



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:47 AM EDT

PDB ID : 4IL6 / pdb_00004il6
Title : Structure of Sr-substituted photosystem II
Authors : Koua, F.H.M.; Umena, Y.; Kawakami, K.; Kamiya, N.; Shen, J.R.
Deposited on : 2012-12-29
Resolution : 2.10 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

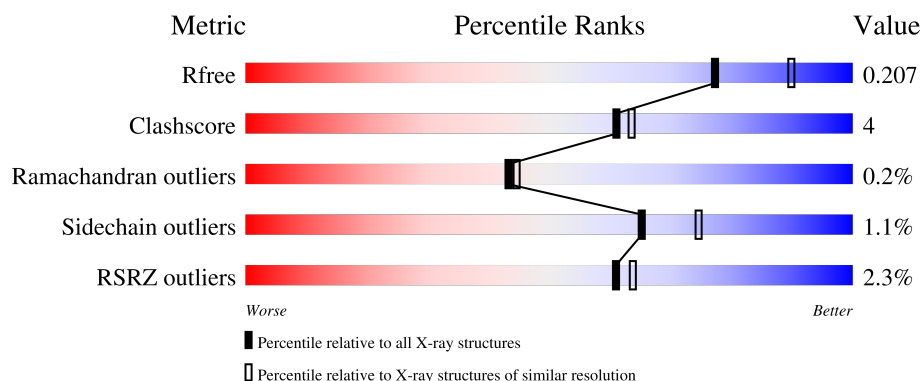
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



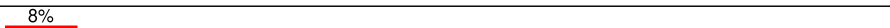
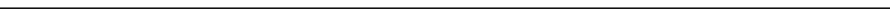
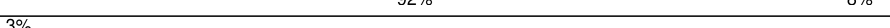
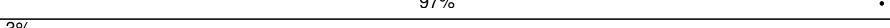
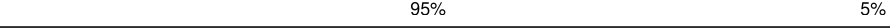
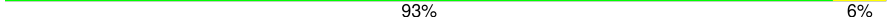
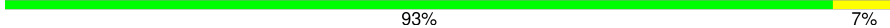
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	334	91% 9%
1	a	334	% 92% 8%
2	B	505	% 94% 6%
2	b	505	3% 93% 6%
3	C	451	% 93% 6%

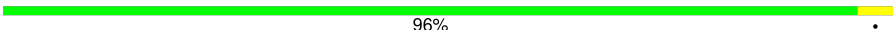
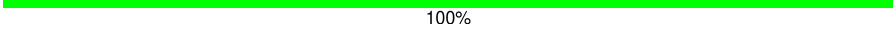
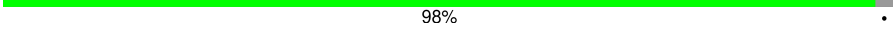
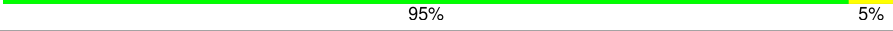
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Mol	Chain	Length	Quality of chain
3	c	451	 90% 9%
4	D	342	 90% 10%
4	d	342	 91% 9%
5	E	80	 84% 16% 8%
5	e	80	 85% 11% 2% ..
6	F	34	 97% .
6	f	34	 82% 12% 6% 6%
7	H	63	 92% 8% 2%
7	h	63	 94% 6% 2%
8	I	36	 94% 6% 3%
8	i	36	 86% 14% 6%
9	J	37	 92% 8% 8%
9	j	37	 97% . 8%
10	K	37	 89% 8% . 3%
10	k	37	 86% 11% . 3%
11	L	37	 92% 8% 3%
11	l	37	 97% . 3%
12	M	34	 79% 15% 6%
12	m	34	 82% 18% 3%
13	O	244	 95% 5% 4%
13	o	244	 93% 6% 2%
14	T	31	 87% 6% 6%
14	t	31	 90% 6% . 3%
15	U	97	 93% 7% 3%
15	u	97	 96% . 3%

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Mol	Chain	Length	Quality of chain
16	V	137	 96%
16	v	137	 93% 7%
17	Y	30	 83% 17% 3%
17	y	30	 87% 7% 7%
18	X	40	 100% 5%
18	x	40	 98% 8%
19	Z	62	 92% 8% 10%
19	z	62	 95% 5% 11%
20	R	34	 82% 18% 79%

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
26	BCR	D	406	-	X	-	-
26	BCR	J	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	d	404	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	y	101	-	X	-	-

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 53568 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	5	0
			2643	1733	431	464	15			
1	a	334	Total	C	N	O	S	0	4	0
			2637	1729	431	462	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 core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	10	0
			4040	2652	674	701	13			
2	b	505	Total	C	N	O	S	0	9	0
			4033	2646	676	698	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3500	2292	584	611	13			
3	c	450	Total	C	N	O	S	0	2	0
			3492	2287	583	609	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O		0	2	0
			660	431	105	124				
5	e	78	Total	C	N	O		0	0	0
			638	418	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
			275	187	45	42	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	1	0
			506	338	83	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	37	Total	C	N	O	S	0	0	0
			266	179	41	45	1			
9	j	37	Total	C	N	O	S	0	0	0
			266	179	41	45	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			
12	m	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

- 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	2	0
			1883	1176	317	386	4			
13	o	243	Total	C	N	O	S	0	1	0
			1868	1167	315	382	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			267	187	38	40	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	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	1	0
			780	495	129	156			
15	u	97	Total	C	N	O	0	1	0
			780	495	129	156			

- 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	3	0
			1081	687	179	211	4			
16	v	137	Total	C	N	O	S	0	2	0
			1076	683	177	212	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	0	0	0
			296	197	47	52			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

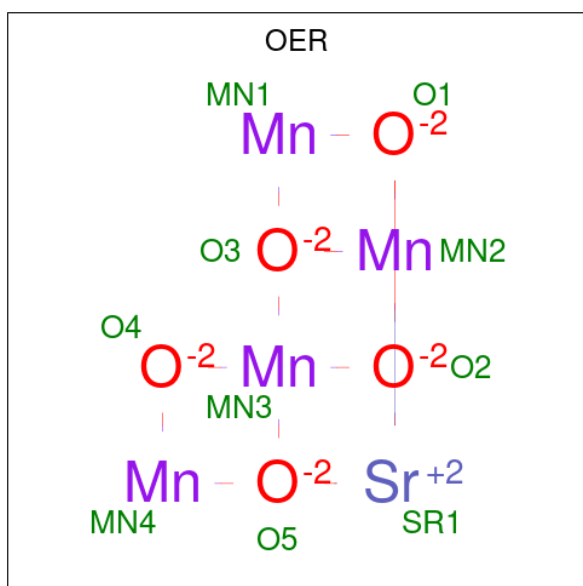
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			
19	z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			

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

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

- Molecule 21 is SR-MN4-O5 CLUSTER (CCD ID: OER) (formula: $\text{Mn}_4\text{O}_5\text{Sr}$).



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

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

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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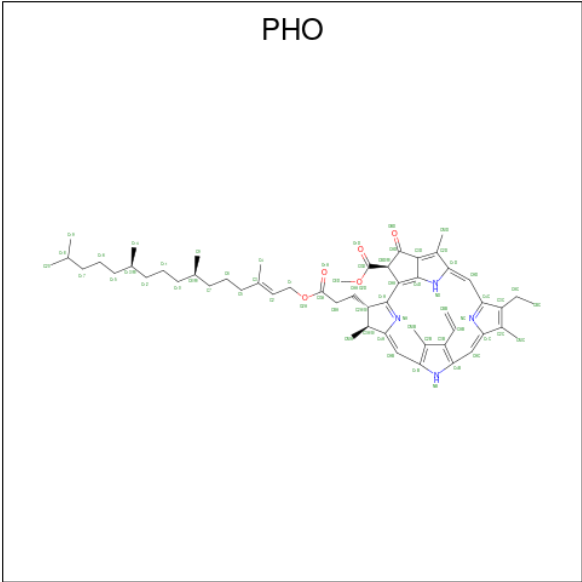
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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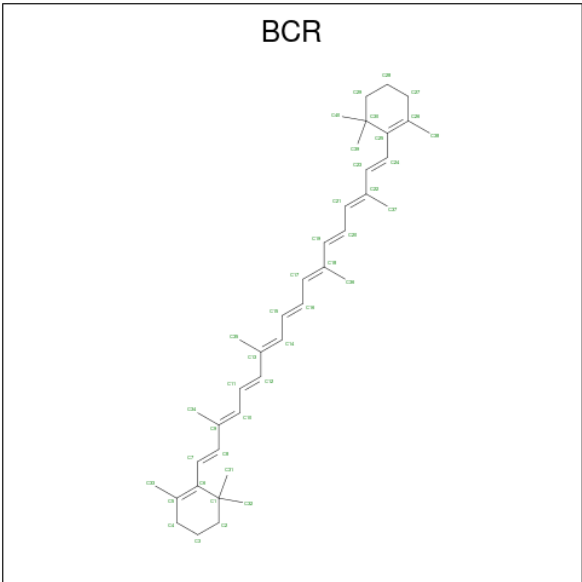
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



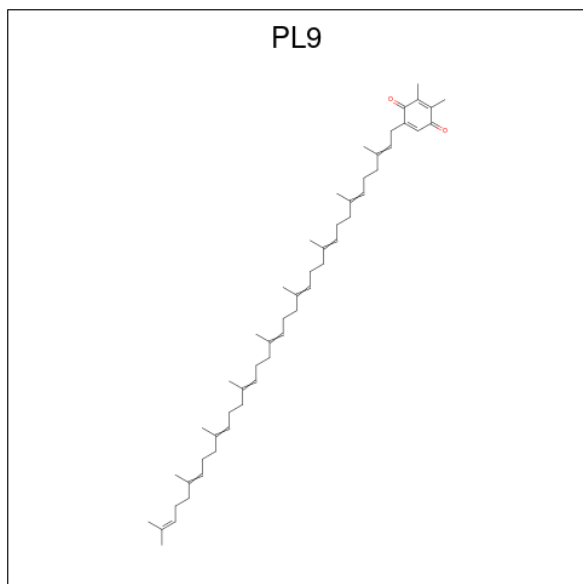
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



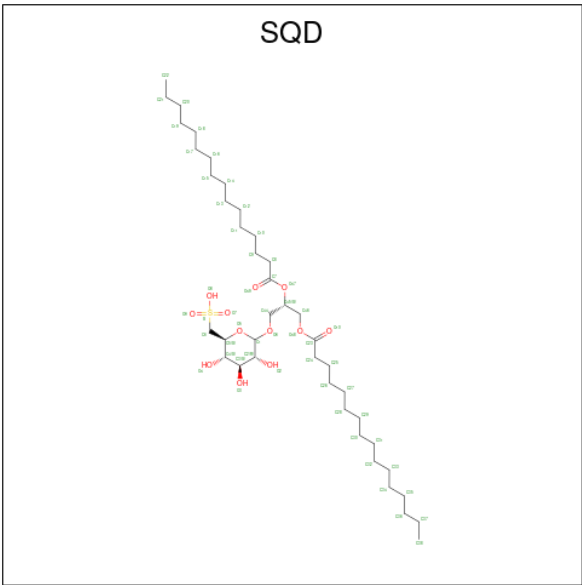
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	J	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

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



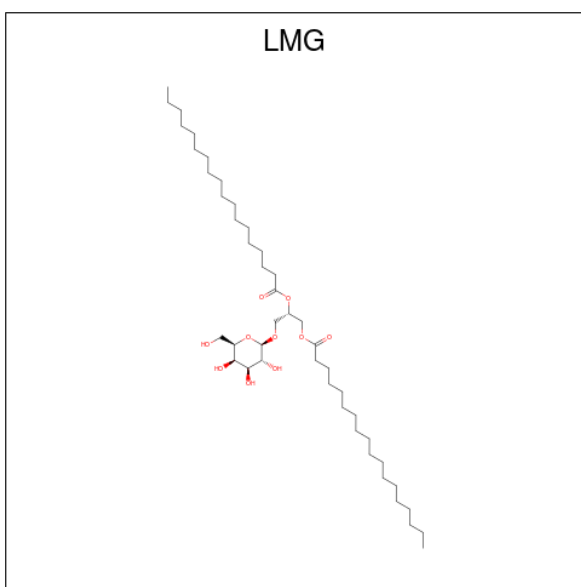
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

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



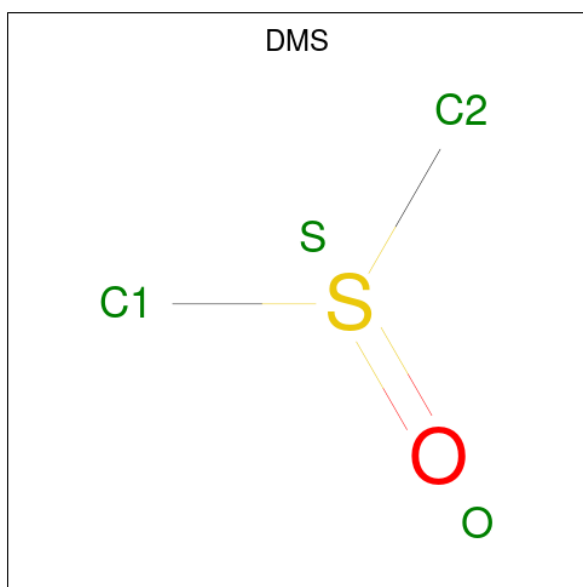
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	B	1	Total	C	O	S	0	1
			108	82	24	2		
28	D	1	Total	C	O	S	0	0
			43	30	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	1
			108	82	24	2		
28	c	1	Total	C	O	S	0	0
			54	41	12	1		
28	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 30 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			4	2	1	1		
30	A	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	D	1	Total	C	O	S	0	0
			4	2	1	1		
30	D	1	Total	C	O	S	0	0
			4	2	1	1		

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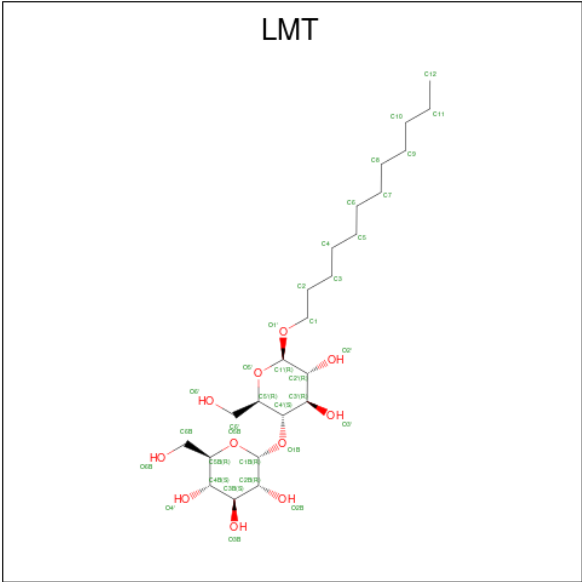
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	U	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	u	1	Total 4	C 2	O 1	S 1	0	0
30	v	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 31 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 28 23 5	0	0
31	B	2	Total C 32 32	0	0
31	D	2	Total C O 56 51 5	0	0
31	I	2	Total C 26 26	0	0
31	J	1	Total C 16 16	0	0
31	K	1	Total C O 34 29 5	0	0
31	L	1	Total C 16 16	0	0
31	Y	1	Total C 16 16	0	0
31	X	1	Total C 16 16	0	0
31	a	1	Total C O 30 25 5	0	0
31	b	2	Total C 32 32	0	0
31	c	1	Total C O 32 27 5	0	0
31	d	2	Total C O 52 47 5	0	0
31	i	1	Total C 16 16	0	0
31	j	1	Total C 16 16	0	0
31	l	1	Total C 16 16	0	0
31	t	1	Total C 16 16	0	0
31	y	1	Total C 16 16	0	0
31	x	1	Total C 16 16	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



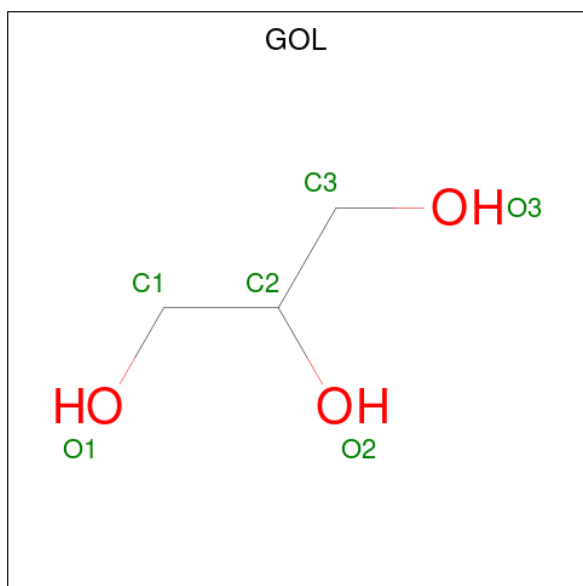
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	C	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	f	1	Total	C	O	0	0
			35	24	11		
32	i	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



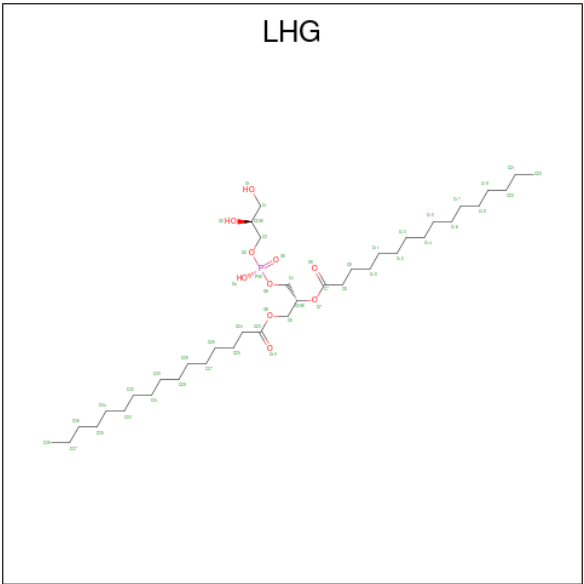
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			6	3	3		
33	B	1	Total	C	O	0	0
			6	3	3		
33	D	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	a	1	Total	C	O	0	0
			6	3	3		
33	b	1	Total	C	O	0	0
			6	3	3		
33	d	1	Total	C	O	0	0
			6	3	3		
33	d	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	v	1	Total	C	O	0	0
			6	3	3		
33	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



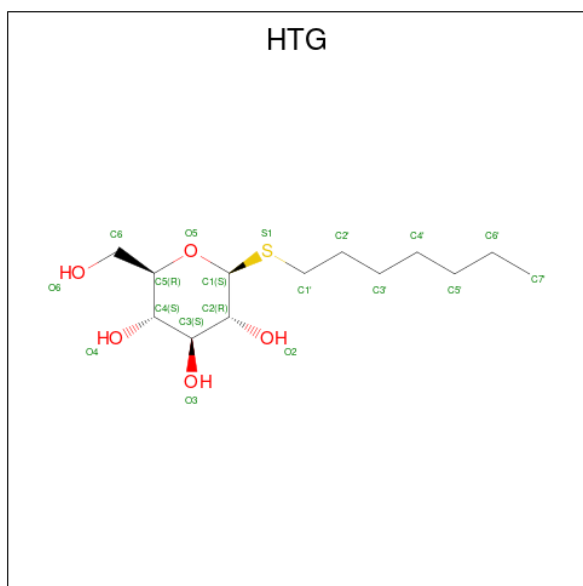
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	E	1	Total	C	O	P	0	0
			49	38	10	1		
34	b	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	e	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



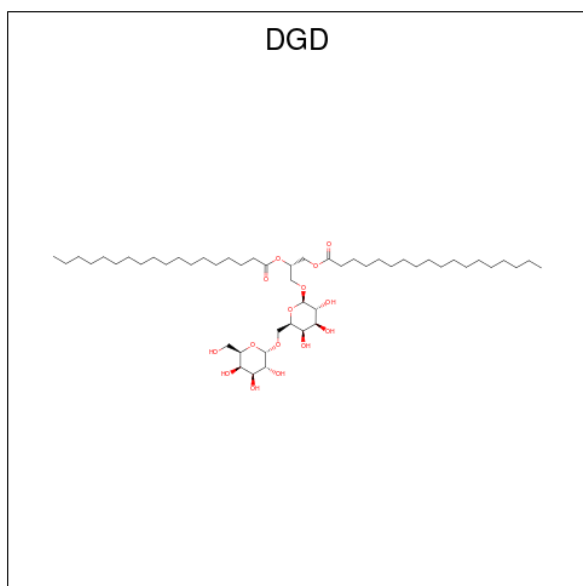
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



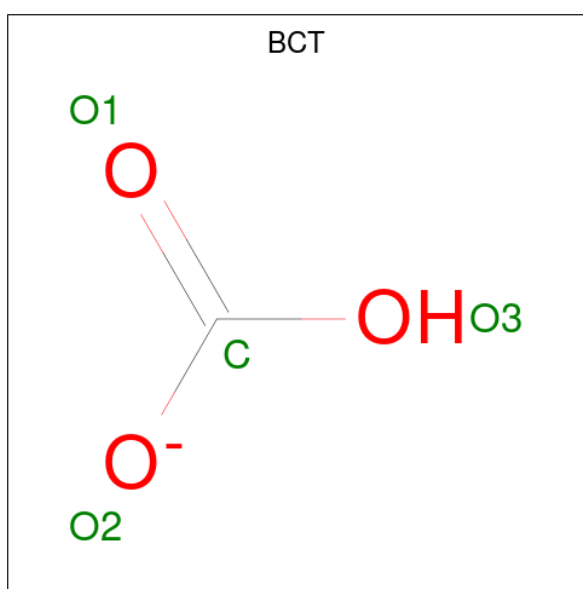
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	H	1	Total	C	O	0	0
			62	47	15		

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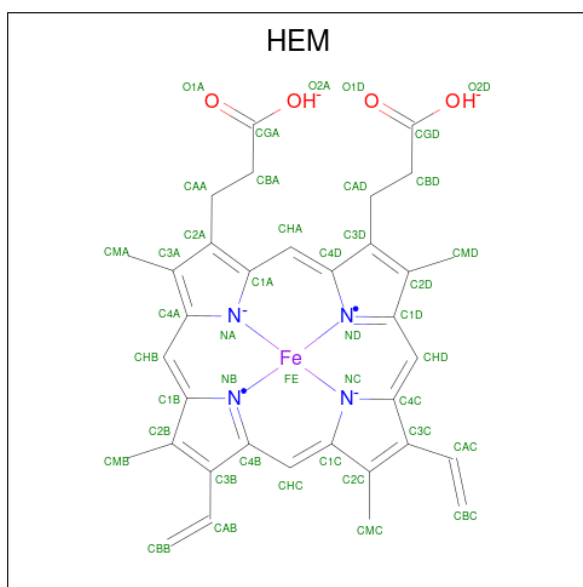
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	134	Total	O		
			134	134	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	B	252	Total 253	O 253	0	1
40	C	168	Total 168	O 168	0	0
40	D	132	Total 132	O 132	0	0
40	E	22	Total 22	O 22	0	0
40	F	6	Total 6	O 6	0	0
40	H	31	Total 31	O 31	0	0
40	I	4	Total 4	O 4	0	0
40	J	7	Total 7	O 7	0	0
40	K	7	Total 7	O 7	0	0
40	L	11	Total 11	O 11	0	0
40	M	6	Total 6	O 6	0	0
40	O	119	Total 119	O 119	0	0
40	T	10	Total 10	O 10	0	0
40	U	63	Total 63	O 63	0	0
40	V	96	Total 96	O 96	0	0
40	Y	1	Total 1	O 1	0	0
40	X	8	Total 8	O 8	0	0
40	Z	1	Total 1	O 1	0	0
40	R	1	Total 1	O 1	0	0
40	a	118	Total 118	O 118	0	0
40	b	209	Total 209	O 209	0	0

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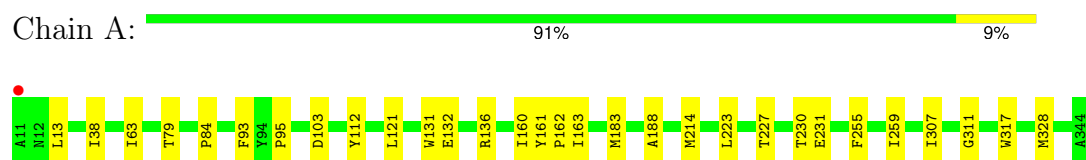
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	c	169	Total 169	O 169	0	0
40	d	121	Total 121	O 121	0	0
40	e	9	Total 9	O 9	0	0
40	f	5	Total 5	O 5	0	0
40	h	23	Total 23	O 23	0	0
40	i	4	Total 4	O 4	0	0
40	j	5	Total 5	O 5	0	0
40	k	3	Total 3	O 3	0	0
40	l	8	Total 8	O 8	0	0
40	m	10	Total 10	O 10	0	0
40	o	112	Total 112	O 112	0	0
40	t	13	Total 13	O 13	0	0
40	u	74	Total 74	O 74	0	0
40	v	65	Total 65	O 65	0	0
40	y	1	Total 1	O 1	0	0
40	x	9	Total 9	O 9	0	0

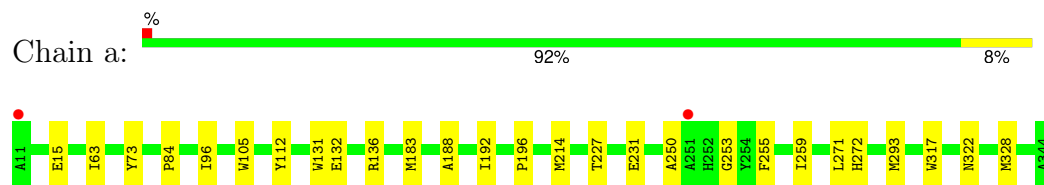
3 Residue-property plots

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

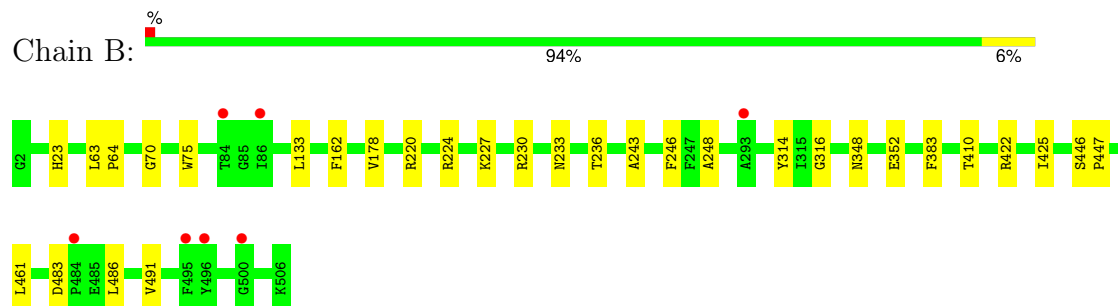
- Molecule 1: Photosystem Q(B) protein



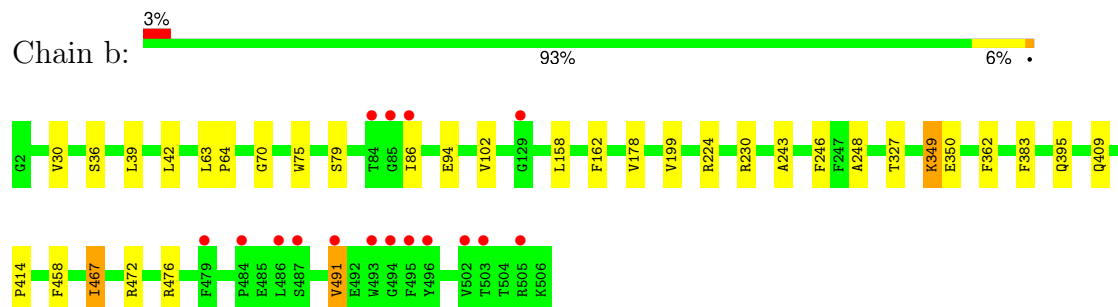
- Molecule 1: Photosystem Q(B) protein



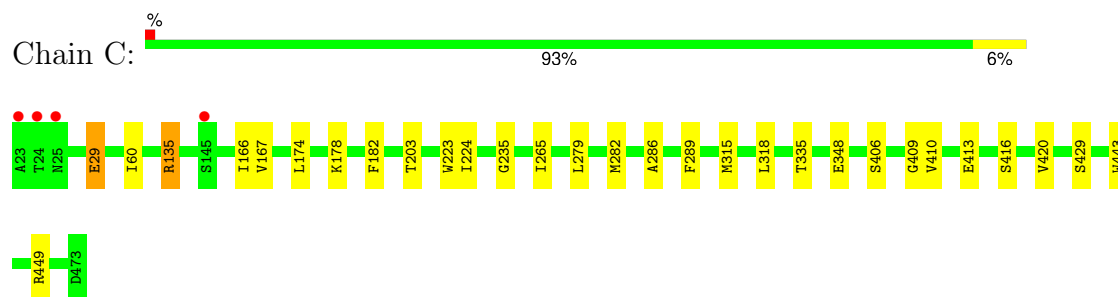
- Molecule 2: Photosystem II core light harvesting protein



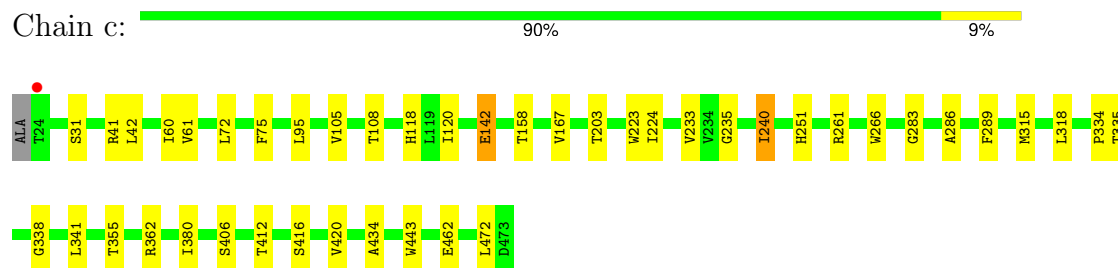
- Molecule 2: Photosystem II core light harvesting protein



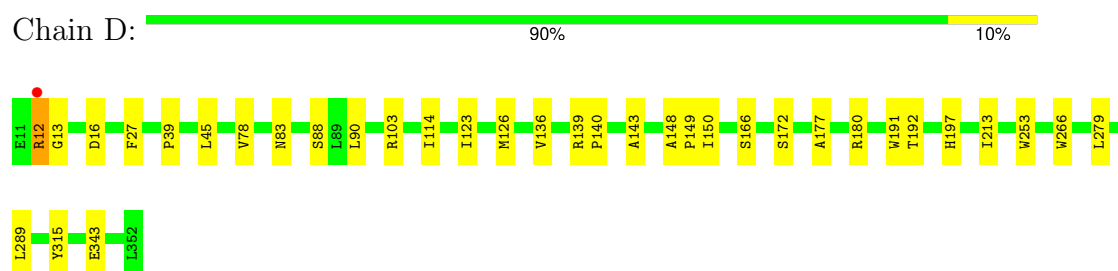
- Molecule 3: Photosystem II CP43 protein



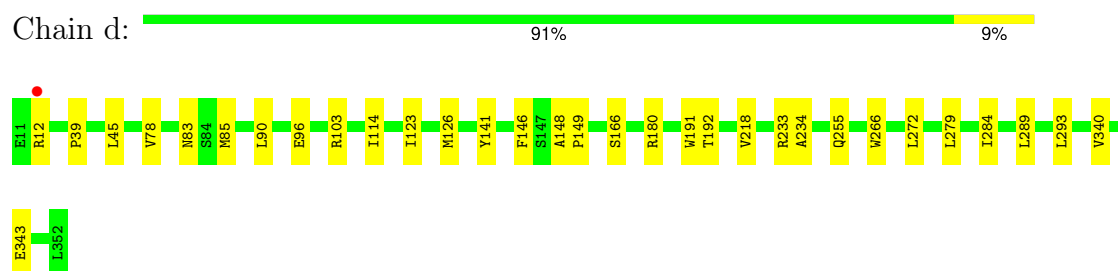
- Molecule 3: Photosystem II CP43 protein



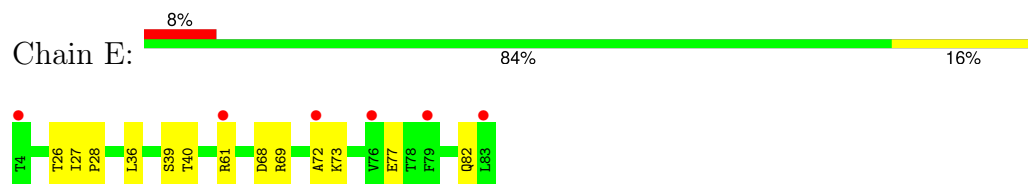
- Molecule 4: Photosystem II D2 protein



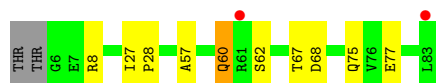
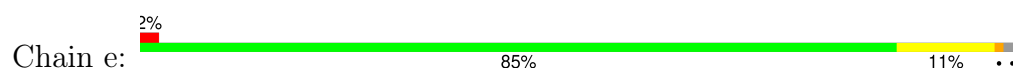
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



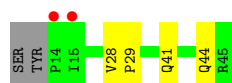
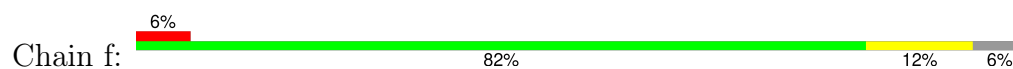
- Molecule 5: Cytochrome b559 subunit alpha



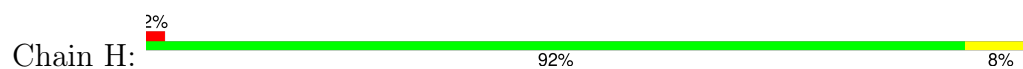
- Molecule 6: Cytochrome b559 subunit beta



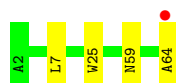
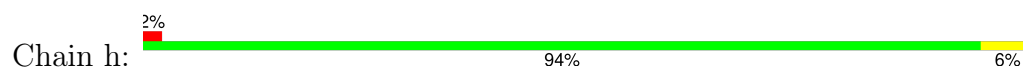
- Molecule 6: Cytochrome b559 subunit beta



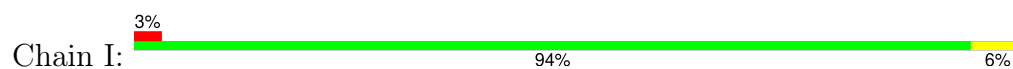
- Molecule 7: Photosystem II reaction center protein H



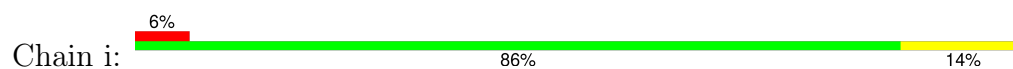
- Molecule 7: Photosystem II reaction center protein H



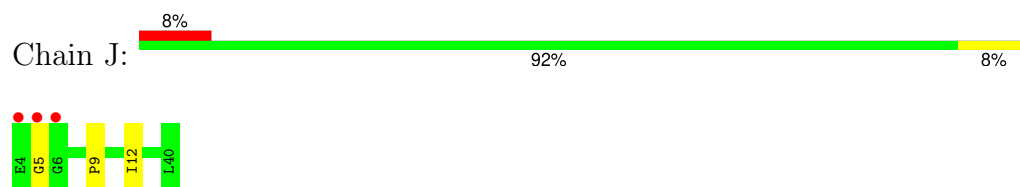
- Molecule 8: Photosystem II reaction center protein I



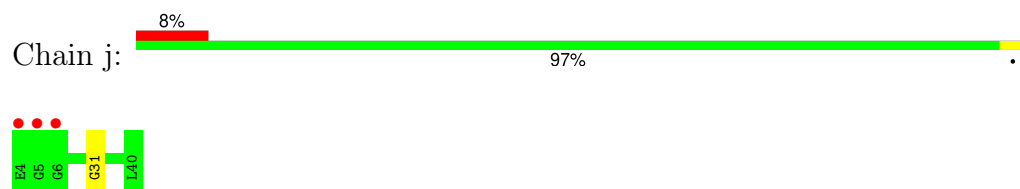
- Molecule 8: Photosystem II reaction center protein I



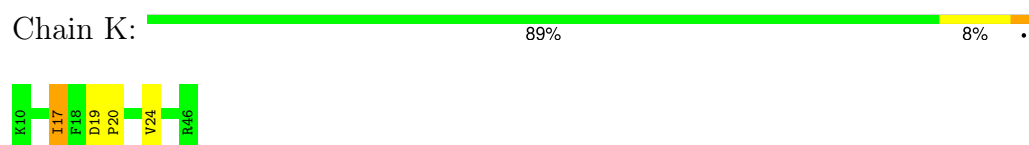
- Molecule 9: Photosystem II reaction center protein J



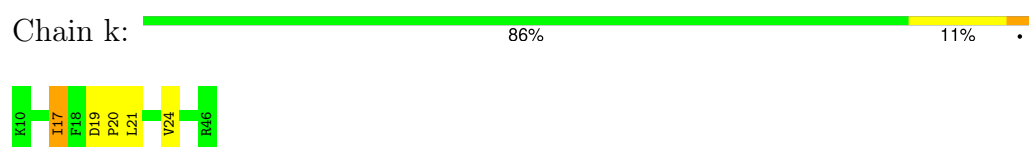
- Molecule 9: Photosystem II reaction center protein J



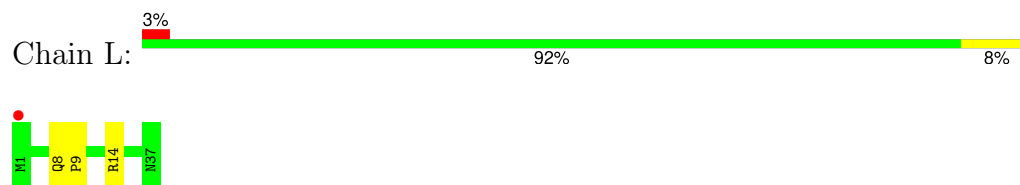
- Molecule 10: Photosystem II reaction center protein K



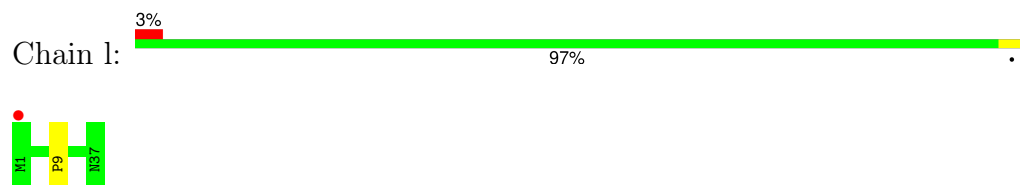
- Molecule 10: Photosystem II reaction center protein K



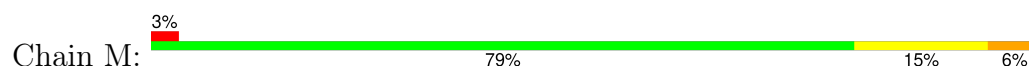
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M





- Molecule 12: Photosystem II reaction center protein M

Chain m: 82% 18%



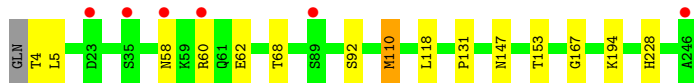
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 4% 95% 5%



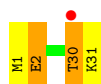
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 2% 93% 6%



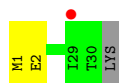
- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 87% 6% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 90% 6% .

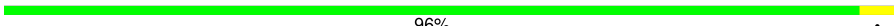


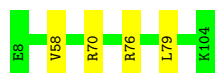
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 93% 7%

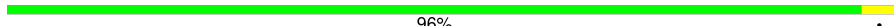


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  96% .



- Molecule 16: Cytochrome c-550

Chain V:  96% .



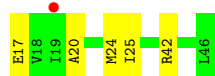
- Molecule 16: Cytochrome c-550

Chain v:  93% 7% .



- Molecule 17: Photosystem II reaction center protein ycf12

Chain Y:  3% 83% 17% .



- Molecule 17: Photosystem II reaction center protein ycf12

Chain y:  87% 7% 7% .



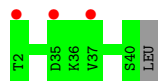
- Molecule 18: Photosystem II reaction center protein X

Chain X:  5% 100% .

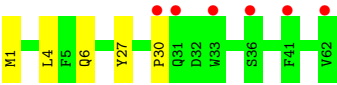


- Molecule 18: Photosystem II reaction center protein X

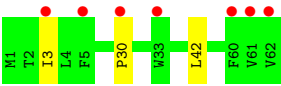
Chain x:  8% 98% .



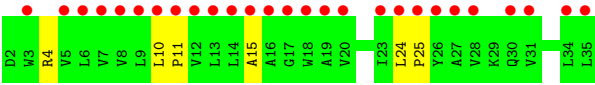
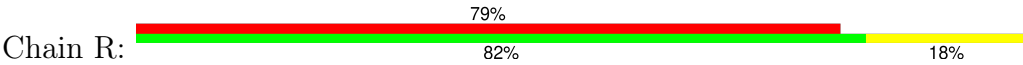
- Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.86Å 228.79Å 285.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.10 19.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.10) 99.8 (19.96-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.205 0.177 , 0.207	Depositor DCC
R_{free} test set	23034 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53568	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LHG, FME, PL9, OER, MG, UNL, HTG, LMT, LMG, CLA, SQD, HEM, BCT, DGD, PHO, DMS, BCR, FE2, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.69	0/2743	0.80	0/3740
1	a	0.68	0/2734	0.81	0/3728
2	B	0.67	0/4210	0.77	0/5731
2	b	0.67	0/4200	0.77	1/5719 (0.0%)
3	C	0.67	0/3622	0.79	0/4931
3	c	0.66	0/3611	0.79	0/4916
4	D	0.67	0/2821	0.79	0/3844
4	d	0.66	0/2821	0.79	0/3844
5	E	0.59	0/685	0.81	0/936
5	e	0.56	0/657	0.77	0/897
6	F	0.69	0/284	0.76	0/387
6	f	0.67	0/265	0.82	0/360
7	H	0.60	0/522	0.76	0/712
7	h	0.60	0/511	0.77	0/697
8	I	0.43	0/293	0.74	0/396
8	i	0.42	0/293	0.74	0/396
9	J	0.57	0/272	0.86	0/368
9	j	0.52	0/272	0.82	0/368
10	K	0.58	0/303	0.80	0/416
10	k	0.58	0/303	0.85	0/416
11	L	0.46	0/311	0.71	0/422
11	l	0.44	0/311	0.78	0/422
12	M	0.40	0/270	0.85	0/368
12	m	0.45	0/270	0.77	0/368
13	O	0.48	0/1920	0.71	0/2603
13	o	0.46	0/1902	0.70	0/2579
14	T	0.45	0/266	0.73	0/360
14	t	0.43	0/257	0.73	0/349
15	U	0.50	0/794	0.71	0/1076
15	u	0.48	0/794	0.74	0/1076
16	V	0.56	0/1111	0.74	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.57	0/1103	0.79	1/1497 (0.1%)
17	Y	0.48	0/225	0.88	0/301
17	y	0.44	0/225	0.87	0/301
18	X	0.39	0/299	0.76	0/403
18	x	0.44	0/290	0.80	0/392
19	Z	0.51	0/482	0.86	0/659
19	z	0.51	0/482	0.88	0/659
20	R	0.66	0/279	0.87	0/383
All	All	0.62	0/43013	0.78	2/58527 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	414	PRO	N-CA-C	5.30	117.17	110.70
16	v	105	ARG	N-CA-C	5.29	117.04	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2643	0	2550	23	0
1	a	2637	0	2544	22	0
2	B	4040	0	3928	25	0
2	b	4033	0	3921	30	0
3	C	3500	0	3429	23	0
3	c	3492	0	3419	26	0
4	D	2726	0	2627	27	0
4	d	2726	0	2627	27	0
5	E	660	0	644	9	0
5	e	638	0	621	6	0
6	F	275	0	282	1	0
6	f	257	0	269	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	506	0	531	3	0
7	h	498	0	518	3	0
8	I	296	0	311	2	0
8	i	296	0	311	4	0
9	J	266	0	274	1	0
9	j	266	0	274	1	0
10	K	293	0	305	4	0
10	k	293	0	305	4	0
11	L	304	0	316	4	0
11	l	304	0	316	1	0
12	M	274	0	299	6	0
12	m	274	0	299	6	0
13	O	1883	0	1857	8	0
13	o	1868	0	1843	8	0
14	T	267	0	274	2	0
14	t	258	0	261	1	0
15	U	780	0	779	3	0
15	u	780	0	779	2	0
16	V	1081	0	1100	9	0
16	v	1076	0	1087	11	0
17	Y	224	0	252	4	0
17	y	224	0	252	4	0
18	X	296	0	328	0	0
18	x	287	0	317	0	0
19	Z	481	0	515	1	0
19	z	481	0	515	0	0
20	R	273	0	305	4	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	195	0	216	9	0
24	B	1040	0	1152	17	0
24	C	845	0	936	28	0
24	D	195	0	216	6	0
24	a	260	0	288	8	0
24	b	1040	0	1152	22	0
24	c	845	0	936	21	0
24	d	130	0	144	3	0
25	A	64	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D	64	0	74	5	0
25	a	128	0	148	3	0
26	A	40	0	48	0	0
26	B	120	0	140	2	0
26	C	40	0	46	2	0
26	D	40	0	46	1	0
26	H	40	0	46	0	0
26	J	40	0	48	1	0
26	K	80	0	95	0	0
26	T	40	0	47	0	0
26	a	40	0	46	0	0
26	b	120	0	141	4	0
26	c	40	0	47	3	0
26	d	40	0	47	1	0
26	h	40	0	48	0	0
26	k	80	0	94	2	0
26	t	40	0	47	0	0
26	y	40	0	46	1	0
27	A	55	0	80	5	0
27	D	55	0	80	0	0
27	a	55	0	80	5	0
27	d	55	0	80	0	0
28	A	108	0	156	3	0
28	B	108	0	156	21	0
28	D	43	0	53	1	0
28	a	54	0	78	0	0
28	b	108	0	156	19	0
28	c	54	0	78	0	0
28	f	43	0	53	1	0
29	A	51	0	72	0	0
29	B	51	0	72	2	0
29	C	102	0	144	0	0
29	D	51	0	72	1	0
29	Z	51	0	72	1	0
29	a	51	0	72	0	0
29	c	153	0	216	2	0
29	d	51	0	72	1	0
29	m	51	0	72	3	0
30	A	8	0	12	3	0
30	B	20	0	30	4	0
30	C	20	0	30	1	0
30	D	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	O	8	0	12	3	0
30	U	4	0	6	0	0
30	V	8	0	12	0	0
30	a	8	0	12	1	0
30	b	20	0	30	3	0
30	c	20	0	30	2	0
30	d	8	0	12	4	0
30	u	4	0	6	0	0
30	v	4	0	6	0	0
31	A	28	0	0	0	0
31	B	32	0	0	0	0
31	D	56	0	0	0	0
31	I	26	0	0	0	0
31	J	16	0	0	0	0
31	K	34	0	0	0	0
31	L	16	0	0	0	0
31	X	16	0	0	0	0
31	Y	16	0	0	0	0
31	a	30	0	0	0	0
31	b	32	0	0	0	0
31	c	32	0	0	0	0
31	d	52	0	0	0	0
31	i	16	0	0	0	0
31	j	16	0	0	0	0
31	l	16	0	0	0	0
31	t	16	0	0	0	0
31	x	16	0	0	0	0
31	y	16	0	0	0	0
32	A	70	0	92	4	0
32	B	35	0	46	0	0
32	C	35	0	46	0	0
32	M	70	0	92	2	0
32	a	70	0	92	3	0
32	b	70	0	92	1	0
32	f	35	0	46	0	0
32	i	35	0	46	1	0
32	m	70	0	92	2	0
32	t	35	0	46	0	0
33	A	6	0	8	0	0
33	B	6	0	8	1	0
33	D	6	0	8	0	0
33	V	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	a	6	0	8	0	0
33	b	6	0	8	1	0
33	d	12	0	16	0	0
33	v	12	0	16	2	0
34	B	49	0	74	1	0
34	D	147	0	222	13	0
34	E	49	0	74	3	0
34	b	49	0	74	3	0
34	d	147	0	222	11	0
34	e	49	0	74	0	0
35	B	57	0	78	1	0
35	C	38	0	52	0	0
35	D	38	0	52	1	0
35	V	19	0	26	0	0
35	b	76	0	104	2	0
35	c	38	0	52	0	0
35	d	38	0	52	0	0
35	o	19	0	26	1	0
36	C	186	0	246	4	0
36	H	62	0	82	1	0
36	c	186	0	246	2	0
36	h	62	0	82	2	0
37	D	4	0	0	0	0
37	d	4	0	0	0	0
38	F	43	0	30	2	0
38	V	43	0	30	7	0
38	f	43	0	30	2	0
38	v	43	0	30	6	0
39	J	1	0	0	0	0
39	K	1	0	0	0	0
39	j	1	0	0	0	0
39	k	1	0	0	0	0
40	A	134	0	0	1	0
40	B	253	0	0	0	0
40	C	168	0	0	2	0
40	D	132	0	0	0	0
40	E	22	0	0	1	0
40	F	6	0	0	0	0
40	H	31	0	0	0	0
40	I	4	0	0	0	0
40	J	7	0	0	0	0
40	K	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	L	11	0	0	0	0
40	M	6	0	0	0	0
40	O	119	0	0	1	0
40	R	1	0	0	0	0
40	T	10	0	0	0	0
40	U	63	0	0	0	0
40	V	96	0	0	0	0
40	X	8	0	0	0	0
40	Y	1	0	0	0	0
40	Z	1	0	0	0	0
40	a	118	0	0	0	0
40	b	209	0	0	0	0
40	c	169	0	0	1	0
40	d	121	0	0	1	0
40	e	9	0	0	0	0
40	f	5	0	0	0	0
40	h	23	0	0	0	0
40	i	4	0	0	0	0
40	j	5	0	0	0	0
40	k	3	0	0	0	0
40	l	8	0	0	0	0
40	m	10	0	0	0	0
40	o	112	0	0	1	0
40	t	13	0	0	0	0
40	u	74	0	0	0	0
40	v	65	0	0	0	0
40	x	9	0	0	0	0
40	y	1	0	0	0	0
All	All	53568	0	52620	436	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 4.

All (436) 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)
16:v:37:CYS:SG	38:v:201:HEM:HAB	1.48	1.53
28:b:623[B]:SQD:H192	28:b:623[B]:SQD:C38	1.46	1.44
28:B:620[B]:SQD:H141	28:B:620[B]:SQD:C38	1.48	1.42
16:V:37:CYS:SG	38:V:201:HEM:HAB	1.58	1.42
28:B:620[B]:SQD:H382	28:B:620[B]:SQD:C14	1.52	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:40:CYS:SG	38:V:201:HEM:CAC	2.14	1.35
16:V:37:CYS:SG	38:V:201:HEM:CAB	2.13	1.35
16:v:37:CYS:SG	38:v:201:HEM:CAB	2.17	1.31
16:V:40:CYS:SG	38:V:201:HEM:HAC	1.72	1.30
28:B:620[A]:SQD:H81	28:B:620[A]:SQD:C46	1.63	1.28
16:v:40:CYS:SG	38:v:201:HEM:HAC	1.73	1.27
16:v:40:CYS:SG	38:v:201:HEM:CAC	2.22	1.26
28:B:620[B]:SQD:C17	28:B:620[B]:SQD:H381	1.64	1.25
28:b:623[B]:SQD:H382	28:b:623[B]:SQD:C19	1.69	1.20
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.20	1.12
28:B:620[A]:SQD:H462	28:B:620[A]:SQD:C8	1.63	1.11
28:b:623[B]:SQD:C38	28:b:623[B]:SQD:C19	2.29	1.07
28:B:620[B]:SQD:H381	28:B:620[B]:SQD:H172	1.06	1.04
28:b:623[B]:SQD:H361	28:b:623[B]:SQD:C18	1.95	0.96
32:a:402:LMT:O2'	35:o:301:HTG:H5	1.65	0.95
28:B:620[B]:SQD:C38	28:B:620[B]:SQD:H172	1.96	0.93
28:B:620[A]:SQD:H81	28:B:620[A]:SQD:H462	0.93	0.92
28:B:620[A]:SQD:C46	28:B:620[A]:SQD:C8	2.26	0.91
32:A:1017:LMT:O2'	35:b:626:HTG:H5	1.72	0.87
4:D:266:TRP:CD1	34:D:410:LHG:HC32	2.09	0.86
28:b:623[A]:SQD:O49	28:b:623[A]:SQD:H461	1.74	0.86
10:K:17:ILE:H	10:K:17:ILE:HD13	1.44	0.82
30:d:413:DMS:H13	40:d:591:HOH:O	1.78	0.82
28:b:623[B]:SQD:H361	28:b:623[B]:SQD:H181	1.61	0.82
17:Y:42:ARG:HG3	17:Y:42:ARG:HH11	1.45	0.81
28:B:620[A]:SQD:H442	28:B:620[A]:SQD:O10	1.82	0.79
34:d:406:LHG:H101	34:d:406:LHG:H351	1.66	0.78
28:b:623[B]:SQD:H192	28:b:623[B]:SQD:H382	0.77	0.76
2:B:230[B]:ARG:HE	30:B:634:DMS:C2	2.00	0.75
24:c:510:CLA:H41	34:d:408:LHG:H383	1.70	0.73
29:m:102:LMG:HC5	32:m:103:LMT:H1'	1.70	0.73
4:d:340:VAL:HG13	30:d:413:DMS:H11	1.71	0.73
28:b:623[B]:SQD:C19	28:b:623[B]:SQD:H383	2.16	0.73
28:b:623[B]:SQD:H361	28:b:623[B]:SQD:C17	2.19	0.72
34:d:408:LHG:H342	34:d:408:LHG:H151	1.70	0.71
32:b:625:LMT:O2B	32:b:625:LMT:H4'	1.88	0.71
1:a:250:ALA:HA	2:b:491:VAL:CG1	2.12	0.71
28:b:623[B]:SQD:H61	28:b:623[B]:SQD:H2	1.72	0.71
16:v:71:GLY:HA2	33:v:203:GOL:H2	1.74	0.69
4:d:266:TRP:CD1	34:d:407:LHG:HC32	2.27	0.69
38:f:101:HEM:HMB1	38:f:101:HEM:HBB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:286:ALA:HB2	24:c:502:CLA:HMD2	1.76	0.68
10:K:24:VAL:HG11	17:Y:25:ILE:HB	1.75	0.67
13:O:55:GLU:H	30:O:301:DMS:H12	1.60	0.67
24:c:503:CLA:HAB	24:c:512:CLA:H41	1.75	0.67
24:b:607:CLA:H43	24:b:608:CLA:H2	1.76	0.66
28:b:623[B]:SQD:H152	28:b:623[B]:SQD:H342	1.79	0.65
4:D:13:GLY:HA3	35:D:413:HTG:H62	1.79	0.65
28:B:620[A]:SQD:C8	28:B:620[A]:SQD:H461	2.22	0.65
28:B:620[A]:SQD:H81	28:B:620[A]:SQD:H461	1.70	0.65
28:B:620[B]:SQD:H461	28:B:620[B]:SQD:H251	1.79	0.64
16:v:40:CYS:SG	38:v:201:HEM:C3C	2.90	0.64
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.78	0.64
5:E:40:THR:HB	20:R:4:ARG:HG2	1.80	0.64
24:c:510:CLA:C4	34:d:408:LHG:H383	2.27	0.64
30:A:1014:DMS:H22	35:b:626:HTG:H1'1	1.80	0.64
3:c:167:VAL:HG21	24:c:512:CLA:HBB	1.79	0.63
28:b:623[B]:SQD:H361	28:b:623[B]:SQD:H172	1.80	0.63
3:C:286:ALA:HB2	24:C:502:CLA:HMD2	1.81	0.63
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.80	0.63
2:B:410:THR:H	33:B:631:GOL:H2	1.61	0.63
7:H:59:ASN:HB3	7:H:64:ALA:HB3	1.81	0.63
16:V:40:CYS:SG	38:V:201:HEM:C3C	2.92	0.62
14:T:30:THR:HG22	14:T:31:LYS:H	1.65	0.62
2:B:162:PHE:O	24:B:606:CLA:HHD	1.99	0.61
12:M:33:GLN:HG3	12:m:33:GLN:HB2	1.83	0.61
28:B:620[B]:SQD:H381	28:B:620[B]:SQD:H171	1.77	0.61
16:V:37:CYS:SG	38:V:201:HEM:C3B	2.93	0.61
24:c:509:CLA:HMB1	24:c:509:CLA:HBB1	1.82	0.61
2:B:230[B]:ARG:HE	30:B:634:DMS:H23	1.66	0.61
2:b:472:ARG:HG2	30:d:414:DMS:H23	1.83	0.60
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.82	0.60
13:o:68:THR:HG22	13:o:110:MET:HE3	1.82	0.60
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.83	0.60
2:B:230[B]:ARG:HE	30:B:634:DMS:H21	1.65	0.60
4:d:192:THR:HG23	24:d:402:CLA:HBC2	1.84	0.60
1:a:15:GLU:HB2	32:a:416:LMT:H6'1	1.83	0.60
34:d:408:LHG:H122	34:d:408:LHG:H381	1.84	0.60
28:B:620[B]:SQD:C38	28:B:620[B]:SQD:C14	2.39	0.59
28:b:623[B]:SQD:C19	28:b:623[B]:SQD:H361	2.33	0.59
28:B:620[B]:SQD:H381	28:B:620[B]:SQD:C16	2.31	0.59
28:b:623[B]:SQD:H342	28:b:623[B]:SQD:C15	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.85	0.59
1:A:223:LEU:HD12	4:D:139:ARG:NH1	2.18	0.58
10:k:17:ILE:HD13	10:k:17:ILE:H	1.69	0.58
24:C:510:CLA:H41	34:D:411:LHG:H381	1.86	0.58
28:b:623[B]:SQD:H383	28:b:623[B]:SQD:H191	1.85	0.58
1:A:223:LEU:HD12	4:D:139:ARG:HH12	1.68	0.58
24:a:407:CLA:CBD	24:a:408:CLA:HAC2	2.33	0.58
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.86	0.57
24:B:614:CLA:H18	29:B:622:LMG:H421	1.86	0.57
28:B:620[B]:SQD:C38	28:B:620[B]:SQD:C17	2.59	0.57
4:d:123:ILE:HD11	36:h:102:DGD:HAH1	1.86	0.56
11:L:9:PRO:HA	32:m:101:LMT:H6D	1.86	0.56
17:Y:42:ARG:HG3	17:Y:42:ARG:NH1	2.19	0.56
24:c:505:CLA:HBB1	24:c:505:CLA:HMB3	1.87	0.56
3:c:60:ILE:HG22	24:c:503:CLA:HHD	1.87	0.56
24:b:613:CLA:HHC	24:b:613:CLA:HBB1	1.87	0.56
1:A:227:THR:HB	1:A:231[A]:GLU:HG3	1.87	0.56
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.88	0.56
4:d:284:ILE:HD13	29:m:102:LMG:H242	1.88	0.55
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.41	0.55
2:B:483:ASP:HB3	2:B:486:LEU:HB2	1.88	0.55
3:C:413[B]:GLU:HG2	40:C:628:HOH:O	2.06	0.55
28:A:1011:SQD:H272	34:D:411:LHG:H141	1.89	0.55
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.41	0.55
8:i:1:FME:H	32:i:102:LMT:H6D	1.70	0.55
24:b:607:CLA:HBA2	24:b:615:CLA:H151	1.89	0.55
24:b:618:CLA:H2	24:b:619:CLA:HBB2	1.89	0.55
2:B:75:TRP:HB3	30:a:418:DMS:H23	1.89	0.55
24:b:616:CLA:HMB1	24:b:616:CLA:HBB1	1.90	0.54
3:C:443:TRP:CZ2	24:C:508:CLA:HMD1	2.43	0.54
30:C:526:DMS:H11	16:V:102:PRO:HG2	1.89	0.54
24:c:506:CLA:HMC2	24:c:507:CLA:H102	1.89	0.54
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.89	0.53
5:e:68:ASP:H	5:e:75:GLN:HE22	1.55	0.53
7:h:59:ASN:HB3	7:h:64:ALA:HB3	1.91	0.53
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.89	0.53
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.90	0.53
12:M:33:GLN:O	12:M:34:LYS:HB2	2.08	0.53
24:b:611:CLA:HAB	4:d:123:ILE:HG12	1.91	0.53
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.44	0.52
5:e:67:THR:H	5:e:75:GLN:HE22	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:37:CYS:SG	38:v:201:HEM:C3B	2.97	0.52
24:A:1005:CLA:CBD	24:D:403:CLA:HAC2	2.40	0.52
2:b:230:ARG:HE	30:b:635:DMS:H12	1.74	0.52
24:a:407:CLA:HBD	24:a:408:CLA:HAC2	1.91	0.52
24:C:506:CLA:HMC2	24:C:507:CLA:H101	1.92	0.52
25:D:404:PHO:HMB1	25:D:404:PHO:HBB1	1.92	0.52
34:b:624:LHG:HC81	34:d:406:LHG:O9	2.10	0.51
24:d:403:CLA:HMB1	24:d:403:CLA:HBB1	1.91	0.51
2:b:248:ALA:HA	24:b:606:CLA:H42	1.91	0.51
2:B:227:LYS:O	2:B:230[B]:ARG:HD3	2.09	0.51
3:c:142:GLU:CD	3:c:142:GLU:H	2.19	0.51
4:d:103:ARG:HH21	5:e:77:GLU:HG3	1.74	0.51
2:B:248:ALA:HA	24:B:603:CLA:H42	1.93	0.51
12:M:8:LEU:HG	12:m:9:ILE:HD13	1.91	0.51
10:K:17:ILE:H	10:K:17:ILE:CD1	2.20	0.51
13:O:55:GLU:HB2	30:O:301:DMS:H23	1.91	0.51
10:k:21:LEU:HD13	17:y:24:MET:HE2	1.91	0.51
3:c:443:TRP:CZ2	24:c:508:CLA:HMD1	2.46	0.51
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.92	0.50
24:c:501:CLA:C4D	24:c:503:CLA:H2	2.41	0.50
24:A:1006:CLA:HBB1	24:D:402:CLA:H102	1.93	0.50
1:a:183:MET:HA	24:a:407:CLA:HMD1	1.92	0.50
38:f:101:HEM:HBB2	38:f:101:HEM:CMB	2.39	0.50
1:a:196:PRO:HB3	36:c:517:DGD:HA82	1.92	0.50
3:c:406:SER:HA	3:c:420:VAL:HG23	1.94	0.50
13:o:92:SER:HB3	13:o:131:PRO:HA	1.93	0.50
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.50
24:b:618:CLA:H161	7:h:7:LEU:HD21	1.93	0.50
4:d:85:MET:CE	4:d:96:GLU:HG2	2.42	0.50
24:C:510:CLA:H52	34:D:411:LHG:H371	1.93	0.50
1:a:84:PRO:HA	1:a:112:TYR:CG	2.47	0.50
24:c:502:CLA:H61	24:c:512:CLA:H42	1.93	0.50
2:B:348:ASN:OD1	2:B:352[B]:GLU:HG3	2.10	0.50
3:C:174:LEU:HB3	24:C:502:CLA:H161	1.93	0.49
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.94	0.49
2:b:162:PHE:O	24:b:609:CLA:HHH	2.12	0.49
2:b:230:ARG:HE	30:b:635:DMS:C1	2.24	0.49
32:M:102:LMT:H6D	11:l:9:PRO:HA	1.94	0.49
4:d:343:GLU:HG2	16:v:135:VAL:HG11	1.94	0.49
2:B:220:ARG:HG3	7:H:20:LYS:HG2	1.95	0.49
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:THR:HG23	24:D:402:CLA:HBC2	1.95	0.49
3:c:42:LEU:HD21	24:c:511:CLA:H2A	1.95	0.49
28:b:623[B]:SQD:H181	28:b:623[B]:SQD:C36	2.38	0.49
24:B:615:CLA:H2	24:B:616:CLA:HBB2	1.94	0.49
5:e:67:THR:H	5:e:75:GLN:NE2	2.10	0.49
1:A:38:ILE:HG12	28:A:1016:SQD:H142	1.95	0.48
28:b:623[B]:SQD:H132	28:b:623[B]:SQD:H162	1.65	0.48
3:c:334:PRO:HA	13:o:153:THR:OG1	2.13	0.48
1:a:250:ALA:CA	2:b:491:VAL:HG11	2.15	0.48
1:A:183:MET:HA	24:A:1005:CLA:HMD1	1.95	0.48
24:B:613:CLA:H18	34:D:409:LHG:H202	1.95	0.48
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.48	0.48
17:y:30:ILE:HD12	17:y:34:MET:HE2	1.96	0.48
3:C:167:VAL:HG21	24:C:512:CLA:HBB	1.95	0.48
24:c:510:CLA:HBC3	24:c:510:CLA:H192	1.95	0.48
24:b:606:CLA:HAB	24:b:608:CLA:H171	1.95	0.48
16:V:40:CYS:SG	38:V:201:HEM:CBC	2.93	0.48
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.49	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.95	0.47
24:c:513:CLA:HAB	26:k:102:BCR:H24C	1.96	0.47
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.96	0.47
16:v:41:HIS:HA	16:v:45:ILE:O	2.14	0.47
24:A:1005:CLA:HMB1	24:A:1005:CLA:HBB1	1.97	0.47
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	1.96	0.47
28:B:620[A]:SQD:H442	28:B:620[A]:SQD:C23	2.45	0.47
26:C:514:BCR:HC32	8:I:23:PHE:HB3	1.95	0.47
4:d:141:TYR:OH	34:d:406:LHG:O4	2.30	0.47
29:c:519:LMG:H152	17:y:25:ILE:HD13	1.96	0.47
27:A:1010:PL9:H512	28:D:408:SQD:H321	1.97	0.47
3:c:203:THR:O	3:c:235:GLY:HA3	2.15	0.47
4:d:123:ILE:HD11	36:h:102:DGD:HAE2	1.97	0.47
32:A:1017:LMT:H42	2:b:39:LEU:HD22	1.96	0.47
3:C:60:ILE:HG22	24:C:503:CLA:HHD	1.97	0.47
3:C:409:GLY:HA3	3:C:413[A]:GLU:HG3	1.97	0.47
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.44	0.47
10:K:19:ASP:HB3	10:K:20:PRO:HD3	1.97	0.47
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.96	0.47
1:A:230:THR:HB	11:L:8:GLN:HE22	1.78	0.47
1:A:103:ASP:OD2	30:A:1014:DMS:H13	2.14	0.47
2:B:461:LEU:HD22	34:D:409:LHG:H301	1.96	0.47
30:c:529:DMS:H11	40:c:715:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:ILE:HD13	24:C:512:CLA:H191	1.97	0.46
2:b:102:VAL:HA	26:b:621:BCR:H402	1.97	0.46
24:b:607:CLA:H42	24:b:615:CLA:H152	1.96	0.46
3:C:410:VAL:HG13	40:C:742:HOH:O	2.15	0.46
25:a:411:PHO:HBC3	4:d:279:LEU:HD22	1.96	0.46
3:c:223:TRP:CG	3:c:224:ILE:H	2.34	0.46
1:a:227:THR:HB	1:a:231[A]:GLU:HG3	1.96	0.46
3:c:472:LEU:HD11	4:d:255:GLN:HG3	1.97	0.46
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.98	0.46
1:A:79:THR:HG22	4:D:315:TYR:HB2	1.98	0.46
2:B:233:ASN:O	2:B:236:THR:HG22	2.16	0.46
24:B:610:CLA:HHC	24:B:610:CLA:HBB1	1.98	0.46
3:C:318:LEU:C	3:C:318:LEU:HD23	2.40	0.46
3:c:61:VAL:HG12	3:c:118:HIS:O	2.16	0.46
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.50	0.46
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.51	0.46
24:c:505:CLA:HBC2	26:c:514:BCR:H341	1.97	0.46
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.98	0.46
24:B:605:CLA:C14	24:B:610:CLA:HED2	2.46	0.46
24:A:1008:CLA:H111	8:I:16:VAL:HG11	1.97	0.45
28:B:620[A]:SQD:H352	28:B:620[A]:SQD:H321	1.81	0.45
24:C:506:CLA:H122	24:C:506:CLA:H161	1.42	0.45
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.97	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.34	0.45
27:A:1010:PL9:H251	34:E:101:LHG:H211	1.98	0.45
5:E:36:LEU:HA	5:E:39:SER:OG	2.15	0.45
24:a:407:CLA:CAD	24:a:408:CLA:HAC2	2.46	0.45
3:c:72:LEU:HD11	3:c:108:THR:HB	1.99	0.45
24:D:403:CLA:HMB1	24:D:403:CLA:HBB1	1.99	0.45
5:E:82:GLN:HB3	40:E:213:HOH:O	2.17	0.45
13:O:33:ASP:OD2	13:O:35:SER:HB3	2.17	0.45
24:a:409:CLA:HED1	36:c:517:DGD:HAE2	1.99	0.45
1:A:121[B]:LEU:HD11	24:C:505:CLA:H152	1.98	0.45
24:C:510:CLA:H41	34:D:411:LHG:C38	2.46	0.45
4:d:340:VAL:HG13	30:d:413:DMS:C1	2.45	0.45
10:k:24:VAL:HB	17:y:25:ILE:HG23	1.98	0.45
34:D:411:LHG:H372	34:D:411:LHG:H142	1.98	0.45
27:a:414:PL9:H302	4:d:45:LEU:HD22	1.99	0.45
27:a:414:PL9:H512	28:f:102:SQD:H301	1.99	0.45
24:C:508:CLA:HBC3	24:C:510:CLA:H71	1.99	0.45
8:i:33:LYS:HA	8:i:33:LYS:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.52	0.45
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.52	0.45
24:A:1005:CLA:HBD	24:D:403:CLA:HAC2	2.00	0.44
24:A:1008:CLA:H152	24:C:505:CLA:H192	1.99	0.44
32:A:1018:LMT:H3'	32:A:1018:LMT:H1B	1.54	0.44
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.99	0.44
29:B:622:LMG:HC5	32:M:101:LMT:H1'	1.99	0.44
4:d:83:ASN:ND2	4:d:166:SER:OG	2.51	0.44
13:o:4:THR:HG23	13:o:5:LEU:H	1.82	0.44
24:a:409:CLA:HAB	24:d:402:CLA:H72	1.99	0.44
2:b:349:LYS:HD2	2:b:350:GLU:N	2.33	0.44
26:c:514:BCR:HC32	8:i:23:PHE:HB3	1.98	0.44
34:d:408:LHG:H331	34:d:408:LHG:H302	1.55	0.44
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.85	0.44
16:v:28:GLU:CD	16:v:31:ARG:HH21	2.25	0.44
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.53	0.44
3:C:348:GLU:OE1	13:O:11:VAL:HA	2.17	0.44
36:C:515:DGD:HA82	36:C:515:DGD:HAE1	1.73	0.44
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.00	0.44
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.81	0.44
13:o:58:ASN:C	13:o:60:ARG:H	2.26	0.44
26:B:617:BCR:H24C	26:B:617:BCR:H371	1.83	0.44
17:Y:20:ALA:O	17:Y:24:MET:HG2	2.18	0.44
29:c:521:LMG:H151	29:c:521:LMG:H322	1.99	0.44
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.17	0.44
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.53	0.44
34:d:408:LHG:H122	34:d:408:LHG:C38	2.48	0.44
2:B:422:ARG:O	2:B:425:ILE:HG12	2.18	0.43
4:D:123:ILE:HD11	36:H:102:DGD:HAE1	2.00	0.43
13:O:137:THR:C	13:O:139:SER:H	2.25	0.43
24:a:409:CLA:H152	27:a:414:PL9:H23	2.00	0.43
4:D:103:ARG:HE	5:E:77:GLU:HG3	1.83	0.43
28:b:623[B]:SQD:C6	28:b:623[B]:SQD:C2	2.96	0.43
1:A:132:GLU:O	1:A:136:ARG:HG2	2.18	0.43
27:A:1010:PL9:H403	6:F:22:ALA:HB2	2.01	0.43
28:A:1011:SQD:H122	34:E:101:LHG:H331	1.99	0.43
24:C:504:CLA:H192	24:C:510:CLA:H72	2.00	0.43
24:c:513:CLA:H171	26:k:102:BCR:H373	2.00	0.43
13:o:147:ASN:HD21	13:o:194:LYS:NZ	2.16	0.43
2:B:70:GLY:HA2	2:B:178:VAL:HG11	2.01	0.43
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:605:CLA:H143	24:B:610:CLA:HED2	2.00	0.43
5:E:68:ASP:O	5:E:72:ALA:HB2	2.18	0.43
13:O:66:VAL:HB	13:O:67:PRO:HD2	2.00	0.43
20:R:24:LEU:N	20:R:25:PRO:HD2	2.33	0.43
2:b:79:SER:HB3	2:b:86:ILE:HG12	2.00	0.43
24:b:615:CLA:CMB	24:b:617:CLA:HBB1	2.48	0.43
4:d:272:LEU:C	4:d:272:LEU:HD23	2.42	0.43
4:D:27:PHE:CD1	34:E:101:LHG:HC12	2.53	0.43
4:D:126:MET:HE3	4:D:143:ALA:O	2.19	0.43
24:b:618:CLA:H2	24:b:619:CLA:CBB	2.47	0.43
26:b:621:BCR:H371	26:b:621:BCR:H24C	1.75	0.43
1:A:160:ILE:HD11	36:C:515:DGD:HBT1	2.00	0.43
24:C:507:CLA:H41	24:C:507:CLA:H61	1.86	0.43
9:J:9:PRO:HD2	9:J:12:ILE:HD12	2.00	0.43
2:b:349:LYS:HG3	2:b:395:GLN:O	2.19	0.43
13:o:228:HIS:HD2	40:o:452:HOH:O	2.00	0.43
3:C:265:ILE:HD11	3:C:449:ARG:HD3	2.01	0.43
34:b:624:LHG:H312	12:m:18:PRO:HB3	2.00	0.43
3:c:362:ARG:HD3	30:c:529:DMS:O	2.18	0.43
24:B:601:CLA:HAB	24:B:601:CLA:H171	2.01	0.43
30:O:302:DMS:H21	40:O:455:HOH:O	2.18	0.43
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.99	0.43
24:b:617:CLA:H41	24:b:617:CLA:H61	1.58	0.43
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.53	0.43
3:C:135:ARG:HG3	19:Z:27:TYR:CD1	2.53	0.43
25:D:404:PHO:HBC2	25:D:404:PHO:HHH	2.01	0.43
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.00	0.43
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.01	0.43
34:B:621:LHG:HC81	34:D:409:LHG:O9	2.19	0.43
1:a:183:MET:HG2	24:a:408:CLA:HBC1	2.01	0.43
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.53	0.43
24:C:513:CLA:HBB1	24:C:513:CLA:HMB3	2.00	0.42
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.01	0.42
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.54	0.42
1:a:132:GLU:O	1:a:136:ARG:HG2	2.19	0.42
27:a:414:PL9:H502	4:d:39:PRO:HG3	2.01	0.42
3:c:233:VAL:HA	26:c:514:BCR:H282	2.01	0.42
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.54	0.42
4:D:279:LEU:HD22	25:D:404:PHO:HBC3	2.00	0.42
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.01	0.42
25:D:404:PHO:HBB1	25:D:404:PHO:CMB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:73:TYR:HA	32:a:402:LMT:H4B	2.01	0.42
25:a:411:PHO:HMB1	25:a:411:PHO:HBB1	2.00	0.42
2:b:458:PHE:HB3	24:b:607:CLA:HBC2	2.00	0.42
2:b:476:ARG:HB3	30:b:635:DMS:H21	2.02	0.42
28:B:620[B]:SQD:H182	28:B:620[B]:SQD:H211	1.86	0.42
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.01	0.42
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.54	0.42
2:b:42:LEU:HD13	2:b:94:GLU:HG3	2.01	0.42
2:b:327:THR:HG21	29:m:102:LMG:HC91	2.01	0.42
24:b:604:CLA:HAB	24:b:604:CLA:H171	2.01	0.42
24:B:604:CLA:C4	24:B:605:CLA:H2	2.49	0.42
38:F:101:HEM:CMB	38:F:101:HEM:HBB2	2.49	0.42
15:U:8:GLU:HB2	15:U:9:LEU:H	1.71	0.42
2:b:36:SER:OG	26:b:621:BCR:H362	2.20	0.42
3:C:29:GLU:CD	3:C:29:GLU:H	2.27	0.42
4:D:83:ASN:ND2	4:D:166:SER:OG	2.53	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.42
5:E:26:THR:HA	20:R:15:ALA:HB1	2.02	0.42
12:M:20:VAL:HG11	12:m:20:VAL:HG22	2.00	0.42
24:b:613:CLA:HHC	24:b:613:CLA:CBB	2.49	0.42
1:A:63:ILE:HB	3:C:335:THR:HG21	2.01	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.01	0.42
1:A:230:THR:HB	11:L:8:GLN:NE2	2.34	0.42
2:B:133:LEU:HD12	30:B:632:DMS:H22	2.00	0.42
24:C:504:CLA:H191	34:D:411:LHG:H362	2.01	0.42
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.42
29:Z:101:LMG:H361	29:Z:101:LMG:H171	2.02	0.42
1:a:322:ASN:OD1	3:c:412:THR:HA	2.20	0.42
24:B:603:CLA:HAB	24:B:605:CLA:H171	2.01	0.42
24:B:607:CLA:H91	24:B:607:CLA:H112	1.87	0.42
24:C:504:CLA:H193	24:C:508:CLA:H91	2.01	0.42
1:a:63:ILE:HB	3:c:335:THR:HG21	2.01	0.42
24:c:505:CLA:HBD	24:c:505:CLA:HAA1	2.01	0.42
24:C:510:CLA:H62	24:C:510:CLA:H2	1.84	0.42
24:C:510:CLA:HBC3	24:C:510:CLA:H192	2.02	0.42
26:b:620:BCR:H24C	26:b:620:BCR:H371	1.83	0.42
3:c:31:SER:CB	3:c:41:ARG:HG2	2.50	0.42
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.91	0.41
2:B:446:SER:HB2	2:B:447:PRO:HD2	2.02	0.41
24:B:606:CLA:H143	35:B:629:HTG:H7'2	2.02	0.41
4:d:146:PHE:C	4:d:149:PRO:HD2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1005:CLA:HBB1	24:A:1005:CLA:CMB	2.50	0.41
15:U:10:VAL:HG11	15:U:15:GLU:OE2	2.20	0.41
24:A:1005:CLA:CAD	24:D:403:CLA:HAC2	2.50	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
24:B:604:CLA:HAB	24:B:611:CLA:H193	2.02	0.41
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.41
4:D:12:ARG:NH1	4:D:16:ASP:HB3	2.36	0.41
34:D:411:LHG:H151	34:D:411:LHG:H332	2.02	0.41
24:b:605:CLA:NC	24:b:605:CLA:ND	2.68	0.41
24:b:607:CLA:C3D	24:b:615:CLA:H161	2.51	0.41
3:c:318:LEU:HD21	3:c:380:ILE:CG2	2.51	0.41
3:c:95:LEU:HD21	24:c:501:CLA:OBD	2.20	0.41
15:u:76:ARG:HA	15:u:79:LEU:HG	2.01	0.41
34:D:409:LHG:H112	34:D:409:LHG:H351	2.03	0.41
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.56	0.41
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.50	0.41
30:A:1014:DMS:H23	2:b:75:TRP:HB3	2.03	0.41
34:b:624:LHG:HC92	34:d:406:LHG:H111	2.02	0.41
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.01	0.41
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.56	0.41
24:C:505:CLA:HBC2	26:C:514:BCR:H341	2.02	0.41
26:D:406:BCR:H383	29:D:412:LMG:H171	2.02	0.41
27:A:1010:PL9:H502	4:D:39:PRO:HG3	2.03	0.41
24:B:612:CLA:CMB	24:B:614:CLA:HBB1	2.51	0.41
26:J:101:BCR:H24C	26:J:101:BCR:H371	1.93	0.41
2:b:30:VAL:HG12	24:b:608:CLA:HHH	2.02	0.41
2:b:63:LEU:N	2:b:64:PRO:HD2	2.36	0.41
2:b:409:GLN:HG2	33:b:632:GOL:H32	2.02	0.41
24:b:606:CLA:H161	24:b:606:CLA:H141	1.75	0.41
24:c:506:CLA:ND	24:c:506:CLA:NC	2.69	0.41
27:A:1010:PL9:H302	4:D:45:LEU:HD22	2.03	0.41
32:A:1017:LMT:H6E	40:A:1189:HOH:O	2.21	0.41
3:C:286:ALA:HB2	24:C:502:CLA:CMD	2.50	0.41
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.02	0.41
4:D:140:PRO:HD2	30:D:417:DMS:H22	2.02	0.41
25:a:411:PHO:ND	25:a:411:PHO:NC	2.67	0.41
3:c:283:GLY:HA3	3:c:434:ALA:HB2	2.03	0.41
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.94	0.41
16:v:71:GLY:CA	33:v:203:GOL:H2	2.49	0.41
1:A:13:LEU:H	1:A:13:LEU:HD12	1.86	0.40
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:158:THR:O	3:c:251:HIS:HB3	2.21	0.40
8:i:2:GLU:O	8:i:6:ILE:HG12	2.21	0.40
3:C:282:MET:CE	24:C:507:CLA:H42	2.51	0.40
3:C:429:SER:HB3	36:C:516:DGD:HB91	2.03	0.40
38:F:101:HEM:HBB2	38:F:101:HEM:HMB2	2.03	0.40
11:L:14:ARG:HD3	28:b:623[A]:SQD:H242	2.02	0.40
3:c:261:ARG:HA	3:c:266:TRP:CZ2	2.56	0.40
2:B:23:HIS:HE1	24:B:610:CLA:H203	1.85	0.40
28:B:620[B]:SQD:C38	28:B:620[B]:SQD:C15	2.97	0.40
3:C:406:SER:HA	3:C:420:VAL:HG23	2.03	0.40
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.03	0.40
1:a:131:TRP:CH2	24:c:505:CLA:HAA2	2.55	0.40
26:d:404:BCR:H272	29:d:409:LMG:H171	2.02	0.40
34:D:411:LHG:H381	34:D:411:LHG:H122	2.04	0.40
24:b:616:CLA:HBB1	24:b:616:CLA:CMB	2.52	0.40
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.02	0.40
1:A:163:ILE:HD11	36:C:515:DGD:HA22	2.03	0.40
25:D:404:PHO:NC	25:D:404:PHO:ND	2.70	0.40
1:a:271:LEU:HD11	27:a:414:PL9:HC71	2.03	0.40
3:c:338:GLY:HA3	3:c:341:LEU:O	2.21	0.40
26:y:101:BCR:H24C	26:y:101:BCR:H371	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	337/334 (101%)	333 (99%)	3 (1%)	1 (0%)	36	36
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	36	36
2	B	513/505 (102%)	505 (98%)	8 (2%)	0	100	100
2	b	512/505 (101%)	506 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	452/451 (100%)	442 (98%)	9 (2%)	1 (0%)	43	44
3	c	450/451 (100%)	441 (98%)	8 (2%)	1 (0%)	43	44
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	333 (98%)	6 (2%)	1 (0%)	36	36
5	E	80/80 (100%)	79 (99%)	1 (1%)	0	100	100
5	e	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	59 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	1
9	j	35/37 (95%)	35 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	244/244 (100%)	240 (98%)	4 (2%)	0	100	100
13	o	242/244 (99%)	234 (97%)	8 (3%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	96/97 (99%)	93 (97%)	3 (3%)	0	100	100
15	u	96/97 (99%)	94 (98%)	2 (2%)	0	100	100
16	V	138/137 (101%)	134 (97%)	4 (3%)	0	100	100
16	v	137/137 (100%)	134 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x	37/40 (92%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5296 (99%)	5151 (98%)	99 (2%)	8 (0%)	43	44

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
9	J	5	GLY
4	d	234	ALA
19	z	30	PRO
19	Z	30	PRO
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/269 (102%)	274 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	413/403 (102%)	413 (100%)	0	100	100
2	b	412/403 (102%)	408 (99%)	4 (1%)	68	76
3	C	355/352 (101%)	351 (99%)	4 (1%)	65	74
3	c	354/352 (101%)	347 (98%)	7 (2%)	48	56
4	D	277/277 (100%)	274 (99%)	3 (1%)	65	74
4	d	277/277 (100%)	274 (99%)	3 (1%)	65	74
5	E	73/71 (103%)	72 (99%)	1 (1%)	59	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	69/71 (97%)	66 (96%)	3 (4%)	26	27
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	26/28 (93%)	25 (96%)	1 (4%)	29	32
7	H	54/53 (102%)	52 (96%)	2 (4%)	30	33
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	32/32 (100%)	32 (100%)	0	100	100
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	25/25 (100%)	25 (100%)	0	100	100
9	j	25/25 (100%)	25 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	37
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	37
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	31/30 (103%)	28 (90%)	3 (10%)	8	5
12	m	31/30 (103%)	31 (100%)	0	100	100
13	O	209/207 (101%)	208 (100%)	1 (0%)	81	88
13	o	207/207 (100%)	204 (99%)	3 (1%)	59	67
14	T	27/27 (100%)	25 (93%)	2 (7%)	13	10
14	t	26/27 (96%)	26 (100%)	0	100	100
15	U	85/84 (101%)	84 (99%)	1 (1%)	63	72
15	u	85/84 (101%)	84 (99%)	1 (1%)	63	72
16	V	120/117 (103%)	119 (99%)	1 (1%)	73	81
16	v	119/117 (102%)	118 (99%)	1 (1%)	73	81
17	Y	23/23 (100%)	22 (96%)	1 (4%)	26	27
17	y	23/23 (100%)	21 (91%)	2 (9%)	9	7
18	X	33/33 (100%)	33 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	51/51 (100%)	49 (96%)	2 (4%)	28	31
19	z	51/51 (100%)	49 (96%)	2 (4%)	28	31
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4364/4323 (101%)	4314 (99%)	50 (1%)	65	74

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	29	GLU
3	C	135	ARG
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	90	LEU
4	D	150	ILE
5	E	61	ARG
7	H	12[A]	ARG
7	H	12[B]	ARG
10	K	17	ILE
12	M	5	GLN
12	M	20	VAL
12	M	33	GLN
13	O	61	GLN
14	T	2	GLU
14	T	30	THR
15	U	70	ARG
16	V	15	GLU
17	Y	17	GLU
19	Z	4	LEU
19	Z	6	GLN
2	b	349	LYS
2	b	362	PHE
2	b	467	ILE
2	b	491	VAL
3	c	120	ILE
3	c	142	GLU
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	462	GLU
4	d	12	ARG
4	d	90	LEU
4	d	233	ARG
5	e	8	ARG
5	e	60	GLN
5	e	62	SER
6	f	44	GLN
10	k	17	ILE
13	o	62	GLU

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Mol	Chain	Res	Type
13	o	110	MET
13	o	118	LEU
15	u	70	ARG
16	v	30	LYS
17	y	25	ILE
17	y	30	ILE
19	z	3	ILE
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
2	B	53	ASN
2	B	281	GLN
2	B	331	ASN
2	B	394	GLN
3	C	25	ASN
3	C	44	ASN
3	C	415	ASN
4	D	83	ASN
4	D	250	ASN
4	D	301	GLN
11	L	8	GLN
12	M	33	GLN
13	O	36	GLN
13	O	61	GLN
13	O	80	GLN
13	O	82	GLN
13	O	124	ASN
13	O	147	ASN
13	O	155	ASN
16	V	34	GLN
16	V	118	HIS
1	a	165	GLN
1	a	296	ASN
1	a	315	ASN
2	b	53	ASN
2	b	281	GLN
2	b	394	GLN
3	c	28	GLN
3	c	415	ASN

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Mol	Chain	Res	Type
3	c	418	ASN
4	d	83	ASN
4	d	186	GLN
4	d	301	GLN
4	d	332	GLN
5	e	75	GLN
12	m	33	GLN
13	o	124	ASN
13	o	147	ASN
15	u	73	GLN
16	v	34	GLN
19	z	6	GLN
19	z	31	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.52	0	8,9,11	1.18	0
12	FME	M	1	12	8,9,10	0.50	0	8,9,11	1.28	1 (12%)
14	FME	t	1	14	8,9,10	0.51	0	8,9,11	1.37	1 (12%)
14	FME	T	1	14	8,9,10	0.55	0	8,9,11	1.54	2 (25%)
8	FME	I	1	8	8,9,10	0.53	0	8,9,11	1.11	0
19	FME	z	1	19	8,9,10	0.49	0	8,9,11	1.46	0
12	FME	m	1	12	8,9,10	0.51	0	8,9,11	1.35	1 (12%)
19	FME	Z	1	19	8,9,10	0.58	0	8,9,11	1.69	4 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
19	FME	z	1	19	-	4/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
19	FME	Z	1	19	-	5/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.82	114.93	109.50
19	Z	1	FME	C-CA-N	2.71	114.73	109.50
14	T	1	FME	O-C-CA	-2.18	119.17	124.77
12	M	1	FME	O1-CN-N	-2.13	119.80	125.32
14	t	1	FME	O-C-CA	-2.13	119.28	124.77
12	m	1	FME	O1-CN-N	-2.13	119.81	125.32
19	Z	1	FME	O1-CN-N	-2.09	119.93	125.32
19	Z	1	FME	O-C-CA	-2.06	119.47	124.77
19	Z	1	FME	CE-SD-CG	2.04	110.90	100.32

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	O1-CN-N-CA
19	Z	1	FME	O1-CN-N-CA
19	Z	1	FME	N-CA-CB-CG
12	m	1	FME	O1-CN-N-CA
14	t	1	FME	O1-CN-N-CA
14	t	1	FME	C-CA-CB-CG
19	z	1	FME	O1-CN-N-CA
19	z	1	FME	C-CA-CB-CG

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	i	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 261 ligands modelled in this entry, 10 are monoatomic and 24 are unknown - leaving 227 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
29	LMG	d	409	39	51,51,55	0.95	2 (3%)	59,59,63	0.87	2 (3%)
30	DMS	a	417	-	3,3,3	2.61	1 (33%)	3,3,3	0.40	0
26	BCR	h	101	-	41,41,41	3.68	14 (34%)	56,56,56	8.60	42 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LHG	D	410	-	48,48,48	0.88	3 (6%)	51,54,54	0.96	4 (7%)
38	HEM	F	101	5,6	50,50,50	2.00	9 (18%)	67,82,82	1.37	6 (8%)
34	LHG	d	408	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
30	DMS	b	628	-	3,3,3	2.57	1 (33%)	3,3,3	0.52	0
24	CLA	C	502	3	69,73,73	2.34	19 (27%)	82,113,113	2.50	24 (29%)
24	CLA	b	618	2	69,73,73	2.44	19 (27%)	82,113,113	2.52	24 (29%)
24	CLA	c	510	3	69,73,73	2.38	19 (27%)	82,113,113	2.45	26 (31%)
25	PHO	A	1007	-	58,69,69	2.63	11 (18%)	55,99,99	2.84	13 (23%)
30	DMS	C	525	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
30	DMS	V	203	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
34	LHG	E	101	-	48,48,48	0.97	2 (4%)	51,54,54	0.97	3 (5%)
28	SQD	B	620[B]	-	52,54,54	0.96	2 (3%)	62,65,65	1.15	5 (8%)
34	LHG	D	411	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
36	DGD	c	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.82	3 (3%)
24	CLA	b	619	2	69,73,73	2.39	19 (27%)	82,113,113	2.48	27 (32%)
26	BCR	a	413	-	41,41,41	3.57	14 (34%)	56,56,56	8.62	41 (73%)
24	CLA	c	507	40	69,73,73	2.48	20 (28%)	82,113,113	2.63	26 (31%)
30	DMS	b	629	-	3,3,3	2.72	1 (33%)	3,3,3	0.46	0
28	SQD	B	620[A]	-	52,54,54	0.98	2 (3%)	62,65,65	1.07	5 (8%)
24	CLA	C	511	3	69,73,73	2.67	21 (30%)	82,113,113	2.53	23 (28%)
24	CLA	a	409	40	69,73,73	2.41	20 (28%)	82,113,113	2.40	25 (30%)
35	HTG	b	602	-	19,19,19	0.94	2 (10%)	23,24,24	1.19	1 (4%)
28	SQD	f	102	-	41,43,54	1.14	3 (7%)	51,54,65	1.34	6 (11%)
35	HTG	B	628	-	19,19,19	0.96	2 (10%)	23,24,24	1.10	1 (4%)
29	LMG	Z	101	-	51,51,55	0.98	2 (3%)	59,59,63	0.99	2 (3%)
24	CLA	C	503	3	69,73,73	2.52	19 (27%)	82,113,113	2.46	24 (29%)
24	CLA	D	402	4	69,73,73	2.19	20 (28%)	82,113,113	2.56	28 (34%)
24	CLA	B	605	2	69,73,73	2.35	20 (28%)	82,113,113	2.44	24 (29%)
35	HTG	c	525	-	19,19,19	0.97	2 (10%)	23,24,24	1.04	1 (4%)
38	HEM	f	101	5,6	50,50,50	1.97	10 (20%)	67,82,82	1.36	6 (8%)
24	CLA	b	611	2	69,73,73	2.35	18 (26%)	82,113,113	2.42	26 (31%)
24	CLA	B	604	2	69,73,73	2.40	18 (26%)	82,113,113	2.48	27 (32%)
32	LMT	M	101	-	36,36,36	0.48	0	47,47,47	0.90	0
24	CLA	B	608	2	69,73,73	2.44	19 (27%)	82,113,113	2.36	22 (26%)
24	CLA	d	403	4	69,73,73	2.49	21 (30%)	82,113,113	2.43	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DMS	C	524	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
28	SQD	a	401	-	52,54,54	0.98	2 (3%)	62,65,65	1.13	4 (6%)
26	BCR	b	620	-	41,41,41	3.64	15 (36%)	56,56,56	8.20	41 (73%)
36	DGD	C	516	-	63,63,67	0.92	3 (4%)	77,77,81	0.94	4 (5%)
30	DMS	C	526	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
26	BCR	B	619	-	41,41,41	3.68	15 (36%)	56,56,56	8.12	38 (67%)
30	DMS	C	527	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0
33	GOL	V	206	-	5,5,5	0.28	0	5,5,5	0.26	0
33	GOL	d	415	-	5,5,5	0.28	0	5,5,5	0.36	0
36	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.84	3 (3%)
24	CLA	b	613	40	69,73,73	2.35	18 (26%)	82,113,113	2.47	22 (26%)
35	HTG	V	202	-	19,19,19	0.90	2 (10%)	23,24,24	1.47	3 (13%)
35	HTG	o	301	-	19,19,19	0.96	1 (5%)	23,24,24	1.16	1 (4%)
24	CLA	b	616	2	69,73,73	2.52	18 (26%)	82,113,113	2.46	26 (31%)
24	CLA	c	502	3	69,73,73	2.41	19 (27%)	82,113,113	2.44	25 (30%)
32	LMT	C	520	-	36,36,36	0.52	1 (2%)	47,47,47	1.04	1 (2%)
32	LMT	m	103	-	36,36,36	0.53	1 (2%)	47,47,47	0.79	1 (2%)
33	GOL	b	632	-	5,5,5	0.22	0	5,5,5	0.32	0
24	CLA	a	407	1	69,73,73	2.33	20 (28%)	82,113,113	2.30	17 (20%)
32	LMT	A	1017	-	36,36,36	0.54	1 (2%)	47,47,47	0.87	2 (4%)
26	BCR	J	101	-	41,41,41	3.70	14 (34%)	56,56,56	8.87	40 (71%)
27	PL9	A	1010	-	55,55,55	0.70	2 (3%)	68,69,69	1.62	18 (26%)
30	DMS	O	302	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
33	GOL	v	203	-	5,5,5	0.34	0	5,5,5	0.34	0
24	CLA	B	606	2	69,73,73	2.57	19 (27%)	82,113,113	2.57	27 (32%)
24	CLA	b	612	2	69,73,73	2.71	20 (28%)	82,113,113	2.44	25 (30%)
32	LMT	m	101	-	36,36,36	0.47	0	47,47,47	0.70	0
33	GOL	v	204	-	5,5,5	0.25	0	5,5,5	0.34	0
30	DMS	d	413	-	3,3,3	2.74	1 (33%)	3,3,3	0.62	0
38	HEM	V	201	16	50,50,50	1.85	10 (20%)	67,82,82	1.33	5 (7%)
29	LMG	D	412	39	51,51,55	0.91	2 (3%)	59,59,63	0.79	1 (1%)
24	CLA	b	617	2	69,73,73	2.70	20 (28%)	82,113,113	2.56	30 (36%)
24	CLA	B	616	2	69,73,73	2.25	17 (24%)	82,113,113	2.52	28 (34%)
26	BCR	B	618	-	41,41,41	3.63	15 (36%)	56,56,56	8.56	41 (73%)
30	DMS	A	1013	-	3,3,3	2.59	1 (33%)	3,3,3	0.59	0
34	LHG	B	621	-	48,48,48	0.93	2 (4%)	51,54,54	0.93	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DMS	a	418	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
26	BCR	b	621	-	41,41,41	3.65	14 (34%)	56,56,56	8.57	43 (76%)
33	GOL	a	420	-	5,5,5	0.28	0	5,5,5	0.31	0
27	PL9	a	414	-	55,55,55	0.71	2 (3%)	68,69,69	1.49	16 (23%)
35	HTG	b	626	-	19,19,19	0.92	1 (5%)	23,24,24	1.06	2 (8%)
24	CLA	A	1005	1	69,73,73	2.27	19 (27%)	82,113,113	2.38	22 (26%)
24	CLA	d	402	4	69,73,73	2.37	19 (27%)	82,113,113	2.45	23 (28%)
28	SQD	b	623[B]	-	52,54,54	0.97	2 (3%)	62,65,65	1.09	7 (11%)
29	LMG	m	102	-	51,51,55	0.99	2 (3%)	59,59,63	1.11	4 (6%)
30	DMS	B	634	-	3,3,3	2.74	1 (33%)	3,3,3	0.49	0
35	HTG	B	624	-	19,19,19	0.95	2 (10%)	23,24,24	1.34	1 (4%)
32	LMT	b	631	-	36,36,36	0.50	0	47,47,47	0.84	2 (4%)
24	CLA	b	609	2	69,73,73	2.68	21 (30%)	82,113,113	2.57	25 (30%)
30	DMS	O	301	-	3,3,3	2.74	1 (33%)	3,3,3	0.55	0
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	0.83	3 (3%)
24	CLA	b	604	40	69,73,73	3.09	21 (30%)	82,113,113	2.48	27 (32%)
30	DMS	B	627	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
24	CLA	c	506	3	69,73,73	2.70	19 (27%)	82,113,113	2.48	25 (30%)
35	HTG	D	413	-	19,19,19	0.96	2 (10%)	23,24,24	1.13	1 (4%)
24	CLA	B	611	2	69,73,73	2.44	19 (27%)	82,113,113	2.44	22 (26%)
30	DMS	V	205	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
30	DMS	b	633	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
30	DMS	d	414	-	3,3,3	2.72	1 (33%)	3,3,3	0.43	0
32	LMT	M	102	-	36,36,36	0.49	0	47,47,47	0.74	0
24	CLA	B	613	2	69,73,73	2.30	19 (27%)	82,113,113	2.48	25 (30%)
24	CLA	c	512	3	69,73,73	2.59	21 (30%)	82,113,113	2.51	25 (30%)
32	LMT	f	103	-	36,36,36	0.52	0	47,47,47	0.67	0
33	GOL	B	631	-	5,5,5	0.24	0	5,5,5	0.29	0
25	PHO	a	411	-	58,69,69	2.77	11 (18%)	55,99,99	2.82	15 (27%)
29	LMG	A	1012	-	51,51,55	0.95	2 (3%)	59,59,63	0.93	2 (3%)
33	GOL	V	207	-	5,5,5	0.24	0	5,5,5	0.39	0
26	BCR	T	101	-	41,41,41	3.71	15 (36%)	56,56,56	8.16	37 (66%)
30	DMS	D	416	-	3,3,3	2.77	1 (33%)	3,3,3	0.77	0
27	PL9	D	407	-	55,55,55	0.75	2 (3%)	68,69,69	1.41	14 (20%)
24	CLA	C	510	3	69,73,73	2.28	18 (26%)	82,113,113	2.53	26 (31%)
26	BCR	D	406	-	41,41,41	3.68	14 (34%)	56,56,56	8.26	45 (80%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	a	415	-	51,51,55	0.96	2 (3%)	59,59,63	0.97	2 (3%)
24	CLA	c	501	3	69,73,73	2.56	19 (27%)	82,113,113	2.54	25 (30%)
24	CLA	b	610	40	69,73,73	2.42	19 (27%)	82,113,113	2.46	26 (31%)
24	CLA	B	612	2	69,73,73	2.42	20 (28%)	82,113,113	2.37	22 (26%)
24	CLA	c	509	3	69,73,73	2.45	20 (28%)	82,113,113	2.52	26 (31%)
34	LHG	e	101	-	48,48,48	0.97	2 (4%)	51,54,54	1.00	2 (3%)
24	CLA	c	504	40	69,73,73	2.49	18 (26%)	82,113,113	2.44	26 (31%)
35	HTG	B	629	-	19,19,19	0.94	1 (5%)	23,24,24	1.18	1 (4%)
26	BCR	d	404	-	41,41,41	3.72	15 (36%)	56,56,56	8.39	41 (73%)
26	BCR	b	622	-	41,41,41	3.71	15 (36%)	56,56,56	8.31	37 (66%)
24	CLA	b	614	2	69,73,73	2.34	19 (27%)	82,113,113	2.42	22 (26%)
24	CLA	c	508	3	69,73,73	2.85	22 (31%)	82,113,113	2.46	24 (29%)
26	BCR	C	514	-	41,41,41	3.74	15 (36%)	56,56,56	8.41	37 (66%)
24	CLA	B	603	2	69,73,73	2.41	20 (28%)	82,113,113	2.54	23 (28%)
28	SQD	D	408	-	41,43,54	1.11	2 (4%)	51,54,65	1.55	9 (17%)
24	CLA	B	610	40	69,73,73	2.23	19 (27%)	82,113,113	2.45	22 (26%)
32	LMT	b	625	-	36,36,36	0.51	0	47,47,47	1.22	5 (10%)
21	OER	a	403	3,1,40	0,14,14	-	-	-	-	-
24	CLA	B	609	2	69,73,73	2.51	19 (27%)	82,113,113	2.44	24 (29%)
26	BCR	A	1009	-	41,41,41	3.64	14 (34%)	56,56,56	8.32	40 (71%)
29	LMG	c	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.07	3 (5%)
26	BCR	t	101	-	41,41,41	3.70	15 (36%)	56,56,56	8.22	41 (73%)
36	DGD	C	517	-	63,63,67	0.86	2 (3%)	77,77,81	0.88	2 (2%)
24	CLA	C	512	3	69,73,73	3.06	21 (30%)	82,113,113	2.42	25 (30%)
24	CLA	C	507	40	69,73,73	2.65	19 (27%)	82,113,113	2.63	26 (31%)
24	CLA	c	511	3	69,73,73	2.70	19 (27%)	82,113,113	2.47	24 (29%)
30	DMS	b	635	-	3,3,3	2.73	1 (33%)	3,3,3	0.46	0
30	DMS	D	417	-	3,3,3	2.74	1 (33%)	3,3,3	0.46	0
24	CLA	C	509	3	69,73,73	2.31	20 (28%)	82,113,113	2.54	26 (31%)
26	BCR	c	514	-	41,41,41	3.72	15 (36%)	56,56,56	8.86	41 (73%)
28	SQD	b	623[A]	-	52,54,54	0.96	2 (3%)	62,65,65	1.11	5 (8%)
24	CLA	b	607	2	69,73,73	2.42	18 (26%)	82,113,113	2.55	23 (28%)
34	LHG	b	624	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
28	SQD	A	1016	-	52,54,54	0.97	2 (3%)	62,65,65	1.13	4 (6%)
25	PHO	D	404	-	58,69,69	2.75	11 (18%)	55,99,99	2.76	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	d	416	-	19,19,19	0.93	1 (5%)	23,24,24	1.39	1 (4%)
37	BCT	D	401	22	3,3,3	0.59	0	2,3,3	0.37	0
24	CLA	C	513	3	69,73,73	2.60	22 (31%)	82,113,113	2.42	27 (32%)
30	DMS	b	634	-	3,3,3	2.78	1 (33%)	3,3,3	0.65	0
24	CLA	A	1008	1	69,73,73	2.39	19 (27%)	82,113,113	2.46	24 (29%)
30	DMS	c	528	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
30	DMS	B	633	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
21	OER	A	1001	3,1,40	0,14,14	-	-	-	-	-
30	DMS	u	201	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
32	LMT	i	102	-	36,36,36	0.51	0	47,47,47	1.04	2 (4%)
26	BCR	K	102	-	41,41,41	3.74	15 (36%)	56,56,56	8.62	39 (69%)
35	HTG	D	419	-	19,19,19	0.93	1 (5%)	23,24,24	1.33	1 (4%)
24	CLA	B	601	40	69,73,73	2.44	20 (28%)	82,113,113	2.54	27 (32%)
26	BCR	k	101	-	41,41,41	3.69	15 (36%)	56,56,56	8.76	40 (71%)
30	DMS	B	632	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
35	HTG	d	410	-	19,19,19	0.96	1 (5%)	23,24,24	1.11	1 (4%)
27	PL9	d	405	-	55,55,55	0.75	2 (3%)	68,69,69	1.37	9 (13%)
34	LHG	d	406	-	48,48,48	0.95	2 (4%)	51,54,54	0.93	3 (5%)
36	DGD	c	516	-	63,63,67	0.92	3 (4%)	77,77,81	0.91	3 (3%)
38	HEM	v	201	16	50,50,50	1.84	10 (20%)	67,82,82	1.27	6 (8%)
29	LMG	C	519	-	51,51,55	0.99	3 (5%)	59,59,63	1.07	4 (6%)
24	CLA	B	607	40	69,73,73	2.46	19 (27%)	82,113,113	2.45	26 (31%)
24	CLA	C	504	40	69,73,73	2.50	20 (28%)	82,113,113	2.48	25 (30%)
24	CLA	C	501	3	69,73,73	2.37	18 (26%)	82,113,113	2.51	25 (30%)
34	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	0.93	3 (5%)
24	CLA	a	412	1	69,73,73	2.21	19 (27%)	82,113,113	2.47	24 (29%)
26	BCR	y	101	-	41,41,41	3.72	15 (36%)	56,56,56	8.97	44 (78%)
24	CLA	a	408	40	69,73,73	2.29	19 (27%)	82,113,113	2.43	24 (29%)
24	CLA	C	506	3	69,73,73	2.41	19 (27%)	82,113,113	2.46	24 (29%)
26	BCR	B	617	-	41,41,41	3.63	15 (36%)	56,56,56	8.26	39 (69%)
32	LMT	t	103	-	36,36,36	0.45	0	47,47,47	1.03	2 (4%)
32	LMT	a	402	-	36,36,36	0.58	1 (2%)	47,47,47	0.87	3 (6%)
37	BCT	d	401	22	3,3,3	0.53	0	2,3,3	0.26	0
35	HTG	C	522	-	19,19,19	0.94	1 (5%)	23,24,24	1.81	5 (21%)
35	HTG	c	522	-	19,19,19	0.92	2 (10%)	23,24,24	1.03	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	k	102	-	41,41,41	3.61	15 (36%)	56,56,56	8.51	37 (66%)
35	HTG	b	630	-	19,19,19	0.99	2 (10%)	23,24,24	1.53	2 (8%)
24	CLA	c	513	3	69,73,73	2.60	22 (31%)	82,113,113	2.39	26 (31%)
36	DGD	c	515	-	63,63,67	0.89	3 (4%)	77,77,81	0.90	2 (2%)
28	SQD	c	518	-	52,54,54	0.98	2 (3%)	62,65,65	1.26	6 (9%)
24	CLA	c	503	3	69,73,73	2.74	22 (31%)	82,113,113	2.47	28 (34%)
29	LMG	B	622	-	51,51,55	0.98	2 (3%)	59,59,63	0.91	2 (3%)
30	DMS	c	524	-	3,3,3	2.64	1 (33%)	3,3,3	0.36	0
30	DMS	U	201	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
33	GOL	V	204	-	5,5,5	0.29	0	5,5,5	0.24	0
24	CLA	b	608	2	69,73,73	2.34	21 (30%)	82,113,113	2.47	23 (28%)
29	LMG	C	518	-	51,51,55	0.98	2 (3%)	59,59,63	0.88	3 (5%)
30	DMS	c	527	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
32	LMT	B	623	-	36,36,36	0.48	0	47,47,47	1.01	2 (4%)
24	CLA	c	505	3	69,73,73	2.38	20 (28%)	82,113,113	2.44	25 (30%)
24	CLA	B	614	2	69,73,73	2.49	18 (26%)	82,113,113	2.60	29 (35%)
33	GOL	A	1019	-	5,5,5	0.26	0	5,5,5	0.34	0
25	PHO	a	410	-	58,69,69	2.69	11 (18%)	55,99,99	2.72	14 (25%)
35	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.07	1 (4%)
24	CLA	C	508	3	69,73,73	2.55	21 (30%)	82,113,113	2.43	24 (29%)
26	BCR	H	101	-	41,41,41	3.65	15 (36%)	56,56,56	8.50	42 (75%)
26	BCR	K	101	-	41,41,41	3.67	15 (36%)	56,56,56	8.14	42 (75%)
30	DMS	B	626	-	3,3,3	2.60	1 (33%)	3,3,3	0.36	0
33	GOL	d	417	-	5,5,5	0.33	0	5,5,5	0.19	0
32	LMT	A	1018	-	36,36,36	0.53	0	47,47,47	1.01	5 (10%)
24	CLA	A	1006	40	69,73,73	2.14	18 (26%)	82,113,113	2.41	24 (29%)
30	DMS	C	523	-	3,3,3	2.60	1 (33%)	3,3,3	0.39	0
24	CLA	b	606	2	69,73,73	2.34	18 (26%)	82,113,113	2.47	25 (30%)
36	DGD	C	515	-	63,63,67	0.87	2 (3%)	77,77,81	0.88	3 (3%)
24	CLA	B	615	2	69,73,73	2.59	22 (31%)	82,113,113	2.54	25 (30%)
34	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	4 (7%)
24	CLA	C	505	3	69,73,73	2.55	18 (26%)	82,113,113	2.44	22 (26%)
30	DMS	v	202	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
24	CLA	b	615	2	69,73,73	2.34	18 (26%)	82,113,113	2.44	24 (29%)
30	DMS	c	529	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	D	403	40	69,73,73	2.10	20 (28%)	82,113,113	2.51	23 (28%)
32	LMT	a	416	-	36,36,36	0.50	0	47,47,47	0.76	1 (2%)
24	CLA	D	405	4	69,73,73	2.50	19 (27%)	82,113,113	2.42	26 (31%)
24	CLA	b	605	2	69,73,73	2.46	20 (28%)	82,113,113	2.40	25 (30%)
33	GOL	D	418	-	5,5,5	0.29	0	5,5,5	0.35	0
35	HTG	b	601	-	19,19,19	0.92	1 (5%)	23,24,24	1.21	1 (4%)
30	DMS	c	526	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
30	DMS	A	1014	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
24	CLA	B	602	2	69,73,73	2.31	18 (26%)	82,113,113	2.39	23 (28%)
28	SQD	A	1011	-	52,54,54	0.96	2 (3%)	62,65,65	1.29	8 (12%)
29	LMG	c	520	-	51,51,55	1.00	3 (5%)	59,59,63	1.03	3 (5%)
29	LMG	c	519	-	51,51,55	0.98	2 (3%)	59,59,63	0.89	3 (5%)

