0/1/1/1
23	CLA	c	908	41	-	8/39/115/115	-
31	GOL	O	304	-	-	2/4/4/4	-
23	CLA	b	612	2	-	2/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	913	3	-	10/39/115/115	-
31	GOL	B	638	-	-	2/4/4/4	-
33	HTG	C	521	-	-	3/10/30/30	0/1/1/1
23	CLA	A	405	1	-	3/39/115/115	-
25	BCR	K	101	-	-	3/29/63/63	0/2/2/2
25	BCR	D	404	-	-	2/29/63/63	0/2/2/2
36	LHG	D	409	-	-	13/53/53/53	-
27	LMG	d	410	39	-	10/46/66/70	0/1/1/1
34	DGD	c	918	-	-	21/51/91/95	0/2/2/2
23	CLA	B	610	2	-	3/39/115/115	-
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
23	CLA	b	610	41	-	2/39/115/115	-
23	CLA	b	613	41	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	416	-	-	20/49/69/69	0/1/1/1
31	GOL	A	423	32	-	0/4/4/4	-
33	HTG	u	201	-	-	6/12/14/30	-
23	CLA	d	402	4	-	1/39/115/115	-
23	CLA	b	611	2	-	1/39/115/115	-
23	CLA	A	407	41	-	7/39/115/115	-
23	CLA	c	904	3	-	1/39/115/115	-
23	CLA	C	509	3	-	6/39/115/115	-
31	GOL	a	422	-	-	0/4/4/4	-
23	CLA	b	619	2	-	6/39/115/115	-
23	CLA	b	604	41	-	14/39/115/115	-
33	HTG	O	303	-	-	3/10/30/30	0/1/1/1
34	DGD	C	516	-	-	17/51/91/95	0/2/2/2
23	CLA	b	609	2	-	10/39/115/115	-
25	BCR	k	102	-	-	3/29/63/63	0/2/2/2
23	CLA	c	911	3	-	6/39/115/115	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
24	PHO	A	409	-	-	3/37/103/103	0/5/6/6
33	HTG	C	522	-	-	2/10/30/30	0/1/1/1
23	CLA	a	410	41	-	3/39/115/115	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
23	CLA	B	615	2	-	11/39/115/115	-
23	CLA	c	907	3	-	12/39/115/115	-
31	GOL	C	525	-	-	0/4/4/4	-
31	GOL	b	636	-	-	2/4/4/4	-
31	GOL	A	421	-	-	0/4/4/4	-
37	HEM	F	101	6,5	-	2/14/54/54	-
34	DGD	h	102	-	-	10/51/91/95	0/2/2/2
34	DGD	H	102	-	-	16/51/91/95	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
38	RRX	H	101	-	-	1/29/65/65	0/2/2/2
25	BCR	c	915	-	-	5/29/63/63	0/2/2/2
30	LMT	a	402	-	-	10/21/61/61	0/2/2/2
31	GOL	B	633	-	-	2/4/4/4	-
23	CLA	B	607	2	-	6/39/115/115	-
23	CLA	B	603	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	A	412	-	-	18/49/69/69	0/1/1/1
34	DGD	C	518	-	-	13/51/91/95	0/2/2/2
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	CLA	A	406	41	-	4/39/115/115	-
33	HTG	b	601	-	-	3/10/30/30	0/1/1/1
23	CLA	C	502	3	-	6/39/115/115	-
30	LMT	b	624	-	-	9/17/37/61	0/1/1/2
23	CLA	B	611	41	-	8/39/115/115	-
33	HTG	B	625	-	-	4/10/30/30	0/1/1/1
31	GOL	v	204	-	-	0/4/4/4	-
36	LHG	d	409	-	-	16/53/53/53	-
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
30	LMT	J	102	-	-	7/15/35/61	0/1/1/2
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	616	2	-	5/39/115/115	-
30	LMT	F	102	-	-	11/21/61/61	0/2/2/2
33	HTG	B	626	-	-	5/10/30/30	0/1/1/1
31	GOL	h	103	-	-	1/4/4/4	-
23	CLA	C	508	3	-	3/39/115/115	-
23	CLA	b	617	2	-	16/39/115/115	-
31	GOL	A	422	-	-	0/4/4/4	-
28	PL9	d	405	-	-	2/53/73/73	0/1/1/1
31	GOL	c	928	-	-	1/4/4/4	-
38	RRX	h	101	-	-	1/29/65/65	0/2/2/2
23	CLA	c	903	3	-	4/39/115/115	-
23	CLA	c	912	3	-	6/39/115/115	-
36	LHG	D	408	-	-	9/53/53/53	-
30	LMT	M	101	-	-	7/21/61/61	0/2/2/2
23	CLA	c	902	3	-	4/39/115/115	-
31	GOL	a	424	-	-	3/4/4/4	-
23	CLA	b	607	2	-	5/39/115/115	-
31	GOL	c	929	-	-	0/4/4/4	-
23	CLA	C	501	3	-	5/39/115/115	-
23	CLA	c	906	3	-	3/39/115/115	-
31	GOL	b	632	-	-	4/4/4/4	-
23	CLA	D	402	4	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	c	919	-	-	16/51/91/95	0/2/2/2
34	DGD	D	406	-	-	26/47/68/95	0/1/1/2
36	LHG	d	407	-	-	6/53/53/53	-
31	GOL	V	203	-	-	2/4/4/4	-
31	GOL	v	203	-	-	2/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	LMG	a	418	-	-	19/46/66/70	0/1/1/1
34	DGD	c	917	-	-	14/51/91/95	0/2/2/2
24	PHO	A	408	-	-	0/37/103/103	0/5/6/6
25	BCR	b	620	-	-	2/29/63/63	0/2/2/2
31	GOL	a	423	-	-	2/4/4/4	-
23	CLA	B	602	41	-	18/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	LMT	m	101	-	-	3/21/61/61	0/2/2/2
30	LMT	c	922	-	-	5/21/61/61	0/2/2/2
31	GOL	B	634	-	-	0/4/4/4	-
37	HEM	v	201	16	-	6/14/54/54	-
23	CLA	B	605	2	-	5/39/115/115	-
30	LMT	b	625	-	-	11/15/35/61	0/1/1/2
23	CLA	C	503	3	-	1/39/115/115	-
23	CLA	B	608	41	-	2/39/115/115	-
31	GOL	b	633	-	-	3/4/4/4	-
23	CLA	a	414	1	-	12/39/115/115	-
23	CLA	c	914	3	-	11/39/115/115	-
24	PHO	a	412	-	-	1/37/103/103	0/5/6/6
34	DGD	C	517	-	-	22/51/91/95	0/2/2/2
23	CLA	b	606	2	-	4/39/115/115	-
23	CLA	b	618	2	-	9/39/115/115	-
30	LMT	B	623	-	-	12/21/61/61	0/2/2/2
33	HTG	c	923	-	-	4/10/30/30	0/1/1/1
26	SQD	a	401	-	-	23/49/69/69	0/1/1/1
25	BCR	a	415	-	-	1/29/63/63	0/2/2/2
23	CLA	b	616	2	-	4/39/115/115	-
30	LMT	C	520	-	-	10/21/61/61	0/2/2/2
33	HTG	b	626	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	A	418	-	-	16/49/69/69	0/1/1/1
30	LMT	M	102	-	-	2/21/61/61	0/2/2/2
37	HEM	V	201	16	-	6/14/54/54	-
23	CLA	A	410	1	-	13/39/115/115	-
23	CLA	D	403	4	-	12/39/115/115	-
23	CLA	C	510	3	-	3/39/115/115	-
23	CLA	B	614	2	-	6/39/115/115	-
37	HEM	f	101	6,5	-	1/14/54/54	-
23	CLA	C	504	41	-	10/39/115/115	-
23	CLA	C	513	3	-	13/39/115/115	-
33	HTG	b	627	-	-	5/10/30/30	0/1/1/1
24	PHO	a	413	-	-	2/37/103/103	0/5/6/6
31	GOL	b	635	-	-	1/4/4/4	-
27	LMG	c	920	-	-	18/46/66/70	0/1/1/1
28	PL9	D	405	-	-	1/53/73/73	0/1/1/1
36	LHG	d	408	-	-	9/53/53/53	-
36	LHG	a	417	-	-	29/44/44/53	-
30	LMT	A	419	-	-	5/21/61/61	0/2/2/2
33	HTG	V	202	-	-	2/4/24/30	0/1/1/1
36	LHG	D	410	-	-	13/50/50/53	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
23	CLA	C	507	41	-	11/39/115/115	-
30	LMT	t	102	-	-	8/15/35/61	0/1/1/2
33	HTG	b	602	-	-	1/10/30/30	0/1/1/1
27	LMG	c	921	-	-	13/46/66/70	0/1/1/1
28	PL9	A	414	-	-	11/53/73/73	0/1/1/1
31	GOL	l	102	-	-	0/4/4/4	-
36	LHG	E	101	-	-	27/53/53/53	-
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
33	HTG	B	624	-	-	2/10/30/30	0/1/1/1
23	CLA	b	608	2	-	3/39/115/115	-
26	SQD	B	621	-	-	29/49/69/69	0/1/1/1
33	HTG	D	414	-	-	2/10/30/30	0/1/1/1
31	GOL	V	204	-	-	0/4/4/4	-
26	SQD	f	102	-	-	13/33/33/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	L	103	-	-	28/49/69/69	0/1/1/1
28	PL9	a	419	-	-	11/53/73/73	0/1/1/1
27	LMG	b	623	-	-	19/46/66/70	0/1/1/1
33	HTG	B	631	-	-	5/10/30/30	0/1/1/1
31	GOL	v	202	-	-	0/4/4/4	-
23	CLA	C	511	3	-	0/39/115/115	-
23	CLA	a	409	1	-	4/39/115/115	-
23	CLA	c	910	3	-	11/39/115/115	-
27	LMG	B	622	-	-	15/46/66/70	0/1/1/1
23	CLA	C	512	3	-	7/39/115/115	-
27	LMG	C	519	-	-	22/46/66/70	0/1/1/1
23	CLA	B	612	2	-	1/39/115/115	-
23	CLA	b	615	2	-	6/39/115/115	-

All (1598) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	MG-NA	12.57	2.36	2.06
23	c	914	CLA	MG-NC	11.74	2.34	2.06
23	C	512	CLA	MG-NA	11.26	2.33	2.06
23	C	511	CLA	MG-NA	11.02	2.32	2.06
23	B	616	CLA	MG-NA	10.89	2.32	2.06
23	B	607	CLA	MG-NA	10.52	2.31	2.06
23	b	615	CLA	MG-NA	10.41	2.31	2.06
23	b	609	CLA	MG-NA	10.30	2.30	2.06
23	C	507	CLA	MG-NA	9.89	2.29	2.06
23	c	904	CLA	MG-NA	9.80	2.29	2.06
23	C	506	CLA	MG-NA	9.65	2.29	2.06
24	A	409	PHO	C1D-C2D	9.64	1.50	1.39
23	A	407	CLA	MG-NA	9.41	2.28	2.06
23	c	913	CLA	MG-NA	9.29	2.28	2.06
23	B	602	CLA	MG-NA	9.21	2.28	2.06
24	a	413	PHO	C1B-C2B	9.16	1.49	1.39
23	C	508	CLA	MG-NA	9.07	2.27	2.06
23	B	613	CLA	MG-NA	9.02	2.27	2.06
23	C	509	CLA	MG-NA	9.00	2.27	2.06
23	c	909	CLA	MG-NA	8.95	2.27	2.06
24	a	413	PHO	C1D-C2D	8.84	1.49	1.39
23	c	905	CLA	MG-NA	8.83	2.27	2.06
23	c	904	CLA	MG-NC	8.66	2.26	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	MG-NA	8.49	2.26	2.06
24	A	408	PHO	C1D-C2D	8.44	1.48	1.39
23	b	618	CLA	MG-NA	8.38	2.26	2.06
23	C	510	CLA	MG-NA	8.38	2.26	2.06
23	B	603	CLA	MG-NA	8.36	2.26	2.06
23	b	614	CLA	MG-NA	8.36	2.26	2.06
23	b	607	CLA	MG-NA	8.25	2.25	2.06
23	c	907	CLA	MG-ND	-8.21	1.89	2.05
23	C	503	CLA	MG-NC	8.19	2.25	2.06
23	c	912	CLA	MG-NA	8.14	2.25	2.06
23	c	902	CLA	MG-NA	8.13	2.25	2.06
23	c	910	CLA	MG-NA	7.80	2.24	2.06
23	b	611	CLA	MG-NA	7.70	2.24	2.06
23	D	403	CLA	MG-NA	7.60	2.24	2.06
24	A	409	PHO	C1B-C2B	7.55	1.47	1.39
23	b	604	CLA	MG-NC	7.53	2.24	2.06
37	v	201	HEM	C3D-C2D	7.49	1.52	1.36
24	a	412	PHO	C1B-C2B	7.40	1.47	1.39
23	c	903	CLA	MG-ND	-7.39	1.91	2.05
23	c	903	CLA	MG-NA	7.39	2.23	2.06
23	c	914	CLA	MG-ND	7.34	2.20	2.05
23	c	910	CLA	MG-ND	-7.34	1.91	2.05
37	f	101	HEM	C3D-C2D	7.29	1.52	1.36
24	A	408	PHO	C1B-C2B	7.14	1.47	1.39
23	b	610	CLA	MG-NA	7.13	2.23	2.06
23	B	614	CLA	MG-NA	7.13	2.23	2.06
23	B	608	CLA	MG-NA	7.13	2.23	2.06
37	F	101	HEM	C3D-C2D	7.05	1.52	1.36
26	f	102	SQD	C6-S	-6.98	1.67	1.77
24	a	413	PHO	C3B-C4B	6.91	1.48	1.41
23	c	905	CLA	MG-ND	-6.89	1.92	2.05
23	c	910	CLA	OBD-CAD	6.88	1.34	1.22
23	B	604	CLA	MG-NA	6.88	2.22	2.06
24	A	409	PHO	C4D-CHA	6.85	1.49	1.39
23	C	504	CLA	MG-NC	6.84	2.22	2.06
23	B	612	CLA	MG-NA	6.78	2.22	2.06
23	b	612	CLA	MG-NC	6.78	2.22	2.06
24	a	412	PHO	C1D-C2D	6.64	1.46	1.39
23	B	606	CLA	MG-NA	6.63	2.22	2.06
23	c	908	CLA	MG-NA	6.58	2.21	2.06
23	c	908	CLA	MG-NC	6.50	2.21	2.06
23	c	911	CLA	MG-NC	6.50	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	913	CLA	MG-NB	6.46	2.18	2.05
23	c	906	CLA	MG-NA	6.43	2.21	2.06
23	b	612	CLA	CHC-C1C	6.40	1.51	1.38
23	a	410	CLA	MG-NA	6.33	2.21	2.06
23	a	409	CLA	MG-NA	6.33	2.21	2.06
23	c	907	CLA	MG-NB	6.32	2.18	2.05
23	C	508	CLA	MG-NB	6.30	2.18	2.05
23	C	509	CLA	MG-NB	-6.27	1.93	2.05
23	B	615	CLA	MG-NA	6.26	2.21	2.06
23	C	508	CLA	MG-NC	6.24	2.21	2.06
26	f	102	SQD	O47-C7	6.24	1.46	1.33
23	b	605	CLA	MG-NC	6.17	2.20	2.06
23	d	403	CLA	MG-NA	6.13	2.20	2.06
23	c	908	CLA	MG-ND	6.10	2.17	2.05
23	b	613	CLA	MG-NA	6.08	2.20	2.06
23	C	508	CLA	C3C-C2C	6.04	1.49	1.36
37	F	101	HEM	FE-NC	6.02	2.15	1.95
23	b	610	CLA	C3C-C2C	5.99	1.49	1.36
23	B	603	CLA	CHC-C1C	5.98	1.50	1.38
23	b	616	CLA	MG-NA	5.97	2.20	2.06
23	B	613	CLA	CHC-C1C	5.96	1.50	1.38
23	b	610	CLA	CHC-C1C	5.93	1.50	1.38
23	c	909	CLA	MG-NC	5.91	2.20	2.06
23	B	611	CLA	MG-NA	5.91	2.20	2.06
37	v	201	HEM	FE-ND	5.91	2.13	1.94
23	b	619	CLA	CHC-C1C	5.90	1.50	1.38
24	A	409	PHO	C3B-C2B	5.90	1.48	1.40
23	B	615	CLA	MG-NC	5.88	2.20	2.06
23	c	905	CLA	C3C-C2C	5.88	1.49	1.36
23	b	605	CLA	C3C-C2C	5.86	1.49	1.36
23	C	502	CLA	CHC-C1C	5.85	1.50	1.38
23	B	603	CLA	C3C-C2C	5.85	1.49	1.36
23	D	403	CLA	MG-NC	5.85	2.20	2.06
37	F	101	HEM	FE-NA	5.83	2.14	1.95
23	b	619	CLA	MG-NA	5.79	2.20	2.06
37	V	201	HEM	C3D-C2D	5.76	1.49	1.36
24	a	413	PHO	C4D-CHA	5.75	1.48	1.39
23	C	509	CLA	CHD-C1D	5.75	1.49	1.38
23	c	913	CLA	C3C-C2C	5.75	1.49	1.36
23	B	609	CLA	MG-NB	-5.73	1.94	2.05
23	b	606	CLA	MG-NA	5.71	2.19	2.06
23	b	610	CLA	MG-NC	5.68	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	CHC-C1C	5.60	1.49	1.38
23	b	612	CLA	O2D-CGD	5.59	1.47	1.33
23	b	604	CLA	MG-NA	5.59	2.19	2.06
23	b	608	CLA	C1D-ND	-5.57	1.30	1.37
23	b	613	CLA	C3C-C2C	5.56	1.48	1.36
23	c	909	CLA	O2D-CGD	5.55	1.46	1.33
23	c	912	CLA	CHD-C1D	5.53	1.49	1.38
23	C	513	CLA	C3C-C2C	5.52	1.48	1.36
24	A	408	PHO	C4D-CHA	5.51	1.47	1.39
23	B	602	CLA	O2A-CGA	5.50	1.49	1.33
23	c	914	CLA	CHC-C1C	5.46	1.49	1.38
23	c	905	CLA	MG-NC	5.45	2.19	2.06
23	b	615	CLA	C3C-C2C	5.45	1.48	1.36
23	c	908	CLA	C3C-C2C	5.44	1.48	1.36
23	B	607	CLA	CHC-C1C	5.44	1.49	1.38
23	b	617	CLA	MG-NA	5.43	2.19	2.06
23	c	907	CLA	O2D-CGD	5.41	1.46	1.33
23	A	405	CLA	CHC-C1C	5.40	1.49	1.38
23	c	904	CLA	C3C-C2C	5.40	1.48	1.36
23	c	913	CLA	O2D-CGD	5.39	1.46	1.33
23	B	611	CLA	CHD-C1D	5.38	1.48	1.38
23	B	613	CLA	C4B-NB	-5.34	1.30	1.37
23	b	609	CLA	MG-NC	5.34	2.18	2.06
23	d	402	CLA	MG-NB	-5.34	1.95	2.05
23	B	604	CLA	CHD-C1D	5.32	1.48	1.38
24	A	408	PHO	C3B-C2B	5.32	1.47	1.40
23	b	612	CLA	C3C-C2C	5.32	1.48	1.36
23	A	405	CLA	MG-NA	5.32	2.18	2.06
23	d	403	CLA	C3C-C2C	5.30	1.48	1.36
23	a	410	CLA	CHC-C1C	5.29	1.49	1.38
23	b	606	CLA	CHC-C1C	5.29	1.49	1.38
23	d	402	CLA	CHD-C1D	5.29	1.48	1.38
23	C	512	CLA	C3C-C2C	5.28	1.48	1.36
23	C	505	CLA	CHD-C1D	5.28	1.48	1.38
23	A	410	CLA	MG-NB	-5.25	1.95	2.05
23	b	607	CLA	CHC-C1C	5.24	1.49	1.38
23	b	604	CLA	O2D-CGD	5.23	1.46	1.33
23	C	507	CLA	C3C-C2C	5.23	1.48	1.36
23	B	615	CLA	C1C-NC	-5.23	1.29	1.37
23	c	913	CLA	MG-NC	5.22	2.18	2.06
23	B	606	CLA	CHC-C1C	5.21	1.48	1.38
23	c	914	CLA	CHD-C1D	5.21	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C3C-C2C	5.20	1.48	1.36
23	C	505	CLA	MG-NA	5.20	2.18	2.06
23	D	402	CLA	C1D-ND	-5.19	1.31	1.37
23	b	606	CLA	C3C-C2C	5.19	1.48	1.36
24	a	412	PHO	C4D-CHA	5.19	1.47	1.39
23	D	403	CLA	MG-NB	-5.19	1.95	2.05
23	B	606	CLA	C3C-C2C	5.19	1.48	1.36
23	c	914	CLA	C3C-C2C	5.18	1.47	1.36
23	d	402	CLA	CHC-C1C	5.18	1.48	1.38
23	C	501	CLA	CHC-C1C	5.17	1.48	1.38
34	D	406	DGD	O2G-C1B	5.17	1.48	1.34
23	C	508	CLA	CHC-C1C	5.14	1.48	1.38
23	D	403	CLA	CHB-C1B	5.14	1.50	1.39
27	Z	101	LMG	O7-C10	5.13	1.48	1.34
26	D	407	SQD	O47-C7	5.12	1.48	1.34
37	f	101	HEM	FE-NB	5.12	2.10	1.94
34	d	406	DGD	O1G-C1A	5.11	1.48	1.33
23	C	510	CLA	C3C-C2C	5.11	1.47	1.36
23	c	909	CLA	CHD-C1D	5.10	1.48	1.38
23	B	611	CLA	CHC-C1C	5.10	1.48	1.38
23	c	914	CLA	O2D-CGD	5.10	1.45	1.33
23	c	913	CLA	CHC-C1C	5.10	1.48	1.38
23	b	604	CLA	O2A-CGA	5.10	1.48	1.33
23	b	613	CLA	O2D-CGD	5.09	1.45	1.33
23	C	504	CLA	MG-NA	5.09	2.18	2.06
23	c	909	CLA	C3C-C2C	5.09	1.47	1.36
23	b	612	CLA	CHD-C1D	5.09	1.48	1.38
23	B	617	CLA	C3C-C2C	5.09	1.47	1.36
23	C	511	CLA	CHB-C1B	5.08	1.50	1.39
23	C	512	CLA	CHC-C1C	5.08	1.48	1.38
23	b	614	CLA	CHD-C1D	5.07	1.48	1.38
23	C	502	CLA	MG-NA	5.06	2.18	2.06
23	b	605	CLA	CHC-C1C	5.05	1.48	1.38
23	b	608	CLA	MG-NA	5.05	2.18	2.06
23	a	414	CLA	MG-NA	5.04	2.18	2.06
23	b	606	CLA	C1D-ND	-5.04	1.31	1.37
26	A	418	SQD	O48-C23	5.04	1.48	1.33
26	a	401	SQD	O47-C7	5.03	1.48	1.34
23	c	911	CLA	O2D-CGD	5.03	1.45	1.33
23	C	508	CLA	O2D-CGD	5.02	1.45	1.33
23	d	402	CLA	MG-NA	5.02	2.18	2.06
24	a	413	PHO	C3D-C4D	-5.02	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	907	CLA	MG-NA	5.02	2.18	2.06
23	C	505	CLA	C3C-C2C	5.02	1.47	1.36
23	A	406	CLA	OBD-CAD	5.01	1.31	1.22
23	c	912	CLA	O2D-CGD	5.01	1.45	1.33
37	V	201	HEM	FE-ND	5.00	2.10	1.94
23	b	605	CLA	OBD-CAD	5.00	1.31	1.22
23	C	502	CLA	O2D-CGD	5.00	1.45	1.33
23	A	410	CLA	CHC-C1C	5.00	1.48	1.38
23	B	602	CLA	O2D-CGD	4.99	1.45	1.33
23	b	616	CLA	O2D-CGD	4.99	1.45	1.33
23	c	903	CLA	O2D-CGD	4.99	1.45	1.33
23	B	610	CLA	CHC-C1C	4.99	1.48	1.38
23	b	607	CLA	C3C-C2C	4.99	1.47	1.36
23	C	503	CLA	CHC-C1C	4.99	1.48	1.38
24	A	409	PHO	OBD-CAD	4.98	1.28	1.22
23	d	403	CLA	MG-NC	4.98	2.18	2.06
23	c	904	CLA	CHC-C1C	4.98	1.48	1.38
23	C	513	CLA	MG-NC	4.98	2.18	2.06
23	C	511	CLA	O2D-CGD	4.97	1.45	1.33
27	c	921	LMG	O7-C10	4.97	1.48	1.34
23	B	607	CLA	C3C-C2C	4.96	1.47	1.36
23	B	614	CLA	CHC-C1C	4.96	1.48	1.38
23	C	504	CLA	CHD-C4C	4.96	1.50	1.39
23	b	608	CLA	CHC-C1C	4.95	1.48	1.38
23	c	913	CLA	CHD-C1D	4.95	1.48	1.38
23	b	608	CLA	O2D-CGD	4.95	1.45	1.33
23	B	610	CLA	MG-NA	4.94	2.18	2.06
23	C	507	CLA	CHD-C1D	4.92	1.48	1.38
23	b	618	CLA	C3C-C2C	4.91	1.47	1.36
23	D	403	CLA	CHC-C1C	4.91	1.48	1.38
23	b	605	CLA	C1D-ND	-4.90	1.31	1.37
23	B	617	CLA	CHC-C1C	4.90	1.48	1.38
23	B	603	CLA	CHD-C1D	4.89	1.48	1.38
24	a	413	PHO	C3D-C2D	4.88	1.48	1.39
26	L	103	SQD	O47-C7	4.86	1.48	1.34
23	c	910	CLA	O2D-CGD	4.86	1.45	1.33
23	B	615	CLA	CHD-C1D	4.85	1.47	1.38
24	a	412	PHO	C3D-C2D	4.85	1.47	1.39
23	B	607	CLA	O2D-CGD	4.85	1.45	1.33
26	B	621	SQD	O47-C7	4.85	1.48	1.34
23	c	908	CLA	CHC-C1C	4.85	1.48	1.38
23	C	506	CLA	CHB-C1B	4.85	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	CLA	OBD-CAD	4.84	1.30	1.22
23	D	402	CLA	MG-NA	4.84	2.17	2.06
23	a	414	CLA	CHC-C1C	4.84	1.48	1.38
23	B	616	CLA	C3C-C2C	4.84	1.47	1.36
23	b	616	CLA	CHC-C1C	4.82	1.48	1.38
23	C	505	CLA	O2D-CGD	4.82	1.45	1.33
23	B	606	CLA	MG-NC	4.82	2.17	2.06
23	C	509	CLA	O2D-CGD	4.81	1.45	1.33
23	b	614	CLA	CHB-C1B	4.81	1.50	1.39
23	B	614	CLA	C3C-C2C	4.80	1.47	1.36
23	B	605	CLA	CHD-C1D	4.80	1.47	1.38
23	b	604	CLA	CHC-C1C	4.78	1.48	1.38
23	c	907	CLA	C3C-C2C	4.78	1.47	1.36
37	f	101	HEM	FE-NC	4.77	2.10	1.95
23	A	410	CLA	C3C-C2C	4.77	1.47	1.36
23	C	508	CLA	CHB-C1B	4.77	1.50	1.39
23	b	613	CLA	CHD-C1D	4.76	1.47	1.38
23	b	608	CLA	C3C-C2C	4.76	1.47	1.36
23	c	912	CLA	CHB-C1B	4.76	1.50	1.39
23	b	604	CLA	CHC-C4B	4.75	1.50	1.39
23	B	613	CLA	C1B-NB	-4.75	1.31	1.37
23	B	610	CLA	MG-NB	4.75	2.15	2.05
26	f	102	SQD	O48-C23	4.75	1.47	1.33
23	a	410	CLA	C3C-C2C	4.75	1.47	1.36
23	B	610	CLA	C3C-C2C	4.74	1.47	1.36
23	B	606	CLA	O2D-CGD	4.74	1.44	1.33
23	b	617	CLA	CHD-C1D	4.74	1.47	1.38
36	a	417	LHG	O8-C23	4.73	1.47	1.33
23	b	619	CLA	C3C-C2C	4.72	1.47	1.36
24	a	412	PHO	O2D-CGD	4.72	1.44	1.33
23	b	604	CLA	CHD-C1D	4.72	1.47	1.38
23	b	619	CLA	O2D-CGD	4.71	1.44	1.33
23	C	505	CLA	C1D-ND	-4.71	1.31	1.37
23	C	512	CLA	CHD-C1D	4.70	1.47	1.38
23	B	602	CLA	C3C-C2C	4.70	1.46	1.36
23	C	501	CLA	MG-NA	4.69	2.17	2.06
23	c	911	CLA	C3C-C2C	4.69	1.46	1.36
23	b	605	CLA	CHD-C4C	4.68	1.49	1.39
23	C	507	CLA	CHC-C1C	4.68	1.47	1.38
23	A	410	CLA	CHB-C1B	4.68	1.49	1.39
23	A	410	CLA	CHD-C1D	4.68	1.47	1.38
23	B	610	CLA	C1D-ND	-4.67	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	414	CLA	CHB-C1B	4.67	1.49	1.39
23	C	513	CLA	CHD-C1D	4.67	1.47	1.38
23	C	512	CLA	O2D-CGD	4.67	1.44	1.33
24	a	412	PHO	C3B-C4B	4.67	1.46	1.41
27	B	622	LMG	O8-C28	4.66	1.46	1.33
23	B	603	CLA	CHB-C1B	4.66	1.49	1.39
36	a	417	LHG	O7-C7	4.66	1.47	1.34
23	A	407	CLA	CHC-C1C	4.65	1.47	1.38
23	C	513	CLA	CHC-C1C	4.65	1.47	1.38
23	b	609	CLA	C3C-C2C	4.65	1.46	1.36
23	B	616	CLA	C1B-NB	-4.65	1.31	1.37
23	c	906	CLA	CHC-C1C	4.64	1.47	1.38
34	D	406	DGD	O1G-C1A	4.64	1.46	1.33
23	c	903	CLA	OBD-CAD	4.64	1.30	1.22
26	a	401	SQD	O48-C23	4.64	1.46	1.33
23	D	403	CLA	C3C-C2C	4.64	1.46	1.36
23	A	410	CLA	CHC-C4B	4.63	1.49	1.39
23	b	619	CLA	C1D-ND	-4.63	1.31	1.37
23	C	513	CLA	O2D-CGD	4.63	1.44	1.33
23	B	608	CLA	CHC-C1C	4.62	1.47	1.38
23	a	409	CLA	C3C-C2C	4.62	1.46	1.36
27	c	920	LMG	O8-C28	4.62	1.46	1.33
34	H	102	DGD	O5D-C1E	4.61	1.47	1.40
23	C	506	CLA	O2D-CGD	4.61	1.44	1.33
23	d	402	CLA	O2A-CGA	4.60	1.46	1.33
23	c	904	CLA	CHD-C1D	4.60	1.47	1.38
23	c	906	CLA	CHD-C4C	4.60	1.49	1.39
23	C	505	CLA	C1B-NB	-4.60	1.31	1.37
24	A	409	PHO	C3B-C4B	4.59	1.46	1.41
23	b	613	CLA	MG-ND	-4.59	1.96	2.05
23	c	904	CLA	CHB-C1B	4.59	1.49	1.39
23	B	615	CLA	C1B-NB	-4.58	1.31	1.37
23	b	618	CLA	OBD-CAD	4.58	1.30	1.22
23	c	906	CLA	CHD-C1D	4.57	1.47	1.38
23	b	618	CLA	O2D-CGD	4.57	1.44	1.33
23	A	405	CLA	CHC-C4B	4.57	1.49	1.39
23	C	510	CLA	CHD-C1D	4.56	1.47	1.38
23	B	615	CLA	CHB-C1B	4.56	1.49	1.39
23	A	405	CLA	C3C-C2C	4.56	1.46	1.36
36	E	101	LHG	O8-C23	4.56	1.46	1.33
23	C	501	CLA	CHD-C1D	4.55	1.47	1.38
23	C	509	CLA	CHC-C1C	4.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	CHB-C1B	4.55	1.49	1.39
23	a	414	CLA	C3C-C2C	4.55	1.46	1.36
23	B	608	CLA	C1B-NB	-4.54	1.31	1.37
23	d	403	CLA	CHD-C1D	4.54	1.47	1.38
23	b	606	CLA	O2D-CGD	4.53	1.44	1.33
23	b	604	CLA	C3C-C2C	4.52	1.46	1.36
23	C	501	CLA	MG-NB	4.52	2.14	2.05
23	b	618	CLA	CHD-C4C	4.52	1.49	1.39
23	C	512	CLA	CHB-C1B	4.51	1.49	1.39
23	c	902	CLA	CHB-C1B	4.51	1.49	1.39
23	c	905	CLA	O2D-CGD	4.50	1.44	1.33
27	A	413	LMG	O7-C10	4.50	1.47	1.34
23	A	407	CLA	C4B-NB	-4.50	1.31	1.37
27	c	921	LMG	O8-C28	4.49	1.46	1.33
23	b	610	CLA	CHD-C1D	4.49	1.47	1.38
23	C	508	CLA	CHD-C1D	4.49	1.47	1.38
23	c	909	CLA	CHC-C1C	4.48	1.47	1.38
23	B	603	CLA	C1B-C2B	4.47	1.53	1.43
23	B	609	CLA	CHD-C1D	4.47	1.47	1.38
27	c	920	LMG	O7-C10	4.47	1.46	1.34
23	B	606	CLA	CHB-C1B	4.47	1.49	1.39
23	C	506	CLA	CHC-C1C	4.46	1.47	1.38
23	c	903	CLA	CHB-C1B	4.46	1.49	1.39
23	c	914	CLA	O2A-CGA	4.46	1.46	1.33
23	a	411	CLA	CHC-C1C	4.46	1.47	1.38
23	c	910	CLA	CHD-C1D	4.46	1.47	1.38
23	b	609	CLA	CHD-C1D	4.45	1.47	1.38
26	D	407	SQD	O48-C23	4.45	1.46	1.33
23	B	609	CLA	O2D-CGD	4.45	1.44	1.33
23	b	614	CLA	O2D-CGD	4.45	1.44	1.33
23	c	912	CLA	C3C-C2C	4.45	1.46	1.36
23	c	914	CLA	CHB-C1B	4.45	1.49	1.39
23	A	406	CLA	CHC-C1C	4.44	1.47	1.38
23	c	911	CLA	MG-NA	4.44	2.16	2.06
23	C	509	CLA	C3C-C2C	4.43	1.46	1.36
23	B	604	CLA	CHB-C1B	4.43	1.49	1.39
23	b	612	CLA	MG-NB	4.43	2.14	2.05
23	B	602	CLA	CHD-C1D	4.42	1.47	1.38
27	C	519	LMG	O8-C28	4.42	1.46	1.33
23	b	611	CLA	C4B-NB	-4.42	1.32	1.37
23	d	403	CLA	MG-NB	-4.41	1.97	2.05
23	c	902	CLA	CHD-C1D	4.40	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	CHC-C1C	4.40	1.47	1.38
27	Z	101	LMG	O8-C28	4.40	1.46	1.33
23	B	608	CLA	CHD-C1D	4.40	1.47	1.38
23	b	617	CLA	O2A-CGA	4.39	1.46	1.33
23	B	608	CLA	C3C-C2C	4.39	1.46	1.36
34	d	406	DGD	O2G-C1B	4.39	1.46	1.34
23	c	903	CLA	CHD-C1D	4.39	1.47	1.38
23	A	406	CLA	C4B-NB	-4.39	1.32	1.37
23	A	407	CLA	C3C-C2C	4.38	1.46	1.36
23	C	506	CLA	O2A-CGA	4.38	1.46	1.33
23	c	913	CLA	O2A-CGA	4.37	1.46	1.33
23	A	406	CLA	C1D-ND	-4.37	1.32	1.37
23	b	607	CLA	MG-ND	-4.37	1.97	2.05
23	c	905	CLA	CHB-C1B	4.36	1.49	1.39
23	b	609	CLA	O2D-CGD	4.36	1.43	1.33
23	C	510	CLA	O2D-CGD	4.35	1.43	1.33
23	d	402	CLA	C3C-C2C	4.35	1.46	1.36
23	B	608	CLA	MG-NC	4.35	2.16	2.06
27	a	418	LMG	O7-C10	4.35	1.46	1.34
23	B	603	CLA	MG-NB	4.35	2.14	2.05
23	c	912	CLA	OBD-CAD	4.34	1.30	1.22
23	b	614	CLA	CHC-C1C	4.34	1.47	1.38
23	B	608	CLA	CHB-C1B	4.34	1.49	1.39
23	b	616	CLA	C3C-C2C	4.33	1.46	1.36
23	C	503	CLA	MG-NA	4.33	2.16	2.06
37	v	201	HEM	CAB-C3B	4.33	1.58	1.47
23	B	616	CLA	CHD-C1D	4.33	1.46	1.38
23	B	609	CLA	C3C-C2C	4.32	1.46	1.36
23	D	403	CLA	CHD-C1D	4.31	1.46	1.38
36	E	101	LHG	O7-C7	4.31	1.46	1.34
23	C	504	CLA	C3C-C2C	4.31	1.46	1.36
23	B	616	CLA	CHD-C4C	4.31	1.49	1.39
23	A	407	CLA	C1B-NB	-4.31	1.32	1.37
23	B	616	CLA	O2D-CGD	4.30	1.43	1.33
23	C	503	CLA	O2A-CGA	4.30	1.45	1.33
23	c	913	CLA	CHC-C4B	4.30	1.49	1.39
23	c	911	CLA	CHC-C1C	4.30	1.47	1.38
23	b	619	CLA	CHD-C1D	4.30	1.46	1.38
23	A	405	CLA	CHD-C4C	4.30	1.49	1.39
23	A	407	CLA	CHD-C1D	4.29	1.46	1.38
23	B	602	CLA	CHC-C1C	4.29	1.47	1.38
23	c	902	CLA	C3C-C2C	4.27	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	619	CLA	O2A-CGA	4.27	1.45	1.33
23	b	611	CLA	CHC-C1C	4.27	1.47	1.38
23	D	402	CLA	O2A-CGA	4.27	1.45	1.33
23	b	617	CLA	CHB-C1B	4.27	1.49	1.39
23	b	605	CLA	CHD-C1D	4.27	1.46	1.38
23	c	904	CLA	O2D-CGD	4.26	1.43	1.33
23	B	605	CLA	C3C-C2C	4.26	1.46	1.36
26	A	418	SQD	O47-C7	4.26	1.46	1.34
24	a	413	PHO	C3B-C2B	4.26	1.46	1.40
23	a	410	CLA	CHD-C1D	4.25	1.46	1.38
23	B	602	CLA	CHC-C4B	4.25	1.48	1.39
23	A	406	CLA	CHC-C4B	4.25	1.48	1.39
23	B	613	CLA	C3C-C2C	4.25	1.45	1.36
23	A	405	CLA	O2D-CGD	4.25	1.43	1.33
23	C	502	CLA	CHD-C1D	4.24	1.46	1.38
23	c	905	CLA	CHD-C1D	4.24	1.46	1.38
23	C	504	CLA	CHC-C1C	4.24	1.47	1.38
23	C	501	CLA	CHC-C4B	4.24	1.48	1.39
23	a	411	CLA	C3C-C2C	4.24	1.45	1.36
23	C	510	CLA	MG-ND	-4.24	1.97	2.05
23	C	502	CLA	C3C-C2C	4.23	1.45	1.36
23	B	611	CLA	CHC-C4B	4.23	1.48	1.39
27	A	413	LMG	O8-C28	4.23	1.45	1.33
24	a	413	PHO	O2D-CGD	4.23	1.43	1.33
23	A	406	CLA	C3C-C2C	4.23	1.45	1.36
23	C	511	CLA	C3C-C2C	4.23	1.45	1.36
23	b	604	CLA	CHB-C1B	4.22	1.48	1.39
23	b	616	CLA	O2A-CGA	4.22	1.45	1.33
24	A	408	PHO	CBD-CGD	-4.22	1.47	1.52
23	D	402	CLA	C4C-C3C	4.22	1.52	1.45
23	a	409	CLA	C4B-NB	-4.22	1.32	1.37
23	b	615	CLA	CHC-C1C	4.21	1.46	1.38
23	b	611	CLA	C3C-C2C	4.20	1.45	1.36
23	B	613	CLA	CHD-C4C	4.20	1.48	1.39
23	B	606	CLA	CHD-C1D	4.20	1.46	1.38
23	c	908	CLA	CHC-C4B	4.19	1.48	1.39
23	c	908	CLA	CHB-C1B	4.19	1.48	1.39
23	C	513	CLA	MG-NB	4.19	2.14	2.05
23	B	605	CLA	CHB-C1B	4.18	1.48	1.39
23	c	913	CLA	CHB-C1B	4.18	1.48	1.39
23	c	910	CLA	C3C-C2C	4.17	1.45	1.36
23	B	612	CLA	CHD-C1D	4.17	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	PHO	C3D-C4D	-4.17	1.35	1.41
23	B	611	CLA	C3C-C2C	4.16	1.45	1.36
23	B	610	CLA	CHC-C4B	4.16	1.48	1.39
23	C	505	CLA	CHC-C1C	4.16	1.46	1.38
23	d	403	CLA	CHC-C1C	4.15	1.46	1.38
23	B	608	CLA	CHD-C4C	4.15	1.48	1.39
23	b	611	CLA	OBD-CAD	4.15	1.29	1.22
23	a	411	CLA	MG-NA	4.14	2.16	2.06
23	d	403	CLA	O2A-CGA	4.14	1.45	1.33
23	C	512	CLA	CHD-C4C	4.14	1.48	1.39
23	C	511	CLA	CHD-C4C	4.14	1.48	1.39
23	c	907	CLA	CHD-C4C	4.14	1.48	1.39
23	B	604	CLA	CHC-C1C	4.14	1.46	1.38
23	C	501	CLA	CHD-C4C	4.13	1.48	1.39
23	C	504	CLA	CHB-C1B	4.13	1.48	1.39
23	C	509	CLA	OBD-CAD	4.13	1.29	1.22
23	c	902	CLA	CHC-C1C	4.13	1.46	1.38
23	c	914	CLA	CHD-C4C	4.12	1.48	1.39
23	B	614	CLA	CHB-C1B	4.11	1.48	1.39
23	C	509	CLA	O2A-CGA	4.11	1.45	1.33
34	c	918	DGD	O1G-C1A	4.11	1.45	1.33
23	b	615	CLA	C1B-C2B	4.10	1.52	1.43
23	c	912	CLA	CHD-C4C	4.10	1.48	1.39
24	a	412	PHO	C3B-C2B	4.09	1.45	1.40
23	c	906	CLA	CHB-C1B	4.09	1.48	1.39
23	B	604	CLA	C3C-C2C	4.08	1.45	1.36
34	h	102	DGD	O5D-C1E	4.08	1.47	1.40
23	d	402	CLA	CHC-C4B	4.07	1.48	1.39
23	C	511	CLA	CHD-C1D	4.06	1.46	1.38
24	a	413	PHO	C3A-C2A	-4.06	1.51	1.54
23	C	501	CLA	C3C-C2C	4.06	1.45	1.36
23	b	609	CLA	CHC-C1C	4.06	1.46	1.38
23	C	505	CLA	MG-NB	4.06	2.13	2.05
23	c	906	CLA	C3C-C2C	4.05	1.45	1.36
23	C	506	CLA	C3C-C2C	4.05	1.45	1.36
23	b	610	CLA	O2D-CGD	4.04	1.43	1.33
23	b	613	CLA	CHC-C1C	4.04	1.46	1.38
23	b	604	CLA	CHD-C4C	4.04	1.48	1.39
23	D	402	CLA	O2D-CGD	4.04	1.43	1.33
23	D	403	CLA	O2A-CGA	4.04	1.45	1.33
23	A	405	CLA	CHB-C1B	4.03	1.48	1.39
27	a	418	LMG	O8-C28	4.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	905	CLA	CHC-C1C	4.02	1.46	1.38
23	c	912	CLA	CHC-C1C	4.02	1.46	1.38
24	A	409	PHO	C3D-C2D	4.01	1.46	1.39
27	b	623	LMG	O8-C28	4.01	1.45	1.33
23	b	607	CLA	O2D-CGD	4.01	1.43	1.33
23	b	609	CLA	CHB-C1B	4.00	1.48	1.39
23	c	911	CLA	CHD-C1D	4.00	1.46	1.38
23	c	911	CLA	CHB-C1B	3.99	1.48	1.39
23	c	907	CLA	O2A-CGA	3.99	1.45	1.33
23	C	511	CLA	CHC-C1C	3.99	1.46	1.38
37	V	201	HEM	CMA-C3A	3.99	1.58	1.50
23	b	607	CLA	CHD-C1D	3.99	1.46	1.38
23	b	604	CLA	MG-ND	3.98	2.13	2.05
23	b	605	CLA	CHB-C1B	3.98	1.48	1.39
23	C	505	CLA	CHC-C4B	3.98	1.48	1.39
23	b	612	CLA	MG-NA	3.98	2.15	2.06
23	b	619	CLA	MG-ND	3.98	2.13	2.05
23	C	511	CLA	O2A-CGA	3.98	1.44	1.33
23	C	510	CLA	CHB-C1B	3.98	1.48	1.39
23	B	610	CLA	CHD-C1D	3.97	1.46	1.38
23	c	911	CLA	O2A-CGA	3.96	1.44	1.33
23	a	410	CLA	CHD-C4C	3.96	1.48	1.39
23	b	613	CLA	C4C-C3C	3.95	1.51	1.45
23	b	610	CLA	MG-NB	3.95	2.13	2.05
23	C	513	CLA	CHD-C4C	3.95	1.48	1.39
23	B	614	CLA	MG-ND	3.95	2.13	2.05
23	c	911	CLA	CHD-C4C	3.95	1.48	1.39
23	b	619	CLA	CHB-C1B	3.94	1.48	1.39
23	b	617	CLA	O2D-CGD	3.94	1.42	1.33
23	B	612	CLA	CHC-C1C	3.94	1.46	1.38
23	c	908	CLA	CHD-C4C	3.94	1.48	1.39
23	b	615	CLA	O2D-CGD	3.94	1.42	1.33
23	b	617	CLA	CHD-C4C	3.94	1.48	1.39
23	b	613	CLA	OBD-CAD	3.94	1.29	1.22
30	B	623	LMT	O6B-C6B	3.94	1.59	1.42
23	C	507	CLA	O2D-CGD	3.93	1.42	1.33
23	b	619	CLA	CHC-C4B	3.93	1.48	1.39
26	A	412	SQD	O47-C7	3.93	1.45	1.34
23	a	409	CLA	MG-NB	-3.93	1.98	2.05
23	c	908	CLA	CHD-C1D	3.93	1.46	1.38
23	b	614	CLA	C3C-C2C	3.92	1.45	1.36
23	C	503	CLA	CHC-C4B	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	912	CLA	MG-NC	3.91	2.15	2.06
23	b	611	CLA	CHB-C1B	3.91	1.48	1.39
23	A	410	CLA	MG-NA	3.91	2.15	2.06
23	c	912	CLA	O2A-CGA	3.90	1.44	1.33
23	C	507	CLA	CHC-C4B	3.90	1.48	1.39
28	D	405	PL9	C21-C19	3.90	1.59	1.51
23	C	504	CLA	C4B-NB	-3.90	1.32	1.37
23	d	403	CLA	CHC-C4B	3.90	1.48	1.39
23	C	503	CLA	CHD-C4C	3.89	1.48	1.39
23	C	507	CLA	MG-ND	3.88	2.13	2.05
23	B	602	CLA	MG-NB	3.87	2.13	2.05
23	C	508	CLA	CHD-C4C	3.87	1.48	1.39
23	c	909	CLA	C4C-C3C	3.87	1.51	1.45
23	A	405	CLA	MG-ND	-3.87	1.98	2.05
23	C	506	CLA	CHC-C4B	3.87	1.48	1.39
23	C	506	CLA	CHD-C1D	3.86	1.46	1.38
23	c	914	CLA	OBD-CAD	3.86	1.29	1.22
23	B	617	CLA	C1D-ND	-3.85	1.32	1.37
27	C	519	LMG	O7-C10	3.85	1.45	1.34
23	a	409	CLA	O2D-CGD	3.85	1.42	1.33
23	C	503	CLA	CHD-C1D	3.85	1.45	1.38
23	b	618	CLA	CHC-C1C	3.85	1.46	1.38
23	b	617	CLA	CHC-C4B	3.84	1.48	1.39
23	B	609	CLA	CHD-C4C	3.84	1.48	1.39
37	V	201	HEM	CMB-C2B	3.84	1.58	1.50
23	c	902	CLA	O2A-CGA	3.84	1.44	1.33
23	B	603	CLA	MG-NC	3.84	2.15	2.06
27	d	410	LMG	O7-C10	3.83	1.45	1.34
37	V	201	HEM	CAB-C3B	3.83	1.57	1.47
23	C	507	CLA	CHD-C4C	3.83	1.47	1.39
23	b	613	CLA	CHD-C4C	3.83	1.47	1.39
23	A	407	CLA	OBD-CAD	3.83	1.29	1.22
23	C	502	CLA	CHB-C1B	3.83	1.48	1.39
26	L	103	SQD	O48-C23	3.82	1.44	1.33
23	C	512	CLA	O2A-CGA	3.82	1.44	1.33
23	c	904	CLA	CHC-C4B	3.82	1.48	1.39
23	b	610	CLA	C3D-C2D	3.82	1.49	1.39
23	b	609	CLA	CHD-C4C	3.82	1.47	1.39
23	B	615	CLA	C3C-C2C	3.82	1.45	1.36
23	c	902	CLA	O2D-CGD	3.82	1.42	1.33
23	c	908	CLA	C4B-NB	-3.81	1.32	1.37
23	c	903	CLA	CHC-C1C	3.81	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	CHB-C1B	3.81	1.48	1.39
26	a	416	SQD	O47-C7	3.81	1.45	1.34
23	B	616	CLA	O2A-CGA	3.81	1.44	1.33
23	B	603	CLA	CHD-C4C	3.81	1.47	1.39
34	C	517	DGD	O1G-C1A	3.81	1.44	1.33
23	c	905	CLA	C1B-NB	-3.80	1.32	1.37
27	D	411	LMG	O7-C10	3.80	1.45	1.34
24	A	409	PHO	O2D-CGD	3.79	1.42	1.33
23	b	607	CLA	CHB-C1B	3.79	1.47	1.39
23	B	613	CLA	CHB-C1B	3.79	1.47	1.39
26	B	621	SQD	O48-C23	3.78	1.44	1.33
23	C	503	CLA	O2D-CGD	3.78	1.42	1.33
23	c	909	CLA	CHB-C1B	3.77	1.47	1.39
23	C	510	CLA	OBD-CAD	3.77	1.29	1.22
23	b	611	CLA	CHD-C1D	3.77	1.45	1.38
23	c	914	CLA	CHC-C4B	3.77	1.47	1.39
23	b	611	CLA	CHD-C4C	3.76	1.47	1.39
23	a	414	CLA	C1D-ND	-3.76	1.32	1.37
23	c	912	CLA	MG-ND	3.75	2.13	2.05
23	C	508	CLA	CHC-C4B	3.75	1.47	1.39
23	C	509	CLA	C4B-NB	-3.75	1.32	1.37
23	C	505	CLA	CHB-C1B	3.75	1.47	1.39
23	C	513	CLA	CHC-C4B	3.75	1.47	1.39
23	c	910	CLA	CHC-C1C	3.75	1.46	1.38
23	d	403	CLA	C4C-C3C	3.74	1.51	1.45
23	C	508	CLA	C4C-C3C	3.74	1.51	1.45
30	A	419	LMT	O1'-C1'	3.73	1.46	1.40
23	B	615	CLA	O2D-CGD	3.73	1.42	1.33
23	c	904	CLA	CHD-C4C	3.73	1.47	1.39
23	C	507	CLA	CHB-C1B	3.72	1.47	1.39
23	b	610	CLA	C1D-ND	-3.71	1.33	1.37
23	b	610	CLA	MG-ND	3.71	2.13	2.05
23	A	406	CLA	MG-NA	3.70	2.15	2.06
23	B	612	CLA	C3C-C2C	3.70	1.44	1.36
23	B	604	CLA	O2D-CGD	3.70	1.42	1.33
23	c	910	CLA	O2A-CGA	3.70	1.44	1.33
23	b	606	CLA	CHD-C1D	3.70	1.45	1.38
23	a	414	CLA	O2A-CGA	3.70	1.44	1.33
23	B	607	CLA	CHB-C1B	3.69	1.47	1.39
23	B	613	CLA	C1D-ND	-3.69	1.33	1.37
23	B	605	CLA	CHC-C1C	3.69	1.45	1.38
23	C	510	CLA	O2A-CGA	3.69	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	O2D-CGD	3.69	1.42	1.33
23	C	506	CLA	CHD-C4C	3.69	1.47	1.39
23	b	610	CLA	CHB-C1B	3.68	1.47	1.39
23	c	913	CLA	CHD-C4C	3.68	1.47	1.39
23	b	604	CLA	C3D-C2D	3.68	1.49	1.39
23	c	911	CLA	CHC-C4B	3.68	1.47	1.39
23	b	618	CLA	C3D-C2D	3.68	1.49	1.39
23	a	414	CLA	CHD-C1D	3.67	1.45	1.38
23	b	612	CLA	O2A-CGA	3.67	1.44	1.33
23	C	505	CLA	CHD-C4C	3.67	1.47	1.39
23	B	609	CLA	MG-NA	3.67	2.15	2.06
23	b	617	CLA	CHC-C1C	3.66	1.45	1.38
36	D	410	LHG	O8-C23	3.66	1.44	1.33
26	a	416	SQD	O48-C23	3.66	1.44	1.33
23	B	617	CLA	MG-NA	3.66	2.15	2.06
23	A	410	CLA	OBD-CAD	3.66	1.28	1.22
23	B	607	CLA	CHD-C1D	3.66	1.45	1.38
23	c	909	CLA	CHC-C4B	3.65	1.47	1.39
23	b	613	CLA	CHC-C4B	3.65	1.47	1.39
23	b	609	CLA	CHC-C4B	3.65	1.47	1.39
24	a	412	PHO	OBD-CAD	3.65	1.27	1.22
23	b	611	CLA	CHC-C4B	3.65	1.47	1.39
23	A	410	CLA	C3D-C4D	-3.65	1.36	1.44
23	B	611	CLA	CHB-C1B	3.65	1.47	1.39
23	b	606	CLA	OBD-CAD	3.65	1.28	1.22
24	A	408	PHO	O2A-CGA	3.64	1.44	1.33
23	D	402	CLA	C4B-NB	-3.64	1.33	1.37
23	C	511	CLA	C3D-C2D	3.63	1.48	1.39
23	c	908	CLA	O2A-CGA	3.63	1.43	1.33
23	b	616	CLA	OBD-CAD	3.63	1.28	1.22
23	B	603	CLA	C1D-ND	-3.62	1.33	1.37
23	B	605	CLA	CHD-C4C	3.62	1.47	1.39
33	B	624	HTG	C1'-S1	-3.62	1.76	1.81
23	b	614	CLA	CHD-C4C	3.62	1.47	1.39
23	c	905	CLA	MG-NB	3.62	2.13	2.05
23	c	906	CLA	C1B-NB	-3.62	1.33	1.37
23	D	403	CLA	CHD-C4C	3.62	1.47	1.39
23	B	602	CLA	CHD-C4C	3.61	1.47	1.39
24	A	408	PHO	C3D-C4D	-3.61	1.36	1.41
23	C	504	CLA	CHD-C1D	3.61	1.45	1.38
23	d	403	CLA	CHB-C1B	3.61	1.47	1.39
23	B	617	CLA	O2D-CGD	3.61	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	MG-NC	3.60	2.14	2.06
24	a	412	PHO	C4B-NB	-3.60	1.32	1.38
23	D	402	CLA	CHC-C4B	3.59	1.47	1.39
23	b	615	CLA	CHD-C1D	3.58	1.45	1.38
27	d	410	LMG	O8-C28	3.58	1.43	1.33
24	a	413	PHO	O2A-CGA	3.57	1.43	1.33
23	c	906	CLA	O2A-CGA	3.57	1.43	1.33
23	B	613	CLA	CHC-C4B	3.57	1.47	1.39
23	c	910	CLA	CHB-C1B	3.57	1.47	1.39
23	B	614	CLA	CHC-C4B	3.56	1.47	1.39
23	b	614	CLA	O2A-CGA	3.56	1.43	1.33
23	C	506	CLA	MG-NB	3.56	2.12	2.05
23	C	512	CLA	C3D-C2D	3.56	1.48	1.39
23	C	504	CLA	O2D-CGD	3.56	1.42	1.33
23	B	602	CLA	CHB-C1B	3.55	1.47	1.39
23	c	902	CLA	CHD-C4C	3.55	1.47	1.39
23	b	606	CLA	C1B-NB	-3.55	1.33	1.37
23	c	907	CLA	CHD-C1D	3.55	1.45	1.38
23	c	908	CLA	O2D-CGD	3.55	1.41	1.33
23	c	913	CLA	MG-ND	-3.55	1.98	2.05
23	B	614	CLA	C3D-C2D	3.54	1.48	1.39
23	B	603	CLA	CHC-C4B	3.54	1.47	1.39
23	b	610	CLA	C1B-C2B	3.54	1.51	1.43
23	B	608	CLA	CHC-C4B	3.54	1.47	1.39
23	d	403	CLA	CHD-C4C	3.54	1.47	1.39
23	b	608	CLA	C1B-NB	-3.53	1.33	1.37
23	c	909	CLA	C3D-C2D	3.53	1.48	1.39
23	c	906	CLA	CHC-C4B	3.53	1.47	1.39
23	a	411	CLA	O2D-CGD	3.53	1.41	1.33
23	B	605	CLA	O2D-CGD	3.53	1.41	1.33
23	B	603	CLA	C4C-C3C	3.53	1.51	1.45
23	b	616	CLA	CHC-C4B	3.53	1.47	1.39
23	c	911	CLA	MG-ND	-3.52	1.98	2.05
23	B	613	CLA	O2D-CGD	3.52	1.41	1.33
23	B	603	CLA	C1B-NB	-3.51	1.33	1.37
23	b	611	CLA	C1B-NB	-3.51	1.33	1.37
34	C	518	DGD	O1G-C1A	3.51	1.43	1.33
23	D	402	CLA	CHD-C4C	3.51	1.47	1.39
23	b	617	CLA	C3C-C2C	3.51	1.44	1.36
23	c	906	CLA	C4B-NB	-3.51	1.33	1.37
23	B	616	CLA	CHB-C1B	3.50	1.47	1.39
23	B	613	CLA	MG-NB	3.50	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	907	CLA	CHC-C1C	3.50	1.45	1.38
23	D	402	CLA	C3C-C2C	3.50	1.44	1.36
23	B	615	CLA	C3B-C4B	3.50	1.52	1.42
23	B	604	CLA	O2A-CGA	3.50	1.43	1.33
23	A	405	CLA	CHD-C1D	3.50	1.45	1.38
34	c	919	DGD	O1G-C1A	3.49	1.43	1.33
23	a	414	CLA	CHD-C4C	3.49	1.47	1.39
23	B	609	CLA	O2A-CGA	3.49	1.43	1.33
23	B	617	CLA	C4B-NB	-3.49	1.33	1.37
23	c	914	CLA	C3D-C2D	3.48	1.48	1.39
23	B	612	CLA	C1D-ND	-3.48	1.33	1.37
23	a	414	CLA	O2D-CGD	3.48	1.41	1.33
23	c	910	CLA	MG-NC	3.48	2.14	2.06
23	B	611	CLA	C3D-C2D	3.48	1.48	1.39
23	B	608	CLA	C1D-ND	-3.48	1.33	1.37
34	C	516	DGD	O2G-C1B	3.48	1.44	1.34
23	B	606	CLA	C4B-NB	-3.48	1.33	1.37
37	V	201	HEM	FE-NB	3.47	2.05	1.94
23	B	617	CLA	O2A-CGA	3.47	1.43	1.33
23	b	613	CLA	CHB-C1B	3.47	1.47	1.39
23	b	615	CLA	CHB-C1B	3.47	1.47	1.39
23	B	611	CLA	MG-NC	3.47	2.14	2.06
23	B	609	CLA	CHB-C1B	3.47	1.47	1.39
34	H	102	DGD	O1G-C1A	3.46	1.43	1.33
23	C	513	CLA	C3D-C2D	3.46	1.48	1.39
34	c	917	DGD	O5D-C1E	3.46	1.46	1.40
23	c	911	CLA	OBD-CAD	3.46	1.28	1.22
23	A	407	CLA	O2D-CGD	3.46	1.41	1.33
23	c	903	CLA	C3C-C2C	3.46	1.44	1.36
23	a	414	CLA	MG-NB	-3.45	1.98	2.05
23	C	507	CLA	O2A-CGA	3.45	1.43	1.33
23	c	909	CLA	C1C-NC	-3.45	1.32	1.37
23	c	902	CLA	CHC-C4B	3.45	1.47	1.39
23	b	612	CLA	C3B-C4B	3.44	1.52	1.42
23	B	614	CLA	CHD-C1D	3.44	1.45	1.38
23	c	913	CLA	C4C-C3C	3.44	1.50	1.45
23	c	902	CLA	C4C-C3C	3.43	1.50	1.45
36	D	408	LHG	O8-C23	3.43	1.43	1.33
23	B	617	CLA	CHC-C4B	3.43	1.47	1.39
23	d	402	CLA	C3D-C2D	3.43	1.48	1.39
36	D	409	LHG	O8-C23	3.42	1.43	1.33
23	b	611	CLA	O2D-CGD	3.42	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	908	CLA	C3D-C2D	3.42	1.48	1.39
33	D	414	HTG	C1'-S1	-3.41	1.76	1.81
23	C	505	CLA	C1B-C2B	3.41	1.51	1.43
23	B	611	CLA	O2D-CGD	3.41	1.41	1.33
23	a	414	CLA	OBD-CAD	3.41	1.28	1.22
23	b	612	CLA	OBD-CAD	3.41	1.28	1.22
26	A	412	SQD	O48-C23	3.40	1.43	1.33
36	D	410	LHG	O7-C7	3.40	1.43	1.34
23	c	905	CLA	C3D-C2D	3.40	1.48	1.39
34	C	516	DGD	O1G-C1A	3.40	1.43	1.33
23	C	501	CLA	OBD-CAD	3.40	1.28	1.22
37	v	201	HEM	CAC-C3C	3.39	1.56	1.47
23	b	613	CLA	MG-NC	3.39	2.14	2.06
23	C	507	CLA	C4D-CHA	3.39	1.50	1.38
23	B	616	CLA	OBD-CAD	3.39	1.28	1.22
23	C	513	CLA	O2A-CGA	3.39	1.43	1.33
23	c	909	CLA	MG-NB	3.39	2.12	2.05
23	B	614	CLA	CHD-C4C	3.38	1.46	1.39
23	c	907	CLA	CHB-C1B	3.38	1.47	1.39
23	c	906	CLA	MG-ND	3.38	2.12	2.05
23	C	510	CLA	CHD-C4C	3.38	1.46	1.39
23	B	605	CLA	C1B-NB	-3.37	1.33	1.37
23	b	605	CLA	O2A-CGA	3.37	1.43	1.33
23	B	604	CLA	CHD-C4C	3.36	1.46	1.39
23	a	411	CLA	C3D-C2D	3.36	1.48	1.39
27	b	623	LMG	O7-C10	3.35	1.43	1.34
23	b	604	CLA	C4D-CHA	3.35	1.49	1.38
37	F	101	HEM	CAB-C3B	3.35	1.56	1.47
23	b	612	CLA	C1B-C2B	3.35	1.51	1.43
23	D	402	CLA	C1B-C2B	3.35	1.51	1.43
23	c	903	CLA	O2A-CGA	3.35	1.43	1.33
23	c	913	CLA	C3D-C2D	3.34	1.48	1.39
23	C	509	CLA	CHB-C1B	3.34	1.46	1.39
23	C	510	CLA	MG-NB	3.34	2.12	2.05
23	B	615	CLA	O2A-CGA	3.34	1.43	1.33
23	c	908	CLA	OBD-CAD	3.34	1.28	1.22
34	D	406	DGD	O3G-C1D	3.34	1.45	1.40
23	C	501	CLA	O2D-CGD	3.34	1.41	1.33
23	D	402	CLA	CHC-C1C	3.33	1.45	1.38
23	B	604	CLA	C3D-C2D	3.33	1.48	1.39
23	a	409	CLA	CHD-C4C	3.33	1.46	1.39
23	B	617	CLA	CHB-C1B	3.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C1B-C2B	3.33	1.50	1.43
23	C	508	CLA	C3D-C2D	3.33	1.48	1.39
23	C	509	CLA	CHC-C4B	3.33	1.46	1.39
23	C	501	CLA	CHB-C1B	3.32	1.46	1.39
30	J	102	LMT	O1'-C1'	3.32	1.45	1.40
23	B	610	CLA	O2A-CGA	3.31	1.43	1.33
23	D	403	CLA	O2D-CGD	3.31	1.41	1.33
23	b	609	CLA	C4D-CHA	3.31	1.49	1.38
33	b	627	HTG	C1'-S1	-3.31	1.76	1.81
34	h	102	DGD	O2G-C1B	3.31	1.43	1.34
23	b	606	CLA	C4B-NB	-3.31	1.33	1.37
23	A	407	CLA	C3D-C2D	3.31	1.48	1.39
23	B	610	CLA	CHB-C1B	3.30	1.46	1.39
24	A	408	PHO	C3B-C4B	3.30	1.44	1.41
23	C	502	CLA	CHC-C4B	3.30	1.46	1.39
23	B	612	CLA	CHD-C4C	3.30	1.46	1.39
23	B	617	CLA	C3D-C2D	3.29	1.48	1.39
23	D	402	CLA	OBD-CAD	3.29	1.28	1.22
23	B	607	CLA	CHD-C4C	3.29	1.46	1.39
23	a	411	CLA	C4D-CHA	3.29	1.49	1.38
23	b	613	CLA	C1B-NB	-3.29	1.33	1.37
23	a	411	CLA	CHB-C1B	3.29	1.46	1.39
34	h	102	DGD	O1G-C1A	3.29	1.42	1.33
23	A	410	CLA	CHD-C4C	3.29	1.46	1.39
23	c	908	CLA	C4D-CHA	3.29	1.49	1.38
23	b	610	CLA	CHC-C4B	3.28	1.46	1.39
23	C	507	CLA	C3D-C2D	3.28	1.47	1.39
23	b	616	CLA	CHD-C1D	3.28	1.44	1.38
23	B	602	CLA	MG-NC	3.28	2.14	2.06
23	C	501	CLA	C3D-C2D	3.27	1.47	1.39
23	B	610	CLA	C4B-NB	-3.26	1.33	1.37
23	A	405	CLA	C1B-NB	-3.26	1.33	1.37
23	b	606	CLA	CHD-C4C	3.26	1.46	1.39
23	B	617	CLA	OBD-CAD	3.26	1.28	1.22
23	b	612	CLA	CHC-C4B	3.26	1.46	1.39
34	C	517	DGD	O2G-C1B	3.26	1.43	1.34
23	b	615	CLA	CHC-C4B	3.25	1.46	1.39
23	c	905	CLA	C4C-C3C	3.25	1.50	1.45
23	C	511	CLA	C4D-CHA	3.24	1.49	1.38
23	B	612	CLA	CHC-C4B	3.24	1.46	1.39
23	b	612	CLA	CHD-C4C	3.23	1.46	1.39
23	C	511	CLA	MG-NB	-3.23	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	C3D-C2D	3.23	1.47	1.39
23	a	410	CLA	C1D-ND	-3.22	1.33	1.37
23	c	914	CLA	C1D-ND	-3.22	1.33	1.37
23	c	905	CLA	C1C-NC	-3.22	1.32	1.37
23	B	611	CLA	O2A-CGA	3.22	1.42	1.33
23	c	905	CLA	O2A-CGA	3.22	1.42	1.33
23	b	610	CLA	C1B-NB	-3.22	1.33	1.37
23	b	606	CLA	CHB-C1B	3.21	1.46	1.39
23	a	410	CLA	CHB-C1B	3.21	1.46	1.39
23	C	506	CLA	C1B-NB	-3.21	1.33	1.37
23	C	505	CLA	C4C-C3C	3.20	1.50	1.45
23	c	904	CLA	O2A-CGA	3.20	1.42	1.33
23	b	617	CLA	MG-ND	-3.20	1.99	2.05
23	A	405	CLA	OBD-CAD	3.20	1.28	1.22
23	b	619	CLA	C4B-NB	-3.20	1.33	1.37
23	B	616	CLA	C4C-C3C	3.20	1.50	1.45
23	b	619	CLA	C3D-C2D	3.19	1.47	1.39
23	a	411	CLA	CHD-C4C	3.19	1.46	1.39
23	c	909	CLA	O2A-CGA	3.18	1.42	1.33
23	c	904	CLA	C4D-CHA	3.17	1.49	1.38
34	c	919	DGD	O2G-C2G	-3.17	1.39	1.46
23	B	616	CLA	C3D-C2D	3.17	1.47	1.39
23	B	616	CLA	C1B-C2B	3.17	1.50	1.43
33	d	401	HTG	C1'-S1	-3.17	1.77	1.81
23	B	604	CLA	C1C-NC	-3.17	1.32	1.37
23	b	607	CLA	CHD-C4C	3.17	1.46	1.39
23	B	602	CLA	OBD-CAD	3.16	1.27	1.22
30	M	101	LMT	O1'-C1'	3.16	1.45	1.40
23	b	612	CLA	C4B-NB	-3.16	1.33	1.37
23	c	903	CLA	CHC-C4B	3.16	1.46	1.39
23	C	505	CLA	C3D-C2D	3.16	1.47	1.39
23	B	607	CLA	C4C-C3C	3.16	1.50	1.45
23	b	615	CLA	O2A-CGA	3.16	1.42	1.33
23	B	602	CLA	C4D-CHA	3.16	1.49	1.38
23	c	905	CLA	CHC-C4B	3.16	1.46	1.39
23	c	912	CLA	C3D-C2D	3.16	1.47	1.39
23	B	604	CLA	OBD-CAD	3.15	1.27	1.22
38	H	101	RRX	C33-C5	3.15	1.56	1.50
23	B	607	CLA	OBD-CAD	3.15	1.27	1.22
37	f	101	HEM	CAB-C3B	3.15	1.55	1.47
23	A	410	CLA	MG-NC	3.15	2.13	2.06
30	a	402	LMT	O1'-C1'	3.15	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	619	CLA	OBD-CAD	3.15	1.27	1.22
23	C	509	CLA	C3D-C2D	3.15	1.47	1.39
23	B	605	CLA	C1B-C2B	3.15	1.50	1.43
23	B	606	CLA	C1B-NB	-3.14	1.33	1.37
23	D	403	CLA	C3D-C2D	3.14	1.47	1.39
37	V	201	HEM	CAC-C3C	3.14	1.55	1.47
23	a	410	CLA	O2A-CGA	3.14	1.42	1.33
34	c	917	DGD	O1G-C1A	3.14	1.42	1.33
27	B	622	LMG	O7-C10	3.14	1.43	1.34
23	c	905	CLA	OBD-CAD	3.14	1.27	1.22
23	A	406	CLA	C3B-C4B	3.13	1.51	1.42
23	B	610	CLA	C1B-C2B	3.13	1.50	1.43
23	C	512	CLA	CHC-C4B	3.13	1.46	1.39
23	D	403	CLA	C1C-NC	-3.13	1.33	1.37
23	c	910	CLA	C3D-C2D	3.13	1.47	1.39
25	b	621	BCR	C5-C6	3.13	1.39	1.34
23	C	501	CLA	O2A-CGA	3.13	1.42	1.33
23	B	606	CLA	O2A-CGA	3.13	1.42	1.33
23	c	903	CLA	CHD-C4C	3.13	1.46	1.39
28	a	419	PL9	C6-C5	3.12	1.50	1.35
36	d	409	LHG	O7-C7	3.12	1.43	1.34
23	b	611	CLA	C1D-ND	-3.12	1.33	1.37
25	a	415	BCR	C8-C9	3.12	1.52	1.46
23	A	410	CLA	O2A-CGA	3.12	1.42	1.33
23	C	512	CLA	C4C-C3C	3.12	1.50	1.45
23	B	608	CLA	O2D-CGD	3.12	1.40	1.33
23	b	618	CLA	CHB-C1B	3.12	1.46	1.39
23	c	902	CLA	OBD-CAD	3.11	1.27	1.22
23	B	607	CLA	CHC-C4B	3.11	1.46	1.39
37	v	201	HEM	FE-NA	3.10	2.05	1.95
23	B	602	CLA	MG-ND	-3.10	1.99	2.05
23	b	614	CLA	C3D-C2D	3.10	1.47	1.39
23	C	512	CLA	C4D-CHA	3.10	1.49	1.38
23	B	608	CLA	MG-ND	3.10	2.11	2.05
23	c	910	CLA	CHC-C4B	3.10	1.46	1.39
23	B	617	CLA	CHD-C4C	3.09	1.46	1.39
23	b	604	CLA	OBD-CAD	3.09	1.27	1.22
23	B	603	CLA	O2D-CGD	3.09	1.40	1.33
28	d	405	PL9	C6-C5	3.09	1.50	1.35
23	A	407	CLA	C3B-C4B	3.08	1.51	1.42
23	B	603	CLA	C3D-C2D	3.08	1.47	1.39
23	b	612	CLA	C3D-C2D	3.08	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	912	CLA	C4D-CHA	3.08	1.48	1.38
23	c	906	CLA	C1B-C2B	3.08	1.50	1.43
23	B	611	CLA	C1C-NC	-3.08	1.33	1.37
23	c	904	CLA	C3D-C2D	3.08	1.47	1.39
23	C	501	CLA	C4D-CHA	3.08	1.48	1.38
36	l	101	LHG	O8-C23	3.08	1.42	1.33
23	B	604	CLA	MG-NB	-3.08	1.99	2.05
23	a	411	CLA	C1D-ND	-3.07	1.33	1.37
23	a	411	CLA	CHC-C4B	3.07	1.46	1.39
23	B	611	CLA	CHD-C4C	3.07	1.46	1.39
23	C	512	CLA	MG-ND	3.07	2.11	2.05
23	b	610	CLA	CHD-C4C	3.06	1.46	1.39
36	d	407	LHG	O8-C23	3.06	1.42	1.33
23	b	608	CLA	C3B-C4B	3.05	1.51	1.42
24	a	412	PHO	CMA-C3A	3.05	1.58	1.53
23	C	501	CLA	MG-ND	3.05	2.11	2.05
23	c	913	CLA	OBD-CAD	3.05	1.27	1.22
23	C	504	CLA	C1D-ND	-3.05	1.33	1.37
23	C	505	CLA	C4B-NB	-3.04	1.33	1.37
23	C	508	CLA	O2A-CGA	3.04	1.42	1.33
23	C	501	CLA	C3B-C4B	3.04	1.51	1.42
23	C	503	CLA	CHB-C1B	3.03	1.46	1.39
23	C	508	CLA	C4B-NB	-3.03	1.33	1.37
23	b	611	CLA	C3B-C4B	3.03	1.51	1.42
23	a	410	CLA	OBD-CAD	3.03	1.27	1.22
23	b	614	CLA	C4D-CHA	3.03	1.48	1.38
23	D	403	CLA	CHC-C4B	3.03	1.46	1.39
23	C	507	CLA	C4B-NB	-3.03	1.33	1.37
23	b	615	CLA	C3D-C2D	3.02	1.47	1.39
23	b	606	CLA	C4D-CHA	3.01	1.48	1.38
23	D	402	CLA	CHD-C1D	3.01	1.44	1.38
28	A	414	PL9	C6-C5	3.01	1.50	1.35
23	b	618	CLA	CHD-C1D	3.01	1.44	1.38
36	d	409	LHG	O8-C23	3.00	1.42	1.33
23	C	502	CLA	O2A-CGA	3.00	1.42	1.33
34	c	918	DGD	O2G-C1B	3.00	1.42	1.34
23	A	406	CLA	CHD-C4C	3.00	1.46	1.39
23	D	403	CLA	OBD-CAD	3.00	1.27	1.22
28	d	405	PL9	C41-C39	2.99	1.57	1.51
23	B	614	CLA	C4C-C3C	2.99	1.50	1.45
23	C	502	CLA	C4B-NB	-2.99	1.33	1.37
23	b	619	CLA	CHD-C4C	2.99	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1C-C2C	2.99	1.50	1.44
23	A	407	CLA	CHD-C4C	2.98	1.46	1.39
23	C	502	CLA	CHD-C4C	2.97	1.46	1.39
23	C	505	CLA	O2A-CGA	2.97	1.42	1.33
23	b	612	CLA	C1D-ND	-2.97	1.34	1.37
23	b	604	CLA	C3B-C4B	2.97	1.51	1.42
23	b	609	CLA	C3D-C2D	2.97	1.47	1.39
23	a	409	CLA	C4D-CHA	2.97	1.48	1.38
23	c	914	CLA	C4D-CHA	2.96	1.48	1.38
23	C	502	CLA	OBD-CAD	2.96	1.27	1.22
23	B	606	CLA	CHD-C4C	2.96	1.45	1.39
23	c	902	CLA	C4D-CHA	2.96	1.48	1.38
23	B	611	CLA	C4D-CHA	2.96	1.48	1.38
23	B	612	CLA	C3D-C2D	2.96	1.47	1.39
23	b	615	CLA	MG-NC	-2.95	1.99	2.06
23	b	604	CLA	MG-NB	-2.95	1.99	2.05
23	b	618	CLA	C4D-CHA	2.95	1.48	1.38
23	b	611	CLA	C4D-CHA	2.95	1.48	1.38
23	C	504	CLA	C3B-C4B	2.95	1.51	1.42
23	B	610	CLA	MG-NC	2.95	2.13	2.06
23	A	405	CLA	MG-NB	2.95	2.11	2.05
23	c	906	CLA	O2D-CGD	2.95	1.40	1.33
23	C	509	CLA	CHD-C4C	2.95	1.45	1.39
23	b	607	CLA	C4B-NB	-2.95	1.34	1.37
23	b	618	CLA	C1B-C2B	2.95	1.50	1.43
28	d	405	PL9	C7-C3	2.95	1.55	1.51
23	a	411	CLA	CHD-C1D	2.95	1.44	1.38
23	B	613	CLA	OBD-CAD	2.95	1.27	1.22
23	c	904	CLA	C4C-C3C	2.95	1.50	1.45
23	C	510	CLA	CHC-C4B	2.95	1.46	1.39
28	D	405	PL9	C6-C5	2.95	1.49	1.35
23	B	613	CLA	CHD-C1D	2.95	1.44	1.38
23	b	610	CLA	C4D-CHA	2.94	1.48	1.38
23	B	608	CLA	C3D-C2D	2.94	1.47	1.39
23	C	509	CLA	C4D-CHA	2.94	1.48	1.38
23	A	406	CLA	C1B-C2B	2.94	1.50	1.43
23	B	610	CLA	C3D-C2D	2.94	1.47	1.39
23	A	406	CLA	O2A-CGA	2.94	1.41	1.33
23	B	607	CLA	O2A-CGA	2.94	1.41	1.33
23	b	606	CLA	C3D-C2D	2.93	1.47	1.39
23	b	615	CLA	C4B-NB	-2.93	1.34	1.37
23	d	402	CLA	C1D-ND	-2.93	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C4D-CHA	2.93	1.48	1.38
23	C	510	CLA	C3D-C2D	2.93	1.47	1.39
23	b	608	CLA	O2A-CGA	2.92	1.41	1.33
37	V	201	HEM	CMC-C2C	2.92	1.56	1.50
23	C	503	CLA	C1B-NB	-2.92	1.34	1.37
23	C	502	CLA	C3D-C2D	2.92	1.47	1.39
23	C	511	CLA	CHC-C4B	2.92	1.46	1.39
23	C	504	CLA	C4D-CHA	2.92	1.48	1.38
36	L	101	LHG	O8-C23	2.91	1.41	1.33
23	C	505	CLA	OBD-CAD	2.91	1.27	1.22
23	a	409	CLA	CHB-C1B	2.91	1.45	1.39
23	c	912	CLA	C3B-C4B	2.91	1.51	1.42
23	b	610	CLA	C3B-C4B	2.90	1.51	1.42
23	c	911	CLA	C4D-CHA	2.90	1.48	1.38
23	a	410	CLA	CHC-C4B	2.90	1.45	1.39
23	D	403	CLA	C4C-C3C	2.90	1.50	1.45
23	B	612	CLA	OBD-CAD	2.90	1.27	1.22
23	b	619	CLA	C1C-C2C	2.90	1.50	1.44
23	B	605	CLA	O2A-CGA	2.89	1.41	1.33
23	c	907	CLA	CHC-C4B	2.89	1.45	1.39
23	b	616	CLA	CHD-C4C	2.89	1.45	1.39
23	a	409	CLA	O2A-CGA	2.89	1.41	1.33
23	c	913	CLA	C4D-CHA	2.89	1.48	1.38
23	c	903	CLA	C4D-CHA	2.89	1.48	1.38
23	c	906	CLA	C3D-C2D	2.88	1.46	1.39
23	b	605	CLA	CHC-C4B	2.88	1.45	1.39
23	b	616	CLA	C1D-ND	-2.88	1.34	1.37
23	C	502	CLA	C4D-CHA	2.88	1.48	1.38
23	C	510	CLA	C1C-NC	-2.88	1.33	1.37
23	b	616	CLA	C3B-C4B	2.88	1.51	1.42
23	b	605	CLA	C1B-NB	-2.88	1.34	1.37
23	B	610	CLA	C1B-NB	-2.87	1.34	1.37
23	a	409	CLA	CHC-C1C	2.87	1.44	1.38
24	A	409	PHO	O2A-CGA	2.87	1.41	1.33
23	b	612	CLA	C4D-CHA	2.87	1.48	1.38
23	C	511	CLA	OBD-CAD	2.87	1.27	1.22
23	a	411	CLA	O2A-CGA	2.86	1.41	1.33
23	c	906	CLA	C4C-C3C	2.86	1.49	1.45
23	b	608	CLA	CHB-C1B	2.86	1.45	1.39
25	a	415	BCR	C26-C25	2.86	1.39	1.34
23	C	510	CLA	C4D-CHA	2.86	1.48	1.38
23	B	616	CLA	CHC-C4B	2.86	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C1B-NB	-2.86	1.34	1.37
23	B	603	CLA	OBD-CAD	2.85	1.27	1.22
26	B	621	SQD	O6-C1	2.85	1.45	1.40
23	c	905	CLA	C4D-CHA	2.85	1.48	1.38
23	a	410	CLA	MG-ND	-2.85	2.00	2.05
23	B	609	CLA	CHC-C1C	2.85	1.44	1.38
24	a	412	PHO	CBD-CGD	-2.84	1.48	1.52
34	H	102	DGD	O2G-C1B	2.84	1.42	1.34
23	c	906	CLA	MG-NB	2.84	2.11	2.05
23	C	503	CLA	C4D-CHA	2.84	1.48	1.38
23	C	506	CLA	C3D-C2D	2.84	1.46	1.39
37	v	201	HEM	FE-NB	2.84	2.03	1.94
23	c	908	CLA	C1D-ND	-2.84	1.34	1.37
23	C	510	CLA	CHC-C1C	2.84	1.44	1.38
23	b	616	CLA	C3D-C2D	2.84	1.46	1.39
23	C	504	CLA	O2A-CGA	2.83	1.41	1.33
23	B	602	CLA	C3B-C4B	2.83	1.51	1.42
36	L	101	LHG	O7-C7	2.83	1.42	1.34
23	b	619	CLA	C4D-CHA	2.83	1.48	1.38
23	B	605	CLA	CHC-C4B	2.82	1.45	1.39
24	A	408	PHO	O2D-CGD	2.82	1.40	1.33
23	b	607	CLA	C3D-C2D	2.82	1.46	1.39
23	D	402	CLA	C3B-C4B	2.82	1.50	1.42
23	c	903	CLA	CBD-CAD	-2.82	1.44	1.56
24	a	412	PHO	C3D-C4D	-2.82	1.37	1.41
23	b	605	CLA	MG-NB	2.81	2.11	2.05
23	C	506	CLA	C4D-CHA	2.81	1.48	1.38
23	c	906	CLA	C4D-CHA	2.81	1.48	1.38
23	B	614	CLA	C1C-NC	-2.81	1.33	1.37
23	B	612	CLA	O2D-CGD	2.81	1.40	1.33
23	C	504	CLA	C1B-NB	-2.80	1.34	1.37
23	c	910	CLA	CHD-C4C	2.80	1.45	1.39
23	C	513	CLA	MG-ND	-2.80	2.00	2.05
23	C	504	CLA	C1C-NC	-2.80	1.33	1.37
23	C	504	CLA	MG-NB	2.80	2.11	2.05
23	d	403	CLA	C4B-NB	-2.80	1.34	1.37
33	B	626	HTG	C1'-S1	-2.80	1.77	1.81
23	B	614	CLA	C4D-CHA	2.80	1.48	1.38
23	b	608	CLA	CHD-C1D	2.80	1.43	1.38
38	H	101	RRX	C5-C6	2.79	1.39	1.34
28	A	414	PL9	C2-C3	2.79	1.41	1.34
23	b	605	CLA	C3B-C4B	2.79	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C3D-C2D	2.78	1.46	1.39
24	A	409	PHO	CBD-CGD	-2.78	1.49	1.52
23	b	604	CLA	C4C-C3C	2.78	1.49	1.45
23	B	617	CLA	C4D-CHA	2.78	1.47	1.38
23	b	608	CLA	OBD-CAD	2.77	1.27	1.22
36	D	409	LHG	O7-C7	2.77	1.42	1.34
23	B	604	CLA	C1B-C2B	2.77	1.49	1.43
23	B	611	CLA	C3B-C4B	2.77	1.50	1.42
33	c	924	HTG	C1'-S1	-2.77	1.77	1.81
23	B	616	CLA	C4B-NB	-2.77	1.34	1.37
23	b	612	CLA	C4C-C3C	2.76	1.49	1.45
27	d	410	LMG	O7-C8	-2.76	1.40	1.46
23	A	410	CLA	C4C-C3C	2.76	1.49	1.45
24	a	413	PHO	OBD-CAD	2.76	1.25	1.22
37	f	101	HEM	CAC-C3C	2.76	1.54	1.47
34	c	918	DGD	O2G-C2G	-2.76	1.40	1.46
23	A	407	CLA	C4D-CHA	2.75	1.47	1.38
38	H	101	RRX	C1-C6	2.75	1.57	1.53
27	D	411	LMG	O8-C28	2.75	1.41	1.33
23	c	911	CLA	MG-NB	-2.74	2.00	2.05
23	D	402	CLA	C4D-CHA	2.74	1.47	1.38
23	c	906	CLA	MG-NC	2.74	2.12	2.06
23	C	503	CLA	C3B-C4B	2.74	1.50	1.42
23	A	405	CLA	C3D-C2D	2.73	1.46	1.39
30	B	623	LMT	O1'-C1'	2.73	1.44	1.40
23	c	911	CLA	C3D-C2D	2.73	1.46	1.39
33	c	923	HTG	C1-S1	-2.73	1.76	1.80
34	c	919	DGD	O2G-C1B	2.73	1.42	1.34
23	A	406	CLA	C1B-NB	-2.73	1.34	1.37
23	b	606	CLA	O2A-CGA	2.73	1.41	1.33
33	B	630	HTG	C1-S1	-2.72	1.76	1.80
23	b	616	CLA	C4D-CHA	2.72	1.47	1.38
23	c	907	CLA	C1C-C2C	2.72	1.50	1.44
30	Z	102	LMT	O1'-C1'	2.72	1.44	1.40
23	a	409	CLA	CHD-C1D	2.72	1.43	1.38
23	b	609	CLA	O2A-CGA	2.72	1.41	1.33
23	C	512	CLA	C1B-C2B	2.72	1.49	1.43
23	c	908	CLA	C1C-C2C	2.72	1.50	1.44
23	b	604	CLA	C1C-C2C	2.71	1.50	1.44
23	B	615	CLA	C3D-C2D	2.71	1.46	1.39
23	b	605	CLA	C4C-C3C	2.71	1.49	1.45
23	c	906	CLA	OBD-CAD	2.71	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C4D-CHA	2.70	1.47	1.38
23	b	613	CLA	C4D-CHA	2.70	1.47	1.38
25	D	404	BCR	C5-C6	2.70	1.39	1.34
25	a	415	BCR	C27-C26	2.70	1.56	1.51
37	v	201	HEM	CMC-C2C	2.69	1.56	1.50
23	C	507	CLA	C4C-C3C	2.69	1.49	1.45
23	C	506	CLA	OBD-CAD	2.69	1.27	1.22
23	C	508	CLA	MG-ND	-2.69	2.00	2.05
23	C	509	CLA	C4C-C3C	2.69	1.49	1.45
23	c	910	CLA	MG-NB	-2.69	2.00	2.05
23	b	608	CLA	CHD-C4C	2.69	1.45	1.39
23	C	508	CLA	C1C-NC	-2.69	1.33	1.37
23	C	513	CLA	OBD-CAD	2.69	1.27	1.22
23	c	909	CLA	C3B-C4B	2.68	1.50	1.42
23	D	402	CLA	CHB-C1B	2.68	1.45	1.39
23	a	410	CLA	C1-C2	2.68	1.56	1.49
23	b	619	CLA	C1C-NC	-2.68	1.33	1.37
23	B	612	CLA	C4D-CHA	2.68	1.47	1.38
23	D	403	CLA	C3D-C4D	-2.67	1.38	1.44
23	C	509	CLA	C1B-NB	-2.67	1.34	1.37
23	B	614	CLA	O2A-CGA	2.66	1.41	1.33
23	C	510	CLA	C4B-NB	-2.66	1.34	1.37
23	b	610	CLA	O2A-CGA	2.66	1.41	1.33
23	b	609	CLA	MG-NB	2.66	2.11	2.05
33	b	601	HTG	C1'-S1	-2.66	1.77	1.81
23	B	609	CLA	C3D-C2D	2.66	1.46	1.39
23	B	606	CLA	C4D-CHA	2.66	1.47	1.38
23	B	611	CLA	OBD-CAD	2.66	1.27	1.22
23	b	618	CLA	MG-NC	2.65	2.12	2.06
23	B	607	CLA	C3D-C2D	2.65	1.46	1.39
23	B	617	CLA	C1B-NB	-2.65	1.34	1.37
23	b	611	CLA	O2A-CGA	2.65	1.41	1.33
23	C	511	CLA	MG-NC	2.65	2.12	2.06
23	c	902	CLA	MG-NB	-2.65	2.00	2.05
37	v	201	HEM	FE-NC	2.64	2.03	1.95
25	D	404	BCR	C30-C25	-2.64	1.50	1.53
23	c	909	CLA	CHD-C4C	2.64	1.45	1.39
23	C	502	CLA	C1C-NC	-2.64	1.33	1.37
23	C	510	CLA	C3D-C4D	-2.64	1.38	1.44
30	b	624	LMT	O1'-C1'	2.64	1.44	1.40
23	B	612	CLA	CBD-CAD	-2.64	1.44	1.56
23	A	405	CLA	C1D-ND	-2.64	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	O2A-CGA	2.64	1.41	1.33
23	C	503	CLA	C1B-C2B	2.64	1.49	1.43
36	d	408	LHG	O7-C7	2.64	1.41	1.34
23	c	910	CLA	C4D-CHA	2.63	1.47	1.38
23	b	607	CLA	C3B-C4B	2.63	1.50	1.42
23	c	905	CLA	CHD-C4C	2.63	1.45	1.39
23	b	609	CLA	OBD-CAD	2.63	1.27	1.22
23	b	607	CLA	C4D-CHA	2.63	1.47	1.38
23	A	407	CLA	CHC-C4B	2.62	1.45	1.39
36	l	101	LHG	O7-C7	2.62	1.41	1.34
23	b	617	CLA	MG-NC	2.62	2.12	2.06
23	b	609	CLA	C3B-C4B	2.62	1.50	1.42
23	A	406	CLA	C4D-CHA	2.62	1.47	1.38
23	b	608	CLA	CHC-C4B	2.62	1.45	1.39
23	B	611	CLA	C3D-C4D	-2.62	1.38	1.44
23	C	503	CLA	C4C-C3C	2.61	1.49	1.45
33	O	303	HTG	O5-C1	2.61	1.46	1.42
30	c	922	LMT	O1'-C1'	2.61	1.44	1.40
23	b	618	CLA	CHC-C4B	2.61	1.45	1.39
23	b	612	CLA	C1B-NB	-2.60	1.34	1.37
23	c	911	CLA	C1B-NB	-2.60	1.34	1.37
23	B	614	CLA	O2D-CGD	2.60	1.39	1.33
23	b	606	CLA	MG-ND	2.60	2.10	2.05
23	C	508	CLA	C4D-CHA	2.60	1.47	1.38
23	B	610	CLA	C4D-CHA	2.60	1.47	1.38
23	a	411	CLA	C4C-C3C	2.60	1.49	1.45
23	a	411	CLA	MG-ND	-2.60	2.00	2.05
23	d	403	CLA	OBD-CAD	2.60	1.27	1.22
33	C	522	HTG	C1'-S1	-2.60	1.77	1.81
23	B	602	CLA	C3D-C2D	2.60	1.46	1.39
23	C	507	CLA	OBD-CAD	2.59	1.26	1.22
23	a	411	CLA	OBD-CAD	2.59	1.26	1.22
23	a	409	CLA	C1B-C2B	2.59	1.49	1.43
23	a	410	CLA	C1B-C2B	2.59	1.49	1.43
23	b	611	CLA	C3D-C2D	2.59	1.46	1.39
23	c	906	CLA	C3B-C4B	2.59	1.50	1.42
23	d	403	CLA	C1B-NB	-2.59	1.34	1.37
23	c	905	CLA	C4B-NB	-2.59	1.34	1.37
24	A	408	PHO	C3D-C2D	2.58	1.44	1.39
23	B	604	CLA	CHC-C4B	2.58	1.45	1.39
33	c	923	HTG	C1'-S1	-2.58	1.77	1.81
23	A	407	CLA	MG-NB	-2.58	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	CLA	CHC-C4B	2.58	1.45	1.39
23	A	407	CLA	O2A-CGA	2.58	1.40	1.33
23	C	507	CLA	C3B-C2B	2.57	1.49	1.41
37	F	101	HEM	CMA-C3A	2.57	1.56	1.50
23	c	914	CLA	MG-NB	-2.57	2.00	2.05
28	D	405	PL9	C41-C39	2.57	1.56	1.51
23	A	407	CLA	C1B-C2B	2.57	1.49	1.43
23	C	504	CLA	CHC-C4B	2.57	1.45	1.39
23	B	615	CLA	CHD-C4C	2.57	1.45	1.39
23	B	606	CLA	C3D-C2D	2.56	1.46	1.39
23	B	606	CLA	C3B-C4B	2.56	1.50	1.42
23	c	913	CLA	C1B-NB	-2.56	1.34	1.37
23	b	614	CLA	C1B-NB	-2.56	1.34	1.37
23	A	410	CLA	C3D-C2D	2.56	1.46	1.39
23	b	605	CLA	C3D-C2D	2.55	1.46	1.39
23	c	903	CLA	C1C-NC	-2.55	1.33	1.37
23	c	914	CLA	C1C-C2C	2.55	1.49	1.44
23	a	414	CLA	C1B-C2B	2.55	1.49	1.43
23	c	908	CLA	C1B-C2B	2.55	1.49	1.43
23	b	618	CLA	C1D-ND	-2.55	1.34	1.37
37	f	101	HEM	CMB-C2B	2.55	1.56	1.50
23	B	605	CLA	MG-ND	2.55	2.10	2.05
23	B	609	CLA	CHC-C4B	2.55	1.45	1.39
23	B	615	CLA	C1B-C2B	2.55	1.49	1.43
23	b	616	CLA	C4C-C3C	2.55	1.49	1.45
28	a	419	PL9	C2-C3	2.54	1.41	1.34
23	c	904	CLA	MG-ND	2.54	2.10	2.05
23	C	510	CLA	C4C-C3C	2.54	1.49	1.45
25	t	101	BCR	C23-C22	2.54	1.51	1.46
23	b	615	CLA	OBD-CAD	2.54	1.26	1.22
36	d	408	LHG	O8-C23	2.54	1.40	1.33
23	c	907	CLA	OBD-CAD	2.54	1.26	1.22
25	C	515	BCR	C1-C6	-2.54	1.50	1.53
23	c	907	CLA	C3D-C2D	2.54	1.45	1.39
23	C	503	CLA	C3D-C2D	2.54	1.45	1.39
23	b	605	CLA	C4D-CHA	2.53	1.47	1.38
23	C	513	CLA	C3B-C4B	2.53	1.50	1.42
23	b	609	CLA	C1C-NC	-2.53	1.33	1.37
23	B	605	CLA	C4D-CHA	2.53	1.47	1.38
23	a	411	CLA	C4B-NB	-2.53	1.34	1.37
23	B	605	CLA	C1D-ND	-2.53	1.34	1.37
28	D	405	PL9	C18-C19	2.53	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	912	CLA	C1B-C2B	2.53	1.49	1.43
23	B	613	CLA	C3D-C2D	2.53	1.45	1.39
23	c	909	CLA	C4D-CHA	2.52	1.47	1.38
23	c	910	CLA	C1C-NC	-2.52	1.33	1.37
23	A	410	CLA	C4D-CHA	2.52	1.47	1.38
23	c	909	CLA	C1C-C2C	2.52	1.49	1.44
23	B	608	CLA	OBD-CAD	2.52	1.26	1.22
23	d	403	CLA	C4D-CHA	2.52	1.47	1.38
23	C	503	CLA	CBD-CAD	-2.51	1.45	1.56
23	C	506	CLA	C1B-C2B	2.51	1.49	1.43
23	a	410	CLA	C1B-NB	-2.51	1.34	1.37
23	c	907	CLA	C1C-NC	-2.51	1.33	1.37
23	c	905	CLA	C3B-C4B	2.51	1.50	1.42
23	B	617	CLA	C4C-C3C	2.50	1.49	1.45
23	b	613	CLA	C3D-C2D	2.50	1.45	1.39
23	B	615	CLA	C4D-CHA	2.50	1.47	1.38
23	c	914	CLA	C4C-C3C	2.49	1.49	1.45
23	b	609	CLA	MG-ND	2.49	2.10	2.05
23	b	615	CLA	C3B-C4B	2.49	1.50	1.42
23	B	617	CLA	CHD-C1D	2.49	1.43	1.38
23	B	615	CLA	CHC-C4B	2.49	1.45	1.39
23	c	913	CLA	C1B-C2B	2.49	1.49	1.43
23	C	505	CLA	C4D-CHA	2.48	1.46	1.38
23	B	607	CLA	C4D-CHA	2.48	1.46	1.38
28	D	405	PL9	C22-C23	2.48	1.58	1.50
23	C	503	CLA	C1C-C2C	2.48	1.49	1.44
23	B	612	CLA	C4C-C3C	2.48	1.49	1.45
23	B	606	CLA	OBD-CAD	2.48	1.26	1.22
23	B	608	CLA	C4C-C3C	2.48	1.49	1.45
33	B	630	HTG	C1'-S1	-2.48	1.78	1.81
23	c	910	CLA	C1B-C2B	2.48	1.48	1.43
23	b	614	CLA	C3B-C4B	2.47	1.49	1.42
34	C	518	DGD	O2G-C1B	2.47	1.41	1.34
23	c	904	CLA	C1D-ND	-2.47	1.34	1.37
23	C	512	CLA	OBD-CAD	2.47	1.26	1.22
23	A	410	CLA	CBD-CAD	-2.47	1.45	1.56
23	B	606	CLA	C1D-ND	-2.47	1.34	1.37
30	z	101	LMT	O1'-C1'	2.47	1.44	1.40
23	b	614	CLA	C1D-ND	-2.47	1.34	1.37
23	b	608	CLA	C4D-CHA	2.46	1.46	1.38
23	b	613	CLA	O2A-CGA	2.46	1.40	1.33
23	B	602	CLA	C4C-C3C	2.46	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C3B-C4B	2.46	1.49	1.42
23	c	913	CLA	C3B-C4B	2.46	1.49	1.42
23	B	610	CLA	C3B-C4B	2.46	1.49	1.42
33	C	521	HTG	C1'-S1	-2.46	1.78	1.81
34	c	918	DGD	O5D-C1E	2.46	1.44	1.40
23	c	902	CLA	MG-NC	2.46	2.12	2.06
23	B	611	CLA	C4C-C3C	2.45	1.49	1.45
23	B	603	CLA	C4D-CHA	2.45	1.46	1.38
23	D	403	CLA	C4D-CHA	2.45	1.46	1.38
36	d	407	LHG	O7-C7	2.45	1.41	1.34
34	c	919	DGD	O5D-C1E	2.45	1.44	1.40
37	f	101	HEM	FE-ND	2.45	2.02	1.94
23	b	607	CLA	MG-NB	2.45	2.10	2.05
23	B	610	CLA	OBD-CAD	2.44	1.26	1.22
25	B	620	BCR	C23-C22	2.44	1.51	1.46
23	c	911	CLA	CBD-CAD	-2.44	1.45	1.56
23	a	410	CLA	O2D-CGD	2.44	1.39	1.33
23	b	608	CLA	C4B-NB	-2.44	1.34	1.37
28	d	405	PL9	C21-C19	2.44	1.56	1.51
23	b	606	CLA	C3B-C4B	2.44	1.49	1.42
23	C	512	CLA	C1D-ND	-2.43	1.34	1.37
23	C	511	CLA	C1C-NC	-2.43	1.34	1.37
23	b	606	CLA	CHC-C4B	2.43	1.44	1.39
23	A	406	CLA	C1-C2	2.43	1.56	1.49
23	C	511	CLA	C1D-ND	-2.43	1.34	1.37
23	c	903	CLA	C4C-C3C	2.42	1.49	1.45
25	B	619	BCR	C24-C25	2.42	1.53	1.45
23	c	903	CLA	C3D-C2D	2.42	1.45	1.39
24	a	413	PHO	CBD-CGD	-2.42	1.49	1.52
23	b	606	CLA	C1B-C2B	2.42	1.48	1.43
34	d	406	DGD	O3G-C1D	2.42	1.44	1.40
23	c	907	CLA	C4D-CHA	2.42	1.46	1.38
23	b	607	CLA	C1C-NC	-2.42	1.34	1.37
23	B	616	CLA	C4D-CHA	2.41	1.46	1.38
23	c	914	CLA	C3B-C4B	2.41	1.49	1.42
23	C	512	CLA	C1B-NB	-2.40	1.34	1.37
23	c	902	CLA	C1B-C2B	2.40	1.48	1.43
23	B	608	CLA	C3B-C4B	2.40	1.49	1.42
23	a	414	CLA	C4D-CHA	2.40	1.46	1.38
25	B	618	BCR	C30-C25	2.39	1.56	1.53
23	A	406	CLA	O2D-CGD	2.39	1.39	1.33
23	C	501	CLA	C4B-NB	-2.39	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	621	BCR	C24-C25	2.39	1.53	1.45
23	B	603	CLA	C3B-C4B	2.39	1.49	1.42
23	B	609	CLA	C4B-NB	-2.39	1.34	1.37
23	A	406	CLA	C4C-C3C	2.39	1.49	1.45
23	c	902	CLA	C3D-C2D	2.39	1.45	1.39
23	b	615	CLA	C4D-CHA	2.38	1.46	1.38
25	D	404	BCR	C12-C13	2.38	1.51	1.46
28	a	419	PL9	C7-C3	2.38	1.54	1.51
23	D	402	CLA	MG-ND	2.38	2.10	2.05
23	b	609	CLA	C1C-C2C	2.38	1.49	1.44
33	O	303	HTG	C1'-S1	-2.38	1.78	1.81
37	f	101	HEM	CMA-C3A	2.38	1.55	1.50
23	c	909	CLA	C1B-C2B	2.38	1.48	1.43
27	C	519	LMG	O7-C8	-2.37	1.41	1.46
37	F	101	HEM	CAC-C3C	2.36	1.53	1.47
25	d	404	BCR	C33-C5	2.36	1.54	1.50
37	V	201	HEM	C4D-ND	-2.36	1.36	1.40
23	B	613	CLA	C3B-C4B	2.36	1.49	1.42
23	c	904	CLA	C1B-NB	-2.36	1.34	1.37
23	A	406	CLA	C3D-C2D	2.36	1.45	1.39
23	D	402	CLA	CAB-C3B	2.35	1.53	1.47
23	b	604	CLA	C1D-ND	-2.35	1.34	1.37
23	b	618	CLA	C4C-C3C	2.35	1.49	1.45
23	C	512	CLA	C3B-C4B	2.35	1.49	1.42
23	b	613	CLA	C4B-NB	-2.35	1.34	1.37
23	C	503	CLA	MG-ND	2.35	2.10	2.05
23	b	616	CLA	C1B-C2B	2.35	1.48	1.43
28	D	405	PL9	C2-C1	-2.35	1.38	1.44
23	b	608	CLA	C1B-C2B	2.34	1.48	1.43
25	d	404	BCR	C12-C13	2.34	1.51	1.46
23	b	618	CLA	C3B-C4B	2.34	1.49	1.42
23	B	613	CLA	O2A-CGA	2.34	1.40	1.33
23	b	608	CLA	MG-NB	2.34	2.10	2.05
23	d	402	CLA	C4D-CHA	2.34	1.46	1.38
33	b	626	HTG	C1'-S1	-2.34	1.78	1.81
23	B	604	CLA	C4D-CHA	2.33	1.46	1.38
23	b	617	CLA	C4D-CHA	2.33	1.46	1.38
28	d	405	PL9	C43-C44	2.33	1.38	1.33
37	f	101	HEM	CMC-C2C	2.33	1.55	1.50
23	A	405	CLA	C4D-CHA	2.33	1.46	1.38
23	c	908	CLA	C1C-NC	-2.33	1.34	1.37
23	B	602	CLA	C1D-ND	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	908	CLA	C4C-C3C	2.32	1.49	1.45
25	b	620	BCR	C23-C22	2.32	1.50	1.46
23	c	910	CLA	C4C-C3C	2.32	1.49	1.45
23	C	506	CLA	C4B-NB	-2.32	1.34	1.37
23	b	615	CLA	CHD-C4C	2.32	1.44	1.39
23	B	608	CLA	C1C-NC	-2.32	1.34	1.37
23	C	513	CLA	C3B-C2B	2.31	1.49	1.41
23	C	505	CLA	C3B-C4B	2.31	1.49	1.42
23	d	403	CLA	MG-ND	2.31	2.10	2.05
23	D	403	CLA	C1B-C2B	2.30	1.48	1.43
23	B	612	CLA	O2A-CGA	2.30	1.40	1.33
33	b	601	HTG	C1-S1	-2.30	1.76	1.80
23	B	613	CLA	C4C-C3C	2.30	1.48	1.45
23	c	914	CLA	C1B-NB	-2.30	1.34	1.37
27	Z	101	LMG	O1-C1	2.29	1.44	1.40
33	B	625	HTG	C1'-S1	-2.29	1.78	1.81
23	B	614	CLA	MG-NC	2.29	2.11	2.06
33	b	627	HTG	C1-S1	-2.28	1.76	1.80
23	b	616	CLA	C3D-C4D	-2.28	1.39	1.44
23	C	511	CLA	C1B-C2B	2.28	1.48	1.43
23	a	414	CLA	C3B-C4B	2.28	1.49	1.42
23	C	511	CLA	CBD-CAD	-2.28	1.46	1.56
28	d	405	PL9	C18-C19	2.28	1.38	1.33
23	c	912	CLA	C4C-C3C	2.28	1.48	1.45
23	a	410	CLA	C4D-CHA	2.28	1.46	1.38
34	C	516	DGD	O5D-C1E	2.27	1.44	1.40
23	d	403	CLA	C1C-NC	-2.27	1.34	1.37
23	B	612	CLA	CHB-C1B	2.27	1.44	1.39
23	b	619	CLA	C3B-C4B	2.27	1.49	1.42
23	a	409	CLA	C3D-C2D	2.26	1.45	1.39
23	c	910	CLA	C3D-C4D	-2.26	1.39	1.44
23	d	402	CLA	O2D-CGD	2.26	1.38	1.33
23	B	602	CLA	C1C-C2C	2.26	1.49	1.44
23	C	510	CLA	C1B-NB	-2.26	1.34	1.37
34	c	919	DGD	O4D-C4D	2.26	1.48	1.43
23	C	511	CLA	C4C-C3C	2.26	1.48	1.45
27	c	921	LMG	O1-C1	2.25	1.44	1.40
25	b	622	BCR	C26-C25	2.25	1.38	1.34
37	F	101	HEM	CMC-C2C	2.25	1.55	1.50
23	a	414	CLA	CBD-CAD	-2.25	1.46	1.56
23	C	513	CLA	C1B-C2B	2.24	1.48	1.43
23	B	615	CLA	C1D-ND	-2.24	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C4C-C3C	2.24	1.48	1.45
23	B	615	CLA	C4B-NB	-2.24	1.34	1.37
37	f	101	HEM	FE-NA	2.24	2.02	1.95
23	C	501	CLA	C4C-C3C	2.24	1.48	1.45
27	c	920	LMG	O1-C1	2.24	1.43	1.40
30	m	102	LMT	O1'-C1'	2.23	1.43	1.40
23	c	914	CLA	C1B-C2B	2.23	1.48	1.43
23	B	607	CLA	C3B-C4B	2.23	1.49	1.42
25	c	916	BCR	C12-C13	2.23	1.50	1.46
23	B	610	CLA	O2D-CGD	2.23	1.38	1.33
23	C	504	CLA	OBD-CAD	2.22	1.26	1.22
23	b	617	CLA	C4B-NB	-2.22	1.34	1.37
23	c	909	CLA	C1B-NB	-2.22	1.34	1.37
23	C	509	CLA	MG-NC	2.22	2.11	2.06
23	B	611	CLA	C1B-NB	-2.22	1.34	1.37
23	c	907	CLA	C1B-C2B	2.22	1.48	1.43
25	B	619	BCR	C5-C6	2.22	1.38	1.34
23	B	610	CLA	CHD-C4C	2.22	1.44	1.39
23	B	617	CLA	MG-ND	2.22	2.10	2.05
23	B	604	CLA	C3B-C4B	2.22	1.49	1.42
23	B	606	CLA	C1B-C2B	2.22	1.48	1.43
23	D	403	CLA	C3B-C4B	2.21	1.49	1.42
23	b	607	CLA	O2A-CGA	2.21	1.39	1.33
23	B	613	CLA	C1B-C2B	2.21	1.48	1.43
23	a	414	CLA	CHC-C4B	2.21	1.44	1.39
23	b	611	CLA	C1B-C2B	2.20	1.48	1.43
28	d	405	PL9	C17-C18	2.20	1.57	1.50
23	B	612	CLA	C3B-C4B	2.20	1.49	1.42
23	b	617	CLA	C4C-C3C	2.20	1.48	1.45
23	C	507	CLA	C3B-C4B	2.19	1.49	1.42
23	B	617	CLA	C3B-C4B	2.19	1.49	1.42
23	c	912	CLA	CBD-CAD	-2.19	1.46	1.56
23	c	914	CLA	C3B-C2B	2.19	1.48	1.41
23	c	903	CLA	C3D-C4D	-2.19	1.39	1.44
23	B	605	CLA	C3D-C2D	2.19	1.45	1.39
23	b	606	CLA	MG-NC	-2.19	2.01	2.06
23	B	611	CLA	MG-ND	-2.19	2.01	2.05
23	A	406	CLA	CHD-C1D	2.18	1.42	1.38
23	c	902	CLA	C3B-C2B	2.18	1.48	1.41
23	C	510	CLA	C1D-ND	-2.18	1.35	1.37
23	C	508	CLA	C3B-C2B	2.18	1.48	1.41
23	b	605	CLA	CBD-CAD	-2.18	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	904	CLA	OBD-CAD	2.18	1.26	1.22
23	C	508	CLA	C1C-C2C	2.18	1.48	1.44
23	b	615	CLA	C1D-ND	-2.18	1.35	1.37
23	c	908	CLA	C1A-CHA	2.18	1.52	1.43
28	d	405	PL9	C2-C3	2.18	1.40	1.34
23	c	910	CLA	C1C-C2C	2.17	1.48	1.44
23	c	912	CLA	CHC-C4B	2.17	1.44	1.39
28	A	414	PL9	C7-C3	2.17	1.54	1.51
23	B	603	CLA	CBD-CAD	-2.17	1.46	1.56
25	K	102	BCR	C12-C13	2.17	1.50	1.46
23	a	410	CLA	C4B-NB	-2.17	1.35	1.37
23	a	411	CLA	CBD-CAD	-2.17	1.46	1.56
23	A	406	CLA	CMC-C2C	2.16	1.55	1.50
23	b	617	CLA	OBD-CAD	2.16	1.26	1.22
25	B	618	BCR	C27-C26	2.16	1.55	1.51
23	C	512	CLA	C1C-C2C	2.16	1.48	1.44
30	C	520	LMT	O1'-C1'	2.16	1.43	1.40
23	B	606	CLA	CHC-C4B	2.16	1.44	1.39
34	C	518	DGD	O2G-C2G	-2.16	1.41	1.46
23	b	612	CLA	MG-ND	2.16	2.10	2.05
23	a	414	CLA	MG-ND	2.16	2.10	2.05
23	C	511	CLA	C3B-C4B	2.16	1.49	1.42
27	c	920	LMG	O3-C3	2.16	1.48	1.43
23	d	402	CLA	C1C-NC	-2.16	1.34	1.37
23	b	616	CLA	C1B-NB	-2.15	1.35	1.37
24	A	408	PHO	C4B-NB	-2.15	1.34	1.38
23	C	501	CLA	C1C-C2C	2.15	1.48	1.44
37	V	201	HEM	CMD-C2D	2.15	1.55	1.50
33	B	631	HTG	C1'-S1	-2.15	1.78	1.81
23	c	913	CLA	C1D-ND	-2.14	1.35	1.37
25	c	915	BCR	C12-C13	2.14	1.50	1.46
23	B	608	CLA	C4D-CHA	2.14	1.45	1.38
23	C	502	CLA	C1B-NB	-2.14	1.35	1.37
25	k	102	BCR	C12-C13	2.14	1.50	1.46
26	D	407	SQD	O6-C1	2.13	1.43	1.40
23	B	617	CLA	C2-C3	2.13	1.38	1.33
37	V	201	HEM	C1B-NB	-2.13	1.36	1.40
23	B	617	CLA	MG-NB	2.13	2.10	2.05
23	a	410	CLA	C4C-C3C	2.13	1.48	1.45
23	C	511	CLA	C3D-C4D	-2.13	1.39	1.44
23	b	607	CLA	C1B-C2B	2.13	1.48	1.43
23	C	507	CLA	C1A-CHA	2.13	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	410	CLA	CMD-C2D	2.13	1.55	1.50
23	b	612	CLA	O2D-CED	-2.13	1.40	1.45
23	B	604	CLA	C1D-ND	-2.13	1.35	1.37
23	d	402	CLA	CHD-C4C	2.12	1.44	1.39
23	b	609	CLA	C4C-C3C	2.12	1.48	1.45
30	F	102	LMT	O1'-C1'	2.12	1.43	1.40
34	c	917	DGD	O2G-C1B	2.12	1.40	1.34
38	h	101	RRX	C30-C25	2.12	1.56	1.53
23	A	405	CLA	CMC-C2C	2.12	1.55	1.50
23	C	505	CLA	MG-ND	2.12	2.10	2.05
23	b	616	CLA	C1-C2	2.12	1.55	1.49
25	B	619	BCR	C23-C22	2.11	1.50	1.46
23	A	410	CLA	O2D-CGD	2.11	1.38	1.33
23	a	414	CLA	C3D-C2D	2.11	1.44	1.39
23	B	613	CLA	CMA-C3A	2.11	1.57	1.53
33	C	522	HTG	O5-C1	2.11	1.45	1.42
23	B	608	CLA	CMA-C3A	2.11	1.57	1.53
23	c	909	CLA	OBD-CAD	2.11	1.26	1.22
23	B	602	CLA	C1D-C2D	2.11	1.49	1.45
23	d	403	CLA	C1C-C2C	2.11	1.48	1.44
37	v	201	HEM	CMD-C2D	2.10	1.55	1.50
25	B	619	BCR	C35-C13	2.10	1.55	1.50
23	B	604	CLA	CBD-CAD	-2.10	1.47	1.56
23	b	611	CLA	CAA-C2A	2.10	1.57	1.54
23	b	609	CLA	C3B-C2B	2.09	1.48	1.41
25	B	618	BCR	C15-C14	2.09	1.49	1.43
25	B	618	BCR	C5-C6	2.09	1.38	1.34
23	c	904	CLA	C1C-C2C	2.09	1.48	1.44
23	B	609	CLA	C1D-ND	-2.09	1.35	1.37
23	a	410	CLA	C3D-C2D	2.09	1.44	1.39
23	b	614	CLA	C3D-C4D	-2.09	1.39	1.44
23	b	614	CLA	MG-NC	2.09	2.11	2.06
23	b	617	CLA	C3D-C2D	2.09	1.44	1.39
23	C	504	CLA	C1B-C2B	2.09	1.48	1.43
25	d	404	BCR	C23-C22	2.09	1.50	1.46
23	d	402	CLA	C1B-NB	-2.09	1.35	1.37
23	B	615	CLA	CMB-C2B	2.09	1.55	1.50
23	C	501	CLA	C1B-C2B	2.09	1.48	1.43
23	C	511	CLA	C1A-CHA	2.08	1.51	1.43
23	B	605	CLA	C3B-C4B	2.08	1.48	1.42
23	a	414	CLA	C4C-C3C	2.08	1.48	1.45
23	c	912	CLA	C1D-ND	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C3B-C2B	2.08	1.48	1.41
23	B	609	CLA	C3B-C4B	2.08	1.48	1.42
23	a	410	CLA	C3B-C4B	2.08	1.48	1.42
23	c	902	CLA	C1C-NC	-2.08	1.34	1.37
23	c	911	CLA	C4C-C3C	2.07	1.48	1.45
23	B	615	CLA	C4C-C3C	2.07	1.48	1.45
34	c	917	DGD	C6E-C5E	2.07	1.58	1.51
23	b	614	CLA	C1B-C2B	2.07	1.48	1.43
23	c	904	CLA	C1B-C2B	2.07	1.48	1.43
23	B	609	CLA	C4C-C3C	2.07	1.48	1.45
23	d	402	CLA	C3B-C4B	2.07	1.48	1.42
23	C	506	CLA	C1C-C2C	2.06	1.48	1.44
23	C	503	CLA	C1C-NC	-2.06	1.34	1.37
28	D	405	PL9	C36-C37	-2.06	1.46	1.53
23	C	506	CLA	C1D-ND	-2.06	1.35	1.37
23	c	911	CLA	C1B-C2B	2.06	1.48	1.43
25	t	101	BCR	C12-C13	2.06	1.50	1.46
26	B	621	SQD	O7-S	2.06	1.50	1.45
23	b	619	CLA	MG-NC	2.06	2.11	2.06
23	c	910	CLA	C3B-C4B	2.06	1.48	1.42
23	b	608	CLA	C1C-NC	-2.06	1.34	1.37
37	f	101	HEM	CAD-C3D	2.05	1.56	1.51
23	D	402	CLA	C3D-C2D	2.05	1.44	1.39
23	d	402	CLA	O2D-CED	-2.05	1.40	1.45
28	d	405	PL9	C13-C14	2.05	1.37	1.33
36	d	409	LHG	C4-C5	2.05	1.57	1.50
23	c	913	CLA	C3D-C4D	-2.04	1.39	1.44
23	B	606	CLA	C4C-C3C	2.04	1.48	1.45
23	A	407	CLA	CBD-CAD	-2.04	1.47	1.56
23	a	411	CLA	C1B-C2B	2.04	1.47	1.43
23	A	410	CLA	C3B-C4B	2.04	1.48	1.42
25	k	102	BCR	C8-C9	2.04	1.50	1.46
23	B	613	CLA	C4D-CHA	2.04	1.45	1.38
23	C	512	CLA	C4B-NB	-2.03	1.35	1.37
23	b	613	CLA	C3B-C4B	2.03	1.48	1.42
37	V	201	HEM	CBB-CAB	2.03	1.40	1.30
25	a	415	BCR	C24-C25	2.03	1.52	1.45
28	D	405	PL9	C28-C29	2.03	1.37	1.33
23	B	610	CLA	C2-C3	2.03	1.37	1.33
25	B	618	BCR	C32-C1	2.03	1.57	1.53
37	F	101	HEM	CAD-C3D	2.03	1.56	1.51
37	F	101	HEM	CMB-C2B	2.02	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	t	101	BCR	C35-C13	2.02	1.54	1.50
23	b	607	CLA	CHC-C4B	2.02	1.44	1.39
23	c	903	CLA	C3B-C2B	2.02	1.48	1.41
23	C	502	CLA	CAA-C2A	2.02	1.57	1.54
23	c	907	CLA	C3D-C4D	-2.02	1.39	1.44
25	b	622	BCR	C12-C13	2.02	1.50	1.46
23	B	603	CLA	CAB-C3B	2.02	1.52	1.47
23	c	902	CLA	CHB-C4A	-2.02	1.32	1.37
23	d	403	CLA	C3B-C2B	2.02	1.48	1.41
25	a	415	BCR	C20-C21	2.02	1.49	1.43
28	D	405	PL9	C16-C14	2.02	1.55	1.51
23	A	407	CLA	CHB-C1B	2.01	1.43	1.39
25	D	404	BCR	C24-C25	2.01	1.52	1.45
23	c	911	CLA	C4B-NB	-2.01	1.35	1.37
23	c	908	CLA	C3B-C4B	2.01	1.48	1.42
23	B	609	CLA	OBD-CAD	2.01	1.25	1.22
23	C	509	CLA	MG-ND	2.01	2.09	2.05
23	a	409	CLA	C1C-NC	-2.01	1.34	1.37
23	c	905	CLA	C1C-C2C	2.00	1.48	1.44
37	f	101	HEM	O1D-CGD	2.00	1.28	1.22
23	C	513	CLA	C1C-C2C	2.00	1.48	1.44