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
29	LMG	d	409	39	-	17/46/66/70	0/1/1/1
26	BCR	h	101	-	-	7/29/63/63	0/2/2/2
34	LHG	D	410	-	-	15/53/53/53	-
38	HEM	F	101	5,6	-	3/14/54/54	-
34	LHG	d	408	-	-	12/53/53/53	-
24	CLA	C	502	3	-	7/39/115/115	-
24	CLA	b	618	2	-	7/39/115/115	-
24	CLA	c	510	3	-	8/39/115/115	-
25	PHO	A	1007	-	-	2/37/103/103	0/5/6/6
34	LHG	E	101	-	-	32/53/53/53	-
28	SQD	B	620[B]	-	-	24/49/69/69	0/1/1/1
34	LHG	D	411	-	-	15/53/53/53	-
36	DGD	c	517	-	-	19/51/91/95	0/2/2/2
24	CLA	b	619	2	-	10/39/115/115	-
26	BCR	a	413	-	-	5/29/63/63	0/2/2/2
24	CLA	c	507	40	-	9/39/115/115	-
28	SQD	B	620[A]	-	-	30/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	511	3	-	6/39/115/115	-
24	CLA	a	409	40	-	10/39/115/115	-
35	HTG	b	602	-	-	2/10/30/30	0/1/1/1
28	SQD	f	102	-	-	24/38/58/69	0/1/1/1
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
29	LMG	Z	101	-	-	29/46/66/70	0/1/1/1
24	CLA	C	503	3	-	4/39/115/115	-
24	CLA	D	402	4	-	5/39/115/115	-
24	CLA	B	605	2	-	4/39/115/115	-
35	HTG	c	525	-	-	4/10/30/30	0/1/1/1
38	HEM	f	101	5,6	-	6/14/54/54	-
24	CLA	b	611	2	-	1/39/115/115	-
24	CLA	B	604	2	-	11/39/115/115	-
32	LMT	M	101	-	-	9/21/61/61	0/2/2/2
24	CLA	B	608	2	-	1/39/115/115	-
24	CLA	d	403	4	-	12/39/115/115	-
28	SQD	a	401	-	-	24/49/69/69	0/1/1/1
26	BCR	b	620	-	-	5/29/63/63	0/2/2/2
36	DGD	C	516	-	-	22/51/91/95	0/2/2/2
26	BCR	B	619	-	-	2/29/63/63	0/2/2/2
33	GOL	V	206	-	-	3/4/4/4	-
33	GOL	d	415	-	-	2/4/4/4	-
36	DGD	h	102	-	-	18/51/91/95	0/2/2/2
24	CLA	b	613	40	-	5/39/115/115	-
35	HTG	V	202	-	-	6/10/30/30	0/1/1/1
35	HTG	o	301	-	-	4/10/30/30	0/1/1/1
24	CLA	b	616	2	-	8/39/115/115	-
24	CLA	c	502	3	-	6/39/115/115	-
32	LMT	C	520	-	-	10/21/61/61	0/2/2/2
32	LMT	m	103	-	-	7/21/61/61	0/2/2/2
33	GOL	b	632	-	-	2/4/4/4	-
24	CLA	a	407	1	-	0/39/115/115	-
32	LMT	A	1017	-	-	10/21/61/61	0/2/2/2
26	BCR	J	101	-	-	12/29/63/63	0/2/2/2
27	PL9	A	1010	-	-	6/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	GOL	v	203	-	-	1/4/4/4	-
24	CLA	B	606	2	-	8/39/115/115	-
24	CLA	b	612	2	-	3/39/115/115	-
32	LMT	m	101	-	-	0/21/61/61	0/2/2/2
33	GOL	v	204	-	-	3/4/4/4	-
38	HEM	V	201	16	-	6/14/54/54	-
29	LMG	D	412	39	-	14/46/66/70	0/1/1/1
24	CLA	b	617	2	-	17/39/115/115	-
24	CLA	B	616	2	-	14/39/115/115	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
34	LHG	B	621	-	-	20/53/53/53	-
26	BCR	b	621	-	-	5/29/63/63	0/2/2/2
33	GOL	a	420	-	-	2/4/4/4	-
27	PL9	a	414	-	-	5/53/73/73	0/1/1/1
35	HTG	b	626	-	-	5/10/30/30	0/1/1/1
24	CLA	A	1005	1	-	0/39/115/115	-
24	CLA	d	402	4	-	5/39/115/115	-
28	SQD	b	623[B]	-	-	29/49/69/69	0/1/1/1
29	LMG	m	102	-	-	21/46/66/70	0/1/1/1
35	HTG	B	624	-	-	7/10/30/30	0/1/1/1
32	LMT	b	631	-	-	10/21/61/61	0/2/2/2
24	CLA	b	609	2	-	7/39/115/115	-
36	DGD	H	102	-	-	16/51/91/95	0/2/2/2
24	CLA	b	604	40	-	19/39/115/115	-
24	CLA	c	506	3	-	12/39/115/115	-
35	HTG	D	413	-	-	5/10/30/30	0/1/1/1
24	CLA	B	611	2	-	5/39/115/115	-
32	LMT	M	102	-	-	6/21/61/61	0/2/2/2
24	CLA	B	613	2	-	5/39/115/115	-
24	CLA	c	512	3	-	15/39/115/115	-
32	LMT	f	103	-	-	15/21/61/61	0/2/2/2
33	GOL	B	631	-	-	0/4/4/4	-
25	PHO	a	411	-	-	4/37/103/103	0/5/6/6
29	LMG	A	1012	-	-	27/46/66/70	0/1/1/1
33	GOL	V	207	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
27	PL9	D	407	-	-	1/53/73/73	0/1/1/1
24	CLA	C	510	3	-	6/39/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
29	LMG	a	415	-	-	24/46/66/70	0/1/1/1
24	CLA	c	501	3	-	3/39/115/115	-
24	CLA	b	610	40	-	6/39/115/115	-
24	CLA	B	612	2	-	4/39/115/115	-
24	CLA	c	509	3	-	10/39/115/115	-
34	LHG	e	101	-	-	28/53/53/53	-
24	CLA	c	504	40	-	13/39/115/115	-
35	HTG	B	629	-	-	2/10/30/30	0/1/1/1
26	BCR	d	404	-	-	10/29/63/63	0/2/2/2
26	BCR	b	622	-	-	6/29/63/63	0/2/2/2
24	CLA	b	614	2	-	3/39/115/115	-
24	CLA	c	508	3	-	12/39/115/115	-
26	BCR	C	514	-	-	5/29/63/63	0/2/2/2
24	CLA	B	603	2	-	5/39/115/115	-
28	SQD	D	408	-	-	22/38/58/69	0/1/1/1
24	CLA	B	610	40	-	8/39/115/115	-
32	LMT	b	625	-	-	10/21/61/61	0/2/2/2
24	CLA	B	609	2	-	2/39/115/115	-
26	BCR	A	1009	-	-	6/29/63/63	0/2/2/2
29	LMG	c	521	-	-	25/46/66/70	0/1/1/1
26	BCR	t	101	-	-	5/29/63/63	0/2/2/2
36	DGD	C	517	-	-	10/51/91/95	0/2/2/2
24	CLA	C	512	3	-	15/39/115/115	-
24	CLA	C	507	40	-	17/39/115/115	-
24	CLA	c	511	3	-	2/39/115/115	-
24	CLA	C	509	3	-	6/39/115/115	-
26	BCR	c	514	-	-	6/29/63/63	0/2/2/2
28	SQD	b	623[A]	-	-	22/49/69/69	0/1/1/1
24	CLA	b	607	2	-	3/39/115/115	-
34	LHG	b	624	-	-	20/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	A	1016	-	-	22/49/69/69	0/1/1/1
25	PHO	D	404	-	-	4/37/103/103	0/5/6/6
35	HTG	d	416	-	-	4/10/30/30	0/1/1/1
24	CLA	C	513	3	-	10/39/115/115	-
24	CLA	A	1008	1	-	7/39/115/115	-
32	LMT	i	102	-	-	12/21/61/61	0/2/2/2
35	HTG	d	410	-	-	4/10/30/30	0/1/1/1
26	BCR	K	102	-	-	8/29/63/63	0/2/2/2
35	HTG	D	419	-	-	7/10/30/30	0/1/1/1
24	CLA	B	601	40	-	14/39/115/115	-
26	BCR	k	101	-	-	14/29/63/63	0/2/2/2
36	DGD	c	516	-	-	27/51/91/95	0/2/2/2
38	HEM	v	201	16	-	6/14/54/54	-
27	PL9	d	405	-	-	1/53/73/73	0/1/1/1
34	LHG	d	406	-	-	16/53/53/53	-
29	LMG	C	519	-	-	22/46/66/70	0/1/1/1
24	CLA	B	607	40	-	2/39/115/115	-
24	CLA	C	504	40	-	9/39/115/115	-
24	CLA	C	501	3	-	4/39/115/115	-
34	LHG	d	407	-	-	14/53/53/53	-
24	CLA	a	412	1	-	14/39/115/115	-
26	BCR	y	101	-	-	11/29/63/63	0/2/2/2
24	CLA	a	408	40	-	1/39/115/115	-
24	CLA	C	506	3	-	13/39/115/115	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
32	LMT	t	103	-	-	16/21/61/61	0/2/2/2
32	LMT	a	402	-	-	7/21/61/61	0/2/2/2
35	HTG	C	522	-	-	5/10/30/30	0/1/1/1
35	HTG	c	522	-	-	5/10/30/30	0/1/1/1
26	BCR	k	102	-	-	9/29/63/63	0/2/2/2
35	HTG	b	630	-	-	7/10/30/30	0/1/1/1
24	CLA	c	513	3	-	20/39/115/115	-
36	DGD	c	515	-	-	23/51/91/95	0/2/2/2
28	SQD	c	518	-	-	19/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	503	3	-	3/39/115/115	-
29	LMG	B	622	-	-	22/46/66/70	0/1/1/1
33	GOL	V	204	-	-	2/4/4/4	-
24	CLA	b	608	2	-	9/39/115/115	-
29	LMG	C	518	-	-	20/46/66/70	0/1/1/1
32	LMT	B	623	-	-	14/21/61/61	0/2/2/2
24	CLA	c	505	3	-	7/39/115/115	-
24	CLA	B	614	2	-	9/39/115/115	-
33	GOL	A	1019	-	-	1/4/4/4	-
25	PHO	a	410	-	-	3/37/103/103	0/5/6/6
35	HTG	C	521	-	-	5/10/30/30	0/1/1/1
24	CLA	C	508	3	-	9/39/115/115	-
26	BCR	H	101	-	-	7/29/63/63	0/2/2/2
26	BCR	K	101	-	-	8/29/63/63	0/2/2/2
33	GOL	d	417	-	-	2/4/4/4	-
32	LMT	A	1018	-	-	12/21/61/61	0/2/2/2
24	CLA	A	1006	40	-	9/39/115/115	-
24	CLA	b	606	2	-	8/39/115/115	-
36	DGD	C	515	-	-	26/51/91/95	0/2/2/2
24	CLA	B	615	2	-	7/39/115/115	-
34	LHG	D	409	-	-	16/53/53/53	-
24	CLA	C	505	3	-	9/39/115/115	-
24	CLA	b	615	2	-	8/39/115/115	-
24	CLA	D	403	40	-	2/39/115/115	-
32	LMT	a	416	-	-	8/21/61/61	0/2/2/2
24	CLA	D	405	4	-	13/39/115/115	-
24	CLA	b	605	2	-	3/39/115/115	-
33	GOL	D	418	-	-	4/4/4/4	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	B	602	2	-	4/39/115/115	-
28	SQD	A	1011	-	-	22/49/69/69	0/1/1/1
29	LMG	c	520	-	-	17/46/66/70	0/1/1/1
29	LMG	c	519	-	-	25/46/66/70	0/1/1/1

All (1931) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	17.54	2.47	2.06
24	b	604	CLA	MG-NC	13.70	2.38	2.06
24	b	617	CLA	MG-NA	13.60	2.38	2.06
24	C	505	CLA	MG-NA	13.03	2.37	2.06
24	C	507	CLA	MG-NA	12.84	2.36	2.06
24	b	616	CLA	MG-NA	12.82	2.36	2.06
24	c	506	CLA	MG-NC	12.80	2.36	2.06
24	B	615	CLA	MG-NA	12.41	2.35	2.06
24	b	609	CLA	MG-NA	12.31	2.35	2.06
24	C	511	CLA	MG-NA	12.27	2.35	2.06
24	B	606	CLA	MG-NA	11.83	2.34	2.06
24	B	611	CLA	MG-NA	11.83	2.34	2.06
24	d	403	CLA	MG-NC	11.58	2.33	2.06
24	D	405	CLA	MG-NC	11.46	2.33	2.06
24	B	607	CLA	MG-NA	11.36	2.33	2.06
24	b	605	CLA	MG-NC	11.06	2.32	2.06
24	c	511	CLA	MG-NC	11.05	2.32	2.06
24	c	504	CLA	MG-NA	11.04	2.32	2.06
24	B	604	CLA	MG-NA	10.91	2.32	2.06
24	c	508	CLA	MG-NC	10.90	2.32	2.06
24	c	509	CLA	MG-NA	10.76	2.31	2.06
24	B	612	CLA	MG-NA	10.61	2.31	2.06
24	c	503	CLA	MG-NA	10.53	2.31	2.06
24	b	612	CLA	MG-NC	10.51	2.31	2.06
24	c	512	CLA	MG-NC	10.48	2.31	2.06
24	b	610	CLA	MG-NA	10.38	2.30	2.06
24	C	504	CLA	MG-NA	10.32	2.30	2.06
24	B	608	CLA	MG-NA	10.10	2.30	2.06
24	c	507	CLA	MG-NC	10.09	2.30	2.06
24	b	619	CLA	MG-NA	10.06	2.30	2.06
24	B	614	CLA	MG-NC	10.06	2.30	2.06
24	C	503	CLA	MG-NA	9.86	2.29	2.06
24	b	612	CLA	MG-NA	9.84	2.29	2.06
24	C	513	CLA	MG-NC	9.76	2.29	2.06
25	D	404	PHO	C1B-C2B	9.70	1.50	1.39
24	b	611	CLA	MG-NA	9.68	2.29	2.06
24	c	511	CLA	MG-NA	9.67	2.29	2.06
24	b	607	CLA	MG-NA	9.65	2.29	2.06
25	a	411	PHO	C1B-C2B	9.63	1.50	1.39
24	B	609	CLA	MG-NC	9.54	2.28	2.06
25	A	1007	PHO	C1B-C2B	9.52	1.50	1.39
25	a	410	PHO	C1D-C2D	9.52	1.50	1.39
24	A	1008	CLA	MG-NA	9.51	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	410	PHO	C1B-C2B	9.50	1.49	1.39
25	a	411	PHO	C1D-C2D	9.49	1.49	1.39
24	c	501	CLA	MG-NA	9.48	2.28	2.06
24	c	503	CLA	MG-NC	9.41	2.28	2.06
25	D	404	PHO	C1D-C2D	9.39	1.49	1.39
24	b	618	CLA	MG-NA	9.16	2.28	2.06
24	b	614	CLA	MG-NA	9.11	2.27	2.06
24	c	513	CLA	MG-NC	9.11	2.27	2.06
24	C	510	CLA	MG-NA	9.08	2.27	2.06
26	c	514	BCR	C8-C9	-9.00	1.26	1.46
24	A	1005	CLA	MG-NC	8.96	2.27	2.06
25	A	1007	PHO	C1D-C2D	8.95	1.49	1.39
26	t	101	BCR	C8-C9	-8.93	1.26	1.46
24	C	509	CLA	MG-NC	8.93	2.27	2.06
26	k	102	BCR	C12-C13	-8.91	1.26	1.46
26	K	101	BCR	C8-C9	-8.91	1.26	1.46
26	D	406	BCR	C19-C18	-8.91	1.26	1.46
26	b	622	BCR	C8-C9	-8.89	1.26	1.46
26	d	404	BCR	C19-C18	-8.88	1.26	1.46
26	B	618	BCR	C8-C9	-8.87	1.27	1.46
26	k	101	BCR	C8-C9	-8.86	1.27	1.46
26	B	619	BCR	C8-C9	-8.86	1.27	1.46
26	C	514	BCR	C8-C9	-8.86	1.27	1.46
26	k	102	BCR	C8-C9	-8.85	1.27	1.46
26	b	622	BCR	C12-C13	-8.83	1.27	1.46
24	C	502	CLA	MG-NA	8.83	2.27	2.06
26	K	102	BCR	C12-C13	-8.82	1.27	1.46
26	C	514	BCR	C19-C18	-8.81	1.27	1.46
26	c	514	BCR	C12-C13	-8.80	1.27	1.46
26	K	102	BCR	C19-C18	-8.80	1.27	1.46
26	t	101	BCR	C19-C18	-8.79	1.27	1.46
26	H	101	BCR	C8-C9	-8.79	1.27	1.46
26	B	617	BCR	C8-C9	-8.79	1.27	1.46
26	y	101	BCR	C12-C13	-8.78	1.27	1.46
26	y	101	BCR	C19-C18	-8.78	1.27	1.46
26	d	404	BCR	C8-C9	-8.77	1.27	1.46
26	T	101	BCR	C8-C9	-8.77	1.27	1.46
26	T	101	BCR	C19-C18	-8.76	1.27	1.46
26	K	102	BCR	C8-C9	-8.75	1.27	1.46
24	b	604	CLA	MG-ND	8.75	2.23	2.05
26	C	514	BCR	C12-C13	-8.73	1.27	1.46
24	a	409	CLA	MG-NA	8.73	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	622	BCR	C19-C18	-8.73	1.27	1.46
26	B	619	BCR	C12-C13	-8.72	1.27	1.46
26	y	101	BCR	C8-C9	-8.72	1.27	1.46
26	h	101	BCR	C19-C18	-8.71	1.27	1.46
26	t	101	BCR	C12-C13	-8.70	1.27	1.46
26	K	101	BCR	C19-C18	-8.70	1.27	1.46
26	k	102	BCR	C19-C18	-8.70	1.27	1.46
26	b	620	BCR	C8-C9	-8.69	1.27	1.46
26	J	101	BCR	C12-C13	-8.68	1.27	1.46
26	k	101	BCR	C19-C18	-8.68	1.27	1.46
26	A	1009	BCR	C8-C9	-8.68	1.27	1.46
26	B	617	BCR	C12-C13	-8.67	1.27	1.46
26	d	404	BCR	C12-C13	-8.67	1.27	1.46
26	h	101	BCR	C8-C9	-8.67	1.27	1.46
26	B	618	BCR	C12-C13	-8.67	1.27	1.46
26	k	101	BCR	C12-C13	-8.66	1.27	1.46
26	T	101	BCR	C12-C13	-8.66	1.27	1.46
26	b	620	BCR	C12-C13	-8.65	1.27	1.46
26	D	406	BCR	C8-C9	-8.65	1.27	1.46
26	h	101	BCR	C12-C13	-8.64	1.27	1.46
26	J	101	BCR	C19-C18	-8.64	1.27	1.46
26	H	101	BCR	C12-C13	-8.63	1.27	1.46
26	J	101	BCR	C8-C9	-8.63	1.27	1.46
26	D	406	BCR	C12-C13	-8.63	1.27	1.46
26	H	101	BCR	C19-C18	-8.62	1.27	1.46
26	b	621	BCR	C8-C9	-8.61	1.27	1.46
26	b	620	BCR	C19-C18	-8.60	1.27	1.46
26	A	1009	BCR	C19-C18	-8.60	1.27	1.46
26	c	514	BCR	C19-C18	-8.59	1.27	1.46
26	A	1009	BCR	C12-C13	-8.58	1.27	1.46
26	b	621	BCR	C19-C18	-8.58	1.27	1.46
26	B	618	BCR	C19-C18	-8.57	1.27	1.46
24	B	605	CLA	MG-NA	8.56	2.26	2.06
26	b	621	BCR	C12-C13	-8.55	1.27	1.46
26	B	619	BCR	C19-C18	-8.54	1.27	1.46
26	K	101	BCR	C12-C13	-8.53	1.27	1.46
26	a	413	BCR	C8-C9	-8.50	1.27	1.46
24	b	604	CLA	MG-NB	-8.48	1.89	2.05
24	B	602	CLA	MG-NC	8.46	2.26	2.06
26	a	413	BCR	C12-C13	-8.46	1.27	1.46
26	B	617	BCR	C19-C18	-8.46	1.27	1.46
24	c	502	CLA	MG-NA	8.35	2.26	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	413	BCR	C19-C18	-8.35	1.28	1.46
24	d	402	CLA	MG-NA	8.26	2.25	2.06
24	B	610	CLA	MG-NC	8.21	2.25	2.06
24	B	601	CLA	MG-NC	8.21	2.25	2.06
24	C	508	CLA	MG-NA	8.18	2.25	2.06
24	c	510	CLA	MG-NA	8.02	2.25	2.06
24	C	508	CLA	MG-NC	7.94	2.25	2.06
24	C	503	CLA	MG-NC	7.94	2.25	2.06
24	b	613	CLA	MG-NA	7.86	2.24	2.06
38	f	101	HEM	C3D-C2D	7.84	1.53	1.36
24	C	506	CLA	MG-NC	7.83	2.24	2.06
24	C	513	CLA	MG-NA	7.80	2.24	2.06
38	F	101	HEM	C3D-C2D	7.75	1.53	1.36
24	C	501	CLA	MG-NA	7.74	2.24	2.06
24	c	513	CLA	MG-NA	7.73	2.24	2.06
24	b	615	CLA	MG-NA	7.71	2.24	2.06
24	c	508	CLA	MG-NB	7.69	2.21	2.05
24	c	505	CLA	MG-NA	7.69	2.24	2.06
26	C	514	BCR	C20-C21	-7.67	1.19	1.43
26	K	102	BCR	C20-C21	-7.66	1.19	1.43
38	v	201	HEM	C3D-C2D	7.65	1.53	1.36
26	y	101	BCR	C20-C21	-7.62	1.19	1.43
24	c	508	CLA	MG-NA	7.60	2.24	2.06
26	K	102	BCR	C16-C17	-7.60	1.19	1.43
26	J	101	BCR	C16-C17	-7.60	1.19	1.43
26	d	404	BCR	C20-C21	-7.59	1.19	1.43
26	D	406	BCR	C20-C21	-7.59	1.19	1.43
26	b	622	BCR	C20-C21	-7.56	1.19	1.43
26	c	514	BCR	C16-C17	-7.54	1.19	1.43
38	V	201	HEM	C3D-C2D	7.54	1.53	1.36
26	B	619	BCR	C20-C21	-7.52	1.19	1.43
26	h	101	BCR	C20-C21	-7.52	1.19	1.43
26	B	618	BCR	C20-C21	-7.51	1.19	1.43
26	H	101	BCR	C20-C21	-7.51	1.19	1.43
26	T	101	BCR	C16-C17	-7.51	1.19	1.43
26	A	1009	BCR	C20-C21	-7.51	1.19	1.43
26	k	101	BCR	C20-C21	-7.50	1.19	1.43
26	C	514	BCR	C16-C17	-7.50	1.19	1.43
26	c	514	BCR	C20-C21	-7.50	1.19	1.43
26	K	101	BCR	C20-C21	-7.50	1.19	1.43
26	b	620	BCR	C20-C21	-7.49	1.19	1.43
26	J	101	BCR	C20-C21	-7.49	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	621	BCR	C20-C21	-7.49	1.20	1.43
26	y	101	BCR	C16-C17	-7.48	1.20	1.43
24	B	601	CLA	MG-NA	7.47	2.24	2.06
26	T	101	BCR	C20-C21	-7.46	1.20	1.43
26	K	101	BCR	C16-C17	-7.46	1.20	1.43
26	B	617	BCR	C16-C17	-7.45	1.20	1.43
26	t	101	BCR	C20-C21	-7.44	1.20	1.43
26	h	101	BCR	C16-C17	-7.43	1.20	1.43
24	b	617	CLA	MG-ND	-7.43	1.91	2.05
26	k	101	BCR	C16-C17	-7.42	1.20	1.43
26	d	404	BCR	C16-C17	-7.41	1.20	1.43
26	D	406	BCR	C16-C17	-7.40	1.20	1.43
26	H	101	BCR	C16-C17	-7.40	1.20	1.43
26	b	622	BCR	C16-C17	-7.39	1.20	1.43
24	c	501	CLA	MG-NC	7.39	2.23	2.06
26	B	619	BCR	C16-C17	-7.39	1.20	1.43
26	t	101	BCR	C16-C17	-7.38	1.20	1.43
24	c	505	CLA	MG-NC	7.38	2.23	2.06
26	b	621	BCR	C16-C17	-7.38	1.20	1.43
26	k	102	BCR	C20-C21	-7.35	1.20	1.43
24	b	606	CLA	MG-NC	7.34	2.23	2.06
26	B	617	BCR	C20-C21	-7.33	1.20	1.43
26	b	620	BCR	C16-C17	-7.28	1.20	1.43
24	B	603	CLA	MG-NB	-7.27	1.91	2.05
24	C	506	CLA	MG-NA	7.26	2.23	2.06
26	a	413	BCR	C16-C17	-7.25	1.20	1.43
26	B	618	BCR	C16-C17	-7.24	1.20	1.43
26	A	1009	BCR	C16-C17	-7.24	1.20	1.43
26	a	413	BCR	C20-C21	-7.23	1.20	1.43
24	C	501	CLA	MG-NC	7.21	2.23	2.06
24	c	502	CLA	MG-NC	7.16	2.23	2.06
24	b	606	CLA	MG-NA	7.16	2.23	2.06
24	A	1006	CLA	MG-NA	7.14	2.23	2.06
24	a	408	CLA	MG-NA	7.13	2.23	2.06
24	b	613	CLA	MG-NC	7.11	2.23	2.06
25	a	411	PHO	C3B-C4B	7.10	1.48	1.41
24	b	607	CLA	MG-NC	7.05	2.23	2.06
24	B	616	CLA	MG-NA	7.05	2.23	2.06
24	b	609	CLA	MG-NC	6.96	2.22	2.06
24	B	613	CLA	MG-NA	6.88	2.22	2.06
24	b	615	CLA	MG-NC	6.86	2.22	2.06
24	b	618	CLA	MG-NC	6.85	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	MG-NA	6.81	2.22	2.06
25	D	404	PHO	C3B-C4B	6.79	1.48	1.41
24	B	613	CLA	MG-NC	6.77	2.22	2.06
24	c	508	CLA	MG-ND	-6.73	1.92	2.05
24	a	407	CLA	MG-NC	6.72	2.22	2.06
24	B	616	CLA	MG-NC	6.72	2.22	2.06
24	C	504	CLA	MG-NC	6.71	2.22	2.06
24	c	512	CLA	MG-NA	6.66	2.22	2.06
24	c	510	CLA	MG-NC	6.63	2.22	2.06
24	B	606	CLA	MG-NC	6.63	2.22	2.06
25	A	1007	PHO	C3B-C4B	6.61	1.48	1.41
24	B	609	CLA	MG-NA	6.60	2.22	2.06
24	a	412	CLA	MG-NA	6.60	2.21	2.06
24	b	608	CLA	MG-NC	6.57	2.21	2.06
25	a	410	PHO	C3B-C4B	6.54	1.48	1.41
24	C	507	CLA	MG-NC	6.52	2.21	2.06
24	c	506	CLA	MG-ND	-6.40	1.93	2.05
24	c	507	CLA	MG-NA	6.35	2.21	2.06
24	B	603	CLA	MG-NC	6.27	2.21	2.06
24	C	512	CLA	MG-ND	-6.22	1.93	2.05
24	D	402	CLA	MG-NC	6.21	2.21	2.06
26	T	101	BCR	C16-C15	-6.17	1.19	1.36
24	b	608	CLA	MG-NB	6.13	2.17	2.05
24	d	402	CLA	MG-NC	6.11	2.20	2.06
26	J	101	BCR	C16-C15	-6.11	1.19	1.36
26	k	102	BCR	C16-C17	-6.10	1.24	1.43
26	c	514	BCR	C16-C15	-6.07	1.19	1.36
26	y	101	BCR	C16-C15	-6.06	1.19	1.36
26	C	514	BCR	C16-C15	-6.06	1.19	1.36
26	K	102	BCR	C16-C15	-6.05	1.19	1.36
26	d	404	BCR	C16-C15	-6.03	1.19	1.36
24	B	614	CLA	MG-NA	6.01	2.20	2.06
26	t	101	BCR	C16-C15	-5.94	1.19	1.36
26	A	1009	BCR	C16-C15	-5.93	1.20	1.36
24	b	614	CLA	MG-NC	5.92	2.20	2.06
26	h	101	BCR	C16-C15	-5.91	1.20	1.36
26	B	619	BCR	C16-C15	-5.90	1.20	1.36
26	H	101	BCR	C16-C15	-5.89	1.20	1.36
26	k	101	BCR	C16-C15	-5.89	1.20	1.36
26	K	101	BCR	C16-C15	-5.89	1.20	1.36
26	b	620	BCR	C16-C15	-5.88	1.20	1.36
26	b	621	BCR	C16-C15	-5.87	1.20	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	514	BCR	C20-C19	-5.87	1.19	1.34
25	D	404	PHO	C4D-CHA	5.86	1.48	1.39
26	b	622	BCR	C16-C15	-5.84	1.20	1.36
26	B	617	BCR	C16-C15	-5.84	1.20	1.36
25	D	404	PHO	C3B-C2B	5.84	1.48	1.40
26	k	102	BCR	C11-C12	-5.84	1.19	1.34
24	A	1008	CLA	MG-NC	5.83	2.20	2.06
26	J	101	BCR	C11-C12	-5.82	1.19	1.34
26	B	619	BCR	C11-C12	-5.80	1.19	1.34
26	D	406	BCR	C16-C15	-5.78	1.20	1.36
26	C	514	BCR	C11-C12	-5.78	1.19	1.34
25	a	411	PHO	C3B-C2B	5.77	1.48	1.40
26	K	102	BCR	C20-C19	-5.77	1.19	1.34
26	t	101	BCR	C11-C12	-5.76	1.19	1.34
26	a	413	BCR	C16-C15	-5.76	1.20	1.36
24	B	605	CLA	MG-NC	5.76	2.19	2.06
26	b	622	BCR	C11-C12	-5.75	1.19	1.34
26	K	102	BCR	C11-C12	-5.74	1.19	1.34
26	h	101	BCR	C20-C19	-5.72	1.19	1.34
26	c	514	BCR	C11-C12	-5.71	1.19	1.34
24	C	502	CLA	MG-NC	5.71	2.19	2.06
25	a	411	PHO	C4D-CHA	5.71	1.48	1.39
26	k	101	BCR	C11-C12	-5.70	1.19	1.34
26	y	101	BCR	C11-C12	-5.70	1.19	1.34
26	y	101	BCR	C20-C19	-5.70	1.19	1.34
26	d	404	BCR	C20-C19	-5.69	1.19	1.34
24	c	513	CLA	MG-NB	-5.69	1.94	2.05
25	A	1007	PHO	C3B-C2B	5.68	1.48	1.40
26	c	514	BCR	C20-C19	-5.68	1.19	1.34
26	T	101	BCR	C20-C19	-5.67	1.19	1.34
26	T	101	BCR	C11-C12	-5.67	1.19	1.34
26	b	621	BCR	C11-C12	-5.66	1.19	1.34
26	K	101	BCR	C20-C19	-5.66	1.19	1.34
26	h	101	BCR	C11-C12	-5.65	1.19	1.34
26	B	618	BCR	C16-C15	-5.65	1.20	1.36
26	B	618	BCR	C11-C12	-5.64	1.19	1.34
26	b	621	BCR	C20-C19	-5.64	1.20	1.34
26	d	404	BCR	C11-C12	-5.64	1.20	1.34
26	K	101	BCR	C11-C12	-5.63	1.20	1.34
26	D	406	BCR	C20-C19	-5.63	1.20	1.34
24	B	602	CLA	MG-NA	5.62	2.19	2.06
26	b	620	BCR	C11-C12	-5.61	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	101	BCR	C20-C19	-5.61	1.20	1.34
26	b	622	BCR	C20-C19	-5.61	1.20	1.34
24	B	608	CLA	MG-NC	5.59	2.19	2.06
26	B	619	BCR	C20-C19	-5.58	1.20	1.34
26	k	101	BCR	C20-C19	-5.57	1.20	1.34
26	D	406	BCR	C11-C12	-5.56	1.20	1.34
24	c	504	CLA	MG-NC	5.55	2.19	2.06
26	H	101	BCR	C20-C19	-5.55	1.20	1.34
26	A	1009	BCR	C11-C12	-5.55	1.20	1.34
26	H	101	BCR	C11-C12	-5.54	1.20	1.34
25	a	410	PHO	C4D-CHA	5.54	1.47	1.39
26	A	1009	BCR	C20-C19	-5.54	1.20	1.34
24	D	402	CLA	MG-NA	5.53	2.19	2.06
24	B	614	CLA	MG-NB	-5.53	1.94	2.05
26	t	101	BCR	C20-C19	-5.51	1.20	1.34
25	A	1007	PHO	C4D-CHA	5.49	1.47	1.39
24	c	501	CLA	MG-ND	-5.49	1.94	2.05
25	a	410	PHO	C3B-C2B	5.49	1.47	1.40
26	B	617	BCR	C11-C12	-5.47	1.20	1.34
26	B	618	BCR	C20-C19	-5.47	1.20	1.34
26	b	620	BCR	C20-C19	-5.47	1.20	1.34
24	b	610	CLA	MG-NC	5.44	2.19	2.06
24	b	604	CLA	MG-NA	5.44	2.19	2.06
24	a	407	CLA	MG-NA	5.43	2.19	2.06
26	a	413	BCR	C11-C12	-5.43	1.20	1.34
24	c	508	CLA	C3C-C2C	5.41	1.48	1.36
24	c	511	CLA	CHC-C1C	5.39	1.49	1.38
24	b	604	CLA	O2D-CGD	5.38	1.46	1.33
24	C	511	CLA	MG-NC	5.37	2.19	2.06
24	C	512	CLA	C3C-C2C	5.37	1.48	1.36
24	b	619	CLA	MG-NC	5.36	2.19	2.06
24	C	513	CLA	C3C-C2C	5.36	1.48	1.36
24	c	501	CLA	C3C-C2C	5.36	1.48	1.36
24	c	504	CLA	O2D-CGD	5.35	1.46	1.33
26	a	413	BCR	C20-C19	-5.35	1.20	1.34
24	c	503	CLA	CHC-C1C	5.35	1.49	1.38
24	c	508	CLA	O2D-CGD	5.35	1.46	1.33
24	a	409	CLA	MG-NC	5.32	2.18	2.06
24	C	511	CLA	C3C-C2C	5.32	1.48	1.36
24	c	503	CLA	C3C-C2C	5.31	1.48	1.36
24	c	512	CLA	C3C-C2C	5.31	1.48	1.36
24	C	503	CLA	CHC-C1C	5.31	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	CLA	MG-ND	-5.31	1.95	2.05
24	b	606	CLA	CHC-C1C	5.30	1.49	1.38
24	b	611	CLA	C3C-C2C	5.30	1.48	1.36
24	c	513	CLA	C3C-C2C	5.30	1.48	1.36
24	B	602	CLA	C3C-C2C	5.30	1.48	1.36
26	B	617	BCR	C20-C19	-5.30	1.20	1.34
24	C	506	CLA	C3C-C2C	5.30	1.48	1.36
26	T	101	BCR	C11-C10	-5.29	1.26	1.43
24	B	608	CLA	C3C-C2C	5.29	1.48	1.36
24	C	512	CLA	MG-NB	5.29	2.16	2.05
24	a	412	CLA	MG-NC	5.29	2.18	2.06
24	a	409	CLA	MG-NB	5.29	2.16	2.05
24	B	610	CLA	C3C-C2C	5.29	1.48	1.36
24	C	504	CLA	C3C-C2C	5.28	1.48	1.36
26	k	102	BCR	C20-C19	-5.28	1.20	1.34
24	D	405	CLA	C3C-C2C	5.28	1.48	1.36
24	B	606	CLA	C3C-C2C	5.28	1.48	1.36
24	C	508	CLA	C3C-C2C	5.28	1.48	1.36
24	c	511	CLA	C3C-C2C	5.27	1.48	1.36
24	C	508	CLA	CHC-C1C	5.27	1.49	1.38
26	k	102	BCR	C11-C10	-5.27	1.26	1.43
24	b	605	CLA	C3C-C2C	5.27	1.48	1.36
24	B	603	CLA	C3C-C2C	5.26	1.48	1.36
24	b	604	CLA	CHC-C1C	5.26	1.49	1.38
24	B	615	CLA	O2D-CGD	5.26	1.46	1.33
24	C	507	CLA	CHC-C1C	5.26	1.49	1.38
24	B	601	CLA	C3C-C2C	5.25	1.48	1.36
24	C	508	CLA	O2D-CGD	5.25	1.46	1.33
24	b	604	CLA	C3C-C2C	5.25	1.48	1.36
26	k	102	BCR	C15-C14	-5.25	1.26	1.43
24	c	512	CLA	CHC-C1C	5.24	1.49	1.38
24	a	407	CLA	C3C-C2C	5.24	1.48	1.36
24	a	408	CLA	MG-NB	5.24	2.16	2.05
24	b	613	CLA	C3C-C2C	5.24	1.48	1.36
24	b	609	CLA	C3C-C2C	5.24	1.48	1.36
24	C	503	CLA	C3C-C2C	5.24	1.48	1.36
24	c	511	CLA	O2D-CGD	5.23	1.46	1.33
24	B	611	CLA	O2D-CGD	5.22	1.46	1.33
26	B	619	BCR	C11-C10	-5.22	1.27	1.43
24	C	509	CLA	C3C-C2C	5.21	1.48	1.36
24	c	506	CLA	C3C-C2C	5.21	1.48	1.36
26	h	101	BCR	C11-C10	-5.21	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	O2D-CGD	5.21	1.46	1.33
24	C	513	CLA	O2D-CGD	5.21	1.46	1.33
26	b	622	BCR	C11-C10	-5.21	1.27	1.43
24	B	601	CLA	O2D-CGD	5.21	1.46	1.33
24	A	1008	CLA	C3C-C2C	5.21	1.48	1.36
26	c	514	BCR	C11-C10	-5.20	1.27	1.43
26	K	102	BCR	C11-C10	-5.20	1.27	1.43
25	a	411	PHO	C3D-C4D	-5.20	1.34	1.41
24	b	606	CLA	O2D-CGD	5.20	1.46	1.33
24	C	507	CLA	C3C-C2C	5.20	1.48	1.36
26	C	514	BCR	C11-C10	-5.20	1.27	1.43
24	b	608	CLA	C3C-C2C	5.20	1.48	1.36
24	B	605	CLA	CHC-C1C	5.19	1.48	1.38
24	C	511	CLA	O2D-CGD	5.19	1.46	1.33
26	k	101	BCR	C11-C10	-5.19	1.27	1.43
24	B	611	CLA	C3C-C2C	5.19	1.48	1.36
24	c	507	CLA	CHC-C1C	5.19	1.48	1.38
24	c	513	CLA	O2D-CGD	5.18	1.46	1.33
24	B	604	CLA	C3C-C2C	5.18	1.47	1.36
24	B	614	CLA	C3C-C2C	5.17	1.47	1.36
26	c	514	BCR	C15-C14	-5.17	1.27	1.43
24	c	505	CLA	C3C-C2C	5.17	1.47	1.36
26	d	404	BCR	C11-C10	-5.17	1.27	1.43
24	b	606	CLA	C3C-C2C	5.17	1.47	1.36
24	c	504	CLA	C3C-C2C	5.17	1.47	1.36
24	d	403	CLA	CHC-C1C	5.17	1.48	1.38
24	D	405	CLA	MG-NA	5.17	2.18	2.06
24	C	513	CLA	CHC-C1C	5.16	1.48	1.38
24	c	510	CLA	C3C-C2C	5.16	1.47	1.36
26	t	101	BCR	C11-C10	-5.16	1.27	1.43
24	b	615	CLA	C3C-C2C	5.16	1.47	1.36
26	y	101	BCR	C11-C10	-5.16	1.27	1.43
26	J	101	BCR	C11-C10	-5.15	1.27	1.43
24	D	405	CLA	CHC-C1C	5.15	1.48	1.38
24	d	402	CLA	C3C-C2C	5.15	1.47	1.36
26	C	514	BCR	C15-C14	-5.15	1.27	1.43
24	b	605	CLA	CHC-C1C	5.15	1.48	1.38
24	C	505	CLA	C3C-C2C	5.15	1.47	1.36
26	K	102	BCR	C15-C14	-5.15	1.27	1.43
24	c	509	CLA	O2D-CGD	5.14	1.45	1.33
26	T	101	BCR	C15-C14	-5.14	1.27	1.43
26	J	101	BCR	C15-C14	-5.14	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	C3C-C2C	5.14	1.47	1.36
24	b	618	CLA	C3C-C2C	5.14	1.47	1.36
24	B	603	CLA	O2D-CGD	5.13	1.45	1.33
24	B	609	CLA	O2D-CGD	5.13	1.45	1.33
24	c	513	CLA	CHC-C1C	5.13	1.48	1.38
24	B	609	CLA	CHC-C1C	5.13	1.48	1.38
24	C	504	CLA	O2D-CGD	5.12	1.45	1.33
24	b	611	CLA	CHC-C1C	5.12	1.48	1.38
26	B	618	BCR	C11-C10	-5.12	1.27	1.43
24	C	506	CLA	CHC-C1C	5.12	1.48	1.38
24	C	508	CLA	MG-ND	-5.12	1.95	2.05
24	b	610	CLA	C3C-C2C	5.12	1.47	1.36
24	C	501	CLA	C3C-C2C	5.11	1.47	1.36
24	B	606	CLA	O2D-CGD	5.11	1.45	1.33
26	A	1009	BCR	C11-C10	-5.11	1.27	1.43
24	b	612	CLA	C3C-C2C	5.11	1.47	1.36
24	c	505	CLA	CHC-C1C	5.11	1.48	1.38
24	c	507	CLA	C3C-C2C	5.10	1.47	1.36
24	C	510	CLA	O2D-CGD	5.10	1.45	1.33
24	C	511	CLA	CHC-C1C	5.10	1.48	1.38
24	c	506	CLA	O2D-CGD	5.09	1.45	1.33
26	h	101	BCR	C15-C14	-5.09	1.27	1.43
24	b	607	CLA	O2D-CGD	5.09	1.45	1.33
25	D	404	PHO	O2D-CGD	5.09	1.45	1.33
26	y	101	BCR	C15-C14	-5.09	1.27	1.43
24	b	613	CLA	O2D-CGD	5.09	1.45	1.33
24	a	412	CLA	C3C-C2C	5.09	1.47	1.36
24	B	601	CLA	CHC-C1C	5.09	1.48	1.38
24	b	617	CLA	C3C-C2C	5.08	1.47	1.36
26	B	619	BCR	C15-C14	-5.08	1.27	1.43
24	C	512	CLA	O2D-CGD	5.08	1.45	1.33
25	a	410	PHO	OBD-CAD	5.08	1.29	1.22
24	B	605	CLA	O2D-CGD	5.08	1.45	1.33
26	k	101	BCR	C15-C14	-5.08	1.27	1.43
26	H	101	BCR	C11-C10	-5.08	1.27	1.43
24	b	615	CLA	O2D-CGD	5.07	1.45	1.33
24	c	510	CLA	O2D-CGD	5.07	1.45	1.33
24	c	501	CLA	CHD-C1D	5.07	1.48	1.38
24	b	608	CLA	O2D-CGD	5.07	1.45	1.33
26	B	617	BCR	C11-C10	-5.07	1.27	1.43
24	b	604	CLA	CHD-C1D	5.07	1.48	1.38
26	K	101	BCR	C11-C10	-5.07	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	404	PHO	C3D-C4D	-5.06	1.34	1.41
26	b	620	BCR	C11-C10	-5.06	1.27	1.43
24	b	613	CLA	CHC-C1C	5.06	1.48	1.38
24	B	613	CLA	CHC-C1C	5.06	1.48	1.38
24	C	512	CLA	CHC-C1C	5.06	1.48	1.38
24	c	502	CLA	CHC-C1C	5.06	1.48	1.38
26	t	101	BCR	C15-C14	-5.05	1.27	1.43
24	B	607	CLA	C3C-C2C	5.05	1.47	1.36
24	B	612	CLA	C3C-C2C	5.04	1.47	1.36
24	c	512	CLA	O2D-CGD	5.04	1.45	1.33
26	D	406	BCR	C11-C10	-5.04	1.27	1.43
26	d	404	BCR	C15-C14	-5.03	1.27	1.43
24	B	607	CLA	MG-NC	5.03	2.18	2.06
24	a	409	CLA	C3C-C2C	5.03	1.47	1.36
26	d	404	BCR	C23-C22	-5.03	1.35	1.46
24	b	612	CLA	CHC-C1C	5.03	1.48	1.38
26	k	102	BCR	C16-C15	-5.03	1.22	1.36
26	B	617	BCR	C15-C14	-5.03	1.27	1.43
26	K	101	BCR	C15-C14	-5.02	1.27	1.43
24	a	408	CLA	C3C-C2C	5.02	1.47	1.36
24	c	504	CLA	CHC-C1C	5.02	1.48	1.38
24	b	609	CLA	CHC-C1C	5.02	1.48	1.38
24	B	605	CLA	C3C-C2C	5.02	1.47	1.36
24	b	612	CLA	O2D-CGD	5.01	1.45	1.33
25	a	411	PHO	O2D-CGD	5.01	1.45	1.33
24	A	1005	CLA	O2D-CGD	5.01	1.45	1.33
24	B	615	CLA	C3C-C2C	5.01	1.47	1.36
24	c	509	CLA	C3C-C2C	5.01	1.47	1.36
26	b	622	BCR	C15-C14	-5.01	1.27	1.43
24	b	610	CLA	O2D-CGD	5.01	1.45	1.33
24	B	611	CLA	CHC-C1C	5.00	1.48	1.38
24	c	507	CLA	O2D-CGD	5.00	1.45	1.33
24	B	612	CLA	O2D-CGD	5.00	1.45	1.33
24	C	501	CLA	CHC-C1C	5.00	1.48	1.38
24	c	513	CLA	CHD-C1D	5.00	1.48	1.38
24	b	612	CLA	CHD-C1D	4.99	1.48	1.38
24	B	609	CLA	C3C-C2C	4.99	1.47	1.36
24	b	611	CLA	MG-NC	4.99	2.18	2.06
24	B	606	CLA	CHC-C1C	4.99	1.48	1.38
26	D	406	BCR	C23-C22	-4.99	1.35	1.46
26	a	413	BCR	C23-C22	-4.99	1.35	1.46
26	b	621	BCR	C15-C14	-4.98	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C3C-C2C	4.98	1.47	1.36
24	b	614	CLA	O2D-CGD	4.98	1.45	1.33
24	a	409	CLA	CHC-C1C	4.98	1.48	1.38
26	b	621	BCR	C11-C10	-4.97	1.27	1.43
24	c	501	CLA	O2D-CGD	4.97	1.45	1.33
24	B	604	CLA	O2D-CGD	4.97	1.45	1.33
24	C	501	CLA	O2D-CGD	4.97	1.45	1.33
24	b	609	CLA	O2D-CGD	4.97	1.45	1.33
24	B	612	CLA	CHC-C1C	4.97	1.48	1.38
24	a	412	CLA	CHC-C1C	4.96	1.48	1.38
26	a	413	BCR	C15-C14	-4.96	1.27	1.43
26	D	406	BCR	C15-C14	-4.96	1.27	1.43
24	C	502	CLA	CHC-C1C	4.95	1.48	1.38
24	b	618	CLA	O2D-CGD	4.95	1.45	1.33
24	d	402	CLA	O2D-CGD	4.95	1.45	1.33
24	b	619	CLA	O2D-CGD	4.94	1.45	1.33
24	C	505	CLA	CHC-C1C	4.94	1.48	1.38
24	A	1006	CLA	C3C-C2C	4.94	1.47	1.36
24	c	503	CLA	CHD-C1D	4.94	1.48	1.38
24	B	616	CLA	C3C-C2C	4.94	1.47	1.36
24	B	610	CLA	CHC-C1C	4.93	1.48	1.38
24	A	1005	CLA	C3C-C2C	4.93	1.47	1.36
24	B	616	CLA	O2D-CGD	4.93	1.45	1.33
24	C	509	CLA	O2D-CGD	4.93	1.45	1.33
24	b	617	CLA	O2D-CGD	4.93	1.45	1.33
24	c	503	CLA	O2D-CGD	4.92	1.45	1.33
24	b	608	CLA	CHC-C1C	4.92	1.48	1.38
24	C	503	CLA	O2D-CGD	4.92	1.45	1.33
26	k	101	BCR	C23-C22	-4.92	1.35	1.46
24	B	614	CLA	O2D-CGD	4.92	1.45	1.33
26	H	101	BCR	C15-C14	-4.92	1.27	1.43
24	a	407	CLA	O2D-CGD	4.92	1.45	1.33
24	d	402	CLA	CHC-C1C	4.92	1.48	1.38
26	k	102	BCR	C23-C22	-4.92	1.35	1.46
24	C	502	CLA	C3C-C2C	4.91	1.47	1.36
24	b	607	CLA	C3C-C2C	4.91	1.47	1.36
24	b	615	CLA	CHC-C1C	4.91	1.48	1.38
26	b	621	BCR	C23-C22	-4.91	1.35	1.46
24	c	502	CLA	O2D-CGD	4.91	1.45	1.33
26	y	101	BCR	C23-C22	-4.91	1.35	1.46
24	C	502	CLA	O2D-CGD	4.91	1.45	1.33
24	b	608	CLA	MG-ND	-4.91	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	411	PHO	OBD-CAD	4.90	1.28	1.22
24	c	504	CLA	CHD-C1D	4.90	1.48	1.38
24	A	1006	CLA	O2D-CGD	4.90	1.45	1.33
24	c	508	CLA	CHC-C1C	4.90	1.48	1.38
24	c	509	CLA	CHC-C1C	4.90	1.48	1.38
24	A	1005	CLA	CHC-C1C	4.90	1.48	1.38
24	b	616	CLA	CHC-C1C	4.90	1.48	1.38
38	F	101	HEM	FE-ND	4.90	2.10	1.94
25	D	404	PHO	OBD-CAD	4.90	1.28	1.22
26	A	1009	BCR	C15-C14	-4.90	1.28	1.43
26	a	413	BCR	C11-C10	-4.90	1.28	1.43
24	A	1008	CLA	O2D-CGD	4.89	1.45	1.33
24	A	1008	CLA	CHC-C1C	4.89	1.48	1.38
26	T	101	BCR	C23-C22	-4.89	1.35	1.46
26	B	618	BCR	C15-C14	-4.88	1.28	1.43
24	B	616	CLA	CHC-C1C	4.88	1.48	1.38
24	d	402	CLA	MG-NB	-4.88	1.96	2.05
26	K	102	BCR	C23-C22	-4.88	1.35	1.46
24	B	613	CLA	C3C-C2C	4.87	1.47	1.36
24	b	614	CLA	C3C-C2C	4.87	1.47	1.36
24	C	505	CLA	O2D-CGD	4.87	1.45	1.33
24	C	510	CLA	C3C-C2C	4.86	1.47	1.36
24	a	412	CLA	O2D-CGD	4.86	1.45	1.33
24	b	618	CLA	CHC-C1C	4.86	1.48	1.38
24	b	611	CLA	O2D-CGD	4.86	1.45	1.33
26	b	620	BCR	C15-C14	-4.86	1.28	1.43
38	f	101	HEM	FE-ND	4.85	2.09	1.94
24	C	501	CLA	CHD-C1D	4.84	1.47	1.38
24	C	505	CLA	CHD-C1D	4.84	1.47	1.38
26	t	101	BCR	C23-C22	-4.84	1.35	1.46
24	c	502	CLA	C3C-C2C	4.84	1.47	1.36
25	a	410	PHO	O2D-CGD	4.84	1.45	1.33
24	b	619	CLA	C3C-C2C	4.83	1.47	1.36
24	b	605	CLA	O2D-CGD	4.83	1.45	1.33
26	B	619	BCR	C23-C22	-4.83	1.35	1.46
24	B	602	CLA	CHC-C1C	4.82	1.48	1.38
24	b	619	CLA	CHC-C1C	4.82	1.48	1.38
24	B	607	CLA	CHD-C1D	4.82	1.47	1.38
26	b	620	BCR	C23-C22	-4.82	1.35	1.46
24	b	617	CLA	CHC-C1C	4.82	1.48	1.38
26	J	101	BCR	C23-C22	-4.82	1.35	1.46
24	D	405	CLA	CHD-C1D	4.82	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	O2D-CGD	4.82	1.45	1.33
24	B	604	CLA	CHC-C1C	4.81	1.48	1.38
24	B	608	CLA	CHD-C1D	4.81	1.47	1.38
25	A	1007	PHO	OBD-CAD	4.81	1.28	1.22
26	H	101	BCR	C23-C22	-4.80	1.35	1.46
24	D	403	CLA	C3C-C2C	4.80	1.47	1.36
24	D	405	CLA	O2D-CGD	4.80	1.45	1.33
24	c	510	CLA	CHC-C1C	4.80	1.48	1.38
24	D	402	CLA	C3C-C2C	4.80	1.47	1.36
24	b	605	CLA	CHD-C1D	4.80	1.47	1.38
24	c	505	CLA	O2D-CGD	4.80	1.45	1.33
24	b	616	CLA	O2D-CGD	4.80	1.45	1.33
38	v	201	HEM	FE-ND	4.79	2.09	1.94
24	A	1006	CLA	CHC-C1C	4.79	1.48	1.38
24	B	608	CLA	O2D-CGD	4.78	1.45	1.33
24	c	506	CLA	CHC-C1C	4.78	1.48	1.38
24	c	506	CLA	CHD-C1D	4.78	1.47	1.38
24	b	614	CLA	CHC-C1C	4.78	1.48	1.38
26	B	617	BCR	C23-C22	-4.77	1.35	1.46
24	b	607	CLA	CHC-C1C	4.77	1.48	1.38
26	K	101	BCR	C23-C22	-4.77	1.35	1.46
24	a	407	CLA	CHC-C1C	4.77	1.48	1.38
24	C	504	CLA	CHC-C1C	4.76	1.48	1.38
24	B	610	CLA	O2D-CGD	4.76	1.44	1.33
26	C	514	BCR	C23-C22	-4.76	1.35	1.46
24	D	403	CLA	MG-NA	4.76	2.17	2.06
26	h	101	BCR	C23-C22	-4.76	1.35	1.46
24	c	509	CLA	CHD-C1D	4.75	1.47	1.38
24	d	403	CLA	O2D-CGD	4.75	1.44	1.33
24	B	613	CLA	O2D-CGD	4.74	1.44	1.33
24	c	505	CLA	CHD-C1D	4.74	1.47	1.38
24	B	614	CLA	CHC-C1C	4.73	1.48	1.38
26	c	514	BCR	C23-C22	-4.72	1.35	1.46
25	A	1007	PHO	C3D-C4D	-4.72	1.34	1.41
26	b	622	BCR	C23-C22	-4.72	1.35	1.46
24	c	511	CLA	CHD-C1D	4.72	1.47	1.38
24	D	402	CLA	O2D-CGD	4.71	1.44	1.33
24	c	502	CLA	CHD-C1D	4.70	1.47	1.38
24	B	615	CLA	CHD-C1D	4.70	1.47	1.38
24	c	501	CLA	CHC-C1C	4.70	1.47	1.38
24	B	602	CLA	CHD-C1D	4.70	1.47	1.38
24	B	601	CLA	CHD-C1D	4.69	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	O2A-CGA	4.68	1.47	1.33
24	a	408	CLA	O2D-CGD	4.68	1.44	1.33
24	C	513	CLA	CHD-C1D	4.67	1.47	1.38
24	a	409	CLA	O2D-CGD	4.67	1.44	1.33
24	B	602	CLA	O2D-CGD	4.67	1.44	1.33
24	b	609	CLA	CHD-C1D	4.66	1.47	1.38
24	B	606	CLA	CHD-C1D	4.66	1.47	1.38
24	d	403	CLA	CHD-C1D	4.66	1.47	1.38
24	B	609	CLA	CHD-C1D	4.66	1.47	1.38
24	C	506	CLA	CHD-C1D	4.66	1.47	1.38
30	b	634	DMS	O-S	4.66	1.81	1.50
24	C	509	CLA	CHD-C1D	4.65	1.47	1.38
24	c	508	CLA	CHD-C1D	4.65	1.47	1.38
24	B	612	CLA	MG-ND	-4.65	1.96	2.05
30	D	416	DMS	O-S	4.65	1.80	1.50
24	B	604	CLA	CHD-C1D	4.64	1.47	1.38
38	F	101	HEM	FE-NC	4.64	2.10	1.95
30	D	417	DMS	O-S	4.63	1.80	1.50
24	D	403	CLA	O2D-CGD	4.63	1.44	1.33
26	B	618	BCR	C23-C22	-4.63	1.36	1.46
30	d	413	DMS	O-S	4.63	1.80	1.50
30	B	634	DMS	O-S	4.62	1.80	1.50
30	B	633	DMS	O-S	4.62	1.80	1.50
30	a	418	DMS	O-S	4.62	1.80	1.50
24	C	508	CLA	CHD-C1D	4.62	1.47	1.38
26	A	1009	BCR	C23-C22	-4.62	1.36	1.46
24	c	510	CLA	CHD-C1D	4.62	1.47	1.38
30	A	1014	DMS	O-S	4.62	1.80	1.50
30	V	203	DMS	O-S	4.62	1.80	1.50
24	a	408	CLA	MG-NC	4.61	2.17	2.06
30	O	301	DMS	O-S	4.60	1.80	1.50
24	b	610	CLA	CHC-C1C	4.60	1.47	1.38
30	c	527	DMS	O-S	4.60	1.80	1.50
24	B	603	CLA	CHC-C1C	4.60	1.47	1.38
24	B	607	CLA	O2D-CGD	4.60	1.44	1.33
30	O	302	DMS	O-S	4.59	1.80	1.50
30	V	205	DMS	O-S	4.59	1.80	1.50
30	b	629	DMS	O-S	4.59	1.80	1.50
30	b	635	DMS	O-S	4.59	1.80	1.50
24	B	615	CLA	CHC-C1C	4.59	1.47	1.38
30	C	525	DMS	O-S	4.58	1.80	1.50
30	b	633	DMS	O-S	4.58	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	CHD-C1D	4.58	1.47	1.38
24	b	615	CLA	CHB-C1B	4.57	1.49	1.39
24	C	510	CLA	CHC-C1C	4.57	1.47	1.38
30	c	528	DMS	O-S	4.57	1.80	1.50
24	b	610	CLA	CHB-C1B	4.57	1.49	1.39
24	B	607	CLA	CHC-C1C	4.57	1.47	1.38
24	C	504	CLA	CHD-C1D	4.57	1.47	1.38
30	C	526	DMS	O-S	4.57	1.80	1.50
30	B	632	DMS	O-S	4.56	1.80	1.50
24	C	509	CLA	CHC-C1C	4.56	1.47	1.38
30	C	527	DMS	O-S	4.56	1.80	1.50
30	d	414	DMS	O-S	4.56	1.80	1.50
24	A	1008	CLA	CHD-C1D	4.56	1.47	1.38
30	c	526	DMS	O-S	4.56	1.80	1.50
24	B	613	CLA	CHB-C1B	4.56	1.49	1.39
29	m	102	LMG	O8-C28	4.55	1.46	1.33
25	A	1007	PHO	O2D-CGD	4.55	1.44	1.33
25	a	410	PHO	C3D-C4D	-4.55	1.35	1.41
30	U	201	DMS	O-S	4.54	1.80	1.50
29	c	521	LMG	O7-C10	4.54	1.47	1.34
38	f	101	HEM	FE-NB	4.54	2.08	1.94
24	b	607	CLA	CHD-C1D	4.53	1.47	1.38
24	C	513	CLA	CHB-C1B	4.53	1.49	1.39
30	u	201	DMS	O-S	4.52	1.80	1.50
29	Z	101	LMG	O8-C28	4.52	1.46	1.33
24	C	511	CLA	CHD-C1D	4.52	1.47	1.38
24	a	412	CLA	CHD-C1D	4.52	1.47	1.38
24	c	510	CLA	CHB-C1B	4.52	1.49	1.39
24	C	508	CLA	MG-NB	4.52	2.14	2.05
29	c	520	LMG	O8-C28	4.51	1.46	1.33
24	d	402	CLA	O2A-CGA	4.51	1.46	1.33
30	v	202	DMS	O-S	4.51	1.80	1.50
38	V	201	HEM	FE-NB	4.51	2.08	1.94
24	B	615	CLA	CHB-C1B	4.51	1.49	1.39
24	D	403	CLA	MG-NC	4.51	2.17	2.06
29	B	622	LMG	O8-C28	4.51	1.46	1.33
24	a	409	CLA	MG-ND	-4.50	1.96	2.05
24	D	402	CLA	CHC-C1C	4.50	1.47	1.38
24	c	512	CLA	MG-ND	-4.50	1.96	2.05
24	B	605	CLA	CHD-C1D	4.49	1.47	1.38
24	b	619	CLA	O2A-CGA	4.48	1.46	1.33
24	c	512	CLA	CHD-C1D	4.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	O2A-CGA	4.48	1.46	1.33
24	a	408	CLA	CHB-C1B	4.48	1.49	1.39
24	C	511	CLA	CHB-C1B	4.48	1.49	1.39
24	b	606	CLA	CHD-C1D	4.48	1.47	1.38
24	b	618	CLA	CHB-C1B	4.47	1.49	1.39
24	B	614	CLA	CHB-C1B	4.47	1.49	1.39
24	c	507	CLA	CHB-C1B	4.47	1.49	1.39
24	C	503	CLA	CHD-C1D	4.47	1.47	1.38
30	c	529	DMS	O-S	4.46	1.79	1.50
24	B	612	CLA	CHB-C1B	4.46	1.49	1.39
24	a	408	CLA	CHC-C1C	4.46	1.47	1.38
29	C	518	LMG	O8-C28	4.46	1.46	1.33
24	b	611	CLA	CHD-C1D	4.46	1.47	1.38
24	C	505	CLA	CHB-C1B	4.45	1.49	1.39
24	C	509	CLA	O2A-CGA	4.45	1.46	1.33
24	C	512	CLA	CHB-C1B	4.45	1.49	1.39
30	c	524	DMS	O-S	4.45	1.79	1.50
29	c	521	LMG	O8-C28	4.45	1.46	1.33
34	d	406	LHG	O8-C23	4.45	1.46	1.33
24	C	507	CLA	CHD-C1D	4.45	1.47	1.38
24	C	512	CLA	CHD-C1D	4.44	1.47	1.38
24	c	507	CLA	CHD-C1D	4.44	1.47	1.38
28	D	408	SQD	O47-C7	4.44	1.46	1.34
24	C	509	CLA	C3D-C4D	-4.44	1.34	1.44
24	C	510	CLA	CHB-C1B	4.44	1.49	1.39
24	c	513	CLA	CHB-C1B	4.44	1.49	1.39
24	c	506	CLA	CHB-C1B	4.43	1.49	1.39
24	b	613	CLA	CHD-C1D	4.43	1.47	1.38
30	B	627	DMS	O-S	4.43	1.79	1.50
24	b	617	CLA	C3D-C4D	-4.43	1.34	1.44
24	c	505	CLA	CHB-C1B	4.43	1.49	1.39
24	c	501	CLA	CHB-C1B	4.43	1.49	1.39
28	f	102	SQD	O48-C23	4.43	1.46	1.33
29	C	519	LMG	O8-C28	4.42	1.46	1.33
24	B	607	CLA	C3D-C4D	-4.42	1.34	1.44
30	C	524	DMS	O-S	4.42	1.79	1.50
24	B	616	CLA	C3D-C4D	-4.42	1.34	1.44
24	b	616	CLA	CHD-C1D	4.42	1.47	1.38
24	C	507	CLA	CHB-C1B	4.42	1.49	1.39
24	c	513	CLA	C3D-C4D	-4.41	1.34	1.44
24	d	403	CLA	O2A-CGA	4.40	1.46	1.33
24	c	505	CLA	C3D-C4D	-4.40	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	MG-ND	-4.40	1.97	2.05
24	c	501	CLA	O2A-CGA	4.40	1.46	1.33
24	a	408	CLA	O2A-CGA	4.40	1.46	1.33
29	c	519	LMG	O7-C10	4.40	1.46	1.34
24	C	510	CLA	C3D-C4D	-4.40	1.34	1.44
24	b	618	CLA	CHD-C1D	4.40	1.47	1.38
24	B	603	CLA	CHD-C1D	4.40	1.47	1.38
24	A	1008	CLA	CHB-C1B	4.39	1.49	1.39
24	C	509	CLA	MG-NA	4.39	2.16	2.06
24	c	509	CLA	CHB-C1B	4.39	1.49	1.39
24	c	507	CLA	O2A-CGA	4.39	1.46	1.33
24	b	619	CLA	CHD-C1D	4.39	1.47	1.38
24	b	614	CLA	C3D-C4D	-4.38	1.34	1.44
24	B	609	CLA	CHB-C1B	4.38	1.49	1.39
24	b	607	CLA	CHB-C1B	4.38	1.49	1.39
24	b	604	CLA	CHB-C1B	4.38	1.49	1.39
24	C	503	CLA	CHB-C1B	4.38	1.49	1.39
34	e	101	LHG	O8-C23	4.38	1.46	1.33
24	C	507	CLA	CHC-C4B	4.38	1.49	1.39
24	b	616	CLA	CHB-C1B	4.38	1.49	1.39
24	D	405	CLA	CHB-C1B	4.37	1.49	1.39
28	a	401	SQD	O48-C23	4.37	1.46	1.33
30	B	626	DMS	O-S	4.37	1.79	1.50
24	c	510	CLA	C3D-C4D	-4.37	1.34	1.44
29	B	622	LMG	O7-C10	4.37	1.46	1.34
24	b	609	CLA	CHB-C1B	4.37	1.49	1.39
29	c	519	LMG	O8-C28	4.37	1.46	1.33
30	a	417	DMS	O-S	4.36	1.79	1.50
24	c	506	CLA	MG-NB	4.36	2.14	2.05
24	b	619	CLA	CHB-C1B	4.36	1.49	1.39
24	C	510	CLA	CHD-C1D	4.36	1.46	1.38
24	a	412	CLA	O2A-CGA	4.36	1.46	1.33
24	C	502	CLA	CHB-C1B	4.36	1.49	1.39
30	C	523	DMS	O-S	4.36	1.79	1.50
34	E	101	LHG	O8-C23	4.36	1.46	1.33
24	b	606	CLA	CHB-C1B	4.36	1.49	1.39
24	c	512	CLA	O2A-CGA	4.36	1.46	1.33
24	a	407	CLA	CHD-C1D	4.36	1.46	1.38
24	B	609	CLA	O2A-CGA	4.36	1.46	1.33
24	A	1005	CLA	CHD-C1D	4.36	1.46	1.38
24	C	513	CLA	CHC-C4B	4.36	1.49	1.39
24	c	503	CLA	MG-NB	-4.35	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	CHB-C1B	4.35	1.49	1.39
24	c	509	CLA	O2A-CGA	4.35	1.46	1.33
24	B	615	CLA	MG-NB	4.35	2.14	2.05
24	C	506	CLA	C3D-C4D	-4.35	1.34	1.44
24	b	613	CLA	CHB-C1B	4.35	1.49	1.39
28	c	518	SQD	O47-C7	4.35	1.46	1.34
24	C	513	CLA	C3D-C4D	-4.35	1.34	1.44
24	C	513	CLA	O2A-CGA	4.34	1.46	1.33
24	b	612	CLA	CHB-C1B	4.34	1.49	1.39
24	B	608	CLA	CHC-C1C	4.34	1.47	1.38
24	B	601	CLA	O2A-CGA	4.34	1.46	1.33
24	B	614	CLA	O2A-CGA	4.34	1.46	1.33
28	D	408	SQD	O48-C23	4.34	1.46	1.33
24	B	610	CLA	CHB-C1B	4.34	1.49	1.39
28	b	623[B]	SQD	O48-C23	4.34	1.46	1.33
24	B	604	CLA	CHB-C1B	4.34	1.49	1.39
29	C	519	LMG	O7-C10	4.34	1.46	1.34
24	b	617	CLA	CHD-C1D	4.34	1.46	1.38
24	c	501	CLA	C3D-C4D	-4.34	1.34	1.44
24	B	611	CLA	CHB-C1B	4.33	1.49	1.39
24	c	504	CLA	CHB-C1B	4.33	1.49	1.39
24	c	512	CLA	CHB-C1B	4.33	1.49	1.39
30	A	1013	DMS	O-S	4.33	1.78	1.50
24	c	503	CLA	CHB-C1B	4.33	1.49	1.39
34	e	101	LHG	O7-C7	4.33	1.46	1.34
29	A	1012	LMG	O8-C28	4.33	1.46	1.33
24	c	511	CLA	CHB-C1B	4.33	1.49	1.39
24	B	606	CLA	CHB-C1B	4.32	1.49	1.39
28	A	1016	SQD	O48-C23	4.32	1.45	1.33
24	B	606	CLA	C3D-C4D	-4.32	1.34	1.44
24	C	506	CLA	O2A-CGA	4.32	1.45	1.33
24	d	403	CLA	C3D-C4D	-4.32	1.34	1.44
24	C	511	CLA	MG-NB	4.32	2.14	2.05
24	B	610	CLA	CHD-C1D	4.32	1.46	1.38
29	a	415	LMG	O7-C10	4.32	1.46	1.34
28	A	1011	SQD	O48-C23	4.32	1.45	1.33
28	a	401	SQD	O47-C7	4.32	1.46	1.34
28	B	620[A]	SQD	O48-C23	4.32	1.45	1.33
24	c	508	CLA	CHB-C1B	4.32	1.49	1.39
24	c	511	CLA	CHC-C4B	4.31	1.49	1.39
24	c	512	CLA	CHC-C4B	4.31	1.49	1.39
24	B	613	CLA	CHD-C1D	4.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	C3D-C4D	-4.31	1.34	1.44
24	C	501	CLA	CHB-C1B	4.31	1.49	1.39
24	B	610	CLA	C3D-C4D	-4.31	1.34	1.44
29	C	518	LMG	O7-C10	4.31	1.46	1.34
24	b	605	CLA	O2A-CGA	4.31	1.45	1.33
24	c	503	CLA	CHC-C4B	4.31	1.49	1.39
24	c	512	CLA	C3D-C4D	-4.30	1.34	1.44
28	B	620[B]	SQD	O48-C23	4.30	1.45	1.33
24	C	504	CLA	CHB-C1B	4.30	1.49	1.39
28	c	518	SQD	O48-C23	4.30	1.45	1.33
24	b	608	CLA	MG-NA	4.30	2.16	2.06
28	A	1016	SQD	O47-C7	4.30	1.46	1.34
24	b	615	CLA	CHD-C1D	4.30	1.46	1.38
24	A	1006	CLA	C3D-C4D	-4.30	1.34	1.44
24	C	506	CLA	CHB-C1B	4.29	1.49	1.39
24	d	403	CLA	CHB-C1B	4.29	1.49	1.39
30	b	628	DMS	O-S	4.29	1.78	1.50
24	b	619	CLA	C3D-C4D	-4.29	1.34	1.44
24	A	1008	CLA	O2A-CGA	4.29	1.45	1.33
36	c	517	DGD	O1G-C1A	4.29	1.45	1.33
24	C	503	CLA	C3D-C4D	-4.29	1.34	1.44
24	C	512	CLA	CHC-C4B	4.29	1.49	1.39
28	b	623[A]	SQD	O48-C23	4.29	1.45	1.33
24	c	507	CLA	CHC-C4B	4.29	1.49	1.39
24	b	604	CLA	CHC-C4B	4.29	1.49	1.39
24	B	603	CLA	CHB-C1B	4.28	1.49	1.39
24	A	1006	CLA	CHB-C1B	4.28	1.49	1.39
24	B	614	CLA	C3D-C4D	-4.28	1.34	1.44
24	c	506	CLA	O2A-CGA	4.28	1.45	1.33
29	a	415	LMG	O8-C28	4.28	1.45	1.33
24	C	503	CLA	CHC-C4B	4.28	1.49	1.39
24	a	409	CLA	CHD-C1D	4.28	1.46	1.38
24	b	614	CLA	CHD-C1D	4.28	1.46	1.38
24	a	408	CLA	CHD-C1D	4.28	1.46	1.38
24	C	511	CLA	C3D-C4D	-4.27	1.34	1.44
24	B	601	CLA	C3D-C4D	-4.27	1.34	1.44
24	B	602	CLA	CHD-C4C	4.27	1.48	1.39
28	f	102	SQD	O47-C7	4.27	1.46	1.34
24	c	509	CLA	C3D-C4D	-4.27	1.34	1.44
24	c	504	CLA	C3D-C4D	-4.27	1.34	1.44
24	C	508	CLA	CHB-C1B	4.27	1.49	1.39
24	b	609	CLA	C3D-C4D	-4.26	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	601	CLA	CHB-C1B	4.26	1.49	1.39
24	c	513	CLA	O2A-CGA	4.26	1.45	1.33
24	b	610	CLA	C3D-C4D	-4.26	1.34	1.44
24	C	512	CLA	C3D-C4D	-4.26	1.34	1.44
24	D	405	CLA	O2A-CGA	4.26	1.45	1.33
24	b	611	CLA	CHB-C1B	4.26	1.49	1.39
24	C	502	CLA	CHD-C1D	4.26	1.46	1.38
24	C	505	CLA	C3D-C4D	-4.26	1.34	1.44
36	c	516	DGD	O1G-C1A	4.26	1.45	1.33
38	F	101	HEM	FE-NA	4.26	2.09	1.95
29	A	1012	LMG	O7-C10	4.26	1.46	1.34
25	D	404	PHO	O2A-CGA	4.26	1.45	1.33
25	a	411	PHO	O2A-CGA	4.26	1.45	1.33
24	D	403	CLA	O2A-CGA	4.25	1.45	1.33
24	B	608	CLA	C3D-C4D	-4.25	1.34	1.44
24	C	508	CLA	O2A-CGA	4.25	1.45	1.33
24	A	1005	CLA	O2A-CGA	4.25	1.45	1.33
24	b	608	CLA	C3D-C4D	-4.25	1.34	1.44
24	B	605	CLA	CHB-C1B	4.25	1.48	1.39
24	b	615	CLA	C3D-C4D	-4.25	1.34	1.44
24	B	616	CLA	O2A-CGA	4.25	1.45	1.33
24	c	513	CLA	CHD-C4C	4.25	1.48	1.39
29	c	520	LMG	O7-C10	4.24	1.46	1.34
29	d	409	LMG	O7-C10	4.24	1.46	1.34
24	c	509	CLA	MG-NC	4.24	2.16	2.06
24	b	617	CLA	CHB-C1B	4.24	1.48	1.39
24	b	606	CLA	C3D-C4D	-4.24	1.34	1.44
24	b	618	CLA	O2A-CGA	4.24	1.45	1.33
34	D	409	LHG	O8-C23	4.24	1.45	1.33
24	B	612	CLA	CHD-C1D	4.24	1.46	1.38
24	c	505	CLA	O2A-CGA	4.24	1.45	1.33
24	c	511	CLA	O2A-CGA	4.24	1.45	1.33
24	D	402	CLA	CHB-C1B	4.23	1.48	1.39
24	C	507	CLA	O2A-CGA	4.23	1.45	1.33
24	D	402	CLA	O2A-CGA	4.23	1.45	1.33
24	C	512	CLA	O2A-CGA	4.23	1.45	1.33
24	B	611	CLA	CHD-C1D	4.23	1.46	1.38
24	b	605	CLA	CHD-C4C	4.23	1.48	1.39
24	b	613	CLA	CHC-C4B	4.23	1.48	1.39
34	E	101	LHG	O7-C7	4.23	1.46	1.34
24	B	613	CLA	C3D-C4D	-4.23	1.34	1.44
24	D	405	CLA	C3D-C4D	-4.23	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	412	CLA	C3D-C4D	-4.23	1.34	1.44
29	d	409	LMG	O8-C28	4.22	1.45	1.33
24	B	614	CLA	CHD-C1D	4.22	1.46	1.38
24	B	614	CLA	CHC-C4B	4.22	1.48	1.39
24	b	609	CLA	O2A-CGA	4.22	1.45	1.33
24	b	604	CLA	C3D-C4D	-4.21	1.34	1.44
24	B	608	CLA	CHB-C1B	4.21	1.48	1.39
24	B	616	CLA	CHD-C1D	4.21	1.46	1.38
24	a	409	CLA	CHB-C1B	4.21	1.48	1.39
36	c	515	DGD	O1G-C1A	4.21	1.45	1.33
28	B	620[A]	SQD	O47-C7	4.21	1.46	1.34
28	b	623[A]	SQD	O47-C7	4.21	1.46	1.34
29	m	102	LMG	O7-C10	4.20	1.46	1.34
24	C	508	CLA	C3D-C4D	-4.20	1.34	1.44
24	c	511	CLA	C3D-C4D	-4.20	1.34	1.44
24	B	603	CLA	C3D-C4D	-4.20	1.34	1.44
25	D	404	PHO	C3D-C2D	4.20	1.46	1.39
34	d	408	LHG	O7-C7	4.20	1.46	1.34
24	b	611	CLA	CHC-C4B	4.20	1.48	1.39
36	h	102	DGD	O1G-C1A	4.20	1.45	1.33
24	C	505	CLA	O2A-CGA	4.20	1.45	1.33
24	b	614	CLA	CHB-C1B	4.19	1.48	1.39
24	D	403	CLA	CHC-C1C	4.19	1.46	1.38
24	c	503	CLA	CHD-C4C	4.19	1.48	1.39
24	c	502	CLA	CHB-C1B	4.19	1.48	1.39
24	C	507	CLA	C3D-C4D	-4.19	1.34	1.44
24	B	609	CLA	MG-NB	4.19	2.14	2.05
34	D	411	LHG	O8-C23	4.19	1.45	1.33
24	b	612	CLA	O2A-CGA	4.19	1.45	1.33
34	d	408	LHG	O8-C23	4.18	1.45	1.33
25	a	410	PHO	C3D-C2D	4.18	1.46	1.39
24	c	510	CLA	O2A-CGA	4.18	1.45	1.33
24	B	602	CLA	CHB-C1B	4.18	1.48	1.39
24	B	616	CLA	CHB-C1B	4.18	1.48	1.39
24	B	605	CLA	C3D-C4D	-4.18	1.34	1.44
24	c	501	CLA	CHC-C4B	4.18	1.48	1.39
24	B	613	CLA	O2A-CGA	4.18	1.45	1.33
24	C	511	CLA	CHC-C4B	4.18	1.48	1.39
24	c	508	CLA	CHC-C4B	4.18	1.48	1.39
29	Z	101	LMG	O7-C10	4.18	1.46	1.34
34	B	621	LHG	O8-C23	4.17	1.45	1.33
24	B	605	CLA	CHC-C4B	4.17	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	CHD-C4C	4.17	1.48	1.39
24	d	402	CLA	C3D-C4D	-4.17	1.34	1.44
24	b	617	CLA	CHC-C4B	4.17	1.48	1.39
36	h	102	DGD	O2G-C1B	4.17	1.46	1.34
24	B	609	CLA	C3D-C4D	-4.17	1.34	1.44
24	C	501	CLA	CHD-C4C	4.17	1.48	1.39
28	B	620[B]	SQD	O47-C7	4.17	1.46	1.34
24	A	1008	CLA	C3D-C4D	-4.17	1.34	1.44
34	b	624	LHG	O8-C23	4.17	1.45	1.33
24	C	501	CLA	C3D-C4D	-4.16	1.34	1.44
24	c	503	CLA	O2A-CGA	4.16	1.45	1.33
24	C	501	CLA	O2A-CGA	4.16	1.45	1.33
24	c	513	CLA	CHC-C4B	4.16	1.48	1.39
24	c	503	CLA	C3D-C4D	-4.16	1.34	1.44
24	a	409	CLA	O2A-CGA	4.16	1.45	1.33
24	c	508	CLA	C3D-C4D	-4.16	1.34	1.44
24	B	612	CLA	C3D-C4D	-4.16	1.34	1.44
24	b	614	CLA	O2A-CGA	4.16	1.45	1.33
28	b	623[B]	SQD	O47-C7	4.16	1.46	1.34
24	c	508	CLA	O2A-CGA	4.15	1.45	1.33
24	b	613	CLA	C3D-C4D	-4.15	1.34	1.44
24	B	611	CLA	O2A-CGA	4.15	1.45	1.33
24	b	617	CLA	O2A-CGA	4.15	1.45	1.33
24	b	612	CLA	MG-NB	4.15	2.14	2.05
24	a	409	CLA	C3D-C4D	-4.15	1.34	1.44
24	b	611	CLA	C3D-C4D	-4.15	1.34	1.44
24	b	616	CLA	C3D-C4D	-4.15	1.34	1.44
24	C	510	CLA	O2A-CGA	4.15	1.45	1.33
25	a	411	PHO	C3D-C2D	4.15	1.46	1.39
24	c	502	CLA	C3D-C4D	-4.15	1.34	1.44
24	B	610	CLA	CHC-C4B	4.15	1.48	1.39
24	a	407	CLA	C3D-C4D	-4.14	1.34	1.44
24	C	511	CLA	O2A-CGA	4.14	1.45	1.33
24	b	618	CLA	C3D-C4D	-4.14	1.34	1.44
38	f	101	HEM	FE-NA	4.14	2.08	1.95
24	D	403	CLA	CHB-C1B	4.14	1.48	1.39
24	c	510	CLA	CHC-C4B	4.13	1.48	1.39
24	B	615	CLA	C3D-C4D	-4.13	1.34	1.44
24	b	604	CLA	CHD-C4C	4.13	1.48	1.39
24	A	1005	CLA	CHB-C1B	4.13	1.48	1.39
24	b	612	CLA	C3D-C4D	-4.13	1.34	1.44
24	B	611	CLA	C3D-C4D	-4.13	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	517	DGD	O2G-C1B	4.13	1.45	1.34
24	a	412	CLA	CHB-C1B	4.12	1.48	1.39
24	c	509	CLA	CHD-C4C	4.12	1.48	1.39
24	b	612	CLA	CHD-C4C	4.11	1.48	1.39
24	a	407	CLA	CHB-C1B	4.11	1.48	1.39
24	b	607	CLA	O2A-CGA	4.11	1.45	1.33
28	A	1011	SQD	O47-C7	4.11	1.45	1.34
24	b	608	CLA	CHB-C1B	4.11	1.48	1.39
24	c	507	CLA	C3D-C4D	-4.11	1.34	1.44
24	b	611	CLA	O2A-CGA	4.11	1.45	1.33
24	c	504	CLA	O2A-CGA	4.11	1.45	1.33
24	C	502	CLA	O2A-CGA	4.11	1.45	1.33
24	d	403	CLA	CHC-C4B	4.10	1.48	1.39
24	b	615	CLA	OBD-CAD	4.10	1.29	1.22
24	C	503	CLA	CHD-C4C	4.10	1.48	1.39
24	D	405	CLA	CHC-C4B	4.10	1.48	1.39
36	c	516	DGD	O2G-C1B	4.10	1.45	1.34
24	C	501	CLA	CHC-C4B	4.10	1.48	1.39
24	b	606	CLA	CHC-C4B	4.09	1.48	1.39
24	C	504	CLA	O2A-CGA	4.09	1.45	1.33
24	c	506	CLA	CHD-C4C	4.09	1.48	1.39
24	b	615	CLA	O2A-CGA	4.09	1.45	1.33
24	B	615	CLA	O2A-CGA	4.09	1.45	1.33
24	b	613	CLA	O2A-CGA	4.09	1.45	1.33
24	B	607	CLA	CHB-C1B	4.09	1.48	1.39
24	c	504	CLA	CHC-C4B	4.09	1.48	1.39
25	a	410	PHO	O2A-CGA	4.09	1.45	1.33
24	B	601	CLA	CHC-C4B	4.08	1.48	1.39
24	B	601	CLA	CHD-C4C	4.08	1.48	1.39
24	A	1006	CLA	CHD-C1D	4.08	1.46	1.38
24	A	1006	CLA	O2A-CGA	4.08	1.45	1.33
24	c	505	CLA	CHC-C4B	4.08	1.48	1.39
24	c	504	CLA	CHD-C4C	4.08	1.48	1.39
24	d	402	CLA	CHB-C1B	4.08	1.48	1.39
24	C	504	CLA	C3D-C4D	-4.08	1.35	1.44
24	b	605	CLA	C3D-C4D	-4.07	1.35	1.44
24	C	503	CLA	O2A-CGA	4.07	1.45	1.33
24	B	608	CLA	MG-NB	-4.07	1.97	2.05
24	b	610	CLA	O2A-CGA	4.07	1.45	1.33
24	B	602	CLA	CHC-C4B	4.06	1.48	1.39
34	D	411	LHG	O7-C7	4.06	1.45	1.34
24	c	502	CLA	O2A-CGA	4.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	O2A-CGA	4.06	1.45	1.33
24	B	611	CLA	CHC-C4B	4.06	1.48	1.39
36	c	517	DGD	O2G-C1B	4.05	1.45	1.34
24	B	606	CLA	CHC-C4B	4.05	1.48	1.39
24	B	609	CLA	CHC-C4B	4.05	1.48	1.39
24	C	504	CLA	CHD-C4C	4.05	1.48	1.39
38	V	201	HEM	FE-ND	4.05	2.07	1.94
34	B	621	LHG	O7-C7	4.05	1.45	1.34
24	D	405	CLA	CHD-C4C	4.05	1.48	1.39
36	C	517	DGD	O1G-C1A	4.04	1.45	1.33
24	b	609	CLA	CHC-C4B	4.04	1.48	1.39
24	b	605	CLA	CHC-C4B	4.04	1.48	1.39
24	b	608	CLA	O2A-CGA	4.04	1.45	1.33
24	b	608	CLA	CHD-C1D	4.03	1.46	1.38
24	b	607	CLA	CHC-C4B	4.03	1.48	1.39
36	C	516	DGD	O1G-C1A	4.03	1.45	1.33
24	C	508	CLA	CHC-C4B	4.03	1.48	1.39
24	c	503	CLA	MG-ND	4.02	2.13	2.05
24	b	612	CLA	CHC-C4B	4.02	1.48	1.39
24	c	505	CLA	CHD-C4C	4.02	1.48	1.39
24	C	506	CLA	CHC-C4B	4.02	1.48	1.39
24	b	614	CLA	CHC-C4B	4.01	1.48	1.39
36	C	515	DGD	O2G-C1B	4.01	1.45	1.34
29	D	412	LMG	O7-C10	4.01	1.45	1.34
24	B	616	CLA	CHC-C4B	4.01	1.48	1.39
24	c	502	CLA	CHC-C4B	4.01	1.48	1.39
24	A	1005	CLA	C3D-C4D	-4.01	1.35	1.44
24	B	604	CLA	C3D-C4D	-4.01	1.35	1.44
36	C	516	DGD	O2G-C1B	4.00	1.45	1.34
24	a	409	CLA	CHD-C4C	4.00	1.48	1.39
24	c	501	CLA	CHD-C4C	4.00	1.48	1.39
29	D	412	LMG	O8-C28	4.00	1.45	1.33
24	b	609	CLA	CHD-C4C	4.00	1.48	1.39
36	H	102	DGD	O1G-C1A	3.99	1.45	1.33
36	C	515	DGD	O1G-C1A	3.99	1.45	1.33
25	A	1007	PHO	O2A-CGA	3.99	1.45	1.33
24	A	1008	CLA	CHC-C4B	3.99	1.48	1.39
24	c	506	CLA	CHC-C4B	3.99	1.48	1.39
24	c	502	CLA	CHD-C4C	3.98	1.48	1.39
24	B	606	CLA	O2A-CGA	3.98	1.44	1.33
24	b	618	CLA	CHD-C4C	3.97	1.48	1.39
36	c	515	DGD	O2G-C1B	3.97	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	CLA	CHC-C4B	3.96	1.48	1.39
24	b	607	CLA	C3D-C4D	-3.96	1.35	1.44
24	b	618	CLA	CHC-C4B	3.96	1.48	1.39
24	b	619	CLA	CHC-C4B	3.96	1.48	1.39
24	D	402	CLA	OBD-CAD	3.96	1.29	1.22
24	b	616	CLA	O2A-CGA	3.96	1.44	1.33
24	c	508	CLA	CHD-C4C	3.96	1.48	1.39
24	B	607	CLA	O2A-CGA	3.95	1.44	1.33
24	B	604	CLA	MG-NC	3.95	2.15	2.06
24	b	616	CLA	CHC-C4B	3.95	1.48	1.39
24	B	604	CLA	O2A-CGA	3.95	1.44	1.33
34	d	407	LHG	O8-C23	3.95	1.44	1.33
24	D	403	CLA	CHD-C4C	3.95	1.48	1.39
24	B	612	CLA	O2A-CGA	3.95	1.44	1.33
24	b	615	CLA	CHC-C4B	3.95	1.48	1.39
24	c	509	CLA	OBD-CAD	3.95	1.29	1.22
24	d	403	CLA	CHD-C4C	3.94	1.48	1.39
24	C	509	CLA	CHB-C1B	3.94	1.48	1.39
24	b	616	CLA	CHD-C4C	3.94	1.48	1.39
24	c	502	CLA	OBD-CAD	3.94	1.29	1.22
24	B	608	CLA	CHD-C4C	3.94	1.48	1.39
24	A	1005	CLA	CHD-C4C	3.93	1.48	1.39
24	A	1005	CLA	OBD-CAD	3.93	1.29	1.22
24	B	610	CLA	O2A-CGA	3.93	1.44	1.33
24	C	513	CLA	CHD-C4C	3.93	1.48	1.39
24	C	506	CLA	CHD-C4C	3.93	1.48	1.39
24	D	403	CLA	C3D-C4D	-3.93	1.35	1.44
25	A	1007	PHO	C3D-C2D	3.92	1.46	1.39
24	a	407	CLA	OBD-CAD	3.92	1.29	1.22
24	B	607	CLA	CHC-C4B	3.92	1.48	1.39
24	a	408	CLA	C3D-C4D	-3.92	1.35	1.44
24	c	512	CLA	CHD-C4C	3.92	1.48	1.39
24	b	606	CLA	O2A-CGA	3.92	1.44	1.33
24	C	505	CLA	CHC-C4B	3.91	1.48	1.39
24	B	612	CLA	CHC-C4B	3.91	1.48	1.39
24	B	611	CLA	OBD-CAD	3.91	1.29	1.22
24	B	602	CLA	C3D-C4D	-3.91	1.35	1.44
24	d	402	CLA	CHD-C1D	3.91	1.46	1.38
24	c	511	CLA	CHD-C4C	3.91	1.48	1.39
24	B	609	CLA	CHD-C4C	3.91	1.48	1.39
24	B	604	CLA	CHD-C4C	3.90	1.48	1.39
24	c	510	CLA	CHD-C4C	3.90	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C3D-C4D	-3.90	1.35	1.44
24	C	509	CLA	CHD-C4C	3.89	1.48	1.39
24	b	613	CLA	CHD-C4C	3.89	1.48	1.39
24	b	611	CLA	CHD-C4C	3.89	1.48	1.39
24	B	610	CLA	MG-NA	3.89	2.15	2.06
24	c	509	CLA	CHC-C4B	3.89	1.48	1.39
24	B	607	CLA	CHD-C4C	3.88	1.48	1.39
24	B	613	CLA	CHC-C4B	3.88	1.48	1.39
24	b	608	CLA	CHD-C4C	3.88	1.48	1.39
24	C	507	CLA	CHD-C4C	3.88	1.48	1.39
34	D	410	LHG	O8-C23	3.88	1.44	1.33
24	b	607	CLA	CHD-C4C	3.88	1.48	1.39
24	B	608	CLA	CHC-C4B	3.87	1.48	1.39
24	C	511	CLA	CHD-C4C	3.87	1.48	1.39
24	B	605	CLA	O2A-CGA	3.86	1.44	1.33
24	D	402	CLA	CHC-C4B	3.86	1.48	1.39
26	D	406	BCR	C21-C22	-3.86	1.26	1.35
24	B	603	CLA	CHD-C4C	3.86	1.48	1.39
24	a	407	CLA	O2A-CGA	3.86	1.44	1.33
24	C	504	CLA	CHC-C4B	3.85	1.48	1.39
24	C	502	CLA	C3D-C4D	-3.85	1.35	1.44
24	A	1006	CLA	CHC-C4B	3.85	1.48	1.39
24	b	615	CLA	CHD-C4C	3.85	1.48	1.39
24	C	502	CLA	CHC-C4B	3.85	1.48	1.39
24	c	512	CLA	MG-NB	3.84	2.13	2.05
24	B	603	CLA	CHC-C4B	3.84	1.48	1.39
36	H	102	DGD	O2G-C1B	3.84	1.45	1.34
24	b	609	CLA	MG-ND	3.84	2.13	2.05
24	B	615	CLA	CHD-C4C	3.84	1.47	1.39
24	b	606	CLA	CHD-C4C	3.83	1.47	1.39
26	K	102	BCR	C21-C22	-3.82	1.27	1.35
24	b	610	CLA	CHC-C4B	3.82	1.48	1.39
24	a	408	CLA	CHD-C4C	3.82	1.47	1.39
34	b	624	LHG	O7-C7	3.82	1.45	1.34
26	d	404	BCR	C21-C22	-3.81	1.27	1.35
34	d	406	LHG	O7-C7	3.81	1.45	1.34
24	B	604	CLA	CHC-C4B	3.81	1.48	1.39
24	d	402	CLA	CHC-C4B	3.81	1.48	1.39
24	C	507	CLA	OBD-CAD	3.81	1.29	1.22
24	d	402	CLA	CHD-C4C	3.81	1.47	1.39
24	b	610	CLA	CHD-C4C	3.80	1.47	1.39
24	a	407	CLA	CHC-C4B	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	OBD-CAD	3.80	1.29	1.22
24	C	510	CLA	CHC-C4B	3.80	1.47	1.39
26	b	622	BCR	C21-C22	-3.80	1.27	1.35
38	F	101	HEM	FE-NB	3.80	2.06	1.94
24	C	510	CLA	OBD-CAD	3.80	1.29	1.22
24	C	510	CLA	MG-NC	3.79	2.15	2.06
24	B	614	CLA	OBD-CAD	3.79	1.29	1.22
24	C	513	CLA	MG-ND	3.79	2.13	2.05
24	A	1006	CLA	CHD-C4C	3.78	1.47	1.39
24	b	608	CLA	CHC-C4B	3.78	1.47	1.39
24	C	510	CLA	CHD-C4C	3.78	1.47	1.39
24	B	603	CLA	O2A-CGA	3.78	1.44	1.33
24	C	509	CLA	CHC-C4B	3.77	1.47	1.39
24	B	606	CLA	CHD-C4C	3.77	1.47	1.39
24	D	402	CLA	CHD-C1D	3.77	1.45	1.38
26	k	102	BCR	C21-C22	-3.76	1.27	1.35
24	C	512	CLA	CHD-C4C	3.76	1.47	1.39
24	c	510	CLA	OBD-CAD	3.76	1.29	1.22
34	d	407	LHG	O7-C7	3.76	1.44	1.34
24	b	609	CLA	OBD-CAD	3.76	1.29	1.22
24	B	605	CLA	CHD-C4C	3.76	1.47	1.39
24	B	604	CLA	OBD-CAD	3.76	1.29	1.22
24	D	403	CLA	MG-NB	3.75	2.13	2.05
24	C	502	CLA	MG-ND	-3.75	1.98	2.05
24	b	616	CLA	OBD-CAD	3.75	1.28	1.22
24	b	604	CLA	OBD-CAD	3.75	1.28	1.22
24	B	610	CLA	CHD-C4C	3.74	1.47	1.39
24	D	403	CLA	CHD-C1D	3.74	1.45	1.38
24	c	508	CLA	OBD-CAD	3.74	1.28	1.22
26	t	101	BCR	C17-C18	-3.74	1.27	1.35
24	C	508	CLA	CHD-C4C	3.73	1.47	1.39
24	B	612	CLA	OBD-CAD	3.73	1.28	1.22
26	c	514	BCR	C17-C18	-3.73	1.27	1.35
24	b	605	CLA	OBD-CAD	3.73	1.28	1.22
24	c	505	CLA	OBD-CAD	3.73	1.28	1.22
24	c	511	CLA	OBD-CAD	3.73	1.28	1.22
26	d	404	BCR	C17-C18	-3.73	1.27	1.35
24	B	602	CLA	OBD-CAD	3.73	1.28	1.22
24	A	1008	CLA	CHD-C4C	3.73	1.47	1.39
24	b	616	CLA	MG-ND	-3.73	1.98	2.05
24	B	615	CLA	OBD-CAD	3.72	1.28	1.22
24	b	612	CLA	OBD-CAD	3.72	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	CHD-C4C	3.72	1.47	1.39
26	T	101	BCR	C17-C18	-3.71	1.27	1.35
26	K	102	BCR	C17-C18	-3.71	1.27	1.35
26	b	621	BCR	C21-C22	-3.71	1.27	1.35
24	c	507	CLA	OBD-CAD	3.71	1.28	1.22
26	A	1009	BCR	C21-C22	-3.71	1.27	1.35
26	C	514	BCR	C21-C22	-3.71	1.27	1.35
24	a	412	CLA	CHD-C4C	3.71	1.47	1.39
24	B	601	CLA	OBD-CAD	3.70	1.28	1.22
34	D	410	LHG	O7-C7	3.70	1.44	1.34
24	c	513	CLA	OBD-CAD	3.70	1.28	1.22
24	B	612	CLA	CHD-C4C	3.70	1.47	1.39
24	a	408	CLA	OBD-CAD	3.70	1.28	1.22
24	B	609	CLA	MG-ND	-3.70	1.98	2.05
24	c	507	CLA	CHD-C4C	3.69	1.47	1.39
24	C	509	CLA	OBD-CAD	3.69	1.28	1.22
26	y	101	BCR	C21-C22	-3.69	1.27	1.35
24	D	403	CLA	OBD-CAD	3.68	1.28	1.22
24	A	1006	CLA	MG-NC	3.68	2.15	2.06
24	C	503	CLA	OBD-CAD	3.68	1.28	1.22
24	d	403	CLA	MG-NA	3.68	2.15	2.06
24	c	506	CLA	OBD-CAD	3.67	1.28	1.22
26	y	101	BCR	C17-C18	-3.67	1.27	1.35
24	b	607	CLA	OBD-CAD	3.67	1.28	1.22
24	a	407	CLA	CHD-C4C	3.67	1.47	1.39
24	a	407	CLA	MG-NB	3.67	2.13	2.05
24	d	403	CLA	OBD-CAD	3.67	1.28	1.22
24	B	605	CLA	MG-NB	-3.67	1.98	2.05
34	D	409	LHG	O7-C7	3.66	1.44	1.34
26	B	617	BCR	C21-C22	-3.66	1.27	1.35
24	C	511	CLA	OBD-CAD	3.66	1.28	1.22
24	C	513	CLA	OBD-CAD	3.66	1.28	1.22
26	T	101	BCR	C21-C22	-3.65	1.27	1.35
26	J	101	BCR	C17-C18	-3.65	1.27	1.35
24	b	619	CLA	CHD-C4C	3.65	1.47	1.39
26	h	101	BCR	C21-C22	-3.65	1.27	1.35
26	b	622	BCR	C17-C18	-3.65	1.27	1.35
26	H	101	BCR	C21-C22	-3.65	1.27	1.35
24	b	614	CLA	CHD-C4C	3.65	1.47	1.39
26	C	514	BCR	C17-C18	-3.65	1.27	1.35
25	a	411	PHO	C3A-C2A	-3.64	1.51	1.54
24	B	611	CLA	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	CLA	CHC-C4B	3.64	1.47	1.39
24	C	508	CLA	OBD-CAD	3.64	1.28	1.22
24	c	512	CLA	OBD-CAD	3.64	1.28	1.22
24	B	615	CLA	CHC-C4B	3.63	1.47	1.39
24	b	618	CLA	OBD-CAD	3.63	1.28	1.22
24	A	1008	CLA	OBD-CAD	3.63	1.28	1.22
26	J	101	BCR	C21-C22	-3.63	1.27	1.35
24	A	1005	CLA	CHC-C4B	3.63	1.47	1.39
24	B	609	CLA	OBD-CAD	3.63	1.28	1.22
24	C	506	CLA	OBD-CAD	3.62	1.28	1.22
24	c	507	CLA	MG-ND	-3.61	1.98	2.05
26	K	101	BCR	C21-C22	-3.61	1.27	1.35
24	b	617	CLA	CHD-C4C	3.61	1.47	1.39
24	a	412	CLA	CHC-C4B	3.61	1.47	1.39
26	k	102	BCR	C17-C18	-3.61	1.27	1.35
24	b	613	CLA	OBD-CAD	3.60	1.28	1.22
24	a	412	CLA	OBD-CAD	3.60	1.28	1.22
26	h	101	BCR	C17-C18	-3.60	1.27	1.35
26	b	621	BCR	C17-C18	-3.59	1.27	1.35
26	k	101	BCR	C17-C18	-3.59	1.27	1.35
24	B	613	CLA	OBD-CAD	3.59	1.28	1.22
24	D	402	CLA	CHD-C4C	3.59	1.47	1.39
24	c	504	CLA	OBD-CAD	3.59	1.28	1.22
26	B	619	BCR	C21-C22	-3.58	1.27	1.35
24	B	614	CLA	CHD-C4C	3.57	1.47	1.39
26	k	101	BCR	C21-C22	-3.57	1.27	1.35
24	C	505	CLA	OBD-CAD	3.56	1.28	1.22
24	D	405	CLA	OBD-CAD	3.56	1.28	1.22
26	t	101	BCR	C21-C22	-3.56	1.27	1.35
26	B	618	BCR	C21-C22	-3.55	1.27	1.35
26	B	619	BCR	C17-C18	-3.54	1.27	1.35
26	A	1009	BCR	C17-C18	-3.54	1.27	1.35
26	b	620	BCR	C21-C22	-3.54	1.27	1.35
24	B	613	CLA	CHD-C4C	3.54	1.47	1.39
26	a	413	BCR	C17-C18	-3.54	1.27	1.35
26	B	617	BCR	C17-C18	-3.53	1.27	1.35
26	c	514	BCR	C21-C22	-3.53	1.27	1.35
24	c	510	CLA	MG-ND	-3.52	1.98	2.05
24	C	501	CLA	OBD-CAD	3.52	1.28	1.22
24	C	506	CLA	MG-NB	-3.52	1.98	2.05
24	c	503	CLA	OBD-CAD	3.51	1.28	1.22
24	b	619	CLA	OBD-CAD	3.51	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H	101	BCR	C17-C18	-3.51	1.27	1.35
24	C	502	CLA	CHD-C4C	3.51	1.47	1.39
26	b	620	BCR	C17-C18	-3.50	1.27	1.35
24	b	606	CLA	OBD-CAD	3.49	1.28	1.22
24	b	618	CLA	MG-ND	3.47	2.12	2.05
26	B	618	BCR	C17-C18	-3.47	1.27	1.35
24	b	611	CLA	OBD-CAD	3.47	1.28	1.22
24	A	1005	CLA	MG-NA	3.46	2.14	2.06
24	c	501	CLA	OBD-CAD	3.45	1.28	1.22
35	o	301	HTG	C1'-S1	-3.44	1.76	1.81
35	b	630	HTG	C1'-S1	-3.43	1.76	1.81
26	D	406	BCR	C17-C18	-3.43	1.27	1.35
24	B	603	CLA	OBD-CAD	3.43	1.28	1.22
26	K	101	BCR	C17-C18	-3.43	1.27	1.35
24	C	504	CLA	OBD-CAD	3.43	1.28	1.22
24	B	610	CLA	OBD-CAD	3.42	1.28	1.22
24	B	603	CLA	MG-ND	3.42	2.12	2.05
24	D	403	CLA	CHC-C4B	3.40	1.47	1.39
24	b	617	CLA	OBD-CAD	3.40	1.28	1.22
24	A	1006	CLA	OBD-CAD	3.40	1.28	1.22
26	a	413	BCR	C21-C22	-3.39	1.28	1.35
24	C	512	CLA	OBD-CAD	3.38	1.28	1.22
24	B	606	CLA	OBD-CAD	3.38	1.28	1.22
35	d	410	HTG	C1'-S1	-3.37	1.76	1.81
24	B	616	CLA	OBD-CAD	3.36	1.28	1.22
24	B	608	CLA	OBD-CAD	3.36	1.28	1.22
24	b	608	CLA	OBD-CAD	3.35	1.28	1.22
35	b	626	HTG	C1'-S1	-3.34	1.76	1.81
24	B	613	CLA	MG-ND	-3.33	1.99	2.05
35	D	413	HTG	C1'-S1	-3.33	1.76	1.81
24	D	402	CLA	C1B-C2B	3.32	1.50	1.43
24	d	402	CLA	OBD-CAD	3.30	1.28	1.22
35	B	628	HTG	C1'-S1	-3.30	1.76	1.81
38	f	101	HEM	FE-NC	3.30	2.06	1.95
35	c	525	HTG	C1'-S1	-3.29	1.76	1.81
35	C	521	HTG	C1'-S1	-3.27	1.76	1.81
35	b	601	HTG	C1'-S1	-3.26	1.76	1.81
38	v	201	HEM	FE-NA	3.26	2.05	1.95
35	B	629	HTG	C1'-S1	-3.24	1.76	1.81
24	b	614	CLA	OBD-CAD	3.24	1.28	1.22
24	B	605	CLA	OBD-CAD	3.23	1.28	1.22
38	v	201	HEM	CAC-C3C	3.22	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	624	HTG	C1'-S1	-3.21	1.76	1.81
24	b	615	CLA	C1B-C2B	3.20	1.50	1.43
38	v	201	HEM	FE-NC	3.20	2.05	1.95
24	c	502	CLA	MG-ND	-3.19	1.99	2.05
24	B	615	CLA	MG-NC	3.19	2.13	2.06
35	D	419	HTG	C1'-S1	-3.19	1.76	1.81
24	B	611	CLA	MG-NC	3.19	2.13	2.06
24	B	615	CLA	C1B-C2B	3.19	1.50	1.43
24	D	403	CLA	C1B-C2B	3.18	1.50	1.43
25	a	410	PHO	C3A-C2A	-3.17	1.52	1.54
35	d	416	HTG	C1'-S1	-3.17	1.77	1.81
24	B	607	CLA	OBD-CAD	3.17	1.27	1.22
24	b	608	CLA	C1B-C2B	3.17	1.50	1.43
35	b	602	HTG	C1'-S1	-3.15	1.77	1.81
24	a	408	CLA	C1B-C2B	3.14	1.50	1.43
38	f	101	HEM	CAB-C3B	3.13	1.55	1.47
38	F	101	HEM	CAB-C3B	3.13	1.55	1.47
24	B	604	CLA	C1B-C2B	3.12	1.50	1.43
24	a	408	CLA	MG-ND	-3.12	1.99	2.05
24	C	504	CLA	MG-NB	3.12	2.12	2.05
24	B	607	CLA	MG-ND	-3.11	1.99	2.05
35	c	522	HTG	C1'-S1	-3.11	1.77	1.81
24	a	412	CLA	MG-NB	-3.11	1.99	2.05
24	b	612	CLA	MG-ND	-3.11	1.99	2.05
24	b	610	CLA	C3D-C2D	3.11	1.47	1.39
35	V	202	HTG	C1'-S1	-3.10	1.77	1.81
38	V	201	HEM	CAB-C3B	3.08	1.55	1.47
25	D	404	PHO	C3A-C2A	-3.08	1.52	1.54
24	D	403	CLA	C3D-C2D	3.07	1.47	1.39
24	b	618	CLA	C1B-C2B	3.06	1.50	1.43
24	C	511	CLA	C3D-C2D	3.06	1.47	1.39
24	C	505	CLA	C1B-C2B	3.06	1.50	1.43
24	B	602	CLA	C3D-C2D	3.06	1.47	1.39
35	C	522	HTG	C1'-S1	-3.04	1.77	1.81
38	V	201	HEM	CAC-C3C	3.03	1.55	1.47
24	c	511	CLA	C4D-CHA	3.03	1.48	1.38
24	a	409	CLA	C3D-C2D	3.03	1.47	1.39
24	C	511	CLA	C1B-C2B	3.02	1.50	1.43
24	C	513	CLA	MG-NB	-3.02	1.99	2.05
24	C	511	CLA	C4D-CHA	3.02	1.48	1.38
24	c	511	CLA	MG-ND	3.01	2.11	2.05
24	b	619	CLA	C1B-C2B	3.01	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C1B-C2B	3.00	1.50	1.43
24	b	610	CLA	OBD-CAD	3.00	1.27	1.22
24	C	503	CLA	C4D-CHA	3.00	1.48	1.38
24	A	1006	CLA	C3D-C2D	2.99	1.47	1.39
24	c	504	CLA	C3D-C2D	2.99	1.47	1.39
24	C	504	CLA	C3D-C2D	2.99	1.47	1.39
24	B	609	CLA	C1B-C2B	2.98	1.50	1.43
24	c	503	CLA	C4D-CHA	2.97	1.48	1.38
24	c	507	CLA	C4D-CHA	2.97	1.48	1.38
38	F	101	HEM	CAC-C3C	2.97	1.55	1.47
24	c	506	CLA	C4D-CHA	2.96	1.48	1.38
24	B	615	CLA	C3D-C2D	2.96	1.47	1.39
24	B	601	CLA	C4D-CHA	2.96	1.48	1.38
24	b	618	CLA	C4D-CHA	2.96	1.48	1.38
24	b	616	CLA	C1B-C2B	2.95	1.50	1.43
24	b	619	CLA	C4D-CHA	2.95	1.48	1.38
24	a	408	CLA	C3D-C2D	2.95	1.47	1.39
24	C	507	CLA	C4D-CHA	2.95	1.48	1.38
24	c	502	CLA	C4D-CHA	2.94	1.48	1.38
24	B	608	CLA	C3D-C2D	2.94	1.47	1.39
24	c	505	CLA	C1B-C2B	2.94	1.50	1.43
24	b	610	CLA	C1B-C2B	2.94	1.50	1.43
38	f	101	HEM	CAC-C3C	2.93	1.55	1.47
24	b	610	CLA	C4D-CHA	2.93	1.48	1.38
24	c	505	CLA	C4D-CHA	2.93	1.48	1.38
24	b	607	CLA	C1B-C2B	2.93	1.50	1.43
24	c	507	CLA	C1B-C2B	2.92	1.50	1.43
24	B	615	CLA	MG-ND	-2.92	2.00	2.05
24	b	605	CLA	MG-NB	2.92	2.11	2.05
24	b	609	CLA	C4D-CHA	2.92	1.48	1.38
24	b	605	CLA	C4D-CHA	2.92	1.48	1.38
24	b	604	CLA	C4D-CHA	2.91	1.48	1.38
24	b	612	CLA	C4D-CHA	2.91	1.48	1.38
24	C	503	CLA	C3D-C2D	2.91	1.46	1.39
24	B	613	CLA	C4D-CHA	2.91	1.48	1.38
24	C	509	CLA	C4D-CHA	2.91	1.48	1.38
24	B	601	CLA	MG-ND	-2.91	2.00	2.05
24	B	613	CLA	C1B-C2B	2.91	1.50	1.43
27	D	407	PL9	C6-C5	2.90	1.49	1.35
27	a	414	PL9	C6-C5	2.90	1.49	1.35
24	a	412	CLA	C3D-C2D	2.90	1.46	1.39
24	C	504	CLA	C4D-CHA	2.90	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C1B-C2B	2.90	1.49	1.43
24	b	612	CLA	C3D-C2D	2.89	1.46	1.39
24	b	609	CLA	C3D-C2D	2.89	1.46	1.39
24	B	602	CLA	C1B-C2B	2.89	1.49	1.43
24	C	501	CLA	C3D-C2D	2.89	1.46	1.39
24	c	513	CLA	C4D-CHA	2.89	1.48	1.38
24	C	512	CLA	C4D-CHA	2.89	1.48	1.38
27	A	1010	PL9	C6-C5	2.88	1.49	1.35
24	C	512	CLA	C3D-C2D	2.88	1.46	1.39
24	a	409	CLA	OBD-CAD	2.88	1.27	1.22
24	b	614	CLA	C3D-C2D	2.88	1.46	1.39
24	C	513	CLA	C1B-C2B	2.88	1.49	1.43
24	A	1005	CLA	C3D-C2D	2.88	1.46	1.39
24	c	506	CLA	C1B-C2B	2.88	1.49	1.43
24	C	501	CLA	C1B-C2B	2.88	1.49	1.43
24	b	608	CLA	C3D-C2D	2.88	1.46	1.39
24	b	607	CLA	C4D-CHA	2.88	1.48	1.38
24	D	402	CLA	MG-ND	-2.87	2.00	2.05
24	d	402	CLA	MG-ND	2.87	2.11	2.05
24	b	613	CLA	C4D-CHA	2.87	1.48	1.38
24	b	614	CLA	C1B-C2B	2.87	1.49	1.43
24	C	509	CLA	C3D-C2D	2.87	1.46	1.39
24	B	612	CLA	C3D-C2D	2.86	1.46	1.39
24	C	510	CLA	C1B-C2B	2.86	1.49	1.43
24	c	502	CLA	C1B-C2B	2.86	1.49	1.43
24	B	606	CLA	C4D-CHA	2.86	1.48	1.38
24	C	505	CLA	C4D-CHA	2.86	1.48	1.38
24	d	403	CLA	C3D-C2D	2.86	1.46	1.39
24	B	616	CLA	C1B-C2B	2.86	1.49	1.43
24	c	503	CLA	C1B-C2B	2.85	1.49	1.43
24	B	608	CLA	C4D-CHA	2.85	1.48	1.38
24	c	513	CLA	C3D-C2D	2.85	1.46	1.39
24	C	509	CLA	C1B-C2B	2.85	1.49	1.43
24	c	501	CLA	C1B-C2B	2.85	1.49	1.43
24	a	412	CLA	C1B-C2B	2.85	1.49	1.43
24	C	507	CLA	C1B-C2B	2.85	1.49	1.43
24	b	616	CLA	C4D-CHA	2.85	1.48	1.38
24	B	607	CLA	C3D-C2D	2.85	1.46	1.39
24	a	407	CLA	C3D-C2D	2.85	1.46	1.39
24	C	502	CLA	C1B-C2B	2.84	1.49	1.43
24	B	606	CLA	C3D-C2D	2.84	1.46	1.39
27	d	405	PL9	C6-C5	2.84	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C3D-C2D	2.84	1.46	1.39
24	B	607	CLA	C4D-CHA	2.84	1.48	1.38
24	C	506	CLA	C4D-CHA	2.84	1.48	1.38
24	D	405	CLA	C1B-C2B	2.83	1.49	1.43
24	A	1006	CLA	C1B-C2B	2.83	1.49	1.43
24	C	506	CLA	C3D-C2D	2.83	1.46	1.39
24	c	502	CLA	C3D-C2D	2.83	1.46	1.39
24	b	605	CLA	C3D-C2D	2.83	1.46	1.39
24	B	609	CLA	C3D-C2D	2.83	1.46	1.39
24	b	604	CLA	C3D-C2D	2.83	1.46	1.39
24	c	508	CLA	C1B-C2B	2.83	1.49	1.43
24	C	513	CLA	C3D-C2D	2.83	1.46	1.39
24	D	405	CLA	C3D-C2D	2.82	1.46	1.39
24	c	508	CLA	C3D-C2D	2.82	1.46	1.39
24	B	607	CLA	C1B-C2B	2.82	1.49	1.43
24	C	513	CLA	C4D-CHA	2.82	1.48	1.38
24	c	506	CLA	C3D-C2D	2.82	1.46	1.39
24	b	605	CLA	C1B-C2B	2.82	1.49	1.43
38	v	201	HEM	CAB-C3B	2.82	1.54	1.47
24	b	609	CLA	C1B-C2B	2.82	1.49	1.43
24	C	503	CLA	C1B-C2B	2.82	1.49	1.43
24	b	607	CLA	C3D-C2D	2.81	1.46	1.39
24	c	503	CLA	C3D-C2D	2.81	1.46	1.39
24	c	509	CLA	C3D-C2D	2.81	1.46	1.39
24	b	617	CLA	C1B-C2B	2.81	1.49	1.43
24	b	606	CLA	C3D-C2D	2.80	1.46	1.39
24	c	501	CLA	C4D-CHA	2.80	1.48	1.38
24	b	618	CLA	C3D-C2D	2.80	1.46	1.39
24	c	509	CLA	C4D-CHA	2.80	1.48	1.38
24	B	605	CLA	C3D-C2D	2.80	1.46	1.39
24	C	505	CLA	C3D-C2D	2.80	1.46	1.39
24	B	602	CLA	C4D-CHA	2.80	1.48	1.38
24	B	606	CLA	C1B-C2B	2.80	1.49	1.43
24	d	403	CLA	C1B-C2B	2.80	1.49	1.43
24	d	403	CLA	MG-NB	-2.80	2.00	2.05
24	b	616	CLA	C3D-C2D	2.80	1.46	1.39
24	C	508	CLA	C4D-CHA	2.79	1.48	1.38
24	B	601	CLA	C1B-C2B	2.79	1.49	1.43
24	C	510	CLA	C3D-C2D	2.79	1.46	1.39
24	c	508	CLA	C4D-CHA	2.79	1.48	1.38
24	c	511	CLA	C1B-C2B	2.79	1.49	1.43
24	B	601	CLA	C3D-C2D	2.79	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C1B-C2B	2.78	1.49	1.43
24	c	504	CLA	C4D-CHA	2.78	1.47	1.38
26	K	101	BCR	C24-C25	-2.77	1.35	1.45
24	a	409	CLA	C1B-C2B	2.77	1.49	1.43
24	b	614	CLA	C4D-CHA	2.77	1.47	1.38
24	B	616	CLA	C4D-CHA	2.77	1.47	1.38
24	A	1008	CLA	C3D-C2D	2.77	1.46	1.39
24	c	509	CLA	MG-NB	-2.77	2.00	2.05
24	c	511	CLA	C3D-C2D	2.77	1.46	1.39
24	B	609	CLA	C4D-CHA	2.77	1.47	1.38
24	b	611	CLA	C3D-C2D	2.77	1.46	1.39
24	B	612	CLA	MG-NB	2.76	2.11	2.05
24	B	611	CLA	C4D-CHA	2.76	1.47	1.38
24	b	619	CLA	C3D-C2D	2.76	1.46	1.39
24	C	504	CLA	C1B-C2B	2.76	1.49	1.43
26	k	102	BCR	C24-C25	-2.76	1.35	1.45
24	C	508	CLA	C3D-C2D	2.76	1.46	1.39
24	B	604	CLA	C3D-C2D	2.76	1.46	1.39
24	C	502	CLA	C3D-C2D	2.76	1.46	1.39
24	c	512	CLA	C1B-C2B	2.76	1.49	1.43
24	B	615	CLA	C4D-CHA	2.76	1.47	1.38
24	C	513	CLA	C1C-C2C	2.76	1.50	1.44
24	b	604	CLA	C1B-C2B	2.75	1.49	1.43
24	C	508	CLA	C1B-C2B	2.74	1.49	1.43
24	c	509	CLA	C1B-C2B	2.74	1.49	1.43
26	y	101	BCR	C24-C25	-2.74	1.35	1.45
24	c	507	CLA	C3D-C2D	2.74	1.46	1.39
24	B	611	CLA	C1B-C2B	2.74	1.49	1.43
24	B	613	CLA	C3D-C2D	2.74	1.46	1.39
24	c	510	CLA	C4D-CHA	2.74	1.47	1.38
24	c	501	CLA	C3D-C2D	2.74	1.46	1.39
24	b	612	CLA	C1B-C2B	2.73	1.49	1.43
24	a	409	CLA	C4D-CHA	2.73	1.47	1.38
24	A	1006	CLA	C4D-CHA	2.73	1.47	1.38
24	A	1008	CLA	C4D-CHA	2.72	1.47	1.38
24	b	611	CLA	C4D-CHA	2.72	1.47	1.38
24	B	614	CLA	C4D-CHA	2.72	1.47	1.38
24	b	606	CLA	C4D-CHA	2.72	1.47	1.38
24	a	412	CLA	C4D-CHA	2.72	1.47	1.38
38	V	201	HEM	FE-NA	2.72	2.04	1.95
24	c	510	CLA	C1B-C2B	2.72	1.49	1.43
24	c	512	CLA	C4D-CHA	2.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	CLA	C4D-CHA	2.71	1.47	1.38
24	B	604	CLA	C4D-CHA	2.71	1.47	1.38
24	B	610	CLA	C4D-CHA	2.71	1.47	1.38
26	K	102	BCR	C24-C25	-2.71	1.35	1.45
24	c	512	CLA	C3D-C2D	2.71	1.46	1.39
24	c	512	CLA	C1C-C2C	2.70	1.50	1.44
24	d	402	CLA	C4D-CHA	2.70	1.47	1.38
24	A	1008	CLA	C1B-C2B	2.70	1.49	1.43
24	D	405	CLA	C4D-CHA	2.70	1.47	1.38
24	b	606	CLA	C1B-C2B	2.70	1.49	1.43
24	b	615	CLA	C3D-C2D	2.69	1.46	1.39
24	C	502	CLA	C4D-CHA	2.69	1.47	1.38
24	c	513	CLA	C1B-C2B	2.69	1.49	1.43
24	a	407	CLA	C1B-C2B	2.69	1.49	1.43
24	b	615	CLA	C4D-CHA	2.69	1.47	1.38
24	c	501	CLA	C1D-C2D	2.69	1.50	1.45
24	c	504	CLA	C1B-C2B	2.69	1.49	1.43
24	d	402	CLA	C1B-C2B	2.69	1.49	1.43
26	J	101	BCR	C24-C25	-2.69	1.35	1.45
24	C	501	CLA	C1D-C2D	2.69	1.50	1.45
24	d	403	CLA	C4D-CHA	2.68	1.47	1.38
24	b	609	CLA	MG-NB	-2.68	2.00	2.05
26	b	621	BCR	C24-C25	-2.68	1.35	1.45
24	D	403	CLA	C4B-NB	-2.68	1.34	1.37
24	A	1005	CLA	C4D-CHA	2.68	1.47	1.38
26	c	514	BCR	C24-C25	-2.68	1.35	1.45
26	d	404	BCR	C24-C25	-2.68	1.35	1.45
24	B	616	CLA	C3D-C2D	2.68	1.46	1.39
24	b	605	CLA	MG-NA	2.68	2.12	2.06
24	C	507	CLA	C3D-C2D	2.68	1.46	1.39
24	b	613	CLA	C3D-C2D	2.67	1.46	1.39
24	a	407	CLA	C4D-CHA	2.67	1.47	1.38
24	B	603	CLA	C3D-C2D	2.66	1.46	1.39
24	B	610	CLA	C3D-C2D	2.66	1.46	1.39
24	b	604	CLA	C1D-C2D	2.65	1.50	1.45
26	b	622	BCR	C24-C25	-2.64	1.36	1.45
24	B	603	CLA	C4D-CHA	2.64	1.47	1.38
26	b	620	BCR	C24-C25	-2.64	1.36	1.45
24	c	505	CLA	C3D-C2D	2.64	1.46	1.39
26	t	101	BCR	C24-C25	-2.64	1.36	1.45
26	k	101	BCR	C24-C25	-2.64	1.36	1.45
24	B	608	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C3D-C2D	2.62	1.46	1.39
24	d	403	CLA	C1D-C2D	2.62	1.50	1.45
24	c	510	CLA	C3D-C2D	2.62	1.46	1.39
24	C	512	CLA	C1C-C2C	2.62	1.49	1.44
26	D	406	BCR	C24-C25	-2.61	1.36	1.45
24	c	504	CLA	C1D-C2D	2.61	1.50	1.45
24	C	510	CLA	C4D-CHA	2.61	1.47	1.38
24	a	408	CLA	C4D-CHA	2.61	1.47	1.38
24	b	613	CLA	C1B-C2B	2.61	1.49	1.43
24	B	614	CLA	C1C-C2C	2.60	1.49	1.44
24	b	608	CLA	C4D-CHA	2.60	1.47	1.38
24	B	614	CLA	C3D-C2D	2.60	1.46	1.39
26	C	514	BCR	C24-C25	-2.60	1.36	1.45
26	h	101	BCR	C24-C25	-2.60	1.36	1.45
24	d	402	CLA	C3D-C2D	2.59	1.46	1.39
24	D	403	CLA	C4D-CHA	2.59	1.47	1.38
24	B	609	CLA	C1D-C2D	2.59	1.50	1.45
24	B	605	CLA	C4D-CHA	2.58	1.47	1.38
24	C	506	CLA	C1B-C2B	2.58	1.49	1.43
24	b	617	CLA	C1C-C2C	2.58	1.49	1.44
26	B	619	BCR	C24-C25	-2.57	1.36	1.45
24	b	617	CLA	C3D-C2D	2.57	1.46	1.39
24	b	611	CLA	C1B-C2B	2.57	1.49	1.43
26	A	1009	BCR	C24-C25	-2.57	1.36	1.45
24	c	513	CLA	C1D-C2D	2.56	1.50	1.45
24	b	612	CLA	C1D-C2D	2.56	1.50	1.45
24	b	617	CLA	C4D-CHA	2.56	1.47	1.38
24	b	609	CLA	C1D-C2D	2.55	1.50	1.45
24	B	603	CLA	C1B-C2B	2.55	1.49	1.43
26	B	618	BCR	C24-C25	-2.55	1.36	1.45
26	B	617	BCR	C24-C25	-2.55	1.36	1.45
24	B	610	CLA	C1B-C2B	2.54	1.49	1.43
24	A	1005	CLA	MG-ND	-2.54	2.00	2.05
38	V	201	HEM	FE-NC	2.54	2.03	1.95
24	D	405	CLA	C1D-C2D	2.53	1.50	1.45
24	c	507	CLA	C1C-C2C	2.53	1.49	1.44
24	B	612	CLA	C4D-CHA	2.53	1.47	1.38
24	B	606	CLA	C1C-C2C	2.52	1.49	1.44
24	a	407	CLA	C4B-NB	-2.52	1.34	1.37
24	C	511	CLA	C1C-C2C	2.52	1.49	1.44
24	B	602	CLA	C1D-C2D	2.51	1.50	1.45
26	a	413	BCR	C24-C25	-2.51	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H	101	BCR	C24-C25	-2.51	1.36	1.45
24	D	403	CLA	C1D-C2D	2.51	1.50	1.45
24	c	503	CLA	C1C-C2C	2.51	1.49	1.44
24	B	606	CLA	C1D-C2D	2.51	1.50	1.45
24	D	402	CLA	C4D-CHA	2.51	1.47	1.38
24	a	408	CLA	C1D-C2D	2.50	1.50	1.45
24	c	503	CLA	C1D-C2D	2.50	1.50	1.45
24	B	613	CLA	MG-NB	2.49	2.10	2.05
24	c	508	CLA	C1D-C2D	2.49	1.50	1.45
24	B	614	CLA	C1B-C2B	2.49	1.49	1.43
24	B	605	CLA	C1C-C2C	2.48	1.49	1.44
24	C	505	CLA	C4C-C3C	2.47	1.49	1.45
26	T	101	BCR	C24-C25	-2.47	1.36	1.45
24	c	506	CLA	C1D-C2D	2.47	1.50	1.45
24	C	506	CLA	C1D-C2D	2.47	1.50	1.45
24	a	409	CLA	C1D-C2D	2.46	1.50	1.45
24	C	507	CLA	C1C-C2C	2.46	1.49	1.44
24	A	1005	CLA	C1D-C2D	2.46	1.50	1.45
24	d	403	CLA	C1C-C2C	2.46	1.49	1.44
24	c	505	CLA	C1D-C2D	2.45	1.50	1.45
24	D	402	CLA	C1C-C2C	2.45	1.49	1.44
24	c	508	CLA	C4C-C3C	2.45	1.49	1.45
24	D	405	CLA	C1C-C2C	2.45	1.49	1.44
24	c	505	CLA	C1C-C2C	2.45	1.49	1.44
24	C	505	CLA	MG-NC	2.45	2.12	2.06
24	C	504	CLA	C1D-C2D	2.45	1.50	1.45
24	A	1005	CLA	C1B-C2B	2.44	1.48	1.43
24	b	605	CLA	C1D-C2D	2.43	1.50	1.45
24	b	605	CLA	C4C-C3C	2.43	1.49	1.45
24	c	513	CLA	C1C-C2C	2.42	1.49	1.44
24	b	606	CLA	C1C-C2C	2.42	1.49	1.44
24	b	614	CLA	MG-NB	2.42	2.10	2.05
24	b	617	CLA	MG-NC	2.42	2.12	2.06
25	A	1007	PHO	C3A-C2A	-2.42	1.52	1.54
27	D	407	PL9	C2-C3	2.41	1.40	1.34
24	b	604	CLA	C1C-C2C	2.41	1.49	1.44
24	b	609	CLA	C4C-C3C	2.41	1.49	1.45
27	A	1010	PL9	C2-C3	2.41	1.40	1.34
36	H	102	DGD	O5D-C1E	2.41	1.44	1.40
24	C	507	CLA	C1D-C2D	2.41	1.50	1.45
24	c	506	CLA	C4C-C3C	2.41	1.49	1.45
24	C	503	CLA	C1C-C2C	2.40	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	C4C-C3C	2.40	1.49	1.45
24	B	601	CLA	C1D-C2D	2.40	1.50	1.45
24	b	609	CLA	C1C-C2C	2.40	1.49	1.44
24	C	513	CLA	C1D-C2D	2.39	1.50	1.45
24	c	508	CLA	C1C-C2C	2.39	1.49	1.44
24	b	607	CLA	C4B-NB	-2.39	1.34	1.37
24	c	511	CLA	C1C-C2C	2.39	1.49	1.44
24	C	508	CLA	C1D-C2D	2.38	1.50	1.45
24	b	605	CLA	C1C-C2C	2.38	1.49	1.44
24	b	606	CLA	C1D-C2D	2.38	1.50	1.45
24	A	1008	CLA	MG-ND	-2.38	2.01	2.05
24	B	615	CLA	C1D-C2D	2.37	1.50	1.45
24	b	607	CLA	C1D-C2D	2.37	1.50	1.45
24	b	618	CLA	C1C-C2C	2.37	1.49	1.44
24	c	504	CLA	C4C-C3C	2.37	1.49	1.45
24	c	509	CLA	C1D-C2D	2.37	1.50	1.45
24	b	608	CLA	C1D-C2D	2.37	1.50	1.45
24	D	402	CLA	C1D-C2D	2.36	1.50	1.45
24	C	505	CLA	C1D-C2D	2.36	1.50	1.45
24	B	608	CLA	C4C-C3C	2.35	1.49	1.45
24	B	602	CLA	C1C-C2C	2.35	1.49	1.44
24	c	501	CLA	C4C-C3C	2.35	1.49	1.45
24	B	606	CLA	C4C-C3C	2.34	1.49	1.45
24	c	503	CLA	C4C-C3C	2.34	1.49	1.45
24	b	611	CLA	C1D-C2D	2.33	1.50	1.45
24	c	513	CLA	C4C-C3C	2.33	1.49	1.45
24	D	405	CLA	C4C-C3C	2.33	1.49	1.45
38	f	101	HEM	CMA-C3A	2.33	1.55	1.50
24	B	607	CLA	C1D-C2D	2.33	1.49	1.45
24	C	501	CLA	C4C-C3C	2.32	1.49	1.45
24	C	506	CLA	C4C-C3C	2.32	1.49	1.45
24	C	508	CLA	C1C-C2C	2.32	1.49	1.44
24	C	509	CLA	C1D-C2D	2.32	1.49	1.45
24	B	601	CLA	C1C-C2C	2.32	1.49	1.44
24	c	510	CLA	C1C-C2C	2.31	1.49	1.44
24	b	610	CLA	C4C-C3C	2.31	1.49	1.45
24	A	1008	CLA	C1C-C2C	2.31	1.49	1.44
24	B	612	CLA	C1C-C2C	2.30	1.49	1.44
38	V	201	HEM	CMC-C2C	2.30	1.55	1.50
27	a	414	PL9	C2-C3	2.30	1.40	1.34
24	c	510	CLA	C1D-C2D	2.29	1.49	1.45
24	b	619	CLA	C1D-C2D	2.28	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C1D-C2D	2.28	1.49	1.45
24	b	617	CLA	MG-NB	2.28	2.10	2.05
24	C	501	CLA	C1C-C2C	2.28	1.49	1.44
24	B	610	CLA	C1C-C2C	2.27	1.49	1.44
24	b	616	CLA	C1D-C2D	2.26	1.49	1.45
38	F	101	HEM	CMB-C2B	2.26	1.55	1.50
24	c	509	CLA	C4C-C3C	2.26	1.48	1.45
28	f	102	SQD	O6-C1	2.25	1.44	1.40
24	b	618	CLA	C1D-C2D	2.25	1.49	1.45
24	d	402	CLA	C1D-C2D	2.25	1.49	1.45
24	c	504	CLA	C1C-C2C	2.25	1.49	1.44
36	h	102	DGD	O5D-C1E	2.24	1.43	1.40
24	A	1006	CLA	C1D-C2D	2.24	1.49	1.45
38	v	201	HEM	CMC-C2C	2.24	1.55	1.50
24	C	505	CLA	C1C-C2C	2.24	1.49	1.44
24	b	616	CLA	MG-NC	2.24	2.11	2.06
24	c	511	CLA	C1D-C2D	2.24	1.49	1.45
38	V	201	HEM	CMA-C3A	2.24	1.55	1.50
24	C	503	CLA	C1D-C2D	2.24	1.49	1.45
35	C	521	HTG	C1-S1	-2.24	1.77	1.80
24	C	510	CLA	C1C-C2C	2.23	1.49	1.44
24	a	412	CLA	C1C-C2C	2.23	1.49	1.44
24	a	407	CLA	C1D-C2D	2.23	1.49	1.45
24	B	615	CLA	C1C-C2C	2.23	1.49	1.44
24	C	509	CLA	C4B-NB	-2.23	1.34	1.37
24	B	615	CLA	C4C-C3C	2.23	1.48	1.45
32	m	103	LMT	O1'-C1'	2.23	1.43	1.40
32	a	402	LMT	O1'-C1'	2.23	1.43	1.40
24	B	602	CLA	C4C-C3C	2.22	1.48	1.45
24	B	611	CLA	C1C-C2C	2.22	1.49	1.44
24	c	507	CLA	C1D-C2D	2.22	1.49	1.45
24	c	513	CLA	MG-ND	2.22	2.10	2.05
27	d	405	PL9	C2-C3	2.22	1.40	1.34
24	b	613	CLA	C1C-C2C	2.21	1.49	1.44
24	B	613	CLA	C1D-C2D	2.21	1.49	1.45
24	C	510	CLA	C1D-C2D	2.21	1.49	1.45
24	c	505	CLA	C4C-C3C	2.21	1.48	1.45
38	F	101	HEM	CMA-C3A	2.21	1.55	1.50
24	B	605	CLA	MG-ND	2.20	2.10	2.05
24	b	615	CLA	C4B-NB	-2.20	1.35	1.37
24	c	502	CLA	C4C-C3C	2.20	1.48	1.45
24	B	605	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C4C-C3C	2.20	1.48	1.45
24	C	504	CLA	C4B-NB	-2.19	1.35	1.37
24	B	613	CLA	C1C-C2C	2.19	1.49	1.44
38	f	101	HEM	CMB-C2B	2.19	1.55	1.50
24	c	511	CLA	C3B-C4B	2.19	1.49	1.42
24	c	502	CLA	C1D-C2D	2.19	1.49	1.45
24	C	506	CLA	C1C-C2C	2.19	1.49	1.44
24	B	612	CLA	C1D-C2D	2.19	1.49	1.45
24	B	607	CLA	C1C-C2C	2.18	1.49	1.44
24	b	611	CLA	C1C-C2C	2.18	1.48	1.44
24	b	619	CLA	C4B-NB	-2.18	1.35	1.37
24	d	402	CLA	C1C-C2C	2.18	1.48	1.44
24	C	502	CLA	C4B-NB	-2.18	1.35	1.37
24	c	506	CLA	C1C-C2C	2.18	1.48	1.44
24	c	501	CLA	C1C-C2C	2.18	1.48	1.44
24	C	502	CLA	C1D-C2D	2.17	1.49	1.45
24	b	614	CLA	C1C-C2C	2.17	1.48	1.44
36	c	515	DGD	O5D-C1E	2.17	1.43	1.40
24	c	510	CLA	C4C-C3C	2.17	1.48	1.45
24	C	507	CLA	C3B-C2B	2.17	1.48	1.41
35	B	628	HTG	C1-S1	-2.17	1.77	1.80
24	A	1008	CLA	C1D-C2D	2.17	1.49	1.45
24	c	509	CLA	C1C-C2C	2.17	1.48	1.44
24	B	604	CLA	C4B-NB	-2.17	1.35	1.37
26	b	622	BCR	C8-C7	-2.16	1.26	1.33
24	C	504	CLA	C4C-C3C	2.16	1.48	1.45
24	C	512	CLA	C3B-C4B	2.16	1.49	1.42
24	B	612	CLA	C3B-C2B	2.16	1.48	1.41
24	B	615	CLA	C1C-NC	-2.16	1.34	1.37
24	B	615	CLA	C3B-C2B	2.16	1.48	1.41
24	b	610	CLA	C1D-C2D	2.16	1.49	1.45
35	b	630	HTG	C1-S1	-2.16	1.77	1.80
24	C	503	CLA	C4B-NB	-2.16	1.35	1.37
24	b	614	CLA	C4B-NB	-2.16	1.35	1.37
24	b	611	CLA	C4B-NB	-2.16	1.35	1.37
35	c	525	HTG	C1-S1	-2.15	1.77	1.80
24	C	504	CLA	C1C-C2C	2.15	1.48	1.44
38	v	201	HEM	CMD-C2D	2.15	1.55	1.50
24	b	612	CLA	C1C-C2C	2.15	1.48	1.44
24	C	513	CLA	C4C-C3C	2.15	1.48	1.45
24	b	610	CLA	C4B-NB	-2.15	1.35	1.37
35	c	522	HTG	C1-S1	-2.15	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	v	201	HEM	CMB-C2B	2.15	1.55	1.50
36	C	516	DGD	O5D-C1E	2.15	1.43	1.40
24	C	512	CLA	C4C-C3C	2.15	1.48	1.45
24	a	408	CLA	C3B-C2B	2.14	1.48	1.41
24	d	403	CLA	C4C-C3C	2.14	1.48	1.45
24	b	615	CLA	C1C-C2C	2.14	1.48	1.44
24	B	608	CLA	C1D-C2D	2.14	1.49	1.45
24	a	409	CLA	C4B-NB	-2.14	1.35	1.37
29	c	520	LMG	O1-C1	2.14	1.43	1.40
24	B	603	CLA	C1D-C2D	2.14	1.49	1.45
24	D	403	CLA	MG-ND	-2.14	2.01	2.05
24	B	601	CLA	C4C-C3C	2.14	1.48	1.45
24	c	512	CLA	C1D-C2D	2.13	1.49	1.45
24	b	608	CLA	C4B-NB	-2.13	1.35	1.37
24	c	512	CLA	C4C-C3C	2.13	1.48	1.45
38	V	201	HEM	CMB-C2B	2.13	1.55	1.50
24	B	609	CLA	C1C-C2C	2.13	1.48	1.44
24	A	1005	CLA	C4B-NB	-2.13	1.35	1.37
26	K	101	BCR	C8-C7	-2.13	1.26	1.33
24	c	503	CLA	C3B-C4B	2.13	1.48	1.42
32	A	1017	LMT	O1'-C1'	2.13	1.43	1.40
26	d	404	BCR	C8-C7	-2.13	1.26	1.33
24	b	607	CLA	C1C-C2C	2.13	1.48	1.44
38	v	201	HEM	CMA-C3A	2.12	1.55	1.50
24	b	606	CLA	MG-ND	-2.12	2.01	2.05
24	B	616	CLA	C1D-C2D	2.12	1.49	1.45
26	K	102	BCR	C8-C7	-2.12	1.26	1.33
24	B	605	CLA	C1D-C2D	2.12	1.49	1.45
26	c	514	BCR	C8-C7	-2.12	1.26	1.33
24	d	403	CLA	C3B-C2B	2.12	1.48	1.41
24	b	609	CLA	C3B-C2B	2.12	1.48	1.41
26	t	101	BCR	C8-C7	-2.12	1.26	1.33
24	C	512	CLA	C1D-C2D	2.11	1.49	1.45
24	b	610	CLA	C1C-C2C	2.11	1.48	1.44
24	B	610	CLA	C4C-C3C	2.11	1.48	1.45
24	A	1008	CLA	C4C-C3C	2.11	1.48	1.45
24	C	513	CLA	C3B-C4B	2.10	1.48	1.42
24	B	604	CLA	C1D-C2D	2.10	1.49	1.45
24	c	507	CLA	C3B-C2B	2.10	1.48	1.41
24	C	511	CLA	C4C-C3C	2.10	1.48	1.45
24	b	608	CLA	C1C-C2C	2.10	1.48	1.44
24	B	612	CLA	MG-NC	2.10	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C1B-NB	-2.10	1.35	1.37
24	b	619	CLA	C3B-C2B	2.10	1.48	1.41
24	b	614	CLA	C1D-C2D	2.10	1.49	1.45
24	C	507	CLA	MG-ND	-2.10	2.01	2.05
24	B	610	CLA	MG-ND	-2.10	2.01	2.05
24	D	402	CLA	C3B-C4B	2.10	1.48	1.42
26	k	101	BCR	C8-C7	-2.10	1.26	1.33
26	C	514	BCR	C8-C7	-2.09	1.26	1.33
24	B	608	CLA	C1C-C2C	2.09	1.48	1.44
35	D	413	HTG	C1-S1	-2.09	1.77	1.80
24	c	508	CLA	C3B-C4B	2.09	1.48	1.42
36	c	516	DGD	O5D-C1E	2.09	1.43	1.40
35	b	602	HTG	C1-S1	-2.08	1.77	1.80
24	b	605	CLA	C3B-C4B	2.08	1.48	1.42
26	B	617	BCR	C8-C7	-2.08	1.26	1.33
24	b	613	CLA	C1D-C2D	2.08	1.49	1.45
26	k	102	BCR	C8-C7	-2.08	1.26	1.33
24	b	615	CLA	C1D-C2D	2.08	1.49	1.45
24	c	509	CLA	C4B-NB	-2.08	1.35	1.37
24	A	1006	CLA	C3B-C2B	2.08	1.48	1.41
24	c	513	CLA	C3B-C4B	2.07	1.48	1.42
24	C	513	CLA	C3B-C2B	2.07	1.48	1.41
26	y	101	BCR	C8-C7	-2.07	1.26	1.33
29	c	521	LMG	O1-C1	2.07	1.43	1.40
24	C	502	CLA	C1C-C2C	2.07	1.48	1.44
24	C	509	CLA	C1C-C2C	2.07	1.48	1.44
24	a	412	CLA	C1D-C2D	2.07	1.49	1.45
26	T	101	BCR	C8-C7	-2.07	1.26	1.33
35	V	202	HTG	C1-S1	-2.07	1.77	1.80
26	B	619	BCR	C8-C7	-2.07	1.27	1.33
24	b	608	CLA	C3B-C4B	2.06	1.48	1.42
24	b	617	CLA	C1D-C2D	2.06	1.49	1.45
24	B	611	CLA	C3B-C4B	2.05	1.48	1.42
24	b	613	CLA	C3B-C4B	2.05	1.48	1.42
24	C	508	CLA	C4C-C3C	2.05	1.48	1.45
24	b	617	CLA	C1C-NC	-2.05	1.34	1.37
24	b	619	CLA	C1C-C2C	2.05	1.48	1.44
24	c	508	CLA	C1C-NC	-2.05	1.34	1.37
24	a	409	CLA	C3B-C4B	2.05	1.48	1.42
24	B	603	CLA	C4B-NB	-2.04	1.35	1.37
24	c	505	CLA	MG-NB	-2.04	2.01	2.05
24	B	614	CLA	C1C-NC	-2.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C1C-C2C	2.04	1.48	1.44
24	b	616	CLA	C1C-C2C	2.04	1.48	1.44
24	C	509	CLA	C4C-C3C	2.04	1.48	1.45
24	d	403	CLA	C3B-C4B	2.04	1.48	1.42
24	b	604	CLA	C3B-C4B	2.04	1.48	1.42
29	C	519	LMG	O1-C1	2.04	1.43	1.40
26	H	101	BCR	C8-C7	-2.04	1.27	1.33
24	B	616	CLA	C1C-C2C	2.03	1.48	1.44
24	c	503	CLA	C3B-C2B	2.03	1.48	1.41
24	B	607	CLA	C4C-C3C	2.03	1.48	1.45
24	a	412	CLA	C4B-NB	-2.03	1.35	1.37
24	B	611	CLA	C4C-C3C	2.03	1.48	1.45
35	B	624	HTG	C1-S1	-2.03	1.77	1.80
24	A	1006	CLA	C1C-C2C	2.03	1.48	1.44
24	C	508	CLA	C1C-NC	-2.03	1.34	1.37
24	C	509	CLA	MG-ND	-2.02	2.01	2.05
38	f	101	HEM	CMD-C2D	2.02	1.54	1.50
24	b	618	CLA	C3B-C2B	2.02	1.48	1.41
24	C	511	CLA	C3B-C2B	2.01	1.48	1.41
24	c	505	CLA	C3B-C2B	2.01	1.48	1.41
24	B	601	CLA	C1C-NC	-2.01	1.34	1.37
24	C	503	CLA	C3B-C2B	2.01	1.48	1.41
24	c	512	CLA	C3B-C2B	2.01	1.48	1.41
24	B	610	CLA	C1D-C2D	2.01	1.49	1.45
24	c	502	CLA	C3B-C4B	2.01	1.48	1.42
24	a	407	CLA	C3B-C2B	2.01	1.48	1.41
24	A	1005	CLA	C1C-C2C	2.01	1.48	1.44
24	D	402	CLA	C4B-NB	-2.01	1.35	1.37
24	C	511	CLA	C1D-C2D	2.01	1.49	1.45
24	B	606	CLA	C3B-C2B	2.01	1.47	1.41
24	C	512	CLA	C3B-C2B	2.01	1.47	1.41
32	C	520	LMT	O1'-C1'	2.01	1.43	1.40
26	B	618	BCR	C8-C7	-2.01	1.27	1.33
24	c	513	CLA	C3B-C2B	2.01	1.47	1.41
24	D	405	CLA	C3B-C4B	2.00	1.48	1.42
24	B	604	CLA	MG-NB	-2.00	2.01	2.05
34	D	410	LHG	O7-C5	-2.00	1.41	1.46
26	b	620	BCR	C8-C7	-2.00	1.27	1.33
24	C	510	CLA	MG-ND	-2.00	2.01	2.05
24	c	507	CLA	C1C-NC	-2.00	1.34	1.37

All (2947) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1009	BCR	C20-C21-C22	28.60	167.39	127.28
26	J	101	BCR	C16-C17-C18	28.55	167.31	127.28
26	y	101	BCR	C20-C21-C22	27.70	166.12	127.28
26	c	514	BCR	C16-C17-C18	27.49	165.84	127.28
26	b	621	BCR	C20-C21-C22	27.46	165.78	127.28
26	h	101	BCR	C20-C21-C22	27.16	165.37	127.28
26	y	101	BCR	C16-C17-C18	27.11	165.30	127.28
26	k	101	BCR	C15-C16-C17	27.03	178.83	123.52
26	B	618	BCR	C20-C21-C22	26.88	164.98	127.28
26	c	514	BCR	C20-C21-C22	26.86	164.94	127.28
26	b	620	BCR	C20-C21-C22	26.66	164.67	127.28
26	d	404	BCR	C20-C21-C22	26.48	164.42	127.28
26	J	101	BCR	C20-C21-C22	26.47	164.40	127.28
26	c	514	BCR	C15-C16-C17	26.39	177.52	123.52
26	C	514	BCR	C15-C16-C17	26.25	177.23	123.52
26	K	102	BCR	C15-C16-C17	26.19	177.10	123.52
26	B	617	BCR	C20-C21-C22	26.12	163.91	127.28
26	d	404	BCR	C15-C16-C17	25.95	176.62	123.52
26	C	514	BCR	C20-C21-C22	25.83	163.51	127.28
26	K	102	BCR	C20-C21-C22	25.70	163.32	127.28
26	h	101	BCR	C16-C17-C18	25.70	163.32	127.28
26	H	101	BCR	C20-C21-C22	25.61	163.20	127.28
26	k	102	BCR	C20-C21-C22	25.57	163.13	127.28
26	y	101	BCR	C15-C16-C17	25.53	175.76	123.52
26	b	622	BCR	C15-C16-C17	25.46	175.61	123.52
26	b	621	BCR	C16-C17-C18	25.36	162.84	127.28
26	B	619	BCR	C20-C21-C22	25.29	162.75	127.28
26	J	101	BCR	C15-C16-C17	25.23	175.15	123.52
26	t	101	BCR	C20-C21-C22	25.13	162.52	127.28
26	k	102	BCR	C15-C16-C17	24.96	174.58	123.52
26	a	413	BCR	C16-C17-C18	24.94	162.26	127.28
26	k	101	BCR	C16-C17-C18	24.81	162.07	127.28
26	b	622	BCR	C20-C21-C22	24.67	161.88	127.28
26	k	102	BCR	C16-C17-C18	24.62	161.80	127.28
26	T	101	BCR	C20-C21-C22	24.60	161.78	127.28
26	D	406	BCR	C20-C21-C22	24.47	161.59	127.28
26	h	101	BCR	C15-C16-C17	24.42	173.49	123.52
26	H	101	BCR	C15-C16-C17	24.32	173.27	123.52
26	H	101	BCR	C16-C17-C18	24.30	161.35	127.28
26	b	621	BCR	C15-C16-C17	24.16	172.95	123.52
26	T	101	BCR	C15-C16-C17	24.15	172.93	123.52
26	k	101	BCR	C20-C21-C22	24.10	161.08	127.28
26	D	406	BCR	C16-C17-C18	23.99	160.92	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C16-C17-C18	23.78	160.62	127.28
26	a	413	BCR	C15-C16-C17	23.19	170.97	123.52
26	t	101	BCR	C15-C16-C17	23.14	170.87	123.52
26	K	101	BCR	C20-C21-C22	23.09	159.66	127.28
26	b	620	BCR	C15-C16-C17	22.91	170.39	123.52
26	B	617	BCR	C16-C17-C18	22.86	159.34	127.28
26	B	618	BCR	C15-C16-C17	22.81	170.19	123.52
26	b	622	BCR	C16-C15-C14	22.79	170.15	123.52
26	T	101	BCR	C16-C15-C14	22.77	170.11	123.52
26	D	406	BCR	C15-C16-C17	22.36	169.28	123.52
26	C	514	BCR	C16-C15-C14	22.34	169.22	123.52
26	a	413	BCR	C20-C21-C22	22.28	158.52	127.28
26	B	619	BCR	C15-C16-C17	22.27	169.09	123.52
26	K	102	BCR	C16-C17-C18	22.24	158.46	127.28
26	b	620	BCR	C16-C17-C18	22.13	158.31	127.28
26	B	617	BCR	C15-C16-C17	21.96	168.46	123.52
26	K	102	BCR	C16-C15-C14	21.93	168.38	123.52
26	K	101	BCR	C15-C16-C17	21.71	167.94	123.52
26	t	101	BCR	C16-C17-C18	21.56	157.52	127.28
26	K	101	BCR	C16-C17-C18	21.47	157.38	127.28
26	A	1009	BCR	C16-C17-C18	21.35	157.22	127.28
26	d	404	BCR	C16-C15-C14	21.22	166.94	123.52
26	C	514	BCR	C16-C17-C18	21.20	157.00	127.28
26	t	101	BCR	C16-C15-C14	21.07	166.63	123.52
26	d	404	BCR	C16-C17-C18	20.97	156.68	127.28
26	B	619	BCR	C16-C17-C18	20.89	156.57	127.28
26	c	514	BCR	C16-C15-C14	20.69	165.86	123.52
26	b	622	BCR	C16-C17-C18	20.68	156.28	127.28
26	y	101	BCR	C16-C15-C14	20.49	165.43	123.52
26	J	101	BCR	C16-C15-C14	20.47	165.41	123.52
26	k	101	BCR	C16-C15-C14	20.45	165.36	123.52
26	T	101	BCR	C16-C17-C18	20.44	155.94	127.28
26	a	413	BCR	C16-C15-C14	20.21	164.87	123.52
26	B	617	BCR	C16-C15-C14	19.96	164.35	123.52
26	h	101	BCR	C16-C15-C14	19.90	164.24	123.52
26	A	1009	BCR	C15-C16-C17	19.80	164.03	123.52
26	k	102	BCR	C16-C15-C14	19.57	163.56	123.52
26	B	618	BCR	C16-C15-C14	19.53	163.48	123.52
26	K	101	BCR	C16-C15-C14	19.51	163.44	123.52
26	B	619	BCR	C16-C15-C14	19.38	163.17	123.52
26	y	101	BCR	C21-C20-C19	19.17	178.74	123.20
26	K	102	BCR	C21-C20-C19	18.92	178.01	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C16-C15-C14	18.80	161.99	123.52
26	A	1009	BCR	C16-C15-C14	18.73	161.83	123.52
26	k	101	BCR	C21-C20-C19	18.65	177.23	123.20
26	b	620	BCR	C16-C15-C14	18.59	161.56	123.52
26	B	618	BCR	C21-C20-C19	18.29	176.20	123.20
26	H	101	BCR	C21-C20-C19	18.14	175.76	123.20
26	h	101	BCR	C21-C20-C19	18.00	175.34	123.20
26	K	101	BCR	C21-C20-C19	17.86	174.96	123.20
26	b	621	BCR	C16-C15-C14	17.63	159.58	123.52
26	T	101	BCR	C21-C20-C19	17.58	174.13	123.20
26	J	101	BCR	C21-C20-C19	17.37	173.53	123.20
26	c	514	BCR	C21-C20-C19	17.24	173.15	123.20
26	b	621	BCR	C21-C20-C19	17.01	172.49	123.20
26	a	413	BCR	C21-C20-C19	17.00	172.44	123.20
26	d	404	BCR	C21-C20-C19	16.95	172.31	123.20
26	B	619	BCR	C21-C20-C19	16.87	172.09	123.20
26	k	102	BCR	C21-C20-C19	16.83	171.96	123.20
26	C	514	BCR	C21-C20-C19	16.61	171.32	123.20
26	B	617	BCR	C21-C20-C19	16.16	170.02	123.20
26	A	1009	BCR	C21-C20-C19	16.14	169.96	123.20
26	D	406	BCR	C16-C15-C14	15.88	156.00	123.52
26	k	102	BCR	C10-C11-C12	15.71	168.72	123.20
26	D	406	BCR	C21-C20-C19	15.66	168.57	123.20
26	b	622	BCR	C21-C20-C19	15.65	168.54	123.20
26	t	101	BCR	C21-C20-C19	15.16	167.12	123.20
26	k	102	BCR	C7-C8-C9	15.02	148.46	126.23
26	b	620	BCR	C21-C20-C19	14.91	166.39	123.20
26	K	102	BCR	C10-C11-C12	14.75	165.95	123.20
26	a	413	BCR	C10-C11-C12	14.53	165.31	123.20
26	t	101	BCR	C11-C12-C13	14.34	165.68	126.36
26	J	101	BCR	C11-C12-C13	14.28	165.52	126.36
26	C	514	BCR	C10-C11-C12	14.21	164.38	123.20
26	B	619	BCR	C10-C11-C12	14.14	164.16	123.20
26	y	101	BCR	C7-C8-C9	14.13	147.14	126.23
26	k	101	BCR	C10-C11-C12	14.01	163.80	123.20
26	y	101	BCR	C20-C19-C18	13.98	164.70	126.36
26	c	514	BCR	C20-C19-C18	13.97	164.66	126.36
26	A	1009	BCR	C20-C19-C18	13.88	164.41	126.36
26	K	102	BCR	C20-C19-C18	13.88	164.41	126.36
26	t	101	BCR	C10-C11-C12	13.84	163.31	123.20
26	K	101	BCR	C11-C12-C13	13.81	164.22	126.36
26	h	101	BCR	C20-C19-C18	13.77	164.13	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	102	BCR	C11-C12-C13	13.49	163.35	126.36
26	b	621	BCR	C11-C10-C9	13.46	146.15	127.28
26	c	514	BCR	C10-C11-C12	13.45	162.17	123.20
26	K	101	BCR	C10-C11-C12	13.39	162.00	123.20
26	B	619	BCR	C11-C12-C13	13.34	162.94	126.36
26	H	101	BCR	C20-C19-C18	13.33	162.91	126.36
26	A	1009	BCR	C19-C18-C17	13.32	139.97	119.01
26	a	413	BCR	C11-C10-C9	13.28	145.91	127.28
26	a	413	BCR	C19-C18-C17	13.25	139.85	119.01
26	K	101	BCR	C15-C14-C13	13.19	145.77	127.28
26	a	413	BCR	C15-C14-C13	13.02	145.54	127.28
26	b	621	BCR	C10-C11-C12	12.97	160.78	123.20
26	a	413	BCR	C20-C19-C18	12.87	161.64	126.36
26	J	101	BCR	C10-C11-C12	12.85	160.42	123.20
26	B	617	BCR	C19-C18-C17	12.83	139.19	119.01
26	K	101	BCR	C20-C19-C18	12.76	161.35	126.36
26	T	101	BCR	C20-C19-C18	12.71	161.21	126.36
26	b	622	BCR	C20-C19-C18	12.60	160.91	126.36
26	t	101	BCR	C20-C19-C18	12.55	160.77	126.36
26	H	101	BCR	C11-C10-C9	12.52	144.83	127.28
26	b	622	BCR	C11-C12-C13	12.52	160.68	126.36
26	C	514	BCR	C20-C19-C18	12.48	160.58	126.36
26	B	618	BCR	C19-C18-C17	12.42	138.55	119.01
26	d	404	BCR	C11-C12-C13	12.38	160.31	126.36
26	k	102	BCR	C20-C19-C18	12.37	160.27	126.36
26	B	617	BCR	C15-C14-C13	12.33	144.57	127.28
26	y	101	BCR	C11-C12-C13	12.31	160.11	126.36
26	k	101	BCR	C11-C12-C13	12.30	160.09	126.36
26	K	102	BCR	C11-C12-C13	12.29	160.07	126.36
24	b	607	CLA	C4A-NA-C1A	12.18	112.24	106.68
26	b	622	BCR	C10-C11-C12	12.11	158.28	123.20
26	A	1009	BCR	C10-C11-C12	12.08	158.21	123.20
26	D	406	BCR	C19-C18-C17	12.06	137.98	119.01
26	d	404	BCR	C20-C19-C18	12.05	159.40	126.36
26	B	617	BCR	C11-C10-C9	12.03	144.15	127.28
26	J	101	BCR	C20-C19-C18	11.98	159.21	126.36
26	D	406	BCR	C15-C14-C13	11.95	144.04	127.28
26	B	617	BCR	C20-C19-C18	11.92	159.04	126.36
26	B	618	BCR	C20-C19-C18	11.89	158.96	126.36
26	B	619	BCR	C19-C18-C17	11.88	137.69	119.01
24	C	511	CLA	C4A-NA-C1A	11.87	112.09	106.68
24	c	507	CLA	C4A-NA-C1A	11.81	112.07	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C20-C19-C18	11.72	158.50	126.36
26	a	413	BCR	C11-C12-C13	11.67	158.38	126.36
26	C	514	BCR	C11-C10-C9	11.63	143.59	127.28
26	y	101	BCR	C10-C11-C12	11.63	156.89	123.20
26	H	101	BCR	C19-C18-C17	11.63	137.30	119.01
26	b	621	BCR	C19-C18-C17	11.62	137.28	119.01
26	D	406	BCR	C7-C8-C9	11.62	143.42	126.23
26	k	101	BCR	C7-C8-C9	11.60	143.40	126.23
26	b	620	BCR	C10-C11-C12	11.55	156.66	123.20
26	T	101	BCR	C10-C11-C12	11.53	156.60	123.20
26	C	514	BCR	C11-C12-C13	11.50	157.88	126.36
26	b	621	BCR	C20-C19-C18	11.49	157.88	126.36
24	C	507	CLA	C4A-NA-C1A	11.45	111.91	106.68
26	B	618	BCR	C7-C8-C9	11.45	143.17	126.23
26	D	406	BCR	C20-C19-C18	11.31	157.38	126.36
26	B	617	BCR	C10-C11-C12	11.24	155.77	123.20
26	A	1009	BCR	C11-C12-C13	11.24	157.19	126.36
26	D	406	BCR	C11-C12-C13	11.23	157.16	126.36
26	A	1009	BCR	C7-C8-C9	11.21	142.82	126.23
26	h	101	BCR	C11-C12-C13	11.16	156.97	126.36
26	a	413	BCR	C7-C8-C9	11.16	142.74	126.23
26	B	619	BCR	C20-C19-C18	11.15	156.95	126.36
26	J	101	BCR	C19-C18-C17	11.12	136.50	119.01
26	k	101	BCR	C15-C14-C13	11.07	142.80	127.28
26	t	101	BCR	C19-C18-C17	11.07	136.42	119.01
26	c	514	BCR	C11-C12-C13	11.06	156.70	126.36
24	b	618	CLA	C4A-NA-C1A	11.05	111.72	106.68
24	C	503	CLA	C4A-NA-C1A	11.04	111.71	106.68
26	B	618	BCR	C10-C11-C12	11.03	155.16	123.20
26	b	620	BCR	C20-C19-C18	11.03	156.60	126.36
26	T	101	BCR	C11-C12-C13	11.02	156.58	126.36
24	B	615	CLA	C4A-NA-C1A	10.97	111.69	106.68
26	d	404	BCR	C7-C8-C9	10.87	142.31	126.23
26	A	1009	BCR	C11-C10-C9	10.84	142.48	127.28
26	H	101	BCR	C11-C12-C13	10.84	156.08	126.36
24	b	609	CLA	C4A-NA-C1A	10.80	111.61	106.68
26	b	620	BCR	C11-C12-C13	10.78	155.91	126.36
26	K	101	BCR	C11-C10-C9	10.75	142.36	127.28
26	b	620	BCR	C15-C14-C13	10.72	142.32	127.28
26	h	101	BCR	C11-C10-C9	10.68	142.26	127.28
26	t	101	BCR	C7-C8-C9	10.64	141.98	126.23
26	B	618	BCR	C15-C14-C13	10.64	142.19	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	C4A-NA-C1A	10.62	111.52	106.68
24	b	612	CLA	C4A-NA-C1A	10.53	111.48	106.68
26	T	101	BCR	C11-C10-C9	10.51	142.02	127.28
26	h	101	BCR	C19-C18-C17	10.49	135.51	119.01
26	b	620	BCR	C19-C18-C17	10.48	135.49	119.01
24	c	511	CLA	C4A-NA-C1A	10.47	111.46	106.68
26	D	406	BCR	C10-C11-C12	10.46	153.49	123.20
26	d	404	BCR	C15-C14-C13	10.43	141.91	127.28
26	K	101	BCR	C7-C8-C9	10.43	141.67	126.23
26	b	622	BCR	C15-C14-C13	10.40	141.87	127.28
26	K	102	BCR	C7-C8-C9	10.40	141.62	126.23
26	b	621	BCR	C11-C12-C13	10.37	154.79	126.36
26	b	620	BCR	C11-C10-C9	10.36	141.81	127.28
26	c	514	BCR	C7-C8-C9	10.36	141.56	126.23
26	J	101	BCR	C7-C8-C9	10.36	141.56	126.23
26	A	1009	BCR	C15-C14-C13	10.34	141.78	127.28
26	D	406	BCR	C11-C10-C9	10.33	141.76	127.28
24	C	505	CLA	C4A-NA-C1A	10.31	111.38	106.68
26	B	619	BCR	C15-C14-C13	10.30	141.72	127.28
26	b	622	BCR	C19-C18-C17	10.29	135.20	119.01
26	b	622	BCR	C7-C8-C9	10.27	141.43	126.23
26	b	621	BCR	C15-C14-C13	10.27	141.68	127.28
24	B	604	CLA	C4A-NA-C1A	10.23	111.35	106.68
26	K	101	BCR	C19-C18-C17	10.20	135.06	119.01
26	H	101	BCR	C15-C14-C13	10.19	141.57	127.28
26	k	101	BCR	C19-C18-C17	10.17	135.00	119.01
26	k	101	BCR	C11-C10-C9	10.13	141.48	127.28
26	B	619	BCR	C7-C8-C9	10.06	141.12	126.23
24	B	606	CLA	C4A-NA-C1A	10.03	111.26	106.68
26	T	101	BCR	C15-C14-C13	10.01	141.31	127.28
24	B	613	CLA	C4A-NA-C1A	9.87	111.18	106.68
26	y	101	BCR	C19-C18-C17	9.86	134.52	119.01
24	c	512	CLA	C4A-NA-C1A	9.86	111.18	106.68
26	K	102	BCR	C15-C14-C13	9.79	141.01	127.28
26	B	618	BCR	C11-C12-C13	9.77	153.16	126.36
24	b	604	CLA	C4A-NA-C1A	9.72	111.11	106.68
26	b	622	BCR	C11-C10-C9	9.69	140.87	127.28
24	c	501	CLA	C4A-NA-C1A	9.68	111.09	106.68
24	c	506	CLA	C4A-NA-C1A	9.66	111.08	106.68
26	B	619	BCR	C11-C10-C9	9.64	140.80	127.28
26	c	514	BCR	C15-C14-C13	9.64	140.79	127.28
26	b	620	BCR	C7-C8-C9	9.63	140.48	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	BCR	C15-C14-C13	9.63	140.78	127.28
25	A	1007	PHO	C3B-C4B-NB	9.62	113.73	107.46
24	B	601	CLA	C4A-NA-C1A	9.61	111.06	106.68
24	c	509	CLA	C4A-NA-C1A	9.59	111.06	106.68
24	b	610	CLA	C4A-NA-C1A	9.59	111.05	106.68
26	t	101	BCR	C15-C14-C13	9.51	140.61	127.28
26	B	618	BCR	C11-C10-C9	9.50	140.60	127.28
26	d	404	BCR	C10-C11-C12	9.46	150.61	123.20
24	B	611	CLA	C4A-NA-C1A	9.43	110.98	106.68
24	C	506	CLA	C4A-NA-C1A	9.41	110.97	106.68
26	b	621	BCR	C7-C8-C9	9.40	140.13	126.23
24	C	512	CLA	C4A-NA-C1A	9.39	110.97	106.68
26	h	101	BCR	C15-C14-C13	9.35	140.39	127.28
24	B	614	CLA	C4A-NA-C1A	9.32	110.93	106.68
24	C	504	CLA	C4A-NA-C1A	9.32	110.93	106.68
24	c	508	CLA	C4A-NA-C1A	9.28	110.91	106.68
24	b	616	CLA	C4A-NA-C1A	9.28	110.91	106.68
24	B	609	CLA	C4A-NA-C1A	9.27	110.91	106.68
26	B	618	BCR	C12-C13-C14	9.24	133.54	119.01
26	c	514	BCR	C19-C18-C17	9.22	133.52	119.01
24	C	501	CLA	C4A-NA-C1A	9.21	110.88	106.68
26	K	102	BCR	C11-C10-C9	9.21	140.19	127.28
26	C	514	BCR	C7-C8-C9	9.16	139.79	126.23
26	h	101	BCR	C10-C11-C12	9.10	149.57	123.20
26	B	617	BCR	C11-C12-C13	9.09	151.30	126.36
26	T	101	BCR	C24-C23-C22	9.09	139.68	126.23
24	c	502	CLA	C4A-NA-C1A	9.08	110.82	106.68
26	K	102	BCR	C19-C18-C17	9.06	133.26	119.01
26	y	101	BCR	C11-C10-C9	9.03	139.94	127.28
24	c	504	CLA	C4A-NA-C1A	9.02	110.80	106.68
25	a	410	PHO	C3B-C4B-NB	9.02	113.34	107.46
24	C	513	CLA	C4A-NA-C1A	8.99	110.78	106.68
26	D	406	BCR	C29-C30-C25	8.94	123.42	110.44
24	b	613	CLA	C4A-NA-C1A	8.93	110.75	106.68
26	B	617	BCR	C23-C22-C21	8.93	133.06	119.01
26	J	101	BCR	C11-C10-C9	8.93	139.80	127.28
24	b	615	CLA	C4A-NA-C1A	8.90	110.74	106.68
24	C	502	CLA	C4A-NA-C1A	8.88	110.73	106.68
26	h	101	BCR	C24-C23-C22	8.88	139.37	126.23
24	C	509	CLA	C4A-NA-C1A	8.88	110.73	106.68
26	H	101	BCR	C12-C13-C14	8.87	132.96	119.01
24	c	505	CLA	C4A-NA-C1A	8.86	110.72	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C7-C8-C9	8.86	139.34	126.23
26	c	514	BCR	C11-C10-C9	8.85	139.69	127.28
26	b	620	BCR	C12-C13-C14	8.82	132.88	119.01
26	T	101	BCR	C7-C8-C9	8.74	139.16	126.23
24	b	605	CLA	C4A-NA-C1A	8.72	110.66	106.68
26	b	621	BCR	C12-C13-C14	8.71	132.71	119.01
24	C	508	CLA	C4A-NA-C1A	8.68	110.64	106.68
25	D	404	PHO	O2D-CGD-CBD	8.66	120.46	110.95
26	T	101	BCR	C19-C18-C17	8.63	132.58	119.01
24	C	510	CLA	C4A-NA-C1A	8.63	110.61	106.68
24	b	606	CLA	C4A-NA-C1A	8.63	110.61	106.68
25	a	411	PHO	C3B-C4B-NB	8.55	113.04	107.46
26	y	101	BCR	C15-C14-C13	8.53	139.25	127.28
26	B	617	BCR	C36-C18-C17	-8.53	108.99	122.82
24	D	402	CLA	C4A-NA-C1A	8.50	110.56	106.68
26	H	101	BCR	C10-C11-C12	8.50	147.83	123.20
26	J	101	BCR	C15-C14-C13	8.50	139.20	127.28
25	D	404	PHO	C3B-C4B-NB	8.48	112.99	107.46
24	b	619	CLA	C4A-NA-C1A	8.47	110.54	106.68
26	D	406	BCR	C36-C18-C19	-8.45	105.18	118.09
26	d	404	BCR	C32-C1-C6	8.42	123.45	110.24
26	d	404	BCR	C19-C18-C17	8.42	132.25	119.01
26	J	101	BCR	C36-C18-C17	-8.40	109.20	122.82
25	a	411	PHO	O2D-CGD-CBD	8.39	120.17	110.95
24	c	513	CLA	C4A-NA-C1A	8.39	110.51	106.68
24	D	405	CLA	C4A-NA-C1A	8.38	110.50	106.68
25	A	1007	PHO	O2D-CGD-CBD	8.35	120.12	110.95
24	B	605	CLA	C4A-NA-C1A	8.30	110.47	106.68
26	a	413	BCR	C24-C23-C22	8.26	138.46	126.23
24	B	607	CLA	C4A-NA-C1A	8.26	110.45	106.68
24	B	602	CLA	C4A-NA-C1A	8.10	110.37	106.68
26	H	101	BCR	C23-C22-C21	8.08	131.72	119.01
24	c	501	CLA	CMD-C2D-C1D	8.08	138.96	124.73
25	A	1007	PHO	C2D-C1D-ND	8.07	115.26	109.43
24	c	506	CLA	CMD-C2D-C1D	8.07	138.94	124.73
24	b	617	CLA	C4A-NA-C1A	8.04	110.34	106.68
25	a	410	PHO	O2D-CGD-CBD	8.03	119.77	110.95
26	k	101	BCR	C23-C22-C21	8.02	131.62	119.01
24	D	403	CLA	C4A-NA-C1A	8.01	110.33	106.68
26	h	101	BCR	C7-C8-C9	7.99	138.06	126.23
24	b	609	CLA	CMD-C2D-C1D	7.99	138.79	124.73
24	A	1008	CLA	C4A-NA-C1A	7.99	110.32	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	CMD-C2D-C1D	7.97	138.77	124.73
24	c	510	CLA	C4A-NA-C1A	7.97	110.31	106.68
26	A	1009	BCR	C12-C13-C14	7.96	131.53	119.01
24	a	409	CLA	C4A-NA-C1A	7.96	110.31	106.68
24	B	606	CLA	CMD-C2D-C1D	7.95	138.72	124.73
24	B	601	CLA	CMD-C2D-C1D	7.90	138.64	124.73
24	d	403	CLA	CMD-C2D-C1D	7.89	138.62	124.73
26	B	617	BCR	C24-C23-C22	7.89	137.90	126.23
24	c	503	CLA	CMD-C2D-C1D	7.85	138.55	124.73
24	c	513	CLA	CMD-C2D-C1D	7.85	138.55	124.73
24	b	614	CLA	C4A-NA-C1A	7.84	110.25	106.68
24	d	403	CLA	C4A-NA-C1A	7.83	110.25	106.68
25	a	411	PHO	C2B-C1B-NB	7.83	115.09	109.43
24	C	501	CLA	CMD-C2D-C1D	7.81	138.47	124.73
24	B	616	CLA	C4A-NA-C1A	7.80	110.24	106.68
26	C	514	BCR	C19-C18-C17	7.79	131.26	119.01
24	C	507	CLA	CMD-C2D-C1D	7.78	138.43	124.73
24	C	510	CLA	CMD-C2D-C1D	7.78	138.43	124.73
24	b	611	CLA	C4A-NA-C1A	7.78	110.23	106.68
26	D	406	BCR	C12-C13-C14	7.78	131.24	119.01
26	a	413	BCR	C23-C22-C21	7.77	131.23	119.01
24	b	617	CLA	CMD-C2D-C1D	7.76	138.40	124.73
26	A	1009	BCR	C23-C22-C21	7.75	131.21	119.01
26	a	413	BCR	C36-C18-C17	-7.75	110.27	122.82
26	d	404	BCR	C11-C10-C9	7.74	138.13	127.28
24	c	505	CLA	CMD-C2D-C1D	7.67	138.24	124.73
24	C	506	CLA	CMD-C2D-C1D	7.67	138.23	124.73
24	B	612	CLA	C1D-ND-C4D	-7.66	100.94	106.31
26	y	101	BCR	C33-C5-C6	7.65	132.83	124.48
24	B	610	CLA	C4A-NA-C1A	7.64	110.16	106.68
24	c	507	CLA	CMD-C2D-C1D	7.63	138.17	124.73
26	B	619	BCR	C29-C30-C25	7.62	121.51	110.44
24	B	603	CLA	C4A-NA-C1A	7.61	110.15	106.68
24	B	614	CLA	C1D-ND-C4D	-7.60	100.98	106.31
24	D	402	CLA	C1D-ND-C4D	-7.59	100.98	106.31
24	C	509	CLA	CMD-C2D-C1D	7.59	138.10	124.73
24	c	509	CLA	CMD-C2D-C1D	7.59	138.09	124.73
25	D	404	PHO	C2D-C1D-ND	7.59	114.92	109.43
24	b	611	CLA	CMD-C2D-C1D	7.59	138.09	124.73
24	d	402	CLA	C1D-ND-C4D	-7.57	101.00	106.31
26	K	101	BCR	C12-C13-C14	7.56	130.91	119.01
26	t	101	BCR	C11-C10-C9	7.56	137.88	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C36-C18-C17	-7.55	110.58	122.82
24	B	610	CLA	CMD-C2D-C1D	7.54	138.01	124.73
24	c	510	CLA	CMD-C2D-C1D	7.52	137.98	124.73
24	b	619	CLA	CMD-C2D-C1D	7.52	137.98	124.73
26	k	102	BCR	C11-C10-C9	7.52	137.83	127.28
24	a	408	CLA	C4A-NA-C1A	7.52	110.11	106.68
24	D	405	CLA	CMD-C2D-C1D	7.51	137.96	124.73
24	B	616	CLA	CMD-C2D-C1D	7.50	137.94	124.73
26	k	102	BCR	C19-C18-C17	7.50	130.80	119.01
26	J	101	BCR	C33-C5-C4	-7.49	97.62	113.60
24	B	614	CLA	CMD-C2D-C1D	7.49	137.91	124.73
25	a	410	PHO	C2D-C1D-ND	7.46	114.82	109.43
24	b	613	CLA	CMD-C2D-C1D	7.46	137.87	124.73
24	C	508	CLA	C1D-ND-C4D	-7.46	101.08	106.31
24	B	608	CLA	C4A-NA-C1A	7.46	110.08	106.68
24	a	412	CLA	C4A-NA-C1A	7.45	110.08	106.68
25	a	411	PHO	C2D-C1D-ND	7.44	114.80	109.43
24	B	612	CLA	C4A-NA-C1A	7.43	110.07	106.68
24	C	503	CLA	CMD-C2D-C1D	7.43	137.81	124.73
24	b	616	CLA	CMD-C2D-C1D	7.41	137.79	124.73
24	b	605	CLA	CMD-C2D-C1D	7.40	137.77	124.73
26	d	404	BCR	C30-C25-C26	-7.40	112.53	122.64
24	B	609	CLA	CMD-C2D-C1D	7.40	137.75	124.73
24	B	603	CLA	CMD-C2D-C1D	7.39	137.74	124.73
24	b	608	CLA	CMD-C2D-C1D	7.37	137.71	124.73
24	C	513	CLA	CMD-C2D-C1D	7.37	137.71	124.73
26	c	514	BCR	C36-C18-C17	-7.37	110.88	122.82
26	d	404	BCR	C12-C13-C14	7.36	130.59	119.01
24	A	1006	CLA	CMD-C2D-C1D	7.35	137.68	124.73
25	A	1007	PHO	C2B-C1B-NB	7.35	114.74	109.43
24	C	502	CLA	C1D-ND-C4D	-7.35	101.15	106.31
24	C	505	CLA	CMD-C2D-C1D	7.35	137.67	124.73
26	T	101	BCR	C8-C7-C6	7.32	146.56	127.00
24	c	508	CLA	CMD-C2D-C1D	7.31	137.61	124.73
24	b	617	CLA	C1D-ND-C4D	-7.31	101.18	106.31
24	C	508	CLA	CMD-C2D-C1D	7.29	137.57	124.73
24	c	504	CLA	CMD-C2D-C1D	7.29	137.56	124.73
24	c	512	CLA	CMD-C2D-C1D	7.28	137.55	124.73
26	h	101	BCR	C23-C22-C21	7.28	130.46	119.01
26	h	101	BCR	C12-C13-C14	7.27	130.45	119.01
24	c	511	CLA	CMD-C2D-C1D	7.27	137.53	124.73
24	d	403	CLA	C1D-ND-C4D	-7.25	101.22	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	CMD-C2D-C1D	7.25	137.50	124.73
24	d	402	CLA	CMD-C2D-C1D	7.25	137.49	124.73
26	b	622	BCR	C23-C22-C21	7.24	130.40	119.01
24	b	606	CLA	CMD-C2D-C1D	7.24	137.48	124.73
26	d	404	BCR	C29-C30-C25	7.21	120.91	110.44
26	A	1009	BCR	C36-C18-C19	-7.21	107.08	118.09
26	C	514	BCR	C23-C22-C21	7.20	130.33	119.01
24	A	1008	CLA	C1D-ND-C4D	-7.19	101.27	106.31
24	A	1005	CLA	CMD-C2D-C1D	7.18	137.36	124.73
26	B	618	BCR	C36-C18-C19	-7.17	107.13	118.09
24	a	412	CLA	C1D-ND-C4D	-7.16	101.29	106.31
24	b	618	CLA	CMD-C2D-C1D	7.16	137.34	124.73
24	B	613	CLA	CMD-C2D-C1D	7.16	137.33	124.73
26	t	101	BCR	C36-C18-C17	-7.16	111.22	122.82
26	C	514	BCR	C37-C22-C21	-7.14	111.25	122.82
25	D	404	PHO	C2B-C1B-NB	7.14	114.59	109.43
25	a	410	PHO	C2B-C1B-NB	7.11	114.57	109.43
24	b	614	CLA	CMD-C2D-C1D	7.10	137.24	124.73
24	c	510	CLA	C1D-ND-C4D	-7.10	101.33	106.31
24	a	408	CLA	C1D-ND-C4D	-7.09	101.34	106.31
24	a	409	CLA	CMD-C2D-C1D	7.09	137.21	124.73
26	B	619	BCR	C24-C23-C22	7.08	136.70	126.23
24	C	504	CLA	CMD-C2D-C1D	7.07	137.17	124.73
24	B	613	CLA	C1D-ND-C4D	-7.05	101.36	106.31
24	B	602	CLA	CMD-C2D-C1D	7.05	137.15	124.73
24	b	613	CLA	C1D-ND-C4D	-7.03	101.38	106.31
24	B	615	CLA	CMD-C2D-C1D	7.03	137.11	124.73
26	K	102	BCR	C38-C26-C25	7.03	132.15	124.48
24	C	510	CLA	C1D-ND-C4D	-7.01	101.39	106.31
24	a	407	CLA	CMD-C2D-C1D	7.01	137.07	124.73
24	B	610	CLA	C1D-ND-C4D	-7.00	101.40	106.31
24	D	402	CLA	CMD-C2D-C1D	6.99	137.04	124.73
26	a	413	BCR	C12-C13-C14	6.99	130.00	119.01
26	c	514	BCR	C24-C23-C22	6.98	136.56	126.23
26	k	102	BCR	C37-C22-C21	-6.98	111.51	122.82
26	B	618	BCR	C23-C22-C21	6.94	129.93	119.01
24	B	616	CLA	C1D-ND-C4D	-6.93	101.45	106.31
24	D	403	CLA	C1D-ND-C4D	-6.93	101.45	106.31
24	d	402	CLA	C4A-NA-C1A	6.92	109.84	106.68
24	B	611	CLA	CMD-C2D-C1D	6.91	136.90	124.73
24	c	512	CLA	C1D-ND-C4D	-6.91	101.47	106.31
24	c	502	CLA	CMD-C2D-C1D	6.91	136.89	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1008	CLA	CMD-C2D-C1D	6.88	136.84	124.73
24	b	608	CLA	C1D-ND-C4D	-6.87	101.49	106.31
24	B	611	CLA	C1D-ND-C4D	-6.86	101.50	106.31
26	H	101	BCR	C8-C7-C6	6.84	145.28	127.00
24	b	608	CLA	C4A-NA-C1A	6.83	109.80	106.68
24	B	603	CLA	C1D-ND-C4D	-6.83	101.52	106.31
24	B	605	CLA	C1D-ND-C4D	-6.83	101.52	106.31
24	a	412	CLA	CMD-C2D-C1D	6.81	136.73	124.73
24	B	605	CLA	CMD-C2D-C1D	6.81	136.72	124.73
24	b	615	CLA	C1D-ND-C4D	-6.81	101.53	106.31
24	C	502	CLA	CMD-C2D-C1D	6.79	136.69	124.73
24	B	609	CLA	C1D-ND-C4D	-6.76	101.57	106.31
26	J	101	BCR	C4-C5-C6	6.74	131.81	122.70
24	a	408	CLA	CMD-C2D-C1D	6.73	136.58	124.73
24	c	508	CLA	C1D-ND-C4D	-6.72	101.59	106.31
26	b	621	BCR	C23-C22-C21	6.72	129.57	119.01
24	D	405	CLA	C1D-ND-C4D	-6.71	101.60	106.31
26	y	101	BCR	C12-C13-C14	6.71	129.56	119.01
26	B	618	BCR	C23-C24-C25	6.70	144.90	127.00
26	b	620	BCR	C23-C22-C21	6.70	129.54	119.01
24	b	606	CLA	C1D-ND-C4D	-6.69	101.61	106.31
24	C	501	CLA	C1D-ND-C4D	-6.68	101.62	106.31
24	b	610	CLA	CMD-C2D-C1D	6.68	136.49	124.73
26	b	620	BCR	C2-C1-C6	6.67	120.12	110.44
26	t	101	BCR	C23-C22-C21	6.66	129.49	119.01
26	D	406	BCR	C2-C1-C6	6.65	120.10	110.44
24	b	615	CLA	CMD-C2D-C1D	6.65	136.44	124.73
24	b	614	CLA	C1D-ND-C4D	-6.65	101.65	106.31
24	B	608	CLA	CMD-C2D-C1D	6.65	136.43	124.73
24	C	507	CLA	C1D-ND-C4D	-6.63	101.66	106.31
24	c	501	CLA	C1D-ND-C4D	-6.62	101.67	106.31
26	b	620	BCR	C38-C26-C27	-6.60	99.52	113.60
24	A	1005	CLA	C1D-ND-C4D	-6.60	101.68	106.31
24	C	512	CLA	CMD-C2D-C1D	6.60	136.35	124.73
24	A	1005	CLA	C4A-NA-C1A	6.60	109.69	106.68
26	k	102	BCR	C38-C26-C25	6.59	131.68	124.48
24	C	512	CLA	C1D-ND-C4D	-6.58	101.70	106.31
24	B	607	CLA	C1D-ND-C4D	-6.57	101.70	106.31
24	c	509	CLA	C1D-ND-C4D	-6.56	101.71	106.31
26	y	101	BCR	C33-C5-C4	-6.55	99.62	113.60
26	C	514	BCR	C8-C7-C6	6.55	144.50	127.00
26	K	102	BCR	C29-C30-C25	6.55	119.95	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C1D-ND-C4D	-6.55	101.72	106.31
26	b	621	BCR	C36-C18-C19	-6.55	108.08	118.09
24	a	407	CLA	C1D-ND-C4D	-6.54	101.72	106.31
26	D	406	BCR	C8-C9-C10	6.54	129.29	119.01
24	C	511	CLA	CMD-C2D-C1D	6.54	136.24	124.73
26	k	101	BCR	C36-C18-C17	-6.53	112.23	122.82
26	b	620	BCR	C38-C26-C25	6.53	131.61	124.48
26	t	101	BCR	C24-C23-C22	6.53	135.89	126.23
26	A	1009	BCR	C24-C23-C22	6.51	135.86	126.23
24	b	607	CLA	CMD-C2D-C1D	6.50	136.18	124.73
26	K	101	BCR	C23-C22-C21	6.50	129.24	119.01
26	k	101	BCR	C12-C13-C14	6.48	129.20	119.01
26	b	622	BCR	C2-C1-C6	6.48	119.85	110.44
26	J	101	BCR	C24-C23-C22	6.47	135.81	126.23
24	b	616	CLA	C1D-ND-C4D	-6.46	101.78	106.31
26	B	618	BCR	C29-C30-C25	6.45	119.81	110.44
26	k	101	BCR	C33-C5-C6	6.45	131.52	124.48
26	B	618	BCR	C24-C23-C22	6.44	135.77	126.23
26	B	617	BCR	C7-C8-C9	6.44	135.76	126.23
26	c	514	BCR	C29-C30-C25	6.43	119.78	110.44
24	B	607	CLA	CMD-C2D-C1D	6.43	136.05	124.73
26	B	618	BCR	C35-C13-C12	-6.42	108.28	118.09
26	H	101	BCR	C36-C18-C19	-6.41	108.30	118.09
26	T	101	BCR	C23-C22-C21	6.40	129.08	119.01
24	A	1006	CLA	C1D-ND-C4D	-6.40	101.82	106.31
26	b	622	BCR	C12-C13-C14	6.38	129.05	119.01
24	D	403	CLA	CMD-C2D-C1D	6.36	135.93	124.73
25	A	1007	PHO	C4D-ND-C1D	-6.35	101.26	108.87
26	k	102	BCR	C15-C14-C13	6.35	136.19	127.28
24	b	618	CLA	C1D-ND-C4D	-6.35	101.86	106.31
24	C	511	CLA	C1D-ND-C4D	-6.34	101.86	106.31
26	h	101	BCR	C37-C22-C21	-6.33	112.56	122.82
24	C	513	CLA	C1D-ND-C4D	-6.32	101.88	106.31
25	A	1007	PHO	C3D-C4D-ND	6.31	115.80	107.71
26	k	101	BCR	C24-C23-C22	6.31	135.57	126.23
24	A	1006	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	b	619	CLA	C1D-ND-C4D	-6.30	101.89	106.31
24	c	502	CLA	C1D-ND-C4D	-6.30	101.89	106.31
26	t	101	BCR	C12-C13-C14	6.28	128.89	119.01
24	D	403	CLA	C2C-C1C-NC	6.26	116.55	109.98
24	B	604	CLA	CMD-C2D-C1D	6.26	135.74	124.73
24	B	606	CLA	C1D-ND-C4D	-6.25	101.92	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C1D-ND-C4D	-6.25	101.93	106.31
24	b	609	CLA	C1D-ND-C4D	-6.23	101.94	106.31
26	c	514	BCR	C38-C26-C25	6.23	131.28	124.48
24	c	504	CLA	C1D-ND-C4D	-6.22	101.95	106.31
26	c	514	BCR	C38-C26-C27	-6.21	100.36	113.60
24	B	601	CLA	C1D-ND-C4D	-6.18	101.97	106.31
24	B	612	CLA	CMD-C2D-C1D	6.17	135.60	124.73
24	a	407	CLA	C4A-NA-C1A	6.17	109.50	106.68
26	B	617	BCR	C12-C13-C14	6.17	128.72	119.01
24	B	603	CLA	O2D-CGD-CBD	6.17	122.02	111.23
24	a	409	CLA	C1D-ND-C4D	-6.16	101.99	106.31
26	k	102	BCR	C33-C5-C6	6.15	131.20	124.48
25	a	410	PHO	C3D-C4D-ND	6.15	115.59	107.71
24	C	504	CLA	C1D-ND-C4D	-6.15	102.00	106.31
24	c	511	CLA	C1D-ND-C4D	-6.14	102.00	106.31
26	B	617	BCR	C8-C7-C6	6.13	143.37	127.00
24	c	505	CLA	C1D-ND-C4D	-6.12	102.02	106.31
26	b	622	BCR	C35-C13-C12	-6.10	108.77	118.09
26	c	514	BCR	C23-C22-C21	6.10	128.60	119.01
26	b	620	BCR	C35-C13-C12	-6.09	108.78	118.09
24	C	509	CLA	C1D-ND-C4D	-6.09	102.04	106.31
24	c	506	CLA	C1D-ND-C4D	-6.09	102.04	106.31
26	A	1009	BCR	C36-C18-C17	-6.09	112.96	122.82
26	a	413	BCR	C33-C5-C6	6.07	131.10	124.48
26	B	619	BCR	C30-C25-C26	-6.06	114.36	122.64
24	b	611	CLA	C1D-ND-C4D	-6.04	102.08	106.31
26	H	101	BCR	C24-C23-C22	6.04	135.16	126.23
26	h	101	BCR	C8-C7-C6	6.02	143.09	127.00
26	b	622	BCR	C8-C7-C6	6.01	143.06	127.00
25	a	411	PHO	C3D-C4D-ND	6.01	115.41	107.71
24	c	507	CLA	C1D-ND-C4D	-6.01	102.09	106.31
26	y	101	BCR	C8-C7-C6	6.01	143.04	127.00
26	B	619	BCR	C12-C13-C14	6.00	128.45	119.01
26	b	620	BCR	C8-C7-C6	6.00	143.03	127.00
26	t	101	BCR	C8-C7-C6	6.00	143.02	127.00
26	y	101	BCR	C29-C30-C25	5.95	119.08	110.44
26	D	406	BCR	C23-C22-C21	5.94	128.36	119.01
26	c	514	BCR	C8-C7-C6	5.91	142.78	127.00
24	b	605	CLA	C1D-ND-C4D	-5.89	102.18	106.31
24	b	607	CLA	C1D-ND-C4D	-5.89	102.18	106.31
26	K	102	BCR	C32-C1-C6	5.89	119.48	110.24
25	a	410	PHO	C4D-ND-C1D	-5.87	101.84	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	PHO	C3D-C4D-ND	5.86	115.23	107.71
26	b	622	BCR	C24-C23-C22	5.86	134.91	126.23
24	B	604	CLA	C1D-ND-C4D	-5.86	102.20	106.31
24	D	402	CLA	C2D-C1D-ND	5.85	115.92	110.13
25	a	411	PHO	C4D-ND-C1D	-5.84	101.87	108.87
26	b	620	BCR	C36-C18-C19	-5.84	109.16	118.09
35	D	419	HTG	C1'-S1-C1	5.84	113.06	100.45
24	b	604	CLA	C1D-ND-C4D	-5.83	102.22	106.31
24	B	615	CLA	C1D-ND-C4D	-5.82	102.23	106.31
35	d	416	HTG	C1'-S1-C1	5.82	113.02	100.45
26	A	1009	BCR	C8-C7-C6	5.82	142.54	127.00
26	b	620	BCR	C24-C23-C22	5.80	134.82	126.23
25	D	404	PHO	C4D-ND-C1D	-5.80	101.92	108.87
26	b	622	BCR	C37-C22-C21	-5.79	113.43	122.82
26	k	102	BCR	C24-C23-C22	5.78	134.79	126.23
26	H	101	BCR	C37-C22-C21	-5.77	113.47	122.82
24	b	612	CLA	C1D-ND-C4D	-5.76	102.27	106.31
24	B	602	CLA	C1D-ND-C4D	-5.75	102.28	106.31
26	h	101	BCR	C29-C30-C25	5.74	118.78	110.44
26	b	621	BCR	C40-C30-C25	5.73	119.22	110.24
24	c	513	CLA	C1D-ND-C4D	-5.73	102.30	106.31
26	k	101	BCR	C38-C26-C25	5.72	130.72	124.48
26	k	101	BCR	C38-C26-C27	-5.68	101.48	113.60
26	K	102	BCR	C38-C26-C27	-5.68	101.50	113.60
24	b	610	CLA	C1D-ND-C4D	-5.67	102.33	106.31
26	C	514	BCR	C12-C13-C14	5.66	127.91	119.01
24	c	505	CLA	O2D-CGD-CBD	5.66	121.12	111.23
24	C	505	CLA	C1D-ND-C4D	-5.65	102.34	106.31
24	D	403	CLA	C2D-C1D-ND	5.65	115.72	110.13
26	d	404	BCR	C36-C18-C19	-5.64	109.48	118.09
24	B	614	CLA	C2D-C1D-ND	5.63	115.70	110.13
26	y	101	BCR	C38-C26-C25	5.63	130.63	124.48
26	k	102	BCR	C33-C5-C4	-5.63	101.60	113.60
24	C	502	CLA	C2D-C1D-ND	5.62	115.69	110.13
26	k	101	BCR	C8-C7-C6	5.61	141.99	127.00
26	B	618	BCR	C30-C25-C26	-5.61	114.97	122.64
26	J	101	BCR	C1-C6-C5	-5.61	114.97	122.64
26	T	101	BCR	C36-C18-C17	-5.60	113.74	122.82
26	J	101	BCR	C23-C22-C21	5.60	127.81	119.01
26	a	413	BCR	C37-C22-C23	-5.59	109.54	118.09
24	B	613	CLA	C2D-C1D-ND	5.59	115.66	110.13
26	b	621	BCR	C8-C7-C6	5.59	141.93	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C37-C22-C21	-5.59	113.77	122.82
26	J	101	BCR	C33-C5-C6	5.58	130.57	124.48
26	K	102	BCR	C8-C7-C6	5.58	141.90	127.00
26	t	101	BCR	C35-C13-C12	-5.56	109.59	118.09
26	J	101	BCR	C40-C30-C25	5.56	118.96	110.24
24	a	408	CLA	C2D-C1D-ND	5.56	115.63	110.13
26	d	404	BCR	C23-C22-C21	5.56	127.75	119.01
26	h	101	BCR	C36-C18-C19	-5.55	109.61	118.09
24	B	616	CLA	O2D-CGD-CBD	5.54	120.92	111.23
38	f	101	HEM	C4D-ND-C1D	5.54	111.77	105.21
26	T	101	BCR	C2-C1-C6	5.54	118.49	110.44
26	d	404	BCR	C8-C7-C6	5.53	141.77	127.00
26	d	404	BCR	C8-C9-C10	5.51	127.67	119.01
26	B	619	BCR	C35-C13-C12	-5.51	109.67	118.09
24	b	610	CLA	C2C-C1C-NC	5.50	115.76	109.98
24	b	608	CLA	C2D-C1D-ND	5.50	115.57	110.13
24	C	509	CLA	C3B-C2B-C1B	-5.50	100.69	107.17
24	B	601	CLA	O2D-CGD-CBD	5.49	120.83	111.23
26	a	413	BCR	C8-C7-C6	5.49	141.67	127.00
24	d	402	CLA	C2D-C1D-ND	5.49	115.56	110.13
26	h	101	BCR	C38-C26-C27	-5.49	101.90	113.60
24	a	408	CLA	C2C-C1C-NC	5.48	115.74	109.98
26	B	619	BCR	C23-C22-C21	5.48	127.62	119.01
38	V	201	HEM	C4D-ND-C1D	5.47	111.68	105.21
24	A	1005	CLA	C2C-C1C-NC	5.47	115.72	109.98
35	b	630	HTG	C1'-S1-C1	5.46	112.24	100.45
24	B	605	CLA	C2D-C1D-ND	5.46	115.53	110.13
24	b	613	CLA	C2D-C1D-ND	5.46	115.53	110.13
26	b	620	BCR	C8-C9-C10	5.45	127.58	119.01
26	k	101	BCR	C33-C5-C4	-5.45	101.98	113.60
26	B	618	BCR	C34-C9-C8	-5.45	109.76	118.09
26	D	406	BCR	C40-C30-C25	5.45	118.78	110.24
26	J	101	BCR	C8-C7-C6	5.44	141.54	127.00
24	D	402	CLA	C2C-C1C-NC	5.42	115.68	109.98
26	B	618	BCR	C38-C26-C27	-5.42	102.03	113.60
24	B	611	CLA	C2D-C1D-ND	5.40	115.47	110.13
24	B	608	CLA	C2C-C1C-NC	5.39	115.64	109.98
26	D	406	BCR	C8-C7-C6	5.39	141.38	127.00
24	B	610	CLA	C2D-C1D-ND	5.38	115.45	110.13
26	h	101	BCR	C32-C1-C6	5.38	118.68	110.24
26	B	619	BCR	C2-C1-C6	5.38	118.25	110.44
24	c	503	CLA	C1D-ND-C4D	-5.38	102.54	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	413	BCR	C36-C18-C19	-5.37	109.88	118.09
24	B	614	CLA	O2D-CGD-CBD	5.36	120.61	111.23
26	k	102	BCR	C36-C18-C17	-5.36	114.13	122.82
24	c	507	CLA	O2D-CGD-CBD	5.36	120.60	111.23
24	B	607	CLA	C2C-C1C-NC	5.35	115.60	109.98
26	K	102	BCR	C24-C23-C22	5.34	134.14	126.23
26	J	101	BCR	C12-C13-C14	5.34	127.42	119.01
26	C	514	BCR	C40-C30-C25	5.34	118.62	110.24
38	F	101	HEM	C4D-ND-C1D	5.34	111.53	105.21
24	c	504	CLA	O2D-CGD-CBD	5.34	120.56	111.23
35	B	624	HTG	C1'-S1-C1	5.33	111.96	100.45
26	C	514	BCR	C36-C18-C19	-5.33	109.95	118.09
24	B	616	CLA	C2D-C1D-ND	5.33	115.40	110.13
26	b	621	BCR	C23-C24-C25	5.33	141.23	127.00
35	C	522	HTG	C1-O5-C5	5.33	122.11	112.56
24	b	614	CLA	C2D-C1D-ND	5.32	115.39	110.13
24	A	1006	CLA	C2D-C1D-ND	5.31	115.38	110.13
24	C	510	CLA	C2C-C1C-NC	5.30	115.55	109.98
24	C	509	CLA	C2B-C1B-NB	5.30	115.82	110.33
24	C	503	CLA	C1D-ND-C4D	-5.28	102.60	106.31
24	a	412	CLA	C2D-C1D-ND	5.28	115.35	110.13
24	B	603	CLA	C2C-C1C-NC	5.28	115.52	109.98
24	D	403	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
26	H	101	BCR	C30-C25-C26	-5.27	115.44	122.64
24	D	403	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
24	B	613	CLA	C3D-C2D-C1D	-5.27	98.65	105.83
26	B	617	BCR	C37-C22-C23	-5.26	110.05	118.09
24	b	611	CLA	O2D-CGD-CBD	5.26	120.43	111.23
26	B	618	BCR	C31-C1-C6	5.26	118.48	110.24
26	k	102	BCR	C2-C1-C6	5.25	118.07	110.44
26	c	514	BCR	C1-C6-C5	-5.25	115.46	122.64
26	B	618	BCR	C36-C18-C17	-5.25	114.31	122.82
26	c	514	BCR	C37-C22-C21	-5.25	114.31	122.82
24	c	503	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
26	y	101	BCR	C38-C26-C27	-5.25	102.41	113.60
26	k	102	BCR	C23-C22-C21	5.24	127.25	119.01
24	b	608	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
26	D	406	BCR	C30-C25-C26	-5.24	115.48	122.64
26	k	101	BCR	C37-C22-C23	-5.24	110.09	118.09
24	B	605	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
24	b	617	CLA	C2D-C1D-ND	5.23	115.30	110.13
24	c	501	CLA	O2D-CGD-CBD	5.23	120.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
26	K	101	BCR	C36-C18-C17	-5.23	114.35	122.82
26	b	622	BCR	C36-C18-C19	-5.22	110.12	118.09
26	A	1009	BCR	C38-C26-C27	-5.22	102.47	113.60
24	C	507	CLA	C2D-C1D-ND	5.21	115.29	110.13
24	A	1006	CLA	C2C-C1C-NC	5.21	115.46	109.98
38	v	201	HEM	C4D-ND-C1D	5.21	111.38	105.21
24	C	503	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
24	B	603	CLA	C2D-C1D-ND	5.20	115.28	110.13
24	D	405	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
26	H	101	BCR	C36-C18-C17	-5.19	114.41	122.82
24	B	612	CLA	C2D-C1D-ND	5.19	115.26	110.13
24	b	604	CLA	O2D-CGD-CBD	5.19	120.30	111.23
24	b	608	CLA	C3B-C2B-C1B	-5.19	101.06	107.17
24	A	1008	CLA	C2D-C1D-ND	5.19	115.26	110.13
24	c	509	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
26	B	619	BCR	C8-C7-C6	5.18	140.83	127.00
26	B	618	BCR	C33-C5-C6	5.17	130.13	124.48
24	B	611	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
26	c	514	BCR	C2-C1-C6	5.15	117.93	110.44
24	b	617	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
24	a	407	CLA	C2C-C1C-NC	5.15	115.39	109.98
26	H	101	BCR	C35-C13-C12	-5.15	110.22	118.09
24	A	1006	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
24	b	618	CLA	C2D-C1D-ND	5.14	115.22	110.13
24	C	508	CLA	C2D-C1D-ND	5.14	115.21	110.13
24	a	409	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
24	c	512	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
26	b	622	BCR	C30-C25-C26	-5.12	115.64	122.64
26	k	102	BCR	C8-C7-C6	5.12	140.68	127.00
24	B	606	CLA	O2D-CGD-CBD	5.12	120.18	111.23
24	c	502	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
24	b	614	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
26	b	621	BCR	C30-C25-C26	-5.11	115.65	122.64
24	c	513	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
24	B	610	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
24	C	509	CLA	C2C-C1C-NC	5.11	115.35	109.98
24	a	408	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
24	A	1005	CLA	C2D-C1D-ND	5.10	115.17	110.13
26	D	406	BCR	C38-C26-C25	5.10	130.04	124.48
24	a	412	CLA	C2C-C1C-NC	5.09	115.33	109.98
24	C	512	CLA	C2D-C1D-ND	5.08	115.15	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1008	CLA	C2C-C1C-NC	5.08	115.31	109.98
24	c	507	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
24	D	402	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
24	B	601	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
24	B	615	CLA	C3B-C2B-C1B	-5.07	101.20	107.17
24	b	614	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
24	C	507	CLA	O2D-CGD-CBD	5.06	120.08	111.23
24	B	616	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
26	K	102	BCR	C2-C1-C6	5.05	117.78	110.44
24	C	513	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
26	H	101	BCR	C32-C1-C6	5.05	118.16	110.24
26	b	621	BCR	C36-C18-C17	-5.05	114.64	122.82
24	C	502	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
24	C	511	CLA	C2D-C1D-ND	5.04	115.11	110.13
24	c	511	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
26	C	514	BCR	C38-C26-C27	-5.04	102.86	113.60
35	b	602	HTG	C1'-S1-C1	5.03	111.32	100.45
26	J	101	BCR	C29-C30-C25	5.03	117.75	110.44
26	t	101	BCR	C2-C1-C6	5.03	117.74	110.44
26	y	101	BCR	C37-C22-C21	-5.02	114.68	122.82
24	b	619	CLA	O2D-CGD-CBD	5.02	120.01	111.23
26	b	622	BCR	C36-C18-C17	-5.02	114.68	122.82
24	b	613	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
24	a	407	CLA	C2D-C1D-ND	5.02	115.09	110.13
24	B	616	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
24	d	403	CLA	C2D-C1D-ND	5.02	115.09	110.13
24	c	507	CLA	C3B-C2B-C1B	-5.02	101.26	107.17
24	B	614	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
26	B	618	BCR	C38-C26-C25	5.02	129.96	124.48
26	c	514	BCR	C30-C25-C26	-5.02	115.78	122.64
24	C	503	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	b	617	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	b	609	CLA	O2D-CGD-CBD	5.01	119.98	111.23
26	h	101	BCR	C30-C25-C26	-5.00	115.80	122.64
24	C	507	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
26	A	1009	BCR	C27-C26-C25	5.00	129.47	122.70
24	B	615	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	a	407	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
24	C	505	CLA	C2C-C1C-NC	5.00	115.23	109.98
24	b	619	CLA	C2D-C1D-ND	4.99	115.07	110.13
26	K	102	BCR	C37-C22-C21	-4.99	114.73	122.82
26	T	101	BCR	C29-C30-C25	4.99	117.69	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C2D-C1D-ND	4.99	115.07	110.13
24	A	1008	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
24	a	412	CLA	O2D-CGD-CBD	4.99	119.95	111.23
24	a	412	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
24	b	613	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
24	b	607	CLA	C2C-C1C-NC	4.99	115.22	109.98
24	C	511	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
24	b	619	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
26	H	101	BCR	C8-C9-C10	4.98	126.84	119.01
24	a	409	CLA	C2D-C1D-ND	4.98	115.05	110.13
26	K	101	BCR	C31-C1-C6	4.98	118.05	110.24
24	b	619	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
24	b	618	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
24	B	615	CLA	C2D-C1D-ND	4.97	115.05	110.13
26	A	1009	BCR	C30-C25-C26	-4.97	115.84	122.64
24	a	409	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
24	c	502	CLA	O2D-CGD-CBD	4.97	119.92	111.23
24	b	604	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
24	b	608	CLA	O2D-CGD-CBD	4.97	119.92	111.23
24	B	615	CLA	C2C-C1C-NC	4.97	115.20	109.98
26	a	413	BCR	C8-C9-C10	4.97	126.82	119.01
24	C	512	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
24	d	403	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	c	506	CLA	C2C-C1C-NC	4.96	115.19	109.98
26	c	514	BCR	C12-C13-C14	4.96	126.81	119.01
24	C	510	CLA	C2D-C1D-ND	4.95	115.03	110.13
24	B	606	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
24	d	403	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
24	b	617	CLA	O2D-CGD-CBD	4.95	119.88	111.23
24	C	502	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
24	b	609	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
24	b	616	CLA	C2D-C1D-ND	4.94	115.02	110.13
24	c	501	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
24	b	606	CLA	C2D-C1D-ND	4.94	115.01	110.13
24	b	615	CLA	C2D-C1D-ND	4.94	115.01	110.13
24	B	603	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
26	y	101	BCR	C36-C18-C17	-4.94	114.82	122.82
26	y	101	BCR	C23-C22-C21	4.94	126.77	119.01
24	C	509	CLA	O2D-CGD-CBD	4.93	119.85	111.23
24	B	604	CLA	C2C-C1C-NC	4.93	115.16	109.98
24	D	403	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
24	b	616	CLA	C2C-C1C-NC	4.92	115.15	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C23-C24-C25	4.92	140.14	127.00
24	C	501	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
24	A	1005	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
26	h	101	BCR	C35-C13-C12	-4.92	110.58	118.09
24	C	510	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
24	B	612	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
24	B	602	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
24	b	611	CLA	C3B-C2B-C1B	-4.91	101.39	107.17
26	A	1009	BCR	C37-C22-C21	-4.91	114.87	122.82
24	d	402	CLA	C2C-C1C-NC	4.90	115.13	109.98
24	b	618	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
26	K	101	BCR	C36-C18-C19	-4.90	110.60	118.09
26	k	101	BCR	C35-C13-C12	-4.90	110.60	118.09
26	h	101	BCR	C36-C18-C17	-4.90	114.88	122.82
24	B	606	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
24	C	502	CLA	O2D-CGD-CBD	4.90	119.80	111.23
24	b	608	CLA	C2C-C1C-NC	4.89	115.12	109.98
26	a	413	BCR	C38-C26-C27	-4.89	103.17	113.60
26	J	101	BCR	C23-C24-C25	4.89	140.06	127.00
24	c	510	CLA	C2D-C1D-ND	4.89	114.97	110.13
24	B	607	CLA	C2D-C1D-ND	4.89	114.96	110.13
24	B	602	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
24	b	612	CLA	C2C-C1C-NC	4.89	115.11	109.98
24	a	407	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
26	a	413	BCR	C33-C5-C4	-4.88	103.19	113.60
24	c	507	CLA	C2D-C1D-ND	4.88	114.96	110.13
24	B	604	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
24	c	508	CLA	C2D-C1D-ND	4.88	114.95	110.13
24	B	608	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
24	c	501	CLA	C2C-C1C-NC	4.87	115.09	109.98
24	B	605	CLA	O2D-CGD-CBD	4.87	119.74	111.23
26	B	618	BCR	C8-C7-C6	4.86	139.99	127.00
24	C	504	CLA	O2D-CGD-CBD	4.86	119.73	111.23
26	y	101	BCR	C36-C18-C19	-4.86	110.66	118.09
24	d	402	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
26	H	101	BCR	C38-C26-C27	-4.86	103.24	113.60
24	C	504	CLA	C2C-C1C-NC	4.86	115.08	109.98
24	c	510	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
24	d	402	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
26	d	404	BCR	C37-C22-C21	-4.85	114.96	122.82
24	b	616	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	b	609	CLA	C3D-C2D-C1D	-4.85	99.21	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C2D-C1D-ND	4.85	114.93	110.13
24	c	508	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
24	b	610	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	C	512	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	B	607	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
26	A	1009	BCR	C37-C22-C23	-4.85	110.69	118.09
24	C	504	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
24	C	506	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
24	c	506	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
29	c	521	LMG	O7-C10-C11	4.84	121.96	111.48
26	b	622	BCR	C38-C26-C27	-4.84	103.27	113.60
24	a	408	CLA	C1C-C2C-C3C	-4.84	101.89	106.98
26	k	102	BCR	C29-C30-C25	4.84	117.46	110.44
26	H	101	BCR	C29-C30-C25	4.83	117.46	110.44
24	b	606	CLA	O2D-CGD-CBD	4.83	119.68	111.23
24	c	505	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
26	k	102	BCR	C38-C26-C27	-4.82	103.31	113.60
24	C	513	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
26	h	101	BCR	C27-C26-C25	4.81	129.21	122.70
24	c	513	CLA	O2D-CGD-CBD	4.81	119.64	111.23
26	T	101	BCR	C38-C26-C27	-4.81	103.35	113.60
24	B	605	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
26	b	621	BCR	C37-C22-C21	-4.80	115.03	122.82
24	c	508	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
24	c	510	CLA	C2C-C1C-NC	4.80	115.02	109.98
24	D	402	CLA	C3C-C4C-NC	4.80	116.58	110.43
24	c	509	CLA	C2C-C1C-NC	4.79	115.01	109.98
24	a	412	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
24	c	512	CLA	O2D-CGD-CBD	4.79	119.60	111.23
24	b	605	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
26	k	101	BCR	C8-C9-C10	4.78	126.53	119.01
24	C	506	CLA	C2D-C1D-ND	4.78	114.85	110.13
26	t	101	BCR	C40-C30-C25	4.77	117.73	110.24
24	C	511	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
26	k	101	BCR	C29-C30-C25	4.77	117.37	110.44
24	d	403	CLA	C2B-C1B-NB	4.77	115.27	110.33
24	b	609	CLA	C2C-C1C-NC	4.77	114.99	109.98
24	B	610	CLA	C2C-C1C-NC	4.77	114.99	109.98
26	b	621	BCR	C32-C1-C6	4.76	117.71	110.24
24	c	503	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
35	d	410	HTG	C1'-S1-C1	4.76	110.73	100.45
24	b	605	CLA	C3D-C2D-C1D	-4.76	99.33	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C2C-C1C-NC	4.76	114.98	109.98
24	A	1005	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
24	b	615	CLA	C2C-C1C-NC	4.76	114.98	109.98
24	C	504	CLA	C2D-C1D-ND	4.75	114.83	110.13
24	b	608	CLA	CHD-C1D-ND	-4.75	118.11	124.80
24	b	607	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
24	C	510	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	C	505	CLA	O2D-CGD-CBD	4.75	119.53	111.23
26	K	102	BCR	C40-C30-C25	4.75	117.69	110.24
26	D	406	BCR	C38-C26-C27	-4.74	103.48	113.60
24	C	513	CLA	C2D-C1D-ND	4.74	114.82	110.13
26	T	101	BCR	C30-C25-C26	-4.74	116.16	122.64
26	d	404	BCR	C24-C23-C22	4.74	133.25	126.23
24	b	606	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	B	609	CLA	C2C-C1C-NC	4.74	114.96	109.98
26	K	102	BCR	C36-C18-C19	-4.74	110.85	118.09
24	B	601	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
24	b	610	CLA	C2D-C1D-ND	4.74	114.81	110.13
24	b	606	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
24	C	502	CLA	C2C-C1C-NC	4.73	114.95	109.98
24	b	611	CLA	C2C-C1C-NC	4.73	114.95	109.98
24	A	1006	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
26	b	621	BCR	C38-C26-C27	-4.73	103.52	113.60
24	b	610	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
26	y	101	BCR	C30-C25-C26	-4.72	116.18	122.64
24	B	607	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
24	C	506	CLA	C2C-C1C-NC	4.72	114.94	109.98
24	c	504	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
26	K	102	BCR	C23-C22-C21	4.72	126.43	119.01
24	C	501	CLA	O2D-CGD-CBD	4.72	119.48	111.23
24	C	501	CLA	C2C-C1C-NC	4.71	114.93	109.98
26	B	617	BCR	C40-C30-C25	4.71	117.64	110.24
26	y	101	BCR	C40-C30-C25	4.71	117.64	110.24
24	c	512	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	c	501	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	D	405	CLA	C2D-C1D-ND	4.71	114.79	110.13
26	J	101	BCR	C35-C13-C12	-4.71	110.89	118.09
26	y	101	BCR	C23-C24-C25	4.71	139.58	127.00
24	A	1008	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	C	508	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	b	607	CLA	O2D-CGD-CBD	4.71	119.46	111.23
24	a	412	CLA	C2B-C1B-NB	4.71	115.21	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C2D-C1D-ND	4.71	114.79	110.13
24	B	602	CLA	C2C-C1C-NC	4.71	114.93	109.98
29	C	519	LMG	O7-C10-C11	4.70	121.66	111.48
24	B	603	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
24	b	615	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
24	b	607	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	C	504	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
24	B	606	CLA	C2C-C1C-NC	4.69	114.91	109.98
24	c	510	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	B	606	CLA	C2D-C1D-ND	4.69	114.77	110.13
26	d	404	BCR	C32-C1-C2	-4.68	90.97	108.95
24	B	607	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
24	b	614	CLA	C2C-C1C-NC	4.68	114.90	109.98
24	c	504	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
24	C	506	CLA	O2D-CGD-CBD	4.67	119.40	111.23
24	B	602	CLA	O2D-CGD-CBD	4.67	119.39	111.23
26	T	101	BCR	C12-C13-C14	4.67	126.35	119.01
24	B	612	CLA	O2D-CGD-CBD	4.67	119.39	111.23
24	C	509	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	D	405	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	b	605	CLA	C2D-C1D-ND	4.64	114.72	110.13
26	H	101	BCR	C39-C30-C25	4.64	117.52	110.24
24	c	509	CLA	C2D-C1D-ND	4.64	114.72	110.13
26	J	101	BCR	C30-C25-C26	-4.64	116.30	122.64
24	B	609	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
26	D	406	BCR	C23-C24-C25	4.63	139.38	127.00
24	c	513	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	B	614	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
24	A	1006	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
24	B	613	CLA	C2C-C1C-NC	4.63	114.85	109.98
24	B	601	CLA	C2D-C1D-ND	4.63	114.71	110.13
24	c	506	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
26	C	514	BCR	C31-C1-C6	4.63	117.50	110.24
24	b	607	CLA	C2D-C1D-ND	4.63	114.71	110.13
24	C	510	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
24	b	611	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
24	c	511	CLA	C2D-C1D-ND	4.63	114.70	110.13
26	B	617	BCR	C23-C24-C25	4.62	139.35	127.00
24	b	604	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
24	C	512	CLA	O2D-CGD-CBD	4.62	119.30	111.23
24	c	511	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
24	C	503	CLA	C2D-C1D-ND	4.61	114.69	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C2B-C1B-NB	4.61	115.11	110.33
26	b	620	BCR	C36-C18-C17	-4.61	115.35	122.82
26	D	406	BCR	C33-C5-C4	-4.61	103.77	113.60
24	B	610	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
24	A	1008	CLA	C2B-C1B-NB	4.61	115.10	110.33
24	C	510	CLA	O2D-CGD-CBD	4.60	119.28	111.23
24	C	506	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
24	a	408	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
26	K	101	BCR	C8-C9-C10	4.60	126.24	119.01
24	A	1008	CLA	O2D-CGD-CBD	4.60	119.27	111.23
24	D	402	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
24	b	617	CLA	C2B-C1B-NB	4.59	115.09	110.33
24	b	609	CLA	C2D-C1D-ND	4.59	114.67	110.13
26	d	404	BCR	C33-C5-C6	4.59	129.49	124.48
24	C	505	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
24	D	405	CLA	C2B-C1B-NB	4.59	115.08	110.33
26	D	406	BCR	C35-C13-C12	-4.59	111.08	118.09
24	b	606	CLA	C2C-C1C-NC	4.58	114.80	109.98
24	c	509	CLA	C2B-C1B-NB	4.58	115.08	110.33
24	C	509	CLA	C2D-C1D-ND	4.58	114.65	110.13
24	c	507	CLA	C2C-C1C-NC	4.57	114.79	109.98
24	B	609	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
24	c	506	CLA	C2D-C1D-ND	4.57	114.65	110.13
24	B	614	CLA	C2C-C1C-NC	4.57	114.78	109.98
24	B	611	CLA	O2D-CGD-CBD	4.57	119.22	111.23
24	A	1005	CLA	C1C-C2C-C3C	-4.57	102.17	106.98
24	b	619	CLA	C2C-C1C-NC	4.57	114.78	109.98
24	c	502	CLA	C2D-C1D-ND	4.56	114.64	110.13
26	b	620	BCR	C27-C26-C25	4.56	128.87	122.70
24	a	409	CLA	C2B-C1B-NB	4.56	115.06	110.33
24	c	509	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	b	612	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
26	t	101	BCR	C38-C26-C27	-4.56	103.88	113.60
24	B	616	CLA	C2B-C1B-NB	4.56	115.05	110.33
26	k	101	BCR	C31-C1-C6	4.55	117.38	110.24
24	b	614	CLA	C2B-C1B-NB	4.55	115.05	110.33
24	B	611	CLA	C2C-C1C-NC	4.55	114.76	109.98
24	c	504	CLA	C2D-C1D-ND	4.55	114.63	110.13
24	c	511	CLA	C2B-C1B-NB	4.54	115.04	110.33
24	b	613	CLA	C2B-C1B-NB	4.54	115.03	110.33
26	t	101	BCR	C33-C5-C6	4.54	129.44	124.48
24	c	501	CLA	C2D-C1D-ND	4.54	114.61	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
26	B	617	BCR	C38-C26-C27	-4.53	103.94	113.60
24	C	508	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	B	603	CLA	C2B-C1B-NB	4.52	115.02	110.33
24	c	502	CLA	C2B-C1B-NB	4.52	115.02	110.33
24	b	612	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
24	C	507	CLA	C2C-C1C-NC	4.52	114.73	109.98
24	C	501	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
24	b	618	CLA	C2C-C1C-NC	4.51	114.72	109.98
24	b	617	CLA	C2C-C1C-NC	4.51	114.72	109.98
24	C	501	CLA	C2D-C1D-ND	4.51	114.59	110.13
26	B	617	BCR	C37-C22-C21	-4.51	115.52	122.82
24	d	403	CLA	C2C-C1C-NC	4.50	114.71	109.98
26	K	102	BCR	C33-C5-C6	4.50	129.40	124.48
24	b	615	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
26	K	101	BCR	C2-C1-C6	4.50	116.97	110.44
24	A	1006	CLA	CHD-C1D-ND	-4.50	118.48	124.80
24	c	508	CLA	C2B-C1B-NB	4.49	114.99	110.33
26	K	102	BCR	C33-C5-C4	-4.49	104.01	113.60
24	c	505	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
35	B	629	HTG	C1'-S1-C1	4.49	110.14	100.45
24	b	611	CLA	C2D-C1D-ND	4.48	114.56	110.13
26	T	101	BCR	C27-C26-C25	4.48	128.76	122.70
24	b	616	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
24	B	601	CLA	C2B-C1B-NB	4.48	114.97	110.33
24	b	615	CLA	O2D-CGD-CBD	4.48	119.06	111.23
26	c	514	BCR	C33-C5-C4	-4.48	104.05	113.60
24	B	616	CLA	C2C-C1C-NC	4.48	114.69	109.98
24	B	604	CLA	C2D-C1D-ND	4.48	114.56	110.13
24	c	510	CLA	C2B-C1B-NB	4.47	114.97	110.33
24	c	503	CLA	C2B-C1B-NB	4.47	114.97	110.33
26	D	406	BCR	C1-C6-C5	-4.47	116.53	122.64
26	t	101	BCR	C37-C22-C23	-4.47	111.26	118.09
24	d	402	CLA	C2B-C1B-NB	4.47	114.96	110.33
24	B	608	CLA	C2D-C1D-ND	4.47	114.55	110.13
24	a	409	CLA	O2D-CGD-CBD	4.47	119.04	111.23
24	A	1005	CLA	C2B-C1B-NB	4.46	114.96	110.33
24	c	504	CLA	C2C-C1C-NC	4.46	114.67	109.98
26	h	101	BCR	C23-C24-C25	4.46	138.92	127.00
24	c	513	CLA	C2B-C1B-NB	4.46	114.95	110.33
28	A	1011	SQD	O47-C7-C8	4.46	121.13	111.48
24	B	611	CLA	C3B-C2B-C1B	-4.46	101.92	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C2B-C1B-NB	4.46	114.95	110.33
24	c	505	CLA	C2C-C1C-NC	4.45	114.66	109.98
24	B	608	CLA	C2B-C1B-NB	4.45	114.94	110.33
35	D	413	HTG	C1'-S1-C1	4.44	110.05	100.45
24	C	505	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	b	612	CLA	O2D-CGD-CBD	4.44	118.99	111.23
26	c	514	BCR	C23-C24-C25	4.44	138.85	127.00
26	b	621	BCR	C29-C30-C25	4.44	116.88	110.44
24	B	601	CLA	C2C-C1C-NC	4.44	114.64	109.98
35	C	521	HTG	C1'-S1-C1	4.44	110.03	100.45
24	c	501	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
24	A	1006	CLA	O2D-CGD-CBD	4.43	118.98	111.23
24	B	606	CLA	C2B-C1B-NB	4.43	114.92	110.33
24	b	610	CLA	O2D-CGD-CBD	4.43	118.97	111.23
24	c	502	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
26	b	622	BCR	C29-C30-C25	4.42	116.86	110.44
24	C	510	CLA	C2B-C1B-NB	4.42	114.91	110.33
28	B	620[A]	SQD	O47-C7-C8	4.42	121.04	111.48
26	a	413	BCR	C2-C1-C6	4.42	116.86	110.44
24	c	502	CLA	C2C-C1C-NC	4.42	114.62	109.98
35	C	522	HTG	C1'-S1-C1	4.42	109.99	100.45
24	A	1008	CLA	C1C-C2C-C3C	-4.42	102.34	106.98
24	B	610	CLA	O2D-CGD-CBD	4.41	118.94	111.23
24	C	501	CLA	C2B-C1B-NB	4.41	114.90	110.33
26	C	514	BCR	C24-C23-C22	4.41	132.76	126.23
24	b	613	CLA	C2C-C1C-NC	4.41	114.61	109.98
26	b	621	BCR	C27-C26-C25	4.41	128.66	122.70
24	C	513	CLA	O2D-CGD-CBD	4.41	118.93	111.23
26	t	101	BCR	C38-C26-C25	4.40	129.29	124.48
24	C	513	CLA	C2B-C1B-NB	4.40	114.89	110.33
24	D	405	CLA	C2C-C1C-NC	4.40	114.60	109.98
35	b	601	HTG	C1'-S1-C1	4.40	109.95	100.45
24	a	407	CLA	C2B-C1B-NB	4.39	114.88	110.33
24	b	610	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
32	C	520	LMT	O1B-C4'-C3'	4.39	118.40	107.23
24	B	603	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
26	k	102	BCR	C32-C1-C6	4.39	117.12	110.24
24	C	511	CLA	O2D-CGD-CBD	4.38	118.89	111.23
26	d	404	BCR	C35-C13-C12	-4.38	111.39	118.09
24	D	402	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
24	b	604	CLA	C2B-C1B-NB	4.38	114.87	110.33
26	K	102	BCR	C12-C13-C14	4.38	125.89	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	101	BCR	C33-C5-C4	-4.38	104.27	113.60
26	K	101	BCR	C34-C9-C8	-4.37	111.41	118.09
26	C	514	BCR	C30-C25-C26	-4.37	116.66	122.64
26	K	101	BCR	C23-C24-C25	4.37	138.67	127.00
24	a	408	CLA	O2D-CGD-CBD	4.36	118.85	111.23
24	c	508	CLA	C2C-C1C-NC	4.36	114.56	109.98
26	J	101	BCR	C38-C26-C25	4.36	129.24	124.48
24	B	609	CLA	O2D-CGD-CBD	4.35	118.84	111.23
24	c	504	CLA	C2B-C1B-NB	4.35	114.84	110.33
24	b	605	CLA	O2D-CGD-CBD	4.35	118.84	111.23
26	D	406	BCR	C4-C5-C6	4.35	128.58	122.70
24	B	612	CLA	C2C-C1C-NC	4.35	114.55	109.98
24	C	502	CLA	C2B-C1B-NB	4.35	114.83	110.33
24	B	608	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
24	C	504	CLA	C2B-C1B-NB	4.34	114.83	110.33
26	b	621	BCR	C35-C13-C12	-4.34	111.46	118.09
24	D	403	CLA	C2B-C1B-NB	4.34	114.83	110.33
24	B	612	CLA	C3C-C4C-NC	4.34	115.99	110.43
24	D	403	CLA	C3B-C4B-NB	4.34	114.40	110.53
26	B	618	BCR	C8-C9-C10	4.33	125.83	119.01
26	B	618	BCR	C37-C22-C21	-4.33	115.80	122.82
26	d	404	BCR	C38-C26-C25	4.33	129.21	124.48
35	B	628	HTG	C1'-S1-C1	4.33	109.79	100.45
26	D	406	BCR	C32-C1-C6	4.32	117.02	110.24
24	c	508	CLA	O2D-CGD-CBD	4.32	118.78	111.23
24	B	612	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
26	b	621	BCR	C35-C13-C14	-4.31	115.83	122.82
24	a	407	CLA	C1C-C2C-C3C	-4.31	102.44	106.98
24	c	505	CLA	C2D-C1D-ND	4.31	114.39	110.13
24	C	508	CLA	C2C-C1C-NC	4.30	114.50	109.98
24	B	615	CLA	C2B-C1B-NB	4.30	114.78	110.33
24	B	605	CLA	C3C-C4C-NC	4.30	115.94	110.43
24	b	611	CLA	C2B-C1B-NB	4.29	114.78	110.33
26	k	102	BCR	C23-C24-C25	4.29	138.46	127.00
35	o	301	HTG	C1'-S1-C1	4.29	109.71	100.45
24	b	612	CLA	C2D-C1D-ND	4.29	114.37	110.13
29	m	102	LMG	O7-C10-C11	4.29	120.76	111.48
24	A	1006	CLA	C2B-C1B-NB	4.29	114.77	110.33
24	B	604	CLA	C3D-C2D-C1D	-4.28	99.98	105.83
26	K	102	BCR	C36-C18-C17	-4.28	115.89	122.82
24	c	501	CLA	C2B-C1B-NB	4.27	114.76	110.33
24	A	1005	CLA	CHD-C1D-ND	-4.27	118.79	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C27-C26-C25	4.27	128.47	122.70
26	K	101	BCR	C30-C25-C26	-4.27	116.81	122.64
24	B	610	CLA	C2B-C1B-NB	4.26	114.75	110.33
36	C	516	DGD	O2G-C1B-C2B	4.26	120.70	111.48
24	D	403	CLA	O2D-CGD-CBD	4.26	118.68	111.23
24	B	612	CLA	C3D-C4D-ND	4.26	116.92	109.99
35	c	522	HTG	C1'-S1-C1	4.26	109.65	100.45
24	B	614	CLA	C3C-C4C-NC	4.26	115.89	110.43
24	c	503	CLA	C2D-C1D-ND	4.26	114.34	110.13
24	B	610	CLA	C3C-C4C-NC	4.26	115.88	110.43
26	d	404	BCR	C33-C5-C4	-4.24	104.55	113.60
24	b	609	CLA	C2B-C1B-NB	4.24	114.72	110.33
24	b	604	CLA	C2C-C1C-NC	4.23	114.43	109.98
24	b	619	CLA	C2B-C1B-NB	4.23	114.71	110.33
28	c	518	SQD	O47-C7-C8	4.23	120.63	111.48
26	C	514	BCR	C29-C30-C25	4.23	116.58	110.44
24	C	507	CLA	C1C-C2C-C3C	-4.23	102.53	106.98
24	b	609	CLA	C1C-C2C-C3C	-4.23	102.53	106.98
26	b	621	BCR	C2-C1-C6	4.22	116.58	110.44
24	B	602	CLA	C2B-C1B-NB	4.22	114.71	110.33
24	C	506	CLA	C2B-C1B-NB	4.22	114.71	110.33
26	k	101	BCR	C30-C25-C26	-4.22	116.87	122.64
24	b	604	CLA	C2D-C1D-ND	4.22	114.30	110.13
24	c	513	CLA	C2C-C1C-NC	4.21	114.40	109.98
24	C	508	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	b	605	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	b	608	CLA	C1C-C2C-C3C	-4.21	102.56	106.98
26	J	101	BCR	C8-C9-C10	4.21	125.62	119.01
24	a	408	CLA	CHD-C1D-ND	-4.21	118.88	124.80
26	b	622	BCR	C27-C26-C25	4.20	128.38	122.70
24	b	606	CLA	C2B-C1B-NB	4.20	114.68	110.33
26	B	617	BCR	C8-C9-C10	4.19	125.61	119.01
24	c	510	CLA	O2D-CGD-CBD	4.19	118.56	111.23
24	b	605	CLA	C2C-C1C-NC	4.19	114.38	109.98
24	d	402	CLA	C3C-C4C-NC	4.19	115.80	110.43
24	a	409	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
24	B	614	CLA	C2B-C1B-NB	4.19	114.67	110.33
26	c	514	BCR	C27-C26-C25	4.19	128.36	122.70
24	B	606	CLA	CHD-C1D-ND	-4.19	118.91	124.80
24	C	502	CLA	C3C-C4C-NC	4.18	115.79	110.43
26	T	101	BCR	C33-C5-C4	-4.18	104.68	113.60
24	C	511	CLA	C2C-C1C-NC	4.18	114.37	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	C1C-C2C-C3C	-4.18	102.59	106.98
24	c	512	CLA	C2C-C1C-NC	4.18	114.37	109.98
28	b	623[B]	SQD	O47-C7-C8	4.17	120.51	111.48
26	B	619	BCR	C36-C18-C19	-4.17	111.72	118.09
24	B	605	CLA	C2C-C1C-NC	4.17	114.36	109.98
24	C	512	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	B	616	CLA	C3C-C4C-NC	4.16	115.76	110.43
24	C	503	CLA	C2C-C1C-NC	4.16	114.35	109.98
26	J	101	BCR	C37-C22-C21	-4.15	116.09	122.82
24	C	503	CLA	C2B-C1B-NB	4.15	114.63	110.33
24	b	606	CLA	C1C-C2C-C3C	-4.15	102.61	106.98
26	C	514	BCR	C2-C1-C6	4.15	116.47	110.44
24	b	616	CLA	C2B-C1B-NB	4.15	114.63	110.33
24	a	412	CLA	C1C-C2C-C3C	-4.15	102.62	106.98
24	C	509	CLA	C1C-C2C-C3C	-4.14	102.62	106.98
24	C	501	CLA	CHD-C1D-ND	-4.14	118.97	124.80
24	c	511	CLA	O2D-CGD-CBD	4.14	118.47	111.23
24	D	403	CLA	C3C-C4C-NC	4.14	115.74	110.43
26	b	621	BCR	C8-C9-C10	4.14	125.52	119.01
24	c	512	CLA	C2B-C1B-NB	4.14	114.62	110.33
26	y	101	BCR	C24-C23-C22	4.14	132.35	126.23
24	C	507	CLA	C2B-C1B-NB	4.14	114.62	110.33
24	C	511	CLA	C2B-C1B-NB	4.14	114.62	110.33
24	c	513	CLA	C2D-C1D-ND	4.14	114.22	110.13
24	B	604	CLA	C2B-C1B-NB	4.14	114.61	110.33
24	c	509	CLA	O2D-CGD-CBD	4.13	118.46	111.23
24	C	505	CLA	C2D-C1D-ND	4.13	114.21	110.13
26	B	617	BCR	C35-C13-C12	-4.13	111.78	118.09
24	a	412	CLA	C3C-C4C-NC	4.13	115.72	110.43
26	T	101	BCR	C33-C5-C6	4.12	128.99	124.48
24	b	616	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
26	d	404	BCR	C40-C30-C29	-4.12	93.14	108.95
26	H	101	BCR	C33-C5-C4	-4.12	104.82	113.60
28	b	623[A]	SQD	O47-C7-C8	4.11	120.38	111.48
24	D	402	CLA	C3D-C4D-ND	4.11	116.68	109.99
24	c	510	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
24	b	614	CLA	C3C-C4C-NC	4.11	115.69	110.43
26	B	617	BCR	C36-C18-C19	-4.10	111.82	118.09
35	c	525	HTG	C1'-S1-C1	4.10	109.30	100.45
26	a	413	BCR	C27-C26-C25	4.09	128.23	122.70
29	Z	101	LMG	O7-C10-C11	4.09	120.33	111.48
26	a	413	BCR	C29-C30-C25	4.09	116.38	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	CLA	C2B-C1B-NB	4.09	114.56	110.33
24	b	615	CLA	C3C-C4C-NC	4.09	115.67	110.43
24	b	618	CLA	CHD-C1D-ND	-4.08	119.05	124.80
26	C	514	BCR	C27-C26-C25	4.08	128.22	122.70
24	B	605	CLA	C2B-C1B-NB	4.08	114.56	110.33
24	a	408	CLA	C2B-C1B-NB	4.08	114.56	110.33
28	f	102	SQD	O47-C7-C8	4.08	120.31	111.48
24	B	606	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
24	B	608	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
24	d	403	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
24	c	503	CLA	C2C-C1C-NC	4.07	114.26	109.98
24	C	501	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
28	B	620[B]	SQD	O47-C7-C8	4.07	120.29	111.48
24	C	504	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
24	c	505	CLA	C2B-C1B-NB	4.07	114.55	110.33
24	b	610	CLA	C2B-C1B-NB	4.07	114.54	110.33
24	b	613	CLA	C3C-C4C-NC	4.07	115.64	110.43
26	b	620	BCR	C30-C25-C26	-4.06	117.08	122.64
26	C	514	BCR	C38-C26-C25	4.06	128.92	124.48
24	c	507	CLA	C2B-C1B-NB	4.06	114.54	110.33
24	B	608	CLA	O2D-CGD-CBD	4.06	118.33	111.23
24	b	618	CLA	C2B-C1B-NB	4.06	114.53	110.33
24	b	616	CLA	O2D-CGD-CBD	4.06	118.32	111.23
26	B	617	BCR	C30-C25-C26	-4.06	117.09	122.64
24	C	512	CLA	C2C-C1C-NC	4.05	114.24	109.98
26	b	620	BCR	C33-C5-C4	-4.05	104.96	113.60
24	B	604	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
24	d	402	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
26	J	101	BCR	C38-C26-C27	-4.05	104.97	113.60
34	e	101	LHG	O7-C7-C8	4.05	120.24	111.48
24	c	507	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
26	D	406	BCR	C37-C22-C21	-4.05	116.26	122.82
24	C	505	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
24	C	511	CLA	C3C-C4C-NC	4.04	115.61	110.43
24	c	507	CLA	C3C-C4C-NC	4.04	115.61	110.43
26	h	101	BCR	C38-C26-C25	4.04	128.89	124.48
24	B	615	CLA	C3C-C4C-NC	4.04	115.60	110.43
24	b	617	CLA	C3C-C4C-NC	4.03	115.60	110.43
24	D	403	CLA	CHD-C1D-ND	-4.03	119.12	124.80
24	B	611	CLA	C3C-C4C-NC	4.03	115.60	110.43
26	B	617	BCR	C29-C30-C25	4.03	116.30	110.44
26	c	514	BCR	C40-C30-C25	4.03	116.57	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	O2D-CGD-CBD	4.03	118.28	111.23
24	B	613	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
24	C	513	CLA	C2C-C1C-NC	4.03	114.22	109.98
26	K	101	BCR	C29-C30-C25	4.03	116.29	110.44
26	A	1009	BCR	C8-C9-C10	4.03	125.35	119.01
26	C	514	BCR	C31-C1-C2	-4.03	93.48	108.95
24	a	407	CLA	C3C-C4C-NC	4.03	115.59	110.43
28	D	408	SQD	O47-C7-C8	4.03	120.19	111.48
24	B	602	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
24	B	612	CLA	C2B-C1B-NB	4.02	114.49	110.33
24	b	617	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
26	C	514	BCR	C1-C6-C5	-4.02	117.15	122.64
24	C	508	CLA	C3C-C4C-NC	4.02	115.57	110.43
24	b	614	CLA	O2D-CGD-CBD	4.02	118.25	111.23
24	B	614	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
24	a	408	CLA	C3B-C4B-NB	4.01	114.11	110.53
24	c	506	CLA	O2D-CGD-CBD	4.01	118.24	111.23
26	T	101	BCR	C37-C22-C21	-4.01	116.32	122.82
24	b	606	CLA	CHD-C1D-ND	-4.01	119.16	124.80
24	b	607	CLA	C3C-C4C-NC	4.00	115.55	110.43
24	c	511	CLA	C2C-C1C-NC	3.99	114.18	109.98
26	a	413	BCR	C30-C25-C26	-3.99	117.18	122.64
26	b	620	BCR	C29-C30-C25	3.99	116.23	110.44
24	b	619	CLA	C3C-C4C-NC	3.98	115.53	110.43
24	b	607	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
35	V	202	HTG	C1'-S1-C1	3.98	109.05	100.45
24	c	503	CLA	CHD-C1D-ND	-3.98	119.20	124.80
26	A	1009	BCR	C35-C13-C14	-3.97	116.38	122.82
24	B	602	CLA	CHD-C1D-ND	-3.97	119.22	124.80
36	c	516	DGD	O2G-C1B-C2B	3.97	120.07	111.48
24	b	614	CLA	CHD-C1D-ND	-3.97	119.22	124.80
24	b	618	CLA	C3C-C4C-NC	3.97	115.51	110.43
26	k	102	BCR	C12-C13-C14	3.96	125.24	119.01
26	k	102	BCR	C40-C30-C25	3.96	116.45	110.24
24	c	506	CLA	C2B-C1B-NB	3.96	114.43	110.33
38	V	201	HEM	CBD-CAD-C3D	-3.95	101.60	112.53
26	y	101	BCR	C1-C6-C5	-3.95	117.23	122.64
26	b	620	BCR	C1-C6-C5	-3.95	117.24	122.64
24	C	513	CLA	C3C-C4C-NC	3.95	115.49	110.43
24	b	611	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
24	B	603	CLA	C3C-C4C-NC	3.94	115.48	110.43
24	A	1008	CLA	C3C-C4C-NC	3.94	115.48	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	408	SQD	O7-S-C6	3.94	112.64	106.76
24	B	613	CLA	C2B-C1B-NB	3.94	114.41	110.33
24	C	503	CLA	O2D-CGD-CBD	3.94	118.11	111.23
24	b	609	CLA	CHD-C1D-ND	-3.93	119.27	124.80
26	A	1009	BCR	C35-C13-C12	-3.93	112.08	118.09
24	C	512	CLA	C3C-C4C-NC	3.93	115.46	110.43
28	D	408	SQD	O6-C1-C2	3.93	114.24	108.27
26	B	618	BCR	C27-C26-C25	3.93	128.01	122.70
26	b	622	BCR	C39-C30-C25	3.92	116.40	110.24
24	c	505	CLA	C1C-C2C-C3C	-3.92	102.85	106.98
24	B	601	CLA	CHD-C1D-ND	-3.92	119.29	124.80
24	c	506	CLA	CHD-C1D-ND	-3.91	119.30	124.80
26	B	619	BCR	C39-C30-C29	-3.91	93.94	108.95
24	b	610	CLA	C3C-C4C-NC	3.91	115.43	110.43
24	C	504	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	B	615	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	c	512	CLA	C3C-C4C-NC	3.90	115.43	110.43
24	B	603	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	c	513	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	C	501	CLA	C3D-C4D-ND	3.90	116.33	109.99
24	b	605	CLA	CHD-C1D-ND	-3.89	119.32	124.80
24	D	405	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
32	b	625	LMT	O1B-C1B-C2B	3.89	117.67	108.09
26	K	101	BCR	C8-C7-C6	3.89	137.39	127.00
24	A	1005	CLA	C3C-C4C-NC	3.89	115.41	110.43
24	B	604	CLA	C3C-C4C-NC	3.88	115.40	110.43
24	c	506	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
26	B	619	BCR	C38-C26-C27	-3.88	105.33	113.60
24	b	618	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
38	f	101	HEM	CBD-CAD-C3D	-3.87	101.82	112.53
26	B	617	BCR	C32-C1-C6	3.87	116.31	110.24
24	b	606	CLA	C3C-C4C-NC	3.87	115.39	110.43
26	A	1009	BCR	C2-C1-C6	3.86	116.05	110.44
24	C	508	CLA	C3D-C4D-ND	3.86	116.26	109.99
24	c	509	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
24	c	504	CLA	CHD-C1D-ND	-3.86	119.38	124.80
24	a	408	CLA	C3D-C4D-ND	3.85	116.25	109.99
24	B	615	CLA	O2D-CGD-CBD	3.85	117.96	111.23
24	c	510	CLA	C3C-C4C-NC	3.85	115.36	110.43
24	B	604	CLA	O2D-CGD-CBD	3.85	117.96	111.23
24	C	506	CLA	C3C-C4C-NC	3.84	115.36	110.43
24	b	613	CLA	O2D-CGD-CBD	3.84	117.95	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C35-C13-C12	-3.84	112.22	118.09
26	K	101	BCR	C35-C13-C14	-3.84	116.59	122.82
24	B	603	CLA	C4-C3-C5	3.84	121.89	115.23
26	K	101	BCR	C38-C26-C27	-3.84	105.41	113.60
24	b	608	CLA	C3C-C4C-NC	3.83	115.34	110.43
24	B	608	CLA	C3C-C4C-NC	3.83	115.33	110.43
36	C	515	DGD	O2G-C1B-C2B	3.83	119.76	111.48
24	d	403	CLA	CHD-C1D-ND	-3.83	119.42	124.80
24	c	512	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
26	b	620	BCR	C37-C22-C21	-3.82	116.62	122.82
24	b	616	CLA	C3C-C4C-NC	3.82	115.33	110.43
34	E	101	LHG	O7-C7-C8	3.82	119.75	111.48
24	c	508	CLA	C3C-C4C-NC	3.82	115.32	110.43
24	b	611	CLA	C3C-C4C-NC	3.82	115.32	110.43
24	C	509	CLA	C3B-C4B-NB	3.82	113.94	110.53
24	D	403	CLA	C3D-C4D-ND	3.82	116.19	109.99
24	B	601	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
26	b	620	BCR	C23-C24-C25	3.81	137.18	127.00
24	B	611	CLA	C2B-C1B-NB	3.81	114.28	110.33
26	t	101	BCR	C1-C6-C5	-3.81	117.43	122.64
24	B	609	CLA	C3D-C4D-ND	3.81	116.18	109.99
26	K	102	BCR	C30-C25-C26	-3.81	117.43	122.64
28	A	1016	SQD	O47-C7-C8	3.81	119.73	111.48
26	A	1009	BCR	C33-C5-C4	-3.81	105.47	113.60
25	D	404	PHO	C1-C2-C3	-3.81	119.95	126.20
26	b	622	BCR	C23-C24-C25	3.81	137.17	127.00
24	b	615	CLA	C3D-C4D-ND	3.80	116.17	109.99
26	C	514	BCR	C35-C13-C12	-3.80	112.28	118.09
24	D	405	CLA	CHD-C1D-ND	-3.80	119.45	124.80
24	B	613	CLA	C3C-C4C-NC	3.80	115.30	110.43
25	a	411	PHO	O2D-CGD-O1D	-3.79	116.47	123.85
24	c	501	CLA	CHD-C1D-ND	-3.79	119.47	124.80
26	K	102	BCR	C35-C13-C12	-3.79	112.30	118.09
24	C	509	CLA	C3C-C4C-NC	3.79	115.29	110.43
24	D	402	CLA	C3B-C4B-NB	3.79	113.91	110.53
24	d	403	CLA	C3D-C4D-ND	3.79	116.14	109.99
24	d	402	CLA	CHD-C1D-ND	-3.79	119.47	124.80
24	B	615	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
24	c	513	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
24	B	606	CLA	C3C-C4C-NC	3.77	115.26	110.43
26	a	413	BCR	C38-C26-C25	3.77	128.60	124.48
26	k	101	BCR	C27-C26-C25	3.77	127.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	C2B-C1B-NB	3.77	114.23	110.33
26	h	101	BCR	C33-C5-C4	-3.77	105.57	113.60
24	B	609	CLA	C3C-C4C-NC	3.76	115.25	110.43
24	B	609	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
24	C	507	CLA	C3C-C4C-NC	3.76	115.25	110.43
24	b	612	CLA	C2B-C1B-NB	3.76	114.22	110.33
24	a	409	CLA	CHD-C1D-ND	-3.76	119.52	124.80
26	t	101	BCR	C36-C18-C19	-3.75	112.36	118.09
24	C	503	CLA	CHD-C1D-ND	-3.75	119.53	124.80
26	d	404	BCR	C40-C30-C39	3.75	119.36	108.63
26	k	102	BCR	C30-C25-C26	-3.74	117.52	122.64
35	b	626	HTG	C1'-S1-C1	3.74	108.54	100.45
24	C	512	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
24	c	509	CLA	C3C-C4C-NC	3.74	115.22	110.43
24	B	607	CLA	O2D-CGD-CBD	3.74	117.76	111.23
24	b	607	CLA	C2B-C1B-NB	3.74	114.20	110.33
26	k	101	BCR	C2-C1-C6	3.73	115.86	110.44
24	c	506	CLA	C3C-C4C-NC	3.73	115.21	110.43
24	C	510	CLA	CHD-C1D-ND	-3.73	119.55	124.80
24	b	615	CLA	C2B-C1B-NB	3.73	114.19	110.33
24	B	611	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
24	a	407	CLA	C3D-C4D-ND	3.72	116.04	109.99
24	d	402	CLA	C3D-C4D-ND	3.72	116.04	109.99
24	c	504	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
26	a	413	BCR	C34-C9-C8	-3.72	112.40	118.09
26	b	620	BCR	C39-C30-C25	3.72	116.08	110.24
24	C	509	CLA	CHD-C1D-ND	-3.72	119.57	124.80
24	b	619	CLA	CHD-C1D-ND	-3.72	119.57	124.80
24	B	609	CLA	C2B-C1B-NB	3.72	114.18	110.33
26	B	617	BCR	C27-C26-C25	3.72	127.73	122.70
26	b	620	BCR	C33-C5-C6	3.72	128.54	124.48
24	D	405	CLA	C3D-C4D-ND	3.72	116.03	109.99
27	D	407	PL9	C40-C39-C41	3.71	121.67	115.23
24	c	503	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
28	c	518	SQD	O9-S-C6	3.71	112.30	106.76
26	h	101	BCR	C39-C30-C25	3.71	116.06	110.24
26	C	514	BCR	C23-C24-C25	3.71	136.91	127.00
24	c	505	CLA	C3C-C4C-NC	3.71	115.18	110.43
34	d	408	LHG	O7-C7-C8	3.71	119.50	111.48
24	C	508	CLA	O2D-CGD-CBD	3.71	117.71	111.23
26	K	101	BCR	C27-C26-C25	3.70	127.71	122.70
24	C	502	CLA	C3D-C4D-ND	3.70	116.00	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C35-C13-C14	-3.70	116.82	122.82
36	h	102	DGD	O2G-C1B-C2B	3.70	119.49	111.48
24	b	619	CLA	C3B-C4B-NB	3.70	113.83	110.53
24	A	1006	CLA	C3C-C4C-NC	3.70	115.17	110.43
24	C	502	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