All (2808) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	13.12	112.67	106.68
24	A	408	PHO	C2D-C1D-ND	12.68	118.60	109.43
23	b	609	CLA	C4A-NA-C1A	11.80	112.06	106.68
24	A	408	PHO	C3B-C4B-NB	11.40	114.89	107.46
23	C	501	CLA	O2D-CGD-O1D	-10.54	103.33	123.85
23	c	904	CLA	C4A-NA-C1A	10.52	111.48	106.68
24	A	409	PHO	C2D-C1D-ND	10.37	116.92	109.43
24	A	409	PHO	C2B-C1B-NB	10.04	116.68	109.43
23	c	902	CLA	C4A-NA-C1A	10.03	111.25	106.68
24	A	409	PHO	C3B-C4B-NB	9.99	113.97	107.46
23	C	507	CLA	C4A-NA-C1A	9.98	111.23	106.68
23	B	602	CLA	C4A-NA-C1A	9.98	111.23	106.68
23	c	912	CLA	C4A-NA-C1A	9.94	111.22	106.68
23	c	909	CLA	C4A-NA-C1A	9.69	111.10	106.68
23	b	607	CLA	C4A-NA-C1A	9.67	111.09	106.68
23	C	513	CLA	C4A-NA-C1A	9.50	111.01	106.68
24	a	413	PHO	C2D-C1D-ND	9.47	116.27	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	413	PHO	O2D-CGD-CBD	9.39	121.26	110.95
23	B	607	CLA	C4A-NA-C1A	9.25	110.90	106.68
24	a	412	PHO	C2D-C1D-ND	8.89	115.86	109.43
24	a	412	PHO	C3B-C4B-NB	8.87	113.24	107.46
23	B	616	CLA	C4A-NA-C1A	8.79	110.69	106.68
23	b	613	CLA	C4A-NA-C1A	8.76	110.67	106.68
23	c	905	CLA	C4A-NA-C1A	8.68	110.64	106.68
23	C	501	CLA	O2D-CGD-CBD	8.66	126.37	111.23
24	a	413	PHO	C3B-C4B-NB	8.63	113.09	107.46
26	a	416	SQD	O6-C1-C2	8.52	121.21	108.27
23	b	617	CLA	C4A-NA-C1A	8.41	110.52	106.68
23	b	615	CLA	CAC-C3C-C4C	8.40	135.72	124.79
26	D	407	SQD	O6-C1-C2	8.20	120.72	108.27
24	a	412	PHO	O2D-CGD-CBD	8.19	119.95	110.95
23	c	908	CLA	C4A-NA-C1A	8.03	110.34	106.68
23	b	604	CLA	C4A-NA-C1A	7.98	110.32	106.68
23	C	510	CLA	C4A-NA-C1A	7.95	110.31	106.68
23	b	614	CLA	C4A-NA-C1A	7.93	110.30	106.68
23	c	903	CLA	C1D-ND-C4D	-7.87	100.79	106.31
23	b	615	CLA	C4A-NA-C1A	7.81	110.24	106.68
24	A	408	PHO	C4D-ND-C1D	-7.75	99.58	108.87
23	C	509	CLA	C4A-NA-C1A	7.72	110.20	106.68
24	A	408	PHO	C2B-C1B-NB	7.48	114.84	109.43
23	c	910	CLA	C4A-NA-C1A	7.33	110.03	106.68
26	B	621	SQD	O6-C1-C2	7.33	119.41	108.27
23	D	403	CLA	C4A-NA-C1A	7.21	109.97	106.68
24	a	413	PHO	C2B-C1B-NB	7.20	114.64	109.43
23	B	604	CLA	C2C-C1C-NC	7.19	117.54	109.98
23	A	406	CLA	C2C-C1C-NC	7.19	117.53	109.98
26	A	412	SQD	O6-C1-C2	7.17	119.16	108.27
24	a	413	PHO	C4D-ND-C1D	-7.16	100.29	108.87
23	c	907	CLA	CHD-C4C-C3C	-7.16	114.33	124.77
24	A	409	PHO	C4D-ND-C1D	-7.11	100.35	108.87
23	c	903	CLA	C2D-C1D-ND	7.02	117.08	110.13
23	B	605	CLA	C2C-C1C-NC	7.02	117.35	109.98
23	b	617	CLA	C4D-CHA-C1A	-7.00	112.89	121.24
23	b	618	CLA	C4A-NA-C1A	6.97	109.86	106.68
23	a	414	CLA	C2C-C1C-NC	6.94	117.27	109.98
23	b	608	CLA	CAC-C3C-C4C	6.94	133.82	124.79
23	A	410	CLA	C1D-ND-C4D	-6.94	101.44	106.31
23	a	409	CLA	CAC-C3C-C4C	6.92	133.80	124.79
23	b	617	CLA	C2D-C1D-ND	6.90	116.96	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	617	CLA	C1D-ND-C4D	-6.88	101.49	106.31
23	b	619	CLA	CHD-C4C-C3C	-6.85	114.78	124.77
23	C	502	CLA	CHD-C4C-C3C	-6.82	114.83	124.77
23	c	913	CLA	C4A-NA-C1A	6.78	109.77	106.68
23	B	609	CLA	C2C-C1C-NC	6.75	117.07	109.98
23	c	903	CLA	C4A-NA-C1A	6.74	109.76	106.68
23	c	905	CLA	C2D-C1D-ND	6.64	116.70	110.13
26	a	416	SQD	O9-S-C6	6.63	116.66	106.76
24	A	409	PHO	C3D-C4D-ND	6.62	116.19	107.71
23	B	604	CLA	CHD-C4C-C3C	-6.61	115.14	124.77
23	b	613	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	d	402	CLA	C2C-C1C-NC	6.56	116.87	109.98
23	c	907	CLA	C4D-CHA-C1A	-6.54	113.44	121.24
23	D	402	CLA	C1D-ND-C4D	6.53	110.89	106.31
23	C	512	CLA	C4A-NA-C1A	6.53	109.66	106.68
23	b	616	CLA	C4A-NA-C1A	6.52	109.66	106.68
23	A	410	CLA	C4D-CHA-C1A	-6.50	113.49	121.24
33	V	202	HTG	C2-C1-S1	6.43	120.99	111.30
23	B	612	CLA	CHD-C4C-C3C	-6.43	115.40	124.77
23	a	411	CLA	C2C-C1C-NC	6.43	116.73	109.98
24	A	408	PHO	C3D-C4D-ND	6.42	115.93	107.71
33	B	631	HTG	C1'-S1-C1	6.40	114.28	100.45
23	b	608	CLA	C2C-C1C-NC	6.40	116.71	109.98
23	c	908	CLA	O2D-CGD-CBD	6.38	122.39	111.23
23	c	906	CLA	C4A-NA-C1A	6.38	109.59	106.68
23	b	617	CLA	O2D-CGD-CBD	6.38	122.38	111.23
23	b	606	CLA	C2C-C1C-NC	6.37	116.67	109.98
23	b	619	CLA	O2D-CGD-CBD	6.32	122.28	111.23
23	C	510	CLA	CHD-C4C-C3C	-6.29	115.60	124.77
33	C	522	HTG	C1'-S1-C1	6.29	114.03	100.45
23	A	406	CLA	C4A-NA-C1A	-6.27	103.82	106.68
23	C	504	CLA	C2C-C1C-NC	6.27	116.57	109.98
23	C	506	CLA	CHD-C4C-C3C	-6.26	115.64	124.77
23	D	402	CLA	CHB-C1B-NB	6.24	133.40	124.05
34	D	406	DGD	O2G-C1B-C2B	6.23	124.96	111.48
23	B	602	CLA	O2D-CGD-CBD	6.23	122.12	111.23
24	a	413	PHO	C3D-C4D-ND	6.21	115.67	107.71
23	c	902	CLA	C1D-ND-C4D	-6.21	101.96	106.31
23	C	508	CLA	C4A-NA-C1A	6.21	109.51	106.68
23	B	604	CLA	C1C-C2C-C3C	-6.18	100.48	106.98
23	C	509	CLA	C2C-C1C-NC	6.18	116.48	109.98
23	c	905	CLA	C1D-ND-C4D	-6.15	101.99	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	909	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	a	411	CLA	CAC-C3C-C4C	6.10	132.73	124.79
38	H	101	RRX	C24-C23-C22	-6.10	117.21	126.23
23	A	407	CLA	CAC-C3C-C4C	6.08	132.71	124.79
33	V	202	HTG	O5-C1-C2	-6.07	101.94	110.32
23	B	617	CLA	C2D-C1D-ND	6.07	116.14	110.13
23	B	611	CLA	C4A-NA-C1A	6.05	109.44	106.68
23	B	612	CLA	C4A-NA-C1A	6.05	109.44	106.68
23	B	607	CLA	CHD-C4C-C3C	-6.04	115.96	124.77
23	b	615	CLA	CHD-C4C-C3C	-6.04	115.97	124.77
23	B	605	CLA	C1C-C2C-C3C	-6.02	100.65	106.98
23	a	414	CLA	CHD-C4C-C3C	-6.00	116.03	124.77
23	b	604	CLA	O2D-CGD-CBD	6.00	121.71	111.23
23	B	612	CLA	C2C-C1C-NC	5.99	116.28	109.98
33	B	626	HTG	C1'-S1-C1	5.98	113.37	100.45
23	C	505	CLA	C2C-C1C-NC	5.97	116.25	109.98
23	B	615	CLA	C4A-NA-C1A	5.96	109.40	106.68
23	B	615	CLA	CAC-C3C-C4C	5.96	132.54	124.79
23	B	607	CLA	C2D-C1D-ND	5.94	116.00	110.13
23	C	506	CLA	C4A-NA-C1A	5.93	109.38	106.68
23	A	406	CLA	C1C-C2C-C3C	-5.93	100.75	106.98
23	c	908	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
23	B	609	CLA	C2B-C1B-NB	5.92	116.46	110.33
33	c	924	HTG	C1-O5-C5	5.91	123.17	112.56
23	C	504	CLA	C1C-C2C-C3C	-5.90	100.78	106.98
23	a	409	CLA	C2D-C1D-ND	5.89	115.95	110.13
33	V	202	HTG	C1-O5-C5	-5.87	102.03	112.56
23	C	506	CLA	O2D-CGD-CBD	5.87	121.49	111.23
23	B	613	CLA	CAC-C3C-C4C	5.86	132.41	124.79
23	B	602	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
23	B	613	CLA	C4A-NA-C1A	5.84	109.34	106.68
23	a	410	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
23	C	504	CLA	C4A-NA-C1A	5.82	109.33	106.68
33	C	522	HTG	C1-O5-C5	5.82	123.00	112.56
23	B	604	CLA	C4A-NA-C1A	5.81	109.33	106.68
23	b	607	CLA	C2C-C1C-NC	5.80	116.08	109.98
23	B	606	CLA	C2C-C1C-NC	5.80	116.07	109.98
23	a	414	CLA	CAC-C3C-C4C	5.80	132.33	124.79
23	C	506	CLA	C2C-C1C-NC	5.79	116.07	109.98
23	c	902	CLA	C2D-C1D-ND	5.78	115.84	110.13
23	B	608	CLA	C2B-C1B-NB	5.77	116.31	110.33
23	A	406	CLA	CAC-C3C-C4C	5.77	132.30	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
23	A	410	CLA	C2C-C1C-NC	5.74	116.01	109.98
24	a	412	PHO	C2B-C1B-NB	5.74	113.58	109.43
23	B	609	CLA	C2D-C1D-ND	5.72	115.79	110.13
25	C	515	BCR	C7-C8-C9	-5.69	117.81	126.23
23	B	609	CLA	O2D-CGD-CBD	5.68	121.17	111.23
26	A	412	SQD	C1-C2-C3	-5.67	98.09	110.01
26	L	103	SQD	O6-C1-C2	5.67	116.88	108.27
26	B	621	SQD	C1-O5-C5	-5.66	102.66	113.72
23	c	903	CLA	C2B-C1B-NB	5.66	116.19	110.33
23	c	910	CLA	C4D-CHA-C1A	-5.65	114.50	121.24
23	A	410	CLA	C2D-C1D-ND	5.64	115.71	110.13
23	b	606	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
23	b	616	CLA	C2C-C1C-NC	5.63	115.90	109.98
23	B	604	CLA	C2B-C1B-NB	5.62	116.15	110.33
23	B	609	CLA	C3B-C4B-NB	5.61	115.54	110.53
23	A	405	CLA	C2D-C1D-ND	5.61	115.68	110.13
23	d	403	CLA	C2B-C1B-NB	5.60	116.14	110.33
33	V	202	HTG	C1-C2-C3	-5.60	99.60	110.55
23	B	611	CLA	C4D-CHA-C1A	-5.58	114.59	121.24
33	c	924	HTG	C1'-S1-C1	5.57	112.47	100.45
26	a	416	SQD	C1-O5-C5	-5.57	102.85	113.72
23	c	913	CLA	O2D-CGD-CBD	5.56	120.94	111.23
25	D	404	BCR	C7-C8-C9	-5.54	118.03	126.23
23	d	402	CLA	C2B-C1B-NB	5.54	116.07	110.33
23	d	403	CLA	O2D-CGD-CBD	5.54	120.92	111.23
27	a	418	LMG	O7-C10-C11	5.53	123.45	111.48
23	b	613	CLA	C2B-C1B-NB	5.51	116.04	110.33
23	c	903	CLA	CHD-C4C-C3C	-5.50	116.76	124.77
23	b	604	CLA	CHD-C4C-C3C	-5.49	116.77	124.77
23	A	407	CLA	C2B-C1B-NB	5.49	116.02	110.33
23	b	615	CLA	C4D-CHA-C1A	-5.48	114.71	121.24
23	C	507	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
23	B	611	CLA	C2D-C1D-ND	5.47	115.54	110.13
23	B	611	CLA	C2B-C1B-NB	5.46	115.99	110.33
23	B	617	CLA	CAC-C3C-C4C	5.46	131.89	124.79
26	A	412	SQD	O47-C7-C8	5.46	123.28	111.48
23	b	616	CLA	CAC-C3C-C4C	5.46	131.89	124.79
26	A	412	SQD	C1-O5-C5	-5.43	103.12	113.72
23	c	910	CLA	C2B-C1B-NB	5.43	115.96	110.33
23	B	604	CLA	C3B-C4B-NB	5.42	115.37	110.53
23	B	602	CLA	C2B-C1B-NB	5.41	115.94	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	401	SQD	C1-O5-C5	-5.41	103.15	113.72
23	c	906	CLA	C3B-C2B-C1B	-5.41	100.79	107.17
23	c	907	CLA	C2D-C1D-ND	5.41	115.48	110.13
26	f	102	SQD	O47-C7-O49	-5.40	118.78	125.70
36	D	408	LHG	O8-C23-O10	-5.40	110.13	123.63
23	c	903	CLA	O2D-CGD-CBD	5.39	120.66	111.23
25	B	620	BCR	C38-C26-C25	-5.38	118.61	124.48
33	b	627	HTG	C1'-S1-C1	5.38	112.07	100.45
23	B	616	CLA	C2C-C1C-NC	5.38	115.63	109.98
23	B	607	CLA	CHD-C1D-ND	-5.37	117.25	124.80
23	B	607	CLA	C2C-C1C-NC	5.35	115.60	109.98
23	b	613	CLA	C1D-ND-C4D	-5.35	102.56	106.31
33	c	923	HTG	C1'-S1-C1	5.33	111.96	100.45
28	d	405	PL9	C40-C39-C41	5.33	124.48	115.23
23	D	402	CLA	CHD-C4C-C3C	-5.32	117.01	124.77
23	A	407	CLA	C2C-C1C-NC	5.32	115.57	109.98
23	B	605	CLA	C4D-CHA-C1A	-5.32	114.90	121.24
23	B	610	CLA	C4A-NA-C1A	5.32	109.11	106.68
23	b	606	CLA	C2B-C1B-NB	5.32	115.84	110.33
37	V	201	HEM	C4D-ND-C1D	5.31	111.50	105.21
30	C	520	LMT	O1B-C4'-C3'	5.31	120.73	107.23
23	C	501	CLA	C2C-C1C-NC	5.30	115.55	109.98
23	b	619	CLA	C4A-NA-C1A	5.30	109.10	106.68
23	d	402	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
23	B	606	CLA	C2D-C1D-ND	5.30	115.37	110.13
37	v	201	HEM	C4D-ND-C1D	5.29	111.48	105.21
23	B	610	CLA	CAC-C3C-C4C	5.29	131.68	124.79
23	B	607	CLA	CMD-C2D-C1D	5.29	134.05	124.73
23	B	611	CLA	C1D-ND-C4D	-5.29	102.60	106.31
24	A	408	PHO	O2D-CGD-CBD	5.29	116.76	110.95
23	b	616	CLA	C1-C2-C3	-5.28	117.54	126.20
23	d	403	CLA	C4D-CHA-C1A	-5.28	114.95	121.24
23	b	618	CLA	C2B-C1B-NB	5.27	115.79	110.33
26	a	416	SQD	C1-C2-C3	-5.27	98.93	110.01
23	B	614	CLA	C2D-C1D-ND	5.26	115.33	110.13
23	A	410	CLA	C4-C3-C5	5.26	124.35	115.23
23	b	612	CLA	CAC-C3C-C4C	5.26	131.63	124.79
26	a	416	SQD	O47-C7-C8	5.25	122.85	111.48
23	c	908	CLA	O2D-CGD-O1D	-5.25	113.64	123.85
23	c	902	CLA	C1C-C2C-C3C	-5.24	101.46	106.98
23	A	405	CLA	C2B-C1B-NB	5.24	115.75	110.33
27	B	622	LMG	O7-C10-C11	5.23	122.79	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	C2D-C1D-ND	5.22	115.29	110.13
26	a	401	SQD	O6-C1-C2	5.22	116.20	108.27
23	a	410	CLA	C2C-C1C-NC	5.22	115.46	109.98
23	D	402	CLA	C2C-C1C-NC	5.20	115.44	109.98
23	B	617	CLA	C2C-C1C-NC	5.19	115.44	109.98
23	B	608	CLA	C4B-C3B-C2B	-5.19	100.84	107.30
23	a	409	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
23	B	609	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
23	c	912	CLA	CHD-C4C-C3C	-5.17	117.23	124.77
26	L	103	SQD	O7-S-C6	5.17	114.47	106.76
28	D	405	PL9	C40-C39-C41	5.16	124.19	115.23
23	b	612	CLA	C2C-C1C-NC	5.16	115.40	109.98
23	A	410	CLA	C2B-C1B-NB	5.16	115.68	110.33
23	b	606	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
23	D	402	CLA	CHA-C4D-ND	5.15	143.17	132.55
23	c	903	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
23	B	604	CLA	O2D-CGD-CBD	5.15	120.23	111.23
23	B	614	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
23	b	618	CLA	C1C-C2C-C3C	-5.14	101.58	106.98
23	d	402	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
23	c	907	CLA	CHD-C4C-NC	5.13	132.18	124.23
23	c	911	CLA	C2D-C1D-ND	5.12	115.20	110.13
33	u	201	HTG	C1'-S1-C1	5.12	111.51	100.45
23	B	610	CLA	C2C-C1C-NC	5.11	115.35	109.98
23	b	618	CLA	C2C-C1C-NC	5.11	115.35	109.98
23	c	907	CLA	C2B-C1B-NB	5.10	115.62	110.33
23	C	501	CLA	C4A-NA-C1A	5.10	109.01	106.68
37	F	101	HEM	CBD-CAD-C3D	-5.09	98.46	112.53
23	B	617	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
23	d	403	CLA	C2D-C1D-ND	5.06	115.14	110.13
23	d	403	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
23	C	509	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
25	b	620	BCR	C33-C5-C6	-5.05	118.97	124.48
23	C	502	CLA	CHD-C4C-NC	5.04	132.05	124.23
23	b	606	CLA	O2D-CGD-O1D	-5.04	114.03	123.85
23	B	612	CLA	C2B-C1B-NB	5.04	115.55	110.33
23	B	609	CLA	C4D-CHA-C1A	-5.04	115.23	121.24
23	c	906	CLA	CHD-C4C-C3C	-5.04	117.43	124.77
23	B	606	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
23	D	403	CLA	C1D-ND-C4D	-5.02	102.79	106.31
30	a	402	LMT	C1'-O5'-C5'	5.02	123.53	113.72
23	c	907	CLA	C3B-C2B-C1B	-5.02	101.25	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	O2D-CGD-CBD	5.01	119.98	111.23
23	C	511	CLA	C2D-C1D-ND	5.01	115.08	110.13
23	C	509	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
23	B	602	CLA	C2D-C1D-ND	4.99	115.06	110.13
23	b	611	CLA	C2C-C1C-NC	4.99	115.22	109.98
23	A	410	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
23	C	509	CLA	C4D-CHA-C1A	-4.98	115.30	121.24
23	a	410	CLA	C2D-C1D-ND	4.98	115.06	110.13
23	C	513	CLA	O2D-CGD-CBD	4.97	119.92	111.23
23	b	615	CLA	C3C-C4C-NC	4.97	116.80	110.43
23	C	509	CLA	CMB-C2B-C1B	4.96	132.97	125.42
23	B	616	CLA	CHD-C4C-C3C	-4.96	117.55	124.77
23	b	616	CLA	C2D-C1D-ND	4.95	115.03	110.13
23	c	908	CLA	C2C-C1C-NC	4.95	115.18	109.98
23	b	607	CLA	C1C-C2C-C3C	-4.95	101.77	106.98
23	c	907	CLA	CMD-C2D-C1D	4.94	133.43	124.73
23	C	505	CLA	CHD-C4C-C3C	-4.94	117.57	124.77
23	b	619	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
25	K	102	BCR	C11-C10-C9	-4.94	120.35	127.28
23	a	409	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
23	B	611	CLA	C2C-C1C-NC	4.93	115.16	109.98
23	c	907	CLA	C1D-ND-C4D	-4.93	102.85	106.31
23	B	615	CLA	C4D-CHA-C1A	-4.93	115.37	121.24
23	c	902	CLA	C4D-CHA-C1A	-4.93	115.37	121.24
23	c	912	CLA	C2C-C1C-NC	4.92	115.15	109.98
23	b	605	CLA	C2D-C1D-ND	4.91	114.98	110.13
27	C	519	LMG	O1-C7-C8	-4.90	98.89	110.82
23	b	606	CLA	CHD-C1D-ND	-4.90	117.91	124.80
23	C	502	CLA	C4D-CHA-C1A	-4.90	115.40	121.24
23	B	611	CLA	CHD-C4C-C3C	-4.90	117.64	124.77
23	B	615	CLA	C2B-C1B-NB	4.89	115.40	110.33
23	c	905	CLA	C4D-CHA-C1A	-4.89	115.41	121.24
23	B	614	CLA	CMD-C2D-C1D	4.89	133.34	124.73
23	B	610	CLA	O2D-CGD-O1D	-4.89	114.33	123.85
23	A	407	CLA	O2D-CGD-CBD	4.89	119.77	111.23
23	c	902	CLA	C2C-C1C-NC	4.89	115.11	109.98
23	B	613	CLA	C2D-C1D-ND	4.88	114.96	110.13
23	b	606	CLA	C4-C3-C5	4.88	123.69	115.23
23	B	616	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
23	c	906	CLA	O2D-CGD-O1D	-4.86	114.38	123.85
23	C	503	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
23	B	612	CLA	O2D-CGD-CBD	4.86	119.73	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	902	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
24	a	413	PHO	O2D-CGD-O1D	-4.85	114.40	123.85
23	b	610	CLA	CHD-C4C-C3C	-4.85	117.70	124.77
23	b	611	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
23	B	608	CLA	C2C-C1C-NC	4.85	115.07	109.98
23	b	617	CLA	C1-C2-C3	-4.85	118.26	126.20
23	b	613	CLA	C2C-C1C-NC	4.84	115.07	109.98
23	b	616	CLA	CHD-C4C-C3C	-4.84	117.71	124.77
23	b	618	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
23	b	617	CLA	O2D-CGD-O1D	-4.84	114.43	123.85
23	a	411	CLA	C1C-C2C-C3C	-4.83	101.89	106.98
23	B	614	CLA	CHD-C4C-C3C	-4.83	117.73	124.77
23	B	617	CLA	CHD-C1D-ND	-4.83	118.00	124.80
23	c	913	CLA	C1-C2-C3	-4.83	118.29	126.20
23	C	503	CLA	CHD-C4C-C3C	-4.81	117.76	124.77
23	b	608	CLA	CHD-C4C-C3C	-4.81	117.76	124.77
27	Z	101	LMG	O7-C10-C11	4.81	121.88	111.48
23	C	510	CLA	C2C-C1C-NC	4.81	115.03	109.98
23	b	606	CLA	C2D-C1D-ND	4.80	114.88	110.13
23	b	615	CLA	C4C-C3C-C2C	-4.80	99.90	106.89
28	a	419	PL9	C7-C3-C4	4.79	120.85	116.91
27	B	622	LMG	O8-C28-C29	4.79	126.42	111.83
23	B	609	CLA	CHD-C4C-C3C	-4.78	117.80	124.77
33	c	924	HTG	O5-C5-C4	4.78	118.31	109.70
26	A	412	SQD	O9-S-C6	4.78	113.89	106.76
24	a	412	PHO	O2D-CGD-O1D	-4.78	114.55	123.85
23	C	503	CLA	C2C-C1C-NC	4.77	115.00	109.98
23	c	910	CLA	CHD-C4C-C3C	-4.77	117.81	124.77
23	D	402	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	C	510	CLA	CHD-C4C-NC	4.77	131.63	124.23
23	b	605	CLA	O2D-CGD-CBD	4.77	119.57	111.23
23	c	909	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	c	914	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
23	b	608	CLA	C4-C3-C5	4.76	123.49	115.23
23	c	902	CLA	O2D-CGD-CBD	4.76	119.55	111.23
23	b	607	CLA	CAC-C3C-C4C	4.75	130.97	124.79
23	b	619	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	c	912	CLA	C1C-C2C-C3C	-4.74	101.99	106.98
23	c	902	CLA	C2B-C1B-NB	4.74	115.24	110.33
23	b	616	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
25	B	620	BCR	C24-C23-C22	-4.73	119.23	126.23
23	c	914	CLA	C4A-NA-C1A	4.73	108.84	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
23	B	610	CLA	CHD-C4C-C3C	-4.73	117.88	124.77
23	A	406	CLA	CHA-C4D-ND	4.73	142.31	132.55
23	c	902	CLA	O2D-CGD-O1D	-4.73	114.64	123.85
23	A	407	CLA	C1C-C2C-C3C	-4.73	102.01	106.98
23	c	905	CLA	C2B-C1B-NB	4.72	115.22	110.33
23	A	405	CLA	CAC-C3C-C4C	4.72	130.93	124.79
23	B	608	CLA	C1-C2-C3	-4.71	118.48	126.20
27	A	413	LMG	O1-C1-C2	4.71	115.42	108.27
23	d	402	CLA	CHC-C4B-NB	4.71	131.11	124.05
27	B	622	LMG	O7-C10-O9	-4.70	112.70	123.70
23	b	608	CLA	C2D-C1D-ND	4.70	114.78	110.13
23	C	502	CLA	C2D-C1D-ND	4.70	114.78	110.13
23	a	411	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	506	CLA	CHC-C4B-NB	4.70	131.10	124.05
23	b	619	CLA	C2D-C1D-ND	4.69	114.77	110.13
23	b	604	CLA	C2B-C1B-NB	4.68	115.18	110.33
23	C	502	CLA	CAC-C3C-C4C	4.68	130.88	124.79
23	b	613	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
36	D	408	LHG	O8-C23-C24	4.67	126.08	111.83
23	c	911	CLA	C4A-NA-C1A	4.67	108.81	106.68
23	b	606	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
23	C	501	CLA	CHD-C4C-C3C	-4.67	117.97	124.77
25	K	101	BCR	C37-C22-C23	4.67	125.22	118.09
23	B	611	CLA	CHB-C4A-NA	4.67	131.13	124.40
23	C	502	CLA	C2C-C1C-NC	4.66	114.88	109.98
23	b	610	CLA	CAC-C3C-C4C	4.66	130.85	124.79
23	d	402	CLA	C4D-CHA-C1A	-4.66	115.69	121.24
23	B	603	CLA	CHD-C4C-C3C	-4.66	117.98	124.77
23	b	618	CLA	CHC-C4B-NB	4.65	131.03	124.05
23	b	612	CLA	O2D-CGD-CBD	4.65	119.36	111.23
23	c	908	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
23	b	607	CLA	C2D-C1D-ND	4.64	114.72	110.13
23	b	605	CLA	C3B-C2B-C1B	-4.64	101.69	107.17
23	B	606	CLA	C2B-C1B-NB	4.64	115.14	110.33
23	C	512	CLA	O2D-CGD-CBD	4.64	119.34	111.23
23	C	507	CLA	CHD-C4C-C3C	-4.64	118.02	124.77
23	d	403	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
23	c	904	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	A	405	CLA	C1D-CHD-C4C	-4.62	116.20	126.02
23	A	410	CLA	C4A-NA-C1A	4.62	108.79	106.68
23	b	609	CLA	C2D-C1D-ND	4.62	114.69	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CHD-C4C-C3C	-4.61	118.05	124.77
23	C	510	CLA	C2B-C1B-NB	4.61	115.11	110.33
23	C	511	CLA	C2B-C1B-NB	4.61	115.11	110.33
23	c	910	CLA	C2C-C1C-NC	4.61	114.82	109.98
23	b	615	CLA	C2D-C1D-ND	4.60	114.68	110.13
23	C	508	CLA	C4D-CHA-C1A	-4.60	115.76	121.24
23	b	615	CLA	C2C-C1C-NC	4.59	114.81	109.98
33	C	521	HTG	C1'-S1-C1	4.59	110.37	100.45
23	B	617	CLA	O2D-CGD-O1D	-4.59	114.91	123.85
23	B	604	CLA	O2D-CGD-O1D	-4.59	114.91	123.85
23	c	909	CLA	C2B-C1B-NB	4.59	115.09	110.33
23	b	611	CLA	CHD-C4C-C3C	-4.59	118.08	124.77
23	c	913	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
25	k	102	BCR	C7-C8-C9	-4.59	119.44	126.23
23	B	613	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	C	512	CLA	C1-O2A-CGA	4.58	127.75	116.65
23	B	604	CLA	CHD-C4C-NC	4.58	131.33	124.23
23	d	402	CLA	O2D-CGD-O1D	-4.58	114.93	123.85
23	a	411	CLA	CHD-C4C-C3C	-4.58	118.10	124.77
23	a	414	CLA	C2D-C1D-ND	4.58	114.66	110.13
23	a	409	CLA	C2C-C1C-NC	4.58	114.79	109.98
23	C	512	CLA	C4D-CHA-C1A	-4.57	115.79	121.24
23	B	604	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
23	b	607	CLA	CHD-C4C-C3C	-4.57	118.11	124.77
36	L	101	LHG	O7-C7-O9	-4.57	113.03	123.70
23	b	608	CLA	O2D-CGD-CBD	4.57	119.21	111.23
23	a	414	CLA	CHC-C4B-NB	4.56	130.89	124.05
23	c	914	CLA	CHD-C4C-C3C	-4.56	118.13	124.77
23	B	613	CLA	CHD-C1D-ND	-4.55	118.39	124.80
24	a	412	PHO	C4D-ND-C1D	-4.55	103.42	108.87
23	d	402	CLA	C4-C3-C5	4.55	123.13	115.23
27	b	623	LMG	O8-C28-C29	4.55	125.71	111.83
23	c	913	CLA	C1-O2A-CGA	4.55	127.66	116.65
23	b	613	CLA	C3B-C2B-C1B	-4.54	101.81	107.17
23	B	615	CLA	C2D-C1D-ND	4.54	114.62	110.13
23	C	504	CLA	C2D-C1D-ND	4.54	114.62	110.13
23	b	618	CLA	C1D-CHD-C4C	-4.54	116.37	126.02
26	B	621	SQD	O7-S-C6	4.53	113.52	106.76
33	d	401	HTG	C1'-S1-C1	4.53	110.23	100.45
23	d	403	CLA	CMB-C2B-C1B	4.53	132.31	125.42
23	a	410	CLA	C1D-CHD-C4C	-4.53	116.40	126.02
23	B	608	CLA	C3B-C4B-NB	4.51	114.55	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CBC-CAC-C3C	-4.51	100.21	112.42
23	c	910	CLA	CHC-C4B-NB	4.50	130.80	124.05
23	B	615	CLA	CHD-C4C-C3C	-4.50	118.22	124.77
23	A	407	CLA	C4A-NA-C1A	4.50	108.73	106.68
23	B	615	CLA	O2D-CGD-CBD	4.50	119.09	111.23
23	C	511	CLA	C2C-C1C-NC	4.49	114.70	109.98
23	C	508	CLA	O2D-CGD-CBD	4.49	119.07	111.23
23	c	903	CLA	C1D-CHD-C4C	-4.47	116.52	126.02
23	c	909	CLA	C1D-ND-C4D	-4.47	103.18	106.31
23	b	614	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
23	C	511	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
23	B	615	CLA	C2C-C1C-NC	4.47	114.67	109.98
23	c	910	CLA	C3B-C2B-C1B	-4.47	101.91	107.17
23	c	902	CLA	CMD-C2D-C1D	4.46	132.59	124.73
23	B	617	CLA	CHC-C4B-NB	4.46	130.75	124.05
23	B	602	CLA	CHD-C1D-ND	-4.46	118.53	124.80
23	b	610	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
23	C	508	CLA	C1C-C2C-C3C	-4.46	102.29	106.98
26	A	418	SQD	O48-C23-C24	4.46	125.43	111.83
25	d	404	BCR	C15-C14-C13	-4.46	121.03	127.28
23	B	609	CLA	CHD-C1D-ND	-4.46	118.53	124.80
23	D	403	CLA	C1C-C2C-C3C	-4.46	102.29	106.98
23	B	612	CLA	CHC-C4B-NB	4.45	130.73	124.05
25	D	404	BCR	C40-C30-C25	-4.45	103.27	110.24
23	C	513	CLA	C3B-C2B-C1B	-4.45	101.93	107.17
23	B	613	CLA	C2C-C1C-NC	4.45	114.65	109.98
23	C	512	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
23	A	406	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
36	d	407	LHG	O8-C23-O10	-4.44	112.52	123.63
23	a	409	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
23	C	512	CLA	C1-C2-C3	-4.44	118.92	126.20
23	D	403	CLA	C4D-CHA-C1A	-4.43	115.96	121.24
23	C	506	CLA	C2D-C1D-ND	4.43	114.51	110.13
23	a	410	CLA	C3B-C2B-C1B	-4.43	101.94	107.17
23	A	406	CLA	O2D-CGD-CBD	4.43	118.98	111.23
23	b	614	CLA	C2C-C1C-NC	4.43	114.63	109.98
25	D	404	BCR	C29-C30-C25	4.42	116.87	110.44
23	b	610	CLA	C4A-NA-C1A	4.42	108.70	106.68
23	B	614	CLA	C2C-C1C-NC	4.42	114.63	109.98
25	b	620	BCR	C7-C8-C9	-4.42	119.69	126.23
23	C	511	CLA	O2D-CGD-CBD	4.42	118.96	111.23
23	C	501	CLA	CMB-C2B-C1B	4.42	132.15	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
23	B	612	CLA	C1D-CHD-C4C	-4.42	116.63	126.02
26	A	418	SQD	O9-S-C6	4.42	113.35	106.76
25	t	101	BCR	C11-C10-C9	-4.41	121.09	127.28
23	c	913	CLA	C4D-CHA-C1A	-4.41	115.98	121.24
23	B	607	CLA	O2D-CGD-O1D	-4.41	115.26	123.85
23	A	410	CLA	CHD-C4C-NC	4.41	131.07	124.23
23	C	506	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	c	912	CLA	O2D-CGD-CBD	4.40	118.93	111.23
23	A	406	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
23	c	902	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
23	C	501	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
23	d	403	CLA	C2C-C1C-NC	4.39	114.59	109.98
23	B	616	CLA	CHA-C4D-ND	4.39	141.60	132.55
23	b	605	CLA	O2D-CGD-O1D	-4.38	115.32	123.85
23	c	905	CLA	C2C-C1C-NC	4.38	114.58	109.98
23	C	511	CLA	C3B-C4B-NB	4.38	114.44	110.53
23	b	608	CLA	CMD-C2D-C1D	4.36	132.41	124.73
23	C	505	CLA	C1D-ND-C4D	4.36	109.37	106.31
23	c	911	CLA	C4D-CHA-C1A	-4.36	116.04	121.24
23	C	503	CLA	C1C-C2C-C3C	-4.36	102.40	106.98
34	d	406	DGD	C3D-C4D-C5D	4.35	116.43	109.81
23	B	608	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
23	c	908	CLA	C1C-C2C-C3C	-4.34	102.41	106.98
23	A	407	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
23	C	502	CLA	C2B-C1B-NB	4.34	114.83	110.33
23	a	414	CLA	O2D-CGD-CBD	4.34	118.81	111.23
23	b	618	CLA	C2D-C1D-ND	4.33	114.41	110.13
23	c	911	CLA	C1D-ND-C4D	-4.33	103.27	106.31
27	d	410	LMG	O7-C10-C11	4.33	120.85	111.48
23	D	403	CLA	C2B-C1B-NB	4.33	114.81	110.33
23	B	612	CLA	O2D-CGD-O1D	-4.33	115.42	123.85
23	C	501	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
23	B	606	CLA	CHD-C4C-C3C	-4.32	118.47	124.77
23	b	617	CLA	CHD-C4C-C3C	-4.32	118.47	124.77
23	C	507	CLA	C1C-C2C-C3C	-4.32	102.43	106.98
23	B	617	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
30	a	402	LMT	C1-O1'-C1'	4.32	121.06	113.68
23	C	503	CLA	CHA-C4D-ND	4.32	141.46	132.55
23	B	613	CLA	CHC-C4B-NB	4.32	130.53	124.05
23	b	614	CLA	C1-C2-C3	-4.32	119.12	126.20
23	B	602	CLA	C1-O2A-CGA	4.32	127.11	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C3B-C4B-NB	4.32	114.38	110.53
23	D	402	CLA	CAC-C3C-C4C	4.32	130.41	124.79
23	b	611	CLA	C2D-C1D-ND	4.31	114.40	110.13
23	B	612	CLA	CMC-C2C-C1C	4.31	131.77	125.03
23	D	403	CLA	CED-O2D-CGD	4.31	125.69	115.92
23	b	604	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
23	D	403	CLA	C3B-C2B-C1B	-4.30	102.09	107.17
23	C	509	CLA	C2B-C1B-NB	4.30	114.79	110.33
23	c	902	CLA	CHD-C1D-ND	-4.30	118.75	124.80
23	B	605	CLA	C3C-C4C-NC	4.30	115.94	110.43
23	B	602	CLA	C1C-C2C-C3C	-4.30	102.46	106.98
34	h	102	DGD	C3E-C4E-C5E	-4.29	102.44	110.23
23	C	512	CLA	C2D-C1D-ND	4.29	114.37	110.13
34	H	102	DGD	O1G-C1A-O1A	-4.29	112.90	123.63
23	d	403	CLA	C1D-ND-C4D	-4.29	103.31	106.31
23	b	614	CLA	CHD-C4C-C3C	-4.28	118.53	124.77
23	B	616	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
23	C	509	CLA	CHC-C4B-NB	4.28	130.47	124.05
23	a	411	CLA	C3C-C4C-NC	4.28	115.91	110.43
23	c	905	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
23	b	618	CLA	O2D-CGD-CBD	4.28	118.71	111.23
23	a	410	CLA	CHC-C4B-NB	4.28	130.46	124.05
23	c	907	CLA	CHD-C1D-ND	-4.27	118.79	124.80
23	B	616	CLA	C2D-C1D-ND	4.27	114.36	110.13
30	b	624	LMT	O5'-C5'-C4'	4.27	118.55	109.72
23	B	604	CLA	CMC-C2C-C1C	4.27	131.70	125.03
26	D	407	SQD	C1-O5-C5	-4.27	105.39	113.72
23	B	602	CLA	C2C-C1C-NC	4.27	114.46	109.98
26	A	418	SQD	O6-C1-C2	4.26	114.74	108.27
23	B	606	CLA	CHC-C4B-NB	4.26	130.44	124.05
23	C	512	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	c	902	CLA	CMB-C2B-C1B	4.26	131.90	125.42
23	b	608	CLA	C3C-C4C-NC	4.25	115.88	110.43
23	C	501	CLA	C2D-C1D-ND	4.25	114.33	110.13
23	c	913	CLA	CMB-C2B-C1B	4.25	131.89	125.42
23	B	607	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
23	a	414	CLA	CHD-C1D-ND	-4.25	118.82	124.80
23	c	910	CLA	C2D-C1D-ND	4.25	114.33	110.13
33	B	630	HTG	C1'-S1-C1	4.24	109.60	100.45
23	B	615	CLA	CHC-C4B-NB	4.24	130.40	124.05
23	C	503	CLA	CHD-C1D-ND	-4.24	118.84	124.80
25	K	102	BCR	C7-C8-C9	-4.23	119.97	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	O2D-CGD-CBD	4.23	118.63	111.23
23	B	610	CLA	C2D-C1D-ND	4.23	114.32	110.13
23	C	508	CLA	C2D-C1D-ND	4.23	114.31	110.13
25	K	101	BCR	C38-C26-C25	-4.22	119.88	124.48
23	B	602	CLA	CMD-C2D-C1D	4.22	132.16	124.73
25	d	404	BCR	C38-C26-C25	-4.22	119.88	124.48
25	c	915	BCR	C33-C5-C6	-4.22	119.88	124.48
23	b	609	CLA	C2B-C1B-NB	4.21	114.70	110.33
37	F	101	HEM	CAD-C3D-C4D	4.21	132.04	124.70
23	c	906	CLA	C2C-C1C-NC	4.21	114.41	109.98
23	a	414	CLA	C1C-C2C-C3C	-4.21	102.55	106.98
23	C	503	CLA	CHC-C4B-NB	4.21	130.36	124.05
26	D	407	SQD	O47-C7-C8	4.21	120.58	111.48
23	c	913	CLA	C2D-C1D-ND	4.20	114.29	110.13
23	c	907	CLA	C3D-C2D-C1D	-4.20	100.09	105.83
23	B	612	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
23	B	608	CLA	C2D-C1D-ND	4.20	114.28	110.13
23	B	606	CLA	CHA-C4D-ND	4.20	141.22	132.55
23	b	612	CLA	C4D-CHA-C1A	-4.20	116.24	121.24
23	c	912	CLA	O2D-CGD-O1D	-4.19	115.69	123.85
23	C	511	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
23	C	513	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
23	b	608	CLA	CHD-C1D-ND	-4.19	118.91	124.80
23	c	909	CLA	C4D-CHA-C1A	-4.19	116.25	121.24
23	B	616	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
23	b	608	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
23	b	608	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
27	b	623	LMG	O8-C28-O10	-4.18	113.17	123.63
25	d	404	BCR	C24-C23-C22	-4.18	120.05	126.23
23	d	403	CLA	CHD-C1D-ND	-4.18	118.92	124.80
23	c	906	CLA	CAC-C3C-C4C	4.17	130.22	124.79
23	D	403	CLA	C2C-C1C-NC	4.17	114.36	109.98
23	c	904	CLA	C1-C2-C3	-4.17	119.36	126.20
23	c	904	CLA	C2D-C1D-ND	4.17	114.25	110.13
23	c	908	CLA	C2D-C1D-ND	4.16	114.25	110.13
23	B	607	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
23	a	410	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
26	B	621	SQD	O48-C23-C24	4.15	124.50	111.83
27	b	623	LMG	O7-C10-C11	4.15	120.46	111.48
26	D	407	SQD	C1-C2-C3	-4.15	101.28	110.01
23	B	613	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	B	602	CLA	C3B-C2B-C1B	-4.15	102.28	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	904	CLA	C2C-C1C-NC	4.14	114.33	109.98
23	A	406	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
23	b	610	CLA	C2C-C1C-NC	4.14	114.33	109.98
23	B	606	CLA	C4D-CHA-C1A	-4.14	116.31	121.24
23	b	619	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
23	C	501	CLA	C4D-CHA-C1A	-4.13	116.31	121.24
23	A	410	CLA	C1C-C2C-C3C	-4.13	102.63	106.98
23	b	617	CLA	C2C-C1C-NC	4.13	114.32	109.98
23	C	507	CLA	C2C-C1C-NC	4.13	114.32	109.98
23	D	402	CLA	CHB-C1B-C2B	-4.13	115.44	127.43
23	B	604	CLA	C2D-C1D-ND	4.13	114.21	110.13
34	c	917	DGD	O3G-C3G-C2G	-4.13	100.77	110.82
23	a	414	CLA	C2B-C1B-NB	4.13	114.61	110.33
23	C	502	CLA	C3B-C2B-C1B	-4.13	102.31	107.17
23	b	605	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
23	C	503	CLA	C2B-C1B-NB	4.12	114.60	110.33
23	b	614	CLA	CHA-C4D-ND	4.12	141.06	132.55
26	a	401	SQD	O47-C7-C8	4.12	120.40	111.48
23	A	407	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
23	B	612	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
23	C	505	CLA	C4D-CHA-C1A	-4.12	116.33	121.24
23	C	505	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
23	B	617	CLA	C2B-C1B-NB	4.11	114.59	110.33
23	B	614	CLA	CHD-C1D-ND	-4.11	119.01	124.80
23	c	912	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
23	B	611	CLA	CAA-CBA-CGA	-4.11	101.53	113.21
23	C	512	CLA	CHA-C4D-ND	4.11	141.03	132.55
23	b	604	CLA	C2C-C1C-NC	4.11	114.30	109.98
23	A	410	CLA	C3B-C2B-C1B	-4.10	102.33	107.17
23	c	905	CLA	C1C-C2C-C3C	-4.10	102.66	106.98
23	C	507	CLA	C2B-C1B-NB	4.09	114.57	110.33
27	C	519	LMG	O7-C10-C11	4.08	120.31	111.48
23	B	616	CLA	C2B-C1B-NB	4.08	114.56	110.33
23	c	904	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
23	C	511	CLA	CHD-C4C-C3C	-4.07	118.83	124.77
23	b	607	CLA	O2D-CGD-CBD	4.07	118.35	111.23
23	b	613	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
23	B	612	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
23	b	618	CLA	CHD-C4C-C3C	-4.07	118.84	124.77
23	b	618	CLA	O2D-CGD-O1D	-4.07	115.93	123.85
36	d	407	LHG	O8-C23-C24	4.07	124.24	111.83
24	A	409	PHO	O2D-CGD-CBD	4.07	115.41	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C1D-ND-C4D	4.06	109.16	106.31
23	c	903	CLA	C2C-C1C-NC	4.06	114.24	109.98
23	d	403	CLA	C3B-C4B-NB	4.06	114.15	110.53
26	L	103	SQD	O9-S-C6	4.05	112.81	106.76
24	a	412	PHO	C3D-C4D-ND	4.05	112.90	107.71
23	b	608	CLA	CMC-C2C-C1C	4.05	131.37	125.03
23	b	614	CLA	C4D-CHA-C1A	-4.05	116.41	121.24
23	b	605	CLA	C2C-C1C-NC	4.05	114.23	109.98
23	B	610	CLA	C4D-CHA-C1A	-4.05	116.42	121.24
24	A	409	PHO	C4B-NB-C1B	-4.05	102.92	108.82
23	B	615	CLA	C3B-C2B-C1B	-4.05	102.40	107.17
23	b	604	CLA	C3B-C2B-C1B	-4.05	102.40	107.17
23	C	511	CLA	C1-O2A-CGA	4.04	126.44	116.65
23	c	906	CLA	O2D-CGD-CBD	4.04	118.30	111.23
23	B	602	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
23	C	512	CLA	C3B-C2B-C1B	-4.04	102.41	107.17
23	c	912	CLA	C4D-CHA-C1A	-4.04	116.43	121.24
23	B	609	CLA	CAC-C3C-C4C	4.04	130.04	124.79
23	c	903	CLA	C4D-CHA-C1A	-4.04	116.43	121.24
27	b	623	LMG	O7-C10-O9	-4.03	114.28	123.70
23	C	510	CLA	CAC-C3C-C4C	4.03	130.03	124.79
23	B	612	CLA	CHA-C4D-ND	4.03	140.86	132.55
25	T	101	BCR	C20-C21-C22	-4.03	121.63	127.28
23	B	602	CLA	CHD-C4C-NC	4.03	130.47	124.23
23	c	906	CLA	C2D-C1D-ND	4.02	114.11	110.13
23	b	606	CLA	C3D-C2D-C1D	-4.02	100.35	105.83
23	B	605	CLA	O2D-CGD-CBD	4.02	118.25	111.23
23	c	913	CLA	C2B-C1B-NB	4.02	114.49	110.33
25	d	404	BCR	C16-C15-C14	-4.01	115.30	123.52
23	C	503	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
23	b	615	CLA	C1-C2-C3	-4.01	119.62	126.20
23	b	608	CLA	C4D-CHA-C1A	-4.01	116.46	121.24
23	C	505	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
23	c	908	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
23	c	904	CLA	C1C-C2C-C3C	-4.01	102.77	106.98
23	b	607	CLA	O2D-CGD-O1D	-4.01	116.05	123.85
27	c	920	LMG	O7-C10-C11	4.01	120.15	111.48
23	A	406	CLA	C1D-ND-C4D	4.00	109.12	106.31
23	B	614	CLA	CHC-C4B-NB	4.00	130.06	124.05
23	b	609	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
23	C	511	CLA	C3B-C2B-C1B	-4.00	102.45	107.17
23	b	604	CLA	C2D-C1D-ND	4.00	114.09	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C1C-C2C-C3C	-4.00	102.78	106.98
23	b	605	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
37	f	101	HEM	CBA-CAA-C2A	-4.00	101.48	112.53
23	B	608	CLA	CBC-CAC-C3C	-4.00	101.58	112.42
23	b	614	CLA	C2D-C1D-ND	4.00	114.08	110.13
34	C	518	DGD	O3G-C3G-C2G	-4.00	101.10	110.82
23	b	609	CLA	C2C-C1C-NC	3.99	114.18	109.98
23	B	609	CLA	C1D-ND-C4D	-3.99	103.51	106.31
36	L	101	LHG	O4-P-O5	3.99	131.02	112.44
23	b	617	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
30	m	102	LMT	O1'-C1'-C2'	3.99	114.33	108.27
23	b	619	CLA	C2C-C1C-NC	3.99	114.17	109.98
23	C	504	CLA	O2D-CGD-CBD	3.98	118.19	111.23
23	c	914	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
25	D	404	BCR	C24-C23-C22	-3.98	120.34	126.23
37	F	101	HEM	CMD-C2D-C1D	3.98	131.25	125.03
23	b	611	CLA	O2D-CGD-O1D	-3.98	116.11	123.85
23	B	612	CLA	C2D-C1D-ND	3.98	114.06	110.13
23	a	414	CLA	C3B-C4B-NB	3.98	114.08	110.53
23	c	910	CLA	C1C-C2C-C3C	-3.98	102.80	106.98
23	C	506	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
23	b	609	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
23	b	614	CLA	C2B-C1B-NB	3.97	114.45	110.33
23	b	616	CLA	C2B-C1B-NB	3.97	114.44	110.33
25	B	618	BCR	C33-C5-C6	-3.96	120.16	124.48
23	b	614	CLA	C4B-C3B-C2B	-3.96	102.37	107.30
23	B	616	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
23	C	505	CLA	CAC-C3C-C4C	3.96	129.94	124.79
23	B	607	CLA	C1D-ND-C4D	-3.96	103.54	106.31
23	B	608	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
23	c	907	CLA	CHB-C4A-NA	3.96	130.11	124.40
23	c	914	CLA	C2B-C1B-NB	3.96	114.43	110.33
23	B	603	CLA	CHA-C4D-ND	3.95	140.70	132.55
23	c	913	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
23	C	513	CLA	C2D-C1D-ND	3.95	114.03	110.13
23	B	615	CLA	O2D-CGD-O1D	-3.95	116.16	123.85
23	c	906	CLA	CBC-CAC-C3C	-3.94	101.73	112.42
24	a	412	PHO	CMB-C2B-C3B	3.94	132.56	124.68
23	c	905	CLA	O2D-CGD-CBD	3.94	118.12	111.23
23	b	619	CLA	O2A-CGA-CBA	3.94	123.85	111.83
23	b	618	CLA	C3D-C2D-C1D	-3.94	100.45	105.83
23	b	611	CLA	C3D-C2D-C1D	-3.94	100.46	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	619	CLA	CAC-C3C-C4C	3.93	129.91	124.79
23	B	617	CLA	O2D-CGD-CBD	3.93	118.11	111.23
23	C	502	CLA	CHA-C4D-ND	3.93	140.65	132.55
23	b	612	CLA	C3B-C2B-C1B	-3.93	102.54	107.17
23	B	605	CLA	CED-O2D-CGD	3.93	124.83	115.92
23	C	504	CLA	CHD-C1D-ND	-3.93	119.28	124.80
27	c	921	LMG	O7-C10-C11	3.93	119.97	111.48
23	c	912	CLA	CHD-C4C-NC	3.93	130.32	124.23
23	c	909	CLA	C3B-C2B-C1B	-3.93	102.54	107.17
23	B	607	CLA	CHD-C4C-NC	3.93	130.32	124.23
23	d	403	CLA	CHD-C4C-C3C	-3.93	119.05	124.77
23	c	905	CLA	CAC-C3C-C4C	3.92	129.90	124.79
23	b	619	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	C	506	CLA	C3B-C2B-C1B	-3.92	102.55	107.17
34	C	516	DGD	O3G-C3G-C2G	-3.92	101.29	110.82
23	B	612	CLA	CHD-C4C-NC	3.92	130.31	124.23
26	A	412	SQD	C45-O47-C7	-3.92	108.42	117.80
23	C	503	CLA	CMD-C2D-C1D	3.91	131.62	124.73
30	A	419	LMT	C1'-O5'-C5'	3.91	121.36	113.72
30	F	102	LMT	O4'-C4B-C5B	3.90	118.94	109.32
23	C	501	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	C	506	CLA	C4D-CHA-C1A	-3.90	116.59	121.24
37	f	101	HEM	CBD-CAD-C3D	-3.90	101.75	112.53
23	C	510	CLA	C3B-C4B-NB	3.90	114.01	110.53
23	D	402	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
34	C	518	DGD	O2G-C1B-C2B	3.90	119.91	111.48
23	A	405	CLA	C3B-C2B-C1B	-3.90	102.58	107.17
34	C	516	DGD	O2G-C1B-C2B	3.89	119.90	111.48
23	C	510	CLA	C2D-C1D-ND	3.89	113.98	110.13
23	A	406	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
23	a	410	CLA	C2B-C1B-NB	3.89	114.36	110.33
23	c	908	CLA	CHC-C4B-NB	3.88	129.88	124.05
23	c	904	CLA	CHA-C4D-ND	3.88	140.56	132.55
23	b	614	CLA	O2D-CGD-CBD	3.88	118.01	111.23
23	C	513	CLA	CHA-C4D-ND	3.87	140.54	132.55
23	b	614	CLA	C3B-C4B-NB	3.87	113.99	110.53
23	C	513	CLA	CHC-C4B-NB	3.87	129.85	124.05
23	B	612	CLA	C1-C2-C3	-3.87	119.86	126.20
23	c	910	CLA	C1D-ND-C4D	-3.86	103.60	106.31
27	C	519	LMG	O8-C28-C29	3.86	123.60	111.83
23	C	510	CLA	CHD-C1D-ND	-3.86	119.37	124.80
23	b	615	CLA	C3D-C2D-C1D	-3.86	100.57	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	913	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	C	513	CLA	CHD-C4C-C3C	-3.86	119.15	124.77
30	A	419	LMT	O2'-C2'-C1'	3.85	119.26	110.08
23	C	501	CLA	CAC-C3C-C4C	3.85	129.80	124.79
27	D	411	LMG	O8-C28-O10	-3.85	113.99	123.63
23	B	602	CLA	CHA-C4D-ND	3.85	140.49	132.55
23	b	605	CLA	C2B-C1B-NB	3.85	114.32	110.33
23	A	406	CLA	CHC-C4B-NB	3.85	129.82	124.05
23	b	606	CLA	CHC-C4B-NB	3.85	129.82	124.05
38	H	101	RRX	C7-C8-C9	-3.84	120.55	126.23
34	d	406	DGD	O2G-C1B-C2B	3.84	119.80	111.48
23	b	611	CLA	C2B-C1B-NB	3.84	114.31	110.33
23	B	609	CLA	C3B-C2B-C1B	-3.84	102.64	107.17
23	D	402	CLA	CHD-C4C-NC	3.84	130.18	124.23
23	b	616	CLA	CMD-C2D-C1D	3.84	131.48	124.73
23	A	407	CLA	C3B-C4B-NB	3.84	113.95	110.53
23	B	617	CLA	C1-O2A-CGA	3.83	125.93	116.65
23	C	503	CLA	C4A-NA-C1A	3.83	108.43	106.68
25	B	618	BCR	C15-C14-C13	-3.83	121.90	127.28
23	a	410	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
23	B	610	CLA	C1-C2-C3	-3.83	119.92	126.20
23	b	615	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
25	D	404	BCR	C38-C26-C25	-3.83	120.31	124.48
23	C	508	CLA	C1D-ND-C4D	-3.83	103.63	106.31
30	m	101	LMT	C3'-C4'-C5'	-3.83	102.44	110.93
23	A	410	CLA	CHC-C4B-NB	3.83	129.79	124.05
23	A	407	CLA	CMD-C2D-C1D	3.82	131.46	124.73
23	B	605	CLA	CHC-C4B-NB	3.82	129.78	124.05
23	a	414	CLA	C1-C2-C3	-3.82	119.94	126.20
37	V	201	HEM	CBD-CAD-C3D	-3.82	101.97	112.53
23	a	411	CLA	C4D-CHA-C1A	-3.82	116.69	121.24
23	d	403	CLA	C4A-NA-C1A	3.82	108.42	106.68
23	C	510	CLA	C4D-CHA-C1A	-3.81	116.69	121.24
23	C	510	CLA	C3B-C2B-C1B	-3.81	102.67	107.17
30	t	102	LMT	O1'-C1'-C2'	3.81	114.06	108.27
26	A	418	SQD	O47-C7-C8	3.81	119.72	111.48
23	b	613	CLA	C4D-CHA-C1A	-3.81	116.70	121.24
23	B	603	CLA	C3D-C2D-C1D	-3.81	100.64	105.83
23	b	610	CLA	CHA-C4D-ND	3.81	140.40	132.55
23	B	609	CLA	O2D-CGD-O1D	-3.81	116.44	123.85
23	c	911	CLA	C2C-C1C-NC	3.80	113.98	109.98
23	c	914	CLA	C4D-CHA-C1A	-3.80	116.71	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	402	LMT	O1'-C1'-C2'	3.80	114.05	108.27
34	c	919	DGD	C6B-C5B-C4B	-3.80	95.15	114.37
23	B	611	CLA	O2A-CGA-O1A	-3.80	114.12	123.63
23	b	607	CLA	C6-C5-C3	-3.80	104.21	113.47
30	B	623	LMT	C1B-O5B-C5B	3.80	121.13	113.72
28	a	419	PL9	C37-C38-C39	-3.79	118.94	127.62
23	c	906	CLA	C2B-C1B-NB	3.79	114.26	110.33
23	b	618	CLA	CAC-C3C-C4C	3.79	129.72	124.79
24	A	409	PHO	C1-C2-C3	-3.79	119.99	126.20
23	B	611	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
23	B	615	CLA	C4-C3-C5	3.79	121.80	115.23
23	c	907	CLA	CMB-C2B-C1B	3.78	131.18	125.42
23	C	508	CLA	C2C-C1C-NC	3.78	113.95	109.98
23	a	410	CLA	C4D-CHA-C1A	-3.78	116.74	121.24
23	a	410	CLA	CHD-C4C-NC	3.78	130.09	124.23
34	C	517	DGD	O2G-C1B-O1B	-3.77	114.89	123.70
23	C	513	CLA	C4D-CHA-C1A	-3.77	116.75	121.24
23	B	610	CLA	O2D-CGD-CBD	3.77	117.82	111.23
23	b	617	CLA	O2A-CGA-O1A	-3.76	114.22	123.63
23	d	403	CLA	CMD-C2D-C1D	3.76	131.35	124.73
23	a	409	CLA	C1D-ND-C4D	-3.76	103.67	106.31
23	C	506	CLA	C3C-C4C-NC	3.76	115.24	110.43
23	c	910	CLA	C3B-C4B-NB	3.76	113.88	110.53
23	B	602	CLA	O2D-CGD-O1D	-3.75	116.54	123.85
23	d	403	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
23	C	511	CLA	CMB-C2B-C1B	3.75	131.13	125.42
23	C	504	CLA	C4-C3-C5	3.75	121.74	115.23
23	B	611	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
23	c	911	CLA	O2D-CGD-CBD	3.75	117.78	111.23
23	D	402	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
23	C	504	CLA	C3D-C2D-C1D	-3.75	100.72	105.83
23	c	912	CLA	C2B-C1B-NB	3.75	114.21	110.33
23	b	604	CLA	C4D-CHA-C1A	-3.75	116.77	121.24
23	b	606	CLA	CHD-C4C-NC	3.75	130.04	124.23
23	B	604	CLA	C4D-CHA-C1A	-3.75	116.78	121.24
23	A	405	CLA	C3B-C4B-NB	3.74	113.87	110.53
23	b	605	CLA	CHD-C4C-C3C	-3.74	119.32	124.77
23	c	911	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
26	f	102	SQD	O9-S-C6	3.74	112.38	106.73
23	c	907	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
23	b	613	CLA	O2D-CGD-CBD	3.74	117.77	111.23
35	a	408	BCT	O3-C-O1	-3.74	110.11	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	411	CLA	C4-C3-C5	3.74	121.72	115.23
23	c	907	CLA	CHA-C4D-ND	3.74	140.26	132.55
23	B	607	CLA	CHC-C4B-NB	3.74	129.66	124.05
23	B	607	CLA	O2D-CGD-CBD	3.74	117.76	111.23
23	b	617	CLA	CMD-C2D-C1D	3.73	131.31	124.73
36	a	417	LHG	O7-C7-C8	3.73	119.56	111.48
23	C	512	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
23	C	502	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
23	c	905	CLA	C4B-C3B-C2B	-3.73	102.66	107.30
23	b	613	CLA	CHD-C4C-C3C	-3.73	119.34	124.77
23	A	407	CLA	CMC-C2C-C1C	3.72	130.85	125.03
23	c	908	CLA	C4-C3-C5	3.72	121.68	115.23
23	C	513	CLA	C3D-C2D-C1D	-3.71	100.76	105.83
30	F	102	LMT	C1B-O5B-C5B	3.71	120.97	113.72
23	B	604	CLA	C1D-CHD-C4C	-3.71	118.13	126.02
23	B	606	CLA	C3D-C2D-C1D	-3.71	100.77	105.83
23	c	907	CLA	CMC-C2C-C1C	3.71	130.83	125.03
23	b	614	CLA	CBC-CAC-C3C	-3.71	102.37	112.42
23	b	609	CLA	CHD-C1D-ND	-3.71	119.58	124.80
23	c	908	CLA	CHD-C1D-ND	-3.71	119.58	124.80
25	b	622	BCR	C24-C23-C22	-3.71	120.75	126.23
28	a	419	PL9	C25-C24-C26	3.70	121.66	115.23
23	d	402	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
23	b	608	CLA	CHC-C4B-NB	3.70	129.60	124.05
23	A	405	CLA	C1D-ND-C4D	-3.70	103.72	106.31
23	C	512	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
23	C	513	CLA	C2B-C1B-NB	3.70	114.16	110.33
23	C	504	CLA	O2D-CGD-O1D	-3.70	116.66	123.85
28	d	405	PL9	C15-C14-C16	3.70	121.64	115.23
30	M	101	LMT	O1'-C1'-C2'	3.69	113.88	108.27
23	b	611	CLA	C4B-C3B-C2B	-3.69	102.71	107.30
25	t	101	BCR	C28-C27-C26	-3.69	107.48	114.06
23	C	503	CLA	O2D-CGD-CBD	3.69	117.68	111.23
23	a	409	CLA	CMB-C2B-C1B	3.69	131.03	125.42
23	b	609	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
23	b	607	CLA	C3C-C4C-NC	3.69	115.15	110.43
23	B	617	CLA	C3C-C4C-NC	3.69	115.15	110.43
23	B	606	CLA	O2A-CGA-O1A	-3.69	114.41	123.63
23	B	603	CLA	C4-C3-C5	3.69	121.62	115.23
23	A	410	CLA	C3D-C2D-C1D	-3.69	100.80	105.83
23	C	511	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
23	c	903	CLA	O2D-CGD-O1D	-3.68	116.68	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CMC-C2C-C1C	3.68	130.79	125.03
23	c	902	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
23	D	403	CLA	CAC-C3C-C4C	3.68	129.58	124.79
23	C	503	CLA	C2D-C1D-ND	3.68	113.77	110.13
23	b	605	CLA	CHD-C1D-ND	-3.68	119.63	124.80
23	B	602	CLA	C4D-CHA-C1A	-3.68	116.86	121.24
23	c	904	CLA	CHD-C4C-C3C	-3.68	119.41	124.77
23	C	512	CLA	C4-C3-C5	3.67	121.61	115.23
23	B	613	CLA	O2D-CGD-CBD	3.67	117.65	111.23
23	C	506	CLA	CHA-C4D-ND	3.67	140.13	132.55
23	b	617	CLA	C2B-C1B-NB	3.67	114.13	110.33
27	c	920	LMG	O8-C28-C29	3.67	123.03	111.83
23	d	403	CLA	C4-C3-C5	3.67	121.59	115.23
23	c	909	CLA	CMB-C2B-C1B	3.67	131.00	125.42
25	T	101	BCR	C35-C13-C12	3.67	123.69	118.09
23	c	912	CLA	C2D-C1D-ND	3.66	113.75	110.13
23	b	607	CLA	CHC-C4B-NB	3.66	129.53	124.05
23	b	619	CLA	O1D-CGD-CBD	-3.66	117.31	124.52
23	B	603	CLA	C2D-C1D-ND	3.65	113.74	110.13
23	b	611	CLA	C3B-C2B-C1B	-3.65	102.86	107.17
23	b	605	CLA	CHA-C4D-ND	3.65	140.08	132.55
23	B	614	CLA	C4D-CHA-C1A	-3.65	116.89	121.24
23	c	903	CLA	C3D-C2D-C1D	-3.65	100.85	105.83
23	C	504	CLA	C4B-C3B-C2B	-3.65	102.77	107.30
23	c	906	CLA	C3D-C2D-C1D	-3.65	100.86	105.83
23	c	914	CLA	O2D-CGD-CBD	3.64	117.60	111.23
23	A	407	CLA	C4D-CHA-C1A	-3.64	116.90	121.24
23	b	604	CLA	C1-O2A-CGA	3.64	125.47	116.65
23	B	604	CLA	CHD-C1D-ND	-3.64	119.67	124.80
23	c	913	CLA	C2C-C1C-NC	3.64	113.81	109.98
23	C	502	CLA	CMD-C2D-C1D	3.64	131.14	124.73
23	B	609	CLA	CHD-C4C-NC	3.64	129.87	124.23
23	A	405	CLA	C3D-C2D-C1D	-3.64	100.87	105.83
23	b	606	CLA	CHA-C4D-ND	3.63	140.05	132.55
23	c	908	CLA	CMB-C2B-C1B	3.63	130.95	125.42
26	D	407	SQD	C44-O6-C1	-3.63	106.02	113.80
23	C	509	CLA	CHD-C4C-C3C	-3.62	119.49	124.77
23	C	505	CLA	CHA-C4D-ND	3.62	140.03	132.55
23	C	501	CLA	C3B-C2B-C1B	-3.62	102.90	107.17
23	C	513	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
23	a	411	CLA	O2D-CGD-CBD	3.62	117.56	111.23
23	C	512	CLA	C2C-C1C-NC	3.62	113.78	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C1-C2-C3	-3.62	120.27	126.20
23	c	903	CLA	C1-C2-C3	-3.62	120.27	126.20
23	b	617	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	B	611	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
37	v	201	HEM	CBD-CAD-C3D	-3.61	102.56	112.53
23	c	911	CLA	C3D-C2D-C1D	-3.61	100.91	105.83
23	d	403	CLA	CHD-C4C-NC	3.61	129.82	124.23
26	A	412	SQD	O7-S-C6	-3.60	101.37	106.76
27	Z	101	LMG	C9-C8-C7	-3.60	103.38	111.78
26	D	407	SQD	O9-S-C6	3.60	112.13	106.76
23	d	403	CLA	O1D-CGD-CBD	-3.60	117.42	124.52
30	M	102	LMT	C1'-O5'-C5'	-3.60	106.69	113.72
26	D	407	SQD	O9-S-O7	-3.59	102.13	113.82
25	t	101	BCR	C35-C13-C12	3.59	123.58	118.09
23	A	405	CLA	CHD-C4C-C3C	-3.59	119.53	124.77
23	D	402	CLA	C2D-C1D-ND	3.59	113.68	110.13
23	c	910	CLA	CMD-C2D-C1D	3.59	131.05	124.73
23	B	615	CLA	CBC-CAC-C3C	-3.59	102.69	112.42
37	F	101	HEM	C4D-ND-C1D	3.59	109.45	105.21
23	B	613	CLA	CHD-C4C-C3C	-3.59	119.54	124.77
23	C	501	CLA	C2B-C1B-NB	3.59	114.05	110.33
23	A	407	CLA	C4-C3-C5	3.59	121.45	115.23
23	A	407	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
37	F	101	HEM	C3B-C2B-C1B	3.58	109.10	106.41
23	C	504	CLA	CAC-C3C-C4C	3.58	129.45	124.79
23	B	609	CLA	C3D-C2D-C1D	-3.58	100.94	105.83
23	b	604	CLA	CHA-C4D-ND	3.58	139.94	132.55
23	C	510	CLA	CMD-C2D-C1D	3.58	131.02	124.73
23	c	904	CLA	CHC-C4B-NB	3.57	129.41	124.05
23	c	912	CLA	C3B-C2B-C1B	-3.57	102.96	107.17
23	c	910	CLA	O2D-CGD-CBD	3.57	117.47	111.23
28	A	414	PL9	C3-C4-C5	3.57	123.02	118.57
36	D	410	LHG	O4-P-O5	3.57	129.05	112.44
23	b	619	CLA	CHD-C4C-NC	3.57	129.76	124.23
23	C	507	CLA	C3D-C2D-C1D	-3.57	100.96	105.83
23	c	902	CLA	C3B-C4B-NB	3.57	113.72	110.53
23	b	607	CLA	CHA-C4D-ND	3.56	139.90	132.55
23	c	908	CLA	CHD-C4C-NC	3.56	129.76	124.23
23	b	615	CLA	C3B-C2B-C1B	-3.56	102.97	107.17
23	A	410	CLA	CAC-C3C-C4C	3.56	129.43	124.79
25	b	621	BCR	C29-C30-C25	3.56	115.61	110.44
23	C	506	CLA	CAC-C3C-C4C	3.56	129.42	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C3B-C2B-C1B	-3.56	102.97	107.17
23	b	604	CLA	O2A-CGA-CBA	3.56	122.69	111.83
23	B	610	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
23	c	903	CLA	CHD-C4C-NC	3.56	129.75	124.23
23	c	911	CLA	CHC-C4B-NB	3.56	129.39	124.05
23	C	508	CLA	C4-C3-C5	3.55	121.40	115.23
25	b	620	BCR	C11-C10-C9	-3.55	122.29	127.28
23	c	907	CLA	C1D-CHD-C4C	-3.55	118.47	126.02
23	c	905	CLA	CHD-C4C-C3C	-3.55	119.59	124.77
33	B	625	HTG	C1'-S1-C1	3.55	108.12	100.45
23	B	602	CLA	C1D-CHD-C4C	-3.55	118.47	126.02
23	c	911	CLA	C4-C3-C5	3.55	121.39	115.23
23	C	508	CLA	C3B-C2B-C1B	-3.55	102.98	107.17
23	A	405	CLA	C2C-C1C-NC	3.55	113.71	109.98
23	b	604	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
23	b	612	CLA	CHD-C4C-C3C	-3.55	119.60	124.77
34	H	102	DGD	O1G-C1A-C2A	3.55	122.65	111.83
23	c	911	CLA	CHD-C4C-C3C	-3.55	119.60	124.77
23	b	609	CLA	O2D-CGD-CBD	3.54	117.43	111.23
24	a	413	PHO	C4-C3-C5	3.54	121.38	115.23
25	t	101	BCR	C38-C26-C25	-3.54	120.62	124.48
23	b	606	CLA	CAC-C3C-C4C	3.54	129.40	124.79
23	c	914	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
23	b	618	CLA	CMC-C2C-C1C	3.54	130.57	125.03
23	c	914	CLA	C2C-C1C-NC	3.54	113.70	109.98
23	A	407	CLA	CHA-C4D-ND	3.54	139.84	132.55
23	a	411	CLA	CMD-C2D-C1D	3.54	130.95	124.73
23	c	905	CLA	C3B-C4B-NB	3.53	113.69	110.53
23	b	614	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
23	b	607	CLA	C2B-C1B-NB	3.53	113.99	110.33
23	c	909	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
25	B	620	BCR	C15-C14-C13	-3.53	122.33	127.28
23	B	614	CLA	C2B-C1B-NB	3.53	113.98	110.33
25	B	619	BCR	C29-C30-C25	3.53	115.56	110.44
23	a	410	CLA	CBC-CAC-C3C	-3.52	102.87	112.42
23	a	414	CLA	C4-C3-C5	3.52	121.34	115.23
23	c	902	CLA	CHD-C4C-NC	3.52	129.68	124.23
38	H	101	RRX	C16-C15-C14	-3.51	116.33	123.52
23	B	605	CLA	C3D-C2D-C1D	-3.51	101.04	105.83
23	B	603	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
23	B	617	CLA	CHA-C4D-ND	3.51	139.79	132.55
23	C	505	CLA	CHC-C4B-NB	3.51	129.31	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	411	CLA	CHA-C4D-ND	3.51	139.78	132.55
23	C	510	CLA	C3D-C2D-C1D	-3.51	101.05	105.83
23	C	507	CLA	CHA-C4D-ND	3.50	139.78	132.55
23	B	608	CLA	CHD-C4C-C3C	-3.50	119.67	124.77
25	A	411	BCR	C15-C16-C17	-3.50	116.35	123.52
23	b	606	CLA	CMC-C2C-C1C	3.50	130.51	125.03
23	B	611	CLA	CMD-C2D-C1D	3.50	130.89	124.73
23	b	614	CLA	C1D-CHD-C4C	-3.50	118.58	126.02
23	c	907	CLA	CHB-C1B-NB	-3.50	118.80	124.05
23	b	611	CLA	C4D-CHA-C1A	-3.49	117.08	121.24
25	a	415	BCR	C28-C27-C26	-3.49	107.83	114.06
23	B	610	CLA	C3D-C2D-C1D	-3.49	101.07	105.83
23	b	614	CLA	C3D-C2D-C1D	-3.49	101.07	105.83
23	B	615	CLA	CHD-C4C-NC	3.49	129.64	124.23
23	b	605	CLA	CMB-C2B-C3B	3.49	134.75	126.55
25	K	102	BCR	C24-C23-C22	-3.48	121.08	126.23
25	D	404	BCR	C28-C27-C26	-3.48	107.85	114.06
23	b	607	CLA	C3B-C2B-C1B	-3.48	103.07	107.17
36	D	408	LHG	O4-P-O5	3.48	128.63	112.44
23	B	603	CLA	O2D-CGD-CBD	3.48	117.31	111.23
34	h	102	DGD	O1G-C1A-O1A	-3.47	114.94	123.63
25	a	415	BCR	C38-C26-C25	-3.47	120.69	124.48
23	c	914	CLA	CHA-C4D-ND	3.47	139.71	132.55
23	c	907	CLA	CHC-C4B-NB	3.47	129.26	124.05
23	B	611	CLA	C3B-C2B-C1B	-3.47	103.08	107.17
36	L	101	LHG	C6-C5-C4	-3.47	103.70	111.78
23	B	615	CLA	CHA-C4D-ND	3.47	139.70	132.55
23	a	411	CLA	C2A-C1A-CHA	-3.47	117.85	123.87
23	B	614	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
23	c	910	CLA	C4D-C3D-CAD	3.47	111.87	108.11
23	b	604	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
23	c	913	CLA	CHA-C4D-ND	3.47	139.70	132.55
23	b	606	CLA	C4D-CHA-C1A	-3.47	117.11	121.24
23	B	603	CLA	C2C-C1C-NC	3.46	113.62	109.98
23	c	911	CLA	C3B-C2B-C1B	-3.46	103.09	107.17
25	A	411	BCR	C8-C7-C6	-3.46	117.75	127.00
23	b	605	CLA	C1-C2-C3	-3.46	120.53	126.20
24	A	408	PHO	C4B-NB-C1B	-3.46	103.77	108.82
23	b	611	CLA	CHA-C4D-ND	3.46	139.69	132.55
23	b	619	CLA	CHD-C1D-ND	-3.46	119.94	124.80
23	b	605	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
33	D	414	HTG	C1'-S1-C1	3.46	107.92	100.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	912	CLA	CHA-C4D-ND	3.45	139.68	132.55
26	a	401	SQD	O48-C23-C24	3.45	122.37	111.83
23	c	909	CLA	CHD-C4C-C3C	-3.45	119.74	124.77
23	B	609	CLA	CHA-C4D-ND	3.45	139.67	132.55
23	B	605	CLA	CHD-C4C-C3C	-3.45	119.74	124.77
23	B	605	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
23	B	615	CLA	CMB-C2B-C1B	3.45	130.67	125.42
23	C	505	CLA	O2D-CGD-CBD	3.45	117.26	111.23
23	c	911	CLA	CHA-C4D-ND	3.45	139.66	132.55
23	c	903	CLA	C1C-C2C-C3C	-3.45	103.36	106.98
23	B	611	CLA	C1D-CHD-C4C	-3.45	118.70	126.02
23	C	502	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
23	B	603	CLA	CHC-C4B-NB	3.44	129.21	124.05
23	B	606	CLA	O2D-CGD-CBD	3.44	117.24	111.23
25	B	618	BCR	C7-C8-C9	-3.44	121.15	126.23
33	b	626	HTG	C1-O5-C5	3.44	118.73	112.56
23	A	407	CLA	C2D-C1D-ND	3.43	113.52	110.13
36	d	409	LHG	O4-P-O5	3.43	128.41	112.44
23	b	606	CLA	C3B-C4B-NB	3.43	113.59	110.53
23	a	414	CLA	C4D-CHA-C1A	-3.43	117.16	121.24
33	V	202	HTG	O2-C2-C1	3.43	116.39	110.30
23	c	907	CLA	C1-C2-C3	-3.43	120.58	126.20
23	b	604	CLA	CHD-C4C-NC	3.43	129.54	124.23
23	c	910	CLA	CHA-C4D-ND	3.42	139.62	132.55
23	C	509	CLA	O2D-CGD-CBD	3.42	117.22	111.23
25	K	102	BCR	C20-C21-C22	-3.42	122.48	127.28
23	B	610	CLA	CBC-CAC-C3C	-3.42	103.15	112.42
23	B	616	CLA	C11-C10-C8	-3.42	104.60	115.97
23	D	402	CLA	CHD-C1D-ND	-3.42	119.99	124.80
23	a	409	CLA	C7-C6-C5	-3.42	104.15	113.26
23	B	614	CLA	CHD-C4C-NC	3.42	129.53	124.23
23	b	612	CLA	C3C-C4C-NC	3.42	114.81	110.43
28	D	405	PL9	C27-C28-C29	-3.41	119.81	127.62
23	A	410	CLA	C3B-C4B-NB	3.41	113.58	110.53
23	C	507	CLA	O2D-CGD-CBD	3.41	117.20	111.23
23	c	907	CLA	C2C-C1C-NC	3.41	113.57	109.98
23	c	909	CLA	C2C-C1C-NC	3.41	113.57	109.98
23	a	411	CLA	CMB-C2B-C1B	3.41	130.61	125.42
23	B	608	CLA	CED-O2D-CGD	3.41	123.65	115.92
23	A	406	CLA	CBC-CAC-C3C	-3.41	103.17	112.42
23	b	618	CLA	CHA-C4D-ND	3.41	139.59	132.55
25	A	411	BCR	C11-C10-C9	-3.41	122.50	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	101	LHG	O7-C7-C8	3.41	118.85	111.48
23	B	615	CLA	C3D-C2D-C1D	-3.41	101.18	105.83
23	a	414	CLA	C3B-C2B-C1B	-3.40	103.16	107.17
23	c	905	CLA	C3B-C2B-C1B	-3.40	103.16	107.17
23	c	906	CLA	CHD-C1D-ND	-3.40	120.02	124.80
23	B	610	CLA	CHC-C4B-NB	3.40	129.15	124.05
23	c	912	CLA	C1-O2A-CGA	3.40	124.88	116.65
23	C	507	CLA	C2D-C1D-ND	3.40	113.49	110.13
23	B	604	CLA	CHC-C1C-NC	-3.40	119.19	124.31
26	L	103	SQD	O47-C7-C8	3.39	118.82	111.48
26	A	412	SQD	O8-S-C6	3.39	112.52	105.97
23	b	616	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
23	B	606	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
23	a	411	CLA	C3B-C2B-C1B	-3.39	103.17	107.17
23	c	913	CLA	CHD-C4C-C3C	-3.39	119.83	124.77
33	V	202	HTG	O5-C1-S1	3.39	119.56	110.30
28	D	405	PL9	C53-C6-C1	3.39	122.22	115.28
23	A	410	CLA	CHB-C4A-NA	3.39	129.29	124.40
23	C	502	CLA	CMB-C2B-C1B	3.39	130.58	125.42
23	b	617	CLA	CMB-C2B-C1B	3.39	130.58	125.42
23	A	410	CLA	O2D-CGD-CBD	3.39	117.15	111.23
23	a	411	CLA	C1-O2A-CGA	3.38	124.84	116.65
23	b	612	CLA	C4C-C3C-C2C	-3.38	101.97	106.89
33	O	303	HTG	C1'-S1-C1	3.38	107.75	100.45
23	B	605	CLA	CHA-C4D-ND	3.38	139.52	132.55
23	B	614	CLA	C1-C2-C3	-3.37	120.67	126.20
23	a	414	CLA	C3C-C4C-NC	3.37	114.75	110.43
23	B	603	CLA	C4A-NA-C1A	3.37	108.22	106.68
23	C	502	CLA	CHD-C1D-ND	-3.37	120.06	124.80
23	a	409	CLA	C1D-CHD-C4C	-3.37	118.86	126.02
36	L	101	LHG	O7-C7-C8	3.37	118.76	111.48
23	B	611	CLA	CHD-C4C-NC	3.36	129.45	124.23
25	c	916	BCR	C38-C26-C25	-3.36	120.81	124.48
25	D	404	BCR	C10-C11-C12	-3.36	113.45	123.20
23	D	403	CLA	CHC-C4B-NB	3.36	129.09	124.05
23	C	509	CLA	CHA-C4D-ND	3.36	139.48	132.55
30	a	402	LMT	O5'-C1'-O1'	-3.36	102.11	110.04
23	c	914	CLA	C1-O2A-CGA	3.35	124.77	116.65
23	B	607	CLA	C2B-C1B-NB	3.35	113.80	110.33
23	B	603	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
23	C	501	CLA	C2A-C1A-CHA	-3.35	118.05	123.87
23	B	606	CLA	CAC-C3C-C4C	3.34	129.14	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C4B-C3B-C2B	-3.34	103.14	107.30
23	A	407	CLA	CHD-C4C-C3C	-3.34	119.91	124.77
23	b	617	CLA	C4-C3-C2	-3.34	115.05	123.63
23	B	616	CLA	C3C-C4C-NC	3.34	114.70	110.43
25	K	102	BCR	C38-C26-C25	-3.34	120.84	124.48
23	c	904	CLA	C1D-CHD-C4C	-3.34	118.93	126.02
30	C	520	LMT	C2'-C3'-C4'	-3.33	102.11	109.68
23	b	612	CLA	C2D-C1D-ND	3.33	113.43	110.13
23	b	609	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
23	D	403	CLA	C3D-C2D-C1D	-3.33	101.29	105.83
23	a	409	CLA	C2B-C1B-NB	3.32	113.77	110.33
25	C	514	BCR	C7-C8-C9	-3.32	121.33	126.23
23	b	608	CLA	C3B-C2B-C1B	-3.32	103.26	107.17
23	b	609	CLA	C4D-CHA-C1A	-3.32	117.29	121.24
25	T	101	BCR	C15-C16-C17	-3.32	116.73	123.52
23	B	611	CLA	O2A-CGA-CBA	3.32	121.95	111.83
23	B	615	CLA	CMD-C2D-C1D	3.31	130.56	124.73
23	c	904	CLA	C2B-C1B-NB	3.31	113.76	110.33
23	C	506	CLA	CHD-C1D-ND	-3.31	120.14	124.80
34	h	102	DGD	O1G-C1A-C2A	3.31	121.93	111.83
23	C	510	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
23	b	615	CLA	CHC-C4B-NB	3.31	129.01	124.05
23	C	507	CLA	CHC-C4B-NB	3.31	129.01	124.05
26	D	407	SQD	O48-C23-C24	3.31	121.92	111.83
23	A	406	CLA	C4-C3-C5	3.30	120.96	115.23
23	c	910	CLA	CMB-C2B-C1B	3.30	130.45	125.42
23	B	610	CLA	C2B-C1B-NB	3.30	113.75	110.33
23	c	905	CLA	CMD-C2D-C1D	3.30	130.54	124.73
23	b	607	CLA	CMD-C2D-C1D	3.30	130.54	124.73
23	B	603	CLA	C3B-C2B-C1B	-3.30	103.28	107.17
23	B	604	CLA	O2A-CGA-O1A	-3.30	115.38	123.63
27	C	519	LMG	O8-C28-O10	-3.30	115.38	123.63
25	B	618	BCR	C10-C11-C12	-3.30	113.64	123.20
23	C	501	CLA	CBC-CAC-C3C	-3.30	103.49	112.42
25	t	101	BCR	C33-C5-C6	-3.29	120.89	124.48
23	b	619	CLA	C4C-C3C-C2C	-3.29	102.10	106.89
23	D	403	CLA	CMA-C3A-C4A	-3.29	102.93	111.77
25	a	415	BCR	C16-C15-C14	-3.29	116.79	123.52
34	c	919	DGD	O1G-C1A-C2A	3.29	121.86	111.83
23	D	402	CLA	CHC-C1C-C2C	-3.29	117.61	126.95
25	T	101	BCR	C2-C1-C6	3.29	115.21	110.44
23	b	618	CLA	CMD-C2D-C3D	3.29	135.22	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	621	SQD	O9-S-C6	3.29	111.66	106.76
26	A	418	SQD	C1-O5-C5	-3.28	107.31	113.72
23	b	617	CLA	C3B-C4B-NB	3.28	113.46	110.53
24	A	409	PHO	O2D-CGD-O1D	-3.28	117.46	123.85
33	V	202	HTG	O5-C5-C6	3.28	114.57	106.44
25	K	102	BCR	C33-C5-C6	-3.28	120.91	124.48
23	A	407	CLA	C4B-C3B-C2B	-3.28	103.22	107.30
23	D	402	CLA	C4B-CHC-C1C	-3.28	118.54	126.25
23	b	607	CLA	C4D-CHA-C1A	-3.28	117.33	121.24
23	c	910	CLA	C4-C3-C5	3.28	120.92	115.23
23	A	405	CLA	CAA-CBA-CGA	-3.28	103.91	113.21
23	A	406	CLA	C2B-C1B-NB	3.28	113.72	110.33
23	C	502	CLA	O2D-CGD-CBD	3.27	116.95	111.23
23	c	914	CLA	CHC-C4B-NB	3.27	128.95	124.05
23	b	610	CLA	C4-C3-C5	3.27	120.90	115.23
23	A	405	CLA	C4D-CHA-C1A	-3.27	117.35	121.24
23	b	609	CLA	CMD-C2D-C1D	3.27	130.48	124.73
25	B	618	BCR	C24-C23-C22	-3.26	121.41	126.23
23	C	513	CLA	C2C-C1C-NC	3.26	113.41	109.98
23	B	609	CLA	O2A-CGA-CBA	3.26	121.79	111.83
23	B	613	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
25	T	101	BCR	C7-C8-C9	-3.26	121.42	126.23
25	b	620	BCR	C35-C13-C12	3.26	123.06	118.09
23	C	505	CLA	C3D-C2D-C1D	-3.26	101.39	105.83
23	A	405	CLA	CMD-C2D-C3D	3.26	135.16	127.69
23	b	616	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
23	A	410	CLA	CHD-C1D-ND	-3.25	120.23	124.80
23	b	604	CLA	C4-C3-C5	3.25	120.87	115.23
23	b	611	CLA	O2A-CGA-O1A	-3.25	115.50	123.63
36	l	101	LHG	O7-C7-O9	-3.24	116.12	123.70
23	D	403	CLA	CHD-C4C-C3C	-3.24	120.05	124.77
23	c	908	CLA	C2B-C1B-NB	3.24	113.69	110.33
23	B	611	CLA	C3B-C4B-NB	3.24	113.42	110.53
30	M	101	LMT	C1-O1'-C1'	3.24	119.21	113.68
37	F	101	HEM	CHC-C4B-NB	3.24	127.91	124.42
23	B	605	CLA	C2D-C1D-ND	3.24	113.33	110.13
23	a	411	CLA	C1D-ND-C4D	3.23	108.58	106.31
23	B	609	CLA	C4B-C3B-C2B	-3.23	103.28	107.30
28	d	405	PL9	C22-C23-C24	-3.23	120.23	127.62
23	C	509	CLA	C1-C2-C3	-3.23	120.91	126.20
23	C	507	CLA	CHD-C4C-NC	3.23	129.24	124.23
30	F	102	LMT	C2'-C3'-C4'	3.23	117.01	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	413	LMG	O6-C1-C2	-3.23	103.73	110.37
34	d	406	DGD	O6D-C1D-O3G	3.23	117.67	110.04
23	b	610	CLA	C2D-C1D-ND	3.22	113.32	110.13
23	c	910	CLA	C1-C2-C3	-3.22	120.92	126.20
23	C	503	CLA	CHC-C1C-NC	-3.22	119.46	124.31
23	c	912	CLA	C4-C3-C5	3.22	120.82	115.23
23	B	602	CLA	O1D-CGD-CBD	-3.22	118.17	124.52
25	t	101	BCR	C1-C6-C7	3.22	124.38	115.65
23	d	402	CLA	OBD-CAD-C3D	-3.22	120.90	128.42
27	C	519	LMG	O5-C6-C5	-3.22	100.38	111.33
23	C	504	CLA	C1-O2A-CGA	3.21	124.43	116.65
28	a	419	PL9	C20-C19-C21	3.21	120.80	115.23
24	A	409	PHO	C4-C3-C5	3.21	120.80	115.23
23	C	510	CLA	CHC-C4B-NB	3.21	128.86	124.05
24	a	413	PHO	C1-C2-C3	-3.21	120.94	126.20
36	d	408	LHG	C34-C33-C32	-3.21	98.17	114.37
23	c	907	CLA	O2A-CGA-O1A	-3.20	115.61	123.63
23	C	504	CLA	CMD-C2D-C1D	3.20	130.37	124.73
23	B	606	CLA	C4-C3-C5	3.20	120.79	115.23
23	c	909	CLA	CMA-C3A-C4A	-3.20	103.16	111.77
26	a	416	SQD	C45-O47-C7	-3.20	110.13	117.80
23	d	402	CLA	CHA-C4D-ND	3.20	139.16	132.55
25	K	102	BCR	C16-C17-C18	-3.20	122.79	127.28
23	b	613	CLA	C1D-CHD-C4C	-3.20	119.22	126.02
25	t	101	BCR	C12-C13-C14	-3.20	113.98	119.01
23	C	512	CLA	C1D-CHD-C4C	-3.20	119.22	126.02
23	C	502	CLA	CHC-C4B-NB	3.20	128.85	124.05
23	B	603	CLA	CHD-C4C-NC	3.20	129.19	124.23
23	c	914	CLA	O2A-CGA-CBA	3.20	121.58	111.83
23	b	615	CLA	O2D-CGD-CBD	3.20	116.82	111.23
23	B	605	CLA	CMD-C2D-C1D	3.19	130.35	124.73
23	B	606	CLA	C2A-C1A-CHA	-3.19	118.33	123.87
33	b	602	HTG	C1'-S1-C1	3.19	107.34	100.45
23	b	613	CLA	CAA-CBA-CGA	-3.19	104.16	113.21
23	C	502	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
23	a	414	CLA	C1D-ND-C4D	-3.19	104.08	106.31
23	b	608	CLA	CHA-C4D-ND	3.18	139.11	132.55
23	b	617	CLA	CHC-C4B-NB	3.18	128.82	124.05
23	a	411	CLA	CBC-CAC-C3C	-3.18	103.80	112.42
23	b	606	CLA	C5-C3-C2	-3.18	114.03	121.17
23	C	509	CLA	O2A-CGA-CBA	3.18	121.53	111.83
23	C	507	CLA	C4-C3-C5	3.18	120.74	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	101	BCR	C38-C26-C25	-3.18	121.02	124.48
24	a	412	PHO	CBA-CAA-C2A	-3.18	104.42	113.78
23	b	616	CLA	C4D-CHA-C1A	-3.18	117.46	121.24
33	B	624	HTG	C3'-C2'-C1'	-3.17	101.08	113.10
23	B	608	CLA	C4A-NA-C1A	3.17	108.13	106.68
23	b	612	CLA	CHC-C4B-NB	3.17	128.81	124.05
25	a	415	BCR	C7-C8-C9	-3.17	121.54	126.23
23	C	509	CLA	C3C-C4C-NC	3.17	114.49	110.43
23	d	402	CLA	C2D-C1D-ND	3.17	113.26	110.13
26	B	621	SQD	C4-C3-C2	3.16	116.38	110.83
23	a	414	CLA	CMC-C2C-C1C	3.16	129.98	125.03
23	a	414	CLA	CHD-C4C-NC	3.16	129.13	124.23
23	a	411	CLA	C2B-C1B-NB	3.16	113.60	110.33
28	A	414	PL9	C22-C23-C24	-3.16	120.39	127.62
23	B	614	CLA	C2A-C1A-CHA	-3.16	118.38	123.87
23	c	902	CLA	CHC-C4B-NB	3.16	128.79	124.05
23	c	906	CLA	CHD-C4C-NC	3.16	129.13	124.23
23	C	509	CLA	O2A-CGA-O1A	-3.16	115.73	123.63
23	D	402	CLA	C4B-C3B-C2B	-3.16	103.38	107.30
34	C	518	DGD	O1G-C1A-C2A	3.16	121.46	111.83
26	f	102	SQD	O48-C23-C24	3.16	121.46	111.83
23	C	504	CLA	CHC-C4B-NB	3.15	128.78	124.05
23	B	606	CLA	C3C-C4C-NC	3.15	114.47	110.43
23	C	509	CLA	CMD-C2D-C1D	3.15	130.28	124.73
23	A	406	CLA	C2D-C1D-ND	3.15	113.24	110.13
23	b	609	CLA	CMC-C2C-C3C	3.15	134.67	126.15
23	a	414	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
23	B	604	CLA	C2A-C1A-CHA	-3.15	118.41	123.87
27	c	920	LMG	O5-C6-C5	-3.15	100.62	111.33
23	C	506	CLA	CHD-C4C-NC	3.15	129.11	124.23
23	B	602	CLA	CMC-C2C-C1C	3.14	129.94	125.03
28	A	414	PL9	C53-C6-C1	3.14	121.71	115.28
23	C	507	CLA	CMD-C2D-C1D	3.14	130.26	124.73
23	c	913	CLA	CMD-C2D-C1D	3.14	130.25	124.73
23	a	410	CLA	CHA-C4D-ND	3.14	139.02	132.55
25	B	618	BCR	C16-C15-C14	-3.14	117.10	123.52
33	b	626	HTG	C1-C2-C3	3.13	116.68	110.55
24	A	408	PHO	CMA-C3A-C4A	-3.13	107.86	114.61
23	A	407	CLA	CHC-C4B-NB	3.13	128.75	124.05
23	C	507	CLA	CHD-C1D-ND	-3.13	120.40	124.80
23	b	616	CLA	C1-O2A-CGA	3.13	124.23	116.65
23	b	618	CLA	C4-C3-C5	3.13	120.66	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	914	CLA	CMC-C2C-C1C	3.13	129.92	125.03
25	b	620	BCR	C24-C23-C22	-3.13	121.61	126.23
30	c	922	LMT	O1'-C1'-C2'	3.13	113.02	108.27
34	c	918	DGD	O6E-C5E-C4E	-3.12	104.07	109.70
23	c	913	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
23	C	506	CLA	CMC-C2C-C1C	3.12	129.91	125.03
25	D	404	BCR	C29-C28-C27	-3.12	104.42	111.28
23	c	908	CLA	CHA-C4D-ND	3.12	138.99	132.55
23	B	617	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
23	B	608	CLA	CHD-C1D-ND	-3.12	120.41	124.80
23	c	905	CLA	C7-C6-C5	-3.12	104.95	113.26
27	Z	101	LMG	C3-C4-C5	3.12	115.88	110.23
23	a	409	CLA	CMD-C2D-C1D	3.12	130.21	124.73
25	b	621	BCR	C8-C7-C6	-3.11	118.68	127.00
23	C	511	CLA	CBC-CAC-C3C	-3.11	103.98	112.42
30	M	102	LMT	C3'-C4'-C5'	-3.11	104.03	110.93
23	c	913	CLA	CHC-C4B-NB	3.11	128.72	124.05
23	B	607	CLA	C4D-CHA-C1A	-3.11	117.53	121.24
23	b	610	CLA	C3B-C2B-C1B	-3.11	103.50	107.17
25	t	101	BCR	C7-C6-C5	-3.11	114.39	121.56
23	B	617	CLA	CMB-C2B-C1B	3.11	130.15	125.42
27	B	622	LMG	C31-C30-C29	-3.10	101.72	113.13
23	c	905	CLA	C4-C3-C5	3.10	120.62	115.23
23	B	606	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
23	B	602	CLA	C1D-ND-C4D	-3.10	104.14	106.31
23	C	506	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
30	b	625	LMT	C3'-C4'-C5'	-3.10	104.61	110.23
23	B	616	CLA	CHC-C4B-NB	3.10	128.70	124.05
23	b	617	CLA	C3B-C2B-C1B	-3.10	103.52	107.17
23	B	603	CLA	C1D-CHD-C4C	-3.10	119.44	126.02
23	B	607	CLA	C1-O2A-CGA	3.10	124.15	116.65
23	B	607	CLA	C3B-C4B-NB	3.10	113.30	110.53
23	b	610	CLA	C2B-C1B-NB	3.10	113.54	110.33
28	a	419	PL9	C42-C43-C44	-3.10	120.54	127.62
23	a	410	CLA	C1D-ND-C4D	-3.10	104.14	106.31
23	B	602	CLA	CHC-C4B-NB	3.09	128.69	124.05
23	A	405	CLA	C4A-NA-C1A	3.09	108.09	106.68
23	B	614	CLA	C3B-C2B-C1B	-3.09	103.52	107.17
28	A	414	PL9	C37-C38-C39	-3.09	120.55	127.62
23	b	612	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
23	b	608	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
25	t	101	BCR	C29-C28-C27	-3.09	104.49	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C3A-C2A-C1A	-3.09	96.72	101.34
25	C	514	BCR	C11-C10-C9	-3.08	122.95	127.28
23	c	911	CLA	C1D-CHD-C4C	-3.08	119.46	126.02
23	B	604	CLA	C3D-C2D-C1D	-3.08	101.62	105.83
23	a	414	CLA	C1D-CHD-C4C	-3.08	119.47	126.02
23	b	617	CLA	CAC-C3C-C4C	3.08	128.80	124.79
23	B	607	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	B	614	CLA	CBC-CAC-C3C	-3.08	104.07	112.42
23	c	909	CLA	C1-C2-C3	-3.08	121.15	126.20
23	b	606	CLA	O2D-CGD-CBD	3.08	116.61	111.23
25	d	404	BCR	C40-C30-C25	-3.08	105.42	110.24
23	C	508	CLA	O2A-CGA-O1A	-3.08	115.93	123.63
26	A	412	SQD	O47-C7-O49	-3.08	116.51	123.70
34	c	919	DGD	O3G-C3G-C2G	-3.08	103.34	110.82
25	k	101	BCR	C24-C23-C22	-3.07	121.69	126.23
23	b	616	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
23	b	608	CLA	CMB-C2B-C1B	3.07	130.10	125.42
23	C	501	CLA	CHA-C4D-ND	3.07	138.88	132.55
23	C	509	CLA	CMC-C2C-C3C	3.07	134.45	126.15
37	f	101	HEM	C4D-ND-C1D	3.07	108.84	105.21
23	b	609	CLA	O2A-CGA-O1A	-3.07	115.95	123.63
23	B	605	CLA	CAA-C2A-C3A	-3.07	104.70	113.00
23	b	612	CLA	C2B-C1B-NB	3.07	113.51	110.33
23	A	405	CLA	CMA-C3A-C4A	-3.07	103.53	111.77
23	C	508	CLA	CHD-C4C-C3C	-3.07	120.30	124.77
23	B	609	CLA	C2A-C1A-CHA	-3.07	118.55	123.87
23	C	512	CLA	C2B-C1B-NB	3.06	113.50	110.33
23	B	611	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	b	604	CLA	CMC-C2C-C1C	3.06	129.82	125.03
23	b	617	CLA	CHB-C4A-NA	3.06	128.82	124.40
23	c	904	CLA	OBD-CAD-C3D	-3.06	121.26	128.42
23	b	617	CLA	C1D-CHD-C4C	-3.06	119.52	126.02
34	c	919	DGD	O1G-C1A-O1A	-3.06	115.98	123.63
25	b	621	BCR	C16-C17-C18	3.06	131.57	127.28
23	b	604	CLA	C3D-C2D-C1D	-3.05	101.66	105.83
23	C	501	CLA	O1D-CGD-CBD	-3.05	118.50	124.52
23	b	615	CLA	C4-C3-C5	3.05	120.53	115.23
26	a	416	SQD	O47-C7-O49	-3.05	116.57	123.70
23	C	504	CLA	C3B-C2B-C1B	-3.05	103.57	107.17
23	B	605	CLA	CGD-CBD-CAD	-3.05	100.97	110.85
23	B	607	CLA	C4B-CHC-C1C	-3.05	119.08	126.25
23	b	617	CLA	C1-O2A-CGA	3.05	124.02	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	h	101	RRX	C16-C17-C18	-3.04	123.01	127.28
23	c	914	CLA	C2D-C1D-ND	3.04	113.14	110.13
27	a	418	LMG	O7-C10-O9	-3.04	116.60	123.70
23	c	909	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
23	B	614	CLA	CAC-C3C-C4C	3.04	128.74	124.79
23	B	615	CLA	O2A-CGA-O1A	-3.04	116.03	123.63
23	C	510	CLA	C4B-C3B-C2B	-3.04	103.53	107.30
23	c	910	CLA	C3C-C4C-NC	3.04	114.32	110.43
24	A	409	PHO	CMB-C2B-C3B	3.03	130.75	124.68
23	C	508	CLA	CHD-C1D-ND	-3.03	120.53	124.80
23	C	506	CLA	C1-C2-C3	-3.03	121.23	126.20
26	B	621	SQD	O48-C23-O10	-3.03	116.04	123.63
30	C	520	LMT	C1B-O5B-C5B	3.03	119.64	113.72
23	B	603	CLA	C1-C2-C3	-3.03	121.23	126.20
23	b	611	CLA	CHD-C1D-ND	-3.03	120.54	124.80
23	d	402	CLA	C4B-CHC-C1C	-3.03	119.12	126.25
27	d	410	LMG	O8-C28-O10	-3.03	116.05	123.63
23	a	411	CLA	C1-C2-C3	-3.03	121.23	126.20
23	D	402	CLA	CMD-C2D-C3D	3.03	134.63	127.69
28	a	419	PL9	C30-C29-C31	3.03	120.48	115.23
23	b	610	CLA	CMD-C2D-C1D	3.02	130.05	124.73
23	C	505	CLA	CMC-C2C-C1C	3.02	129.76	125.03
23	b	614	CLA	CMC-C2C-C1C	3.02	129.76	125.03
23	C	502	CLA	CMC-C2C-C1C	3.02	129.75	125.03
23	a	414	CLA	C3D-C2D-C1D	-3.02	101.71	105.83
36	d	408	LHG	O8-C23-O10	-3.02	116.08	123.63
23	b	613	CLA	CMB-C2B-C1B	3.02	130.01	125.42
37	v	201	HEM	C2A-C1A-NA	-3.01	106.81	110.15
23	D	402	CLA	O2A-CGA-O1A	-3.01	116.09	123.63
23	b	605	CLA	CMD-C2D-C3D	3.01	134.59	127.69
33	c	924	HTG	C3-C4-C5	3.01	115.69	110.23
23	b	609	CLA	CHD-C4C-NC	3.01	128.89	124.23
25	C	515	BCR	C33-C5-C6	-3.01	121.20	124.48
23	C	509	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
23	b	607	CLA	O2A-CGA-O1A	-3.00	116.11	123.63
23	B	610	CLA	C3C-C4C-NC	3.00	114.28	110.43
23	B	605	CLA	C4-C3-C5	3.00	120.44	115.23
34	H	102	DGD	C6D-C5D-C4D	3.00	118.37	112.07
23	B	612	CLA	C3C-C4C-NC	3.00	114.28	110.43
23	b	610	CLA	C1C-C2C-C3C	-3.00	103.82	106.98
28	a	419	PL9	C35-C34-C36	3.00	120.44	115.23
23	C	501	CLA	CMD-C2D-C1D	3.00	130.01	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C4-C3-C5	3.00	120.43	115.23
27	B	622	LMG	O8-C28-O10	-3.00	116.13	123.63
26	a	416	SQD	O9-S-O7	-3.00	104.08	113.82
23	b	617	CLA	CHA-C4D-ND	3.00	138.73	132.55
23	b	608	CLA	C2B-C1B-NB	3.00	113.43	110.33
23	B	607	CLA	C4-C3-C5	2.99	120.43	115.23
23	C	510	CLA	C1C-C2C-C3C	-2.99	103.83	106.98
23	C	504	CLA	CHD-C4C-C3C	-2.99	120.41	124.77
30	B	623	LMT	O5B-C5B-C4B	2.99	115.09	109.70
23	C	512	CLA	CHC-C4B-NB	2.99	128.53	124.05
23	B	616	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
23	b	617	CLA	CHD-C4C-NC	2.99	128.86	124.23
31	C	524	GOL	O3-C3-C2	-2.99	96.94	110.38
23	C	505	CLA	C4A-NA-C1A	2.99	108.04	106.68
25	t	101	BCR	C20-C21-C22	-2.98	123.09	127.28
23	a	409	CLA	CHD-C4C-NC	2.98	128.86	124.23
23	b	616	CLA	C2A-C1A-CHA	-2.98	118.69	123.87
25	A	411	BCR	C7-C8-C9	-2.98	121.82	126.23
25	T	101	BCR	C23-C24-C25	-2.98	119.03	127.00
23	b	608	CLA	CHC-C1C-NC	-2.98	119.83	124.31
23	B	609	CLA	C1D-CHD-C4C	-2.97	119.70	126.02
23	d	402	CLA	CHC-C4B-C3B	-2.97	114.48	127.37
23	B	607	CLA	C1-C2-C3	-2.97	121.33	126.20
23	b	616	CLA	C3B-C2B-C1B	-2.97	103.67	107.17
23	b	605	CLA	C4D-CHA-C1A	-2.97	117.70	121.24
23	C	507	CLA	C4D-CHA-C1A	-2.97	117.70	121.24
34	c	918	DGD	C3E-C4E-C5E	2.97	115.61	110.23
23	C	505	CLA	CHD-C4C-NC	2.97	128.83	124.23
23	B	605	CLA	C3B-C2B-C1B	-2.97	103.67	107.17
25	K	101	BCR	C40-C30-C25	-2.96	105.60	110.24
23	b	610	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	B	611	CLA	CMB-C2B-C1B	2.96	129.93	125.42
23	D	403	CLA	O2D-CGD-CBD	2.96	116.41	111.23
34	C	516	DGD	C3G-C2G-C1G	-2.96	104.88	111.78
23	D	402	CLA	CAA-CBA-CGA	-2.96	104.81	113.21
30	J	102	LMT	C3'-C4'-C5'	-2.96	104.87	110.23
23	c	910	CLA	C3D-C2D-C1D	-2.96	101.80	105.83
23	B	615	CLA	CHD-C1D-ND	-2.96	120.64	124.80
34	c	917	DGD	O2G-C1B-O1B	-2.96	116.80	123.70
23	a	409	CLA	CHC-C4B-NB	2.96	128.48	124.05
23	C	511	CLA	CHD-C1D-ND	-2.95	120.65	124.80
23	c	903	CLA	CAC-C3C-C4C	2.95	128.63	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C4D-CHA-C1A	-2.95	117.72	121.24
23	c	911	CLA	C2B-C1B-NB	2.95	113.39	110.33
23	b	613	CLA	CHA-C4D-ND	2.95	138.64	132.55
23	C	503	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
23	b	613	CLA	CHB-C4A-NA	2.95	128.66	124.40
23	b	616	CLA	CHC-C4B-NB	2.95	128.47	124.05
26	A	418	SQD	C1-C2-C3	-2.95	103.81	110.01
23	B	606	CLA	C4A-NA-C1A	2.95	108.02	106.68
23	c	912	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
30	m	101	LMT	O1'-C1'-C2'	2.94	112.75	108.27
23	b	616	CLA	CHD-C1D-ND	-2.94	120.66	124.80
28	d	405	PL9	C40-C39-C38	-2.94	116.08	123.63
28	a	419	PL9	C40-C39-C41	2.94	120.33	115.23
23	c	902	CLA	CBC-CAC-C3C	-2.94	104.45	112.42
23	C	511	CLA	C3A-C2A-C1A	2.93	105.73	101.34
23	B	605	CLA	C2A-C1A-CHA	-2.93	118.78	123.87
25	T	101	BCR	C12-C13-C14	-2.93	114.40	119.01
23	b	611	CLA	CAC-C3C-C4C	2.93	128.60	124.79
27	c	921	LMG	O1-C1-C2	2.93	112.72	108.27
38	H	101	RRX	C10-C11-C12	-2.93	114.72	123.20
23	B	605	CLA	CAC-C3C-C4C	2.93	128.60	124.79
23	C	511	CLA	CHA-C4D-ND	2.93	138.59	132.55
23	c	903	CLA	CMB-C2B-C1B	2.93	129.87	125.42
34	d	406	DGD	O1G-C1G-C2G	2.92	116.83	108.40
24	a	413	PHO	CMA-C3A-C4A	-2.92	108.32	114.61
23	c	914	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
23	b	618	CLA	CHD-C4C-NC	2.92	128.76	124.23
23	A	405	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
23	c	905	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	B	604	CLA	C6-C5-C3	2.92	120.58	113.47
28	D	405	PL9	C42-C41-C39	-2.92	103.51	113.19
23	B	617	CLA	C2A-C1A-CHA	-2.92	118.80	123.87
23	b	605	CLA	C2A-C3A-C4A	-2.92	97.16	101.87
23	B	613	CLA	C4-C3-C5	2.91	120.29	115.23
34	C	517	DGD	O2G-C1B-C2B	2.91	117.78	111.48
26	D	407	SQD	O7-S-C6	2.91	111.11	106.76
23	b	608	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
23	D	403	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
23	B	607	CLA	CMB-C2B-C1B	2.91	129.85	125.42
23	C	504	CLA	CHA-C4D-ND	2.91	138.55	132.55
23	c	914	CLA	CHD-C4C-NC	2.91	128.74	124.23
23	c	910	CLA	O2D-CGD-O1D	-2.91	118.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C3C-C4C-NC	2.90	114.15	110.43
23	C	509	CLA	C2D-C1D-ND	2.90	113.00	110.13
23	b	619	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
23	c	903	CLA	CHA-C4D-ND	2.90	138.53	132.55
26	a	401	SQD	O9-S-C6	2.90	111.08	106.76
25	B	620	BCR	C7-C8-C9	-2.89	121.95	126.23
23	c	909	CLA	C3B-C4B-NB	2.89	113.11	110.53
23	B	608	CLA	CMA-C3A-C4A	-2.89	104.00	111.77
27	B	622	LMG	O5-C6-C5	-2.89	101.49	111.33
23	c	910	CLA	C1D-CHD-C4C	-2.89	119.87	126.02
23	b	611	CLA	C3C-C4C-NC	2.89	114.13	110.43
23	b	615	CLA	C3B-C4B-NB	2.89	113.11	110.53
23	a	411	CLA	CHB-C1B-C2B	-2.89	119.04	127.43
23	C	505	CLA	CED-O2D-CGD	2.89	122.47	115.92
26	a	416	SQD	O5-C1-C2	-2.89	104.44	110.37
23	a	409	CLA	CAC-C3C-C2C	-2.89	122.25	127.56
36	a	417	LHG	O8-C23-C24	2.89	120.64	111.83
23	C	508	CLA	CMC-C2C-C3C	2.89	133.96	126.15
23	b	610	CLA	CHD-C4C-NC	2.89	128.71	124.23
23	B	612	CLA	C2A-C1A-CHA	-2.88	118.87	123.87
25	D	404	BCR	C30-C25-C26	-2.88	118.70	122.64
23	D	402	CLA	C2A-C1A-CHA	-2.88	118.87	123.87
23	b	610	CLA	CHD-C1D-ND	-2.88	120.75	124.80
23	C	502	CLA	C1D-CHD-C4C	-2.87	119.91	126.02
26	A	418	SQD	O48-C23-O10	-2.87	116.44	123.63
23	b	609	CLA	C1-O2A-CGA	2.87	123.61	116.65
26	A	412	SQD	O48-C23-O10	-2.87	116.44	123.63
25	c	916	BCR	C15-C16-C17	-2.87	117.64	123.52
23	c	912	CLA	C3D-C2D-C1D	-2.87	101.91	105.83
23	d	402	CLA	C3C-C4C-NC	2.87	114.11	110.43
23	b	616	CLA	C3B-C4B-NB	2.87	113.09	110.53
23	c	908	CLA	C3C-C4C-NC	2.87	114.10	110.43
23	c	909	CLA	C4B-C3B-C2B	-2.87	103.74	107.30
34	c	918	DGD	O1G-C1A-O1A	-2.87	116.46	123.63
30	C	520	LMT	O3'-C3'-C4'	2.87	117.28	109.94
23	b	619	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	B	620	BCR	C32-C1-C6	-2.86	105.75	110.24
24	a	413	PHO	C4B-NB-C1B	-2.86	104.65	108.82
24	A	408	PHO	CMB-C2B-C3B	2.86	130.40	124.68
23	b	605	CLA	CMA-C3A-C4A	-2.86	104.09	111.77
28	D	405	PL9	C40-C39-C38	-2.86	116.29	123.63
23	b	611	CLA	C3B-C4B-NB	2.86	113.08	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	412	PHO	CMC-C2C-C1C	2.85	129.87	124.73
28	D	405	PL9	C22-C23-C24	-2.85	121.09	127.62
23	B	616	CLA	C4-C3-C5	2.85	120.18	115.23
23	c	906	CLA	CHA-C4D-ND	2.85	138.43	132.55
23	b	608	CLA	C2A-C1A-CHA	-2.85	118.92	123.87
25	A	411	BCR	C24-C23-C22	-2.85	122.02	126.23
28	d	405	PL9	C37-C36-C34	-2.85	103.75	113.19
23	C	504	CLA	C5-C3-C2	-2.85	114.78	121.17
23	B	611	CLA	CHA-C4D-ND	2.85	138.42	132.55
37	V	201	HEM	C1D-C2D-C3D	-2.84	103.99	106.98
34	c	919	DGD	C3E-C4E-C5E	-2.84	105.08	110.23
23	a	414	CLA	CHC-C4B-C3B	-2.84	115.03	127.37
23	B	607	CLA	C3B-C2B-C1B	-2.84	103.82	107.17
23	c	903	CLA	C3B-C4B-NB	2.84	113.07	110.53
23	B	613	CLA	C3C-C4C-NC	2.84	114.07	110.43
23	a	411	CLA	C2D-C1D-ND	2.84	112.94	110.13
28	A	414	PL9	C2-C1-C6	2.84	122.37	119.00
23	b	605	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
23	B	613	CLA	C1C-C2C-C3C	-2.84	104.00	106.98
26	L	103	SQD	O5-C1-C2	-2.84	104.54	110.37
25	D	404	BCR	C30-C25-C24	2.84	123.34	115.65
34	c	918	DGD	O2G-C1B-C2B	2.83	117.61	111.48
23	c	906	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
28	A	414	PL9	C30-C29-C31	2.83	120.15	115.23
23	b	619	CLA	C1-O2A-CGA	2.83	123.51	116.65
23	c	907	CLA	CED-O2D-CGD	2.83	122.34	115.92
27	C	519	LMG	O7-C10-O9	-2.83	117.08	123.70
30	M	102	LMT	O1'-C1-C2	-2.83	99.77	109.37
25	b	620	BCR	C15-C14-C13	-2.83	123.31	127.28
23	A	406	CLA	C3C-C4C-NC	2.83	114.05	110.43
23	b	612	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
23	C	513	CLA	C4-C3-C5	2.82	120.13	115.23
23	C	503	CLA	CHD-C4C-NC	2.82	128.61	124.23
23	B	616	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
23	a	411	CLA	C3B-C4B-NB	2.82	113.05	110.53
23	c	905	CLA	CHD-C1D-ND	-2.82	120.83	124.80
23	b	609	CLA	C3B-C4B-NB	2.82	113.05	110.53
25	B	620	BCR	C2-C1-C6	2.82	114.53	110.44
25	c	915	BCR	C15-C14-C13	-2.82	123.33	127.28
23	a	414	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
23	c	910	CLA	CED-O2D-CGD	2.81	122.29	115.92
24	a	412	PHO	CAA-CBA-CGA	-2.81	105.24	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	405	PL9	C53-C6-C1	2.81	121.03	115.28
23	B	614	CLA	C4A-NA-C1A	2.81	107.96	106.68
23	c	907	CLA	C3B-C4B-NB	2.80	113.03	110.53
23	A	410	CLA	C4B-CHC-C1C	-2.80	119.65	126.25
23	b	606	CLA	C2A-C1A-CHA	-2.80	119.00	123.87
23	c	908	CLA	CBC-CAC-C3C	-2.80	104.82	112.42
23	C	506	CLA	C1D-CHD-C4C	-2.80	120.06	126.02
24	a	412	PHO	CMA-C3A-C4A	-2.80	108.57	114.61
23	c	907	CLA	O2D-CGD-CBD	2.80	116.13	111.23
23	c	902	CLA	C3D-C4D-ND	2.80	114.54	109.99
23	b	618	CLA	C3B-C4B-NB	2.80	113.03	110.53
23	C	503	CLA	CMB-C2B-C3B	2.80	133.14	126.55
36	d	408	LHG	O7-C7-O9	-2.80	117.16	123.70
23	A	406	CLA	CAC-C3C-C2C	-2.80	122.41	127.56
23	A	405	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
23	b	609	CLA	C1D-ND-C4D	-2.80	104.35	106.31
23	C	502	CLA	C4-C3-C5	2.80	120.09	115.23
23	A	406	CLA	CMD-C2D-C3D	2.80	134.11	127.69
30	a	402	LMT	O2'-C2'-C1'	2.80	116.74	110.08
23	B	615	CLA	C4C-C3C-C2C	-2.79	102.82	106.89
23	c	906	CLA	C1D-CHD-C4C	-2.79	120.09	126.02
26	D	407	SQD	C46-C45-C44	-2.79	105.28	111.78
23	A	410	CLA	CMB-C2B-C1B	2.79	129.66	125.42
24	a	413	PHO	O2A-CGA-O1A	-2.78	116.66	123.63
25	K	101	BCR	C15-C16-C17	-2.78	117.83	123.52
23	c	910	CLA	CHC-C1C-NC	-2.78	120.12	124.31
23	d	403	CLA	CBC-CAC-C3C	-2.78	104.88	112.42
23	c	910	CLA	CHC-C4B-C3B	-2.78	115.31	127.37
36	D	408	LHG	O7-C7-O9	-2.78	117.21	123.70
34	c	917	DGD	C6D-O5D-C1E	-2.78	107.84	113.80
34	c	919	DGD	C4A-C3A-C2A	-2.78	102.93	113.13
23	B	610	CLA	CHA-C4D-ND	2.78	138.28	132.55
23	b	606	CLA	C1D-CHD-C4C	-2.78	120.12	126.02
34	D	406	DGD	O2G-C1B-O1B	-2.78	117.22	123.70
23	b	613	CLA	CHD-C4C-NC	2.77	128.53	124.23
23	B	612	CLA	CMB-C2B-C1B	2.77	129.64	125.42
23	C	511	CLA	CHC-C4B-NB	2.77	128.21	124.05
23	C	512	CLA	CHD-C4C-NC	2.77	128.53	124.23
25	d	404	BCR	C21-C20-C19	-2.77	115.17	123.20
23	C	512	CLA	CED-O2D-CGD	2.77	122.20	115.92
23	b	604	CLA	CMB-C2B-C1B	2.77	129.64	125.42
23	c	903	CLA	C3D-C4D-ND	2.77	114.49	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	411	BCR	C28-C27-C26	-2.77	109.12	114.06
23	d	402	CLA	CHD-C4C-NC	2.77	128.52	124.23
23	b	613	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
23	B	609	CLA	CMC-C2C-C1C	2.76	129.35	125.03
23	D	403	CLA	CMD-C2D-C1D	2.76	129.60	124.73
23	B	605	CLA	C1D-CHD-C4C	-2.76	120.14	126.02
30	B	623	LMT	O1B-C4'-C3'	2.76	114.25	107.23
37	F	101	HEM	CBA-CAA-C2A	-2.76	104.89	112.53
23	b	613	CLA	CMD-C2D-C1D	2.76	129.59	124.73
23	b	604	CLA	CHD-C1D-ND	-2.76	120.92	124.80
30	A	419	LMT	C1-O1'-C1'	2.76	118.39	113.68
23	B	617	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
23	b	610	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
23	c	914	CLA	CHC-C1C-NC	-2.76	120.16	124.31
23	D	403	CLA	CHD-C1D-ND	-2.76	120.92	124.80
23	b	617	CLA	C4B-C3B-C2B	-2.76	103.88	107.30
25	d	404	BCR	C7-C8-C9	-2.76	122.16	126.23
23	B	605	CLA	O2A-CGA-O1A	-2.75	116.74	123.63
23	b	618	CLA	CMB-C2B-C3B	2.75	133.03	126.55
23	c	906	CLA	C4D-CHA-C1A	-2.75	117.96	121.24
23	B	608	CLA	CHD-C4C-NC	2.75	128.50	124.23
23	a	409	CLA	CHD-C1D-ND	-2.75	120.93	124.80
23	C	508	CLA	C2B-C1B-NB	2.75	113.18	110.33
30	B	623	LMT	O1'-C1'-C2'	2.75	112.45	108.27
23	c	910	CLA	CHB-C4A-NA	2.75	128.37	124.40
36	L	101	LHG	O8-C23-O10	-2.75	116.76	123.63
23	c	908	CLA	O2A-CGA-CBA	2.75	120.21	111.83
23	b	619	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
23	b	617	CLA	C4-C3-C5	2.74	119.99	115.23
23	b	612	CLA	CHD-C1D-ND	-2.74	120.94	124.80
23	b	610	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
23	A	406	CLA	OBD-CAD-C3D	-2.74	122.01	128.42
23	D	402	CLA	CHC-C4B-NB	2.74	128.16	124.05
23	B	602	CLA	O2A-CGA-CBA	2.74	120.19	111.83
23	A	406	CLA	C16-C17-C18	-2.74	103.71	115.94
23	a	409	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
23	C	506	CLA	C4-C3-C5	2.73	119.97	115.23
23	b	614	CLA	C14-C13-C15	-2.73	101.53	111.27
23	a	409	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	A	411	BCR	C27-C26-C25	2.73	126.39	122.70
26	A	418	SQD	O5-C1-C2	-2.73	104.76	110.37
25	c	915	BCR	C38-C26-C25	-2.73	121.51	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	CHA-C4D-ND	2.73	138.18	132.55
23	B	617	CLA	CBC-CAC-C3C	-2.73	105.03	112.42
23	a	411	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
34	d	406	DGD	O2G-C1B-O1B	-2.73	117.33	123.70
23	B	606	CLA	C1D-CHD-C4C	-2.73	120.22	126.02
36	d	407	LHG	C6-O8-C23	2.73	127.08	117.12
23	b	612	CLA	C7-C6-C5	-2.72	106.00	113.26
23	b	615	CLA	O2A-CGA-CBA	2.72	120.14	111.83
23	b	610	CLA	O2D-CGD-CBD	2.72	115.99	111.23
23	B	603	CLA	CHD-C1D-ND	-2.72	120.97	124.80
23	B	614	CLA	C14-C13-C15	-2.72	101.57	111.27
23	C	511	CLA	CAC-C3C-C4C	2.72	128.33	124.79
25	t	101	BCR	C2-C3-C4	-2.72	105.30	111.28
23	B	603	CLA	CAA-CBA-CGA	-2.72	105.49	113.21
23	B	617	CLA	CHD-C4C-NC	2.72	128.44	124.23
23	c	907	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
23	b	610	CLA	C4D-CHA-C1A	-2.71	118.01	121.24
34	c	917	DGD	O5D-C6D-C5D	-2.71	103.31	109.42
25	b	622	BCR	C3-C4-C5	-2.71	109.22	114.06
23	B	609	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
23	a	410	CLA	CMB-C2B-C1B	2.71	129.55	125.42
25	c	916	BCR	C11-C10-C9	-2.71	123.48	127.28
23	D	403	CLA	C3B-C4B-NB	2.71	112.95	110.53
23	B	608	CLA	CHA-C4D-ND	2.71	138.13	132.55
23	b	619	CLA	CHA-C4D-ND	2.70	138.12	132.55
23	C	501	CLA	C1-O2A-CGA	2.70	123.18	116.65
23	c	914	CLA	CHD-C1D-ND	-2.70	121.01	124.80
27	c	921	LMG	O8-C28-C29	2.70	120.06	111.83
23	B	614	CLA	CHA-C4D-ND	2.70	138.11	132.55
23	b	617	CLA	CBC-CAC-C3C	-2.69	105.11	112.42
23	C	508	CLA	C3D-C4D-ND	2.69	114.36	109.99
23	A	407	CLA	CHD-C1D-ND	-2.69	121.01	124.80
36	d	408	LHG	C32-C31-C30	-2.69	100.78	114.37
34	D	406	DGD	O6D-C5D-C6D	2.69	112.03	106.69
23	C	508	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
23	b	617	CLA	C4B-CHC-C1C	-2.69	119.93	126.25
30	z	101	LMT	O5B-C5B-C6B	2.69	113.10	106.44
25	A	411	BCR	C33-C5-C6	-2.69	121.55	124.48
23	b	616	CLA	O2A-CGA-CBA	2.69	120.03	111.83
28	A	414	PL9	C7-C8-C9	-2.68	122.21	126.83
23	a	411	CLA	CHC-C4B-NB	2.68	128.07	124.05
37	f	101	HEM	CHC-C1C-NC	2.68	127.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	BCR	C30-C25-C24	2.68	122.92	115.65
23	d	402	CLA	C5-C3-C2	-2.68	115.15	121.17
23	c	909	CLA	CHD-C1D-ND	-2.68	121.03	124.80
23	A	407	CLA	CMB-C2B-C3B	2.68	132.85	126.55
23	b	607	CLA	CED-O2D-CGD	2.68	121.99	115.92
36	d	409	LHG	O7-C7-C8	2.68	117.27	111.48
34	d	406	DGD	O1G-C1A-C2A	2.68	120.00	111.83
23	C	505	CLA	C2B-C1B-NB	2.68	113.10	110.33
23	c	912	CLA	CBC-CAC-C3C	-2.67	105.17	112.42
23	b	608	CLA	C4A-NA-C1A	-2.67	105.46	106.68
23	d	403	CLA	CED-O2D-CGD	2.67	121.98	115.92
27	Z	101	LMG	O8-C28-C29	2.67	119.99	111.83
37	v	201	HEM	C1D-C2D-C3D	-2.67	104.17	106.98
23	B	611	CLA	CAC-C3C-C4C	2.67	128.27	124.79
23	C	513	CLA	C1D-CHD-C4C	-2.67	120.34	126.02
28	a	419	PL9	C45-C44-C46	2.67	119.87	115.23
23	C	504	CLA	C4D-CHA-C1A	-2.67	118.06	121.24
27	b	623	LMG	C13-C12-C11	2.67	122.94	113.13
23	b	616	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
23	b	613	CLA	CHC-C4B-NB	2.67	128.06	124.05
25	b	622	BCR	C8-C7-C6	-2.67	119.87	127.00
23	a	411	CLA	CBA-CAA-C2A	-2.67	105.85	113.79
23	B	613	CLA	CED-O2D-CGD	2.67	121.96	115.92
23	A	406	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
23	d	403	CLA	CAC-C3C-C4C	2.67	128.26	124.79
23	b	605	CLA	CHC-C4B-NB	2.67	128.05	124.05
30	A	419	LMT	O5'-C1'-C2'	-2.67	104.89	110.37
23	B	604	CLA	C1D-ND-C4D	-2.67	104.44	106.31
23	b	612	CLA	CHA-C4D-ND	2.66	138.05	132.55
34	D	406	DGD	O2D-C2D-C3D	-2.66	104.10	110.38
23	d	403	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
28	a	419	PL9	C53-C6-C1	2.66	120.73	115.28
23	C	510	CLA	CHB-C4A-NA	2.66	128.24	124.40
23	C	512	CLA	CBA-CAA-C2A	-2.66	105.89	113.79
37	v	201	HEM	C3B-C2B-C1B	2.66	108.41	106.41
23	B	609	CLA	CHB-C1B-C2B	-2.66	119.72	127.43
23	b	617	CLA	O2A-CGA-CBA	2.66	119.93	111.83
23	C	504	CLA	C2B-C1B-NB	2.65	113.08	110.33
27	C	519	LMG	O8-C9-C8	2.65	116.04	108.40
23	c	904	CLA	CBC-CAC-C3C	-2.65	105.23	112.42
23	b	617	CLA	CHD-C1D-ND	-2.65	121.07	124.80
23	C	513	CLA	O2A-CGA-CBA	2.65	119.92	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	411	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
30	m	101	LMT	O4'-C4B-C3B	2.65	116.62	110.38
23	b	606	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
23	C	501	CLA	C3C-C4C-NC	2.65	113.82	110.43
23	A	410	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
25	D	404	BCR	C32-C1-C6	2.65	114.40	110.24
23	b	606	CLA	C7-C6-C5	-2.65	106.20	113.26
26	a	401	SQD	C3-C4-C5	2.65	115.03	110.23
23	B	607	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
23	C	511	CLA	C4D-CHA-C1A	-2.65	118.09	121.24
34	c	918	DGD	O2G-C1B-O1B	-2.65	117.52	123.70
25	k	101	BCR	C23-C24-C25	-2.65	119.93	127.00
23	B	603	CLA	CMD-C2D-C1D	2.65	129.39	124.73
23	c	913	CLA	C6-C5-C3	-2.64	107.03	113.47
23	D	403	CLA	C6-C7-C8	-2.64	107.18	115.97
23	C	503	CLA	C1D-CHD-C4C	-2.64	120.40	126.02
34	C	518	DGD	O2G-C1B-O1B	-2.64	117.53	123.70
26	L	103	SQD	C4-C3-C2	2.64	115.46	110.83
23	A	405	CLA	CHA-C4D-ND	2.64	137.99	132.55
23	b	607	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
23	C	510	CLA	C4-C3-C5	2.64	119.81	115.23
23	b	618	CLA	CHC-C4B-C3B	-2.63	115.94	127.37
30	M	101	LMT	O2'-C2'-C1'	2.63	116.35	110.08
23	b	611	CLA	C1D-CHD-C4C	-2.63	120.42	126.02
23	c	905	CLA	CHA-C4D-ND	2.63	137.98	132.55
23	b	612	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
23	D	403	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
23	c	905	CLA	C3D-C4D-ND	2.63	114.26	109.99
24	A	409	PHO	CED-O2D-CGD	2.63	121.88	115.92
23	A	410	CLA	C1D-CHD-C4C	-2.63	120.43	126.02
23	A	407	CLA	CAC-C3C-C2C	-2.63	122.73	127.56
28	A	414	PL9	C45-C44-C46	2.62	119.78	115.23
25	c	915	BCR	C11-C10-C9	-2.62	123.60	127.28
30	b	624	LMT	C3'-C4'-C5'	2.62	116.75	110.93
37	v	201	HEM	C3D-C4D-ND	-2.62	107.30	110.17
23	c	907	CLA	C6-C5-C3	-2.62	107.08	113.47
26	B	621	SQD	O47-C7-C8	2.62	117.15	111.48
38	h	101	RRX	C38-C26-C25	-2.62	121.62	124.48
34	H	102	DGD	O6E-C5E-C6E	2.62	112.94	106.44
25	D	404	BCR	C21-C20-C19	-2.62	115.61	123.20
26	L	103	SQD	O9-S-O7	-2.62	105.30	113.82
23	B	610	CLA	C4C-C3C-C2C	-2.62	103.08	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	PHO	CBA-CAA-C2A	-2.62	106.06	113.78
34	h	102	DGD	O2G-C1B-C2B	2.62	117.15	111.48
34	C	516	DGD	C1E-O6E-C5E	2.62	118.83	113.72
23	C	510	CLA	C4C-C3C-C2C	-2.62	103.08	106.89
37	F	101	HEM	C4A-NA-C1A	2.62	110.09	105.82
23	C	503	CLA	C4-C3-C5	2.62	119.77	115.23
23	a	414	CLA	CHA-C4D-ND	2.62	137.95	132.55
33	B	625	HTG	C1-C2-C3	2.61	115.66	110.55
36	l	101	LHG	O7-C7-C8	2.61	117.14	111.48
34	d	406	DGD	C4D-C3D-C2D	2.61	115.42	110.83
25	k	102	BCR	C24-C23-C22	-2.61	122.37	126.23
23	B	609	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
23	b	613	CLA	CHD-C1D-ND	-2.61	121.13	124.80
23	a	411	CLA	C3A-C2A-C1A	-2.61	97.43	101.34
23	c	913	CLA	CHB-C1B-NB	-2.60	120.14	124.05
23	b	613	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
23	B	608	CLA	CGD-CBD-CAD	-2.60	102.42	110.85
23	B	608	CLA	C7-C6-C5	-2.60	106.33	113.26
23	B	613	CLA	C1-O2A-CGA	2.60	122.95	116.65
23	c	906	CLA	CMC-C2C-C1C	2.60	129.10	125.03
34	C	516	DGD	O1G-C1G-C2G	-2.60	100.91	108.40
23	D	403	CLA	CHA-C4D-ND	2.60	137.90	132.55
23	C	502	CLA	C6-C5-C3	-2.59	107.15	113.47
33	C	522	HTG	O5-C5-C4	2.59	114.37	109.70
28	a	419	PL9	C15-C14-C16	2.59	119.73	115.23
23	c	906	CLA	CMB-C2B-C3B	2.59	132.64	126.55
23	B	616	CLA	CAC-C3C-C2C	2.59	132.31	127.56
25	b	620	BCR	C21-C20-C19	-2.59	115.70	123.20
25	c	916	BCR	C8-C7-C6	-2.59	120.09	127.00
25	t	101	BCR	C23-C24-C25	-2.59	120.09	127.00
23	c	912	CLA	O2A-CGA-CBA	2.59	119.72	111.83
23	b	606	CLA	CMB-C2B-C3B	2.58	132.63	126.55
23	B	604	CLA	CHA-C4D-ND	2.58	137.87	132.55
25	A	411	BCR	C35-C13-C12	2.58	122.03	118.09
23	C	507	CLA	C1D-CHD-C4C	-2.58	120.54	126.02
23	C	504	CLA	C7-C6-C5	-2.58	106.39	113.26
23	C	510	CLA	CMC-C2C-C1C	2.58	129.06	125.03
30	c	922	LMT	O5'-C5'-C6'	2.58	112.83	106.44
25	K	101	BCR	C10-C11-C12	-2.58	115.74	123.20
26	a	401	SQD	O48-C46-C45	2.57	115.82	108.40
23	B	608	CLA	C2A-C1A-CHA	-2.57	119.40	123.87
23	B	603	CLA	C14-C13-C12	-2.57	102.10	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	PHO	CAC-C3C-C4C	2.57	130.64	124.03
26	B	621	SQD	O5-C5-C4	-2.57	105.06	109.70
25	B	620	BCR	C23-C24-C25	-2.57	120.12	127.00
23	b	618	CLA	CMA-C3A-C4A	-2.57	104.86	111.77
23	B	611	CLA	CHB-C1B-NB	-2.57	120.19	124.05
36	l	101	LHG	O4-P-O5	2.57	124.41	112.44
23	c	910	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
23	b	605	CLA	CHD-C4C-NC	2.57	128.22	124.23
23	A	406	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
23	B	604	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
23	c	910	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
23	C	512	CLA	C2A-C1A-CHA	-2.57	119.41	123.87
34	H	102	DGD	O3G-C3G-C2G	-2.57	104.57	110.82
27	c	920	LMG	O8-C28-O10	-2.57	117.21	123.63
23	B	605	CLA	C4A-NA-C1A	2.57	107.85	106.68
23	b	610	CLA	CBC-CAC-C3C	-2.57	105.46	112.42
37	V	201	HEM	C1B-NB-C4B	2.57	108.25	105.21
23	C	502	CLA	C16-C17-C18	-2.57	104.48	115.94
36	D	409	LHG	O8-C23-C24	2.56	119.65	111.83
34	C	516	DGD	O6E-C5E-C6E	2.56	112.79	106.44
23	D	402	CLA	C4-C3-C5	2.56	119.67	115.23
23	a	410	CLA	C4A-NA-C1A	-2.56	105.51	106.68
23	c	909	CLA	O2D-CGD-CBD	2.56	115.70	111.23
24	A	408	PHO	O2D-CGD-O1D	-2.56	118.87	123.85
34	H	102	DGD	O4D-C4D-C3D	-2.55	104.36	110.38
27	B	622	LMG	C35-C34-C33	-2.55	101.46	114.37
27	a	418	LMG	O8-C28-C29	2.55	119.62	111.83
25	b	620	BCR	C39-C30-C25	2.55	114.24	110.24
23	B	611	CLA	C4C-C3C-C2C	-2.55	103.18	106.89
23	c	902	CLA	C4-C3-C5	2.55	119.66	115.23
23	D	402	CLA	C3B-C4B-NB	2.55	112.81	110.53
37	f	101	HEM	C4D-C3D-C2D	-2.55	103.18	106.89
23	C	507	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
23	C	501	CLA	CHD-C4C-NC	2.55	128.19	124.23
23	B	615	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
23	b	619	CLA	C4D-CHA-C1A	-2.55	118.20	121.24
23	b	616	CLA	C11-C10-C8	-2.55	107.50	115.97
23	B	612	CLA	CHD-C1D-ND	-2.55	121.22	124.80
23	b	604	CLA	C2A-C1A-CHA	-2.55	119.45	123.87
23	B	602	CLA	CMB-C2B-C1B	2.54	129.29	125.42
23	b	614	CLA	CHD-C4C-NC	2.54	128.18	124.23
23	d	402	CLA	C1D-CHD-C4C	-2.54	120.62	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	101	LMG	O8-C28-O10	-2.54	117.27	123.63
23	B	613	CLA	CAA-CBA-CGA	-2.54	105.99	113.21
23	B	603	CLA	C4B-C3B-C2B	-2.54	104.14	107.30
31	B	633	GOL	O3-C3-C2	-2.54	98.94	110.38
30	b	624	LMT	C2'-C3'-C4'	2.54	115.44	109.68
26	A	418	SQD	O48-C46-C45	2.54	115.72	108.40
23	B	614	CLA	C4C-C3C-C2C	-2.54	103.20	106.89
23	C	510	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
25	T	101	BCR	C23-C22-C21	-2.54	115.02	119.01
26	a	416	SQD	O5-C1-O6	2.54	116.04	110.04
23	b	617	CLA	CED-O2D-CGD	2.54	121.67	115.92
23	b	619	CLA	CED-O2D-CGD	2.54	121.67	115.92
23	b	619	CLA	CBC-CAC-C3C	-2.54	105.55	112.42
33	b	602	HTG	C1-O5-C5	2.53	117.11	112.56
23	B	607	CLA	C3C-C4C-NC	2.53	113.68	110.43
23	b	604	CLA	C3C-C4C-NC	2.53	113.68	110.43
23	c	907	CLA	C4A-NA-C1A	2.53	107.83	106.68
36	d	408	LHG	O7-C7-C8	2.53	116.96	111.48
23	D	403	CLA	CBC-CAC-C3C	-2.53	105.55	112.42
30	m	101	LMT	C1'-O5'-C5'	-2.53	108.78	113.72
23	b	616	CLA	C12-C11-C10	-2.53	101.94	113.28
23	B	610	CLA	CMD-C2D-C3D	2.53	133.49	127.69
27	c	920	LMG	O8-C9-C8	2.53	115.68	108.40
36	d	408	LHG	C13-C12-C11	-2.53	101.59	114.37
23	a	410	CLA	C1-O2A-CGA	2.53	122.77	116.65
24	A	408	PHO	C16-C17-C18	-2.53	104.66	115.94
23	c	904	CLA	C7-C6-C5	-2.53	106.53	113.26
25	D	404	BCR	C40-C30-C39	2.53	115.86	108.63
34	c	918	DGD	O3D-C3D-C2D	-2.52	104.43	110.38
23	B	608	CLA	O2D-CGD-CBD	2.52	115.64	111.23
23	d	403	CLA	C2A-C1A-CHA	-2.52	119.49	123.87
34	c	918	DGD	O1G-C1A-C2A	2.52	119.52	111.83
36	l	101	LHG	O8-C23-O10	-2.52	117.32	123.63
23	b	618	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
23	b	607	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
23	B	603	CLA	C4C-C3C-C2C	-2.52	103.23	106.89
23	C	510	CLA	O2D-CGD-CBD	2.52	115.63	111.23
23	c	908	CLA	CAC-C3C-C4C	2.52	128.06	124.79
23	c	909	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
34	C	518	DGD	O1G-C1A-O1A	-2.52	117.33	123.63
23	c	914	CLA	C1D-CHD-C4C	-2.51	120.67	126.02
36	D	409	LHG	O8-C23-O10	-2.51	117.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CBC-CAC-C3C	-2.51	105.61	112.42
23	A	407	CLA	CED-O2D-CGD	2.51	121.61	115.92
25	D	404	BCR	C15-C14-C13	-2.51	123.75	127.28
23	b	607	CLA	C7-C6-C5	-2.51	106.57	113.26
24	A	408	PHO	C7-C6-C5	-2.51	106.57	113.26
23	C	508	CLA	C3D-C2D-C1D	-2.51	102.41	105.83
23	c	913	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
23	C	508	CLA	CMD-C2D-C1D	2.51	129.14	124.73
23	b	614	CLA	CMD-C2D-C1D	2.51	129.14	124.73
23	c	909	CLA	C3D-C4D-ND	2.51	114.06	109.99
23	C	508	CLA	C2A-C1A-CHA	-2.51	119.52	123.87
26	D	407	SQD	C3-C4-C5	2.50	114.77	110.23
23	a	414	CLA	C4C-C3C-C2C	-2.50	103.25	106.89
23	c	904	CLA	CHD-C1D-ND	-2.50	121.28	124.80
25	k	101	BCR	C8-C9-C10	-2.50	115.07	119.01
23	A	406	CLA	C3A-C2A-C1A	-2.50	97.59	101.34
34	D	406	DGD	O3G-C3G-C2G	2.50	116.90	110.82
23	A	405	CLA	C4C-C3C-C2C	-2.50	103.25	106.89
23	c	913	CLA	CHD-C4C-NC	2.50	128.11	124.23
25	B	619	BCR	C15-C16-C17	-2.50	118.40	123.52
23	B	613	CLA	CHA-C4D-ND	2.50	137.71	132.55
34	C	517	DGD	O1G-C1A-O1A	-2.50	117.38	123.63
23	B	605	CLA	CMC-C2C-C1C	2.50	128.94	125.03
25	d	404	BCR	C30-C25-C26	-2.50	119.22	122.64
26	a	416	SQD	C44-O6-C1	-2.50	108.44	113.80
23	b	606	CLA	CHC-C4B-C3B	-2.50	116.53	127.37
23	d	403	CLA	CHC-C4B-NB	2.50	127.79	124.05
38	H	101	RRX	C36-C18-C17	2.50	126.86	122.82
23	B	615	CLA	C1-C2-C3	-2.50	122.11	126.20
23	C	503	CLA	C3C-C4C-NC	2.49	113.63	110.43
23	a	410	CLA	C3C-C4C-NC	2.49	113.63	110.43
23	c	902	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
36	D	409	LHG	C34-C33-C32	-2.49	101.76	114.37
25	K	101	BCR	C23-C22-C21	-2.49	115.09	119.01
23	B	610	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	b	605	CLA	O2A-CGA-CBA	2.49	119.43	111.83
23	B	612	CLA	CAC-C3C-C4C	2.49	128.03	124.79
23	B	609	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
25	T	101	BCR	C21-C20-C19	-2.49	115.98	123.20
23	b	610	CLA	CGD-CBD-CAD	-2.49	102.78	110.85
23	b	612	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
23	b	616	CLA	CHD-C4C-NC	2.49	128.09	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	419	PL9	C2-C1-C6	2.49	121.95	119.00
34	c	917	DGD	C1D-O6D-C5D	-2.49	108.86	113.72
34	c	917	DGD	C1E-C2E-C3E	-2.49	104.78	110.01
23	b	606	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
23	c	914	CLA	CED-O2D-CGD	2.48	121.55	115.92
23	D	403	CLA	C3D-C4D-ND	2.48	114.02	109.99
38	H	101	RRX	C34-C9-C8	2.48	121.88	118.09
23	C	512	CLA	CMD-C2D-C1D	2.48	129.10	124.73
30	b	625	LMT	C1-O1'-C1'	2.48	117.92	113.68
30	M	101	LMT	O5'-C5'-C6'	2.48	112.59	106.44
26	A	412	SQD	O2-C2-C1	2.48	115.99	110.08
23	D	402	CLA	C3B-C2B-C1B	-2.48	104.25	107.17
36	d	407	LHG	O7-C7-O9	-2.48	117.91	123.70
23	b	615	CLA	C4B-CHC-C1C	-2.48	120.42	126.25
23	d	403	CLA	CHA-C4D-ND	2.48	137.66	132.55
25	a	415	BCR	C15-C14-C13	-2.48	123.80	127.28
23	C	513	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
23	a	411	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
23	A	410	CLA	CHC-C4B-C3B	-2.48	116.63	127.37
33	B	631	HTG	O5-C5-C6	2.47	112.57	106.44
25	K	101	BCR	C29-C28-C27	-2.47	105.84	111.28
25	A	411	BCR	C20-C21-C22	-2.47	123.81	127.28
23	c	903	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
27	Z	101	LMG	O6-C5-C4	2.47	114.15	109.70
26	a	401	SQD	O48-C23-O10	-2.47	117.45	123.63
23	c	903	CLA	C16-C17-C18	-2.47	104.91	115.94
37	F	101	HEM	CAD-C3D-C2D	-2.47	123.24	127.87
23	b	613	CLA	C3B-C4B-NB	2.47	112.73	110.53
23	B	617	CLA	C1D-CHD-C4C	-2.47	120.77	126.02
23	C	505	CLA	C3C-C4C-NC	2.47	113.59	110.43
23	A	407	CLA	C3C-C4C-NC	2.47	113.59	110.43
23	a	414	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
34	h	102	DGD	O6E-C1E-C2E	-2.47	105.31	110.37
24	a	413	PHO	C4D-CHA-CBD	2.46	109.64	108.45
23	C	501	CLA	C1D-CHD-C4C	-2.46	120.78	126.02
25	C	515	BCR	C23-C24-C25	-2.46	120.42	127.00
23	A	410	CLA	C5-C3-C2	-2.46	115.64	121.17
27	d	410	LMG	O8-C28-C29	2.46	119.34	111.83
23	B	616	CLA	C2A-C1A-CHA	-2.46	119.59	123.87
23	C	502	CLA	C4B-CHC-C1C	-2.46	120.46	126.25
23	c	911	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
24	A	408	PHO	CBA-CAA-C2A	-2.46	106.53	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	407	SQD	O48-C23-O10	-2.46	117.48	123.63
23	C	509	CLA	C1D-CHD-C4C	-2.46	120.80	126.02
34	C	518	DGD	C4B-C3B-C2B	-2.46	104.10	113.13
23	c	904	CLA	CED-O2D-CGD	2.46	121.49	115.92
23	C	502	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	b	610	CLA	C7-C6-C5	-2.45	106.72	113.26
23	B	614	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
23	A	405	CLA	CHD-C1D-C2D	-2.45	120.39	125.49
28	D	405	PL9	C2-C1-C6	2.45	121.91	119.00
27	c	921	LMG	O8-C9-C8	2.45	115.46	108.40
27	Z	101	LMG	O1-C7-C8	2.45	116.78	110.82
23	b	616	CLA	CHA-C4D-ND	2.45	137.60	132.55
23	C	505	CLA	CHD-C1D-ND	-2.45	121.36	124.80
23	B	615	CLA	CHC-C1C-NC	-2.45	120.62	124.31
25	T	101	BCR	C24-C23-C22	-2.45	122.61	126.23
25	d	404	BCR	C34-C9-C8	2.45	121.83	118.09
23	B	616	CLA	C3B-C4B-NB	2.45	112.71	110.53
23	b	605	CLA	C2A-C1A-CHA	-2.45	119.62	123.87
23	c	906	CLA	CHC-C4B-NB	2.45	127.72	124.05
23	c	909	CLA	CMC-C2C-C3C	2.44	132.76	126.15
25	c	916	BCR	C35-C13-C12	2.44	121.82	118.09
25	b	620	BCR	C20-C21-C22	-2.44	123.85	127.28
36	d	407	LHG	C11-C10-C9	-2.44	102.03	114.37
23	c	908	CLA	CMD-C2D-C1D	2.44	129.03	124.73
25	B	619	BCR	C30-C25-C26	-2.44	119.30	122.64
37	f	101	HEM	C4C-NC-C1C	2.44	109.80	105.82
23	c	902	CLA	C2A-C1A-CHA	-2.44	119.64	123.87
23	B	612	CLA	CAA-CBA-CGA	-2.44	106.29	113.21
34	h	102	DGD	O3G-C3G-C2G	-2.43	104.90	110.82
23	B	613	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
23	C	505	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
34	h	102	DGD	C6D-C5D-C4D	2.43	117.17	112.07
27	B	622	LMG	C9-C8-C7	-2.43	106.11	111.78
27	C	519	LMG	C8-O7-C10	-2.43	111.97	117.80
23	C	506	CLA	CMD-C2D-C1D	2.43	129.01	124.73
23	b	610	CLA	CHC-C4B-NB	2.43	127.69	124.05
23	B	611	CLA	C4-C3-C5	2.43	119.44	115.23
23	c	909	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
28	D	405	PL9	C12-C13-C14	-2.43	122.07	127.62
28	d	405	PL9	C3-C4-C5	2.43	121.60	118.57
23	C	502	CLA	C5-C3-C2	-2.43	115.72	121.17
25	B	620	BCR	C10-C11-C12	-2.43	116.17	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C4D-C3D-CAD	2.43	110.74	108.11
25	K	101	BCR	C39-C30-C25	-2.42	106.44	110.24
23	d	402	CLA	CHB-C4A-NA	2.42	127.90	124.40
23	c	908	CLA	C4C-C3C-C2C	-2.42	103.36	106.89
33	b	601	HTG	C1'-S1-C1	2.42	105.68	100.45
23	B	604	CLA	CHC-C4B-NB	2.42	127.68	124.05
23	A	406	CLA	C4D-CHA-C1A	-2.42	118.36	121.24
23	c	911	CLA	C4C-C3C-C2C	-2.42	103.37	106.89
24	a	412	PHO	C7-C6-C5	-2.42	106.81	113.26
23	C	511	CLA	C4B-C3B-C2B	-2.42	104.30	107.30
23	a	409	CLA	C1-C2-C3	-2.42	122.24	126.20
28	A	414	PL9	C17-C18-C19	-2.42	122.09	127.62
23	c	906	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
34	c	919	DGD	O3G-C1D-C2D	-2.42	104.61	108.27
23	c	903	CLA	CHD-C1D-ND	-2.41	121.40	124.80
23	b	609	CLA	CMB-C2B-C1B	2.41	129.10	125.42
23	b	611	CLA	CMD-C2D-C1D	2.41	128.98	124.73
23	B	615	CLA	C1C-C2C-C3C	-2.41	104.44	106.98
23	A	410	CLA	CHA-C4D-ND	2.41	137.53	132.55
23	C	509	CLA	CHC-C4B-C3B	-2.41	116.90	127.37
23	b	605	CLA	C16-C17-C18	-2.41	105.17	115.94
34	C	516	DGD	CDB-CCB-CBB	-2.41	102.18	114.37
23	C	511	CLA	C1D-CHD-C4C	-2.41	120.90	126.02
23	b	615	CLA	CED-O2D-CGD	2.41	121.38	115.92
38	h	101	RRX	C7-C8-C9	-2.41	122.67	126.23
23	B	607	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
30	B	623	LMT	C1B-C2B-C3B	-2.41	104.94	110.01
23	B	604	CLA	CHC-C4B-C3B	-2.41	116.92	127.37
33	B	624	HTG	O3-C3-C4	-2.41	104.70	110.38
23	B	617	CLA	C4D-CHA-C1A	-2.41	118.38	121.24
23	B	607	CLA	CHC-C4B-C3B	-2.41	116.93	127.37
23	c	906	CLA	C4C-C3C-C2C	-2.40	103.39	106.89
23	D	402	CLA	C4C-C3C-C2C	-2.40	103.39	106.89
23	C	501	CLA	C1-C2-C3	-2.40	122.26	126.20
23	d	402	CLA	O2D-CGD-CBD	2.40	115.43	111.23
25	C	514	BCR	C2-C1-C6	2.40	113.93	110.44
36	D	409	LHG	O7-C7-O9	-2.40	118.09	123.70
30	M	102	LMT	O6'-C6'-C5'	-2.40	103.16	111.33
23	C	508	CLA	C4C-C3C-C2C	-2.40	103.40	106.89
24	A	409	PHO	C16-C15-C13	-2.40	107.99	115.97
34	C	516	DGD	C3D-C4D-C5D	-2.40	105.89	110.23
23	c	909	CLA	CMD-C2D-C3D	2.40	133.19	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	514	BCR	C37-C22-C23	2.40	121.75	118.09
23	B	606	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
25	a	415	BCR	C35-C13-C12	2.40	121.75	118.09
34	c	919	DGD	C8B-C7B-C6B	-2.39	102.26	114.37
30	A	419	LMT	O1'-C1'-C2'	2.39	111.91	108.27
24	a	413	PHO	OBD-CAD-C3D	-2.39	124.16	127.89
36	D	408	LHG	C11-C10-C9	-2.39	102.27	114.37
25	k	102	BCR	C3-C4-C5	-2.39	109.79	114.06
25	C	514	BCR	C23-C22-C21	-2.39	115.24	119.01
23	C	513	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
23	B	604	CLA	C3C-C4C-NC	2.39	113.49	110.43
23	C	509	CLA	CHB-C4A-NA	2.39	127.85	124.40
28	a	419	PL9	C17-C18-C19	-2.39	122.16	127.62
23	b	610	CLA	C3C-C4C-NC	2.39	113.49	110.43
23	B	616	CLA	C4D-CHA-C1A	-2.39	118.40	121.24
23	B	612	CLA	CHB-C1B-C2B	-2.39	120.50	127.43
23	b	609	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
37	F	101	HEM	C2A-C1A-NA	-2.39	107.50	110.15
23	c	903	CLA	C4C-C3C-C2C	-2.39	103.42	106.89
25	b	621	BCR	C16-C15-C14	-2.39	118.64	123.52
23	B	613	CLA	C2B-C1B-NB	2.38	112.80	110.33
36	d	408	LHG	O8-C23-C24	2.38	119.10	111.83
38	H	101	RRX	C16-C17-C18	-2.38	123.94	127.28
34	C	516	DGD	O2G-C1B-O1B	-2.38	118.14	123.70
23	c	907	CLA	C3C-C4C-NC	2.38	113.48	110.43
23	d	402	CLA	CHD-C1D-ND	-2.38	121.46	124.80
23	C	508	CLA	CHC-C4B-NB	2.38	127.61	124.05
23	A	410	CLA	CMD-C2D-C1D	2.38	128.91	124.73
23	c	913	CLA	O2A-CGA-CBA	2.38	119.08	111.83
23	b	610	CLA	C1-C2-C3	-2.38	122.30	126.20
30	B	623	LMT	O4'-C4B-C3B	-2.37	104.79	110.38
23	b	610	CLA	C3B-C4B-NB	2.37	112.64	110.53
23	a	411	CLA	O2A-CGA-CBA	2.37	119.06	111.83
23	A	410	CLA	C3D-C4D-ND	2.37	113.83	109.99
27	d	410	LMG	O7-C10-O9	-2.37	118.17	123.70
23	B	615	CLA	C1-O2A-CGA	2.37	122.38	116.65
34	D	406	DGD	O1G-C1A-C2A	2.37	119.05	111.83
23	C	510	CLA	CHC-C4B-C3B	-2.37	117.10	127.37
36	d	408	LHG	O2-C2-C1	-2.37	99.39	109.18
23	b	614	CLA	C7-C6-C5	-2.36	106.96	113.26
26	A	412	SQD	O9-S-O7	-2.36	106.13	113.82
30	B	623	LMT	O1'-C1-C2	2.36	117.39	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	904	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
23	B	614	CLA	CHC-C1C-NC	-2.36	120.75	124.31
23	C	504	CLA	CHD-C4C-NC	2.36	127.89	124.23
23	B	608	CLA	CAC-C3C-C4C	2.36	127.86	124.79
26	f	102	SQD	O6-C44-C45	2.36	114.83	109.42
23	A	405	CLA	C7-C6-C5	-2.36	106.97	113.26
34	D	406	DGD	O6D-C5D-C4D	2.36	113.95	109.70
25	b	620	BCR	C39-C30-C29	-2.36	99.90	108.95
23	D	402	CLA	OBD-CAD-C3D	-2.36	122.91	128.42
23	D	402	CLA	CHB-C4A-NA	-2.36	121.00	124.40
33	B	631	HTG	C1-O5-C5	2.36	116.79	112.56
38	H	101	RRX	C21-C20-C19	-2.36	116.37	123.20
36	D	409	LHG	C13-C12-C11	-2.36	102.46	114.37
23	B	616	CLA	CMB-C2B-C1B	2.36	129.00	125.42
23	C	503	CLA	C4D-CHA-C1A	-2.36	118.44	121.24
23	c	912	CLA	CMC-C2C-C1C	2.35	128.71	125.03
23	b	615	CLA	CMB-C2B-C1B	2.35	129.00	125.42
30	m	101	LMT	C3B-C4B-C5B	-2.35	105.97	110.23
34	H	102	DGD	C2G-O2G-C1B	-2.35	112.17	117.80
27	c	920	LMG	C8-O7-C10	-2.35	112.17	117.80
28	D	405	PL9	C51-C49-C50	2.35	119.99	114.59
36	D	410	LHG	O7-C7-C8	2.35	116.56	111.48
26	A	412	SQD	C9-C8-C7	-2.35	105.09	113.69
23	c	911	CLA	CAC-C3C-C4C	2.35	127.84	124.79
33	B	624	HTG	C1'-S1-C1	2.35	105.52	100.45
23	c	911	CLA	C2A-C1A-CHA	-2.35	119.80	123.87
23	c	903	CLA	C3C-C4C-NC	2.35	113.44	110.43
25	K	101	BCR	C7-C8-C9	-2.35	122.77	126.23
23	c	913	CLA	CHD-C1D-ND	-2.35	121.50	124.80
23	b	608	CLA	C14-C13-C12	-2.35	102.91	111.27
23	c	910	CLA	CHD-C4C-NC	2.34	127.87	124.23
23	B	614	CLA	C4-C3-C5	2.34	119.30	115.23
26	a	416	SQD	O48-C23-O10	-2.34	117.77	123.63
23	b	614	CLA	C3B-C2B-C1B	-2.34	104.41	107.17
23	c	910	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
23	b	608	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
37	F	101	HEM	C4C-NC-C1C	2.34	109.64	105.82
23	c	911	CLA	C4-C3-C2	-2.34	117.62	123.63
23	b	619	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
27	A	413	LMG	O8-C28-C29	2.34	118.97	111.83
23	B	605	CLA	C5-C3-C2	-2.34	115.92	121.17
23	b	604	CLA	CED-O2D-CGD	2.34	121.22	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	620	BCR	C16-C17-C18	-2.34	124.00	127.28
23	c	906	CLA	C3C-C4C-NC	2.34	113.42	110.43
26	L	103	SQD	O47-C7-O49	-2.34	118.25	123.70
25	C	514	BCR	C40-C30-C25	-2.34	106.58	110.24
25	b	622	BCR	C40-C30-C25	-2.34	106.58	110.24
34	H	102	DGD	C3E-C4E-C5E	-2.33	106.00	110.23
23	c	912	CLA	C3B-C4B-NB	2.33	112.61	110.53
23	C	512	CLA	OBD-CAD-C3D	-2.33	122.96	128.42
23	c	905	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
23	C	509	CLA	C3B-C4B-NB	2.33	112.61	110.53
23	c	912	CLA	C4D-C3D-CAD	2.33	110.64	108.11
23	B	609	CLA	C11-C12-C13	-2.33	108.22	115.97
23	c	904	CLA	O2A-CGA-CBA	2.33	118.94	111.83
23	B	604	CLA	C4-C3-C5	2.33	119.27	115.23
36	L	101	LHG	C34-C33-C32	-2.33	102.59	114.37
23	B	610	CLA	CHD-C4C-NC	2.33	127.84	124.23
25	k	101	BCR	C1-C6-C7	2.33	121.97	115.65
23	B	610	CLA	CHD-C1D-ND	-2.33	121.53	124.80
23	c	910	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
23	b	612	CLA	CBC-CAC-C3C	-2.33	106.11	112.42
23	B	602	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
23	D	402	CLA	CMC-C2C-C1C	2.33	128.67	125.03
23	b	619	CLA	CHC-C4B-NB	2.33	127.54	124.05
23	A	407	CLA	C1D-CHD-C4C	-2.33	121.08	126.02
23	B	615	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
23	a	409	CLA	O2A-CGA-CBA	2.32	118.92	111.83
33	B	625	HTG	O4-C4-C5	2.32	115.05	109.32
23	A	406	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
23	A	407	CLA	CHC-C4B-C3B	-2.32	117.30	127.37
23	a	409	CLA	CMC-C2C-C3C	2.32	132.42	126.15
23	C	501	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
23	a	410	CLA	CHC-C4B-C3B	-2.32	117.31	127.37
23	B	612	CLA	C3A-C2A-C1A	-2.32	97.87	101.34
23	C	509	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
23	c	905	CLA	C1D-CHD-C4C	-2.32	121.09	126.02
26	A	412	SQD	C44-O6-C1	-2.32	108.83	113.80
23	b	619	CLA	CMB-C2B-C3B	2.32	132.00	126.55
23	c	908	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	B	610	CLA	CED-O2D-CGD	2.32	121.17	115.92
30	a	402	LMT	O4'-C4B-C3B	-2.32	104.92	110.38
23	C	506	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	C	510	CLA	CHA-C4D-ND	2.32	137.33	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	409	LHG	O8-C23-O10	-2.32	117.84	123.63
34	c	919	DGD	C4E-C3E-C2E	2.31	114.89	110.83
23	c	912	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	C	514	BCR	C29-C30-C25	2.31	113.80	110.44
25	k	101	BCR	C15-C16-C17	-2.31	118.79	123.52
23	A	407	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
23	b	612	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
23	C	511	CLA	CHC-C4B-C3B	-2.31	117.35	127.37
26	B	621	SQD	O9-S-O7	-2.31	106.31	113.82
23	b	608	CLA	C1-C2-C3	-2.31	122.42	126.20
23	a	414	CLA	C4B-CHC-C1C	-2.31	120.82	126.25
23	B	605	CLA	C4B-C3B-C2B	-2.31	104.44	107.30
23	b	617	CLA	C2A-C1A-CHA	-2.31	119.87	123.87
23	B	616	CLA	CHB-C1B-NB	-2.30	120.59	124.05
34	c	917	DGD	O2G-C1B-C2B	2.30	116.47	111.48
23	C	506	CLA	O1D-CGD-CBD	-2.30	119.97	124.52
23	c	911	CLA	C1-C2-C3	-2.30	122.42	126.20
28	a	419	PL9	C3-C4-C5	2.30	121.44	118.57
23	A	407	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
34	H	102	DGD	O5D-C6D-C5D	-2.30	104.23	109.42
23	A	406	CLA	CMB-C2B-C1B	2.30	128.92	125.42
23	a	409	CLA	C3B-C4B-NB	2.30	112.58	110.53
25	B	620	BCR	C38-C26-C27	2.30	118.50	113.60
23	B	612	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
23	C	511	CLA	CHD-C4C-NC	2.30	127.79	124.23
23	C	512	CLA	CAC-C3C-C4C	2.30	127.78	124.79
25	d	404	BCR	C10-C11-C12	-2.30	116.55	123.20
27	D	411	LMG	O8-C28-C29	2.29	118.83	111.83
23	c	912	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
23	b	618	CLA	C1-O2A-CGA	2.29	122.20	116.65
23	B	607	CLA	CBC-CAC-C3C	-2.29	106.20	112.42
23	b	611	CLA	CHD-C4C-NC	2.29	127.79	124.23
38	h	101	RRX	C11-C10-C9	-2.29	124.06	127.28
23	B	602	CLA	C4B-C3B-C2B	-2.29	104.45	107.30
23	C	511	CLA	CMD-C2D-C1D	2.29	128.76	124.73
23	b	618	CLA	C11-C10-C8	-2.29	108.35	115.97
23	c	904	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
23	a	414	CLA	O2A-CGA-CBA	2.29	118.81	111.83
25	b	620	BCR	C15-C16-C17	-2.29	118.84	123.52
23	c	909	CLA	CHB-C1B-NB	-2.29	120.62	124.05
23	b	614	CLA	CAC-C3C-C4C	2.28	127.76	124.79
23	C	513	CLA	CHD-C1D-ND	-2.28	121.59	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C28-C27-C26	-2.28	109.99	114.06
23	c	902	CLA	CHC-C4B-C3B	-2.28	117.48	127.37
23	C	509	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
25	A	411	BCR	C35-C13-C14	-2.28	119.12	122.82
23	c	903	CLA	C6-C5-C3	-2.28	107.92	113.47
23	A	405	CLA	CHC-C1C-C2C	-2.28	120.48	126.95
23	B	606	CLA	CHB-C1B-C2B	-2.27	120.82	127.43
23	C	513	CLA	CHD-C4C-NC	2.27	127.76	124.23
23	B	605	CLA	CHC-C1C-NC	-2.27	120.89	124.31
23	b	609	CLA	O2A-CGA-CBA	2.27	118.76	111.83
23	c	903	CLA	O2A-CGA-CBA	2.27	118.76	111.83
25	K	102	BCR	C34-C9-C8	2.27	121.56	118.09
23	c	911	CLA	C3C-C4C-NC	2.27	113.34	110.43
25	B	618	BCR	C24-C25-C26	2.27	126.79	121.56
23	A	410	CLA	C4B-C3B-C2B	-2.27	104.48	107.30
23	A	407	CLA	CHB-C1B-C2B	-2.27	120.83	127.43
34	c	917	DGD	C3G-C2G-C1G	-2.27	106.49	111.78
23	B	609	CLA	C4B-CHC-C1C	-2.27	120.91	126.25
23	c	911	CLA	CHD-C1D-ND	-2.27	121.61	124.80
23	C	506	CLA	CBB-CAB-C3B	-2.27	116.19	127.53
23	b	617	CLA	C3D-C4D-ND	2.27	113.67	109.99
23	B	607	CLA	C4C-C3C-C2C	-2.27	103.59	106.89
26	D	407	SQD	O6-C44-C45	2.27	116.33	110.82
28	d	405	PL9	C25-C24-C26	2.27	119.16	115.23
23	B	615	CLA	C4-C3-C2	-2.27	117.81	123.63
25	B	619	BCR	C37-C22-C23	2.27	121.55	118.09
23	B	616	CLA	CHD-C4C-NC	2.27	127.74	124.23
23	A	406	CLA	C2A-C1A-CHA	-2.27	119.94	123.87
23	c	908	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
23	b	604	CLA	CHC-C4B-NB	2.26	127.44	124.05
34	h	102	DGD	C6D-O5D-C1E	2.26	118.64	113.80
25	B	618	BCR	C15-C16-C17	-2.26	118.89	123.52
23	b	615	CLA	C4B-C3B-C2B	-2.26	104.49	107.30
38	h	101	RRX	C20-C21-C22	-2.26	124.11	127.28
23	c	908	CLA	C1-O2A-CGA	2.26	122.11	116.65
23	C	506	CLA	C4C-C3C-C2C	-2.26	103.61	106.89
23	C	508	CLA	CHD-C4C-NC	2.26	127.73	124.23
23	c	908	CLA	C4D-CHA-C1A	-2.26	118.55	121.24
23	A	407	CLA	CGD-CBD-CAD	-2.26	103.54	110.85
23	A	410	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
23	B	611	CLA	C6-C5-C3	-2.26	107.97	113.47
23	C	511	CLA	C4-C3-C5	2.26	119.14	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	906	CLA	C4-C3-C5	2.26	119.14	115.23
23	b	606	CLA	C3C-C4C-NC	2.26	113.32	110.43
23	c	911	CLA	CMB-C2B-C1B	2.26	128.85	125.42
23	c	911	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
23	B	613	CLA	C4B-CHC-C1C	-2.25	120.95	126.25
23	B	604	CLA	C3D-C4D-ND	2.25	113.65	109.99
26	L	103	SQD	O48-C23-C24	2.25	118.70	111.83
25	a	415	BCR	C8-C7-C6	-2.25	120.98	127.00
23	a	411	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
38	h	101	RRX	C33-C5-C6	-2.25	122.03	124.48
25	T	101	BCR	C29-C28-C27	-2.25	106.33	111.28
25	b	622	BCR	C23-C22-C21	-2.25	115.47	119.01
30	t	102	LMT	C1-O1'-C1'	-2.25	109.84	113.68
23	b	609	CLA	CHA-C4D-ND	2.25	137.19	132.55
23	c	913	CLA	CBA-CAA-C2A	-2.25	107.10	113.79
23	b	605	CLA	CED-O2D-CGD	2.25	121.01	115.92
34	c	917	DGD	CDB-CCB-CBB	-2.25	103.02	114.37
23	d	402	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
27	b	623	LMG	C1-O6-C5	-2.25	109.33	113.72
28	D	405	PL9	C50-C49-C48	-2.24	115.92	122.66
34	C	516	DGD	O6E-C1E-C2E	-2.24	105.76	110.37
23	c	909	CLA	C4-C3-C5	2.24	119.12	115.23
25	k	101	BCR	C33-C5-C6	-2.24	122.04	124.48
23	b	615	CLA	C2B-C1B-NB	2.24	112.65	110.33
23	c	907	CLA	CHC-C4B-C3B	-2.24	117.65	127.37
23	C	509	CLA	C4C-C3C-C2C	-2.24	103.63	106.89
25	k	101	BCR	C29-C30-C25	2.24	113.69	110.44
25	K	101	BCR	C4-C5-C6	2.24	125.73	122.70
23	c	906	CLA	C11-C12-C13	-2.24	108.52	115.97
25	b	621	BCR	C11-C12-C13	-2.24	120.23	126.36
25	b	620	BCR	C40-C30-C25	-2.24	106.73	110.24
24	a	413	PHO	C3D-CAD-CBD	2.24	110.55	107.61
23	b	617	CLA	C4D-C3D-CAD	2.24	110.54	108.11
26	A	412	SQD	O3-C3-C4	2.24	115.65	110.38
23	c	913	CLA	C4C-C3C-C2C	-2.24	103.64	106.89
23	b	613	CLA	O2A-CGA-CBA	2.24	118.65	111.83
23	c	905	CLA	C2A-C1A-CHA	-2.24	119.99	123.87
23	B	608	CLA	C1-O2A-CGA	2.23	122.06	116.65
38	h	101	RRX	C24-C23-C22	-2.23	122.93	126.23
23	B	617	CLA	C4A-NA-C1A	2.23	107.70	106.68
23	B	612	CLA	C4B-CHC-C1C	-2.23	121.00	126.25
23	D	402	CLA	C1C-C2C-C3C	-2.23	104.63	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	CHD-C1D-ND	-2.23	121.66	124.80
23	c	912	CLA	CHB-C4A-NA	2.23	127.62	124.40
23	B	612	CLA	CHC-C4B-C3B	-2.23	117.69	127.37
23	C	502	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
27	c	921	LMG	O6-C1-C2	-2.23	105.79	110.37
23	d	403	CLA	CHB-C1B-NB	-2.23	120.70	124.05
26	D	407	SQD	O5-C1-O6	2.23	115.31	110.04
23	c	902	CLA	C7-C6-C5	-2.23	107.32	113.26
25	D	404	BCR	C32-C1-C2	-2.23	100.39	108.95
25	b	621	BCR	C8-C9-C10	-2.23	115.51	119.01
30	a	402	LMT	O5B-C5B-C6B	2.23	111.95	106.44
23	C	510	CLA	C1D-ND-C4D	-2.22	104.75	106.31
23	b	617	CLA	CHC-C4B-C3B	-2.22	117.72	127.37
28	D	405	PL9	C27-C26-C24	-2.22	105.81	113.19
38	h	101	RRX	C34-C9-C8	2.22	121.49	118.09
23	b	607	CLA	C3B-C4B-NB	2.22	112.52	110.53
23	C	505	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
25	a	415	BCR	C15-C16-C17	-2.22	118.97	123.52
34	c	918	DGD	O5D-C1E-C2E	-2.22	104.90	108.27
30	b	625	LMT	C1'-C2'-C3'	2.22	114.68	110.01
25	c	915	BCR	C35-C13-C12	2.22	121.48	118.09
38	H	101	RRX	C23-C24-C25	-2.22	121.07	127.00
23	c	914	CLA	CAA-CBA-CGA	-2.22	106.91	113.21
23	c	902	CLA	O2A-CGA-CBA	2.22	118.60	111.83
23	C	503	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
23	B	602	CLA	C3C-C4C-NC	2.22	113.27	110.43
23	a	411	CLA	C4B-CHC-C1C	-2.22	121.03	126.25
30	m	102	LMT	O2'-C2'-C1'	2.22	115.36	110.08
23	b	611	CLA	C6-C5-C3	-2.22	108.07	113.47
25	d	404	BCR	C32-C1-C2	-2.22	100.44	108.95
23	B	605	CLA	CHB-C1B-NB	-2.21	120.73	124.05
30	C	520	LMT	C3'-C4'-C5'	-2.21	106.03	110.93
26	f	102	SQD	C46-O48-C23	2.21	125.20	117.12
36	d	407	LHG	O4-P-O5	2.21	122.73	112.44
25	k	101	BCR	C16-C15-C14	-2.21	118.99	123.52
24	A	408	PHO	CAC-C3C-C4C	2.21	129.71	124.03
25	B	619	BCR	C7-C8-C9	-2.21	122.96	126.23
23	A	410	CLA	CED-O2D-CGD	2.21	120.93	115.92
23	a	411	CLA	CED-O2D-CGD	2.21	120.93	115.92
26	a	416	SQD	O48-C23-C24	2.21	118.57	111.83
23	b	615	CLA	CMC-C2C-C1C	2.21	128.48	125.03
34	C	518	DGD	C3D-C4D-C5D	-2.21	106.23	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	620	BCR	C16-C15-C14	-2.21	119.00	123.52
23	A	405	CLA	CHB-C4A-NA	2.21	127.58	124.40
23	D	403	CLA	CHD-C4C-NC	2.21	127.65	124.23
23	c	907	CLA	O2A-CGA-CBA	2.21	118.56	111.83
23	b	615	CLA	CHC-C4B-C3B	-2.20	117.80	127.37
23	C	504	CLA	CMC-C2C-C1C	2.20	128.48	125.03
34	H	102	DGD	O3G-C1D-C2D	-2.20	104.93	108.27
25	K	102	BCR	C37-C22-C23	2.20	121.45	118.09
23	B	608	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
25	k	101	BCR	C2-C3-C4	-2.20	106.43	111.28
23	B	614	CLA	CHC-C4B-C3B	-2.20	117.81	127.37
23	C	502	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
23	B	611	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
23	B	609	CLA	CHC-C4B-C3B	-2.20	117.83	127.37
23	C	513	CLA	CMC-C2C-C1C	2.20	128.47	125.03
30	M	101	LMT	O2'-C2'-C3'	-2.20	105.20	110.38
28	D	405	PL9	C2-C3-C4	2.20	121.73	118.78
23	a	411	CLA	C1D-CHD-C4C	-2.20	121.35	126.02
23	C	509	CLA	C6-C5-C3	-2.20	108.12	113.47
25	C	515	BCR	C40-C30-C25	-2.20	106.80	110.24
23	c	902	CLA	C1-O2A-CGA	2.20	121.97	116.65
23	c	908	CLA	CHC-C4B-C3B	-2.19	117.85	127.37
23	C	507	CLA	C1-O2A-CGA	2.19	121.96	116.65
28	a	419	PL9	C7-C3-C2	-2.19	120.80	123.39
23	A	406	CLA	C11-C10-C8	-2.19	108.67	115.97
34	H	102	DGD	O2G-C1B-C2B	2.19	116.23	111.48
23	a	410	CLA	CGD-CBD-CAD	-2.19	103.75	110.85
23	B	608	CLA	C3B-C2B-C1B	-2.19	104.58	107.17
23	A	406	CLA	CHD-C4C-NC	2.19	127.63	124.23
23	b	614	CLA	CHD-C1D-ND	-2.19	121.72	124.80
23	a	410	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
25	d	404	BCR	C34-C9-C10	-2.19	119.27	122.82
23	B	606	CLA	CMB-C2B-C1B	2.19	128.75	125.42
36	d	409	LHG	O8-C23-C24	2.19	118.51	111.83
30	B	623	LMT	O2'-C2'-C1'	2.19	115.29	110.08
23	A	406	CLA	CHC-C4B-C3B	-2.19	117.88	127.37
25	t	101	BCR	C21-C20-C19	-2.19	116.86	123.20
26	B	621	SQD	O47-C45-C46	2.19	116.19	108.34
23	B	602	CLA	CBC-CAC-C3C	-2.19	106.49	112.42
23	d	402	CLA	CHB-C1B-C2B	-2.19	121.08	127.43
28	d	405	PL9	C16-C14-C13	-2.19	116.26	121.17
23	a	410	CLA	O2D-CGD-O1D	-2.19	119.59	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	626	HTG	O4-C4-C5	2.19	114.71	109.32
23	B	603	CLA	CBC-CAC-C3C	-2.19	106.50	112.42
23	B	607	CLA	C14-C13-C12	-2.19	103.48	111.27
23	B	603	CLA	CMA-C3A-C4A	-2.18	105.90	111.77
23	c	910	CLA	O2A-CGA-CBA	2.18	118.50	111.83
23	a	414	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
23	c	913	CLA	CED-O2D-CGD	2.18	120.86	115.92
34	C	518	DGD	C3A-C2A-C1A	-2.18	105.71	113.69
23	B	612	CLA	CMD-C2D-C3D	2.18	132.69	127.69
23	B	603	CLA	C1-O2A-CGA	2.18	121.93	116.65
36	L	101	LHG	C13-C12-C11	-2.18	103.37	114.37
23	B	613	CLA	O2A-CGA-CBA	2.18	118.47	111.83
27	a	418	LMG	O1-C1-C2	2.18	111.58	108.27
23	b	607	CLA	CHC-C4B-C3B	-2.17	117.93	127.37
30	M	101	LMT	C2'-C3'-C4'	2.17	114.61	109.68
25	D	404	BCR	C39-C30-C25	-2.17	106.84	110.24
23	c	908	CLA	C11-C12-C13	-2.17	108.74	115.97
23	D	403	CLA	CHC-C4B-C3B	-2.17	117.94	127.37
25	d	404	BCR	C35-C13-C12	2.17	121.41	118.09
23	C	502	CLA	CMA-C3A-C4A	-2.17	105.94	111.77
23	d	402	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
23	d	403	CLA	C5-C3-C2	-2.17	116.29	121.17
25	D	404	BCR	C34-C9-C8	2.17	121.40	118.09
23	A	406	CLA	C7-C6-C5	-2.17	107.48	113.26
28	d	405	PL9	C50-C49-C48	-2.17	116.14	122.66
23	d	402	CLA	CMD-C2D-C3D	2.17	132.66	127.69
25	T	101	BCR	C19-C18-C17	-2.17	115.60	119.01
27	c	920	LMG	O1-C7-C8	-2.17	105.55	110.82
23	a	411	CLA	C4B-C3B-C2B	-2.17	104.61	107.30
23	A	405	CLA	C1C-C2C-C3C	-2.17	104.70	106.98
23	c	904	CLA	CHD-C4C-NC	2.17	127.59	124.23
23	b	613	CLA	C4D-C3D-CAD	2.16	110.46	108.11
23	B	602	CLA	C3B-C4B-NB	2.16	112.46	110.53
23	C	511	CLA	C3C-C4C-NC	2.16	113.20	110.43
23	C	513	CLA	CHC-C1C-NC	-2.16	121.05	124.31
23	a	410	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
30	m	101	LMT	C6'-C5'-C4'	2.16	119.46	113.38
26	a	401	SQD	C1-C2-C3	-2.16	105.47	110.01
23	b	614	CLA	C3C-C4C-NC	2.16	113.19	110.43
23	B	604	CLA	CHB-C1B-C2B	-2.16	121.17	127.43
23	D	402	CLA	O2D-CGD-CBD	2.16	115.00	111.23
24	a	413	PHO	CMB-C2B-C3B	2.16	128.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	CLA	O2A-C1-C2	2.16	116.41	108.11
23	c	907	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
23	B	606	CLA	CHC-C4B-C3B	-2.15	118.02	127.37
23	B	617	CLA	CHC-C4B-C3B	-2.15	118.02	127.37
34	H	102	DGD	C3D-C4D-C5D	-2.15	106.33	110.23
23	C	511	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
23	C	506	CLA	CHC-C1C-NC	-2.15	121.07	124.31
23	b	614	CLA	C17-C16-C15	-2.15	103.63	113.28
23	b	614	CLA	C2A-C1A-CHA	-2.15	120.13	123.87
23	b	612	CLA	CMB-C2B-C1B	2.15	128.70	125.42
26	D	407	SQD	O4-C4-C3	-2.15	105.30	110.38
23	d	403	CLA	CGD-CBD-CAD	-2.15	103.88	110.85
28	a	419	PL9	C11-C9-C8	-2.15	116.34	121.17
23	b	619	CLA	C3B-C4B-NB	2.15	112.45	110.53
23	A	405	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
27	d	410	LMG	O1-C7-C8	-2.15	105.59	110.82
30	a	402	LMT	C8-C7-C6	-2.15	103.50	114.37
23	b	606	CLA	C1-C2-C3	-2.15	122.67	126.20
23	a	411	CLA	OBD-CAD-C3D	-2.15	123.39	128.42
26	A	412	SQD	O5-C1-C2	-2.15	105.96	110.37
24	A	409	PHO	O2A-CGA-O1A	-2.15	118.26	123.63
23	d	403	CLA	CHC-C4B-C3B	-2.15	118.05	127.37
28	a	419	PL9	C10-C9-C11	2.15	118.95	115.23
23	A	405	CLA	CMB-C2B-C3B	2.14	131.59	126.55
27	C	519	LMG	C9-C8-C7	-2.14	106.78	111.78
23	c	914	CLA	CMB-C2B-C3B	2.14	131.59	126.55
23	c	905	CLA	CHC-C4B-NB	2.14	127.26	124.05
26	L	103	SQD	C1-O5-C5	-2.14	109.54	113.72
25	c	916	BCR	C19-C18-C17	-2.14	115.64	119.01
23	c	912	CLA	CHC-C4B-NB	2.14	127.26	124.05
34	h	102	DGD	C3B-C2B-C1B	-2.14	105.85	113.69
34	C	518	DGD	C7B-C6B-C5B	-2.14	103.55	114.37
23	B	611	CLA	CHD-C1D-ND	-2.14	121.79	124.80
25	k	101	BCR	C20-C21-C22	-2.14	124.28	127.28
23	b	609	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
33	u	201	HTG	O3-C3-C2	-2.14	106.67	111.16
33	c	923	HTG	C1-O5-C5	2.14	116.40	112.56
23	C	512	CLA	C3C-C4C-NC	2.14	113.17	110.43
30	b	624	LMT	C1'-O5'-C5'	2.14	117.89	113.72
36	l	101	LHG	O3-P-O5	-2.13	100.47	108.94
37	v	201	HEM	C1B-NB-C4B	2.13	107.73	105.21
23	c	909	CLA	C7-C6-C5	-2.13	107.58	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	411	CLA	CHB-C1B-NB	2.13	127.25	124.05
23	B	609	CLA	C11-C10-C8	-2.13	108.88	115.97
33	B	624	HTG	O5-C5-C6	2.13	111.73	106.44
23	c	904	CLA	O2D-CGD-CBD	2.13	114.96	111.23
23	b	618	CLA	CBB-CAB-C3B	-2.13	116.87	127.53
28	d	405	PL9	C36-C37-C38	-2.13	101.47	112.02
23	c	902	CLA	C4B-C3B-C2B	-2.13	104.65	107.30
23	b	605	CLA	C17-C16-C15	-2.13	103.73	113.28
23	c	912	CLA	C3A-C2A-C1A	2.13	104.53	101.34
25	C	514	BCR	C38-C26-C25	-2.13	122.16	124.48
25	c	916	BCR	C7-C8-C9	-2.13	123.08	126.23
23	c	904	CLA	C2A-C1A-CHA	-2.13	120.17	123.87
25	B	619	BCR	C2-C1-C6	2.13	113.53	110.44
23	c	909	CLA	CAC-C3C-C2C	2.13	131.47	127.56
27	c	920	LMG	O7-C10-O9	-2.13	118.73	123.70
25	c	915	BCR	C8-C7-C6	-2.13	121.31	127.00
34	d	406	DGD	O6D-C5D-C6D	2.13	111.46	106.74
34	C	516	DGD	C6D-O5D-C1E	-2.13	109.23	113.80
23	C	506	CLA	O2A-CGA-CBA	2.13	118.32	111.83
28	A	414	PL9	C25-C24-C23	-2.13	118.16	123.63
24	A	408	PHO	CMD-C2D-C3D	2.13	128.93	124.68
25	B	619	BCR	C29-C28-C27	-2.12	106.61	111.28
23	B	605	CLA	C6-C5-C3	-2.12	108.29	113.47
23	a	409	CLA	C6-C5-C3	-2.12	108.30	113.47
37	v	201	HEM	CBB-CAB-C3B	-2.12	116.92	127.53
23	C	505	CLA	CMD-C2D-C3D	2.12	132.56	127.69
28	d	405	PL9	C7-C8-C9	-2.12	123.17	126.83
23	C	503	CLA	CED-O2D-CGD	2.12	120.73	115.92
26	a	416	SQD	O8-S-C6	2.12	110.07	105.97
23	b	609	CLA	C1-C2-C3	-2.12	122.72	126.20
26	A	412	SQD	O48-C23-C24	2.12	118.30	111.83
33	B	625	HTG	O2-C2-C3	-2.12	105.38	110.38
23	C	504	CLA	C2A-C1A-CHA	-2.12	120.19	123.87
37	V	201	HEM	CBB-CAB-C3B	-2.12	116.94	127.53
24	A	408	PHO	CBC-CAC-C3C	-2.12	109.84	112.87
23	B	612	CLA	C15-C13-C12	-2.12	101.34	112.07
34	h	102	DGD	O2G-C1B-O1B	-2.12	118.75	123.70
27	c	920	LMG	C3-C4-C5	2.12	114.07	110.23
33	B	624	HTG	O5-C5-C4	-2.12	105.88	109.70
23	c	913	CLA	CAC-C3C-C4C	2.12	127.54	124.79
23	b	609	CLA	C4-C3-C5	2.12	118.90	115.23
25	t	101	BCR	C15-C16-C17	-2.12	119.19	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	CHC-C1C-C2C	-2.12	120.94	126.95
23	C	507	CLA	CHB-C4A-NA	2.12	127.45	124.40
23	b	611	CLA	C6-C7-C8	-2.12	108.94	115.97
31	D	415	GOL	O2-C2-C1	-2.11	100.42	109.18
33	B	630	HTG	O2-C2-C3	2.11	115.36	110.38
23	B	610	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
23	c	904	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
23	D	403	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
23	C	512	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
23	c	902	CLA	CHA-C4D-ND	2.11	136.90	132.55
23	a	410	CLA	CMD-C2D-C3D	2.11	132.53	127.69
23	d	403	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
23	B	605	CLA	CHC-C4B-C3B	-2.10	118.24	127.37
23	C	503	CLA	CBB-CAB-C3B	-2.10	117.01	127.53
37	f	101	HEM	C2A-C1A-NA	-2.10	107.82	110.15
23	B	616	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
23	B	604	CLA	CMD-C2D-C1D	2.10	128.43	124.73
23	B	608	CLA	CMC-C2C-C3C	2.10	131.84	126.15
23	c	914	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
23	A	405	CLA	C3C-C4C-NC	2.10	113.12	110.43
23	B	605	CLA	O2A-CGA-CBA	2.10	118.24	111.83
26	A	418	SQD	C44-O6-C1	2.10	118.30	113.80
23	c	910	CLA	CMC-C2C-C1C	2.10	128.32	125.03
34	C	516	DGD	O6D-C1D-O3G	-2.10	105.08	110.04
23	c	908	CLA	CHC-C1C-NC	-2.10	121.15	124.31
30	z	101	LMT	O1B-C4'-C3'	2.10	112.57	107.23
23	c	914	CLA	C3C-C4C-NC	2.10	113.12	110.43
23	B	607	CLA	CHA-C4D-ND	2.10	136.88	132.55
25	k	102	BCR	C20-C21-C22	-2.10	124.33	127.28
23	C	501	CLA	C7-C6-C5	-2.10	107.67	113.26
30	M	102	LMT	C3B-C4B-C5B	-2.10	106.43	110.23
23	C	501	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
23	c	911	CLA	CHC-C4B-C3B	-2.10	118.27	127.37
23	b	607	CLA	C1D-CHD-C4C	-2.10	121.56	126.02
25	d	404	BCR	C15-C16-C17	-2.10	119.23	123.52
23	c	905	CLA	C16-C15-C13	2.10	122.94	115.97
23	b	615	CLA	CHA-C4D-ND	2.10	136.87	132.55
23	b	613	CLA	C4B-C3B-C2B	-2.10	104.70	107.30
23	b	606	CLA	CHC-C1C-NC	-2.10	121.16	124.31
23	C	502	CLA	C3C-C4C-NC	2.10	113.11	110.43
23	B	610	CLA	CMB-C2B-C3B	2.10	131.48	126.55
23	b	608	CLA	CAC-C3C-C2C	-2.10	123.71	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CAC-C3C-C4C	2.09	127.51	124.79
23	B	606	CLA	CHC-C1C-NC	-2.09	121.16	124.31
23	b	618	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
23	B	615	CLA	CHC-C4B-C3B	-2.09	118.29	127.37
25	b	620	BCR	C33-C5-C4	2.09	118.06	113.60
23	c	910	CLA	C1-O2A-CGA	2.09	121.71	116.65
24	a	413	PHO	CBA-CAA-C2A	-2.09	107.62	113.78
24	a	413	PHO	C16-C15-C13	-2.09	109.02	115.97
33	b	601	HTG	C2'-C1'-S1	-2.09	105.33	112.36
23	B	606	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
23	B	610	CLA	C4B-CHC-C1C	-2.09	121.34	126.25
23	D	403	CLA	CMB-C2B-C1B	2.09	128.60	125.42
23	B	602	CLA	OBD-CAD-C3D	-2.09	123.54	128.42
23	b	615	CLA	CMD-C2D-C1D	2.09	128.40	124.73
23	d	403	CLA	CMC-C2C-C3C	2.09	131.79	126.15
36	D	410	LHG	O7-C5-C4	2.09	115.83	108.34
37	f	101	HEM	CMC-C2C-C1C	-2.09	121.06	124.73
23	c	912	CLA	CMB-C2B-C1B	2.09	128.59	125.42
23	C	504	CLA	CBB-CAB-C3B	-2.08	117.11	127.53
27	d	410	LMG	O2-C2-C1	-2.08	105.11	110.08
23	c	909	CLA	CHD-C4C-NC	2.08	127.46	124.23
23	C	513	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
23	c	906	CLA	C11-C10-C8	-2.08	109.04	115.97
23	B	614	CLA	CAA-CBA-CGA	-2.08	107.30	113.21
23	B	613	CLA	CMD-C2D-C1D	2.08	128.39	124.73
23	b	605	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
25	t	101	BCR	C29-C30-C25	-2.08	107.42	110.44
38	H	101	RRX	C38-C26-C25	-2.08	122.22	124.48
25	k	102	BCR	C21-C20-C19	-2.08	117.18	123.20
23	d	402	CLA	CAC-C3C-C4C	2.08	127.49	124.79
30	M	102	LMT	O4'-C4B-C3B	2.08	115.27	110.38
26	A	418	SQD	C46-O48-C23	2.08	124.71	117.12
23	C	513	CLA	C3C-C4C-NC	2.08	113.09	110.43
23	b	614	CLA	C16-C15-C13	2.07	122.86	115.97
23	B	613	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
37	V	201	HEM	C4C-C3C-C2C	2.07	108.61	106.81
23	C	505	CLA	CHC-C4B-C3B	-2.07	118.38	127.37
25	D	404	BCR	C31-C1-C2	2.07	116.90	108.95
30	m	101	LMT	C10-C9-C8	-2.07	103.90	114.37
26	L	103	SQD	C28-C27-C26	-2.07	103.91	114.37
23	C	505	CLA	C4C-C3C-C2C	-2.07	103.88	106.89
27	d	410	LMG	C9-C8-C7	-2.07	106.96	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
23	B	608	CLA	CAA-CBA-CGA	-2.07	107.33	113.21
23	a	409	CLA	O2D-CGD-CBD	2.07	114.84	111.23
23	c	911	CLA	C3D-C4D-ND	2.07	113.35	109.99
25	C	515	BCR	C11-C12-C13	-2.07	120.69	126.36
23	B	615	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
33	B	626	HTG	O5-C5-C4	-2.07	105.98	109.70
23	d	403	CLA	C3D-C4D-ND	2.07	113.34	109.99
23	B	608	CLA	CMD-C2D-C3D	2.07	132.43	127.69
23	b	612	CLA	CBB-CAB-C3B	-2.07	117.21	127.53
23	C	507	CLA	O2A-CGA-CBA	2.06	118.13	111.83
23	B	616	CLA	CHC-C4B-C3B	-2.06	118.42	127.37
30	b	625	LMT	O1'-C1'-C2'	-2.06	105.14	108.27
23	c	914	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
27	b	623	LMG	C38-C37-C36	-2.06	103.95	114.37
23	c	903	CLA	CHC-C4B-NB	2.06	127.14	124.05
23	b	616	CLA	CHC-C4B-C3B	-2.06	118.43	127.37
23	A	406	CLA	CED-O2D-CGD	2.06	120.59	115.92
23	C	501	CLA	C6-C5-C3	-2.06	108.45	113.47
23	b	616	CLA	C6-C7-C8	-2.06	109.12	115.97
30	c	922	LMT	O3B-C3B-C4B	2.06	115.23	110.38
23	C	507	CLA	CMB-C2B-C3B	2.06	131.39	126.55
23	B	616	CLA	CMD-C2D-C1D	2.06	128.35	124.73
37	V	201	HEM	CAD-CBD-CGD	-2.06	108.21	113.67
23	C	505	CLA	C2D-C1D-ND	2.06	112.16	110.13
25	k	102	BCR	C28-C27-C26	-2.05	110.39	114.06
30	a	402	LMT	O2'-C2'-C3'	-2.05	105.53	110.38
23	b	615	CLA	C2A-C1A-CHA	-2.05	120.30	123.87
30	z	101	LMT	O1B-C1B-C2B	2.05	113.14	108.09
23	b	609	CLA	C3C-C4C-NC	2.05	113.06	110.43
30	a	402	LMT	O5'-C1'-C2'	-2.05	106.16	110.37
23	b	618	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
23	c	904	CLA	CMD-C2D-C3D	2.05	132.39	127.69
24	A	409	PHO	CMA-C3A-C4A	-2.05	110.19	114.61
27	A	413	LMG	O2-C2-C3	-2.05	105.55	110.38
23	b	607	CLA	O2A-CGA-CBA	2.05	118.08	111.83
23	a	414	CLA	C2A-C1A-CHA	-2.05	120.31	123.87
23	C	504	CLA	CHC-C4B-C3B	-2.05	118.48	127.37
23	C	509	CLA	C1-O2A-CGA	2.05	121.61	116.65
30	M	102	LMT	O2B-C2B-C1B	-2.05	105.20	110.08
23	A	410	CLA	O2A-CGA-CBA	2.05	118.08	111.83
23	B	613	CLA	C2A-C3A-C4A	-2.05	98.56	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	921	LMG	O6-C5-C4	2.05	113.39	109.70
23	d	403	CLA	CBB-CAB-C3B	-2.05	117.30	127.53
34	h	102	DGD	O4E-C4E-C5E	2.05	114.36	109.32
23	B	607	CLA	C9-C8-C10	-2.05	103.98	111.27
23	D	403	CLA	C4-C3-C5	2.05	118.78	115.23
25	T	101	BCR	C16-C17-C18	-2.05	124.41	127.28
23	B	614	CLA	O2A-CGA-CBA	2.04	118.07	111.83
23	b	611	CLA	C2A-C1A-CHA	-2.04	120.32	123.87
23	B	610	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
36	D	408	LHG	C6-O8-C23	2.04	124.59	117.12
23	c	906	CLA	O2A-CGA-CBA	2.04	118.06	111.83
34	c	919	DGD	O5D-C6D-C5D	-2.04	104.82	109.42
23	B	603	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
23	b	604	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
30	t	102	LMT	O5'-C1'-O1'	-2.04	105.22	110.04
27	B	622	LMG	O4-C4-C3	-2.04	105.57	110.38
23	b	609	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
25	b	622	BCR	C20-C19-C18	-2.04	120.77	126.36
23	a	414	CLA	OBD-CAD-C3D	-2.04	123.65	128.42
25	B	620	BCR	C24-C25-C26	-2.04	116.86	121.56
23	b	609	CLA	C4B-CHC-C1C	-2.04	121.46	126.25
26	L	103	SQD	C25-C24-C23	-2.04	106.23	113.69
23	c	912	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
36	d	408	LHG	O3-P-O5	2.04	117.01	108.94
23	C	505	CLA	OBD-CAD-C3D	-2.04	123.66	128.42
28	a	419	PL9	C27-C28-C29	-2.04	122.96	127.62
28	A	414	PL9	C10-C9-C11	2.04	118.76	115.23
23	c	910	CLA	CHB-C1B-NB	-2.04	121.00	124.05
23	c	908	CLA	C5-C3-C2	-2.03	116.60	121.17
23	c	909	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
24	A	409	PHO	OBD-CAD-C3D	-2.03	124.72	127.89
27	a	418	LMG	C30-C29-C28	-2.03	106.24	113.69
25	K	101	BCR	C34-C9-C8	2.03	121.19	118.09
34	D	406	DGD	C3D-C4D-C5D	2.03	113.92	110.23
23	B	611	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
23	c	913	CLA	CBB-CAB-C3B	-2.03	117.37	127.53
30	C	520	LMT	O1'-C1'-C2'	2.03	111.36	108.27
30	b	624	LMT	O5'-C5'-C6'	2.03	111.47	106.44
33	B	630	HTG	C4-C3-C2	2.03	114.40	110.83
30	J	102	LMT	C1'-C2'-C3'	2.03	114.28	110.01
36	E	101	LHG	O8-C23-C24	2.03	118.03	111.83
23	b	614	CLA	CHC-C4B-NB	2.03	127.09	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C1D-CHD-C4C	-2.03	121.70	126.02
23	b	619	CLA	CHC-C1C-NC	-2.03	121.25	124.31
26	A	418	SQD	C9-C8-C7	-2.03	106.25	113.69
23	c	911	CLA	C3B-C4B-NB	2.03	112.34	110.53
33	b	601	HTG	O5-C5-C4	2.03	113.36	109.70
23	B	605	CLA	CMB-C2B-C1B	2.03	128.51	125.42
25	T	101	BCR	C36-C18-C19	2.03	121.19	118.09
23	b	606	CLA	CBB-CAB-C3B	-2.03	117.39	127.53
34	d	406	DGD	O2G-C2G-C1G	2.03	115.62	108.34
23	a	409	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
23	B	606	CLA	CHD-C1D-ND	-2.03	121.95	124.80
23	C	512	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
25	B	620	BCR	C16-C17-C18	-2.03	124.44	127.28
23	b	612	CLA	C4-C3-C5	2.03	118.74	115.23
23	B	616	CLA	C4B-C3B-C2B	-2.02	104.78	107.30
25	b	620	BCR	C37-C22-C23	2.02	121.18	118.09
25	B	619	BCR	C32-C1-C6	-2.02	107.07	110.24
37	F	101	HEM	CHB-C1B-NB	2.02	126.87	124.37
25	B	618	BCR	C23-C22-C21	-2.02	115.83	119.01
33	B	624	HTG	C1-O5-C5	2.02	116.19	112.56
23	B	613	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
25	C	514	BCR	C34-C9-C8	2.02	121.17	118.09
30	C	520	LMT	O3B-C3B-C2B	-2.02	105.61	110.38
23	b	615	CLA	C1D-ND-C4D	-2.02	104.89	106.31
23	b	612	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	a	412	PHO	CAA-C2A-C3A	-2.02	107.54	113.00
30	m	102	LMT	C1'-O5'-C5'	2.02	117.66	113.72
23	B	612	CLA	CBC-CAC-C3C	-2.02	106.95	112.42
31	B	637	GOL	O3-C3-C2	-2.02	101.29	110.38
25	K	101	BCR	C24-C23-C22	-2.02	123.25	126.23
23	b	605	CLA	C4D-C3D-CAD	2.02	110.30	108.11
23	D	402	CLA	C3A-C2A-C1A	-2.01	98.32	101.34
23	a	414	CLA	C4A-NA-C1A	2.01	107.60	106.68
23	A	406	CLA	CMC-C2C-C1C	2.01	128.18	125.03
25	C	515	BCR	C24-C23-C22	-2.01	123.26	126.23
23	B	603	CLA	C4D-CHA-C1A	-2.01	118.84	121.24
23	a	414	CLA	C3A-C2A-C1A	2.01	104.35	101.34
25	k	101	BCR	C7-C6-C5	-2.01	116.92	121.56
28	d	405	PL9	C11-C9-C8	-2.01	116.65	121.17
34	c	918	DGD	O5D-C6D-C5D	2.01	113.95	109.42
23	b	607	CLA	CBB-CAB-C3B	-2.01	117.48	127.53
23	C	508	CLA	CMA-C3A-C4A	-2.01	106.37	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	C1-O2A-CGA	2.01	121.52	116.65
23	B	607	CLA	C6-C5-C3	-2.01	108.57	113.47
25	b	621	BCR	C7-C8-C9	-2.01	123.26	126.23
30	m	101	LMT	C1B-O5B-C5B	2.01	117.64	113.72
25	k	102	BCR	C34-C9-C8	2.01	121.16	118.09
26	B	621	SQD	C45-O47-C7	2.01	122.60	117.80
30	z	101	LMT	C4B-C3B-C2B	-2.01	107.31	110.83
23	c	906	CLA	CED-O2D-CGD	2.01	120.47	115.92
23	B	603	CLA	CHC-C4B-C3B	-2.01	118.66	127.37
23	c	904	CLA	CBB-CAB-C3B	-2.01	117.51	127.53
23	c	906	CLA	C2A-C1A-CHA	-2.00	120.39	123.87
23	b	604	CLA	CMD-C2D-C3D	2.00	132.28	127.69
23	B	607	CLA	C11-C12-C13	-2.00	109.30	115.97
23	c	905	CLA	C3C-C4C-NC	2.00	113.00	110.43
23	b	617	CLA	C6-C5-C3	-2.00	108.59	113.47
23	B	614	CLA	C4B-C3B-C2B	-2.00	104.81	107.30
25	C	515	BCR	C29-C30-C25	2.00	113.35	110.44
37	f	101	HEM	CMD-C2D-C1D	2.00	128.16	125.03
34	c	918	DGD	O4E-C4E-C3E	-2.00	105.66	110.38