24	b	613	CLA	CHD-C1D-ND	-3.69	119.60	124.80
28	a	401	SQD	O47-C7-C8	3.69	119.47	111.48
26	c	514	BCR	C4-C5-C6	3.69	127.69	122.70
24	c	501	CLA	C3D-C4D-ND	3.69	115.99	109.99
24	C	503	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
26	D	406	BCR	C36-C18-C17	-3.69	116.84	122.82
24	B	602	CLA	C3C-C4C-NC	3.69	115.15	110.43
24	C	503	CLA	C3C-C4C-NC	3.69	115.15	110.43
24	C	506	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
26	t	101	BCR	C23-C24-C25	3.69	136.84	127.00
24	C	510	CLA	C3D-C4D-ND	3.68	115.97	109.99
24	c	511	CLA	C3C-C4C-NC	3.68	115.15	110.43
24	c	503	CLA	O2D-CGD-CBD	3.68	117.66	111.23
26	H	101	BCR	C23-C24-C25	3.68	136.82	127.00
24	B	614	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
24	b	606	CLA	C3D-C4D-ND	3.67	115.96	109.99
26	K	101	BCR	C24-C23-C22	3.67	131.67	126.23
26	a	413	BCR	C35-C13-C12	-3.67	112.48	118.09
24	b	613	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
28	A	1011	SQD	O6-C1-C2	3.66	113.84	108.27
24	B	610	CLA	CHD-C1D-ND	-3.66	119.65	124.80
24	b	617	CLA	C4-C3-C5	3.66	121.58	115.23
26	K	101	BCR	C35-C13-C12	-3.66	112.50	118.09
24	c	504	CLA	C3D-C4D-ND	3.65	115.92	109.99
26	T	101	BCR	C23-C24-C25	3.64	136.72	127.00
24	C	510	CLA	C3C-C4C-NC	3.64	115.09	110.43
24	B	603	CLA	C3B-C4B-NB	3.64	113.78	110.53
24	C	507	CLA	CHD-C1D-ND	-3.64	119.68	124.80
24	b	617	CLA	C3D-C4D-ND	3.64	115.90	109.99
24	c	508	CLA	C3D-C4D-ND	3.64	115.90	109.99
26	h	101	BCR	C39-C30-C29	-3.63	95.00	108.95
24	b	615	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	D	402	CLA	CHD-C1D-ND	-3.63	119.70	124.80
24	b	616	CLA	C3B-C4B-NB	3.63	113.77	110.53
24	C	504	CLA	C3C-C4C-NC	3.63	115.07	110.43
24	B	607	CLA	C3D-C4D-ND	3.62	115.88	109.99
24	A	1008	CLA	C3D-C4D-ND	3.62	115.88	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	102	LMT	C1'-O5'-C5'	3.62	120.79	113.72
26	D	406	BCR	C40-C30-C29	-3.62	95.05	108.95
24	b	611	CLA	CHD-C1D-ND	-3.62	119.71	124.80
24	C	513	CLA	C1C-C2C-C3C	-3.62	103.18	106.98
26	K	102	BCR	C40-C30-C29	-3.62	95.07	108.95
24	B	610	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
28	c	518	SQD	O6-C1-C2	3.61	113.76	108.27
24	a	407	CLA	CHD-C1D-ND	-3.61	119.72	124.80
24	c	510	CLA	C3D-C4D-ND	3.61	115.86	109.99
24	B	616	CLA	CHD-C1D-ND	-3.61	119.72	124.80
24	C	505	CLA	C3C-C4C-NC	3.61	115.05	110.43
24	b	604	CLA	C3C-C4C-NC	3.61	115.05	110.43
24	a	412	CLA	C3D-C4D-ND	3.61	115.85	109.99
35	b	630	HTG	C1-O5-C5	3.60	119.03	112.56
24	c	502	CLA	C3C-C4C-NC	3.60	115.05	110.43
26	y	101	BCR	C32-C1-C6	3.60	115.89	110.24
26	y	101	BCR	C8-C9-C10	3.60	124.67	119.01
24	b	604	CLA	C1C-C2C-C3C	-3.60	103.20	106.98
24	b	608	CLA	C3D-C4D-ND	3.60	115.83	109.99
29	c	519	LMG	O7-C10-C11	3.60	119.26	111.48
36	c	515	DGD	O2G-C1B-C2B	3.59	119.25	111.48
24	A	1005	CLA	C3D-C4D-ND	3.59	115.83	109.99
26	A	1009	BCR	C29-C30-C25	3.59	115.65	110.44
26	y	101	BCR	C4-C5-C6	3.58	127.55	122.70
24	b	610	CLA	CHD-C1D-ND	-3.58	119.76	124.80
24	C	508	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
24	b	610	CLA	C3B-C4B-NB	3.58	113.73	110.53
26	k	102	BCR	C39-C30-C25	3.58	115.86	110.24
24	D	405	CLA	C3C-C4C-NC	3.58	115.02	110.43
24	B	608	CLA	C3B-C4B-NB	3.58	113.73	110.53
24	C	506	CLA	CHD-C1D-ND	-3.58	119.76	124.80
24	B	605	CLA	CHD-C1D-ND	-3.57	119.78	124.80
24	c	511	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
26	H	101	BCR	C34-C9-C10	-3.57	117.04	122.82
24	B	601	CLA	C3C-C4C-NC	3.57	115.00	110.43
24	C	510	CLA	C3B-C4B-NB	3.56	113.71	110.53
24	B	613	CLA	O2D-CGD-CBD	3.56	117.46	111.23
24	a	409	CLA	C3C-C4C-NC	3.56	114.99	110.43
24	B	607	CLA	C3C-C4C-NC	3.56	114.99	110.43
24	B	609	CLA	CHD-C1D-ND	-3.56	119.80	124.80
24	C	504	CLA	C3B-C4B-NB	3.55	113.70	110.53
24	d	403	CLA	C3C-C4C-NC	3.55	114.98	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C3B-C4B-NB	3.55	113.70	110.53
26	b	622	BCR	C38-C26-C25	3.55	128.35	124.48
24	c	502	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
24	a	409	CLA	C3D-C4D-ND	3.55	115.75	109.99
24	B	616	CLA	C1C-C2C-C3C	-3.54	103.26	106.98
24	b	605	CLA	C1C-C2C-C3C	-3.54	103.26	106.98
24	B	608	CLA	C3D-C4D-ND	3.54	115.73	109.99
26	D	406	BCR	C34-C9-C8	-3.53	112.69	118.09
24	c	508	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
26	c	514	BCR	C31-C1-C2	-3.53	95.38	108.95
24	A	1006	CLA	C3B-C4B-NB	3.53	113.68	110.53
26	B	617	BCR	C38-C26-C25	3.53	128.33	124.48
26	k	101	BCR	C39-C30-C25	3.53	115.77	110.24
26	a	413	BCR	C31-C1-C6	3.52	115.77	110.24
24	B	613	CLA	CHD-C1D-ND	-3.52	119.84	124.80
24	B	614	CLA	C3D-C4D-ND	3.52	115.70	109.99
24	b	609	CLA	C3C-C4C-NC	3.52	114.94	110.43
24	c	507	CLA	CHD-C1D-ND	-3.52	119.85	124.80
24	c	502	CLA	CAC-C3C-C4C	3.51	129.36	124.79
24	a	412	CLA	C3B-C4B-NB	3.51	113.67	110.53
24	c	509	CLA	CHD-C1D-ND	-3.51	119.86	124.80
24	B	605	CLA	C4-C3-C5	3.51	121.32	115.23
24	c	509	CLA	C3D-C4D-ND	3.51	115.69	109.99
24	c	512	CLA	C3D-C4D-ND	3.50	115.68	109.99
29	d	409	LMG	O7-C10-C11	3.50	119.06	111.48
24	a	408	CLA	C3C-C4C-NC	3.50	114.92	110.43
26	A	1009	BCR	C1-C6-C5	-3.50	117.85	122.64
36	c	517	DGD	O2G-C1B-C2B	3.50	119.05	111.48
24	A	1006	CLA	C3D-C4D-ND	3.49	115.67	109.99
29	a	415	LMG	O7-C10-C11	3.49	119.04	111.48
24	b	618	CLA	O2D-CGD-CBD	3.49	117.33	111.23
26	H	101	BCR	C38-C26-C25	3.49	128.29	124.48
26	k	101	BCR	C36-C18-C19	-3.49	112.76	118.09
24	b	612	CLA	C3C-C4C-NC	3.48	114.89	110.43
24	B	611	CLA	C3D-C4D-ND	3.48	115.65	109.99
24	b	614	CLA	C3D-C4D-ND	3.48	115.64	109.99
24	B	613	CLA	C3B-C4B-NB	3.47	113.63	110.53
24	C	511	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
29	A	1012	LMG	O7-C10-C11	3.47	118.99	111.48
24	b	614	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
26	C	514	BCR	C8-C9-C10	3.47	124.46	119.01
24	b	615	CLA	CHD-C1D-ND	-3.46	119.93	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	BCR	C33-C5-C6	3.46	128.26	124.48
24	c	502	CLA	C3D-C4D-ND	3.46	115.60	109.99
24	B	612	CLA	C1C-C2C-C3C	-3.45	103.35	106.98
24	b	604	CLA	CHD-C1D-ND	-3.45	119.94	124.80
24	B	605	CLA	C3D-C4D-ND	3.45	115.59	109.99
29	m	102	LMG	O8-C28-C29	3.45	122.35	111.83
24	c	505	CLA	C3D-C4D-ND	3.45	115.59	109.99
24	a	412	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
24	C	506	CLA	C3D-C4D-ND	3.44	115.58	109.99
29	c	520	LMG	O7-C10-C11	3.44	118.92	111.48
24	B	606	CLA	C3D-C4D-ND	3.44	115.57	109.99
38	F	101	HEM	CBD-CAD-C3D	-3.44	103.03	112.53
24	b	605	CLA	C3C-C4C-NC	3.43	114.83	110.43
24	b	619	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
24	A	1005	CLA	C3B-C4B-NB	3.42	113.59	110.53
26	d	404	BCR	C2-C1-C6	3.42	115.41	110.44
24	B	616	CLA	C3D-C4D-ND	3.42	115.55	109.99
24	c	505	CLA	CHD-C1D-ND	-3.42	119.99	124.80
35	V	202	HTG	O5-C1-C2	-3.41	105.61	110.32
24	c	502	CLA	CHD-C1D-ND	-3.41	120.00	124.80
24	D	402	CLA	O2D-CGD-CBD	3.41	117.19	111.23
24	B	607	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
24	B	613	CLA	C3D-C4D-ND	3.40	115.52	109.99
24	c	504	CLA	C3C-C4C-NC	3.40	114.79	110.43
24	c	503	CLA	C3C-C4C-NC	3.40	114.79	110.43
26	D	406	BCR	C39-C30-C25	-3.40	104.91	110.24
24	b	606	CLA	C4-C3-C5	3.40	121.12	115.23
24	C	513	CLA	C3D-C4D-ND	3.40	115.51	109.99
29	C	518	LMG	O7-C10-C11	3.39	118.81	111.48
24	B	612	CLA	CHD-C1D-ND	-3.39	120.03	124.80
24	b	609	CLA	C3D-C4D-ND	3.39	115.50	109.99
24	C	513	CLA	CHD-C1D-ND	-3.39	120.04	124.80
24	C	502	CLA	CHD-C1D-ND	-3.38	120.04	124.80
26	c	514	BCR	C35-C13-C12	-3.38	112.92	118.09
24	b	611	CLA	C3D-C4D-ND	3.38	115.47	109.99
24	D	405	CLA	O2D-CGD-CBD	3.38	117.13	111.23
26	B	617	BCR	C2-C1-C6	3.38	115.34	110.44
27	A	1010	PL9	C37-C38-C39	-3.37	119.90	127.62
26	a	413	BCR	C37-C22-C21	-3.37	117.35	122.82
24	c	508	CLA	CHD-C1D-ND	-3.37	120.06	124.80
34	D	411	LHG	O7-C7-C8	3.37	118.77	111.48
24	B	603	CLA	C3D-C4D-ND	3.37	115.46	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C4-C5-C6	3.37	127.25	122.70
27	A	1010	PL9	C7-C3-C4	3.36	119.68	116.91
24	C	505	CLA	C3D-C4D-ND	3.36	115.45	109.99
26	b	622	BCR	C1-C6-C5	-3.36	118.05	122.64
26	K	101	BCR	C31-C1-C2	-3.36	96.06	108.95
24	b	613	CLA	C3D-C4D-ND	3.36	115.44	109.99
24	b	612	CLA	CHD-C1D-ND	-3.36	120.08	124.80
24	B	611	CLA	CHD-C1D-ND	-3.35	120.08	124.80
24	a	407	CLA	C3B-C4B-NB	3.35	113.52	110.53
24	b	615	CLA	C3B-C4B-NB	3.35	113.52	110.53
26	b	620	BCR	C40-C30-C25	3.34	115.49	110.24
24	c	508	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
24	C	505	CLA	CHD-C1D-ND	-3.34	120.11	124.80
24	b	612	CLA	C3D-C4D-ND	3.34	115.41	109.99
26	B	619	BCR	C38-C26-C25	3.34	128.12	124.48
24	b	610	CLA	C3D-C4D-ND	3.34	115.41	109.99
24	c	513	CLA	C3C-C4C-NC	3.33	114.70	110.43
24	C	512	CLA	C3D-C4D-ND	3.33	115.41	109.99
24	B	612	CLA	C4C-C3C-C2C	-3.33	102.05	106.89
24	B	615	CLA	C3B-C4B-NB	3.33	113.50	110.53
26	k	102	BCR	C4-C5-C6	3.33	127.20	122.70
24	C	509	CLA	C3D-C4D-ND	3.32	115.39	109.99
24	C	508	CLA	CHD-C1D-ND	-3.32	120.13	124.80
24	C	508	CLA	C3B-C4B-NB	3.32	113.49	110.53
24	B	610	CLA	C3D-C4D-ND	3.32	115.38	109.99
26	H	101	BCR	C39-C30-C29	-3.32	96.21	108.95
29	B	622	LMG	O7-C10-C11	3.32	118.66	111.48
24	C	504	CLA	C3D-C4D-ND	3.31	115.37	109.99
26	B	618	BCR	C40-C30-C25	3.31	115.44	110.24
24	C	501	CLA	C3C-C4C-NC	3.31	114.67	110.43
24	b	614	CLA	C3B-C4B-NB	3.31	113.48	110.53
24	A	1005	CLA	O2D-CGD-CBD	3.30	117.01	111.23
24	B	604	CLA	C3B-C4B-NB	3.30	113.48	110.53
24	D	402	CLA	CMC-C2C-C1C	3.30	130.19	125.03
24	B	605	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
24	C	508	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
24	B	607	CLA	C4-C3-C5	3.29	120.95	115.23
24	B	605	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
26	A	1009	BCR	C38-C26-C25	3.28	128.06	124.48
24	b	619	CLA	CAC-C3C-C4C	3.27	129.05	124.79
24	B	608	CLA	CAC-C3C-C4C	3.27	129.05	124.79
24	B	604	CLA	C3D-C4D-ND	3.27	115.31	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	413	BCR	C35-C13-C14	-3.27	117.52	122.82
24	b	608	CLA	C4-C3-C5	3.27	120.90	115.23
32	t	103	LMT	C2'-C3'-C4'	3.27	117.10	109.68
24	B	602	CLA	C3D-C4D-ND	3.26	115.29	109.99
24	C	511	CLA	C3D-C4D-ND	3.26	115.28	109.99
24	b	616	CLA	C3D-C4D-ND	3.26	115.28	109.99
24	c	513	CLA	C3D-C4D-ND	3.26	115.28	109.99
24	B	610	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
26	d	404	BCR	C23-C24-C25	3.25	135.69	127.00
26	c	514	BCR	C28-C27-C26	3.25	119.86	114.06
24	C	511	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
24	c	504	CLA	CAC-C3C-C4C	3.24	129.01	124.79
26	y	101	BCR	C39-C30-C29	-3.24	96.51	108.95
26	k	101	BCR	C39-C30-C29	-3.24	96.52	108.95
26	B	617	BCR	C33-C5-C6	3.24	128.01	124.48
24	c	506	CLA	C3B-C4B-NB	3.23	113.42	110.53
26	c	514	BCR	C31-C1-C6	3.23	115.31	110.24
24	b	607	CLA	C3D-C4D-ND	3.23	115.24	109.99
24	B	615	CLA	C3D-C4D-ND	3.23	115.23	109.99
24	B	615	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
24	d	403	CLA	C3B-C4B-NB	3.22	113.41	110.53
24	C	501	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
26	T	101	BCR	C1-C6-C5	-3.22	118.24	122.64
24	c	506	CLA	C3D-C4D-ND	3.22	115.22	109.99
24	c	509	CLA	C3B-C4B-NB	3.22	113.40	110.53
26	C	514	BCR	C33-C5-C4	-3.22	106.74	113.60
24	b	618	CLA	C3D-C4D-ND	3.22	115.21	109.99
24	c	501	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
24	C	513	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
24	B	616	CLA	C4C-C3C-C2C	-3.21	102.21	106.89
24	C	506	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
24	c	501	CLA	C3C-C4C-NC	3.21	114.54	110.43
24	A	1008	CLA	C3B-C4B-NB	3.21	113.39	110.53
24	C	502	CLA	C3B-C4B-NB	3.20	113.39	110.53
24	b	619	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
26	c	514	BCR	C39-C30-C29	-3.20	96.65	108.95
24	b	607	CLA	CAC-C3C-C4C	3.20	128.96	124.79
26	b	622	BCR	C32-C1-C6	3.20	115.26	110.24
27	A	1010	PL9	C25-C24-C26	3.20	120.78	115.23
24	b	619	CLA	C3D-C4D-ND	3.19	115.17	109.99
26	K	101	BCR	C33-C5-C4	-3.19	106.79	113.60
26	B	618	BCR	C39-C30-C29	-3.19	96.70	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	CAC-C3C-C4C	3.18	128.93	124.79
26	y	101	BCR	C2-C1-C6	3.18	115.06	110.44
26	b	621	BCR	C31-C1-C6	3.18	115.23	110.24
26	h	101	BCR	C1-C6-C5	-3.18	118.29	122.64
24	a	412	CLA	CHD-C1D-ND	-3.18	120.33	124.80
24	c	511	CLA	C3D-C4D-ND	3.18	115.15	109.99
24	C	507	CLA	C3D-C4D-ND	3.17	115.14	109.99
34	d	406	LHG	O8-C23-C24	3.17	121.51	111.83
24	b	604	CLA	C3D-C4D-ND	3.17	115.14	109.99
26	D	406	BCR	C35-C13-C14	-3.17	117.68	122.82
24	B	614	CLA	CHD-C1D-ND	-3.17	120.34	124.80
26	B	618	BCR	C33-C5-C4	-3.17	106.84	113.60
26	K	102	BCR	C39-C30-C29	-3.17	96.79	108.95
24	C	501	CLA	C3B-C4B-NB	3.16	113.35	110.53
24	b	614	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
25	A	1007	PHO	CBC-CAC-C3C	-3.16	108.35	112.87
24	b	613	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
24	B	601	CLA	O2A-CGA-CBA	3.16	121.46	111.83
24	B	616	CLA	C3B-C4B-NB	3.16	113.35	110.53
26	H	101	BCR	C33-C5-C6	3.16	127.93	124.48
26	b	621	BCR	C34-C9-C8	-3.15	113.27	118.09
27	d	405	PL9	C7-C8-C9	-3.15	121.40	126.83
26	y	101	BCR	C27-C26-C25	3.15	126.96	122.70
24	B	614	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
24	b	615	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
24	C	502	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
27	a	414	PL9	C7-C3-C4	3.15	119.50	116.91
24	b	616	CLA	CHD-C1D-ND	-3.15	120.38	124.80
24	B	607	CLA	CHD-C1D-ND	-3.14	120.38	124.80
24	B	601	CLA	C3D-C4D-ND	3.14	115.09	109.99
24	d	403	CLA	O2D-CGD-O1D	-3.14	117.75	123.85
26	B	618	BCR	C31-C1-C2	-3.13	96.92	108.95
24	c	504	CLA	C3B-C4B-NB	3.13	113.33	110.53
24	d	402	CLA	C3B-C4B-NB	3.13	113.32	110.53
32	i	102	LMT	O5'-C5'-C4'	3.13	116.19	109.72
24	b	605	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
35	V	202	HTG	C1-C2-C3	-3.12	104.44	110.55
24	B	603	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
24	c	510	CLA	CHD-C1D-ND	-3.12	120.41	124.80
28	D	408	SQD	C1-O5-C5	-3.12	107.62	113.72
24	B	609	CLA	CAC-C3C-C4C	3.12	128.85	124.79
26	T	101	BCR	C38-C26-C25	3.12	127.89	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
24	A	1005	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
36	C	517	DGD	O2G-C1B-C2B	3.12	118.22	111.48
24	c	511	CLA	CHD-C1D-ND	-3.12	120.42	124.80
24	D	402	CLA	C1-C2-C3	-3.12	121.09	126.20
26	B	617	BCR	C39-C30-C25	3.12	115.13	110.24
24	b	614	CLA	CAC-C3C-C4C	3.11	128.84	124.79
24	c	512	CLA	CHD-C1D-ND	-3.11	120.42	124.80
34	b	624	LHG	O7-C7-C8	3.11	118.21	111.48
24	C	505	CLA	C3B-C4B-NB	3.11	113.31	110.53
24	b	604	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
24	c	508	CLA	C3B-C4B-NB	3.11	113.30	110.53
28	f	102	SQD	C3-C4-C5	3.11	115.86	110.23
24	B	611	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
26	a	413	BCR	C23-C24-C25	3.10	135.29	127.00
32	b	631	LMT	C1B-O5B-C5B	3.10	119.78	113.72
26	B	618	BCR	C39-C30-C25	3.10	115.11	110.24
24	B	609	CLA	CMB-C2B-C1B	3.10	130.14	125.42
26	b	622	BCR	C39-C30-C29	-3.10	97.05	108.95
24	B	604	CLA	CAC-C3C-C4C	3.10	128.82	124.79
26	k	102	BCR	C39-C30-C29	-3.10	97.06	108.95
34	D	409	LHG	O8-C23-C24	3.09	121.27	111.83
24	A	1008	CLA	CHD-C1D-ND	-3.09	120.46	124.80
24	C	509	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	B	604	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
26	A	1009	BCR	C4-C5-C6	3.08	126.87	122.70
24	b	605	CLA	C3D-C4D-ND	3.08	114.99	109.99
29	B	622	LMG	O8-C28-C29	3.08	121.22	111.83
26	h	101	BCR	C8-C9-C10	3.07	123.84	119.01
24	c	506	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
24	b	615	CLA	C4-C3-C5	3.07	120.55	115.23
34	B	621	LHG	O7-C7-C8	3.07	118.11	111.48
24	b	609	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
26	t	101	BCR	C39-C30-C25	3.06	115.05	110.24
24	D	402	CLA	C4-C3-C5	3.06	120.54	115.23
25	D	404	PHO	O2D-CGD-O1D	-3.06	117.89	123.85
24	c	512	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
24	c	511	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
26	J	101	BCR	C34-C9-C10	-3.06	117.86	122.82
35	C	522	HTG	O5-C5-C4	3.06	115.21	109.70
24	c	510	CLA	C3B-C4B-NB	3.06	113.26	110.53
26	b	621	BCR	C38-C26-C25	3.06	127.82	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	101	BCR	C27-C26-C25	3.05	126.83	122.70
28	A	1011	SQD	O9-S-C6	3.05	111.31	106.76
24	b	615	CLA	CAC-C3C-C4C	3.05	128.76	124.79
24	B	612	CLA	C3B-C4B-NB	3.05	113.25	110.53
24	B	606	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	A	1006	CLA	CMC-C2C-C1C	3.05	129.80	125.03
24	B	606	CLA	C1-O2A-CGA	3.04	124.01	116.65
24	C	511	CLA	CHD-C1D-ND	-3.04	120.53	124.80
26	H	101	BCR	C28-C27-C26	3.04	119.47	114.06
26	k	101	BCR	C34-C9-C8	-3.03	113.45	118.09
25	A	1007	PHO	O1D-CGD-CBD	-3.03	120.12	124.72
24	B	604	CLA	CED-O2D-CGD	3.03	122.80	115.92
35	C	522	HTG	O5-C1-C2	3.03	114.49	110.32
27	A	1010	PL9	C32-C33-C34	-3.03	120.69	127.62
38	v	201	HEM	CBD-CAD-C3D	-3.03	104.16	112.53
34	D	409	LHG	O7-C7-C8	3.02	118.02	111.48
24	b	617	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
24	B	608	CLA	CHD-C1D-ND	-3.01	120.56	124.80
24	c	502	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
24	a	409	CLA	C3B-C4B-NB	3.00	113.21	110.53
24	b	608	CLA	C3B-C4B-NB	3.00	113.20	110.53
26	h	101	BCR	C33-C5-C6	2.99	127.75	124.48
36	c	515	DGD	O1G-C1A-C2A	2.99	120.96	111.83
24	b	612	CLA	CAC-C3C-C4C	2.99	128.68	124.79
24	B	608	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
24	D	402	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
28	b	623[A]	SQD	O48-C23-C24	2.99	120.95	111.83
25	a	411	PHO	C4-C3-C5	2.99	120.42	115.23
24	b	607	CLA	C3B-C4B-NB	2.99	113.20	110.53
24	B	608	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
24	B	606	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
26	d	404	BCR	C39-C30-C29	-2.98	97.52	108.95
24	d	402	CLA	C4-C3-C5	2.98	120.39	115.23
24	c	509	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
24	b	612	CLA	CMB-C2B-C1B	2.97	129.95	125.42
26	t	101	BCR	C1-C6-C7	2.97	123.71	115.65
24	d	402	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
24	C	502	CLA	CAC-C3C-C4C	2.97	128.65	124.79
24	B	606	CLA	C3B-C4B-NB	2.97	113.18	110.53
24	c	503	CLA	C3D-C4D-ND	2.97	114.81	109.99
24	b	617	CLA	C3B-C4B-NB	2.97	113.18	110.53
24	B	601	CLA	C4C-C3C-C2C	-2.96	102.58	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	406	BCR	C34-C9-C10	-2.96	118.02	122.82
24	b	618	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
24	c	510	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
26	d	404	BCR	C35-C13-C14	-2.96	118.02	122.82
24	c	507	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
26	b	620	BCR	C31-C1-C2	-2.96	97.59	108.95
26	B	619	BCR	C23-C24-C25	2.96	134.90	127.00
26	d	404	BCR	C34-C9-C8	-2.96	113.57	118.09
24	a	407	CLA	O2D-CGD-CBD	2.95	116.39	111.23
24	B	614	CLA	O1D-CGD-CBD	-2.95	118.70	124.52
24	c	509	CLA	CAC-C3C-C4C	2.95	128.62	124.79
26	K	101	BCR	C39-C30-C25	2.95	114.86	110.24
24	B	616	CLA	O2A-CGA-CBA	2.95	120.82	111.83
24	b	604	CLA	O2A-CGA-CBA	2.94	120.81	111.83
26	b	621	BCR	C33-C5-C4	-2.94	107.32	113.60
24	b	611	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
26	h	101	BCR	C4-C5-C6	2.94	126.68	122.70
24	c	509	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
24	C	511	CLA	CMB-C2B-C1B	2.94	129.89	125.42
24	b	607	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
36	c	517	DGD	O1G-C1A-C2A	2.94	120.78	111.83
24	c	501	CLA	C3B-C4B-NB	2.93	113.15	110.53
26	b	621	BCR	C33-C5-C6	2.93	127.69	124.48
34	E	101	LHG	O8-C23-C24	2.93	120.78	111.83
26	H	101	BCR	C2-C1-C6	2.93	114.70	110.44
24	C	503	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
27	A	1010	PL9	C10-C9-C11	2.93	120.32	115.23
25	a	410	PHO	O1D-CGD-CBD	-2.93	120.28	124.72
24	B	604	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
24	C	509	CLA	C4C-C3C-C2C	-2.92	102.63	106.89
24	B	604	CLA	O1D-CGD-CBD	-2.92	118.75	124.52
28	b	623[B]	SQD	O48-C23-C24	2.92	120.74	111.83
26	t	101	BCR	C8-C9-C10	2.92	123.60	119.01
34	D	410	LHG	O7-C7-C8	2.92	117.80	111.48
24	C	510	CLA	CMB-C2B-C1B	2.92	129.86	125.42
26	K	101	BCR	C33-C5-C6	2.92	127.67	124.48
24	C	501	CLA	CAC-C3C-C4C	2.92	128.59	124.79
24	a	407	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
24	B	615	CLA	CED-O2D-CGD	2.92	122.53	115.92
26	b	620	BCR	C37-C22-C23	-2.91	113.64	118.09
24	C	510	CLA	CBC-CAC-C3C	-2.91	104.52	112.42
26	A	1009	BCR	C33-C5-C6	2.91	127.66	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	CBC-CAC-C3C	-2.91	104.52	112.42
24	b	605	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
24	C	512	CLA	C4-C3-C5	2.91	120.28	115.23
24	C	504	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
26	d	404	BCR	C30-C25-C24	2.91	123.53	115.65
24	b	607	CLA	O2A-CGA-CBA	2.91	120.69	111.83
24	C	503	CLA	C3D-C4D-ND	2.91	114.71	109.99
36	H	102	DGD	O2G-C1B-C2B	2.90	117.77	111.48
24	B	609	CLA	C3B-C4B-NB	2.90	113.12	110.53
24	D	405	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	c	505	CLA	CAC-C3C-C4C	2.90	128.56	124.79
24	D	405	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
24	c	508	CLA	C4-C3-C5	2.90	120.26	115.23
24	c	510	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
28	f	102	SQD	O6-C1-C2	2.90	112.67	108.27
26	D	406	BCR	C33-C5-C6	2.90	127.64	124.48
34	d	406	LHG	O7-C7-C8	2.90	117.74	111.48
24	b	610	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
24	c	507	CLA	C3D-C4D-ND	2.89	114.69	109.99
24	d	402	CLA	O2A-CGA-CBA	2.89	120.64	111.83
24	B	609	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
26	T	101	BCR	C36-C18-C19	-2.89	113.68	118.09
24	c	503	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
24	b	610	CLA	CED-O2D-CGD	2.88	122.46	115.92
24	c	504	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
24	c	512	CLA	C4-C3-C5	2.88	120.23	115.23
26	T	101	BCR	C8-C9-C10	2.88	123.53	119.01
24	b	617	CLA	CHD-C1D-ND	-2.87	120.76	124.80
26	K	102	BCR	C4-C5-C6	2.87	126.59	122.70
27	a	414	PL9	C25-C24-C26	2.87	120.22	115.23
27	d	405	PL9	C40-C39-C41	2.87	120.21	115.23
24	a	412	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
24	D	403	CLA	CBC-CAC-C3C	-2.87	104.64	112.42
26	D	406	BCR	C32-C1-C2	-2.87	97.94	108.95
24	c	505	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
24	A	1008	CLA	C4-C3-C5	2.86	120.20	115.23
26	B	618	BCR	C35-C13-C14	-2.86	118.18	122.82
26	k	101	BCR	C31-C1-C2	-2.86	97.96	108.95
29	c	521	LMG	O8-C28-C29	2.86	120.56	111.83
26	B	619	BCR	C37-C22-C21	-2.86	118.18	122.82
24	C	504	CLA	CAC-C3C-C4C	2.86	128.51	124.79
24	B	607	CLA	CMC-C2C-C1C	2.86	129.50	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	617	BCR	C33-C5-C4	-2.86	107.50	113.60
24	b	606	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	D	407	PL9	C25-C24-C26	2.85	120.17	115.23
24	C	504	CLA	C4-C3-C5	2.85	120.17	115.23
24	b	609	CLA	C3B-C4B-NB	2.85	113.07	110.53
26	H	101	BCR	C1-C6-C5	-2.85	118.75	122.64
26	B	619	BCR	C27-C26-C25	2.84	126.55	122.70
24	C	505	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
26	y	101	BCR	C35-C13-C14	-2.84	118.22	122.82
26	B	619	BCR	C31-C1-C2	-2.84	98.05	108.95
26	A	1009	BCR	C32-C1-C6	2.84	114.69	110.24
24	B	602	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
24	B	602	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	b	620	BCR	C34-C9-C8	-2.83	113.76	118.09
28	a	401	SQD	O9-S-C6	2.83	110.98	106.76
24	a	412	CLA	CAC-C3C-C4C	2.83	128.47	124.79
27	A	1010	PL9	C35-C34-C36	2.83	120.14	115.23
24	c	513	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
24	c	502	CLA	C3B-C4B-NB	2.83	113.06	110.53
24	C	505	CLA	CMB-C2B-C1B	2.83	129.73	125.42
26	T	101	BCR	C35-C13-C12	-2.83	113.77	118.09
24	b	605	CLA	C1-O2A-CGA	2.83	123.49	116.65
26	b	621	BCR	C1-C6-C5	-2.82	118.78	122.64
24	b	609	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
24	b	616	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
24	c	512	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
29	C	518	LMG	O8-C28-C29	2.82	120.43	111.83
26	D	406	BCR	C39-C30-C29	-2.82	98.13	108.95
24	B	613	CLA	CMC-C2C-C1C	2.82	129.44	125.03
24	B	610	CLA	C3B-C4B-NB	2.82	113.04	110.53
26	k	101	BCR	C37-C22-C21	-2.82	118.25	122.82
32	A	1018	LMT	C1B-O5B-C5B	2.81	119.22	113.72
26	K	102	BCR	C8-C9-C10	2.81	123.43	119.01
26	k	101	BCR	C4-C5-C6	2.81	126.50	122.70
26	b	620	BCR	C4-C5-C6	2.81	126.50	122.70
26	J	101	BCR	C40-C30-C29	-2.81	98.17	108.95
24	A	1006	CLA	C4-C3-C5	2.81	120.10	115.23
32	B	623	LMT	C2'-C3'-C4'	2.81	116.05	109.68
28	A	1016	SQD	O48-C23-C24	2.81	120.39	111.83
29	A	1012	LMG	O8-C28-C29	2.81	120.39	111.83
28	A	1016	SQD	O6-C1-C2	2.81	112.53	108.27
24	D	403	CLA	CMC-C2C-C1C	2.80	129.42	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C3B-C4B-NB	2.80	113.03	110.53
24	b	617	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
24	C	506	CLA	C3B-C4B-NB	2.80	113.03	110.53
24	C	513	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
34	D	411	LHG	O8-C23-C24	2.80	120.38	111.83
26	d	404	BCR	C36-C18-C17	-2.80	118.28	122.82
24	B	616	CLA	CAC-C3C-C4C	2.80	128.43	124.79
26	b	622	BCR	C32-C1-C2	-2.80	98.20	108.95
24	b	619	CLA	CBC-CAC-C3C	-2.80	104.84	112.42
24	B	610	CLA	O2A-CGA-CBA	2.79	120.36	111.83
26	D	406	BCR	C27-C26-C25	2.79	126.48	122.70
24	c	506	CLA	CAC-C3C-C4C	2.79	128.42	124.79
24	B	616	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	b	615	CLA	CED-O2D-CGD	2.79	122.24	115.92
24	A	1008	CLA	C4C-C3C-C2C	-2.79	102.84	106.89
26	h	101	BCR	C2-C1-C6	2.79	114.49	110.44
24	a	409	CLA	CMB-C2B-C1B	2.79	129.66	125.42
24	B	603	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
24	b	606	CLA	C3B-C4B-NB	2.78	113.02	110.53
25	a	411	PHO	CMB-C2B-C3B	2.78	130.24	124.68
26	y	101	BCR	C34-C9-C8	-2.78	113.84	118.09
28	A	1016	SQD	O9-S-C6	2.78	110.91	106.76
24	B	610	CLA	C4-C3-C5	2.78	120.05	115.23
24	b	606	CLA	CMC-C2C-C1C	2.78	129.38	125.03
24	B	615	CLA	C1-O2A-CGA	2.78	123.37	116.65
24	B	606	CLA	C4-C3-C5	2.78	120.05	115.23
24	B	612	CLA	CAC-C3C-C4C	2.77	128.40	124.79
24	c	511	CLA	C4-C3-C5	2.77	120.04	115.23
26	b	622	BCR	C8-C9-C10	2.77	123.37	119.01
24	B	611	CLA	C1-C2-C3	-2.77	121.66	126.20
24	B	614	CLA	C4-C3-C5	2.77	120.04	115.23
24	B	615	CLA	CAC-C3C-C4C	2.77	128.40	124.79
24	c	505	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
29	a	415	LMG	O8-C28-C29	2.77	120.28	111.83
24	B	601	CLA	CMB-C2B-C1B	2.77	129.63	125.42
24	b	604	CLA	C1-O2A-CGA	2.77	123.35	116.65
26	b	620	BCR	C35-C13-C14	-2.76	118.34	122.82
27	a	414	PL9	C37-C38-C39	-2.76	121.30	127.62
24	B	612	CLA	C4-C3-C5	2.76	120.02	115.23
24	C	506	CLA	CAC-C3C-C4C	2.76	128.38	124.79
24	C	501	CLA	C1-O2A-CGA	2.76	123.33	116.65
28	a	401	SQD	O48-C23-C24	2.75	120.23	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	C4D-C3D-CAD	2.75	111.10	108.11
24	b	604	CLA	C4D-C3D-CAD	2.75	111.10	108.11
24	c	513	CLA	O2A-CGA-CBA	2.75	120.22	111.83
24	B	604	CLA	O2A-CGA-CBA	2.75	120.22	111.83
24	b	614	CLA	C1-C2-C3	-2.75	121.69	126.20
24	b	606	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
28	f	102	SQD	O48-C23-C24	2.74	120.20	111.83
24	C	511	CLA	C3B-C4B-NB	2.74	112.98	110.53
24	c	501	CLA	CAC-C3C-C4C	2.74	128.36	124.79
24	B	611	CLA	C3B-C4B-NB	2.74	112.98	110.53
24	c	508	CLA	C1-C2-C3	-2.74	121.71	126.20
24	c	507	CLA	O1D-CGD-CBD	-2.74	119.12	124.52
24	d	403	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
24	c	507	CLA	C3B-C4B-NB	2.73	112.97	110.53
26	C	514	BCR	C4-C5-C6	2.73	126.40	122.70
24	b	608	CLA	CMB-C2B-C1B	2.73	129.58	125.42
29	Z	101	LMG	O8-C28-C29	2.73	120.17	111.83
28	B	620[B]	SQD	O48-C23-C24	2.73	120.16	111.83
24	c	508	CLA	CAC-C3C-C4C	2.73	128.34	124.79
24	b	604	CLA	CMB-C2B-C1B	2.73	129.58	125.42
24	B	601	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
27	A	1010	PL9	C7-C3-C2	-2.73	120.17	123.39
32	b	625	LMT	C3B-C4B-C5B	2.73	115.17	110.23
24	b	615	CLA	O2A-CGA-CBA	2.73	120.15	111.83
24	d	403	CLA	C1-O2A-CGA	2.73	123.25	116.65
24	C	509	CLA	CAC-C3C-C4C	2.73	128.34	124.79
29	c	520	LMG	O1-C1-C2	2.72	112.41	108.27
26	y	101	BCR	C28-C27-C26	2.72	118.91	114.06
24	B	605	CLA	CMB-C2B-C1B	2.72	129.56	125.42
24	C	512	CLA	O2A-CGA-CBA	2.72	120.13	111.83
24	c	501	CLA	CMB-C2B-C1B	2.72	129.56	125.42
24	c	510	CLA	O2A-CGA-CBA	2.72	120.13	111.83
28	B	620[A]	SQD	O48-C23-C24	2.72	120.13	111.83
24	c	501	CLA	C4-C3-C5	2.72	119.94	115.23
24	D	405	CLA	C3B-C4B-NB	2.72	112.95	110.53
24	C	510	CLA	O2A-CGA-CBA	2.71	120.11	111.83
26	A	1009	BCR	C23-C24-C25	2.71	134.25	127.00
26	J	101	BCR	C2-C1-C6	2.71	114.38	110.44
29	C	519	LMG	O8-C28-C29	2.71	120.10	111.83
25	a	411	PHO	O1D-CGD-CBD	-2.71	120.61	124.72
24	C	510	CLA	C4-C3-C5	2.71	119.93	115.23
24	b	615	CLA	CMC-C2C-C1C	2.71	129.27	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	408	SQD	O9-S-C6	2.71	110.80	106.76
26	K	101	BCR	C28-C27-C26	2.71	118.88	114.06
24	c	513	CLA	CAC-C3C-C4C	2.70	128.31	124.79
29	D	412	LMG	O7-C10-C11	2.70	117.33	111.48
24	D	403	CLA	CHD-C4C-C3C	-2.70	120.83	124.77
24	C	503	CLA	C4-C3-C5	2.70	119.92	115.23
26	K	102	BCR	C27-C26-C25	2.70	126.35	122.70
24	b	610	CLA	CMB-C2B-C1B	2.70	129.53	125.42
25	a	410	PHO	CMA-C3A-C4A	-2.70	108.80	114.61
29	c	520	LMG	O8-C28-C29	2.70	120.06	111.83
24	B	605	CLA	CAC-C3C-C4C	2.70	128.30	124.79
24	B	616	CLA	C4D-C3D-CAD	2.70	111.03	108.11
24	b	617	CLA	CMC-C2C-C1C	2.69	129.24	125.03
34	e	101	LHG	O8-C23-C24	2.69	120.05	111.83
26	K	101	BCR	C39-C30-C29	-2.69	98.61	108.95
24	b	617	CLA	C4D-C3D-CAD	2.69	111.03	108.11
26	b	620	BCR	C39-C30-C29	-2.69	98.62	108.95
24	c	502	CLA	C1-C2-C3	-2.69	121.79	126.20
24	c	505	CLA	C3B-C4B-NB	2.69	112.93	110.53
36	C	517	DGD	O1G-C1A-C2A	2.69	120.04	111.83
24	c	504	CLA	C4-C3-C5	2.69	119.89	115.23
24	b	612	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
38	V	201	HEM	C1B-NB-C4B	2.69	108.39	105.21
26	k	102	BCR	C1-C6-C5	-2.69	118.96	122.64
24	a	412	CLA	CMC-C2C-C1C	2.69	129.23	125.03
24	B	604	CLA	CMB-C2B-C1B	2.69	129.51	125.42
26	T	101	BCR	C4-C5-C6	2.68	126.33	122.70
26	B	617	BCR	C39-C30-C29	-2.68	98.66	108.95
27	A	1010	PL9	C53-C6-C1	2.68	120.77	115.28
24	B	602	CLA	O2A-CGA-CBA	2.68	120.00	111.83
24	C	507	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
24	C	501	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
24	C	507	CLA	O2A-CGA-CBA	2.67	119.99	111.83
24	C	502	CLA	CMB-C2B-C1B	2.67	129.49	125.42
24	c	510	CLA	C1-C2-C3	-2.67	121.82	126.20
24	C	501	CLA	C4-C3-C5	2.67	119.87	115.23
27	a	414	PL9	C53-C6-C1	2.67	120.75	115.28
24	B	613	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
26	K	102	BCR	C32-C1-C2	-2.67	98.70	108.95
24	B	614	CLA	C1-O2A-CGA	2.67	123.11	116.65
26	b	621	BCR	C37-C22-C23	-2.67	114.01	118.09
24	C	512	CLA	CMC-C2C-C1C	2.67	129.20	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	102	BCR	C23-C24-C25	2.67	134.12	127.00
24	c	512	CLA	O2A-CGA-CBA	2.67	119.96	111.83
24	b	616	CLA	C1-C2-C3	-2.66	121.83	126.20
24	b	605	CLA	O2A-CGA-CBA	2.66	119.95	111.83
26	a	413	BCR	C1-C6-C5	-2.66	119.00	122.64
36	h	102	DGD	O1G-C1A-C2A	2.66	119.95	111.83
24	b	612	CLA	C1-O2A-CGA	2.66	123.09	116.65
24	c	507	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
26	t	101	BCR	C4-C5-C6	2.66	126.30	122.70
24	B	605	CLA	CMC-C2C-C1C	2.66	129.19	125.03
24	a	412	CLA	C4-C3-C5	2.66	119.84	115.23
24	A	1006	CLA	CBC-CAC-C3C	-2.66	105.22	112.42
24	D	405	CLA	C4-C3-C5	2.65	119.84	115.23
24	b	616	CLA	CMC-C2C-C1C	2.65	129.18	125.03
24	C	507	CLA	C4-C3-C5	2.65	119.83	115.23
26	A	1009	BCR	C40-C30-C29	-2.65	98.76	108.95
34	d	407	LHG	O8-C23-C24	2.65	119.92	111.83
24	C	512	CLA	CHD-C1D-ND	-2.65	121.07	124.80
29	c	519	LMG	O8-C28-C29	2.65	119.91	111.83
24	b	612	CLA	C3B-C4B-NB	2.65	112.89	110.53
24	B	604	CLA	C4-C3-C5	2.65	119.83	115.23
24	c	505	CLA	C4D-C3D-CAD	2.64	110.98	108.11
24	b	616	CLA	O2A-CGA-CBA	2.64	119.89	111.83
24	a	408	CLA	CMC-C2C-C1C	2.64	129.16	125.03
24	c	501	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
34	d	407	LHG	O7-C7-C8	2.64	117.19	111.48
24	B	601	CLA	C4D-C3D-CAD	2.64	110.97	108.11
27	a	414	PL9	C40-C39-C41	2.64	119.81	115.23
24	B	604	CLA	CHD-C1D-ND	-2.64	121.09	124.80
24	a	409	CLA	CMC-C2C-C1C	2.64	129.15	125.03
24	b	611	CLA	CAC-C3C-C4C	2.63	128.22	124.79
24	A	1005	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
24	B	602	CLA	C1-O2A-CGA	2.63	123.03	116.65
24	b	604	CLA	CAC-C3C-C4C	2.63	128.22	124.79
24	B	601	CLA	C3B-C4B-NB	2.63	112.88	110.53
24	b	608	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
24	B	611	CLA	CAC-C3C-C4C	2.63	128.21	124.79
26	b	621	BCR	C28-C29-C30	2.63	123.73	114.43
24	c	501	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
24	b	605	CLA	C3B-C4B-NB	2.63	112.87	110.53
24	C	510	CLA	CMC-C2C-C1C	2.62	129.13	125.03
24	c	503	CLA	C4D-CHA-C1A	2.62	124.37	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	413	BCR	C3-C4-C5	2.62	118.73	114.06
26	D	406	BCR	C37-C22-C23	-2.62	114.09	118.09
26	B	619	BCR	C1-C6-C5	-2.61	119.06	122.64
26	c	514	BCR	C34-C9-C8	-2.61	114.09	118.09
26	t	101	BCR	C31-C1-C2	-2.61	98.92	108.95
24	C	511	CLA	C4-C3-C5	2.61	119.76	115.23
24	A	1008	CLA	CMB-C2B-C1B	2.61	129.39	125.42
25	a	411	PHO	CMA-C3A-C4A	-2.61	108.99	114.61
24	b	604	CLA	CMD-C2D-C3D	-2.61	121.71	127.69
25	a	410	PHO	CBC-CAC-C3C	-2.61	109.14	112.87
26	K	102	BCR	C1-C6-C5	-2.61	119.07	122.64
24	d	402	CLA	CMC-C2C-C1C	2.61	129.11	125.03
24	a	409	CLA	C4-C3-C5	2.61	119.75	115.23
24	b	617	CLA	CED-O2D-CGD	2.61	121.83	115.92
26	k	102	BCR	C8-C9-C10	2.61	123.11	119.01
28	D	408	SQD	C44-O6-C1	-2.60	108.21	113.80
24	A	1008	CLA	CED-O2D-CGD	2.60	121.82	115.92
27	a	414	PL9	C10-C9-C11	2.60	119.75	115.23
24	B	614	CLA	C3B-C4B-NB	2.60	112.85	110.53
24	b	611	CLA	C6-C5-C3	-2.60	107.13	113.47
24	c	505	CLA	C1-O2A-CGA	2.60	122.95	116.65
29	C	519	LMG	O7-C10-O9	-2.60	117.62	123.70
24	c	510	CLA	C4D-C3D-CAD	2.60	110.93	108.11
24	c	503	CLA	C4-C3-C5	2.60	119.74	115.23
27	A	1010	PL9	C30-C29-C31	2.60	119.74	115.23
24	c	509	CLA	C4D-C3D-CAD	2.60	110.93	108.11
24	b	604	CLA	CED-O2D-CGD	2.60	121.81	115.92
24	b	610	CLA	C4-C3-C5	2.59	119.73	115.23
24	b	609	CLA	CAC-C3C-C4C	2.59	128.16	124.79
27	a	414	PL9	C35-C34-C36	2.59	119.73	115.23
32	A	1018	LMT	C2'-C3'-C4'	2.59	115.56	109.68
24	c	512	CLA	CMC-C2C-C1C	2.59	129.08	125.03
24	c	505	CLA	CMC-C2C-C1C	2.59	129.08	125.03
24	C	506	CLA	C4-C3-C5	2.59	119.72	115.23
24	c	511	CLA	C1-O2A-CGA	2.59	122.91	116.65
24	B	616	CLA	C4-C3-C5	2.59	119.72	115.23
24	b	613	CLA	C4D-C3D-CAD	2.58	110.91	108.11
24	c	512	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
34	D	410	LHG	O8-C23-C24	2.58	119.70	111.83
26	t	101	BCR	C34-C9-C8	-2.58	114.15	118.09
27	D	407	PL9	C37-C38-C39	-2.58	121.72	127.62
26	h	101	BCR	C32-C1-C31	-2.58	101.26	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	O2A-CGA-CBA	2.58	119.69	111.83
25	D	404	PHO	CMA-C3A-C4A	-2.57	109.06	114.61
26	a	413	BCR	C40-C30-C25	2.57	114.28	110.24
26	b	621	BCR	C31-C1-C2	-2.57	99.07	108.95
34	d	408	LHG	O8-C23-C24	2.57	119.68	111.83
24	b	610	CLA	CAC-C3C-C4C	2.57	128.13	124.79
26	b	620	BCR	C34-C9-C10	-2.57	118.66	122.82
26	h	101	BCR	C34-C9-C10	-2.57	118.66	122.82
24	C	507	CLA	C3B-C4B-NB	2.57	112.82	110.53
24	c	512	CLA	C4D-C3D-CAD	2.57	110.89	108.11
27	d	405	PL9	C25-C24-C26	2.57	119.68	115.23
24	C	510	CLA	C4D-C3D-CAD	2.57	110.89	108.11
25	D	404	PHO	CED-O2D-CGD	2.56	121.72	115.92
24	a	407	CLA	CAC-C3C-C4C	2.56	128.12	124.79
24	a	408	CLA	C4-C3-C5	2.56	119.67	115.23
27	d	405	PL9	C22-C23-C24	-2.56	121.77	127.62
24	c	506	CLA	C4-C3-C5	2.56	119.67	115.23
26	B	619	BCR	C34-C9-C8	-2.55	114.19	118.09
25	D	404	PHO	C4-C3-C5	2.55	119.66	115.23
24	c	512	CLA	CMB-C2B-C1B	2.55	129.31	125.42
24	B	603	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
24	b	618	CLA	CMC-C2C-C1C	2.55	129.02	125.03
26	K	102	BCR	C29-C28-C27	2.55	116.89	111.28
24	c	511	CLA	C4D-C3D-CAD	2.55	110.88	108.11
24	c	506	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
27	d	405	PL9	C35-C34-C36	2.55	119.65	115.23
26	k	102	BCR	C35-C13-C12	-2.55	114.19	118.09
24	a	409	CLA	C4C-C3C-C2C	-2.55	103.18	106.89
24	b	618	CLA	CMB-C2B-C1B	2.55	129.30	125.42
24	B	602	CLA	C3B-C4B-NB	2.55	112.80	110.53
26	B	619	BCR	C37-C22-C23	-2.55	114.20	118.09
24	C	501	CLA	CMD-C2D-C3D	-2.54	121.85	127.69
24	c	504	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
26	T	101	BCR	C3-C4-C5	2.54	118.59	114.06
26	T	101	BCR	C30-C25-C24	2.54	122.55	115.65
24	c	512	CLA	C1-C2-C3	-2.54	122.03	126.20
24	C	507	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
24	c	509	CLA	C1-O2A-CGA	2.54	122.80	116.65
24	b	613	CLA	C3B-C4B-NB	2.54	112.80	110.53
24	B	603	CLA	O2A-CGA-CBA	2.54	119.58	111.83
24	C	505	CLA	C1-O2A-CGA	2.54	122.80	116.65
24	c	506	CLA	O2D-CGD-O1D	-2.54	118.91	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	411	PHO	C1-C2-C3	-2.54	122.04	126.20
24	b	606	CLA	O2A-CGA-CBA	2.54	119.57	111.83
24	B	616	CLA	CBC-CAC-C3C	-2.54	105.55	112.42
26	c	514	BCR	C8-C9-C10	2.54	123.00	119.01
26	K	101	BCR	C30-C25-C24	2.53	122.53	115.65
24	B	613	CLA	O2A-CGA-CBA	2.53	119.55	111.83
24	C	513	CLA	C4D-C3D-CAD	2.53	110.85	108.11
36	C	515	DGD	O1G-C1A-C2A	2.53	119.54	111.83
24	B	607	CLA	C1-O2A-CGA	2.52	122.76	116.65
24	B	605	CLA	CED-O2D-CGD	2.52	121.64	115.92
24	C	501	CLA	CMB-C2B-C1B	2.52	129.26	125.42
24	c	511	CLA	CMB-C2B-C1B	2.52	129.26	125.42
24	B	601	CLA	C4-C3-C5	2.52	119.60	115.23
24	c	503	CLA	CAC-C3C-C4C	2.52	128.06	124.79
26	B	618	BCR	C2-C1-C6	2.52	114.09	110.44
27	a	414	PL9	C32-C33-C34	-2.51	121.87	127.62
25	D	404	PHO	CMB-C2B-C3B	2.51	129.71	124.68
24	C	502	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
24	B	604	CLA	C4D-C3D-CAD	2.51	110.83	108.11
24	C	513	CLA	C3B-C4B-NB	2.51	112.77	110.53
26	d	404	BCR	C34-C9-C10	-2.51	118.75	122.82
24	b	611	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
26	h	101	BCR	C28-C27-C26	2.51	118.52	114.06
24	c	506	CLA	O2A-CGA-CBA	2.51	119.48	111.83
27	D	407	PL9	C22-C23-C24	-2.51	121.89	127.62
24	c	513	CLA	CMD-C2D-C3D	-2.50	121.94	127.69
26	H	101	BCR	C32-C1-C2	-2.50	99.35	108.95
26	B	618	BCR	C37-C22-C23	-2.50	114.27	118.09
25	A	1007	PHO	C4B-NB-C1B	-2.50	105.17	108.82
24	b	616	CLA	CAC-C3C-C4C	2.50	128.04	124.79
24	C	502	CLA	C4-C3-C5	2.50	119.57	115.23
24	B	616	CLA	CMB-C2B-C1B	2.50	129.22	125.42
26	b	621	BCR	C24-C23-C22	2.50	129.93	126.23
26	k	102	BCR	C2-C3-C4	2.50	116.77	111.28
27	D	407	PL9	C20-C19-C21	2.50	119.56	115.23
26	k	102	BCR	C30-C25-C24	2.50	122.42	115.65
24	a	409	CLA	CAC-C3C-C4C	2.49	128.03	124.79
24	b	608	CLA	CMC-C2C-C1C	2.49	128.93	125.03
24	b	607	CLA	CHD-C1D-ND	-2.49	121.30	124.80
24	B	612	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
24	b	614	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
24	B	607	CLA	C4C-C3C-C2C	-2.49	103.27	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	408	SQD	O48-C23-C24	2.49	119.43	111.83
27	d	405	PL9	C53-C6-C1	2.49	120.38	115.28
24	a	408	CLA	C4B-C3B-C2B	-2.49	104.21	107.30
36	H	102	DGD	O1G-C1A-O1A	-2.49	117.40	123.63
24	A	1008	CLA	CMC-C2C-C1C	2.49	128.92	125.03
38	V	201	HEM	C3B-C4B-NB	-2.49	107.68	109.47
24	C	513	CLA	O2A-CGA-CBA	2.49	119.42	111.83
24	c	502	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
24	C	504	CLA	CED-O2D-CGD	2.49	121.55	115.92
24	B	601	CLA	CMD-C2D-C3D	-2.49	121.99	127.69
26	k	101	BCR	C40-C30-C25	2.49	114.14	110.24
26	C	514	BCR	C36-C18-C17	-2.48	118.79	122.82
32	b	625	LMT	C4B-C3B-C2B	2.48	115.19	110.83
24	c	509	CLA	CED-O2D-CGD	2.48	121.55	115.92
26	t	101	BCR	C3-C4-C5	2.48	118.48	114.06
24	b	609	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
36	H	102	DGD	O1G-C1A-C2A	2.48	119.40	111.83
26	J	101	BCR	C36-C18-C19	-2.48	114.30	118.09
27	A	1010	PL9	C40-C39-C41	2.48	119.53	115.23
24	c	504	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
24	b	618	CLA	CAC-C3C-C4C	2.48	128.02	124.79
24	D	405	CLA	CAC-C3C-C4C	2.48	128.02	124.79
27	a	414	PL9	C30-C29-C31	2.48	119.53	115.23
24	C	513	CLA	CMC-C2C-C1C	2.48	128.91	125.03
24	C	507	CLA	C4D-C3D-CAD	2.48	110.80	108.11
25	a	410	PHO	CMB-C2B-C3B	2.48	129.64	124.68
24	B	602	CLA	CMC-C2C-C1C	2.48	128.91	125.03
24	b	617	CLA	CAC-C3C-C4C	2.48	128.01	124.79
27	A	1010	PL9	C42-C43-C44	-2.48	121.95	127.62
24	C	503	CLA	CMB-C2B-C1B	2.48	129.19	125.42
24	B	603	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
24	C	512	CLA	CAC-C3C-C4C	2.47	128.01	124.79
26	t	101	BCR	C40-C30-C29	-2.47	99.47	108.95
24	C	511	CLA	C1-O2A-CGA	2.47	122.62	116.65
36	c	516	DGD	O1G-C1A-C2A	2.47	119.36	111.83
24	C	509	CLA	C1-O2A-CGA	2.47	122.62	116.65
26	c	514	BCR	C28-C29-C30	2.46	123.15	114.43
24	A	1005	CLA	O2A-CGA-CBA	2.46	119.35	111.83
24	b	611	CLA	O2A-CGA-CBA	2.46	119.35	111.83
24	C	507	CLA	CED-O2D-CGD	2.46	121.50	115.92
24	D	405	CLA	CMB-C2B-C1B	2.46	129.16	125.42
26	B	617	BCR	C34-C9-C10	-2.46	118.83	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	518	SQD	O5-C1-C2	-2.46	105.32	110.37
24	b	611	CLA	C3B-C4B-NB	2.46	112.72	110.53
24	c	509	CLA	C4-C3-C5	2.46	119.50	115.23
24	c	507	CLA	CMC-C2C-C1C	2.46	128.88	125.03
26	B	619	BCR	C30-C25-C24	2.46	122.31	115.65
24	c	505	CLA	CMD-C2D-C3D	-2.46	122.06	127.69
24	b	607	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
26	B	619	BCR	C31-C1-C6	2.46	114.09	110.24
24	b	607	CLA	CMC-C2C-C1C	2.45	128.87	125.03
28	b	623[A]	SQD	O7-S-C6	2.45	110.42	106.76
24	a	408	CLA	CHD-C4C-C3C	-2.45	121.20	124.77
24	C	510	CLA	C4C-C3C-C2C	-2.45	103.32	106.89
24	b	617	CLA	CBC-CAC-C3C	-2.45	105.77	112.42
24	b	607	CLA	CMB-C2B-C1B	2.45	129.15	125.42
26	y	101	BCR	C3-C4-C5	2.45	118.43	114.06
32	A	1018	LMT	C1'-C2'-C3'	2.45	115.17	110.01
24	B	606	CLA	CAC-C3C-C4C	2.45	127.98	124.79
24	a	409	CLA	C1-O2A-CGA	2.45	122.58	116.65
24	C	505	CLA	CMC-C2C-C1C	2.45	128.86	125.03
24	b	617	CLA	O2A-CGA-CBA	2.45	119.31	111.83
24	b	616	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
24	B	612	CLA	CMC-C2C-C1C	2.45	128.86	125.03
24	b	610	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
24	c	504	CLA	CED-O2D-CGD	2.45	121.46	115.92
28	B	620[B]	SQD	O6-C1-C2	2.45	111.99	108.27
24	c	511	CLA	C3B-C4B-NB	2.44	112.71	110.53
24	C	511	CLA	CAC-C3C-C4C	2.44	127.97	124.79
24	c	510	CLA	C4-C3-C5	2.44	119.47	115.23
26	D	406	BCR	C28-C27-C26	2.44	118.40	114.06
24	B	609	CLA	C1-C2-C3	-2.44	122.20	126.20
24	B	609	CLA	C1-O2A-CGA	2.44	122.55	116.65
24	c	503	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
24	c	513	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
27	d	405	PL9	C20-C19-C21	2.43	119.45	115.23
24	b	618	CLA	C4-C3-C5	2.43	119.45	115.23
24	b	605	CLA	C1-C2-C3	-2.43	122.21	126.20
24	C	506	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
24	C	508	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
24	b	605	CLA	CAC-C3C-C4C	2.43	127.95	124.79
24	C	509	CLA	C4-C3-C5	2.43	119.45	115.23
24	C	504	CLA	C1-O2A-CGA	2.43	122.53	116.65
27	A	1010	PL9	C45-C44-C46	2.43	119.44	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
24	D	403	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
27	A	1010	PL9	C20-C19-C21	2.43	119.44	115.23
24	C	507	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
24	B	602	CLA	CAC-C3C-C4C	2.42	127.94	124.79
24	D	402	CLA	O2A-CGA-CBA	2.42	119.22	111.83
24	b	610	CLA	C1-O2A-CGA	2.42	122.52	116.65
24	c	503	CLA	CMB-C2B-C1B	2.42	129.11	125.42
24	B	606	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
24	b	609	CLA	C1-O2A-CGA	2.42	122.50	116.65
24	B	607	CLA	CED-O2D-CGD	2.42	121.40	115.92
24	a	409	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
24	b	613	CLA	O2A-CGA-CBA	2.42	119.20	111.83
24	B	608	CLA	C4-C3-C5	2.42	119.42	115.23
32	A	1017	LMT	C3'-C4'-C5'	-2.41	105.58	110.93
27	D	407	PL9	C10-C9-C11	2.41	119.42	115.23
26	c	514	BCR	C7-C6-C5	2.41	127.11	121.56
28	f	102	SQD	C4-C3-C2	2.41	115.06	110.83
24	d	402	CLA	C4D-C3D-CAD	2.41	110.72	108.11
24	c	510	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
24	C	507	CLA	CMC-C2C-C1C	2.41	128.80	125.03
26	d	404	BCR	C4-C5-C6	2.41	125.96	122.70
26	H	101	BCR	C37-C22-C23	-2.41	114.41	118.09
26	k	101	BCR	C1-C6-C5	-2.41	119.35	122.64
24	b	608	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
26	t	101	BCR	C37-C22-C21	-2.41	118.92	122.82
24	c	513	CLA	CMC-C2C-C1C	2.40	128.79	125.03
28	a	401	SQD	O6-C1-C2	2.40	111.92	108.27
26	T	101	BCR	C37-C22-C23	-2.40	114.42	118.09
24	b	617	CLA	CMB-C2B-C1B	2.40	129.08	125.42
32	b	625	LMT	O1'-C1'-C2'	2.40	111.92	108.27
26	H	101	BCR	C30-C25-C24	2.40	122.16	115.65
24	b	609	CLA	CMC-C2C-C1C	2.40	128.78	125.03
26	B	618	BCR	C32-C1-C6	2.40	114.00	110.24
26	d	404	BCR	C38-C26-C27	-2.39	108.49	113.60
24	c	507	CLA	C4-C3-C5	2.39	119.38	115.23
26	d	404	BCR	C3-C2-C1	2.39	122.90	114.43
24	B	607	CLA	CHC-C1C-NC	-2.39	120.71	124.31
32	t	103	LMT	C1'-C2'-C3'	2.39	115.04	110.01
24	c	513	CLA	C4-C3-C5	2.39	119.38	115.23
24	B	613	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
25	a	410	PHO	CED-O2D-CGD	2.39	121.34	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
24	c	506	CLA	CED-O2D-CGD	2.39	121.34	115.92
24	b	604	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
26	k	102	BCR	C31-C1-C2	-2.39	99.78	108.95
24	b	605	CLA	C4B-CHC-C1C	2.39	131.86	126.25
24	A	1005	CLA	CMC-C2C-C1C	2.39	128.76	125.03
24	c	506	CLA	C4D-C3D-CAD	2.39	110.70	108.11
24	C	512	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
26	y	101	BCR	C31-C1-C6	2.38	113.98	110.24
24	c	511	CLA	CAC-C3C-C4C	2.38	127.89	124.79
24	C	510	CLA	CMD-C2D-C3D	-2.38	122.22	127.69
24	b	609	CLA	CMB-C2B-C1B	2.38	129.05	125.42
24	b	619	CLA	C4D-C3D-CAD	2.38	110.69	108.11
24	b	613	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
24	C	513	CLA	CAC-C3C-C4C	2.38	127.89	124.79
24	B	610	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
26	y	101	BCR	C30-C25-C24	2.38	122.10	115.65
26	A	1009	BCR	C32-C1-C2	-2.38	99.82	108.95
36	C	516	DGD	O1G-C1A-C2A	2.38	119.08	111.83
24	D	402	CLA	CHD-C4C-C3C	-2.38	121.31	124.77
38	F	101	HEM	C2A-C1A-NA	-2.37	107.52	110.15
24	B	602	CLA	C1-C2-C3	-2.37	122.31	126.20
26	h	101	BCR	C35-C13-C14	-2.37	118.97	122.82
24	A	1008	CLA	O2A-CGA-CBA	2.37	119.07	111.83
26	b	621	BCR	C32-C1-C31	-2.37	101.84	108.63
24	b	617	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
24	d	403	CLA	CMC-C2C-C1C	2.37	128.74	125.03
24	c	501	CLA	C4D-C3D-CAD	2.37	110.68	108.11
24	C	508	CLA	CED-O2D-CGD	2.37	121.29	115.92
24	b	610	CLA	CBC-CAC-C3C	-2.37	106.00	112.42
24	C	512	CLA	C1-C2-C3	-2.37	122.32	126.20
24	B	611	CLA	CMB-C2B-C1B	2.36	129.02	125.42
38	F	101	HEM	CBA-CAA-C2A	-2.36	105.99	112.53
24	b	606	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
24	C	513	CLA	CED-O2D-CGD	2.36	121.28	115.92
24	b	619	CLA	O2A-CGA-CBA	2.36	119.04	111.83
24	b	614	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
24	C	504	CLA	CHD-C4C-NC	-2.36	120.57	124.23
26	c	514	BCR	C39-C30-C25	2.36	113.95	110.24
24	c	509	CLA	O2A-CGA-CBA	2.36	119.04	111.83
24	D	402	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	b	613	CLA	CMB-C2B-C1B	2.36	129.01	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	C4-C3-C5	2.36	119.33	115.23
38	f	101	HEM	CHC-C1C-NC	2.36	127.02	124.45
24	b	609	CLA	C4-C3-C5	2.36	119.33	115.23
24	a	408	CLA	O2A-CGA-CBA	2.36	119.03	111.83
36	C	516	DGD	O2G-C1B-O1B	-2.36	118.19	123.70
24	b	611	CLA	C4-C3-C5	2.36	119.32	115.23
24	b	610	CLA	C1-C2-C3	-2.36	122.34	126.20
24	b	613	CLA	C4-C3-C5	2.36	119.32	115.23
24	d	402	CLA	CED-O2D-CGD	2.35	121.26	115.92
24	C	509	CLA	C4D-C3D-CAD	2.35	110.66	108.11
24	c	510	CLA	CMC-C2C-C1C	2.35	128.71	125.03
24	C	505	CLA	C4D-C3D-CAD	2.35	110.66	108.11
24	C	509	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
24	D	402	CLA	CMB-C2B-C1B	2.35	129.00	125.42
25	a	410	PHO	O2D-CGD-O1D	-2.35	119.27	123.85
24	c	509	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
24	B	601	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
24	b	606	CLA	C1-O2A-CGA	2.35	122.34	116.65
24	b	616	CLA	CED-O2D-CGD	2.35	121.24	115.92
26	B	618	BCR	C3-C4-C5	2.35	118.24	114.06
27	a	414	PL9	C7-C3-C2	-2.35	120.62	123.39
24	d	403	CLA	C4D-C3D-CAD	2.35	110.65	108.11
34	D	410	LHG	C5-O7-C7	-2.34	112.19	117.80
24	b	604	CLA	C4B-CHC-C1C	2.34	131.76	126.25
24	b	619	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
26	y	101	BCR	C1-C6-C7	2.34	122.01	115.65
26	b	621	BCR	C30-C25-C24	2.34	122.01	115.65
24	B	603	CLA	C4D-C3D-CAD	2.34	110.65	108.11
28	f	102	SQD	O7-S-C6	2.34	110.25	106.76
27	d	405	PL9	C10-C9-C11	2.34	119.29	115.23
24	d	403	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
24	C	503	CLA	CMC-C2C-C1C	2.34	128.69	125.03
24	C	509	CLA	CMB-C2B-C1B	2.34	128.98	125.42
24	c	513	CLA	CED-O2D-CGD	2.34	121.22	115.92
24	c	502	CLA	CMC-C2C-C1C	2.34	128.69	125.03
24	C	501	CLA	CED-O2D-CGD	2.34	121.22	115.92
24	B	614	CLA	CMC-C2C-C1C	2.34	128.69	125.03
24	D	402	CLA	C1-O2A-CGA	2.34	122.31	116.65
24	C	509	CLA	O2A-CGA-CBA	2.34	118.96	111.83
24	B	609	CLA	CMC-C2C-C1C	2.34	128.69	125.03
24	a	412	CLA	C4D-C3D-CAD	2.34	110.64	108.11
24	b	605	CLA	C4D-C3D-CAD	2.34	110.64	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C4-C3-C5	2.33	119.28	115.23
24	c	502	CLA	C4-C3-C5	2.33	119.28	115.23
24	b	608	CLA	C1-O2A-CGA	2.33	122.30	116.65
24	d	402	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
24	C	503	CLA	CAC-C3C-C4C	2.33	127.82	124.79
24	c	512	CLA	C1-O2A-CGA	2.33	122.29	116.65
36	C	516	DGD	O1G-C1A-O1A	-2.33	117.80	123.63
26	A	1009	BCR	C3-C4-C5	2.33	118.21	114.06
24	B	608	CLA	CMC-C2C-C1C	2.33	128.67	125.03
24	A	1008	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
24	b	604	CLA	C3B-C4B-NB	2.33	112.61	110.53
27	A	1010	PL9	C15-C14-C16	2.33	119.27	115.23
34	b	624	LHG	O8-C23-C24	2.33	118.93	111.83
24	c	511	CLA	CMC-C2C-C1C	2.32	128.66	125.03
26	h	101	BCR	C40-C30-C25	2.32	113.88	110.24
32	A	1018	LMT	O1B-C4'-C3'	2.32	113.13	107.23
24	b	608	CLA	CED-O2D-CGD	2.32	121.18	115.92
24	D	402	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
24	C	511	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
28	B	620[B]	SQD	C45-O47-C7	-2.32	112.25	117.80
26	D	406	BCR	C40-C30-C39	2.32	115.27	108.63
24	b	614	CLA	CMB-C2B-C1B	2.32	128.94	125.42
24	C	503	CLA	O2A-CGA-CBA	2.31	118.89	111.83
24	c	502	CLA	CMB-C2B-C1B	2.31	128.94	125.42
26	h	101	BCR	C30-C25-C24	2.31	121.92	115.65
32	a	402	LMT	C1B-O5B-C5B	2.31	118.24	113.72
24	C	508	CLA	C4D-C3D-CAD	2.31	110.62	108.11
34	d	407	LHG	O8-C23-O10	-2.31	117.85	123.63
28	A	1011	SQD	C45-O47-C7	-2.31	112.27	117.80
24	b	614	CLA	CED-O2D-CGD	2.31	121.16	115.92
24	B	615	CLA	C4-C3-C5	2.31	119.24	115.23
24	C	508	CLA	C1-C2-C3	-2.31	122.41	126.20
24	c	507	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
24	b	611	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
24	b	611	CLA	CMC-C2C-C1C	2.31	128.64	125.03
27	D	407	PL9	C53-C6-C1	2.31	120.00	115.28
26	J	101	BCR	C1-C6-C7	2.31	121.91	115.65
24	B	607	CLA	CMB-C2B-C1B	2.31	128.93	125.42
24	A	1008	CLA	C4D-C3D-CAD	2.31	110.61	108.11
24	c	509	CLA	CMB-C2B-C1B	2.31	128.93	125.42
24	D	403	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
26	A	1009	BCR	C34-C9-C8	-2.30	114.58	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C4D-C3D-CAD	2.30	110.60	108.11
24	c	509	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
24	C	509	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
24	b	604	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
24	a	412	CLA	CMB-C2B-C1B	2.30	128.92	125.42
24	B	615	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
24	d	403	CLA	O2D-CGD-CBD	2.30	115.24	111.23
26	c	514	BCR	C40-C30-C29	-2.29	100.14	108.95
38	F	101	HEM	C3B-C2B-C1B	2.29	108.13	106.41
24	D	405	CLA	C1-O2A-CGA	2.29	122.20	116.65
24	B	604	CLA	CHD-C4C-NC	-2.29	120.68	124.23
28	A	1011	SQD	O5-C1-C2	-2.29	105.66	110.37
26	a	413	BCR	C31-C1-C2	-2.29	100.15	108.95
24	c	509	CLA	CMC-C2C-C1C	2.29	128.61	125.03
24	C	509	CLA	CED-O2D-CGD	2.29	121.11	115.92
25	a	410	PHO	C4B-NB-C1B	-2.29	105.48	108.82
24	C	501	CLA	C4D-C3D-CAD	2.29	110.59	108.11
26	J	101	BCR	C27-C26-C25	2.29	125.80	122.70
24	B	611	CLA	CED-O2D-CGD	2.29	121.11	115.92
24	B	612	CLA	O2A-CGA-CBA	2.29	118.81	111.83
26	t	101	BCR	C30-C25-C26	-2.29	119.51	122.64
24	b	614	CLA	CMC-C2C-C1C	2.29	128.61	125.03
25	A	1007	PHO	CMB-C2B-C3B	2.29	129.25	124.68
38	v	201	HEM	C1B-NB-C4B	2.28	107.91	105.21
26	D	406	BCR	C31-C1-C2	-2.28	100.18	108.95
24	B	611	CLA	CBC-CAC-C3C	-2.28	106.23	112.42
26	C	514	BCR	C34-C9-C8	-2.28	114.60	118.09
28	D	408	SQD	O5-C1-C2	-2.28	105.68	110.37
24	c	513	CLA	C4D-C3D-CAD	2.28	110.58	108.11
24	c	501	CLA	CMC-C2C-C1C	2.28	128.60	125.03
24	b	617	CLA	CHC-C1C-NC	-2.28	120.88	124.31
26	b	622	BCR	C30-C25-C24	2.28	121.83	115.65
36	c	517	DGD	O1G-C1A-O1A	-2.28	117.93	123.63
24	C	506	CLA	O2A-CGA-CBA	2.28	118.78	111.83
26	K	101	BCR	C1-C6-C7	2.28	121.82	115.65
26	A	1009	BCR	C1-C6-C7	2.27	121.82	115.65
28	A	1011	SQD	O48-C23-C24	2.27	118.77	111.83
27	a	414	PL9	C20-C19-C21	2.27	119.18	115.23
24	B	616	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
24	b	604	CLA	C4-C3-C5	2.27	119.17	115.23
24	B	613	CLA	C1-O2A-CGA	2.27	122.14	116.65
32	a	402	LMT	C3'-C4'-C5'	-2.27	105.91	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	601	CLA	CAC-C3C-C4C	2.27	127.74	124.79
24	B	614	CLA	O2A-CGA-CBA	2.27	118.74	111.83
24	C	513	CLA	C1-O2A-CGA	2.26	122.13	116.65
24	A	1006	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
24	C	506	CLA	C4D-C3D-CAD	2.26	110.56	108.11
24	A	1005	CLA	C4D-C3D-CAD	2.26	110.56	108.11
24	B	614	CLA	C1-C2-C3	-2.26	122.49	126.20
26	J	101	BCR	C32-C1-C6	2.26	113.79	110.24
24	B	610	CLA	CMB-C2B-C1B	2.26	128.86	125.42
24	c	503	CLA	CMC-C2C-C1C	2.26	128.56	125.03
26	C	514	BCR	C30-C25-C24	2.26	121.77	115.65
25	a	411	PHO	C4B-NB-C1B	-2.26	105.53	108.82
24	c	511	CLA	O2A-CGA-CBA	2.26	118.71	111.83
34	d	406	LHG	O8-C23-O10	-2.26	117.98	123.63
24	b	616	CLA	C4-C3-C5	2.25	119.14	115.23
24	D	403	CLA	C4C-C3C-C2C	-2.25	103.61	106.89
26	t	101	BCR	C31-C1-C6	2.25	113.77	110.24
24	D	405	CLA	O2A-CGA-CBA	2.25	118.70	111.83
24	D	403	CLA	CHC-C1C-C2C	-2.25	120.55	126.95
24	C	502	CLA	CMC-C2C-C1C	2.25	128.55	125.03
28	c	518	SQD	O48-C23-C24	2.25	118.69	111.83
24	c	501	CLA	O2A-CGA-CBA	2.25	118.69	111.83
26	T	101	BCR	C1-C6-C7	2.25	121.74	115.65
24	B	616	CLA	C1-C2-C3	-2.25	122.52	126.20
24	b	611	CLA	C4D-C3D-CAD	2.24	110.54	108.11
26	y	101	BCR	C40-C30-C29	-2.24	100.34	108.95
24	C	508	CLA	CAC-C3C-C4C	2.24	127.71	124.79
24	A	1006	CLA	C4B-C3B-C2B	-2.24	104.52	107.30
24	B	615	CLA	CMB-C2B-C1B	2.24	128.83	125.42
24	B	607	CLA	CAC-C3C-C4C	2.24	127.70	124.79
24	D	405	CLA	CMC-C2C-C1C	2.24	128.53	125.03
24	c	504	CLA	CHD-C4C-NC	-2.24	120.76	124.23
24	C	506	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
24	D	405	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
24	b	618	CLA	C1-O2A-CGA	2.24	122.07	116.65
24	c	508	CLA	O2A-CGA-CBA	2.24	118.66	111.83
24	c	503	CLA	C4D-C3D-CAD	2.24	110.54	108.11
27	a	414	PL9	C45-C44-C46	2.24	119.11	115.23
24	C	505	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
26	h	101	BCR	C28-C29-C30	2.24	122.35	114.43
26	J	101	BCR	C39-C30-C29	-2.24	100.36	108.95
24	c	505	CLA	O1D-CGD-CBD	-2.24	120.11	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	407	PL9	C35-C34-C36	2.24	119.11	115.23
24	B	615	CLA	CMC-C2C-C1C	2.23	128.52	125.03
24	D	402	CLA	CED-O2D-CGD	2.23	120.98	115.92
26	y	101	BCR	C39-C30-C25	2.23	113.74	110.24
24	B	613	CLA	CAC-C3C-C4C	2.23	127.69	124.79
27	A	1010	PL9	C27-C28-C29	-2.23	122.52	127.62
24	B	610	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
24	C	508	CLA	C4-C3-C5	2.23	119.10	115.23
24	C	504	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
24	b	612	CLA	CMC-C2C-C1C	2.23	128.51	125.03
24	A	1008	CLA	C1-O2A-CGA	2.23	122.04	116.65
24	B	613	CLA	CED-O2D-CGD	2.23	120.97	115.92
26	b	621	BCR	C40-C30-C29	-2.23	100.40	108.95
24	c	502	CLA	C4B-CHC-C1C	2.23	131.48	126.25
26	a	413	BCR	C1-C6-C7	2.23	121.69	115.65
24	C	504	CLA	C4B-C3B-C2B	-2.23	104.53	107.30
24	C	512	CLA	CMB-C2B-C1B	2.23	128.81	125.42
24	C	512	CLA	C1-O2A-CGA	2.22	122.03	116.65
24	c	510	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
26	a	413	BCR	C4-C5-C6	2.22	125.71	122.70
27	D	407	PL9	C7-C3-C4	2.22	118.74	116.91
24	B	601	CLA	CED-O2D-CGD	2.22	120.95	115.92
29	d	409	LMG	O8-C28-C29	2.22	118.59	111.83
28	B	620[B]	SQD	O8-S-C6	2.22	110.25	105.97
24	b	615	CLA	C1-C2-C3	-2.21	122.57	126.20
24	B	612	CLA	CED-O2D-CGD	2.21	120.94	115.92
24	c	507	CLA	C4D-C3D-CAD	2.21	110.51	108.11
24	b	617	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
24	b	615	CLA	CMB-C2B-C1B	2.21	128.79	125.42
27	D	407	PL9	C42-C43-C44	-2.21	122.56	127.62
24	B	608	CLA	CHD-C4C-NC	-2.21	120.80	124.23
24	A	1006	CLA	C4C-C3C-C2C	-2.21	103.67	106.89
24	B	613	CLA	C4-C3-C5	2.21	119.06	115.23
24	C	512	CLA	C3B-C4B-NB	2.21	112.50	110.53
24	c	512	CLA	CAC-C3C-C4C	2.21	127.67	124.79
24	b	617	CLA	C1-O2A-CGA	2.21	122.00	116.65
34	B	621	LHG	O8-C23-C24	2.21	118.57	111.83
26	K	101	BCR	C40-C30-C25	2.21	113.70	110.24
24	c	513	CLA	C3B-C4B-NB	2.21	112.50	110.53
26	B	619	BCR	C28-C27-C26	2.20	117.99	114.06
24	c	503	CLA	C3B-C4B-NB	2.20	112.50	110.53
25	a	411	PHO	CED-O2D-CGD	2.20	120.92	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CHC-C1C-NC	-2.20	120.99	124.31
24	b	604	CLA	CHD-C4C-NC	-2.20	120.82	124.23
26	D	406	BCR	C3-C4-C5	2.20	117.98	114.06
24	B	601	CLA	C4B-CHC-C1C	2.20	131.42	126.25
24	b	616	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
34	D	409	LHG	O8-C23-O10	-2.20	118.12	123.63
24	A	1006	CLA	C1-O2A-CGA	2.20	121.98	116.65
24	B	604	CLA	CMC-C2C-C1C	2.20	128.47	125.03
24	b	619	CLA	CED-O2D-CGD	2.20	120.90	115.92
27	a	414	PL9	C51-C49-C50	2.20	119.65	114.59
24	C	506	CLA	CED-O2D-CGD	2.20	120.90	115.92
24	c	502	CLA	C4D-C3D-CAD	2.20	110.49	108.11
24	c	505	CLA	CMB-C2B-C1B	2.20	128.76	125.42
24	a	412	CLA	O2A-CGA-CBA	2.20	118.53	111.83
26	K	101	BCR	C38-C26-C25	2.19	126.88	124.48
24	c	501	CLA	C1-O2A-CGA	2.19	121.96	116.65
24	b	606	CLA	C4D-C3D-CAD	2.19	110.49	108.11
28	b	623[A]	SQD	C45-O47-C7	-2.19	112.55	117.80
26	T	101	BCR	C31-C1-C2	-2.19	100.53	108.95
38	f	101	HEM	C1B-NB-C4B	2.19	107.80	105.21
24	B	605	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	c	510	CLA	CAC-C3C-C4C	2.19	127.64	124.79
24	c	502	CLA	CHD-C4C-NC	-2.19	120.84	124.23
24	c	508	CLA	C4D-C3D-CAD	2.19	110.48	108.11
24	C	502	CLA	O2A-CGA-CBA	2.19	118.50	111.83
24	A	1008	CLA	CAC-C3C-C4C	2.19	127.64	124.79
24	b	617	CLA	C1-C2-C3	-2.19	122.61	126.20
24	b	612	CLA	CED-O2D-CGD	2.19	120.87	115.92
24	c	508	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
24	B	603	CLA	C5-C3-C2	-2.18	116.26	121.17
24	B	606	CLA	CMC-C2C-C1C	2.18	128.45	125.03
24	b	605	CLA	CED-O2D-CGD	2.18	120.87	115.92
26	C	514	BCR	C33-C5-C6	2.18	126.86	124.48
24	B	604	CLA	C1-C2-C3	-2.18	122.62	126.20
24	c	505	CLA	CED-O2D-CGD	2.18	120.86	115.92
24	b	618	CLA	CED-O2D-CGD	2.18	120.86	115.92
24	b	616	CLA	CMB-C2B-C1B	2.18	128.74	125.42
24	C	508	CLA	O2A-CGA-CBA	2.18	118.48	111.83
24	c	507	CLA	CMB-C2B-C1B	2.18	128.74	125.42
24	d	403	CLA	CAC-C3C-C4C	2.18	127.62	124.79
24	C	508	CLA	C4B-C3B-C2B	-2.18	104.59	107.30
24	B	614	CLA	CED-O2D-CGD	2.18	120.85	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	CED-O2D-CGD	2.18	120.85	115.92
24	B	613	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
26	K	101	BCR	C2-C3-C4	2.17	116.05	111.28
24	B	608	CLA	O2A-CGA-CBA	2.17	118.45	111.83
24	c	502	CLA	O2A-CGA-CBA	2.17	118.45	111.83
24	a	408	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
24	B	601	CLA	CMC-C2C-C1C	2.17	128.42	125.03
24	c	501	CLA	CHD-C4C-NC	-2.17	120.87	124.23
24	b	615	CLA	C4D-C3D-CAD	2.17	110.46	108.11
24	c	513	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
24	C	501	CLA	CMC-C2C-C1C	2.17	128.42	125.03
24	a	409	CLA	C1-C2-C3	-2.16	122.65	126.20
24	c	506	CLA	CMB-C2B-C1B	2.16	128.71	125.42
24	b	609	CLA	C4D-C3D-CAD	2.16	110.46	108.11
36	c	516	DGD	O1G-C1A-O1A	-2.16	118.22	123.63
26	b	622	BCR	C28-C27-C26	2.16	117.91	114.06
24	C	505	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
24	B	609	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
24	a	408	CLA	C4C-C3C-C2C	-2.16	103.75	106.89
24	B	610	CLA	C4D-C3D-CAD	2.16	110.45	108.11
24	b	606	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
29	m	102	LMG	O8-C28-O10	-2.16	118.23	123.63
24	B	615	CLA	O2A-CGA-CBA	2.15	118.41	111.83
27	D	407	PL9	C12-C13-C14	-2.15	122.69	127.62
24	B	608	CLA	C6-C5-C3	-2.15	108.23	113.47
24	a	408	CLA	CED-O2D-CGD	2.15	120.79	115.92
26	K	102	BCR	C39-C30-C25	2.15	113.61	110.24
24	D	402	CLA	CAC-C3C-C4C	2.14	127.58	124.79
24	a	408	CLA	CMB-C2B-C1B	2.14	128.68	125.42
32	m	103	LMT	O1'-C1'-C2'	2.14	111.53	108.27
32	B	623	LMT	C1B-O5B-C5B	2.14	117.91	113.72
24	b	612	CLA	O2A-CGA-CBA	2.14	118.37	111.83
24	B	605	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
25	A	1007	PHO	CED-O2D-CGD	2.14	120.77	115.92
24	c	503	CLA	CHD-C4C-NC	-2.14	120.91	124.23
24	b	619	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
28	b	623[B]	SQD	C45-O47-C7	-2.14	112.67	117.80
32	b	631	LMT	O5B-C5B-C6B	2.14	111.74	106.44
32	A	1018	LMT	O5B-C5B-C4B	2.14	113.55	109.70
24	c	507	CLA	C1-O2A-CGA	2.14	121.83	116.65
24	C	512	CLA	CED-O2D-CGD	2.14	120.77	115.92
24	b	606	CLA	CMB-C2B-C1B	2.14	128.67	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C4B-C3B-C2B	-2.13	104.65	107.30
24	d	402	CLA	CAC-C3C-C4C	2.13	127.56	124.79
24	b	610	CLA	CMC-C2C-C1C	2.13	128.37	125.03
24	B	606	CLA	CMB-C2B-C1B	2.13	128.66	125.42
28	A	1011	SQD	C1-O5-C5	-2.13	109.56	113.72
24	b	606	CLA	CAC-C3C-C4C	2.13	127.56	124.79
38	F	101	HEM	C1B-NB-C4B	2.13	107.73	105.21
24	B	613	CLA	C4B-C3B-C2B	-2.13	104.66	107.30
24	C	503	CLA	C3B-C4B-NB	2.13	112.43	110.53
24	B	606	CLA	O2A-CGA-CBA	2.13	118.32	111.83
24	B	616	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
27	A	1010	PL9	C51-C49-C50	2.13	119.48	114.59
24	b	612	CLA	C1-C2-C3	-2.13	122.71	126.20
24	B	609	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
24	a	412	CLA	CED-O2D-CGD	2.12	120.73	115.92
24	C	501	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
38	v	201	HEM	CMD-C2D-C1D	2.12	128.35	125.03
24	C	513	CLA	C4-C3-C5	2.12	118.91	115.23
24	c	510	CLA	CMB-C2B-C1B	2.12	128.65	125.42
24	B	616	CLA	CMC-C2C-C1C	2.12	128.34	125.03
26	b	622	BCR	C31-C1-C2	-2.12	100.82	108.95
24	B	615	CLA	CHB-C1B-NB	-2.12	120.87	124.05
24	A	1006	CLA	CHD-C4C-C3C	-2.12	121.69	124.77
28	B	620[A]	SQD	O9-S-C6	2.12	109.92	106.76
24	C	510	CLA	CAC-C3C-C4C	2.12	127.54	124.79
26	b	621	BCR	C40-C30-C39	-2.12	102.57	108.63
24	C	504	CLA	CMB-C2B-C1B	2.12	128.64	125.42
24	B	602	CLA	CMB-C2B-C1B	2.12	128.64	125.42
24	C	507	CLA	CMB-C2B-C1B	2.11	128.64	125.42
28	c	518	SQD	O9-S-O7	-2.11	106.95	113.82
32	a	416	LMT	C1B-O5B-C5B	2.11	117.85	113.72
24	C	513	CLA	CHC-C1C-NC	-2.11	121.13	124.31
25	A	1007	PHO	O2D-CGD-O1D	-2.11	119.74	123.85
24	b	618	CLA	C4D-CHA-C1A	2.11	123.76	121.24
24	C	502	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
28	A	1011	SQD	O47-C7-O49	-2.11	118.77	123.70
38	v	201	HEM	C3B-C4B-NB	-2.11	107.95	109.47
24	C	509	CLA	CHD-C4C-NC	-2.11	120.96	124.23
24	B	609	CLA	CED-O2D-CGD	2.11	120.70	115.92
24	D	405	CLA	C4D-C3D-CAD	2.11	110.39	108.11
26	H	101	BCR	C28-C29-C30	2.11	121.89	114.43
24	B	611	CLA	CMC-C2C-C1C	2.11	128.33	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	CMB-C2B-C1B	2.10	128.62	125.42
24	b	618	CLA	O2A-CGA-CBA	2.10	118.25	111.83
24	b	609	CLA	O2A-CGA-CBA	2.10	118.24	111.83
24	c	513	CLA	C1-C2-C3	-2.10	122.75	126.20
24	C	507	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
24	C	510	CLA	CED-O2D-CGD	2.10	120.68	115.92
24	B	616	CLA	C1-O2A-CGA	2.10	121.73	116.65
24	a	408	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
24	b	611	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
26	K	101	BCR	C4-C5-C6	2.10	125.54	122.70
26	B	618	BCR	C40-C30-C29	-2.10	100.90	108.95
24	b	619	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
24	b	613	CLA	CED-O2D-CGD	2.10	120.67	115.92
29	m	102	LMG	O7-C10-O9	-2.10	118.81	123.70
24	b	608	CLA	CAC-C3C-C4C	2.09	127.52	124.79
24	b	612	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
24	C	512	CLA	C4D-C3D-CAD	2.09	110.38	108.11
28	B	620[A]	SQD	O47-C7-O49	-2.09	118.81	123.70
24	D	405	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
24	b	605	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
25	a	410	PHO	C1-O2A-CGA	2.09	121.71	116.65
25	D	404	PHO	O1D-CGD-CBD	-2.09	121.56	124.72
24	C	503	CLA	C4D-C3D-CAD	2.09	110.37	108.11
24	C	503	CLA	CED-O2D-CGD	2.09	120.65	115.92
24	A	1006	CLA	CED-O2D-CGD	2.09	120.65	115.92
24	B	613	CLA	CHD-C4C-C3C	-2.09	121.73	124.77
29	c	521	LMG	O7-C10-O9	-2.08	118.83	123.70
24	D	403	CLA	O2A-CGA-CBA	2.08	118.19	111.83
24	C	504	CLA	CMC-C2C-C1C	2.08	128.29	125.03
27	A	1010	PL9	C17-C18-C19	-2.08	122.86	127.62
29	C	519	LMG	O6-C5-C6	2.08	111.59	106.44
24	c	513	CLA	CMB-C2B-C1B	2.08	128.59	125.42
24	b	619	CLA	C4D-CHA-C1A	2.08	123.72	121.24
24	c	507	CLA	CHA-C1A-NA	-2.08	121.68	126.39
24	c	507	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
24	C	506	CLA	C1-O2A-CGA	2.08	121.68	116.65
24	B	606	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
27	a	414	PL9	C27-C28-C29	-2.08	122.87	127.62
34	D	410	LHG	O8-C23-O10	-2.08	118.43	123.63
24	D	402	CLA	CHC-C1C-NC	-2.08	121.18	124.31
24	c	511	CLA	CED-O2D-CGD	2.08	120.63	115.92
24	A	1006	CLA	O2D-CGD-O1D	-2.08	119.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	623[B]	SQD	O48-C23-O10	-2.07	118.44	123.63
24	C	507	CLA	C1-O2A-CGA	2.07	121.67	116.65
26	d	404	BCR	C31-C1-C6	2.07	113.49	110.24
24	c	504	CLA	C1-C2-C3	-2.07	122.80	126.20
24	c	511	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
27	A	1010	PL9	C7-C8-C9	-2.07	123.26	126.83
27	d	405	PL9	C51-C49-C50	2.07	119.35	114.59
28	b	623[B]	SQD	O47-C7-O49	-2.07	118.87	123.70
24	d	403	CLA	CED-O2D-CGD	2.07	120.61	115.92
24	A	1005	CLA	C4-C3-C5	2.07	118.82	115.23
24	c	508	CLA	CHD-C4C-NC	-2.07	121.03	124.23
24	b	616	CLA	C4D-C3D-CAD	2.07	110.35	108.11
24	D	405	CLA	C1-C2-C3	-2.07	122.81	126.20
25	D	404	PHO	C4B-NB-C1B	-2.07	105.80	108.82
35	C	522	HTG	O5-C5-C6	2.07	111.56	106.44
26	B	619	BCR	C32-C1-C2	-2.07	101.02	108.95
32	A	1017	LMT	C1B-O1B-C4'	-2.07	113.08	117.98
24	b	619	CLA	CMB-C2B-C1B	2.07	128.56	125.42
24	C	510	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
24	b	613	CLA	C4B-CHC-C1C	2.06	131.10	126.25
28	B	620[A]	SQD	C45-O47-C7	-2.06	112.86	117.80
25	A	1007	PHO	CMA-C3A-C4A	-2.06	110.17	114.61
24	a	412	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
24	a	407	CLA	C4-C3-C5	2.06	118.81	115.23
24	B	614	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
24	c	504	CLA	CMC-C2C-C1C	2.06	128.25	125.03
24	B	604	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
36	h	102	DGD	O1G-C1A-O1A	-2.06	118.47	123.63
24	B	605	CLA	CHD-C4C-C3C	-2.06	121.77	124.77
24	c	505	CLA	O2A-CGA-CBA	2.06	118.12	111.83
24	d	403	CLA	CBC-CAC-C3C	-2.06	106.84	112.42
24	D	402	CLA	CBC-CAC-C3C	-2.06	106.84	112.42
24	b	619	CLA	CMD-C2D-C3D	-2.06	122.98	127.69
38	f	101	HEM	CMD-C2D-C1D	2.05	128.24	125.03
24	C	511	CLA	CED-O2D-CGD	2.05	120.57	115.92
26	k	101	BCR	C32-C1-C6	2.05	113.46	110.24
24	c	503	CLA	C1-O2A-CGA	2.05	121.61	116.65
27	a	414	PL9	C42-C43-C44	-2.05	122.93	127.62
24	a	409	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
38	v	201	HEM	CHC-C4B-NB	2.05	126.63	124.42
24	B	606	CLA	CHD-C4C-NC	-2.05	121.06	124.23
26	B	617	BCR	C35-C13-C14	-2.05	119.50	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	611	CLA	C1-C2-C3	-2.05	122.84	126.20
24	B	605	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
24	c	504	CLA	CMB-C2B-C1B	2.05	128.54	125.42
24	b	607	CLA	CHD-C4C-NC	-2.05	121.06	124.23
25	a	411	PHO	OBD-CAD-C3D	-2.05	124.70	127.89
24	c	508	CLA	CMB-C2B-C1B	2.05	128.53	125.42
28	b	623[A]	SQD	O48-C23-O10	-2.04	118.51	123.63
24	b	616	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
24	c	503	CLA	O2A-CGA-CBA	2.04	118.07	111.83
24	b	610	CLA	O2A-CGA-CBA	2.04	118.06	111.83
24	C	502	CLA	C4D-C3D-CAD	2.04	110.33	108.11
24	B	601	CLA	C4-C3-C2	-2.04	118.38	123.63
24	C	503	CLA	C4B-CHC-C1C	2.04	131.04	126.25
24	c	503	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
24	B	607	CLA	C4B-C3B-C2B	-2.04	104.77	107.30
24	b	608	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
24	b	612	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
24	B	614	CLA	CMB-C2B-C1B	2.04	128.52	125.42
28	b	623[B]	SQD	O9-S-C6	2.04	109.80	106.76
24	a	409	CLA	O2A-CGA-CBA	2.04	118.04	111.83
27	a	414	PL9	C15-C14-C16	2.03	118.76	115.23
24	C	508	CLA	CMD-C2D-C3D	-2.03	123.02	127.69
24	A	1005	CLA	CMB-C2B-C3B	2.03	131.33	126.55
24	b	615	CLA	C4B-C3B-C2B	-2.03	104.77	107.30
34	E	101	LHG	O8-C23-O10	-2.03	118.54	123.63
36	C	515	DGD	O1G-C1A-O1A	-2.03	118.54	123.63
24	B	614	CLA	CAC-C3C-C4C	2.03	127.43	124.79
32	a	402	LMT	O5'-C5'-C6'	2.03	111.48	106.44
24	C	502	CLA	C1-C2-C3	-2.03	122.87	126.20
26	a	413	BCR	C39-C30-C25	2.03	113.43	110.24
24	C	506	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
24	C	513	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
24	b	610	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
24	C	513	CLA	CHD-C4C-NC	-2.03	121.09	124.23
24	C	510	CLA	C1-O2A-CGA	2.03	121.56	116.65
26	B	617	BCR	C1-C6-C7	2.03	121.15	115.65
26	t	101	BCR	C29-C30-C25	2.03	113.38	110.44
24	D	403	CLA	C4-C3-C5	2.03	118.74	115.23
24	a	409	CLA	O1D-CGD-CBD	-2.02	120.52	124.52
24	c	503	CLA	C4B-CHC-C1C	2.02	131.01	126.25
24	B	605	CLA	C3B-C4B-NB	2.02	112.34	110.53
24	c	504	CLA	CMD-C2D-C3D	-2.02	123.05	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
29	c	519	LMG	O8-C28-O10	-2.02	118.57	123.63
26	J	101	BCR	C30-C25-C24	2.02	121.14	115.65
26	b	620	BCR	C1-C6-C7	2.02	121.14	115.65
26	b	622	BCR	C1-C6-C7	2.02	121.14	115.65
27	D	407	PL9	C27-C28-C29	-2.02	123.00	127.62
28	b	623[B]	SQD	O8-S-C6	2.02	109.87	105.97
26	J	101	BCR	C28-C27-C26	2.02	117.66	114.06
24	C	503	CLA	C4D-CHA-C1A	2.02	123.65	121.24
24	d	403	CLA	C4-C3-C5	2.02	118.73	115.23
24	C	511	CLA	C4D-C3D-CAD	2.02	110.30	108.11
24	c	504	CLA	C4D-C3D-CAD	2.02	110.30	108.11
26	B	617	BCR	C2-C3-C4	2.02	115.71	111.28
28	D	408	SQD	C1-C2-C3	-2.02	105.77	110.01
24	b	619	CLA	C1-O2A-CGA	2.02	121.53	116.65
24	c	506	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
34	D	409	LHG	C5-O7-C7	-2.02	112.97	117.80
26	B	619	BCR	C1-C6-C7	2.02	121.12	115.65
24	B	610	CLA	O1D-CGD-CBD	-2.01	120.54	124.52
35	b	626	HTG	O5-C5-C6	2.01	111.43	106.44
38	f	101	HEM	C2A-C1A-NA	-2.01	107.92	110.15
24	B	612	CLA	CMB-C2B-C1B	2.01	128.49	125.42
24	C	504	CLA	C7-C6-C5	-2.01	107.89	113.26
32	b	625	LMT	O5B-C5B-C6B	2.01	111.43	106.44
24	C	511	CLA	CMC-C2C-C1C	2.01	128.18	125.03
24	b	607	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
24	B	616	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
24	C	507	CLA	CHA-C1A-NA	-2.01	121.84	126.39
24	B	606	CLA	C4D-C3D-CAD	2.01	110.29	108.11
24	B	611	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
29	C	518	LMG	O8-C28-O10	-2.01	118.60	123.63
24	C	513	CLA	CMB-C2B-C1B	2.01	128.48	125.42
38	V	201	HEM	CHA-C4D-ND	2.01	126.85	124.37
24	B	609	CLA	O2A-CGA-CBA	2.01	117.96	111.83
24	b	609	CLA	CED-O2D-CGD	2.01	120.47	115.92
24	b	612	CLA	C4D-C3D-CAD	2.01	110.28	108.11
24	b	618	CLA	C4D-C3D-CAD	2.01	110.28	108.11
24	B	615	CLA	C4D-C3D-CAD	2.01	110.28	108.11
24	c	510	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
24	B	614	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
26	B	619	BCR	C32-C1-C6	2.00	113.39	110.24
24	A	1005	CLA	CAC-C3C-C4C	2.00	127.40	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	611	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
24	c	506	CLA	C4B-C3B-C2B	-2.00	104.81	107.30
27	D	407	PL9	C51-C49-C50	2.00	119.19	114.59
24	B	607	CLA	C1-C2-C3	-2.00	122.92	126.20
27	D	407	PL9	C7-C8-C9	-2.00	123.38	126.83
24	B	614	CLA	CMD-C2D-C3D	-2.00	123.10	127.69