There are no chirality outliers.

All (1412) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	C11-C10-C8-C9
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	B	617	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	a	411	CLA	C2B-C3B-CAB-CBB
23	a	411	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C2-C1-O2A-CGA
23	b	604	CLA	C14-C13-C15-C16
23	b	608	CLA	C4-C3-C5-C6
23	b	617	CLA	CAD-CBD-CGD-O1D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	c	903	CLA	CAD-CBD-CGD-O1D
23	c	908	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	c	910	CLA	CHA-CBD-CGD-O1D
25	K	102	BCR	C7-C8-C9-C10
25	K	102	BCR	C7-C8-C9-C34
25	d	404	BCR	C21-C22-C23-C24
25	d	404	BCR	C37-C22-C23-C24
25	k	102	BCR	C7-C8-C9-C10
26	B	621	SQD	C5-C6-S-O7
26	B	621	SQD	C5-C6-S-O8
26	B	621	SQD	C5-C6-S-O9
26	L	103	SQD	O49-C7-O47-C45
26	L	103	SQD	O5-C5-C6-S
26	a	401	SQD	C2-C1-O6-C44
26	f	102	SQD	C44-C45-O47-C7
26	f	102	SQD	O49-C7-O47-C45
27	a	418	LMG	O6-C1-O1-C7
27	a	418	LMG	O1-C7-C8-O7
28	a	419	PL9	C14-C16-C17-C18
30	B	623	LMT	C2-C1-O1'-C1'
30	M	101	LMT	O5'-C1'-O1'-C1
30	m	102	LMT	O5'-C1'-O1'-C1
31	B	635	GOL	O1-C1-C2-C3
31	C	524	GOL	C1-C2-C3-O3
31	a	423	GOL	C1-C2-C3-O3
31	a	424	GOL	O1-C1-C2-C3
31	b	633	GOL	O1-C1-C2-C3
31	b	636	GOL	O1-C1-C2-C3
31	c	927	GOL	C1-C2-C3-O3
31	c	930	GOL	O1-C1-C2-O2
31	c	930	GOL	O1-C1-C2-C3
31	c	930	GOL	C1-C2-C3-O3
33	B	625	HTG	C2'-C1'-S1-C1
33	B	626	HTG	O5-C1-S1-C1'
33	V	202	HTG	C2-C1-S1-C1'
33	V	202	HTG	O5-C1-S1-C1'
33	b	627	HTG	C2-C1-S1-C1'
33	b	627	HTG	O5-C1-S1-C1'
33	u	201	HTG	O2-C2-C3-O3
34	D	406	DGD	C2B-C1B-O2G-C2G
34	d	406	DGD	O6D-C1D-O3G-C3G
36	D	409	LHG	O1-C1-C2-C3
36	D	409	LHG	C3-O3-P-O5
36	D	409	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
36	D	409	LHG	C4-O6-P-O4
36	E	101	LHG	C3-O3-P-O4
36	E	101	LHG	C3-O3-P-O6
36	L	101	LHG	C4-O6-P-O3
36	L	101	LHG	C4-O6-P-O4
36	a	417	LHG	O2-C2-C3-O3
36	a	417	LHG	C3-O3-P-O5
36	a	417	LHG	C3-O3-P-O6
36	a	417	LHG	C4-O6-P-O3
36	a	417	LHG	C4-O6-P-O5
36	d	408	LHG	C3-O3-P-O5
36	l	101	LHG	C4-O6-P-O3
36	l	101	LHG	C4-O6-P-O4
37	v	201	HEM	C2C-C3C-CAC-CBC
23	b	604	CLA	O1A-CGA-O2A-C1
26	D	407	SQD	O10-C23-O48-C46
26	D	407	SQD	C24-C23-O48-C46
30	C	520	LMT	C3'-C4'-O1B-C1B
26	D	407	SQD	O49-C7-O47-C45
34	D	406	DGD	O1B-C1B-O2G-C2G
23	B	615	CLA	C3-C5-C6-C7
23	b	617	CLA	C3-C5-C6-C7
23	b	604	CLA	CBA-CGA-O2A-C1
23	c	914	CLA	CBD-CGD-O2D-CED
26	D	407	SQD	C8-C7-O47-C45
26	L	103	SQD	C8-C7-O47-C45
23	A	410	CLA	C4-C3-C5-C6
23	B	606	CLA	C4-C3-C5-C6
28	a	419	PL9	C30-C29-C31-C32
23	A	410	CLA	C2-C3-C5-C6
23	b	608	CLA	C2-C3-C5-C6
23	B	602	CLA	C3-C5-C6-C7
23	b	607	CLA	C3-C5-C6-C7
33	u	201	HTG	C1-C2-C3-O3
27	c	921	LMG	O6-C5-C6-O5
23	c	913	CLA	C3-C5-C6-C7
26	L	103	SQD	C31-C32-C33-C34
26	a	416	SQD	C17-C18-C19-C20
36	D	409	LHG	O2-C2-C3-O3
36	d	408	LHG	O2-C2-C3-O3
34	D	406	DGD	C2A-C1A-O1G-C1G
30	C	520	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
30	z	101	LMT	O5B-C5B-C6B-O6B
33	d	401	HTG	O5-C5-C6-O6
30	J	102	LMT	O5'-C5'-C6'-O6'
23	C	513	CLA	CBD-CGD-O2D-CED
33	C	521	HTG	S1-C1'-C2'-C3'
33	c	923	HTG	S1-C1'-C2'-C3'
33	u	201	HTG	S1-C1'-C2'-C3'
23	c	912	CLA	O1D-CGD-O2D-CED
23	B	606	CLA	C2-C3-C5-C6
23	b	617	CLA	C2-C3-C5-C6
28	a	419	PL9	C28-C29-C31-C32
27	Z	101	LMG	O6-C5-C6-O5
33	B	631	HTG	O5-C5-C6-O6
28	A	414	PL9	C9-C11-C12-C13
28	A	414	PL9	C19-C21-C22-C23
28	A	414	PL9	C24-C26-C27-C28
28	a	419	PL9	C9-C11-C12-C13
28	a	419	PL9	C24-C26-C27-C28
30	z	101	LMT	C4B-C5B-C6B-O6B
33	b	627	HTG	O5-C5-C6-O6
33	d	401	HTG	C4-C5-C6-O6
34	D	406	DGD	O1A-C1A-O1G-C1G
34	D	406	DGD	O6D-C1D-O3G-C3G
23	C	501	CLA	CBD-CGD-O2D-CED
30	m	101	LMT	O5'-C5'-C6'-O6'
27	A	413	LMG	C20-C21-C22-C23
30	F	102	LMT	O5'-C5'-C6'-O6'
30	m	102	LMT	O5'-C5'-C6'-O6'
36	D	409	LHG	C1-C2-C3-O3
36	E	101	LHG	C1-C2-C3-O3
27	c	920	LMG	C29-C28-O8-C9
26	A	412	SQD	C18-C19-C20-C21
30	Z	102	LMT	C4B-C5B-C6B-O6B
30	b	624	LMT	C4'-C5'-C6'-O6'
30	m	102	LMT	C4'-C5'-C6'-O6'
23	C	513	CLA	O1D-CGD-O2D-CED
23	b	617	CLA	C4-C3-C5-C6
28	A	414	PL9	C30-C29-C31-C32
23	B	602	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C12-C13-C14
23	C	502	CLA	C14-C13-C15-C16
23	C	504	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C11-C10-C8-C9
23	c	907	CLA	C6-C7-C8-C9
23	c	910	CLA	C11-C10-C8-C9
23	c	912	CLA	C14-C13-C15-C16
23	c	913	CLA	C6-C7-C8-C9
27	c	921	LMG	C4-C5-C6-O5
34	D	406	DGD	C2D-C1D-O3G-C3G
34	d	406	DGD	C2D-C1D-O3G-C3G
30	z	101	LMT	C2B-C1B-O1B-C4'
33	B	631	HTG	C4-C5-C6-O6
25	k	102	BCR	C7-C8-C9-C34
33	C	522	HTG	S1-C1'-C2'-C3'
33	b	626	HTG	S1-C1'-C2'-C3'
33	b	627	HTG	C4-C5-C6-O6
34	C	517	DGD	C1B-C2B-C3B-C4B
27	c	920	LMG	O10-C28-O8-C9
30	Z	102	LMT	O5B-C5B-C6B-O6B
30	F	102	LMT	C4'-C5'-C6'-O6'
26	A	418	SQD	O6-C44-C45-O47
26	a	401	SQD	O6-C44-C45-O47
36	E	101	LHG	C24-C23-O8-C6
23	B	617	CLA	C8-C10-C11-C12
26	A	418	SQD	C23-C24-C25-C26
23	B	617	CLA	C2-C1-O2A-CGA
30	J	102	LMT	C4'-C5'-C6'-O6'
23	A	410	CLA	C13-C15-C16-C17
23	C	506	CLA	C5-C6-C7-C8
23	b	607	CLA	C13-C15-C16-C17
34	c	918	DGD	C1A-C2A-C3A-C4A
23	B	614	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C12-C13-C15
23	D	402	CLA	C12-C13-C15-C16
23	a	414	CLA	C12-C13-C15-C16
23	b	609	CLA	C11-C12-C13-C15
23	c	905	CLA	C12-C13-C15-C16
23	c	907	CLA	C12-C13-C15-C16
26	a	401	SQD	C15-C16-C17-C18
34	d	406	DGD	C7B-C8B-C9B-CAB
30	z	101	LMT	O5B-C1B-O1B-C4'
23	A	410	CLA	C10-C11-C12-C13
25	T	101	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	O1D-CGD-O2D-CED
28	a	419	PL9	C19-C21-C22-C23
30	B	623	LMT	C4B-C5B-C6B-O6B
26	B	621	SQD	C31-C32-C33-C34
26	a	401	SQD	C23-C24-C25-C26
27	c	920	LMG	C28-C29-C30-C31
34	c	919	DGD	C1A-C2A-C3A-C4A
36	D	408	LHG	C23-C24-C25-C26
36	l	101	LHG	C7-C8-C9-C10
23	B	614	CLA	C8-C10-C11-C12
23	b	617	CLA	C5-C6-C7-C8
23	b	619	CLA	C13-C15-C16-C17
23	c	910	CLA	C13-C15-C16-C17
30	b	624	LMT	O5'-C5'-C6'-O6'
23	C	512	CLA	C10-C11-C12-C13
23	c	914	CLA	C10-C11-C12-C13
26	L	103	SQD	C7-C8-C9-C10
34	D	406	DGD	C1B-C2B-C3B-C4B
34	d	406	DGD	C1B-C2B-C3B-C4B
36	a	417	LHG	C23-C24-C25-C26
36	d	407	LHG	C23-C24-C25-C26
26	a	401	SQD	O5-C1-O6-C44
30	B	623	LMT	O1'-C1-C2-C3
23	A	410	CLA	C15-C16-C17-C18
23	B	607	CLA	C10-C11-C12-C13
23	C	509	CLA	C13-C15-C16-C17
23	c	914	CLA	C5-C6-C7-C8
36	E	101	LHG	O2-C2-C3-O3
27	c	921	LMG	C10-C11-C12-C13
23	C	506	CLA	C13-C15-C16-C17
23	b	619	CLA	C15-C16-C17-C18
26	B	621	SQD	O49-C7-O47-C45
23	a	414	CLA	C15-C16-C17-C18
23	c	907	CLA	C10-C11-C12-C13
30	M	101	LMT	O5'-C5'-C6'-O6'
34	c	919	DGD	C2B-C3B-C4B-C5B
23	a	414	CLA	C10-C11-C12-C13
26	B	621	SQD	C24-C23-O48-C46
26	B	621	SQD	C8-C7-O47-C45
30	b	625	LMT	O1'-C1-C2-C3
36	E	101	LHG	O10-C23-O8-C6
33	U	201	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
27	d	410	LMG	C10-C11-C12-C13
23	A	410	CLA	C3-C5-C6-C7
23	a	409	CLA	C15-C16-C17-C18
23	b	606	CLA	C5-C6-C7-C8
24	a	413	PHO	C2C-C3C-CAC-CBC
30	m	102	LMT	O1'-C1-C2-C3
36	a	417	LHG	C1-C2-C3-O3
36	d	408	LHG	C1-C2-C3-O3
33	D	414	HTG	C1'-C2'-C3'-C4'
23	B	616	CLA	C5-C6-C7-C8
23	C	509	CLA	C8-C10-C11-C12
23	a	414	CLA	C8-C10-C11-C12
23	B	607	CLA	O1D-CGD-O2D-CED
23	B	614	CLA	C15-C16-C17-C18
23	B	616	CLA	C10-C11-C12-C13
30	M	102	LMT	O5'-C5'-C6'-O6'
23	B	615	CLA	C5-C6-C7-C8
23	D	403	CLA	C8-C10-C11-C12
27	A	413	LMG	C29-C28-O8-C9
23	c	908	CLA	O1D-CGD-O2D-CED
26	A	418	SQD	C2-C1-O6-C44
30	Z	102	LMT	C2'-C1'-O1'-C1
30	t	102	LMT	C2'-C1'-O1'-C1
33	U	201	HTG	C1'-C2'-C3'-C4'
23	c	912	CLA	C16-C17-C18-C20
30	C	520	LMT	C4B-C5B-C6B-O6B
23	b	609	CLA	C13-C15-C16-C17
30	Z	102	LMT	O5B-C1B-O1B-C4'
23	B	607	CLA	C2A-CAA-CBA-CGA
23	b	618	CLA	C10-C11-C12-C13
23	c	911	CLA	C8-C10-C11-C12
31	B	633	GOL	C1-C2-C3-O3
31	B	635	GOL	C1-C2-C3-O3
31	B	638	GOL	O1-C1-C2-C3
31	D	415	GOL	C1-C2-C3-O3
31	b	632	GOL	O1-C1-C2-C3
31	b	632	GOL	C1-C2-C3-O3
31	b	633	GOL	C1-C2-C3-O3
31	f	104	GOL	C1-C2-C3-O3
31	v	203	GOL	O1-C1-C2-C3
36	D	408	LHG	O1-C1-C2-C3
36	a	417	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	a	401	SQD	C7-C8-C9-C10
26	B	621	SQD	C46-C45-O47-C7
23	C	506	CLA	C16-C17-C18-C20
30	Z	102	LMT	O1'-C1-C2-C3
30	Z	102	LMT	C2B-C1B-O1B-C4'
26	A	418	SQD	O5-C1-O6-C44
30	Z	102	LMT	O5'-C1'-O1'-C1
28	A	414	PL9	C28-C29-C31-C32
30	b	624	LMT	C1-C2-C3-C4
24	A	409	PHO	O1D-CGD-O2D-CED
23	B	617	CLA	C16-C17-C18-C19
23	C	507	CLA	C16-C17-C18-C20
23	b	609	CLA	C16-C17-C18-C19
26	L	103	SQD	C15-C16-C17-C18
27	a	418	LMG	C15-C16-C17-C18
30	z	101	LMT	C5-C6-C7-C8
30	J	102	LMT	C1-C2-C3-C4
30	m	102	LMT	C1-C2-C3-C4
26	L	103	SQD	C29-C30-C31-C32
26	a	416	SQD	C33-C34-C35-C36
27	A	413	LMG	C14-C15-C16-C17
27	A	413	LMG	C17-C18-C19-C20
34	C	518	DGD	C8B-C9B-CAB-CBB
34	c	918	DGD	C2B-C3B-C4B-C5B
36	a	417	LHG	C14-C15-C16-C17
26	A	412	SQD	C16-C17-C18-C19
27	A	413	LMG	C36-C37-C38-C39
30	J	102	LMT	C7-C8-C9-C10
34	D	406	DGD	CCB-CDB-CEB-CFB
36	l	101	LHG	C27-C28-C29-C30
34	C	516	DGD	O6D-C5D-C6D-O5D
27	A	413	LMG	C21-C22-C23-C24
27	B	622	LMG	C36-C37-C38-C39
27	C	519	LMG	C15-C16-C17-C18
27	d	410	LMG	C20-C21-C22-C23
30	F	102	LMT	C3-C4-C5-C6
34	D	406	DGD	C5A-C6A-C7A-C8A
34	D	406	DGD	C9A-CAA-CBA-CCA
34	H	102	DGD	C7A-C8A-C9A-CAA
34	d	406	DGD	C6B-C7B-C8B-C9B
36	d	409	LHG	C31-C32-C33-C34
30	F	102	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
31	B	635	GOL	O1-C1-C2-O2
31	B	638	GOL	O1-C1-C2-O2
31	C	524	GOL	O2-C2-C3-O3
31	a	423	GOL	O2-C2-C3-O3
31	b	633	GOL	O1-C1-C2-O2
31	b	636	GOL	O1-C1-C2-O2
31	c	927	GOL	O2-C2-C3-O3
31	c	930	GOL	O2-C2-C3-O3
36	D	409	LHG	O1-C1-C2-O2
27	b	623	LMG	C20-C21-C22-C23
27	d	410	LMG	C34-C35-C36-C37
33	O	303	HTG	C3'-C4'-C5'-C6'
34	C	516	DGD	C4B-C5B-C6B-C7B
34	C	517	DGD	CBA-CCA-CDA-CEA
34	c	917	DGD	C4B-C5B-C6B-C7B
36	D	408	LHG	C30-C31-C32-C33
36	D	410	LHG	C28-C29-C30-C31
23	B	614	CLA	C13-C15-C16-C17
23	c	913	CLA	C4B-C3B-CAB-CBB
27	C	519	LMG	C10-C11-C12-C13
33	B	625	HTG	C1'-C2'-C3'-C4'
23	C	506	CLA	C16-C17-C18-C19
23	C	507	CLA	C16-C17-C18-C19
23	c	903	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
24	A	409	PHO	C2C-C3C-CAC-CBC
23	C	506	CLA	C10-C11-C12-C13
30	Z	102	LMT	C1-C2-C3-C4
27	A	413	LMG	C11-C10-O7-C8
27	a	418	LMG	C20-C21-C22-C23
23	b	609	CLA	C6-C7-C8-C10
23	b	616	CLA	C11-C12-C13-C15
26	D	407	SQD	C11-C10-C9-C8
27	B	622	LMG	C30-C31-C32-C33
27	c	920	LMG	C32-C33-C34-C35
34	C	516	DGD	C7A-C8A-C9A-CAA
26	A	412	SQD	C7-C8-C9-C10
34	D	406	DGD	C1A-C2A-C3A-C4A
23	a	411	CLA	C13-C15-C16-C17
27	Z	101	LMG	C29-C30-C31-C32
27	a	418	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	b	623	LMG	C14-C15-C16-C17
27	c	920	LMG	C13-C14-C15-C16
30	F	102	LMT	C4-C5-C6-C7
36	a	417	LHG	C16-C17-C18-C19
36	d	408	LHG	C32-C33-C34-C35
36	l	101	LHG	C31-C32-C33-C34
23	b	604	CLA	C3-C5-C6-C7
26	f	102	SQD	C28-C29-C30-C31
27	d	410	LMG	C35-C36-C37-C38
30	b	624	LMT	C6-C7-C8-C9
33	B	625	HTG	C2'-C3'-C4'-C5'
34	C	516	DGD	C4A-C5A-C6A-C7A
34	c	919	DGD	CCB-CDB-CEB-CFB
36	d	409	LHG	C15-C16-C17-C18
36	d	409	LHG	C17-C18-C19-C20
23	B	602	CLA	C10-C11-C12-C13
23	B	607	CLA	C15-C16-C17-C18
23	B	615	CLA	C10-C11-C12-C13
23	c	905	CLA	C8-C10-C11-C12
23	c	907	CLA	C15-C16-C17-C18
23	C	502	CLA	C16-C17-C18-C20
23	c	903	CLA	C16-C17-C18-C19
23	c	912	CLA	C16-C17-C18-C19
30	F	102	LMT	C1-C2-C3-C4
26	B	621	SQD	O10-C23-O48-C46
27	A	413	LMG	O10-C28-O8-C9
26	B	621	SQD	C11-C10-C9-C8
30	F	102	LMT	C5-C6-C7-C8
26	f	102	SQD	O5-C1-O6-C44
27	Z	101	LMG	C31-C32-C33-C34
26	A	412	SQD	O6-C44-C45-C46
26	a	416	SQD	O6-C44-C45-C46
34	D	406	DGD	O1G-C1G-C2G-C3G
26	B	621	SQD	C15-C16-C17-C18
26	a	416	SQD	C34-C35-C36-C37
30	z	101	LMT	C6-C7-C8-C9
36	L	101	LHG	C12-C13-C14-C15
26	A	418	SQD	C7-C8-C9-C10
26	B	621	SQD	C29-C30-C31-C32
26	D	407	SQD	C33-C34-C35-C36
27	A	413	LMG	C12-C13-C14-C15
27	d	410	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	A	419	LMT	C6-C7-C8-C9
34	C	518	DGD	CBA-CCA-CDA-CEA
34	D	406	DGD	CAA-CBA-CCA-CDA
34	c	919	DGD	CBA-CCA-CDA-CEA
36	a	417	LHG	C13-C14-C15-C16
36	d	407	LHG	C27-C28-C29-C30
36	l	101	LHG	C33-C34-C35-C36
34	c	918	DGD	C8B-C9B-CAB-CBB
33	B	631	HTG	S1-C1'-C2'-C3'
23	b	614	CLA	O1D-CGD-O2D-CED
26	a	416	SQD	C14-C15-C16-C17
27	B	622	LMG	C31-C32-C33-C34
33	B	630	HTG	C2'-C3'-C4'-C5'
36	E	101	LHG	C25-C26-C27-C28
36	a	417	LHG	C24-C25-C26-C27
36	d	407	LHG	C29-C30-C31-C32
23	c	907	CLA	C16-C17-C18-C19
30	M	101	LMT	O1'-C1-C2-C3
25	B	618	BCR	C1-C6-C7-C8
27	b	623	LMG	C38-C39-C40-C41
27	c	921	LMG	C38-C39-C40-C41
30	M	101	LMT	C2-C3-C4-C5
34	d	406	DGD	C2B-C1B-O2G-C2G
23	C	507	CLA	C5-C6-C7-C8
26	A	418	SQD	C35-C36-C37-C38
27	b	623	LMG	C19-C20-C21-C22
27	b	623	LMG	C21-C22-C23-C24
34	c	918	DGD	C3B-C4B-C5B-C6B
27	D	411	LMG	C19-C20-C21-C22
27	c	920	LMG	C29-C30-C31-C32
34	c	918	DGD	CBB-CCB-CDB-CEB
27	Z	101	LMG	C28-C29-C30-C31
36	E	101	LHG	C18-C19-C20-C21
23	a	409	CLA	C2C-C3C-CAC-CBC
34	C	516	DGD	C5B-C6B-C7B-C8B
34	c	918	DGD	C5B-C6B-C7B-C8B
27	A	413	LMG	O9-C10-O7-C8
34	d	406	DGD	O1B-C1B-O2G-C2G
26	L	103	SQD	C11-C10-C9-C8
23	b	611	CLA	C13-C15-C16-C17
27	A	413	LMG	C32-C33-C34-C35
27	C	519	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
27	c	920	LMG	C19-C20-C21-C22
34	D	406	DGD	C9B-CAB-CBB-CCB
36	E	101	LHG	C14-C15-C16-C17
36	d	407	LHG	C30-C31-C32-C33
33	B	630	HTG	C1'-C2'-C3'-C4'
34	C	517	DGD	C1A-C2A-C3A-C4A
26	L	103	SQD	C10-C11-C12-C13
27	b	623	LMG	C15-C16-C17-C18
30	t	102	LMT	C11-C10-C9-C8
34	c	917	DGD	C2B-C3B-C4B-C5B
36	D	409	LHG	C32-C33-C34-C35
36	L	101	LHG	C10-C11-C12-C13
36	d	409	LHG	C10-C11-C12-C13
27	A	413	LMG	C13-C14-C15-C16
27	a	418	LMG	C16-C17-C18-C19
27	c	920	LMG	C35-C36-C37-C38
30	B	623	LMT	C6-C7-C8-C9
34	C	517	DGD	C9B-CAB-CBB-CCB
34	D	406	DGD	C8B-C9B-CAB-CBB
34	c	917	DGD	C8A-C9A-CAA-CBA
27	b	623	LMG	C40-C41-C42-C43
33	C	522	HTG	O5-C5-C6-O6
26	A	412	SQD	C11-C12-C13-C14
27	C	519	LMG	C38-C39-C40-C41
27	c	920	LMG	C18-C19-C20-C21
34	H	102	DGD	CBA-CCA-CDA-CEA
30	a	402	LMT	C1-C2-C3-C4
26	a	401	SQD	C13-C14-C15-C16
34	C	517	DGD	CAA-CBA-CCA-CDA
36	E	101	LHG	C33-C34-C35-C36
27	D	411	LMG	C12-C13-C14-C15
34	d	406	DGD	C5B-C6B-C7B-C8B
25	c	915	BCR	C19-C20-C21-C22
23	B	617	CLA	C16-C17-C18-C20
30	b	625	LMT	C4'-C5'-C6'-O6'
26	a	401	SQD	C26-C27-C28-C29
27	C	519	LMG	C32-C33-C34-C35
27	Z	101	LMG	C39-C40-C41-C42
27	a	418	LMG	C36-C37-C38-C39
34	H	102	DGD	C9B-CAB-CBB-CCB
36	D	408	LHG	C29-C30-C31-C32
36	D	410	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	c	921	LMG	C35-C36-C37-C38
26	B	621	SQD	C17-C18-C19-C20
36	L	101	LHG	C7-C8-C9-C10
36	L	101	LHG	C11-C12-C13-C14
23	c	907	CLA	C3-C5-C6-C7
27	a	418	LMG	C29-C28-O8-C9
27	Z	101	LMG	C8-C7-O1-C1
34	C	517	DGD	C2G-C3G-O3G-C1D
34	c	918	DGD	C2G-C3G-O3G-C1D
23	a	414	CLA	C16-C17-C18-C19
23	b	609	CLA	C16-C17-C18-C20
23	b	617	CLA	C16-C17-C18-C20
33	b	626	HTG	C2'-C3'-C4'-C5'
37	V	201	HEM	C2C-C3C-CAC-CBC
34	c	917	DGD	O6D-C5D-C6D-O5D
26	D	407	SQD	C24-C25-C26-C27
26	a	401	SQD	C9-C10-C11-C12
27	a	418	LMG	C11-C12-C13-C14
27	b	623	LMG	C29-C30-C31-C32
34	H	102	DGD	CBB-CCB-CDB-CEB
23	B	612	CLA	C15-C16-C17-C18
36	E	101	LHG	C30-C31-C32-C33
33	U	201	HTG	C2'-C1'-S1-C1
27	B	622	LMG	C15-C16-C17-C18
27	b	623	LMG	C17-C18-C19-C20
23	b	615	CLA	C13-C15-C16-C17
26	A	412	SQD	C15-C16-C17-C18
26	a	416	SQD	C9-C10-C11-C12
26	B	621	SQD	C24-C25-C26-C27
26	L	103	SQD	C34-C35-C36-C37
23	d	403	CLA	C8-C10-C11-C12
37	v	201	HEM	C4C-C3C-CAC-CBC
23	b	619	CLA	C16-C17-C18-C19
26	D	407	SQD	C26-C27-C28-C29
26	a	401	SQD	C14-C15-C16-C17
27	B	622	LMG	C34-C35-C36-C37
34	C	517	DGD	C3A-C4A-C5A-C6A
34	C	518	DGD	C2A-C3A-C4A-C5A
23	a	410	CLA	C2C-C3C-CAC-CBC
30	B	623	LMT	C1-C2-C3-C4
23	b	614	CLA	C13-C15-C16-C17
23	c	910	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	d	409	LHG	C18-C19-C20-C21
23	b	606	CLA	CBD-CGD-O2D-CED
26	A	412	SQD	O6-C44-C45-O47
26	D	407	SQD	O6-C44-C45-O47
26	a	416	SQD	O6-C44-C45-O47
34	d	406	DGD	O1G-C1G-C2G-O2G
33	B	624	HTG	C3'-C4'-C5'-C6'
26	f	102	SQD	C27-C28-C29-C30
34	C	517	DGD	C9A-CAA-CBA-CCA
34	c	918	DGD	C5A-C6A-C7A-C8A
34	h	102	DGD	C7A-C8A-C9A-CAA
36	a	417	LHG	C10-C11-C12-C13
36	d	409	LHG	C34-C35-C36-C37
23	D	403	CLA	C10-C11-C12-C13
23	c	902	CLA	O1D-CGD-O2D-CED
30	a	402	LMT	C4B-C5B-C6B-O6B
26	a	401	SQD	C28-C29-C30-C31
27	B	622	LMG	C17-C18-C19-C20
34	C	517	DGD	C4B-C5B-C6B-C7B
26	B	621	SQD	C27-C28-C29-C30
26	a	401	SQD	C34-C35-C36-C37
27	Z	101	LMG	C18-C19-C20-C21
30	c	922	LMT	C6-C7-C8-C9
34	D	406	DGD	C7A-C8A-C9A-CAA
23	b	605	CLA	C16-C17-C18-C19
23	c	910	CLA	C16-C17-C18-C19
26	A	412	SQD	C28-C29-C30-C31
33	d	401	HTG	C3'-C4'-C5'-C6'
23	d	403	CLA	C4-C3-C5-C6
36	E	101	LHG	C9-C10-C11-C12
27	C	519	LMG	C31-C32-C33-C34
36	D	410	LHG	C30-C31-C32-C33
36	l	101	LHG	C11-C10-C9-C8
36	l	101	LHG	C25-C26-C27-C28
34	c	917	DGD	C4D-C5D-C6D-O5D
27	a	418	LMG	C30-C31-C32-C33
36	E	101	LHG	C17-C18-C19-C20
34	H	102	DGD	C9A-CAA-CBA-CCA
36	D	408	LHG	C27-C28-C29-C30
31	a	424	GOL	O1-C1-C2-O2
27	b	623	LMG	C39-C40-C41-C42
34	h	102	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
26	A	418	SQD	C29-C30-C31-C32
30	a	402	LMT	C2-C3-C4-C5
23	c	914	CLA	C1A-C2A-CAA-CBA
26	a	401	SQD	C31-C32-C33-C34
30	t	102	LMT	C4-C5-C6-C7
34	c	917	DGD	O6E-C5E-C6E-O5E
30	a	402	LMT	O1'-C1-C2-C3
26	A	418	SQD	C26-C27-C28-C29
23	A	410	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C12-C13-C15
23	C	504	CLA	C11-C12-C13-C15
23	C	506	CLA	C6-C7-C8-C10
23	c	904	CLA	C6-C7-C8-C10
23	c	905	CLA	C11-C10-C8-C7
23	c	908	CLA	C11-C10-C8-C7
23	d	403	CLA	C11-C12-C13-C15
26	a	416	SQD	C27-C28-C29-C30
27	b	623	LMG	C18-C19-C20-C21
23	a	414	CLA	C16-C17-C18-C20
26	f	102	SQD	C24-C25-C26-C27
23	c	912	CLA	C13-C15-C16-C17
26	a	416	SQD	C26-C27-C28-C29
33	B	630	HTG	C4-C5-C6-O6
27	B	622	LMG	C39-C40-C41-C42
26	B	621	SQD	C16-C17-C18-C19
34	c	917	DGD	C9A-CAA-CBA-CCA
23	D	402	CLA	C2C-C3C-CAC-CBC
23	B	605	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C2A-CAA-CBA-CGA
23	b	609	CLA	C2A-CAA-CBA-CGA
23	A	410	CLA	C11-C10-C8-C9
23	B	607	CLA	C11-C10-C8-C9
23	B	615	CLA	C11-C10-C8-C9
23	B	617	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C9
23	D	402	CLA	C14-C13-C15-C16
23	a	414	CLA	C14-C13-C15-C16
23	c	905	CLA	C11-C10-C8-C9
23	d	403	CLA	C11-C12-C13-C14
30	B	623	LMT	C5-C6-C7-C8
34	c	918	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
36	D	408	LHG	C24-C25-C26-C27
27	D	411	LMG	O6-C5-C6-O5
26	f	102	SQD	C29-C30-C31-C32
34	c	917	DGD	C6A-C7A-C8A-C9A
23	c	914	CLA	CBA-CGA-O2A-C1
23	C	504	CLA	C13-C15-C16-C17
27	d	410	LMG	O6-C5-C6-O5
34	d	406	DGD	CAA-CBA-CCA-CDA
36	a	417	LHG	C17-C18-C19-C20
36	l	101	LHG	C34-C35-C36-C37
26	A	418	SQD	O6-C44-C45-C46
26	B	621	SQD	C44-C45-C46-O48
26	D	407	SQD	O6-C44-C45-C46
26	L	103	SQD	C44-C45-C46-O48
26	a	401	SQD	O6-C44-C45-C46
27	a	418	LMG	O1-C7-C8-C9
27	a	418	LMG	C7-C8-C9-O8
34	d	406	DGD	C1G-C2G-C3G-O3G
30	m	101	LMT	C4'-C5'-C6'-O6'
27	D	411	LMG	C35-C36-C37-C38
27	Z	101	LMG	C30-C31-C32-C33
27	b	623	LMG	C37-C38-C39-C40
23	D	403	CLA	C16-C17-C18-C19
23	b	605	CLA	C16-C17-C18-C20
26	a	401	SQD	C11-C12-C13-C14
27	Z	101	LMG	C37-C38-C39-C40
30	A	419	LMT	C7-C8-C9-C10
34	c	919	DGD	C6A-C7A-C8A-C9A
36	d	408	LHG	C11-C10-C9-C8
26	a	401	SQD	C16-C17-C18-C19
27	c	920	LMG	C16-C17-C18-C19
36	D	410	LHG	C17-C18-C19-C20
36	E	101	LHG	C7-C8-C9-C10
27	a	418	LMG	O10-C28-O8-C9
30	a	402	LMT	O5'-C5'-C6'-O6'
26	a	416	SQD	C12-C13-C14-C15
27	B	622	LMG	C18-C19-C20-C21
23	c	907	CLA	C16-C17-C18-C20
34	C	516	DGD	O6E-C5E-C6E-O5E
23	c	914	CLA	O1A-CGA-O2A-C1
26	a	401	SQD	C27-C28-C29-C30
33	b	602	HTG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
26	B	621	SQD	C10-C11-C12-C13
23	b	617	CLA	O1D-CGD-O2D-CED
26	A	418	SQD	C24-C23-O48-C46
27	B	622	LMG	C16-C17-C18-C19
30	Z	102	LMT	C4-C5-C6-C7
30	b	625	LMT	C1-C2-C3-C4
34	D	406	DGD	CBA-CCA-CDA-CEA
25	k	102	BCR	C19-C20-C21-C22
30	t	102	LMT	C3-C4-C5-C6
27	C	519	LMG	C29-C28-O8-C9
34	h	102	DGD	CBB-CCB-CDB-CEB
33	b	601	HTG	C4'-C5'-C6'-C7'
36	d	409	LHG	C19-C20-C21-C22
26	B	621	SQD	C32-C33-C34-C35
23	C	507	CLA	C4-C3-C5-C6
28	A	414	PL9	C23-C24-C26-C27
34	d	406	DGD	CDB-CEB-CFB-CGB
36	D	410	LHG	C16-C17-C18-C19
26	L	103	SQD	C35-C36-C37-C38
26	B	621	SQD	O47-C45-C46-O48
34	d	406	DGD	CDA-CEA-CFA-CGA
26	A	412	SQD	C10-C11-C12-C13
26	f	102	SQD	C26-C27-C28-C29
34	C	516	DGD	CCA-CDA-CEA-CFA
36	d	409	LHG	C13-C14-C15-C16
30	b	624	LMT	C9-C10-C11-C12
23	B	605	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
34	C	518	DGD	CDA-CEA-CFA-CGA
36	D	410	LHG	C32-C33-C34-C35
23	c	910	CLA	C16-C17-C18-C20
34	c	917	DGD	CDA-CEA-CFA-CGA
36	E	101	LHG	C19-C20-C21-C22
34	d	406	DGD	C2A-C3A-C4A-C5A
34	d	406	DGD	C4B-C5B-C6B-C7B
33	D	414	HTG	C4'-C5'-C6'-C7'
26	L	103	SQD	C18-C19-C20-C21
34	D	406	DGD	CBB-CCB-CDB-CEB
33	O	303	HTG	C1'-C2'-C3'-C4'
27	A	413	LMG	C22-C23-C24-C25
26	A	418	SQD	C27-C28-C29-C30
27	Z	101	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
36	d	409	LHG	C12-C13-C14-C15
27	Z	101	LMG	C40-C41-C42-C43
33	u	201	HTG	C4'-C5'-C6'-C7'
36	a	417	LHG	C26-C27-C28-C29
30	b	625	LMT	C5-C6-C7-C8
30	b	625	LMT	C9-C10-C11-C12
36	a	417	LHG	C19-C20-C21-C22
34	C	516	DGD	C1B-C2B-C3B-C4B
36	d	409	LHG	C35-C36-C37-C38
23	a	414	CLA	C5-C6-C7-C8
23	b	618	CLA	C16-C17-C18-C20
34	C	517	DGD	C4A-C5A-C6A-C7A
27	c	920	LMG	C12-C13-C14-C15
27	C	519	LMG	C39-C40-C41-C42
27	c	920	LMG	C37-C38-C39-C40
27	d	410	LMG	C29-C30-C31-C32
34	C	517	DGD	C7A-C8A-C9A-CAA
30	b	624	LMT	C2-C1-O1'-C1'
31	f	104	GOL	O2-C2-C3-O3
31	h	103	GOL	O2-C2-C3-O3
23	B	611	CLA	C14-C13-C15-C16
23	B	615	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	c	908	CLA	C11-C10-C8-C9
23	B	617	CLA	C13-C15-C16-C17
23	b	612	CLA	C4B-C3B-CAB-CBB
27	D	411	LMG	C15-C16-C17-C18
30	B	623	LMT	C7-C8-C9-C10
33	B	626	HTG	C3'-C4'-C5'-C6'
33	c	923	HTG	C2'-C3'-C4'-C5'
26	L	103	SQD	C24-C25-C26-C27
34	d	406	DGD	CBB-CCB-CDB-CEB
27	C	519	LMG	C22-C23-C24-C25
30	F	102	LMT	C9-C10-C11-C12
27	a	418	LMG	C12-C13-C14-C15
34	d	406	DGD	CBA-CCA-CDA-CEA
36	d	409	LHG	C16-C17-C18-C19
23	b	618	CLA	C5-C6-C7-C8
26	a	416	SQD	C10-C11-C12-C13
27	B	622	LMG	C14-C15-C16-C17
27	C	519	LMG	C17-C18-C19-C20
27	Z	101	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
34	c	919	DGD	C7A-C8A-C9A-CAA
36	E	101	LHG	C11-C12-C13-C14
36	d	409	LHG	C24-C25-C26-C27
27	B	622	LMG	C40-C41-C42-C43
27	c	920	LMG	C36-C37-C38-C39
23	B	602	CLA	C11-C10-C8-C7
23	B	611	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C11-C10-C8-C7
23	a	411	CLA	C11-C10-C8-C7
23	b	609	CLA	C12-C13-C15-C16
23	b	614	CLA	C12-C13-C15-C16
23	c	913	CLA	C11-C10-C8-C7
30	c	922	LMT	O1'-C1-C2-C3
26	D	407	SQD	C23-C24-C25-C26
26	B	621	SQD	C13-C14-C15-C16
30	J	102	LMT	C9-C10-C11-C12
23	c	905	CLA	C3A-C2A-CAA-CBA
23	c	911	CLA	C2-C3-C5-C6
33	B	625	HTG	C4'-C5'-C6'-C7'
34	C	516	DGD	C5A-C6A-C7A-C8A
27	C	519	LMG	O10-C28-O8-C9
23	d	403	CLA	C15-C16-C17-C18
34	c	919	DGD	C2A-C1A-O1G-C1G
34	d	406	DGD	C6A-C7A-C8A-C9A
25	t	101	BCR	C13-C14-C15-C16
27	A	413	LMG	C15-C16-C17-C18
34	C	517	DGD	CCB-CDB-CEB-CFB
27	d	410	LMG	C40-C41-C42-C43
33	c	923	HTG	C3'-C4'-C5'-C6'
27	A	413	LMG	C7-C8-C9-O8
34	d	406	DGD	O1G-C1G-C2G-C3G
27	A	413	LMG	C31-C32-C33-C34
36	a	417	LHG	C9-C10-C11-C12
23	C	507	CLA	C13-C15-C16-C17
30	C	520	LMT	C6-C7-C8-C9
34	D	406	DGD	C4A-C5A-C6A-C7A
27	d	410	LMG	C36-C37-C38-C39
34	C	517	DGD	C7B-C8B-C9B-CAB
30	A	419	LMT	C1-C2-C3-C4
23	C	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	C	516	DGD	CAA-CBA-CCA-CDA
23	c	911	CLA	C4-C3-C5-C6
28	A	414	PL9	C25-C24-C26-C27
23	a	409	CLA	C4C-C3C-CAC-CBC
26	a	416	SQD	C29-C30-C31-C32
34	h	102	DGD	CDB-CEB-CFB-CGB
36	a	417	LHG	O6-C4-C5-O7
30	J	102	LMT	C5-C6-C7-C8
25	B	618	BCR	C5-C6-C7-C8
25	b	620	BCR	C1-C6-C7-C8
36	E	101	LHG	C8-C7-O7-C5
36	D	410	LHG	C2-C3-O3-P
23	b	618	CLA	O1D-CGD-O2D-CED
26	A	418	SQD	C28-C29-C30-C31
27	D	411	LMG	C36-C37-C38-C39
34	c	919	DGD	C9B-CAB-CBB-CCB
36	a	417	LHG	C25-C26-C27-C28
34	h	102	DGD	O2G-C1B-C2B-C3B
23	B	613	CLA	C13-C15-C16-C17
27	A	413	LMG	O7-C8-C9-O8
27	a	418	LMG	O7-C8-C9-O8
34	d	406	DGD	O2G-C2G-C3G-O3G
28	A	414	PL9	C4-C3-C7-C8
28	a	419	PL9	C4-C3-C7-C8
26	L	103	SQD	C27-C28-C29-C30
23	c	908	CLA	C5-C6-C7-C8
23	a	410	CLA	C4C-C3C-CAC-CBC
26	L	103	SQD	C17-C18-C19-C20
26	A	412	SQD	C33-C34-C35-C36
23	b	604	CLA	C10-C11-C12-C13
34	H	102	DGD	CDB-CEB-CFB-CGB
26	A	418	SQD	C25-C26-C27-C28
30	b	625	LMT	C3-C4-C5-C6
33	b	601	HTG	C3'-C4'-C5'-C6'
34	C	518	DGD	C6A-C7A-C8A-C9A
36	D	409	LHG	C11-C10-C9-C8
36	l	101	LHG	C10-C11-C12-C13
27	C	519	LMG	C14-C15-C16-C17
27	C	519	LMG	C29-C30-C31-C32
34	h	102	DGD	C5B-C6B-C7B-C8B
23	C	509	CLA	C11-C10-C8-C9
23	D	403	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	609	CLA	C11-C12-C13-C14
23	b	613	CLA	C11-C12-C13-C14
23	c	913	CLA	C11-C10-C8-C9
33	C	521	HTG	C2'-C3'-C4'-C5'
34	C	516	DGD	C3B-C4B-C5B-C6B
34	D	406	DGD	CDB-CEB-CFB-CGB
27	A	413	LMG	C19-C20-C21-C22
27	c	921	LMG	C11-C12-C13-C14
36	D	409	LHG	C16-C17-C18-C19
23	b	618	CLA	C16-C17-C18-C19
34	C	517	DGD	CAB-CBB-CCB-CDB
33	B	626	HTG	C4-C5-C6-O6
36	d	409	LHG	C27-C28-C29-C30
26	a	416	SQD	C35-C36-C37-C38
31	L	104	GOL	O1-C1-C2-O2
31	b	632	GOL	O1-C1-C2-O2
31	c	928	GOL	O1-C1-C2-O2
36	a	417	LHG	O1-C1-C2-O2
23	B	611	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
26	A	418	SQD	O10-C23-O48-C46
30	C	520	LMT	C5-C6-C7-C8
36	E	101	LHG	C11-C10-C9-C8
34	C	518	DGD	CDB-CEB-CFB-CGB
23	D	403	CLA	C16-C17-C18-C20
23	b	617	CLA	C16-C17-C18-C19
23	b	619	CLA	C16-C17-C18-C20
23	B	617	CLA	C5-C6-C7-C8
23	C	503	CLA	C8-C10-C11-C12
23	b	617	CLA	C10-C11-C12-C13
25	c	915	BCR	C36-C18-C19-C20
23	B	602	CLA	C11-C12-C13-C15
23	B	607	CLA	C11-C10-C8-C7
23	B	614	CLA	C11-C12-C13-C15
23	B	617	CLA	C11-C12-C13-C15
23	C	513	CLA	C6-C7-C8-C10
23	D	403	CLA	C6-C7-C8-C10
23	a	414	CLA	C11-C10-C8-C7
23	b	607	CLA	C6-C7-C8-C10
23	c	907	CLA	C11-C10-C8-C7
34	C	517	DGD	CCA-CDA-CEA-CFA
34	D	406	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
34	H	102	DGD	CCA-CDA-CEA-CFA
26	a	401	SQD	C24-C25-C26-C27
23	a	414	CLA	C13-C15-C16-C17
23	c	905	CLA	C15-C16-C17-C18
25	D	404	BCR	C21-C22-C23-C24
27	b	623	LMG	C36-C37-C38-C39
36	E	101	LHG	C15-C16-C17-C18
26	B	621	SQD	C45-C44-O6-C1
26	L	103	SQD	C45-C44-O6-C1
27	c	921	LMG	C8-C7-O1-C1
34	C	517	DGD	C5D-C6D-O5D-C1E
34	c	918	DGD	C5D-C6D-O5D-C1E
30	a	402	LMT	C4'-C5'-C6'-O6'
36	D	410	LHG	C24-C25-C26-C27
23	A	410	CLA	C16-C17-C18-C20
27	A	413	LMG	C39-C40-C41-C42
34	C	517	DGD	C6B-C7B-C8B-C9B
23	d	403	CLA	C2-C3-C5-C6
37	V	201	HEM	C2B-C3B-CAB-CBB
37	v	201	HEM	C2B-C3B-CAB-CBB
23	B	609	CLA	C13-C15-C16-C17
31	O	304	GOL	C1-C2-C3-O3
31	V	203	GOL	O1-C1-C2-C3
30	t	102	LMT	C6-C7-C8-C9
34	c	917	DGD	C5B-C6B-C7B-C8B
30	B	623	LMT	O5B-C5B-C6B-O6B
23	C	513	CLA	O2A-C1-C2-C3
23	A	405	CLA	C2C-C3C-CAC-CBC
30	C	520	LMT	C9-C10-C11-C12
26	a	416	SQD	C7-C8-C9-C10
23	C	508	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	C16-C17-C18-C20
26	f	102	SQD	O5-C5-C6-S
26	L	103	SQD	O5-C1-O6-C44
30	t	102	LMT	O5'-C1'-O1'-C1
23	C	508	CLA	C16-C17-C18-C19
26	L	103	SQD	C19-C20-C21-C22
34	C	516	DGD	C4D-C5D-C6D-O5D
33	U	201	HTG	C2'-C3'-C4'-C5'
34	H	102	DGD	CCB-CDB-CEB-CFB
26	L	103	SQD	O47-C45-C46-O48
26	f	102	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
27	A	413	LMG	O1-C7-C8-O7
34	H	102	DGD	O1G-C1G-C2G-O2G
23	a	411	CLA	C6-C7-C8-C9
23	a	411	CLA	C11-C10-C8-C9
23	A	410	CLA	C16-C17-C18-C19
23	C	512	CLA	C16-C17-C18-C20
27	C	519	LMG	C30-C31-C32-C33
33	b	626	HTG	C3'-C4'-C5'-C6'
26	a	401	SQD	C25-C26-C27-C28
27	d	410	LMG	C17-C18-C19-C20
30	B	623	LMT	C11-C10-C9-C8
23	B	605	CLA	C13-C15-C16-C17
23	B	611	CLA	C8-C10-C11-C12
36	E	101	LHG	C13-C14-C15-C16
33	B	630	HTG	C3'-C4'-C5'-C6'
34	c	917	DGD	C7A-C8A-C9A-CAA
23	B	602	CLA	O1A-CGA-O2A-C1
36	D	410	LHG	C29-C30-C31-C32
30	c	922	LMT	C11-C10-C9-C8
34	C	517	DGD	C2E-C1E-O5D-C6D
23	c	914	CLA	C16-C17-C18-C19
23	A	410	CLA	C8-C10-C11-C12
36	E	101	LHG	O9-C7-O7-C5
27	C	519	LMG	C19-C20-C21-C22
34	c	918	DGD	C3A-C4A-C5A-C6A
23	B	602	CLA	CBA-CGA-O2A-C1
34	c	919	DGD	CDB-CEB-CFB-CGB
30	Z	102	LMT	C2-C1-O1'-C1'
31	B	633	GOL	O2-C2-C3-O3
34	c	918	DGD	CBA-CCA-CDA-CEA
33	d	401	HTG	C4'-C5'-C6'-C7'
23	C	501	CLA	C4B-C3B-CAB-CBB
26	B	621	SQD	C14-C15-C16-C17
27	c	920	LMG	C40-C41-C42-C43
27	B	622	LMG	O8-C28-C29-C30
27	a	418	LMG	C17-C18-C19-C20
26	B	621	SQD	C19-C20-C21-C22
27	Z	101	LMG	C33-C34-C35-C36
26	A	412	SQD	C27-C28-C29-C30
27	D	411	LMG	C37-C38-C39-C40
23	A	407	CLA	C12-C13-C15-C16
23	B	615	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	C	504	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	b	604	CLA	C11-C10-C8-C7
23	b	617	CLA	C11-C10-C8-C7
23	c	907	CLA	C6-C7-C8-C10
23	c	908	CLA	C11-C12-C13-C15
23	c	913	CLA	C6-C7-C8-C10
34	c	918	DGD	CCA-CDA-CEA-CFA
34	c	918	DGD	C6B-C7B-C8B-C9B
34	H	102	DGD	C6B-C7B-C8B-C9B
23	B	602	CLA	C8-C10-C11-C12
34	C	516	DGD	CBA-CCA-CDA-CEA
23	C	502	CLA	C15-C16-C17-C18
36	E	101	LHG	C2-C3-O3-P
26	B	621	SQD	C28-C29-C30-C31
26	a	416	SQD	C16-C17-C18-C19
27	A	413	LMG	C11-C12-C13-C14
34	d	406	DGD	C8B-C9B-CAB-CBB
36	E	101	LHG	C34-C35-C36-C37
23	C	502	CLA	C16-C17-C18-C19
30	Z	102	LMT	C2-C3-C4-C5
34	d	406	DGD	C8A-C9A-CAA-CBA
23	A	406	CLA	C2C-C3C-CAC-CBC
30	F	102	LMT	O1'-C1-C2-C3
26	A	412	SQD	C34-C35-C36-C37
23	C	507	CLA	C11-C10-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	C	513	CLA	C11-C12-C13-C14
23	a	414	CLA	C11-C10-C8-C9
23	b	607	CLA	C6-C7-C8-C9
23	b	609	CLA	C14-C13-C15-C16
23	c	907	CLA	C11-C10-C8-C9
25	a	415	BCR	C19-C20-C21-C22
30	b	625	LMT	C2-C3-C4-C5
26	a	401	SQD	O5-C5-C6-S
36	l	101	LHG	C26-C27-C28-C29
23	b	618	CLA	C13-C15-C16-C17
23	a	414	CLA	O1D-CGD-O2D-CED
27	C	519	LMG	O1-C7-C8-O7
34	D	406	DGD	O1G-C1G-C2G-O2G
27	A	413	LMG	O1-C7-C8-C9
30	C	520	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C8-C10-C11-C12
23	c	907	CLA	C13-C15-C16-C17
30	b	625	LMT	C11-C10-C9-C8
27	Z	101	LMG	C4-C5-C6-O5
34	D	406	DGD	C7B-C8B-C9B-CAB
23	B	602	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	CAD-CBD-CGD-O2D
23	B	608	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	903	CLA	CAD-CBD-CGD-O2D
23	c	905	CLA	CAD-CBD-CGD-O2D
23	A	410	CLA	O1D-CGD-O2D-CED
27	C	519	LMG	C16-C17-C18-C19
34	H	102	DGD	C5B-C6B-C7B-C8B
26	a	416	SQD	C31-C32-C33-C34
26	a	401	SQD	C12-C13-C14-C15
36	D	408	LHG	C13-C14-C15-C16
26	L	103	SQD	C12-C13-C14-C15
30	F	102	LMT	C2B-C1B-O1B-C4'
23	B	606	CLA	CAD-CBD-CGD-O1D
23	B	610	CLA	CAD-CBD-CGD-O1D
23	B	611	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	b	604	CLA	CAD-CBD-CGD-O1D
23	b	608	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
23	b	619	CLA	CHA-CBD-CGD-O1D
23	c	902	CLA	CHA-CBD-CGD-O1D
23	c	905	CLA	CAD-CBD-CGD-O1D
23	c	907	CLA	CAD-CBD-CGD-O1D
23	c	908	CLA	CHA-CBD-CGD-O2D
24	A	409	PHO	CHA-CBD-CGD-O1D
36	D	409	LHG	C3-O3-P-O4
36	D	409	LHG	C4-O6-P-O5
36	E	101	LHG	C4-O6-P-O5
36	L	101	LHG	C4-O6-P-O5
36	a	417	LHG	C3-O3-P-O4
36	a	417	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
36	d	408	LHG	C3-O3-P-O4
36	d	408	LHG	C3-O3-P-O6
36	d	408	LHG	C4-O6-P-O5
36	l	101	LHG	C4-O6-P-O5
23	c	914	CLA	C3-C5-C6-C7
34	C	518	DGD	CBB-CCB-CDB-CEB
23	C	501	CLA	C2B-C3B-CAB-CBB
30	a	402	LMT	C7-C8-C9-C10
33	B	626	HTG	O5-C5-C6-O6
36	a	417	LHG	C2-C3-O3-P
36	d	409	LHG	C2-C3-O3-P
23	B	602	CLA	CBD-CGD-O2D-CED
26	A	412	SQD	C14-C15-C16-C17
30	b	624	LMT	C2-C3-C4-C5
26	D	407	SQD	C10-C11-C12-C13
26	L	103	SQD	C32-C33-C34-C35
23	c	912	CLA	CBD-CGD-O2D-CED
26	a	401	SQD	C11-C10-C9-C8
31	B	635	GOL	O2-C2-C3-O3
31	V	203	GOL	O1-C1-C2-O2
31	b	632	GOL	O2-C2-C3-O3
23	c	913	CLA	C15-C16-C17-C18
34	c	919	DGD	O1A-C1A-O1G-C1G
27	A	413	LMG	C38-C39-C40-C41
27	b	623	LMG	C16-C17-C18-C19
30	b	625	LMT	O5'-C5'-C6'-O6'
26	L	103	SQD	C46-C45-O47-C7
26	A	418	SQD	C24-C25-C26-C27
34	c	918	DGD	C7B-C8B-C9B-CAB
28	d	405	PL9	C39-C41-C42-C43
23	b	609	CLA	C15-C16-C17-C18
30	m	102	LMT	C11-C10-C9-C8
38	h	101	RRX	C9-C10-C11-C12
36	E	101	LHG	C35-C36-C37-C38
23	B	617	CLA	C11-C10-C8-C9
23	B	617	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C12-C13-C14
23	b	617	CLA	C6-C7-C8-C9
23	c	905	CLA	C14-C13-C15-C16
23	c	908	CLA	C11-C12-C13-C14
30	M	101	LMT	C9-C10-C11-C12
23	b	617	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
34	C	517	DGD	CBB-CCB-CDB-CEB
36	D	410	LHG	C14-C15-C16-C17
36	D	408	LHG	C25-C26-C27-C28
23	b	610	CLA	C3-C5-C6-C7
26	D	407	SQD	C28-C29-C30-C31
30	J	102	LMT	C4-C5-C6-C7
23	C	507	CLA	C2-C3-C5-C6
30	C	520	LMT	C11-C10-C9-C8
23	B	604	CLA	C16-C17-C18-C20
23	B	611	CLA	C16-C17-C18-C19
36	D	410	LHG	C12-C13-C14-C15
30	b	625	LMT	C4-C5-C6-C7
30	a	402	LMT	C11-C10-C9-C8
27	c	921	LMG	C36-C37-C38-C39
36	l	101	LHG	C28-C29-C30-C31
34	h	102	DGD	CDA-CEA-CFA-CGA
34	H	102	DGD	O2G-C1B-C2B-C3B
23	C	509	CLA	C2-C1-O2A-CGA
23	c	910	CLA	C2-C1-O2A-CGA
34	C	518	DGD	CCB-CDB-CEB-CFB
23	B	616	CLA	C16-C17-C18-C19
23	D	403	CLA	C13-C15-C16-C17
34	c	918	DGD	C9A-CAA-CBA-CCA
25	D	404	BCR	C37-C22-C23-C24
36	L	101	LHG	C9-C10-C11-C12
34	D	406	DGD	C2G-C3G-O3G-C1D
27	D	411	LMG	C30-C31-C32-C33
23	C	501	CLA	C2A-CAA-CBA-CGA
36	d	409	LHG	C28-C29-C30-C31
23	B	602	CLA	CAA-CBA-CGA-O2A
28	d	405	PL9	C43-C44-C46-C47
34	c	918	DGD	CAA-CBA-CCA-CDA
33	b	627	HTG	S1-C1'-C2'-C3'
34	C	517	DGD	C8B-C9B-CAB-CBB
28	a	419	PL9	C2-C3-C7-C8
26	L	103	SQD	C28-C29-C30-C31
30	M	101	LMT	C2-C1-O1'-C1'
30	b	625	LMT	C2-C1-O1'-C1'
33	B	631	HTG	C4'-C5'-C6'-C7'
23	B	602	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	C	504	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C11-C12-C13-C14
23	b	618	CLA	C14-C13-C15-C16
27	Z	101	LMG	C29-C28-O8-C9
27	b	623	LMG	C32-C33-C34-C35
23	D	402	CLA	C16-C17-C18-C19
27	Z	101	LMG	O10-C28-O8-C9
30	Z	102	LMT	O5'-C5'-C6'-O6'
36	d	409	LHG	C25-C26-C27-C28
27	B	622	LMG	C29-C30-C31-C32
28	a	419	PL9	C39-C41-C42-C43
37	V	201	HEM	C4B-C3B-CAB-CBB
37	v	201	HEM	C4B-C3B-CAB-CBB
33	c	924	HTG	C4'-C5'-C6'-C7'
30	A	419	LMT	C11-C10-C9-C8
23	B	617	CLA	C12-C13-C15-C16
23	b	617	CLA	C15-C16-C17-C18
34	c	919	DGD	C3B-C4B-C5B-C6B
23	b	615	CLA	CBA-CGA-O2A-C1
27	a	418	LMG	O8-C28-C29-C30
36	l	101	LHG	C32-C33-C34-C35
23	c	914	CLA	C16-C17-C18-C20
34	h	102	DGD	CCB-CDB-CEB-CFB
26	B	621	SQD	C35-C36-C37-C38
30	M	101	LMT	C4'-C5'-C6'-O6'
34	c	918	DGD	CAB-CBB-CCB-CDB
36	l	101	LHG	C9-C10-C11-C12
34	c	919	DGD	O6D-C5D-C6D-O5D
27	Z	101	LMG	C38-C39-C40-C41
27	c	921	LMG	C33-C34-C35-C36
23	c	911	CLA	O1D-CGD-O2D-CED
36	d	408	LHG	C16-C17-C18-C19
23	D	402	CLA	C2-C1-O2A-CGA
25	C	514	BCR	C19-C20-C21-C22
30	t	102	LMT	C2-C3-C4-C5
26	L	103	SQD	C14-C15-C16-C17
34	c	919	DGD	CAA-CBA-CCA-CDA
27	a	418	LMG	C22-C23-C24-C25
34	D	406	DGD	C8A-C9A-CAA-CBA
23	c	910	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	C10-C11-C12-C13
36	D	410	LHG	C13-C14-C15-C16
23	C	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C11-C10-C8-C9
23	b	617	CLA	C11-C10-C8-C9
23	c	910	CLA	C14-C13-C15-C16
27	C	519	LMG	C11-C12-C13-C14
27	D	411	LMG	C34-C35-C36-C37
26	f	102	SQD	C23-C24-C25-C26
23	B	605	CLA	C16-C17-C18-C20
26	A	418	SQD	C30-C31-C32-C33
30	B	623	LMT	C3-C4-C5-C6
27	c	920	LMG	C11-C12-C13-C14
31	D	415	GOL	O2-C2-C3-O3
31	O	304	GOL	O2-C2-C3-O3
27	c	920	LMG	C14-C15-C16-C17
30	C	520	LMT	C4-C5-C6-C7
34	H	102	DGD	CAA-CBA-CCA-CDA
23	A	405	CLA	C4C-C3C-CAC-CBC
23	c	913	CLA	C2B-C3B-CAB-CBB
25	K	101	BCR	C5-C6-C7-C8
25	b	620	BCR	C5-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C30
26	f	102	SQD	C31-C32-C33-C34
27	c	920	LMG	C21-C22-C23-C24
34	c	917	DGD	C5A-C6A-C7A-C8A
27	C	519	LMG	C12-C13-C14-C15
27	Z	101	LMG	C14-C15-C16-C17
26	B	621	SQD	C25-C26-C27-C28
30	A	419	LMT	C4-C5-C6-C7
30	B	623	LMT	C3'-C4'-O1B-C1B
23	A	407	CLA	C11-C10-C8-C7
23	A	410	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	a	411	CLA	C6-C7-C8-C10
23	b	618	CLA	C12-C13-C15-C16
23	c	910	CLA	C12-C13-C15-C16
23	c	914	CLA	C6-C7-C8-C10
23	b	613	CLA	C16-C17-C18-C20
26	a	416	SQD	C32-C33-C34-C35
27	c	921	LMG	O7-C8-C9-O8
27	B	622	LMG	C32-C33-C34-C35
27	b	623	LMG	C30-C31-C32-C33
34	d	406	DGD	C3B-C4B-C5B-C6B
37	F	101	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	c	915	BCR	C37-C22-C23-C24
23	C	513	CLA	C4-C3-C5-C6
30	z	101	LMT	C7-C8-C9-C10
23	B	611	CLA	C13-C15-C16-C17
34	C	516	DGD	C6B-C7B-C8B-C9B
37	V	201	HEM	CAD-CBD-CGD-O2D
37	v	201	HEM	CAD-CBD-CGD-O2D
23	A	407	CLA	C16-C17-C18-C19
23	a	410	CLA	C15-C16-C17-C18
27	Z	101	LMG	C10-C11-C12-C13
30	F	102	LMT	O5B-C1B-O1B-C4'
23	C	507	CLA	C2A-CAA-CBA-CGA
37	F	101	HEM	CAD-CBD-CGD-O1D
23	C	508	CLA	C15-C16-C17-C18
27	c	921	LMG	C34-C35-C36-C37
36	E	101	LHG	C31-C32-C33-C34
34	c	919	DGD	C8B-C9B-CAB-CBB
27	b	623	LMG	C22-C23-C24-C25
34	D	406	DGD	C2A-C3A-C4A-C5A
26	A	412	SQD	C30-C31-C32-C33
27	A	413	LMG	C29-C30-C31-C32
34	C	518	DGD	C4A-C5A-C6A-C7A
34	C	518	DGD	O6D-C5D-C6D-O5D
30	b	624	LMT	C3-C4-C5-C6
27	C	519	LMG	O1-C7-C8-C9
28	D	405	PL9	C39-C41-C42-C43
34	H	102	DGD	O1G-C1G-C2G-C3G
23	b	613	CLA	C2A-CAA-CBA-CGA
27	b	623	LMG	C12-C13-C14-C15
27	C	519	LMG	C13-C14-C15-C16
30	B	623	LMT	C5'-C4'-O1B-C1B
23	A	406	CLA	C13-C15-C16-C17
31	v	203	GOL	O1-C1-C2-O2
23	B	617	CLA	C4-C3-C5-C6
23	B	606	CLA	C10-C11-C12-C13
26	a	416	SQD	O10-C23-O48-C46
23	b	604	CLA	CAA-CBA-CGA-O2A
33	b	626	HTG	C1'-C2'-C3'-C4'
33	u	201	HTG	C1'-C2'-C3'-C4'
27	a	418	LMG	C21-C22-C23-C24
36	D	409	LHG	C26-C27-C28-C29
26	f	102	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	C16-C17-C18-C19
24	a	413	PHO	CHA-CBD-CGD-O2D
37	V	201	HEM	CAD-CBD-CGD-O1D
34	h	102	DGD	C9B-CAB-CBB-CCB
30	t	102	LMT	C7-C8-C9-C10
34	H	102	DGD	CDA-CEA-CFA-CGA
36	a	417	LHG	O6-C4-C5-C6
27	A	413	LMG	O6-C1-O1-C7
34	C	517	DGD	O6E-C1E-O5D-C6D
23	c	902	CLA	C13-C15-C16-C17
23	D	403	CLA	C11-C10-C8-C7
34	C	516	DGD	C2B-C3B-C4B-C5B
27	C	519	LMG	C20-C21-C22-C23
37	v	201	HEM	CAD-CBD-CGD-O1D
23	B	617	CLA	C6-C7-C8-C9
30	M	102	LMT	C3-C4-C5-C6
34	c	917	DGD	C5D-C6D-O5D-C1E
23	d	402	CLA	C2-C1-O2A-CGA
34	C	518	DGD	CCA-CDA-CEA-CFA
23	b	618	CLA	C3A-C2A-CAA-CBA
36	E	101	LHG	C23-C24-C25-C26
33	b	601	HTG	C1'-C2'-C3'-C4'
27	c	921	LMG	C40-C41-C42-C43
34	d	406	DGD	O1A-C1A-O1G-C1G
36	l	101	LHG	C16-C17-C18-C19
30	z	101	LMT	O5'-C1'-O1'-C1
23	D	402	CLA	C4C-C3C-CAC-CBC
30	C	520	LMT	C2-C3-C4-C5
36	a	417	LHG	C5-C4-O6-P
36	D	408	LHG	C15-C16-C17-C18
23	D	403	CLA	O1D-CGD-O2D-CED
28	A	414	PL9	C39-C41-C42-C43
33	O	303	HTG	C2'-C3'-C4'-C5'
37	V	201	HEM	C4C-C3C-CAC-CBC
23	B	605	CLA	C16-C17-C18-C19
31	a	424	GOL	O2-C2-C3-O3
31	b	635	GOL	O1-C1-C2-O2
36	L	101	LHG	C28-C29-C30-C31
26	B	621	SQD	C30-C31-C32-C33
23	B	602	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
34	C	517	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
26	a	401	SQD	O47-C45-C46-O48
23	C	505	CLA	C14-C13-C15-C16
23	c	914	CLA	C6-C7-C8-C9
27	Z	101	LMG	O9-C10-O7-C8
23	C	513	CLA	C2-C3-C5-C6
33	B	624	HTG	C4'-C5'-C6'-C7'
23	B	604	CLA	C6-C7-C8-C10
23	B	617	CLA	C6-C7-C8-C10
23	D	403	CLA	C12-C13-C15-C16
36	l	101	LHG	C17-C18-C19-C20
23	A	407	CLA	C2B-C3B-CAB-CBB
23	B	608	CLA	C2B-C3B-CAB-CBB
23	b	612	CLA	C2B-C3B-CAB-CBB
25	K	101	BCR	C1-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C26
25	k	101	BCR	C5-C6-C7-C8
38	H	101	RRX	C23-C24-C25-C30
27	Z	101	LMG	C16-C17-C18-C19
27	Z	101	LMG	C11-C10-O7-C8
36	a	417	LHG	O7-C7-C8-C9
23	b	617	CLA	C2-C1-O2A-CGA
34	c	918	DGD	O6E-C1E-O5D-C6D
26	L	103	SQD	C11-C12-C13-C14
23	C	512	CLA	CAA-CBA-CGA-O2A
23	B	610	CLA	C2-C3-C5-C6
23	c	906	CLA	C2-C3-C5-C6
28	a	419	PL9	C13-C14-C16-C17
27	B	622	LMG	O9-C10-O7-C8
33	B	631	HTG	C2'-C1'-S1-C1
33	C	521	HTG	C2'-C1'-S1-C1
33	c	923	HTG	C2'-C1'-S1-C1
33	d	401	HTG	C2'-C1'-S1-C1
30	c	922	LMT	C5-C6-C7-C8
30	a	402	LMT	C4-C5-C6-C7
23	b	619	CLA	C8-C10-C11-C12
23	C	513	CLA	O1A-CGA-O2A-C1
23	A	406	CLA	C4C-C3C-CAC-CBC
28	a	419	PL9	C15-C14-C16-C17
23	A	407	CLA	C13-C15-C16-C17
23	b	606	CLA	C13-C15-C16-C17
27	Z	101	LMG	C19-C20-C21-C22
34	c	919	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C15-C16-C17-C18
34	C	518	DGD	O1G-C1A-C2A-C3A
30	m	101	LMT	C2-C1-O1'-C1'
23	b	604	CLA	C6-C7-C8-C9
30	a	402	LMT	O5B-C5B-C6B-O6B
27	b	623	LMG	C34-C35-C36-C37
34	C	516	DGD	O6E-C1E-O5D-C6D
26	a	416	SQD	O47-C45-C46-O48
25	K	101	BCR	C21-C22-C23-C24
25	C	514	BCR	C15-C16-C17-C18
23	B	606	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	C16-C17-C18-C19
23	b	606	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C8-C10-C11-C12
36	D	410	LHG	C10-C11-C12-C13
23	B	610	CLA	C4-C3-C5-C6
23	C	512	CLA	C4-C3-C5-C6
23	c	906	CLA	C4-C3-C5-C6
23	C	506	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C10-C8-C7
23	c	910	CLA	C11-C10-C8-C7
23	c	909	CLA	C16-C17-C18-C19
23	c	911	CLA	C16-C17-C18-C20
23	c	913	CLA	O2A-C1-C2-C3
27	Z	101	LMG	C32-C33-C34-C35
23	C	513	CLA	C10-C11-C12-C13
23	C	501	CLA	C13-C15-C16-C17
23	B	613	CLA	C8-C10-C11-C12
26	A	412	SQD	O47-C7-C8-C9
26	L	103	SQD	C9-C10-C11-C12
23	c	906	CLA	CAA-CBA-CGA-O2A
27	Z	101	LMG	C15-C16-C17-C18
36	d	407	LHG	C25-C26-C27-C28
26	a	416	SQD	C24-C23-O48-C46
36	d	407	LHG	C11-C10-C9-C8
23	C	512	CLA	CAA-CBA-CGA-O1A
36	a	417	LHG	O9-C7-C8-C9
23	b	607	CLA	C16-C17-C18-C19
36	L	101	LHG	C5-C6-O8-C23

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Mol	Chain	Res	Type	Atoms
23	B	611	CLA	C2A-CAA-CBA-CGA
23	A	407	CLA	C14-C13-C15-C16
23	B	604	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	A	407	CLA	C16-C17-C18-C20
28	A	414	PL9	C20-C19-C21-C22
34	C	518	DGD	O1A-C1A-C2A-C3A
28	A	414	PL9	C18-C19-C21-C22
33	B	626	HTG	S1-C1'-C2'-C3'
26	B	621	SQD	O5-C5-C6-S
37	f	101	HEM	CAD-CBD-CGD-O1D
26	A	412	SQD	C29-C30-C31-C32
23	b	614	CLA	C16-C17-C18-C20
23	c	911	CLA	C16-C17-C18-C19
25	c	915	BCR	C17-C18-C19-C20
25	c	915	BCR	C21-C22-C23-C24
34	C	516	DGD	C5D-C6D-O5D-C1E
34	h	102	DGD	C2G-C3G-O3G-C1D
34	c	918	DGD	C9B-CAB-CBB-CCB
26	A	412	SQD	C32-C33-C34-C35
36	a	417	LHG	C18-C19-C20-C21
23	A	406	CLA	C15-C16-C17-C18
23	B	603	CLA	C8-C10-C11-C12
26	L	103	SQD	O48-C23-C24-C25
30	Z	102	LMT	C4'-C5'-C6'-O6'
27	c	921	LMG	C37-C38-C39-C40
23	A	405	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
24	a	412	PHO	CAD-CBD-CGD-O2D
23	a	411	CLA	C2C-C3C-CAC-CBC
30	b	624	LMT	C11-C10-C9-C8
33	u	201	HTG	C3'-C4'-C5'-C6'
27	c	920	LMG	C30-C31-C32-C33
34	H	102	DGD	C3B-C4B-C5B-C6B
34	d	406	DGD	C2A-C1A-O1G-C1G
23	b	616	CLA	C16-C17-C18-C19
23	c	905	CLA	C5-C6-C7-C8
23	c	902	CLA	CAA-CBA-CGA-O2A
23	c	913	CLA	CAA-CBA-CGA-O2A
34	c	919	DGD	O1G-C1A-C2A-C3A
34	d	406	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
36	a	417	LHG	C11-C10-C9-C8
26	A	412	SQD	O49-C7-C8-C9
34	c	918	DGD	C1B-C2B-C3B-C4B
30	c	922	LMT	O5B-C5B-C6B-O6B
34	c	917	DGD	O2G-C1B-C2B-C3B
23	C	513	CLA	CBA-CGA-O2A-C1
23	B	603	CLA	C13-C15-C16-C17
23	b	616	CLA	C8-C10-C11-C12

There are no ring outliers.