There are no chirality outliers.

All (1830) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	607	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	a	409	CLA	C2B-C3B-CAB-CBB
24	a	409	CLA	C4B-C3B-CAB-CBB
24	b	604	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	C2B-C3B-CAB-CBB
24	b	612	CLA	C4B-C3B-CAB-CBB
24	b	617	CLA	CAD-CBD-CGD-O1D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	C4B-C3B-CAB-CBB
26	A	1009	BCR	C14-C15-C16-C17
26	A	1009	BCR	C18-C19-C20-C21
26	A	1009	BCR	C19-C20-C21-C22
26	B	619	BCR	C10-C11-C12-C13
26	C	514	BCR	C14-C15-C16-C17
26	D	406	BCR	C37-C22-C23-C24
26	D	406	BCR	C22-C23-C24-C25
26	H	101	BCR	C10-C11-C12-C13
26	H	101	BCR	C14-C15-C16-C17
26	H	101	BCR	C18-C19-C20-C21
26	H	101	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
26	J	101	BCR	C10-C11-C12-C13
26	J	101	BCR	C11-C12-C13-C14
26	J	101	BCR	C11-C12-C13-C35
26	J	101	BCR	C14-C15-C16-C17
26	J	101	BCR	C18-C19-C20-C21
26	K	101	BCR	C10-C11-C12-C13
26	K	101	BCR	C18-C19-C20-C21
26	K	102	BCR	C14-C15-C16-C17
26	K	102	BCR	C18-C19-C20-C21
26	T	101	BCR	C14-C15-C16-C17
26	T	101	BCR	C18-C19-C20-C21
26	a	413	BCR	C14-C15-C16-C17
26	a	413	BCR	C18-C19-C20-C21
26	a	413	BCR	C19-C20-C21-C22
26	b	622	BCR	C14-C15-C16-C17
26	b	622	BCR	C15-C16-C17-C18
26	c	514	BCR	C14-C15-C16-C17
26	c	514	BCR	C18-C19-C20-C21
26	d	404	BCR	C14-C15-C16-C17
26	d	404	BCR	C18-C19-C20-C21
26	d	404	BCR	C37-C22-C23-C24
26	h	101	BCR	C18-C19-C20-C21
26	k	101	BCR	C10-C11-C12-C13
26	k	101	BCR	C18-C19-C20-C21
26	k	101	BCR	C19-C20-C21-C22
26	k	101	BCR	C21-C22-C23-C24
26	k	102	BCR	C10-C11-C12-C13
26	k	102	BCR	C14-C15-C16-C17
26	k	102	BCR	C18-C19-C20-C21
26	t	101	BCR	C14-C15-C16-C17
26	t	101	BCR	C18-C19-C20-C21
26	y	101	BCR	C10-C11-C12-C13
26	y	101	BCR	C18-C19-C20-C21
26	y	101	BCR	C19-C20-C21-C22
26	y	101	BCR	C20-C21-C22-C37
28	A	1016	SQD	O6-C44-C45-O47
28	B	620[A]	SQD	O5-C1-O6-C44
28	B	620[A]	SQD	O49-C7-O47-C45
28	B	620[A]	SQD	C8-C7-O47-C45
28	B	620[A]	SQD	O5-C5-C6-S
28	B	620[B]	SQD	O49-C7-O47-C45
28	B	620[B]	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
28	B	620[B]	SQD	O5-C5-C6-S
28	a	401	SQD	O6-C44-C45-O47
28	b	623[A]	SQD	C46-C45-O47-C7
28	b	623[A]	SQD	C8-C7-O47-C45
28	b	623[A]	SQD	O5-C5-C6-S
28	b	623[B]	SQD	O49-C7-O47-C45
28	b	623[B]	SQD	C5-C6-S-O7
28	b	623[B]	SQD	C5-C6-S-O8
28	b	623[B]	SQD	C5-C6-S-O9
28	f	102	SQD	C8-C7-O47-C45
29	C	519	LMG	O9-C10-O7-C8
29	c	520	LMG	C2-C1-O1-C7
29	c	520	LMG	O6-C1-O1-C7
29	c	521	LMG	O6-C1-O1-C7
29	c	521	LMG	C11-C10-O7-C8
32	B	623	LMT	C2'-C1'-O1'-C1
32	B	623	LMT	C2-C1-O1'-C1'
32	b	625	LMT	C2B-C1B-O1B-C4'
32	f	103	LMT	C2-C1-O1'-C1'
33	D	418	GOL	O1-C1-C2-C3
33	V	206	GOL	C1-C2-C3-O3
33	d	415	GOL	C1-C2-C3-O3
34	B	621	LHG	C4-O6-P-O3
34	B	621	LHG	C4-O6-P-O4
34	B	621	LHG	C4-O6-P-O5
34	D	410	LHG	C4-O6-P-O3
34	D	410	LHG	C4-O6-P-O4
34	E	101	LHG	C4-O6-P-O3
34	E	101	LHG	C4-O6-P-O4
34	b	624	LHG	C4-O6-P-O3
34	b	624	LHG	C4-O6-P-O4
34	b	624	LHG	C4-O6-P-O5
34	d	407	LHG	C4-O6-P-O3
34	d	407	LHG	C4-O6-P-O4
34	e	101	LHG	C4-O6-P-O3
34	e	101	LHG	C4-O6-P-O4
34	e	101	LHG	C8-C7-O7-C5
35	D	419	HTG	O5-C1-S1-C1'
35	V	202	HTG	C2-C1-S1-C1'
35	V	202	HTG	O5-C1-S1-C1'
35	b	630	HTG	O5-C1-S1-C1'
35	c	522	HTG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
35	d	416	HTG	O5-C1-S1-C1'
38	V	201	HEM	C2B-C3B-CAB-CBB
38	v	201	HEM	C2B-C3B-CAB-CBB
38	v	201	HEM	C4B-C3B-CAB-CBB
32	A	1018	LMT	C3'-C4'-O1B-C1B
24	c	513	CLA	CBD-CGD-O2D-CED
32	b	631	LMT	O5B-C1B-O1B-C4'
28	B	620[B]	SQD	O10-C23-O48-C46
29	m	102	LMG	O10-C28-O8-C9
24	b	615	CLA	C13-C15-C16-C17
32	C	520	LMT	C3'-C4'-O1B-C1B
24	C	513	CLA	CBD-CGD-O2D-CED
28	b	623[A]	SQD	O49-C7-O47-C45
28	f	102	SQD	O49-C7-O47-C45
29	c	521	LMG	O9-C10-O7-C8
34	e	101	LHG	O9-C7-O7-C5
24	b	617	CLA	C3-C5-C6-C7
28	D	408	SQD	C24-C23-O48-C46
29	m	102	LMG	C29-C28-O8-C9
28	b	623[B]	SQD	C8-C7-O47-C45
29	C	519	LMG	C11-C10-O7-C8
24	C	513	CLA	O1D-CGD-O2D-CED
32	A	1018	LMT	O5'-C5'-C6'-O6'
24	c	512	CLA	O1D-CGD-O2D-CED
34	E	101	LHG	O10-C23-O8-C6
24	B	614	CLA	C3-C5-C6-C7
28	B	620[B]	SQD	C24-C23-O48-C46
29	a	415	LMG	C29-C28-O8-C9
34	e	101	LHG	C24-C23-O8-C6
26	C	514	BCR	C19-C20-C21-C22
26	J	101	BCR	C15-C16-C17-C18
26	J	101	BCR	C19-C20-C21-C22
26	K	101	BCR	C19-C20-C21-C22
26	K	102	BCR	C19-C20-C21-C22
26	T	101	BCR	C19-C20-C21-C22
26	b	620	BCR	C19-C20-C21-C22
26	h	101	BCR	C15-C16-C17-C18
24	B	616	CLA	O1A-CGA-O2A-C1
28	D	408	SQD	O10-C23-O48-C46
29	a	415	LMG	O10-C28-O8-C9
29	c	519	LMG	O10-C28-O8-C9
35	D	419	HTG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
24	c	512	CLA	CBD-CGD-O2D-CED
34	D	410	LHG	O2-C2-C3-O3
34	d	407	LHG	O2-C2-C3-O3
24	B	616	CLA	CBA-CGA-O2A-C1
34	E	101	LHG	C24-C23-O8-C6
32	a	402	LMT	O5B-C5B-C6B-O6B
32	A	1018	LMT	C4'-C5'-C6'-O6'
32	a	402	LMT	C4B-C5B-C6B-O6B
32	i	102	LMT	C4'-C5'-C6'-O6'
35	d	410	HTG	C4-C5-C6-O6
32	A	1017	LMT	O5'-C5'-C6'-O6'
32	C	520	LMT	O5B-C5B-C6B-O6B
35	d	410	HTG	O5-C5-C6-O6
26	y	101	BCR	C14-C15-C16-C17
25	a	411	PHO	O1D-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
24	c	508	CLA	CBD-CGD-O2D-CED
29	C	519	LMG	O6-C5-C6-O5
35	B	629	HTG	O5-C5-C6-O6
32	f	103	LMT	C4B-C5B-C6B-O6B
35	B	624	HTG	S1-C1'-C2'-C3'
35	C	521	HTG	S1-C1'-C2'-C3'
35	D	419	HTG	S1-C1'-C2'-C3'
35	c	522	HTG	S1-C1'-C2'-C3'
29	c	519	LMG	C29-C28-O8-C9
29	c	521	LMG	C29-C28-O8-C9
24	b	617	CLA	C4-C3-C5-C6
24	b	617	CLA	C2-C3-C5-C6
34	e	101	LHG	O10-C23-O8-C6
29	c	521	LMG	O6-C5-C6-O5
27	A	1010	PL9	C24-C26-C27-C28
27	a	414	PL9	C24-C26-C27-C28
24	C	502	CLA	CBD-CGD-O2D-CED
35	D	419	HTG	C4-C5-C6-O6
29	c	521	LMG	O10-C28-O8-C9
32	A	1017	LMT	O5'-C1'-O1'-C1
32	B	623	LMT	O5'-C1'-O1'-C1
32	a	402	LMT	O5'-C1'-O1'-C1
32	t	103	LMT	O5'-C1'-O1'-C1
29	A	1012	LMG	C29-C28-O8-C9
35	B	624	HTG	O5-C5-C6-O6
32	b	631	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
32	m	103	LMT	O5B-C5B-C6B-O6B
24	C	502	CLA	O1D-CGD-O2D-CED
32	f	103	LMT	C4'-C5'-C6'-O6'
28	D	408	SQD	C8-C7-O47-C45
28	B	620[B]	SQD	C30-C31-C32-C33
26	B	617	BCR	C19-C20-C21-C22
24	B	601	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	CBA-CGA-O2A-C1
28	B	620[A]	SQD	C24-C23-O48-C46
32	b	631	LMT	C4B-C5B-C6B-O6B
29	A	1012	LMG	O10-C28-O8-C9
24	C	513	CLA	C3-C5-C6-C7
24	B	610	CLA	C14-C13-C15-C16
24	C	507	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C12-C13-C14
24	c	509	CLA	C6-C7-C8-C9
24	c	513	CLA	C14-C13-C15-C16
32	m	103	LMT	C4B-C5B-C6B-O6B
35	B	624	HTG	C4-C5-C6-O6
35	B	629	HTG	C4-C5-C6-O6
28	b	623[B]	SQD	C2-C1-O6-C44
32	A	1017	LMT	C2'-C1'-O1'-C1
32	a	402	LMT	C2'-C1'-O1'-C1
32	i	102	LMT	C2'-C1'-O1'-C1
32	t	103	LMT	C2'-C1'-O1'-C1
35	b	630	HTG	O5-C5-C6-O6
24	B	601	CLA	O1A-CGA-O2A-C1
26	K	102	BCR	C37-C22-C23-C24
26	k	101	BCR	C37-C22-C23-C24
32	f	103	LMT	O5B-C5B-C6B-O6B
24	c	513	CLA	O1A-CGA-O2A-C1
24	b	604	CLA	CBA-CGA-O2A-C1
24	b	604	CLA	C2-C1-O2A-CGA
24	c	510	CLA	O1D-CGD-O2D-CED
26	B	618	BCR	C14-C15-C16-C17
24	B	601	CLA	C5-C6-C7-C8
24	C	506	CLA	C15-C16-C17-C18
24	D	405	CLA	C10-C11-C12-C13
33	D	418	GOL	O1-C1-C2-O2
33	D	418	GOL	O2-C2-C3-O3
25	a	411	PHO	CBD-CGD-O2D-CED
32	A	1017	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
32	f	103	LMT	O5'-C5'-C6'-O6'
24	C	506	CLA	C12-C13-C15-C16
24	c	508	CLA	C13-C15-C16-C17
28	b	623[B]	SQD	C7-C8-C9-C10
29	C	518	LMG	C28-C29-C30-C31
26	c	514	BCR	C15-C16-C17-C18
26	d	404	BCR	C13-C14-C15-C16
32	C	520	LMT	O1'-C1-C2-C3
28	D	408	SQD	O49-C7-O47-C45
24	B	614	CLA	C5-C6-C7-C8
29	c	521	LMG	C4-C5-C6-O5
28	A	1016	SQD	C23-C24-C25-C26
28	B	620[A]	SQD	C23-C24-C25-C26
29	C	518	LMG	C10-C11-C12-C13
29	m	102	LMG	C28-C29-C30-C31
36	C	516	DGD	C1B-C2B-C3B-C4B
28	B	620[A]	SQD	O10-C23-O48-C46
24	b	614	CLA	C13-C15-C16-C17
24	b	617	CLA	C8-C10-C11-C12
38	f	101	HEM	C2A-CAA-CBA-CGA
24	c	513	CLA	O1D-CGD-O2D-CED
26	D	406	BCR	C18-C19-C20-C21
26	b	620	BCR	C10-C11-C12-C13
26	b	622	BCR	C18-C19-C20-C21
24	B	606	CLA	C10-C11-C12-C13
24	B	606	CLA	C15-C16-C17-C18
24	C	509	CLA	C15-C16-C17-C18
24	b	609	CLA	C15-C16-C17-C18
24	b	619	CLA	C10-C11-C12-C13
24	c	506	CLA	C5-C6-C7-C8
24	c	509	CLA	C13-C15-C16-C17
35	b	626	HTG	C4-C5-C6-O6
28	f	102	SQD	C23-C24-C25-C26
29	c	519	LMG	C28-C29-C30-C31
36	C	515	DGD	C1B-C2B-C3B-C4B
35	b	601	HTG	S1-C1'-C2'-C3'
28	b	623[B]	SQD	O5-C1-O6-C44
32	i	102	LMT	O5'-C1'-O1'-C1
34	d	408	LHG	C30-C31-C32-C33
32	i	102	LMT	O5'-C5'-C6'-O6'
35	C	522	HTG	O5-C5-C6-O6
24	B	606	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C5-C6-C7-C8
24	C	506	CLA	C13-C15-C16-C17
24	C	508	CLA	C10-C11-C12-C13
24	b	604	CLA	C15-C16-C17-C18
24	c	508	CLA	C10-C11-C12-C13
34	e	101	LHG	C23-C24-C25-C26
36	c	517	DGD	C1A-C2A-C3A-C4A
24	C	509	CLA	C10-C11-C12-C13
24	b	619	CLA	C5-C6-C7-C8
32	b	625	LMT	O1'-C1-C2-C3
24	A	1008	CLA	C10-C11-C12-C13
24	B	616	CLA	C15-C16-C17-C18
32	f	103	LMT	O1'-C1-C2-C3
24	d	403	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C5-C6-C7-C8
24	b	619	CLA	C13-C15-C16-C17
24	c	513	CLA	C15-C16-C17-C18
24	C	512	CLA	CBA-CGA-O2A-C1
29	Z	101	LMG	C11-C10-O7-C8
24	C	511	CLA	O1D-CGD-O2D-CED
24	B	601	CLA	C3-C5-C6-C7
24	B	607	CLA	C3-C5-C6-C7
32	A	1018	LMT	O1'-C1-C2-C3
26	C	514	BCR	C15-C16-C17-C18
26	K	102	BCR	C15-C16-C17-C18
26	k	102	BCR	C15-C16-C17-C18
26	k	102	BCR	C19-C20-C21-C22
36	H	102	DGD	C6B-C7B-C8B-C9B
29	Z	101	LMG	O9-C10-O7-C8
34	d	407	LHG	C1-C2-C3-O3
24	a	412	CLA	CBA-CGA-O2A-C1
24	B	604	CLA	C13-C15-C16-C17
24	B	610	CLA	C8-C10-C11-C12
24	a	412	CLA	C8-C10-C11-C12
24	b	604	CLA	C10-C11-C12-C13
24	c	506	CLA	C15-C16-C17-C18
32	b	631	LMT	O1'-C1-C2-C3
34	D	411	LHG	C31-C32-C33-C34
24	c	508	CLA	O1D-CGD-O2D-CED
24	B	615	CLA	C5-C6-C7-C8
24	D	405	CLA	C8-C10-C11-C12
24	b	616	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	b	619	CLA	C15-C16-C17-C18
29	d	409	LMG	O6-C5-C6-O5
35	b	626	HTG	O5-C5-C6-O6
35	o	301	HTG	S1-C1'-C2'-C3'
24	B	613	CLA	C13-C15-C16-C17
24	b	609	CLA	C10-C11-C12-C13
24	b	617	CLA	C5-C6-C7-C8
24	c	504	CLA	C10-C11-C12-C13
24	c	508	CLA	C15-C16-C17-C18
28	b	623[A]	SQD	C24-C23-O48-C46
24	c	506	CLA	O1D-CGD-O2D-CED
24	A	1008	CLA	C8-C10-C11-C12
28	f	102	SQD	C2-C1-O6-C44
29	m	102	LMG	C2-C1-O1-C7
32	A	1018	LMT	C2'-C1'-O1'-C1
32	a	416	LMT	C2'-C1'-O1'-C1
32	b	631	LMT	C2'-C1'-O1'-C1
35	C	521	HTG	C1'-C2'-C3'-C4'
34	e	101	LHG	O2-C2-C3-O3
26	A	1009	BCR	C16-C17-C18-C36
26	B	617	BCR	C20-C21-C22-C37
26	B	618	BCR	C20-C21-C22-C37
26	C	514	BCR	C20-C21-C22-C37
26	a	413	BCR	C16-C17-C18-C36
26	b	622	BCR	C20-C21-C22-C37
26	k	101	BCR	C20-C21-C22-C37
26	k	102	BCR	C16-C17-C18-C36
26	k	102	BCR	C20-C21-C22-C37
26	k	101	BCR	C7-C8-C9-C34
26	y	101	BCR	C11-C12-C13-C35
26	d	404	BCR	C21-C22-C23-C24
24	b	604	CLA	O1A-CGA-O2A-C1
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	609	CLA	C2A-CAA-CBA-CGA
33	D	418	GOL	C1-C2-C3-O3
33	V	204	GOL	C1-C2-C3-O3
33	V	207	GOL	O1-C1-C2-C3
33	a	420	GOL	C1-C2-C3-O3
33	d	417	GOL	O1-C1-C2-C3
34	D	409	LHG	O1-C1-C2-C3
34	d	406	LHG	O1-C1-C2-C3
34	d	408	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	B	620[A]	SQD	C46-C45-O47-C7
28	B	620[B]	SQD	C46-C45-O47-C7
26	c	514	BCR	C19-C20-C21-C22
24	A	1006	CLA	C16-C17-C18-C19
24	B	604	CLA	C16-C17-C18-C20
24	B	606	CLA	C16-C17-C18-C20
24	b	616	CLA	C16-C17-C18-C19
24	C	506	CLA	O1D-CGD-O2D-CED
24	B	604	CLA	C3-C5-C6-C7
32	b	625	LMT	O5B-C5B-C6B-O6B
24	b	611	CLA	C13-C15-C16-C17
26	A	1009	BCR	C16-C17-C18-C19
26	A	1009	BCR	C20-C21-C22-C23
26	B	618	BCR	C20-C21-C22-C23
26	C	514	BCR	C20-C21-C22-C23
26	K	101	BCR	C20-C21-C22-C23
26	K	102	BCR	C20-C21-C22-C23
26	a	413	BCR	C16-C17-C18-C19
26	k	101	BCR	C20-C21-C22-C23
26	k	102	BCR	C16-C17-C18-C19
26	y	101	BCR	C20-C21-C22-C23
28	b	623[B]	SQD	C13-C14-C15-C16
29	m	102	LMG	O6-C1-O1-C7
32	b	631	LMT	O5'-C1'-O1'-C1
29	c	519	LMG	C11-C10-O7-C8
32	A	1017	LMT	C4'-C5'-C6'-O6'
28	D	408	SQD	C23-C24-C25-C26
34	e	101	LHG	C7-C8-C9-C10
24	B	604	CLA	C16-C17-C18-C19
24	C	508	CLA	C16-C17-C18-C20
24	a	409	CLA	C16-C17-C18-C19
24	b	605	CLA	C16-C17-C18-C19
24	b	607	CLA	C16-C17-C18-C19
24	b	607	CLA	C16-C17-C18-C20
24	b	619	CLA	C16-C17-C18-C19
24	C	512	CLA	O1A-CGA-O2A-C1
24	b	606	CLA	C5-C6-C7-C8
28	B	620[B]	SQD	C12-C13-C14-C15
29	A	1012	LMG	C15-C16-C17-C18
29	B	622	LMG	C32-C33-C34-C35
29	C	519	LMG	C33-C34-C35-C36
29	Z	101	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	a	415	LMG	C16-C17-C18-C19
29	a	415	LMG	C30-C31-C32-C33
32	A	1018	LMT	C11-C10-C9-C8
32	i	102	LMT	C7-C8-C9-C10
32	i	102	LMT	C11-C10-C9-C8
32	t	103	LMT	C6-C7-C8-C9
35	B	628	HTG	C2'-C3'-C4'-C5'
36	C	515	DGD	CBA-CCA-CDA-CEA
36	c	516	DGD	C5B-C6B-C7B-C8B
26	k	101	BCR	C14-C15-C16-C17
28	A	1011	SQD	C32-C33-C34-C35
28	a	401	SQD	C17-C18-C19-C20
29	Z	101	LMG	C15-C16-C17-C18
29	Z	101	LMG	C34-C35-C36-C37
29	d	409	LMG	C36-C37-C38-C39
29	m	102	LMG	C31-C32-C33-C34
32	b	625	LMT	C3-C4-C5-C6
32	t	103	LMT	C5-C6-C7-C8
34	D	410	LHG	C14-C15-C16-C17
34	D	411	LHG	C26-C27-C28-C29
34	e	101	LHG	C11-C10-C9-C8
34	e	101	LHG	C13-C14-C15-C16
36	C	516	DGD	C9A-CAA-CBA-CCA
36	c	515	DGD	CBA-CCA-CDA-CEA
36	c	516	DGD	C7B-C8B-C9B-CAB
36	c	516	DGD	C9B-CAB-CBB-CCB
24	c	507	CLA	C5-C6-C7-C8
24	c	513	CLA	C13-C15-C16-C17
28	b	623[B]	SQD	C14-C15-C16-C17
29	C	518	LMG	C33-C34-C35-C36
29	Z	101	LMG	C18-C19-C20-C21
32	b	625	LMT	C7-C8-C9-C10
34	E	101	LHG	C9-C10-C11-C12
34	E	101	LHG	C18-C19-C20-C21
35	o	301	HTG	C3'-C4'-C5'-C6'
36	c	515	DGD	C3A-C4A-C5A-C6A
28	B	620[B]	SQD	C31-C32-C33-C34
28	D	408	SQD	C32-C33-C34-C35
28	a	401	SQD	C10-C11-C12-C13
28	c	518	SQD	C12-C13-C14-C15
28	c	518	SQD	C31-C32-C33-C34
29	A	1012	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	C11-C12-C13-C14
29	a	415	LMG	C39-C40-C41-C42
29	d	409	LMG	C15-C16-C17-C18
29	d	409	LMG	C20-C21-C22-C23
32	f	103	LMT	C2-C3-C4-C5
34	E	101	LHG	C32-C33-C34-C35
34	b	624	LHG	C13-C14-C15-C16
34	d	406	LHG	C11-C12-C13-C14
34	e	101	LHG	C10-C11-C12-C13
34	e	101	LHG	C34-C35-C36-C37
36	C	516	DGD	C3B-C4B-C5B-C6B
36	c	515	DGD	C5A-C6A-C7A-C8A
36	c	517	DGD	C7B-C8B-C9B-CAB
29	D	412	LMG	O6-C5-C6-O5
29	c	519	LMG	O9-C10-O7-C8
33	V	206	GOL	O2-C2-C3-O3
33	d	415	GOL	O2-C2-C3-O3
34	d	406	LHG	O1-C1-C2-O2
28	a	401	SQD	C26-C27-C28-C29
28	a	401	SQD	C30-C31-C32-C33
29	A	1012	LMG	C19-C20-C21-C22
29	c	519	LMG	C14-C15-C16-C17
29	d	409	LMG	C35-C36-C37-C38
32	B	623	LMT	C6-C7-C8-C9
36	C	515	DGD	C5B-C6B-C7B-C8B
36	c	516	DGD	C4A-C5A-C6A-C7A
24	B	609	CLA	C4B-C3B-CAB-CBB
24	C	505	CLA	C4B-C3B-CAB-CBB
24	b	608	CLA	C4B-C3B-CAB-CBB
28	A	1011	SQD	C7-C8-C9-C10
29	C	519	LMG	C10-C11-C12-C13
28	b	623[A]	SQD	C34-C35-C36-C37
28	c	518	SQD	C9-C10-C11-C12
29	B	622	LMG	C34-C35-C36-C37
29	c	521	LMG	C11-C12-C13-C14
32	b	631	LMT	C5-C6-C7-C8
34	B	621	LHG	C14-C15-C16-C17
34	b	624	LHG	C12-C13-C14-C15
35	C	522	HTG	C2'-C3'-C4'-C5'
36	C	517	DGD	CCB-CDB-CEB-CFB
24	B	606	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C16-C17-C18-C20
24	C	508	CLA	C16-C17-C18-C19
24	b	616	CLA	C16-C17-C18-C20
24	d	403	CLA	C16-C17-C18-C19
24	d	403	CLA	C16-C17-C18-C20
24	a	412	CLA	O1A-CGA-O2A-C1
28	c	518	SQD	C30-C31-C32-C33
34	E	101	LHG	C25-C26-C27-C28
32	b	631	LMT	C1-C2-C3-C4
29	A	1012	LMG	C11-C10-O7-C8
29	C	518	LMG	C19-C20-C21-C22
29	a	415	LMG	C32-C33-C34-C35
24	A	1008	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	B	616	CLA	C11-C12-C13-C15
24	c	513	CLA	C11-C10-C8-C7
35	b	626	HTG	S1-C1'-C2'-C3'
29	a	415	LMG	C29-C30-C31-C32
34	e	101	LHG	C27-C28-C29-C30
35	V	202	HTG	C3'-C4'-C5'-C6'
36	C	515	DGD	CAB-CBB-CCB-CDB
24	a	409	CLA	C13-C15-C16-C17
24	b	607	CLA	C13-C15-C16-C17
32	C	520	LMT	C1-C2-C3-C4
32	i	102	LMT	C1-C2-C3-C4
28	A	1011	SQD	C14-C15-C16-C17
28	f	102	SQD	C24-C25-C26-C27
29	C	519	LMG	C39-C40-C41-C42
29	Z	101	LMG	C20-C21-C22-C23
29	m	102	LMG	C30-C31-C32-C33
34	d	406	LHG	C30-C31-C32-C33
36	C	516	DGD	C8A-C9A-CAA-CBA
28	f	102	SQD	C30-C31-C32-C33
29	C	519	LMG	C35-C36-C37-C38
29	c	519	LMG	C33-C34-C35-C36
34	e	101	LHG	C17-C18-C19-C20
35	c	522	HTG	C2'-C3'-C4'-C5'
29	B	622	LMG	C21-C22-C23-C24
32	m	103	LMT	C5-C6-C7-C8
36	C	517	DGD	C8B-C9B-CAB-CBB
36	c	516	DGD	CBA-CCA-CDA-CEA
24	B	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	C10-C11-C12-C13
32	t	103	LMT	C7-C8-C9-C10
34	e	101	LHG	C31-C32-C33-C34
26	D	406	BCR	C13-C14-C15-C16
26	K	101	BCR	C9-C10-C11-C12
24	b	619	CLA	C16-C17-C18-C20
36	c	515	DGD	O6D-C5D-C6D-O5D
32	M	101	LMT	O5B-C5B-C6B-O6B
32	M	101	LMT	C2B-C1B-O1B-C4'
28	A	1011	SQD	C18-C19-C20-C21
29	C	518	LMG	C21-C22-C23-C24
29	Z	101	LMG	C37-C38-C39-C40
32	f	103	LMT	C6-C7-C8-C9
36	c	515	DGD	C2B-C3B-C4B-C5B
36	c	515	DGD	C4B-C5B-C6B-C7B
28	B	620[A]	SQD	C34-C35-C36-C37
34	D	410	LHG	C1-C2-C3-O3
29	C	518	LMG	C29-C28-O8-C9
32	B	623	LMT	C1-C2-C3-C4
28	B	620[B]	SQD	C29-C30-C31-C32
28	a	401	SQD	C15-C16-C17-C18
28	a	401	SQD	C25-C26-C27-C28
29	a	415	LMG	C36-C37-C38-C39
34	E	101	LHG	C30-C31-C32-C33
34	d	408	LHG	C31-C32-C33-C34
36	c	516	DGD	CAA-CBA-CCA-CDA
35	D	419	HTG	C1'-C2'-C3'-C4'
28	b	623[A]	SQD	C7-C8-C9-C10
28	c	518	SQD	C23-C24-C25-C26
29	C	519	LMG	C28-C29-C30-C31
28	A	1011	SQD	C15-C16-C17-C18
28	A	1011	SQD	C28-C29-C30-C31
28	D	408	SQD	C28-C29-C30-C31
28	c	518	SQD	C33-C34-C35-C36
29	B	622	LMG	C35-C36-C37-C38
29	C	518	LMG	C34-C35-C36-C37
29	C	519	LMG	C30-C31-C32-C33
29	D	412	LMG	C35-C36-C37-C38
29	a	415	LMG	C20-C21-C22-C23
29	c	519	LMG	C19-C20-C21-C22
29	c	519	LMG	C21-C22-C23-C24
29	c	519	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
34	B	621	LHG	C33-C34-C35-C36
34	E	101	LHG	C14-C15-C16-C17
34	e	101	LHG	C14-C15-C16-C17
34	e	101	LHG	C15-C16-C17-C18
36	C	515	DGD	C8B-C9B-CAB-CBB
36	C	516	DGD	CCA-CDA-CEA-CFA
36	c	515	DGD	C9A-CAA-CBA-CCA
36	c	516	DGD	C6A-C7A-C8A-C9A
36	c	516	DGD	C2B-C3B-C4B-C5B
36	C	515	DGD	O6E-C5E-C6E-O5E
28	b	623[A]	SQD	O10-C23-O48-C46
32	C	520	LMT	C4B-C5B-C6B-O6B
28	A	1016	SQD	C29-C30-C31-C32
28	b	623[B]	SQD	C28-C29-C30-C31
29	d	409	LMG	C13-C14-C15-C16
29	d	409	LMG	C29-C30-C31-C32
34	D	411	LHG	C32-C33-C34-C35
34	E	101	LHG	C29-C30-C31-C32
34	b	624	LHG	C27-C28-C29-C30
36	c	517	DGD	C6B-C7B-C8B-C9B
28	D	408	SQD	C25-C26-C27-C28
29	a	415	LMG	C17-C18-C19-C20
32	b	625	LMT	C5-C6-C7-C8
34	e	101	LHG	C24-C25-C26-C27
36	H	102	DGD	C7A-C8A-C9A-CAA
36	c	517	DGD	C2A-C3A-C4A-C5A
28	B	620[B]	SQD	C11-C12-C13-C14
28	B	620[B]	SQD	C24-C25-C26-C27
29	B	622	LMG	C31-C32-C33-C34
29	D	412	LMG	C12-C13-C14-C15
29	D	412	LMG	C18-C19-C20-C21
34	e	101	LHG	C25-C26-C27-C28
36	H	102	DGD	C9B-CAB-CBB-CCB
24	A	1006	CLA	C16-C17-C18-C20
34	B	621	LHG	C7-C8-C9-C10
24	B	609	CLA	C2B-C3B-CAB-CBB
24	b	608	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C2B-C3B-CAB-CBB
26	b	620	BCR	C1-C6-C7-C8
26	b	620	BCR	C5-C6-C7-C8
29	d	409	LMG	C39-C40-C41-C42
34	D	410	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	D	404	PHO	CBD-CGD-O2D-CED
24	B	616	CLA	C3-C5-C6-C7
29	c	521	LMG	C19-C20-C21-C22
34	D	409	LHG	C32-C33-C34-C35
34	E	101	LHG	C11-C12-C13-C14
28	B	620[A]	SQD	C15-C16-C17-C18
29	c	520	LMG	C31-C32-C33-C34
29	c	521	LMG	C39-C40-C41-C42
36	c	517	DGD	C9B-CAB-CBB-CCB
32	t	103	LMT	O1'-C1-C2-C3
24	B	613	CLA	C15-C16-C17-C18
28	b	623[A]	SQD	C32-C33-C34-C35
29	B	622	LMG	C14-C15-C16-C17
27	A	1010	PL9	C4-C3-C7-C8
29	C	519	LMG	C37-C38-C39-C40
36	C	516	DGD	C7A-C8A-C9A-CAA
29	A	1012	LMG	O9-C10-O7-C8
28	a	401	SQD	C16-C17-C18-C19
32	a	416	LMT	C5-C6-C7-C8
36	C	516	DGD	C3A-C4A-C5A-C6A
36	c	516	DGD	C8A-C9A-CAA-CBA
36	c	517	DGD	C8A-C9A-CAA-CBA
26	B	618	BCR	C18-C19-C20-C21
26	b	620	BCR	C18-C19-C20-C21
26	b	622	BCR	C10-C11-C12-C13
26	d	404	BCR	C10-C11-C12-C13
28	A	1016	SQD	C14-C15-C16-C17
28	A	1016	SQD	C34-C35-C36-C37
28	b	623[B]	SQD	C29-C30-C31-C32
29	Z	101	LMG	C29-C30-C31-C32
29	m	102	LMG	C35-C36-C37-C38
32	t	103	LMT	C11-C10-C9-C8
34	D	411	LHG	C29-C30-C31-C32
36	c	517	DGD	C7A-C8A-C9A-CAA
35	B	624	HTG	C1'-C2'-C3'-C4'
35	b	630	HTG	C1'-C2'-C3'-C4'
28	A	1011	SQD	C12-C13-C14-C15
29	Z	101	LMG	C16-C17-C18-C19
29	c	521	LMG	C18-C19-C20-C21
34	D	409	LHG	C25-C26-C27-C28
36	C	515	DGD	C5A-C6A-C7A-C8A
36	H	102	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
24	B	611	CLA	C15-C16-C17-C18
28	b	623[A]	SQD	C31-C32-C33-C34
29	C	518	LMG	C31-C32-C33-C34
29	a	415	LMG	C15-C16-C17-C18
29	c	521	LMG	C13-C14-C15-C16
34	B	621	LHG	C30-C31-C32-C33
32	M	101	LMT	O5B-C1B-O1B-C4'
32	a	416	LMT	O5'-C1'-O1'-C1
32	f	103	LMT	O5'-C1'-O1'-C1
28	A	1011	SQD	C25-C26-C27-C28
28	A	1016	SQD	C27-C28-C29-C30
29	Z	101	LMG	C33-C34-C35-C36
29	c	519	LMG	C11-C12-C13-C14
32	B	623	LMT	C11-C10-C9-C8
32	m	103	LMT	C7-C8-C9-C10
34	B	621	LHG	C13-C14-C15-C16
34	D	409	LHG	C11-C10-C9-C8
34	e	101	LHG	C18-C19-C20-C21
24	B	608	CLA	C13-C15-C16-C17
24	C	504	CLA	C13-C15-C16-C17
29	C	518	LMG	C36-C37-C38-C39
32	t	103	LMT	C1-C2-C3-C4
28	b	623[B]	SQD	C15-C16-C17-C18
29	B	622	LMG	C30-C31-C32-C33
29	Z	101	LMG	C17-C18-C19-C20
36	h	102	DGD	C6A-C7A-C8A-C9A
28	A	1011	SQD	C13-C14-C15-C16
28	c	518	SQD	C16-C17-C18-C19
29	A	1012	LMG	C29-C30-C31-C32
32	a	416	LMT	C7-C8-C9-C10
34	D	410	LHG	C11-C10-C9-C8
34	b	624	LHG	C11-C10-C9-C8
34	d	407	LHG	C34-C35-C36-C37
35	D	419	HTG	C3'-C4'-C5'-C6'
35	V	202	HTG	C2'-C3'-C4'-C5'
36	h	102	DGD	C9A-CAA-CBA-CCA
26	b	621	BCR	C19-C20-C21-C22
24	a	409	CLA	C16-C17-C18-C20
24	b	618	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C19
24	c	513	CLA	C16-C17-C18-C19
28	A	1011	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C8-C7-O7-C5
29	c	520	LMG	C28-C29-C30-C31
36	h	102	DGD	CAA-CBA-CCA-CDA
32	a	402	LMT	C1-C2-C3-C4
24	C	507	CLA	C5-C6-C7-C8
24	C	508	CLA	C13-C15-C16-C17
24	c	513	CLA	C8-C10-C11-C12
28	c	518	SQD	C14-C15-C16-C17
28	f	102	SQD	C33-C34-C35-C36
29	B	622	LMG	C36-C37-C38-C39
29	c	521	LMG	C36-C37-C38-C39
34	E	101	LHG	C26-C27-C28-C29
36	C	515	DGD	C7A-C8A-C9A-CAA
29	A	1012	LMG	C36-C37-C38-C39
32	C	520	LMT	C6-C7-C8-C9
34	d	407	LHG	C14-C15-C16-C17
24	D	405	CLA	C13-C15-C16-C17
28	f	102	SQD	C29-C30-C31-C32
29	c	519	LMG	C39-C40-C41-C42
34	d	406	LHG	C29-C30-C31-C32
29	C	519	LMG	C8-C7-O1-C1
29	C	519	LMG	C4-C5-C6-O5
32	t	103	LMT	C4'-C5'-C6'-O6'
28	b	623[A]	SQD	C30-C31-C32-C33
29	B	622	LMG	C38-C39-C40-C41
34	E	101	LHG	C15-C16-C17-C18
24	C	502	CLA	C16-C17-C18-C19
24	b	605	CLA	C16-C17-C18-C20
24	b	618	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C19
29	D	412	LMG	C36-C37-C38-C39
34	d	407	LHG	C30-C31-C32-C33
36	C	517	DGD	C2A-C3A-C4A-C5A
28	B	620[A]	SQD	C12-C13-C14-C15
28	B	620[B]	SQD	C32-C33-C34-C35
28	b	623[B]	SQD	C24-C25-C26-C27
29	A	1012	LMG	C37-C38-C39-C40
32	i	102	LMT	C2-C3-C4-C5
24	b	616	CLA	C8-C10-C11-C12
24	c	512	CLA	C15-C16-C17-C18
29	Z	101	LMG	C38-C39-C40-C41
36	H	102	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
29	B	622	LMG	C39-C40-C41-C42
36	C	517	DGD	C9B-CAB-CBB-CCB
36	C	517	DGD	CAB-CBB-CCB-CDB
29	C	518	LMG	O10-C28-O8-C9
24	c	513	CLA	C3-C5-C6-C7
24	C	512	CLA	C8-C10-C11-C12
29	Z	101	LMG	C12-C13-C14-C15
28	D	408	SQD	C24-C25-C26-C27
29	D	412	LMG	C20-C21-C22-C23
24	b	609	CLA	CBD-CGD-O2D-CED
38	V	201	HEM	C4B-C3B-CAB-CBB
28	c	518	SQD	C29-C30-C31-C32
29	A	1012	LMG	C18-C19-C20-C21
34	d	406	LHG	C25-C26-C27-C28
35	C	522	HTG	C1'-C2'-C3'-C4'
28	c	518	SQD	C11-C12-C13-C14
29	A	1012	LMG	C21-C22-C23-C24
34	D	411	LHG	C33-C34-C35-C36
36	h	102	DGD	C9B-CAB-CBB-CCB
24	B	603	CLA	C5-C6-C7-C8
24	c	506	CLA	C10-C11-C12-C13
28	A	1011	SQD	C33-C34-C35-C36
28	b	623[B]	SQD	C9-C10-C11-C12
32	M	101	LMT	C3-C4-C5-C6
36	C	515	DGD	C7B-C8B-C9B-CAB
36	c	515	DGD	C2A-C3A-C4A-C5A
36	c	515	DGD	O6E-C5E-C6E-O5E
24	a	412	CLA	C3-C5-C6-C7
34	e	101	LHG	O7-C5-C6-O8
28	c	518	SQD	C34-C35-C36-C37
29	A	1012	LMG	C38-C39-C40-C41
29	D	412	LMG	C30-C31-C32-C33
29	c	520	LMG	C37-C38-C39-C40
34	D	409	LHG	C29-C30-C31-C32
35	b	626	HTG	C3'-C4'-C5'-C6'
25	D	404	PHO	O1D-CGD-O2D-CED
28	D	408	SQD	C34-C35-C36-C37
29	c	521	LMG	C16-C17-C18-C19
35	d	410	HTG	C3'-C4'-C5'-C6'
32	A	1018	LMT	O5B-C5B-C6B-O6B
29	c	519	LMG	C30-C31-C32-C33
29	m	102	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
32	a	416	LMT	C11-C10-C9-C8
28	a	401	SQD	C11-C12-C13-C14
32	A	1017	LMT	C4-C5-C6-C7
24	c	509	CLA	C2-C1-O2A-CGA
24	C	503	CLA	C8-C10-C11-C12
29	c	520	LMG	C4-C5-C6-O5
29	A	1012	LMG	C32-C33-C34-C35
29	d	409	LMG	C14-C15-C16-C17
32	f	103	LMT	C5-C6-C7-C8
34	D	411	LHG	C14-C15-C16-C17
28	A	1011	SQD	O49-C7-O47-C45
28	B	620[B]	SQD	C34-C35-C36-C37
29	a	415	LMG	C19-C20-C21-C22
36	c	517	DGD	CBB-CCB-CDB-CEB
26	h	101	BCR	C14-C15-C16-C17
29	A	1012	LMG	C20-C21-C22-C23
32	b	625	LMT	C1-C2-C3-C4
29	C	519	LMG	C31-C32-C33-C34
35	d	410	HTG	C2'-C3'-C4'-C5'
36	C	515	DGD	O6D-C5D-C6D-O5D
34	e	101	LHG	C26-C27-C28-C29
36	c	516	DGD	C9A-CAA-CBA-CCA
33	V	207	GOL	O1-C1-C2-O2
33	a	420	GOL	O2-C2-C3-O3
36	c	517	DGD	CBA-CCA-CDA-CEA
32	f	103	LMT	C1-C2-C3-C4
28	B	620[A]	SQD	C28-C29-C30-C31
32	A	1018	LMT	C6-C7-C8-C9
32	C	520	LMT	C11-C10-C9-C8
24	C	503	CLA	C1A-C2A-CAA-CBA
24	C	506	CLA	C1A-C2A-CAA-CBA
24	c	506	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
24	C	505	CLA	C13-C15-C16-C17
24	c	503	CLA	C8-C10-C11-C12
29	A	1012	LMG	C34-C35-C36-C37
29	c	520	LMG	C38-C39-C40-C41
32	t	103	LMT	C3-C4-C5-C6
34	E	101	LHG	C34-C35-C36-C37
34	e	101	LHG	C29-C30-C31-C32
36	C	516	DGD	C5B-C6B-C7B-C8B
24	b	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	A	1016	SQD	C15-C16-C17-C18
32	C	520	LMT	C3-C4-C5-C6
36	c	516	DGD	C1A-C2A-C3A-C4A
24	a	412	CLA	O1D-CGD-O2D-CED
24	a	409	CLA	C6-C7-C8-C10
24	b	614	CLA	C12-C13-C15-C16
24	b	615	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	b	617	CLA	C6-C7-C8-C10
24	b	619	CLA	C11-C12-C13-C15
24	b	619	CLA	C12-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C15
32	b	631	LMT	C7-C8-C9-C10
24	c	507	CLA	C16-C17-C18-C19
29	C	518	LMG	C15-C16-C17-C18
29	m	102	LMG	C10-C11-C12-C13
28	f	102	SQD	C34-C35-C36-C37
36	C	515	DGD	C3B-C4B-C5B-C6B
24	c	510	CLA	C4-C3-C5-C6
34	D	411	LHG	C9-C10-C11-C12
36	c	515	DGD	C8A-C9A-CAA-CBA
24	a	412	CLA	C13-C15-C16-C17
24	B	614	CLA	C14-C13-C15-C16
24	B	615	CLA	C14-C13-C15-C16
24	B	616	CLA	C11-C12-C13-C14
24	B	616	CLA	C14-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C10-C8-C9
24	D	405	CLA	C6-C7-C8-C9
24	D	405	CLA	C14-C13-C15-C16
24	a	409	CLA	C11-C10-C8-C9
24	b	604	CLA	C11-C10-C8-C9
24	b	614	CLA	C14-C13-C15-C16
24	b	617	CLA	C14-C13-C15-C16
24	b	619	CLA	C11-C12-C13-C14
24	b	619	CLA	C14-C13-C15-C16
28	a	401	SQD	C28-C29-C30-C31
32	t	103	LMT	O5'-C5'-C6'-O6'
34	E	101	LHG	C11-C10-C9-C8
32	f	103	LMT	C2'-C1'-O1'-C1
32	m	103	LMT	C2'-C1'-O1'-C1
28	b	623[A]	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
29	A	1012	LMG	C7-C8-C9-O8
29	C	519	LMG	C7-C8-C9-O8
29	c	519	LMG	C7-C8-C9-O8
29	c	520	LMG	C7-C8-C9-O8
34	E	101	LHG	C4-C5-C6-O8
28	B	620[A]	SQD	C27-C28-C29-C30
29	m	102	LMG	C29-C30-C31-C32
34	D	409	LHG	C15-C16-C17-C18
29	c	519	LMG	C18-C19-C20-C21
36	C	516	DGD	C5A-C6A-C7A-C8A
32	B	623	LMT	O5B-C1B-O1B-C4'
24	b	604	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C20
28	f	102	SQD	C32-C33-C34-C35
34	D	411	LHG	C34-C35-C36-C37
36	c	515	DGD	CAB-CBB-CCB-CDB
32	m	103	LMT	C1-C2-C3-C4
24	c	505	CLA	C15-C16-C17-C18
36	C	516	DGD	CAA-CBA-CCA-CDA
36	H	102	DGD	CCB-CDB-CEB-CFB
25	a	411	PHO	CHA-CBD-CGD-O2D
24	c	509	CLA	C15-C16-C17-C18
34	b	624	LHG	C14-C15-C16-C17
28	B	620[A]	SQD	C16-C17-C18-C19
24	c	510	CLA	C2-C3-C5-C6
26	k	101	BCR	C11-C12-C13-C35
36	h	102	DGD	C7A-C8A-C9A-CAA
24	b	606	CLA	C16-C17-C18-C20
28	a	401	SQD	C32-C33-C34-C35
28	b	623[B]	SQD	C17-C18-C19-C20
36	H	102	DGD	C5B-C6B-C7B-C8B
26	k	101	BCR	C7-C8-C9-C10
26	y	101	BCR	C11-C12-C13-C14
24	B	615	CLA	C10-C11-C12-C13
24	c	509	CLA	C8-C10-C11-C12
29	Z	101	LMG	C19-C20-C21-C22
28	D	408	SQD	C27-C28-C29-C30
28	a	401	SQD	C31-C32-C33-C34
34	d	408	LHG	C29-C30-C31-C32
32	B	623	LMT	C3'-C4'-O1B-C1B
36	c	515	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
29	m	102	LMG	C16-C17-C18-C19
29	m	102	LMG	C33-C34-C35-C36
34	E	101	LHG	C13-C14-C15-C16
29	a	415	LMG	C10-C11-C12-C13
34	b	624	LHG	C7-C8-C9-C10
28	A	1016	SQD	C24-C25-C26-C27
28	a	401	SQD	C24-C23-O48-C46
26	B	619	BCR	C18-C19-C20-C21
28	b	623[A]	SQD	C10-C11-C12-C13
29	d	409	LMG	C38-C39-C40-C41
32	M	101	LMT	C7-C8-C9-C10
34	d	408	LHG	C17-C18-C19-C20
26	h	101	BCR	C9-C10-C11-C12
26	k	101	BCR	C15-C16-C17-C18
26	t	101	BCR	C19-C20-C21-C22
24	C	502	CLA	C16-C17-C18-C20
24	c	502	CLA	C16-C17-C18-C20
29	c	520	LMG	C33-C34-C35-C36
29	d	409	LMG	C19-C20-C21-C22
29	A	1012	LMG	C10-C11-C12-C13
34	D	410	LHG	C34-C35-C36-C37
26	J	101	BCR	C20-C21-C22-C23
29	m	102	LMG	C34-C35-C36-C37
24	c	511	CLA	CBA-CGA-O2A-C1
28	f	102	SQD	C26-C27-C28-C29
29	c	520	LMG	C30-C31-C32-C33
29	D	412	LMG	C17-C18-C19-C20
34	D	410	LHG	C10-C11-C12-C13
28	A	1011	SQD	C9-C10-C11-C12
29	B	622	LMG	C12-C13-C14-C15
34	d	408	LHG	C9-C10-C11-C12
29	C	519	LMG	C34-C35-C36-C37
32	C	520	LMT	C5-C6-C7-C8
36	C	515	DGD	C4A-C5A-C6A-C7A
36	c	516	DGD	C8B-C9B-CAB-CBB
28	c	518	SQD	C19-C20-C21-C22
28	b	623[B]	SQD	O6-C44-C45-O47
29	C	519	LMG	O7-C8-C9-O8
29	Z	101	LMG	O7-C8-C9-O8
29	a	415	LMG	O7-C8-C9-O8
29	c	520	LMG	O7-C8-C9-O8
36	H	102	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
36	c	517	DGD	CDB-CEB-CFB-CGB
36	h	102	DGD	CCB-CDB-CEB-CFB
32	a	416	LMT	C9-C10-C11-C12
34	D	411	LHG	C35-C36-C37-C38
28	A	1016	SQD	C16-C17-C18-C19
29	c	519	LMG	C17-C18-C19-C20
28	b	623[A]	SQD	C35-C36-C37-C38
36	H	102	DGD	O2G-C1B-C2B-C3B
29	D	412	LMG	C21-C22-C23-C24
29	c	519	LMG	C31-C32-C33-C34
24	C	509	CLA	C2-C1-O2A-CGA
28	D	408	SQD	C35-C36-C37-C38
29	C	518	LMG	C40-C41-C42-C43
29	C	519	LMG	C40-C41-C42-C43
36	c	517	DGD	CDA-CEA-CFA-CGA
28	B	620[A]	SQD	C35-C36-C37-C38
36	c	516	DGD	C1B-C2B-C3B-C4B
24	b	608	CLA	CBA-CGA-O2A-C1
29	c	520	LMG	C29-C28-O8-C9
36	c	517	DGD	C2A-C1A-O1G-C1G
32	i	102	LMT	C4B-C5B-C6B-O6B
36	h	102	DGD	CDB-CEB-CFB-CGB
28	A	1011	SQD	C10-C11-C12-C13
29	B	622	LMG	C15-C16-C17-C18
29	a	415	LMG	C13-C14-C15-C16
28	b	623[B]	SQD	C33-C34-C35-C36
24	C	512	CLA	O1D-CGD-O2D-CED
34	E	101	LHG	C23-C24-C25-C26
29	B	622	LMG	C40-C41-C42-C43
29	C	518	LMG	C22-C23-C24-C25
24	d	403	CLA	C10-C11-C12-C13
26	H	101	BCR	C15-C16-C17-C18
26	h	101	BCR	C19-C20-C21-C22
26	y	101	BCR	C15-C16-C17-C18
24	B	603	CLA	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C20
29	A	1012	LMG	C30-C31-C32-C33
24	C	503	CLA	CBA-CGA-O2A-C1
34	B	621	LHG	C17-C18-C19-C20
25	D	404	PHO	C2C-C3C-CAC-CBC
28	B	620[A]	SQD	C18-C19-C20-C21
34	D	411	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
36	H	102	DGD	C7B-C8B-C9B-CAB
34	E	101	LHG	O9-C7-O7-C5
32	b	625	LMT	C2-C1-O1'-C1'
33	v	203	GOL	O2-C2-C3-O3
24	A	1006	CLA	C11-C10-C8-C9
24	A	1008	CLA	C11-C12-C13-C14
24	C	506	CLA	C6-C7-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	C	506	CLA	C14-C13-C15-C16
24	a	409	CLA	C6-C7-C8-C9
24	b	616	CLA	C11-C10-C8-C9
24	b	617	CLA	C6-C7-C8-C9
24	c	507	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C12-C13-C14
24	c	513	CLA	C11-C10-C8-C9
24	d	402	CLA	C11-C12-C13-C14
34	b	624	LHG	C32-C33-C34-C35
24	c	503	CLA	O1D-CGD-O2D-CED
24	c	509	CLA	O1D-CGD-O2D-CED
29	c	521	LMG	C40-C41-C42-C43
24	b	610	CLA	C4B-C3B-CAB-CBB
24	b	618	CLA	C4B-C3B-CAB-CBB
24	c	504	CLA	C4B-C3B-CAB-CBB
28	A	1016	SQD	C18-C19-C20-C21
34	B	621	LHG	C12-C13-C14-C15
36	C	516	DGD	C8B-C9B-CAB-CBB
34	E	101	LHG	C35-C36-C37-C38
36	c	515	DGD	CCB-CDB-CEB-CFB
24	D	405	CLA	C16-C17-C18-C19
28	A	1011	SQD	C19-C20-C21-C22
28	b	623[B]	SQD	C35-C36-C37-C38
29	c	521	LMG	C34-C35-C36-C37
34	b	624	LHG	C28-C29-C30-C31
32	M	101	LMT	C2'-C1'-O1'-C1
36	C	516	DGD	C2E-C1E-O5D-C6D
34	D	409	LHG	C9-C10-C11-C12
36	C	516	DGD	C7B-C8B-C9B-CAB
36	C	517	DGD	CBB-CCB-CDB-CEB
28	A	1011	SQD	C35-C36-C37-C38
28	f	102	SQD	C11-C10-C9-C8
24	A	1006	CLA	C11-C10-C8-C7
24	B	614	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C12-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C10
24	C	506	CLA	C11-C12-C13-C15
24	C	507	CLA	C11-C12-C13-C15
24	C	508	CLA	C11-C10-C8-C7
24	C	508	CLA	C11-C12-C13-C15
24	C	512	CLA	C11-C10-C8-C7
24	C	513	CLA	C6-C7-C8-C10
24	D	405	CLA	C6-C7-C8-C10
24	D	405	CLA	C12-C13-C15-C16
24	a	409	CLA	C11-C10-C8-C7
24	b	617	CLA	C12-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C7
24	c	504	CLA	C12-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C15
24	c	507	CLA	C11-C10-C8-C7
24	c	508	CLA	C11-C12-C13-C15
24	c	512	CLA	C11-C10-C8-C7
24	d	403	CLA	C12-C13-C15-C16
28	B	620[B]	SQD	C19-C20-C21-C22
35	V	202	HTG	C4'-C5'-C6'-C7'
28	c	518	SQD	C17-C18-C19-C20
34	D	409	LHG	C10-C11-C12-C13
35	o	301	HTG	C4'-C5'-C6'-C7'
34	d	406	LHG	C7-C8-C9-C10
35	d	416	HTG	C1'-C2'-C3'-C4'
32	B	623	LMT	C5'-C4'-O1B-C1B
28	b	623[A]	SQD	C17-C18-C19-C20
28	B	620[A]	SQD	C17-C18-C19-C20
24	C	513	CLA	C15-C16-C17-C18
24	b	618	CLA	C10-C11-C12-C13
36	c	516	DGD	C6B-C7B-C8B-C9B
34	d	406	LHG	C34-C35-C36-C37
26	B	618	BCR	C15-C16-C17-C18
26	H	101	BCR	C9-C10-C11-C12
26	k	101	BCR	C9-C10-C11-C12
26	k	102	BCR	C9-C10-C11-C12
24	b	604	CLA	C3-C5-C6-C7
24	b	604	CLA	C16-C17-C18-C19
28	D	408	SQD	C31-C32-C33-C34
35	b	630	HTG	C4-C5-C6-O6
24	b	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	B	622	LMG	C20-C21-C22-C23
34	E	101	LHG	C19-C20-C21-C22
29	B	622	LMG	C37-C38-C39-C40
34	d	407	LHG	C12-C13-C14-C15
28	A	1016	SQD	O6-C44-C45-C46
29	Z	101	LMG	C7-C8-C9-O8
29	c	519	LMG	O1-C7-C8-C9
34	e	101	LHG	C4-C5-C6-O8
24	B	613	CLA	C3-C5-C6-C7
32	a	416	LMT	C4B-C5B-C6B-O6B
28	f	102	SQD	C27-C28-C29-C30
29	A	1012	LMG	C16-C17-C18-C19
29	a	415	LMG	C38-C39-C40-C41
34	D	409	LHG	C24-C25-C26-C27
25	a	410	PHO	C8-C10-C11-C12
24	c	505	CLA	C4-C3-C5-C6
28	A	1016	SQD	C19-C20-C21-C22
28	a	401	SQD	O10-C23-O48-C46
28	A	1011	SQD	C11-C10-C9-C8
29	Z	101	LMG	C13-C14-C15-C16
35	B	624	HTG	C2'-C3'-C4'-C5'
24	B	601	CLA	C16-C17-C18-C20
24	b	606	CLA	C16-C17-C18-C19
24	b	617	CLA	C16-C17-C18-C20
29	a	415	LMG	C22-C23-C24-C25
32	m	103	LMT	C4-C5-C6-C7
36	c	515	DGD	CDA-CEA-CFA-CGA
26	B	617	BCR	C1-C6-C7-C8
26	K	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
36	h	102	DGD	CCA-CDA-CEA-CFA
29	d	409	LMG	C34-C35-C36-C37
36	C	515	DGD	C4D-C5D-C6D-O5D
35	B	628	HTG	C4'-C5'-C6'-C7'
24	C	501	CLA	O1D-CGD-O2D-CED
28	B	620[A]	SQD	C24-C25-C26-C27
29	m	102	LMG	C12-C13-C14-C15
34	B	621	LHG	C10-C11-C12-C13
34	d	408	LHG	C28-C29-C30-C31
24	b	606	CLA	C13-C15-C16-C17
29	c	519	LMG	O1-C7-C8-O7
29	c	519	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
29	c	521	LMG	O1-C7-C8-O7
27	a	414	PL9	C4-C3-C7-C8
35	B	624	HTG	O5-C1-S1-C1'
36	C	515	DGD	CCA-CDA-CEA-CFA
29	c	521	LMG	C28-C29-C30-C31
34	D	409	LHG	C7-C8-C9-C10
24	c	511	CLA	O1A-CGA-O2A-C1
24	b	609	CLA	O1D-CGD-O2D-CED
32	t	103	LMT	C4-C5-C6-C7
24	b	608	CLA	C13-C15-C16-C17
29	c	521	LMG	C31-C32-C33-C34
34	d	406	LHG	C24-C25-C26-C27
36	C	515	DGD	C9A-CAA-CBA-CCA
36	c	515	DGD	C5B-C6B-C7B-C8B
24	c	508	CLA	C16-C17-C18-C20
28	D	408	SQD	C30-C31-C32-C33
29	m	102	LMG	C37-C38-C39-C40
34	D	409	LHG	C23-C24-C25-C26
28	B	620[A]	SQD	C26-C27-C28-C29
36	c	515	DGD	CBB-CCB-CDB-CEB
24	B	604	CLA	C6-C7-C8-C9
24	C	513	CLA	C6-C7-C8-C9
24	b	615	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C9
24	c	505	CLA	C14-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C14
29	Z	101	LMG	C4-C5-C6-O5
34	D	410	LHG	C12-C13-C14-C15
32	a	402	LMT	C4-C5-C6-C7
32	A	1018	LMT	O5'-C1'-O1'-C1
29	B	622	LMG	C22-C23-C24-C25
26	D	406	BCR	C14-C15-C16-C17
28	B	620[B]	SQD	C10-C11-C12-C13
28	B	620[B]	SQD	C14-C15-C16-C17
32	B	623	LMT	C9-C10-C11-C12
24	C	504	CLA	C3-C5-C6-C7
24	c	510	CLA	C8-C10-C11-C12
32	M	102	LMT	C3-C4-C5-C6
34	d	406	LHG	C17-C18-C19-C20
27	A	1010	PL9	C19-C21-C22-C23
27	a	414	PL9	C14-C16-C17-C18
27	a	414	PL9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
29	a	415	LMG	C14-C15-C16-C17
24	B	604	CLA	O1D-CGD-O2D-CED
34	E	101	LHG	C31-C32-C33-C34
32	f	103	LMT	C9-C10-C11-C12
24	C	506	CLA	C10-C11-C12-C13
33	A	1019	GOL	O2-C2-C3-O3
33	d	417	GOL	O1-C1-C2-O2
35	c	525	HTG	S1-C1'-C2'-C3'
24	c	505	CLA	C2-C3-C5-C6
34	D	411	LHG	C17-C18-C19-C20
29	d	409	LMG	C17-C18-C19-C20
36	h	102	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	CBB-CCB-CDB-CEB
34	d	406	LHG	C1-C2-C3-O3
29	C	518	LMG	C13-C14-C15-C16
26	J	101	BCR	C20-C21-C22-C37
24	C	503	CLA	O1A-CGA-O2A-C1
35	C	521	HTG	C2'-C3'-C4'-C5'
24	C	509	CLA	C13-C15-C16-C17
28	A	1011	SQD	C34-C35-C36-C37
34	D	409	LHG	C33-C34-C35-C36
24	B	606	CLA	C11-C10-C8-C7
24	C	504	CLA	C6-C7-C8-C10
24	C	507	CLA	C12-C13-C15-C16
24	b	604	CLA	C6-C7-C8-C10
24	b	609	CLA	C11-C10-C8-C7
24	c	505	CLA	C12-C13-C15-C16
24	d	403	CLA	C11-C12-C13-C15
28	D	408	SQD	C7-C8-C9-C10
34	D	409	LHG	C34-C35-C36-C37
34	d	406	LHG	C18-C19-C20-C21
36	C	515	DGD	C8A-C9A-CAA-CBA
24	C	510	CLA	C8-C10-C11-C12
26	D	406	BCR	C21-C22-C23-C24
29	c	520	LMG	C8-C7-O1-C1
36	C	516	DGD	C2G-C3G-O3G-C1D
36	C	516	DGD	C5D-C6D-O5D-C1E
36	c	516	DGD	C2G-C3G-O3G-C1D
36	c	516	DGD	C5D-C6D-O5D-C1E
29	B	622	LMG	C10-C11-C12-C13
36	C	516	DGD	C1A-C2A-C3A-C4A
28	b	623[A]	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
29	A	1012	LMG	C13-C14-C15-C16
34	b	624	LHG	C17-C18-C19-C20
24	b	608	CLA	O1A-CGA-O2A-C1
38	V	201	HEM	C2C-C3C-CAC-CBC
38	v	201	HEM	C2C-C3C-CAC-CBC
34	B	621	LHG	C28-C29-C30-C31
33	V	206	GOL	O1-C1-C2-C3
33	v	204	GOL	O1-C1-C2-C3
34	E	101	LHG	O1-C1-C2-C3
34	D	411	LHG	C24-C23-O8-C6
29	d	409	LMG	C30-C31-C32-C33
24	c	506	CLA	C13-C15-C16-C17
28	b	623[B]	SQD	C46-C45-O47-C7
29	c	521	LMG	C7-C8-O7-C10
35	D	413	HTG	C1'-C2'-C3'-C4'
29	c	520	LMG	O10-C28-O8-C9
32	t	103	LMT	C2B-C1B-O1B-C4'
28	b	623[B]	SQD	C26-C27-C28-C29
29	C	518	LMG	C35-C36-C37-C38
26	T	101	BCR	C20-C21-C22-C23
26	t	101	BCR	C20-C21-C22-C23
28	f	102	SQD	O5-C1-O6-C44
32	M	101	LMT	O5'-C1'-O1'-C1
36	C	516	DGD	O6E-C1E-O5D-C6D
28	a	401	SQD	C9-C10-C11-C12
27	d	405	PL9	C39-C41-C42-C43
28	D	408	SQD	C44-C45-C46-O48
28	a	401	SQD	O6-C44-C45-C46
29	C	519	LMG	O1-C7-C8-C9
29	c	521	LMG	O1-C7-C8-C9
32	a	416	LMT	C4'-C5'-C6'-O6'
24	D	405	CLA	C16-C17-C18-C20
36	C	516	DGD	CDA-CEA-CFA-CGA
36	c	516	DGD	C3B-C4B-C5B-C6B
36	c	517	DGD	O1A-C1A-O1G-C1G
35	C	522	HTG	C2-C1-S1-C1'
35	D	419	HTG	C2-C1-S1-C1'
35	b	630	HTG	C2-C1-S1-C1'
35	c	522	HTG	C2-C1-S1-C1'
36	c	516	DGD	CBB-CCB-CDB-CEB
34	E	101	LHG	O7-C5-C6-O8
24	B	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	B	606	CLA	C11-C10-C8-C9
24	C	504	CLA	C6-C7-C8-C9
24	b	609	CLA	C11-C10-C8-C9
32	t	103	LMT	O5B-C1B-O1B-C4'
24	B	611	CLA	C16-C17-C18-C20
34	d	407	LHG	C26-C27-C28-C29
24	C	511	CLA	CBA-CGA-O2A-C1
28	B	620[A]	SQD	C11-C10-C9-C8
35	b	626	HTG	C2'-C3'-C4'-C5'
36	c	517	DGD	CAA-CBA-CCA-CDA
29	D	412	LMG	C40-C41-C42-C43
28	A	1011	SQD	C30-C31-C32-C33
28	A	1016	SQD	C26-C27-C28-C29
34	b	624	LHG	C30-C31-C32-C33
34	d	408	LHG	C34-C35-C36-C37
35	C	521	HTG	C3'-C4'-C5'-C6'
28	b	623[B]	SQD	C30-C31-C32-C33
32	A	1017	LMT	C11-C10-C9-C8
32	M	102	LMT	C7-C8-C9-C10
35	b	630	HTG	S1-C1'-C2'-C3'
32	B	623	LMT	C3-C4-C5-C6
34	B	621	LHG	C11-C12-C13-C14
29	Z	101	LMG	C40-C41-C42-C43
36	c	516	DGD	C2E-C1E-O5D-C6D
24	B	612	CLA	C8-C10-C11-C12
24	C	504	CLA	C15-C16-C17-C18
28	B	620[B]	SQD	C15-C16-C17-C18
34	B	621	LHG	C11-C10-C9-C8
28	B	620[A]	SQD	C32-C33-C34-C35
36	H	102	DGD	C2B-C3B-C4B-C5B
34	d	406	LHG	C23-C24-C25-C26
35	D	413	HTG	O5-C5-C6-O6
24	C	505	CLA	C16-C17-C18-C20
24	B	601	CLA	C15-C16-C17-C18
32	A	1018	LMT	C1-C2-C3-C4
34	B	621	LHG	C25-C26-C27-C28
34	E	101	LHG	C28-C29-C30-C31
34	d	407	LHG	C28-C29-C30-C31
35	d	416	HTG	S1-C1'-C2'-C3'
29	d	409	LMG	C10-C11-C12-C13
29	d	409	LMG	C21-C22-C23-C24
28	b	623[A]	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
29	B	622	LMG	C28-C29-C30-C31
24	B	601	CLA	C16-C17-C18-C19
24	B	603	CLA	C16-C17-C18-C19
24	D	402	CLA	C16-C17-C18-C20
24	b	617	CLA	C10-C11-C12-C13
35	b	601	HTG	O5-C5-C6-O6
33	b	632	GOL	O1-C1-C2-O2
33	v	204	GOL	O1-C1-C2-O2
34	E	101	LHG	O1-C1-C2-O2
24	b	616	CLA	C3-C5-C6-C7
26	K	102	BCR	C7-C8-C9-C34
24	B	601	CLA	C4B-C3B-CAB-CBB
24	b	604	CLA	C4B-C3B-CAB-CBB
24	c	503	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
27	A	1010	PL9	C15-C14-C16-C17
26	k	101	BCR	C11-C12-C13-C14
34	D	410	LHG	C32-C33-C34-C35
24	b	605	CLA	C3-C5-C6-C7
34	b	624	LHG	O6-C4-C5-C6
28	a	401	SQD	O49-C7-O47-C45
29	C	519	LMG	C32-C33-C34-C35
36	c	516	DGD	C4B-C5B-C6B-C7B
24	B	605	CLA	O1D-CGD-O2D-CED
28	f	102	SQD	C5-C6-S-O7
24	A	1006	CLA	C12-C13-C15-C16
24	B	604	CLA	C11-C12-C13-C15
24	B	615	CLA	C11-C10-C8-C7
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C10
24	C	512	CLA	C11-C12-C13-C15
24	a	412	CLA	C11-C10-C8-C7
24	b	604	CLA	C11-C12-C13-C15
24	b	617	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
24	c	507	CLA	C11-C12-C13-C15
24	c	513	CLA	C6-C7-C8-C10
24	c	513	CLA	C11-C12-C13-C15
28	b	623[B]	SQD	C25-C26-C27-C28
29	C	518	LMG	C18-C19-C20-C21
36	c	516	DGD	C3A-C4A-C5A-C6A
36	c	516	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
34	D	411	LHG	O10-C23-O8-C6
29	c	519	LMG	C10-C11-C12-C13
34	D	411	LHG	C2-C3-O3-P
34	d	408	LHG	C2-C3-O3-P
35	o	301	HTG	C4-C5-C6-O6
24	b	617	CLA	C16-C17-C18-C19
29	D	412	LMG	C22-C23-C24-C25
29	Z	101	LMG	C22-C23-C24-C25
29	c	520	LMG	O6-C5-C6-O5
24	d	403	CLA	C14-C13-C15-C16
36	C	515	DGD	CBB-CCB-CDB-CEB
36	h	102	DGD	C6B-C7B-C8B-C9B
26	d	404	BCR	C19-C20-C21-C22
34	b	624	LHG	C31-C32-C33-C34
36	C	515	DGD	C6B-C7B-C8B-C9B
28	f	102	SQD	C31-C32-C33-C34
35	D	413	HTG	C3'-C4'-C5'-C6'
29	c	520	LMG	C40-C41-C42-C43
36	H	102	DGD	CDA-CEA-CFA-CGA
28	a	401	SQD	C18-C19-C20-C21
34	D	410	LHG	C26-C27-C28-C29
24	C	511	CLA	O1A-CGA-O2A-C1
28	B	620[A]	SQD	O6-C44-C45-O47
28	D	408	SQD	O47-C45-C46-O48
29	A	1012	LMG	O7-C8-C9-O8
24	C	501	CLA	C13-C15-C16-C17
36	c	516	DGD	C2A-C3A-C4A-C5A
28	b	623[B]	SQD	O6-C44-C45-C46
29	a	415	LMG	C12-C13-C14-C15
32	M	102	LMT	C9-C10-C11-C12
35	B	628	HTG	C1'-C2'-C3'-C4'
24	B	605	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	CAD-CBD-CGD-O2D
24	b	610	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	C13-C15-C16-C17
24	b	617	CLA	CBD-CGD-O2D-CED
24	b	615	CLA	C16-C17-C18-C20
24	c	508	CLA	C16-C17-C18-C19
25	a	411	PHO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	m	102	LMG	C13-C14-C15-C16
24	B	604	CLA	CHA-CBD-CGD-O1D
24	B	605	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CHA-CBD-CGD-O1D
24	B	616	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	b	604	CLA	CAD-CBD-CGD-O1D
24	b	608	CLA	CAD-CBD-CGD-O1D
24	b	612	CLA	CAD-CBD-CGD-O1D
24	b	613	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
34	D	410	LHG	C4-O6-P-O5
34	d	407	LHG	C4-O6-P-O5
36	C	517	DGD	C7A-C8A-C9A-CAA
24	B	601	CLA	C2B-C3B-CAB-CBB
24	C	505	CLA	C2B-C3B-CAB-CBB
24	b	610	CLA	C2B-C3B-CAB-CBB
28	b	623[B]	SQD	C11-C10-C9-C8
26	b	621	BCR	C37-C22-C23-C24
26	h	101	BCR	C37-C22-C23-C24
32	B	623	LMT	C2B-C1B-O1B-C4'
29	C	518	LMG	C32-C33-C34-C35
36	h	102	DGD	CBA-CCA-CDA-CEA
24	C	510	CLA	C16-C17-C18-C19
24	D	403	CLA	C2C-C3C-CAC-CBC
33	v	204	GOL	C1-C2-C3-O3
29	c	519	LMG	C32-C33-C34-C35
24	B	614	CLA	C13-C15-C16-C17
29	c	519	LMG	C34-C35-C36-C37
32	i	102	LMT	O5B-C5B-C6B-O6B
24	d	402	CLA	C16-C17-C18-C20
24	b	618	CLA	C5-C6-C7-C8
24	A	1006	CLA	C6-C7-C8-C9
24	C	504	CLA	C11-C12-C13-C14
24	C	505	CLA	C11-C12-C13-C14
24	C	508	CLA	C11-C12-C13-C14
24	C	512	CLA	C11-C12-C13-C14
24	D	405	CLA	C11-C10-C8-C9
24	b	604	CLA	C6-C7-C8-C9
24	c	512	CLA	C11-C10-C8-C9
24	B	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	C	505	CLA	C11-C12-C13-C15
24	D	405	CLA	C11-C10-C8-C7
24	d	403	CLA	C6-C7-C8-C10
34	b	624	LHG	O6-C4-C5-O7
28	b	623[A]	SQD	C14-C15-C16-C17
24	C	505	CLA	C16-C17-C18-C19
24	D	402	CLA	C16-C17-C18-C19
28	a	401	SQD	C8-C7-O47-C45
36	c	515	DGD	CAA-CBA-CCA-CDA
24	A	1008	CLA	C13-C15-C16-C17
24	b	613	CLA	C15-C16-C17-C18
24	C	510	CLA	C4-C3-C5-C6
25	a	410	PHO	C4-C3-C5-C6
24	c	512	CLA	O1A-CGA-O2A-C1
24	B	611	CLA	C16-C17-C18-C19
24	c	510	CLA	C16-C17-C18-C19
29	Z	101	LMG	C36-C37-C38-C39
32	A	1017	LMT	C3-C4-C5-C6
28	A	1016	SQD	C35-C36-C37-C38
35	D	413	HTG	C2'-C3'-C4'-C5'
28	b	623[A]	SQD	O47-C45-C46-O48
29	A	1012	LMG	O1-C7-C8-O7
28	a	401	SQD	C23-C24-C25-C26
28	D	408	SQD	C11-C10-C9-C8
32	M	102	LMT	O1'-C1-C2-C3
34	E	101	LHG	C24-C25-C26-C27
36	h	102	DGD	CDA-CEA-CFA-CGA
24	C	507	CLA	C4-C3-C5-C6
24	C	512	CLA	C16-C17-C18-C20
36	h	102	DGD	O2G-C1B-C2B-C3B
29	B	622	LMG	C13-C14-C15-C16
36	C	517	DGD	CBA-CCA-CDA-CEA
27	D	407	PL9	C39-C41-C42-C43
29	a	415	LMG	C7-C8-C9-O8
34	d	408	LHG	C11-C10-C9-C8
35	b	602	HTG	C4-C5-C6-O6
28	D	408	SQD	C33-C34-C35-C36
29	B	622	LMG	O8-C28-C29-C30
24	c	512	CLA	CBA-CGA-O2A-C1
32	t	103	LMT	C9-C10-C11-C12
28	b	623[A]	SQD	C45-C44-O6-C1
29	D	412	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
24	D	405	CLA	O1A-CGA-O2A-C1
35	D	413	HTG	C4'-C5'-C6'-C7'
26	J	101	BCR	C13-C14-C15-C16
26	t	101	BCR	C9-C10-C11-C12
24	C	513	CLA	C16-C17-C18-C19
34	e	101	LHG	C33-C34-C35-C36
35	b	601	HTG	C1'-C2'-C3'-C4'
25	a	410	PHO	C2-C3-C5-C6
36	c	515	DGD	CDB-CEB-CFB-CGB
29	c	519	LMG	C12-C13-C14-C15
24	a	412	CLA	C10-C11-C12-C13
32	M	102	LMT	C2-C1-O1'-C1'
24	C	505	CLA	C14-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C14
24	a	412	CLA	C11-C10-C8-C9
24	b	617	CLA	C11-C10-C8-C9
24	D	405	CLA	CBA-CGA-O2A-C1
24	b	616	CLA	C15-C16-C17-C18
29	a	415	LMG	C40-C41-C42-C43
32	f	103	LMT	C11-C10-C9-C8
34	D	409	LHG	C11-C12-C13-C14
24	B	610	CLA	C10-C11-C12-C13
24	c	510	CLA	O1A-CGA-O2A-C1
24	b	608	CLA	C4-C3-C5-C6
29	m	102	LMG	C21-C22-C23-C24
38	v	201	HEM	C4C-C3C-CAC-CBC
24	b	615	CLA	C16-C17-C18-C19
34	d	408	LHG	C12-C13-C14-C15
36	H	102	DGD	O1B-C1B-C2B-C3B
28	A	1016	SQD	C10-C11-C12-C13
29	C	519	LMG	C36-C37-C38-C39
24	A	1006	CLA	C6-C7-C8-C10
24	a	412	CLA	C11-C12-C13-C15
24	c	502	CLA	C11-C12-C13-C15
24	c	513	CLA	C12-C13-C15-C16
32	A	1018	LMT	C5-C6-C7-C8
32	M	101	LMT	C1-C2-C3-C4
24	d	402	CLA	C16-C17-C18-C19
28	b	623[B]	SQD	O47-C45-C46-O48
36	c	517	DGD	C9A-CAA-CBA-CCA
24	c	512	CLA	C3A-C2A-CAA-CBA
34	E	101	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	C2-C3-C5-C6
29	C	518	LMG	C12-C13-C14-C15
24	C	501	CLA	C15-C16-C17-C18
28	A	1011	SQD	C16-C17-C18-C19
29	Z	101	LMG	C32-C33-C34-C35
26	d	404	BCR	C15-C16-C17-C18
34	B	621	LHG	C34-C35-C36-C37
34	D	409	LHG	C26-C27-C28-C29
27	A	1010	PL9	C13-C14-C16-C17
28	A	1016	SQD	C25-C26-C27-C28
36	c	517	DGD	C6A-C7A-C8A-C9A
24	C	507	CLA	C8-C10-C11-C12
34	D	409	LHG	C30-C31-C32-C33
24	B	615	CLA	C11-C10-C8-C9
24	C	512	CLA	C14-C13-C15-C16
24	a	412	CLA	C11-C12-C13-C14
24	a	412	CLA	C14-C13-C15-C16
24	b	613	CLA	C11-C12-C13-C14
24	c	502	CLA	C11-C12-C13-C14
24	c	504	CLA	C14-C13-C15-C16
32	t	103	LMT	C4B-C5B-C6B-O6B
28	a	401	SQD	C34-C35-C36-C37
34	D	411	LHG	C27-C28-C29-C30
28	A	1016	SQD	O49-C7-O47-C45
36	C	515	DGD	C2A-C3A-C4A-C5A
34	d	406	LHG	C26-C27-C28-C29
36	H	102	DGD	CBB-CCB-CDB-CEB
33	V	204	GOL	O2-C2-C3-O3
24	B	602	CLA	C3-C5-C6-C7
35	c	525	HTG	C4-C5-C6-O6
24	C	513	CLA	C1A-C2A-CAA-CBA
24	c	513	CLA	C1A-C2A-CAA-CBA
24	b	610	CLA	CBA-CGA-O2A-C1
29	m	102	LMG	C14-C15-C16-C17
24	b	604	CLA	C2B-C3B-CAB-CBB
24	b	618	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C5-C6-C7-C8
26	J	101	BCR	C1-C6-C7-C8
26	K	101	BCR	C5-C6-C7-C8
26	K	101	BCR	C23-C24-C25-C30
26	b	621	BCR	C23-C24-C25-C30
26	d	404	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	d	404	BCR	C23-C24-C25-C30
26	y	101	BCR	C1-C6-C7-C8
35	c	525	HTG	C4'-C5'-C6'-C7'
36	C	515	DGD	C6A-C7A-C8A-C9A
34	d	406	LHG	C31-C32-C33-C34
38	f	101	HEM	CAA-CBA-CGA-O1A
24	c	510	CLA	CBA-CGA-O2A-C1
24	B	601	CLA	C6-C7-C8-C10
24	B	610	CLA	C11-C12-C13-C15
24	B	616	CLA	C11-C10-C8-C7
24	C	512	CLA	C12-C13-C15-C16
24	D	402	CLA	C11-C12-C13-C15
24	b	606	CLA	C11-C10-C8-C7
24	c	504	CLA	C11-C12-C13-C15
24	c	509	CLA	C6-C7-C8-C10
24	C	510	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C20
29	C	519	LMG	O1-C7-C8-O7
34	b	624	LHG	C33-C34-C35-C36
32	A	1017	LMT	C4B-C5B-C6B-O6B
28	f	102	SQD	C25-C26-C27-C28
24	d	403	CLA	C15-C16-C17-C18
38	F	101	HEM	CAD-CBD-CGD-O1D
32	b	625	LMT	C2-C3-C4-C5
26	K	102	BCR	C7-C8-C9-C10
28	A	1016	SQD	C28-C29-C30-C31
29	D	412	LMG	C38-C39-C40-C41
29	Z	101	LMG	C30-C31-C32-C33
24	B	613	CLA	C10-C11-C12-C13
24	C	502	CLA	C15-C16-C17-C18
38	f	101	HEM	CAA-CBA-CGA-O2A
38	f	101	HEM	CAD-CBD-CGD-O1D
34	E	101	LHG	C2-C3-O3-P
24	b	610	CLA	O1A-CGA-O2A-C1
38	F	101	HEM	CAD-CBD-CGD-O2D
38	f	101	HEM	CAD-CBD-CGD-O2D
27	A	1010	PL9	C9-C11-C12-C13
29	A	1012	LMG	O1-C7-C8-C9
36	h	102	DGD	O1G-C1G-C2G-C3G
32	A	1018	LMT	C5'-C4'-O1B-C1B
24	C	512	CLA	C16-C17-C18-C19
35	b	602	HTG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
29	Z	101	LMG	C31-C32-C33-C34
28	c	518	SQD	O49-C7-O47-C45
24	B	616	CLA	C10-C11-C12-C13
34	B	621	LHG	C18-C19-C20-C21
29	d	409	LMG	C4-C5-C6-O5
24	B	601	CLA	CAA-CBA-CGA-O2A
36	c	516	DGD	C7A-C8A-C9A-CAA
24	B	602	CLA	C8-C10-C11-C12
28	c	518	SQD	C15-C16-C17-C18
24	b	604	CLA	CAA-CBA-CGA-O2A
36	C	516	DGD	CCB-CDB-CEB-CFB
34	d	407	LHG	C32-C33-C34-C35
25	A	1007	PHO	CHA-CBD-CGD-O1D
25	D	404	PHO	CHA-CBD-CGD-O2D
26	c	514	BCR	C20-C21-C22-C37
35	b	630	HTG	C2'-C3'-C4'-C5'
34	D	410	LHG	O6-C4-C5-C6
34	d	407	LHG	O6-C4-C5-C6
34	e	101	LHG	O6-C4-C5-C6
28	B	620[B]	SQD	O47-C45-C46-O48
28	a	401	SQD	O5-C1-O6-C44
36	c	515	DGD	O6E-C1E-O5D-C6D
36	c	516	DGD	O6E-C1E-O5D-C6D
24	C	508	CLA	C15-C16-C17-C18
24	A	1008	CLA	C11-C10-C8-C7
24	a	412	CLA	C12-C13-C15-C16
24	b	606	CLA	C6-C7-C8-C10
38	V	201	HEM	CAD-CBD-CGD-O1D
38	V	201	HEM	CAD-CBD-CGD-O2D
29	c	521	LMG	C12-C13-C14-C15
26	H	101	BCR	C13-C14-C15-C16
28	b	623[A]	SQD	C15-C16-C17-C18
36	c	517	DGD	C4A-C5A-C6A-C7A
24	C	511	CLA	C8-C10-C11-C12
36	H	102	DGD	C9A-CAA-CBA-CCA
24	B	603	CLA	C6-C7-C8-C9
24	B	614	CLA	C11-C12-C13-C14
24	b	604	CLA	C11-C12-C13-C14
24	b	606	CLA	C6-C7-C8-C9
24	c	506	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C10-C8-C9
28	A	1011	SQD	C45-C44-O6-C1

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Mol	Chain	Res	Type	Atoms
28	D	408	SQD	C45-C44-O6-C1
28	f	102	SQD	C5-C6-S-O8
36	C	515	DGD	C5D-C6D-O5D-C1E
36	c	515	DGD	C5D-C6D-O5D-C1E
32	B	623	LMT	O5'-C5'-C6'-O6'
24	B	610	CLA	C2A-CAA-CBA-CGA
36	c	517	DGD	O6D-C5D-C6D-O5D
32	i	102	LMT	C9-C10-C11-C12
28	b	623[B]	SQD	C32-C33-C34-C35
24	B	615	CLA	C8-C10-C11-C12
28	c	518	SQD	C10-C11-C12-C13
38	f	101	HEM	C2C-C3C-CAC-CBC
33	b	632	GOL	O1-C1-C2-C3
28	B	620[B]	SQD	C23-C24-C25-C26
34	b	624	LHG	C11-C12-C13-C14
28	a	401	SQD	C2-C1-O6-C44
36	c	515	DGD	C2E-C1E-O5D-C6D
26	b	621	BCR	C18-C19-C20-C21
24	C	513	CLA	C16-C17-C18-C20
38	v	201	HEM	CAD-CBD-CGD-O2D
29	c	519	LMG	C35-C36-C37-C38
28	B	620[A]	SQD	C31-C32-C33-C34
28	B	620[B]	SQD	C18-C19-C20-C21
28	A	1016	SQD	O5-C1-O6-C44
35	c	525	HTG	C2'-C3'-C4'-C5'
38	v	201	HEM	CAD-CBD-CGD-O1D
28	B	620[A]	SQD	O6-C44-C45-C46
28	b	623[B]	SQD	C44-C45-C46-O48
24	B	612	CLA	O1A-CGA-O2A-C1
24	A	1008	CLA	C15-C16-C17-C18
24	B	605	CLA	C13-C15-C16-C17
38	V	201	HEM	C4C-C3C-CAC-CBC
36	C	516	DGD	C6A-C7A-C8A-C9A
36	C	516	DGD	CAB-CBB-CCB-CDB
29	C	518	LMG	C39-C40-C41-C42
24	C	507	CLA	C2-C3-C5-C6
24	b	608	CLA	C2-C3-C5-C6
34	B	621	LHG	C9-C10-C11-C12
34	d	408	LHG	C32-C33-C34-C35
35	d	416	HTG	C2-C1-S1-C1'
28	B	620[A]	SQD	C11-C12-C13-C14
28	b	623[A]	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
28	c	518	SQD	C25-C26-C27-C28
32	a	402	LMT	C5-C6-C7-C8
36	C	515	DGD	O2G-C1B-C2B-C3B
32	f	103	LMT	C3-C4-C5-C6
28	B	620[B]	SQD	O6-C44-C45-O47
29	m	102	LMG	O1-C7-C8-O7
24	C	507	CLA	C6-C7-C8-C9
24	b	606	CLA	C11-C10-C8-C9
24	c	505	CLA	C11-C12-C13-C14
24	c	507	CLA	C11-C12-C13-C14
24	c	513	CLA	C6-C7-C8-C9
24	d	403	CLA	C11-C12-C13-C14
24	b	613	CLA	C16-C17-C18-C19
34	b	624	LHG	C16-C17-C18-C19
28	B	620[A]	SQD	O48-C23-C24-C25
32	M	102	LMT	O5'-C5'-C6'-O6'
24	C	512	CLA	CAA-CBA-CGA-O2A
24	A	1006	CLA	C11-C12-C13-C15
24	B	603	CLA	C6-C7-C8-C10
24	B	614	CLA	C11-C12-C13-C15
24	c	504	CLA	C6-C7-C8-C10
24	c	508	CLA	C11-C10-C8-C7
24	d	403	CLA	C11-C10-C8-C7
24	B	602	CLA	C2B-C3B-CAB-CBB
24	C	504	CLA	C2B-C3B-CAB-CBB
24	D	402	CLA	C2B-C3B-CAB-CBB
24	c	501	CLA	C2B-C3B-CAB-CBB
24	c	504	CLA	C2B-C3B-CAB-CBB
26	J	101	BCR	C5-C6-C7-C8
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C26
28	B	620[A]	SQD	C19-C20-C21-C22
24	B	601	CLA	C2-C1-O2A-CGA
24	B	616	CLA	C2-C1-O2A-CGA
24	D	402	CLA	C2-C1-O2A-CGA
24	d	402	CLA	C2-C1-O2A-CGA
32	b	625	LMT	O5'-C1'-O1'-C1
28	b	623[B]	SQD	C27-C28-C29-C30
24	B	612	CLA	CBA-CGA-O2A-C1
24	B	610	CLA	C15-C16-C17-C18
29	Z	101	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
34	D	410	LHG	C30-C31-C32-C33
35	B	624	HTG	C2'-C1'-S1-C1
35	C	521	HTG	C2'-C1'-S1-C1
35	C	522	HTG	C2'-C1'-S1-C1
35	c	522	HTG	C2'-C1'-S1-C1
29	c	520	LMG	C12-C13-C14-C15
28	A	1016	SQD	C8-C7-O47-C45
28	c	518	SQD	C8-C7-O47-C45
24	C	507	CLA	C15-C16-C17-C18
24	c	504	CLA	C15-C16-C17-C18
29	a	415	LMG	O7-C10-C11-C12
36	C	517	DGD	O1G-C1A-C2A-C3A
28	a	401	SQD	C27-C28-C29-C30
24	b	613	CLA	C16-C17-C18-C20
32	i	102	LMT	C5-C6-C7-C8
29	D	412	LMG	C34-C35-C36-C37
29	c	521	LMG	O8-C28-C29-C30
28	f	102	SQD	C7-C8-C9-C10
32	M	101	LMT	C4-C5-C6-C7
34	b	624	LHG	C29-C30-C31-C32
24	C	513	CLA	C4-C3-C5-C6
26	b	621	BCR	C20-C21-C22-C37
26	c	514	BCR	C16-C17-C18-C36
36	h	102	DGD	CAB-CBB-CCB-CDB
32	B	623	LMT	C2-C3-C4-C5
24	C	507	CLA	C2A-CAA-CBA-CGA
29	C	518	LMG	C29-C30-C31-C32
24	a	412	CLA	C5-C6-C7-C8
32	b	631	LMT	C2-C1-O1'-C1'
36	h	102	DGD	C7B-C8B-C9B-CAB
24	c	504	CLA	C6-C7-C8-C9
24	C	512	CLA	C2C-C3C-CAC-CBC
26	b	622	BCR	C37-C22-C23-C24
32	A	1017	LMT	C9-C10-C11-C12
28	B	620[B]	SQD	O6-C44-C45-C46
28	B	620[B]	SQD	C44-C45-C46-O48
29	m	102	LMG	O1-C7-C8-C9
24	B	602	CLA	C4B-C3B-CAB-CBB
24	c	501	CLA	C4B-C3B-CAB-CBB
36	C	515	DGD	O6E-C1E-O5D-C6D
24	c	512	CLA	CAA-CBA-CGA-O2A
36	h	102	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
28	f	102	SQD	O47-C7-C8-C9
36	c	516	DGD	O2G-C1B-C2B-C3B
24	b	615	CLA	O1A-CGA-O2A-C1
34	d	406	LHG	C9-C10-C11-C12
28	B	620[A]	SQD	C7-C8-C9-C10
29	A	1012	LMG	C40-C41-C42-C43
28	f	102	SQD	C5-C6-S-O9
34	e	101	LHG	C1-C2-C3-O3
24	c	501	CLA	C13-C15-C16-C17
24	B	610	CLA	C12-C13-C15-C16
24	B	611	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	c	505	CLA	C11-C12-C13-C15
24	c	509	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C12-C13-C15
24	a	408	CLA	C15-C16-C17-C18
28	A	1016	SQD	O10-C23-O48-C46
36	C	515	DGD	O1G-C1A-C2A-C3A
24	C	507	CLA	C10-C11-C12-C13
24	b	610	CLA	C16-C17-C18-C20
29	Z	101	LMG	O10-C28-C29-C30
36	C	515	DGD	O1B-C1B-C2B-C3B
36	C	517	DGD	O1A-C1A-C2A-C3A
24	a	409	CLA	C3-C5-C6-C7
34	d	407	LHG	C11-C10-C9-C8
36	H	102	DGD	C3B-C4B-C5B-C6B
24	C	512	CLA	CAA-CBA-CGA-O1A
24	c	513	CLA	C5-C6-C7-C8
32	C	520	LMT	C5'-C4'-O1B-C1B
28	f	102	SQD	O10-C23-O48-C46
28	B	620[A]	SQD	O10-C23-C24-C25
29	A	1012	LMG	C33-C34-C35-C36
28	A	1016	SQD	C24-C23-O48-C46
28	f	102	SQD	C24-C23-O48-C46
24	A	1006	CLA	C14-C13-C15-C16
24	B	611	CLA	C14-C13-C15-C16
24	B	616	CLA	C11-C10-C8-C9
24	C	511	CLA	C6-C7-C8-C9
24	c	512	CLA	C11-C12-C13-C14
24	c	513	CLA	C11-C12-C13-C14
24	d	403	CLA	C6-C7-C8-C9
28	c	518	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	c	521	LMG	O10-C28-C29-C30
35	V	202	HTG	C4-C5-C6-O6
24	D	403	CLA	C15-C16-C17-C18
29	a	415	LMG	O9-C10-C11-C12
24	b	615	CLA	C10-C11-C12-C13
28	B	620[A]	SQD	C45-C44-O6-C1
29	Z	101	LMG	C8-C7-O1-C1
29	B	622	LMG	O9-C10-O7-C8
29	a	415	LMG	O1-C7-C8-O7
29	c	521	LMG	O7-C8-C9-O8
29	A	1012	LMG	C22-C23-C24-C25
38	F	101	HEM	CAA-CBA-CGA-O2A
24	C	501	CLA	C2A-CAA-CBA-CGA
29	B	622	LMG	C33-C34-C35-C36
28	f	102	SQD	O49-C7-C8-C9
27	a	414	PL9	C36-C37-C38-C39
24	B	612	CLA	C10-C11-C12-C13
24	b	608	CLA	CAD-CBD-CGD-O2D
25	A	1007	PHO	CAD-CBD-CGD-O2D
28	D	408	SQD	C29-C30-C31-C32
34	B	621	LHG	O6-C4-C5-C6
24	c	512	CLA	CAA-CBA-CGA-O1A
34	E	101	LHG	O7-C7-C8-C9
29	Z	101	LMG	O6-C5-C6-O5
24	C	510	CLA	CAA-CBA-CGA-O2A
36	c	515	DGD	O2G-C1B-C2B-C3B
24	B	613	CLA	C16-C17-C18-C19
36	c	515	DGD	O1B-C1B-C2B-C3B
34	B	621	LHG	C5-C6-O8-C23
28	A	1011	SQD	O47-C7-C8-C9
28	D	408	SQD	O47-C7-C8-C9
36	c	517	DGD	O1G-C1A-C2A-C3A
36	C	515	DGD	O1A-C1A-C2A-C3A
36	c	516	DGD	O1B-C1B-C2B-C3B
36	C	516	DGD	O6D-C5D-C6D-O5D

There are no ring outliers.

137 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	409	LMG	1	0
34	D	410	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	F	101	HEM	2	0
34	d	408	LHG	6	0
24	C	502	CLA	3	0
24	b	618	CLA	3	0
24	c	510	CLA	3	0
34	E	101	LHG	3	0
28	B	620[B]	SQD	12	0
34	D	411	LHG	8	0
36	c	517	DGD	2	0
24	b	619	CLA	2	0
24	c	507	CLA	1	0
28	B	620[A]	SQD	9	0
24	a	409	CLA	3	0
28	f	102	SQD	1	0
29	Z	101	LMG	1	0
24	C	503	CLA	2	0
24	D	402	CLA	2	0
24	B	605	CLA	4	0
38	f	101	HEM	2	0
24	b	611	CLA	1	0
24	B	604	CLA	2	0
32	M	101	LMT	1	0
24	d	403	CLA	1	0
26	b	620	BCR	1	0
36	C	516	DGD	1	0
30	C	526	DMS	1	0
36	h	102	DGD	2	0
24	b	613	CLA	2	0
35	o	301	HTG	1	0
24	b	616	CLA	2	0
24	c	502	CLA	2	0
32	m	103	LMT	1	0
33	b	632	GOL	1	0
24	a	407	CLA	4	0
32	A	1017	LMT	3	0
26	J	101	BCR	1	0
27	A	1010	PL9	5	0
30	O	302	DMS	1	0
33	v	203	GOL	2	0
24	B	606	CLA	2	0
32	m	101	LMT	1	0
30	d	413	DMS	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	V	201	HEM	7	0
29	D	412	LMG	1	0
24	b	617	CLA	2	0
24	B	616	CLA	1	0
26	B	618	BCR	1	0
34	B	621	LHG	1	0
30	a	418	DMS	1	0
26	b	621	BCR	3	0
27	a	414	PL9	5	0
35	b	626	HTG	2	0
24	A	1005	CLA	6	0
24	d	402	CLA	2	0
28	b	623[B]	SQD	17	0
29	m	102	LMG	3	0
30	B	634	DMS	3	0
24	b	609	CLA	1	0
30	O	301	DMS	2	0
36	H	102	DGD	1	0
24	b	604	CLA	1	0
24	c	506	CLA	2	0
35	D	413	HTG	1	0
24	B	611	CLA	1	0
30	d	414	DMS	1	0
32	M	102	LMT	1	0
24	B	613	CLA	2	0
24	c	512	CLA	3	0
33	B	631	GOL	1	0
25	a	411	PHO	3	0
24	C	510	CLA	7	0
26	D	406	BCR	1	0
24	c	501	CLA	2	0
24	B	612	CLA	1	0
24	c	509	CLA	1	0
35	B	629	HTG	1	0
26	d	404	BCR	1	0
24	c	508	CLA	1	0
26	C	514	BCR	2	0
24	B	603	CLA	2	0
28	D	408	SQD	1	0
24	B	610	CLA	4	0
32	b	625	LMT	1	0
29	c	521	LMG	1	0

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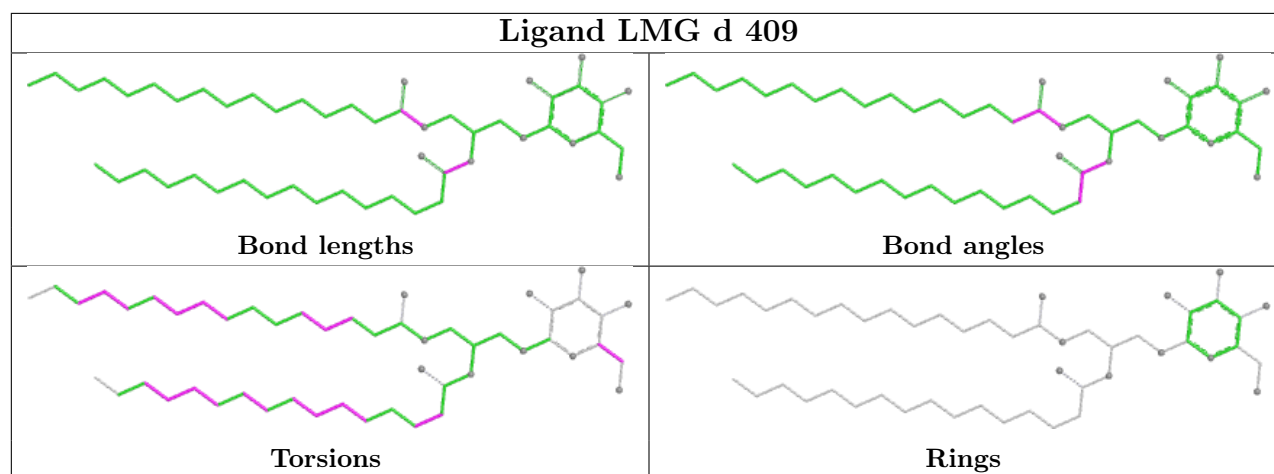
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24	C	507	CLA	3	0
24	c	511	CLA	1	0
30	b	635	DMS	3	0
30	D	417	DMS	1	0
24	C	509	CLA	2	0
26	c	514	BCR	3	0
28	b	623[A]	SQD	2	0
24	b	607	CLA	5	0
34	b	624	LHG	3	0
28	A	1016	SQD	1	0
25	D	404	PHO	5	0
24	C	513	CLA	1	0
24	A	1008	CLA	2	0
32	i	102	LMT	1	0
24	B	601	CLA	1	0
30	B	632	DMS	1	0
34	d	406	LHG	4	0
38	v	201	HEM	6	0
24	B	607	CLA	1	0
24	C	504	CLA	3	0
24	C	501	CLA	1	0
34	d	407	LHG	1	0
26	y	101	BCR	1	0
24	a	408	CLA	4	0
24	C	506	CLA	2	0
26	B	617	BCR	1	0
32	a	402	LMT	2	0
26	k	102	BCR	2	0
24	c	513	CLA	2	0
24	c	503	CLA	3	0
29	B	622	LMG	2	0
24	b	608	CLA	3	0
24	c	505	CLA	4	0
24	B	614	CLA	2	0
24	C	508	CLA	3	0
32	A	1018	LMT	1	0
24	A	1006	CLA	1	0
24	b	606	CLA	3	0
36	C	515	DGD	3	0
24	B	615	CLA	1	0
34	D	409	LHG	4	0

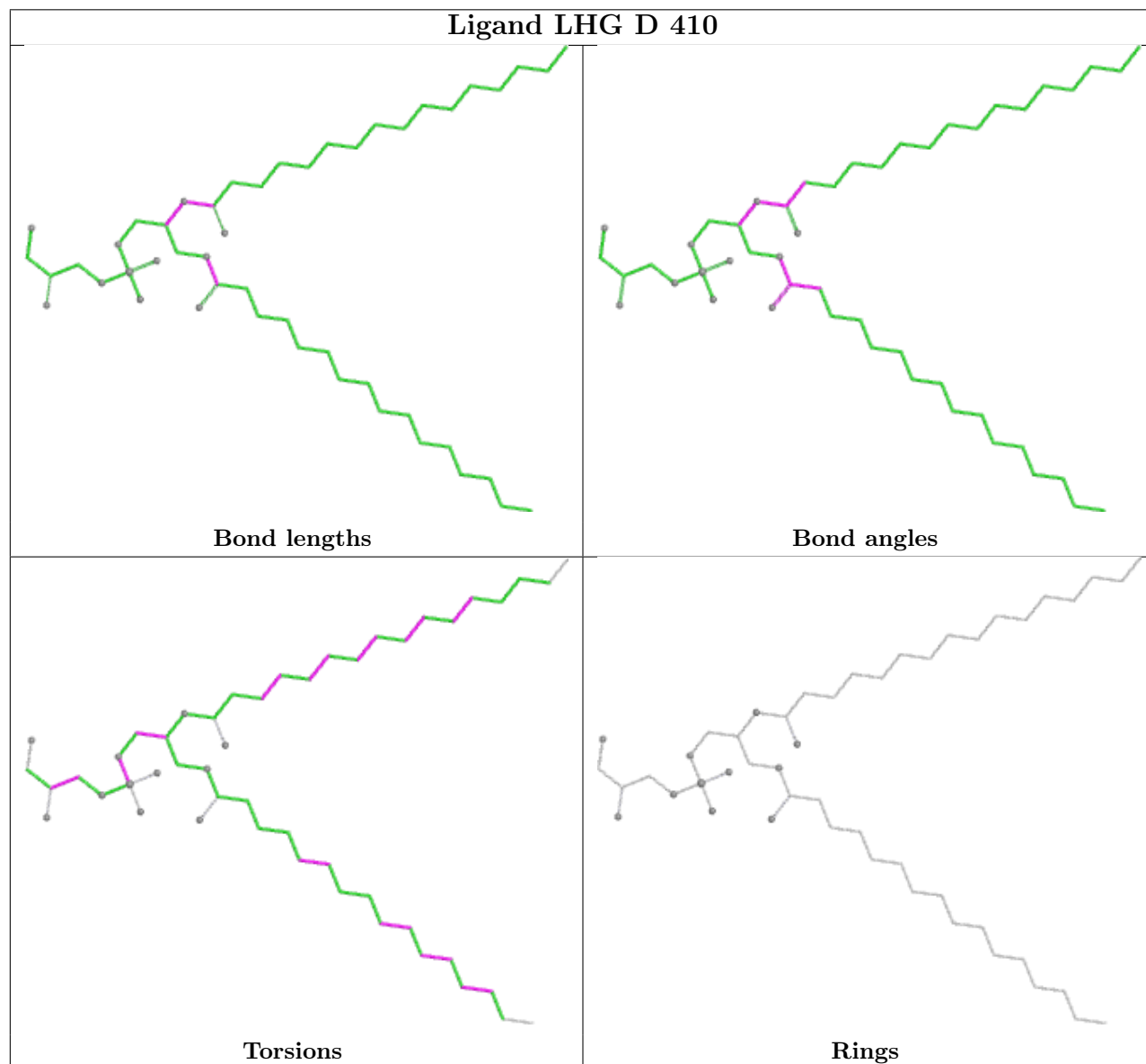
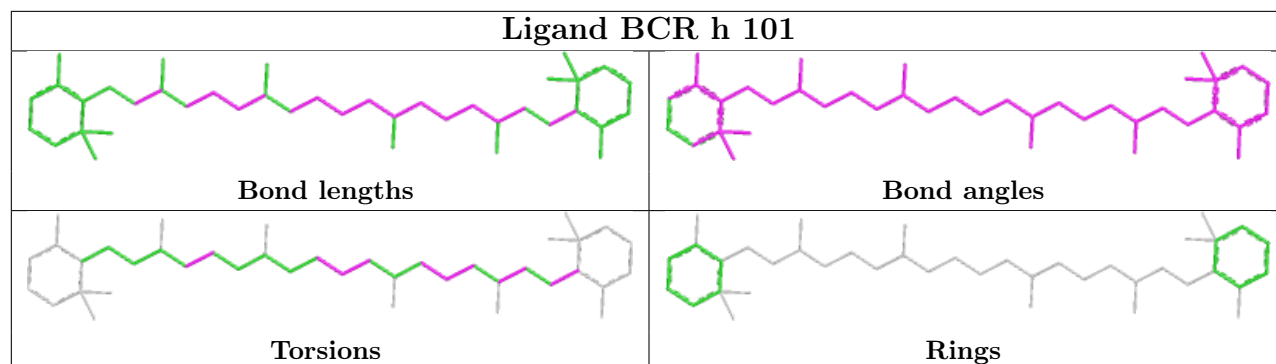
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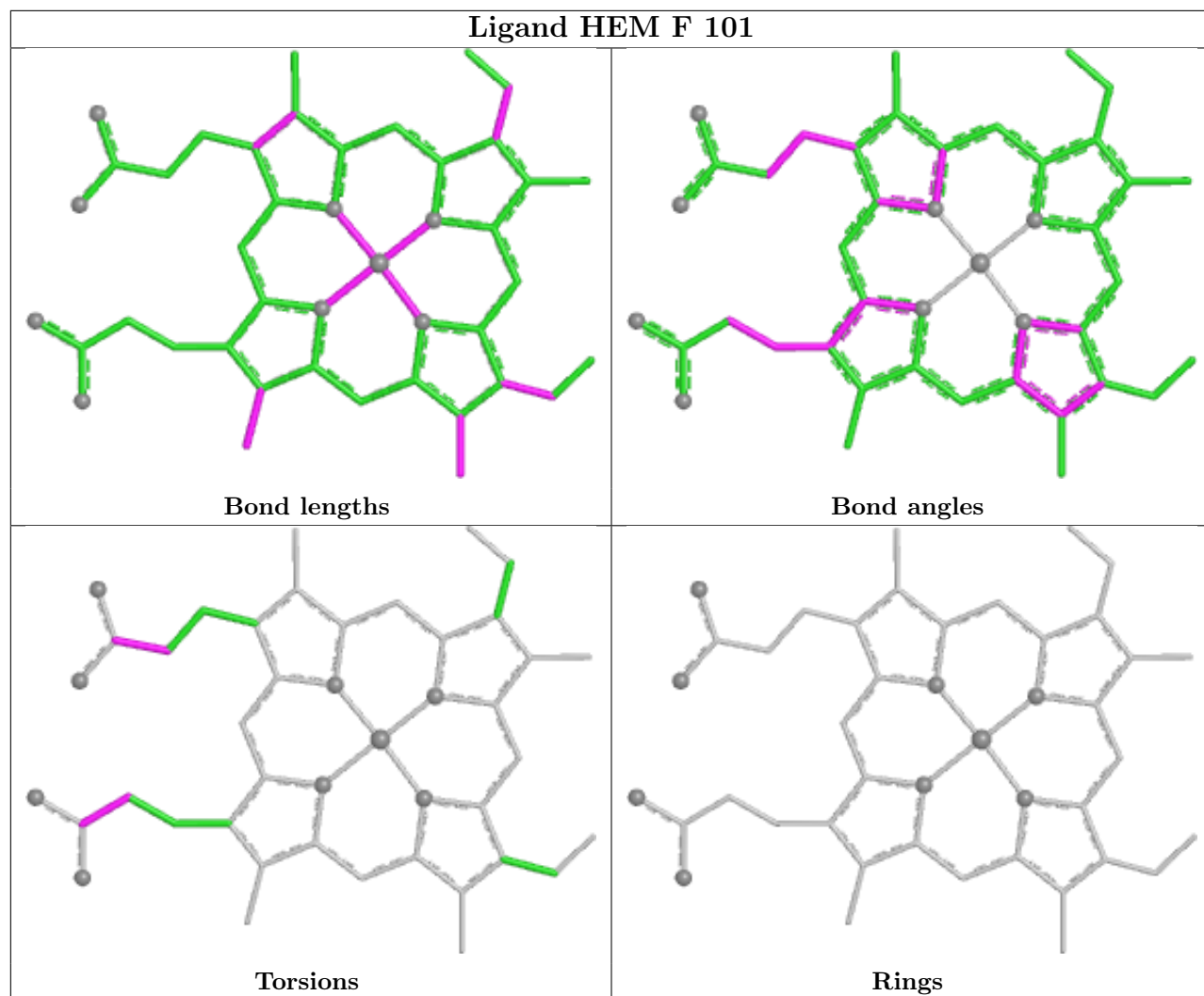
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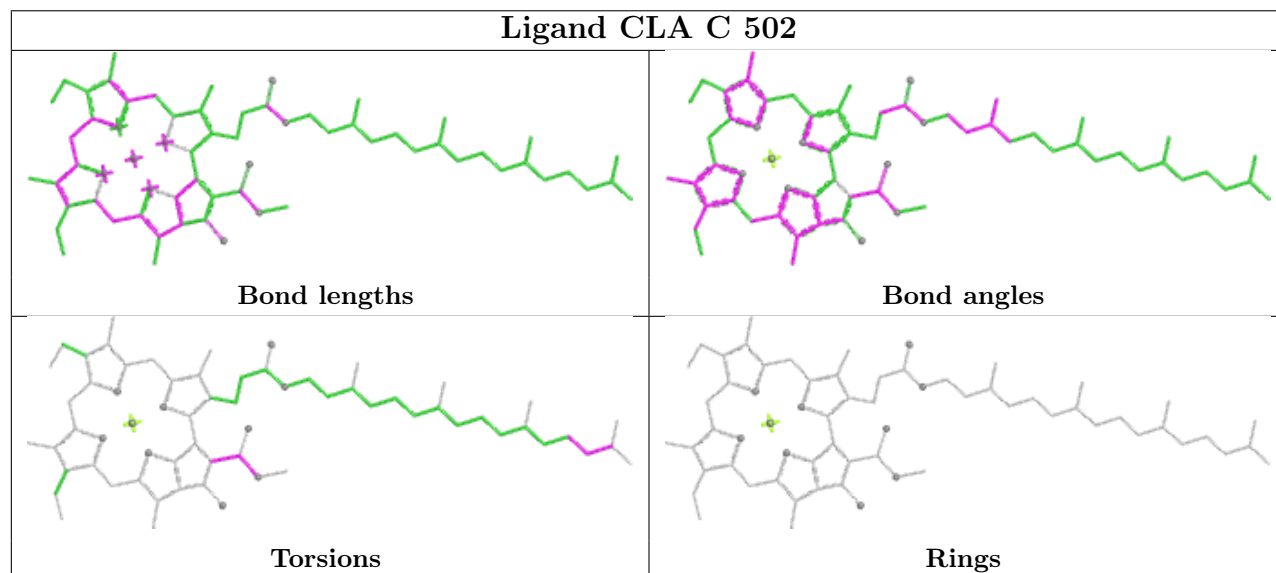
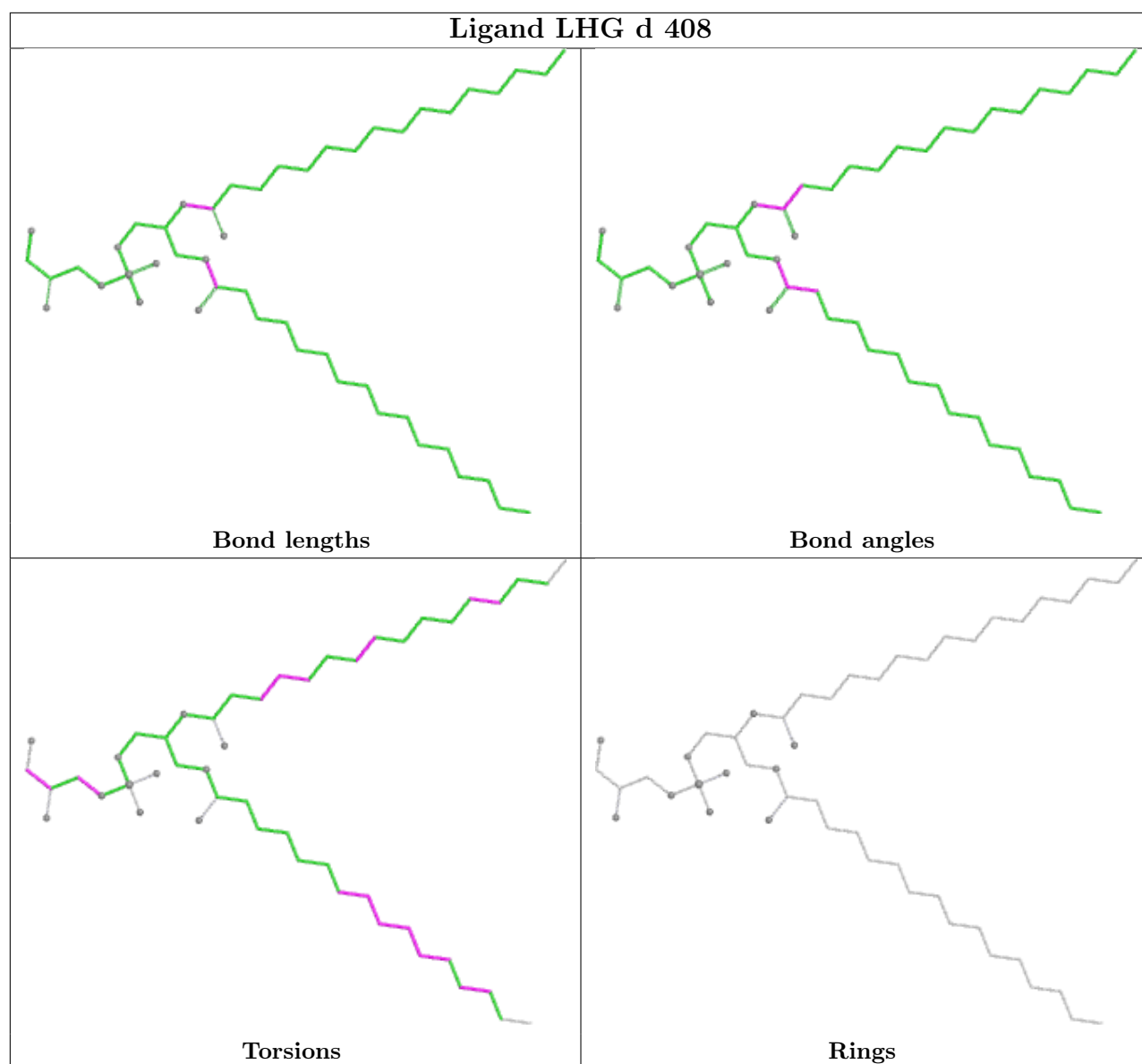
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	505	CLA	4	0
24	b	615	CLA	4	0
30	c	529	DMS	2	0
24	D	403	CLA	4	0
32	a	416	LMT	1	0
24	b	605	CLA	1	0
30	A	1014	DMS	3	0
28	A	1011	SQD	2	0
29	c	519	LMG	1	0

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.

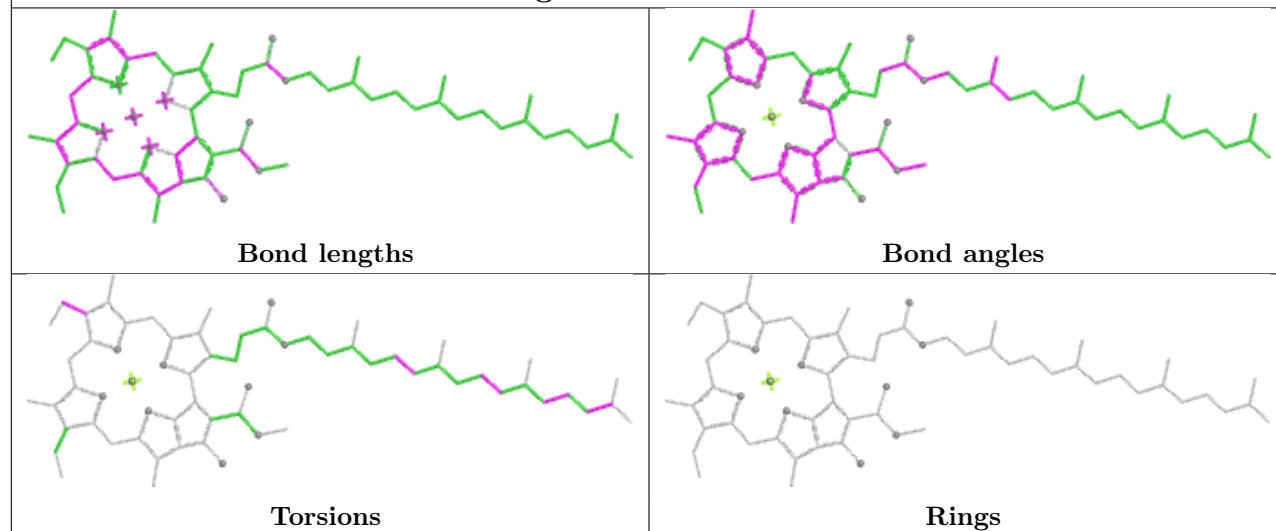




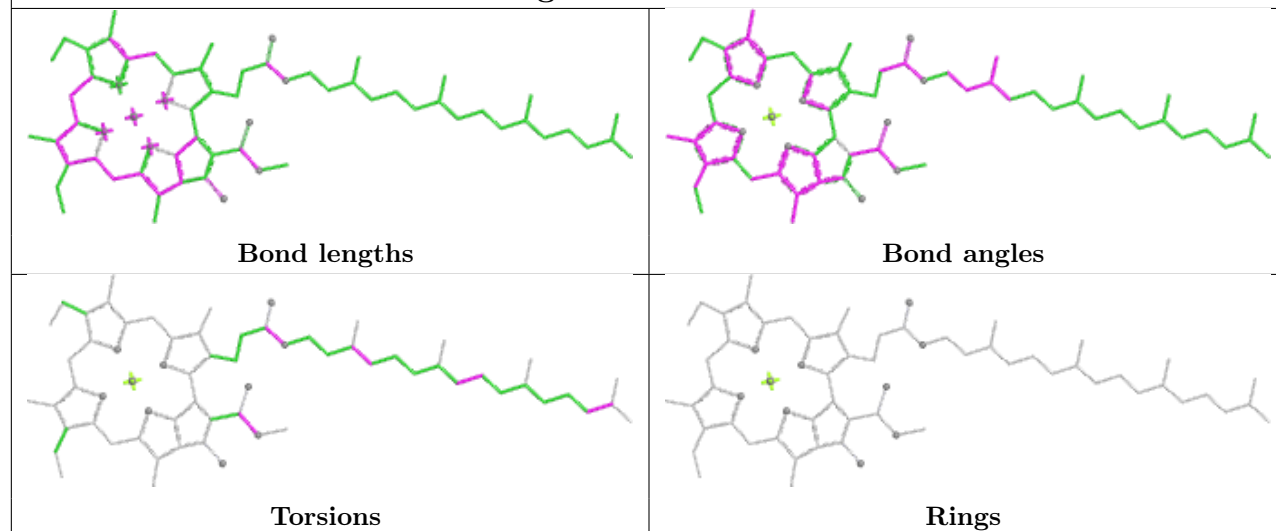




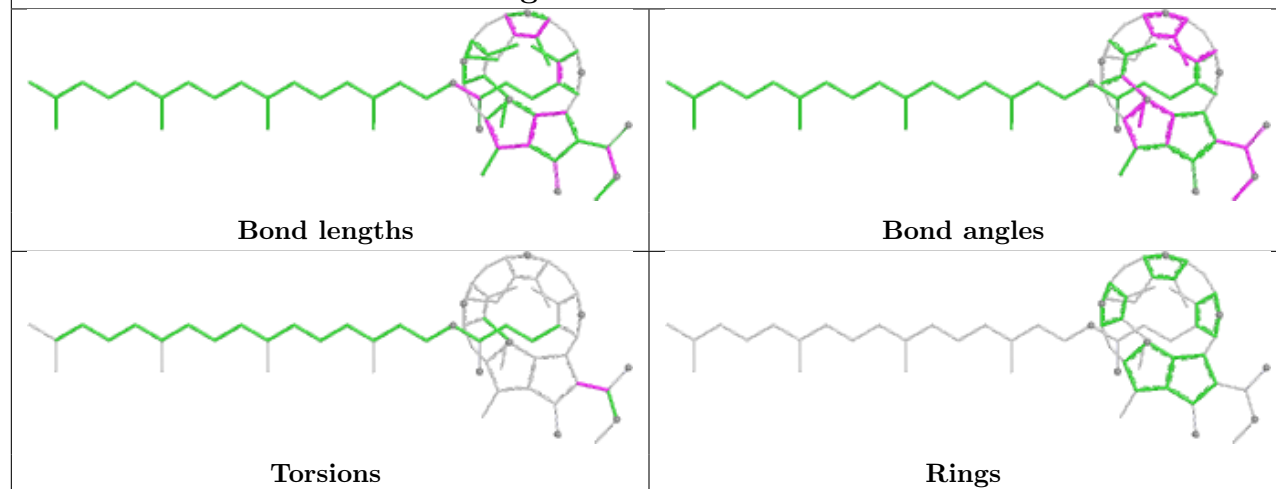
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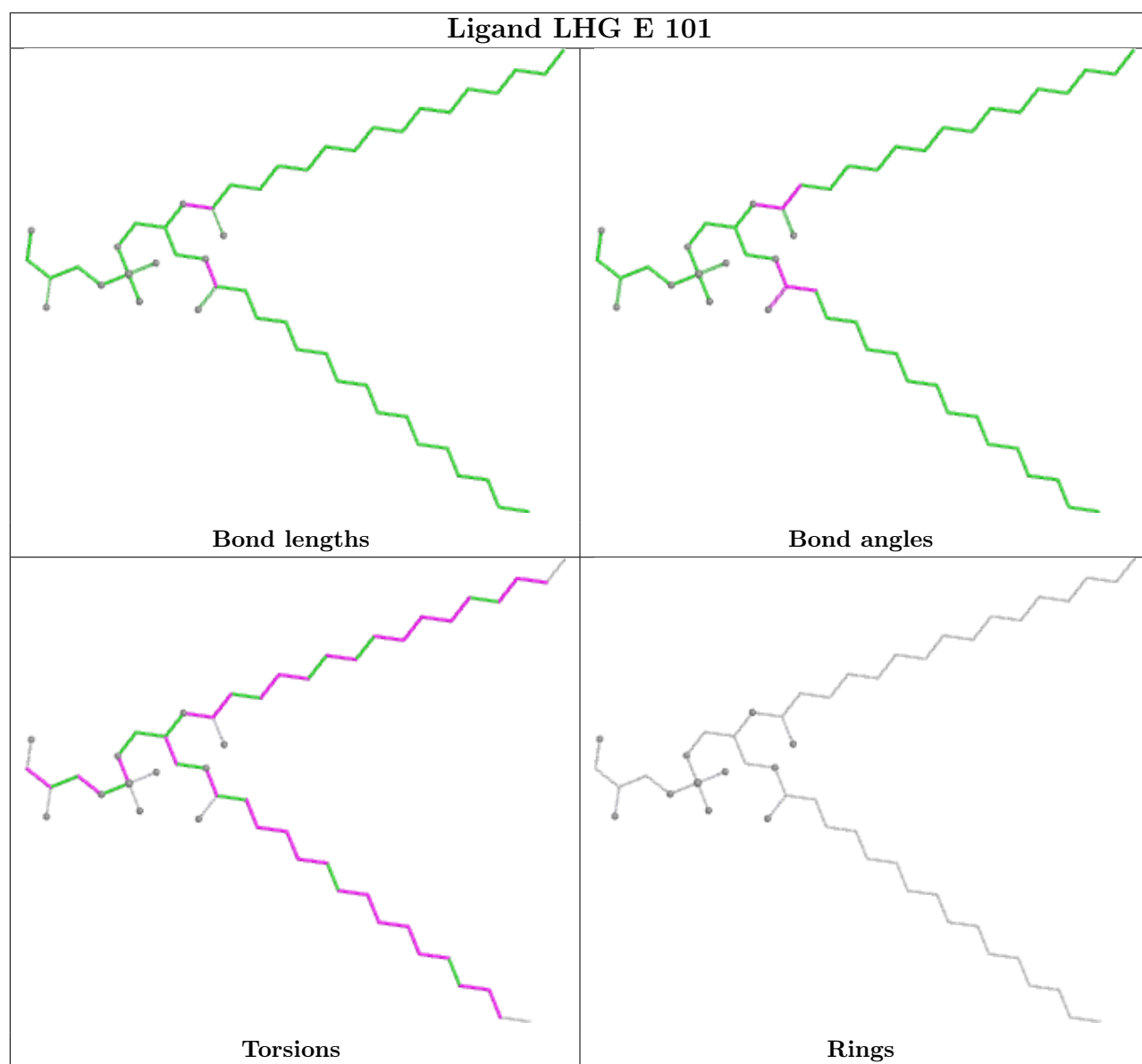


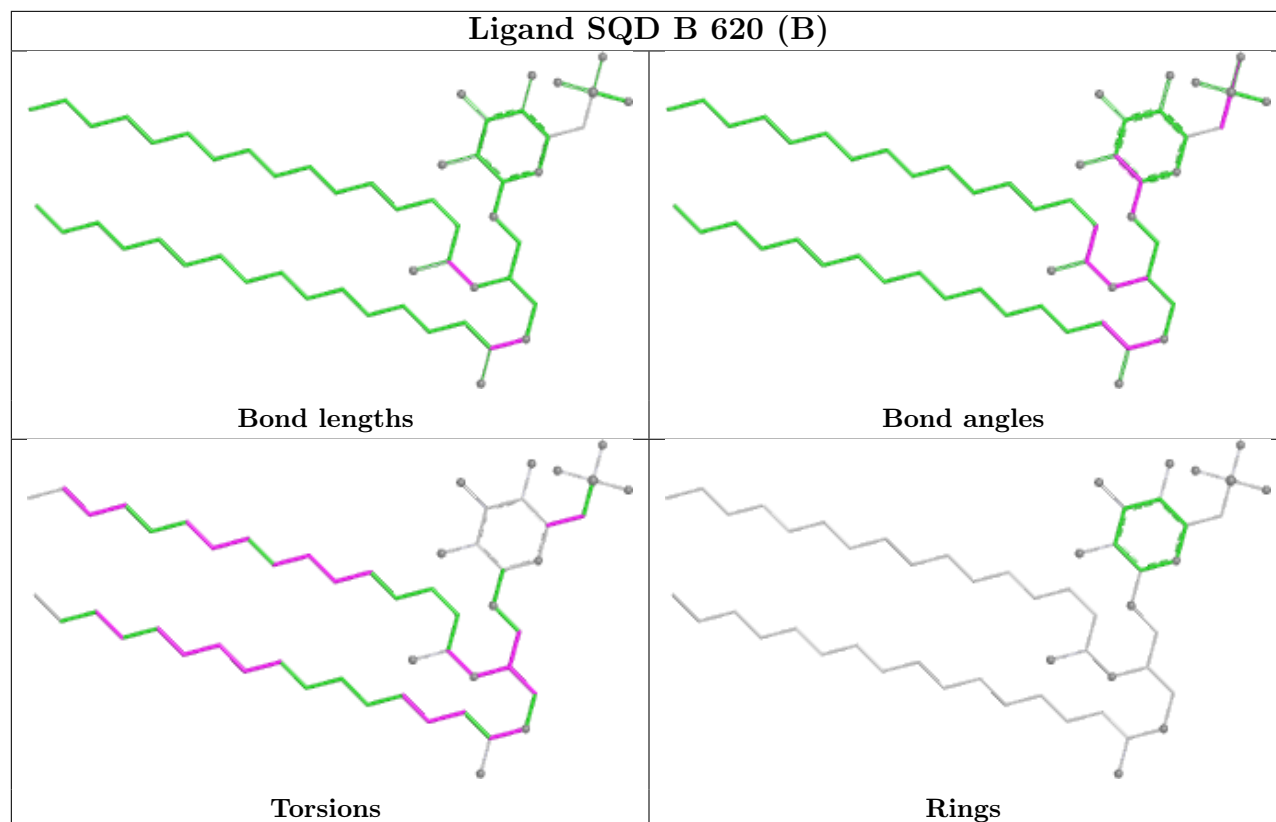
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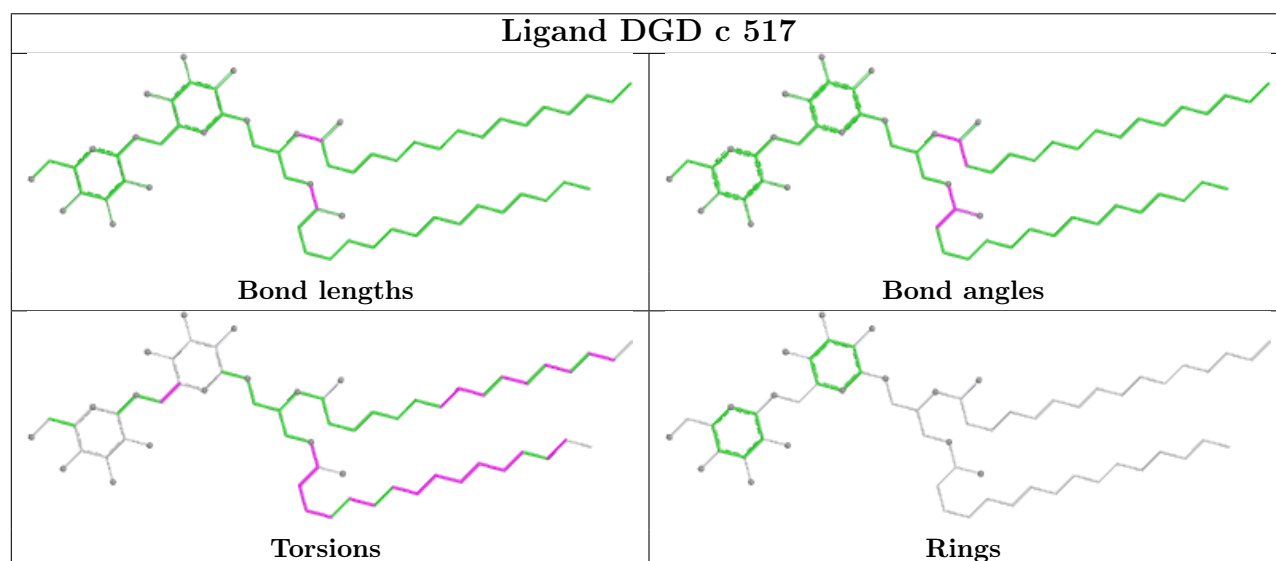
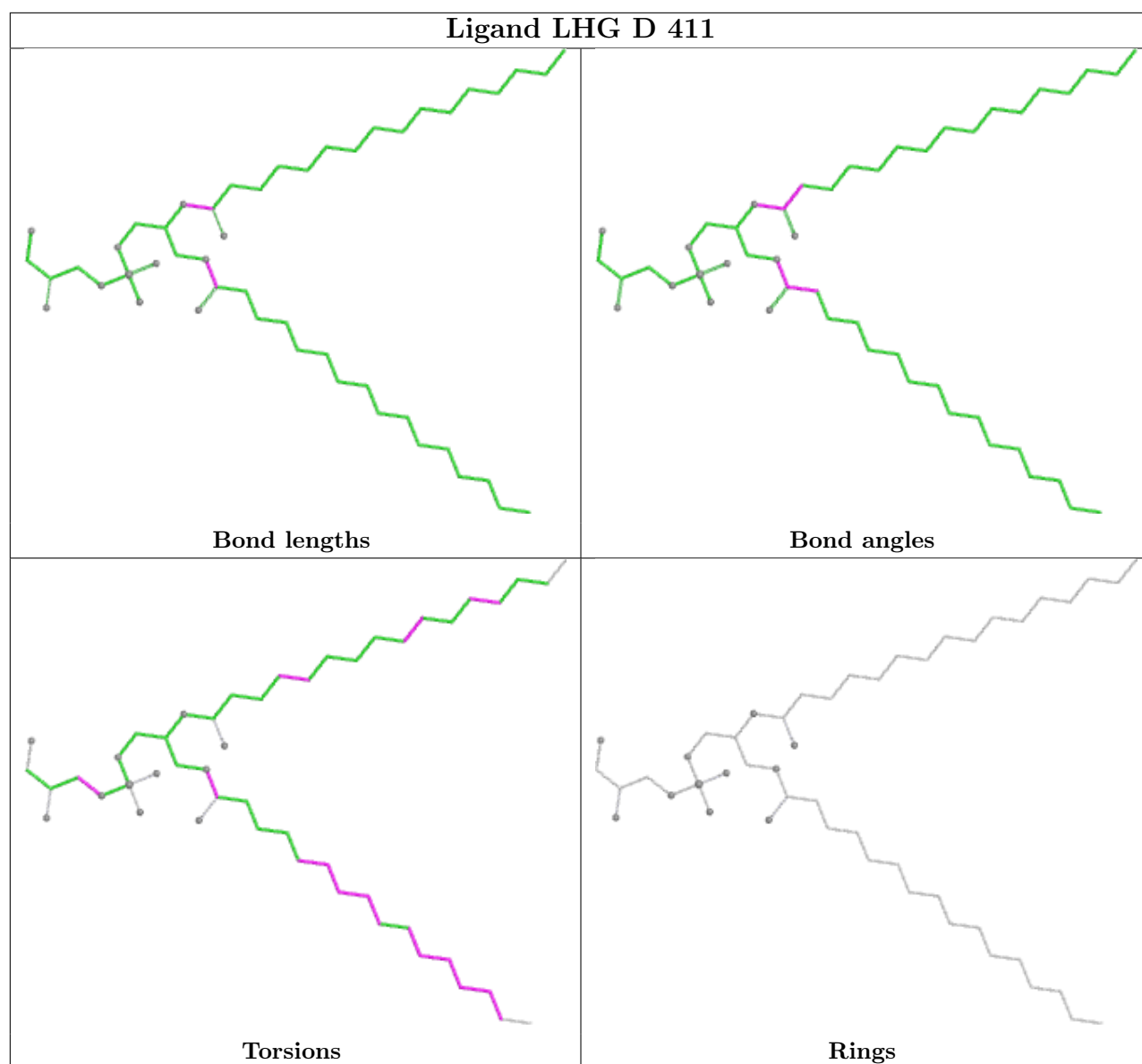


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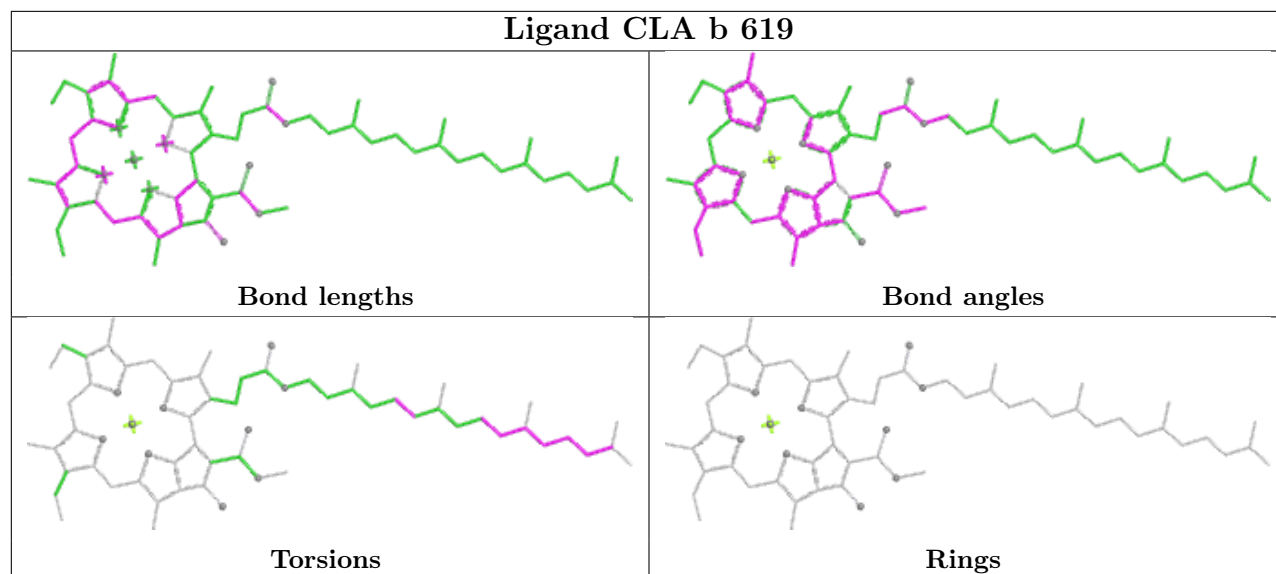




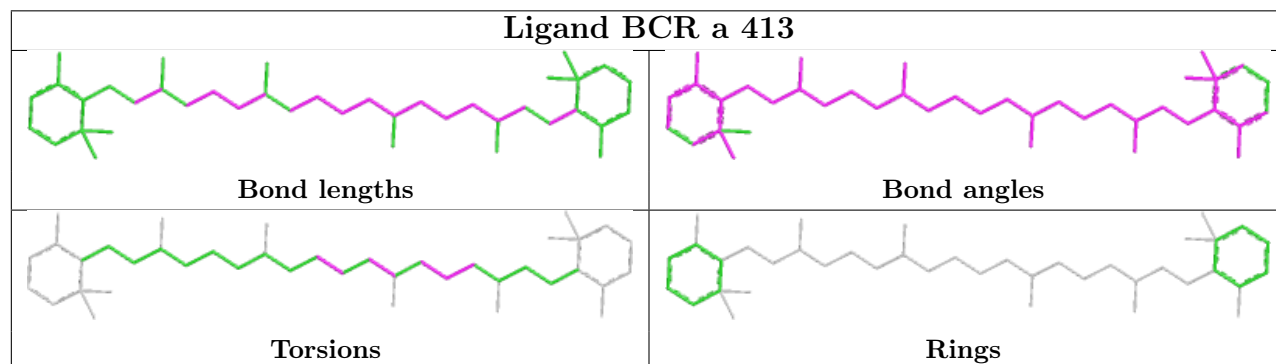




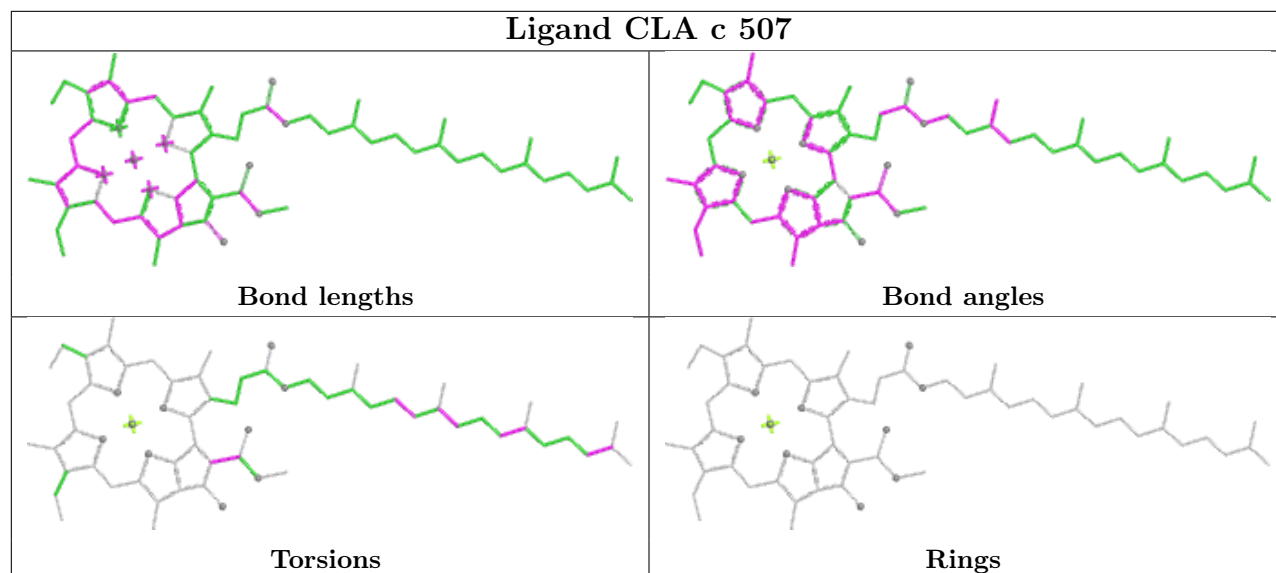
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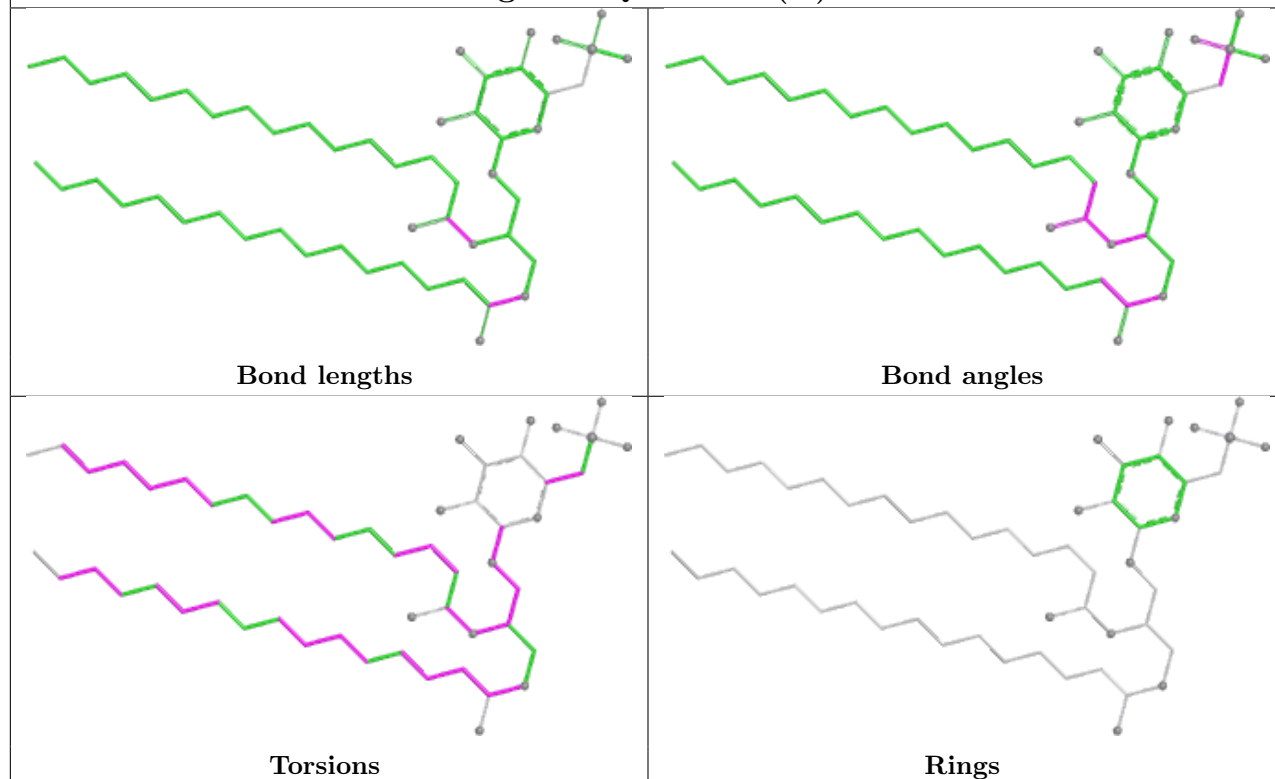
Ligand BCR a 413