152 monomers are involved in 343 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	617	CLA	7	0
31	c	927	GOL	2	0
31	D	415	GOL	3	0
34	d	406	DGD	3	0
26	D	407	SQD	3	0
23	B	613	CLA	1	0
27	D	411	LMG	2	0
25	C	514	BCR	1	0
23	c	905	CLA	3	0
23	c	909	CLA	3	0
23	C	506	CLA	3	0
23	B	604	CLA	2	0
23	d	403	CLA	4	0
25	k	101	BCR	3	0
31	L	104	GOL	1	0
23	B	609	CLA	1	0
31	B	635	GOL	1	0
33	U	201	HTG	1	0
36	l	101	LHG	2	0
30	Z	102	LMT	2	0
23	a	411	CLA	1	0
25	K	102	BCR	3	0
23	B	606	CLA	4	0
36	L	101	LHG	2	0
31	C	524	GOL	4	0
27	A	413	LMG	3	0
33	d	401	HTG	1	0
23	c	908	CLA	2	0
23	b	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	T	101	BCR	5	0
23	c	913	CLA	3	0
33	C	521	HTG	1	0
23	A	405	CLA	4	0
25	K	101	BCR	3	0
25	D	404	BCR	2	0
36	D	409	LHG	1	0
27	d	410	LMG	1	0
34	c	918	DGD	3	0
23	B	610	CLA	1	0
25	c	916	BCR	6	0
23	b	610	CLA	1	0
23	b	613	CLA	5	0
26	a	416	SQD	7	0
23	d	402	CLA	1	0
23	c	904	CLA	4	0
23	C	509	CLA	5	0
23	b	619	CLA	2	0
23	b	604	CLA	1	0
23	b	609	CLA	2	0
25	k	102	BCR	2	0
23	c	911	CLA	2	0
25	d	404	BCR	5	0
24	A	409	PHO	2	0
25	B	620	BCR	2	0
23	B	615	CLA	3	0
23	c	907	CLA	5	0
31	b	636	GOL	1	0
37	F	101	HEM	2	0
34	h	102	DGD	1	0
34	H	102	DGD	1	0
25	b	622	BCR	2	0
38	H	101	RRX	2	0
30	a	402	LMT	1	0
23	B	607	CLA	1	0
26	A	412	SQD	4	0
25	b	621	BCR	1	0
23	A	406	CLA	4	0
23	C	502	CLA	2	0
30	b	624	LMT	2	0
23	B	611	CLA	5	0
36	d	409	LHG	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	z	101	LMT	5	0
30	J	102	LMT	1	0
25	t	101	BCR	7	0
23	B	616	CLA	1	0
23	C	508	CLA	2	0
23	b	617	CLA	3	0
31	A	422	GOL	1	0
31	c	928	GOL	3	0
38	h	101	RRX	3	0
23	c	903	CLA	2	0
23	c	912	CLA	3	0
36	D	408	LHG	1	0
30	M	101	LMT	2	0
23	c	902	CLA	3	0
23	b	607	CLA	1	0
23	C	501	CLA	3	0
23	c	906	CLA	7	0
34	c	919	DGD	2	0
34	D	406	DGD	6	0
36	d	407	LHG	1	0
25	C	515	BCR	3	0
27	a	418	LMG	7	0
34	c	917	DGD	1	0
24	A	408	PHO	1	0
31	a	423	GOL	3	0
23	B	602	CLA	1	0
25	B	619	BCR	3	0
30	m	101	LMT	1	0
30	c	922	LMT	1	0
23	B	605	CLA	3	0
23	C	503	CLA	2	0
31	b	633	GOL	2	0
23	a	414	CLA	3	0
23	c	914	CLA	5	0
24	a	412	PHO	1	0
34	C	517	DGD	2	0
23	b	606	CLA	2	0
23	b	618	CLA	4	0
30	B	623	LMT	4	0
33	c	923	HTG	1	0
26	a	401	SQD	3	0
25	a	415	BCR	2	0

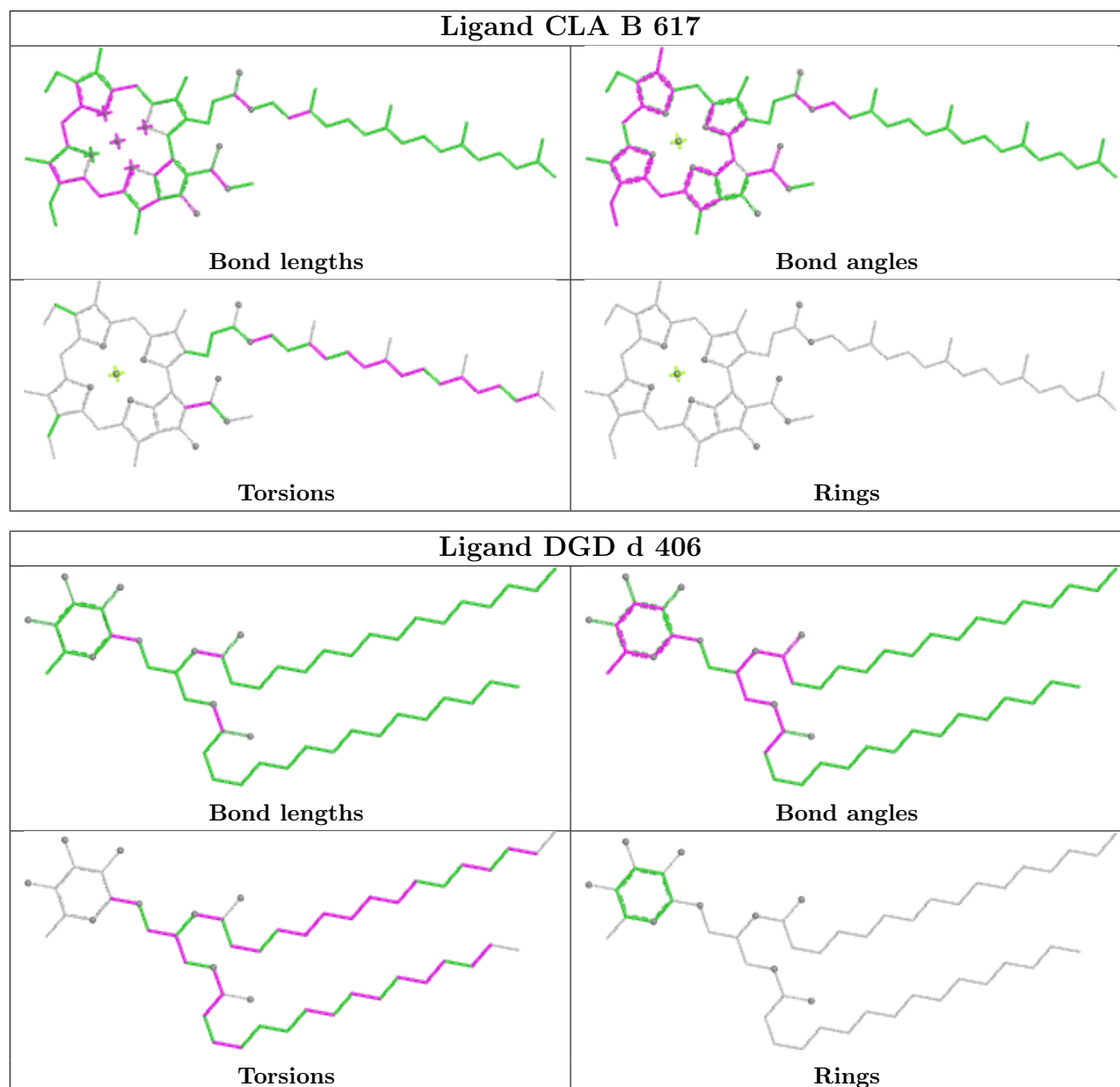
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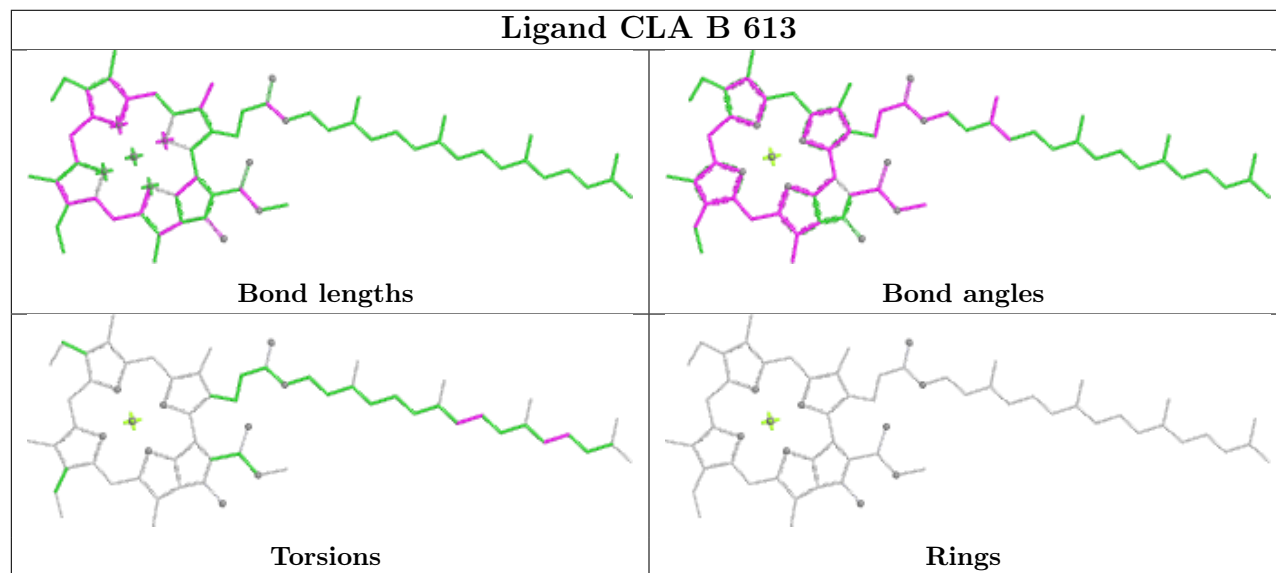
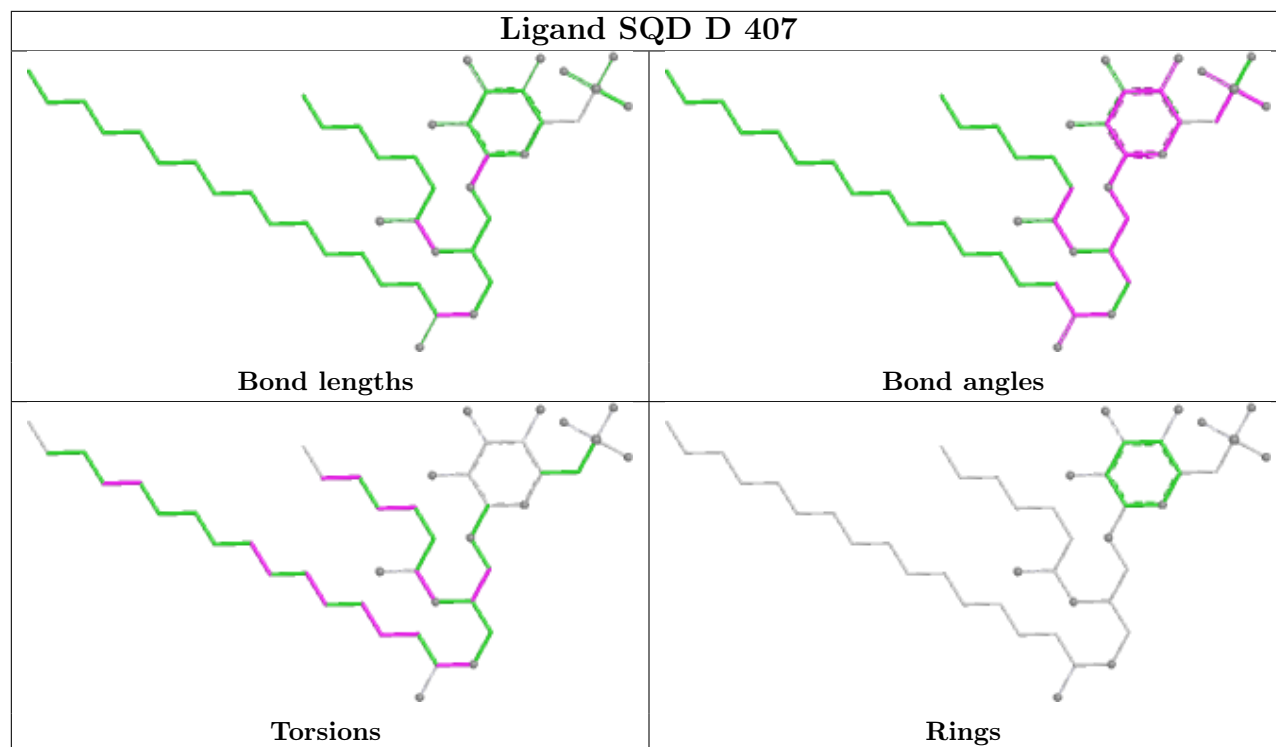
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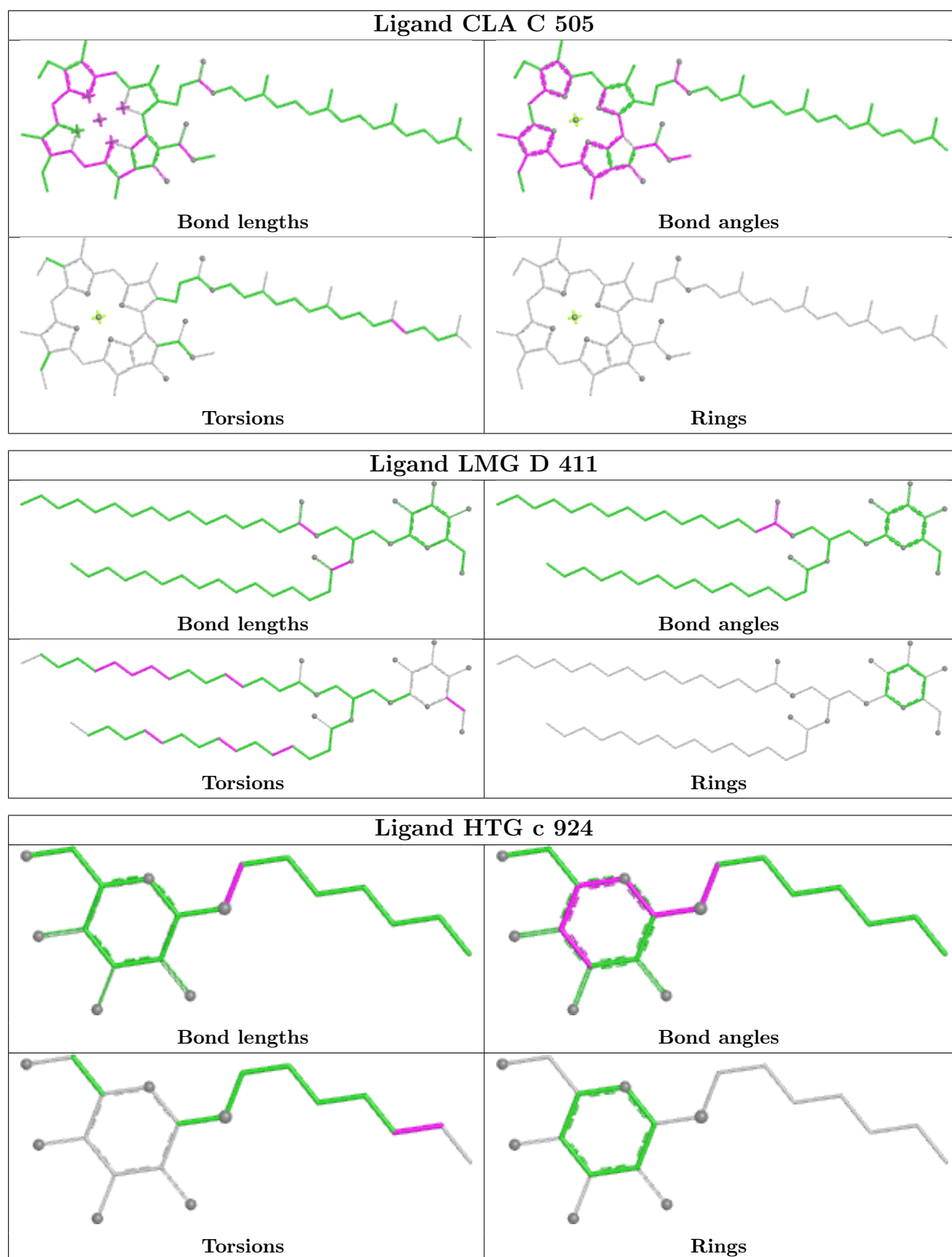
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	616	CLA	5	0
30	C	520	LMT	4	0
33	b	626	HTG	2	0
26	A	418	SQD	1	0
37	V	201	HEM	1	0
23	A	410	CLA	1	0
23	D	403	CLA	1	0
23	C	510	CLA	1	0
23	B	614	CLA	2	0
37	f	101	HEM	3	0
23	C	504	CLA	4	0
23	C	513	CLA	2	0
33	b	627	HTG	1	0
24	a	413	PHO	2	0
27	c	920	LMG	1	0
36	d	408	LHG	1	0
36	a	417	LHG	1	0
36	D	410	LHG	13	0
23	C	507	CLA	1	0
27	c	921	LMG	1	0
28	A	414	PL9	10	0
36	E	101	LHG	3	0
25	A	411	BCR	2	0
23	b	608	CLA	2	0
26	B	621	SQD	5	0
33	D	414	HTG	2	0
26	f	102	SQD	2	0
26	L	103	SQD	5	0
28	a	419	PL9	9	0
27	b	623	LMG	3	0
33	B	631	HTG	1	0
23	C	511	CLA	4	0
23	a	409	CLA	2	0
23	c	910	CLA	2	0
27	B	622	LMG	4	0
23	C	512	CLA	3	0
27	C	519	LMG	2	0
23	B	612	CLA	3	0
23	b	615	CLA	1	0

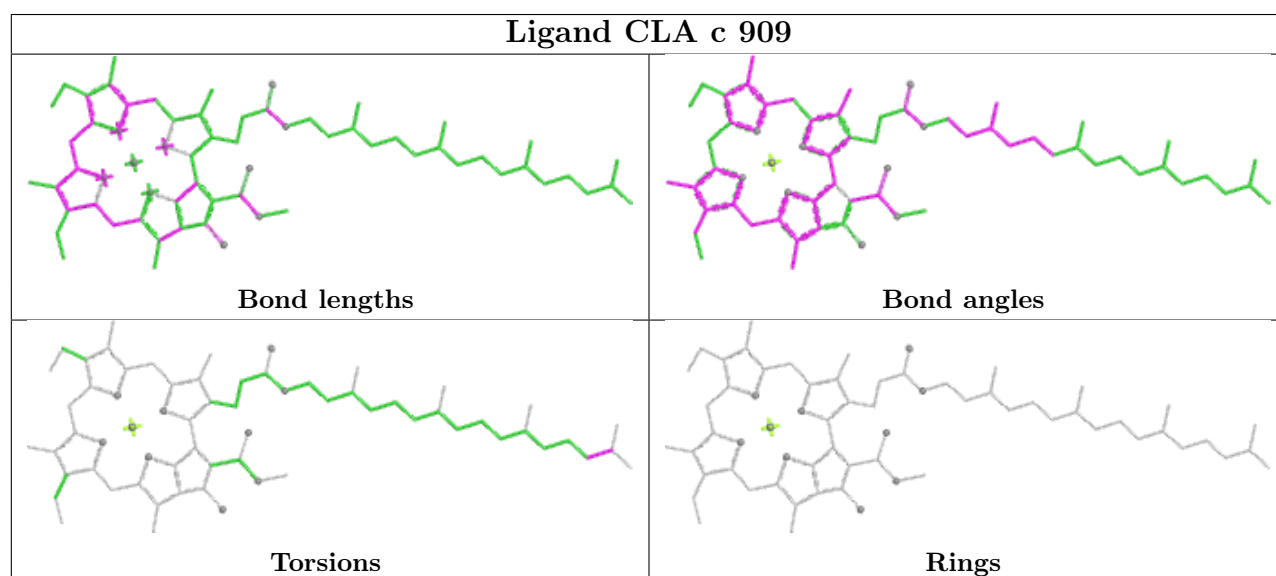
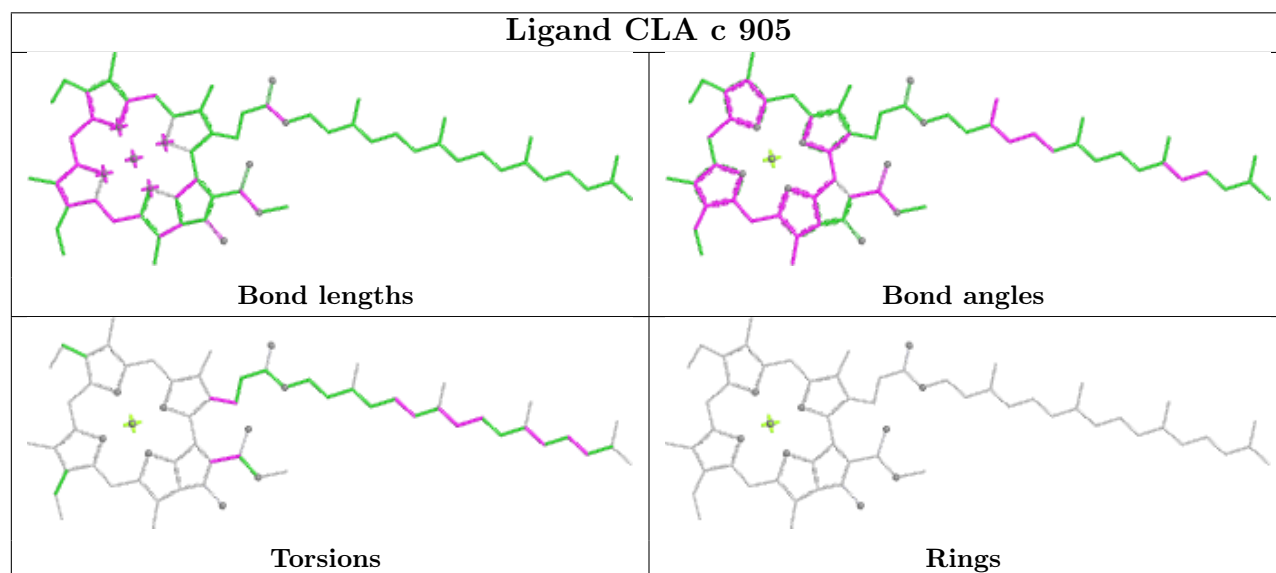
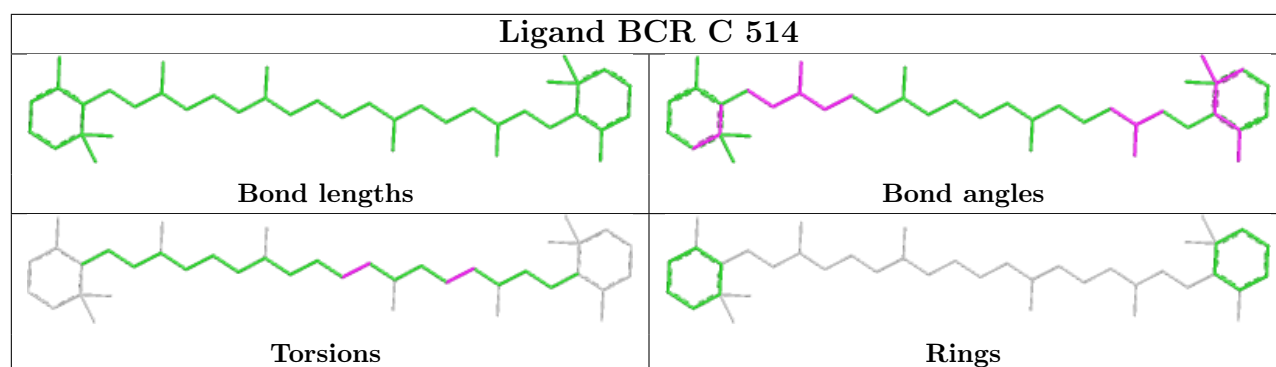
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

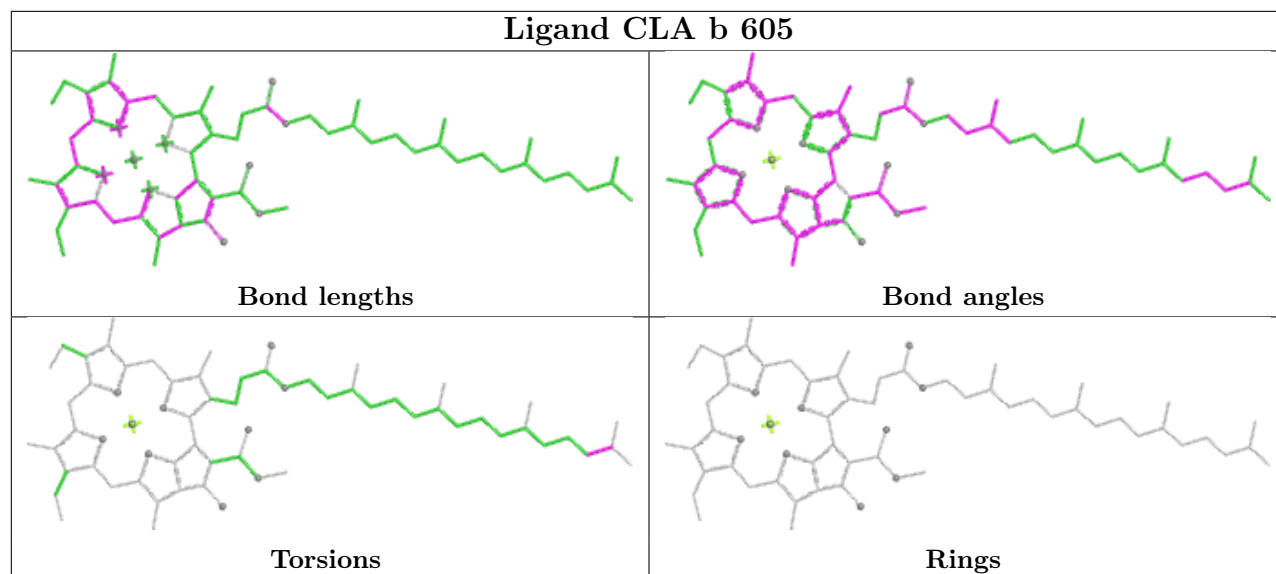




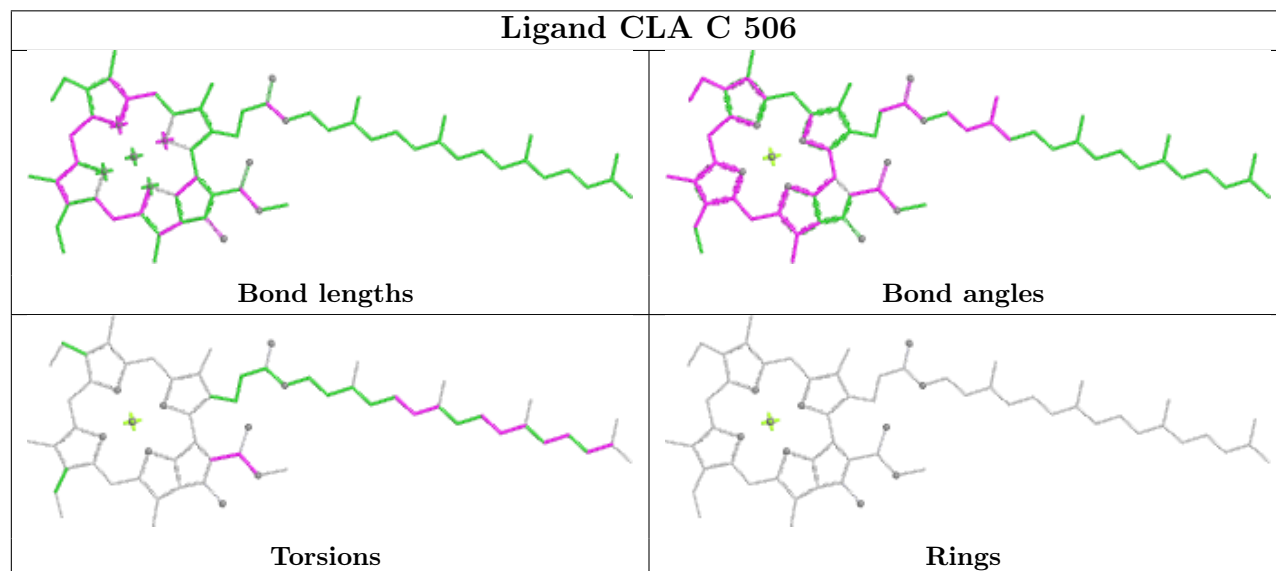




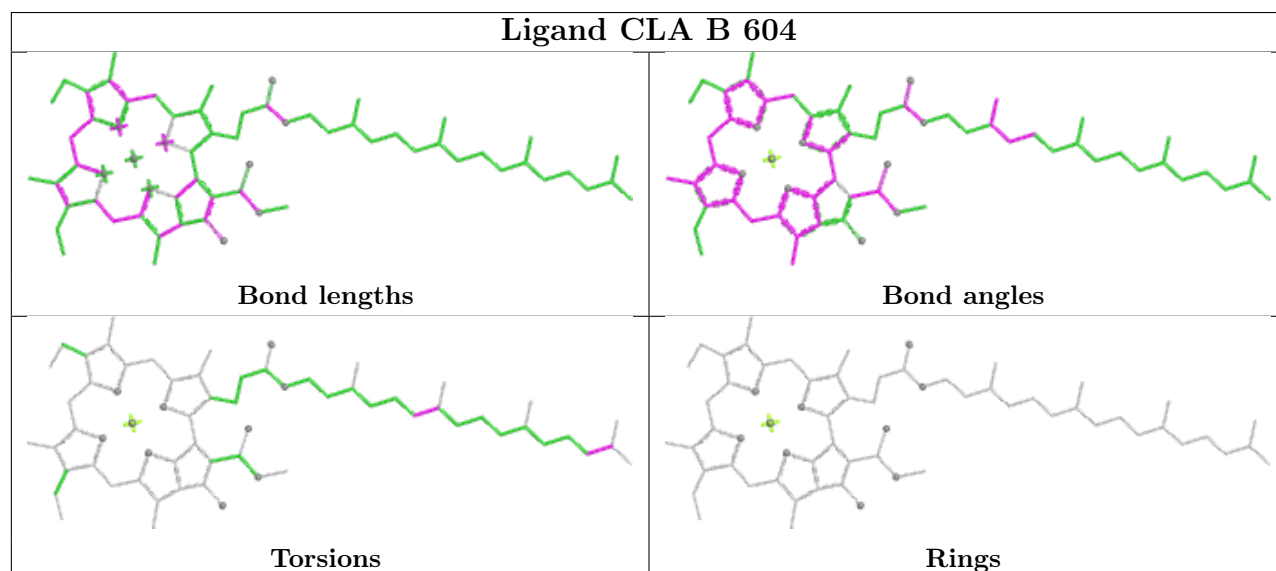
Ligand CLA b 605



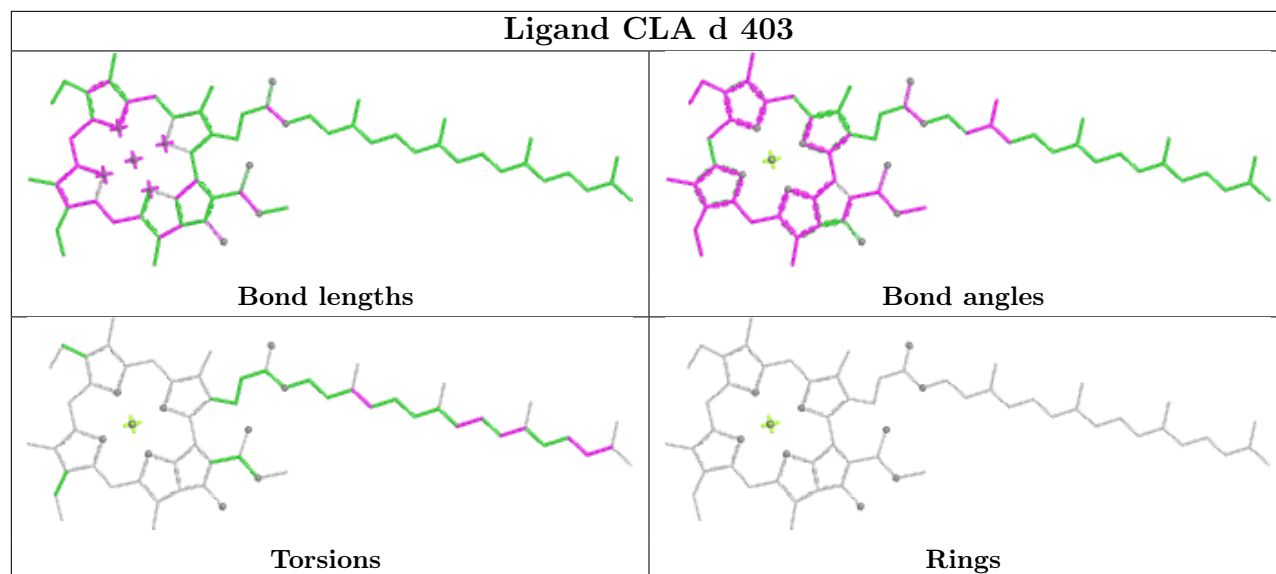
Ligand CLA C 506



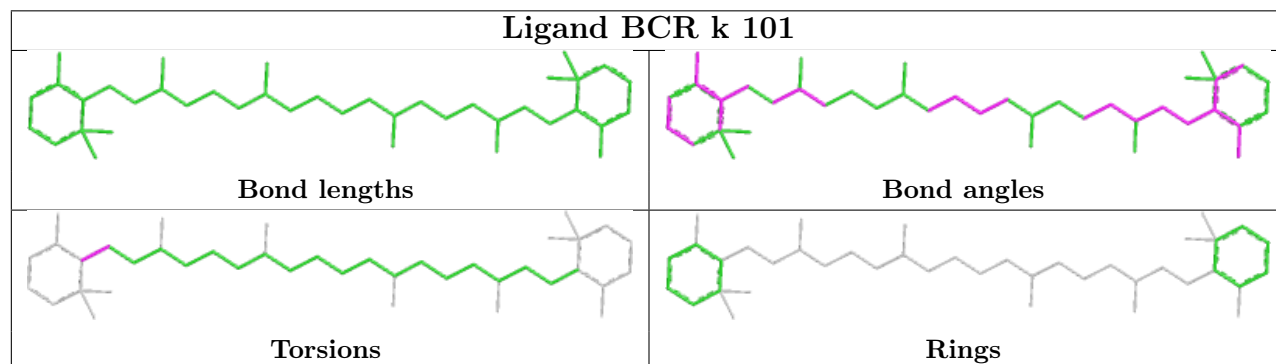
Ligand CLA B 604



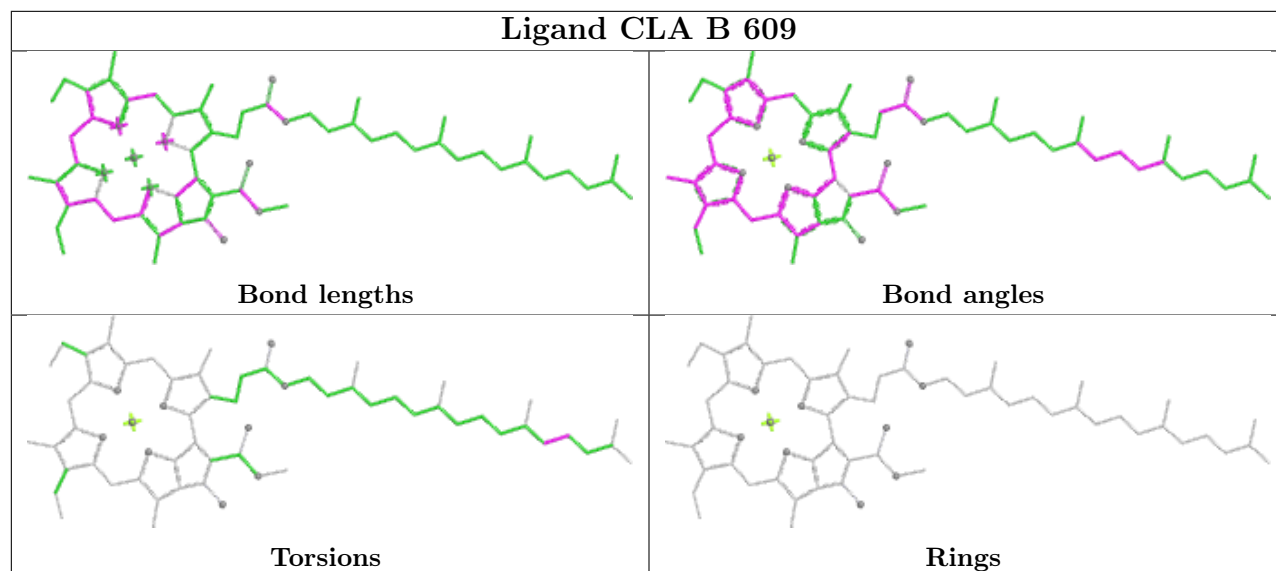
Ligand CLA d 403

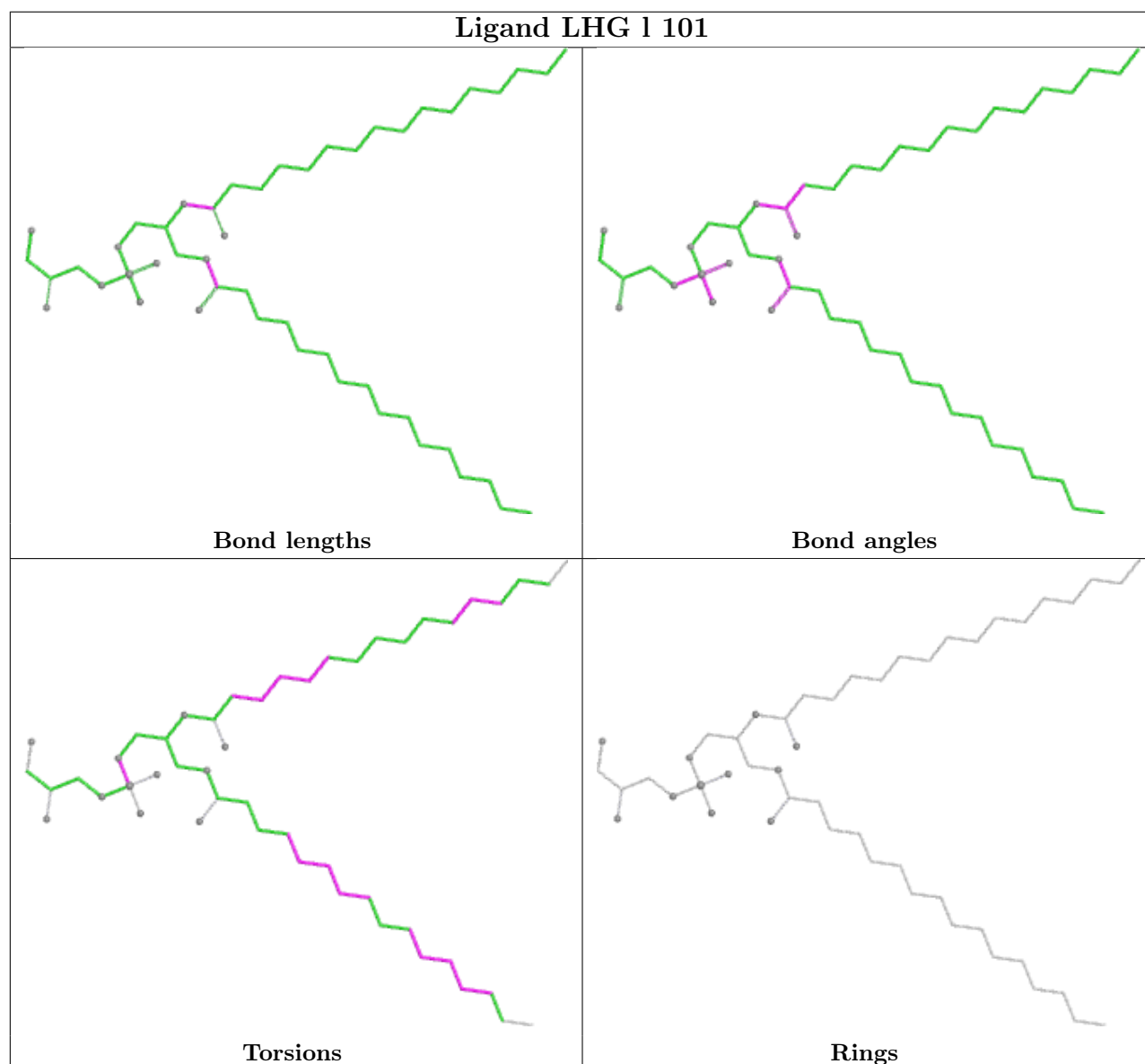
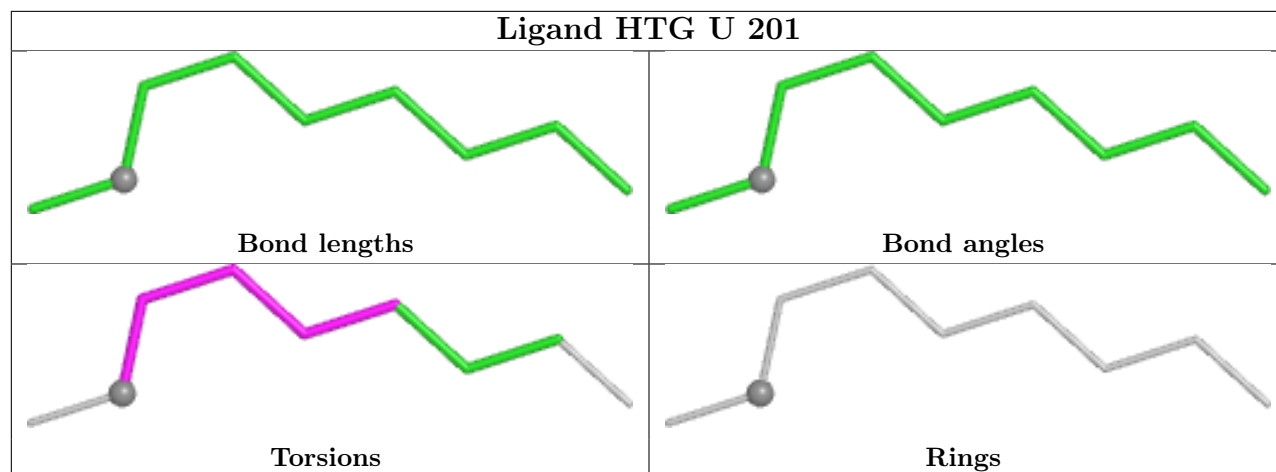


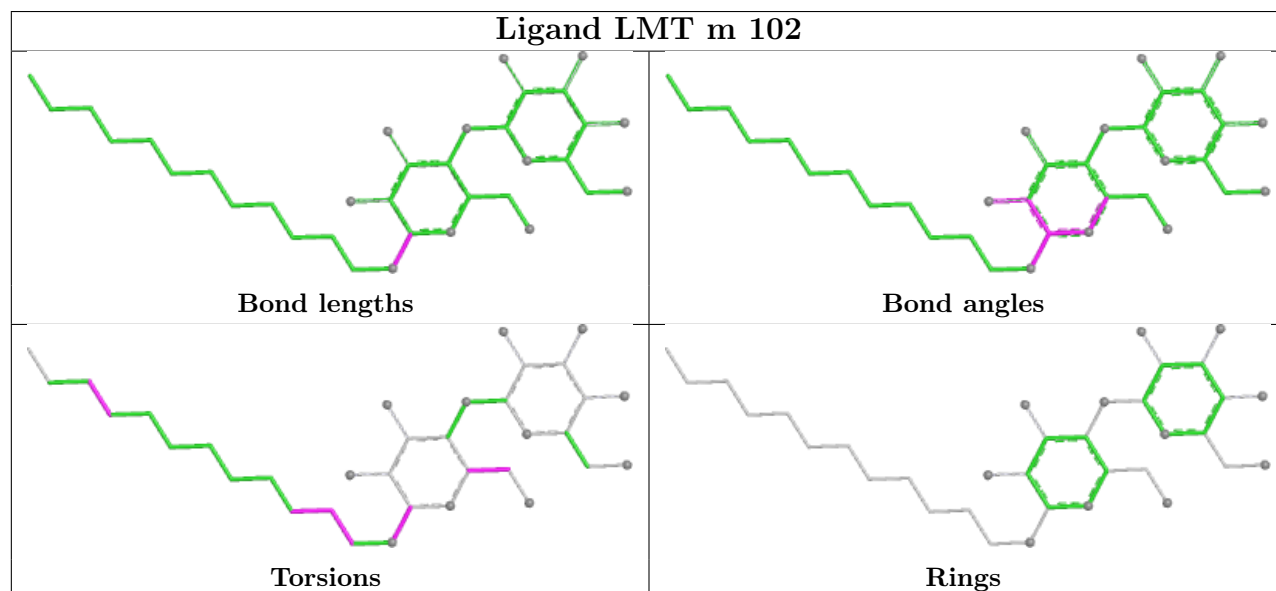
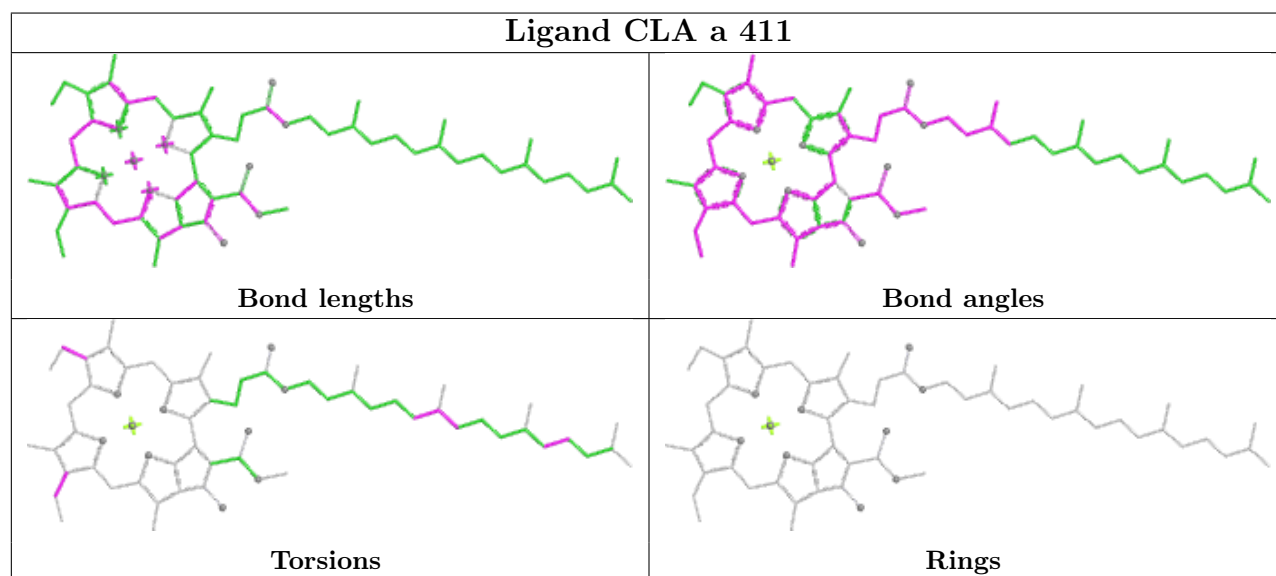
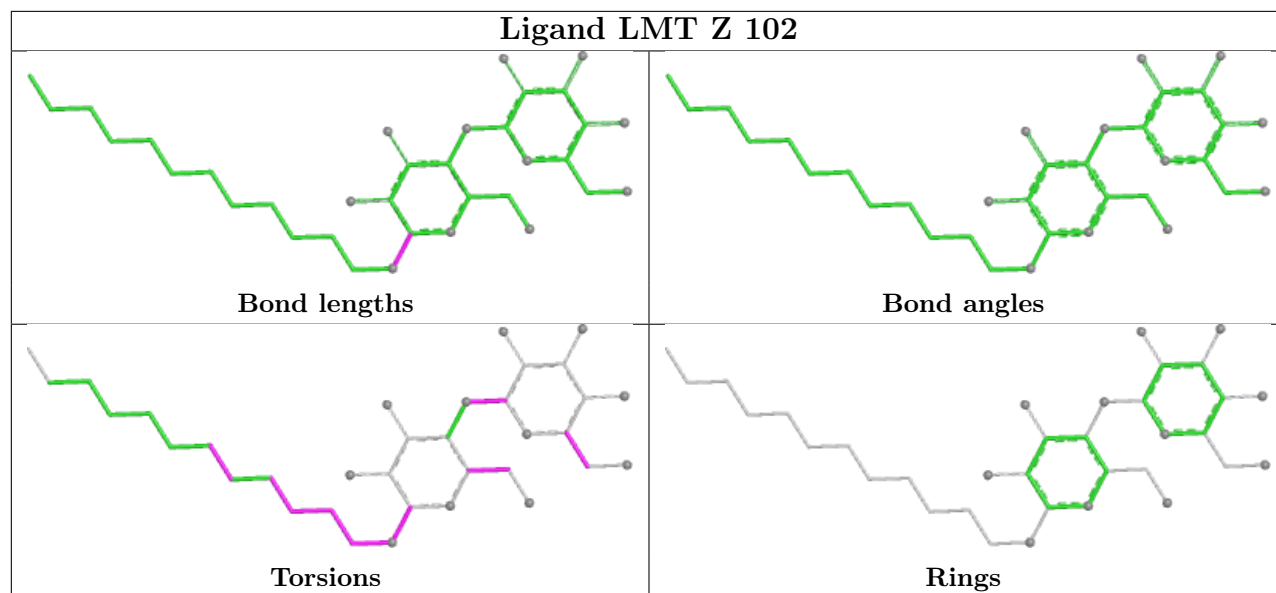
Ligand BCR k 101

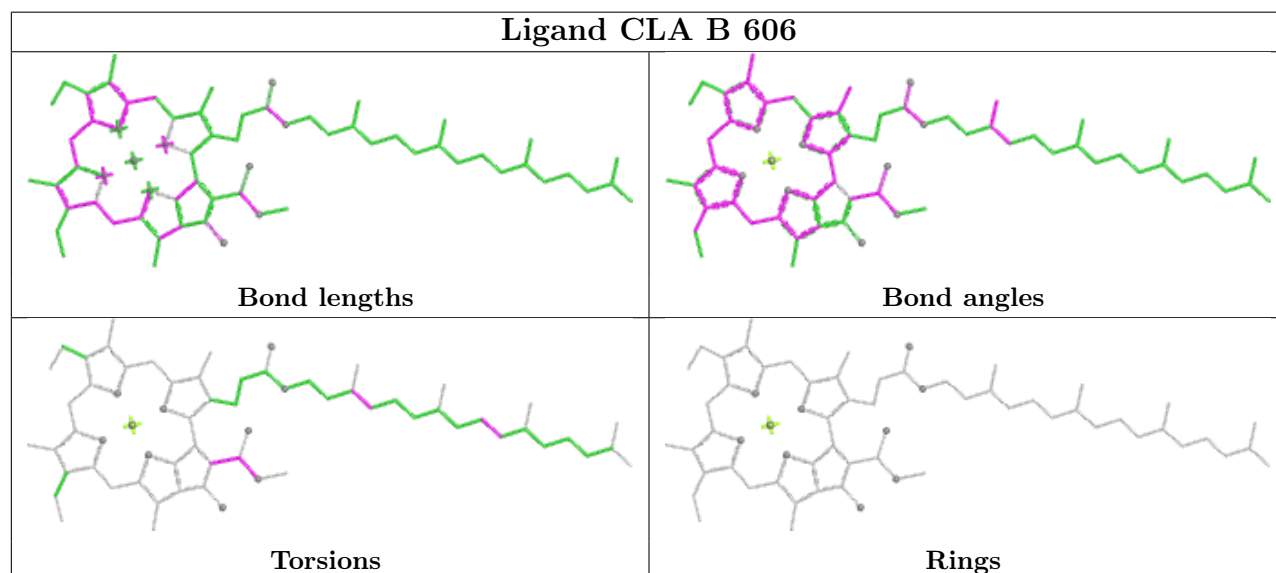
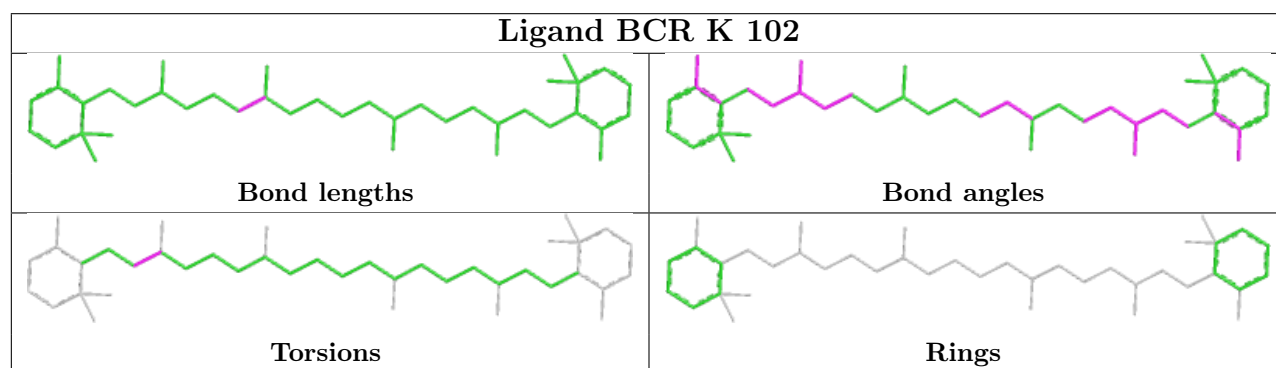
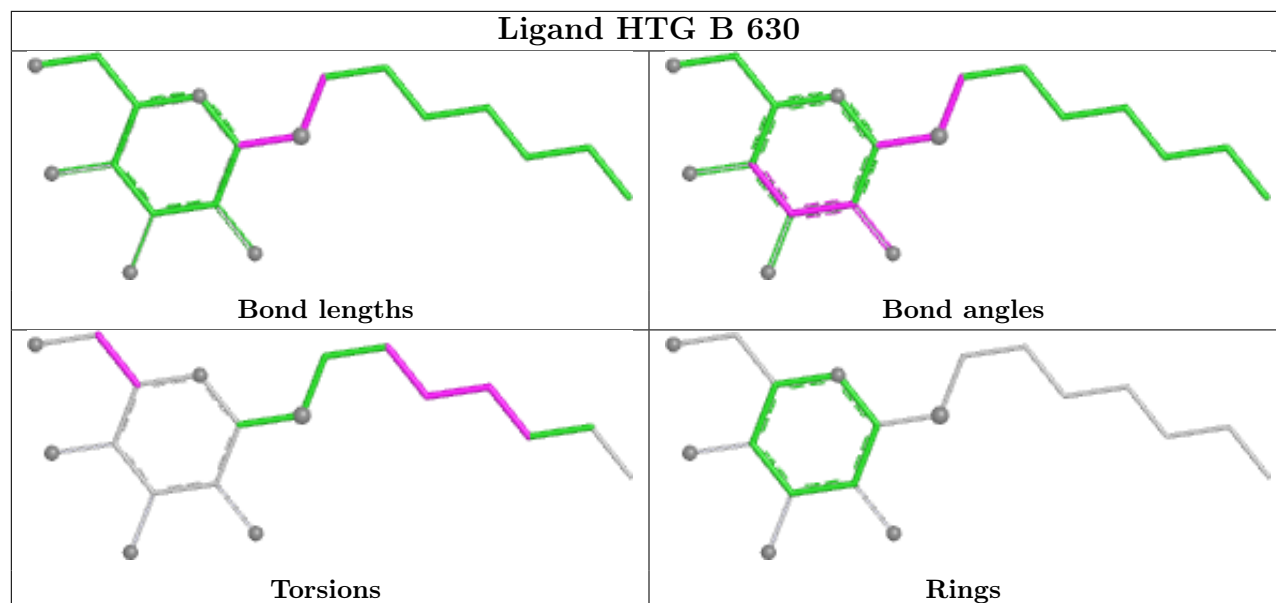


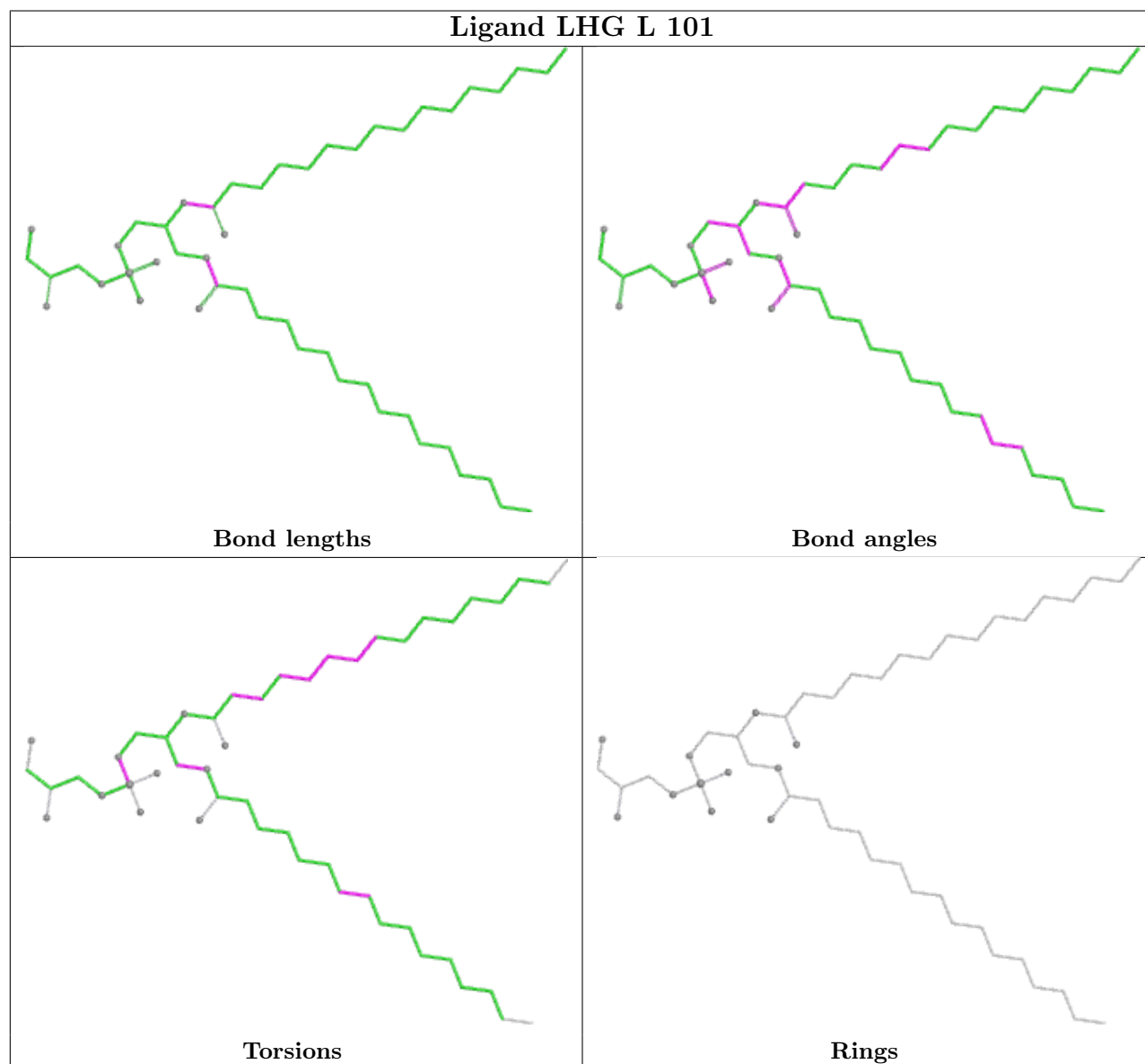
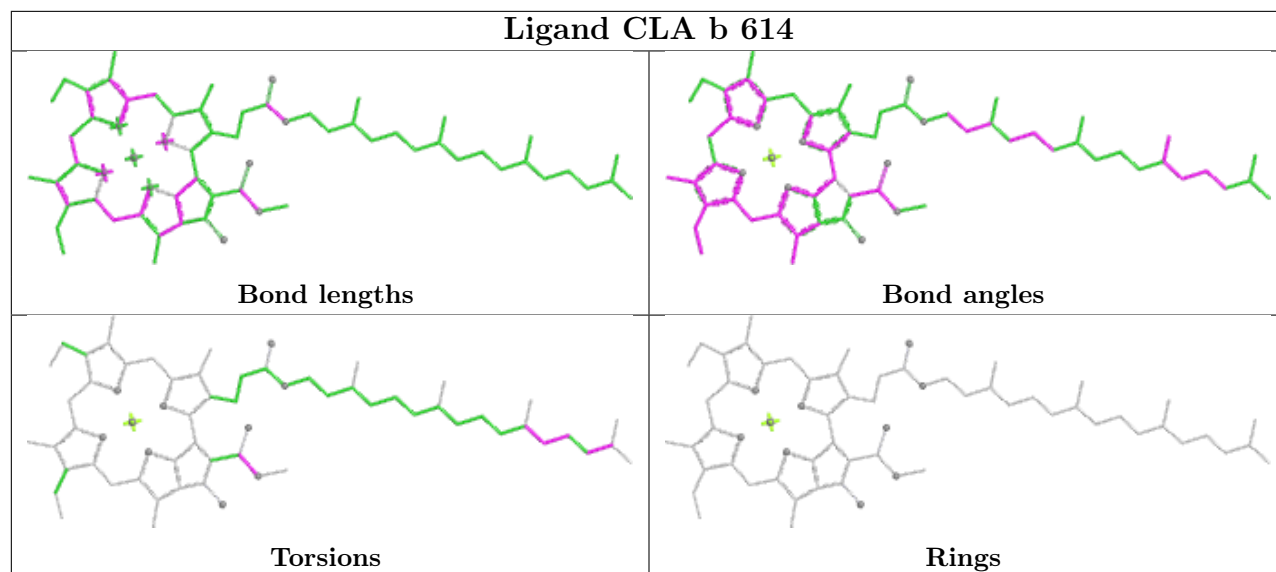
Ligand CLA B 609

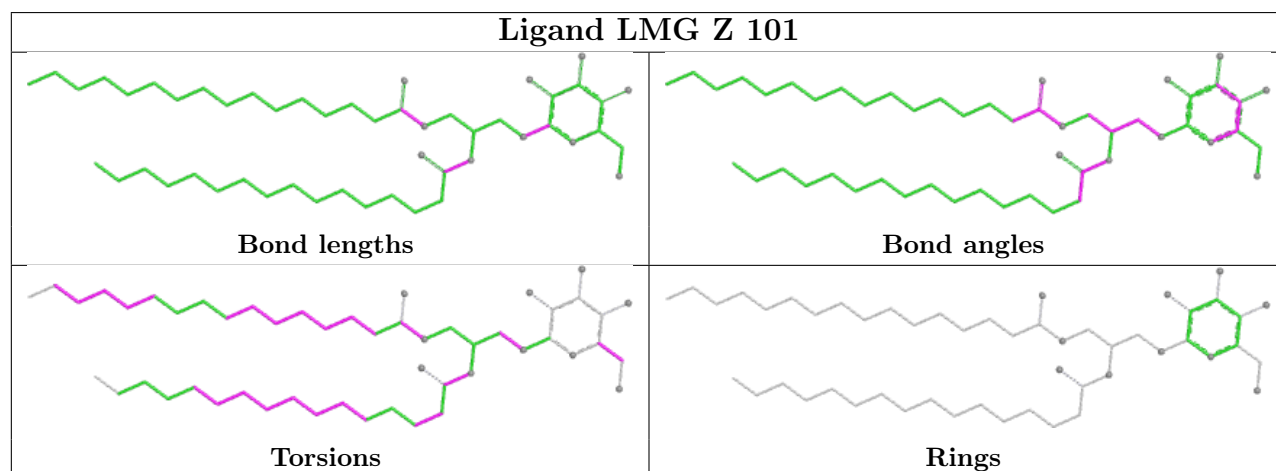
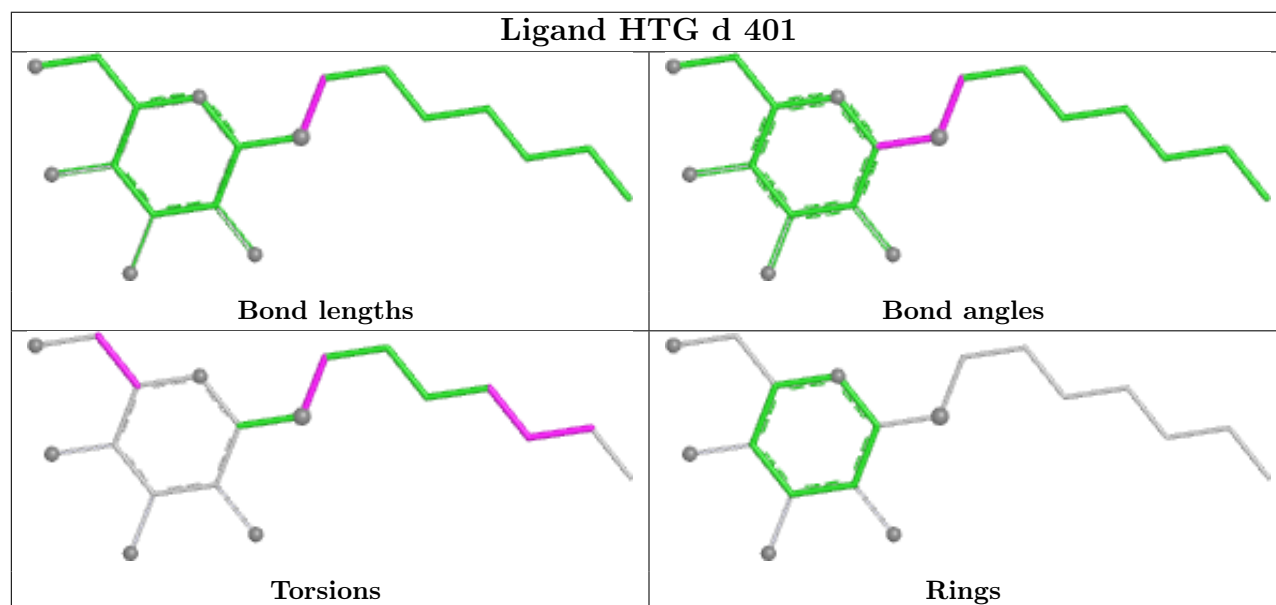
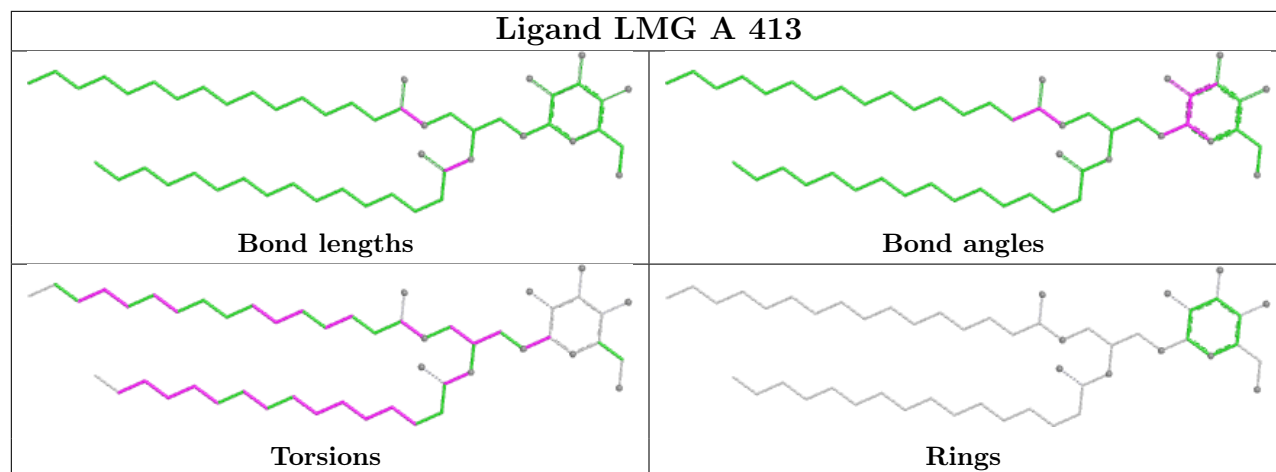


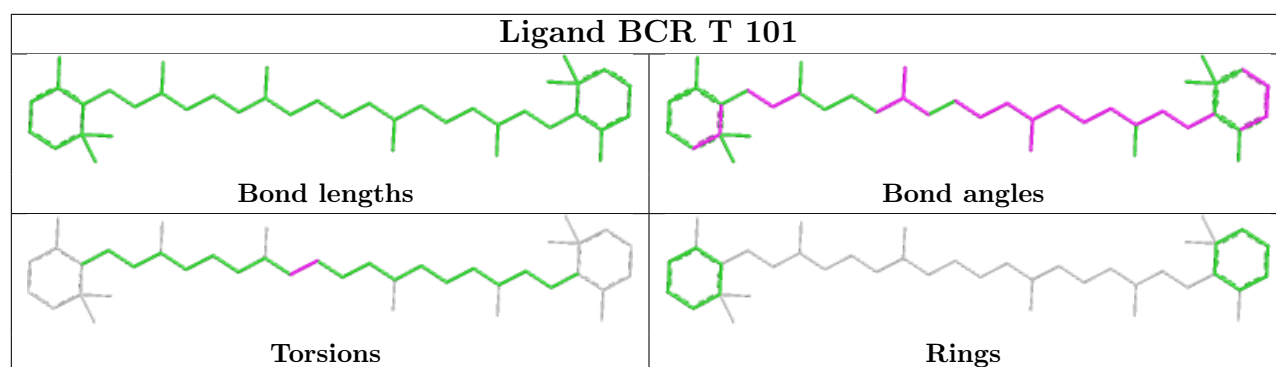
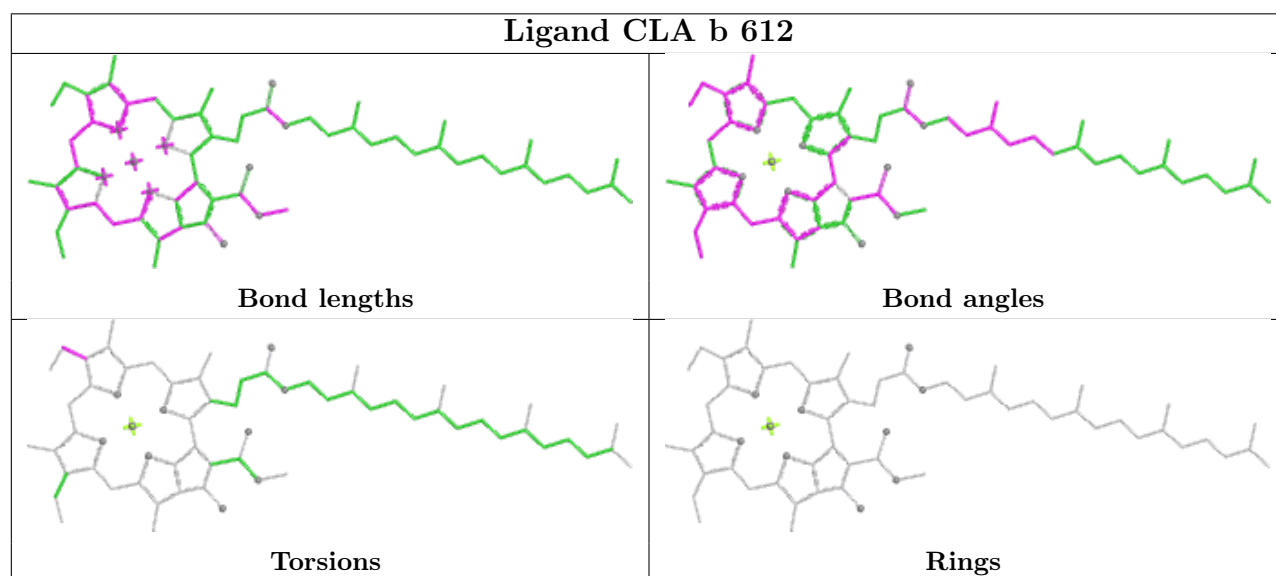
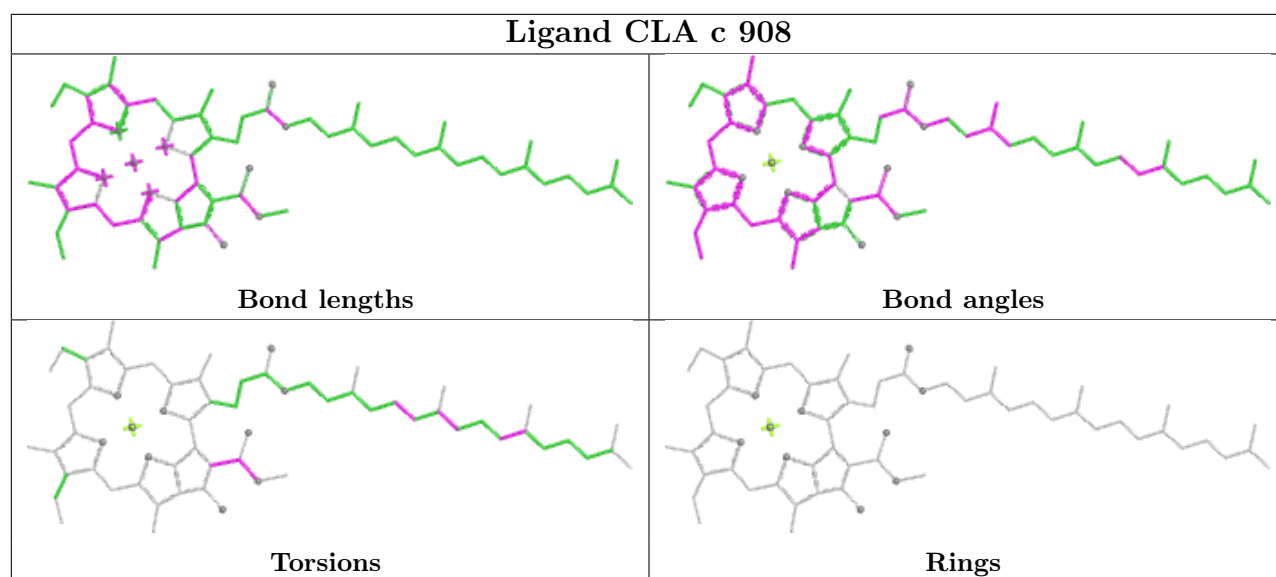




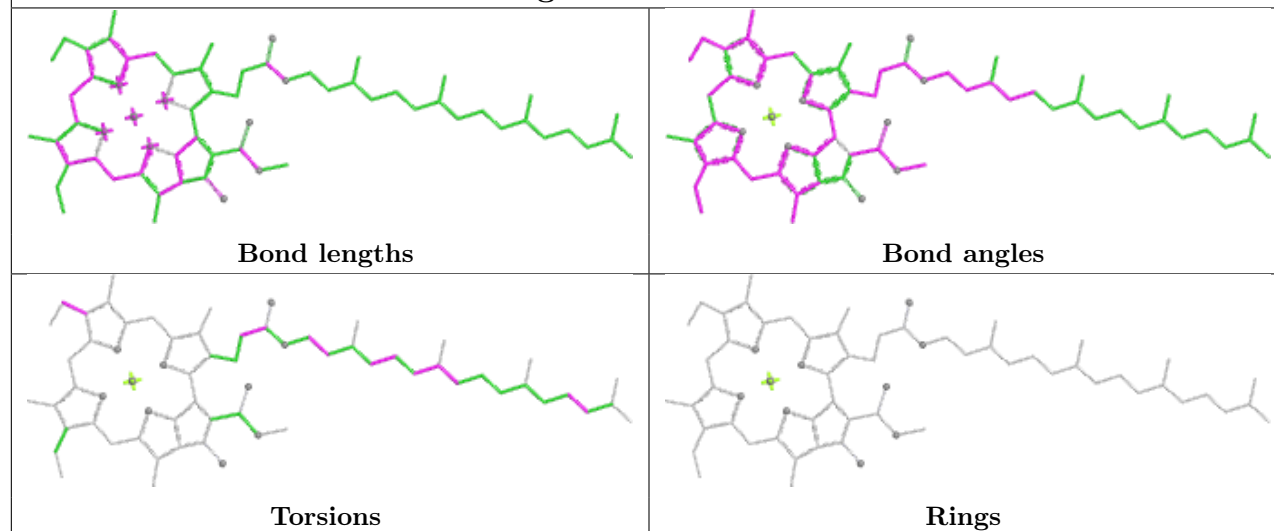




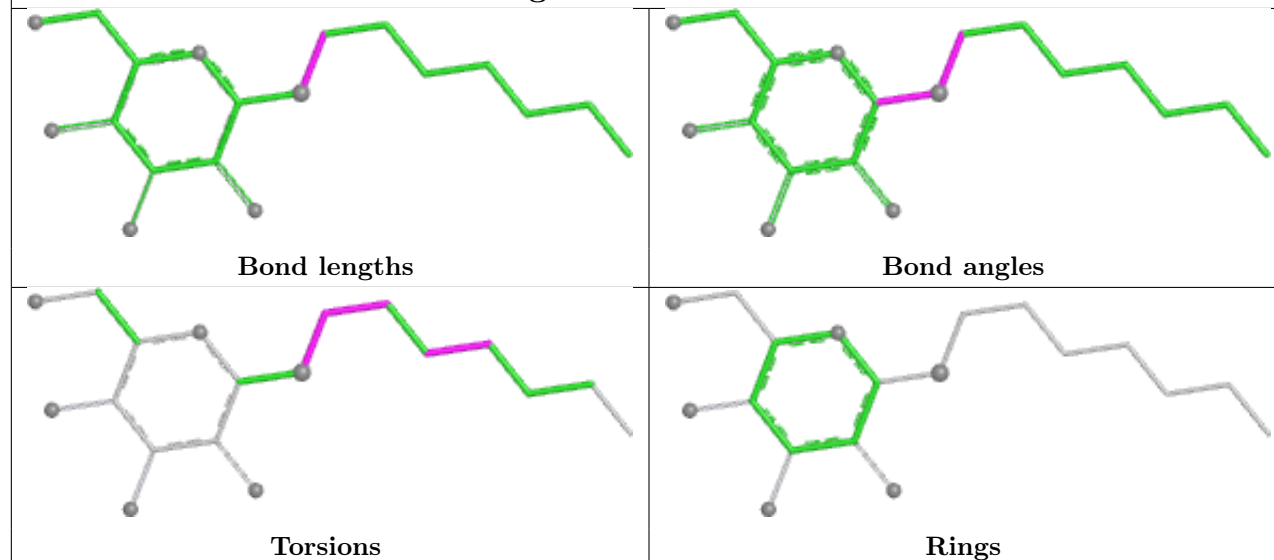




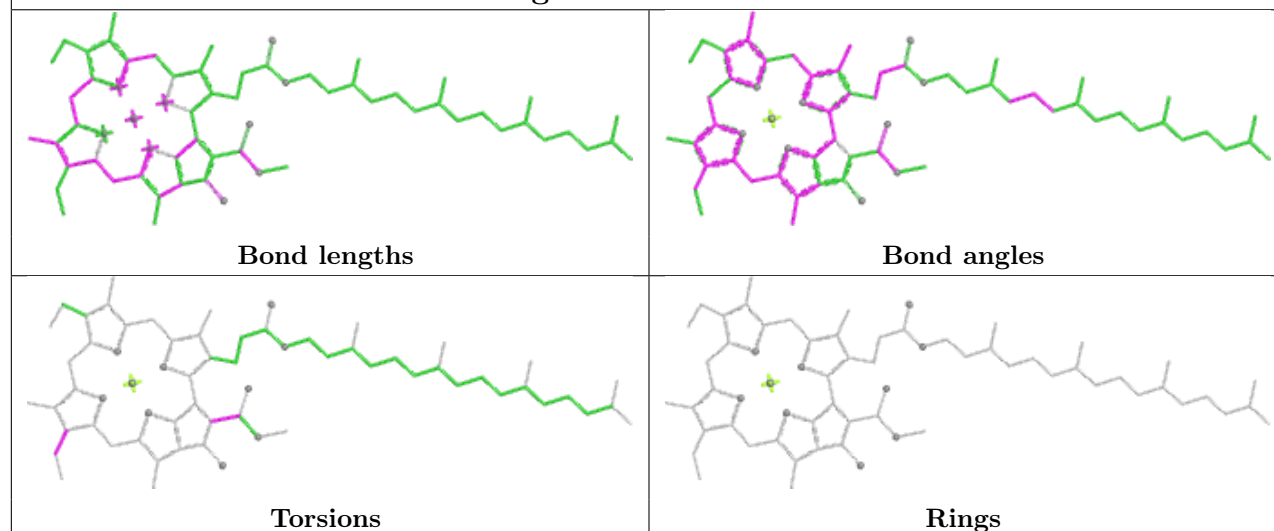
Ligand CLA c 913

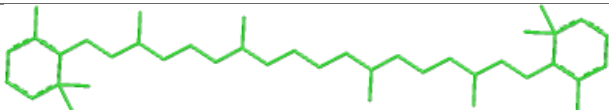
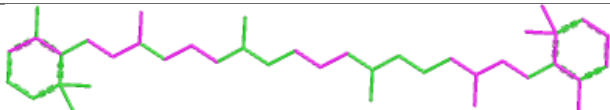
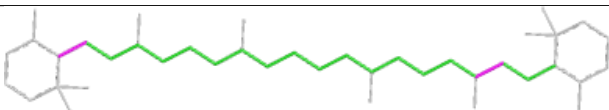
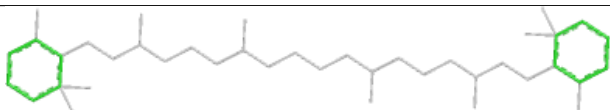


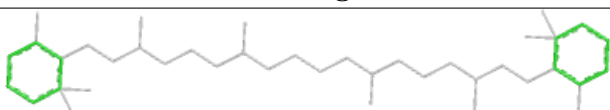
Ligand HTG C 521

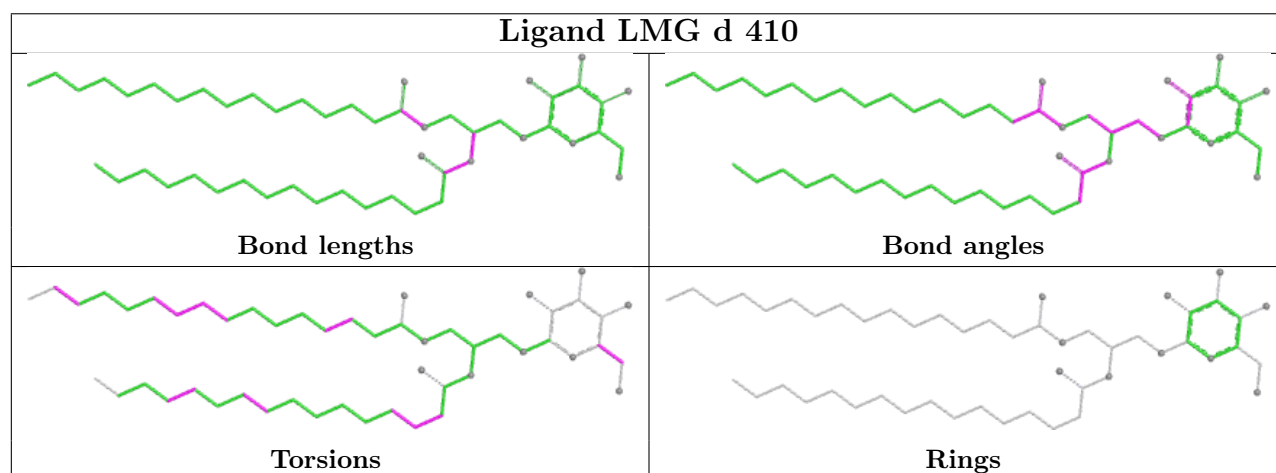
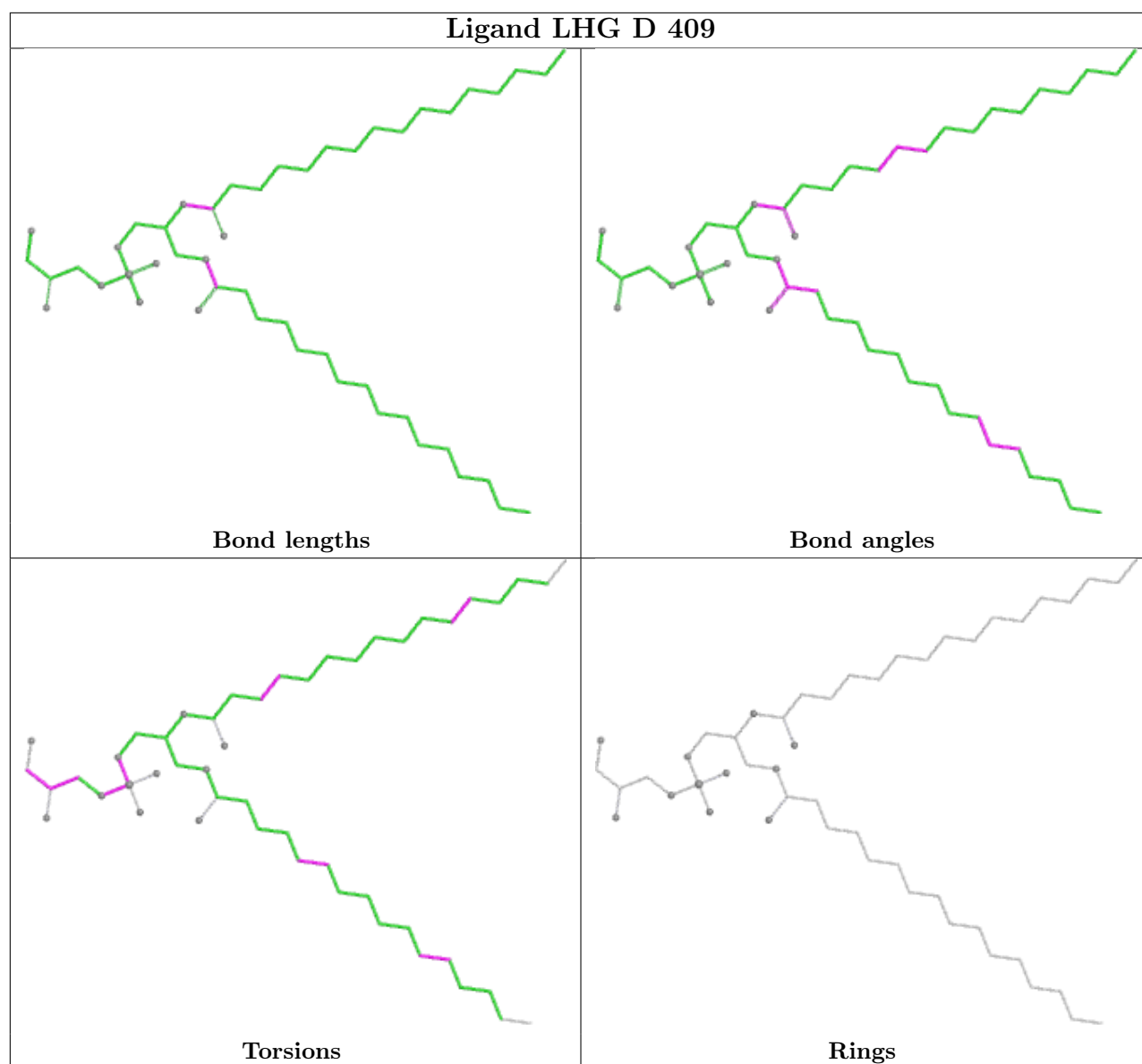


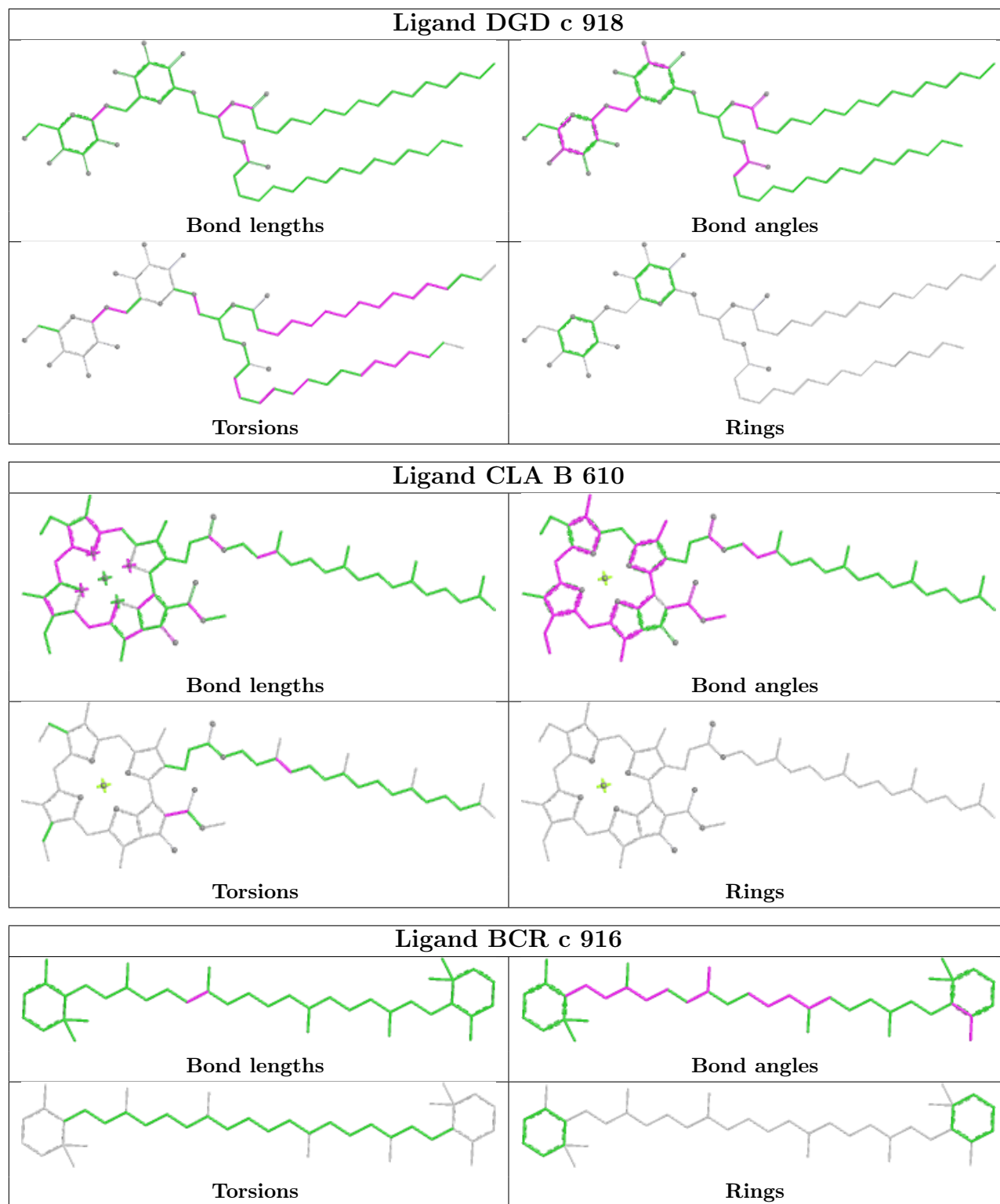
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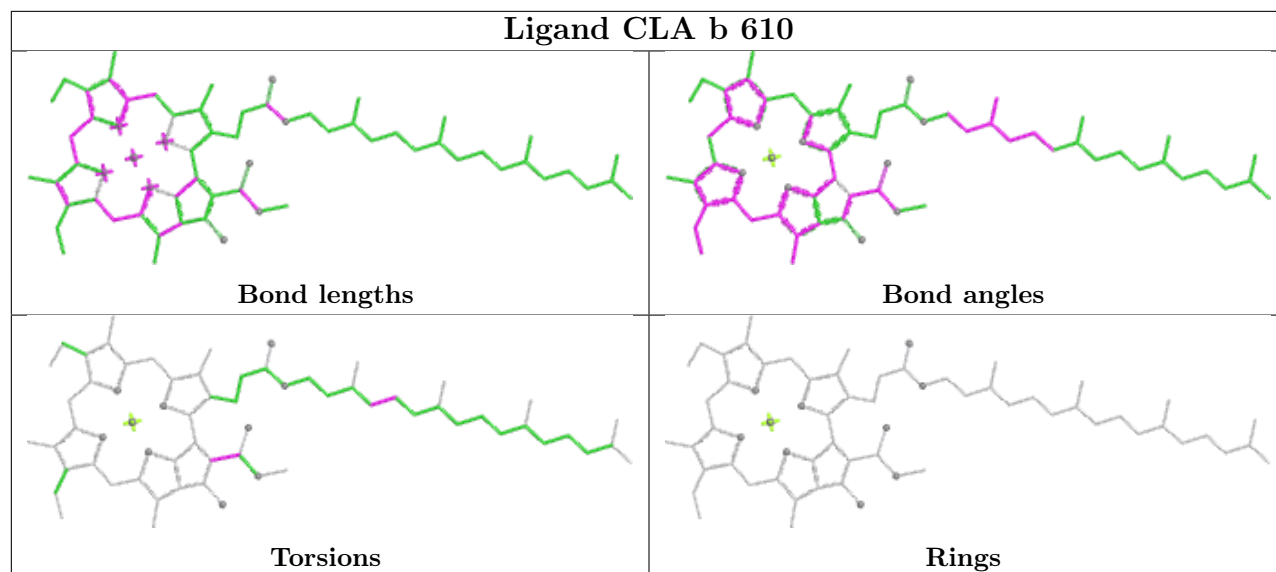
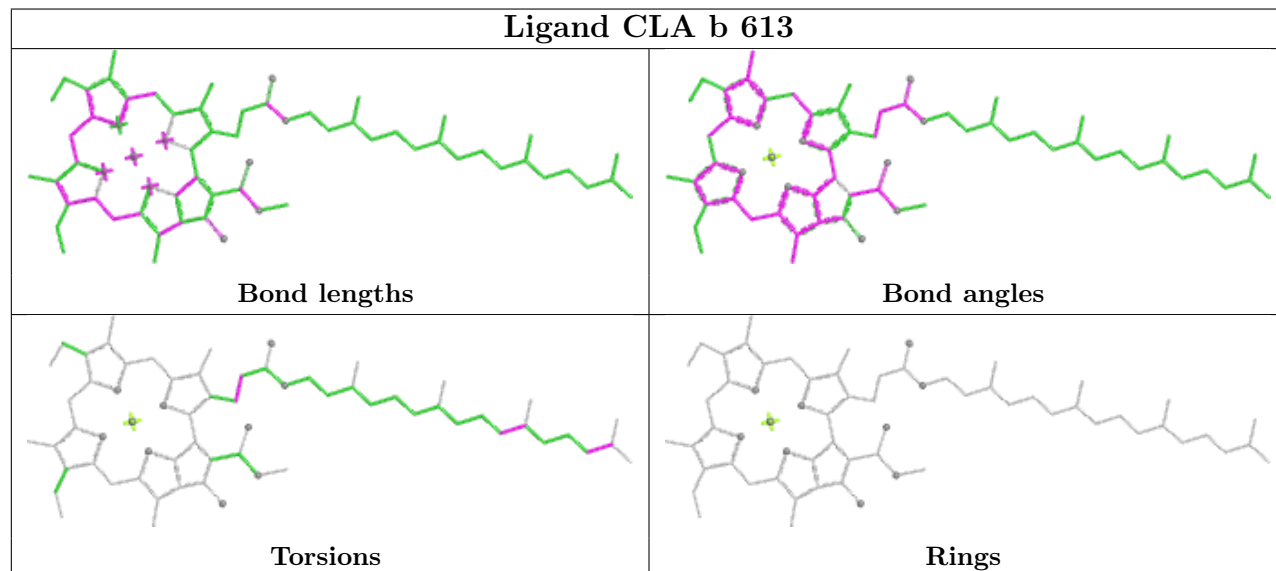


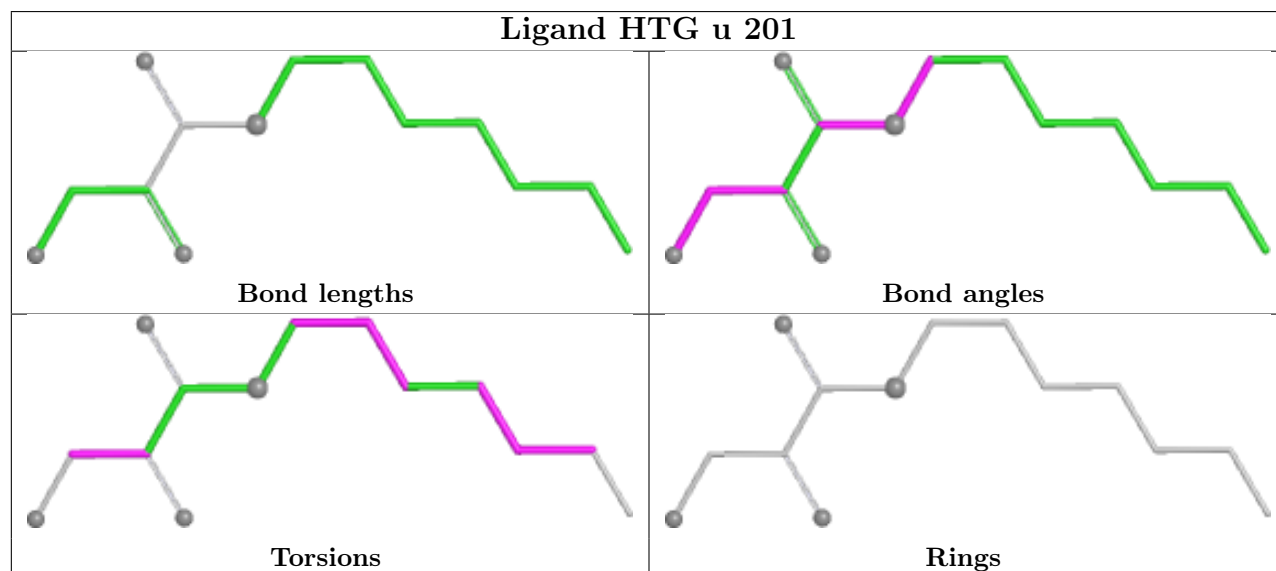
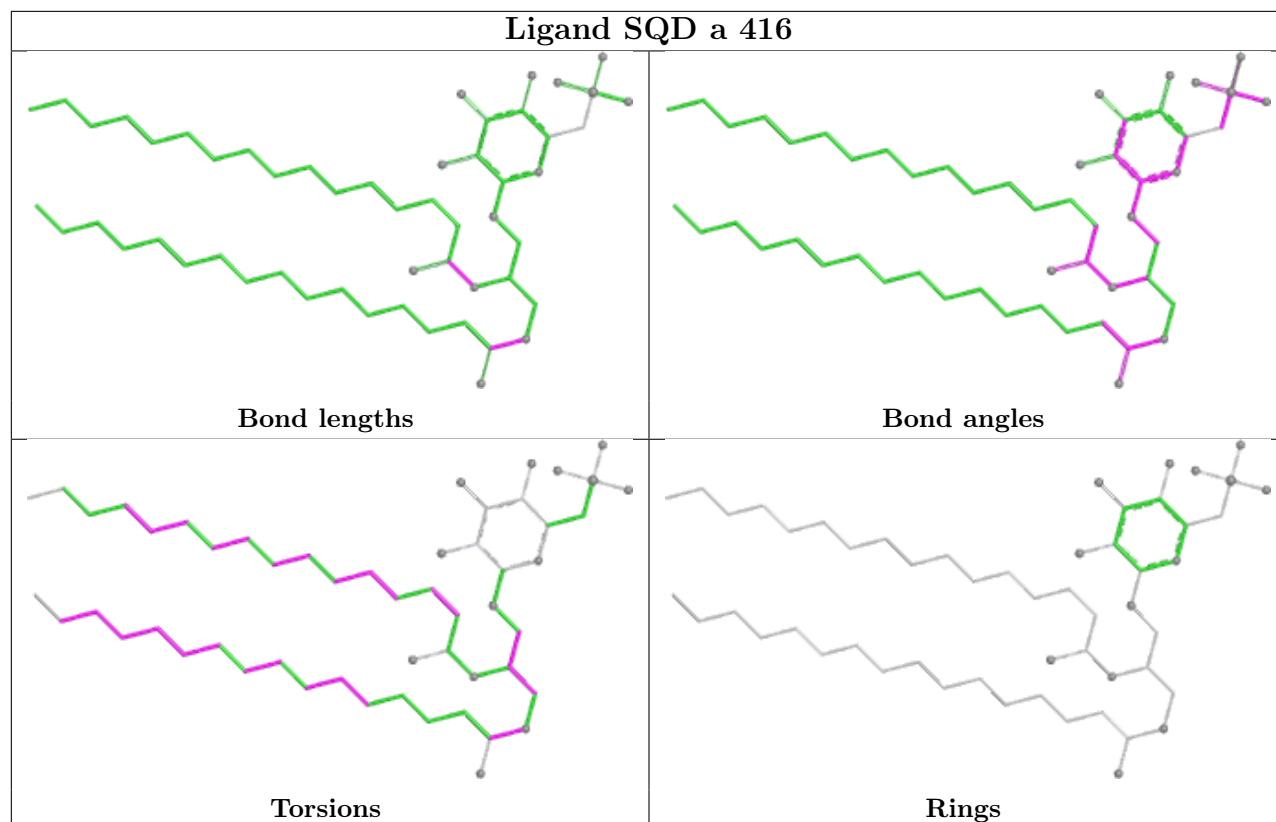
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

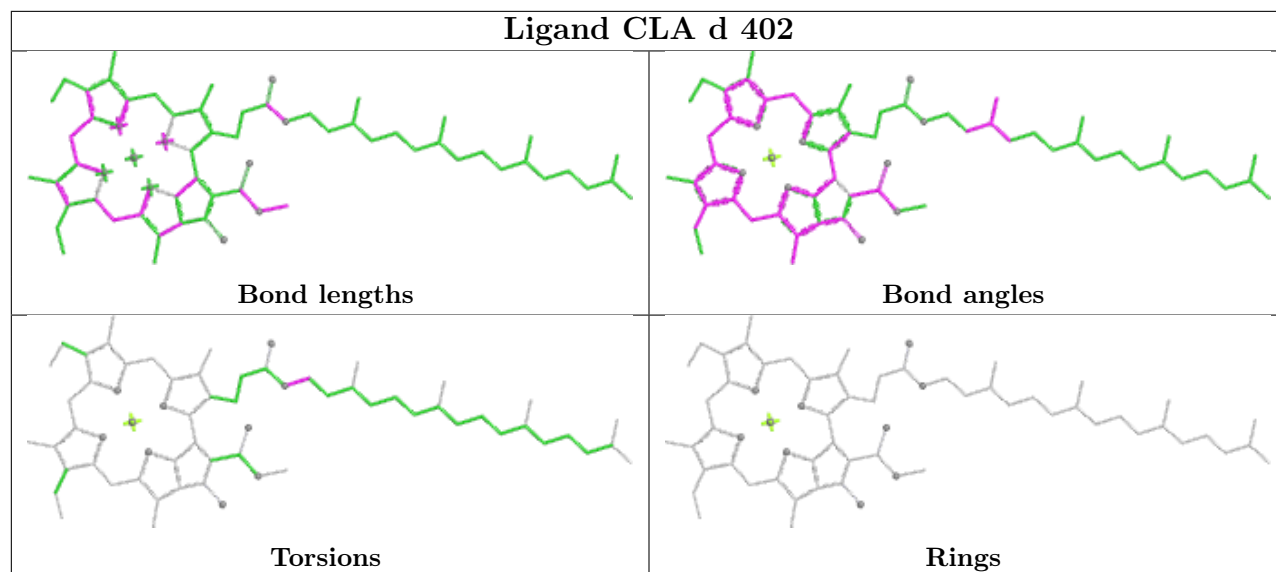




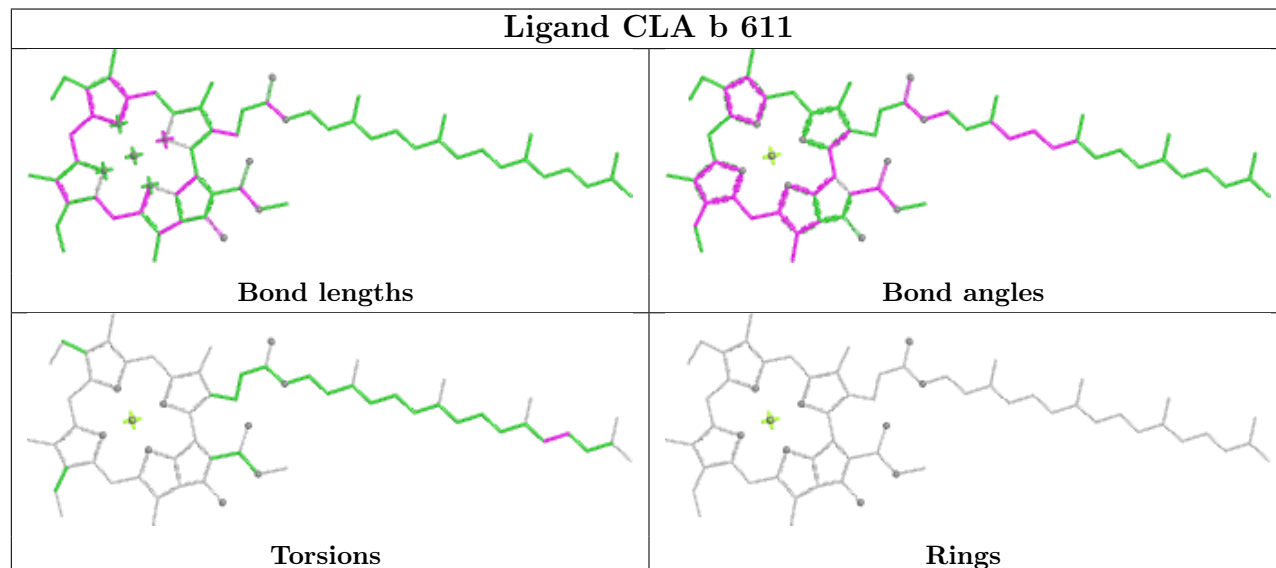
Ligand CLA b 610**Ligand CLA b 613**



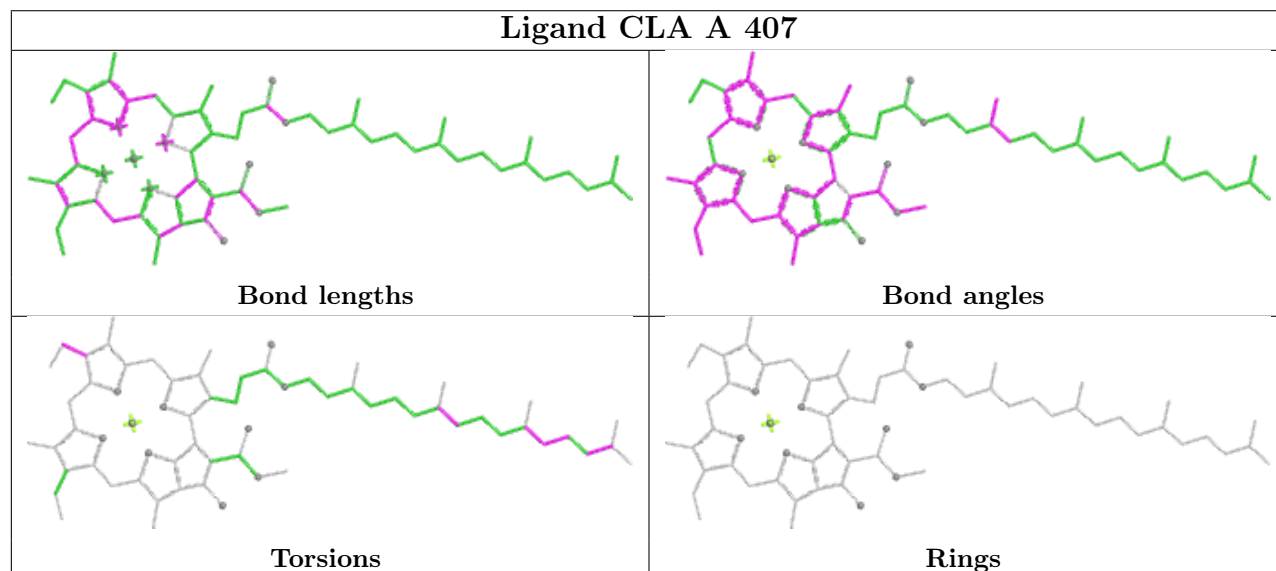
Ligand CLA d 402



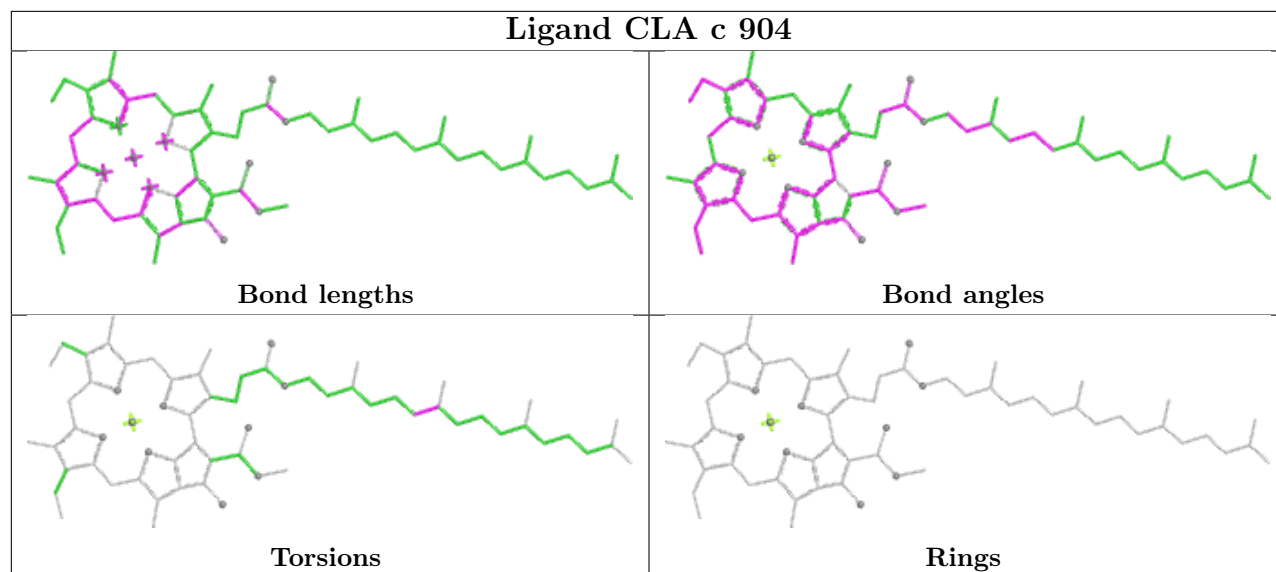
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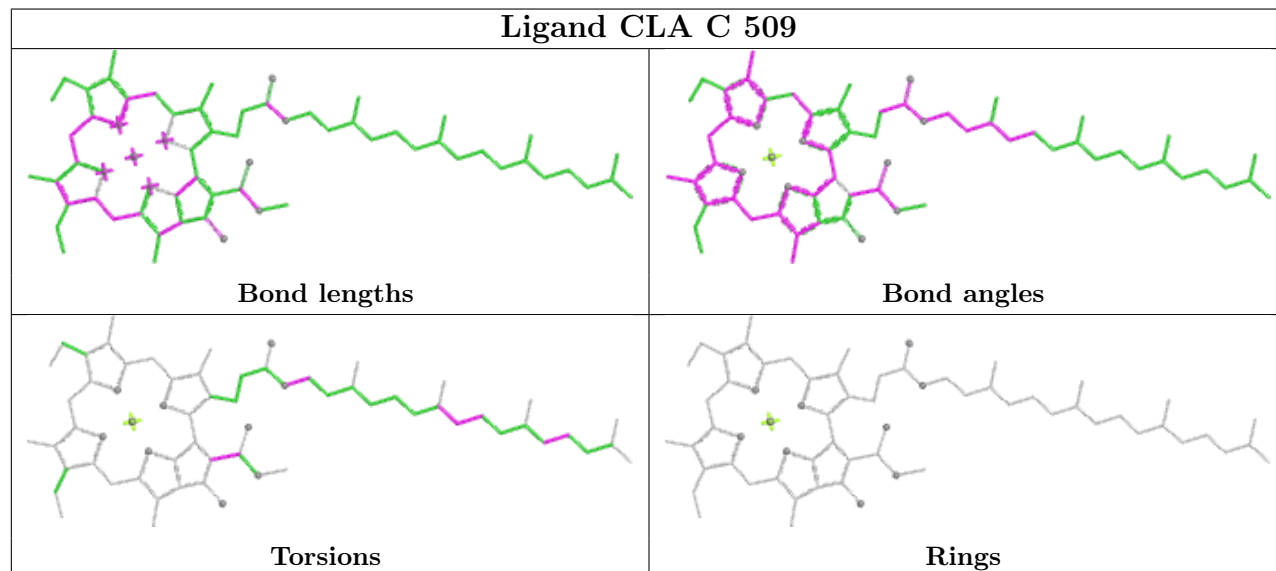
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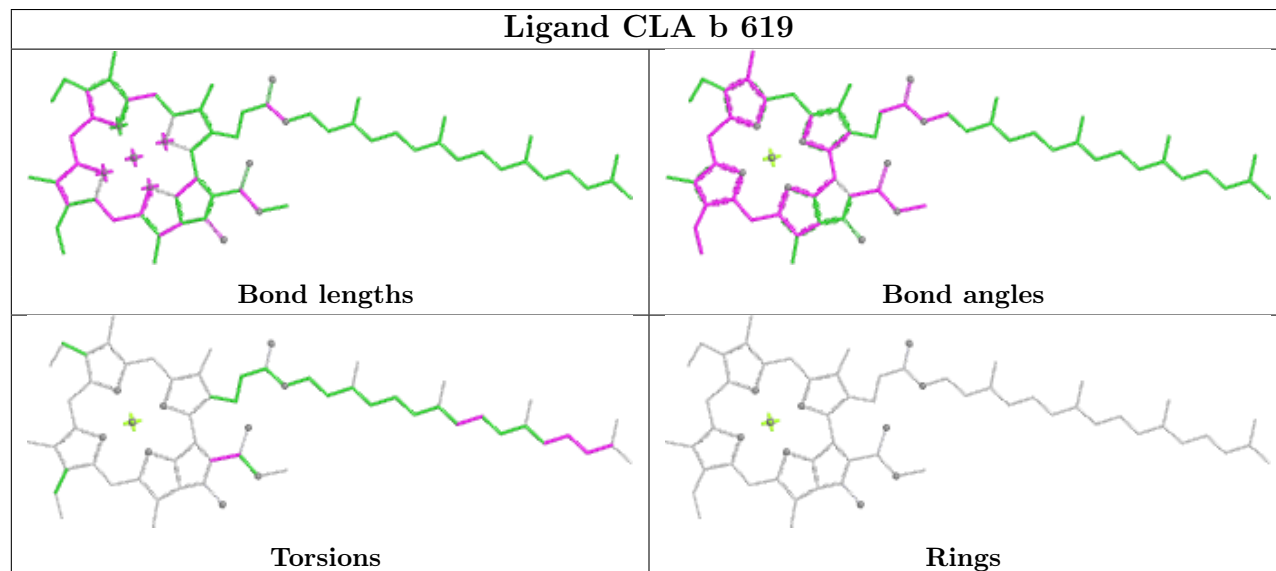
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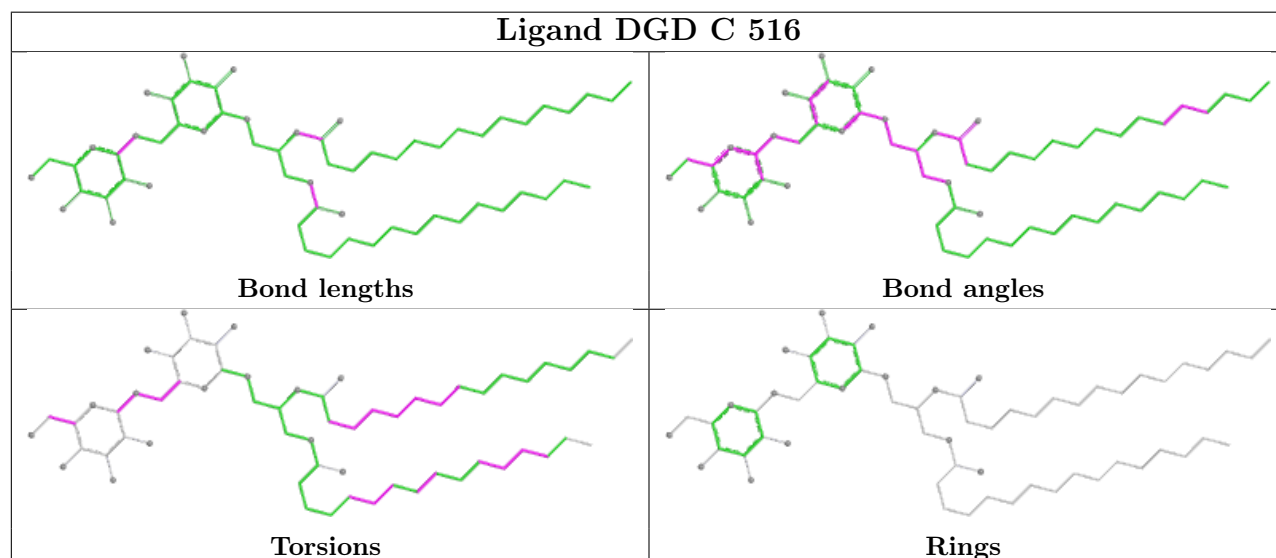
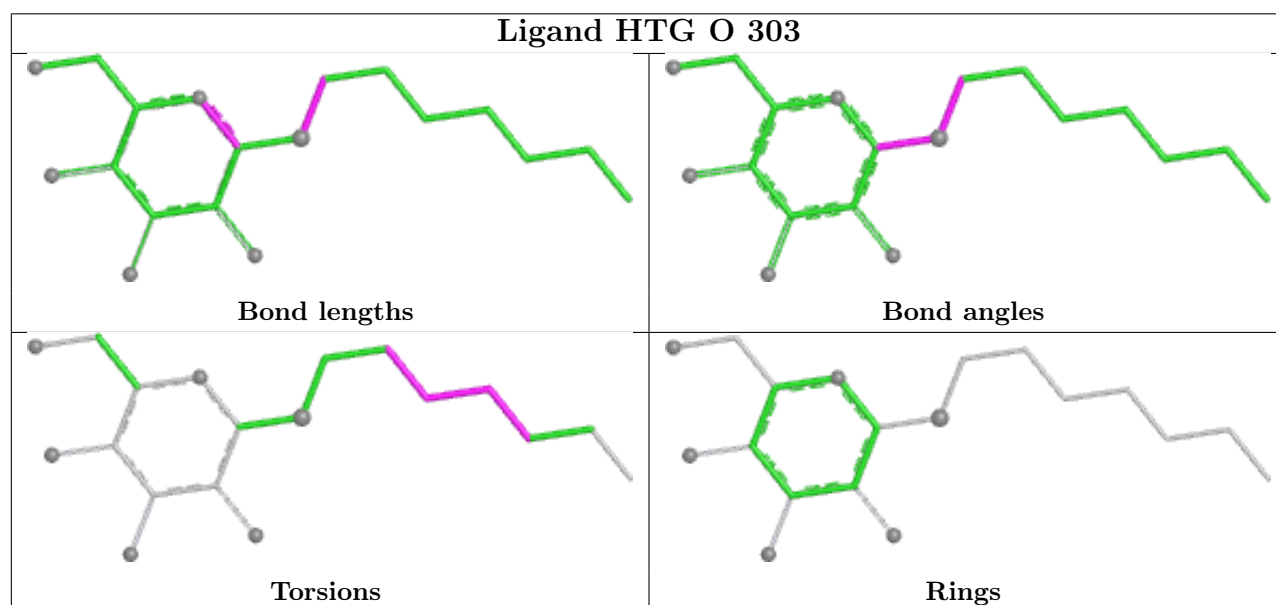
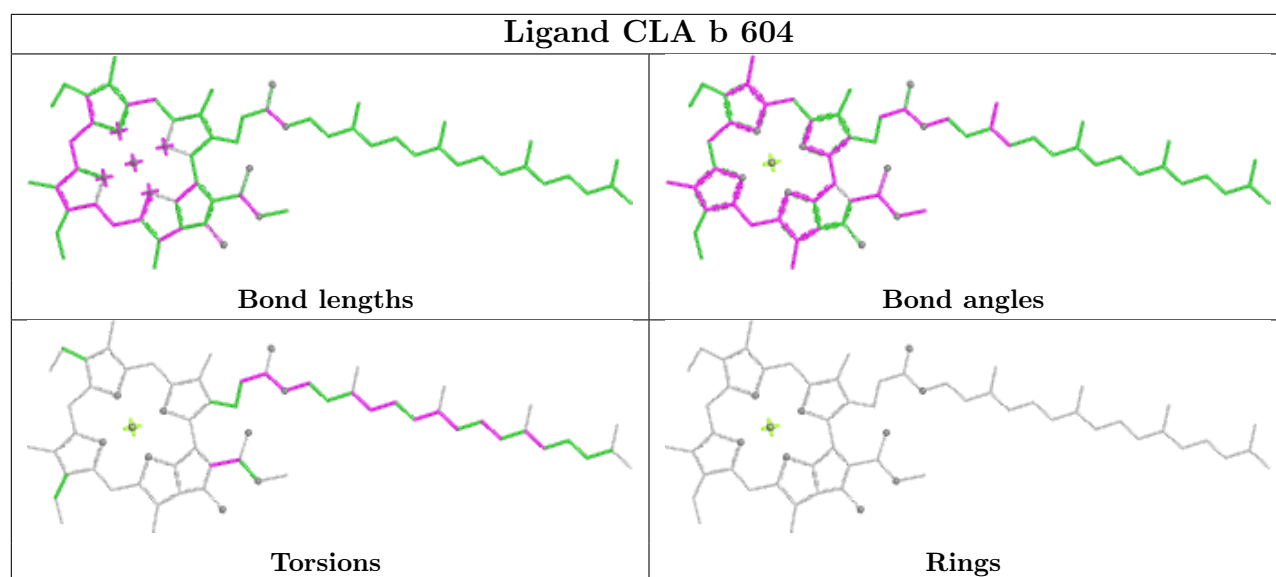


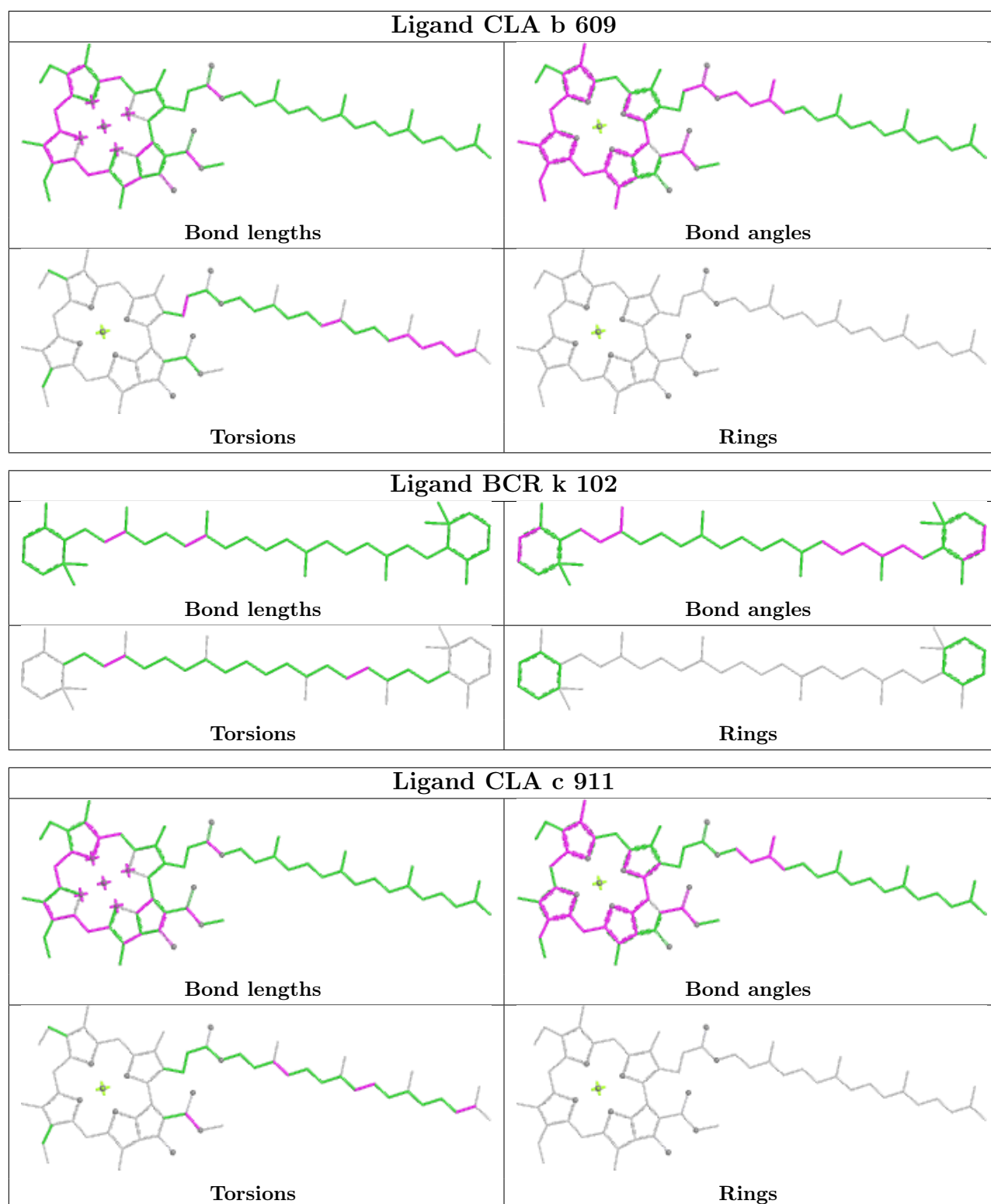
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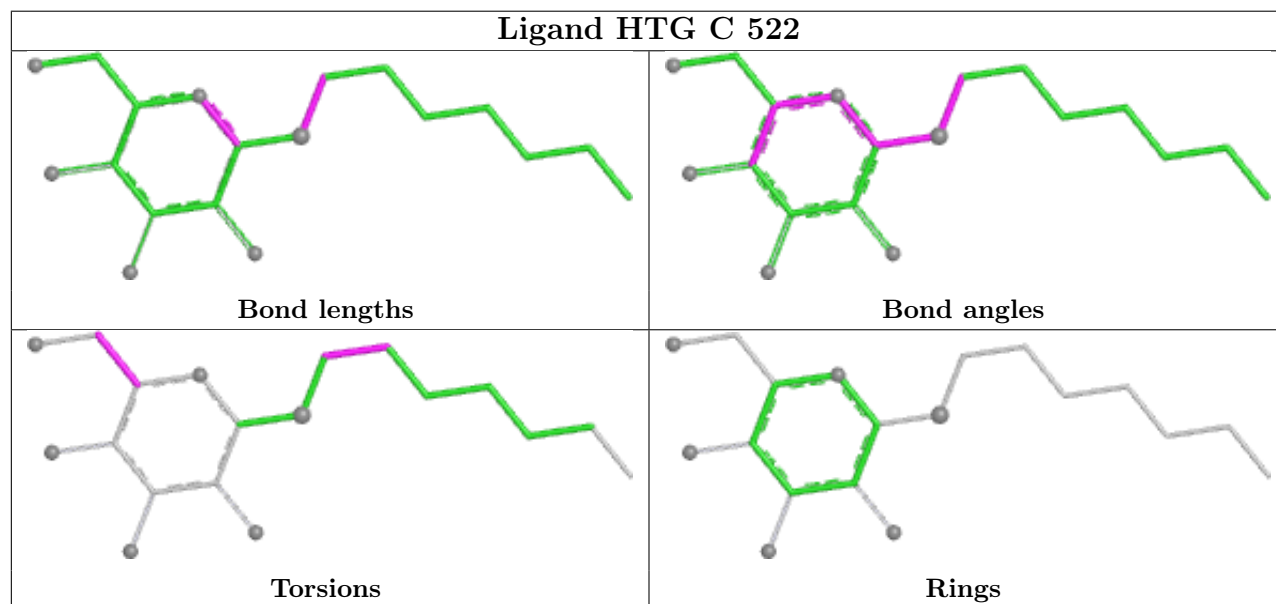
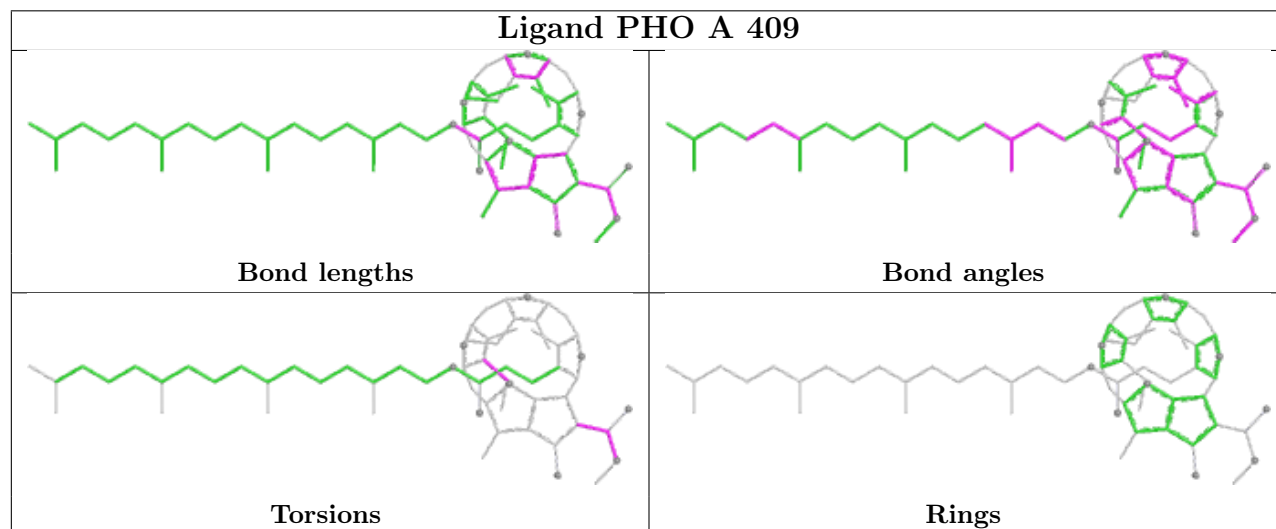
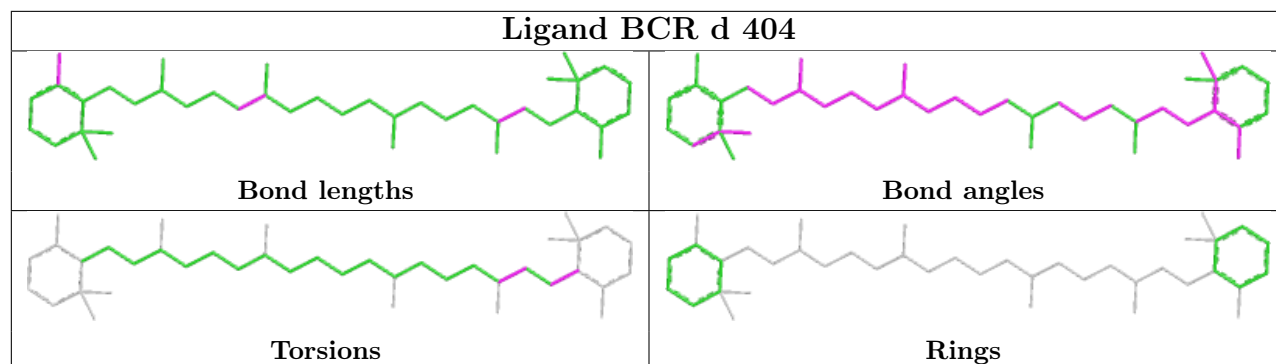


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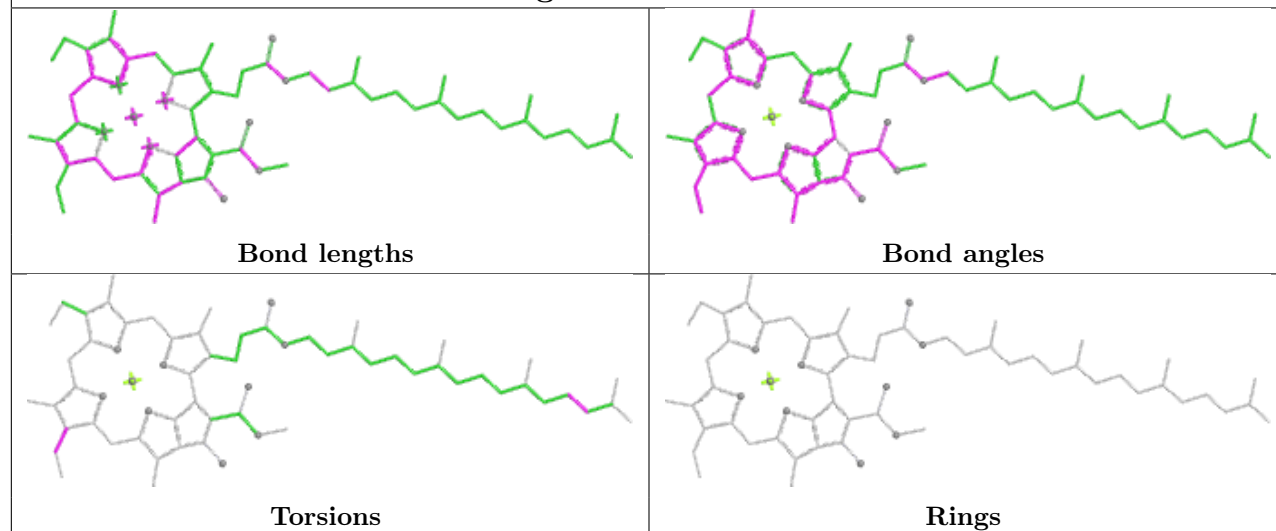