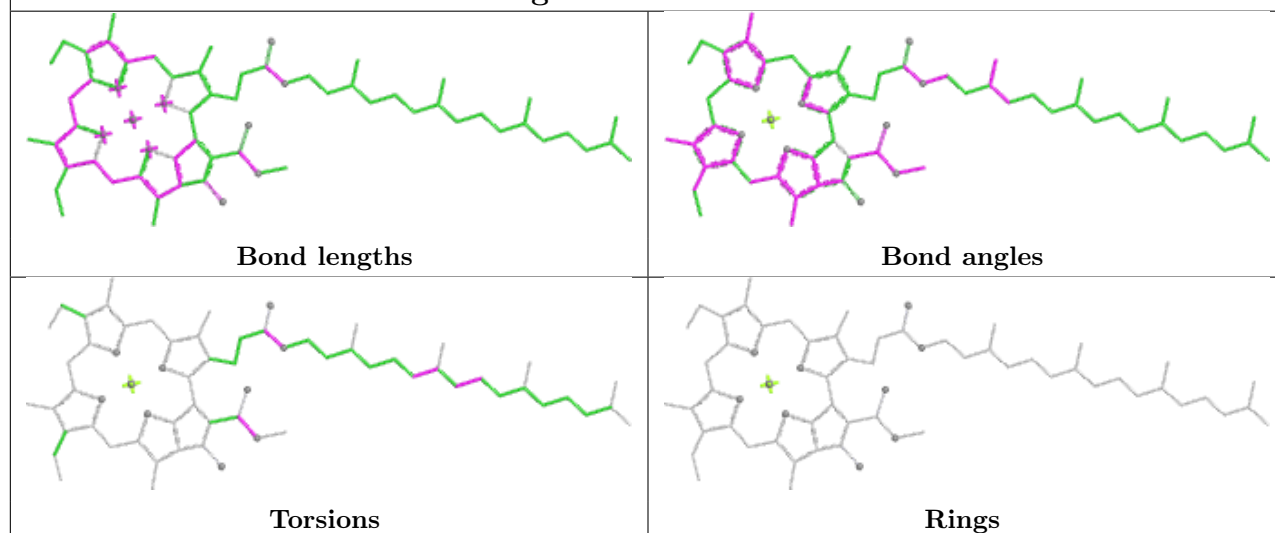
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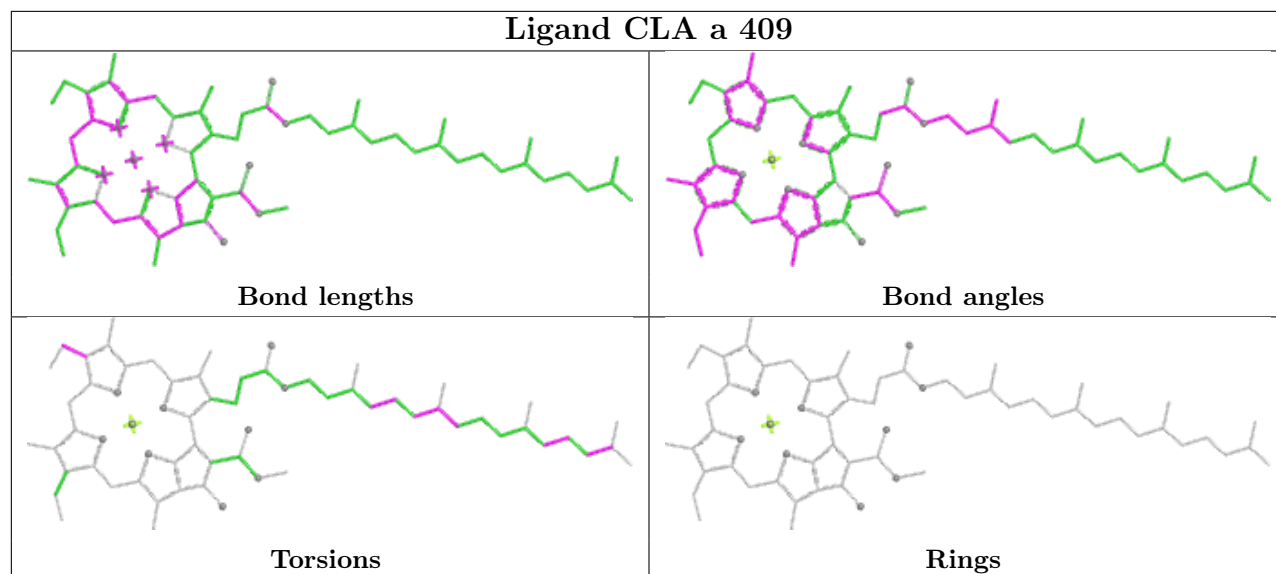
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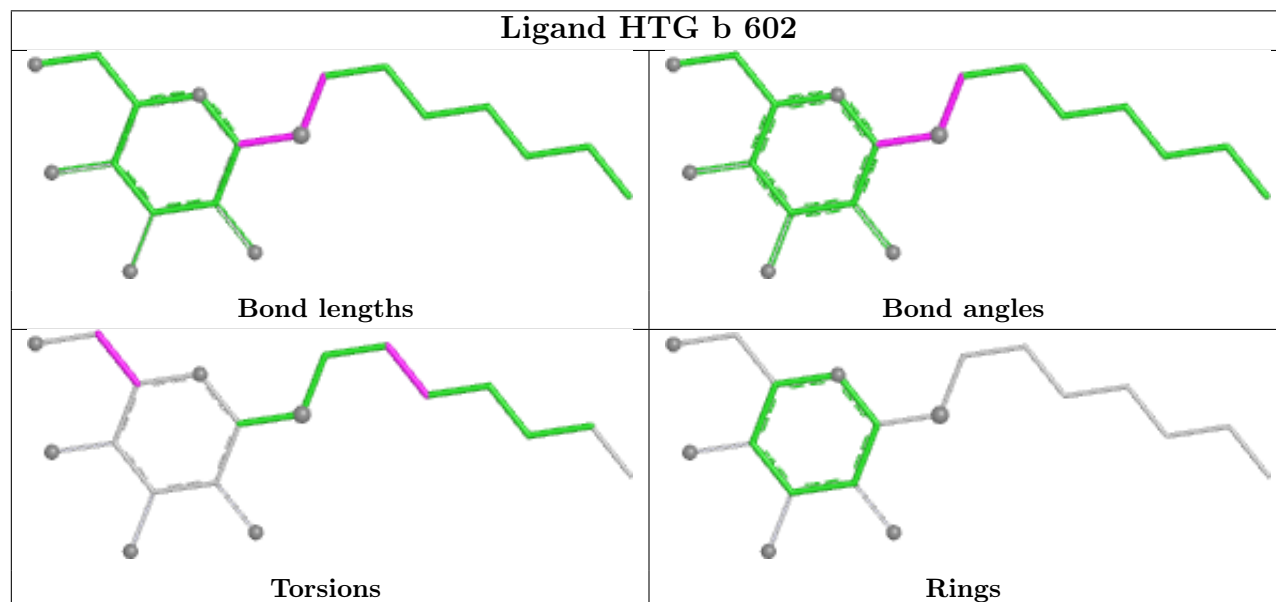
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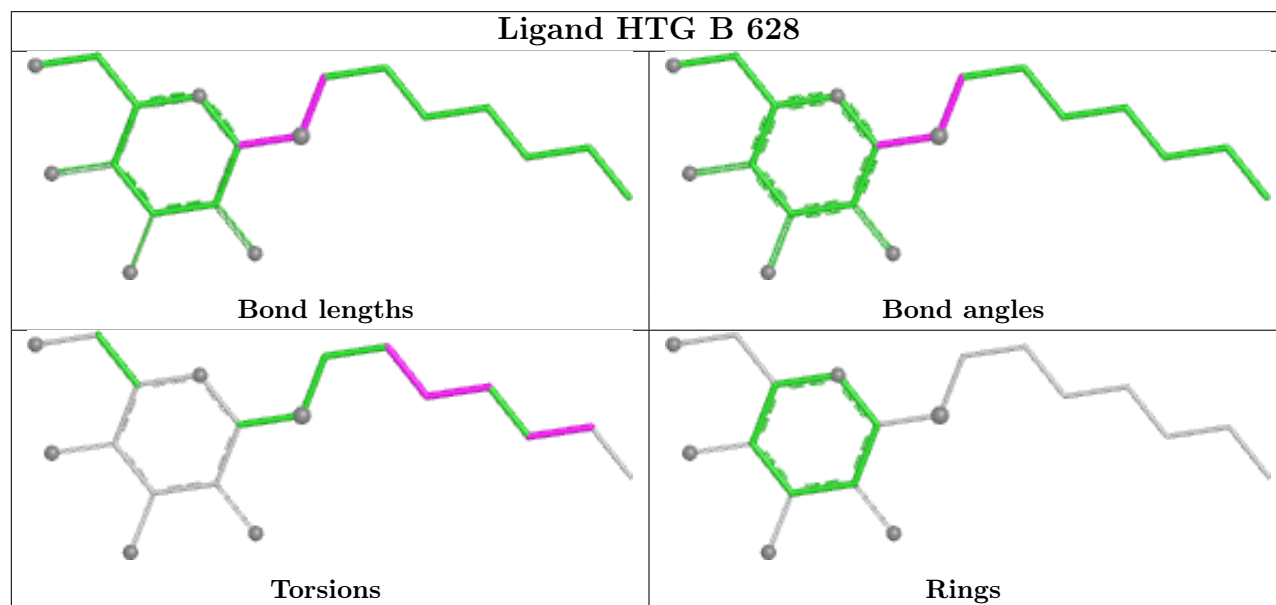
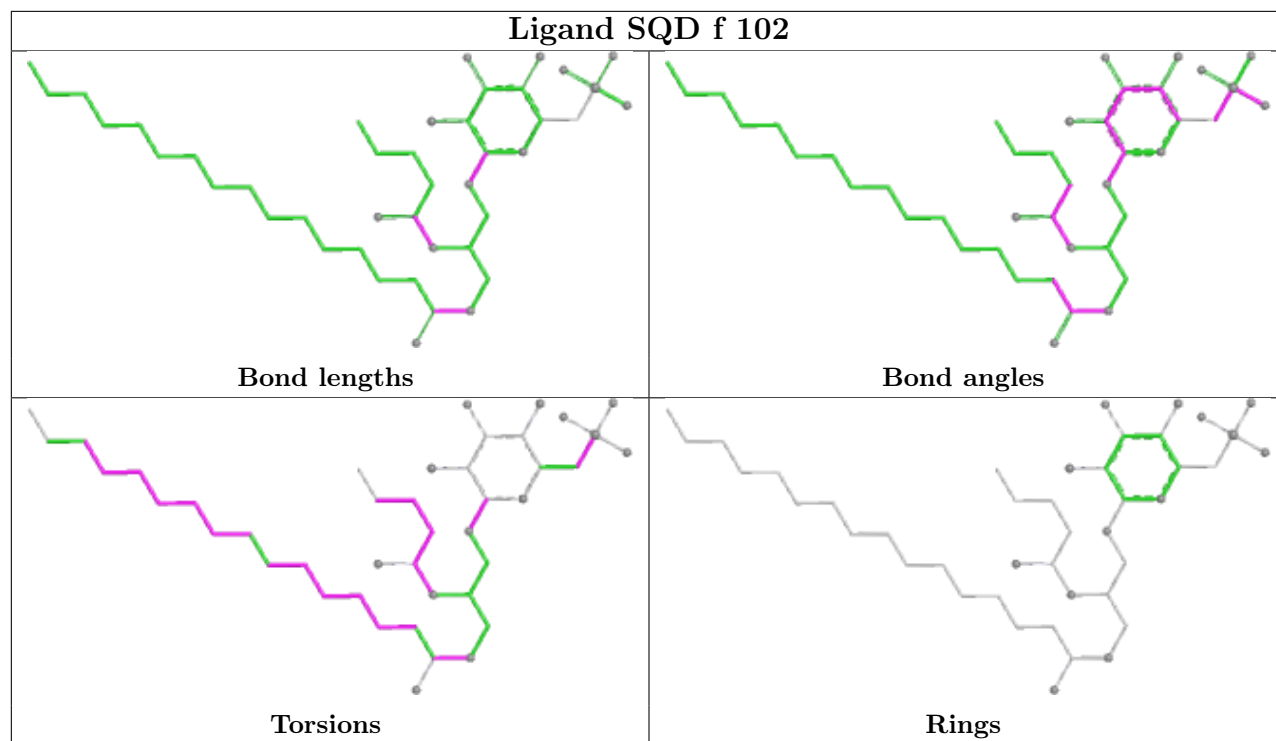


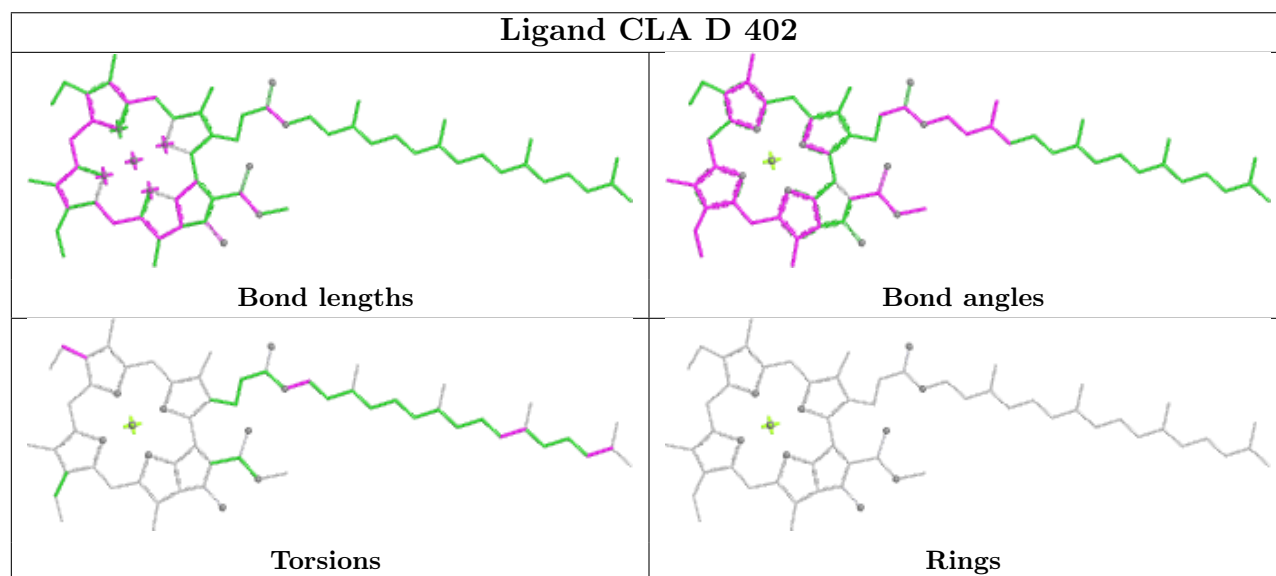
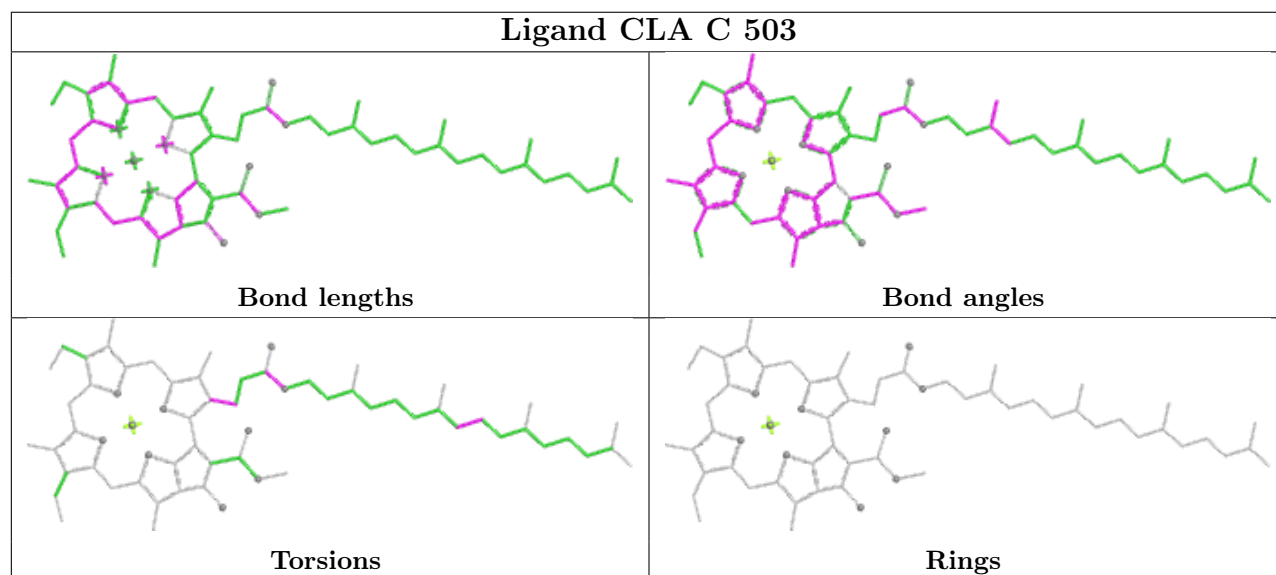
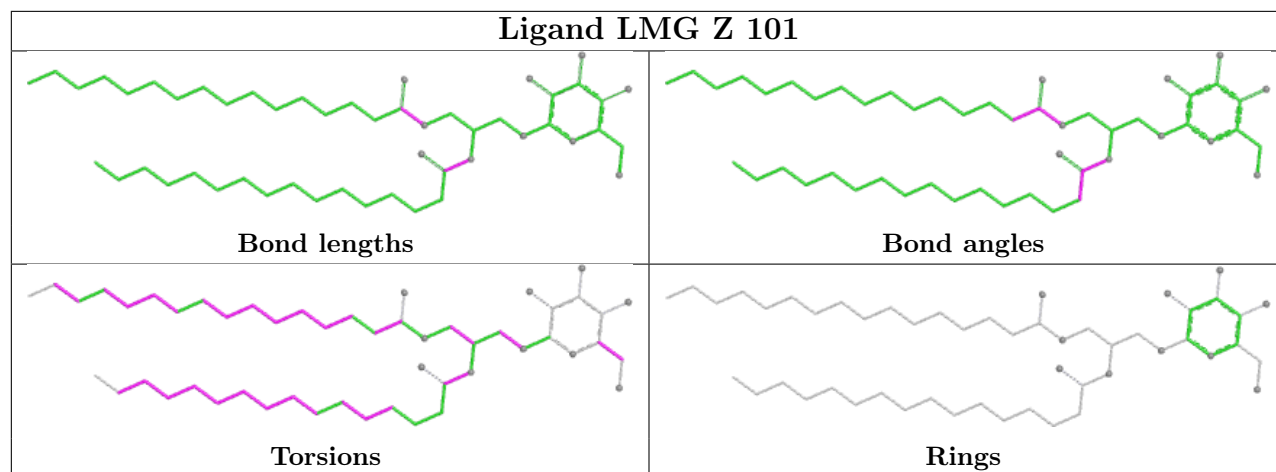
Ligand CLA a 409



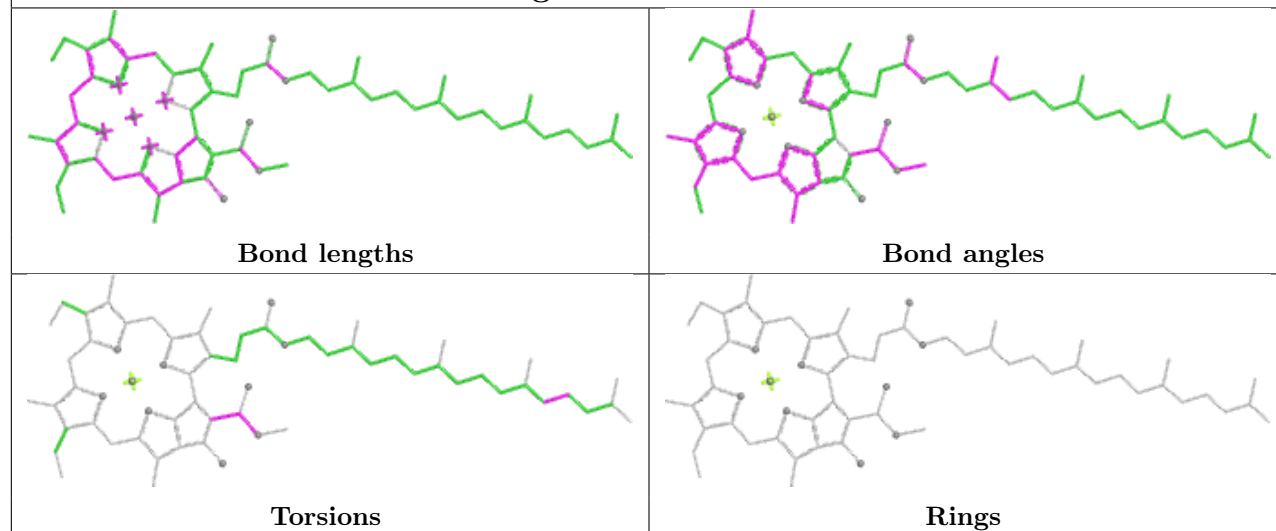
Ligand HTG b 602



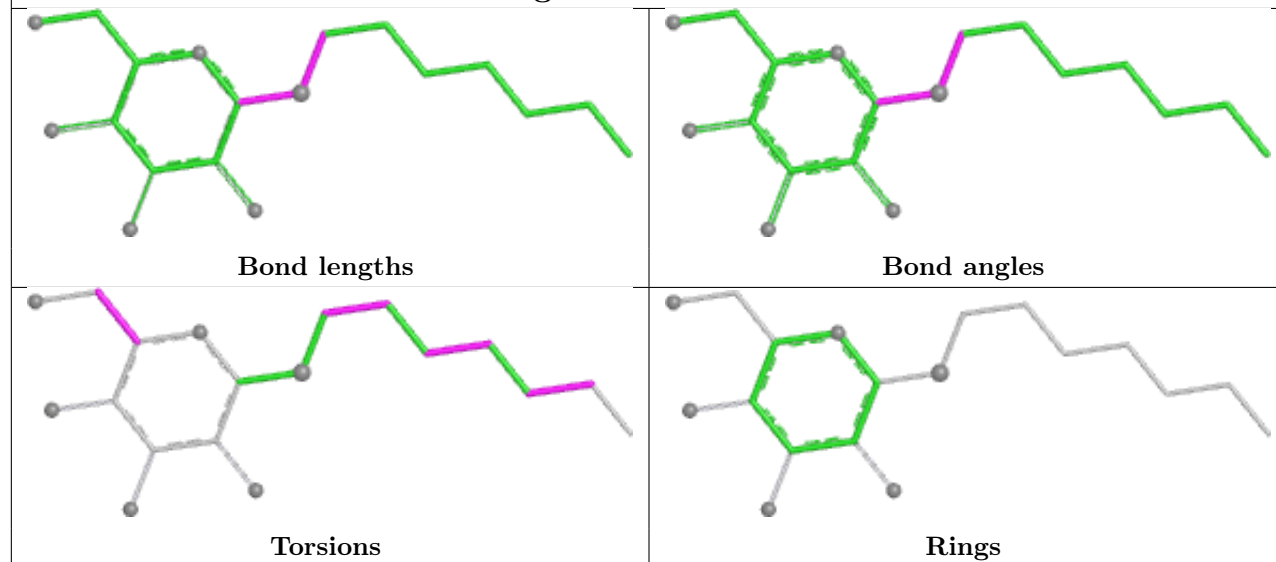




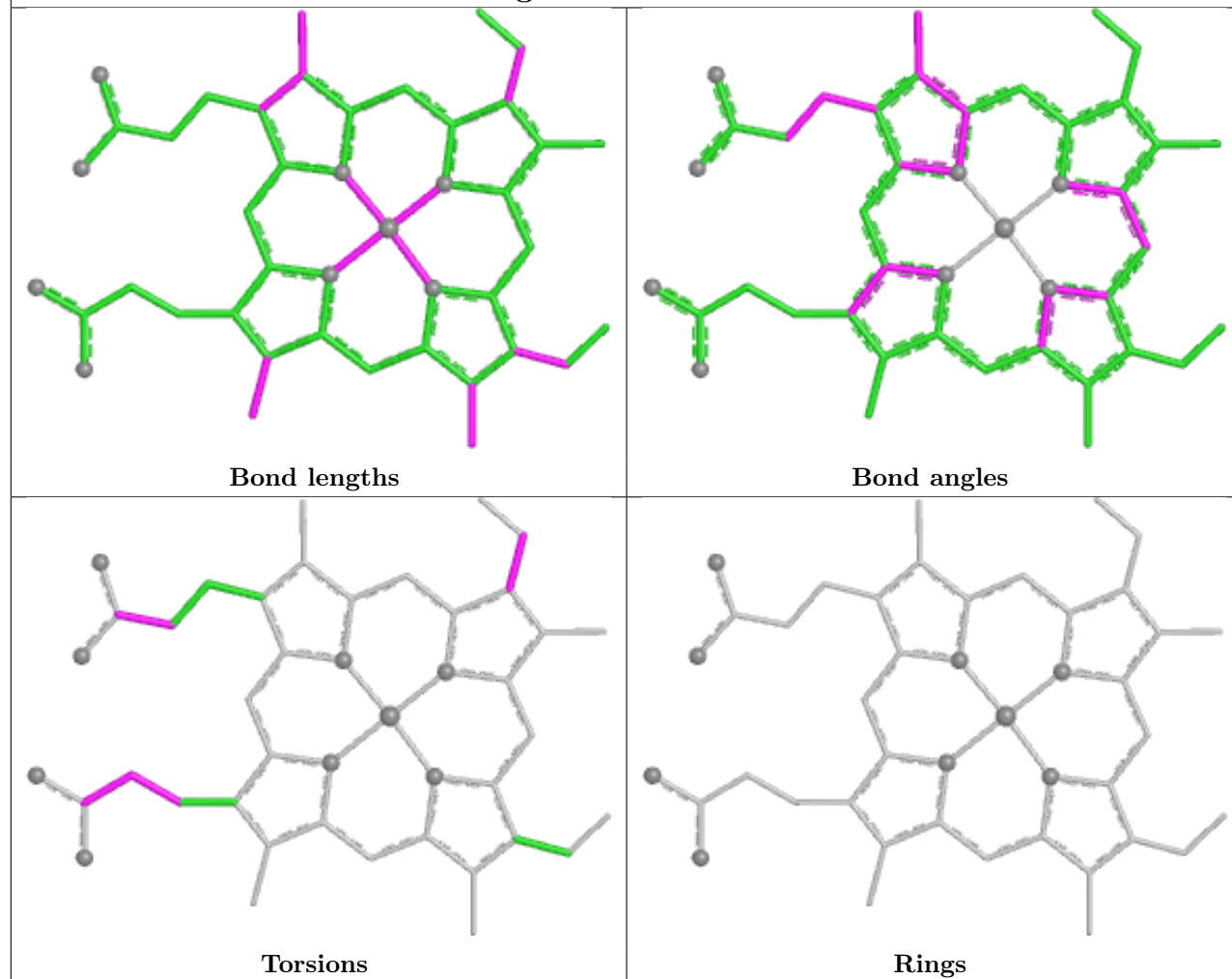
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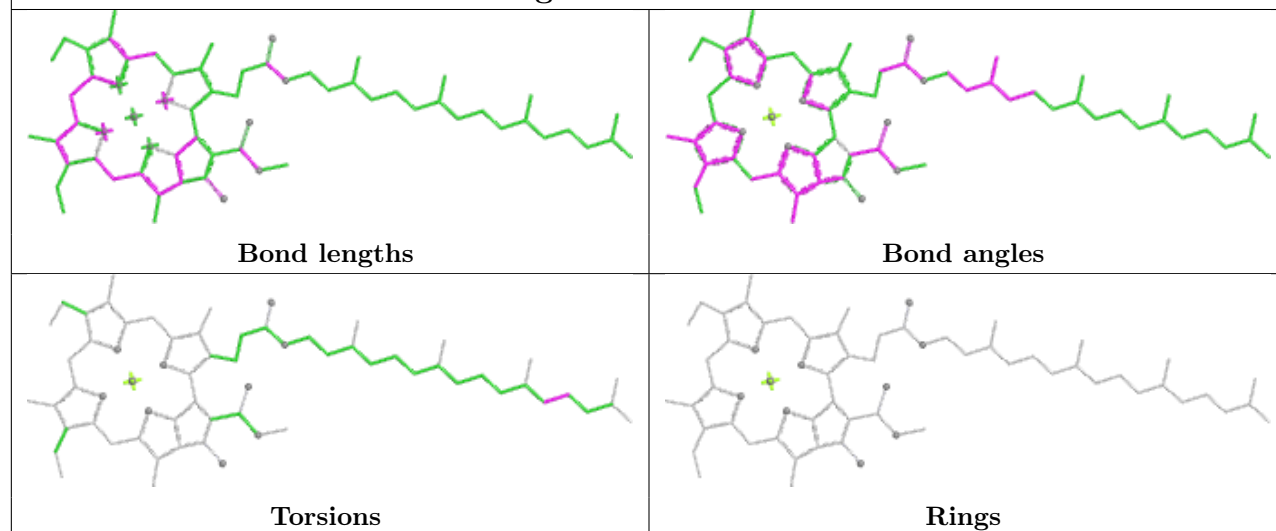
Ligand HTG c 525



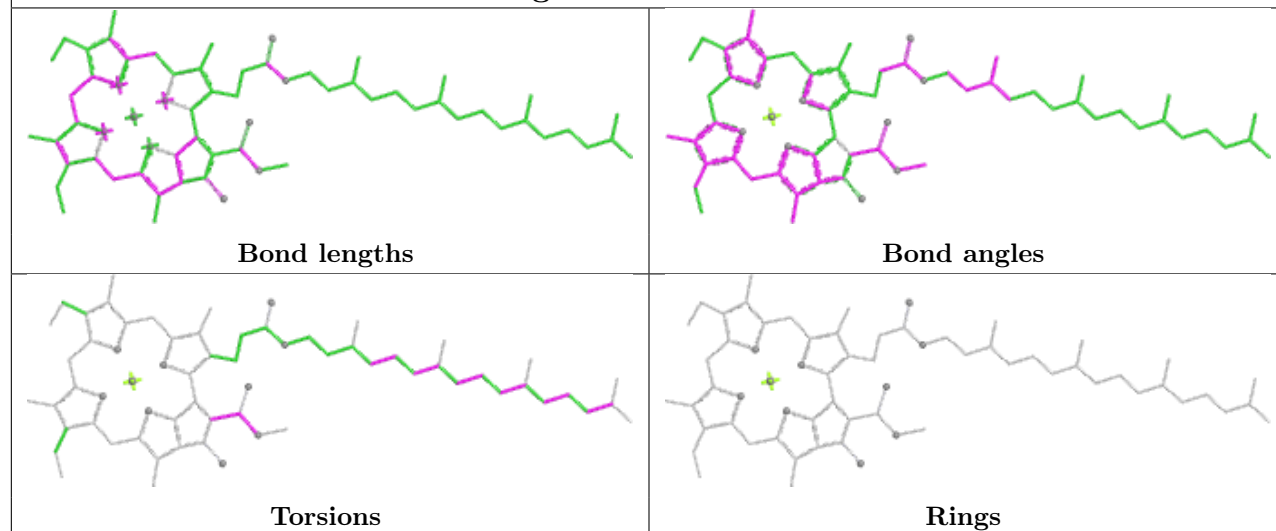
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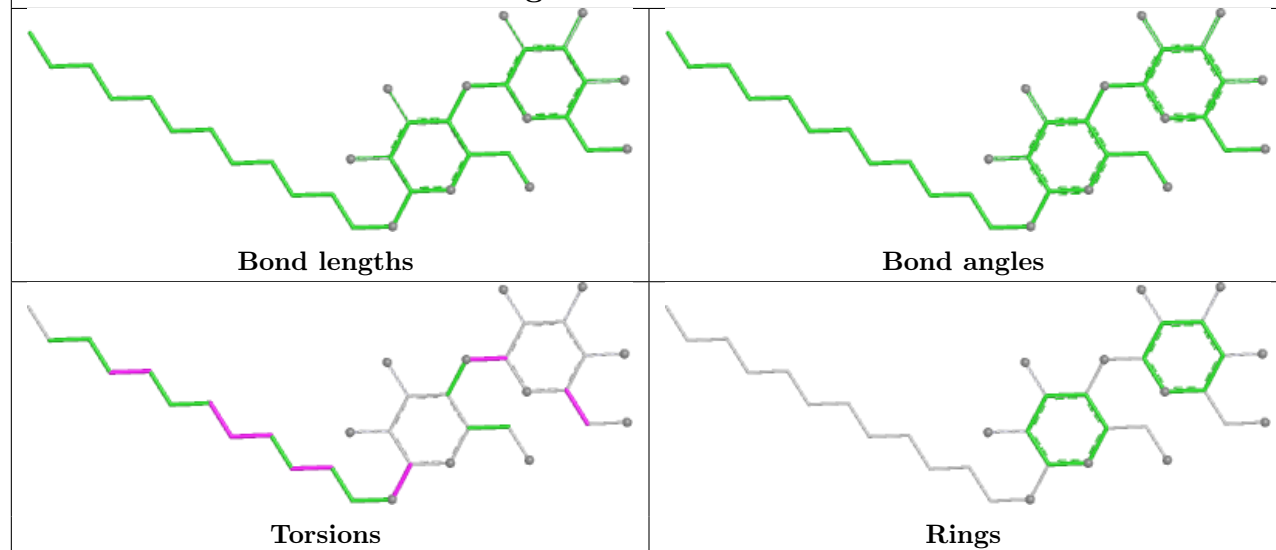
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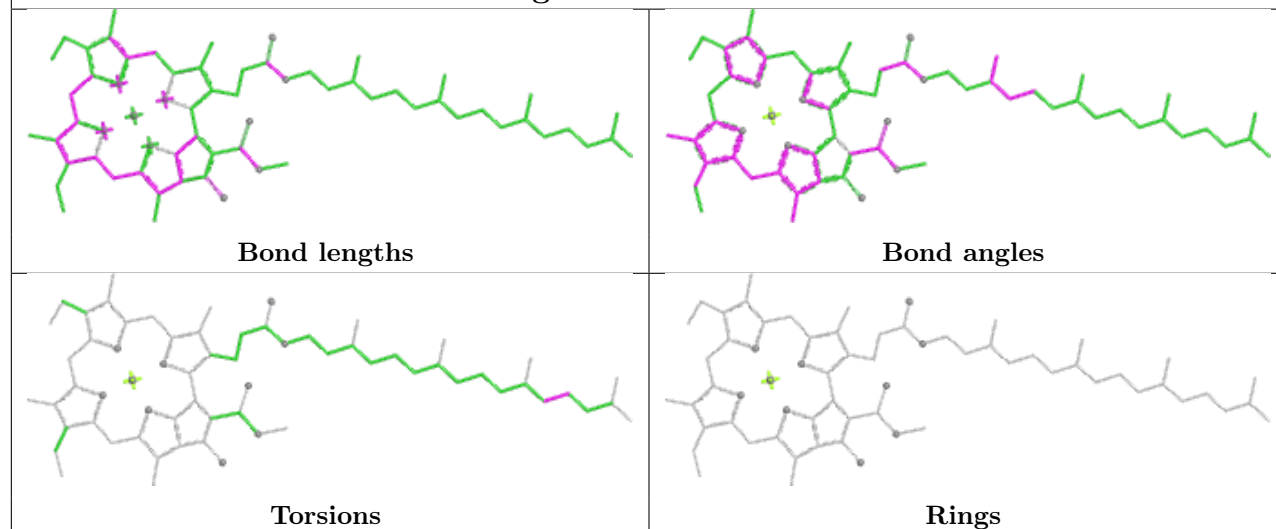
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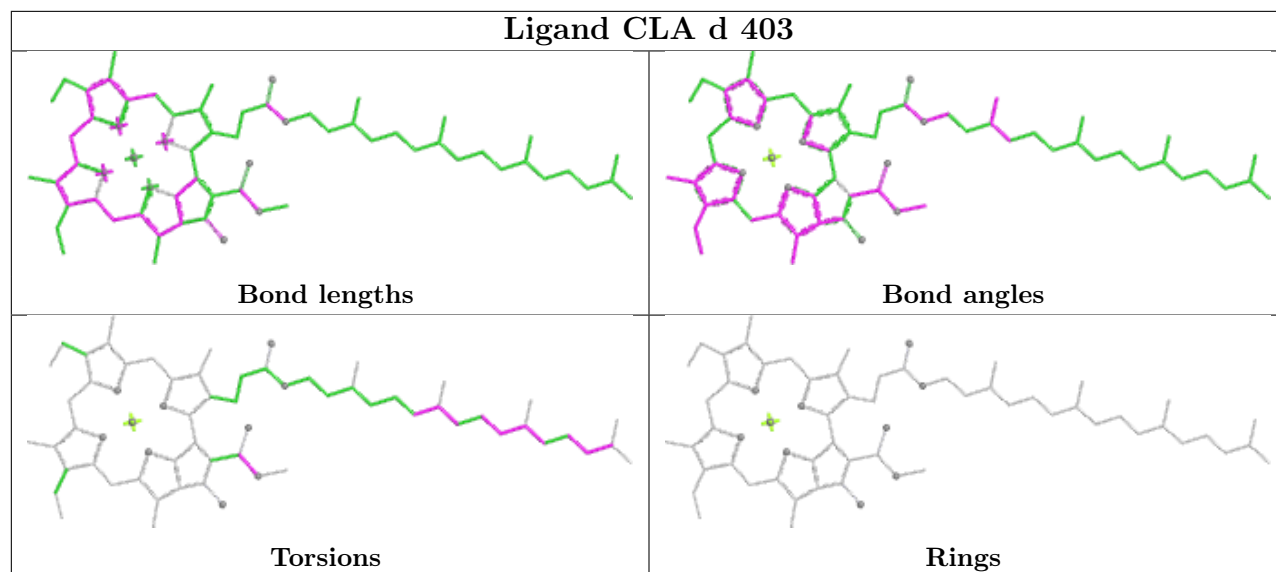
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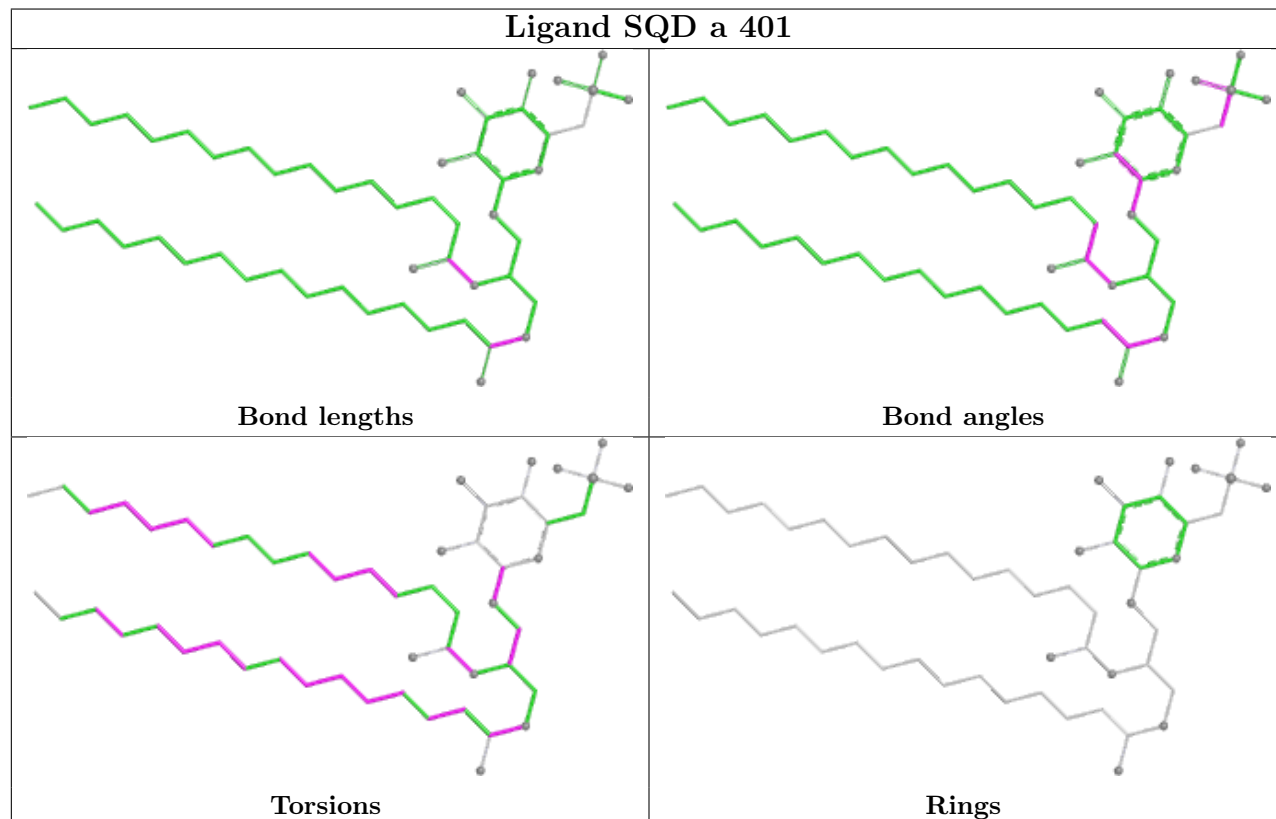
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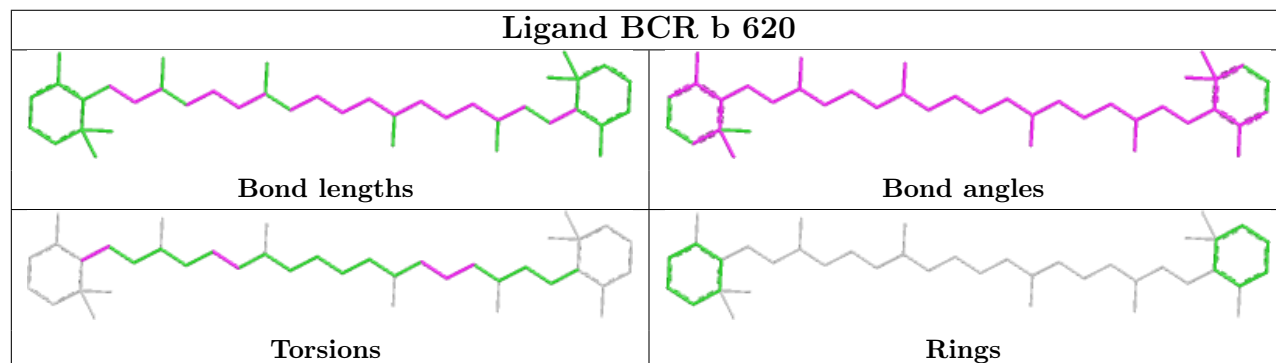
Ligand CLA d 403

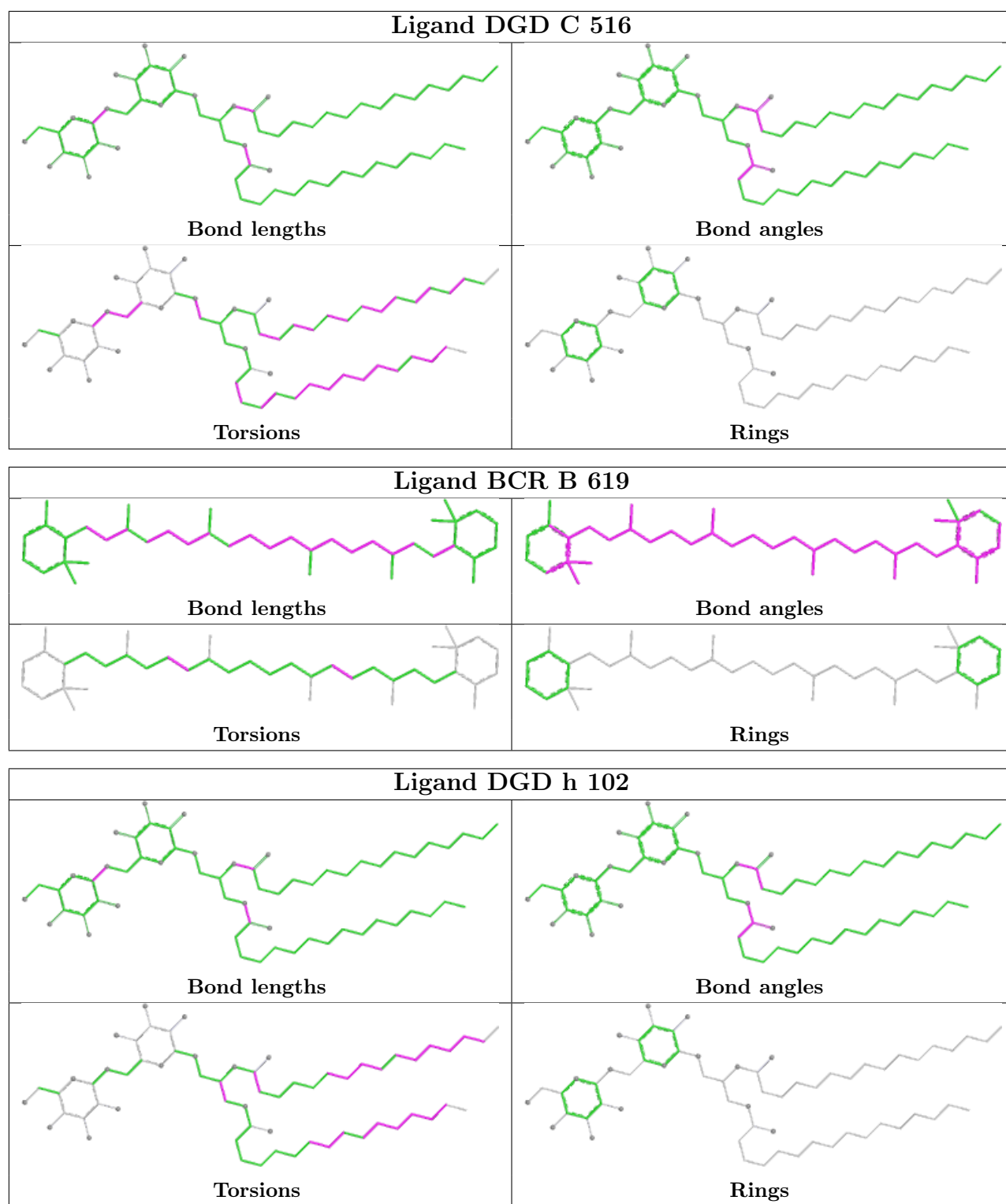


Ligand SQD a 401

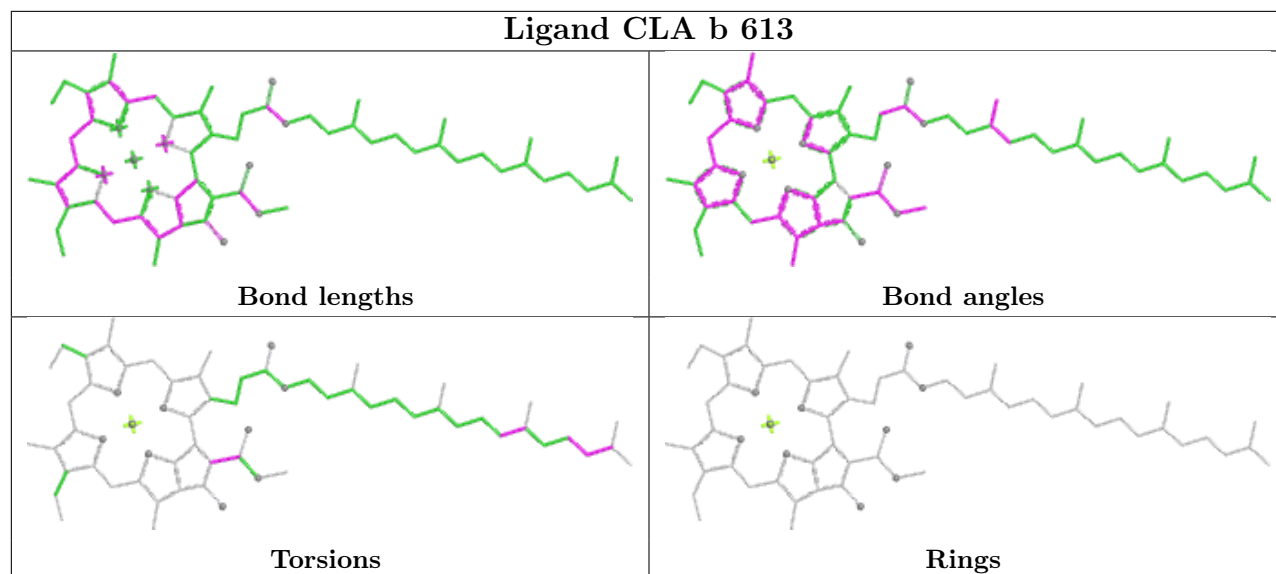


Ligand BCR b 620

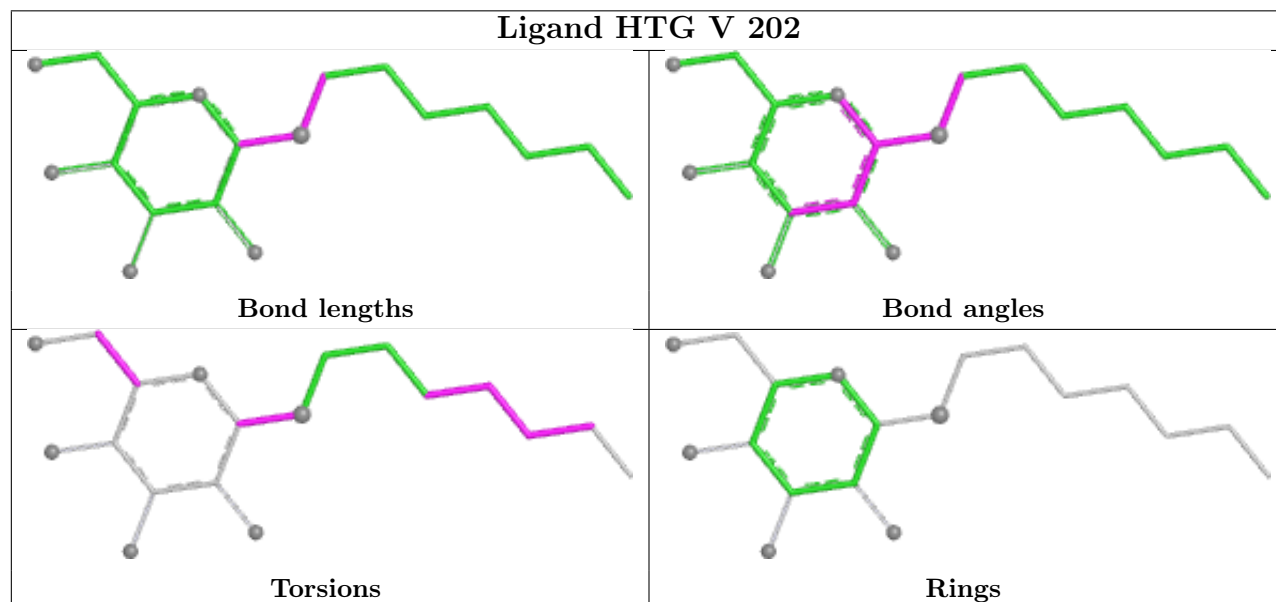




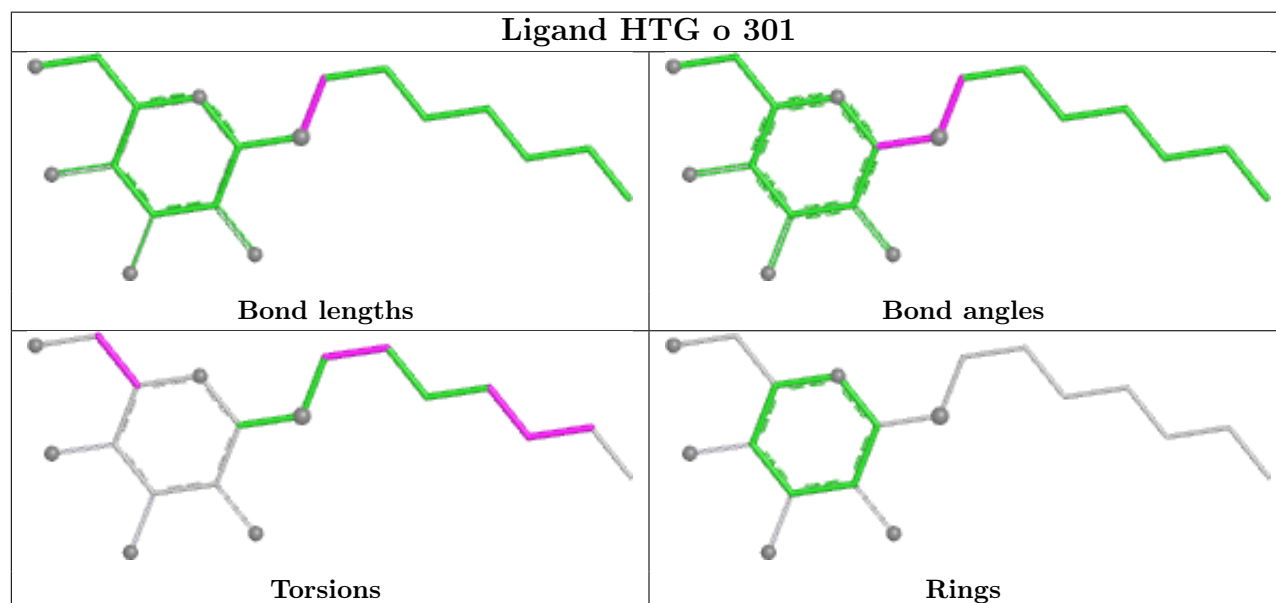
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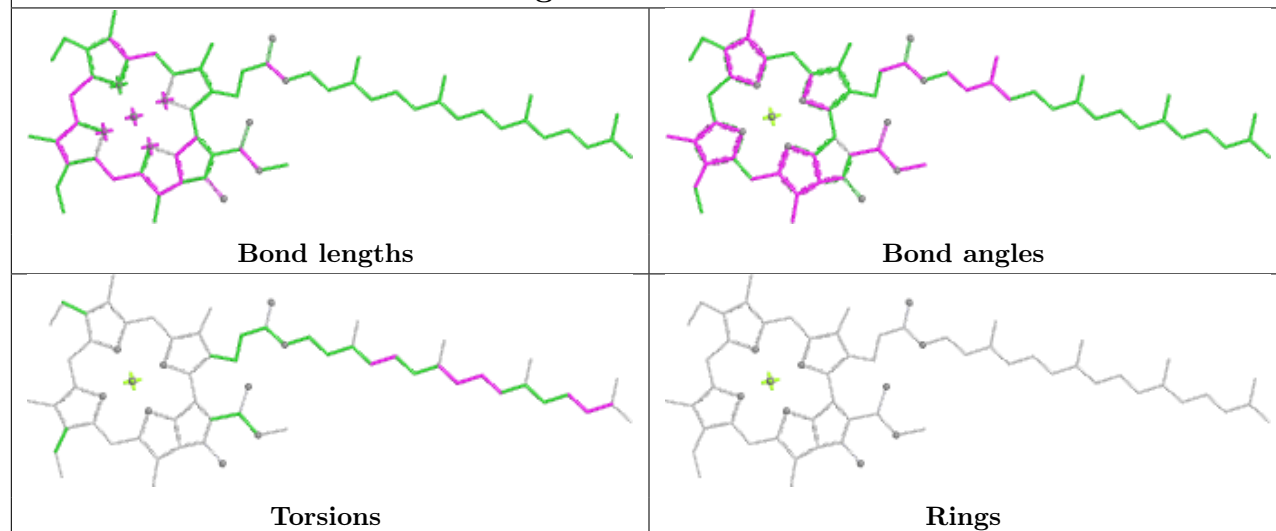
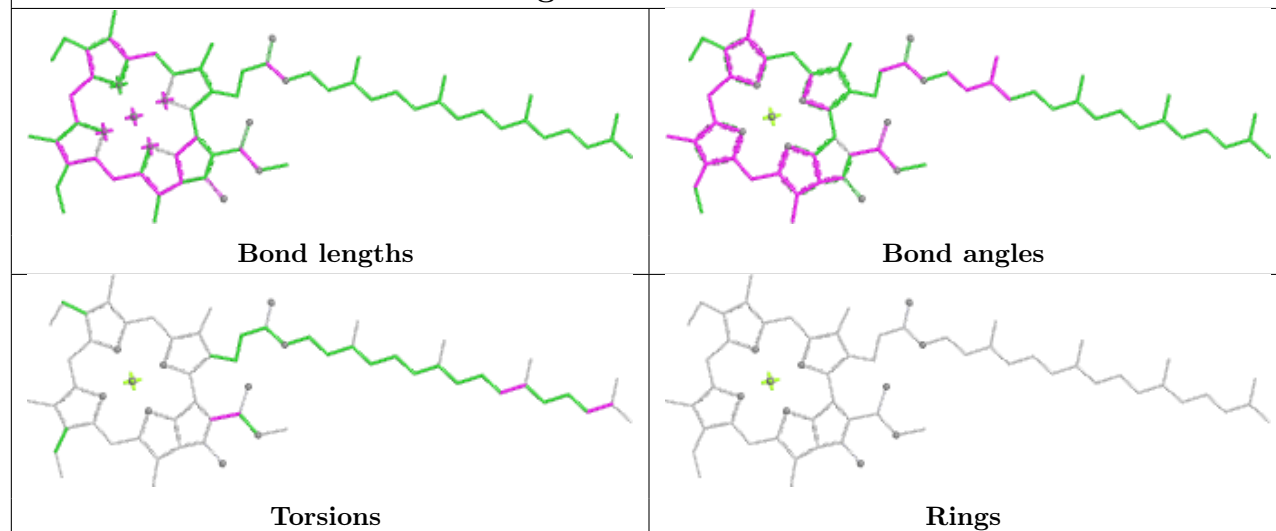
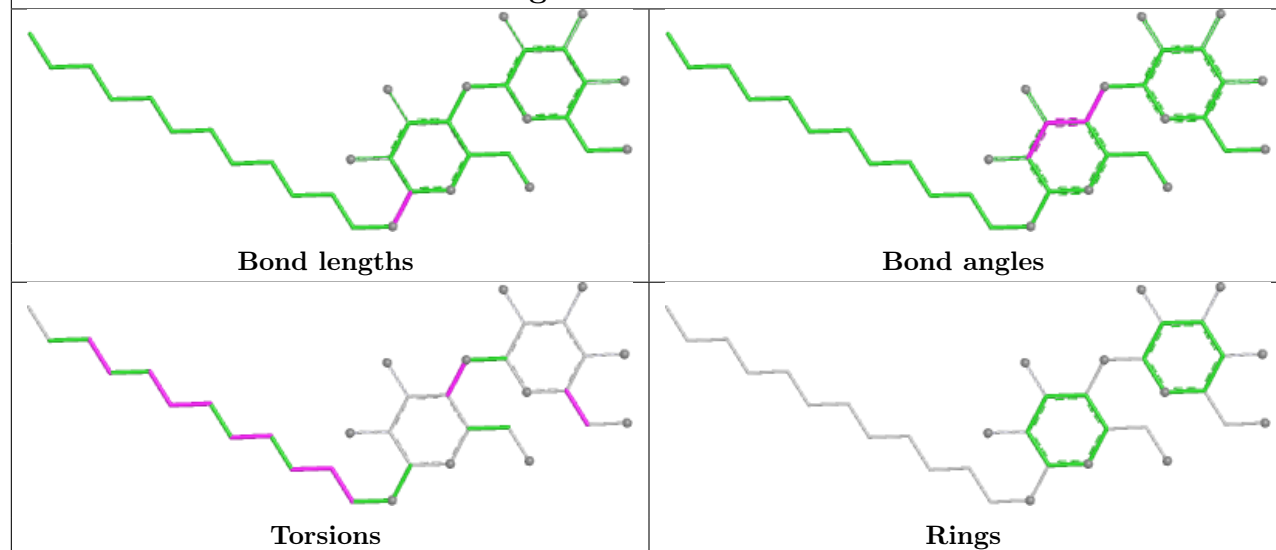


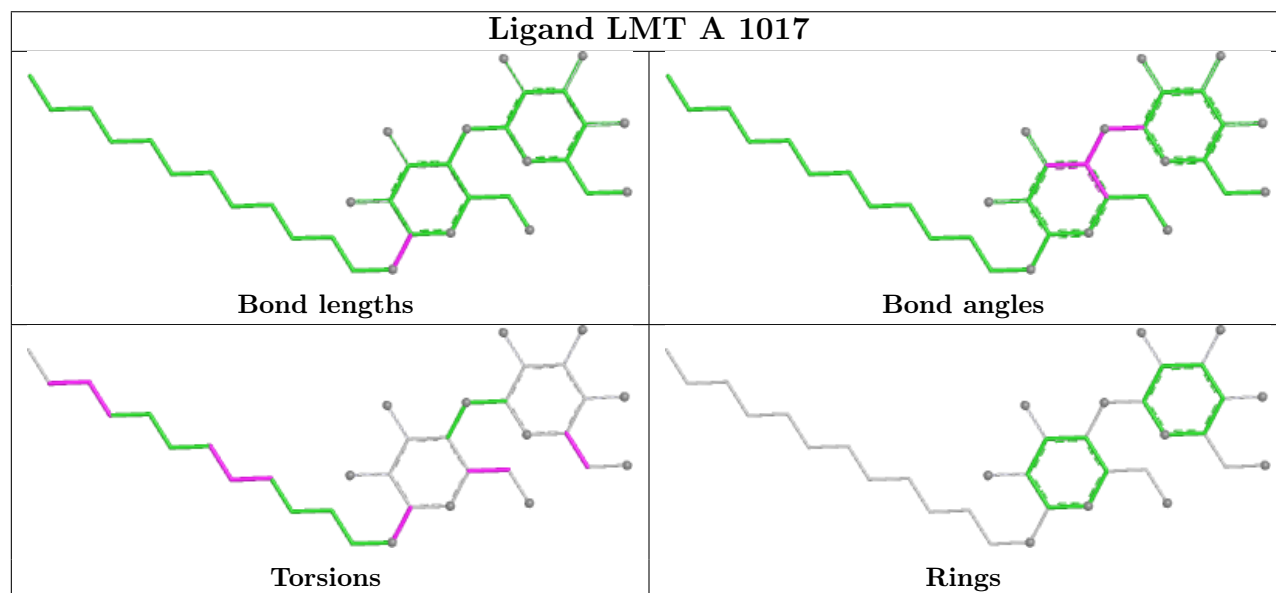
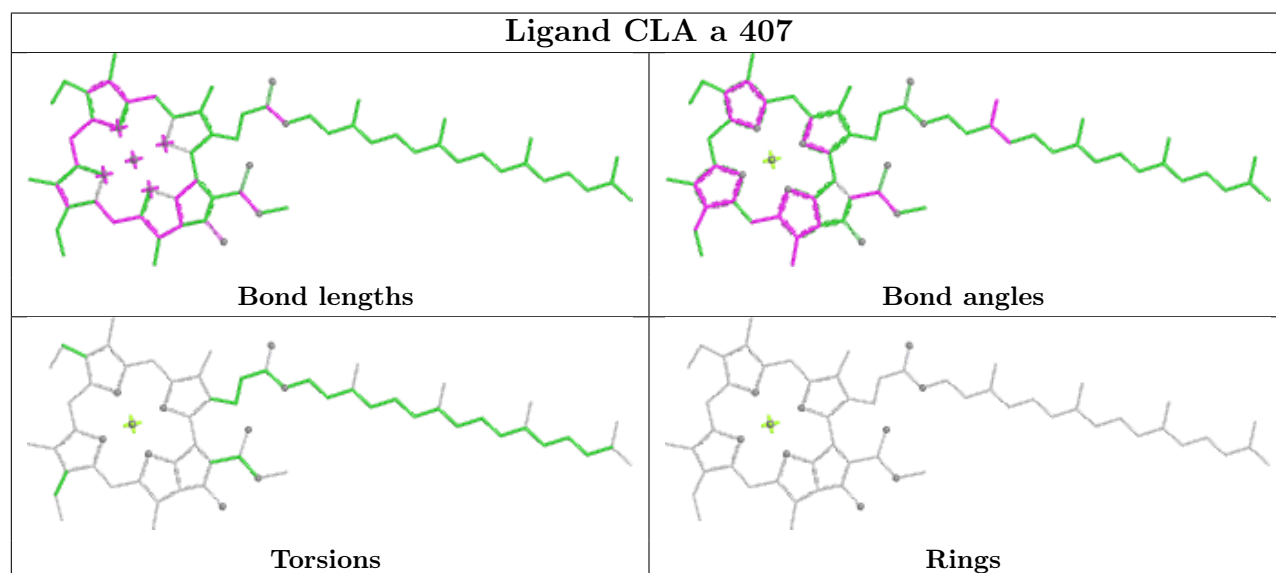
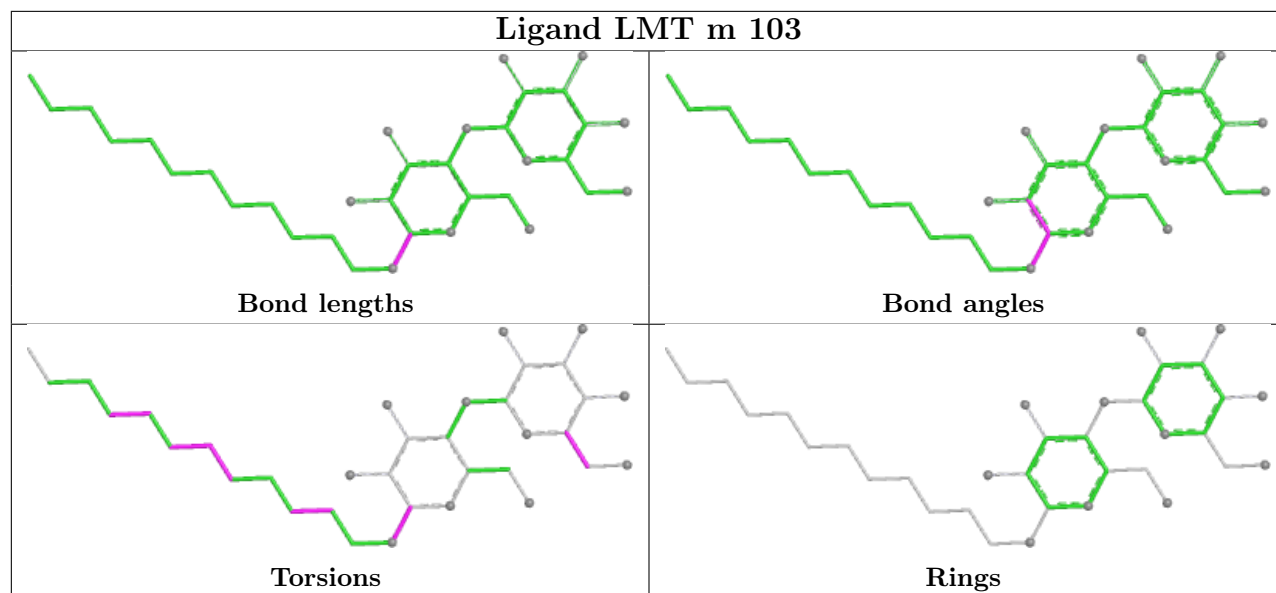
Ligand HTG V 202

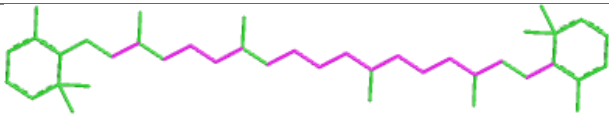
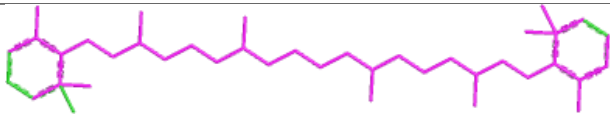
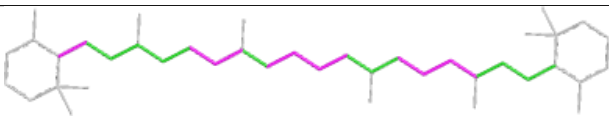
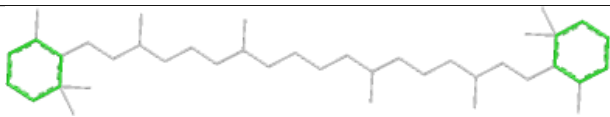


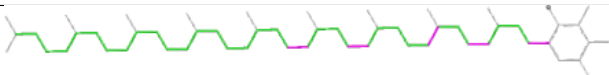
Ligand HTG o 301

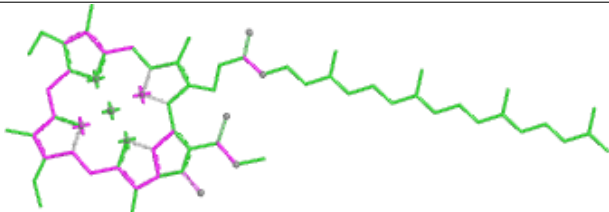
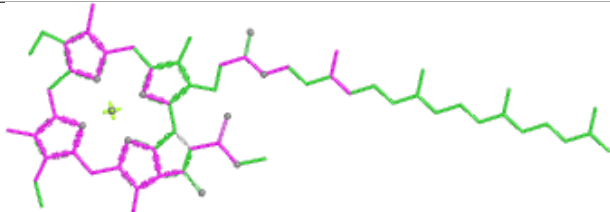
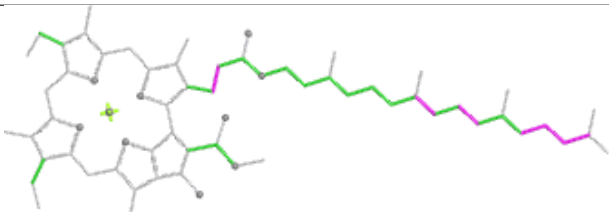
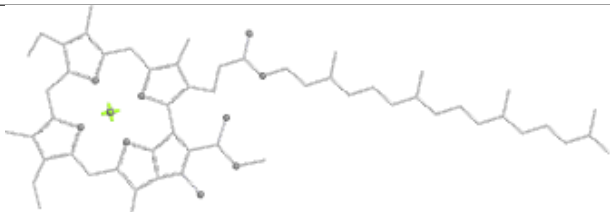


Ligand CLA b 616**Ligand CLA c 502****Ligand LMT C 520**

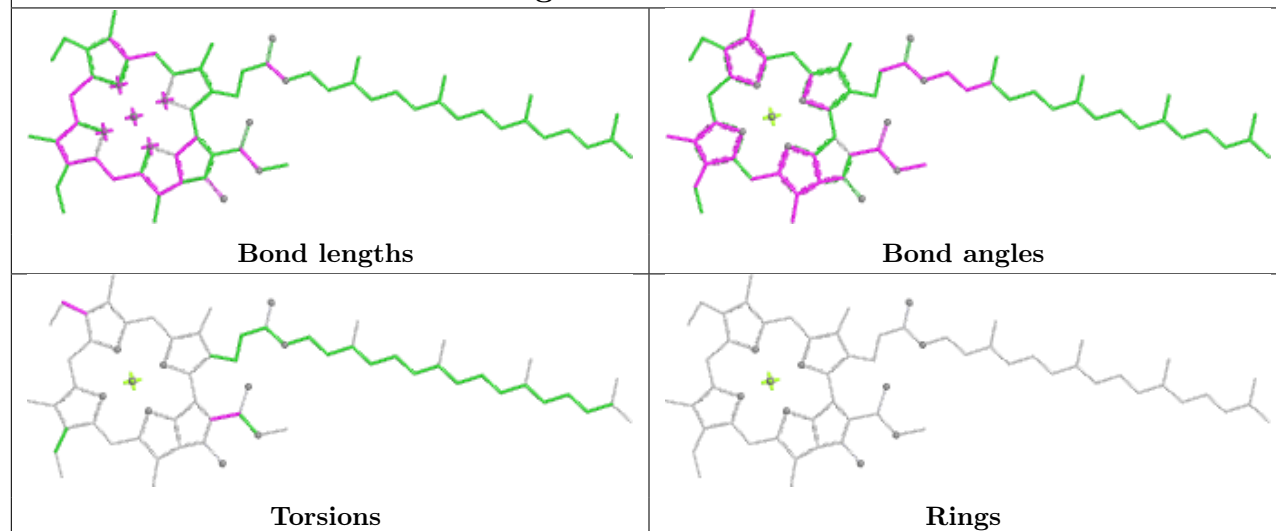


Ligand BCR J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

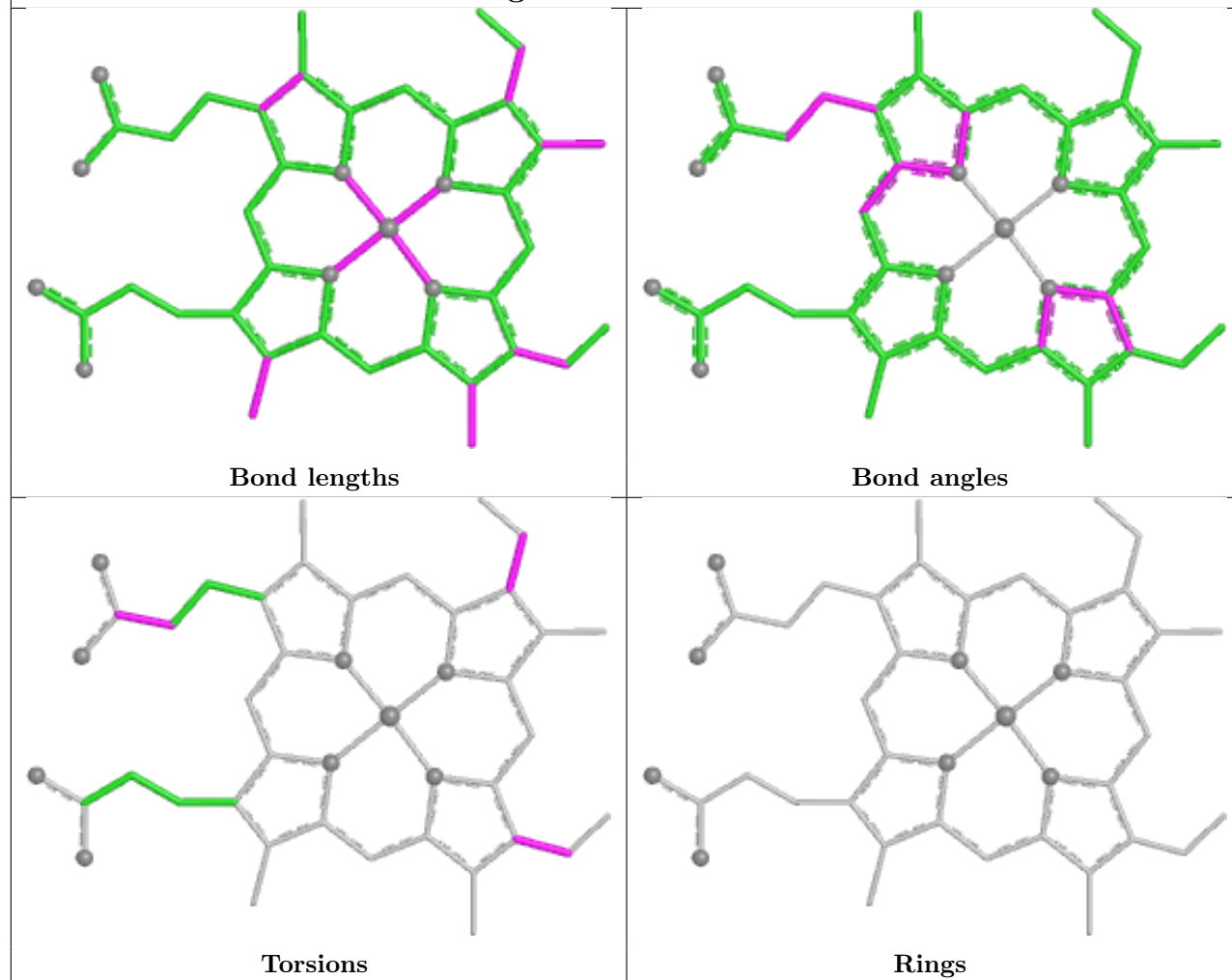
Ligand PL9 A 1010	
	
Bond lengths	Bond angles
	
Torsions	Rings

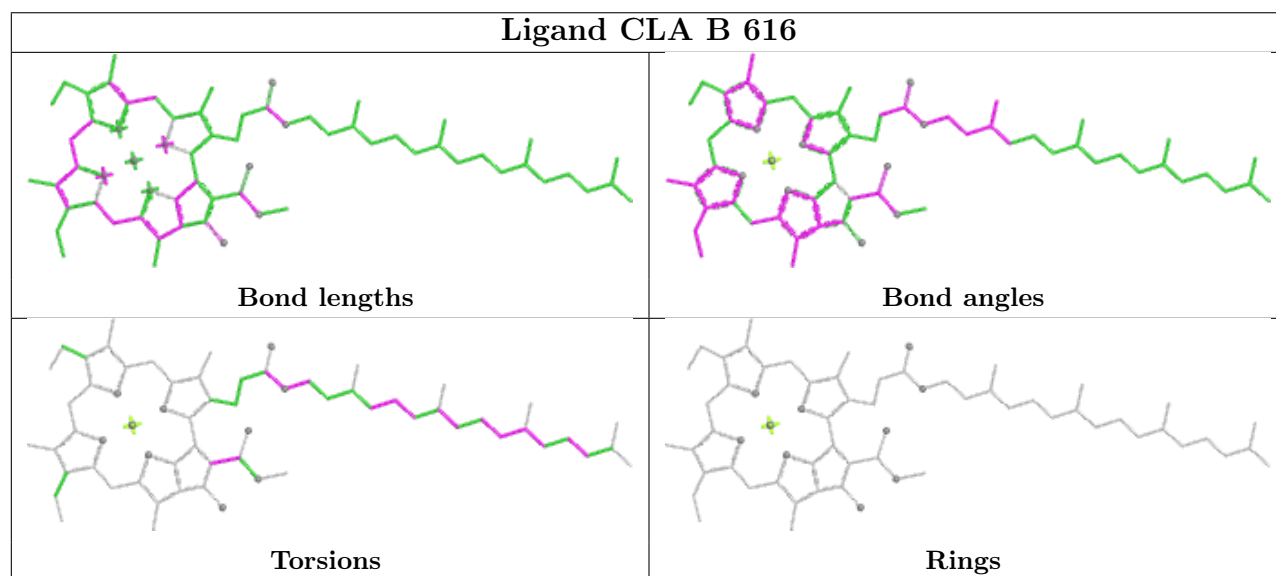
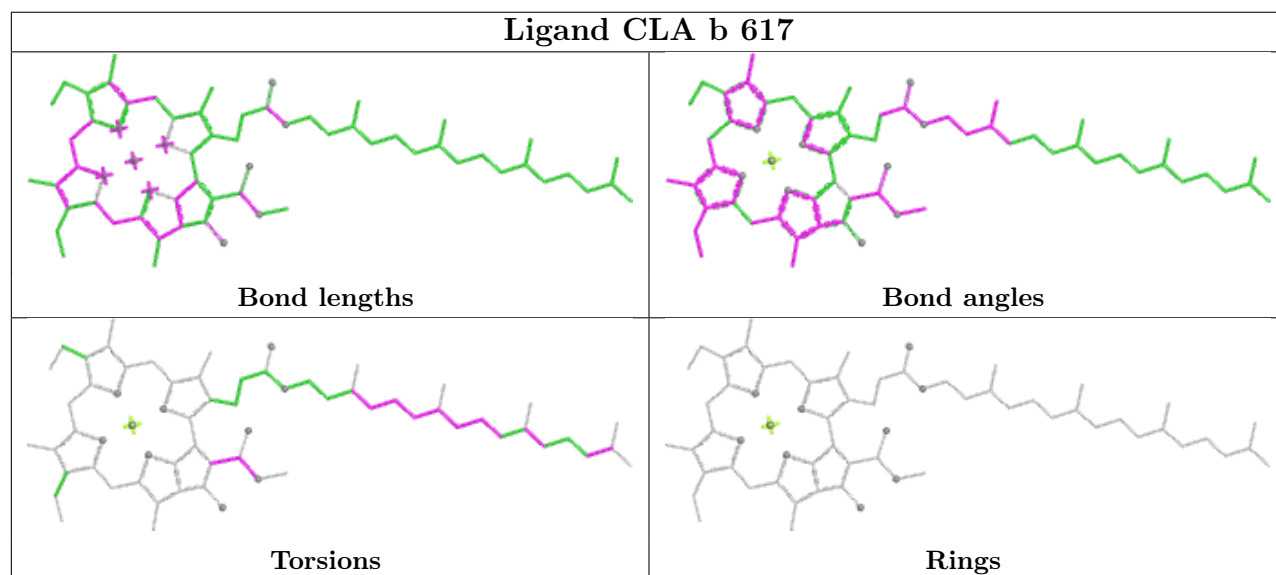
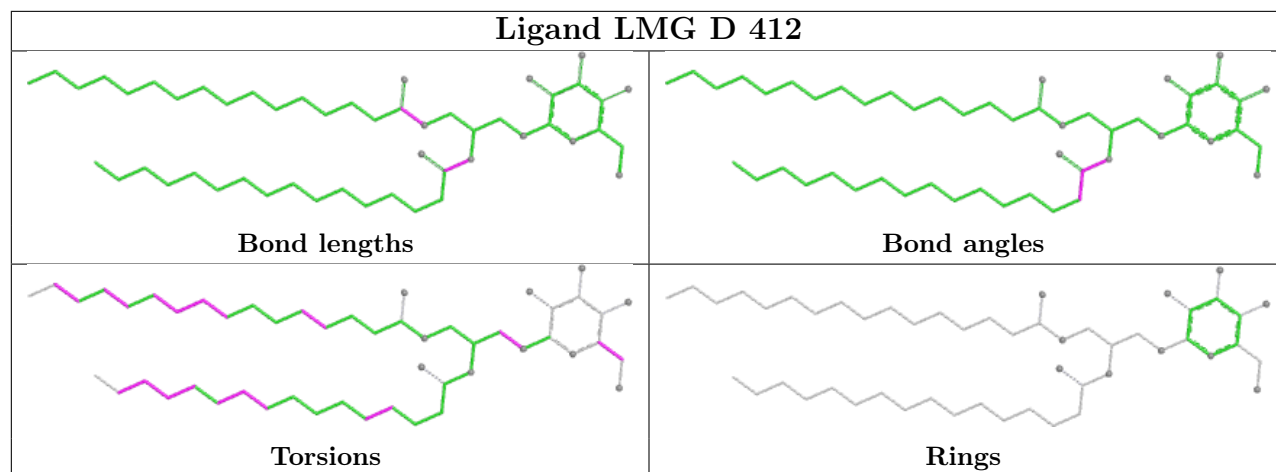
Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

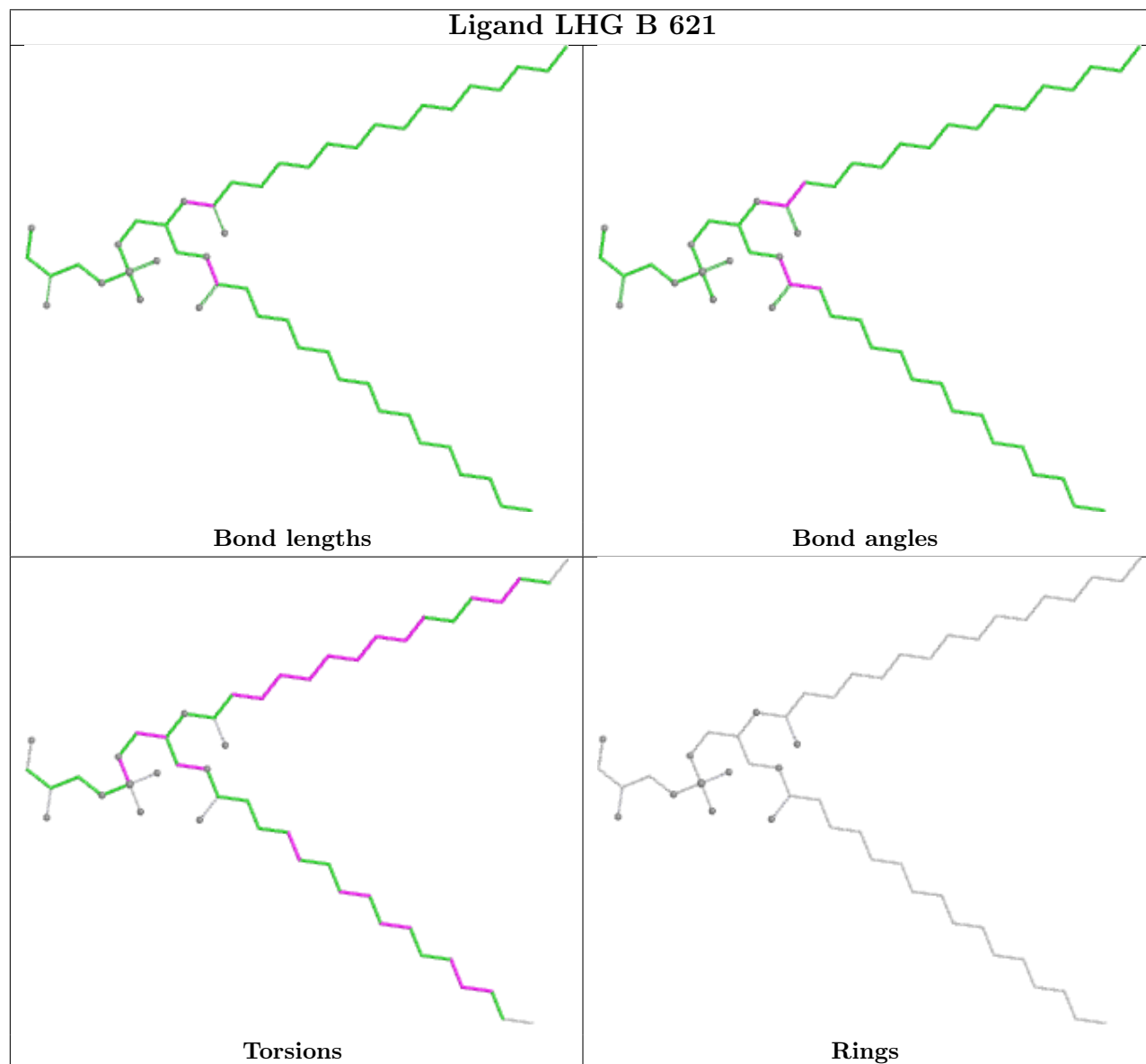
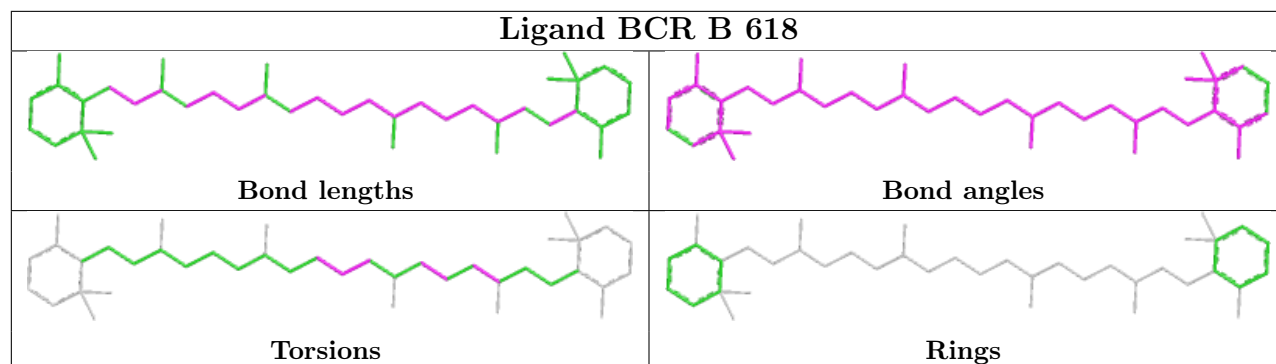
Ligand CLA b 612

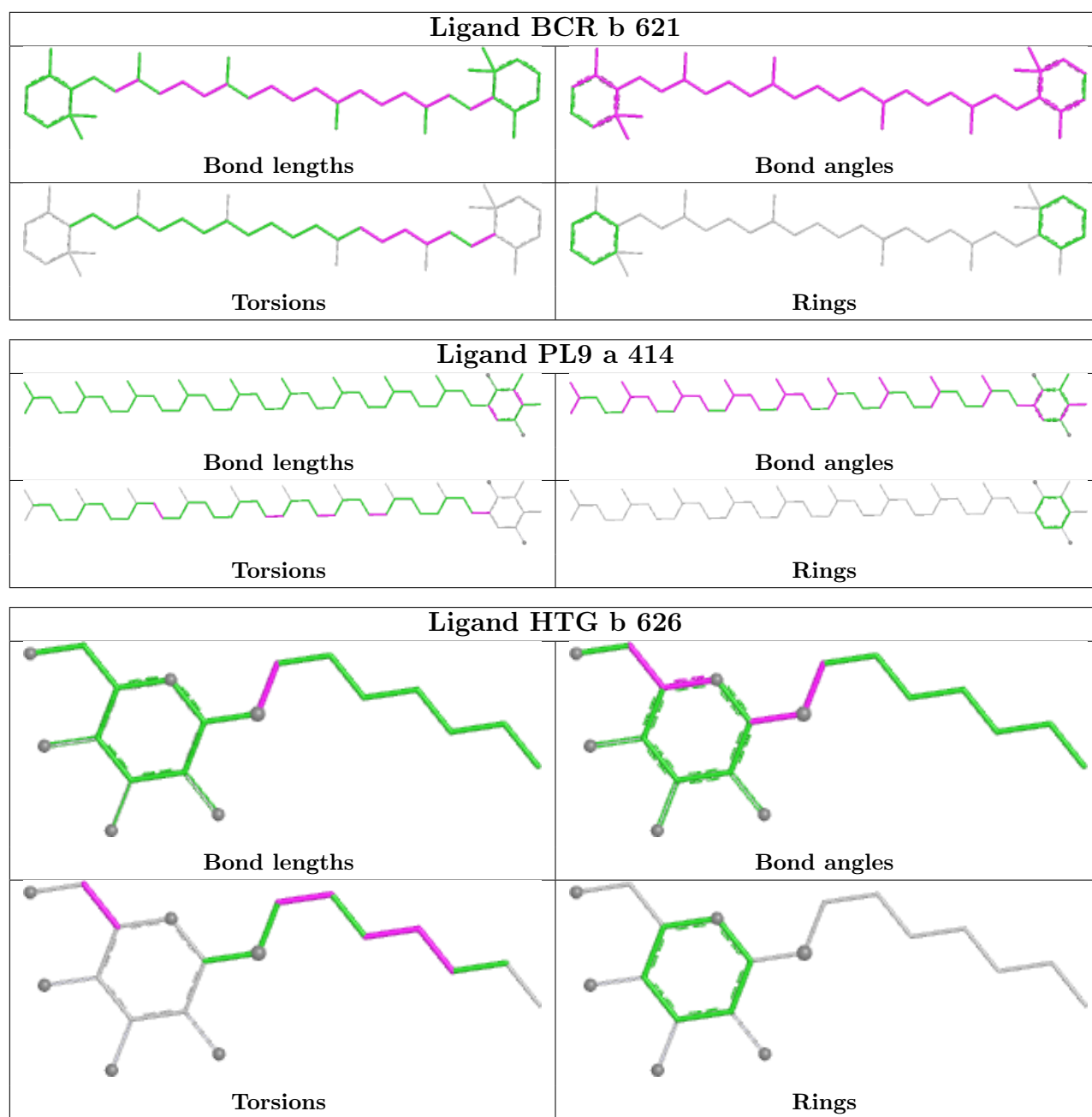


Ligand HEM V 201

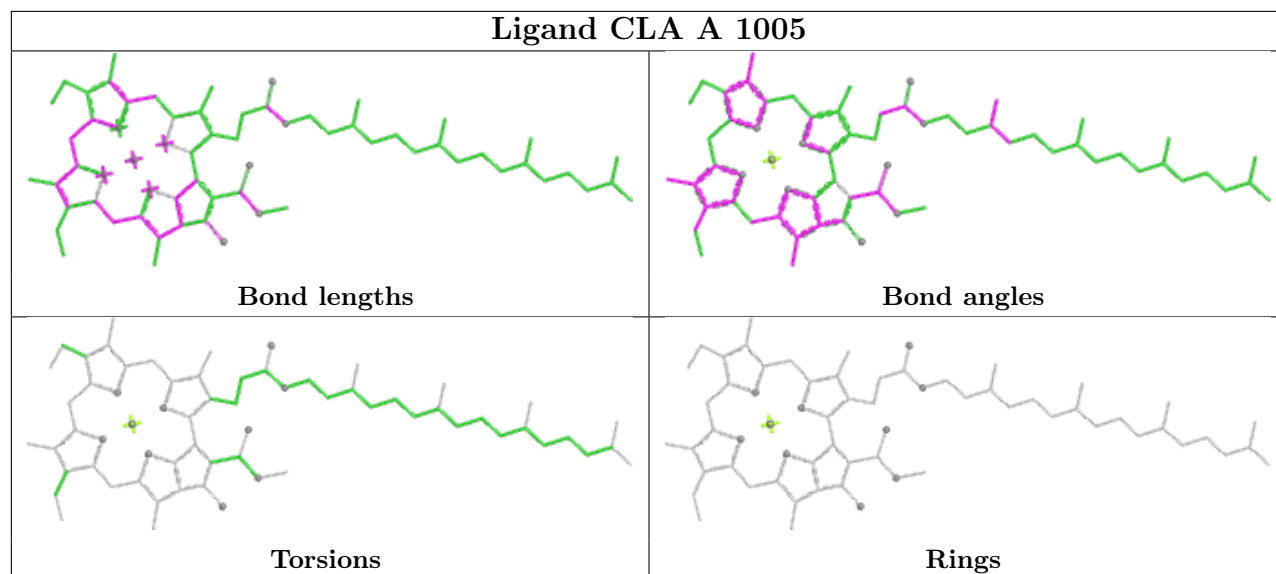




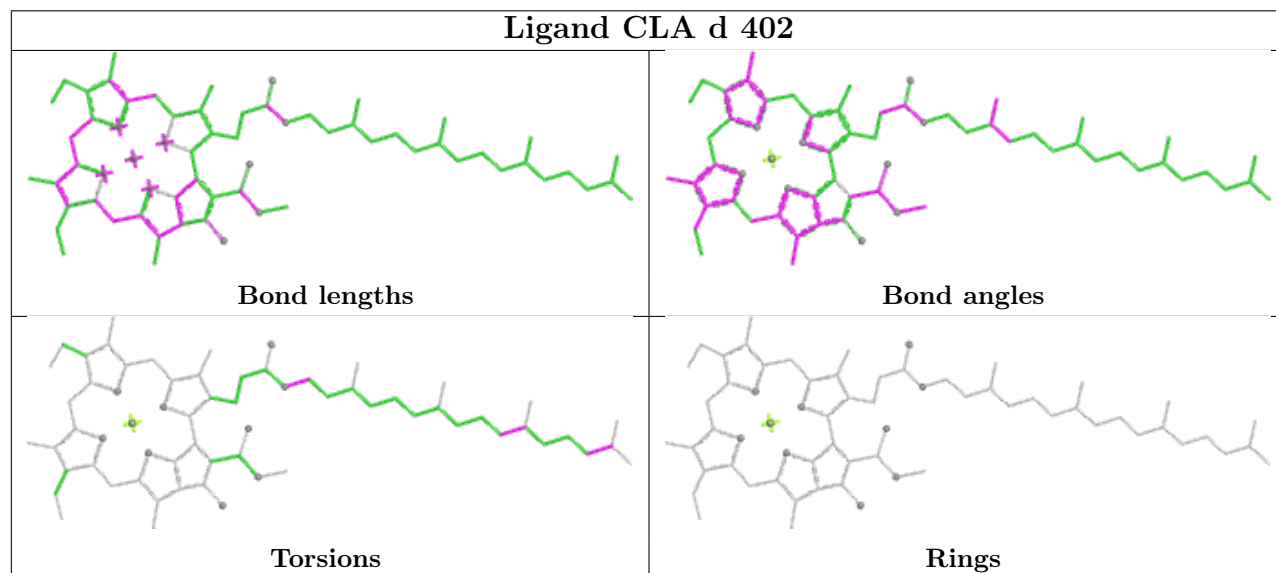


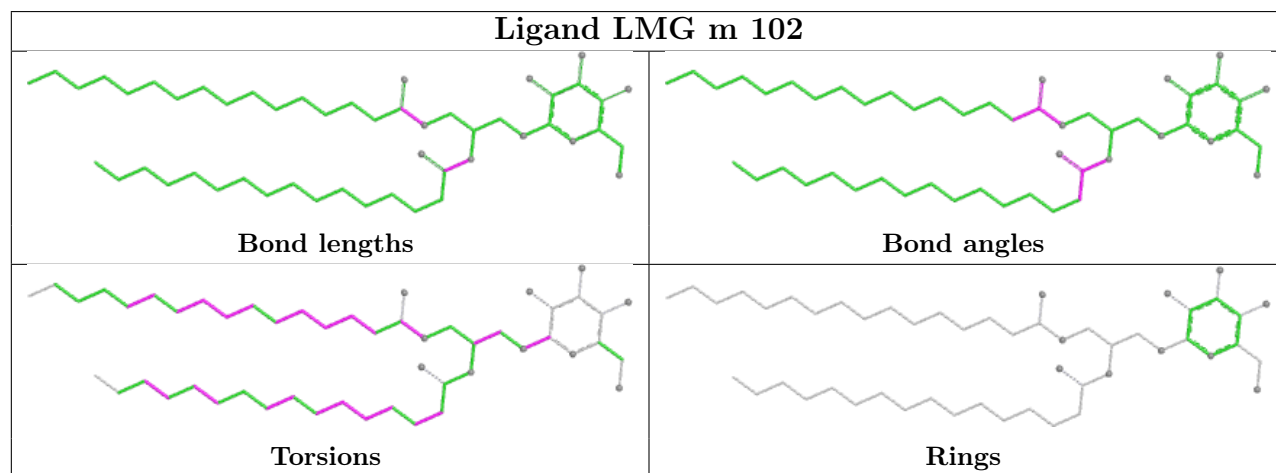
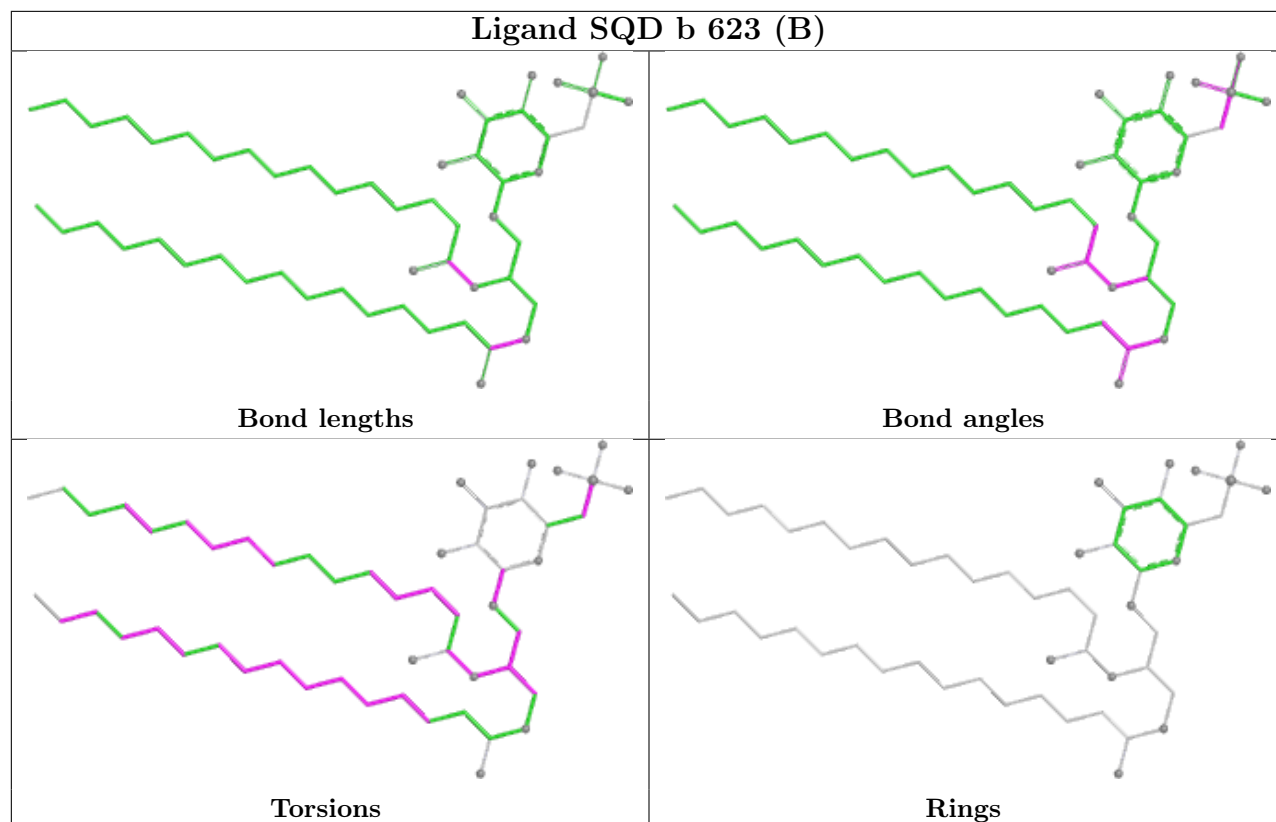


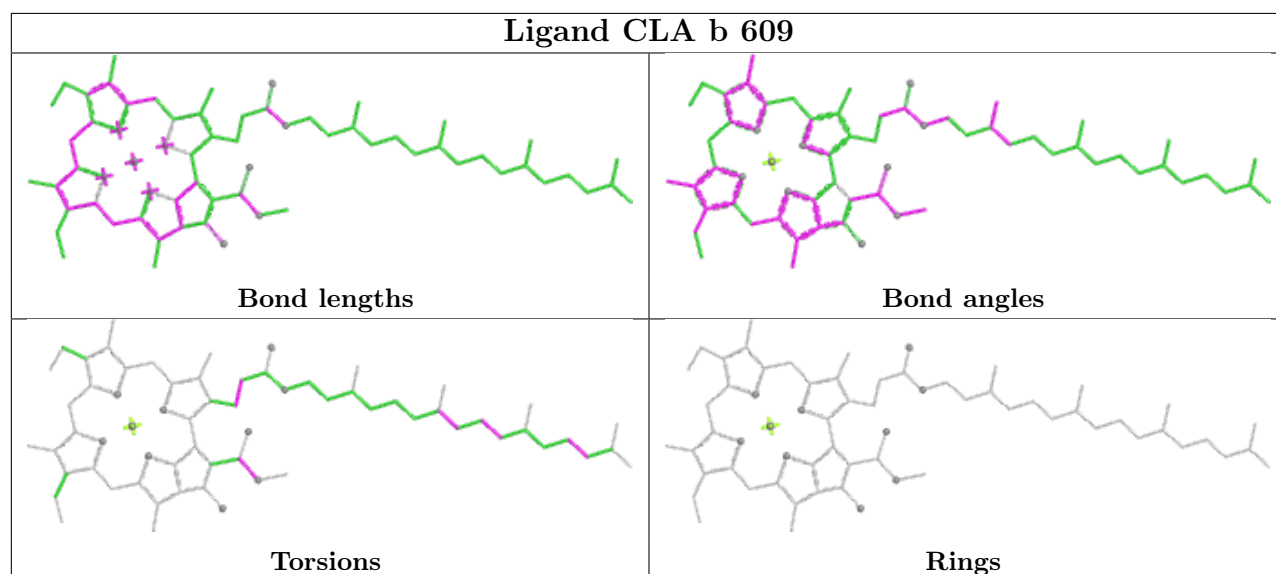
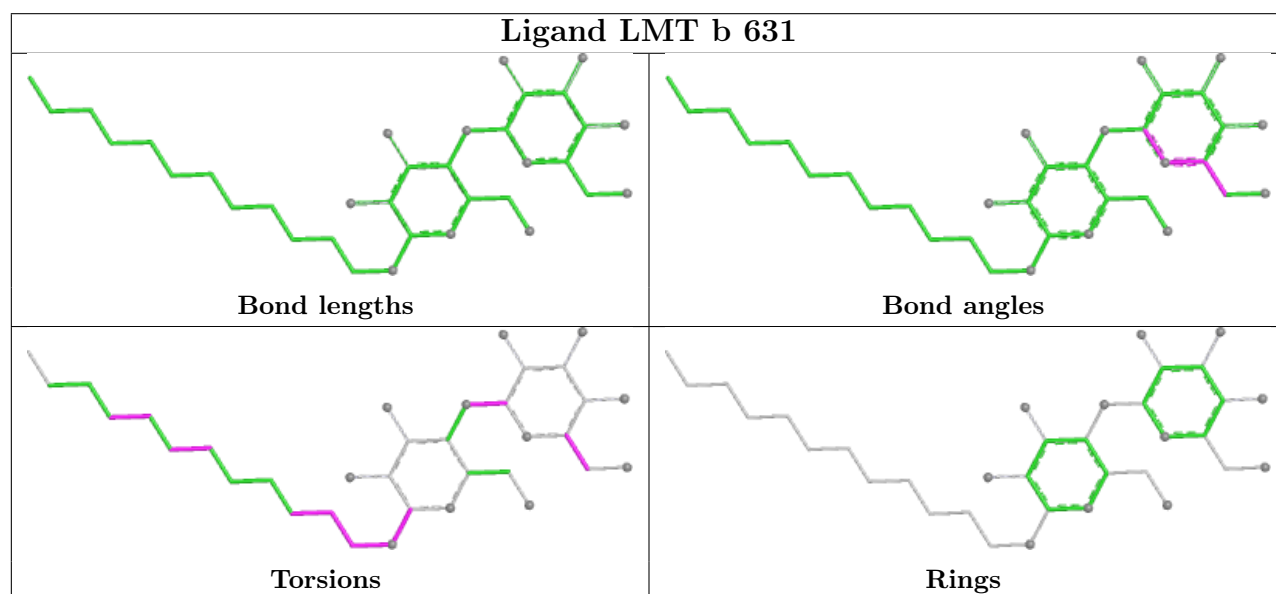
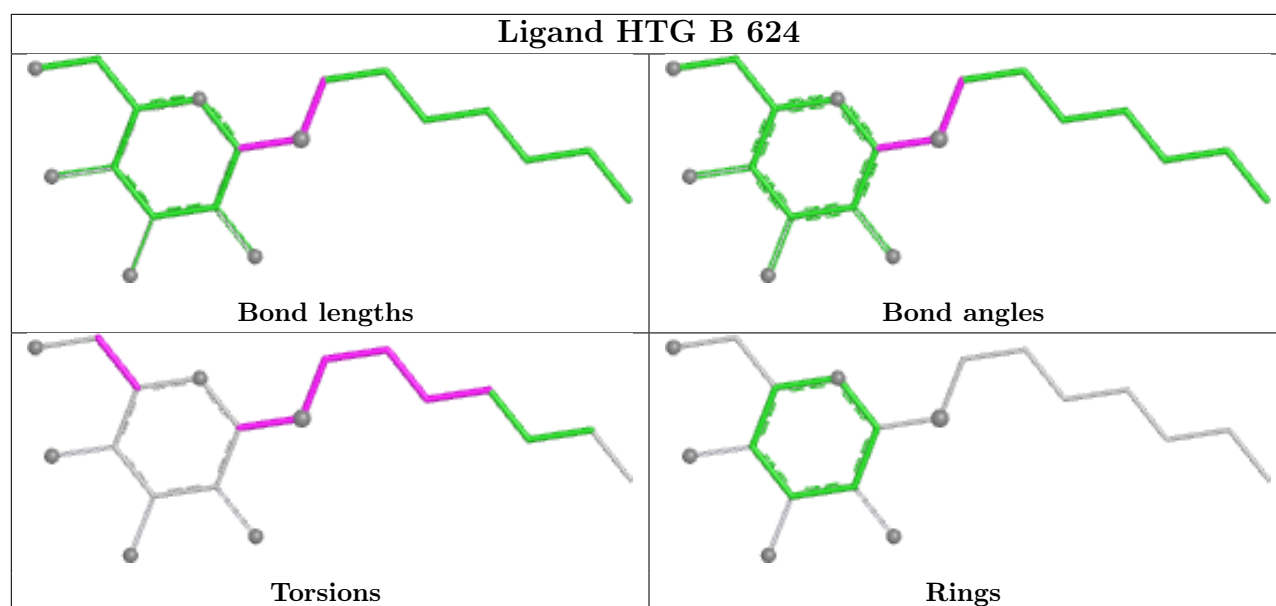
Ligand CLA A 1005