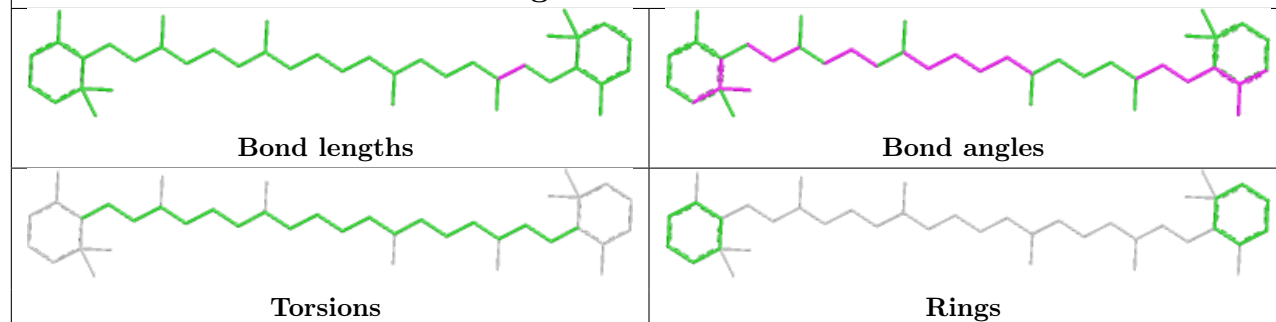




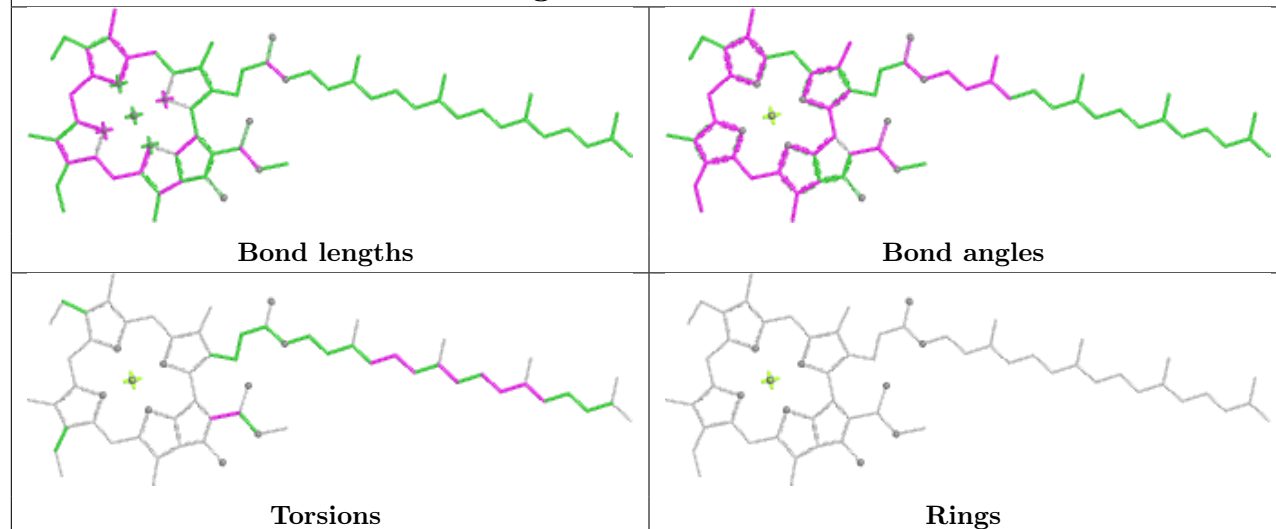
Ligand CLA a 410



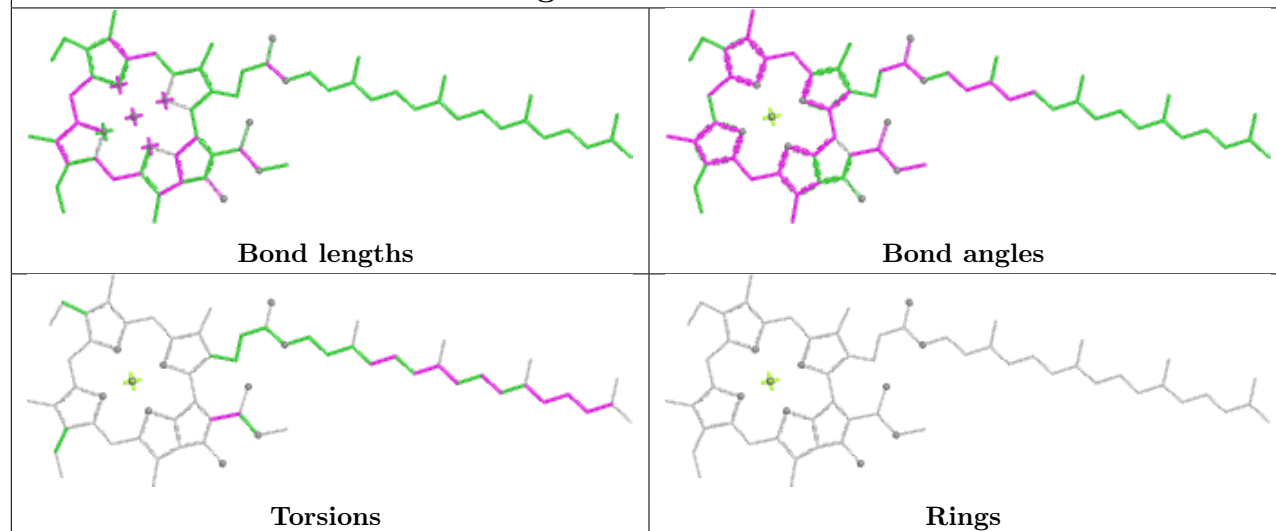
Ligand BCR B 620



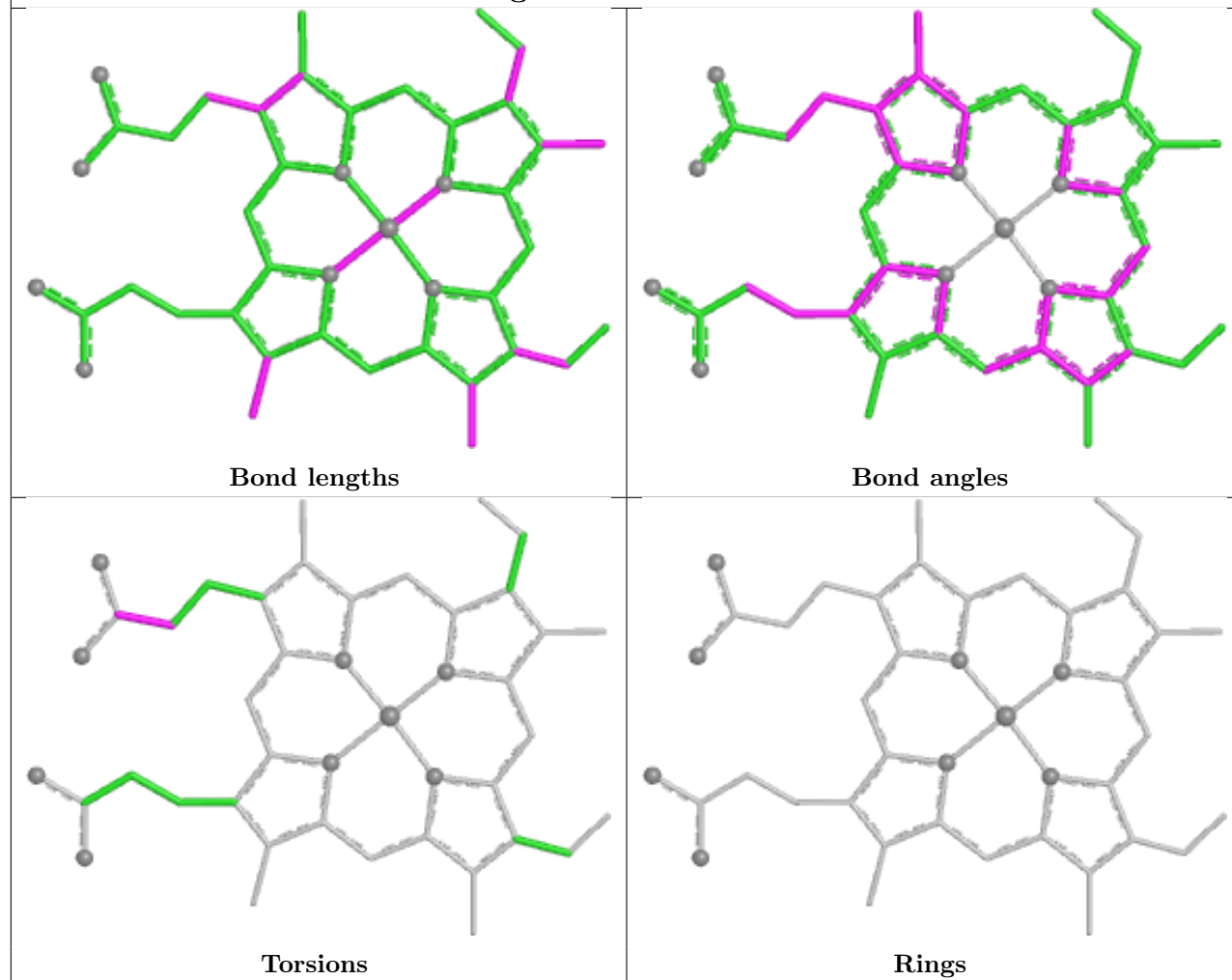
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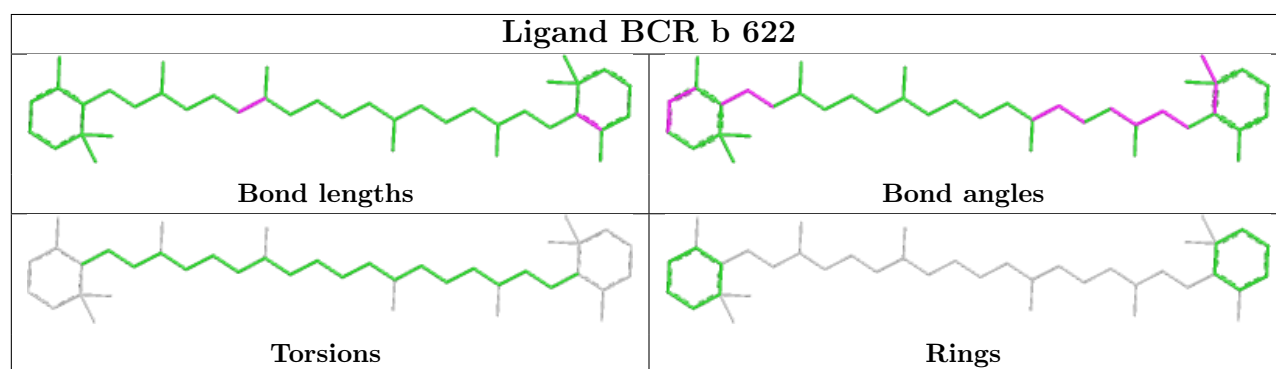
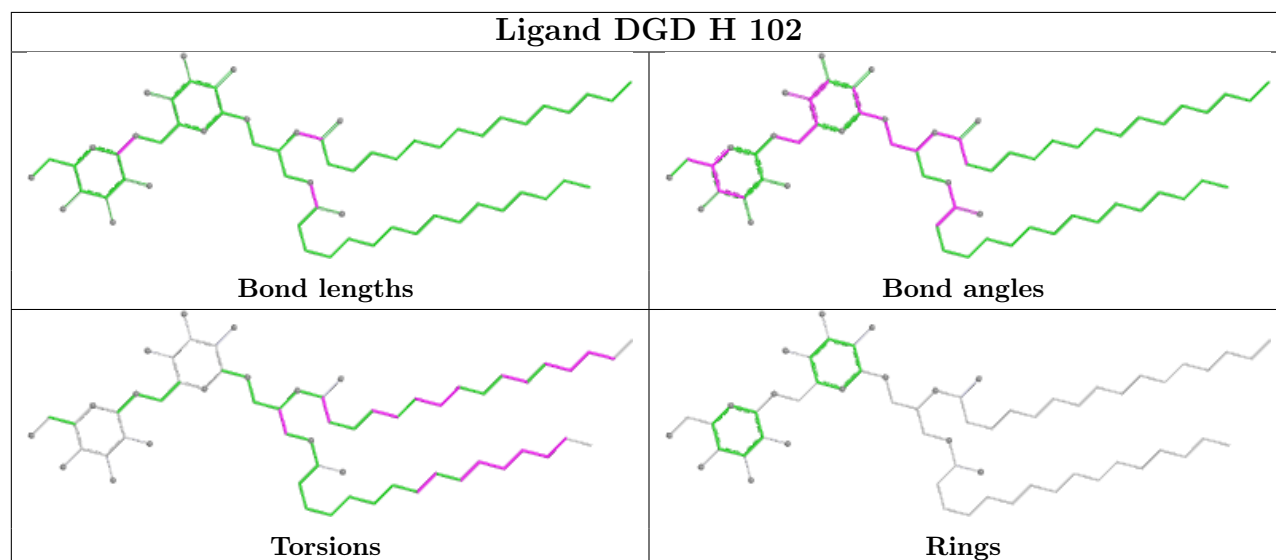
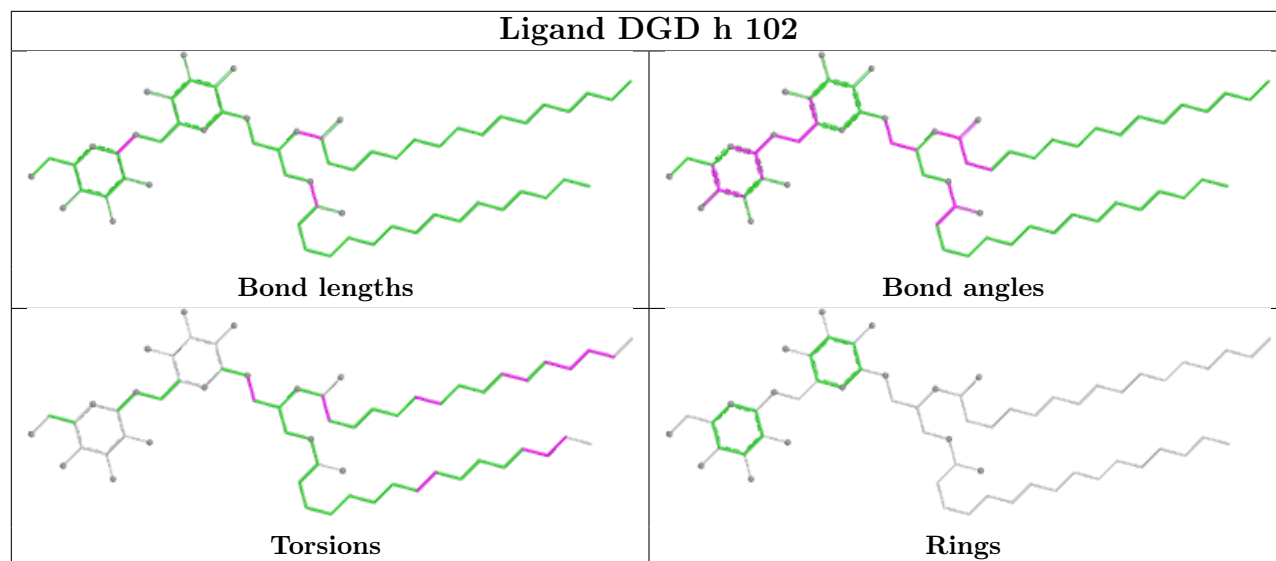


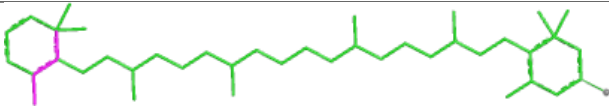
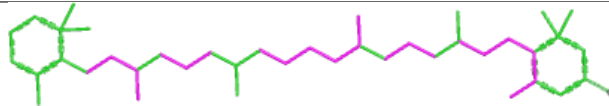
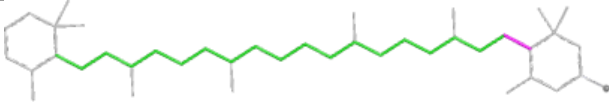
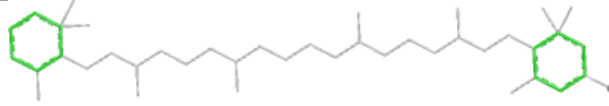
Ligand CLA c 907

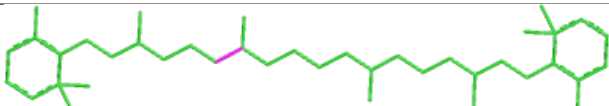
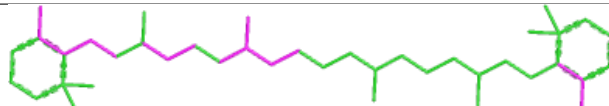
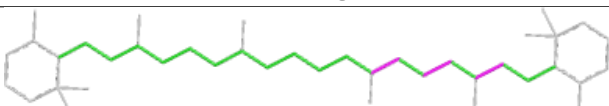
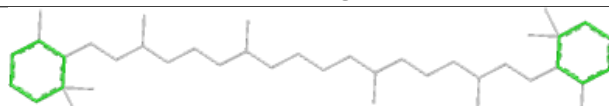


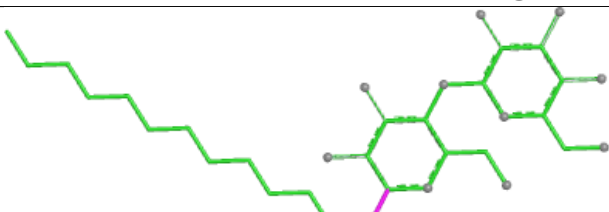
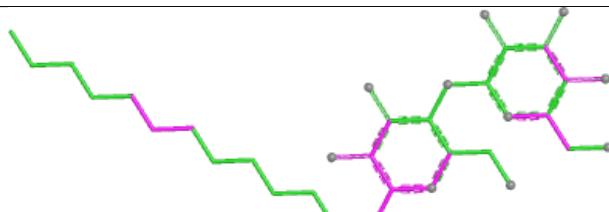
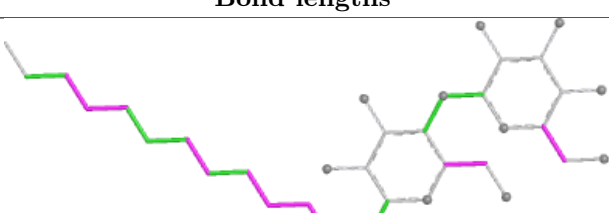
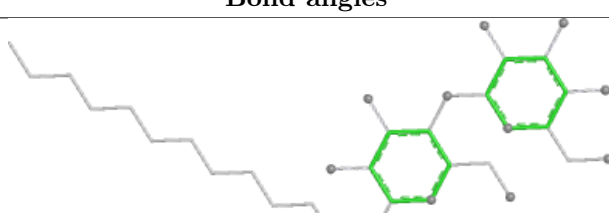
Ligand HEM F 101

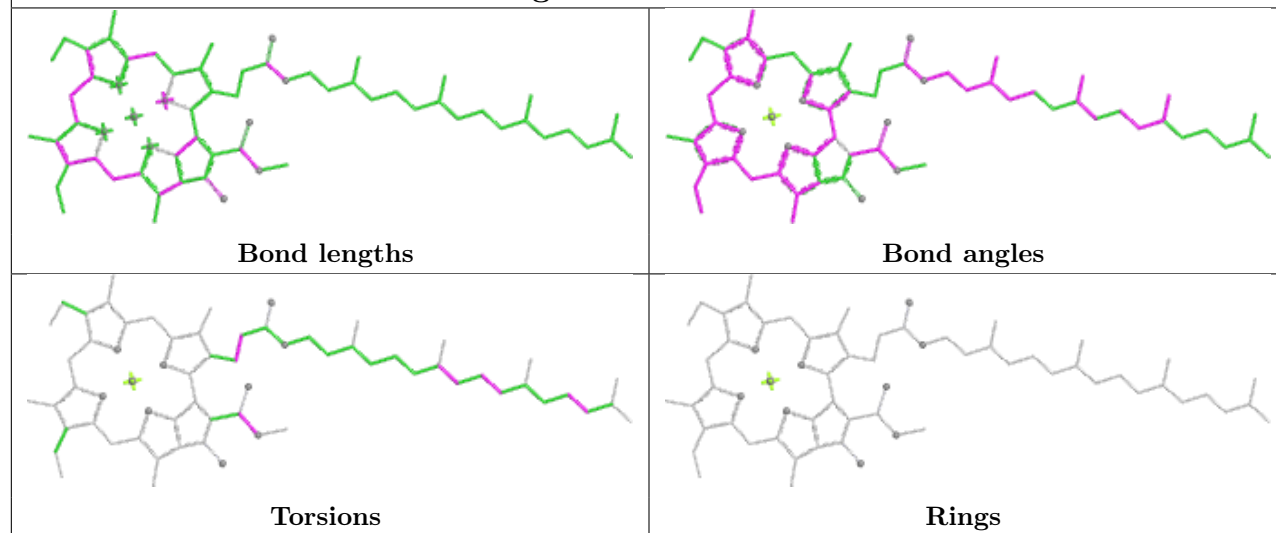
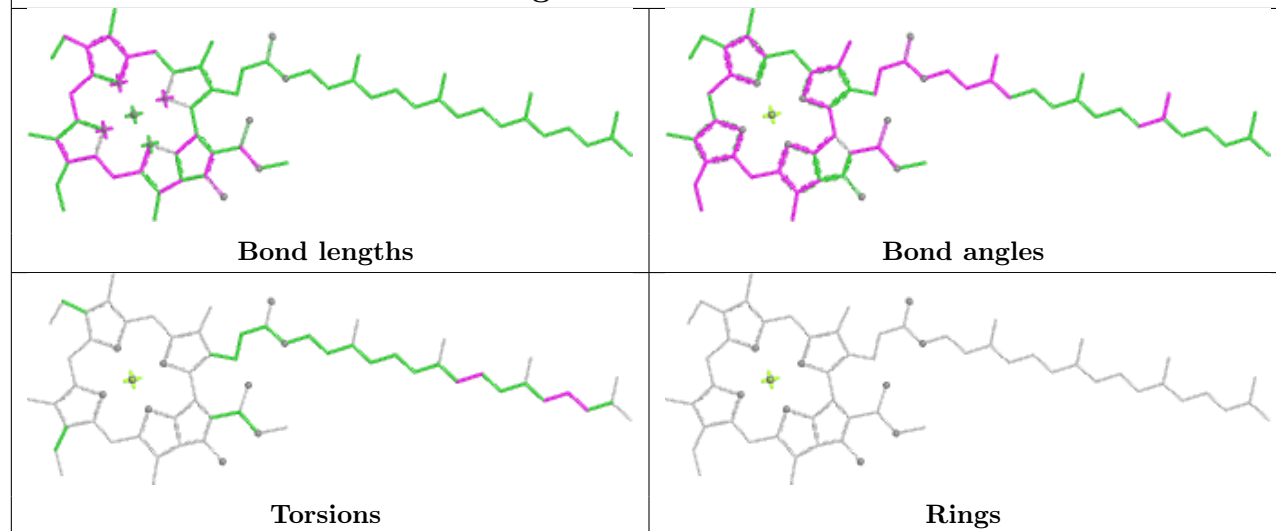


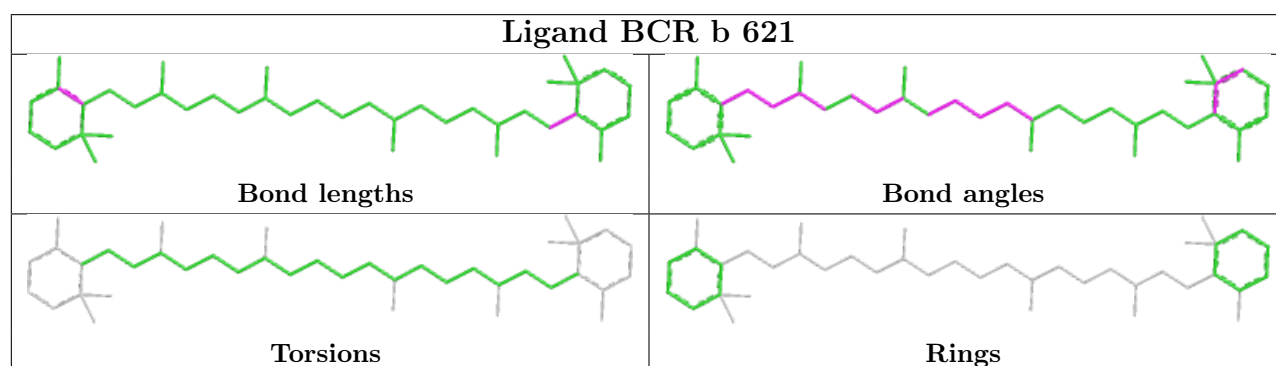
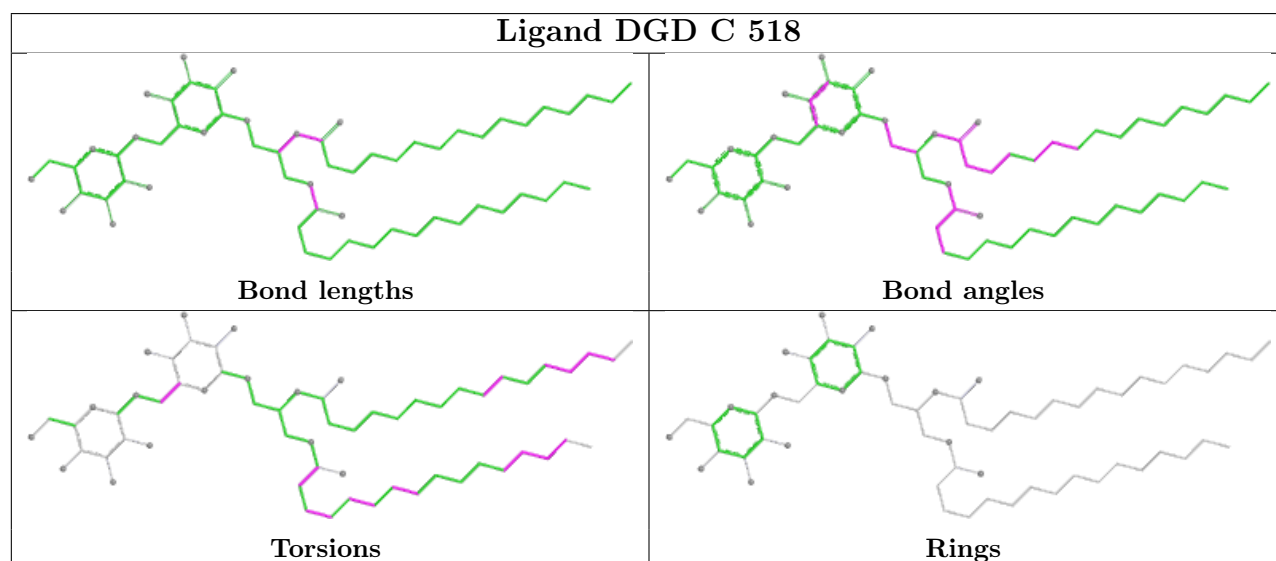
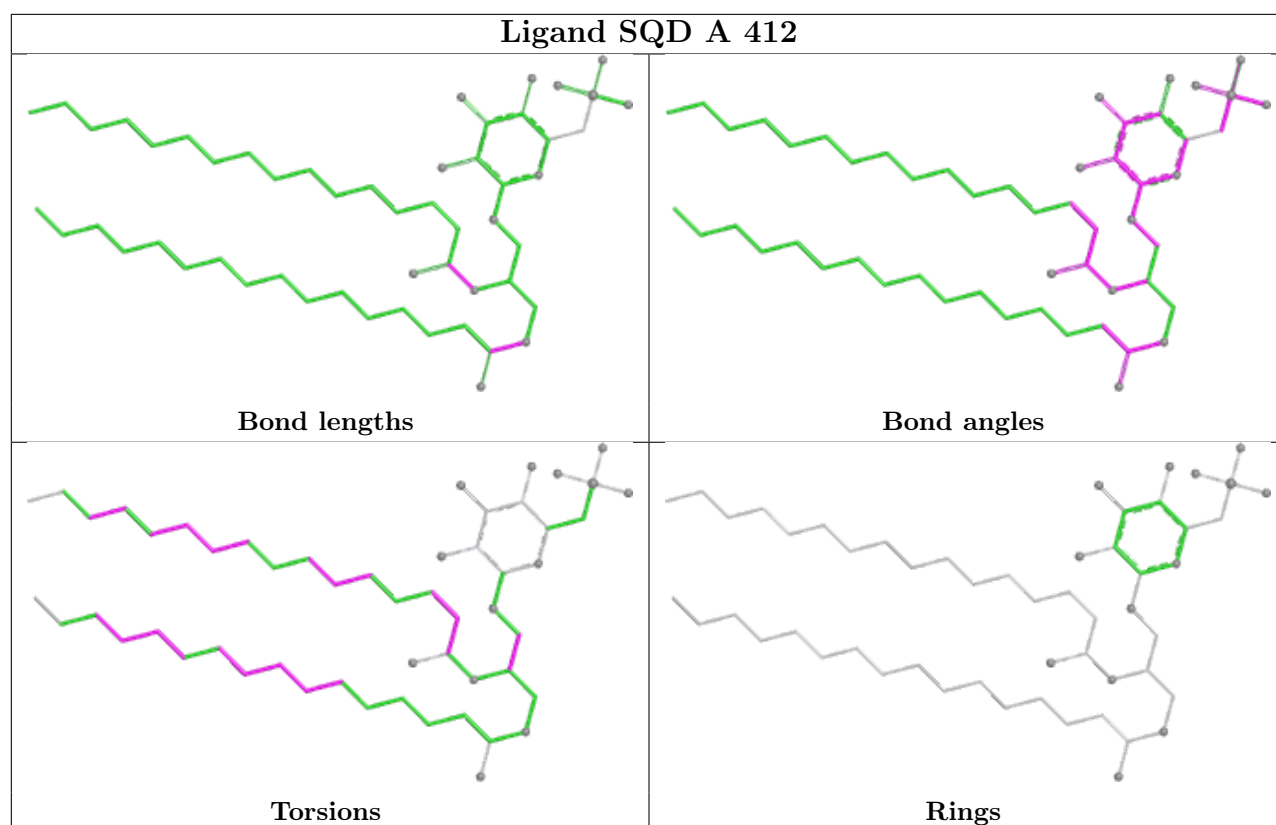


Ligand RRX H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

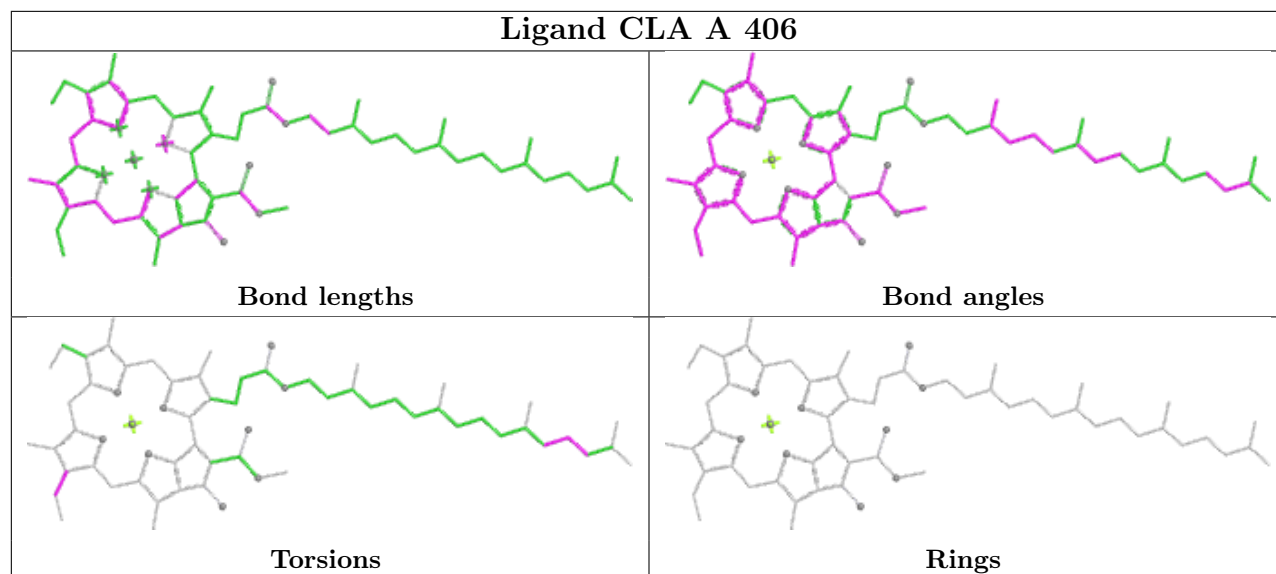
Ligand BCR c 915	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT a 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

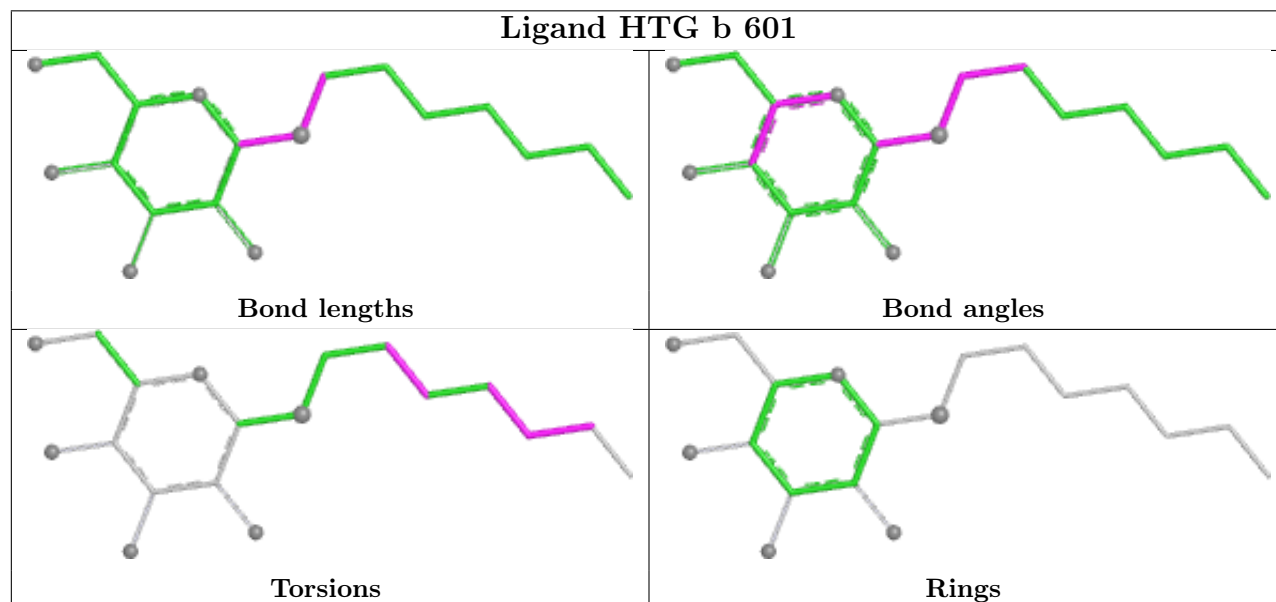
Ligand CLA B 607**Ligand CLA B 603**



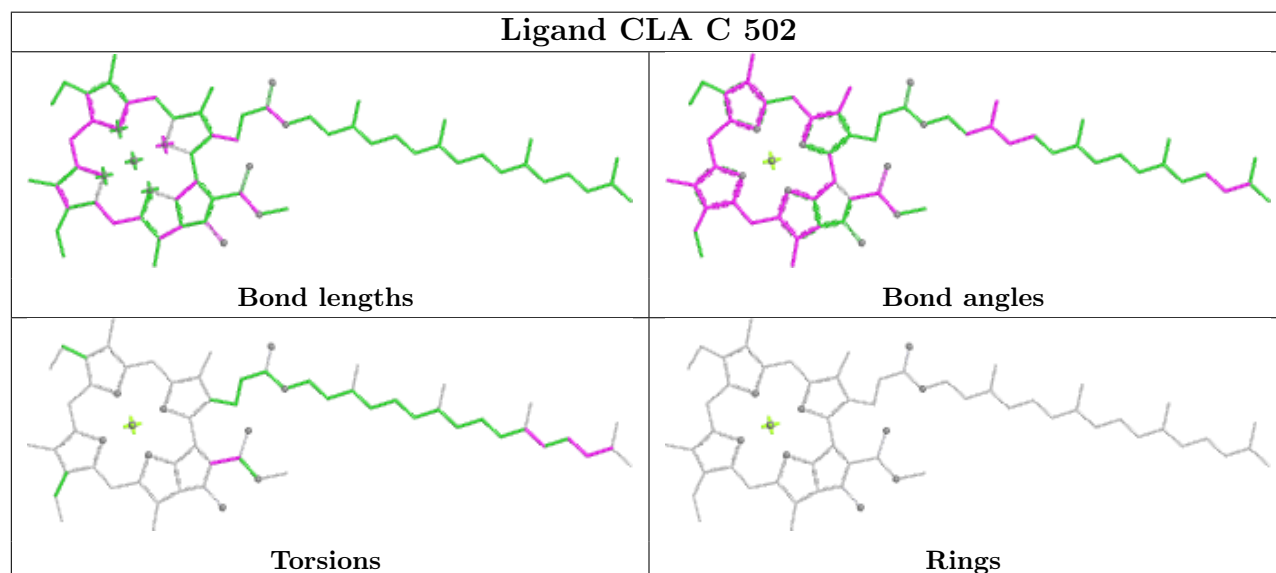
Ligand CLA A 406

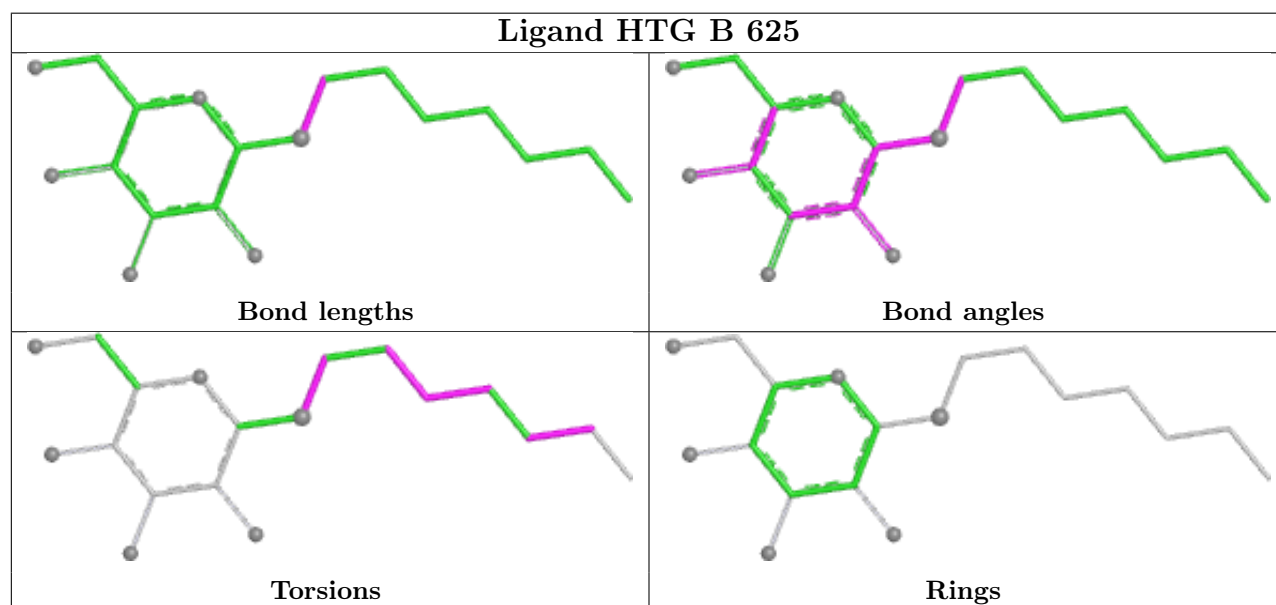
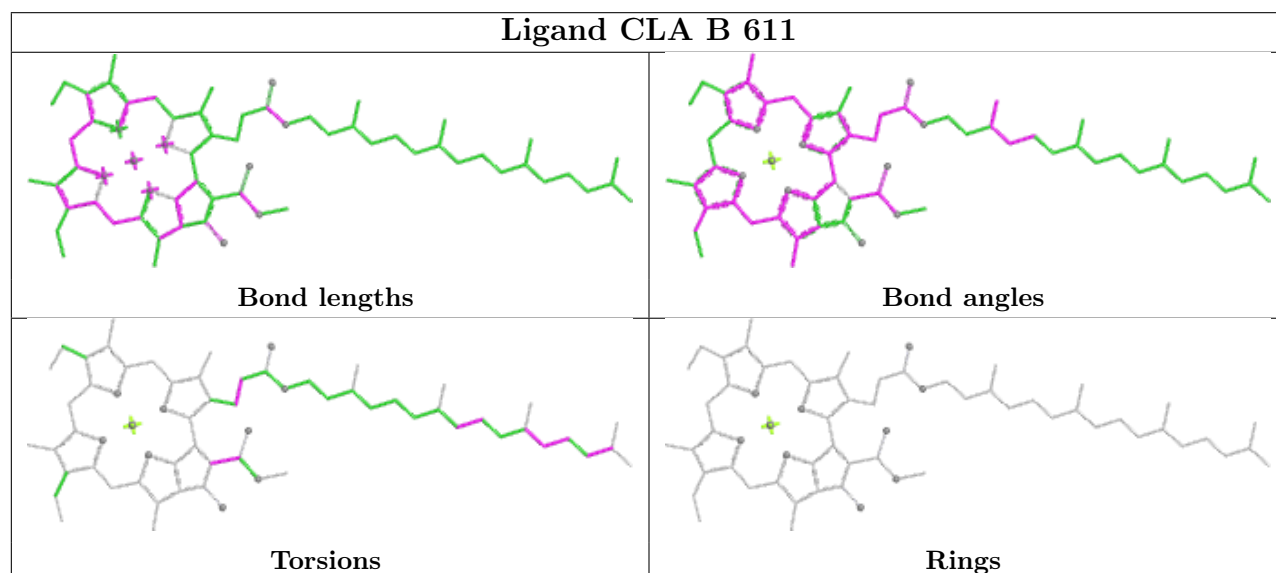
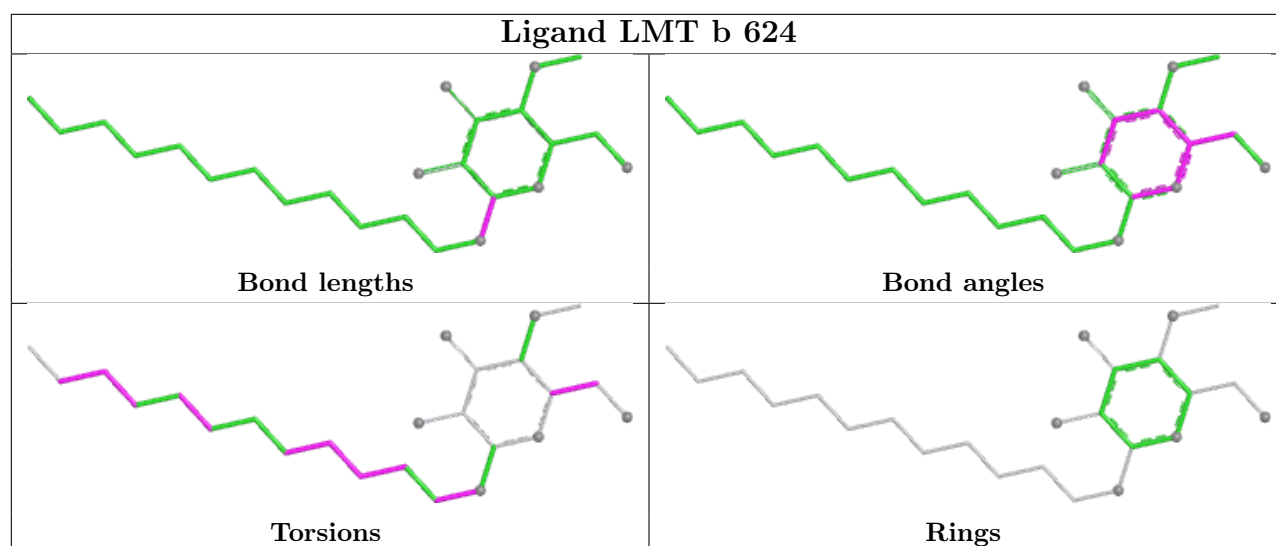


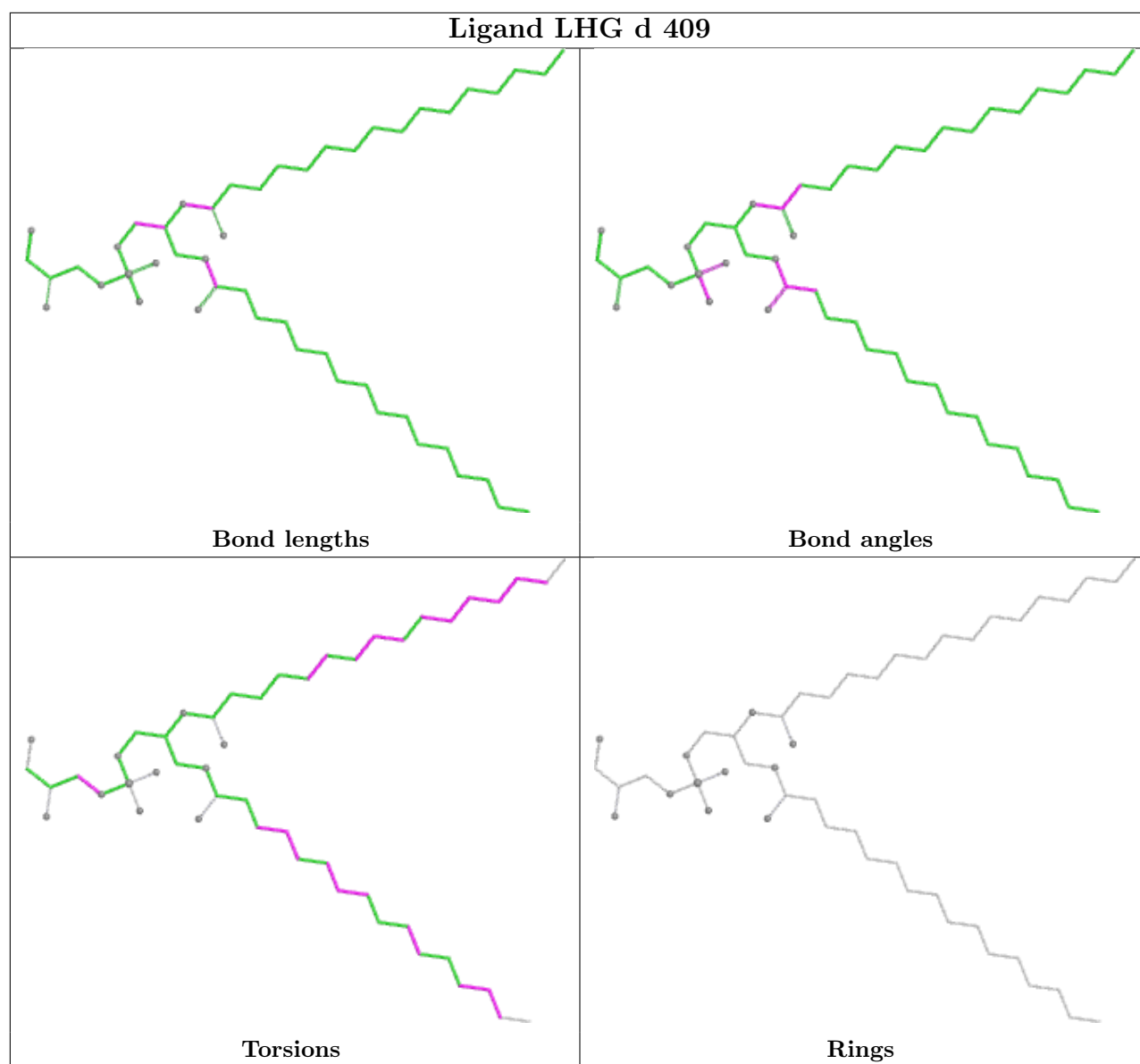
Ligand HTG b 601

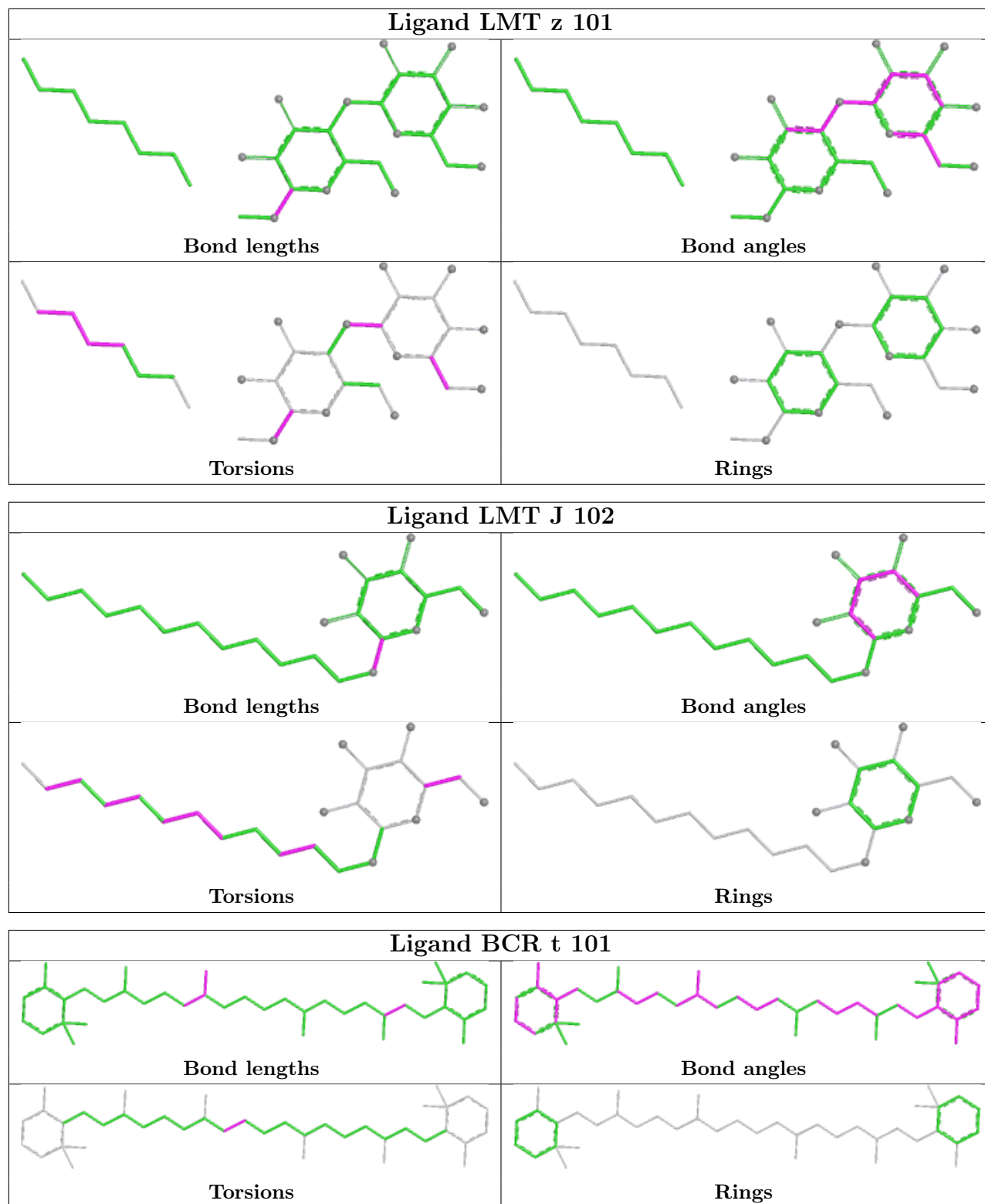


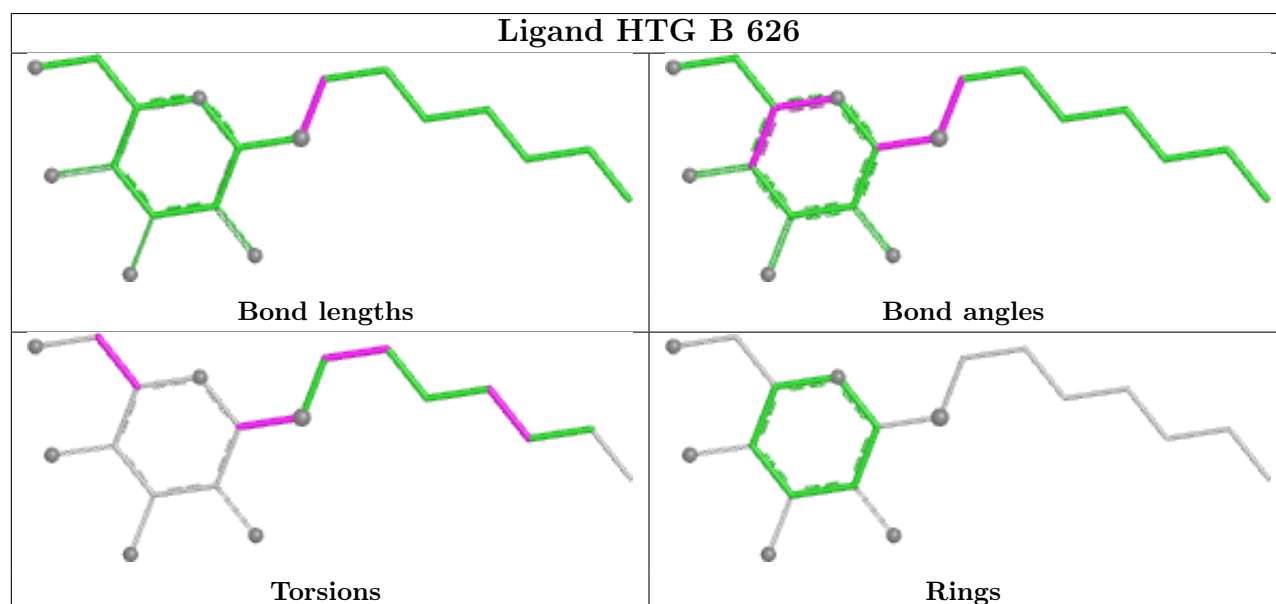
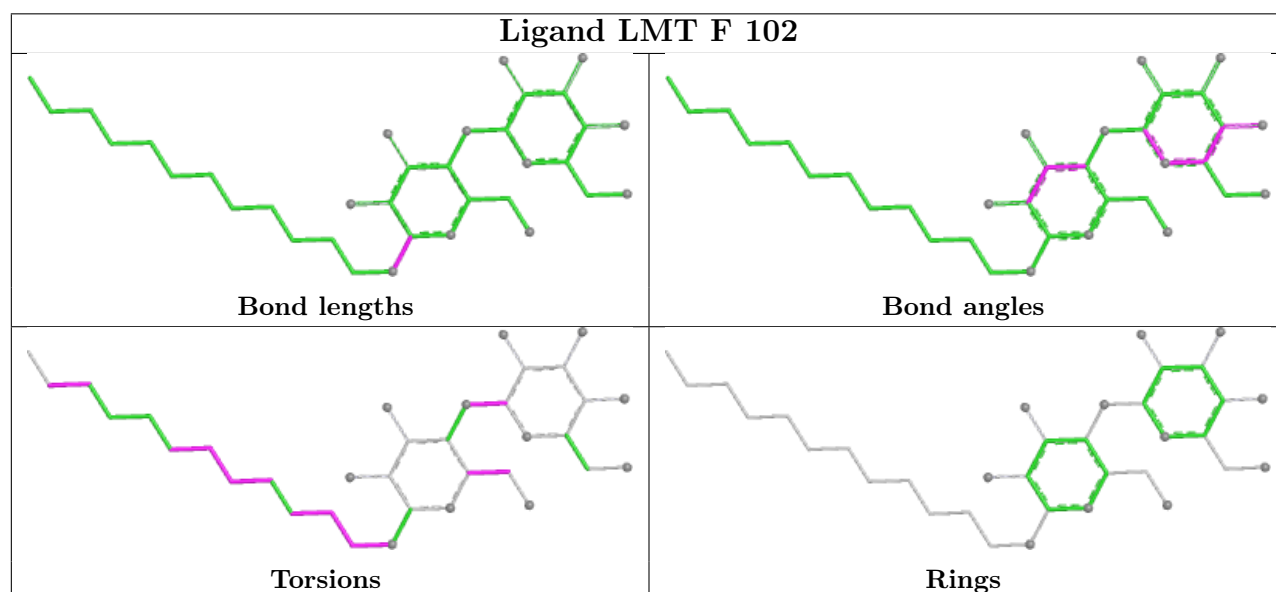
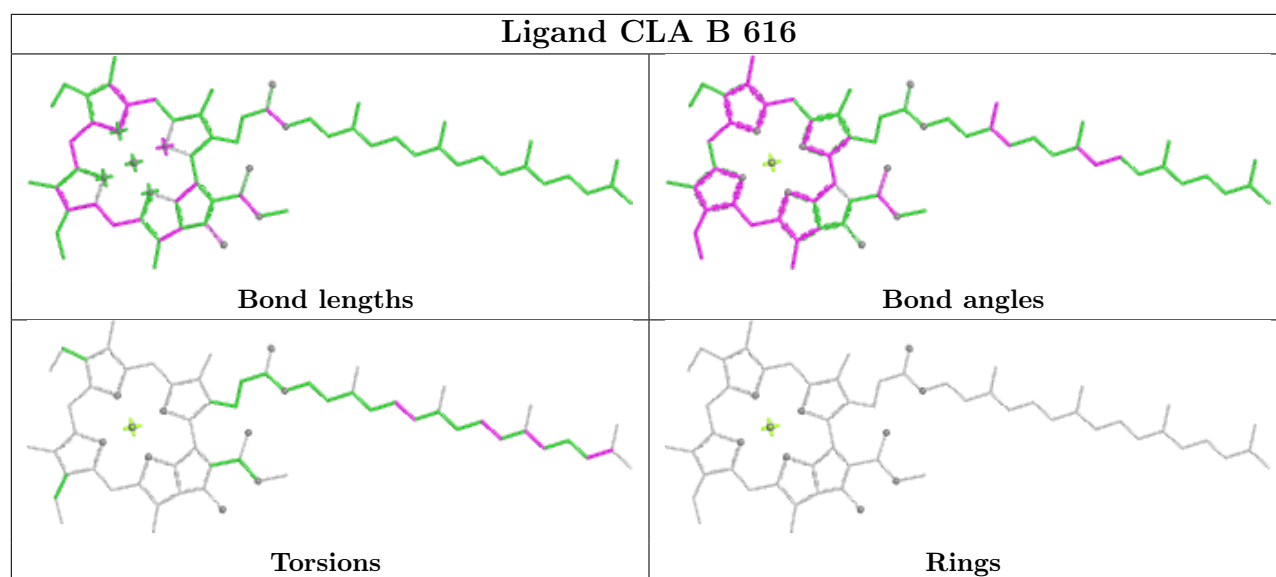
Ligand CLA C 502

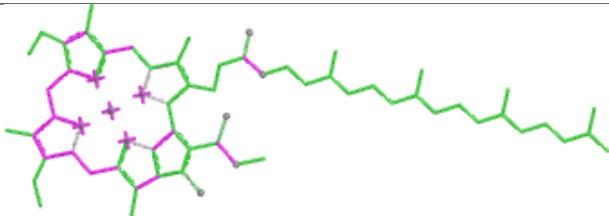
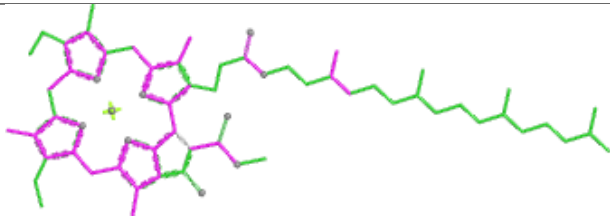
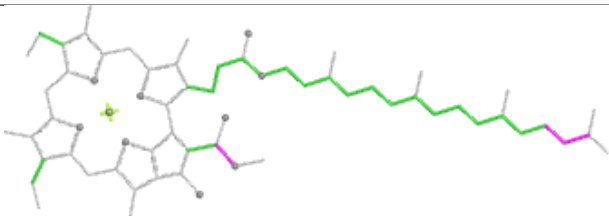
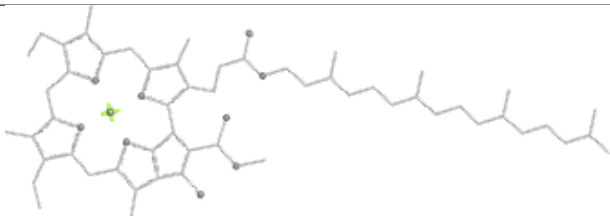


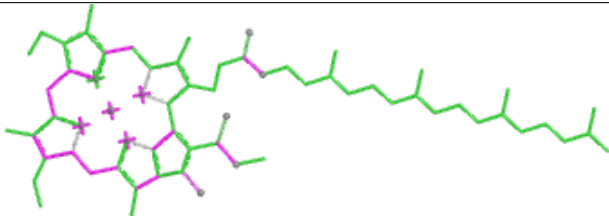
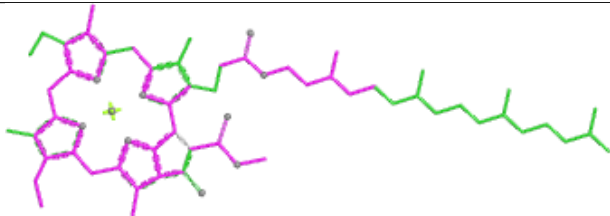
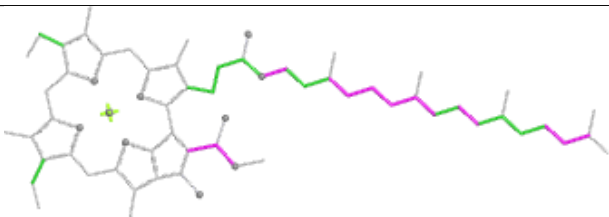
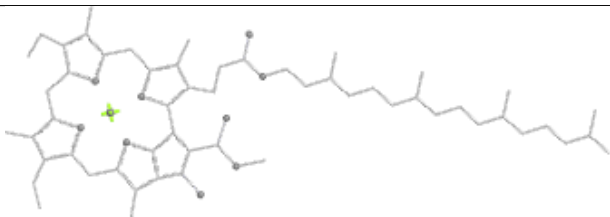


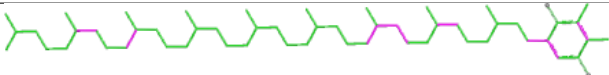
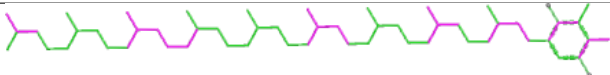
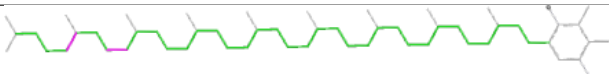


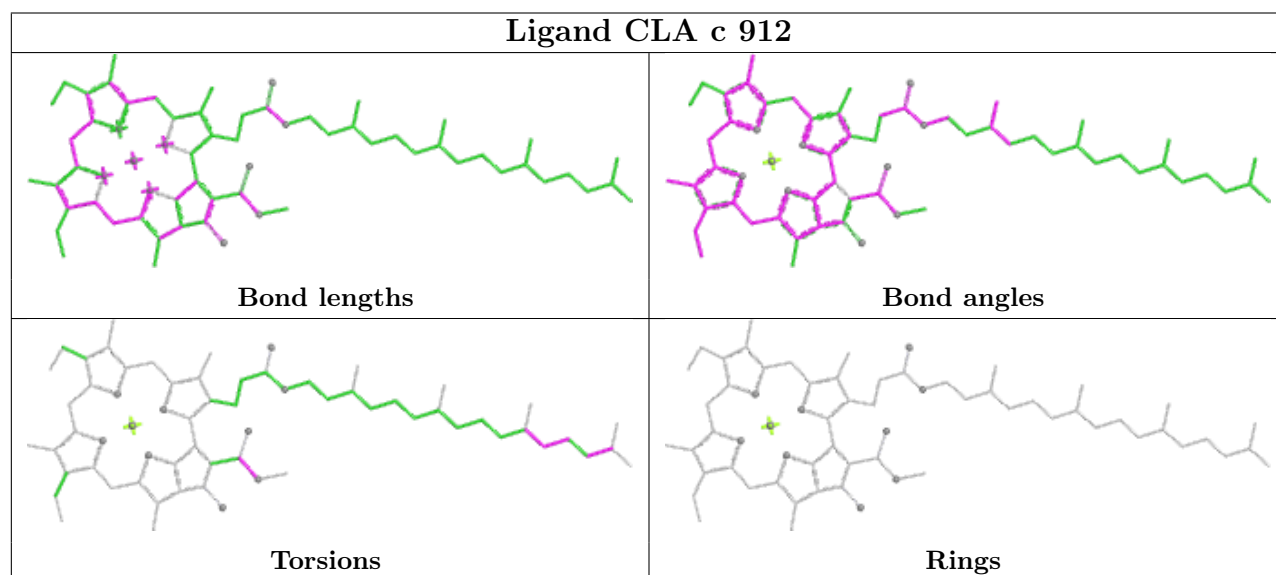
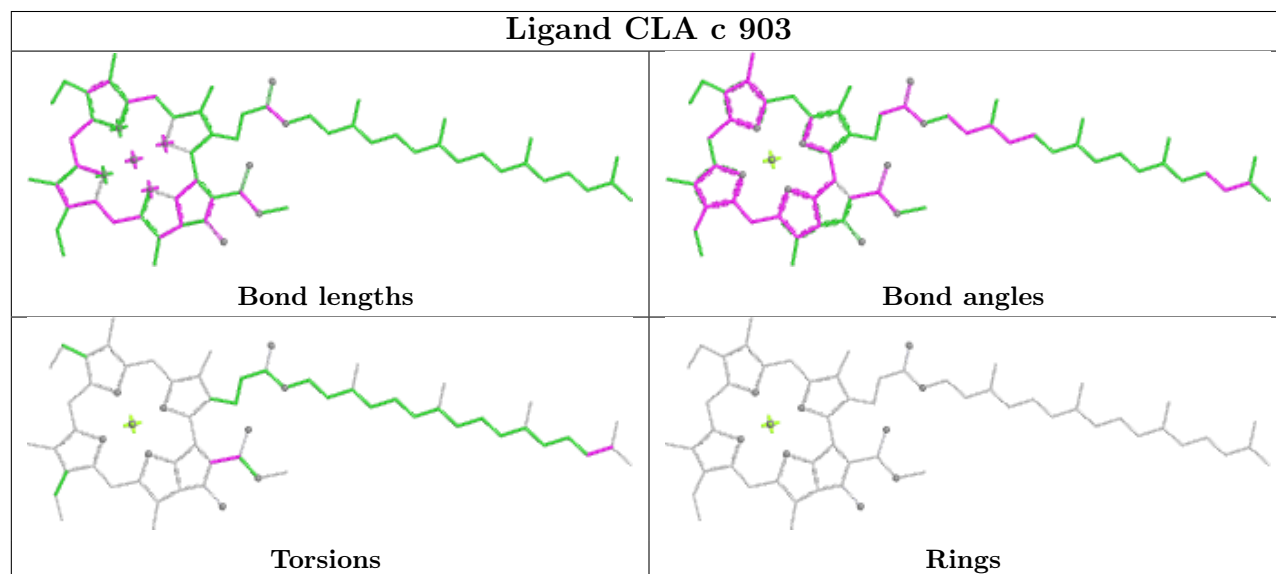
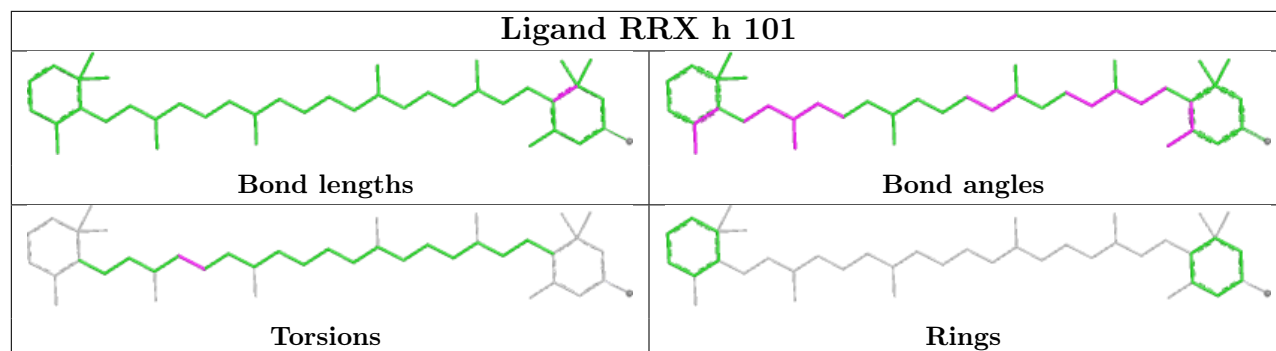


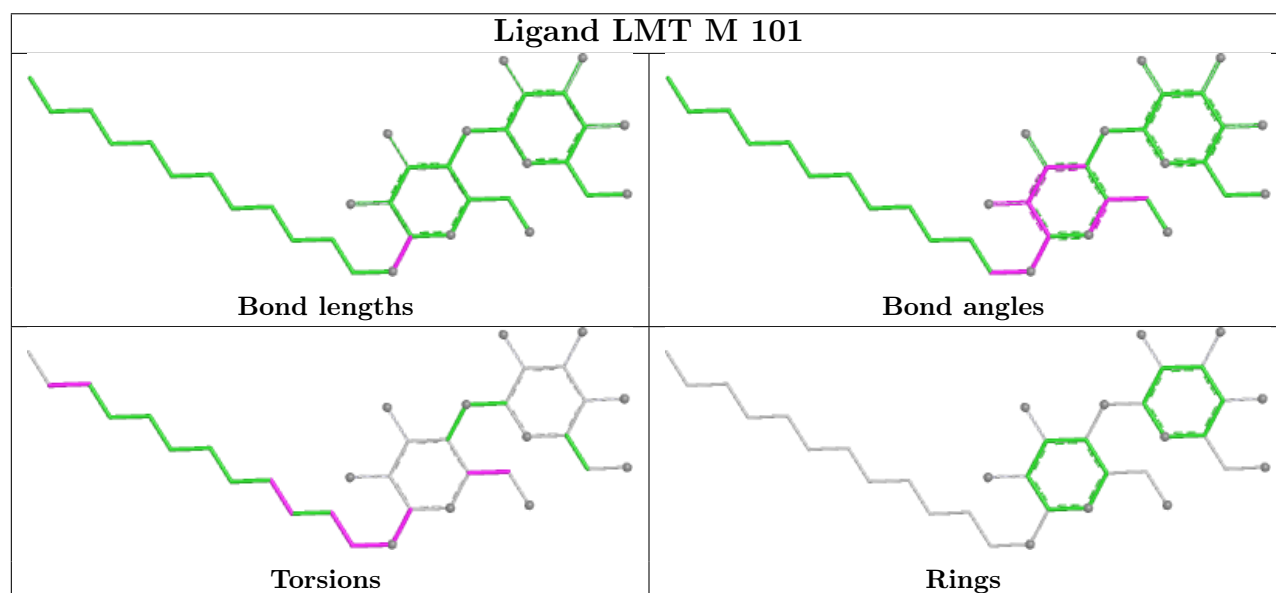
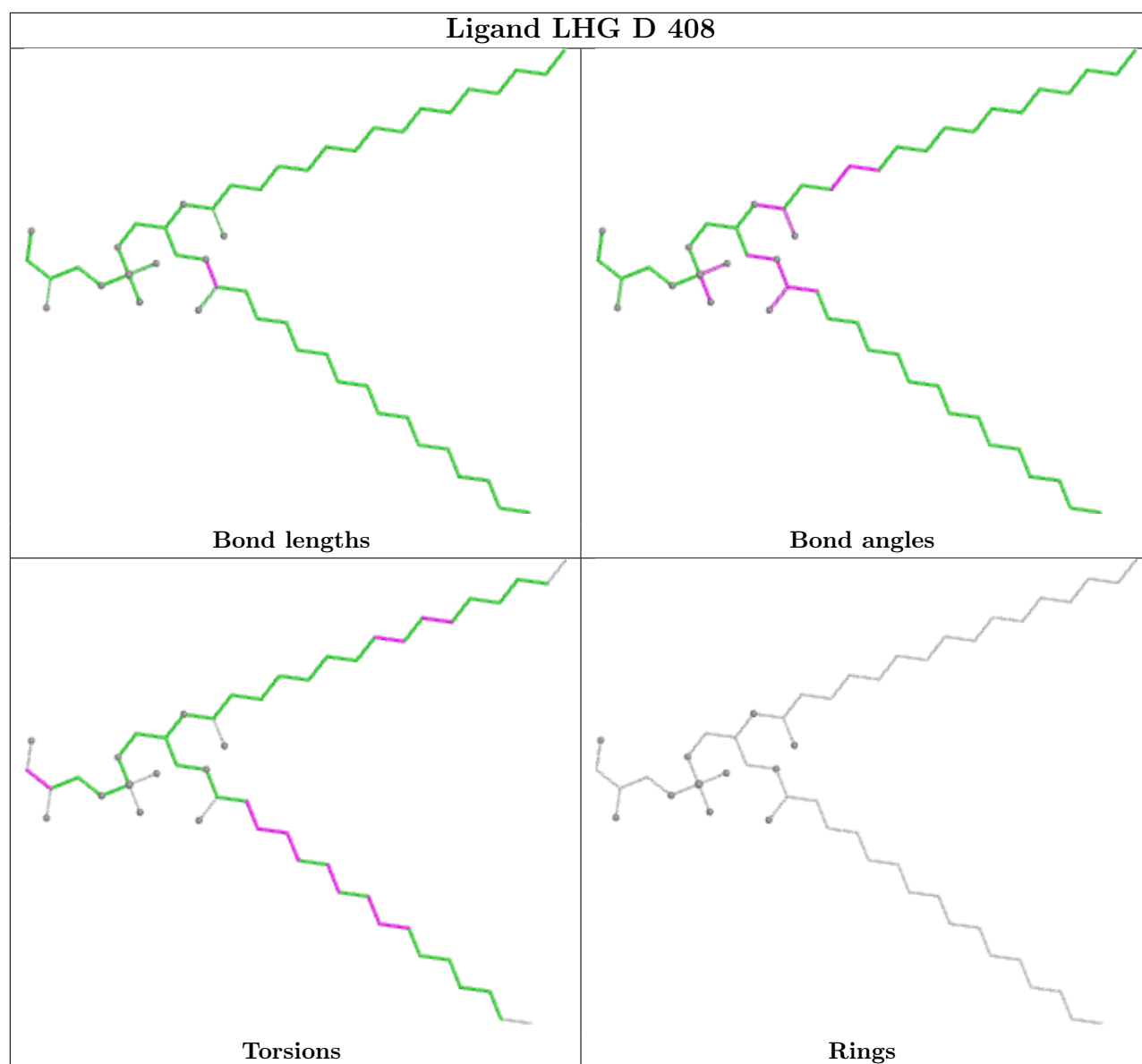


Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

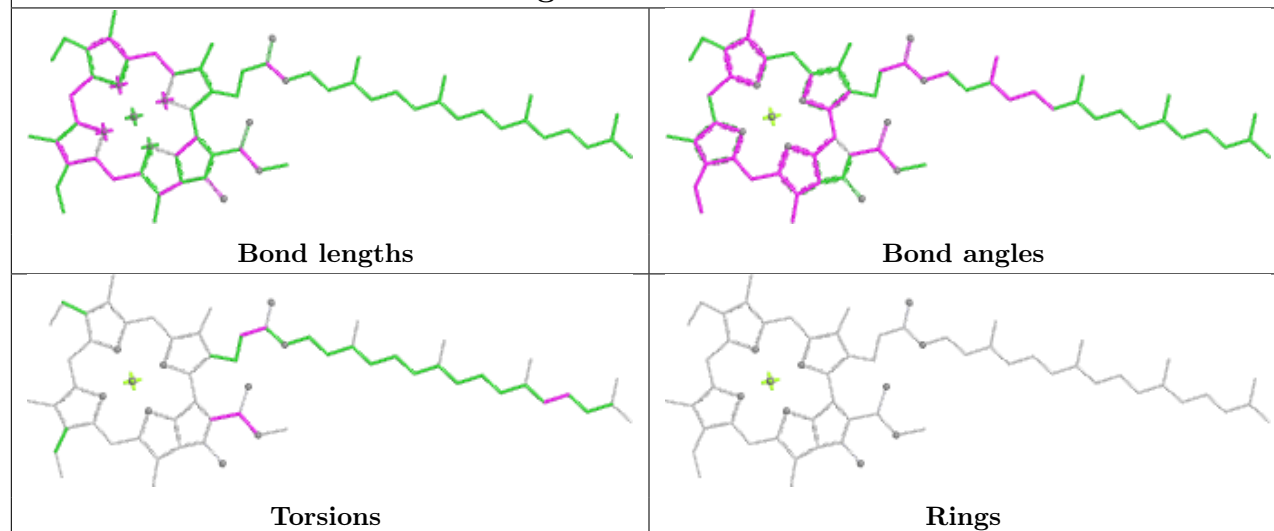
Ligand CLA b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

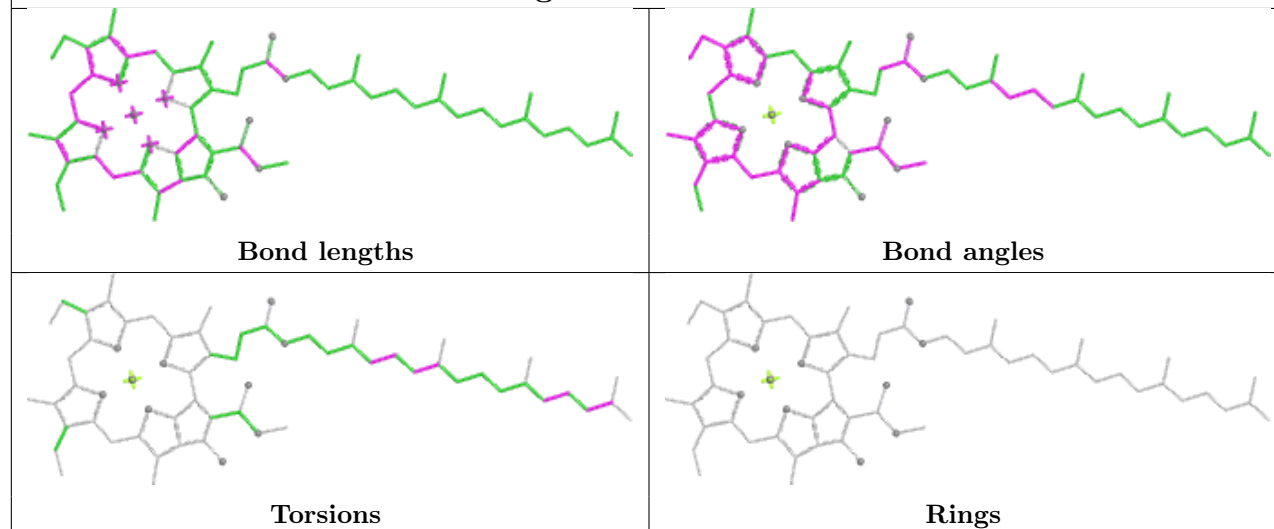




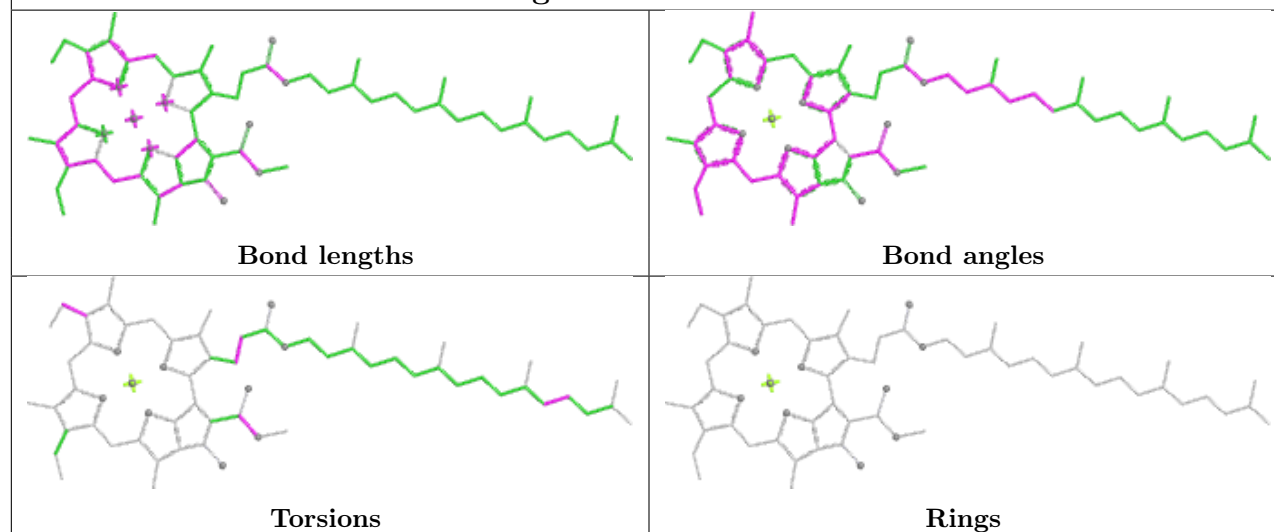
Ligand CLA c 902

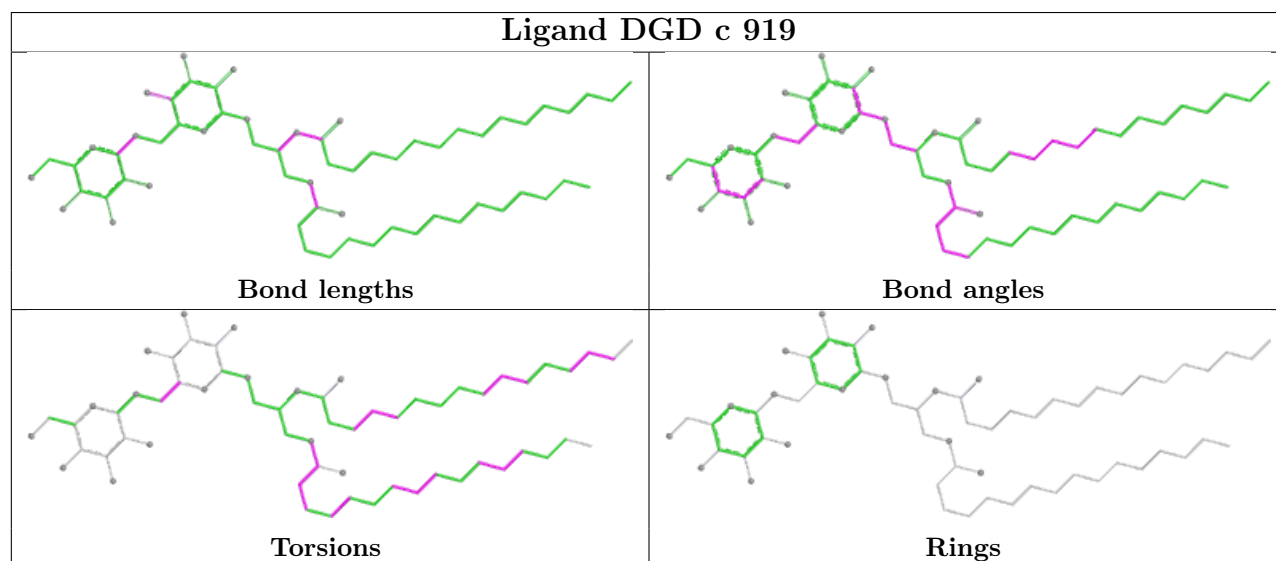
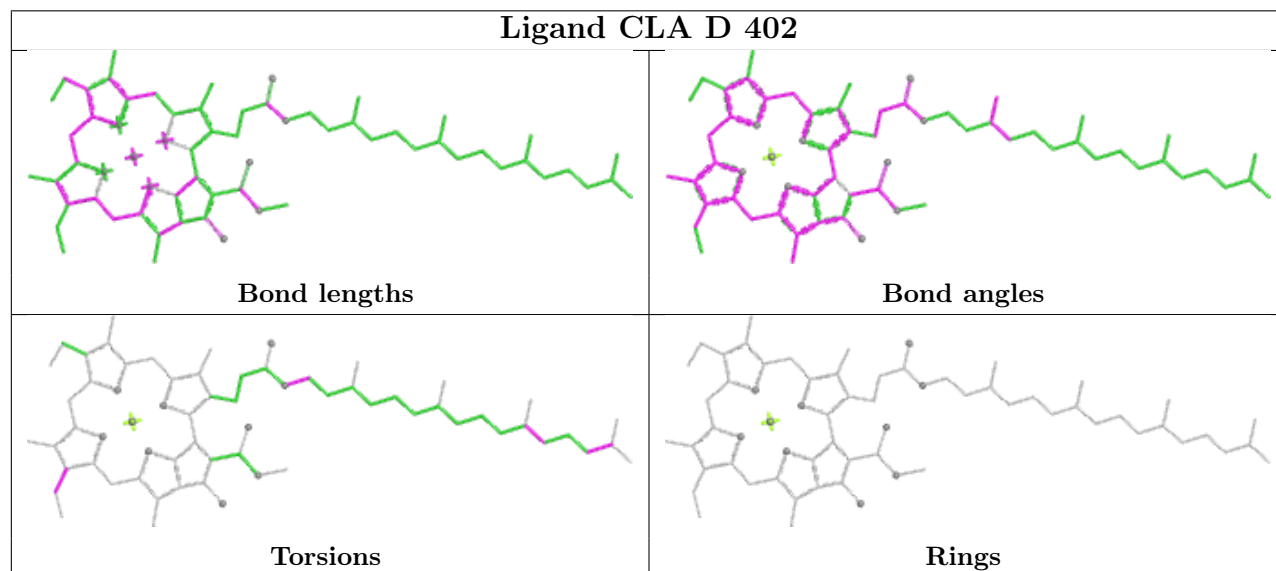
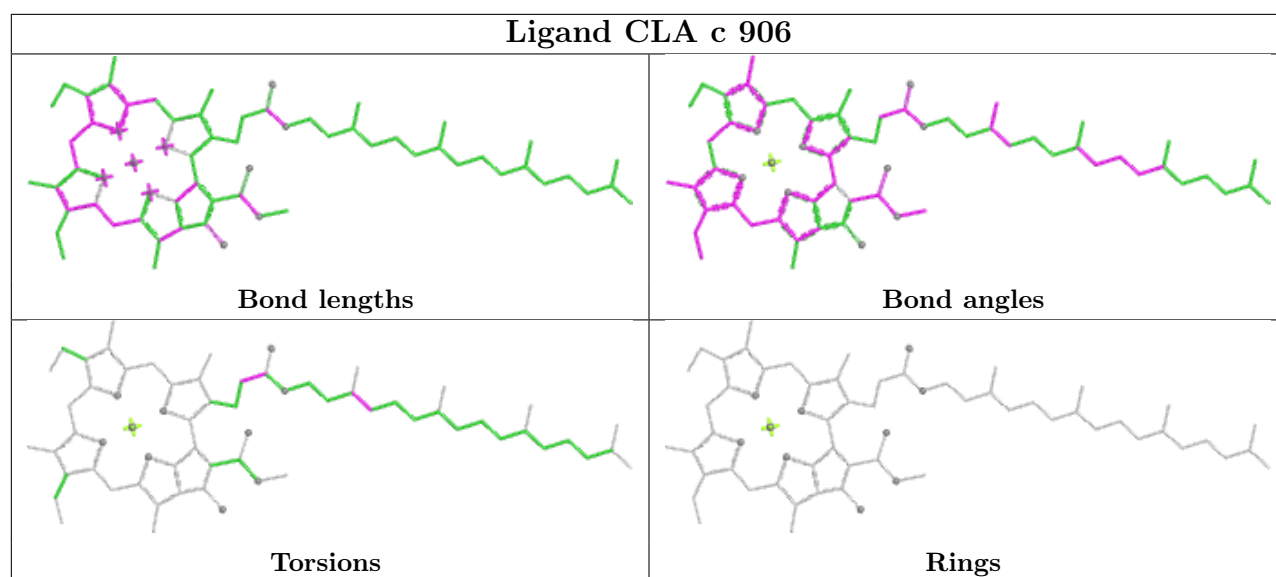


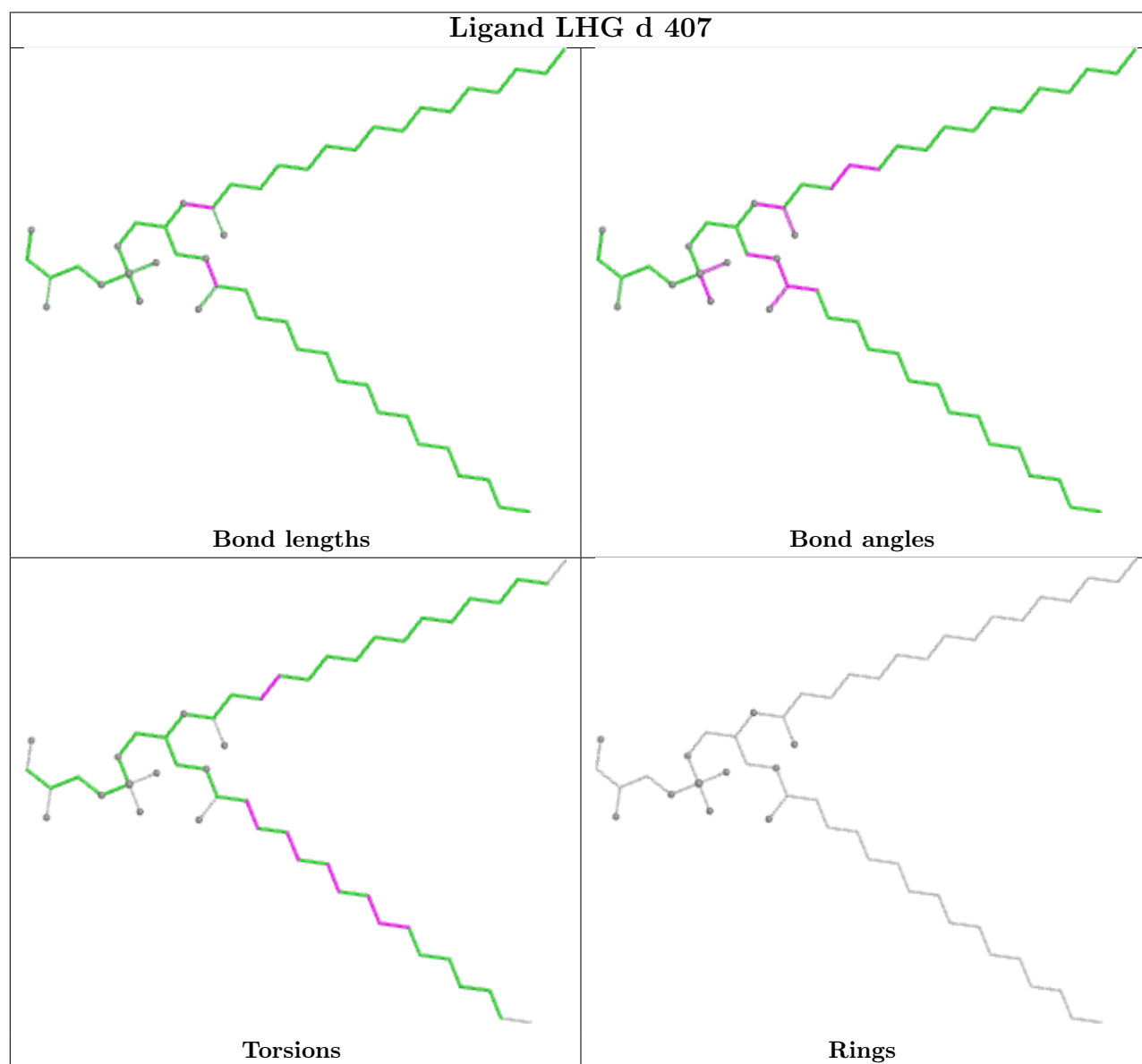
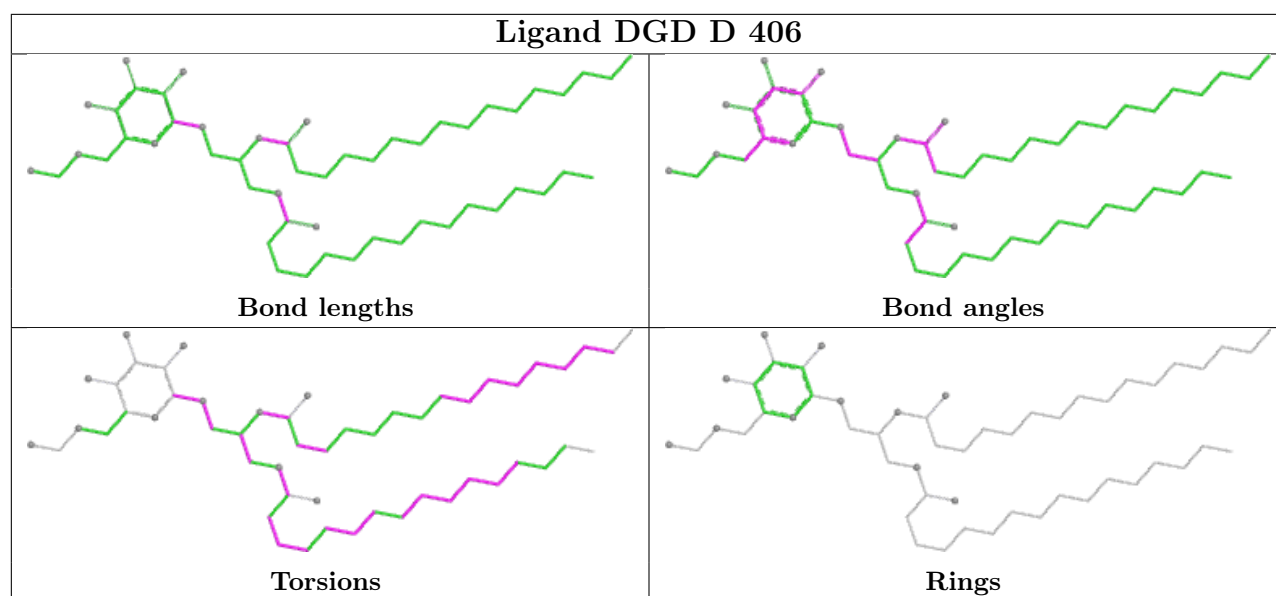
Ligand CLA b 607

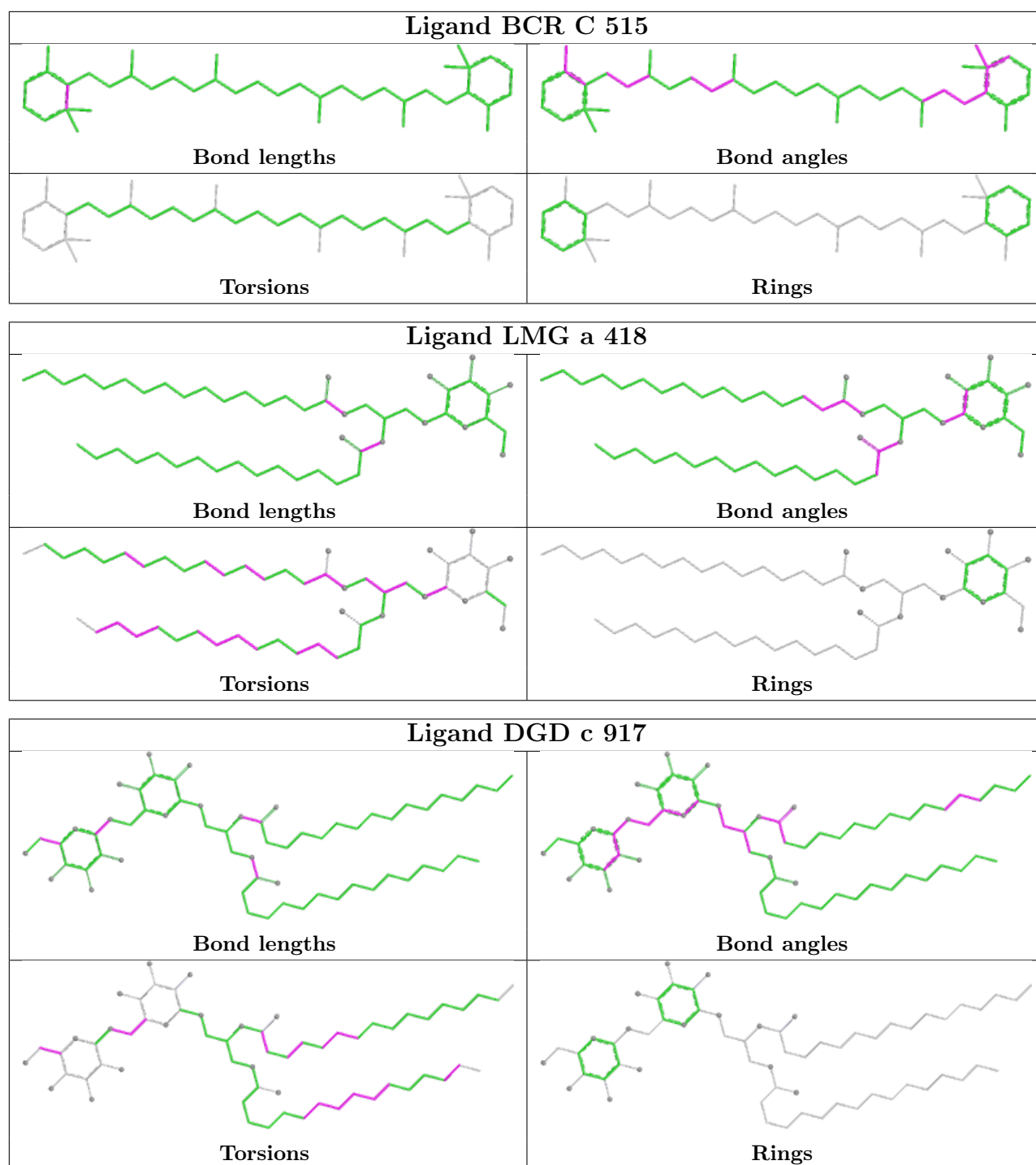


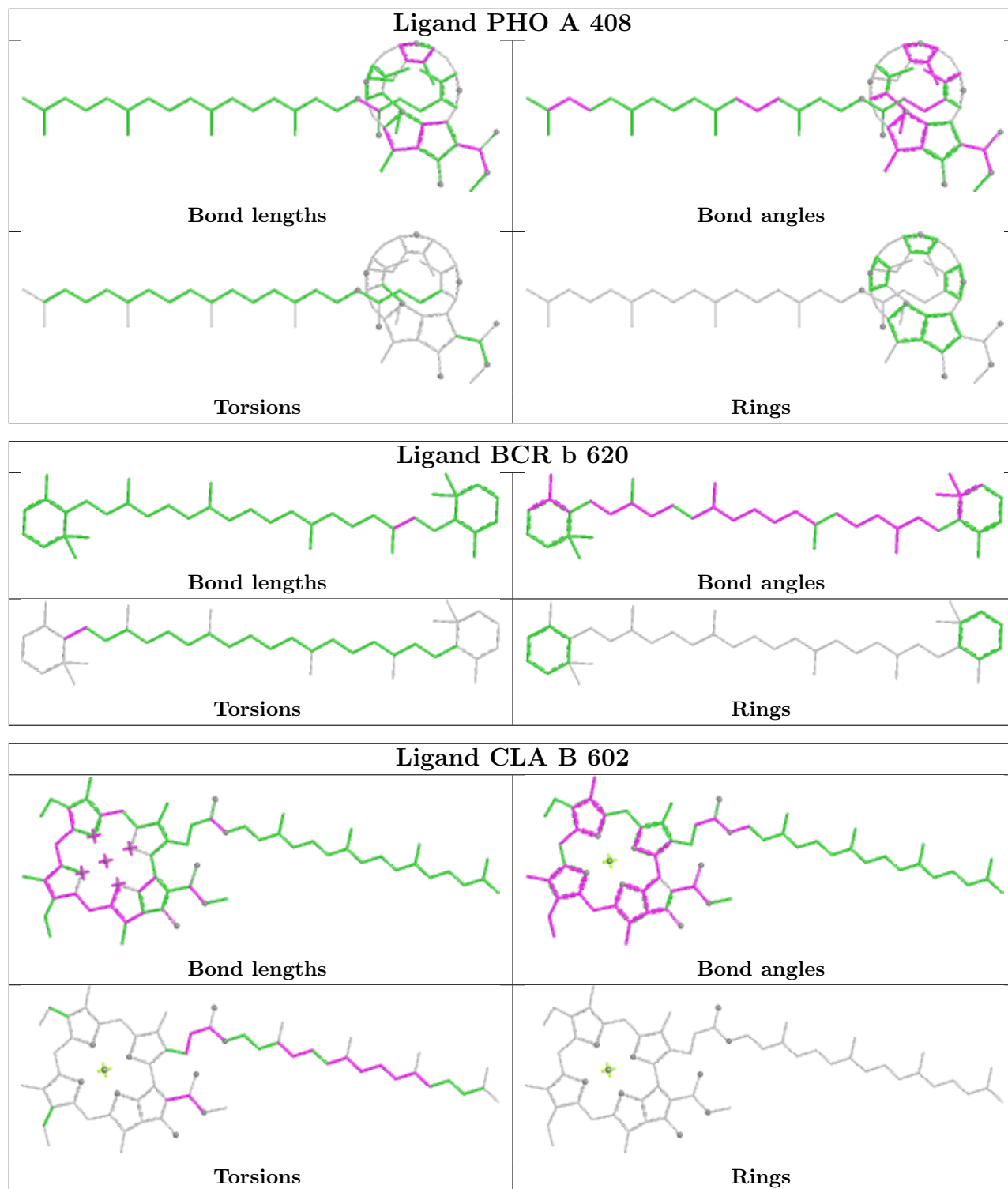
Ligand CLA C 501

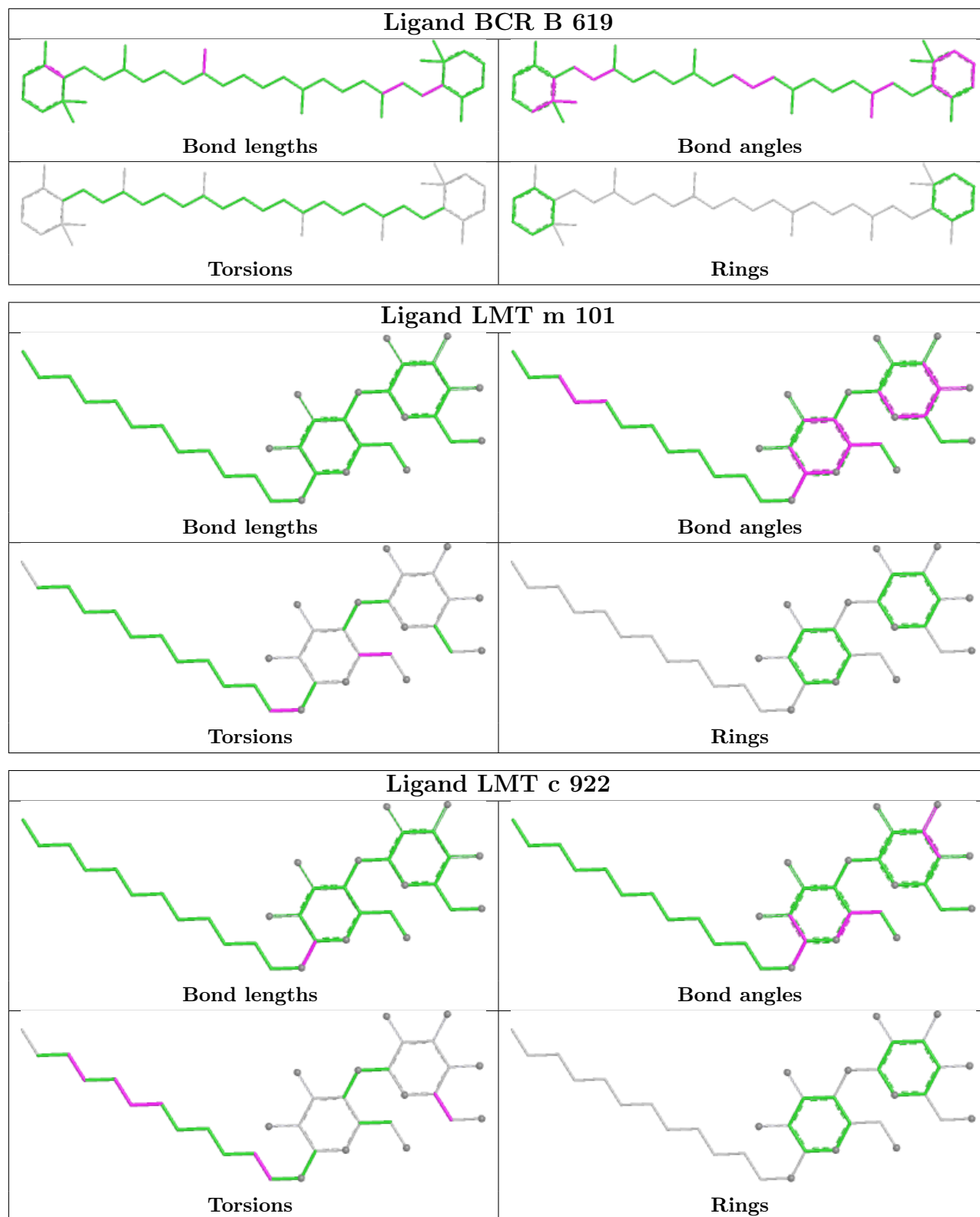


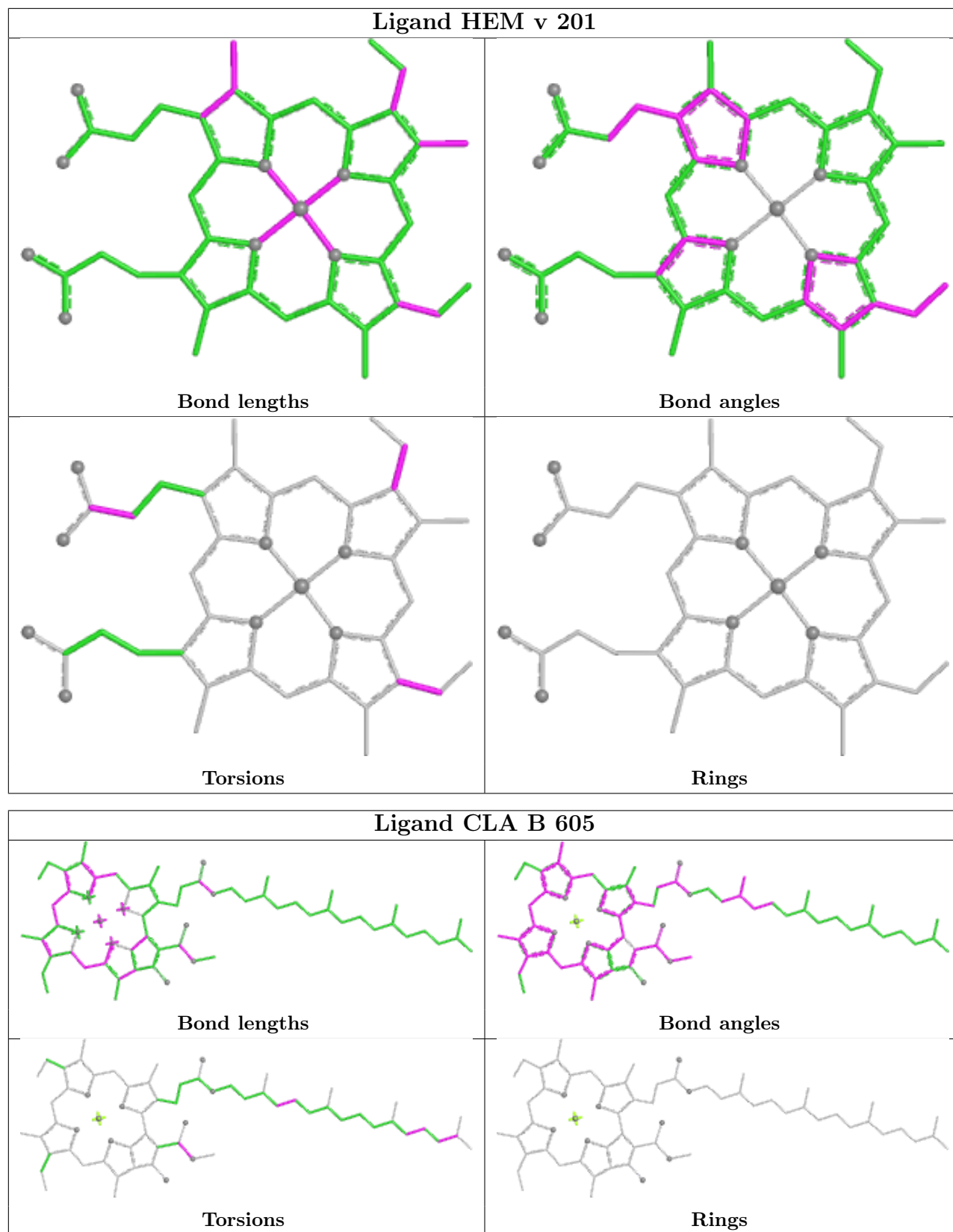


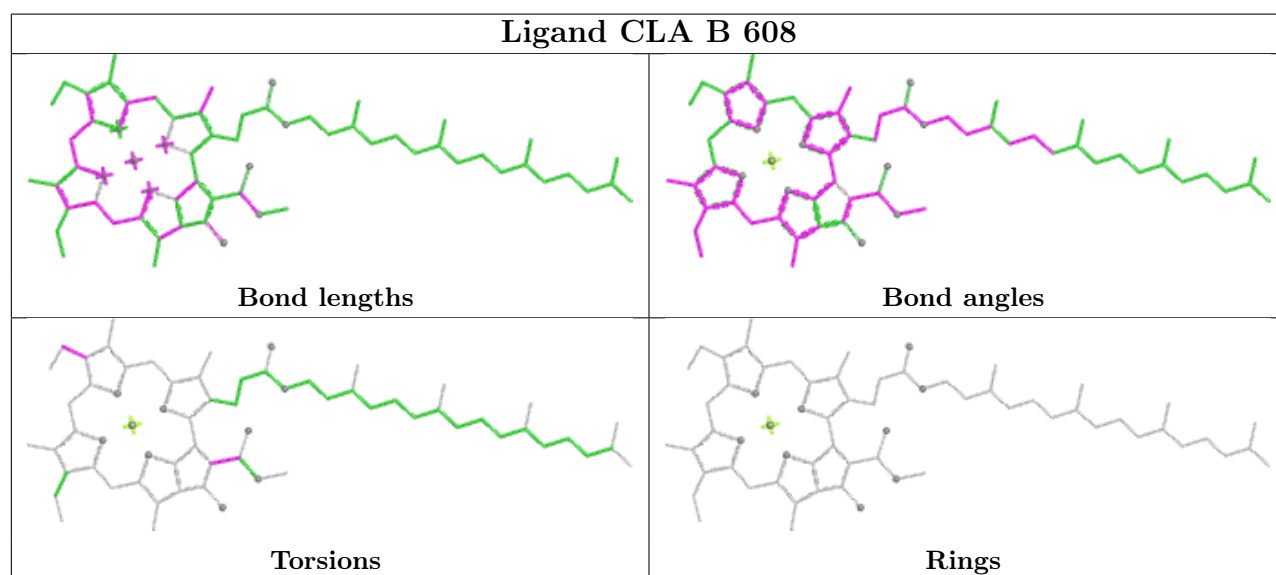
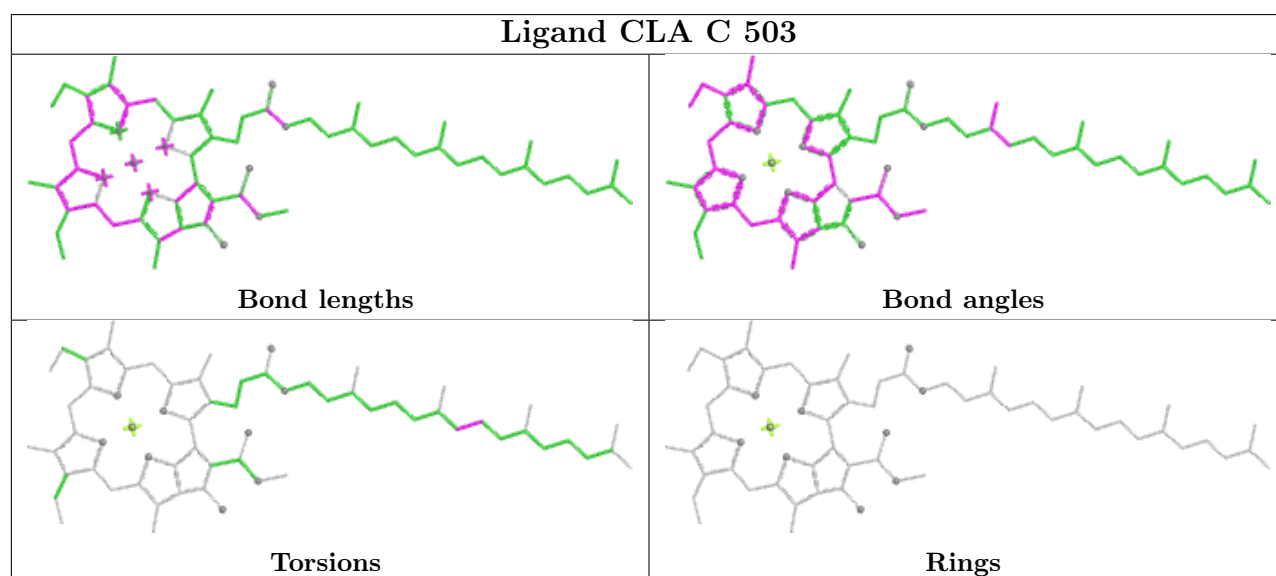
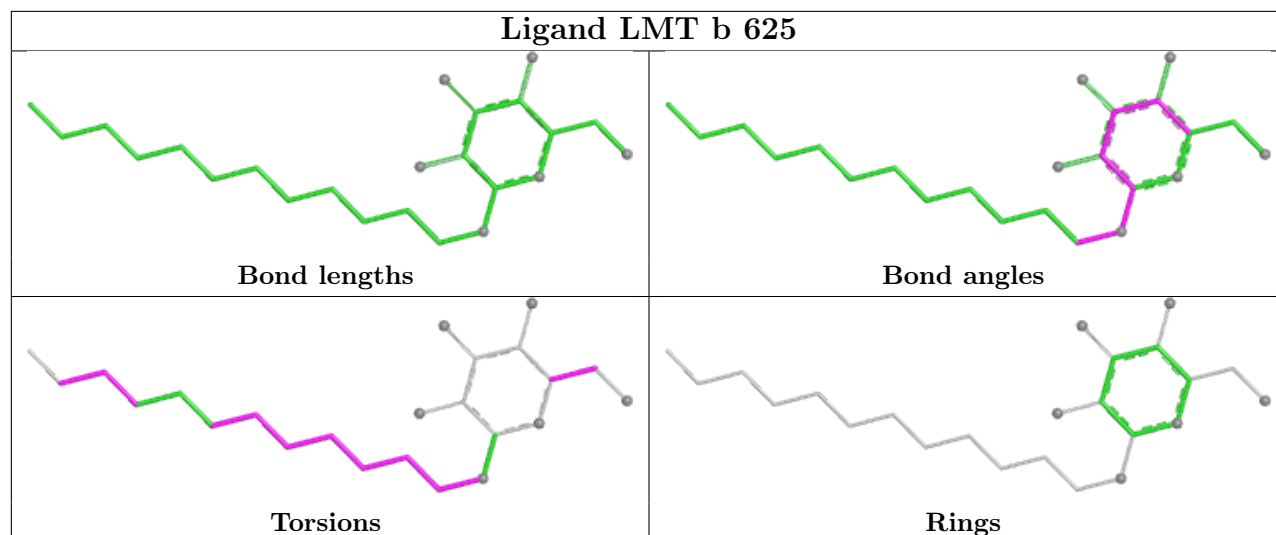


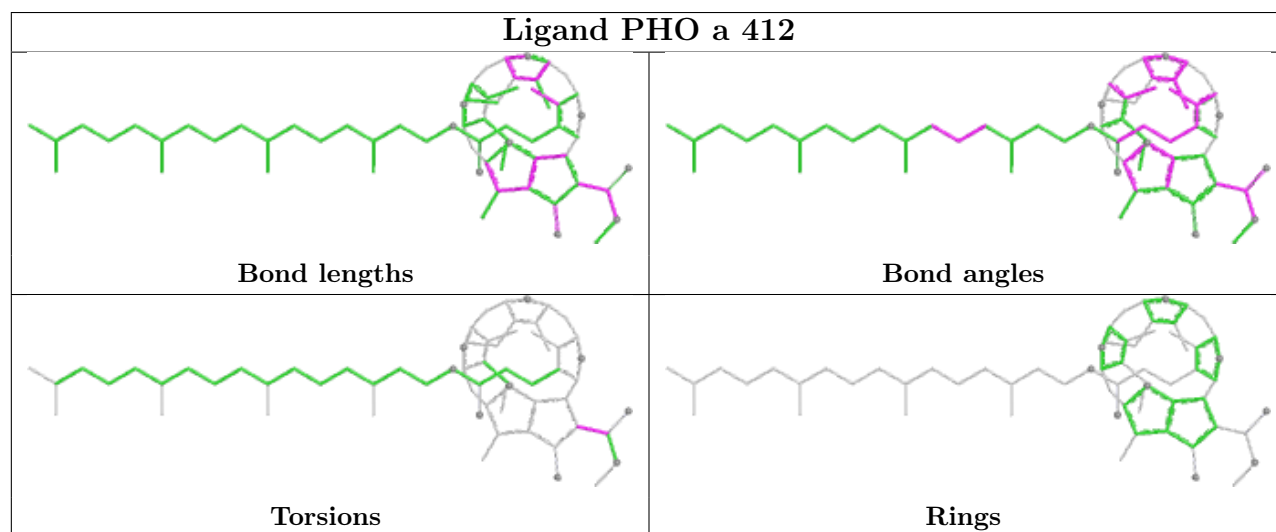
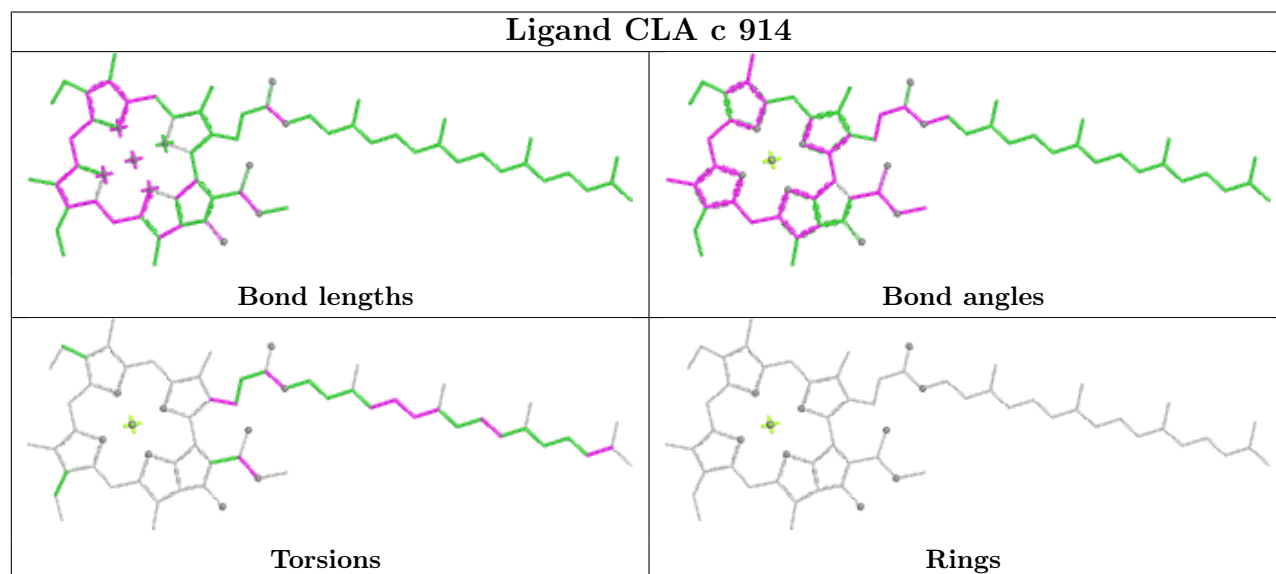
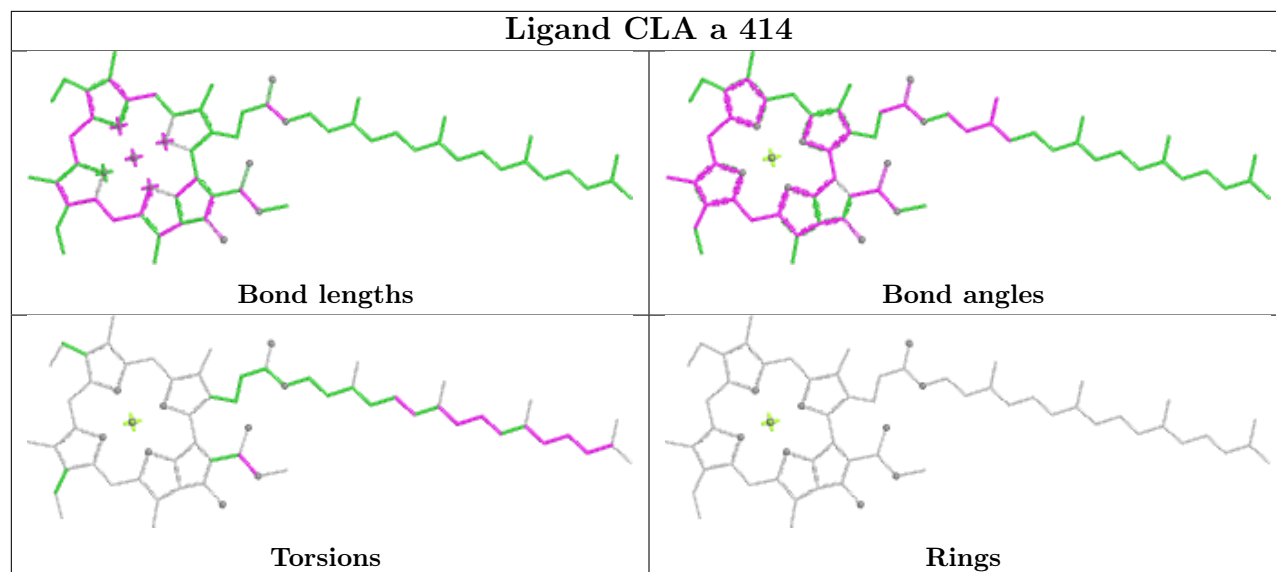


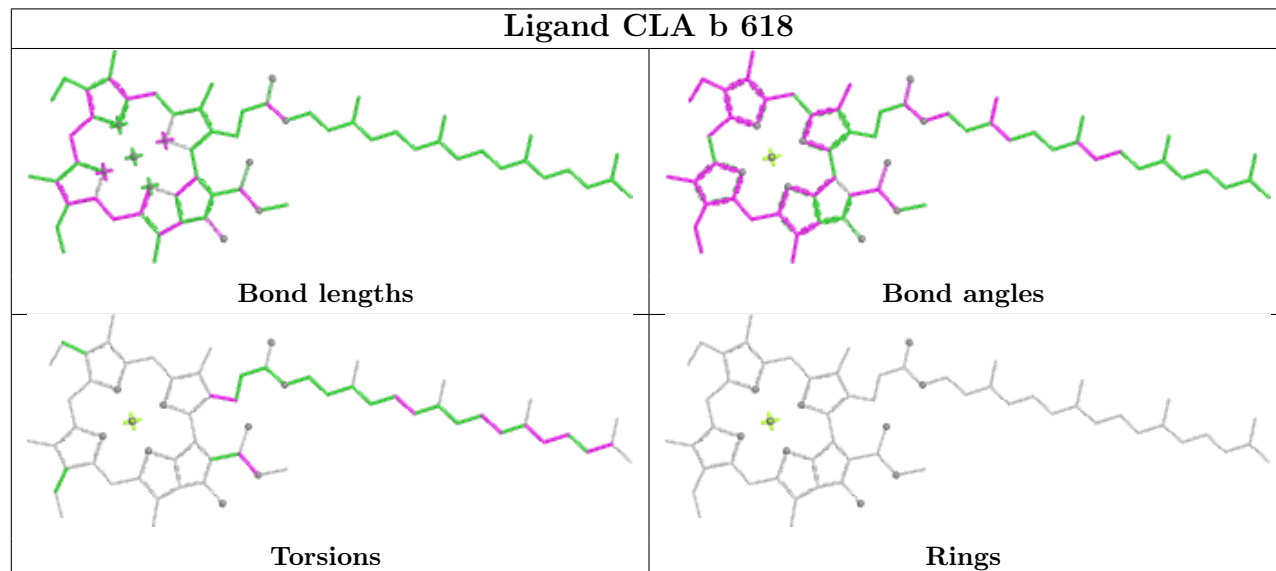
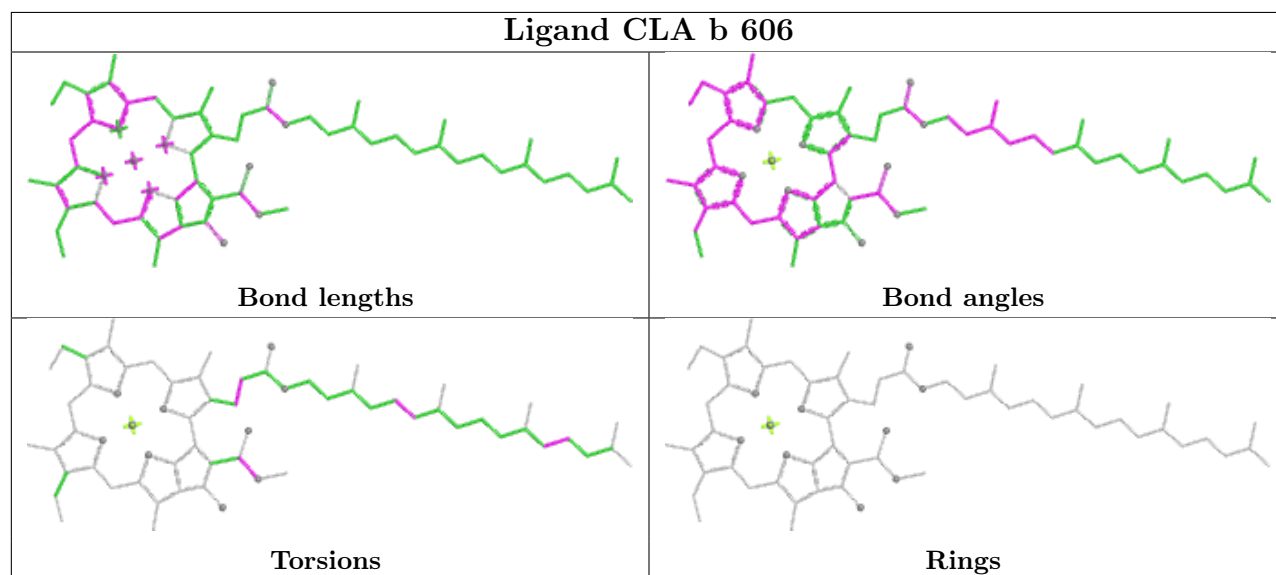
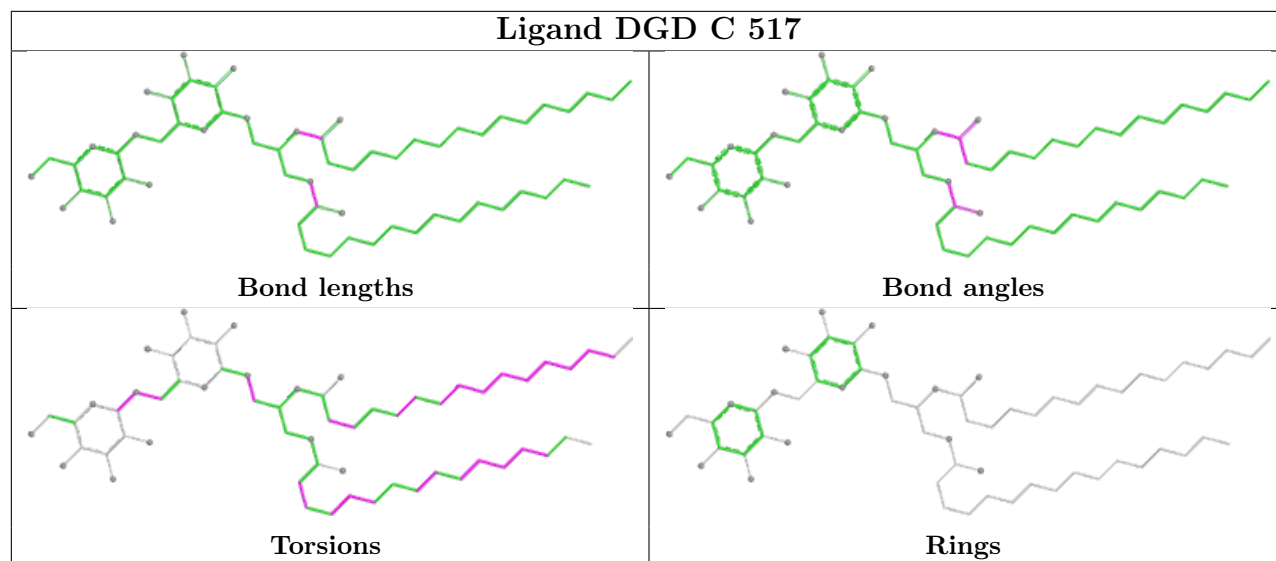


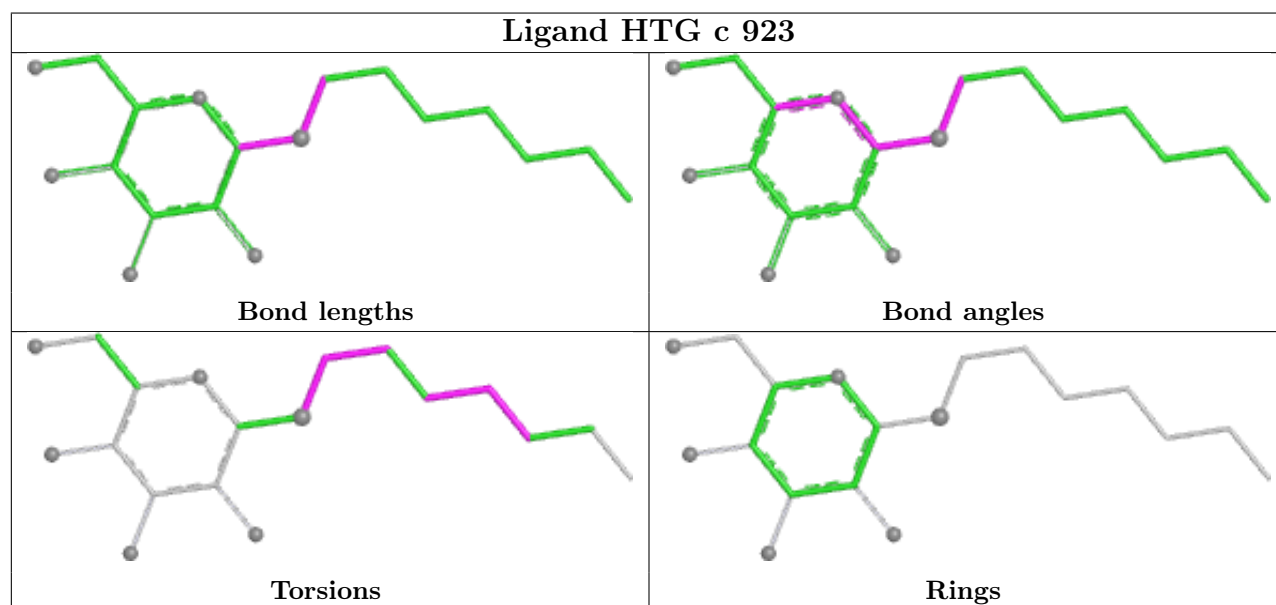
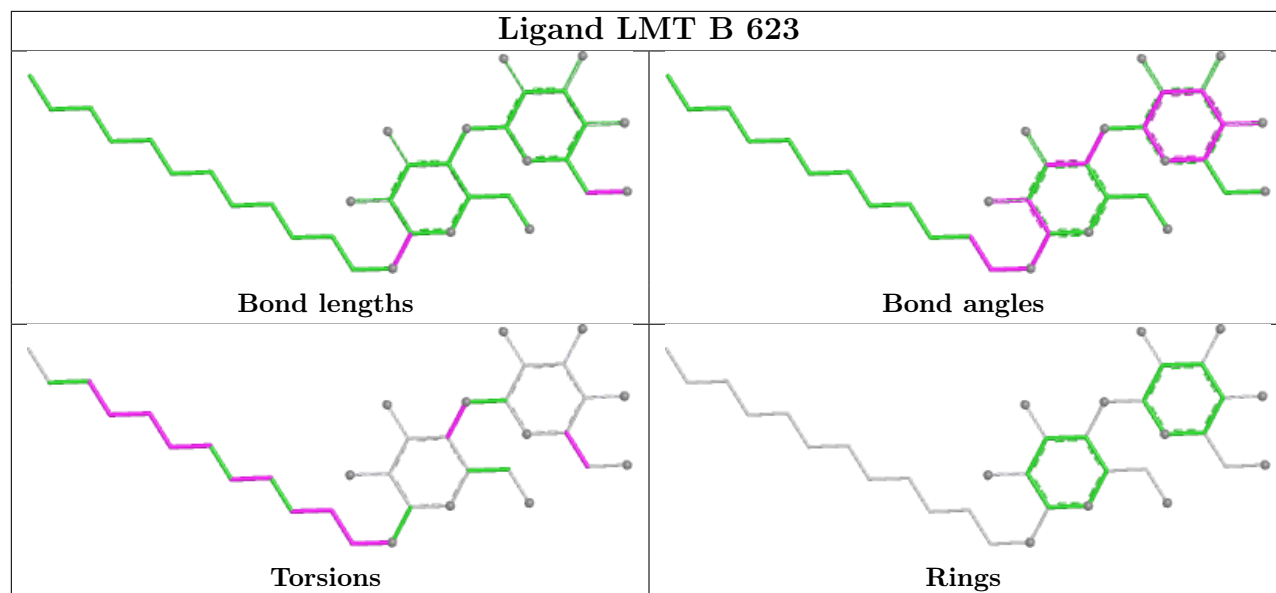


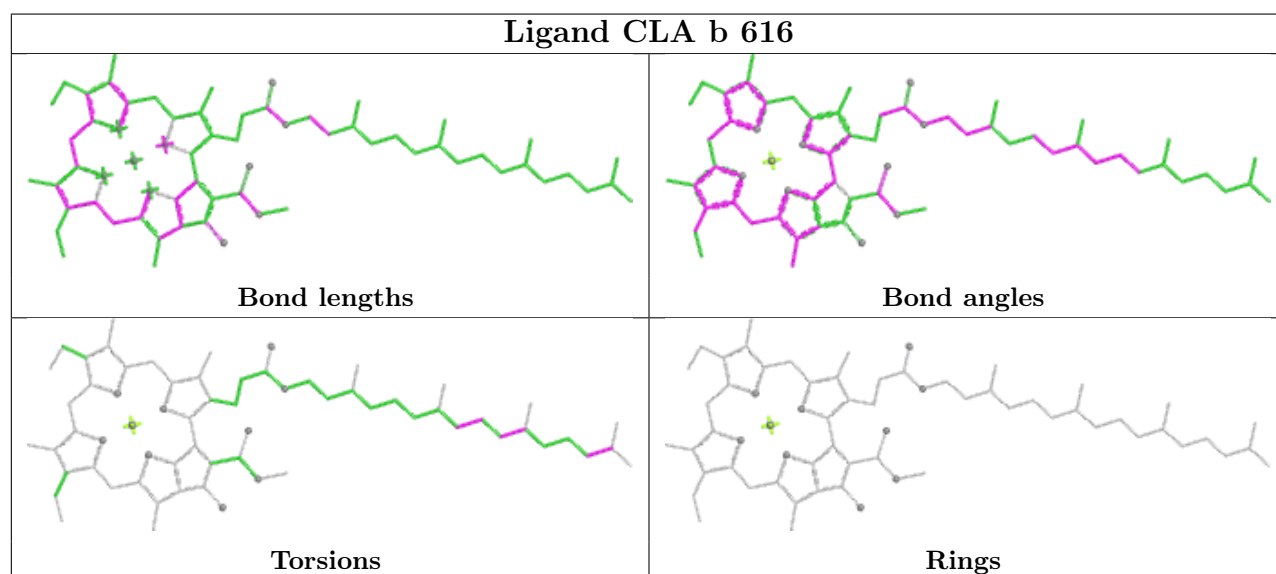
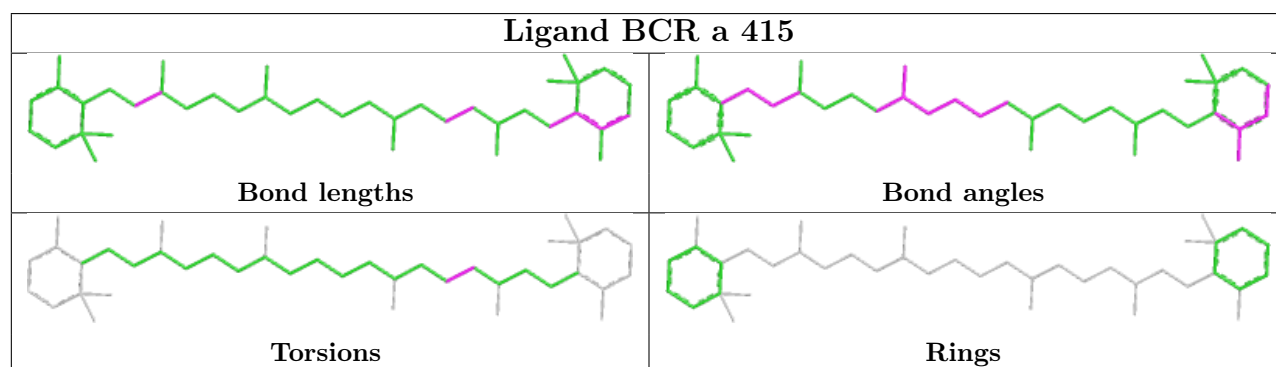
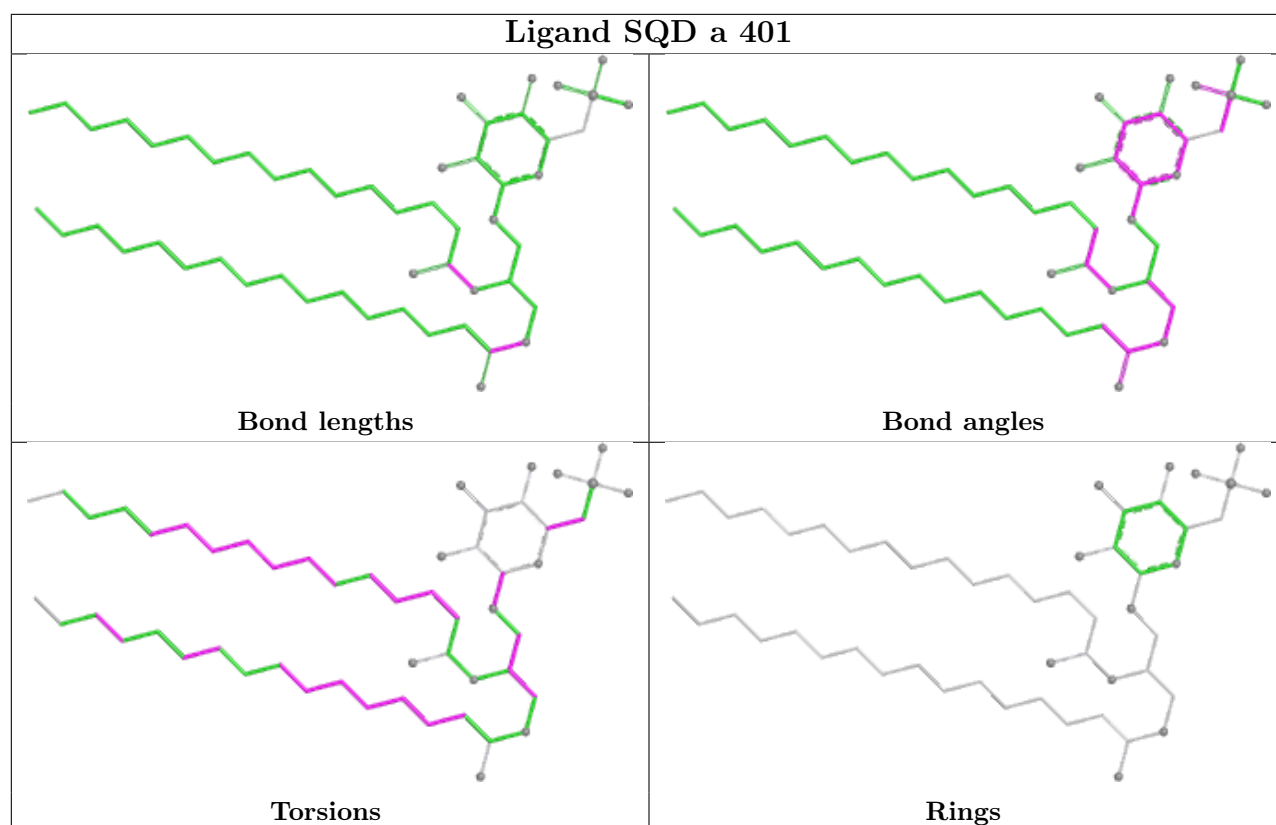


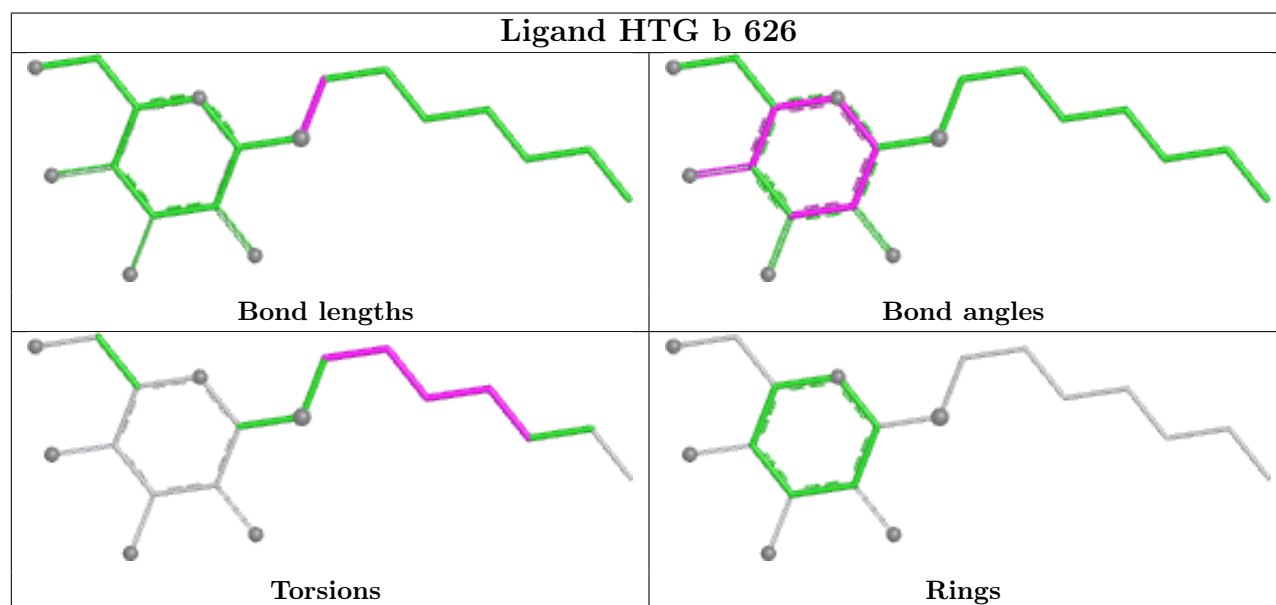
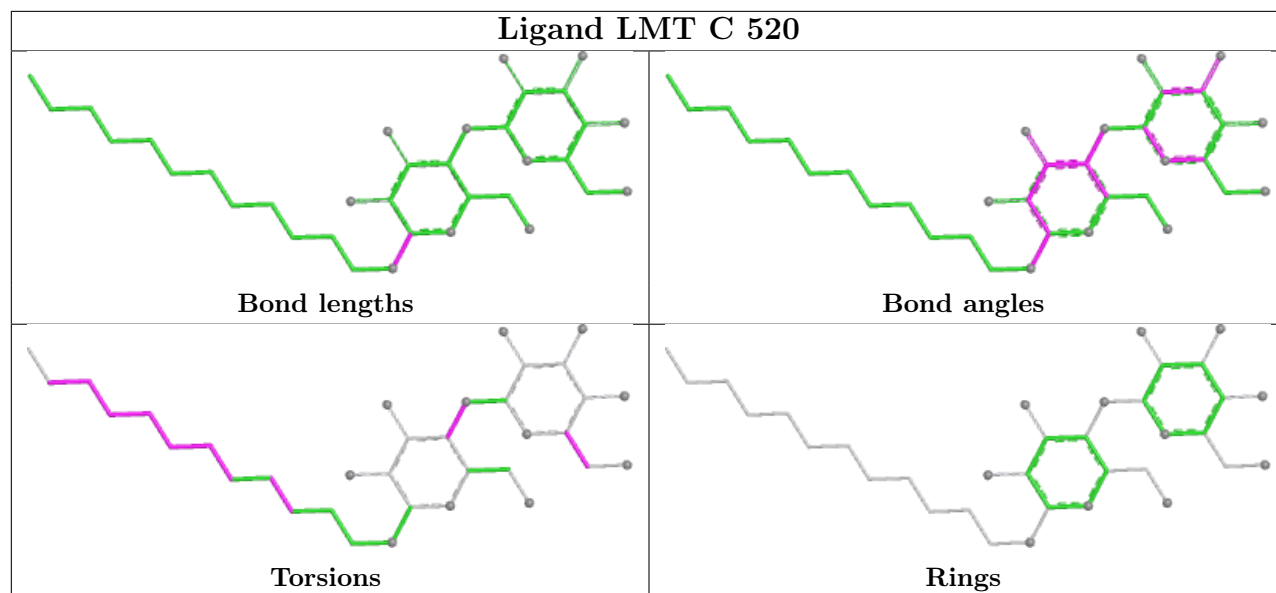


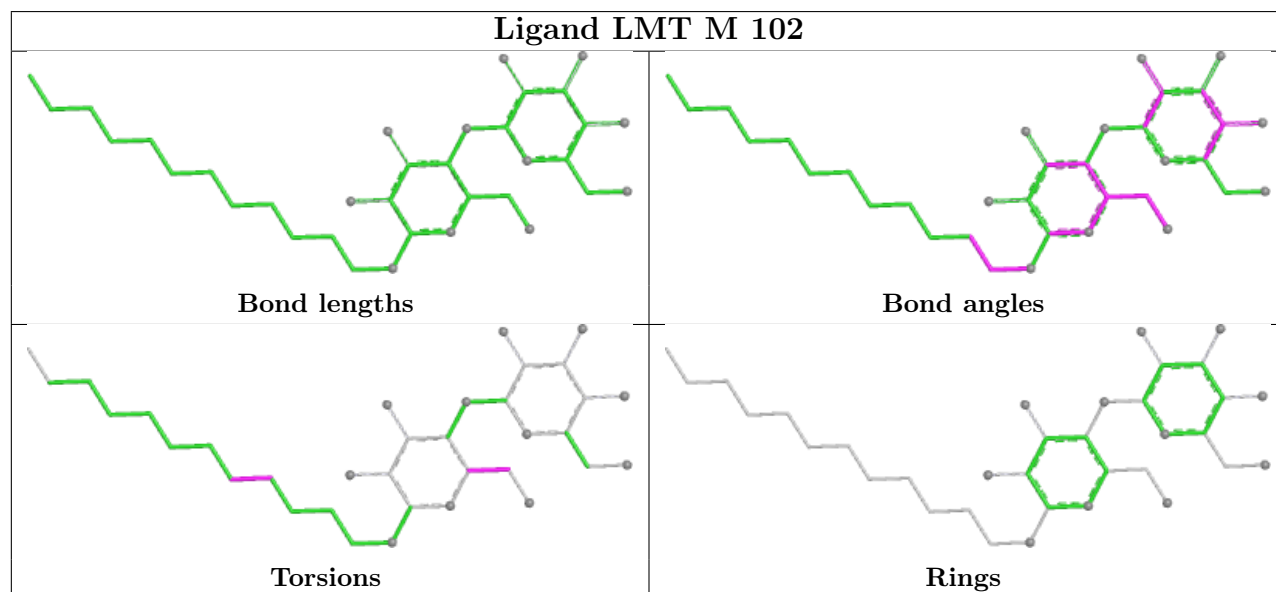
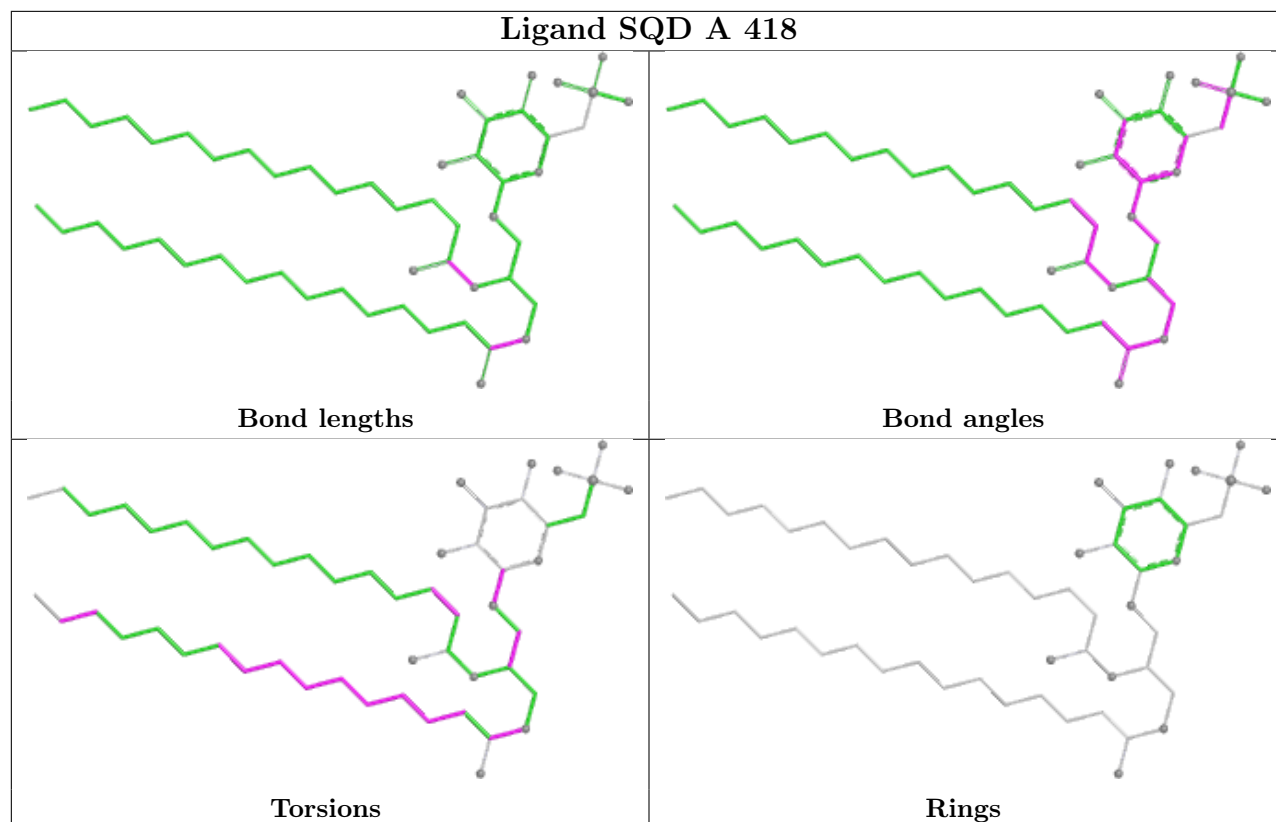


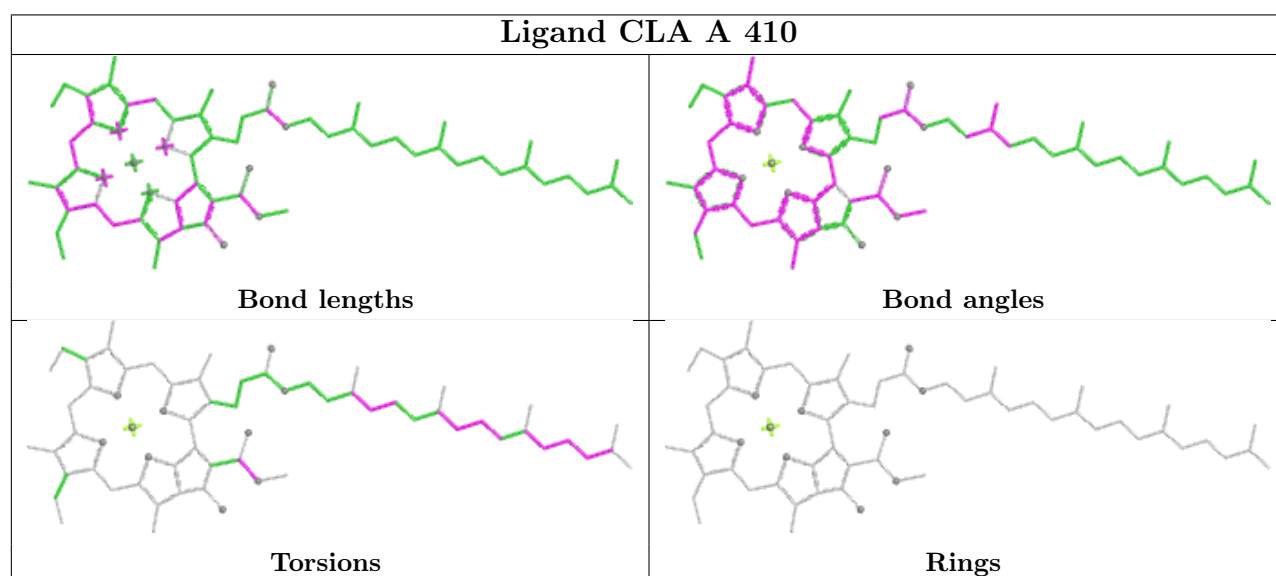
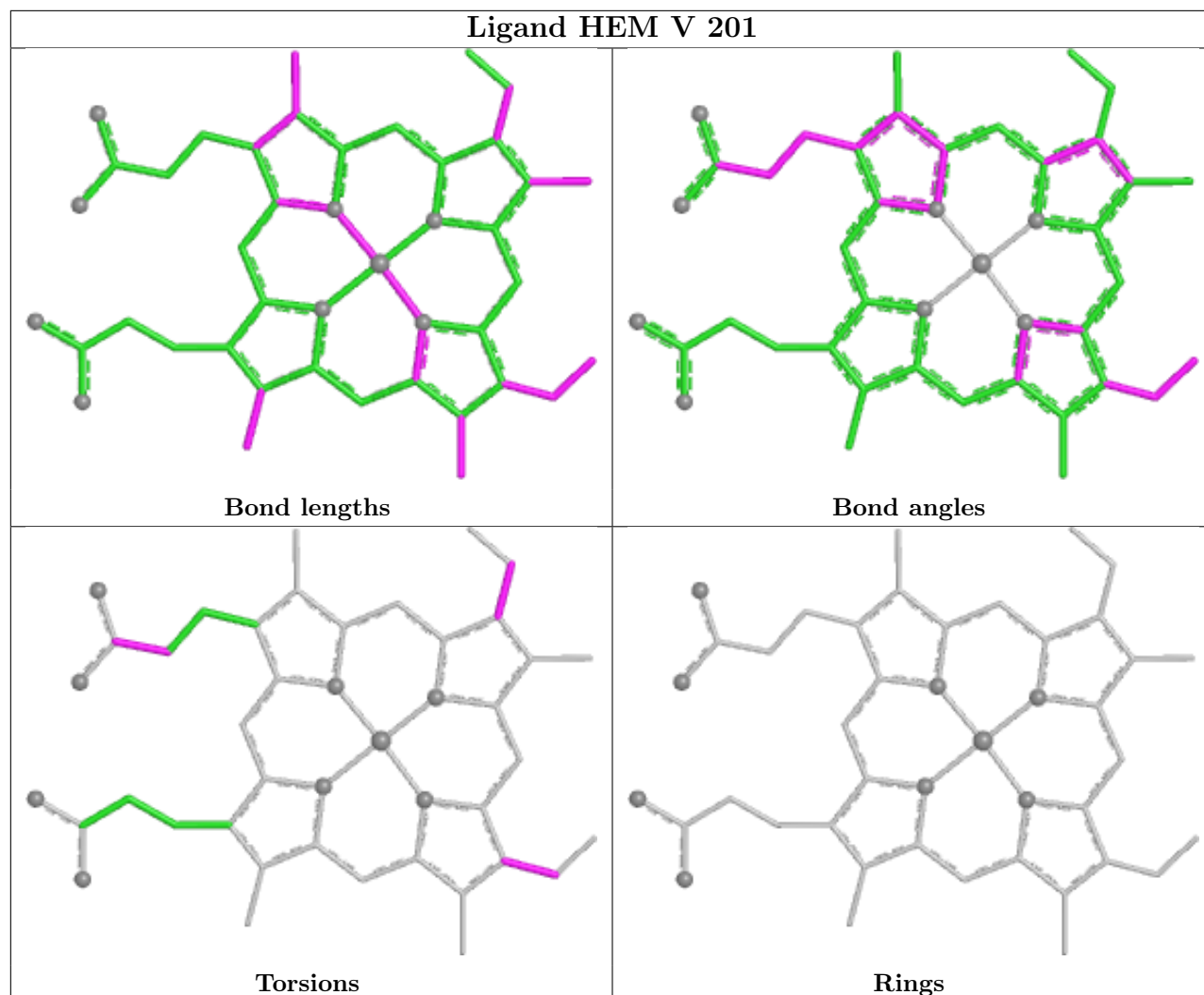




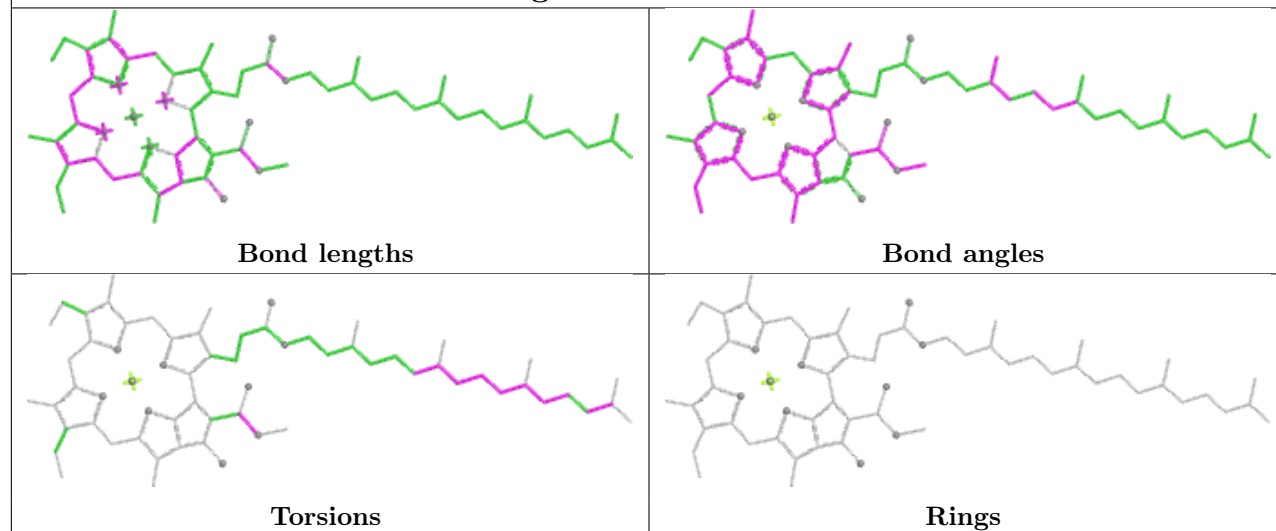




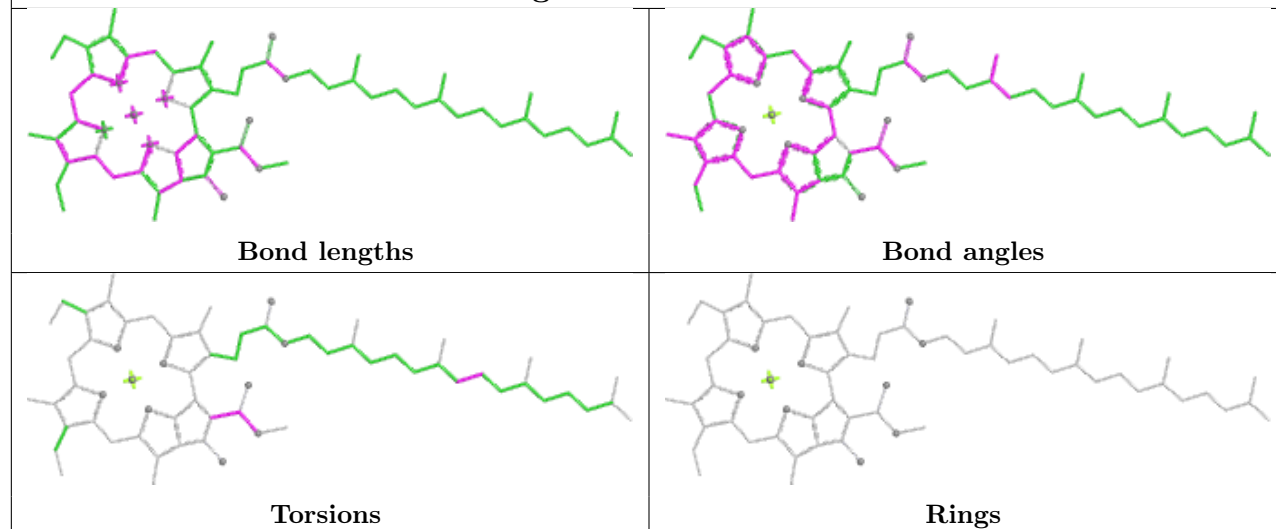




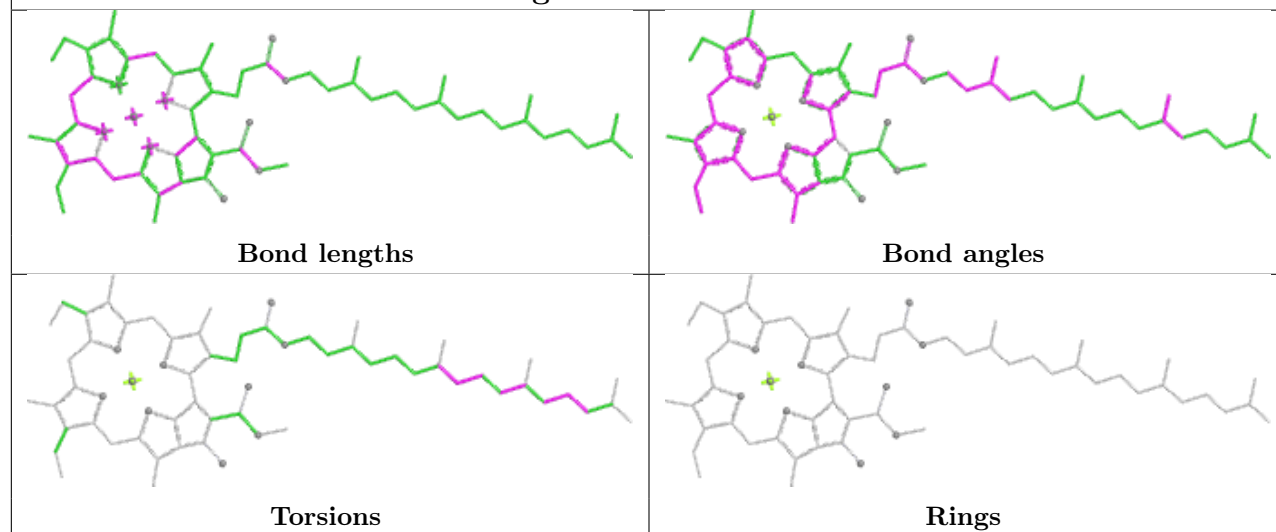
Ligand CLA D 403



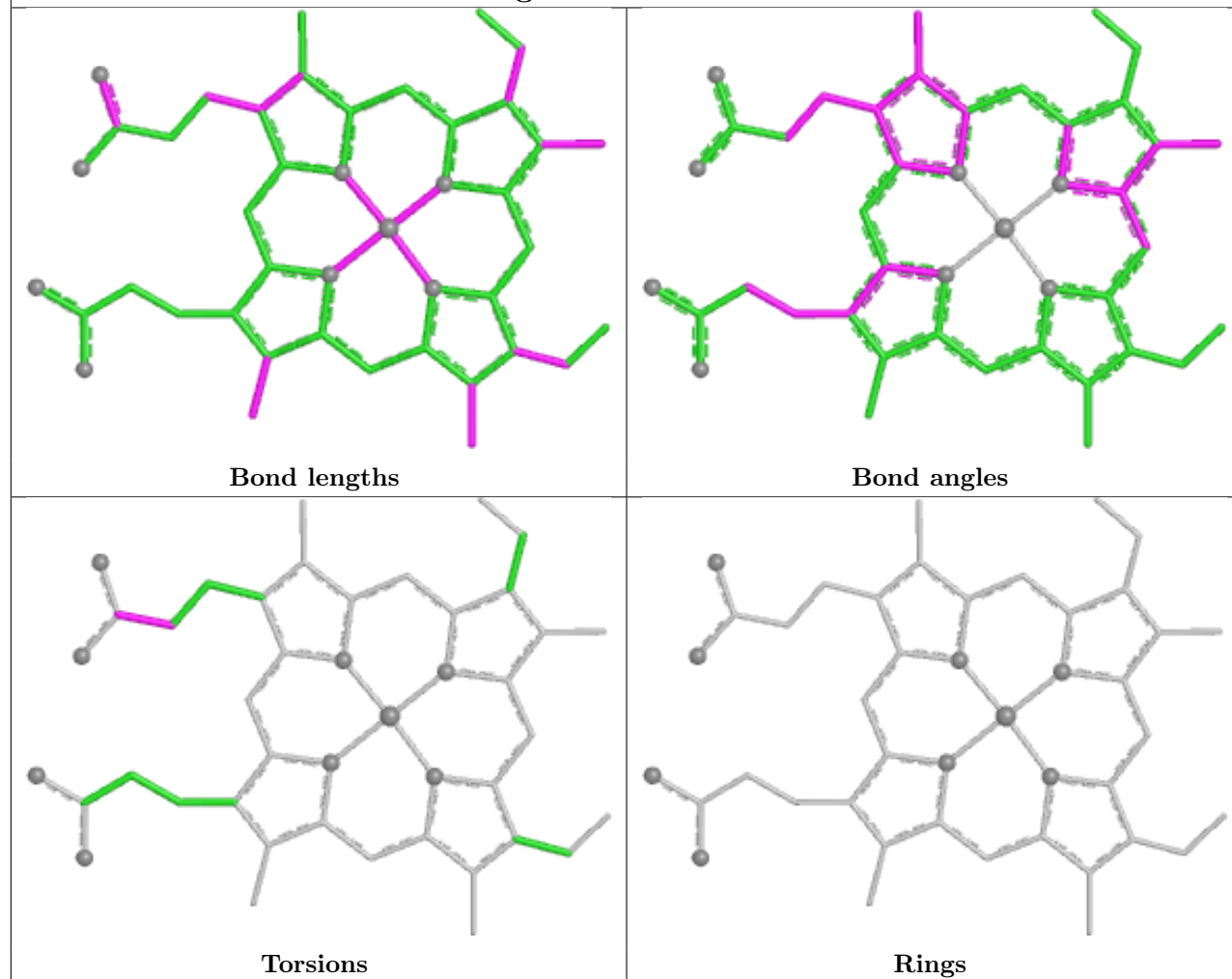
Ligand CLA C 510



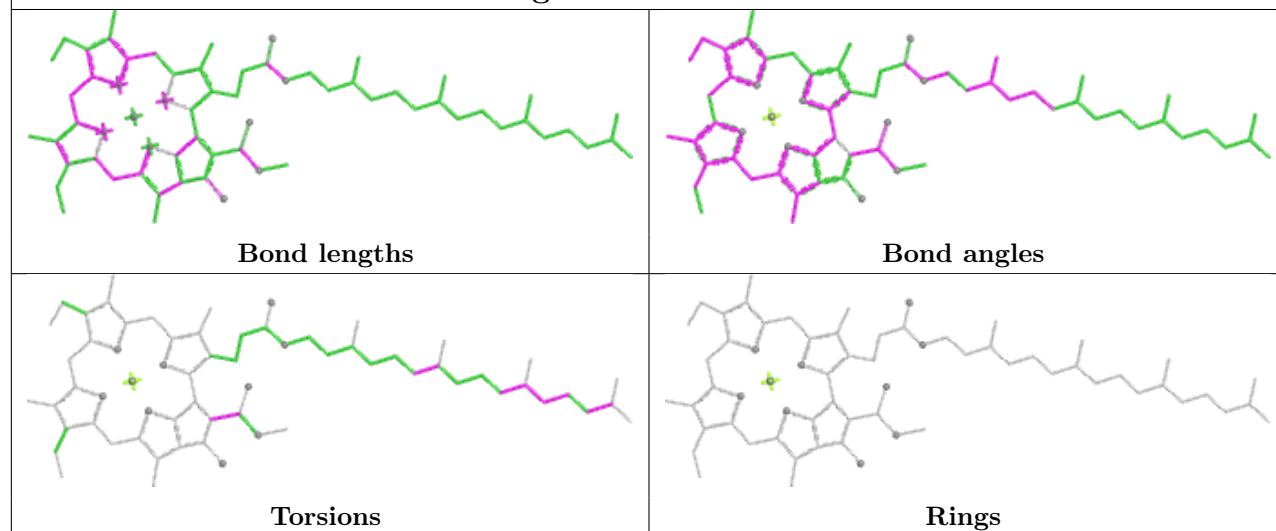
Ligand CLA B 614

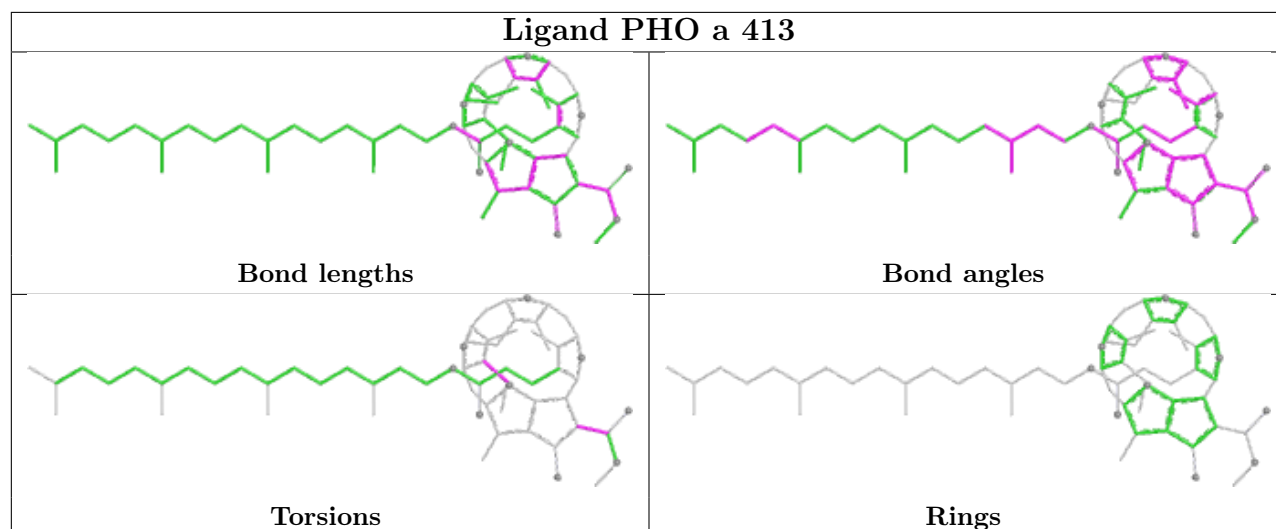
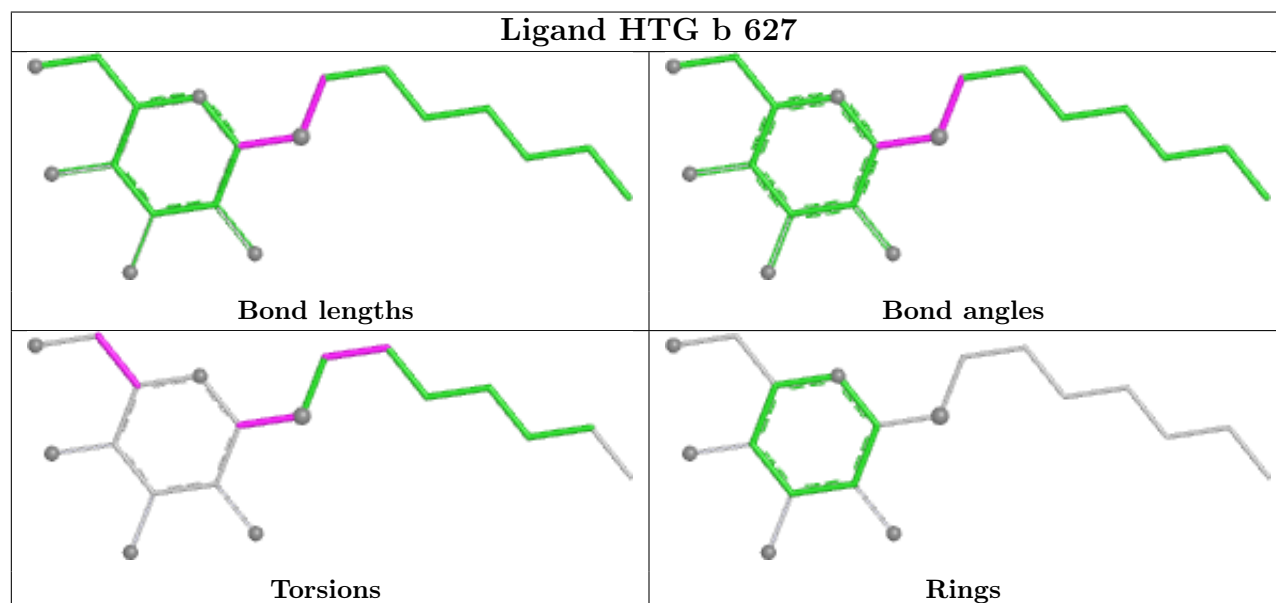
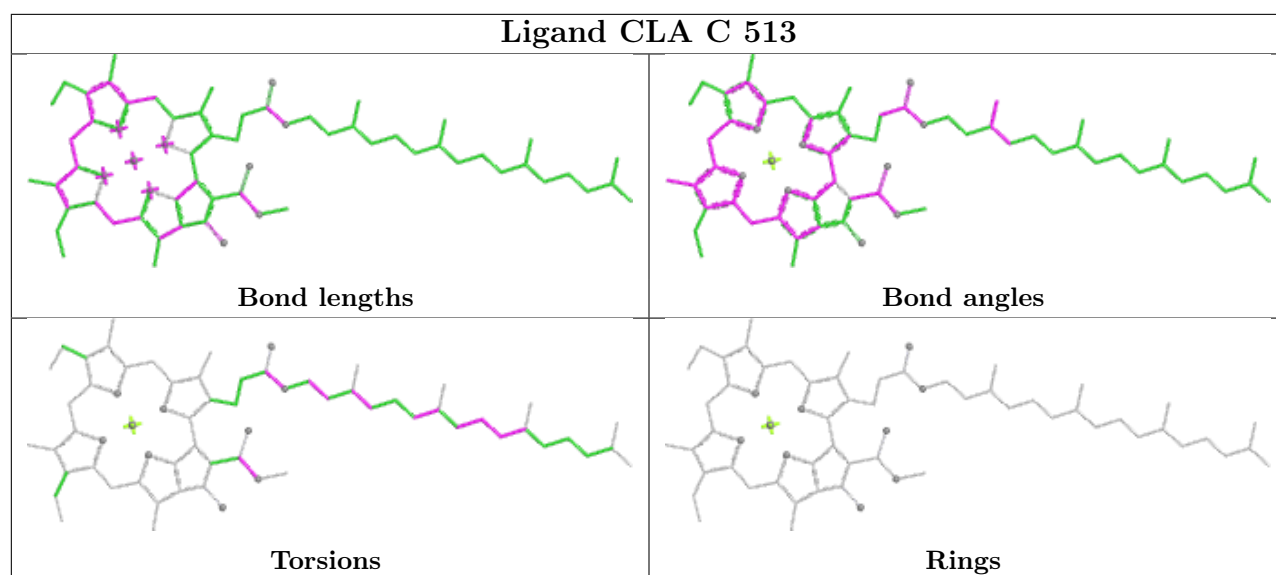


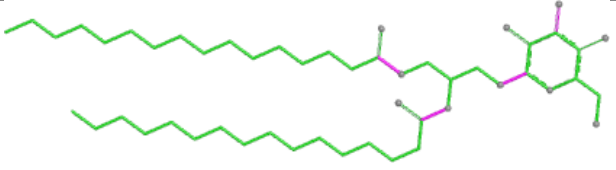
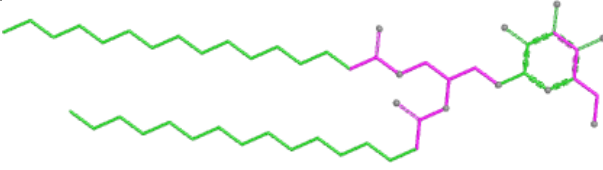
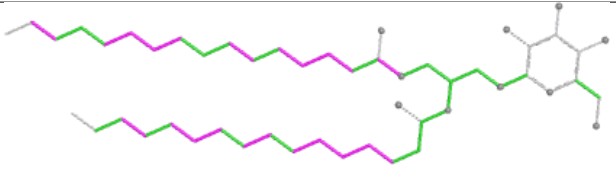
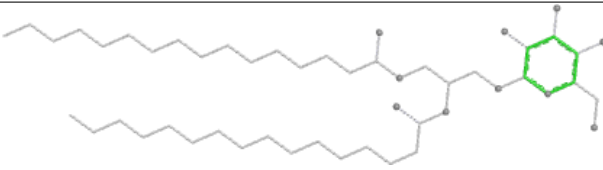
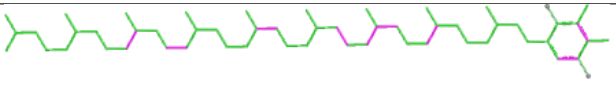
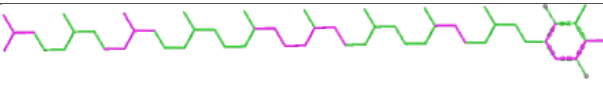
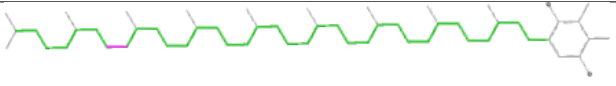
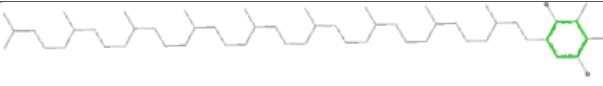
Ligand HEM f 101

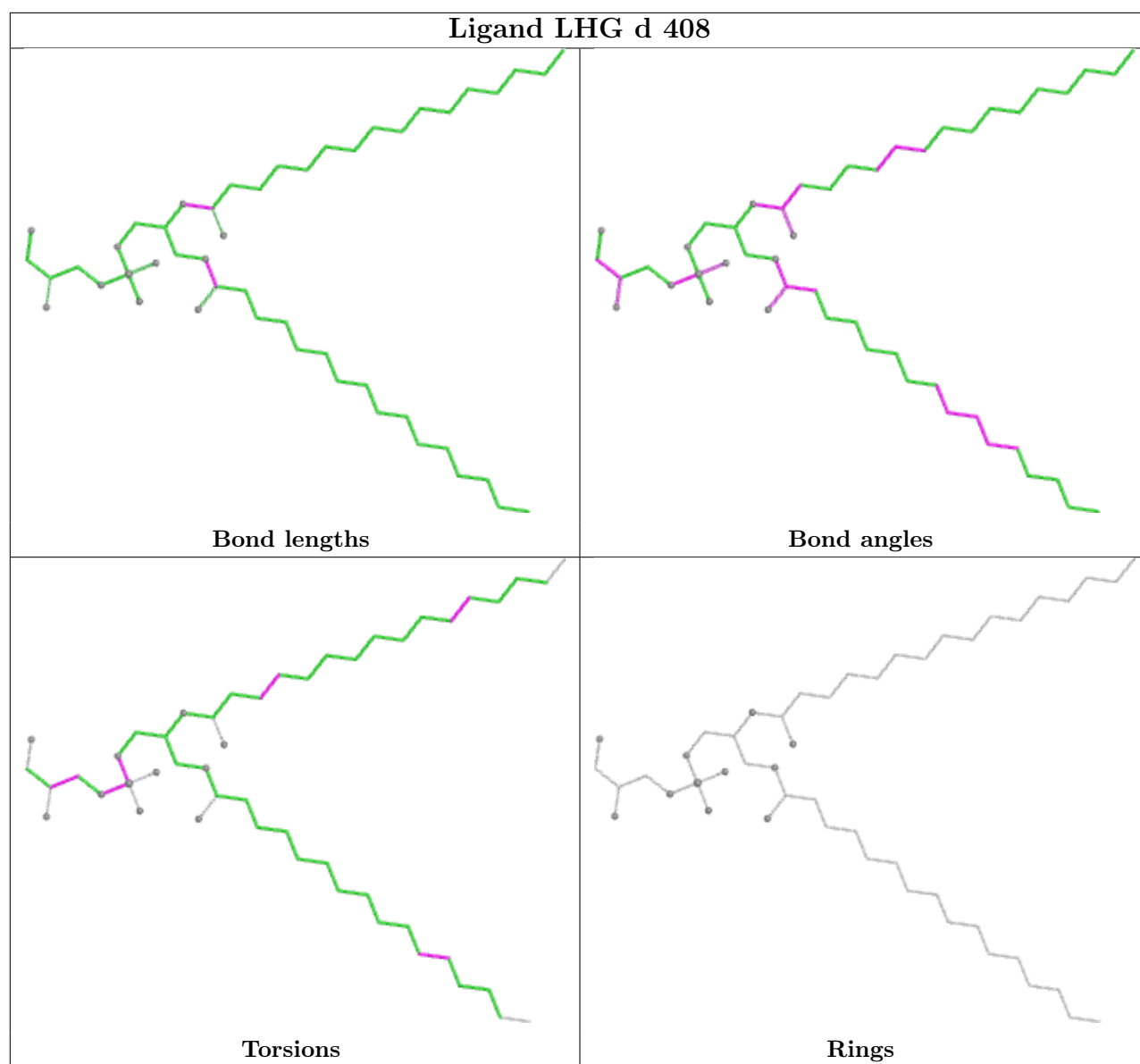


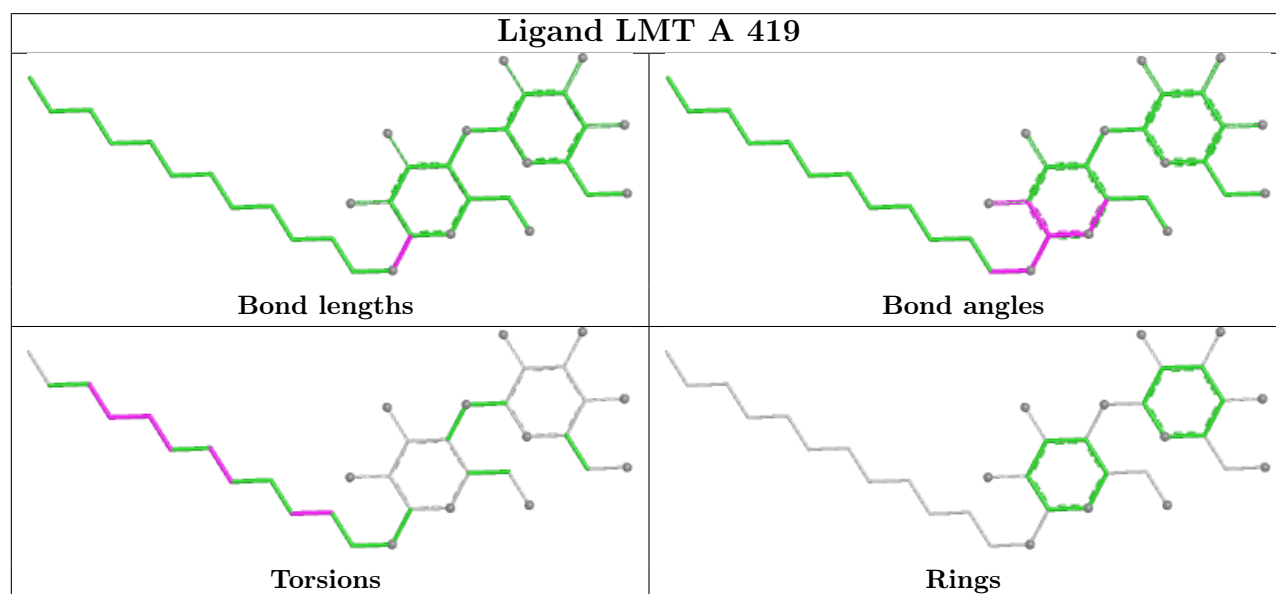
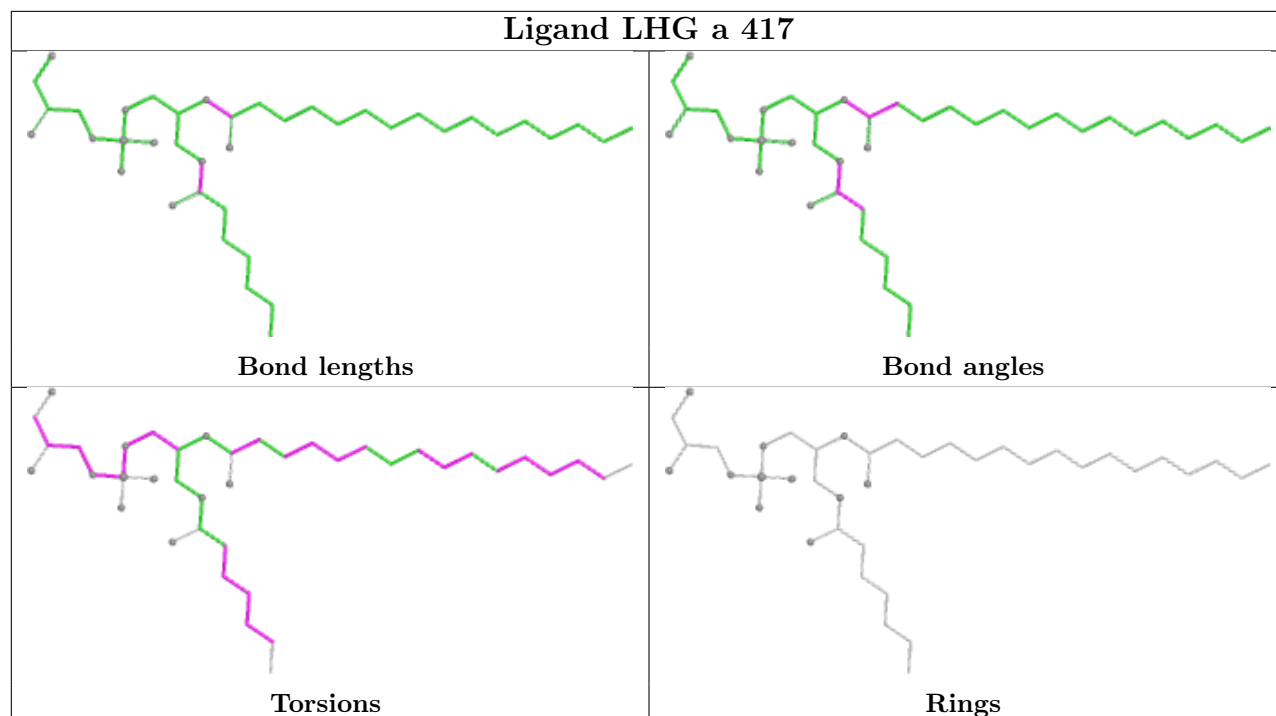
Ligand CLA C 504

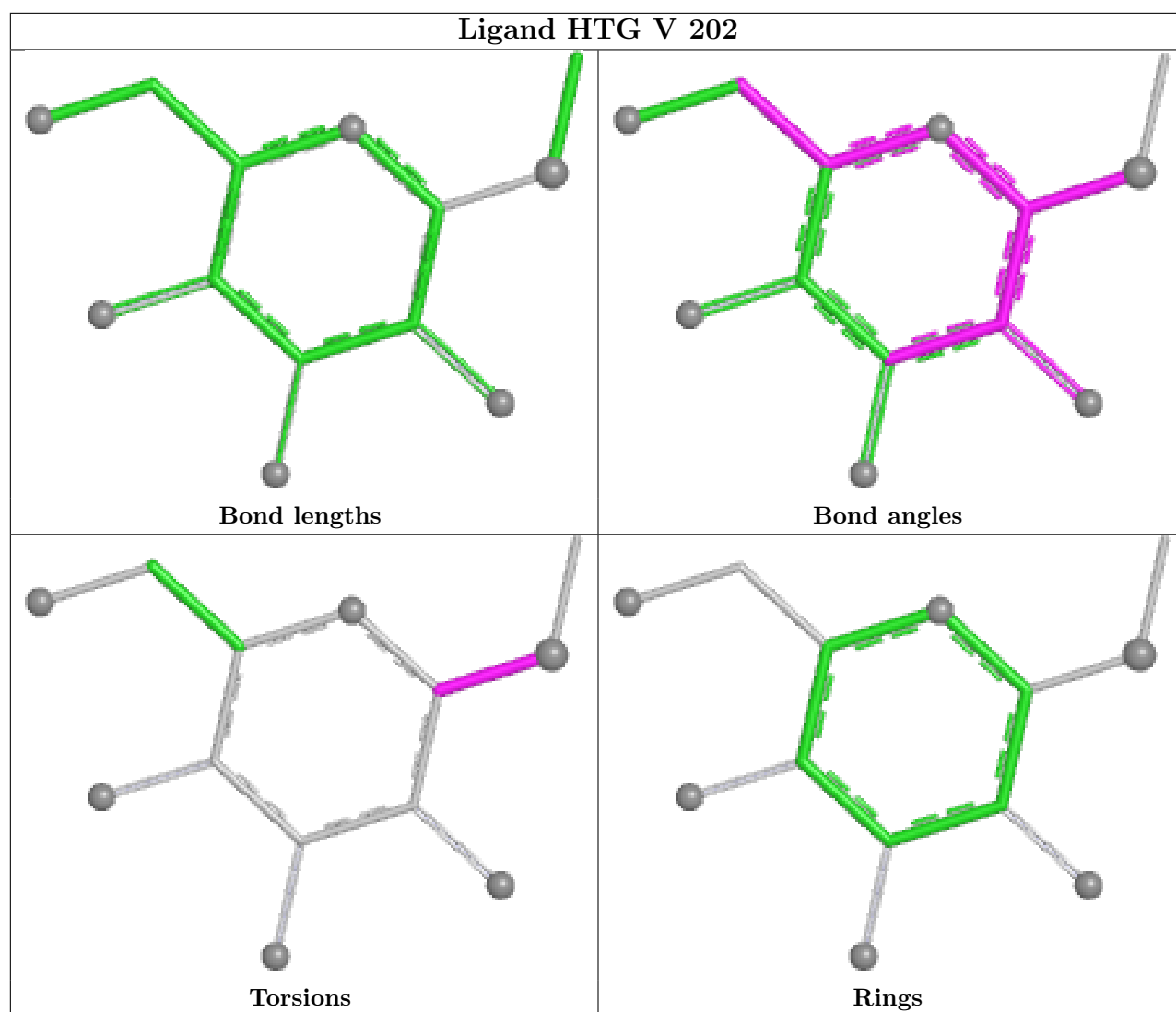


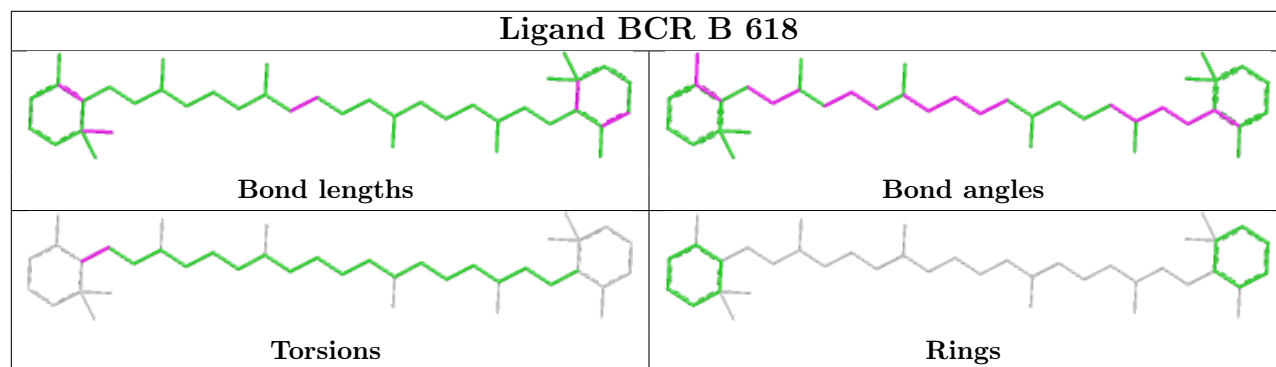
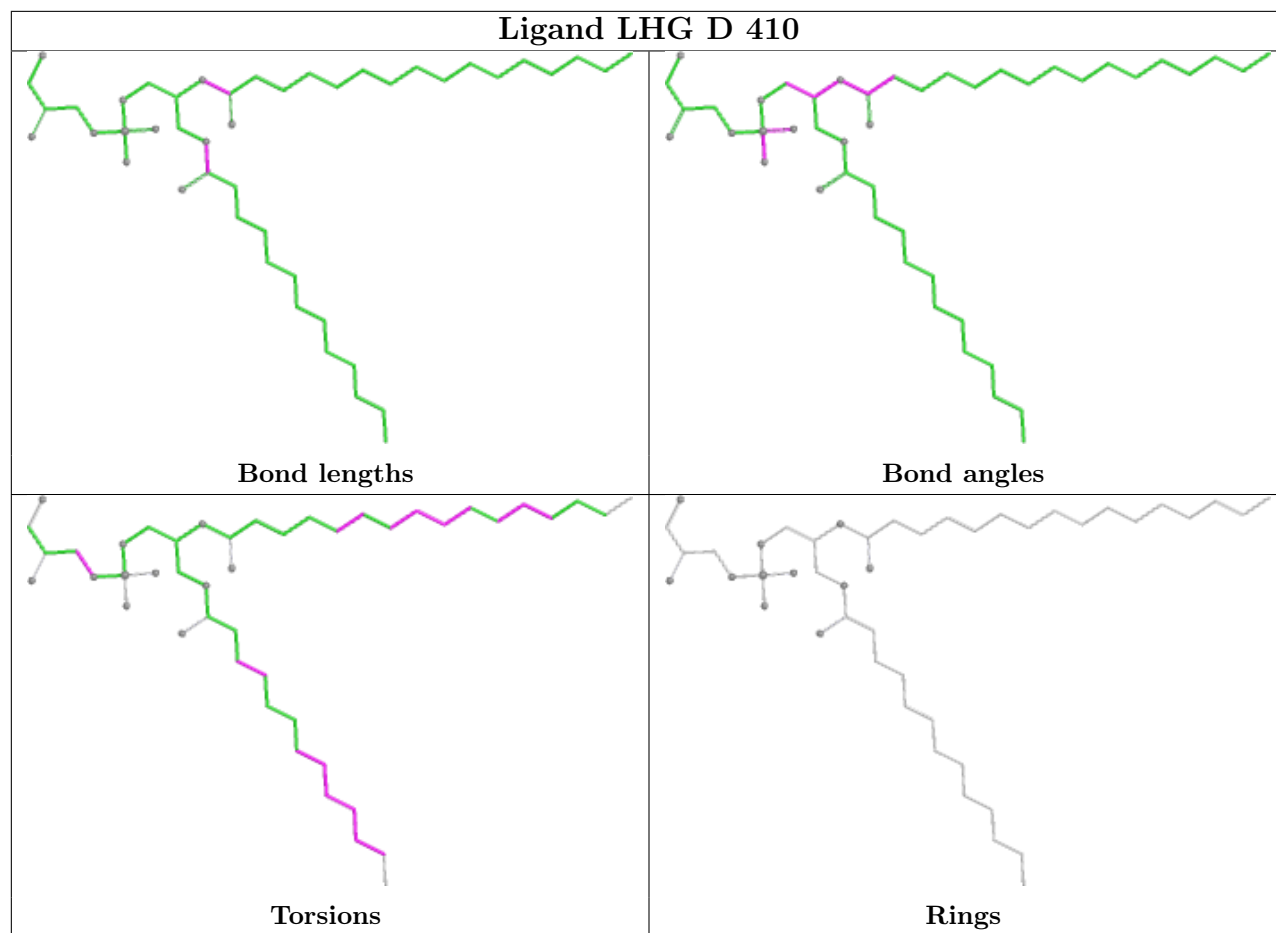


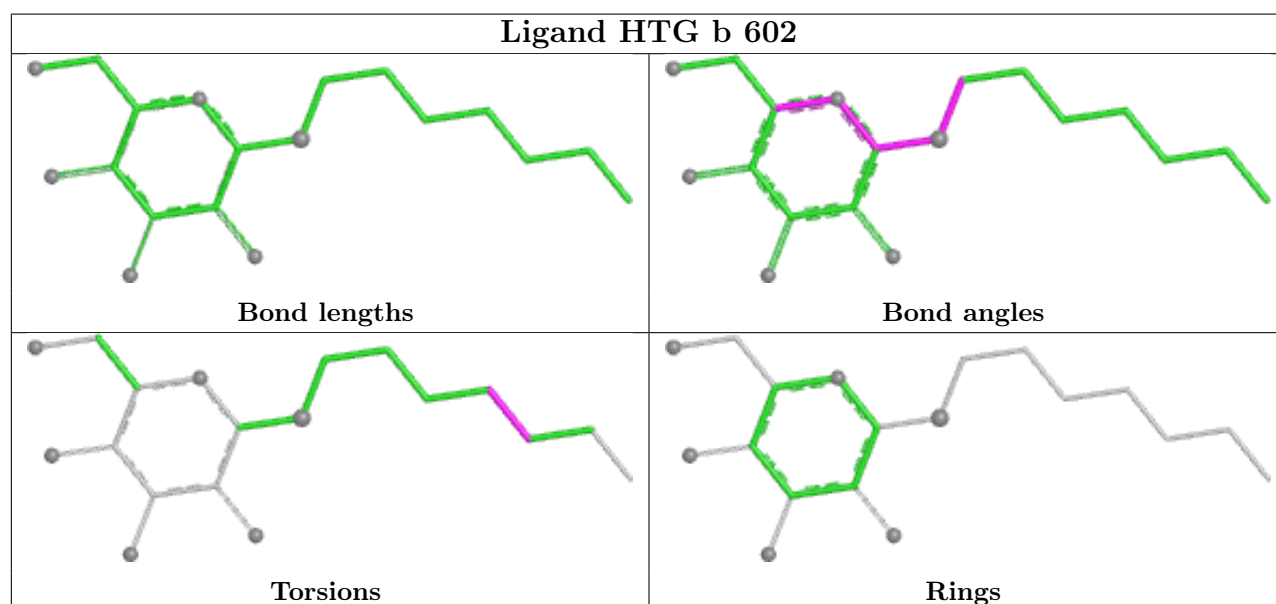
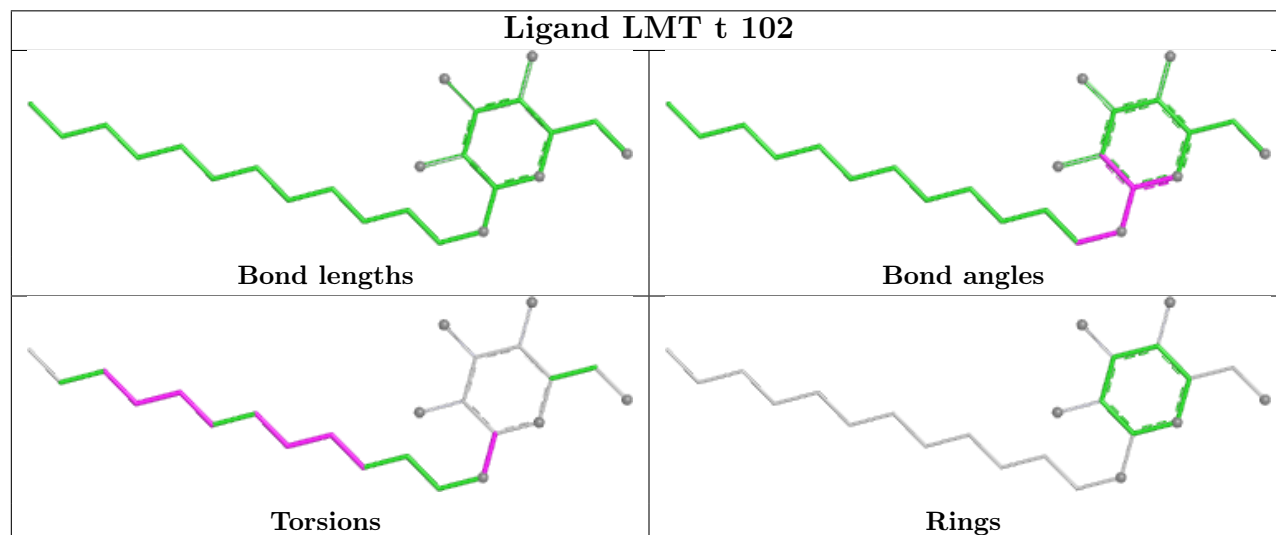
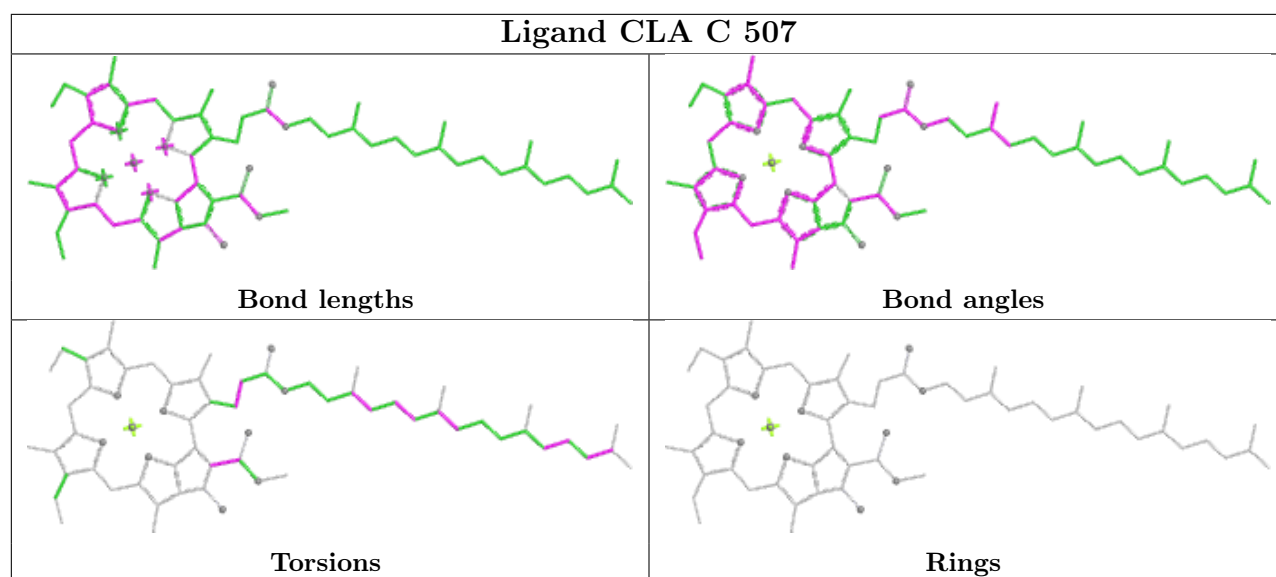
Ligand LMG c 920	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

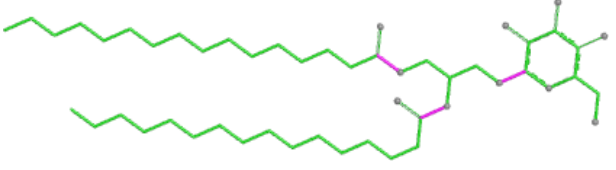
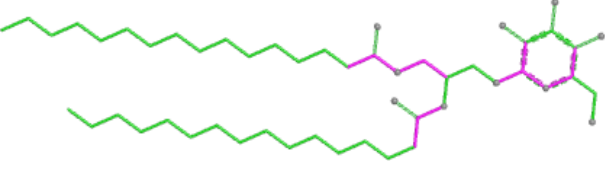
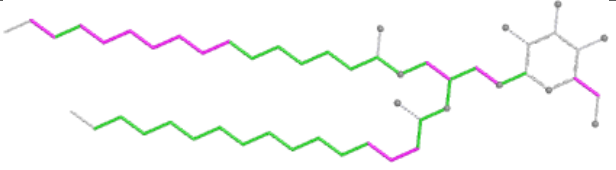
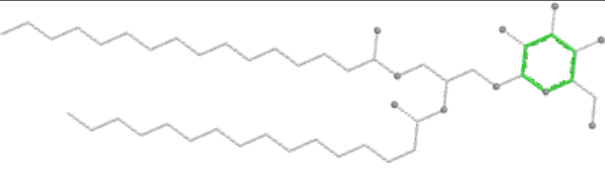


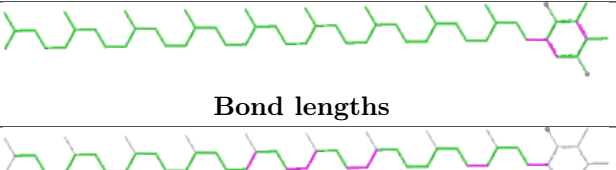
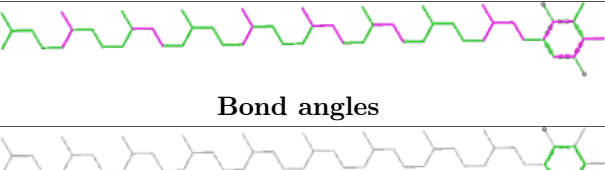
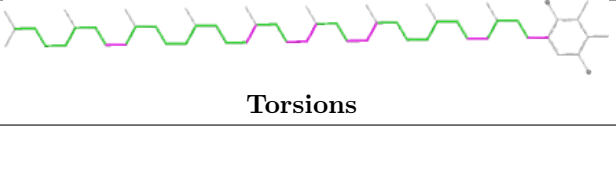
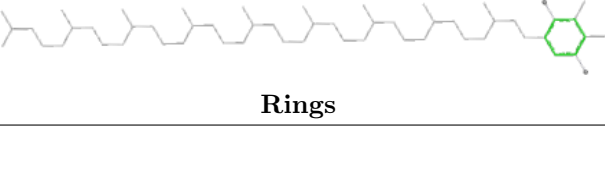


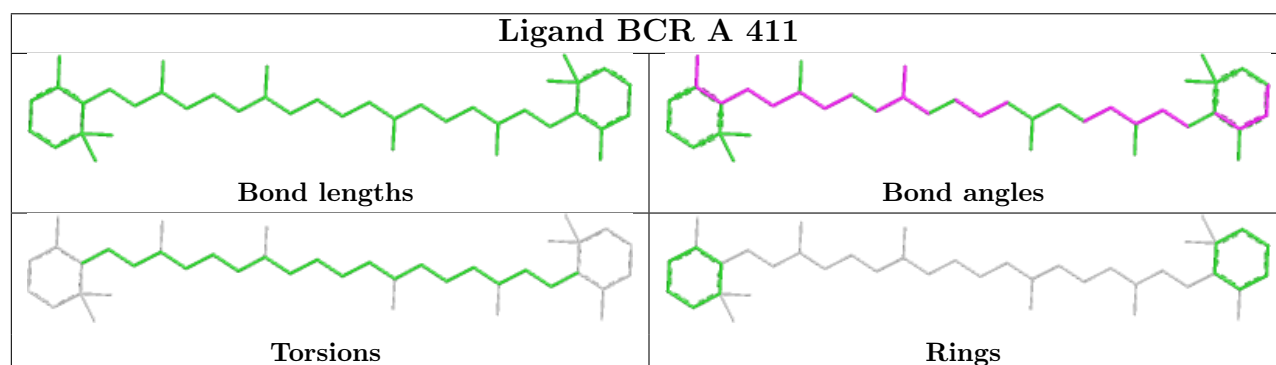
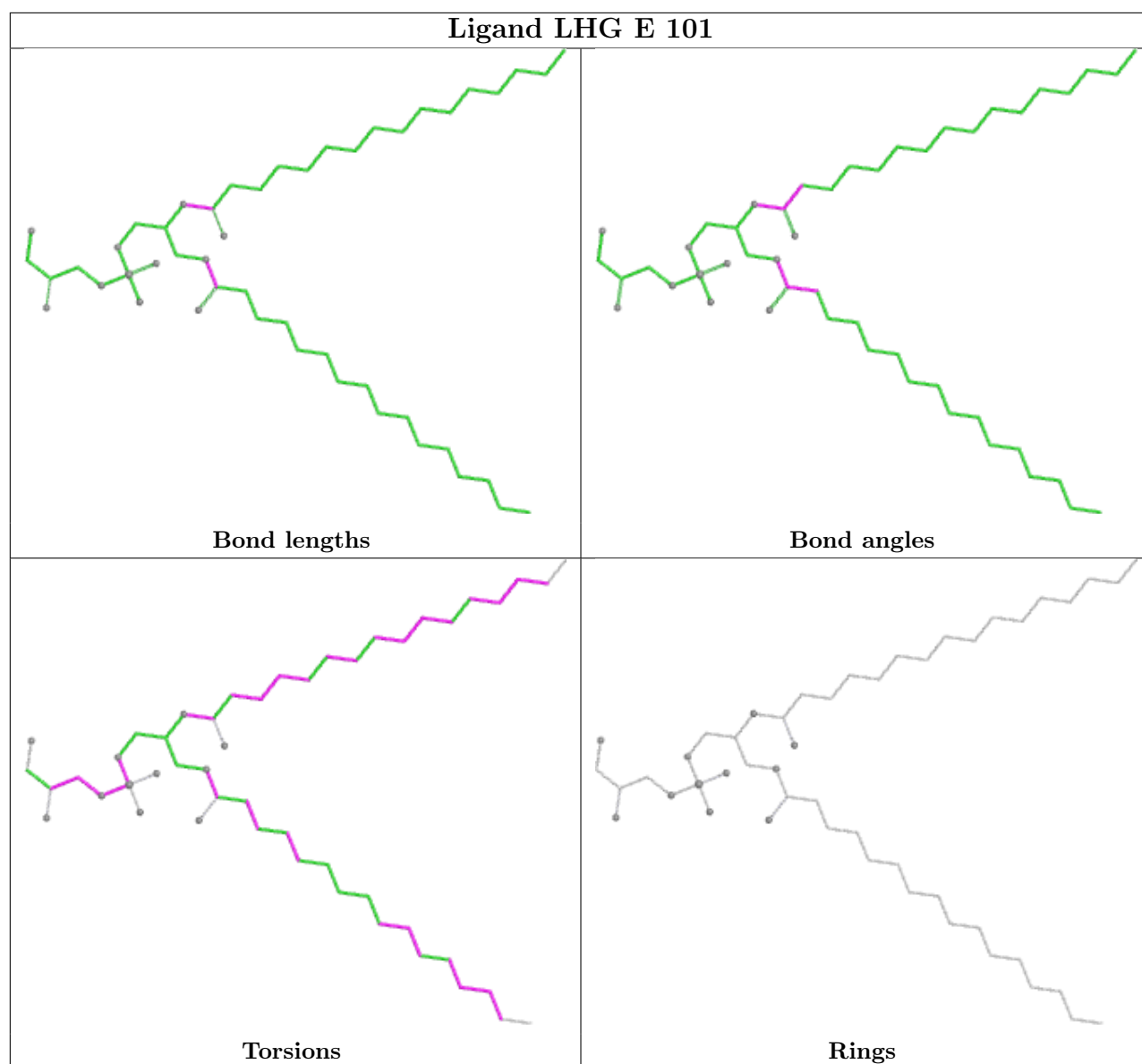


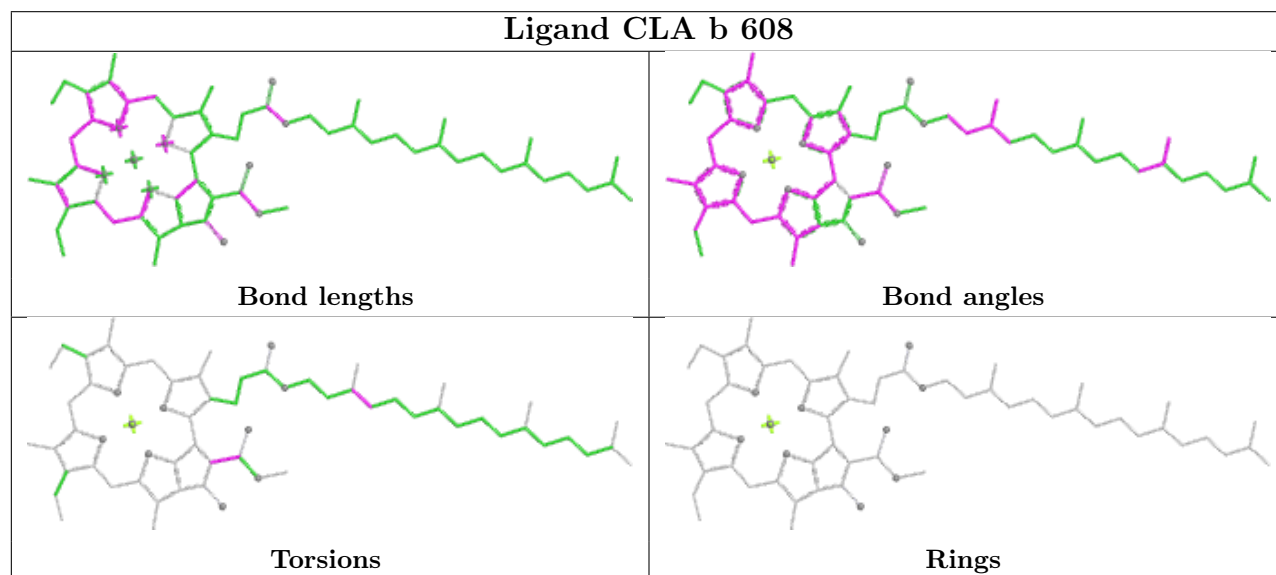
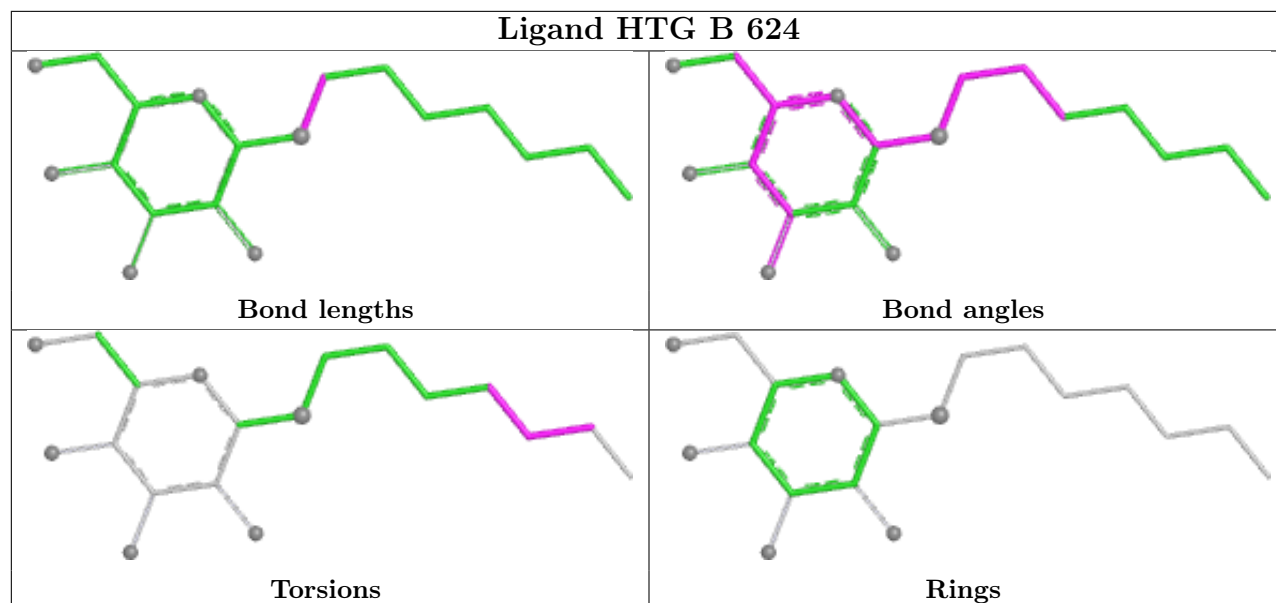


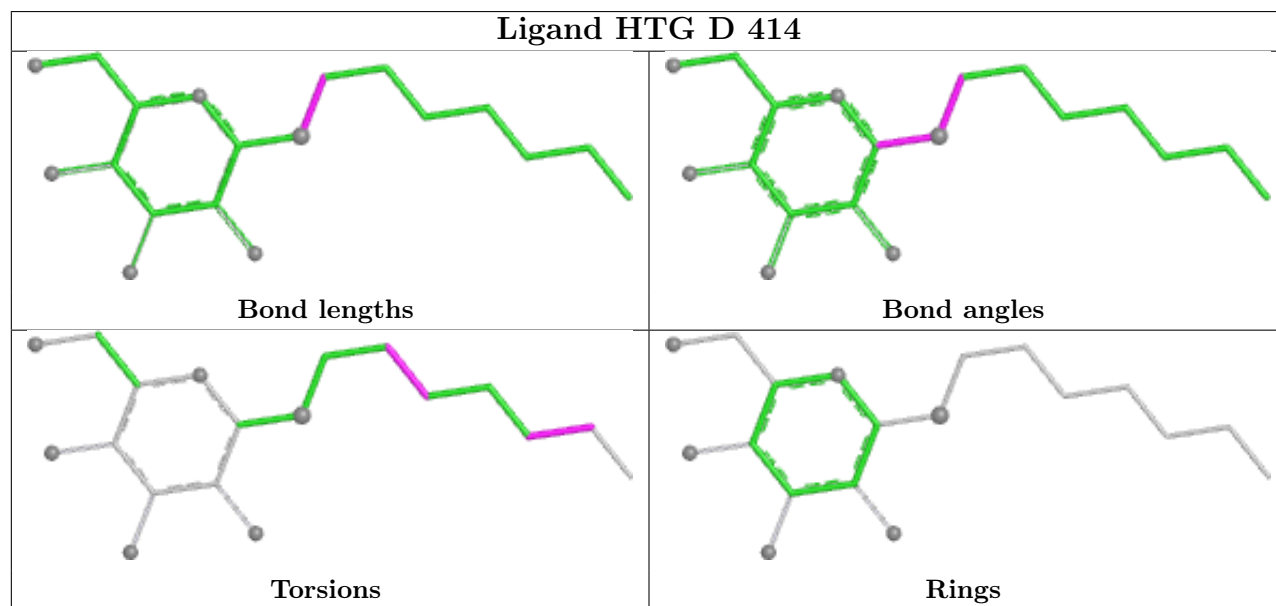
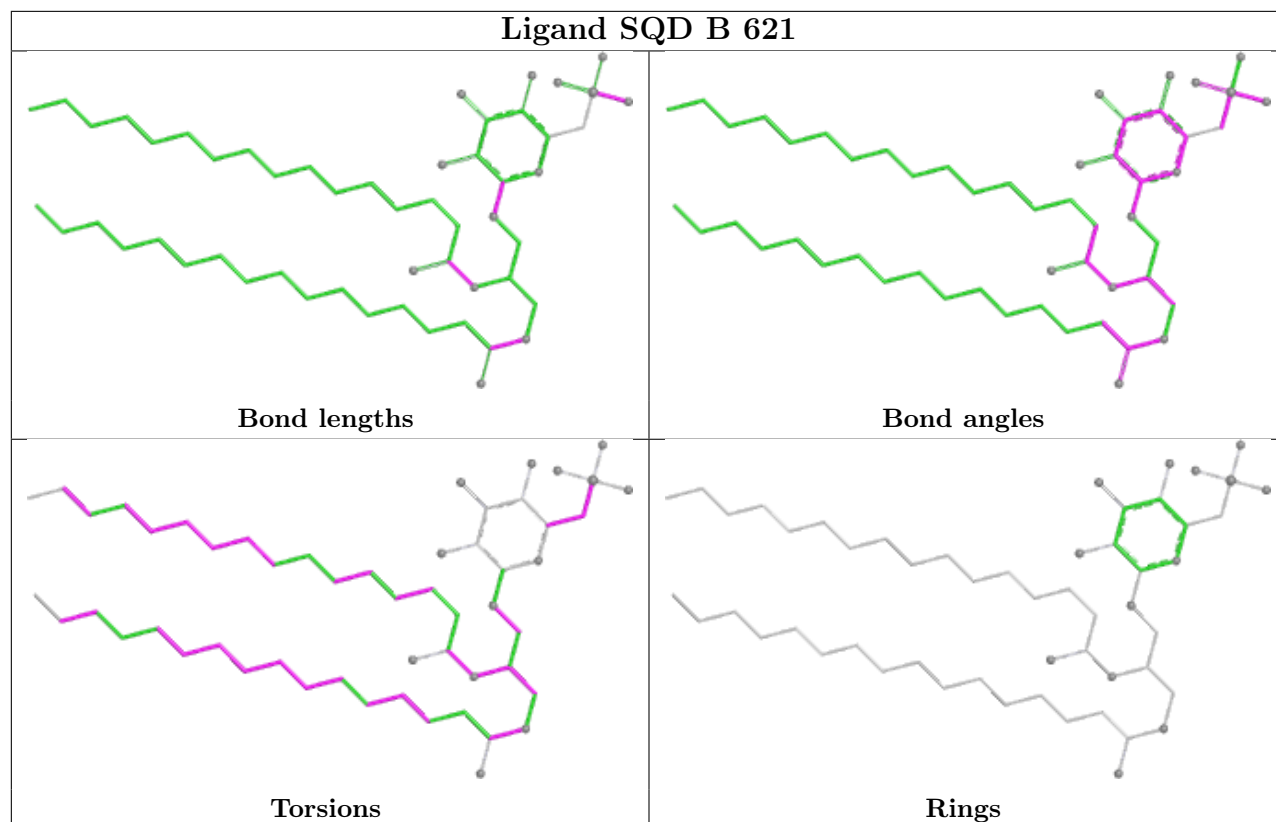


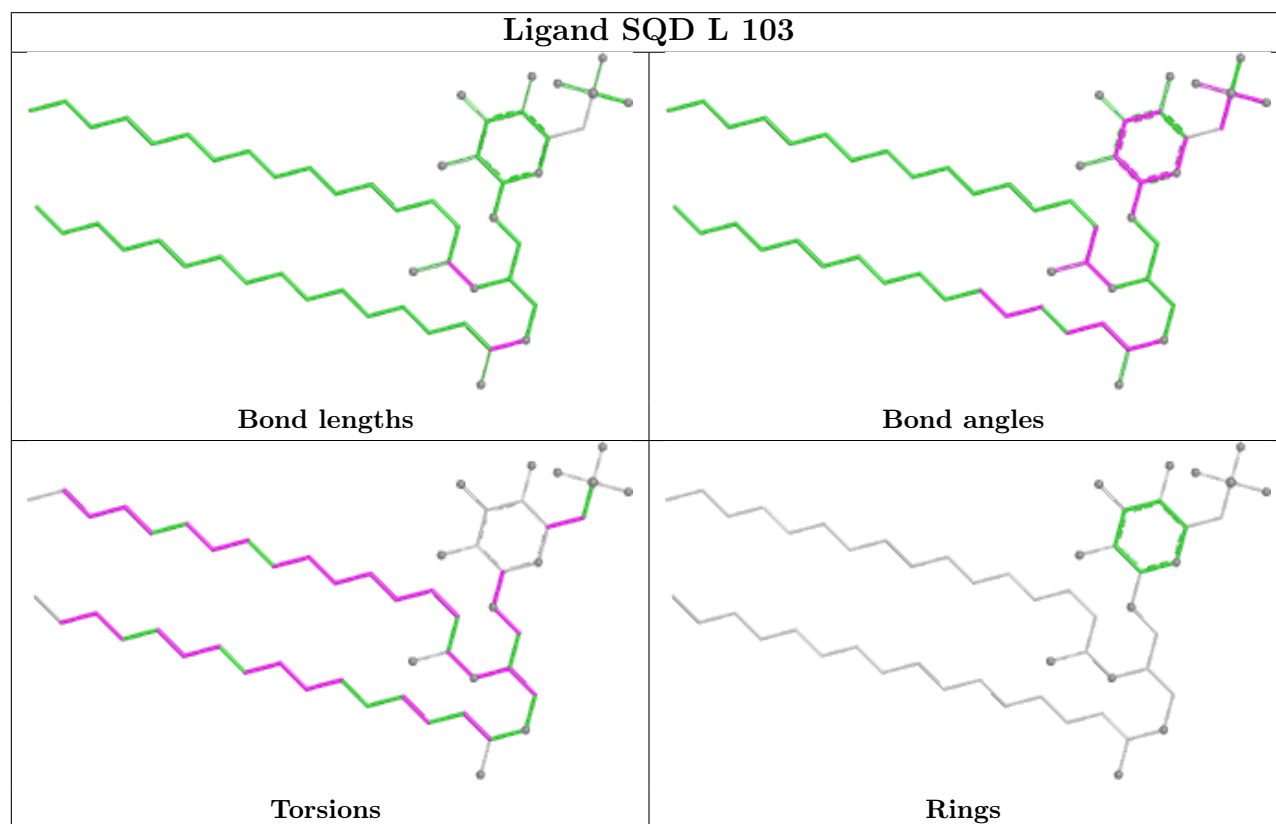
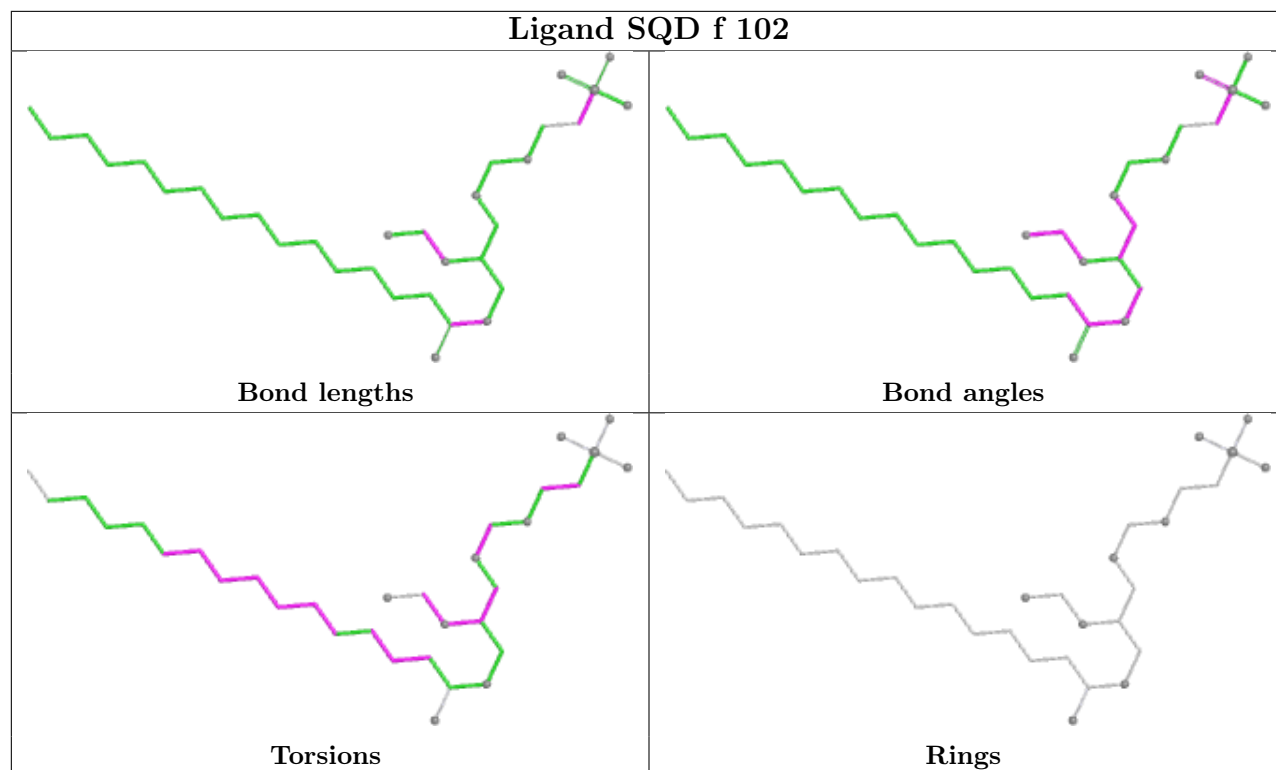
Ligand LMG c 921			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

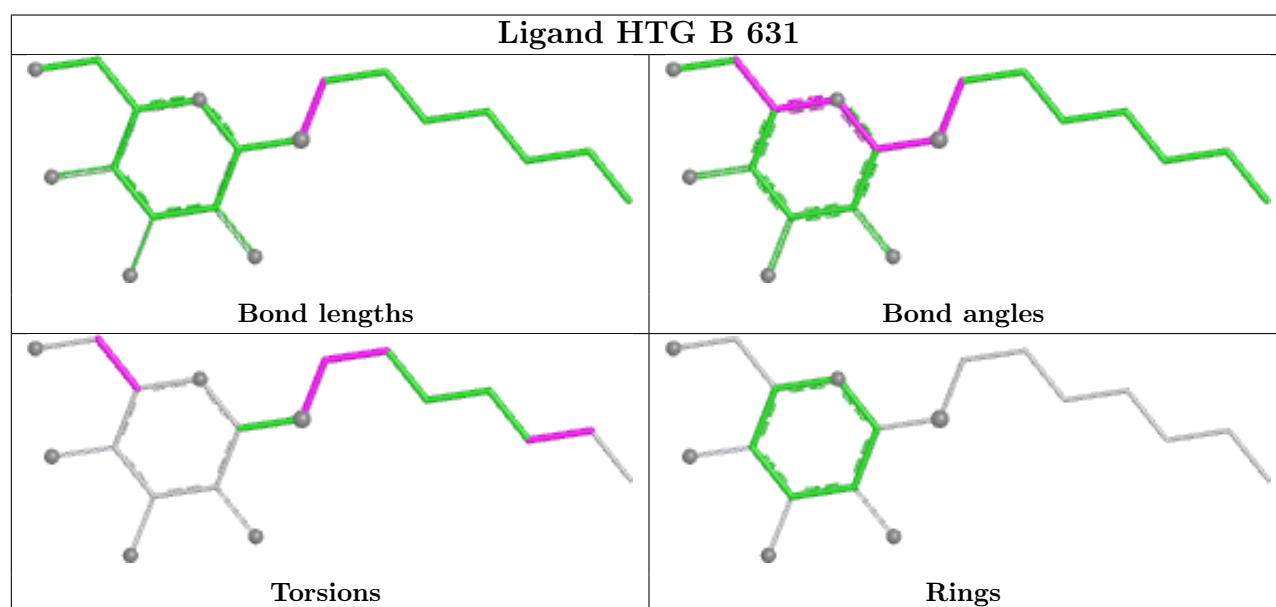
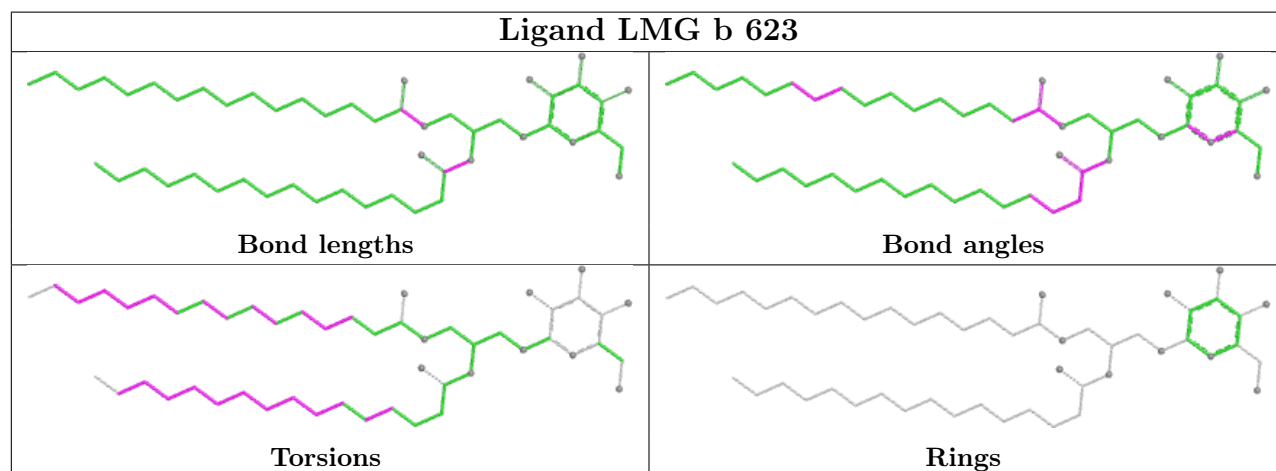
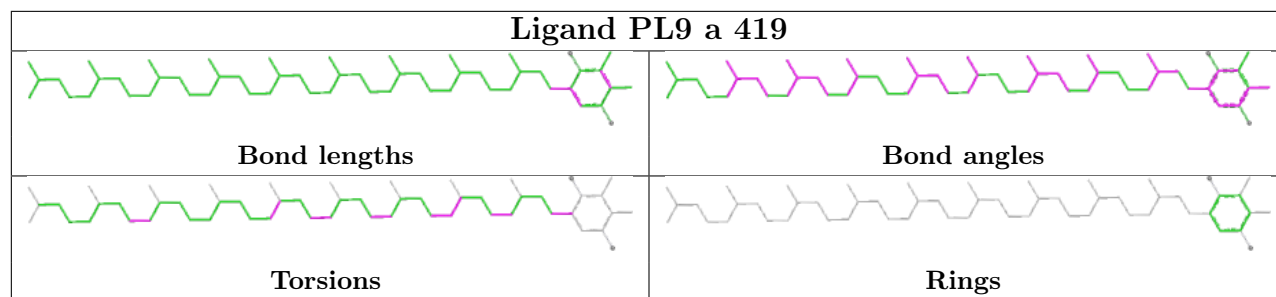
Ligand PL9 A 414			
			
Bond lengths		Bond angles	
			
Torsions		Rings	



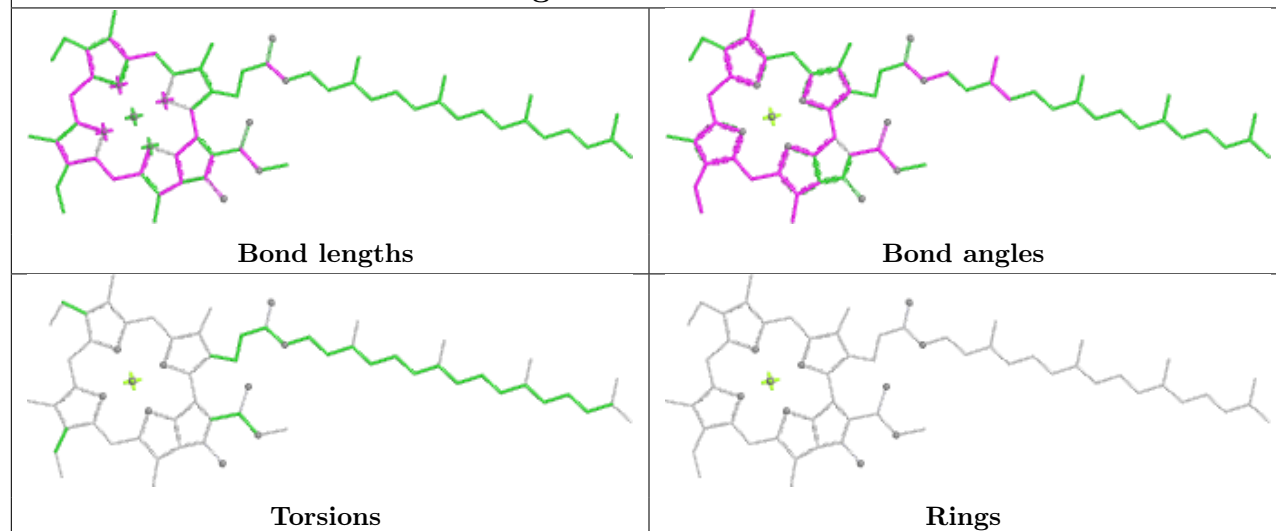




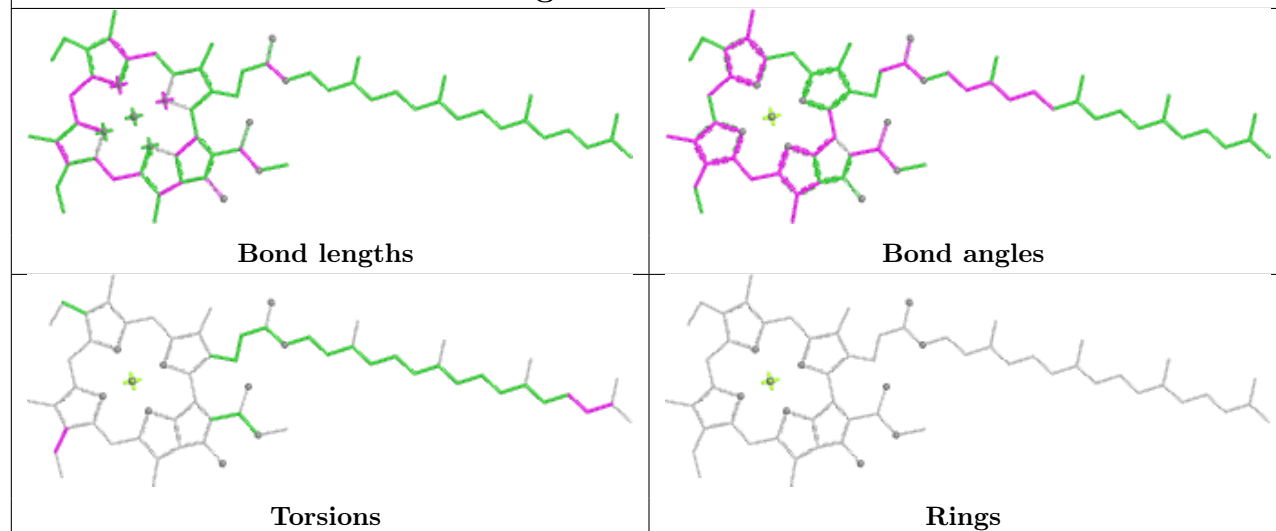




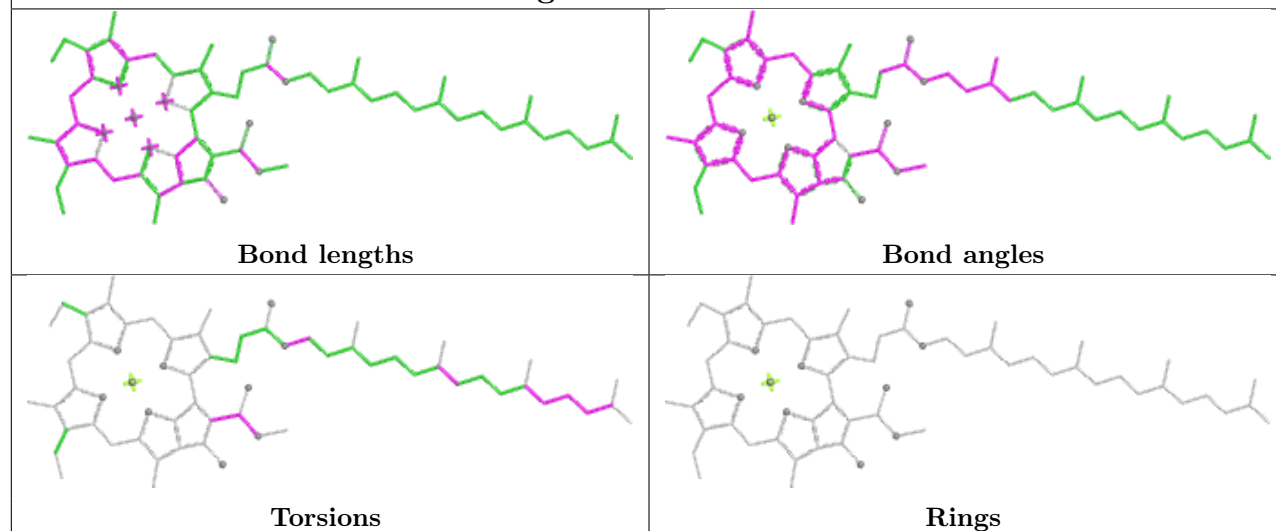
Ligand CLA C 511

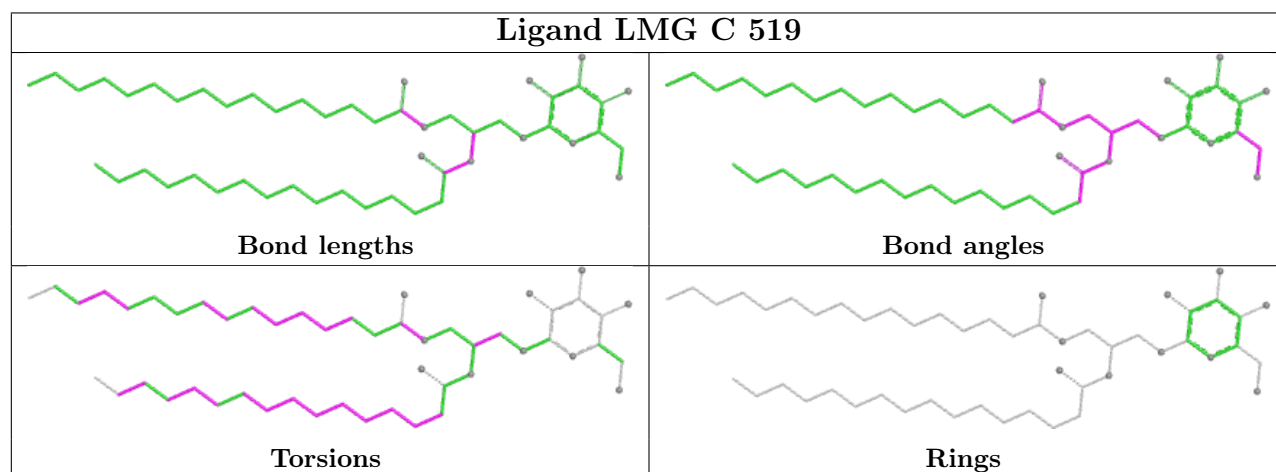
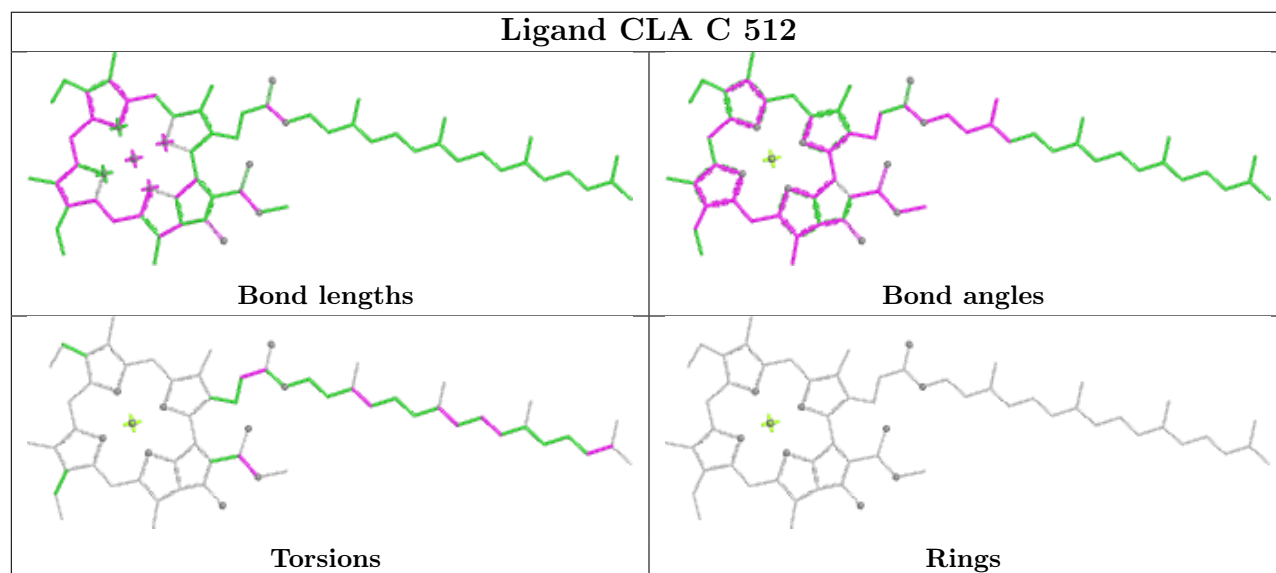
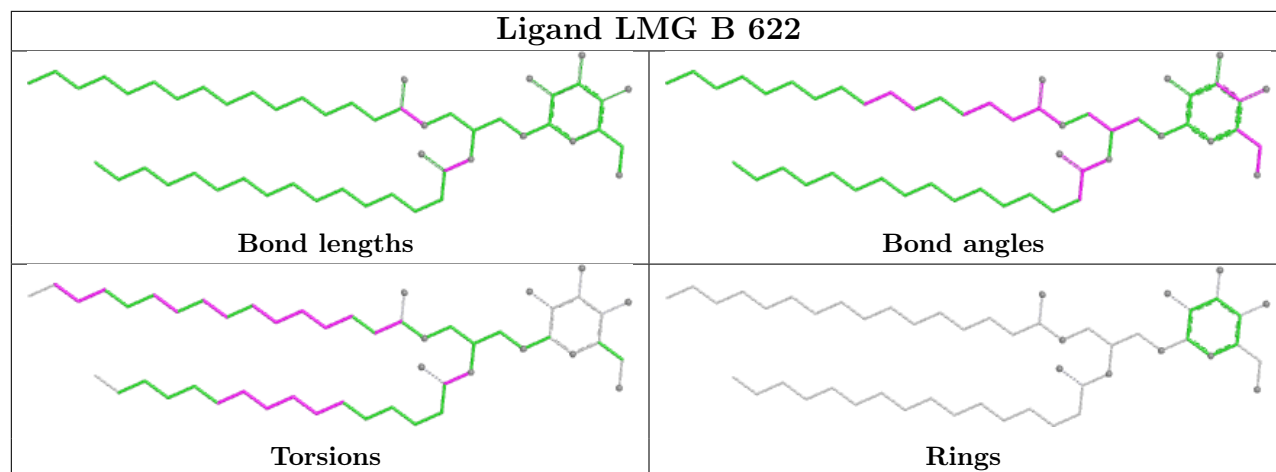


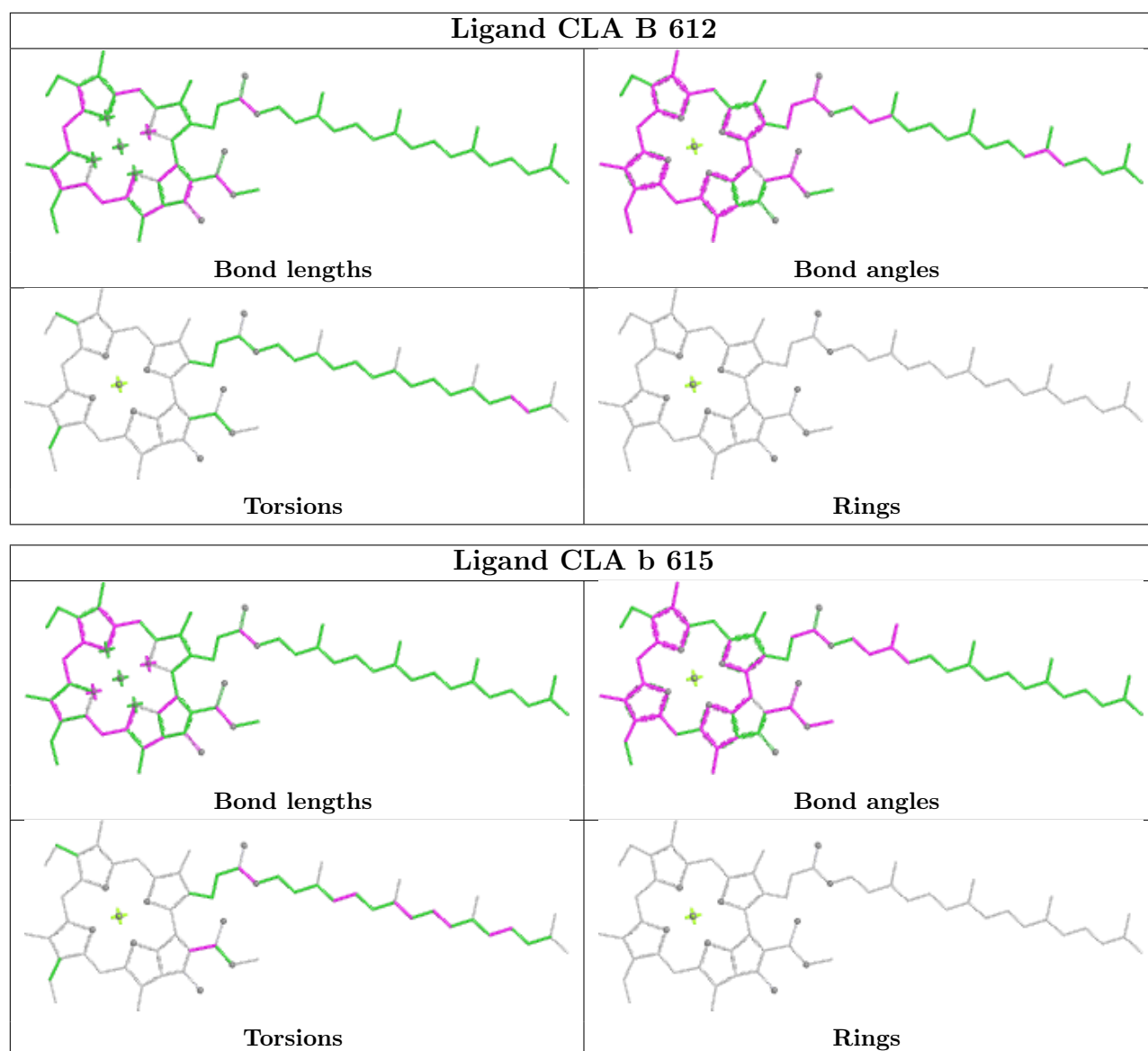
Ligand CLA a 409



Ligand CLA c 910







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%)	-0.68	0 100 100	15, 23, 46, 69	4 (1%)
1	a	334/344 (97%)	-0.62	1 (0%) 90 91	17, 24, 50, 76	4 (1%)
2	B	504/504 (100%)	-0.48	8 (1%) 70 74	14, 27, 54, 88	10 (1%)
2	b	501/504 (99%)	-0.35	17 (3%) 48 51	16, 29, 58, 119	11 (2%)
3	C	451/455 (99%)	-0.42	0 100 100	17, 31, 46, 81	3 (0%)
3	c	455/455 (100%)	-0.27	0 100 100	21, 34, 48, 79	4 (0%)
4	D	340/342 (99%)	-0.74	0 100 100	13, 24, 40, 70	1 (0%)
4	d	340/342 (99%)	-0.67	0 100 100	13, 26, 45, 80	3 (0%)
5	E	81/83 (97%)	0.10	1 (1%) 76 79	27, 40, 62, 82	0
5	e	79/83 (95%)	0.30	0 100 100	32, 44, 72, 82	0
6	F	34/44 (77%)	-0.09	1 (2%) 53 57	26, 34, 63, 74	0
6	f	32/44 (72%)	0.05	3 (9%) 14 14	29, 37, 76, 86	0
7	H	63/63 (100%)	-0.19	1 (1%) 70 74	24, 33, 43, 70	0
7	h	63/63 (100%)	0.03	1 (1%) 70 74	27, 37, 51, 81	0
8	I	35/38 (92%)	-0.05	0 100 100	27, 34, 64, 86	0
8	i	37/38 (97%)	-0.03	2 (5%) 31 33	26, 34, 71, 83	0
9	J	36/40 (90%)	-0.13	2 (5%) 30 32	26, 38, 65, 79	0
9	j	39/40 (97%)	0.28	2 (5%) 33 36	30, 42, 68, 84	0
10	K	37/37 (100%)	-0.30	0 100 100	24, 38, 47, 63	1 (2%)
10	k	37/37 (100%)	0.06	0 100 100	36, 42, 55, 69	0
11	L	37/37 (100%)	-0.63	0 100 100	11, 22, 65, 75	1 (2%)
11	l	37/37 (100%)	-0.65	1 (2%) 56 60	13, 23, 64, 95	2 (5%)
12	M	32/36 (88%)	-0.68	0 100 100	13, 24, 40, 56	1 (3%)
12	m	33/36 (91%)	-0.55	1 (3%) 52 56	13, 25, 48, 68	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.30	3 (1%) 76 79	17, 33, 66, 120	5 (2%)
13	o	241/244 (98%)	-0.15	4 (1%) 69 72	17, 34, 71, 87	5 (2%)
14	T	29/32 (90%)	-0.61	1 (3%) 48 51	19, 23, 49, 85	0
14	t	29/32 (90%)	-0.59	1 (3%) 48 51	20, 23, 47, 72	0
15	U	97/104 (93%)	-0.39	0 100 100	23, 30, 52, 58	0
15	u	97/104 (93%)	-0.47	1 (1%) 79 82	20, 30, 40, 66	1 (1%)
16	V	137/137 (100%)	-0.62	0 100 100	16, 28, 42, 51	2 (1%)
16	v	137/137 (100%)	-0.10	0 100 100	19, 37, 52, 72	1 (0%)
17	Y	27/30 (90%)	0.59	2 (7%) 20 22	37, 47, 70, 77	0
17	y	28/30 (93%)	0.79	1 (3%) 46 49	45, 55, 73, 77	0
18	X	38/40 (95%)	0.30	1 (2%) 57 61	23, 39, 65, 69	1 (2%)
18	x	38/40 (95%)	0.53	4 (10%) 11 12	26, 42, 83, 94	1 (2%)
19	Z	62/62 (100%)	0.64	8 (12%) 7 7	37, 46, 75, 92	0
19	z	60/62 (96%)	1.24	8 (13%) 7 7	47, 57, 88, 95	0
All	All	5235/5344 (97%)	-0.36	75 (1%) 73 76	11, 30, 59, 120	63 (1%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	64	ALA	5.7
2	B	494	GLY	4.3
2	b	502	VAL	4.2
2	b	499	VAL	4.2
19	z	3	ILE	4.0
2	b	490	GLN	4.0
19	z	2	THR	3.9
18	x	37	VAL	3.8
14	T	30	THR	3.7
19	z	36	SER	3.5
2	b	491	VAL	3.4
2	b	500	GLY	3.4
19	z	33	TRP	3.3
2	b	495	PHE	3.2
19	Z	62	VAL	3.2
13	O	60	ARG	3.2
19	Z	32	ASP	3.2
17	Y	22	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	b	488	PRO	3.1
14	t	30	THR	3.1
9	J	5	GLY	3.0
9	j	5	GLY	3.0
13	O	58	ASN	3.0
2	B	501	ASP	2.9
6	f	14	PRO	2.9
2	b	86	ILE	2.9
19	Z	1	MET	2.9
8	i	36	ASP	2.9
2	B	495	PHE	2.8
2	B	86	ILE	2.8
13	o	4	THR	2.8
11	l	1	MET	2.8
2	b	496	TYR	2.7
18	x	38	GLN	2.7
2	b	493	TRP	2.7
19	Z	33	TRP	2.7
5	E	4	THR	2.6
19	z	61	VAL	2.6
2	b	504	THR	2.6
2	B	483	ASP	2.6
19	Z	3	ILE	2.6
2	b	484	PRO	2.5
17	y	19	ILE	2.5
6	F	16	PHE	2.5
19	z	60	PHE	2.5
18	x	36	LYS	2.5
2	b	85	GLY	2.4
6	f	15	ILE	2.4
2	B	500	GLY	2.4
9	J	6	GLY	2.4
8	i	37	LEU	2.4
2	B	479	PHE	2.4
2	b	479	PHE	2.4
13	o	59	LYS	2.4
15	u	8	GLU	2.4
13	o	246	ALA	2.3
13	o	62	GLU	2.3
17	Y	23	THR	2.3
12	m	33	GLN	2.2
2	b	489	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
19	z	34	ASP	2.2
13	O	56	PRO	2.2
2	B	496	TYR	2.1
19	Z	7	LEU	2.1
18	x	35	ASP	2.1
2	b	503	THR	2.1
18	X	2	THR	2.1
2	b	497	GLN	2.1
1	a	11	ALA	2.1
7	H	64	ALA	2.1
6	f	16	PHE	2.0
19	Z	41	PHE	2.0
9	j	6	GLY	2.0
19	Z	31	GLN	2.0
19	z	50	LEU	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
12	FME	m	1	10/11	0.93	0.11	31,38,54,60	0
14	FME	t	1	10/11	0.93	0.08	20,23,41,50	0
12	FME	M	1	10/11	0.95	0.08	27,34,51,59	0
4	HSK	d	336[B]	11/12	0.96	0.08	30,31,37,38	8
14	FME	T	1	10/11	0.96	0.06	24,27,43,50	0
4	HSK	d	336[A]	10/12	0.96	0.08	30,33,40,44	7
4	HSK	D	336[A]	10/12	0.97	0.06	26,28,31,34	7
4	HSK	D	336[B]	11/12	0.97	0.06	23,26,27,29	8
8	FME	I	1	10/11	0.97	0.07	27,34,38,39	0
8	FME	i	1	10/11	0.98	0.06	30,32,37,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	DGD	d	406	50/66	0.60	0.17	56,75,94,97	0
29	UNL	b	630	16/-	0.66	0.15	51,62,73,74	0
34	DGD	D	406	53/66	0.67	0.15	53,77,92,103	0
29	UNL	b	631	16/-	0.69	0.17	59,66,77,79	0
29	UNL	E	103	12/-	0.70	0.16	65,73,83,88	0
29	UNL	B	629	14/-	0.71	0.17	61,70,89,90	0
36	LHG	a	417	40/49	0.71	0.14	60,109,148,151	0
29	UNL	i	103	13/-	0.72	0.16	58,65,76,78	0
29	UNL	a	420	40/-	0.72	0.16	53,72,88,94	0
29	UNL	j	103	12/-	0.73	0.14	55,65,70,71	0
29	UNL	E	102	15/-	0.74	0.20	57,64,83,83	0
29	UNL	c	926	10/-	0.74	0.14	65,67,71,72	0
29	UNL	Z	103	16/-	0.74	0.16	48,63,81,81	0
29	UNL	j	102	16/-	0.74	0.17	52,61,69,69	0
29	UNL	A	415	36/-	0.75	0.15	58,67,75,79	0
29	UNL	i	104	10/-	0.75	0.12	67,72,77,78	0
30	LMT	F	102	35/35	0.75	0.13	53,84,91,96	0
33	HTG	d	401	19/19	0.76	0.14	55,101,111,114	0
29	UNL	z	102	16/-	0.77	0.17	51,70,89,92	0
29	UNL	C	523	34/-	0.77	0.14	52,77,88,93	0
29	UNL	H	103	10/-	0.77	0.16	60,69,74,76	0
29	UNL	T	102	13/-	0.77	0.14	66,70,83,87	0
29	UNL	B	628	10/-	0.77	0.15	52,56,70,74	0
29	UNL	t	103	16/-	0.77	0.14	63,74,94,95	0
29	UNL	e	800	11/-	0.78	0.16	53,60,68,68	0
33	HTG	B	631	19/19	0.78	0.14	49,111,120,125	0
29	UNL	J	103	14/-	0.79	0.14	61,66,73,76	0
33	HTG	C	522	19/19	0.79	0.12	50,79,92,94	0
33	HTG	U	201	9/19	0.79	0.17	54,59,82,98	0
26	SQD	f	102	33/54	0.79	0.15	63,73,113,114	0
29	UNL	B	632	16/-	0.79	0.15	50,59,73,73	0
30	LMT	c	922	35/35	0.79	0.12	61,73,85,90	0
31	GOL	h	103	6/6	0.79	0.12	78,83,83,84	0
40	SO4	O	302	5/5	0.79	0.12	78,87,95,105	0
30	LMT	M	101	35/35	0.80	0.12	43,61,77,90	0
33	HTG	b	627	19/19	0.80	0.14	53,94,104,105	0
33	HTG	c	924	19/19	0.80	0.12	53,85,97,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	PL9	a	419	55/55	0.80	0.15	52,74,98,109	0
30	LMT	z	101	32/35	0.80	0.12	46,85,90,100	0
29	UNL	A	417	13/-	0.80	0.15	56,59,66,66	0
29	UNL	c	925	30/-	0.80	0.14	59,72,89,95	0
29	UNL	L	102	14/-	0.80	0.15	52,58,66,69	0
33	HTG	b	602	19/19	0.81	0.13	50,93,111,117	0
27	LMG	c	921	51/55	0.81	0.13	38,80,95,111	0
33	HTG	c	923	19/19	0.81	0.11	64,75,82,83	0
31	GOL	O	304	6/6	0.81	0.10	52,60,61,63	0
30	LMT	B	623	35/35	0.81	0.14	43,79,117,129	0
29	UNL	b	629	16/-	0.81	0.15	43,48,56,60	0
26	SQD	B	621	54/54	0.81	0.14	48,65,108,109	0
33	HTG	D	414	19/19	0.81	0.12	66,93,106,107	0
29	UNL	J	104	12/-	0.81	0.15	53,65,72,74	0
29	UNL	A	420	4/-	0.82	0.13	64,66,66,66	0
28	PL9	A	414	55/55	0.82	0.14	47,66,93,96	0
29	UNL	D	412	40/-	0.82	0.13	39,60,96,99	0
36	LHG	E	101	49/49	0.82	0.13	50,80,94,97	0
29	UNL	x	101	16/-	0.82	0.16	36,45,70,73	0
26	SQD	D	407	45/54	0.82	0.14	50,78,94,101	0
29	UNL	a	421	10/-	0.83	0.13	53,57,61,64	0
33	HTG	u	201	14/19	0.83	0.14	46,64,90,96	0
26	SQD	L	103	54/54	0.83	0.12	43,64,89,96	0
30	LMT	J	102	24/35	0.83	0.12	45,55,79,83	0
33	HTG	B	626	19/19	0.83	0.10	48,87,92,93	0
27	LMG	Z	101	51/55	0.83	0.14	41,76,102,113	0
29	UNL	d	411	16/-	0.83	0.12	39,49,63,66	0
29	UNL	M	103	16/-	0.84	0.13	49,58,77,79	0
32	CA	B	601	1/1	0.84	0.08	81,81,81,81	0
29	UNL	i	101	16/-	0.84	0.13	40,46,56,62	0
29	UNL	b	628	36/-	0.84	0.13	44,65,101,106	0
30	LMT	Z	102	35/35	0.84	0.14	41,87,102,107	0
29	UNL	a	403	6/-	0.84	0.09	57,62,66,66	0
29	UNL	I	102	11/-	0.84	0.12	62,65,66,68	0
30	LMT	C	520	35/35	0.84	0.11	52,71,83,89	0
31	GOL	b	636	6/6	0.84	0.12	45,56,58,60	0
31	GOL	b	635	6/6	0.85	0.12	40,43,46,48	0
30	LMT	b	624	25/35	0.85	0.11	51,71,94,98	0
31	GOL	c	928	6/6	0.85	0.10	42,51,54,54	0
29	UNL	I	101	13/-	0.85	0.10	44,53,61,63	0
29	UNL	D	413	16/-	0.85	0.12	39,47,65,65	0
31	GOL	C	524	6/6	0.85	0.19	36,45,47,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	SQD	A	418	54/54	0.85	0.11	42,59,81,86	0
31	GOL	c	927	6/6	0.86	0.12	43,53,60,68	0
30	LMT	b	625	24/35	0.86	0.14	35,61,99,100	0
26	SQD	a	401	54/54	0.86	0.11	45,59,85,90	0
30	LMT	t	102	24/35	0.86	0.12	33,55,94,95	0
29	UNL	i	102	16/-	0.86	0.11	54,65,83,84	0
30	LMT	m	102	35/35	0.87	0.10	41,54,72,84	0
29	UNL	A	416	16/-	0.87	0.12	41,46,73,73	0
29	UNL	X	101	16/-	0.87	0.12	34,39,58,60	0
31	GOL	A	422	6/6	0.87	0.11	42,55,58,67	0
30	LMT	A	419	35/35	0.88	0.10	37,56,73,94	0
31	GOL	l	102	6/6	0.88	0.13	37,55,57,57	0
33	HTG	V	202	13/19	0.88	0.09	43,48,76,84	0
30	LMT	a	402	35/35	0.88	0.10	37,54,69,80	0
27	LMG	A	413	51/55	0.88	0.10	42,57,76,78	0
29	UNL	B	627	16/-	0.88	0.12	43,47,69,69	0
30	LMT	M	102	35/35	0.88	0.10	35,52,60,63	0
31	GOL	b	633	6/6	0.90	0.10	41,46,49,52	0
31	GOL	B	638	6/6	0.90	0.10	35,47,49,53	0
27	LMG	a	418	51/55	0.90	0.09	43,60,68,73	0
31	GOL	L	104	6/6	0.90	0.11	44,52,54,55	0
30	LMT	m	101	35/35	0.90	0.09	32,51,61,62	0
32	CA	b	603	1/1	0.91	0.06	82,82,82,82	0
27	LMG	C	519	51/55	0.91	0.11	29,59,97,105	0
33	HTG	B	630	19/19	0.91	0.10	39,52,66,79	0
31	GOL	C	526	6/6	0.91	0.09	38,43,51,57	0
33	HTG	C	521	19/19	0.91	0.09	56,63,76,80	0
27	LMG	c	920	51/55	0.91	0.10	30,65,100,104	0
31	GOL	B	633	6/6	0.91	0.10	34,39,47,52	0
31	GOL	B	637	6/6	0.91	0.10	36,38,45,54	0
31	GOL	v	204	6/6	0.91	0.09	46,50,61,62	0
23	CLA	c	914	65/65	0.91	0.10	38,53,90,98	0
31	GOL	b	632	6/6	0.92	0.09	35,42,46,47	0
23	CLA	B	602	65/65	0.92	0.10	29,41,78,95	0
33	HTG	B	625	19/19	0.92	0.12	31,38,71,75	0
27	LMG	B	622	51/55	0.92	0.08	28,37,53,63	0
25	BCR	c	915	40/40	0.92	0.08	44,51,59,60	0
23	CLA	C	506	65/65	0.92	0.09	25,38,94,97	0
23	CLA	b	604	65/65	0.92	0.09	34,47,73,81	0
31	GOL	f	104	6/6	0.92	0.08	46,51,51,54	0
31	GOL	B	635	6/6	0.92	0.08	38,47,49,50	0
31	GOL	a	422	6/6	0.92	0.09	30,38,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	GOL	a	424	6/6	0.92	0.10	42,56,59,74	0
25	BCR	d	404	40/40	0.93	0.07	25,33,56,58	0
25	BCR	k	101	40/40	0.93	0.07	33,39,47,49	0
25	BCR	k	102	40/40	0.93	0.07	29,41,48,50	0
26	SQD	A	412	54/54	0.93	0.09	35,54,71,74	0
26	SQD	a	416	54/54	0.93	0.09	37,55,88,90	0
27	LMG	b	623	51/55	0.93	0.08	30,39,52,63	0
31	GOL	A	421	6/6	0.93	0.09	30,37,38,41	0
33	HTG	b	601	19/19	0.93	0.08	43,51,62,68	0
25	BCR	C	514	40/40	0.93	0.07	33,42,46,46	0
38	RRX	H	101	41/41	0.93	0.07	25,30,44,47	0
38	RRX	h	101	41/41	0.93	0.07	27,35,49,54	0
33	HTG	b	626	19/19	0.93	0.12	29,40,73,75	0
31	GOL	A	423	6/6	0.94	0.10	39,43,45,53	0
23	CLA	C	512	65/65	0.94	0.07	34,41,69,74	0
25	BCR	D	404	40/40	0.94	0.07	24,29,55,57	0
25	BCR	T	101	40/40	0.94	0.06	24,32,47,53	0
23	CLA	b	609	65/65	0.94	0.08	23,31,57,63	0
23	CLA	c	907	65/65	0.94	0.07	28,36,76,80	0
23	CLA	c	913	65/65	0.94	0.07	33,45,67,72	0
34	DGD	c	918	62/66	0.94	0.08	27,35,79,91	0
31	GOL	c	930	6/6	0.94	0.07	49,54,57,59	0
35	BCT	D	401	4/4	0.94	0.08	32,35,41,51	0
31	GOL	D	415	6/6	0.94	0.12	35,36,42,46	0
23	CLA	C	513	65/65	0.94	0.08	35,46,78,83	0
25	BCR	t	101	40/40	0.94	0.06	23,30,42,44	0
31	GOL	v	203	6/6	0.94	0.10	31,35,41,43	0
27	LMG	d	410	51/55	0.94	0.09	29,36,80,91	0
25	BCR	K	101	40/40	0.95	0.06	30,35,40,43	0
31	GOL	V	203	6/6	0.95	0.08	26,32,36,38	0
31	GOL	V	204	6/6	0.95	0.07	39,52,59,59	0
31	GOL	V	205	6/6	0.95	0.09	33,36,37,41	0
27	LMG	D	411	51/55	0.95	0.09	23,35,91,99	0
31	GOL	a	423	6/6	0.95	0.09	33,34,35,45	0
25	BCR	K	102	40/40	0.95	0.07	28,31,39,42	0
23	CLA	b	612	65/65	0.95	0.06	26,30,36,38	0
34	DGD	H	102	62/66	0.95	0.07	24,31,40,45	0
31	GOL	B	636	6/6	0.95	0.09	33,43,47,56	0
34	DGD	c	919	62/66	0.95	0.07	25,35,60,71	0
31	GOL	b	634	6/6	0.95	0.08	32,39,44,46	0
34	DGD	h	102	62/66	0.95	0.07	27,35,45,52	0
23	CLA	c	908	65/65	0.95	0.07	26,32,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	BCT	a	408	4/4	0.95	0.07	30,32,37,46	0
36	LHG	D	408	49/49	0.95	0.07	26,35,45,45	0
23	CLA	c	912	65/65	0.95	0.07	29,37,45,50	0
23	CLA	b	617	65/65	0.95	0.07	20,25,71,83	0
36	LHG	d	409	49/49	0.95	0.09	27,32,85,91	0
23	CLA	c	902	65/65	0.95	0.07	27,34,46,50	0
23	CLA	c	904	65/65	0.95	0.06	24,37,42,42	0
23	CLA	c	905	65/65	0.95	0.06	24,31,64,66	0
23	CLA	c	909	65/65	0.96	0.06	25,30,82,98	0
23	CLA	c	911	65/65	0.96	0.06	24,30,41,45	0
23	CLA	B	615	65/65	0.96	0.07	19,24,67,74	0
23	CLA	D	403	65/65	0.96	0.07	22,28,73,79	0
23	CLA	B	616	65/65	0.96	0.06	23,28,48,50	0
23	CLA	d	403	65/65	0.96	0.07	25,32,83,90	0
25	BCR	A	411	40/40	0.96	0.05	21,26,33,36	0
25	BCR	B	619	40/40	0.96	0.06	19,26,42,45	0
25	BCR	B	620	40/40	0.96	0.06	22,31,41,44	0
23	CLA	b	605	65/65	0.96	0.06	24,29,36,39	0
25	BCR	C	515	40/40	0.96	0.06	28,34,41,44	0
23	CLA	C	503	65/65	0.96	0.06	26,31,38,39	0
23	CLA	C	505	65/65	0.96	0.06	26,31,47,51	0
23	CLA	b	613	65/65	0.96	0.06	24,28,35,40	0
23	CLA	b	615	65/65	0.96	0.06	19,27,33,38	0
25	BCR	a	415	40/40	0.96	0.05	21,25,30,31	0
34	DGD	C	516	62/66	0.96	0.07	22,32,85,87	0
34	DGD	C	517	62/66	0.96	0.07	22,31,78,92	0
34	DGD	C	518	62/66	0.96	0.06	20,30,68,75	0
28	PL9	D	405	55/55	0.96	0.05	18,23,31,38	0
25	BCR	b	621	40/40	0.96	0.06	21,28,43,46	0
34	DGD	c	917	62/66	0.96	0.07	24,33,77,80	0
25	BCR	b	622	40/40	0.96	0.06	25,33,43,45	0
23	CLA	B	607	65/65	0.96	0.07	21,27,55,61	0
25	BCR	c	916	40/40	0.96	0.06	28,36,45,47	0
23	CLA	b	618	65/65	0.96	0.06	24,30,49,53	0
23	CLA	b	619	65/65	0.96	0.08	25,32,89,97	0
31	GOL	v	202	6/6	0.96	0.08	35,36,40,41	0
23	CLA	C	507	65/65	0.96	0.06	26,33,56,61	0
36	LHG	D	410	46/49	0.96	0.07	24,32,82,87	0
23	CLA	C	508	65/65	0.96	0.06	24,29,73,81	0
36	LHG	L	101	49/49	0.96	0.06	22,31,44,49	0
23	CLA	C	509	65/65	0.96	0.06	27,31,47,51	0
36	LHG	d	407	49/49	0.96	0.06	27,36,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	CA	O	301	1/1	0.96	0.07	49,49,49,49	0
36	LHG	l	101	49/49	0.96	0.07	22,31,47,57	0
23	CLA	C	511	65/65	0.96	0.06	27,34,40,42	0
32	CA	o	301	1/1	0.96	0.06	51,51,51,51	0
23	CLA	B	610	65/65	0.96	0.06	23,28,33,35	0
23	CLA	C	501	65/65	0.97	0.05	25,32,46,53	0
23	CLA	C	502	65/65	0.97	0.05	21,26,39,48	0
23	CLA	b	606	65/65	0.97	0.05	20,26,37,42	0
23	CLA	b	607	65/65	0.97	0.06	20,25,54,59	0
24	PHO	A	408	64/64	0.97	0.04	16,21,25,27	0
24	PHO	A	409	64/64	0.97	0.04	19,22,29,37	0
24	PHO	a	413	64/64	0.97	0.05	19,25,30,35	0
23	CLA	b	608	65/65	0.97	0.05	20,24,33,34	0
25	BCR	B	618	40/40	0.97	0.05	20,26,29,30	0
23	CLA	A	410	65/65	0.97	0.08	20,24,99,105	0
23	CLA	b	611	65/65	0.97	0.04	22,27,39,43	0
23	CLA	C	504	65/65	0.97	0.06	23,28,62,68	0
23	CLA	B	608	65/65	0.97	0.05	17,20,34,37	0
23	CLA	B	603	65/65	0.97	0.05	23,26,34,37	0
23	CLA	b	616	65/65	0.97	0.05	20,24,46,50	0
23	CLA	B	611	65/65	0.97	0.05	19,25,34,39	0
23	CLA	B	612	65/65	0.97	0.05	18,21,34,37	0
23	CLA	B	613	65/65	0.97	0.05	19,24,31,34	0
25	BCR	b	620	40/40	0.97	0.04	23,27,33,33	0
28	PL9	d	405	55/55	0.97	0.05	19,25,30,34	0
23	CLA	C	510	65/65	0.97	0.05	22,28,38,41	0
23	CLA	c	903	65/65	0.97	0.06	22,29,42,55	0
23	CLA	B	614	65/65	0.97	0.05	18,23,48,54	0
32	CA	F	103	1/1	0.97	0.10	55,55,55,55	0
31	GOL	B	634	6/6	0.97	0.08	29,29,34,37	0
23	CLA	B	604	65/65	0.97	0.05	17,22,34,41	0
32	CA	c	901	1/1	0.97	0.06	46,46,46,46	0
32	CA	f	103	1/1	0.97	0.11	56,56,56,56	0
23	CLA	c	906	65/65	0.97	0.05	26,31,46,50	0
33	HTG	B	624	19/19	0.97	0.06	27,33,41,51	0
36	LHG	d	408	49/49	0.97	0.06	22,27,42,47	0
23	CLA	B	606	65/65	0.97	0.05	17,23,35,40	0
23	CLA	B	617	65/65	0.97	0.08	20,28,79,83	0
37	HEM	f	101	43/43	0.97	0.08	39,47,61,77	0
23	CLA	a	411	65/65	0.97	0.07	18,23,106,117	0
23	CLA	c	910	65/65	0.97	0.06	25,31,49,52	0
23	CLA	a	414	65/65	0.97	0.08	19,25,99,104	0

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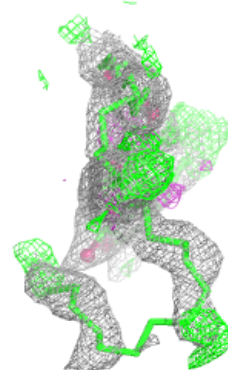
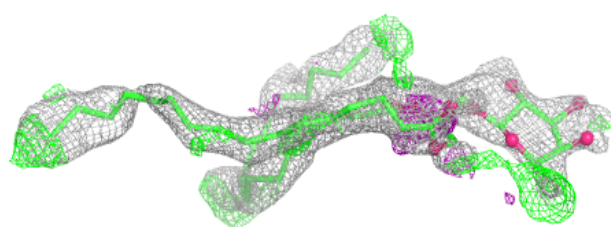
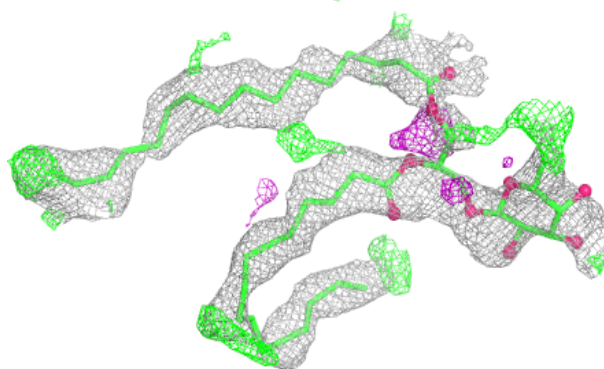
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	GOL	c	929	6/6	0.98	0.04	25,27,30,30	0
23	CLA	B	609	65/65	0.98	0.04	18,24,31,34	0
23	CLA	b	614	65/65	0.98	0.05	20,24,36,45	0
36	LHG	D	409	49/49	0.98	0.05	22,28,40,44	0
23	CLA	B	605	65/65	0.98	0.05	19,22,53,55	0
24	PHO	a	412	64/64	0.98	0.04	17,22,26,27	0
23	CLA	D	402	65/65	0.98	0.04	13,18,36,39	0
23	CLA	A	406	65/65	0.98	0.04	13,18,29,39	0
23	CLA	a	409	65/65	0.98	0.04	18,21,31,43	0
23	CLA	a	410	65/65	0.98	0.04	17,20,28,34	0
33	HTG	O	303	19/19	0.98	0.06	27,32,50,52	0
31	GOL	C	525	6/6	0.98	0.04	26,26,27,29	0
37	HEM	F	101	43/43	0.98	0.07	36,42,49,52	0
23	CLA	b	610	65/65	0.98	0.04	18,23,32,35	0
37	HEM	v	201	43/43	0.98	0.06	25,31,35,38	0
23	CLA	A	407	65/65	0.98	0.06	18,21,80,92	0
23	CLA	A	405	65/65	0.98	0.04	14,19,25,42	0
39	MG	J	101	1/1	0.98	0.05	28,28,28,28	0
39	MG	j	101	1/1	0.98	0.09	35,35,35,35	0
23	CLA	d	402	65/65	0.98	0.04	18,21,39,44	0
37	HEM	V	201	43/43	0.99	0.04	22,24,28,33	0
22	CL	a	406	1/1	0.99	0.06	29,29,29,29	0
22	CL	A	403	1/1	0.99	0.04	25,25,25,25	0
22	CL	A	404	1/1	0.99	0.02	22,22,22,22	0
21	FE2	A	402	1/1	1.00	0.01	26,26,26,26	0
22	CL	a	407	1/1	1.00	0.02	27,27,27,27	0
21	FE2	a	405	1/1	1.00	0.01	27,27,27,27	0
20	OEX	A	401	10/10	1.00	0.03	21,23,27,28	0
20	OEX	a	404	10/10	1.00	0.02	22,26,28,29	0

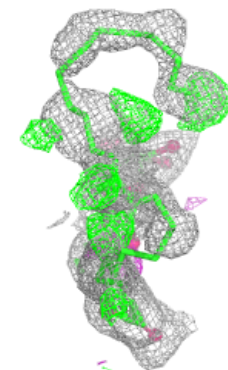
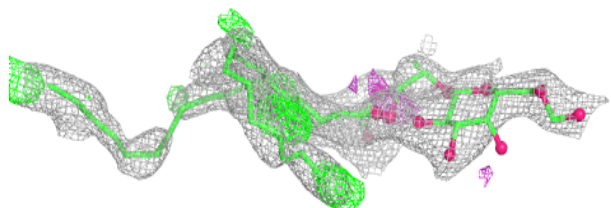
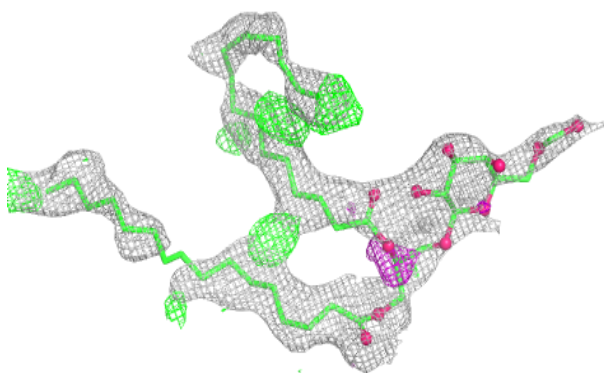
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD 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)

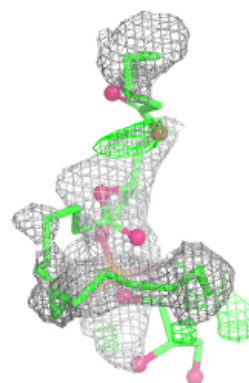
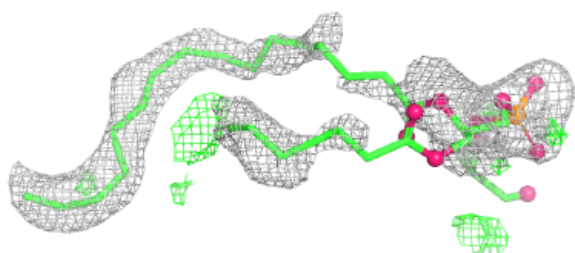
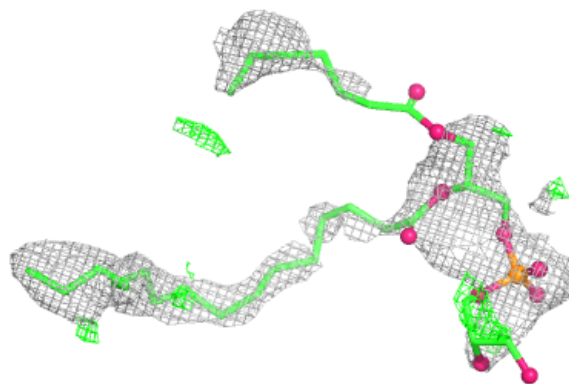
**Electron density around DGD D 406:**

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

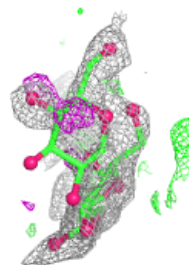
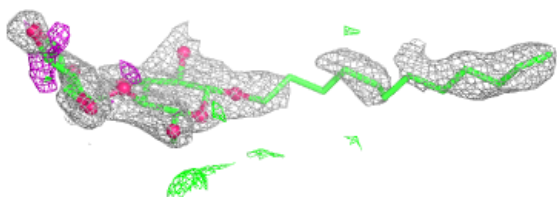
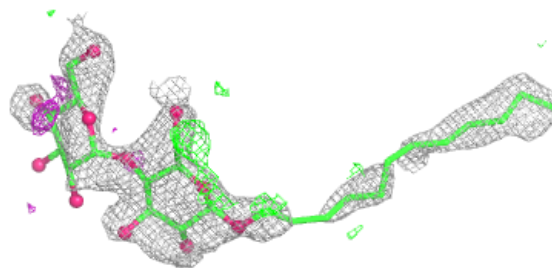


Electron density around LHG a 417:

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

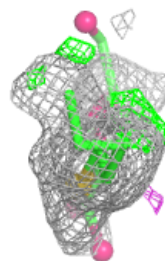
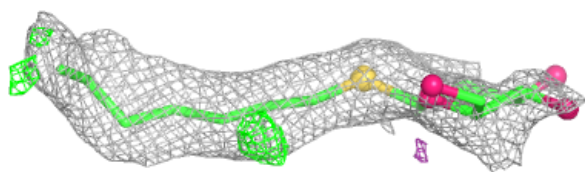
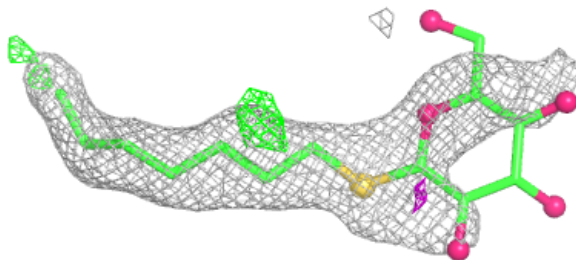
**Electron density around LMT F 102:**

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

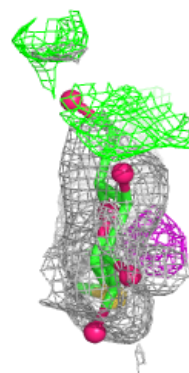
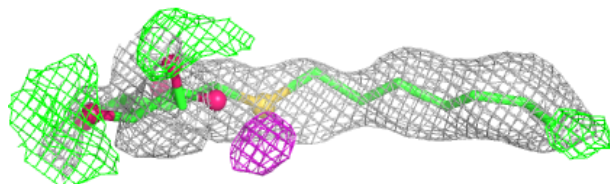
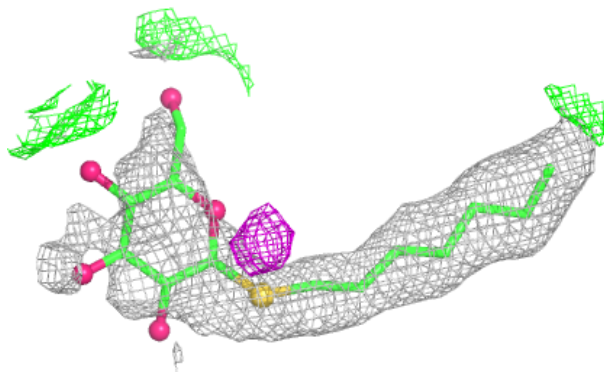


Electron density around HTG d 401:

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

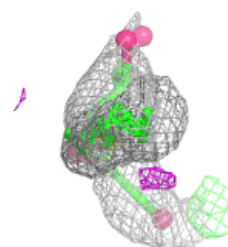
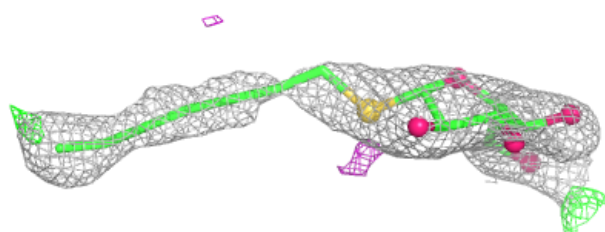
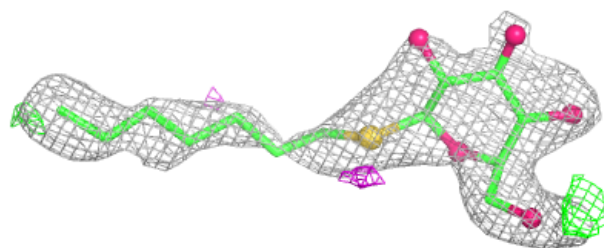
**Electron density around HTG B 631:**

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

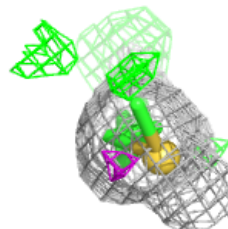
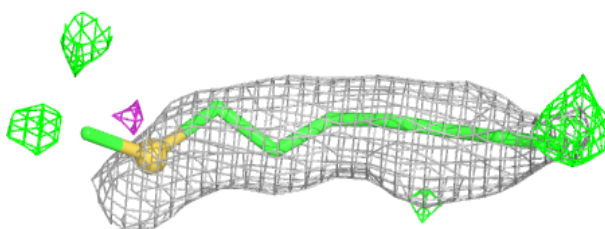
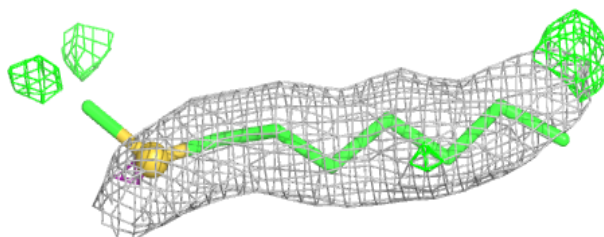


Electron density around HTG C 522:

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

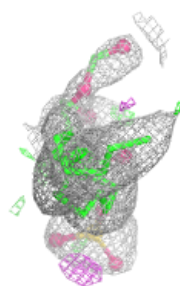
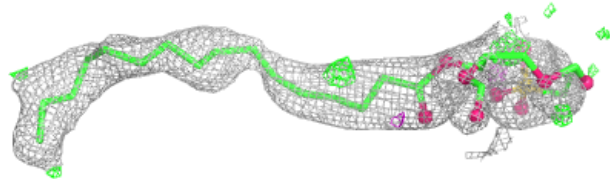
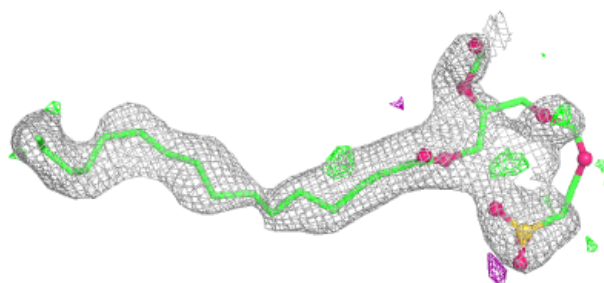
**Electron density around HTG U 201:**

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

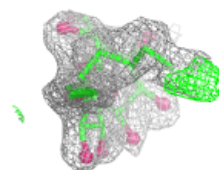
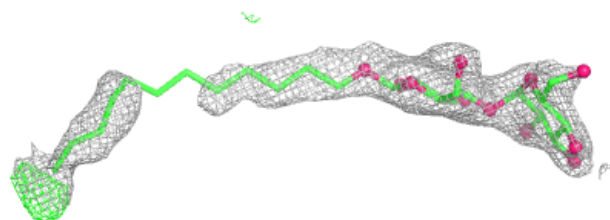
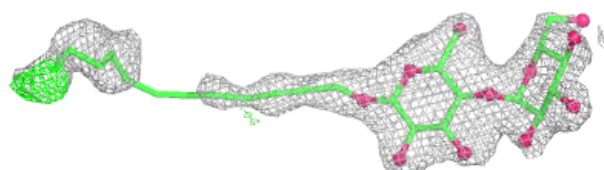


Electron density around SQD f 102:

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

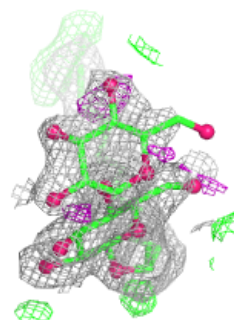
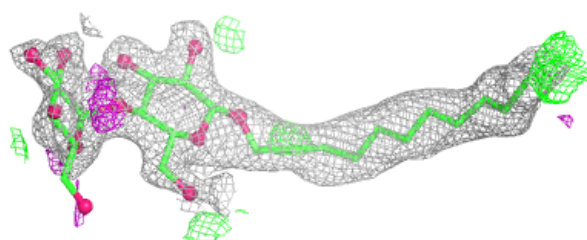
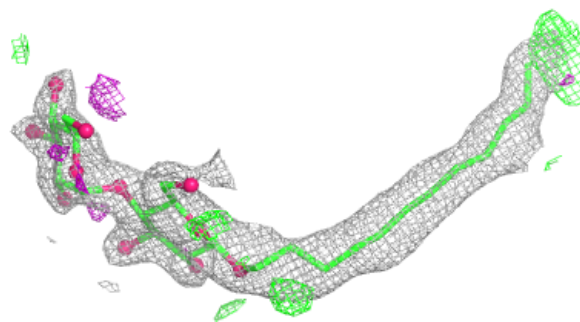
**Electron density around LMT c 922:**

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

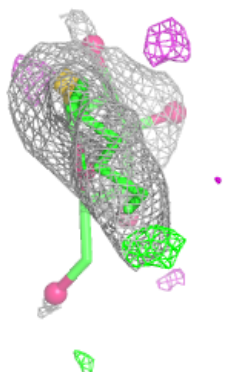
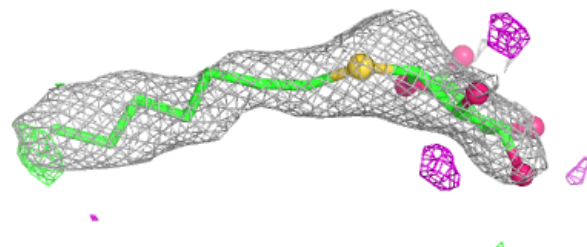
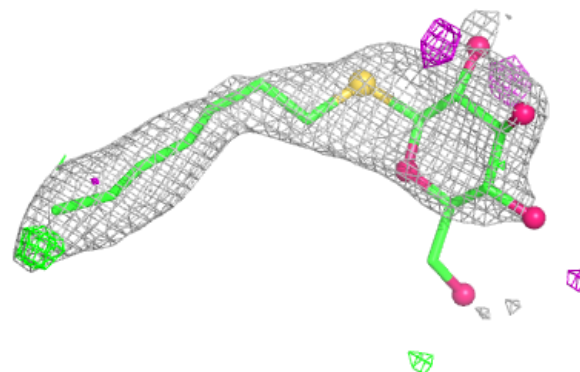


Electron density around LMT M 101:

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

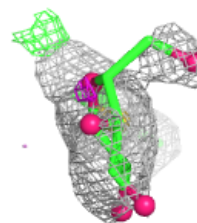
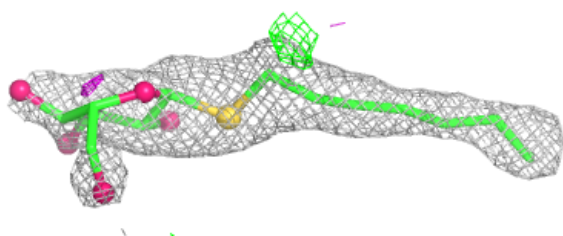
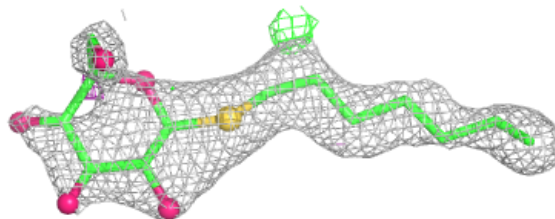
**Electron density around HTG b 627:**

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

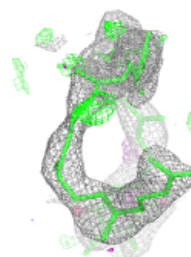
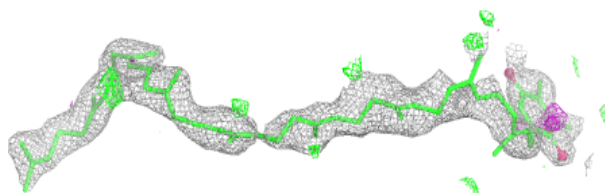
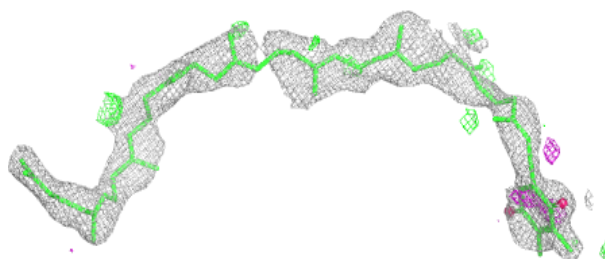


Electron density around HTG c 924:

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

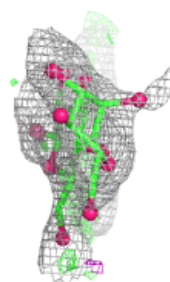
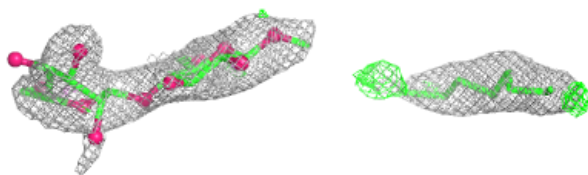
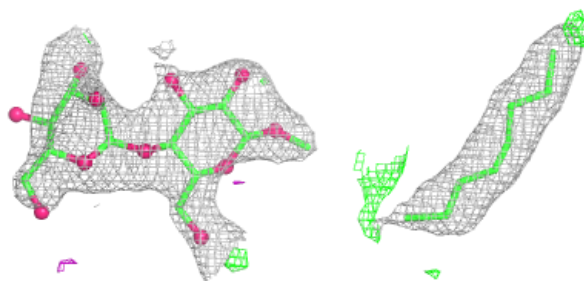
**Electron density around PL9 a 419:**

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

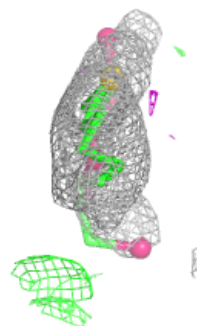
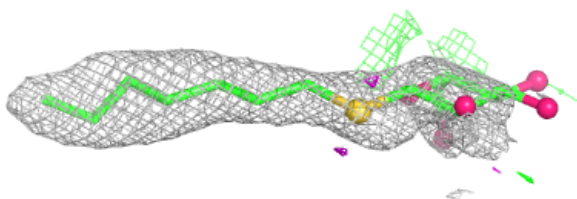
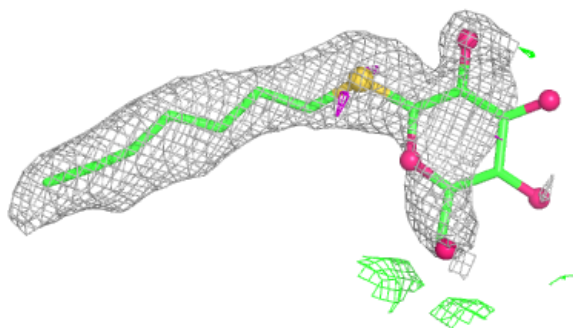


Electron density around LMT z 101:

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

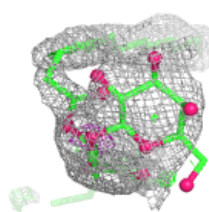
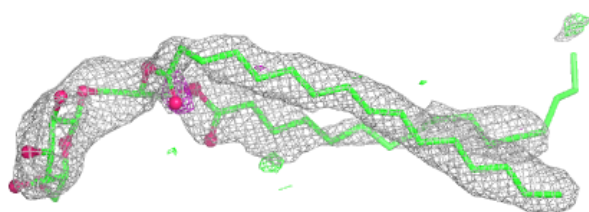
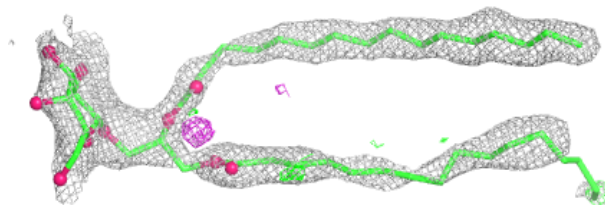
**Electron density around HTG b 602:**

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

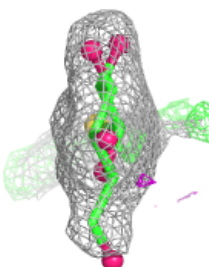
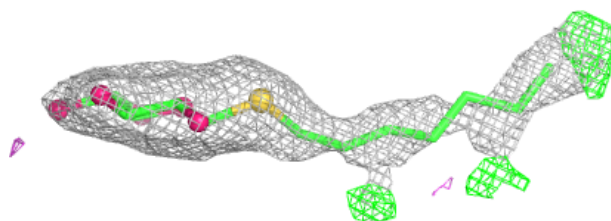
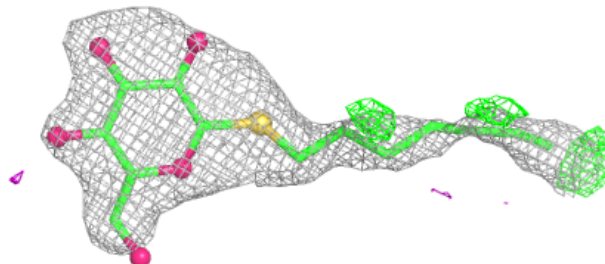


Electron density around LMG c 921:

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

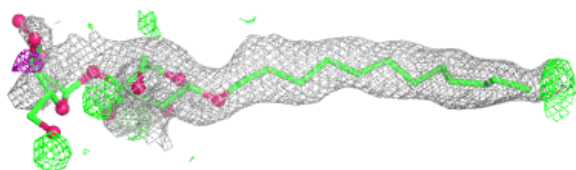
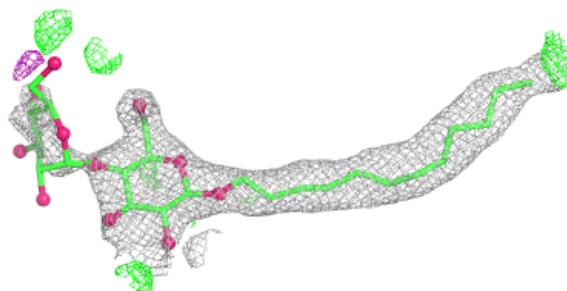
**Electron density around HTG c 923:**

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

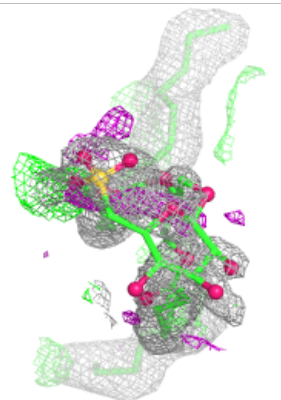
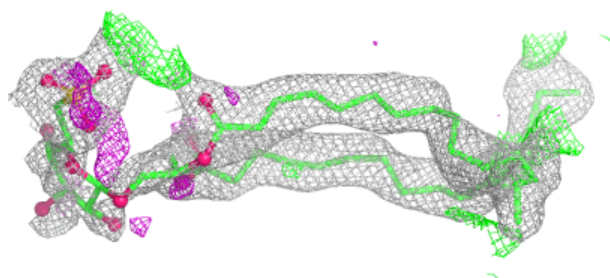
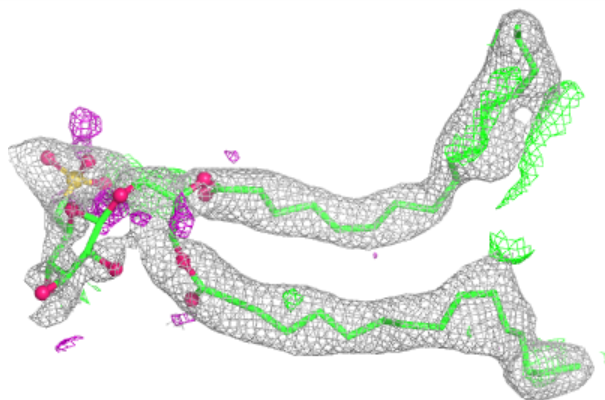


Electron density around LMT B 623:

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

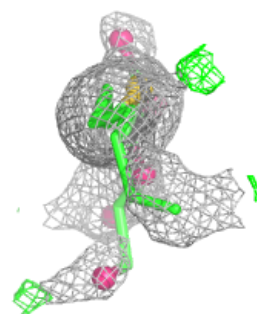
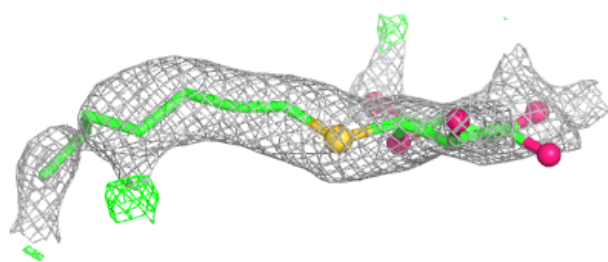
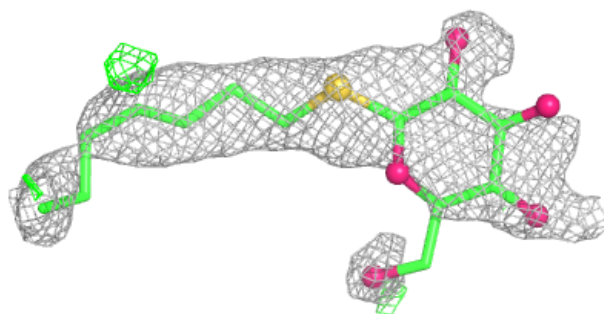
**Electron density around SQD B 621:**

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

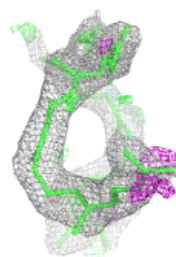
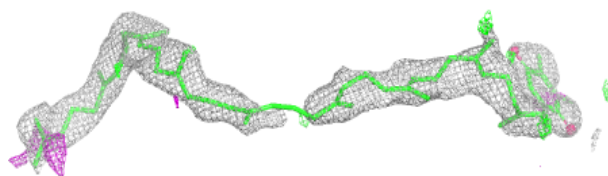
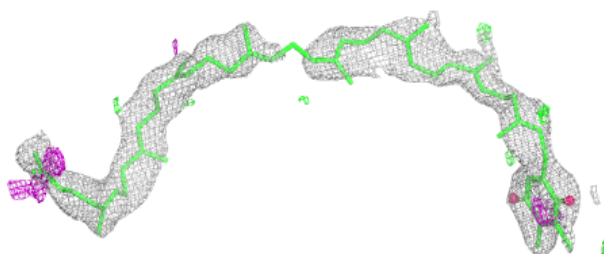


Electron density around HTG D 414:

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

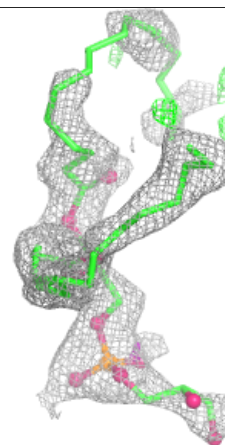
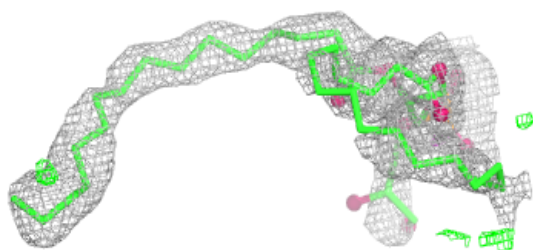
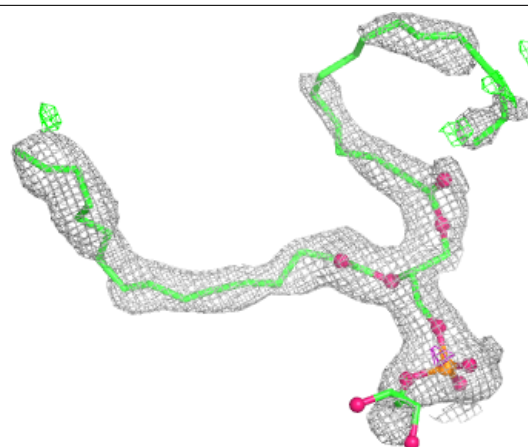
**Electron density around PL9 A 414:**

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

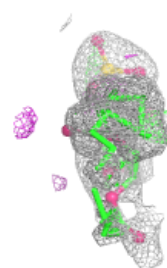
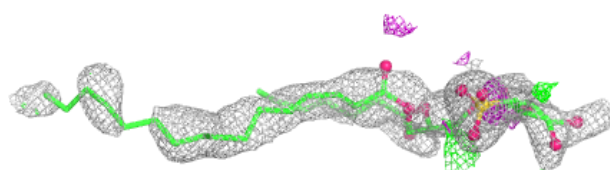
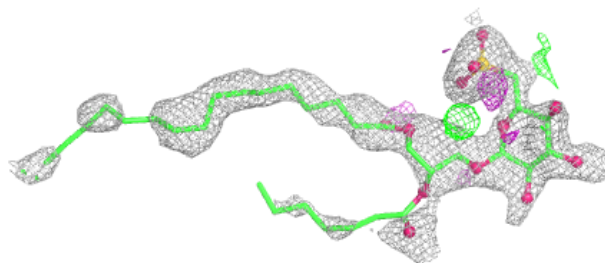


Electron density around LHG E 101:

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

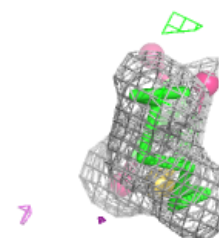
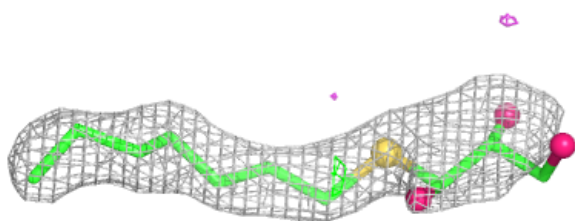
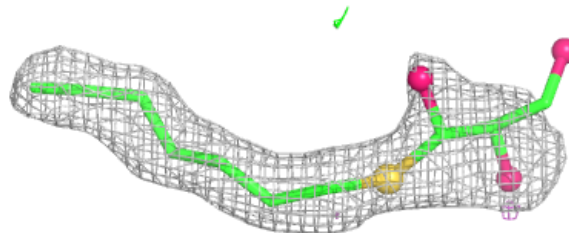
**Electron density around SQD D 407:**

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

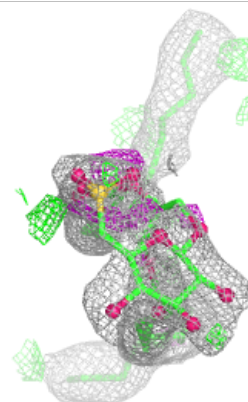
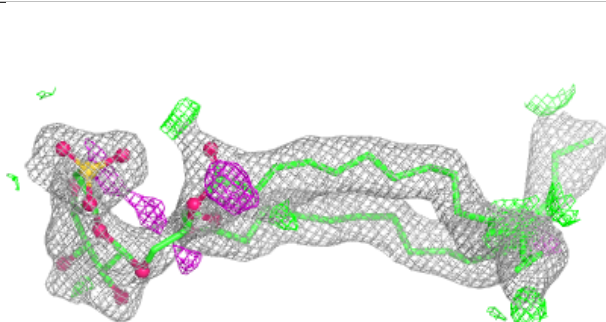
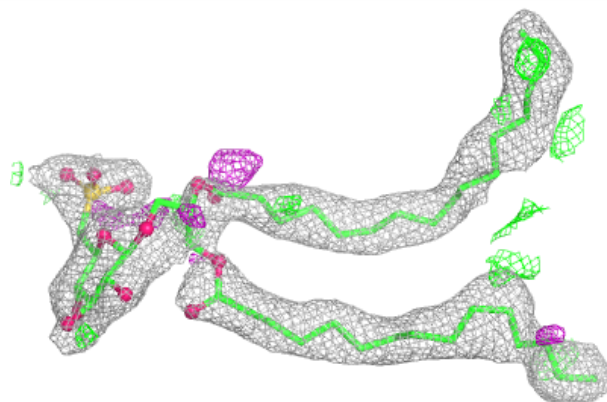


Electron density around HTG u 201:

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

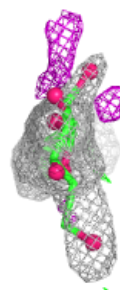
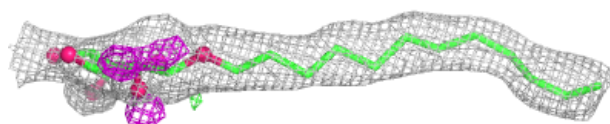
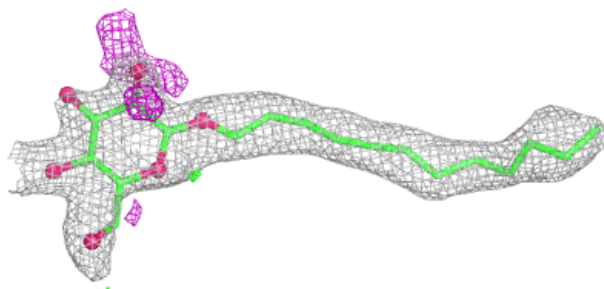
**Electron density around SQD L 103:**

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

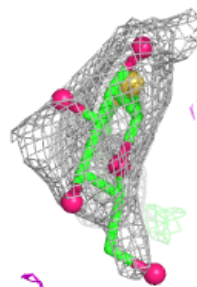
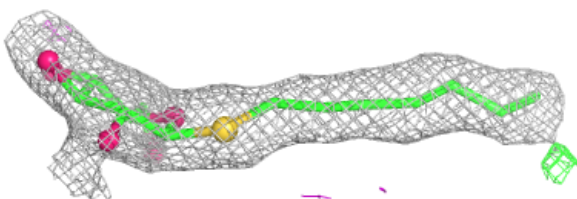
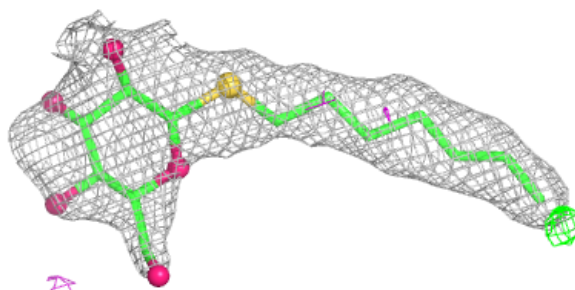


Electron density around LMT J 102:

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

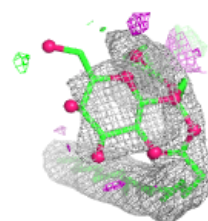
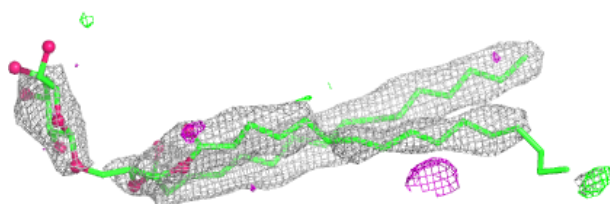
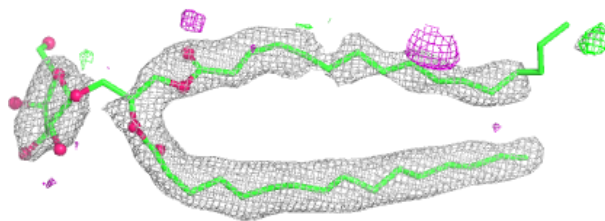
**Electron density around HTG B 626:**

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

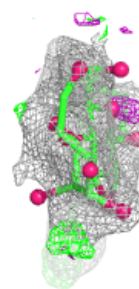
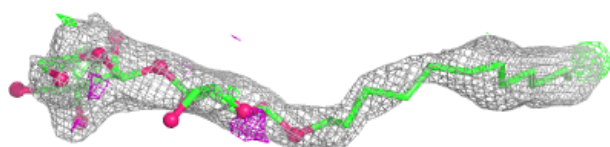
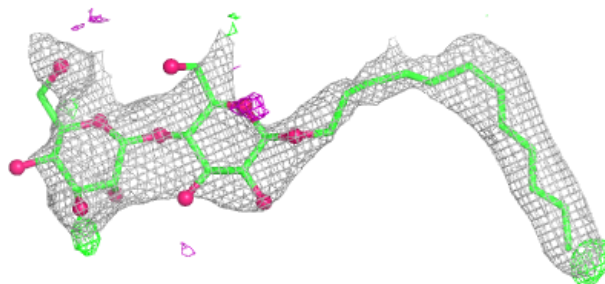


Electron density around LMG Z 101:

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

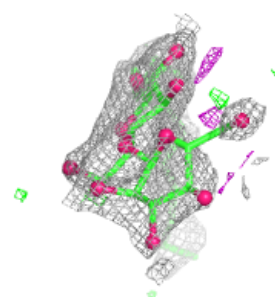
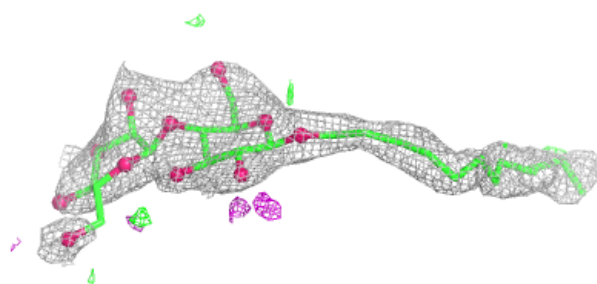
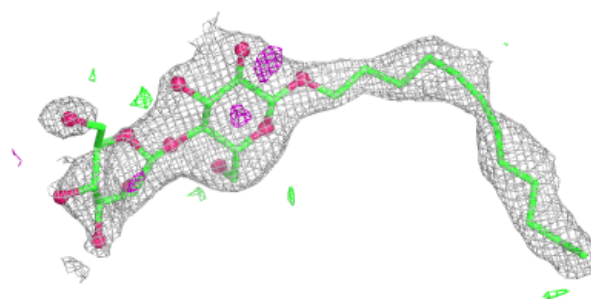
**Electron density around LMT Z 102:**

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

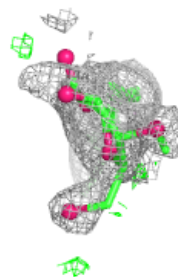
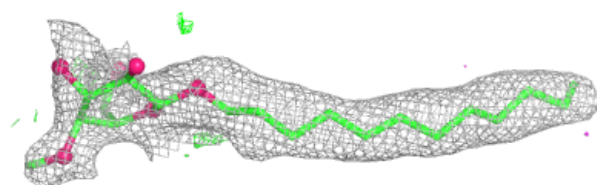
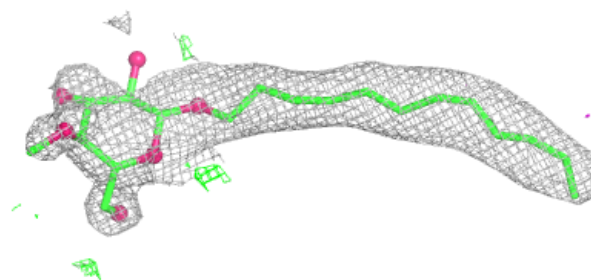


Electron density around LMT C 520:

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

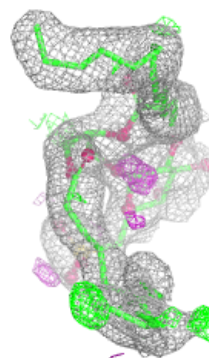
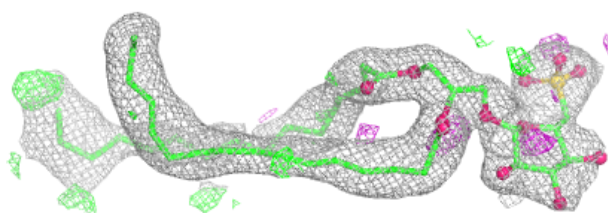
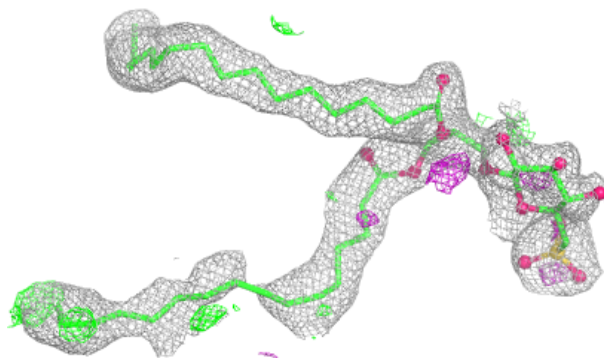
**Electron density around LMT b 624:**

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

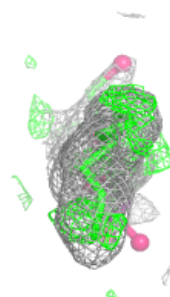
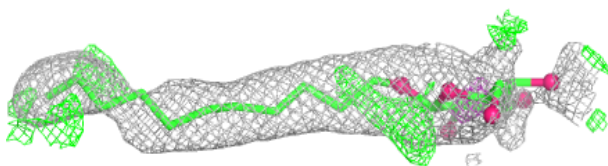
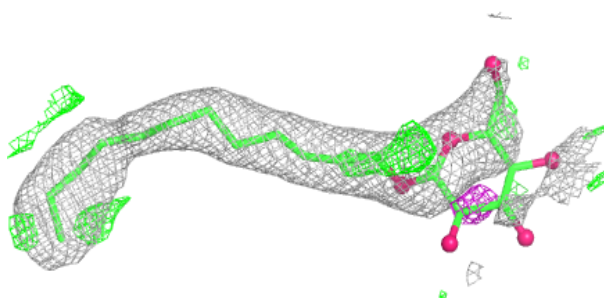


Electron density around SQD A 418:

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

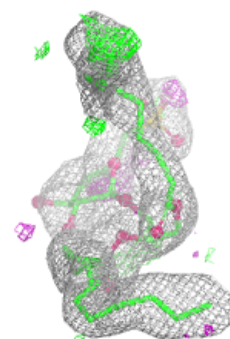
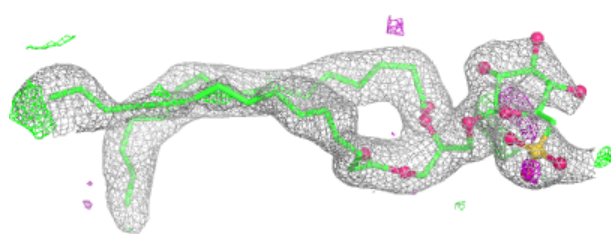
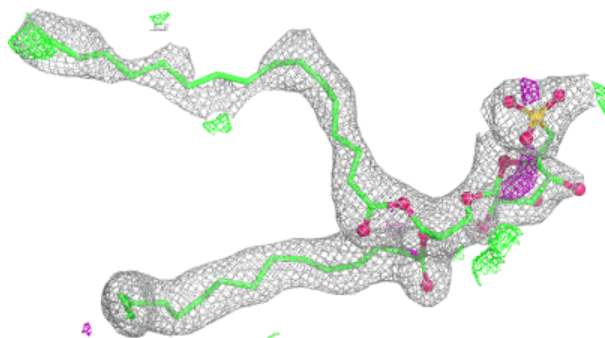
**Electron density around LMT b 625:**

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

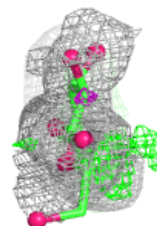
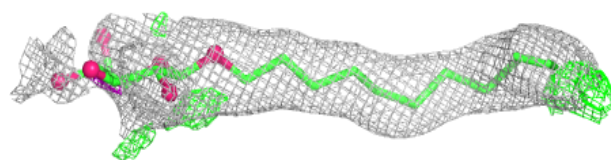
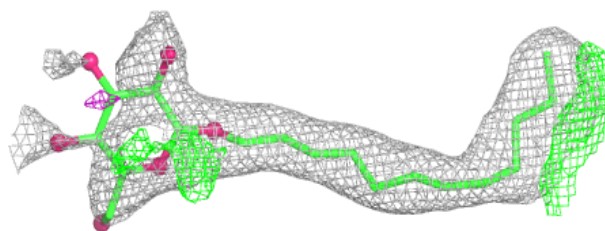


Electron density around SQD a 401:

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

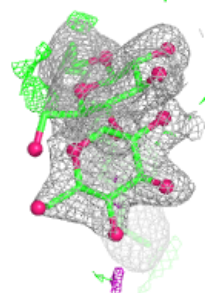
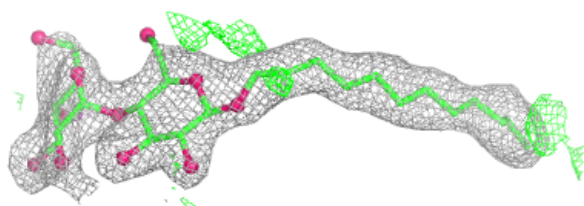
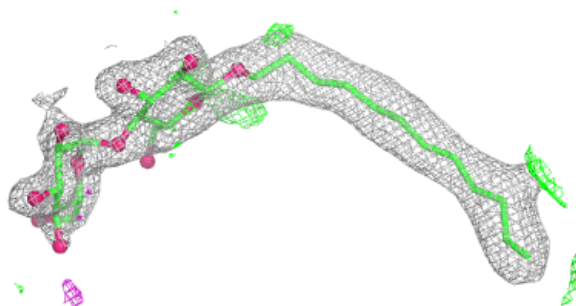
**Electron density around LMT t 102:**

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

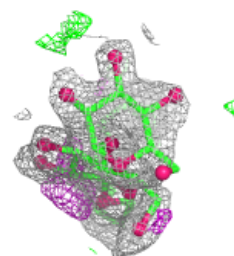
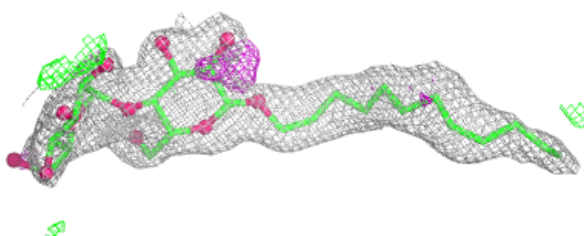
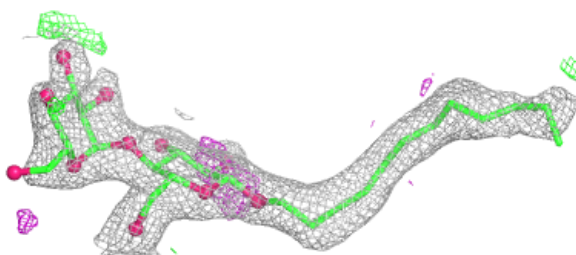


Electron density around LMT m 102:

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

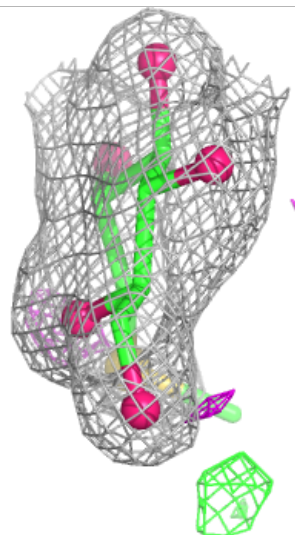
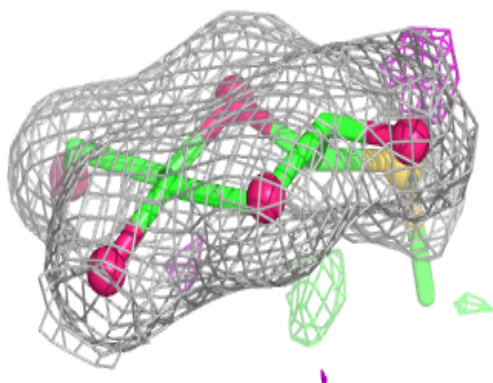
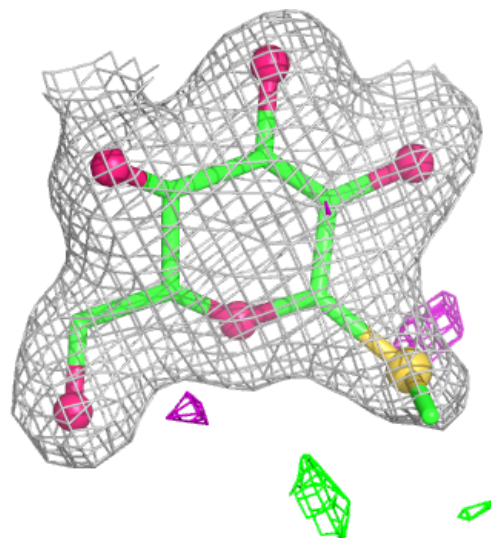
**Electron density around LMT A 419:**

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



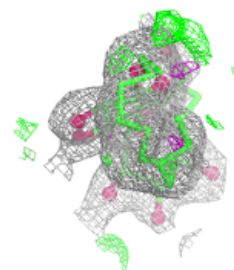
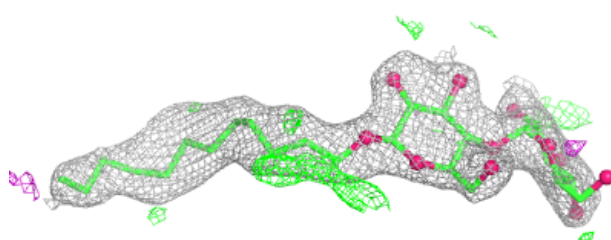
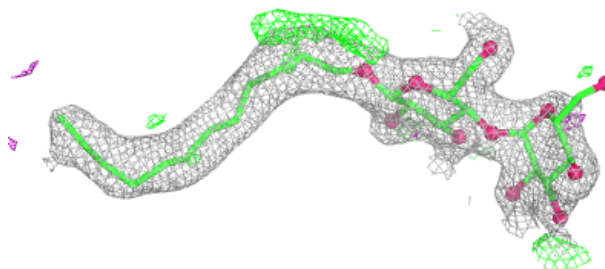
Electron density around HTG V 202:

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

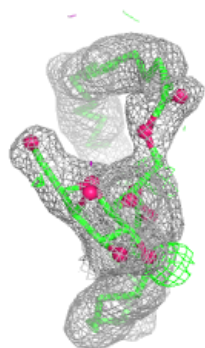
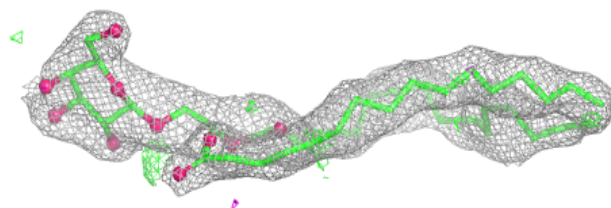
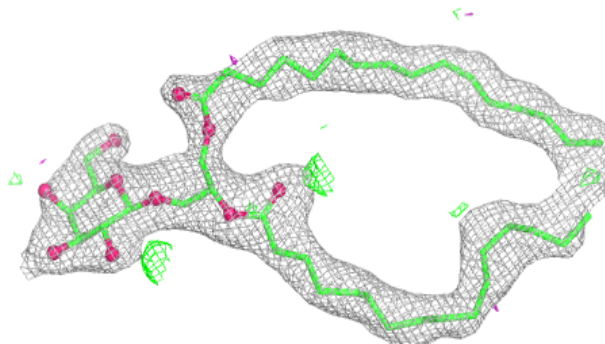


Electron density around LMT a 402:

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

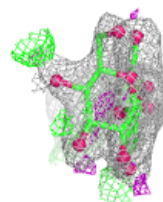
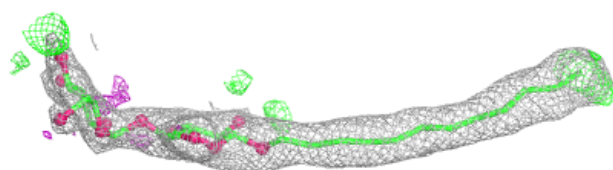
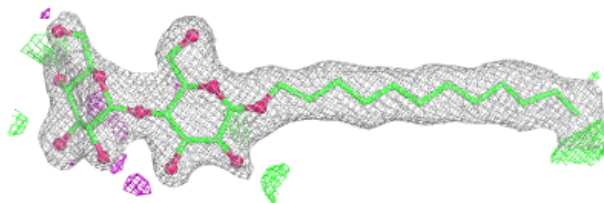
**Electron density around LMG A 413:**

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

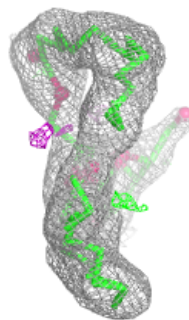
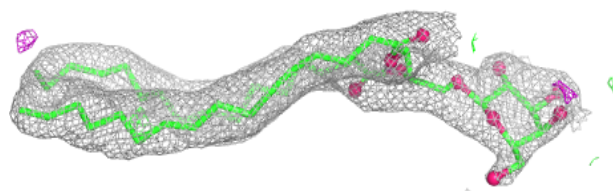
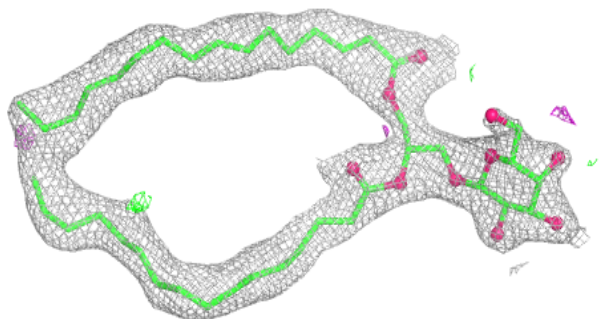


Electron density around LMT M 102:

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

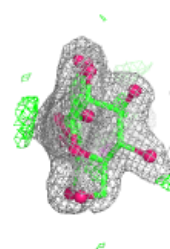
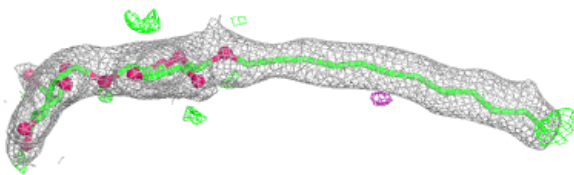
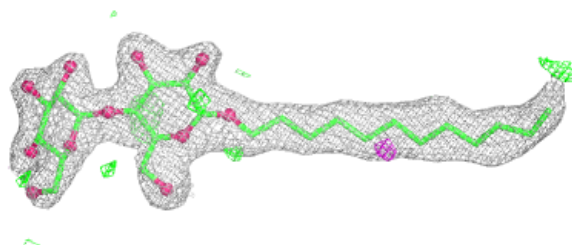
**Electron density around LMG a 418:**

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



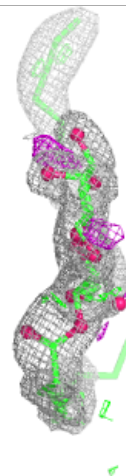
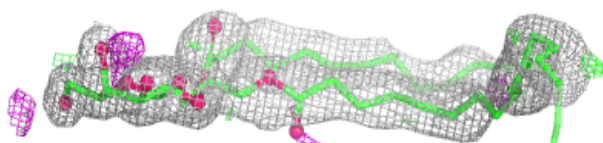
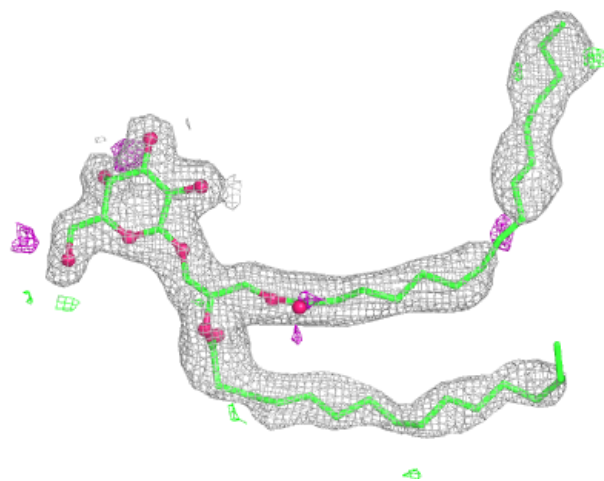
Electron density around LMT m 101:

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



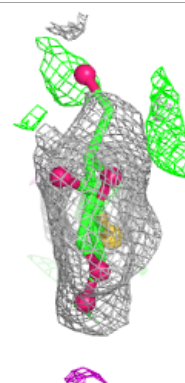
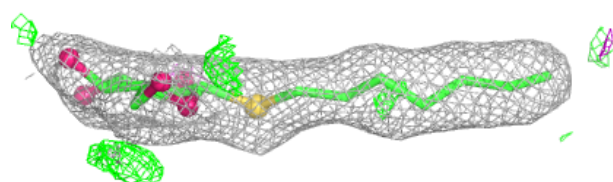
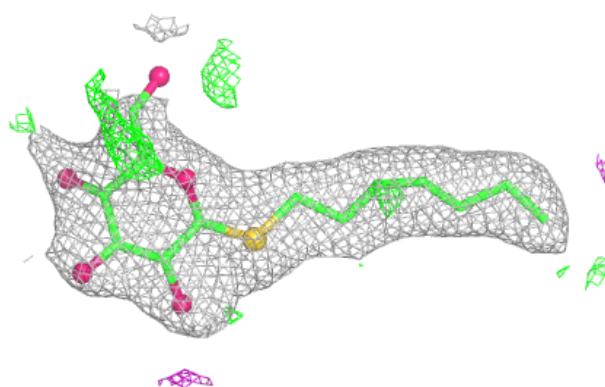
Electron density around LMG C 519:

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

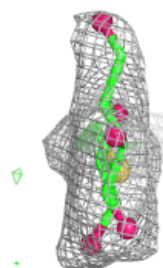
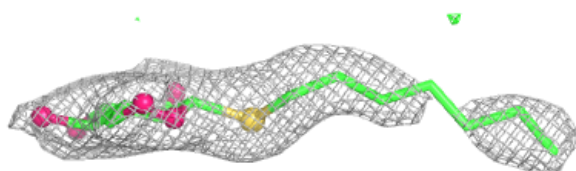
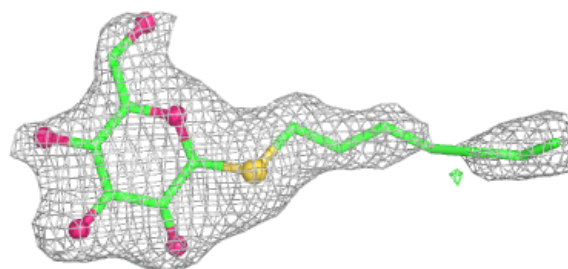


Electron density around HTG B 630:

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

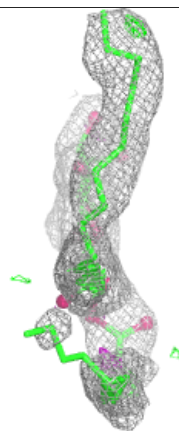
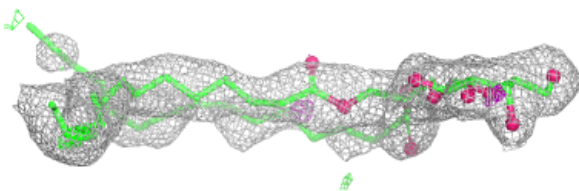
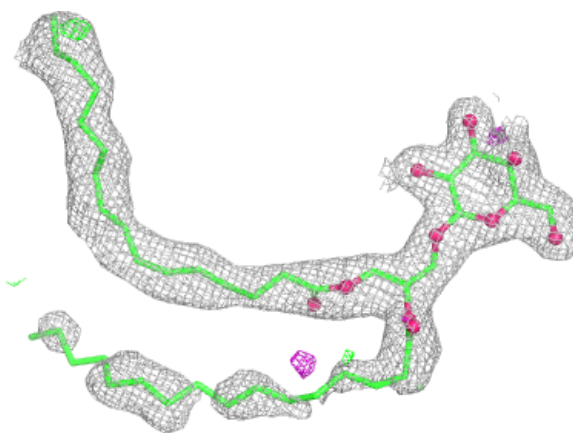
**Electron density around HTG C 521:**

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

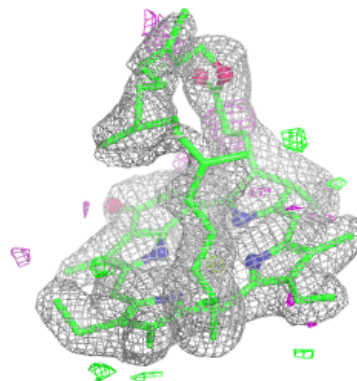
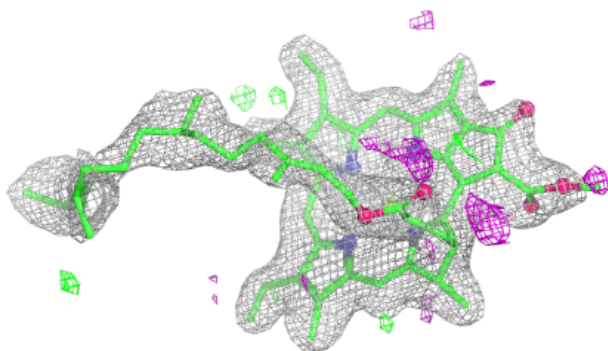
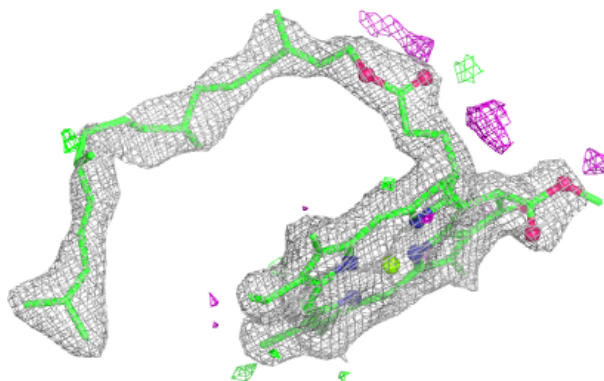


Electron density around LMG c 920:

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

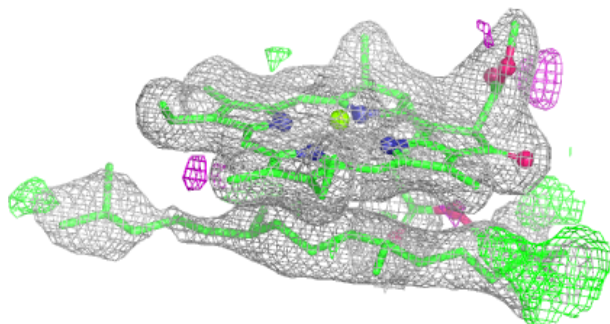
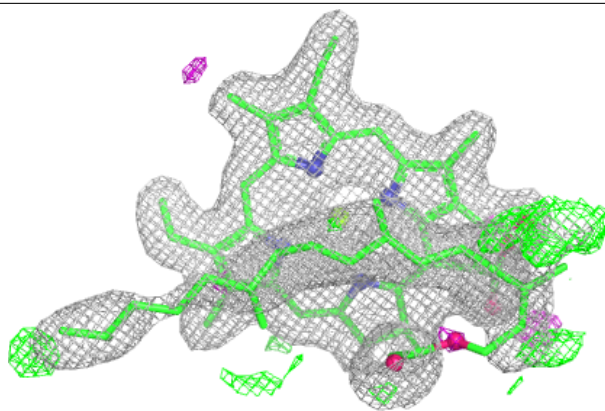
**Electron density around CLA c 914:**

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

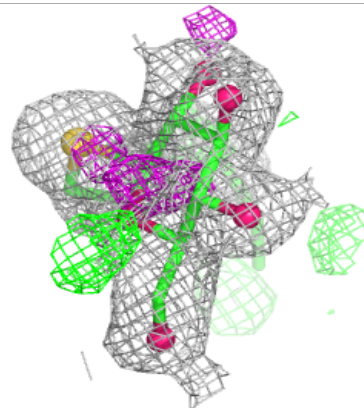
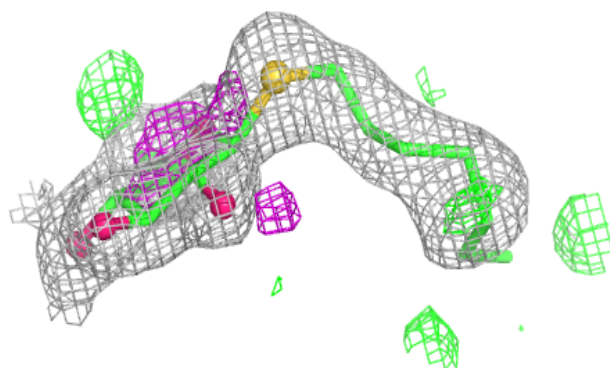
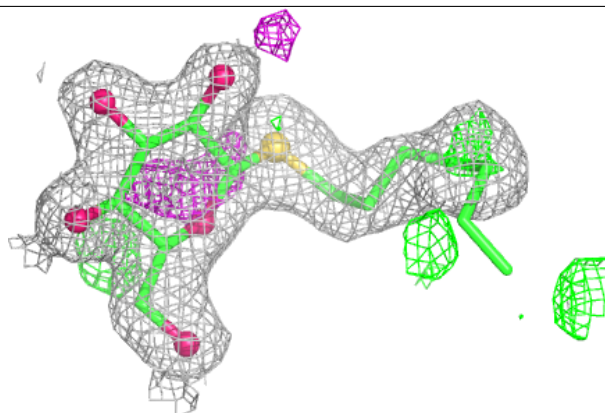


Electron density around CLA B 602:

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

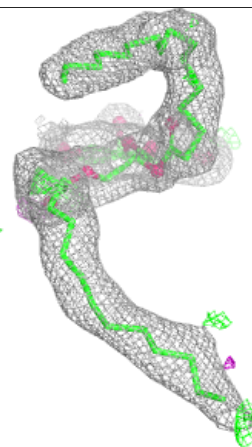
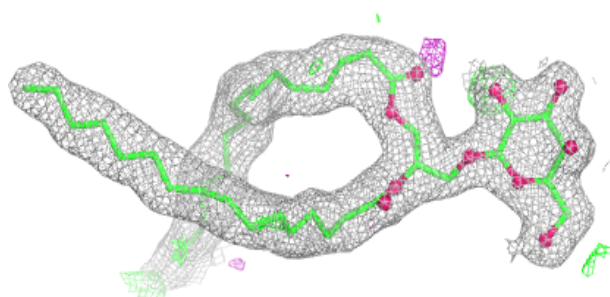
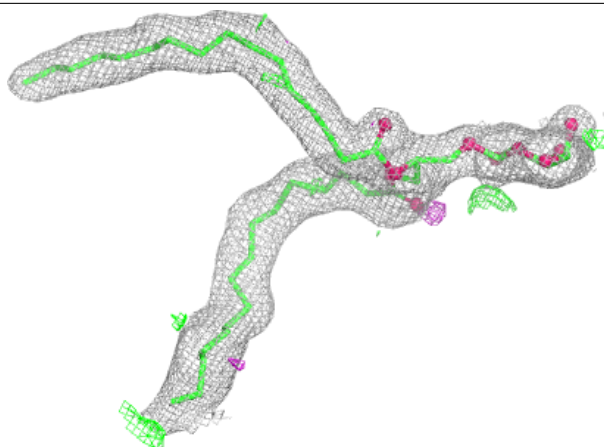
**Electron density around HTG B 625:**

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

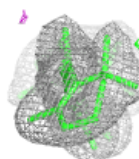
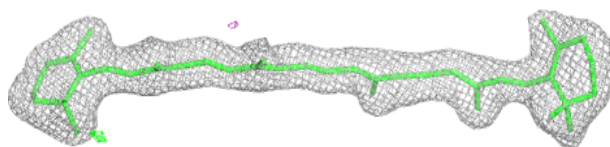
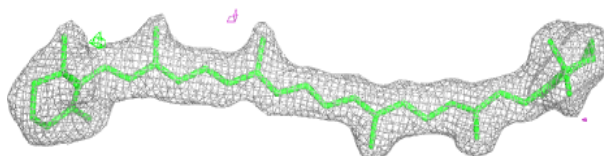


Electron density around LMG B 622:

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

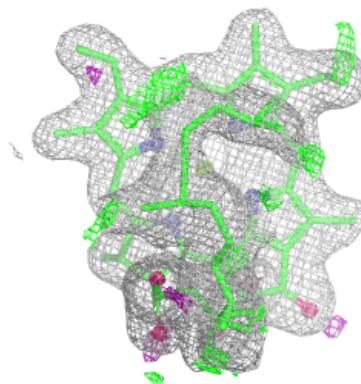
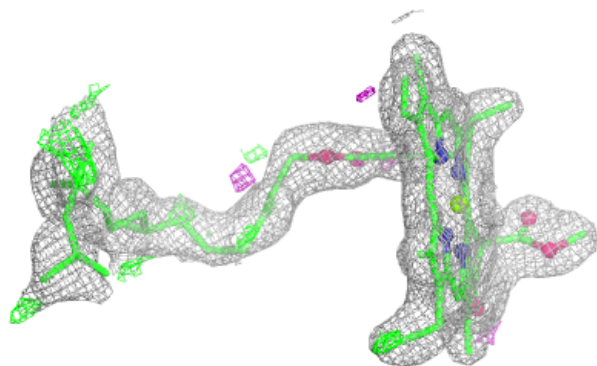
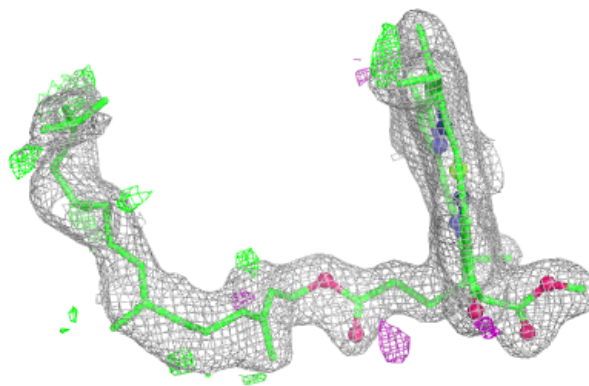
**Electron density around BCR c 915:**

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



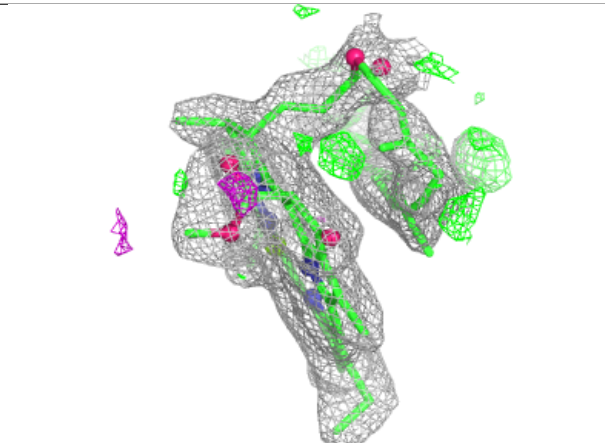
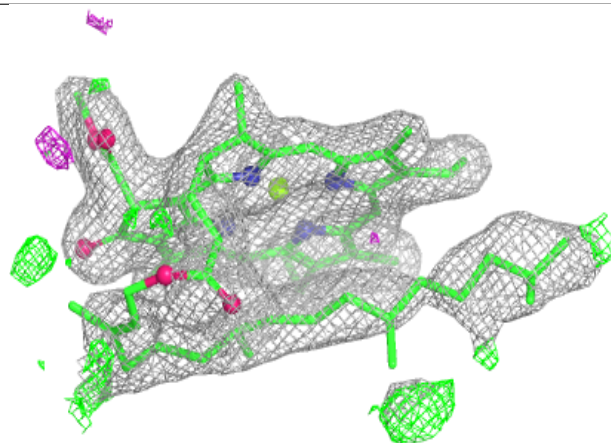
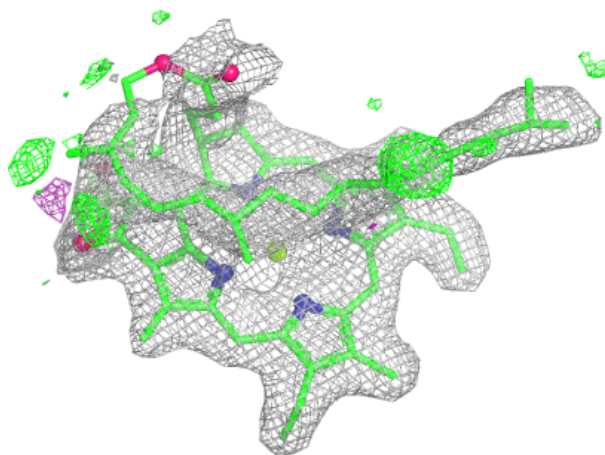
Electron density around CLA C 506:

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



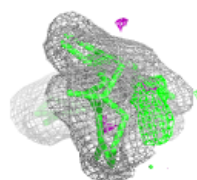
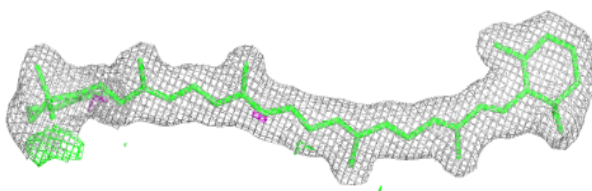
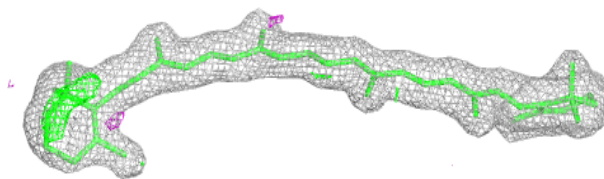
Electron density around CLA b 604:

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

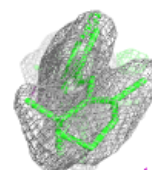
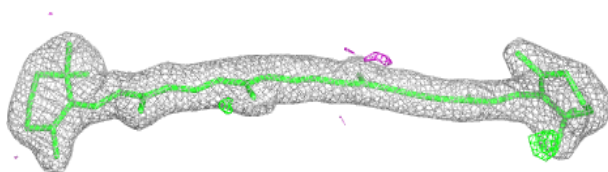
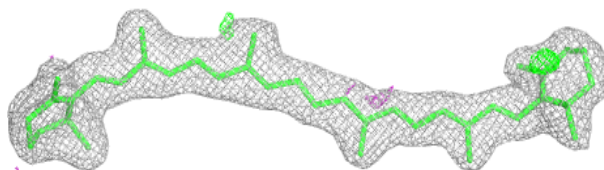


Electron density around BCR d 404:

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

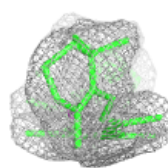
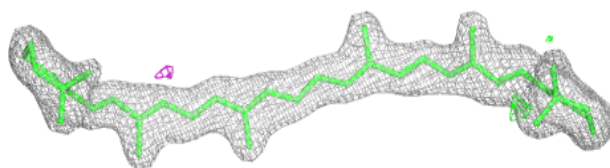
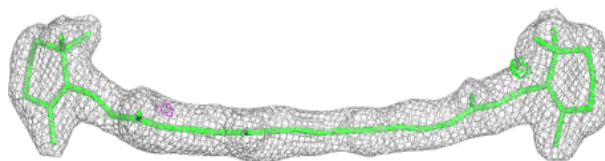
**Electron density around BCR k 101:**

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



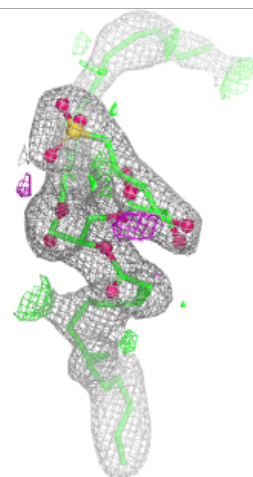
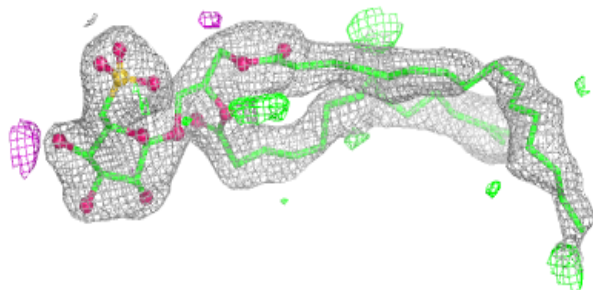
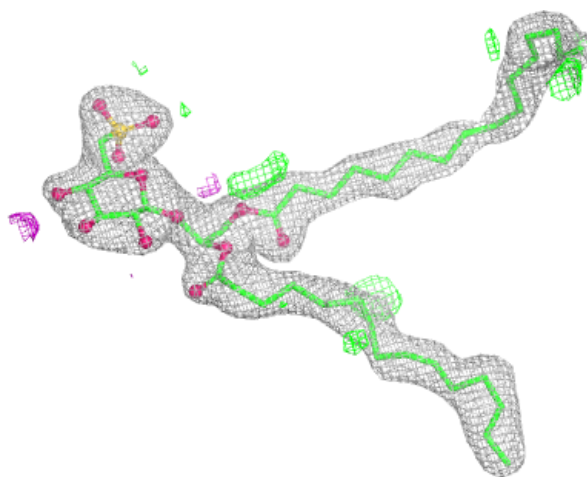
Electron density around BCR k 102:

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



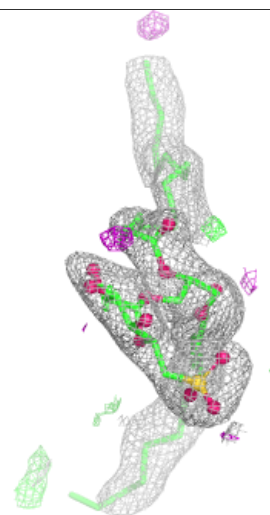
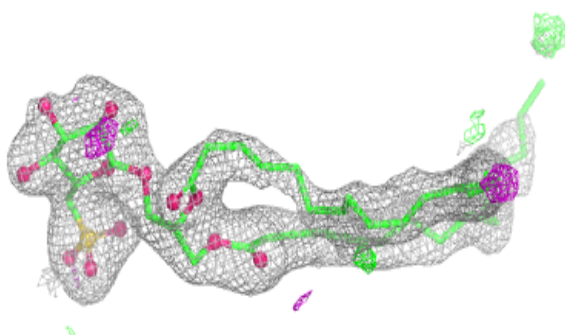
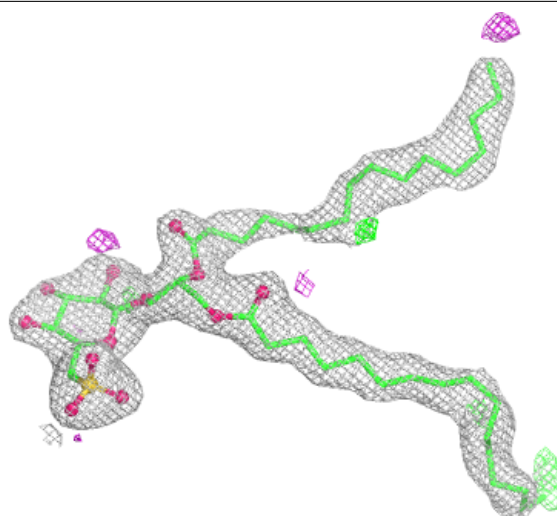
Electron density around SQD A 412:

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



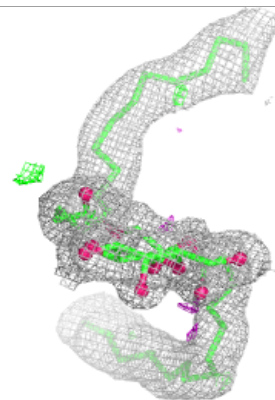
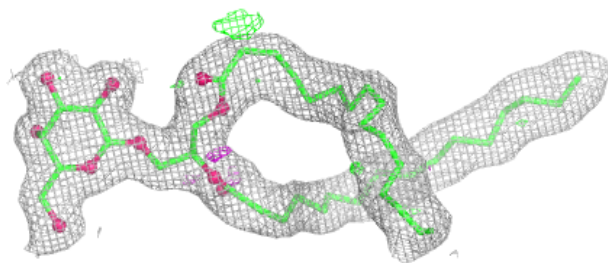
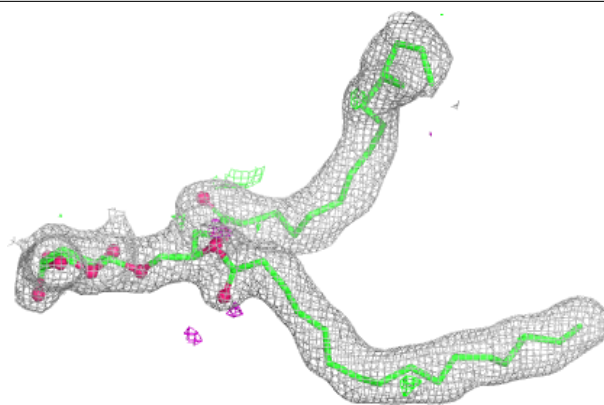
Electron density around SQD a 416:

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

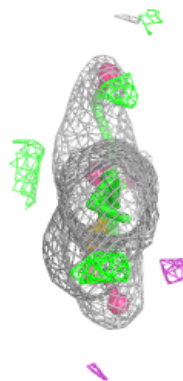
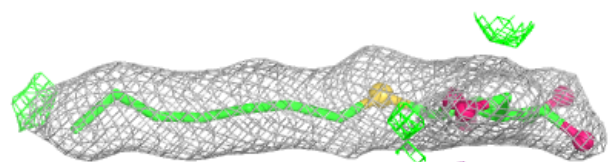
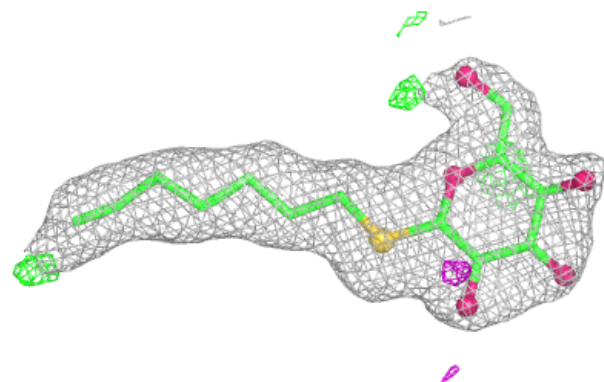


Electron density around LMG b 623:

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

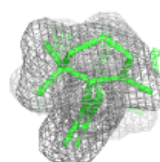
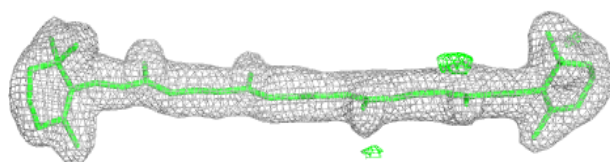
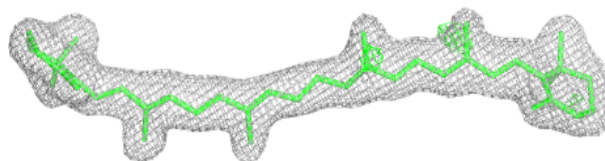
**Electron density around HTG b 601:**

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

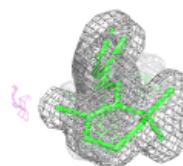
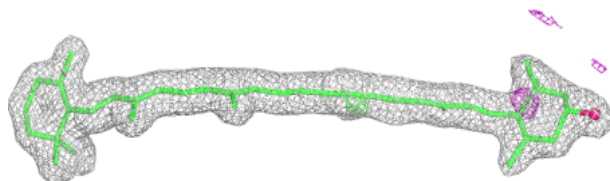
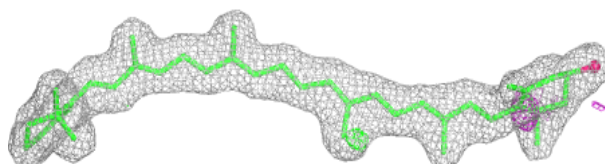


Electron density around BCR C 514:

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

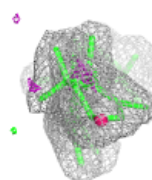
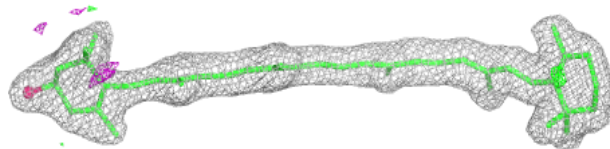
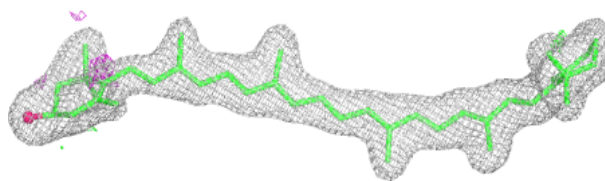
**Electron density around RRX H 101:**

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

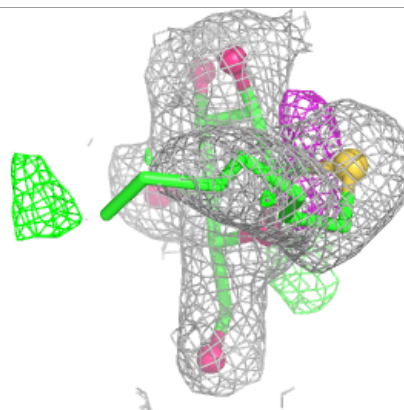
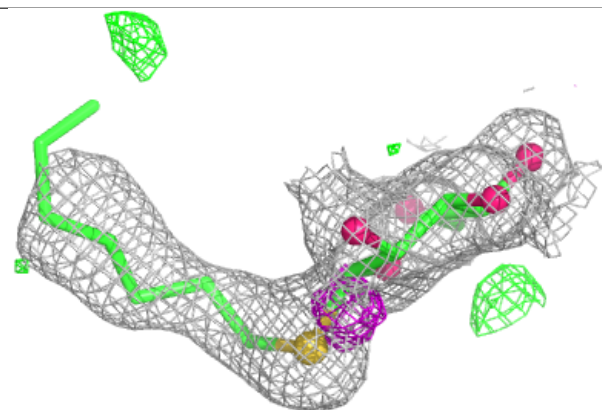
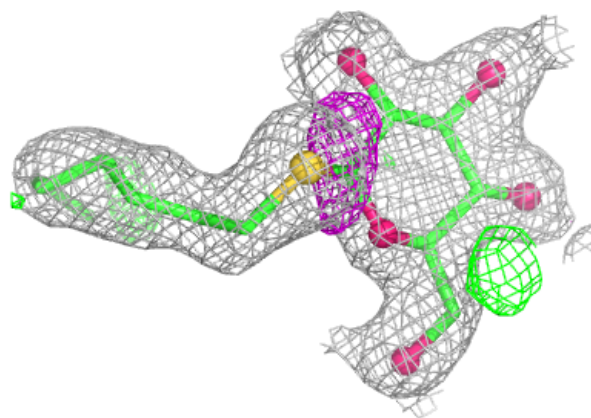


Electron density around RRX h 101:

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

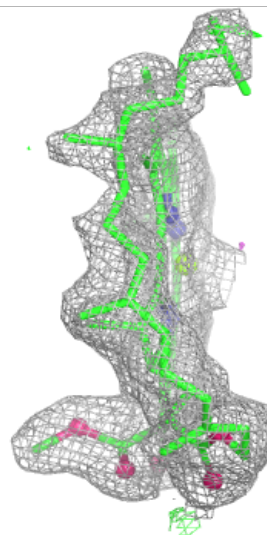
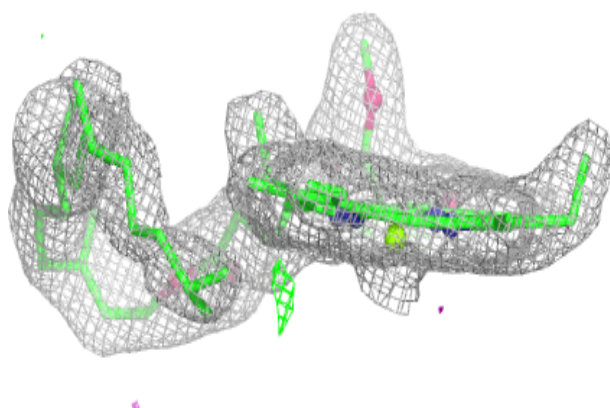
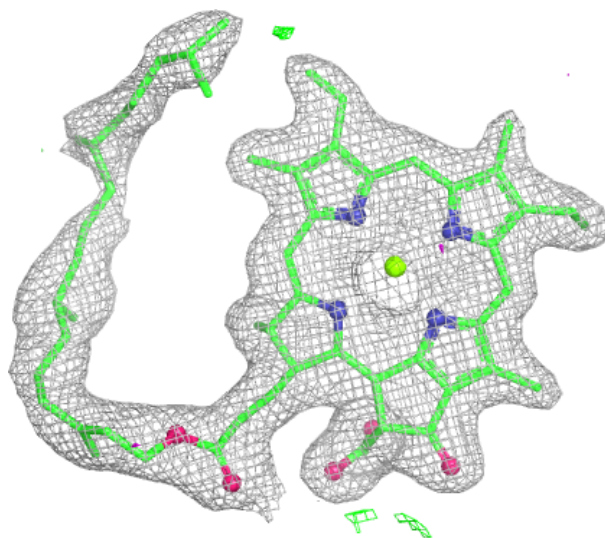
**Electron density around HTG b 626:**

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



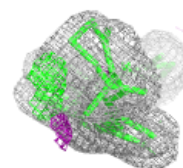
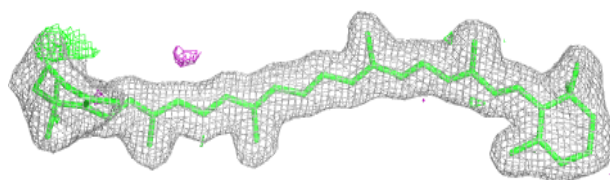
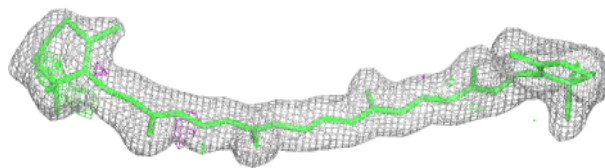
Electron density around CLA C 512:

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

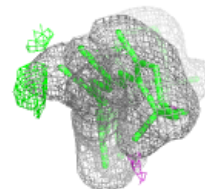
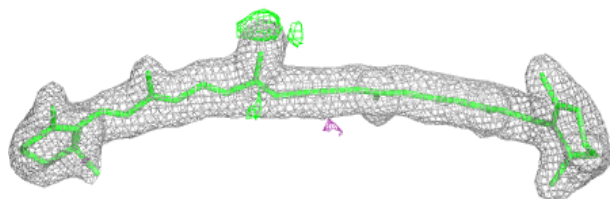
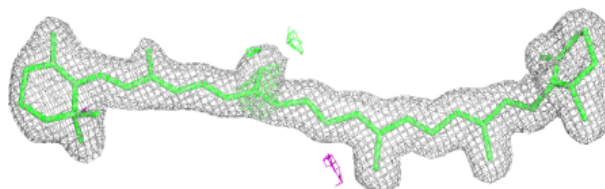


Electron density around BCR D 404:

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

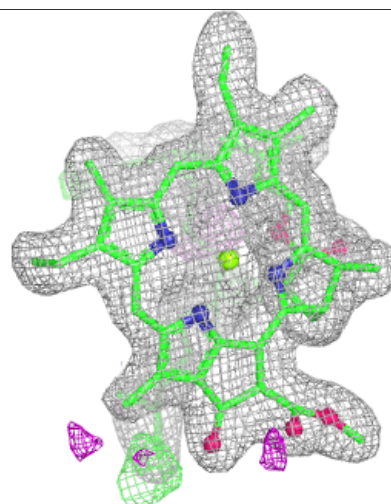
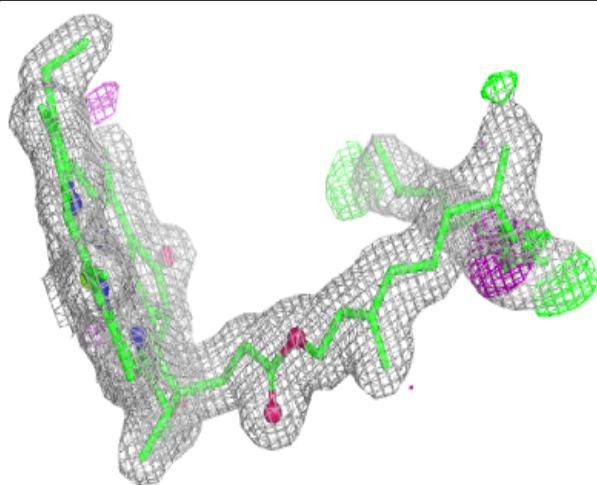
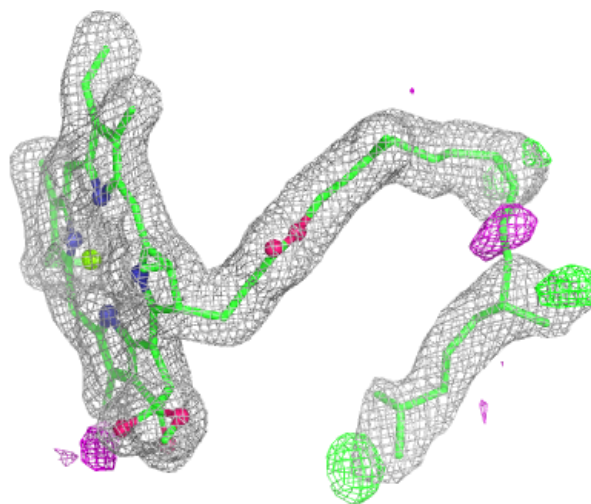
**Electron density around BCR T 101:**

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



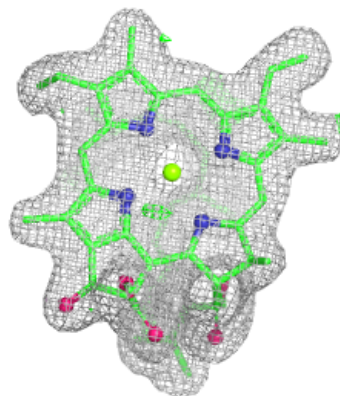
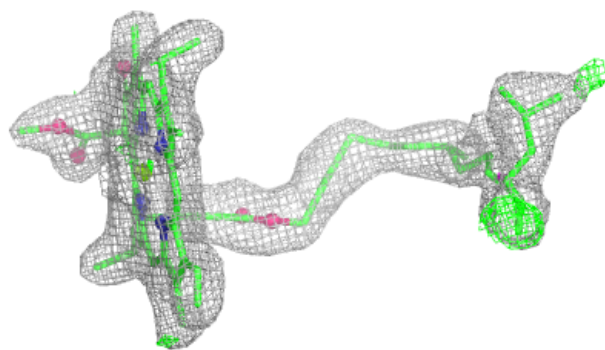
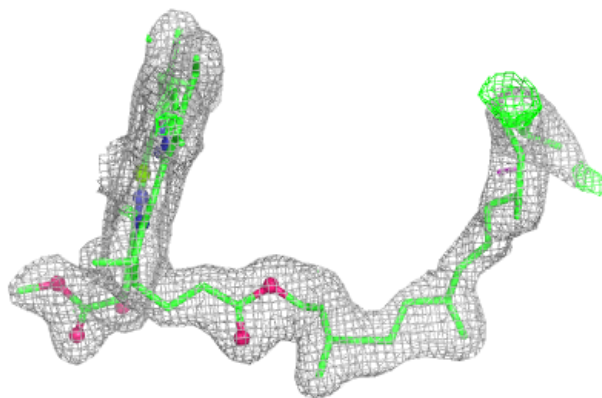
Electron density around CLA b 609:

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



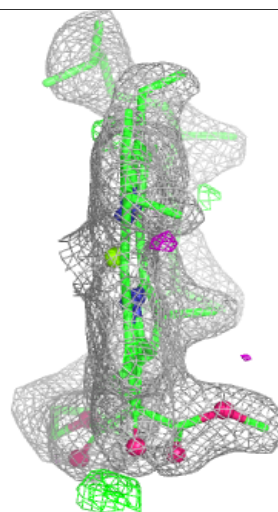
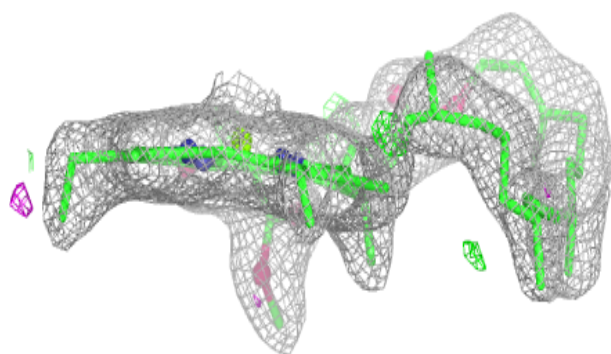
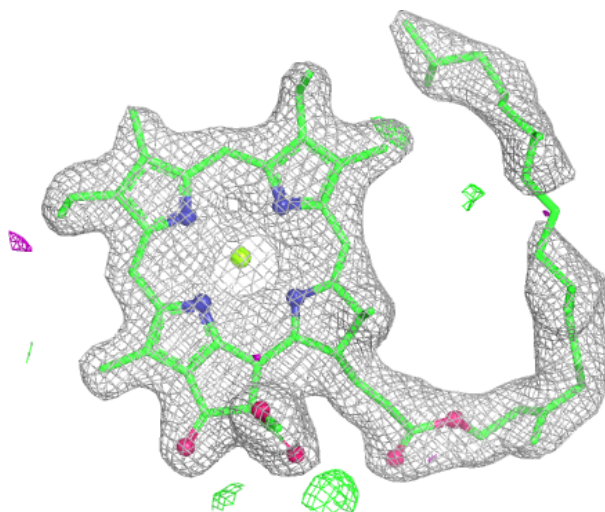
Electron density around CLA c 907:

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



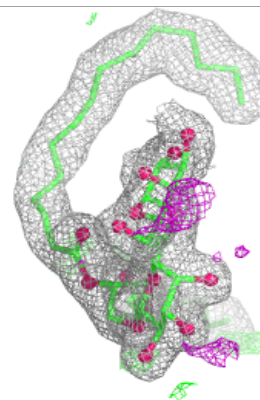
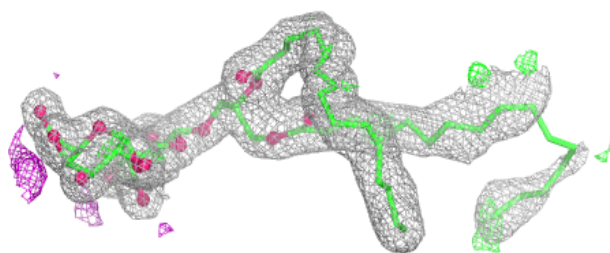
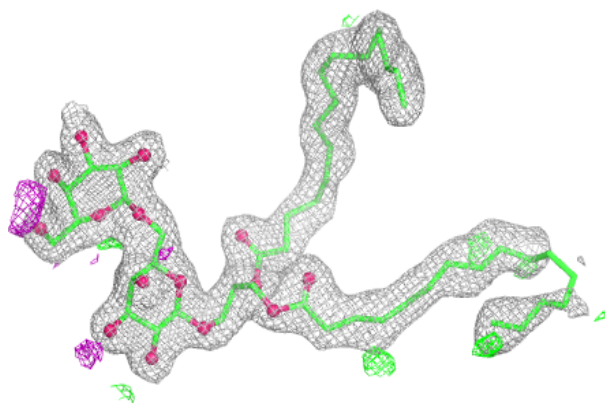
Electron density around CLA c 913:

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

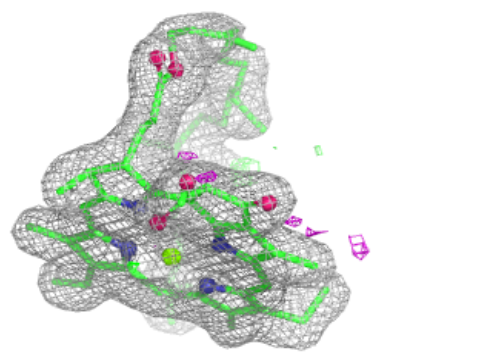
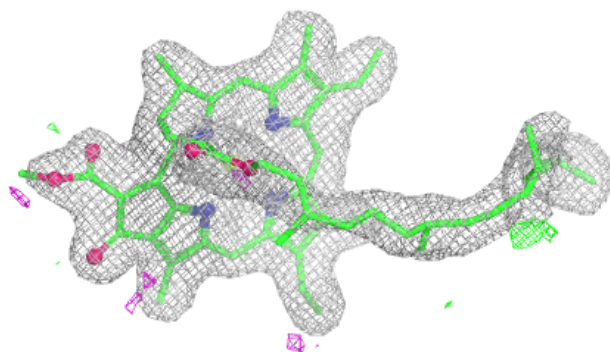
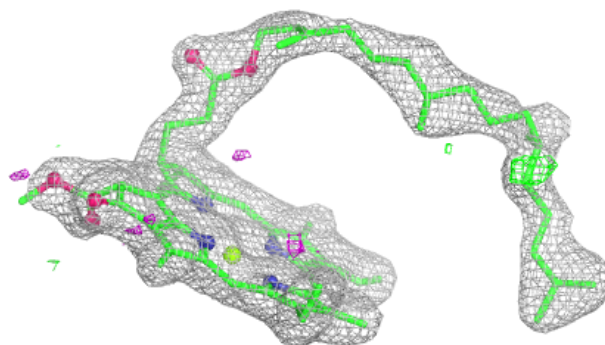


Electron density around DGD c 918:

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

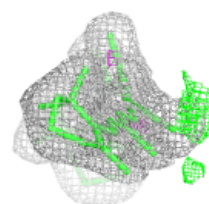
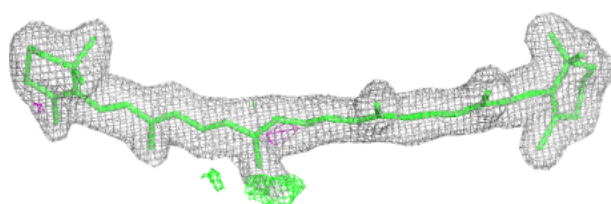
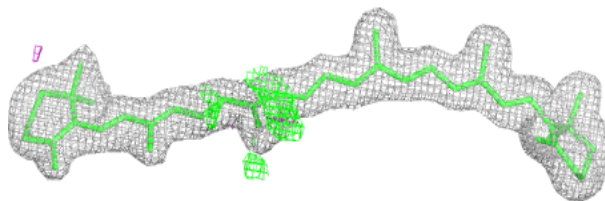
**Electron density around CLA C 513:**

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

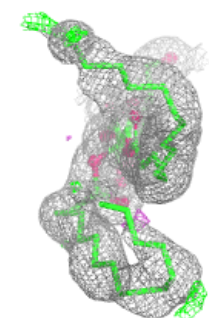
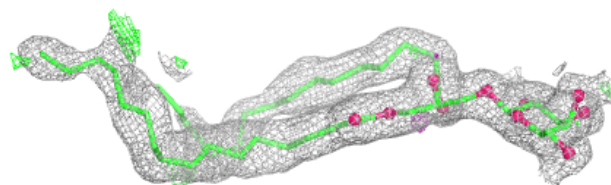
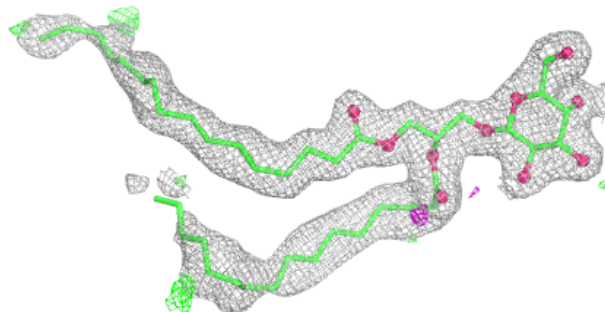


Electron density around BCR t 101:

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

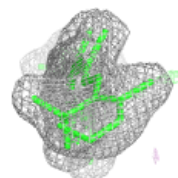
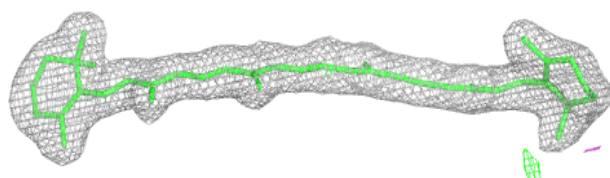
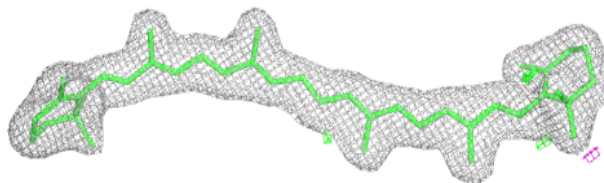
**Electron density around LMG d 410:**

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

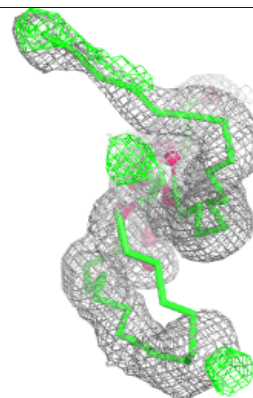
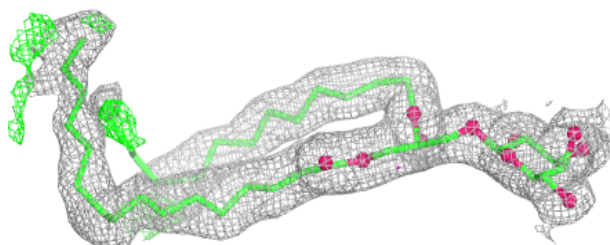
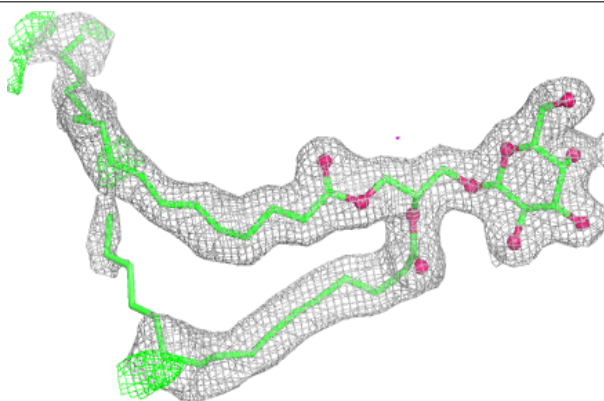


Electron density around BCR K 101:

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

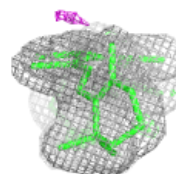
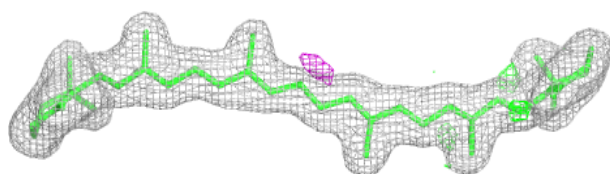
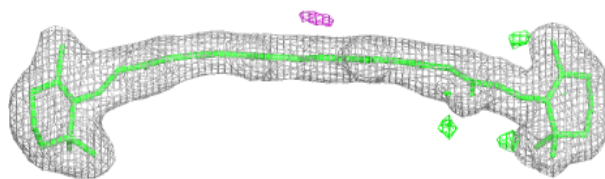
**Electron density around LMG D 411:**

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

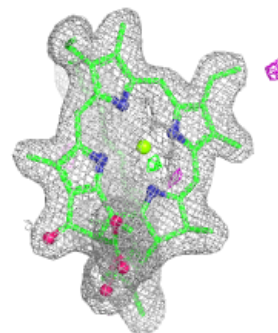
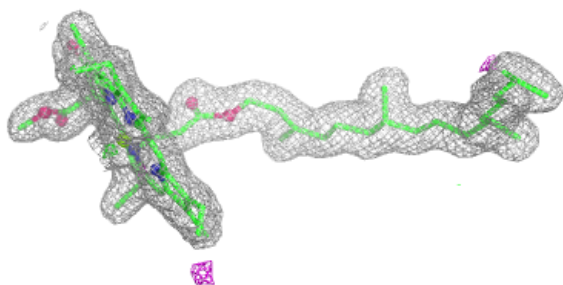
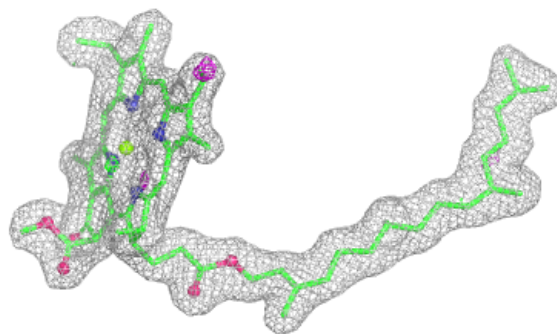


Electron density around BCR K 102:

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

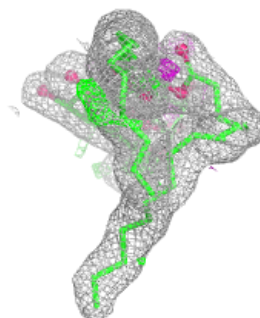
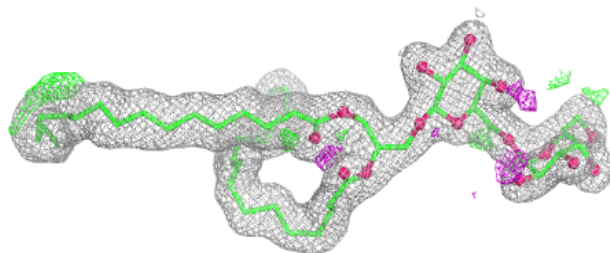
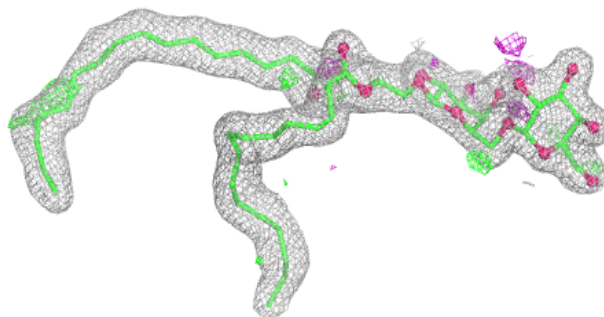
**Electron density around CLA b 612:**

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

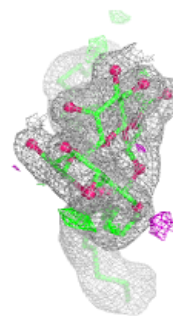
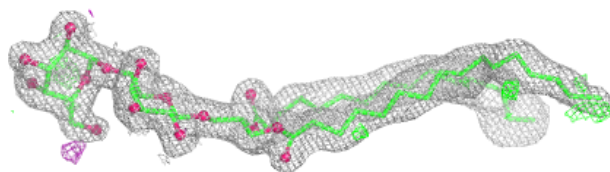
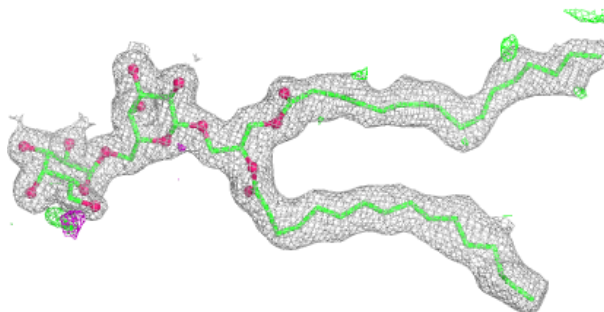


Electron density around DGD H 102:

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

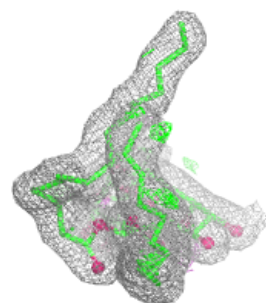
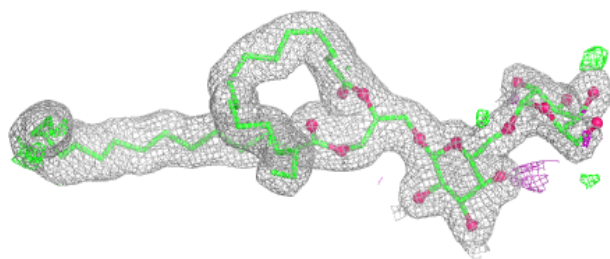
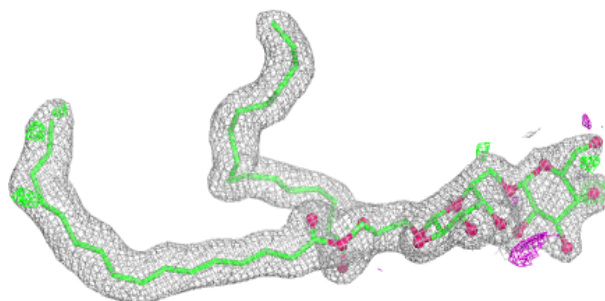
**Electron density around DGD c 919:**

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



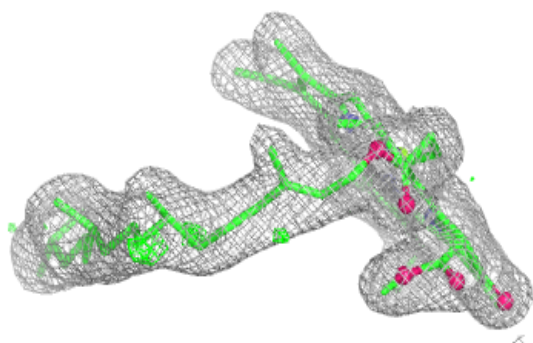
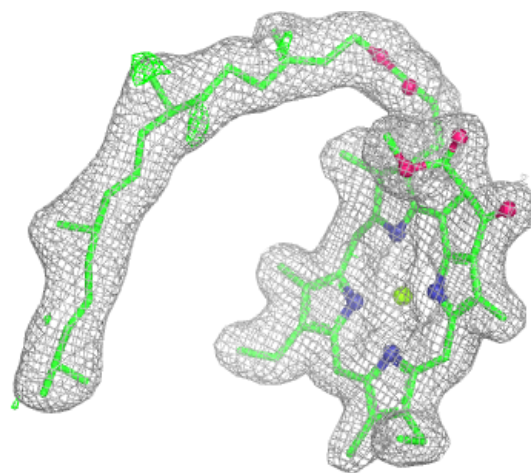
Electron density around DGD h 102:

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



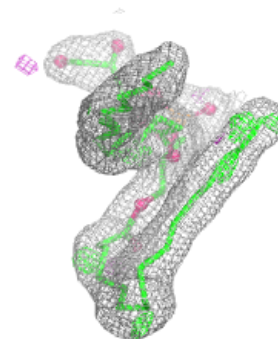
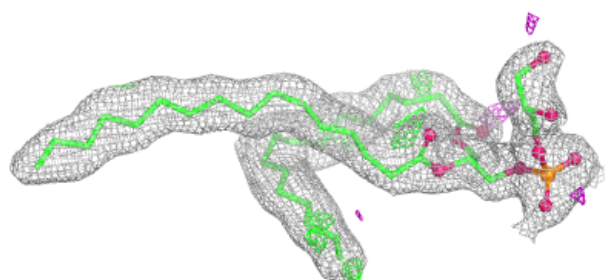
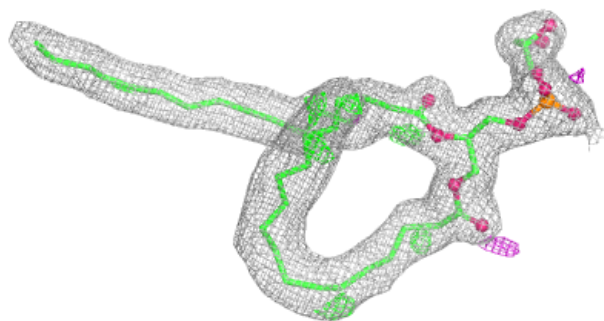
Electron density around CLA c 908:

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

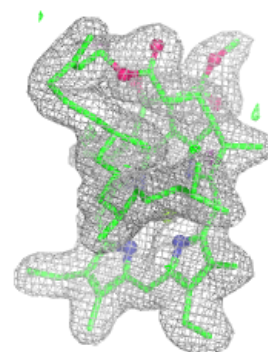
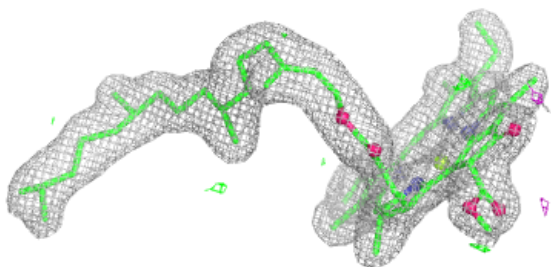
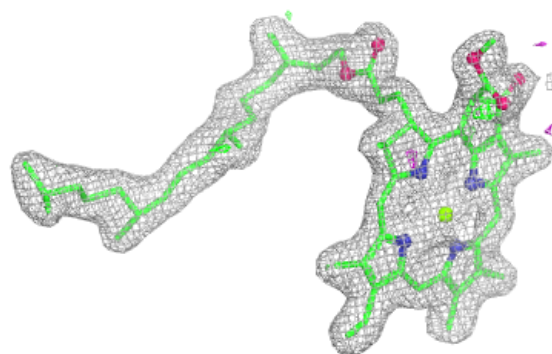


Electron density around LHG D 408:

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

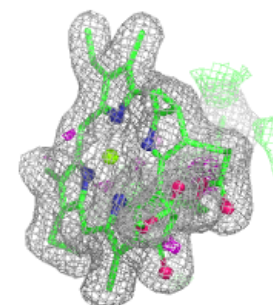
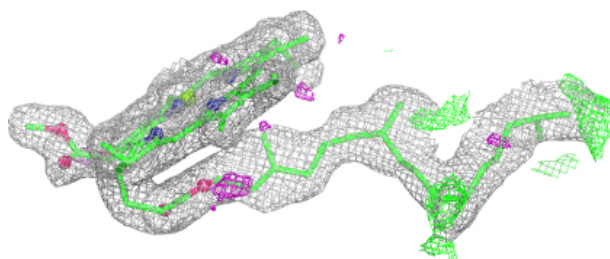
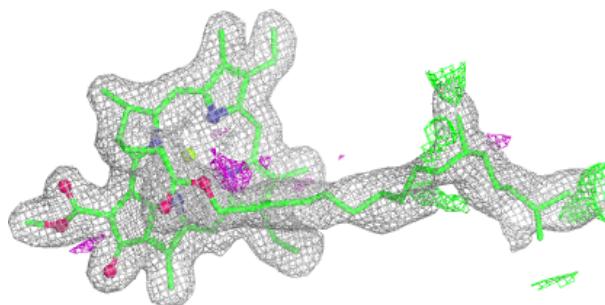
**Electron density around CLA c 912:**

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

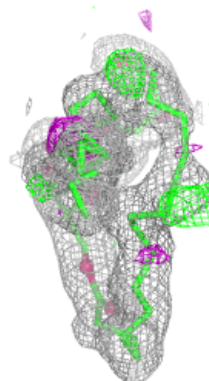
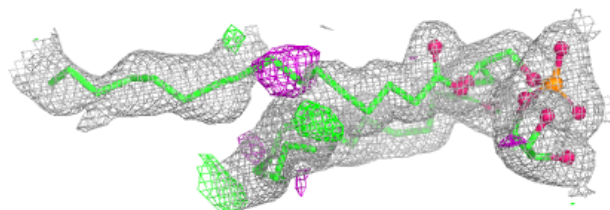
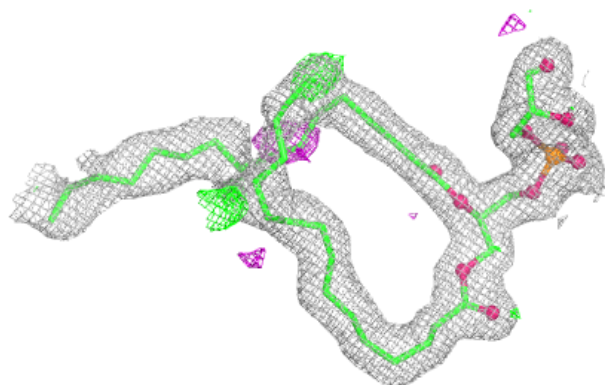


Electron density around CLA b 617:

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

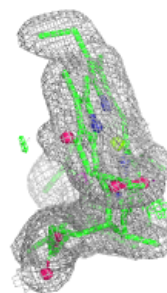
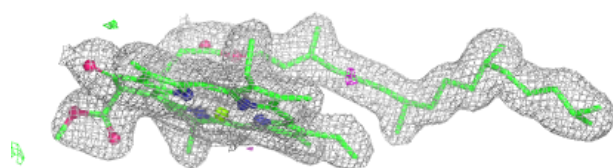
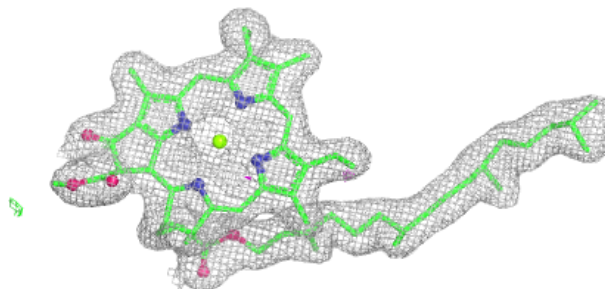
**Electron density around LHG d 409:**

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

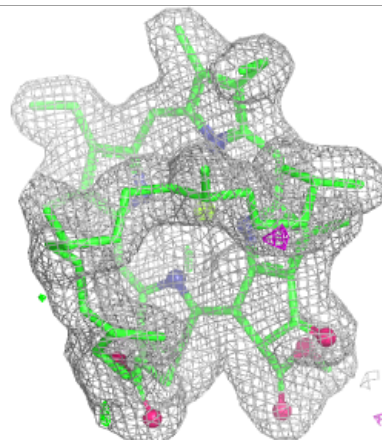
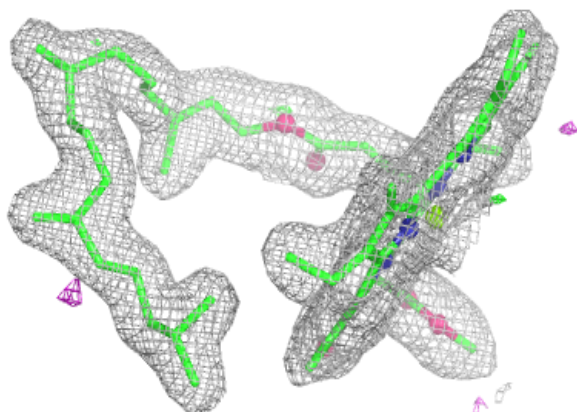
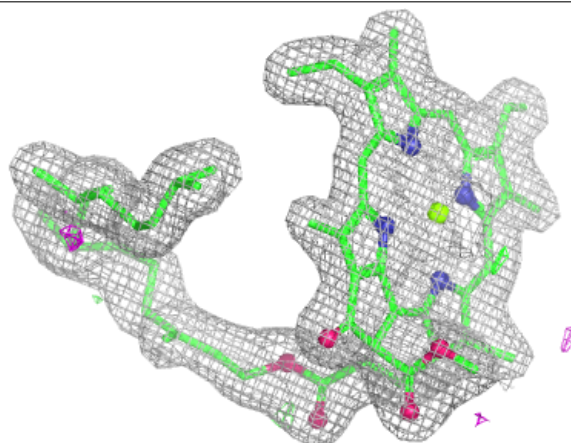


Electron density around CLA c 902:

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

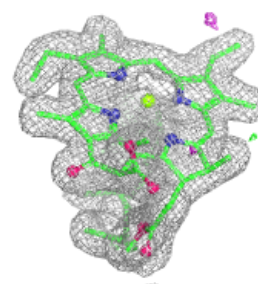
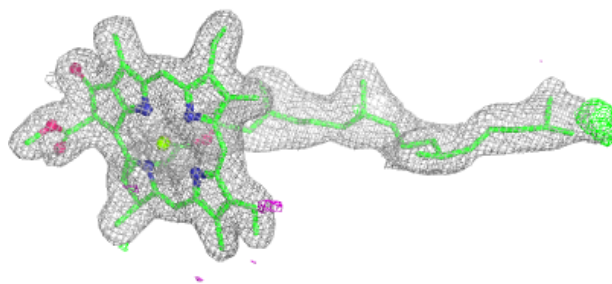
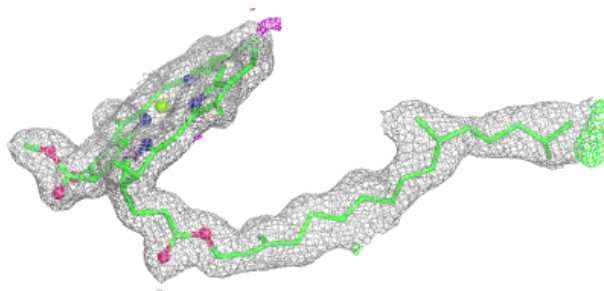
**Electron density around CLA c 904:**

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

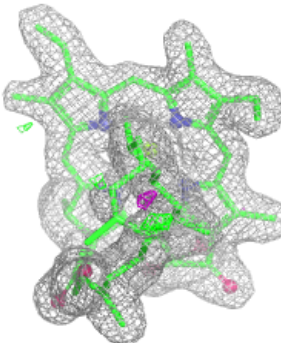
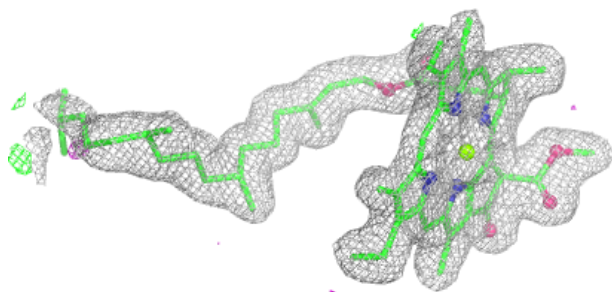
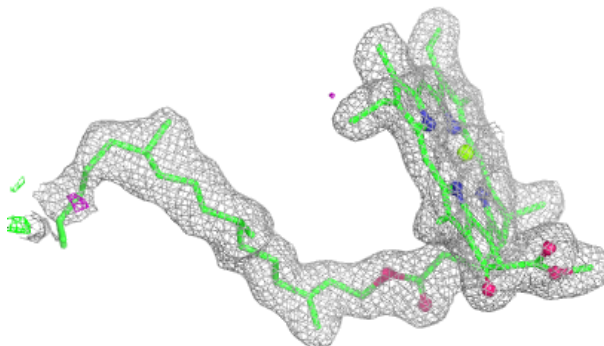


Electron density around CLA c 905:

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

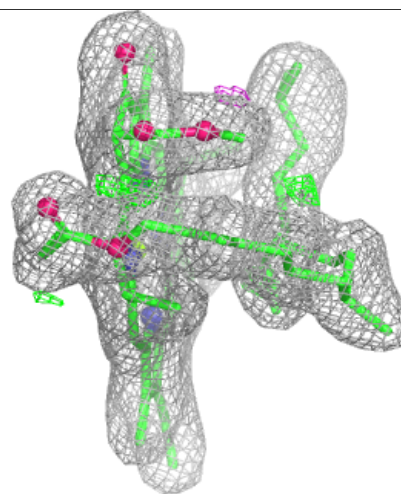
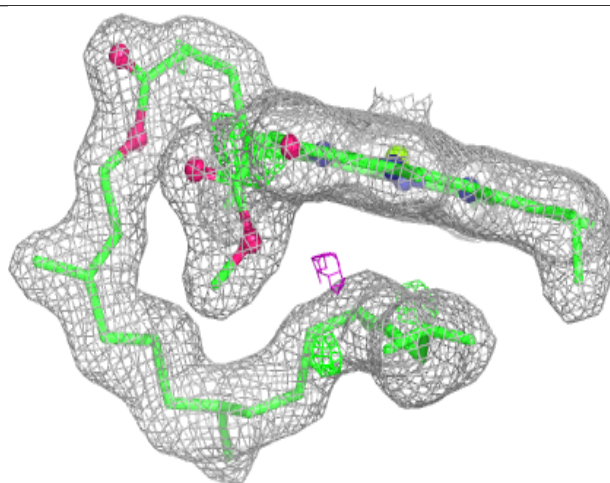
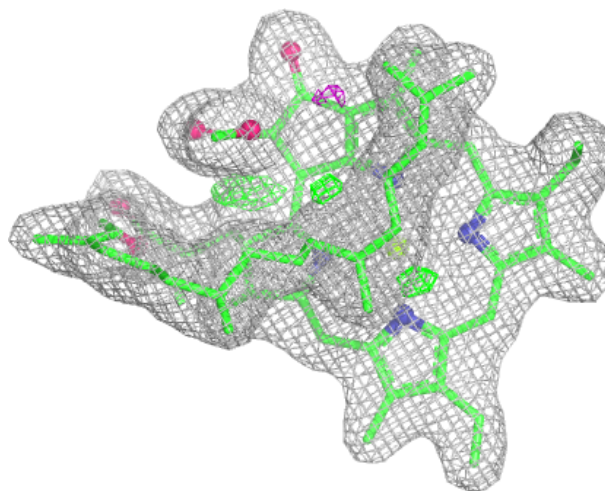
**Electron density around CLA c 909:**

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



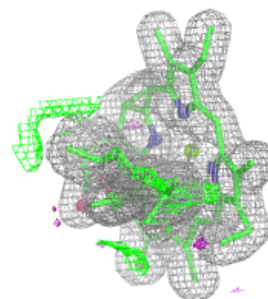
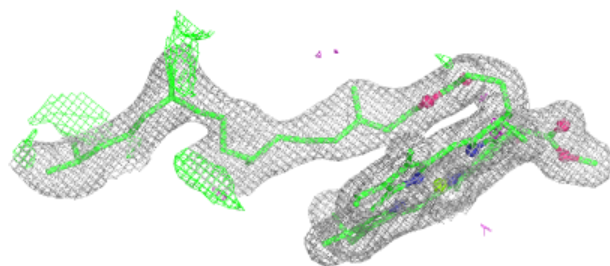
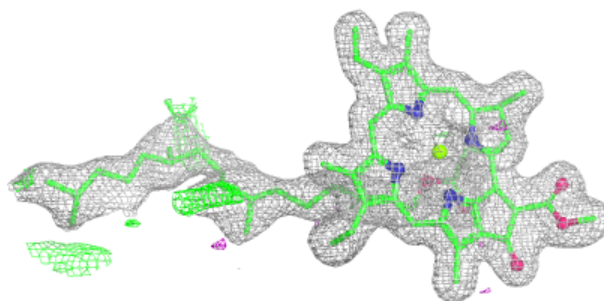
Electron density around CLA c 911:

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

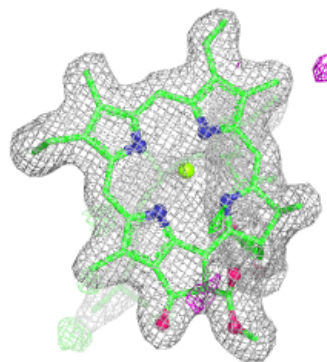
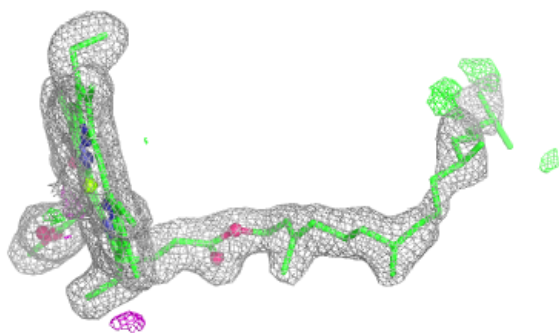
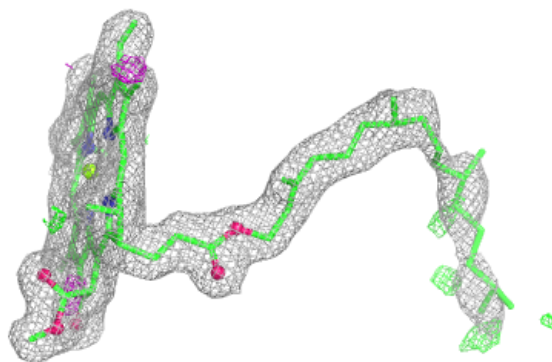


Electron density around CLA B 615:

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

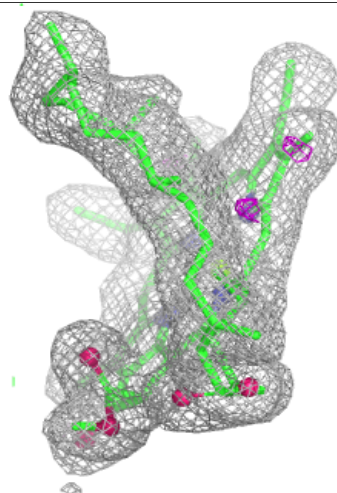
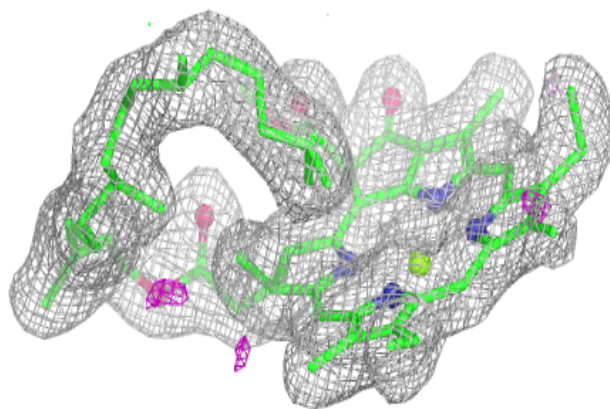
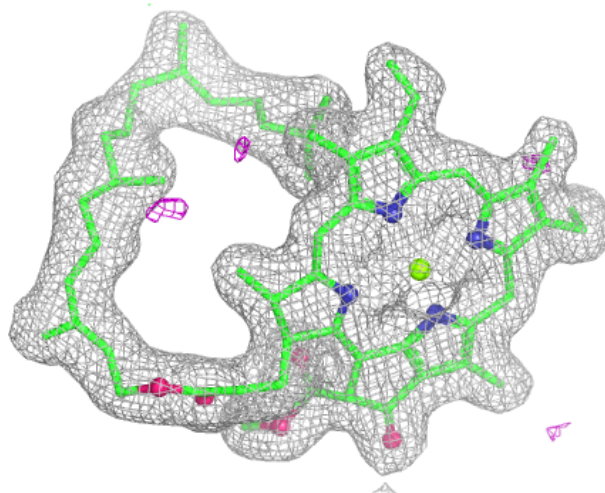
**Electron density around CLA D 403:**

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



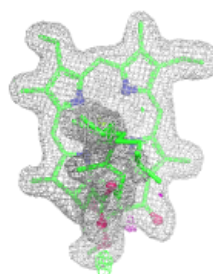
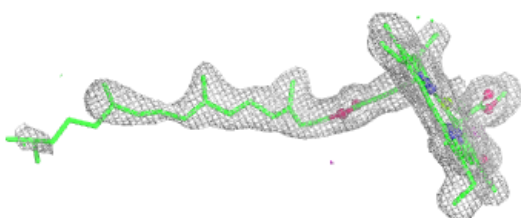
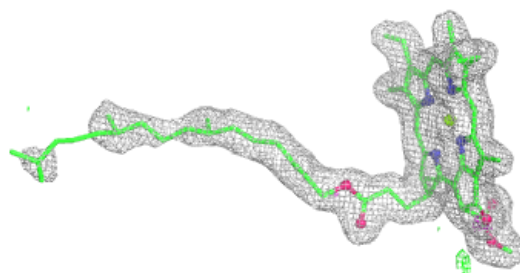
Electron density around CLA B 616:

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

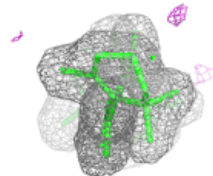
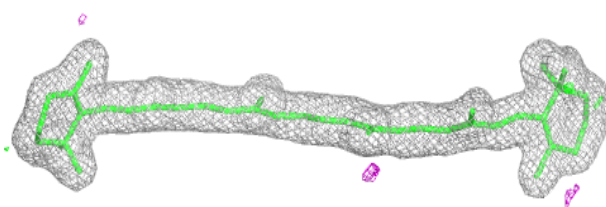
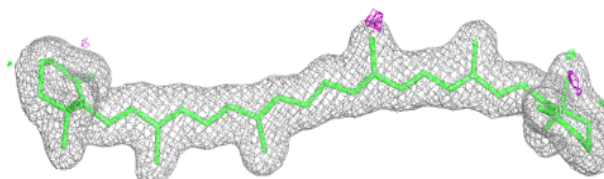


Electron density around CLA d 403:

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

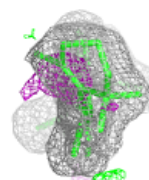
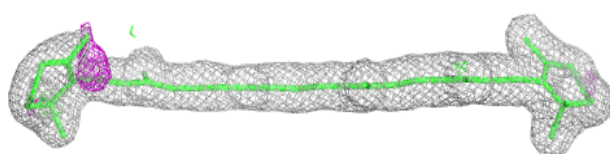
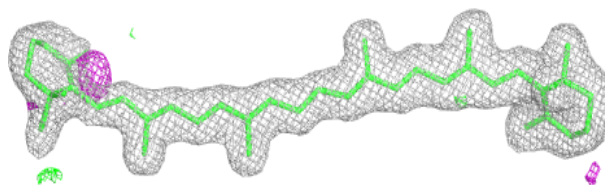
**Electron density around BCR A 411:**

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

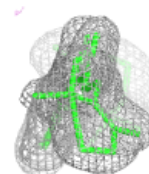
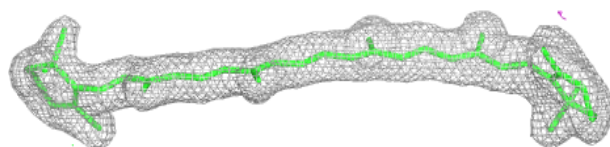
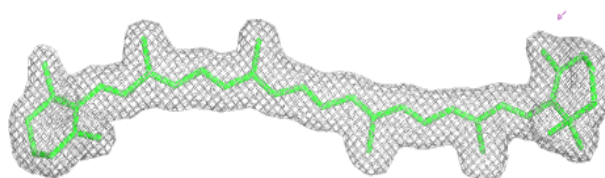


Electron density around BCR B 619:

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

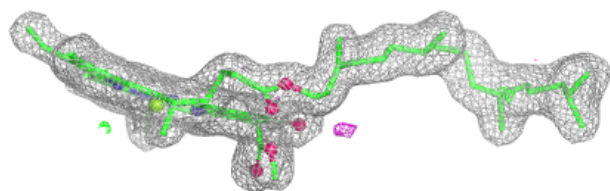
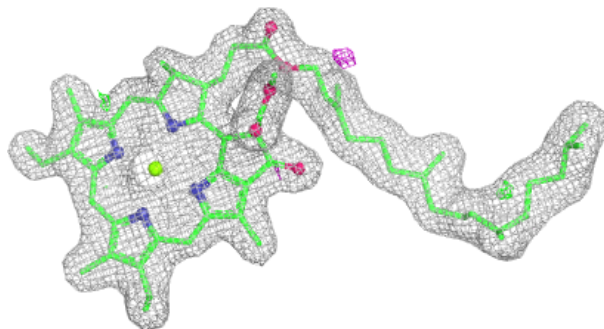
**Electron density around BCR B 620:**

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

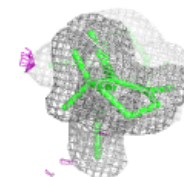
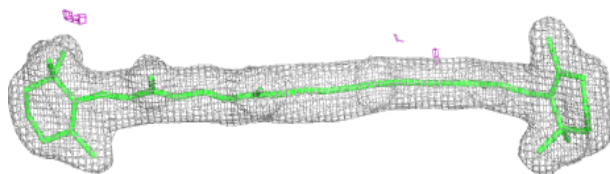
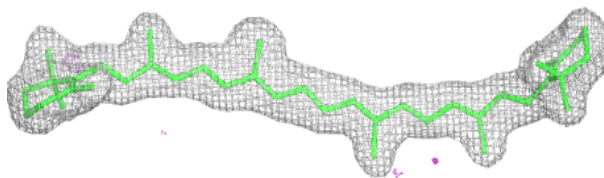


Electron density around CLA b 605:

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

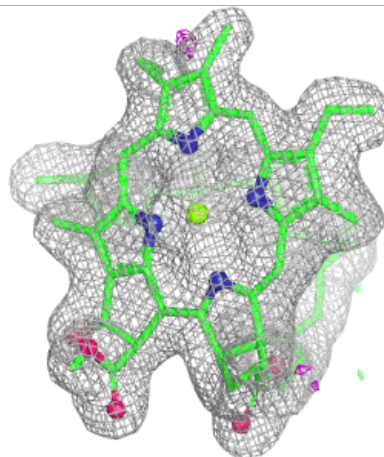
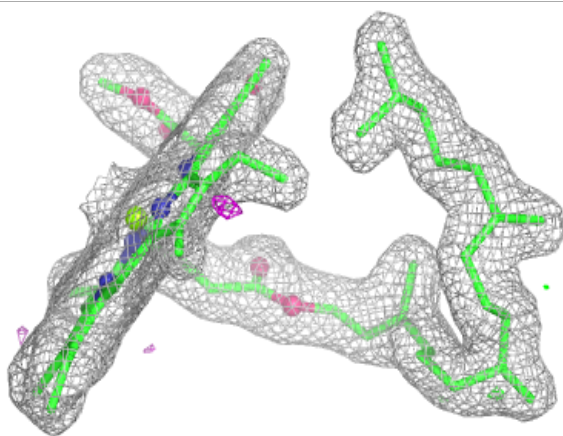
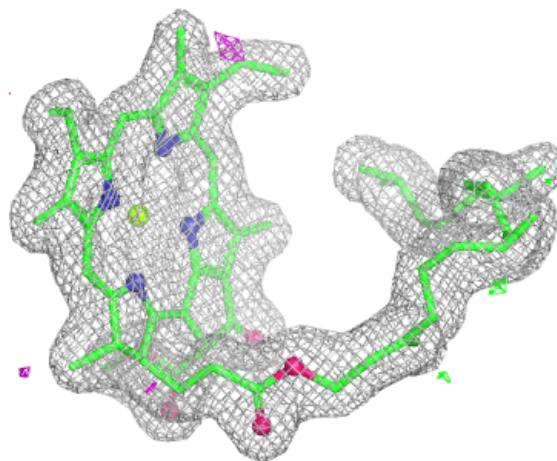
**Electron density around BCR C 515:**

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



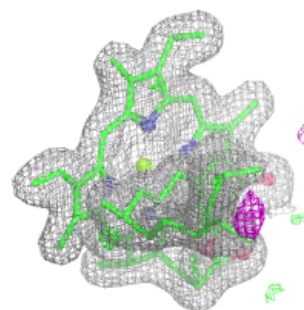
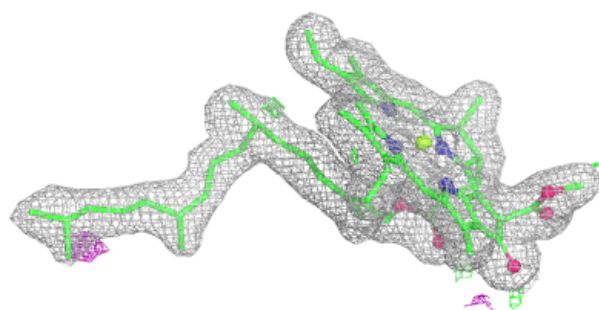
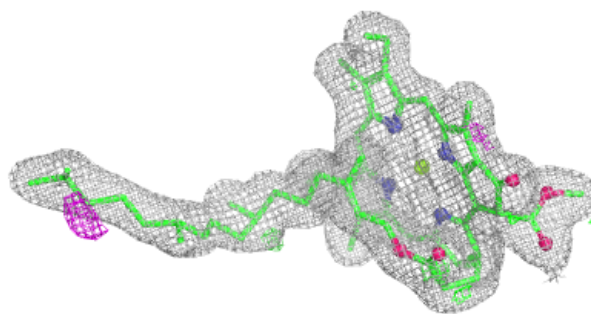
Electron density around CLA C 503:

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



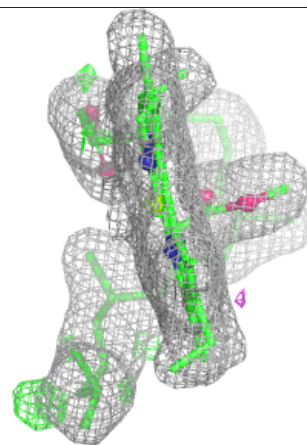
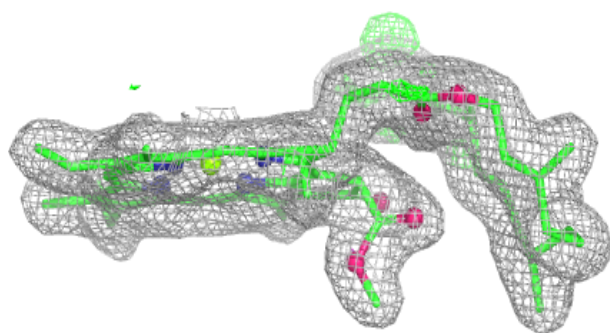
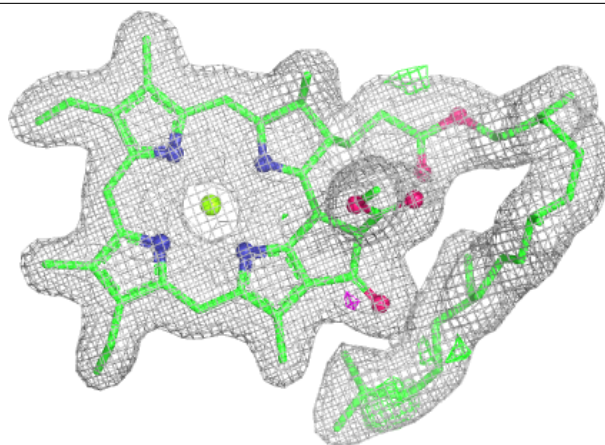
Electron density around CLA C 505:

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

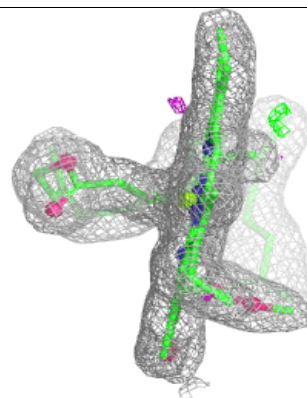
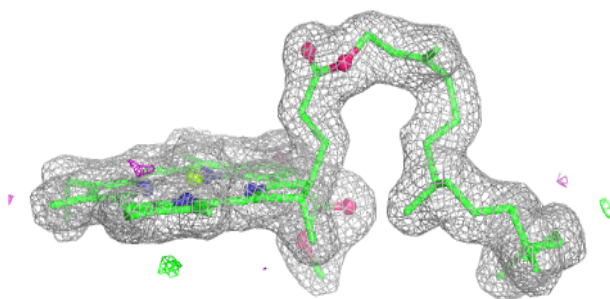
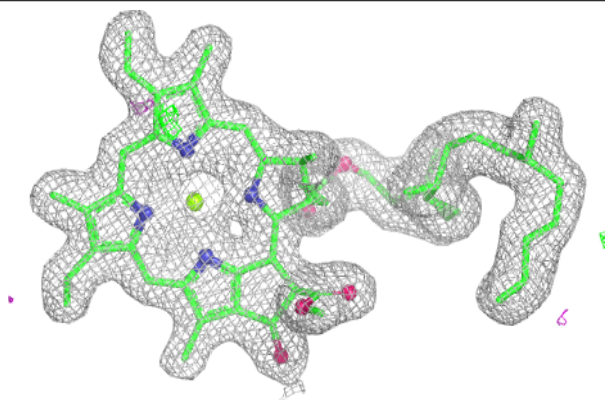


Electron density around CLA b 613:

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

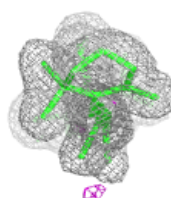
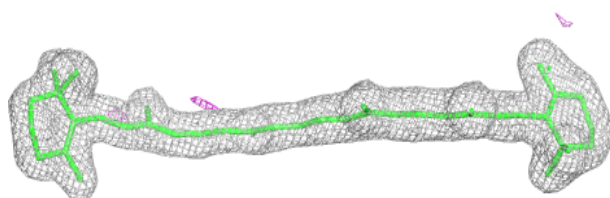
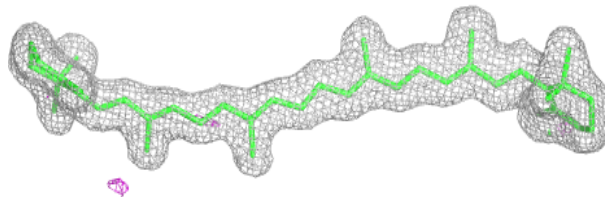
**Electron density around CLA b 615:**

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

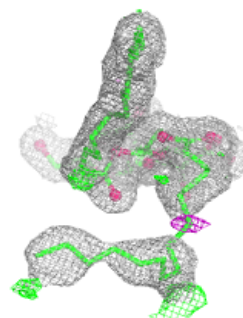
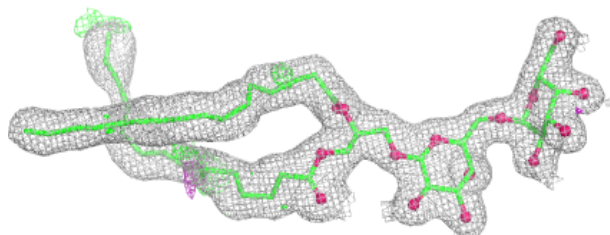
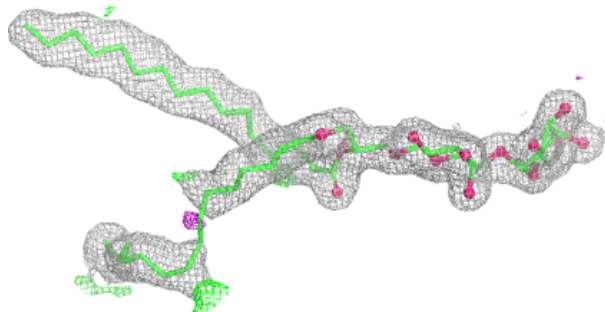


Electron density around BCR a 415:

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

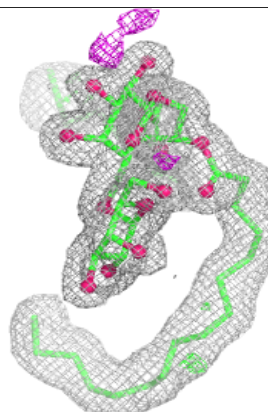
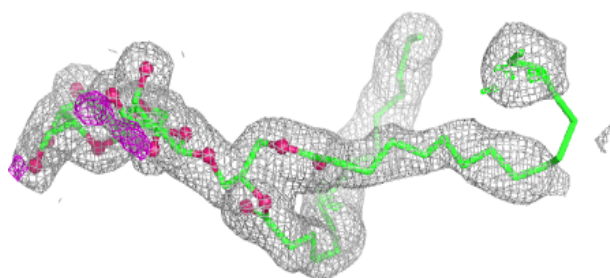
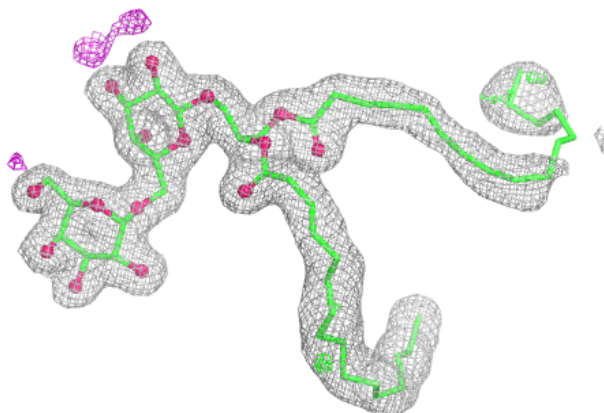
**Electron density around DGD C 516:**

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

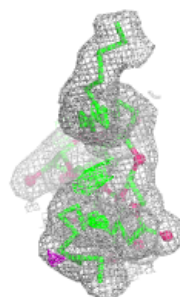
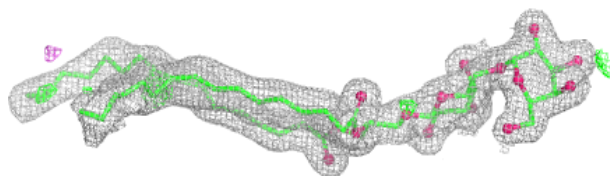
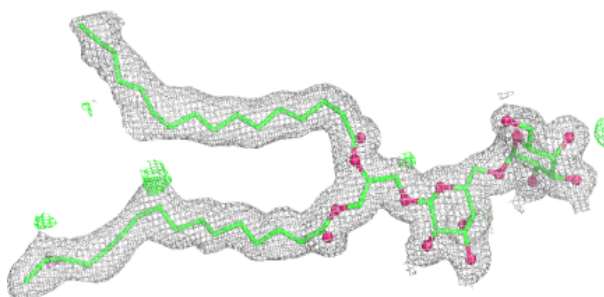


Electron density around DGD C 517:

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

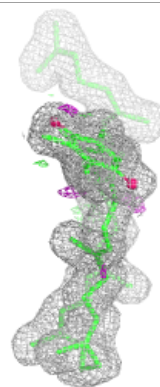
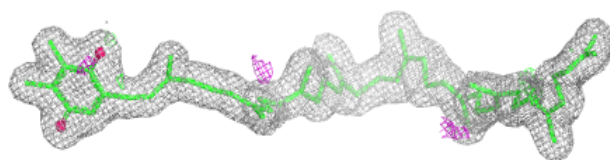
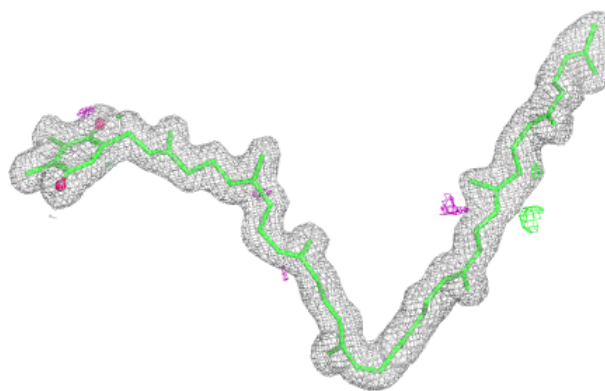
**Electron density around DGD C 518:**

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

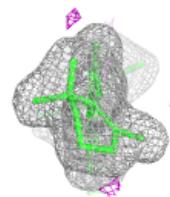
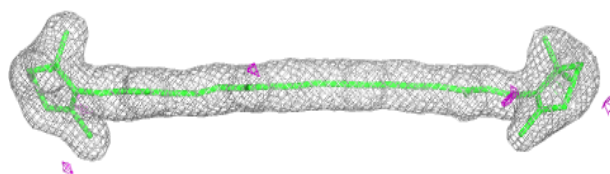
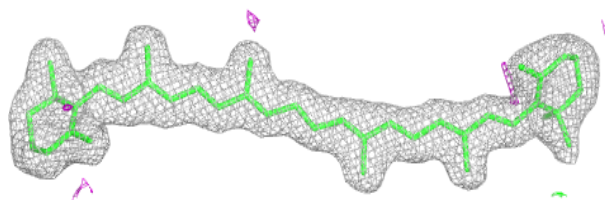


Electron density around PL9 D 405:

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

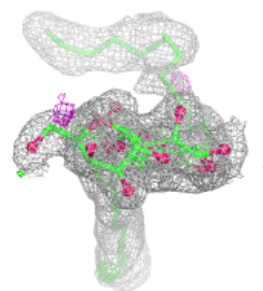
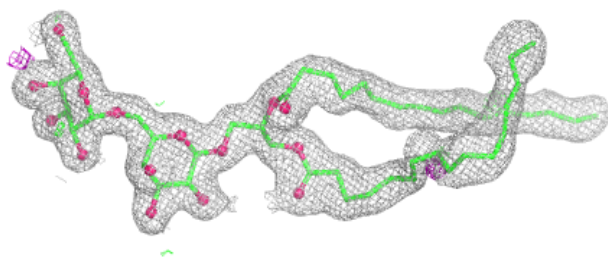
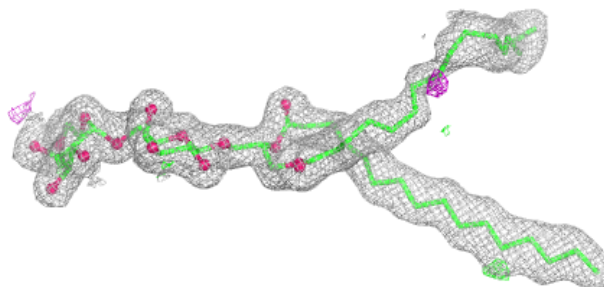
**Electron density around BCR b 621:**

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

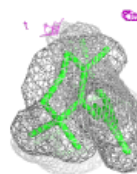
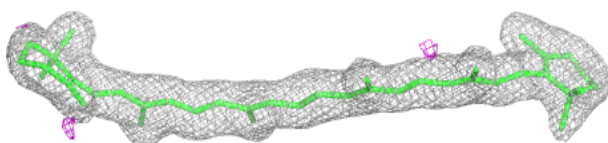
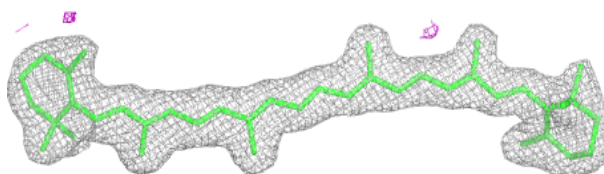


Electron density around DGD c 917:

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

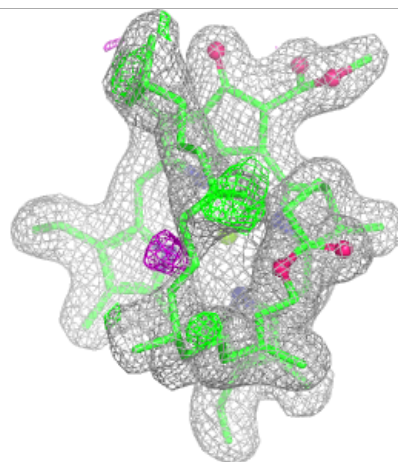
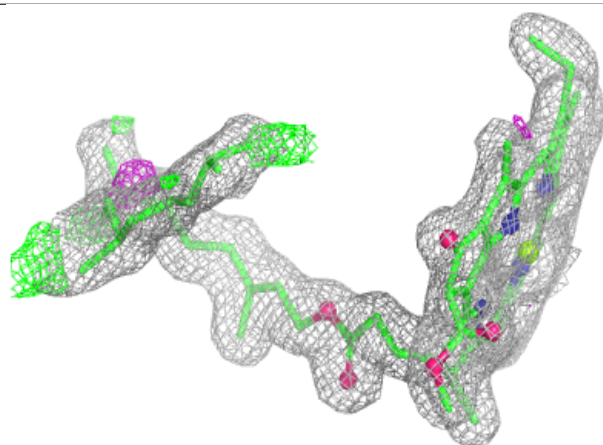
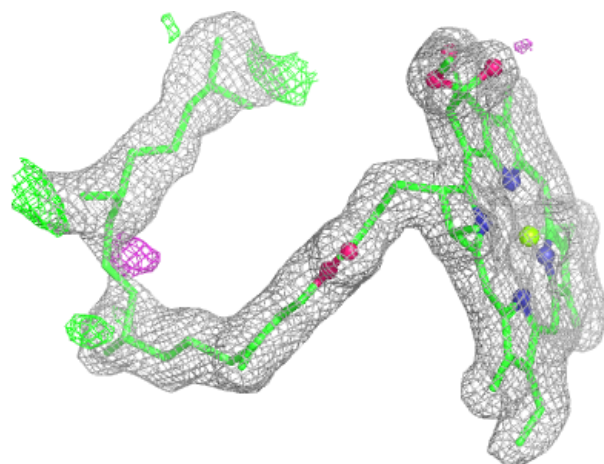
**Electron density around BCR b 622:**

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



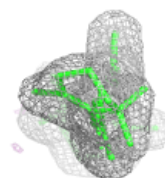
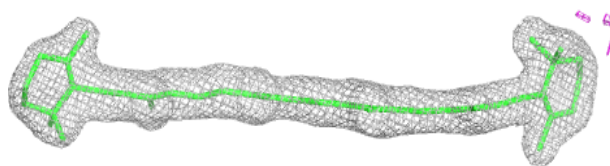
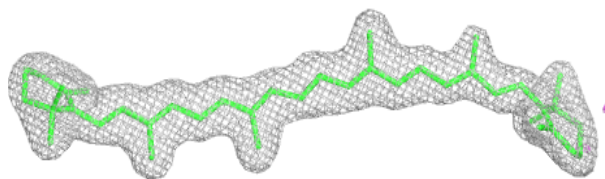
Electron density around CLA B 607:

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



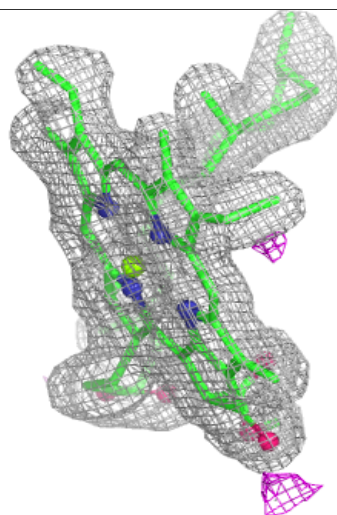
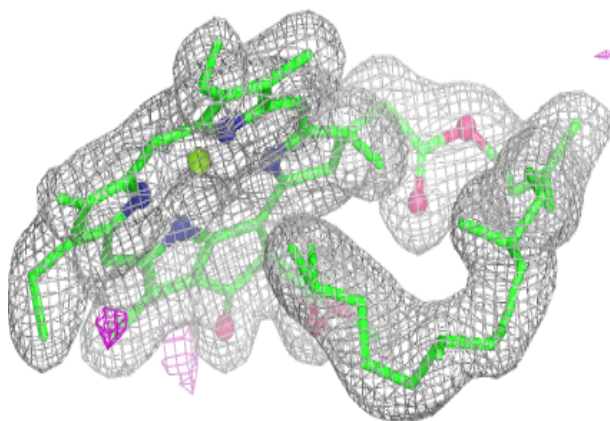
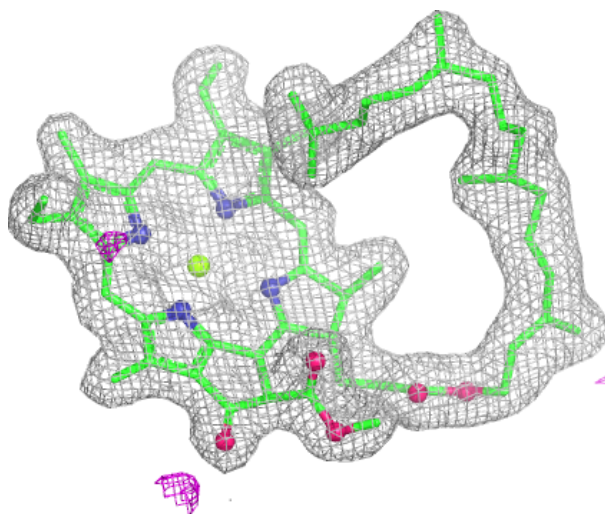
Electron density around BCR c 916:

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



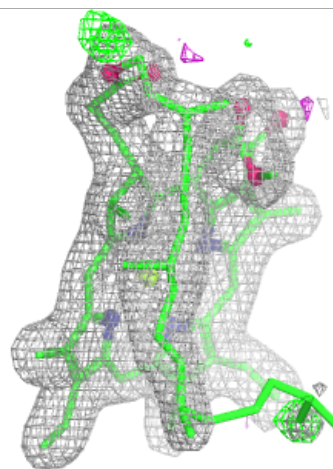
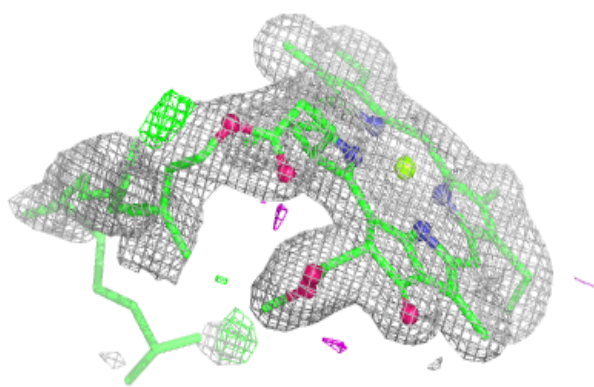
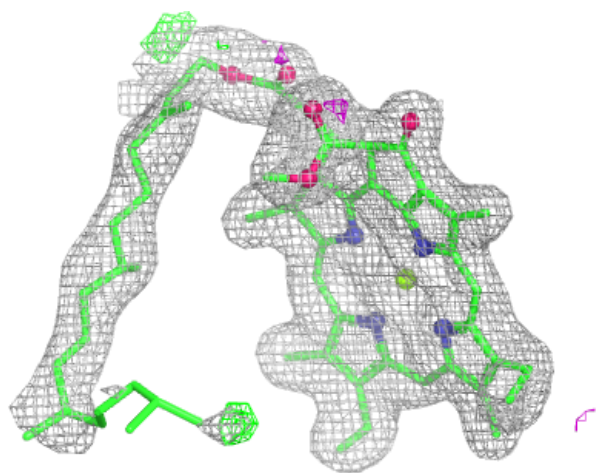
Electron density around CLA b 618:

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



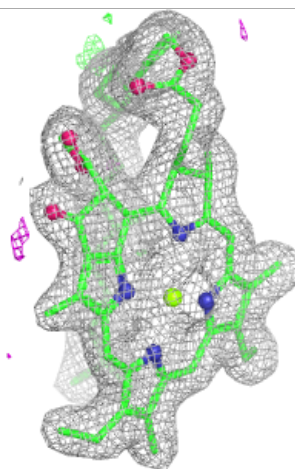
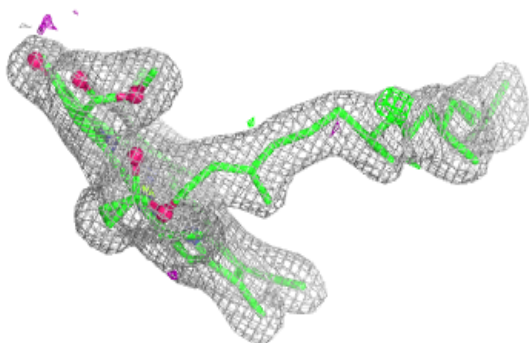
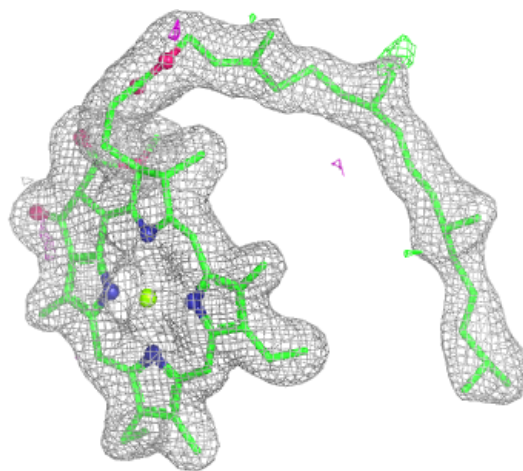
Electron density around CLA b 619:

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



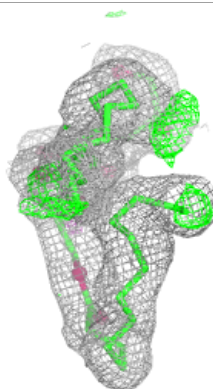
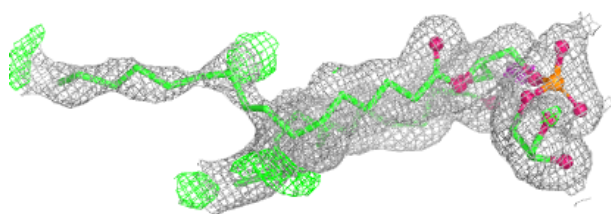
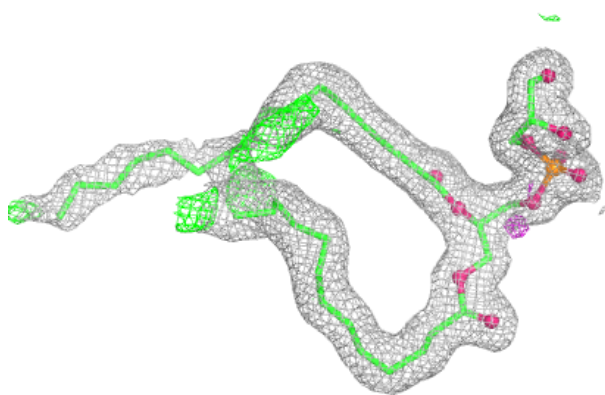
Electron density around CLA C 507:

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

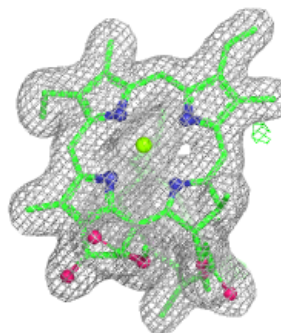
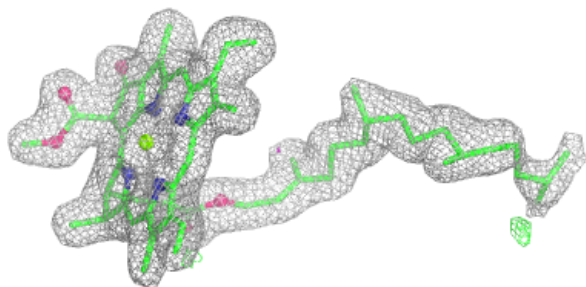
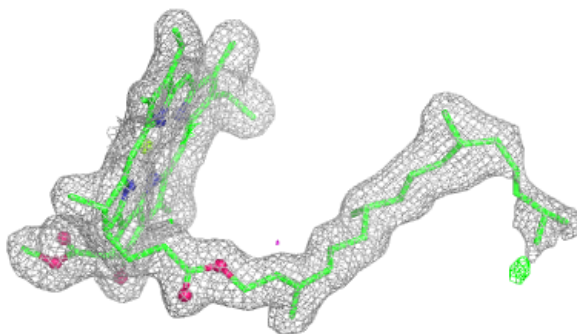


Electron density around LHG D 410:

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

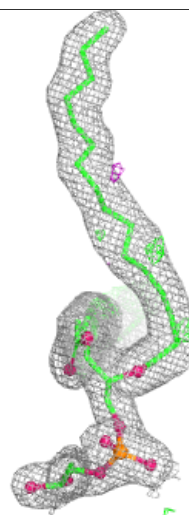
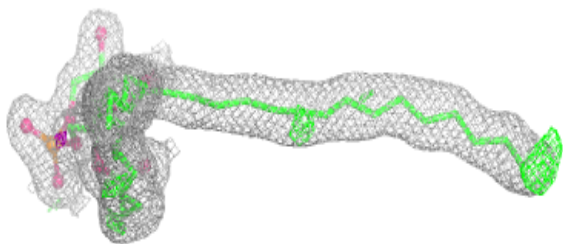
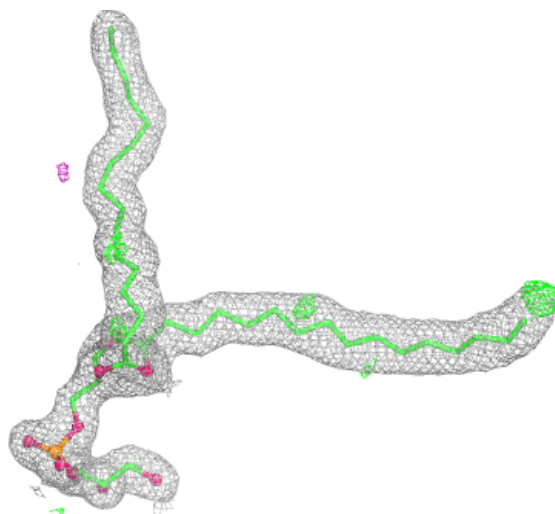
**Electron density around CLA C 508:**

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



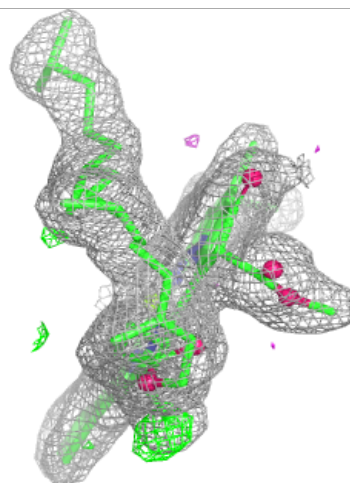
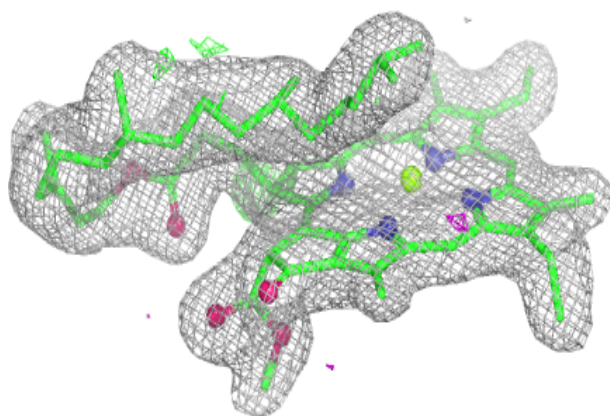
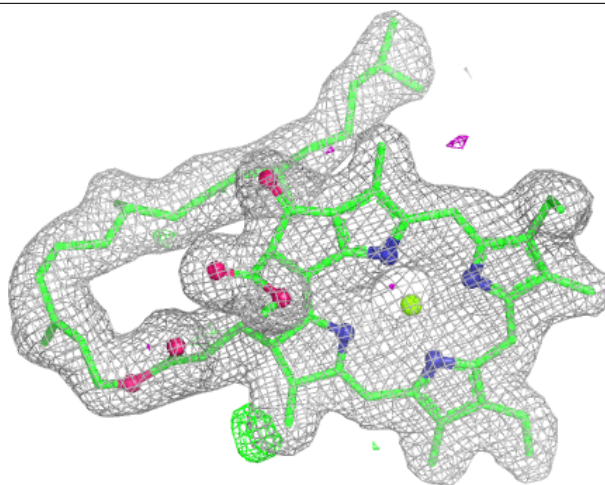
Electron density around LHG L 101:

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



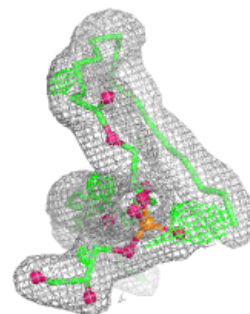
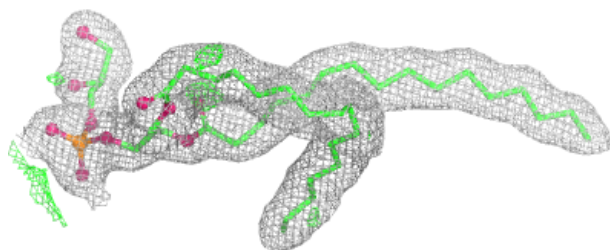
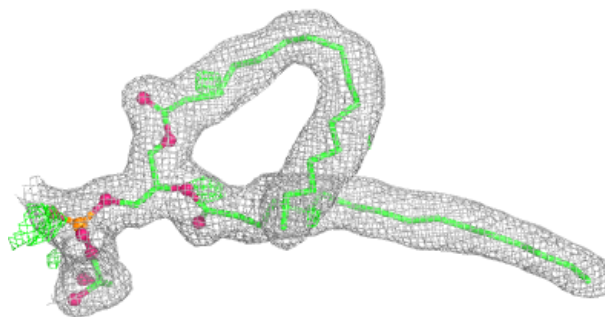
Electron density around CLA C 509:

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



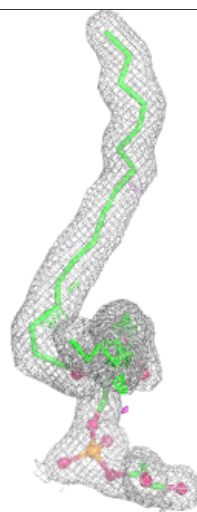
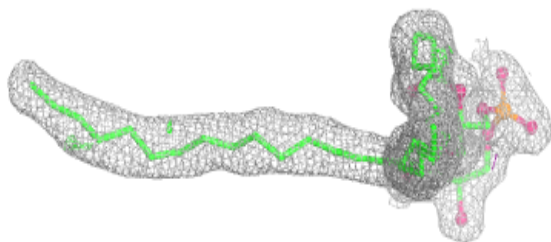
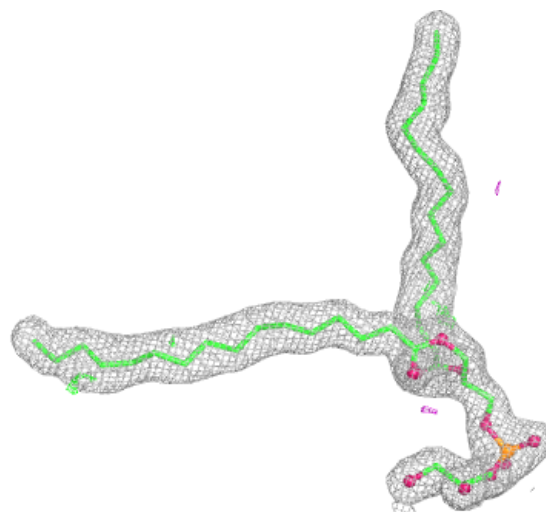
Electron density around LHG d 407:

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



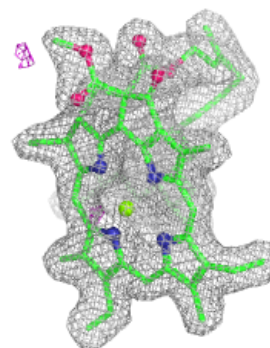
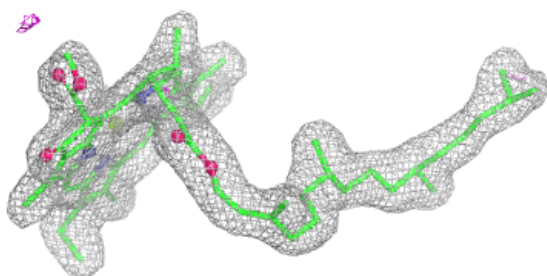
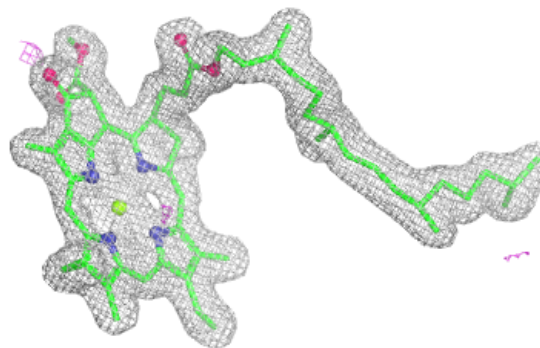
Electron density around LHG 1 101:

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

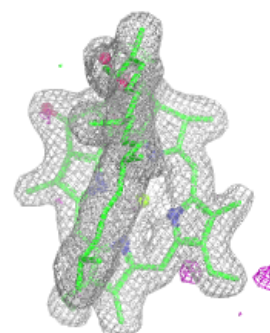
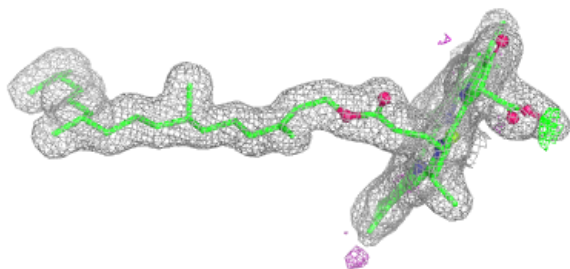
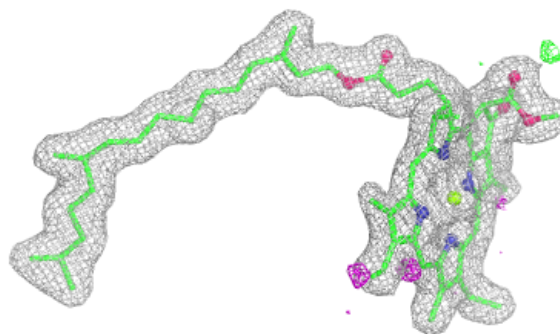


Electron density around CLA C 511:

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

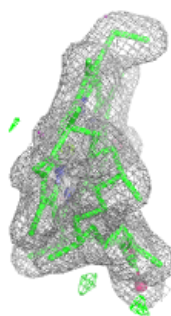
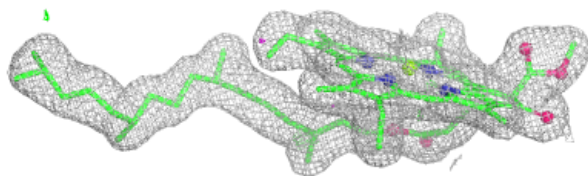
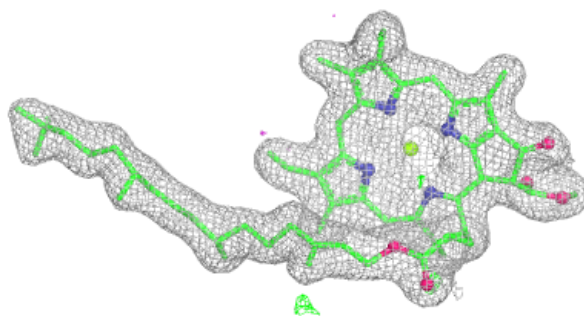
**Electron density around CLA B 610:**

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

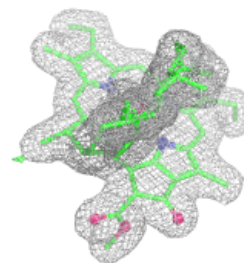
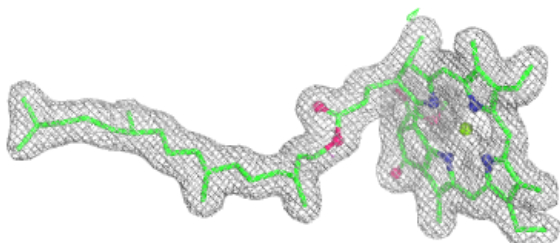
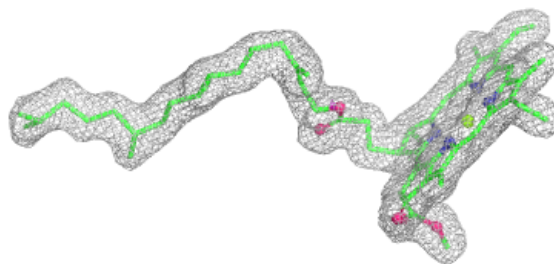


Electron density around CLA C 501:

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

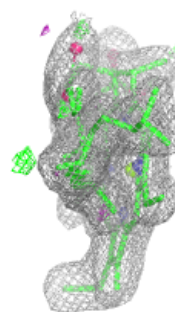
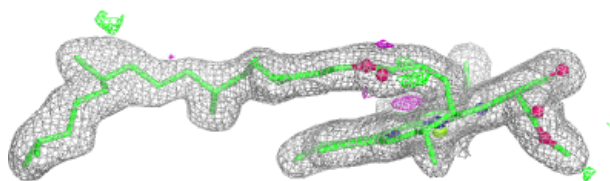
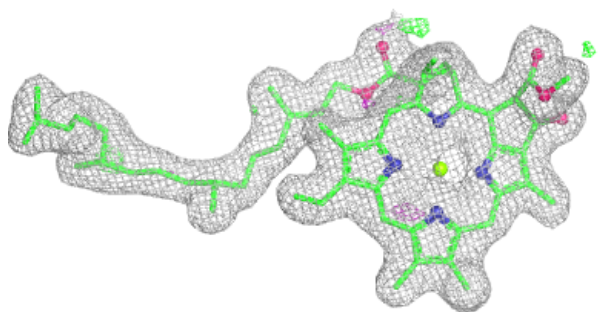
**Electron density around CLA C 502:**

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

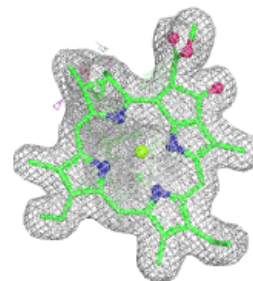
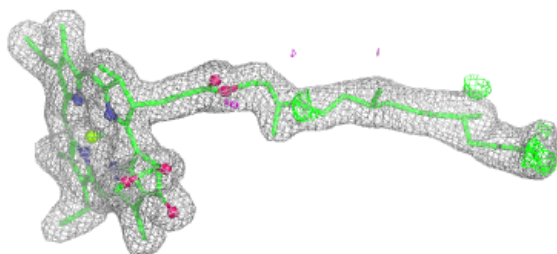
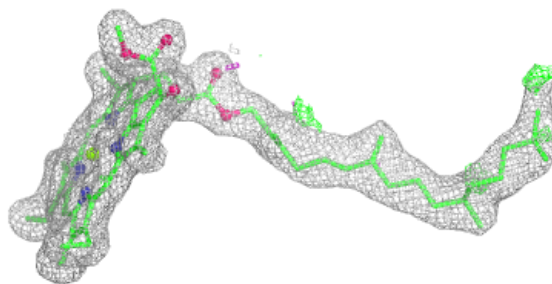


Electron density around CLA b 606:

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

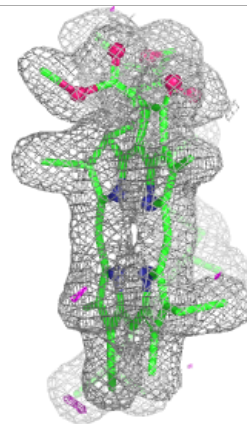
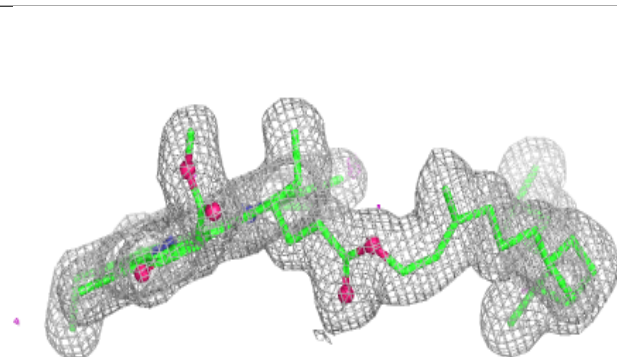
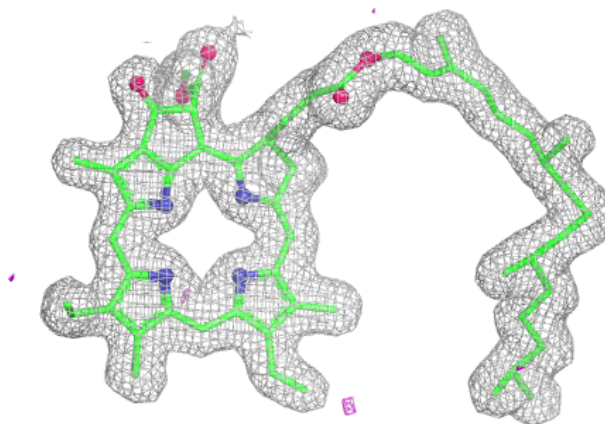
**Electron density around CLA b 607:**

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



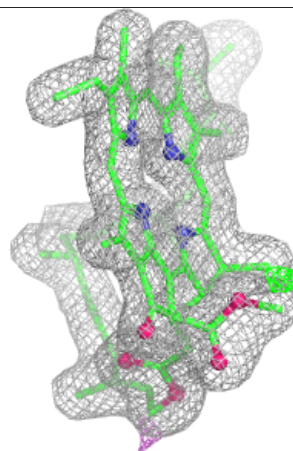
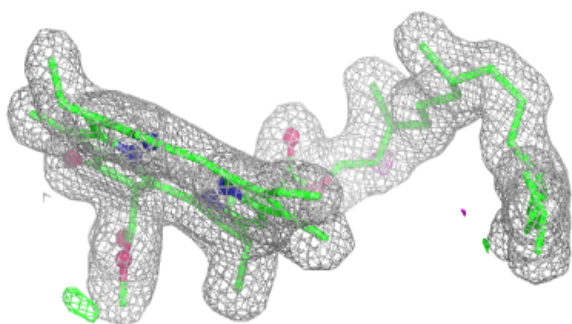
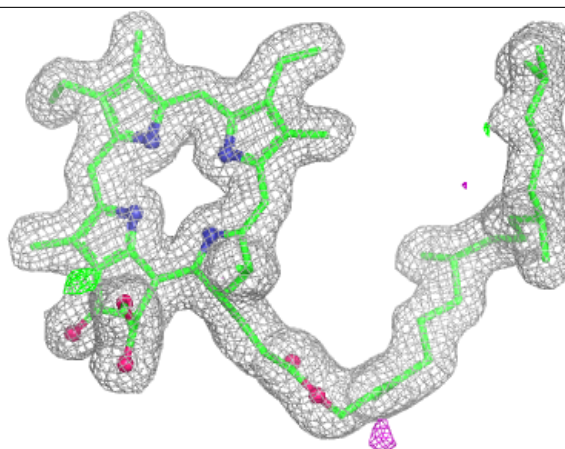
Electron density around PHO A 408:

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



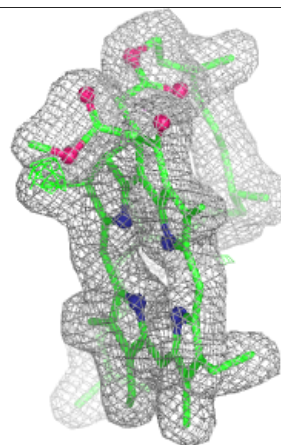
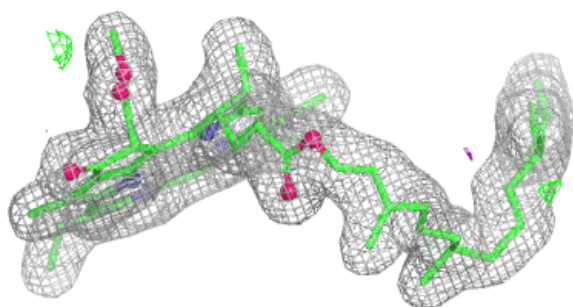
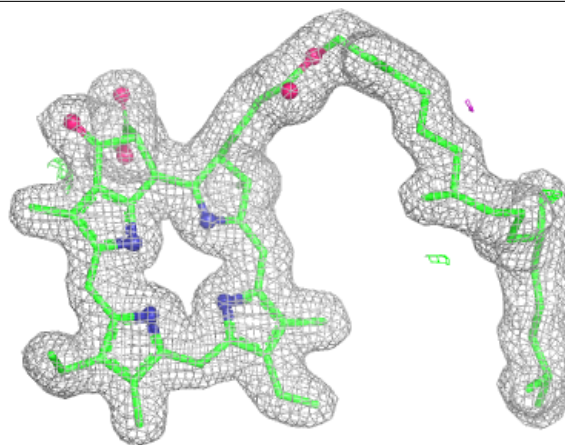
Electron density around PHO A 409:

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



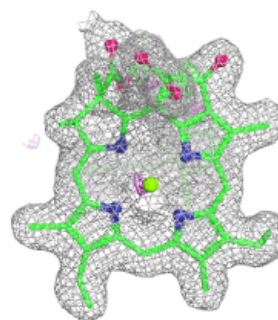
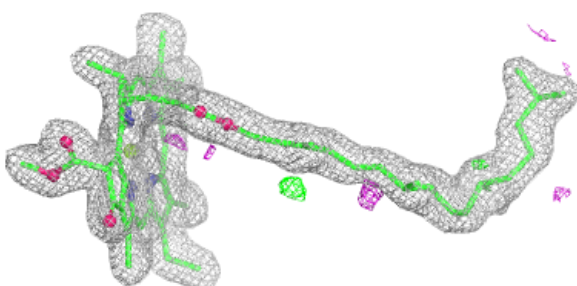
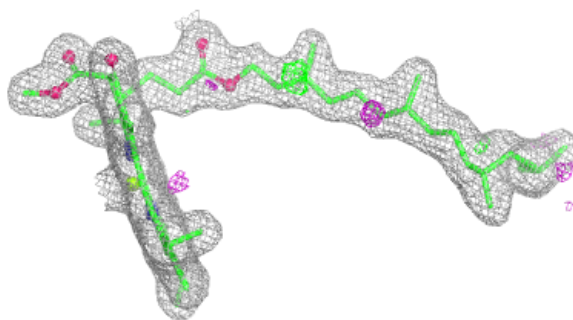
Electron density around PHO a 413:

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

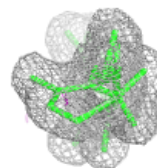
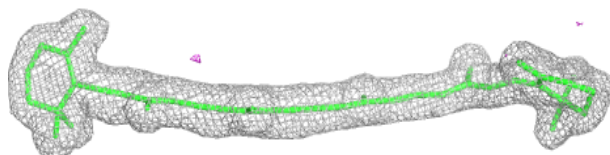
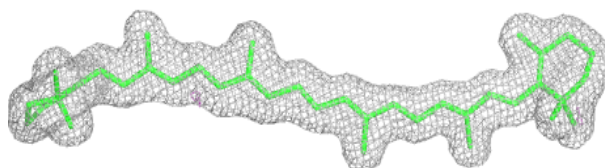


Electron density around CLA b 608:

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

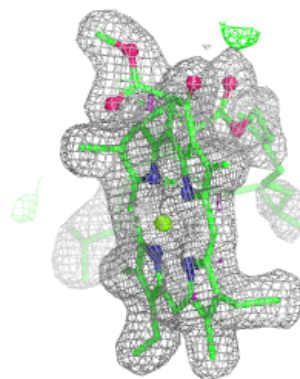
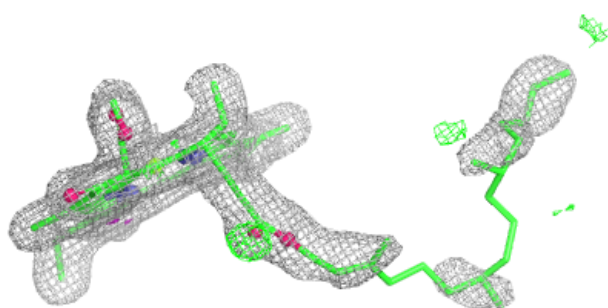
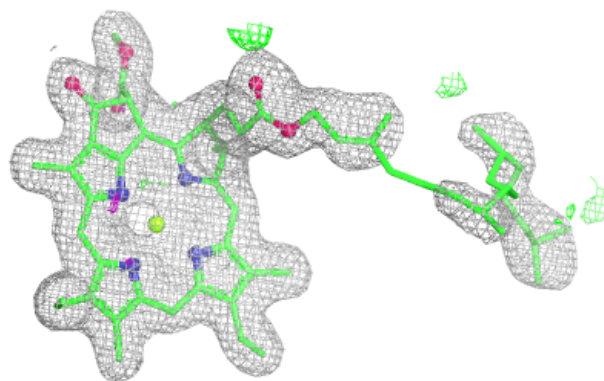
**Electron density around BCR B 618:**

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

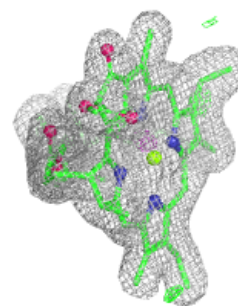
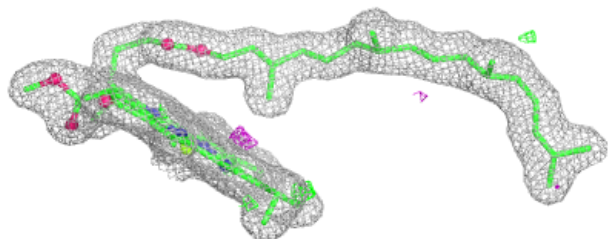
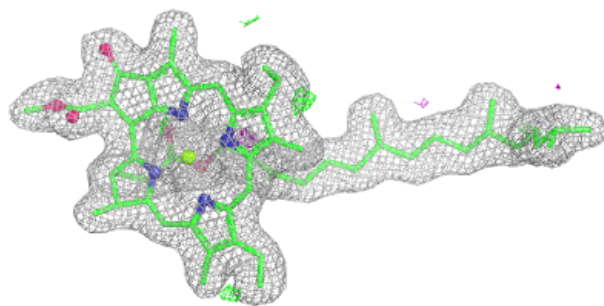


Electron density around CLA A 410:

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

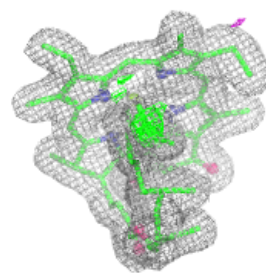
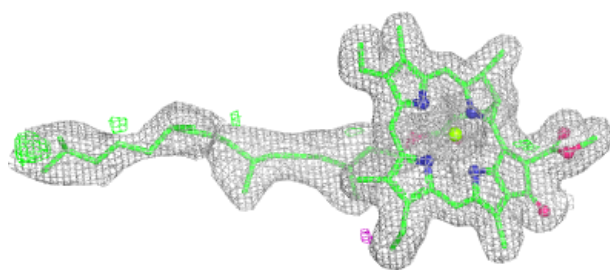
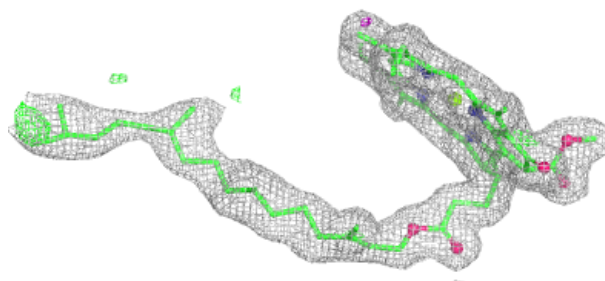
**Electron density around CLA b 611:**

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

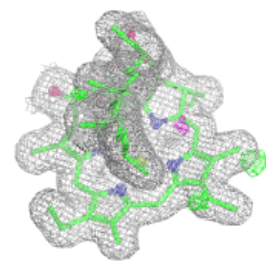
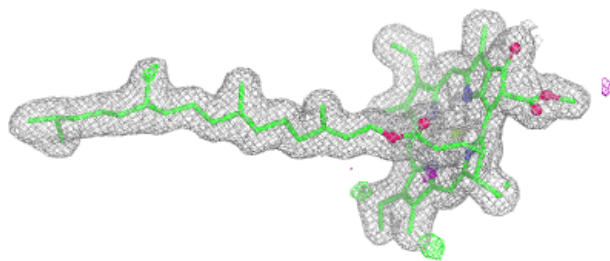
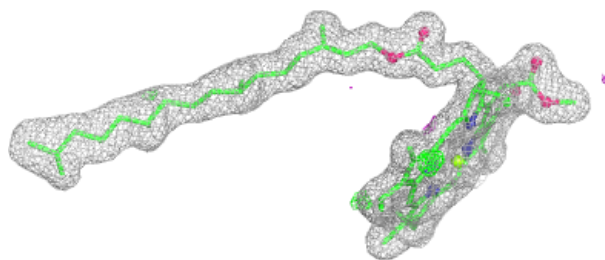


Electron density around CLA C 504:

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

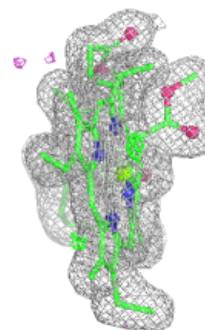
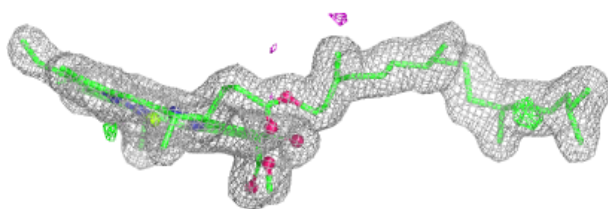
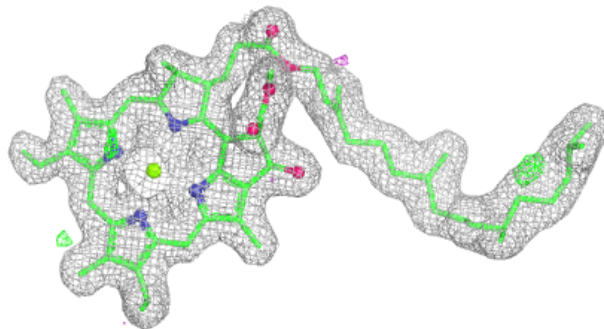
**Electron density around CLA B 608:**

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



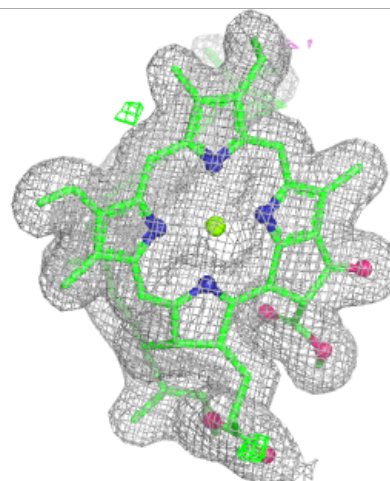
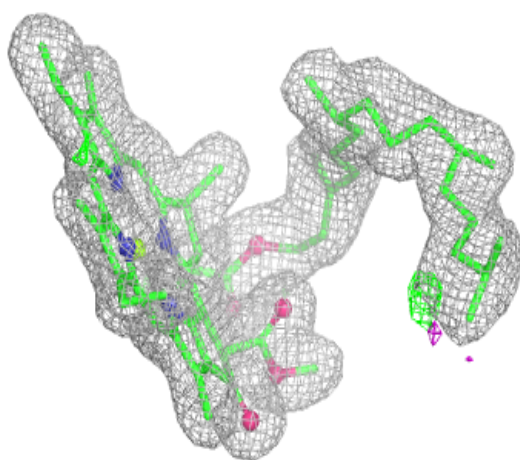
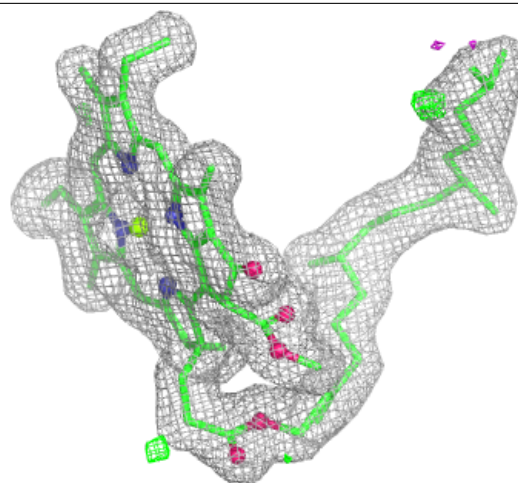
Electron density around CLA B 603:

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



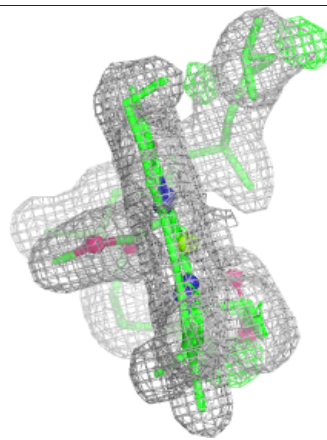
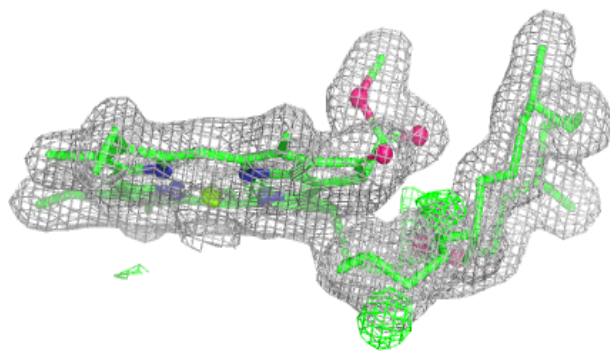
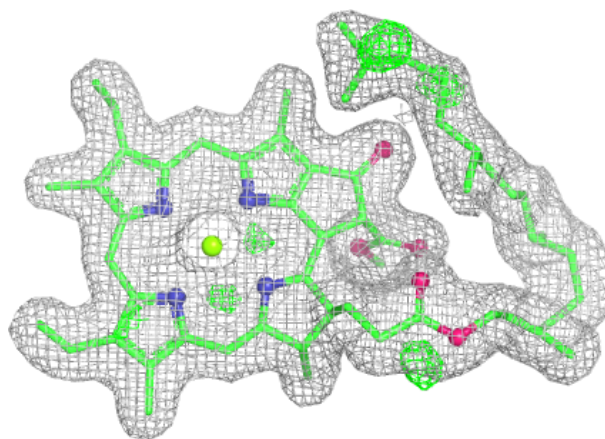
Electron density around CLA b 616:

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



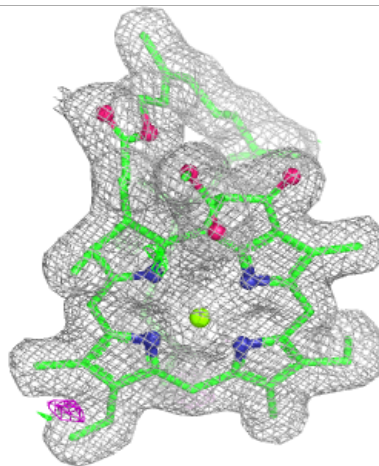
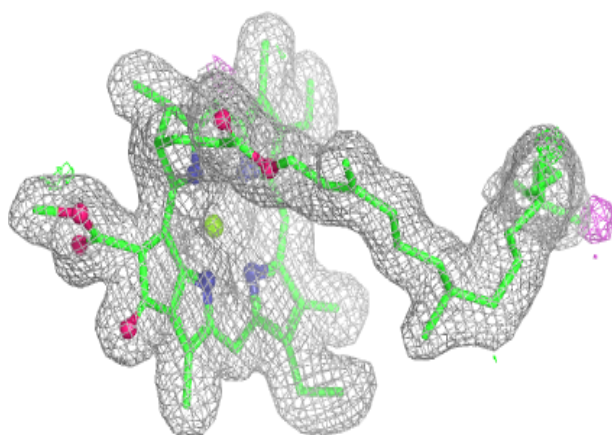
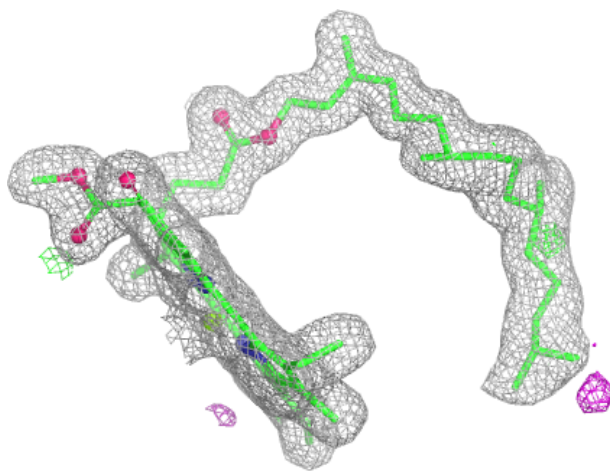
Electron density around CLA B 611:

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



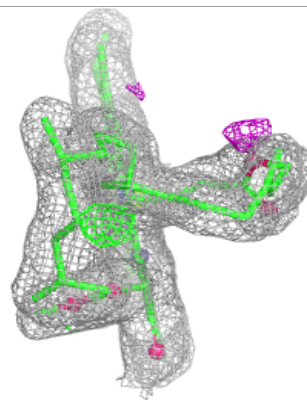
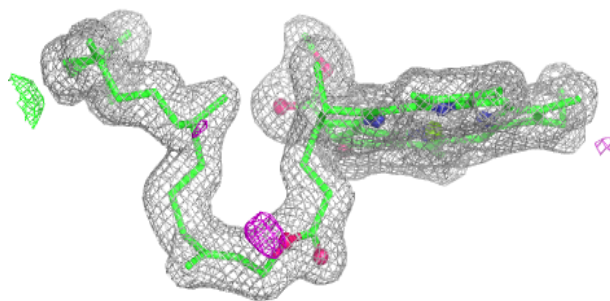
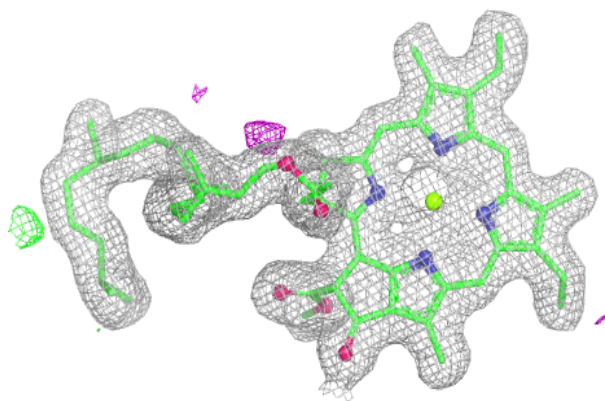
Electron density around CLA B 612:

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

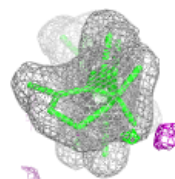
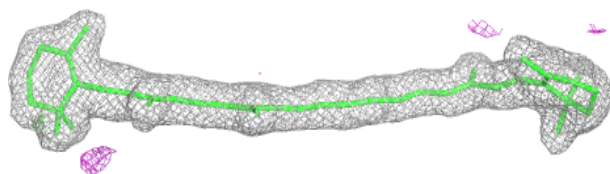
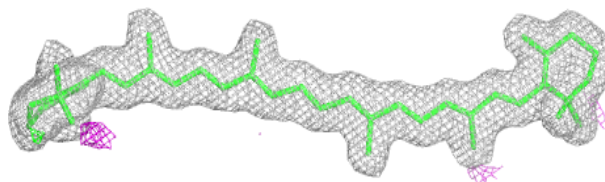


Electron density around CLA B 613:

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

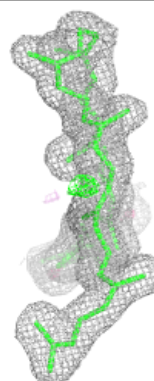
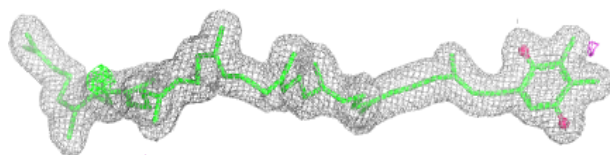
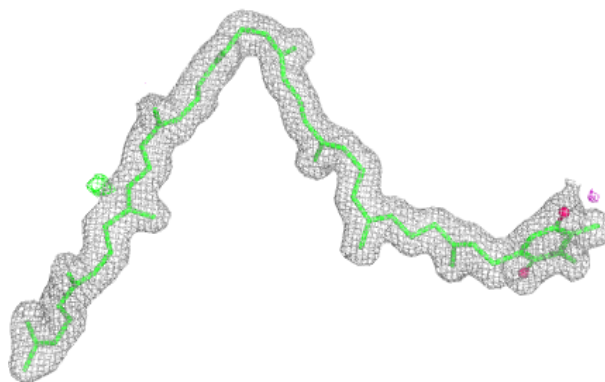
**Electron density around BCR b 620:**

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



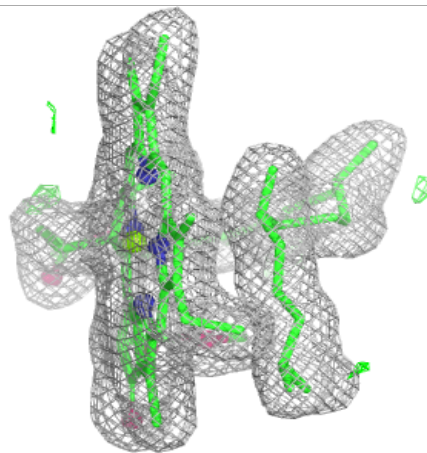
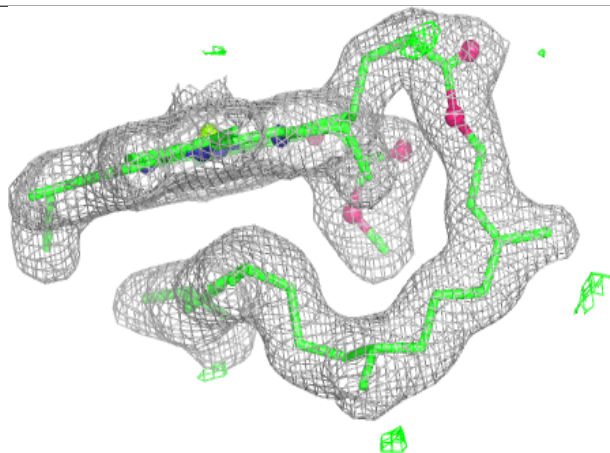
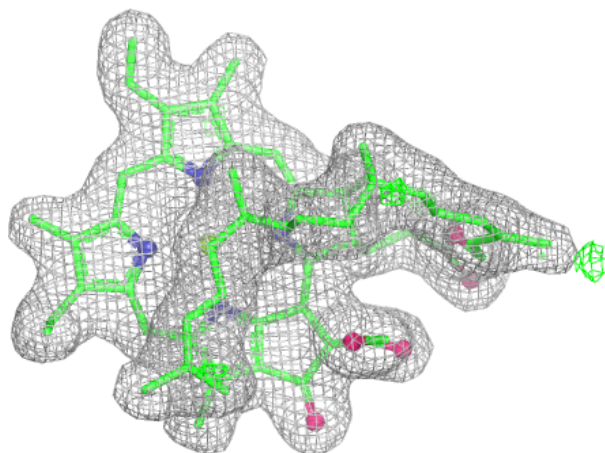
Electron density around PL9 d 405:

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



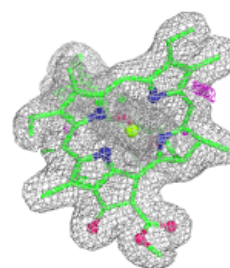
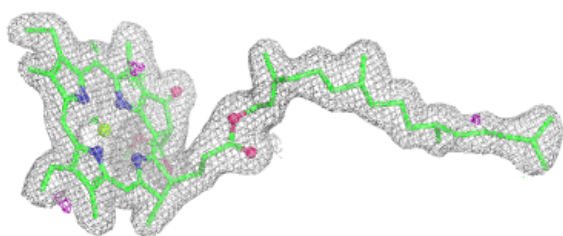
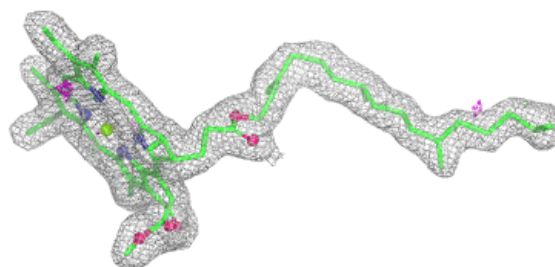
Electron density around CLA C 510:

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



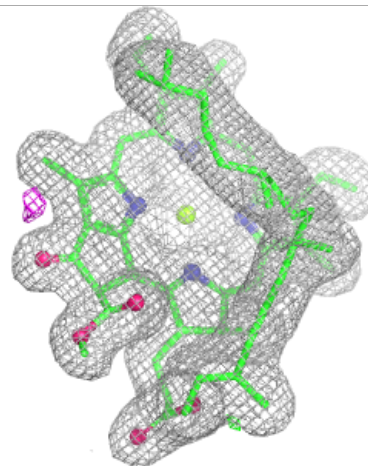
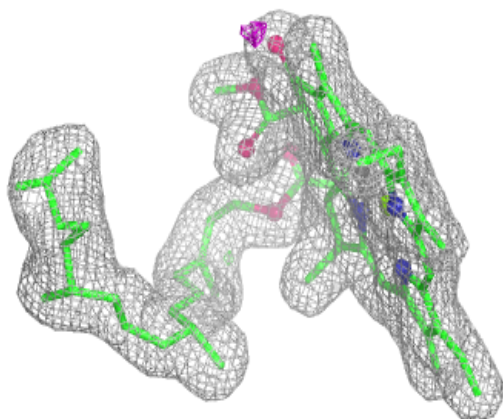
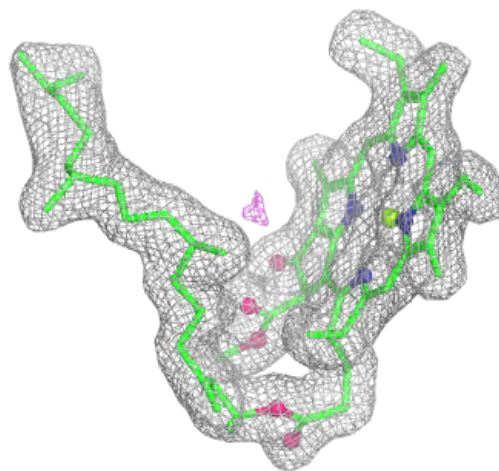
Electron density around CLA c 903:

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



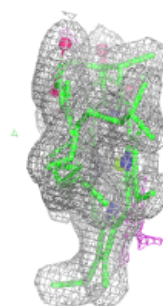
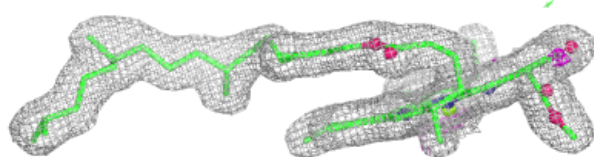
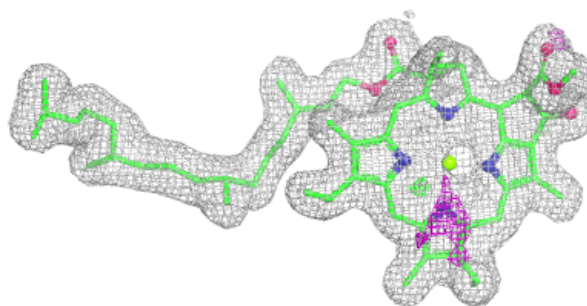
Electron density around CLA B 614:

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

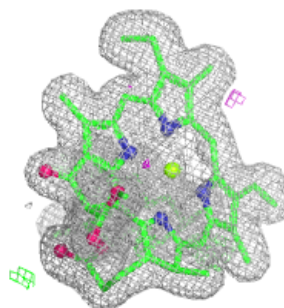
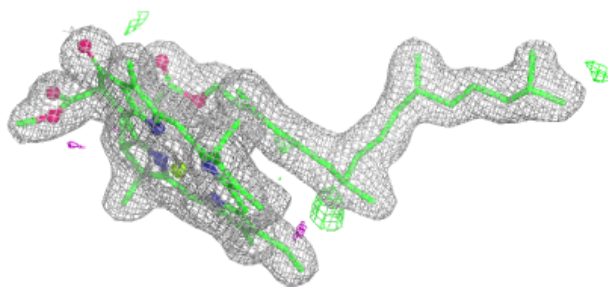
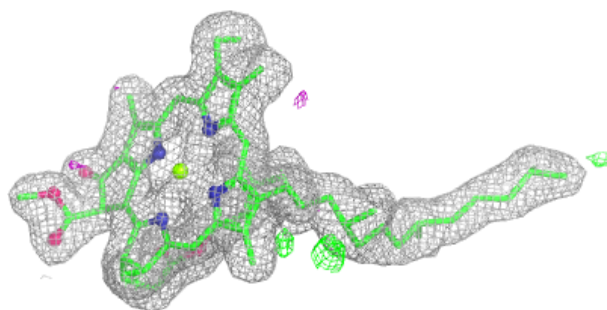


Electron density around CLA B 604:

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

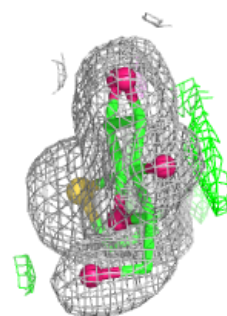
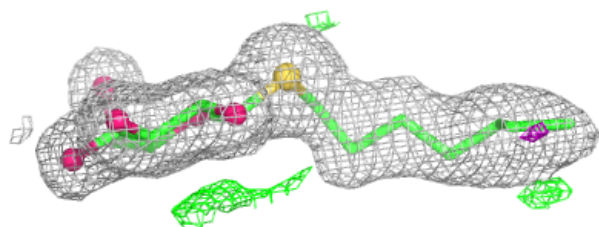
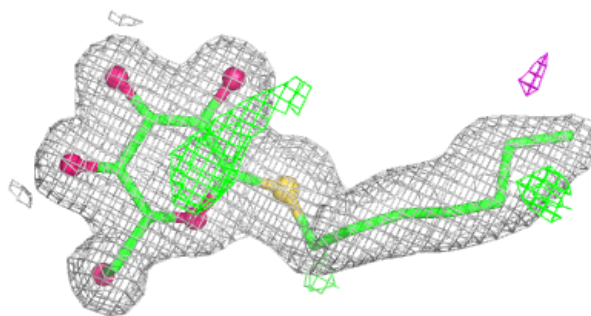
**Electron density around CLA c 906:**

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



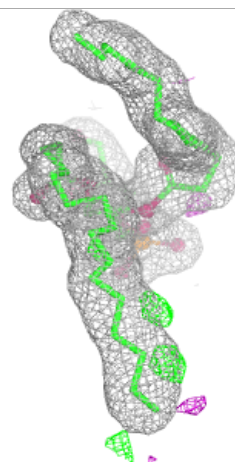
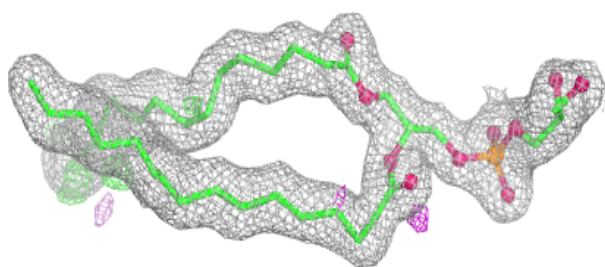
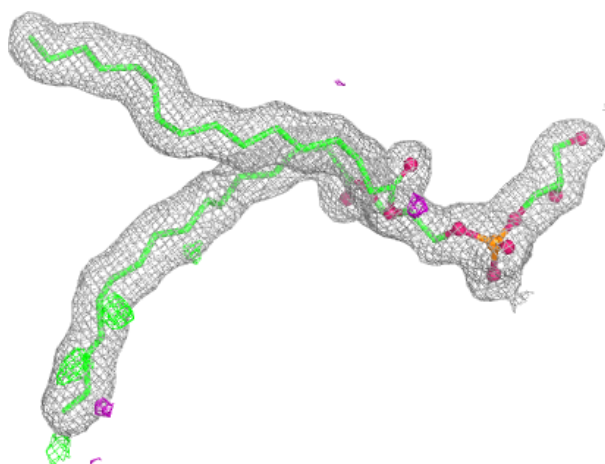
Electron density around HTG B 624:

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



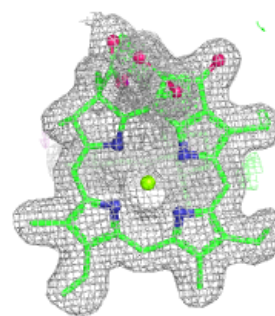
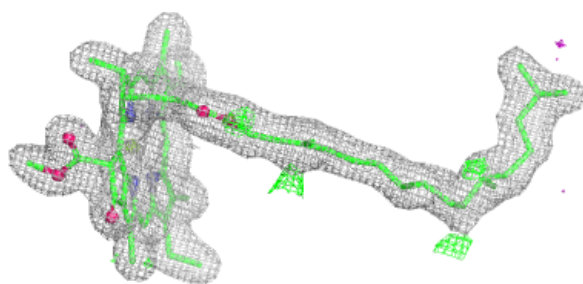
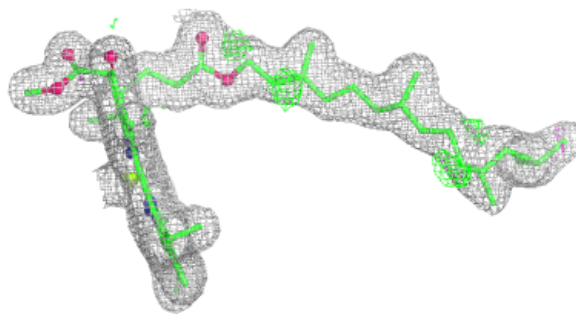
Electron density around LHG d 408:

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



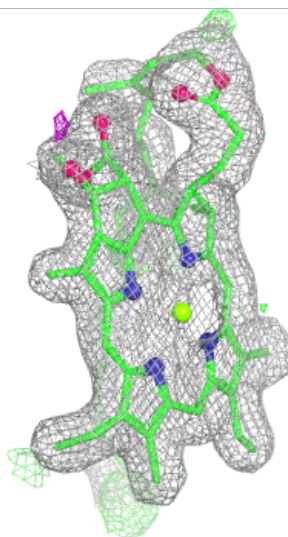
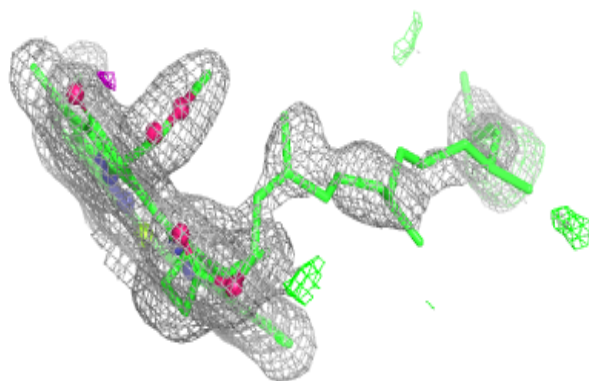
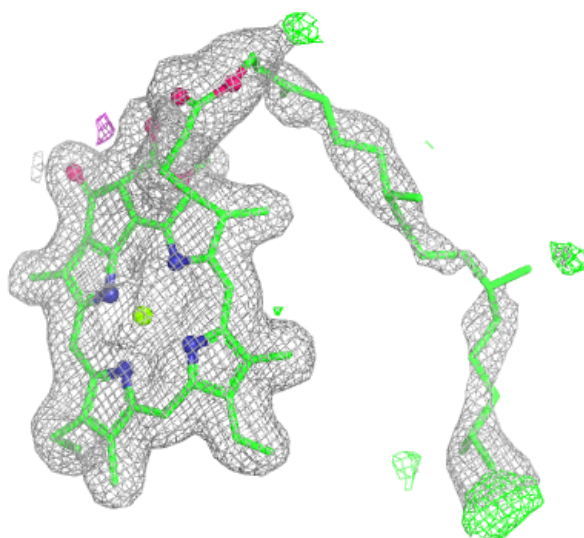
Electron density around CLA B 606:

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



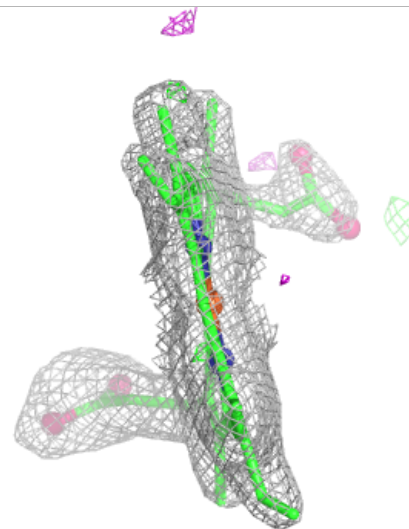
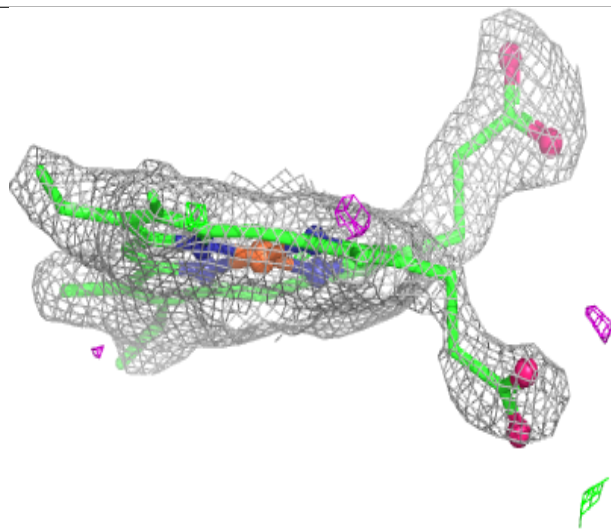
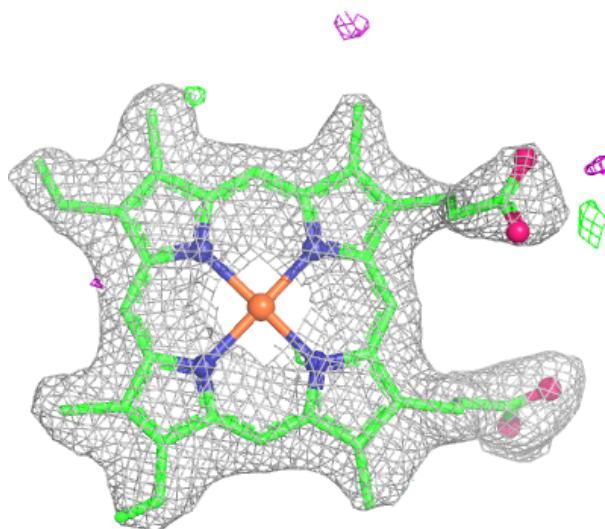
Electron density around CLA B 617:

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



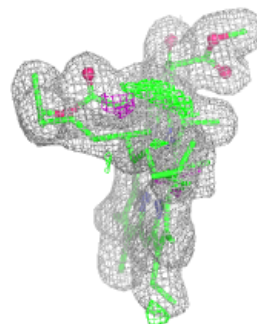
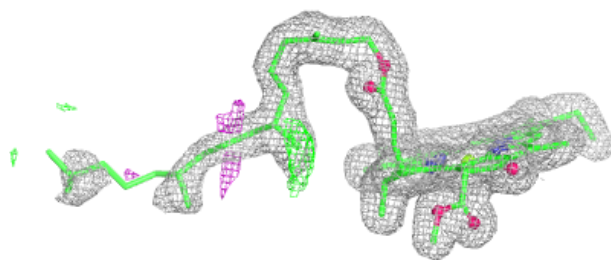
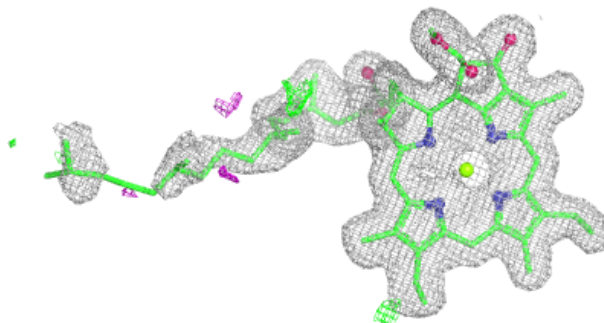
Electron density around HEM f 101:

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



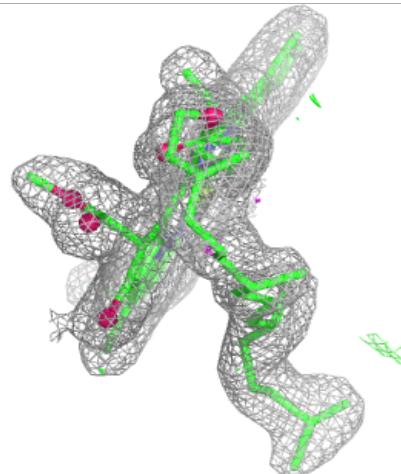
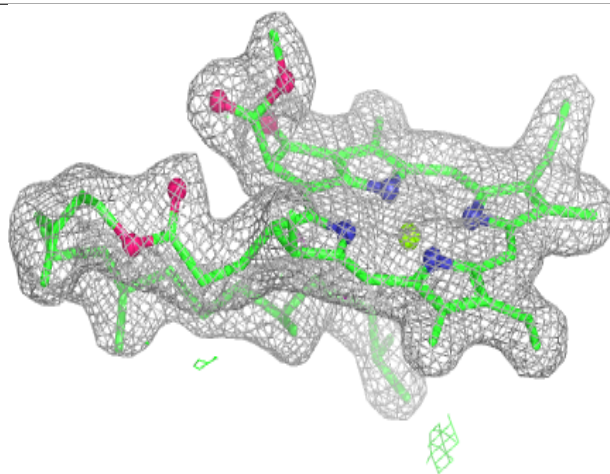
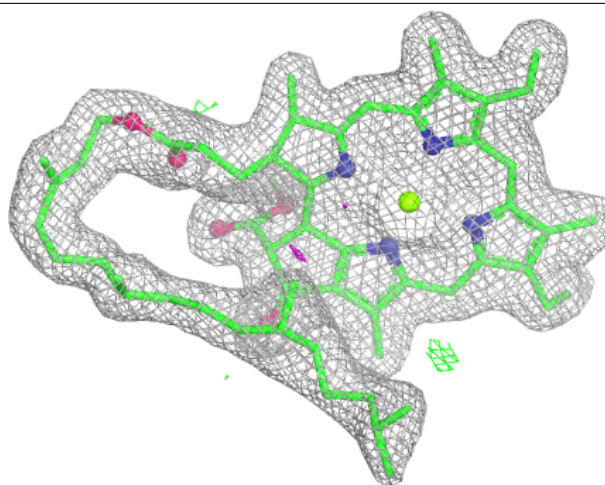
Electron density around CLA a 411:

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



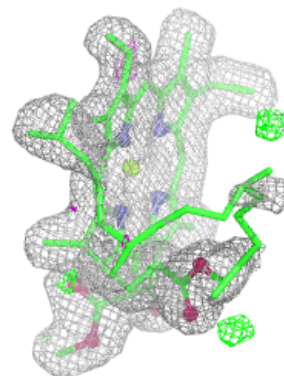
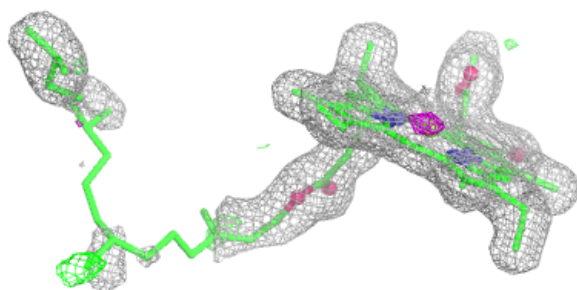
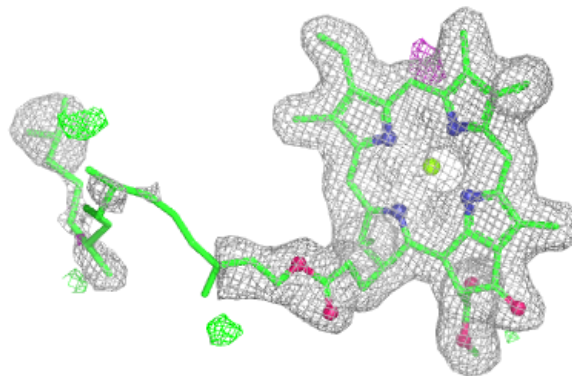
Electron density around CLA c 910:

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

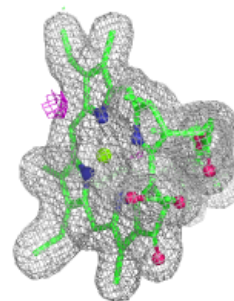
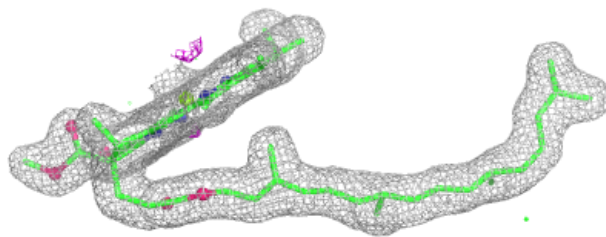
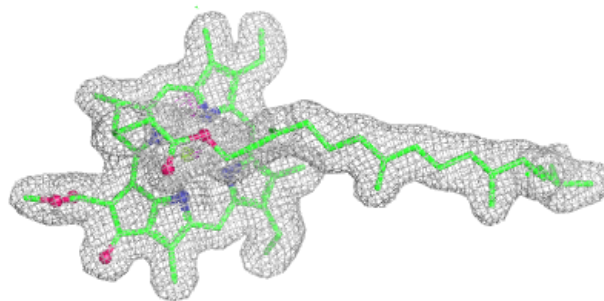


Electron density around CLA a 414:

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

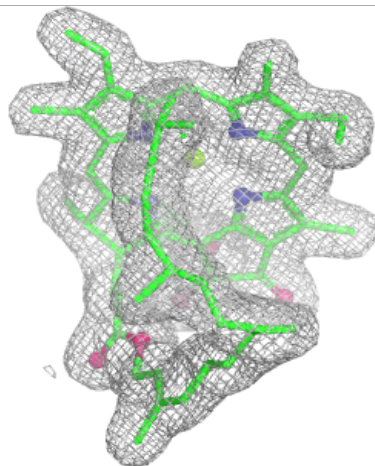
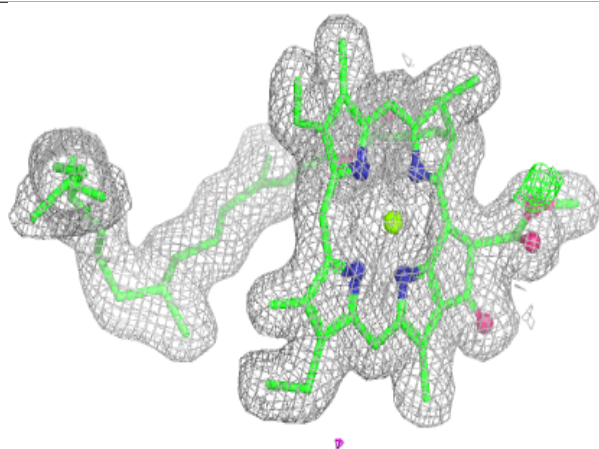
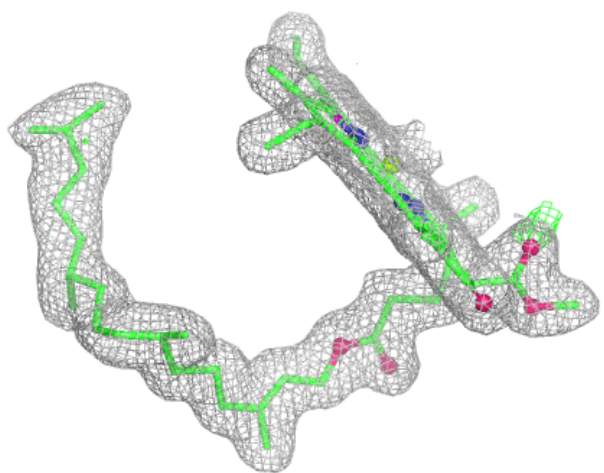
**Electron density around CLA B 609:**

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



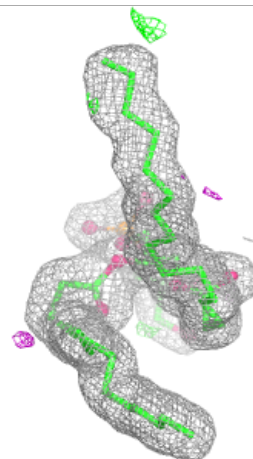
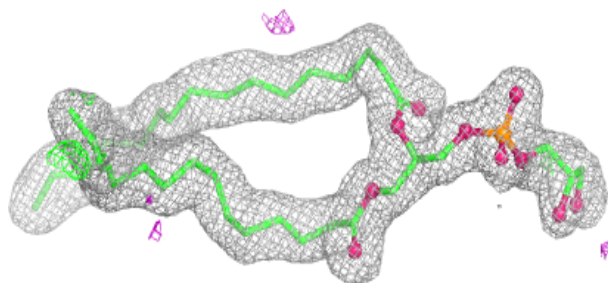
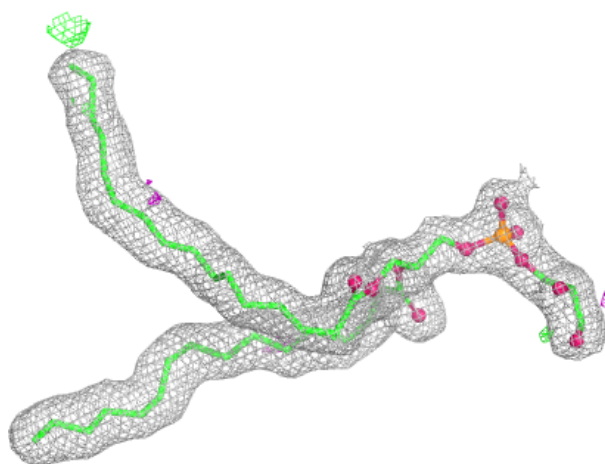
Electron density around CLA b 614:

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



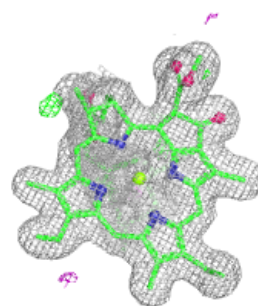
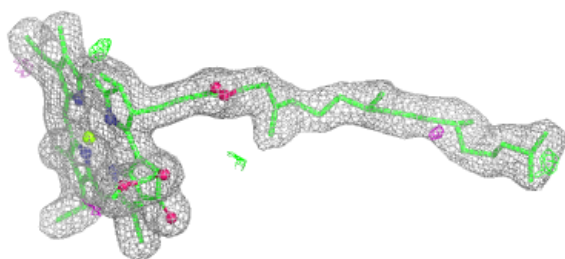
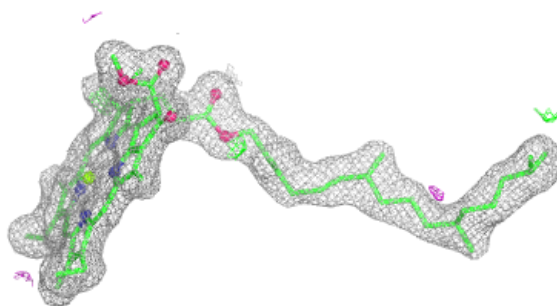
Electron density around LHG D 409:

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



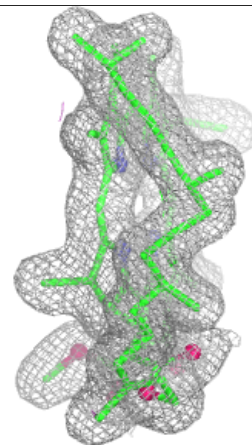
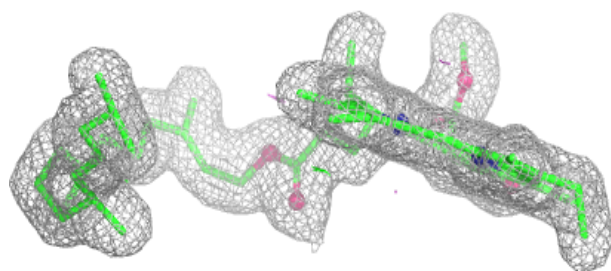
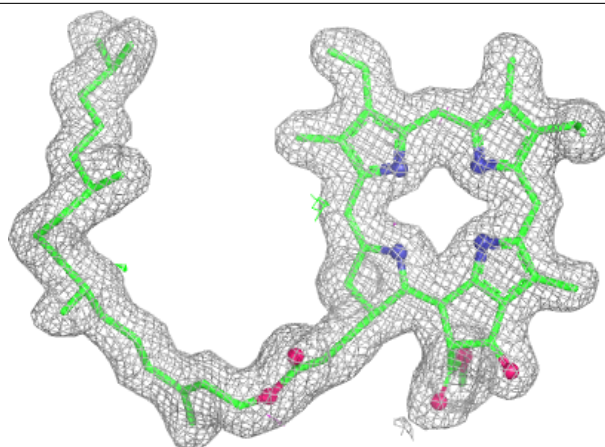
Electron density around CLA B 605:

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



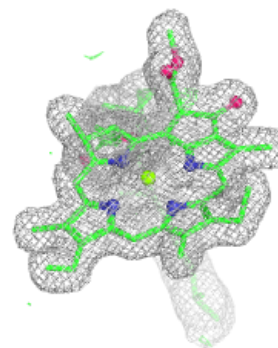
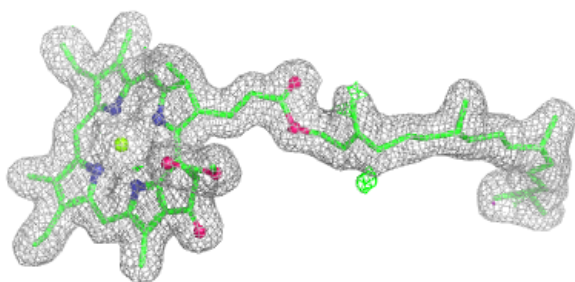
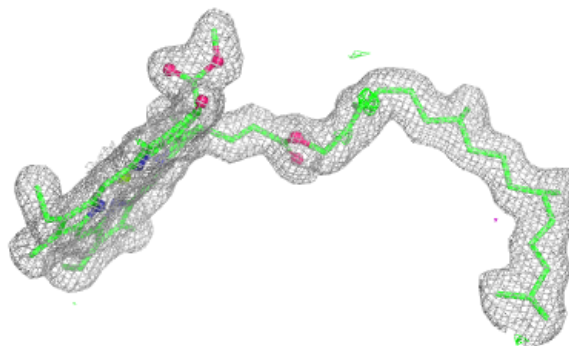
Electron density around PHO a 412:

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

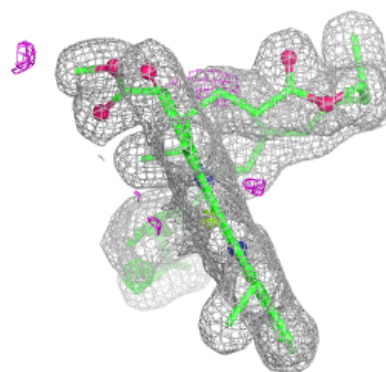
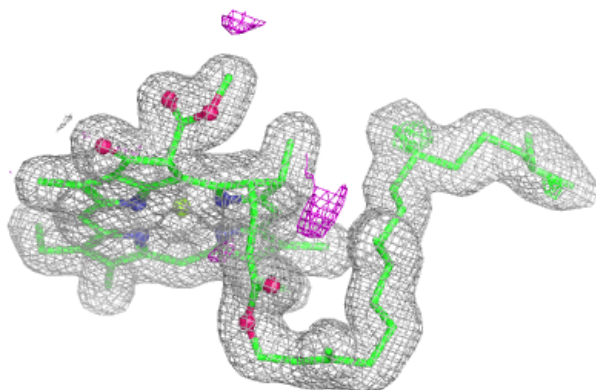
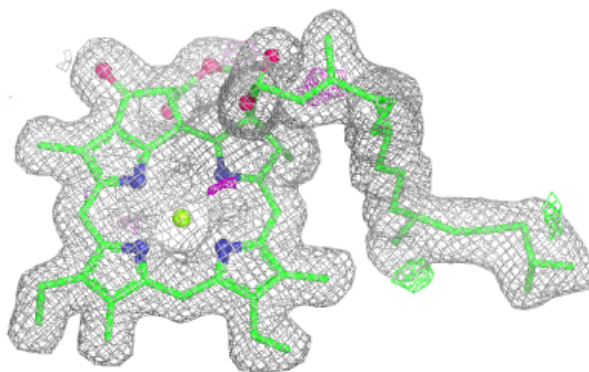


Electron density around CLA D 402:

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

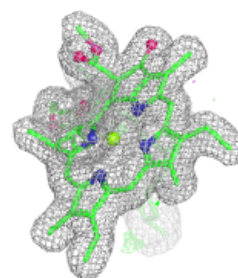
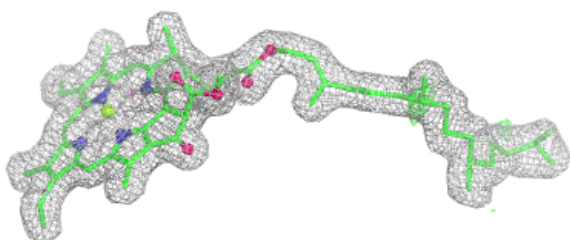
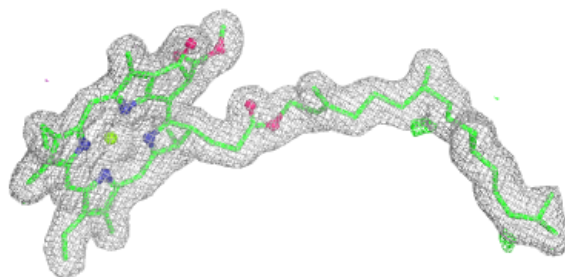
**Electron density around CLA A 406:**

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

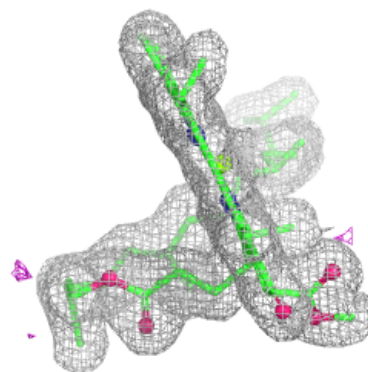
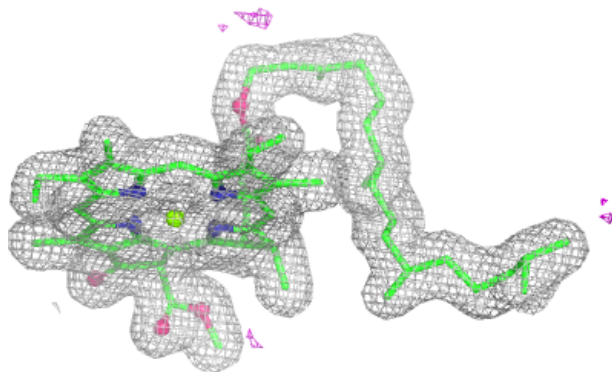
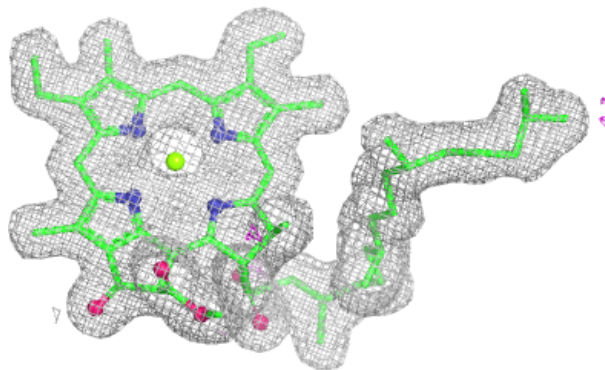


Electron density around CLA a 409:

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

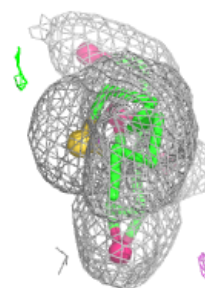
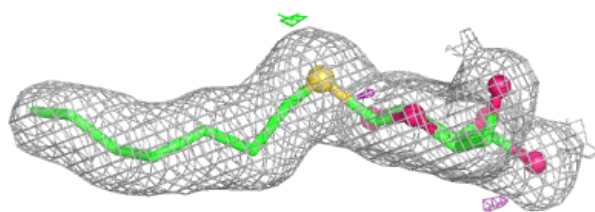
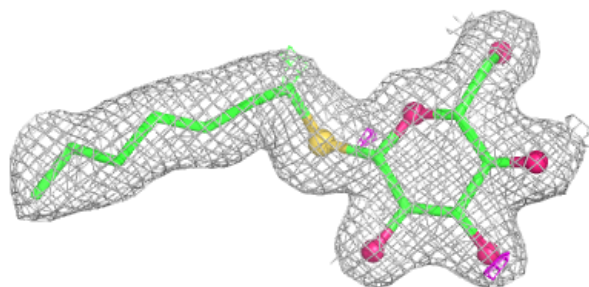
**Electron density around CLA a 410:**

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



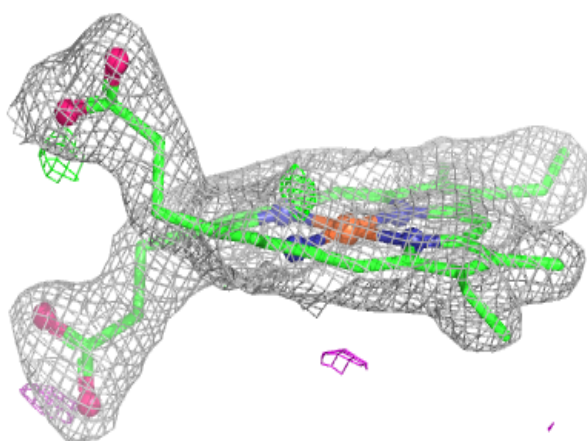
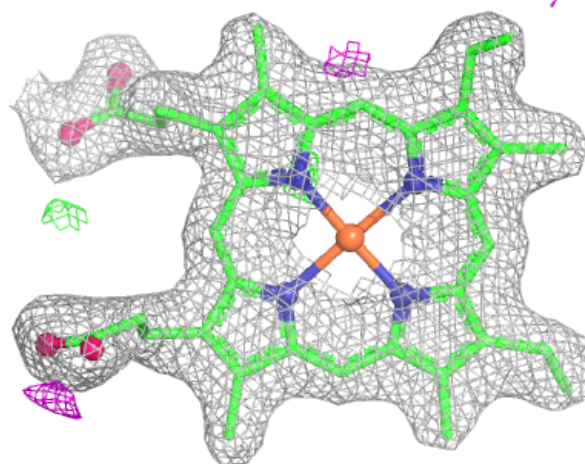
Electron density around HTG O 303:

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



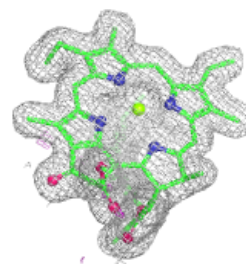
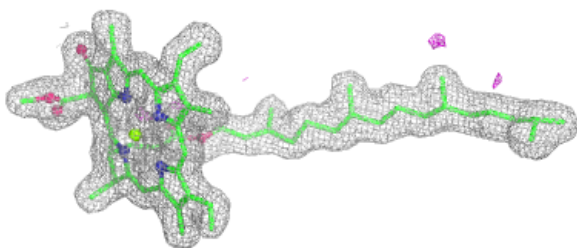
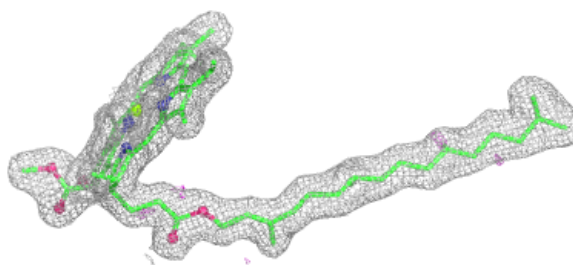
Electron density around HEM F 101:

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



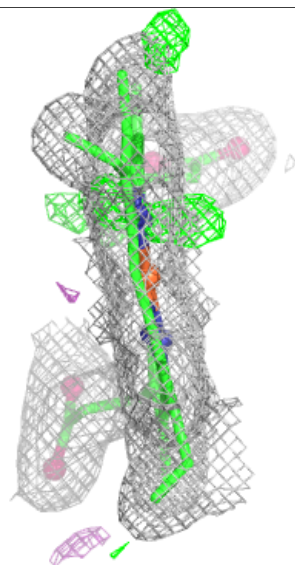
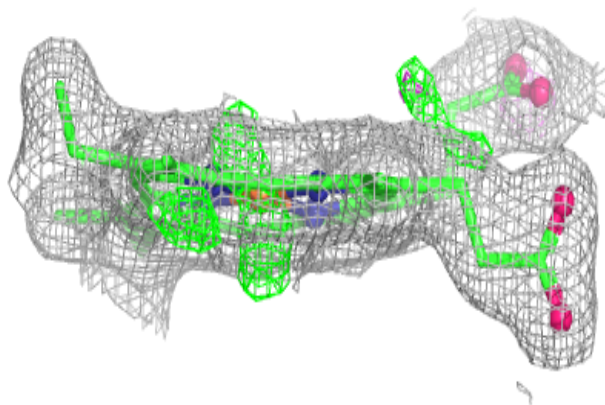
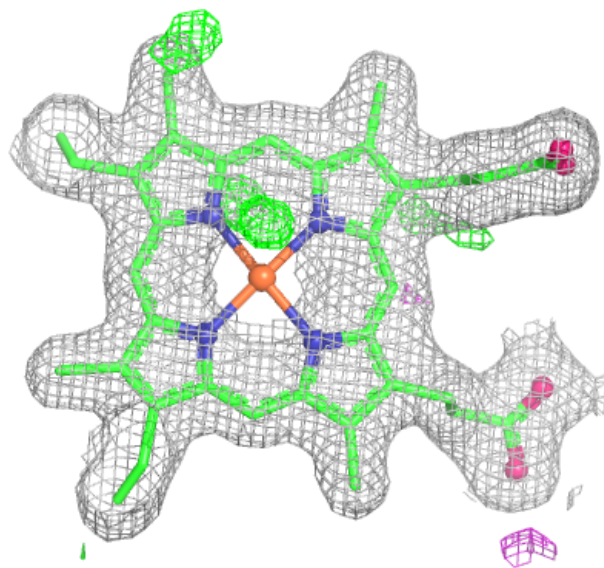
Electron density around CLA b 610:

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



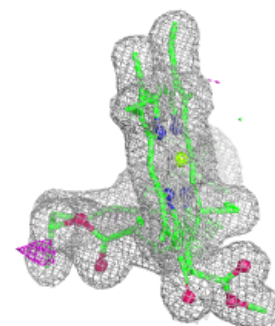
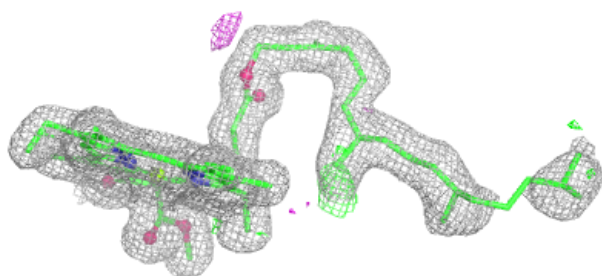
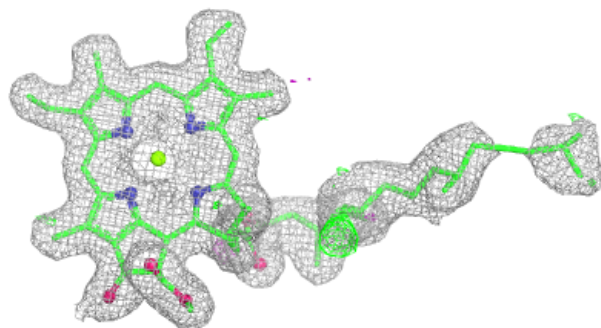
Electron density around HEM v 201:

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

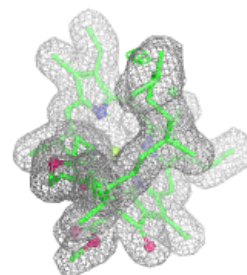
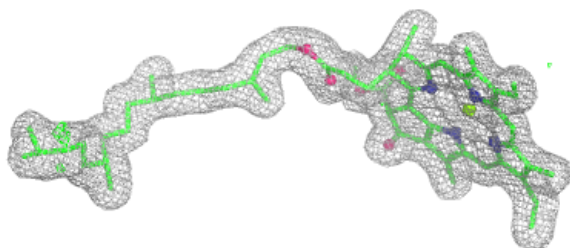
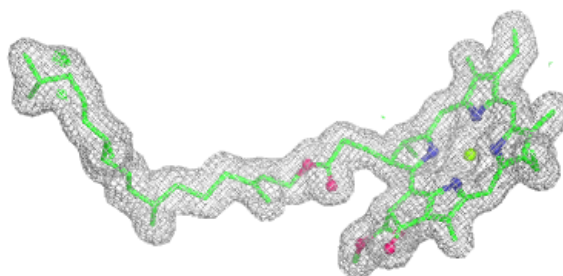


Electron density around CLA A 407:

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

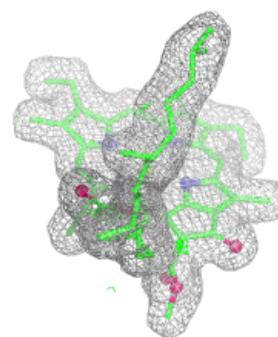
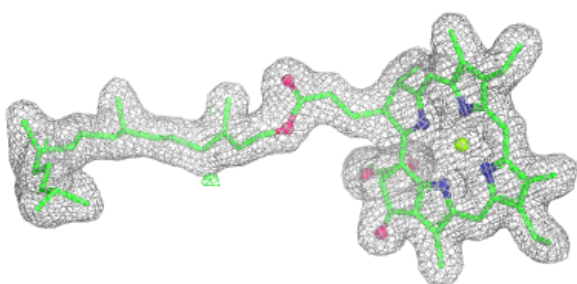
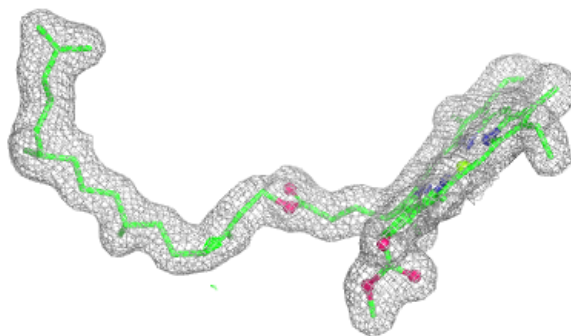
**Electron density around CLA A 405:**

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



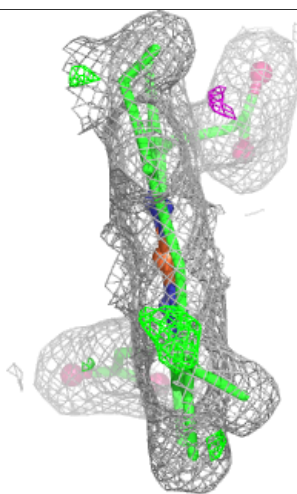
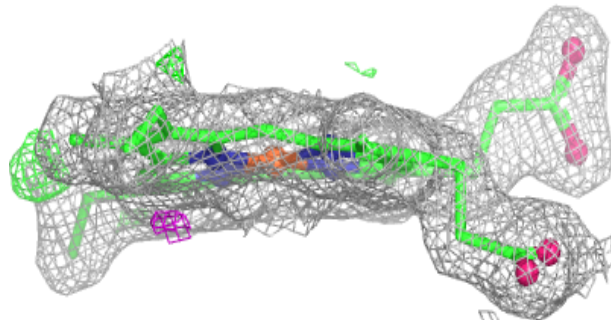
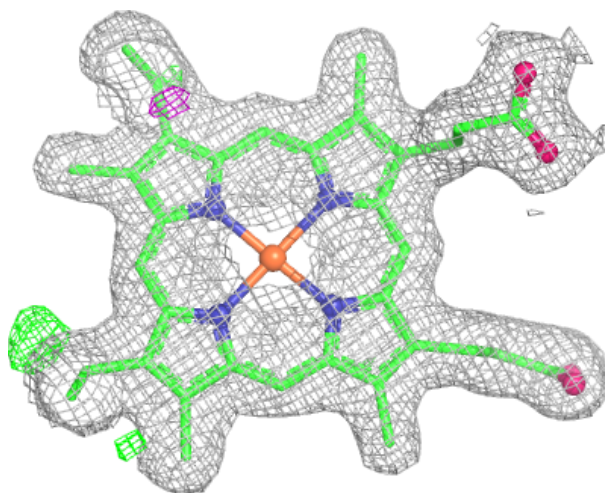
Electron density around CLA d 402:

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



Electron density around HEM V 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.