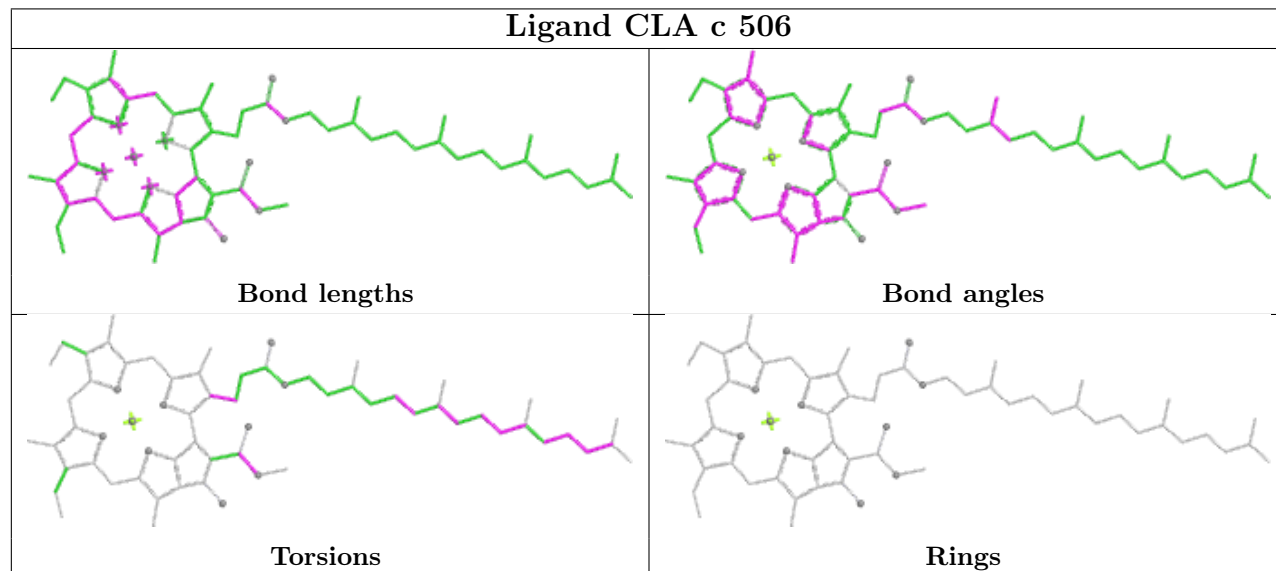
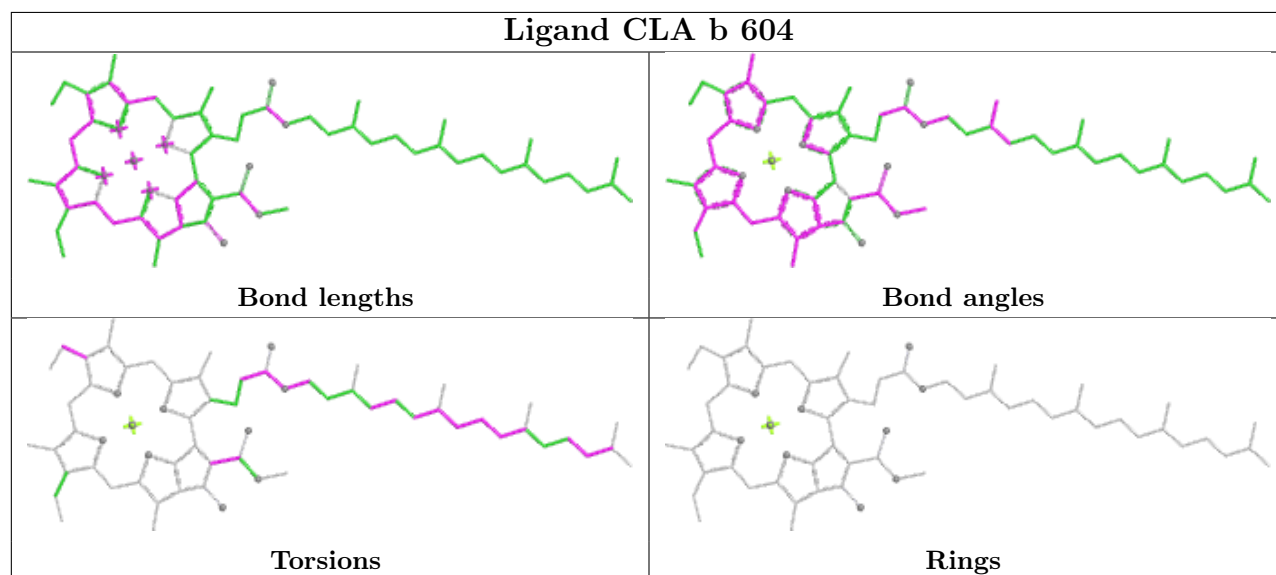
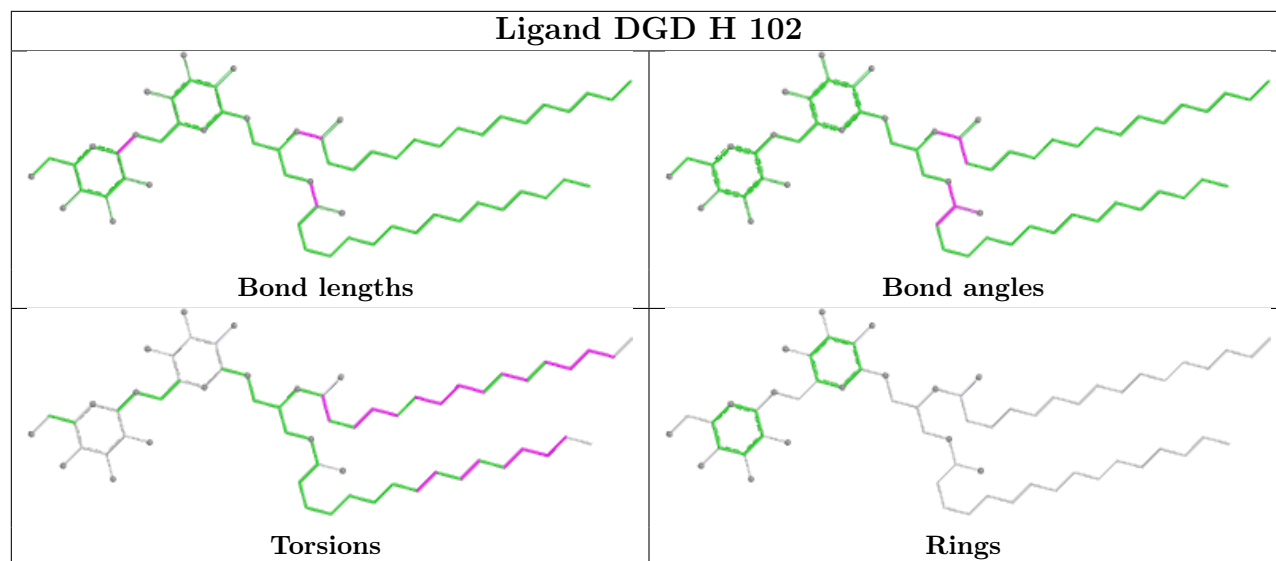


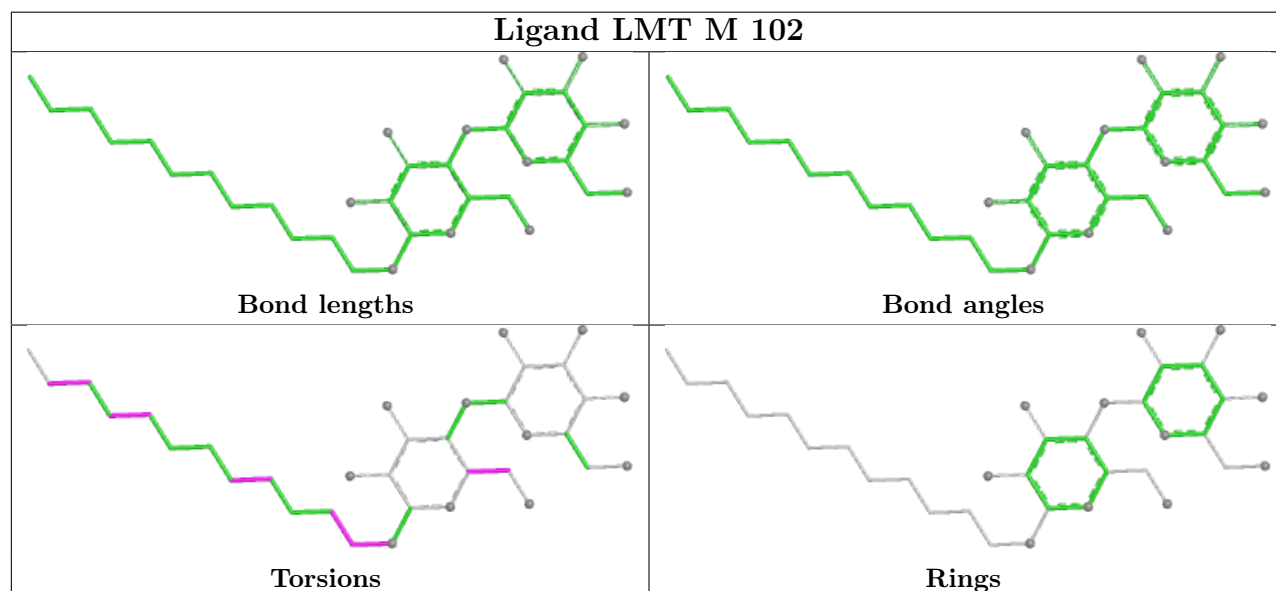
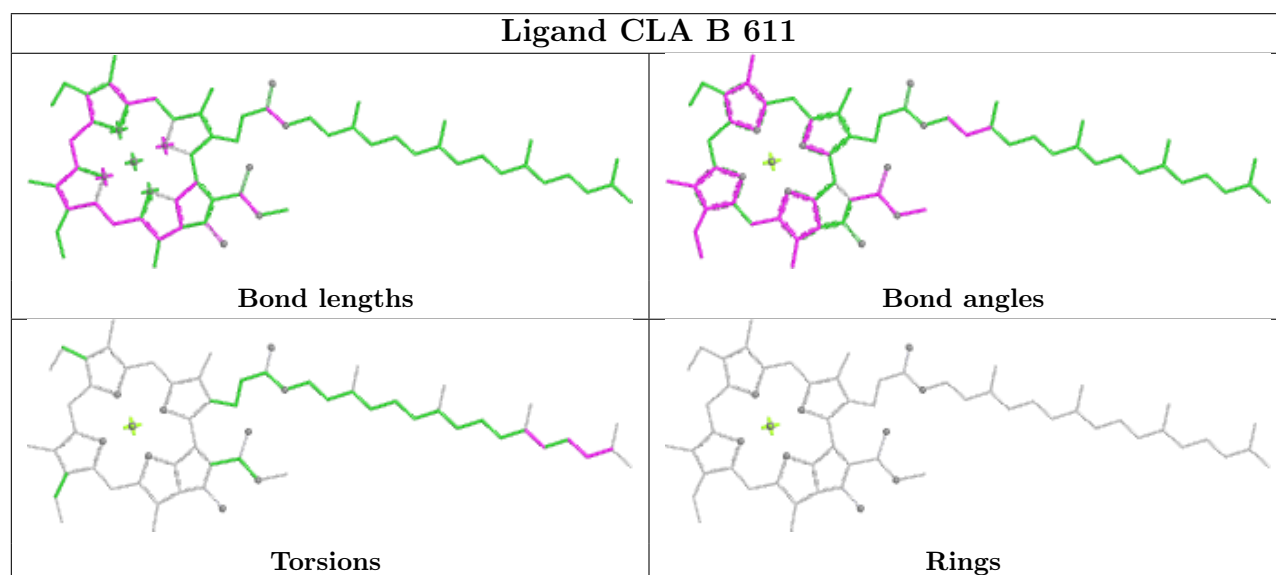
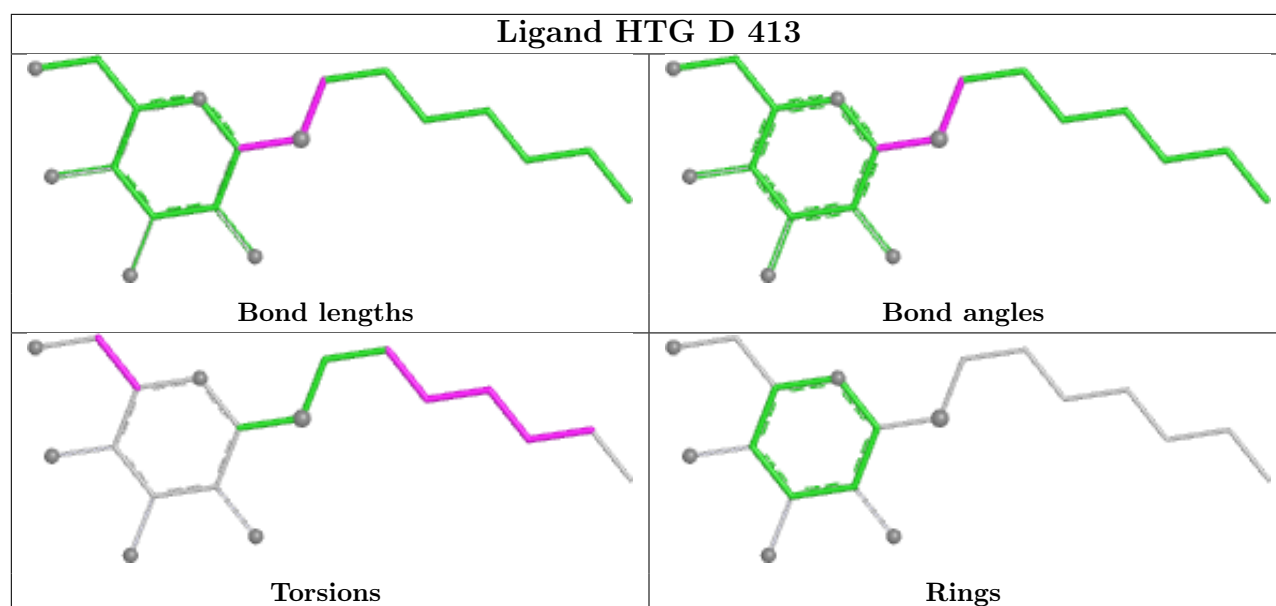
Ligand CLA d 402

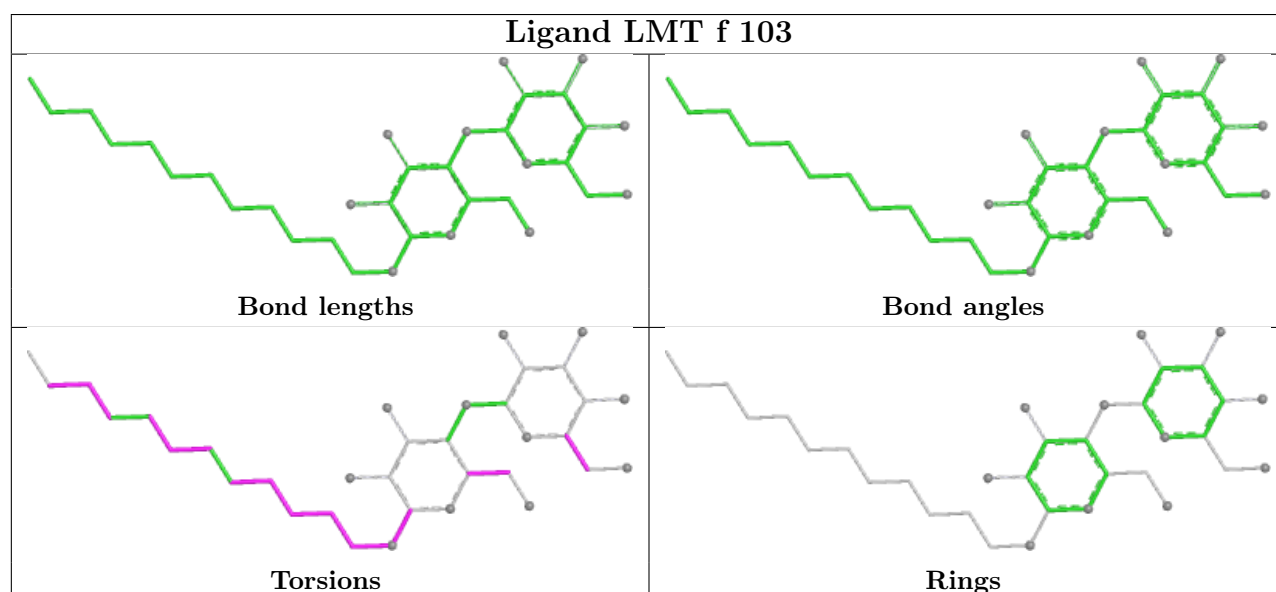
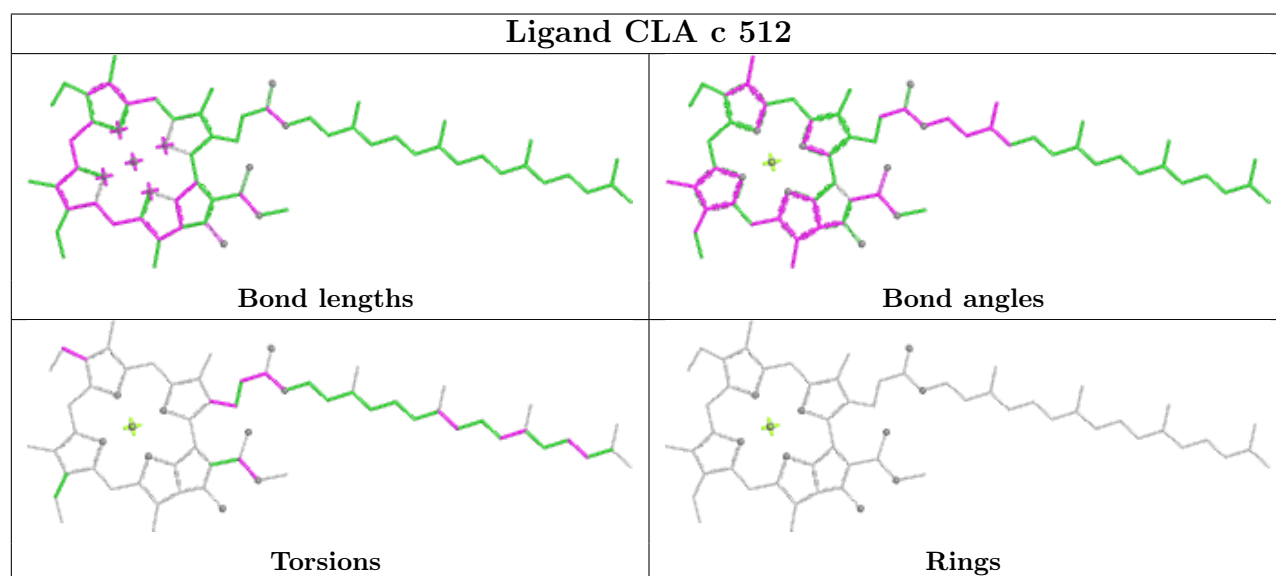
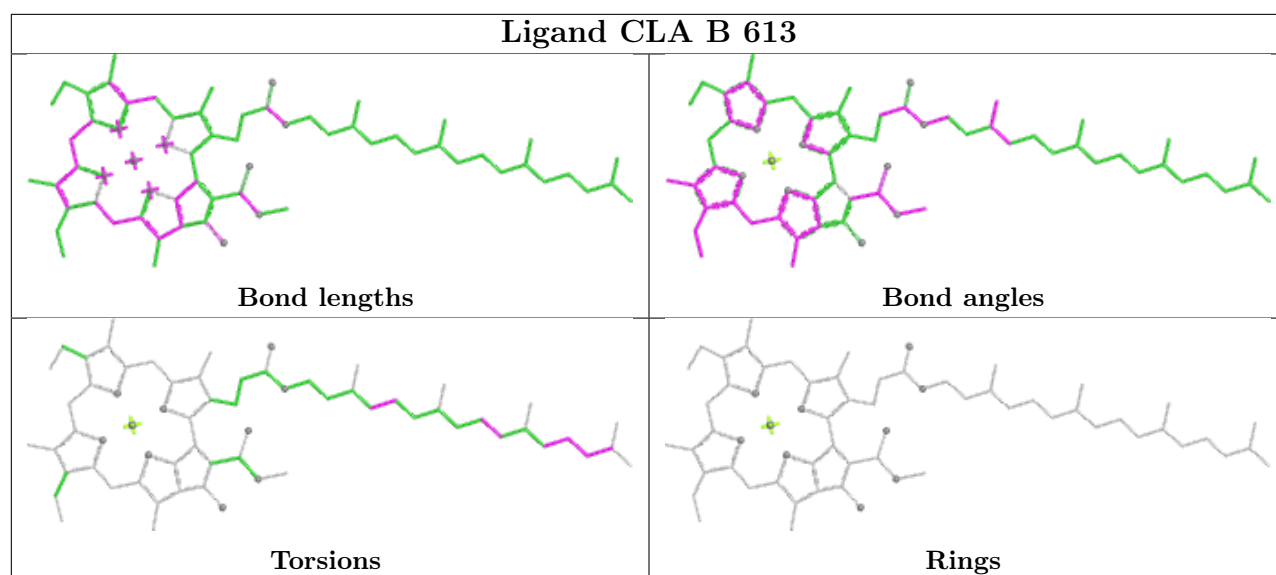


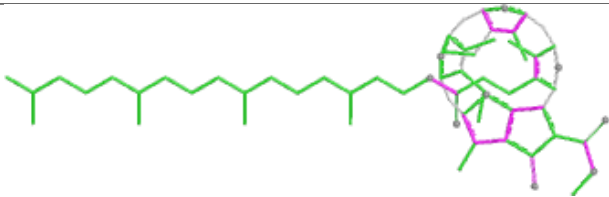
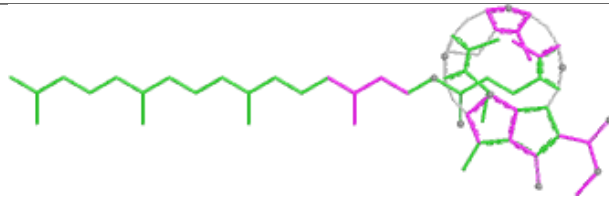
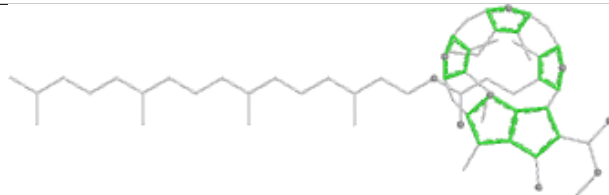


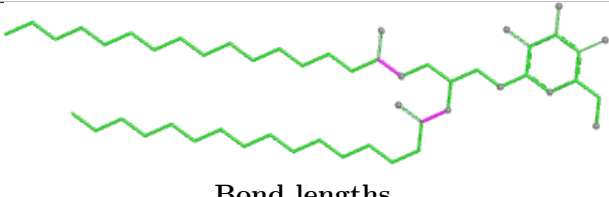
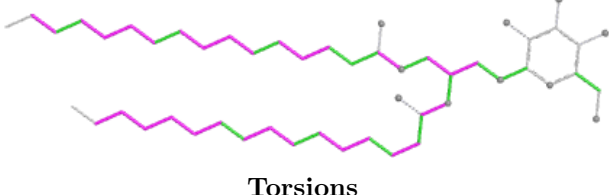
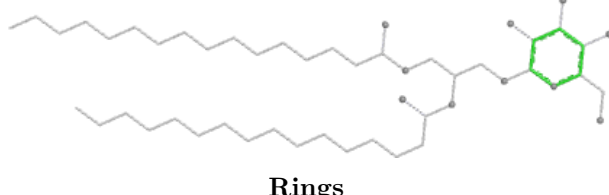


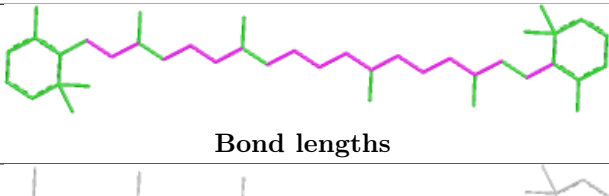
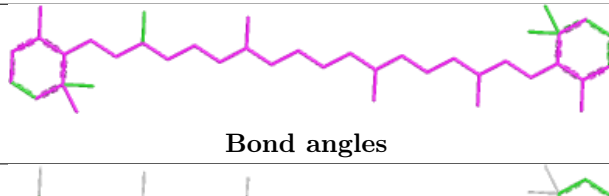
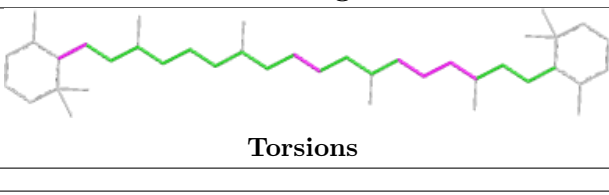
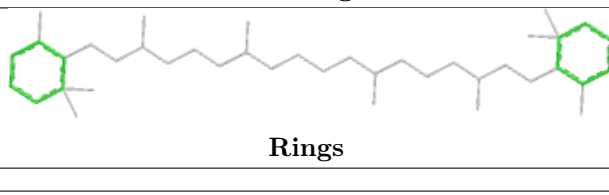


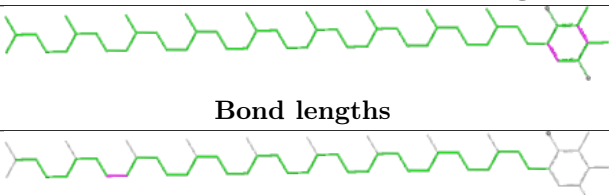
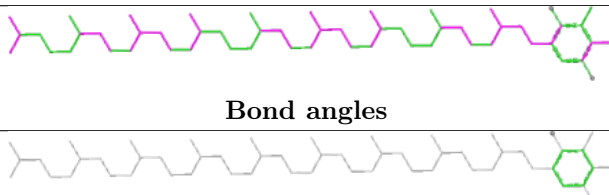
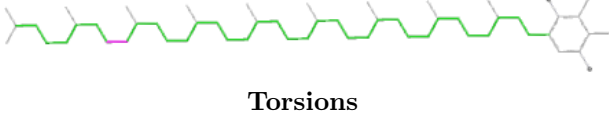
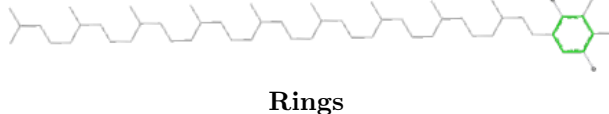


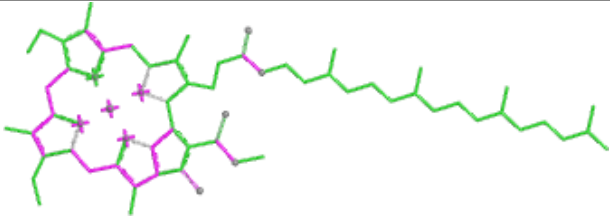
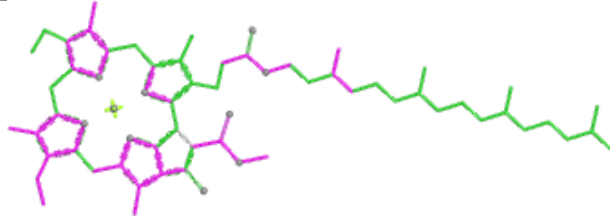
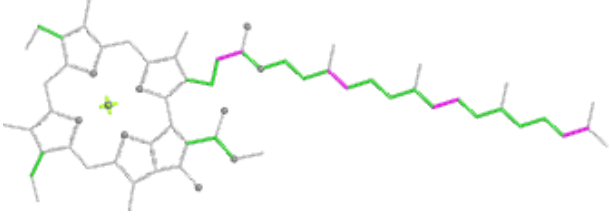
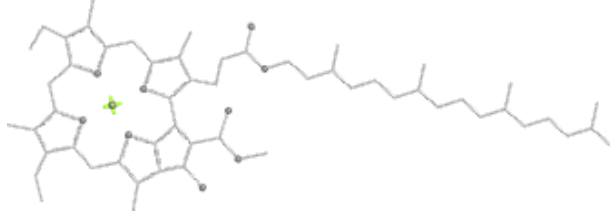
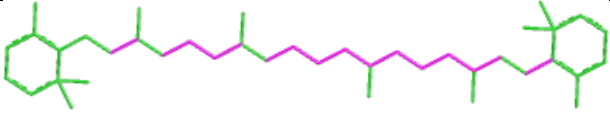
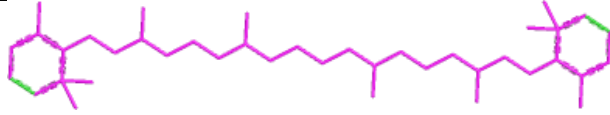
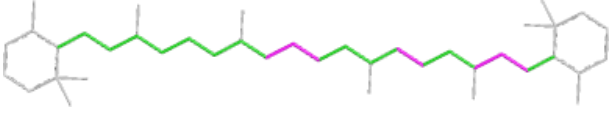
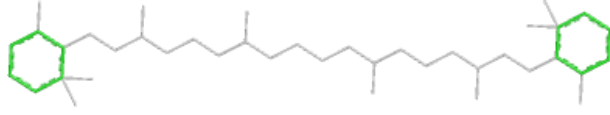
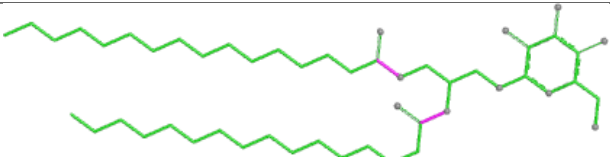
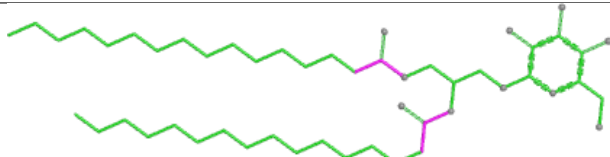
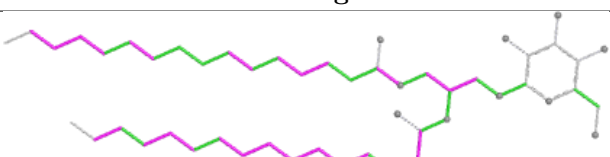
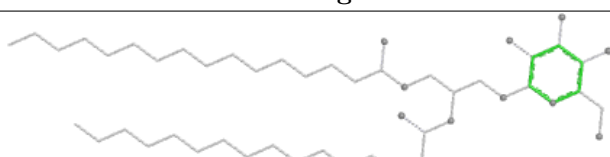


Ligand PHO a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

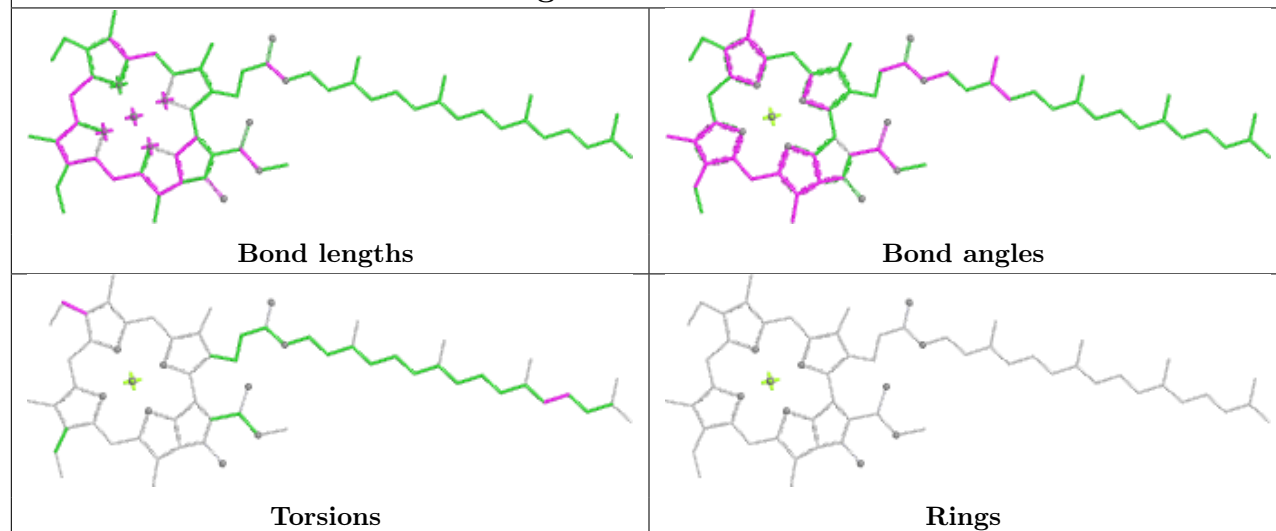
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

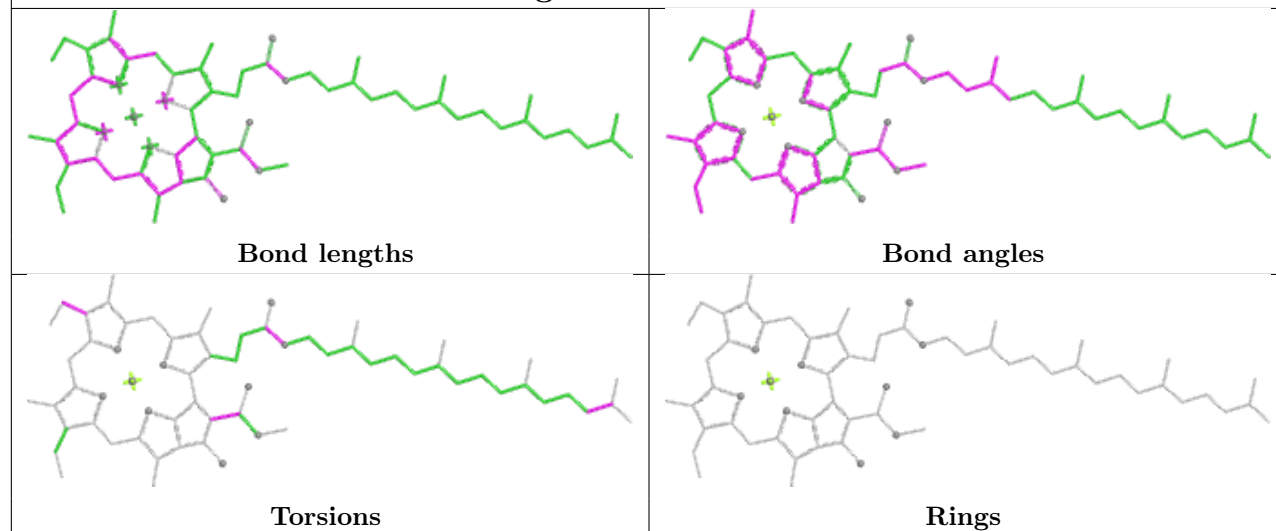
Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings

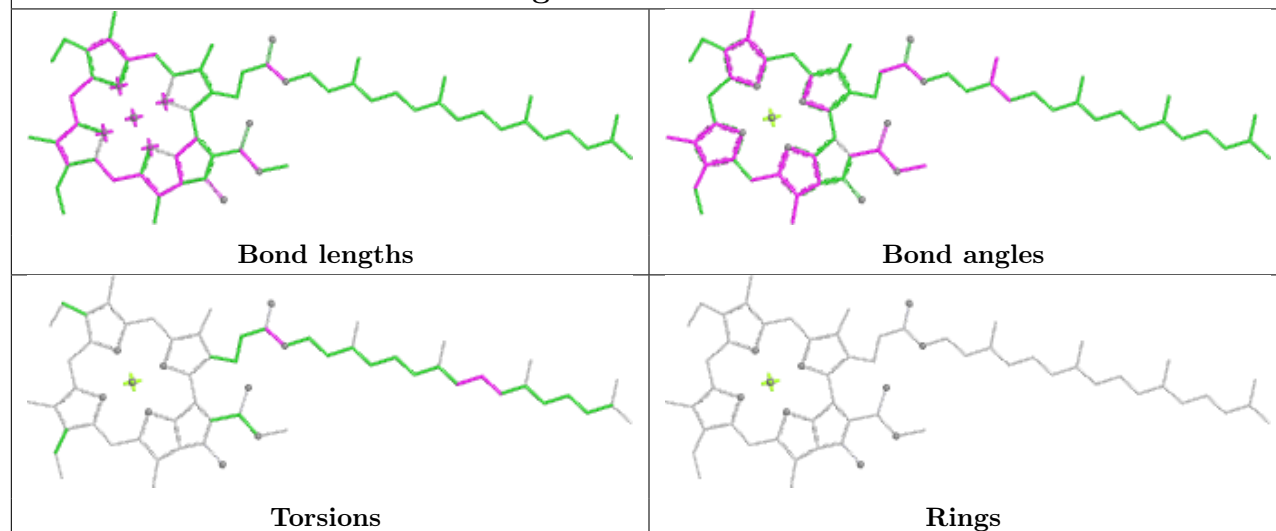
Ligand CLA c 501

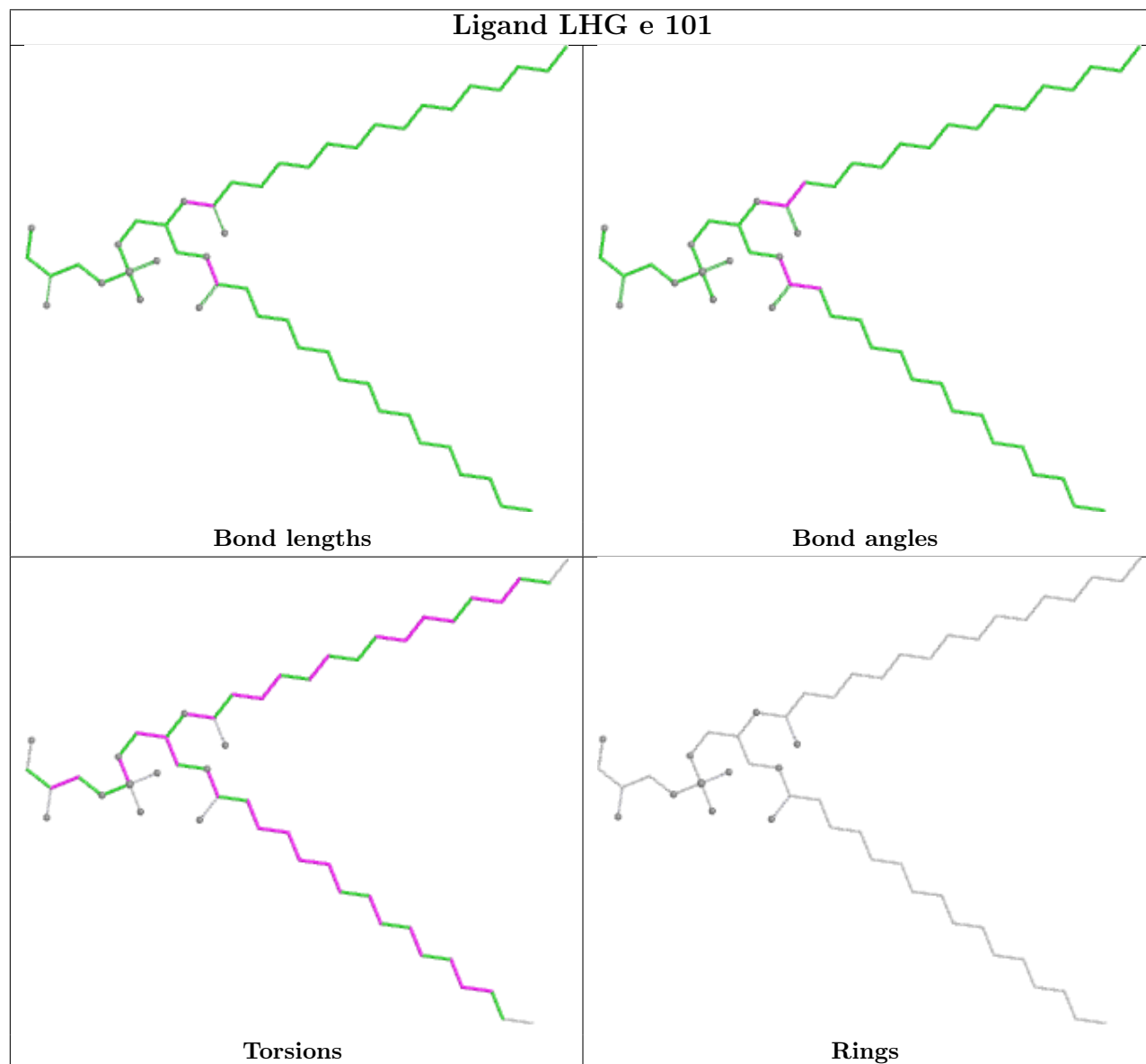
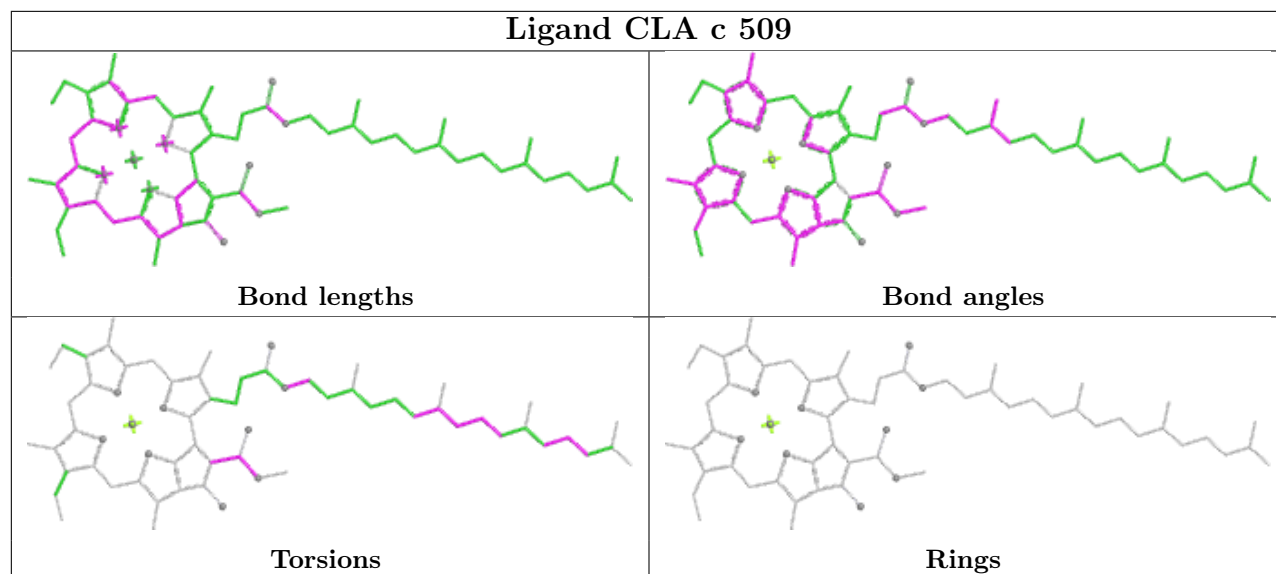


Ligand CLA b 610

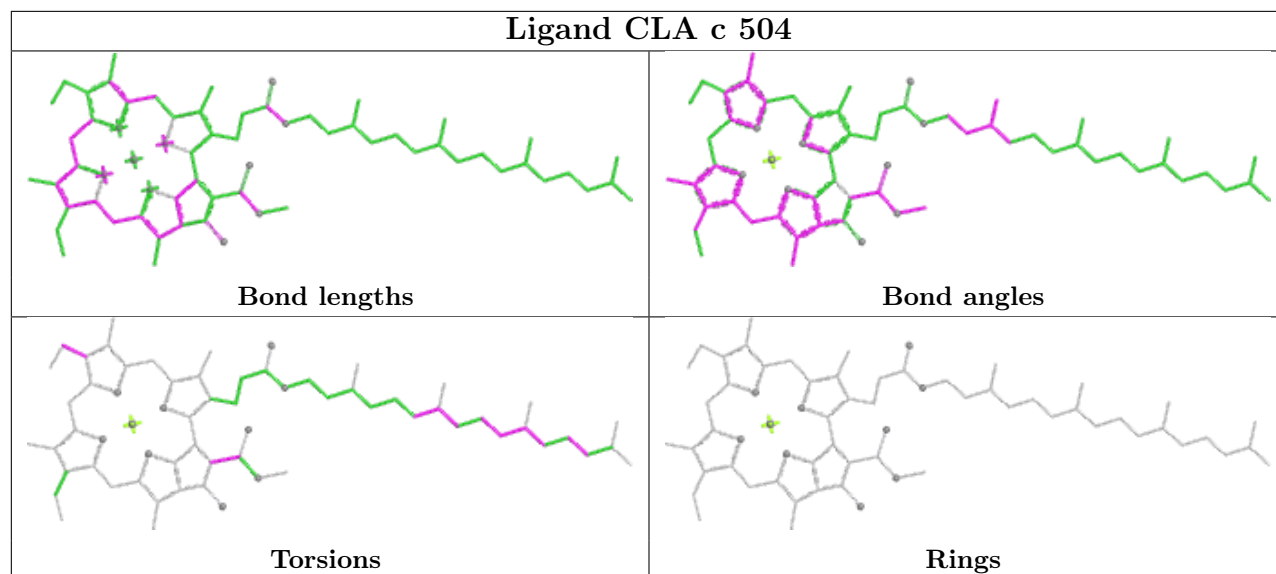


Ligand CLA B 612

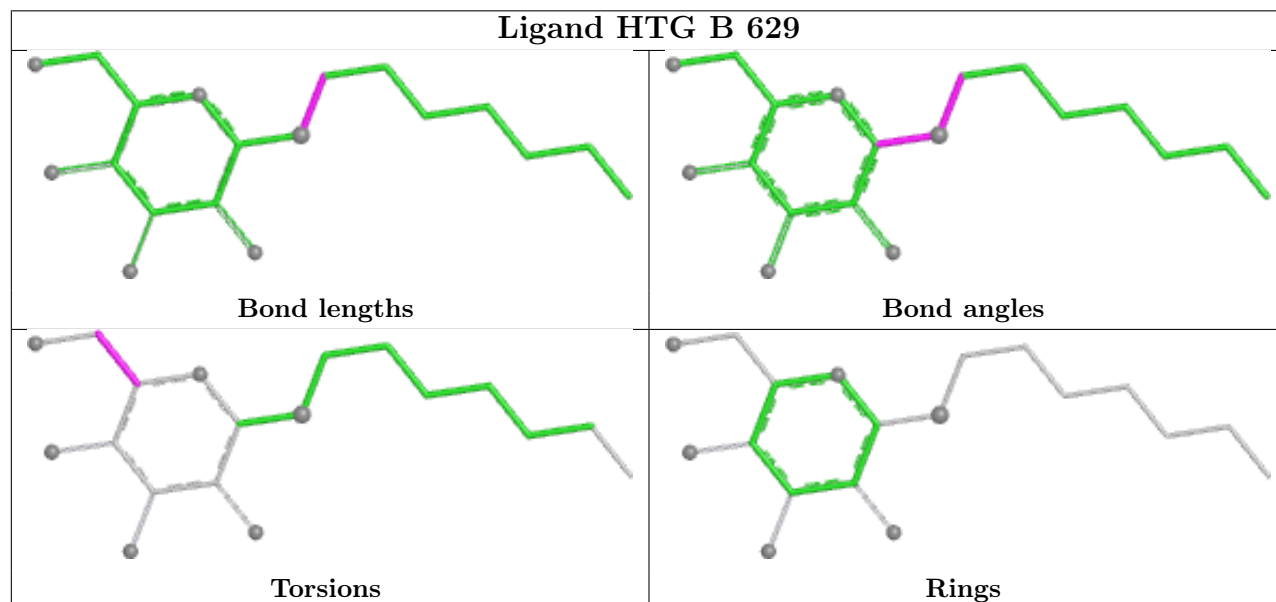




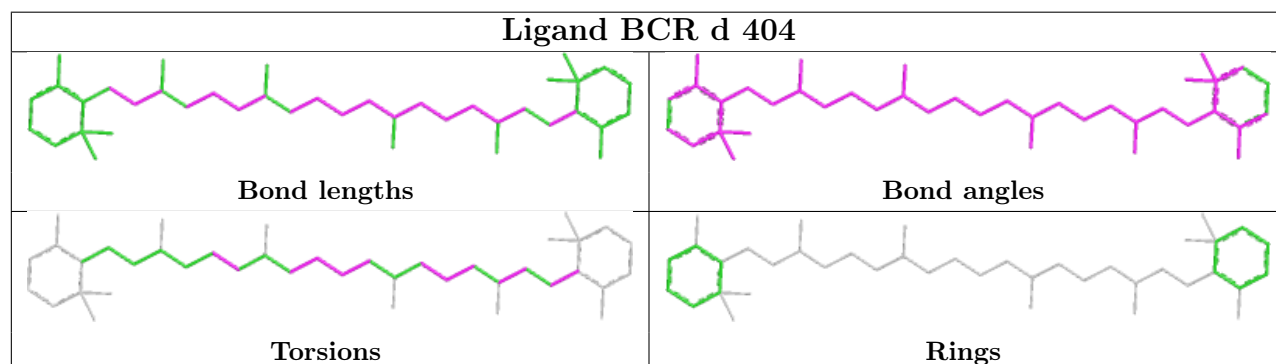
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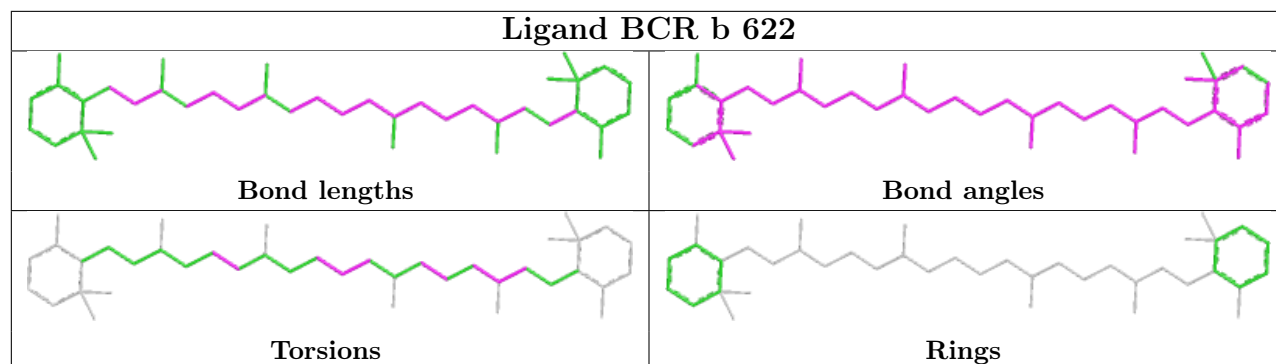
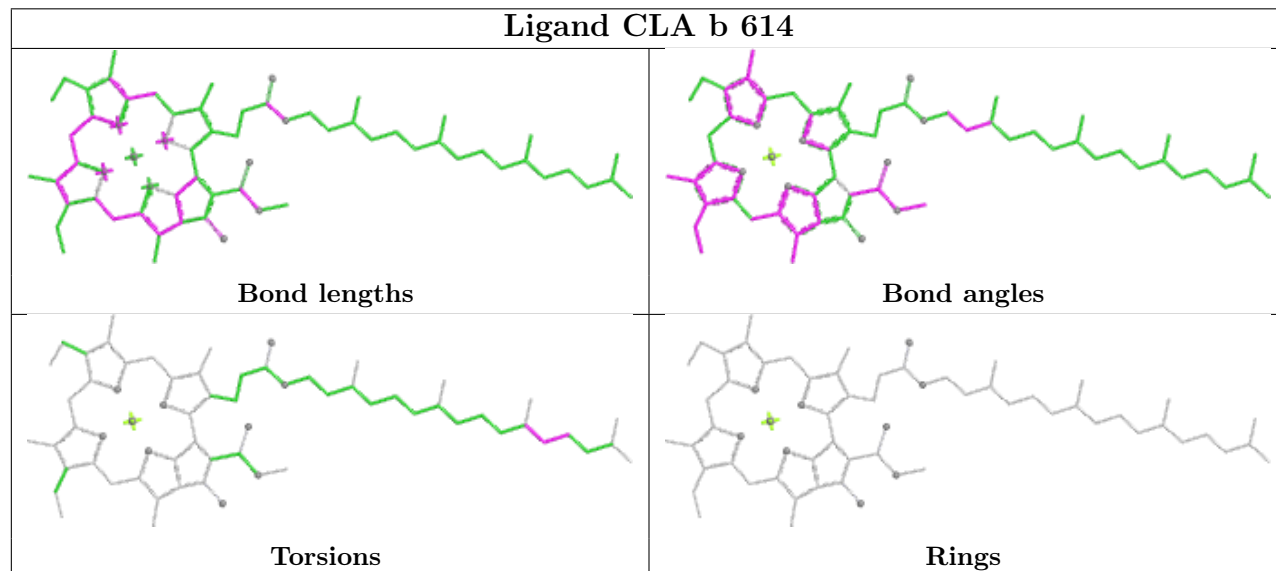
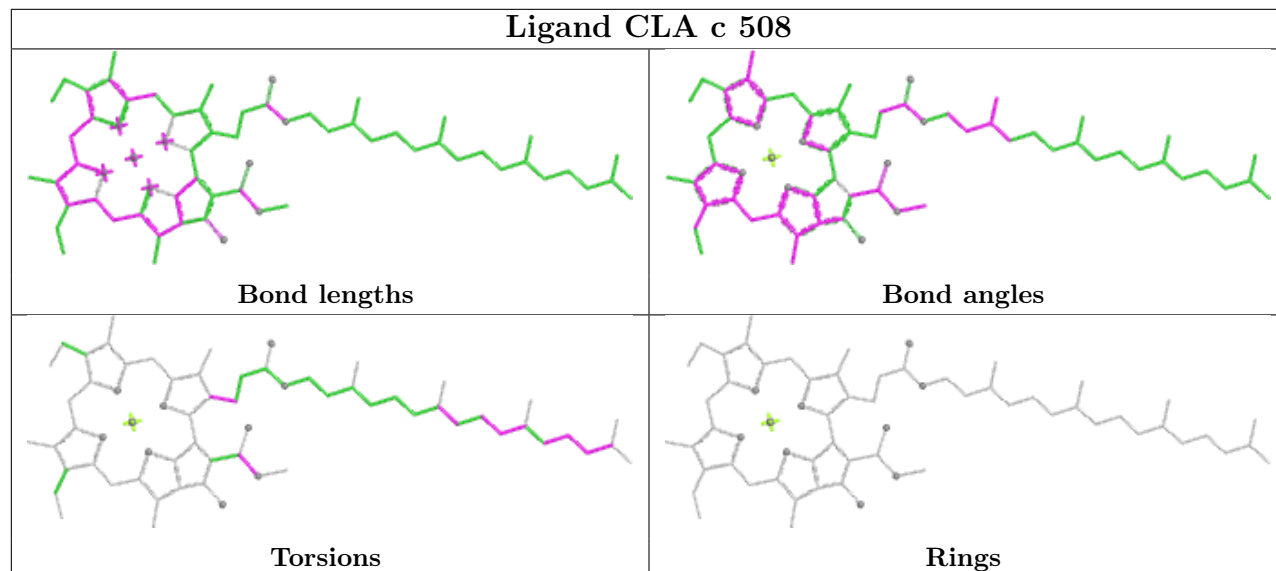


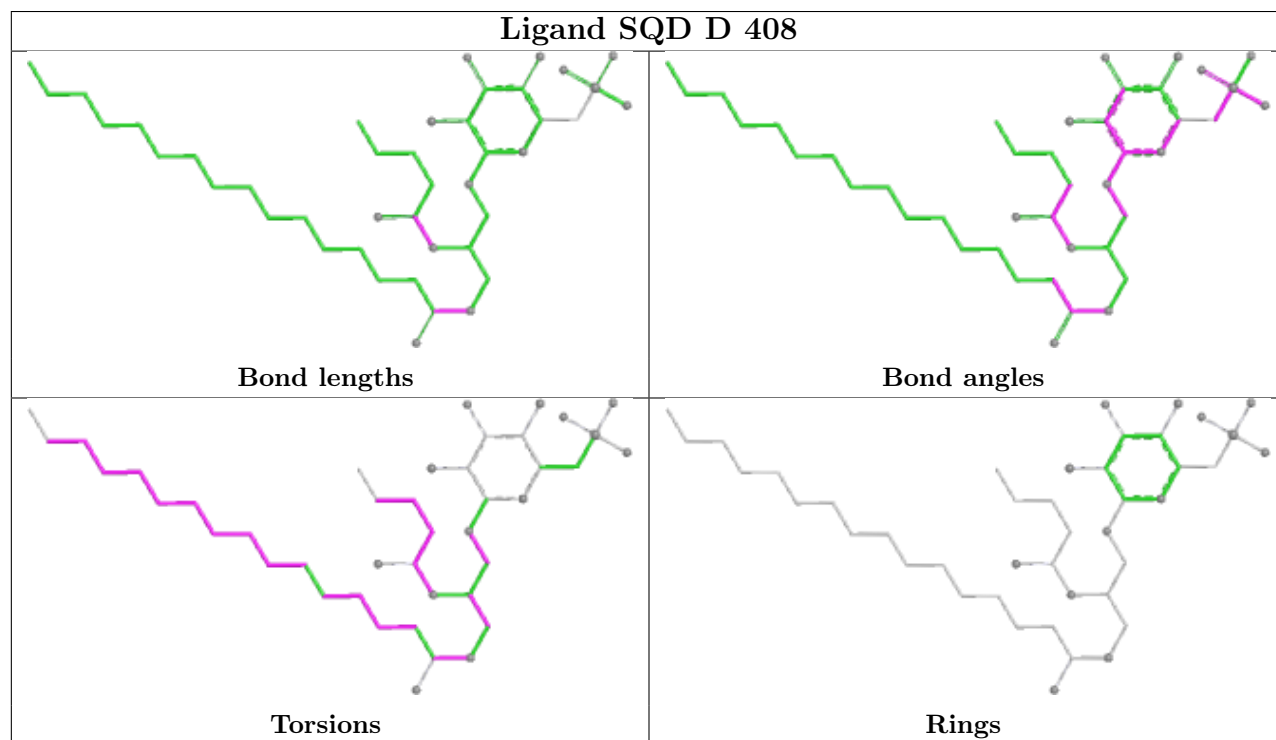
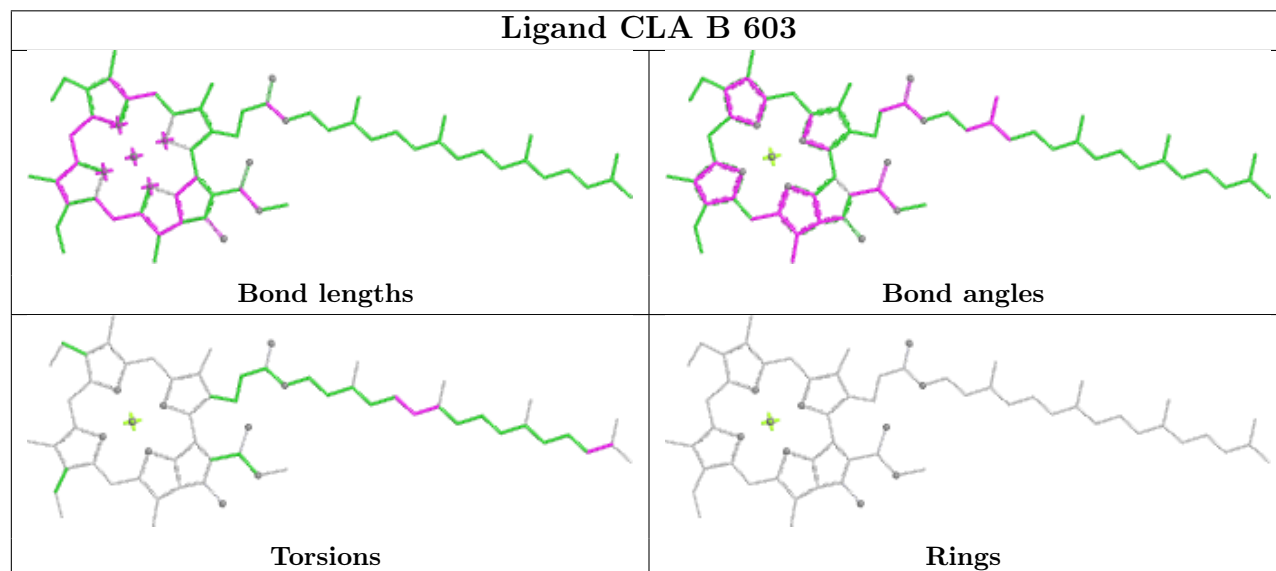
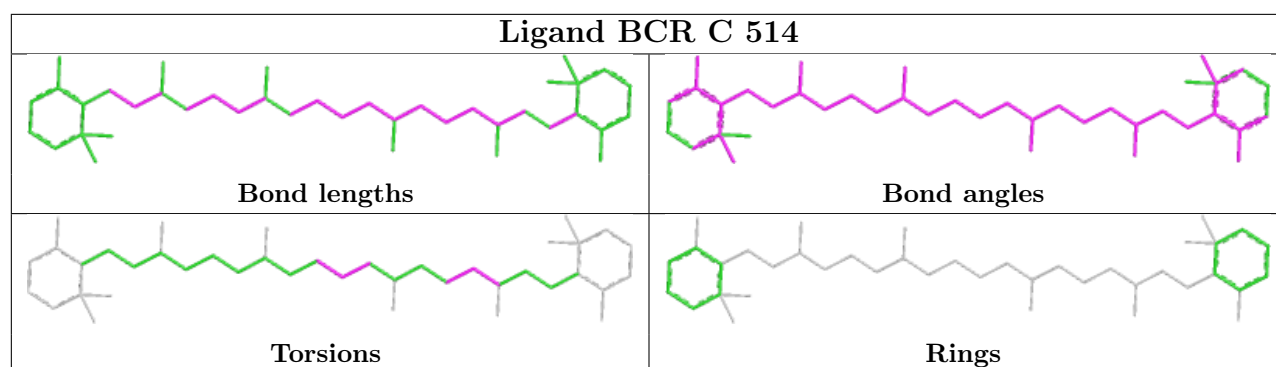
Ligand HTG B 629

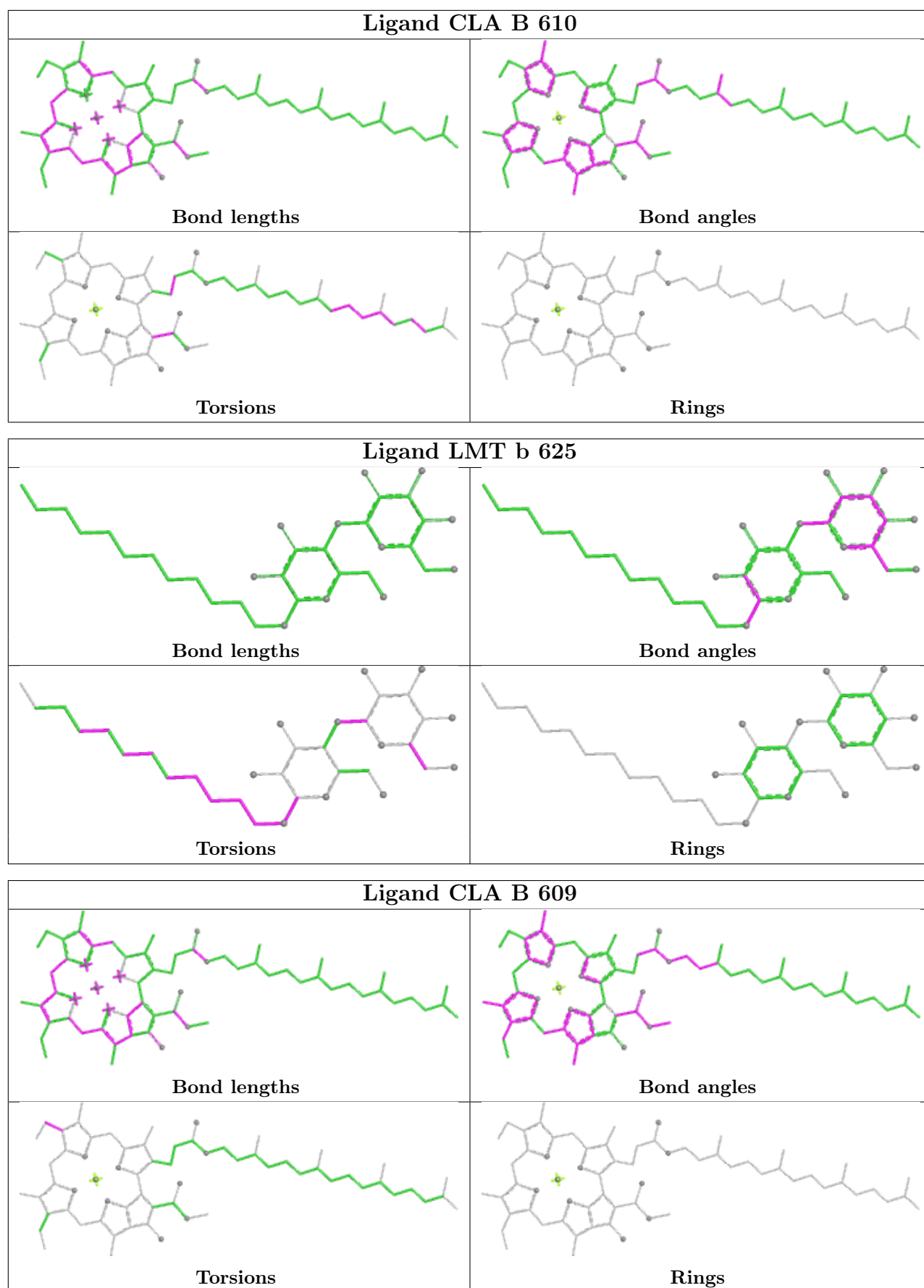


Ligand BCR d 404

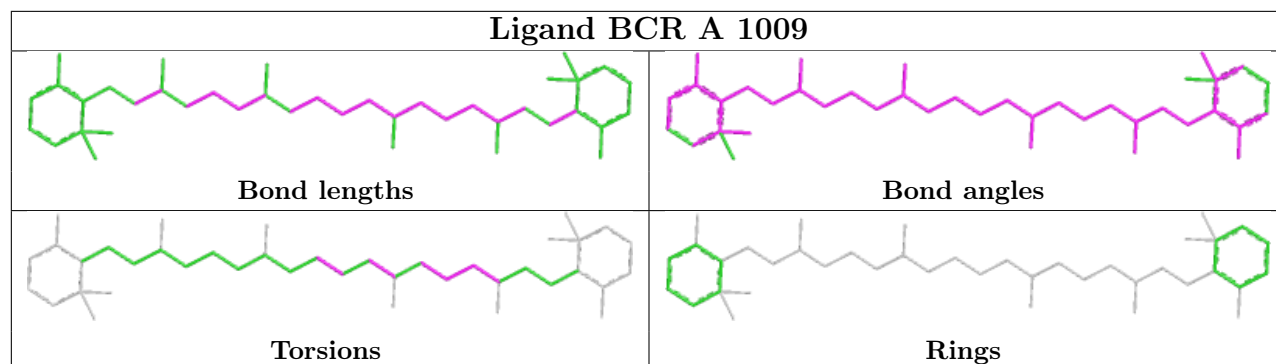


Ligand BCR b 622**Ligand CLA b 614****Ligand CLA c 508**

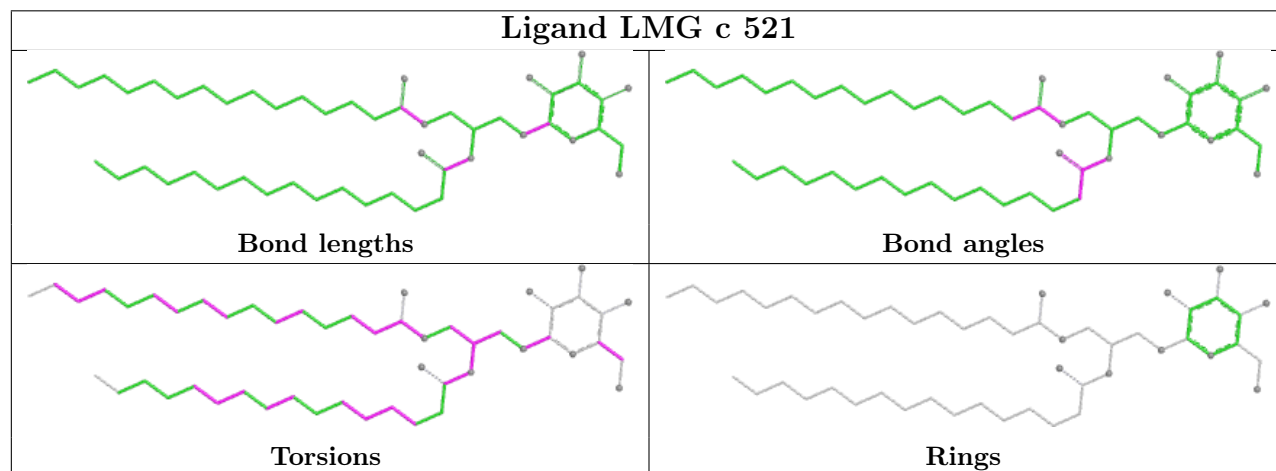




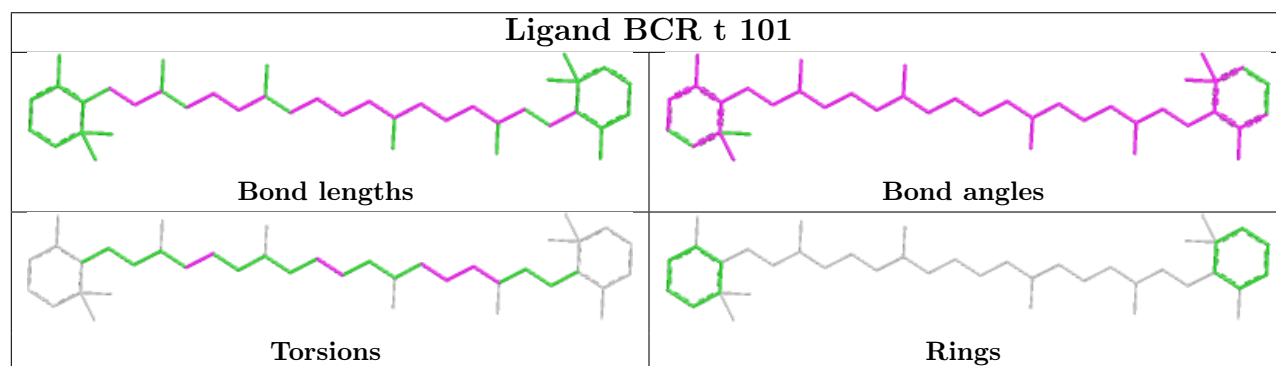
Ligand BCR A 1009



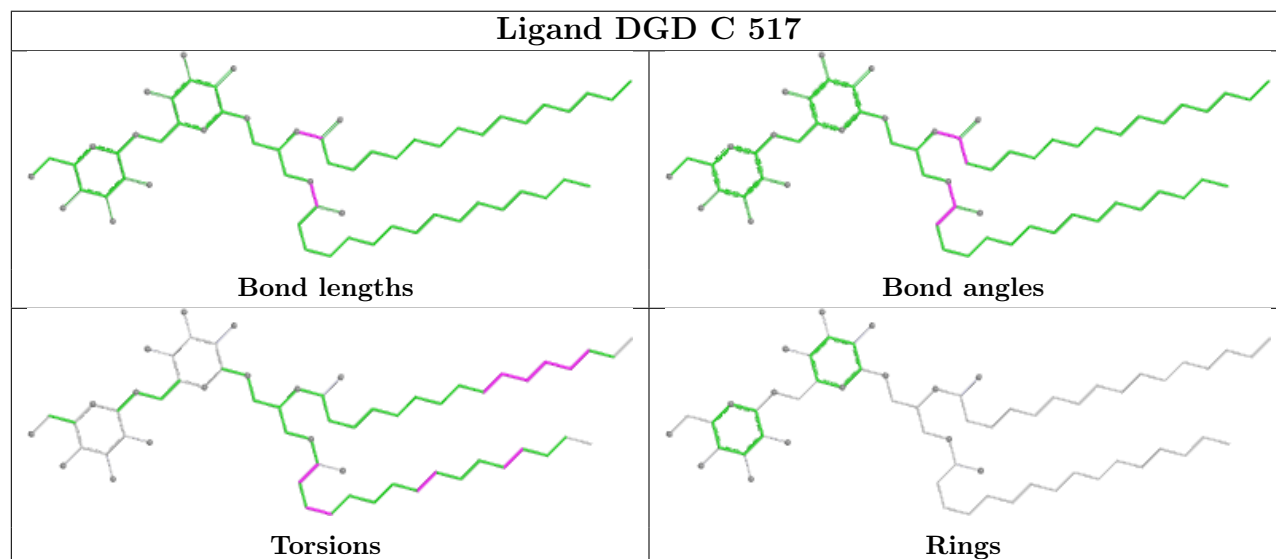
Ligand LMG c 521



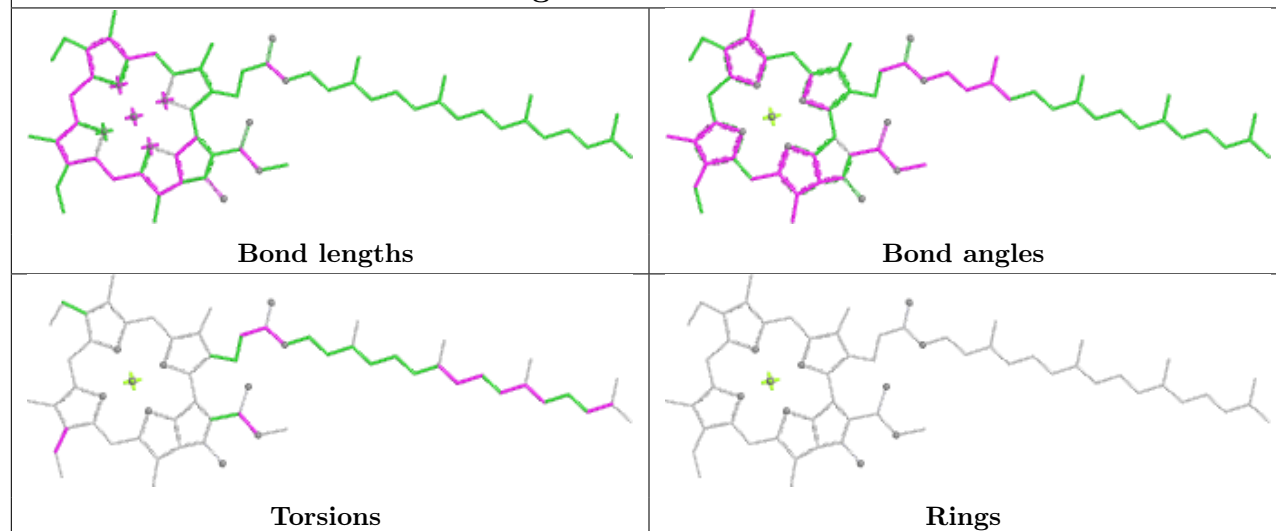
Ligand BCR t 101



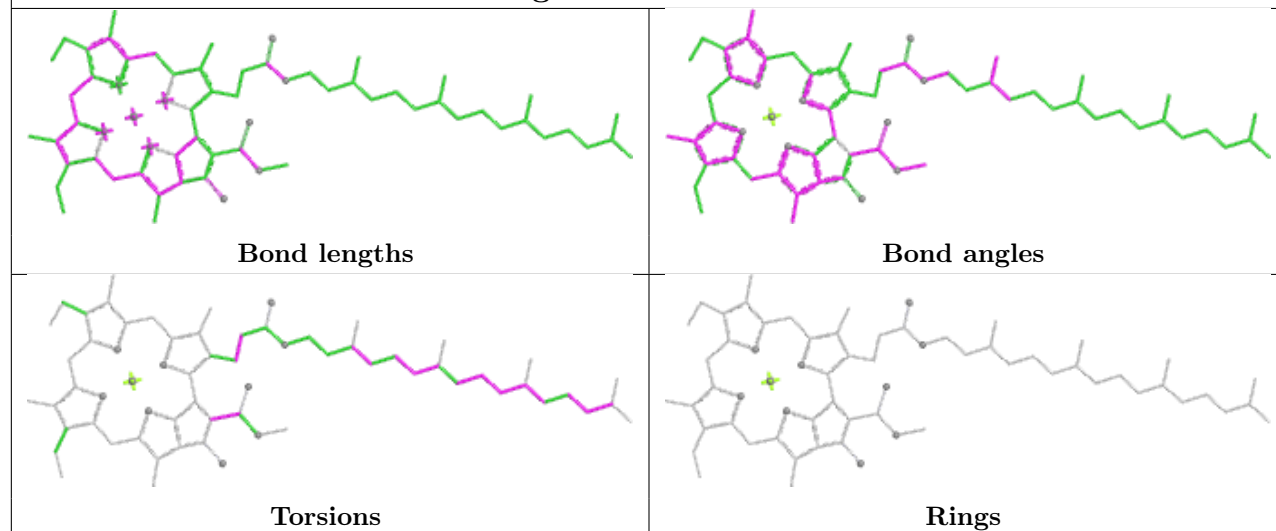
Ligand DGD C 517



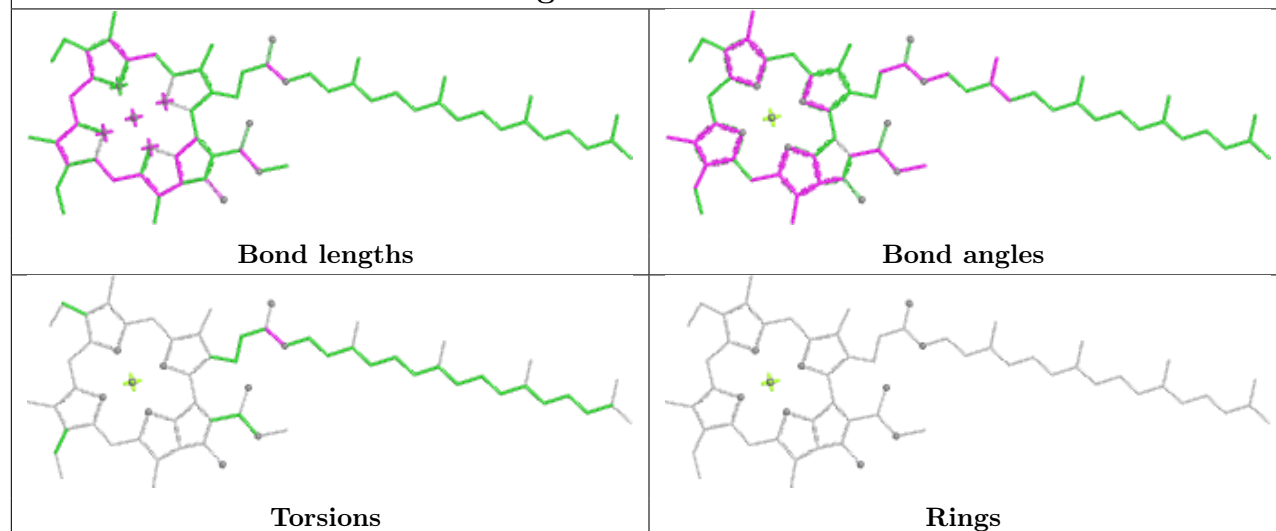
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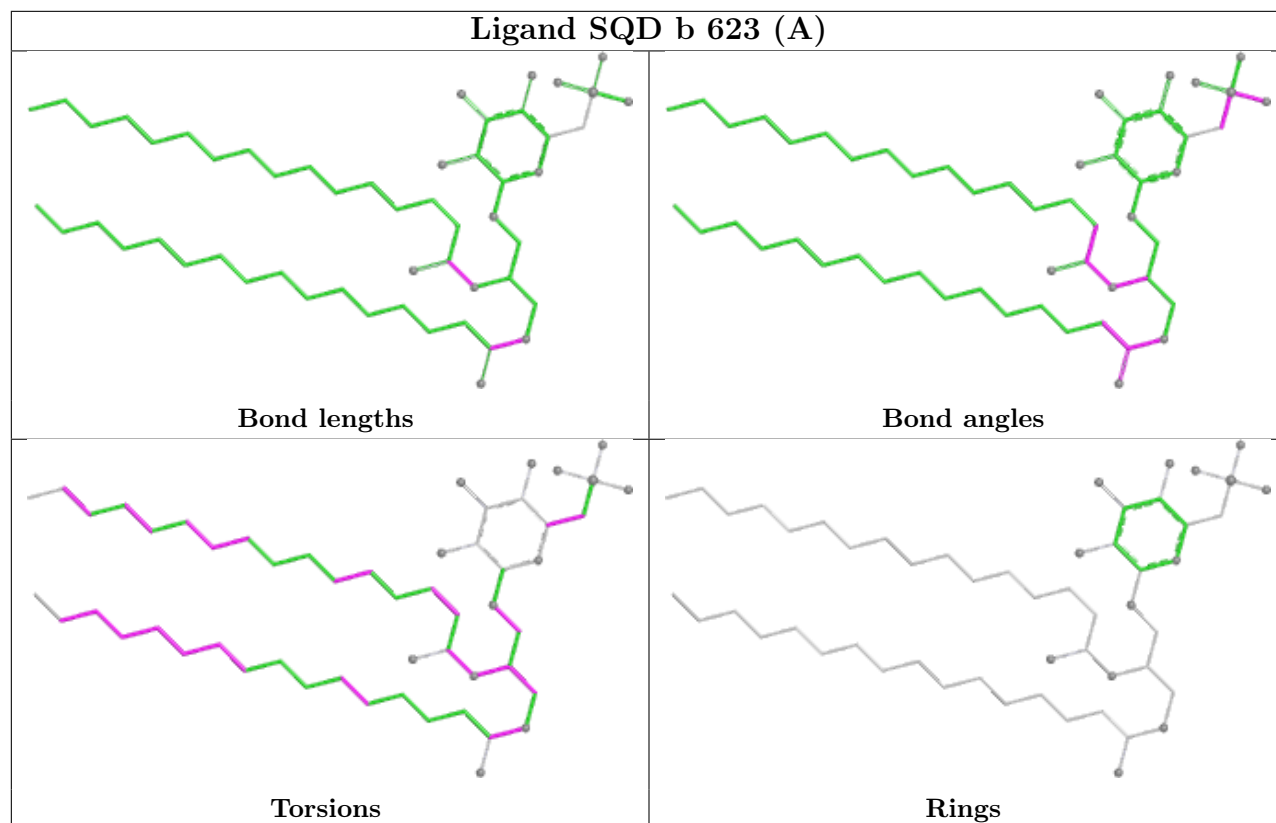
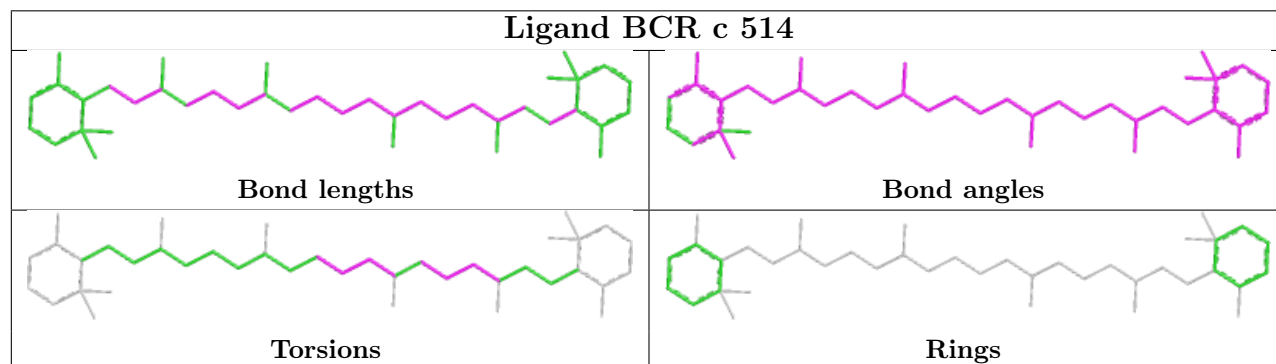
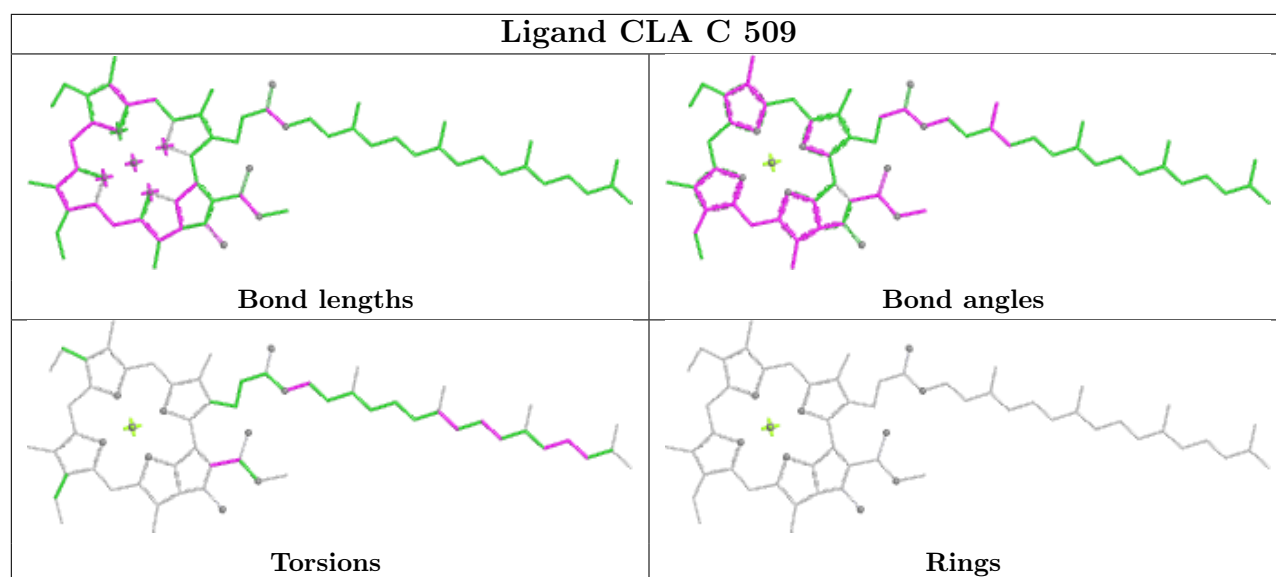


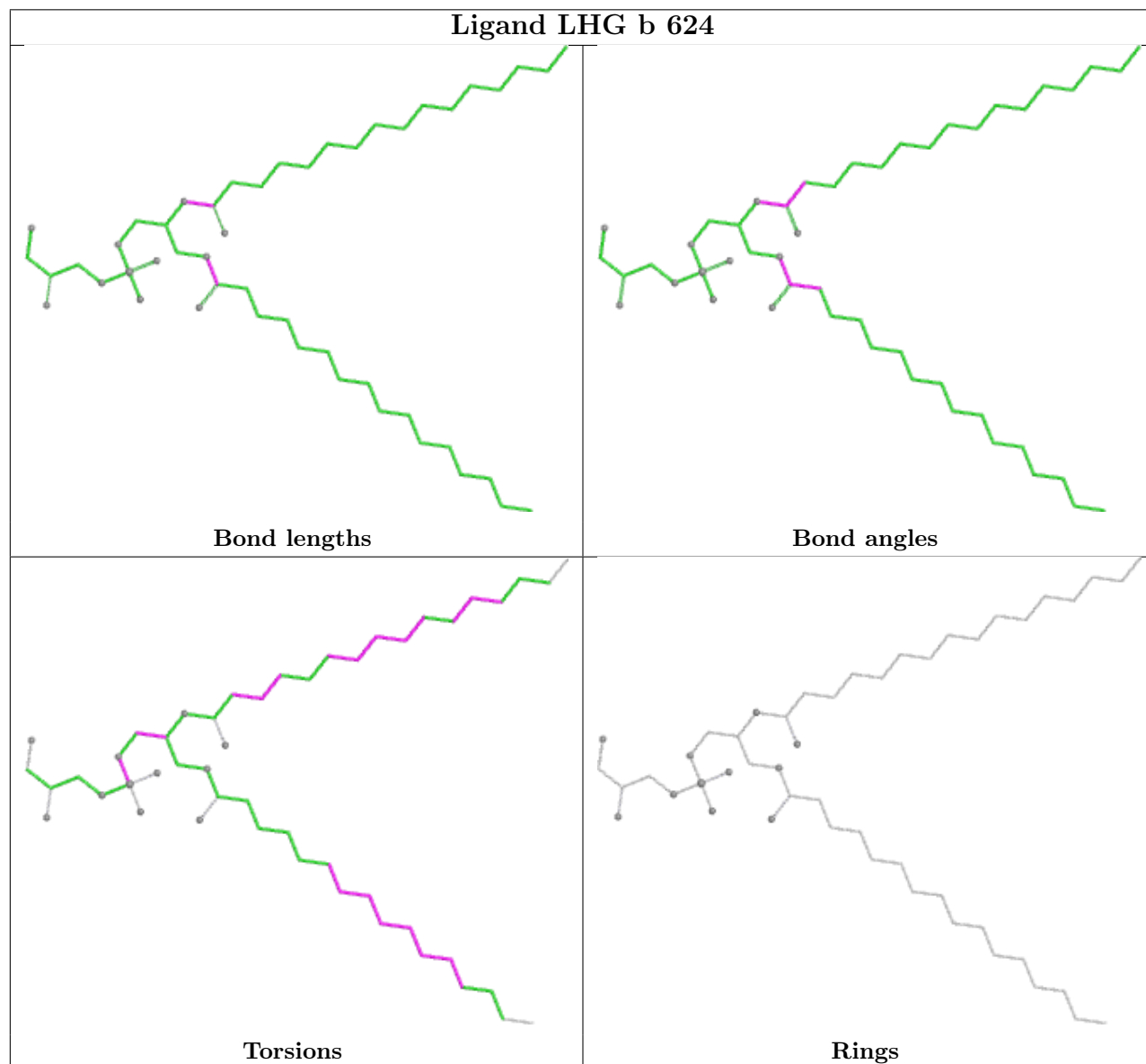
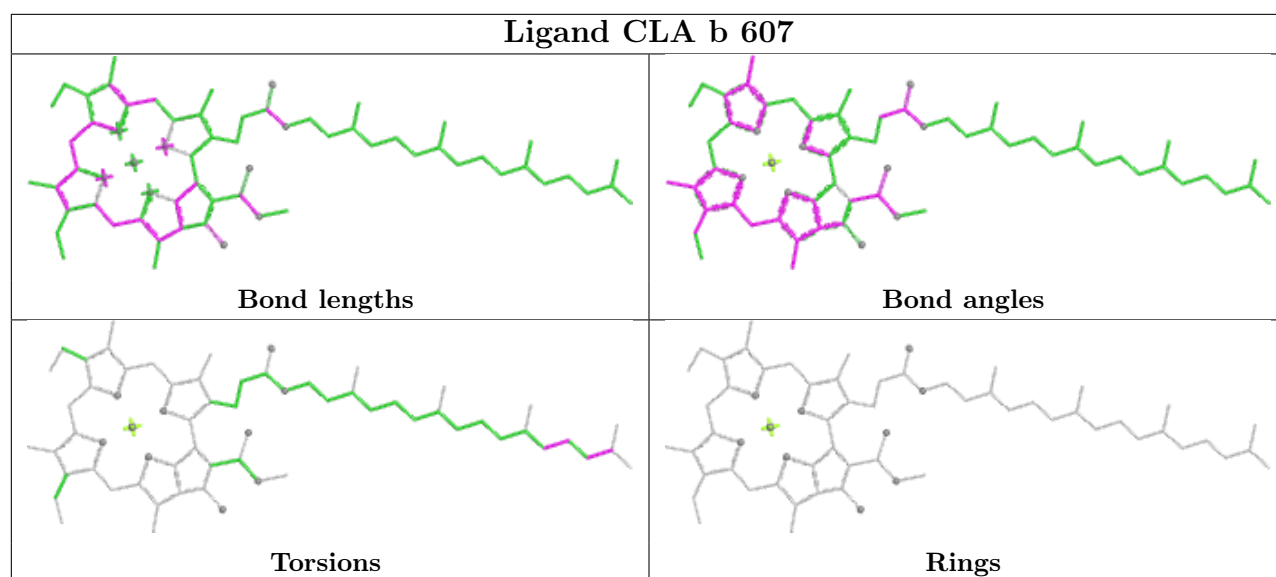
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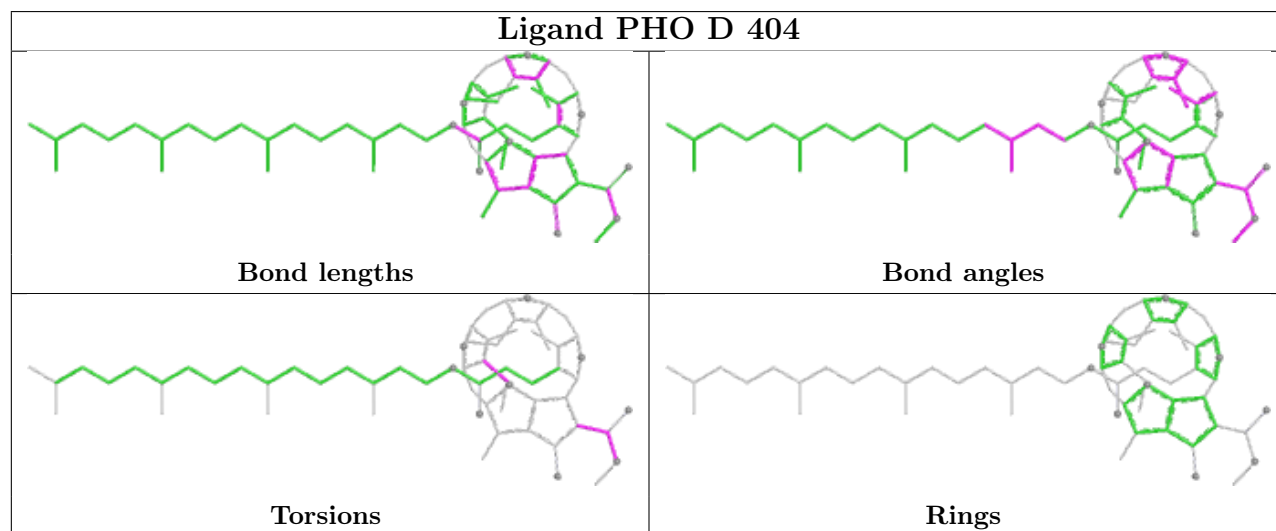
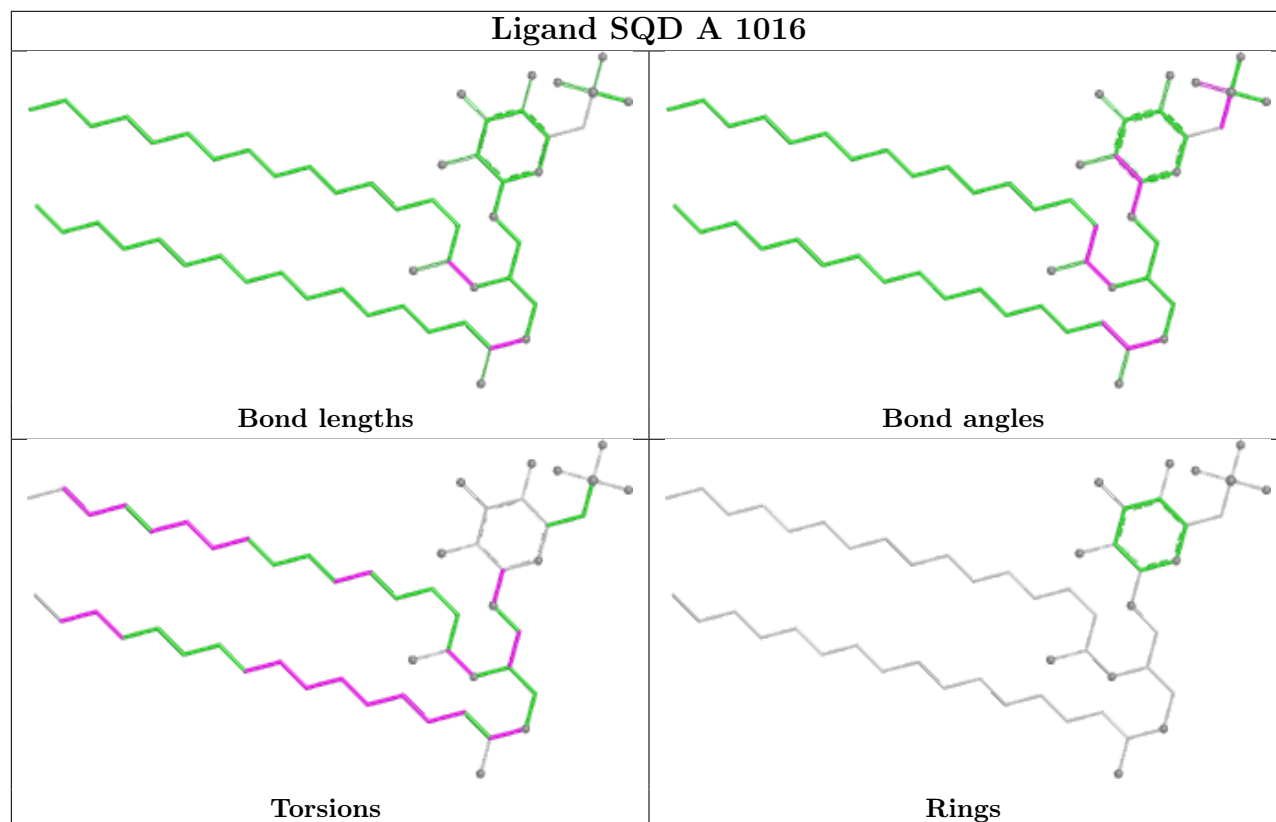


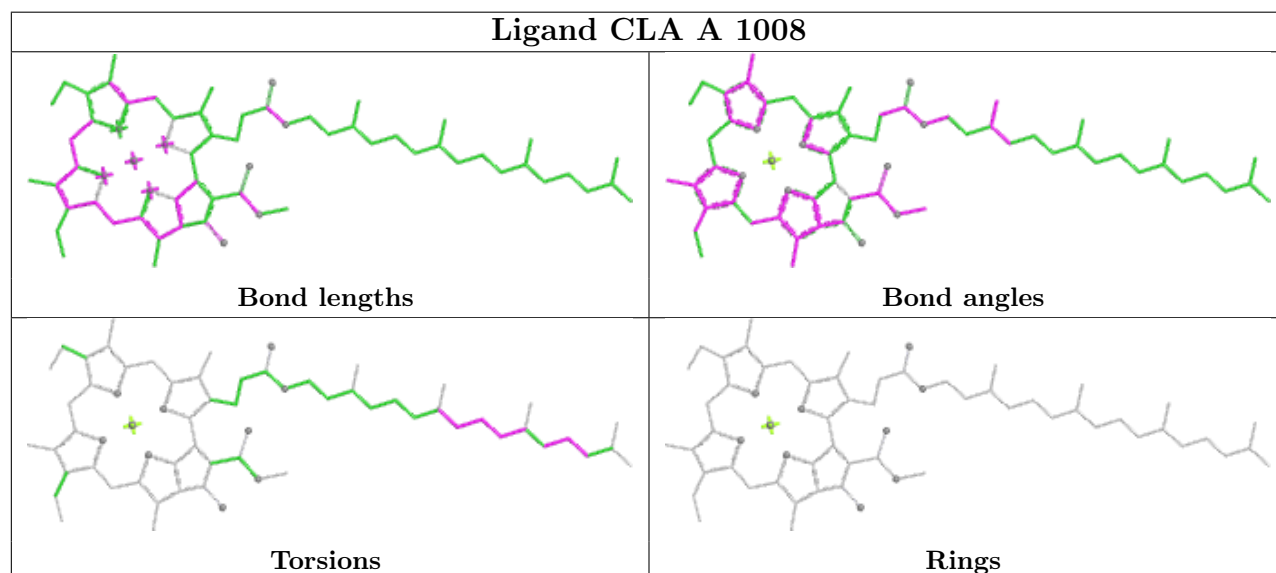
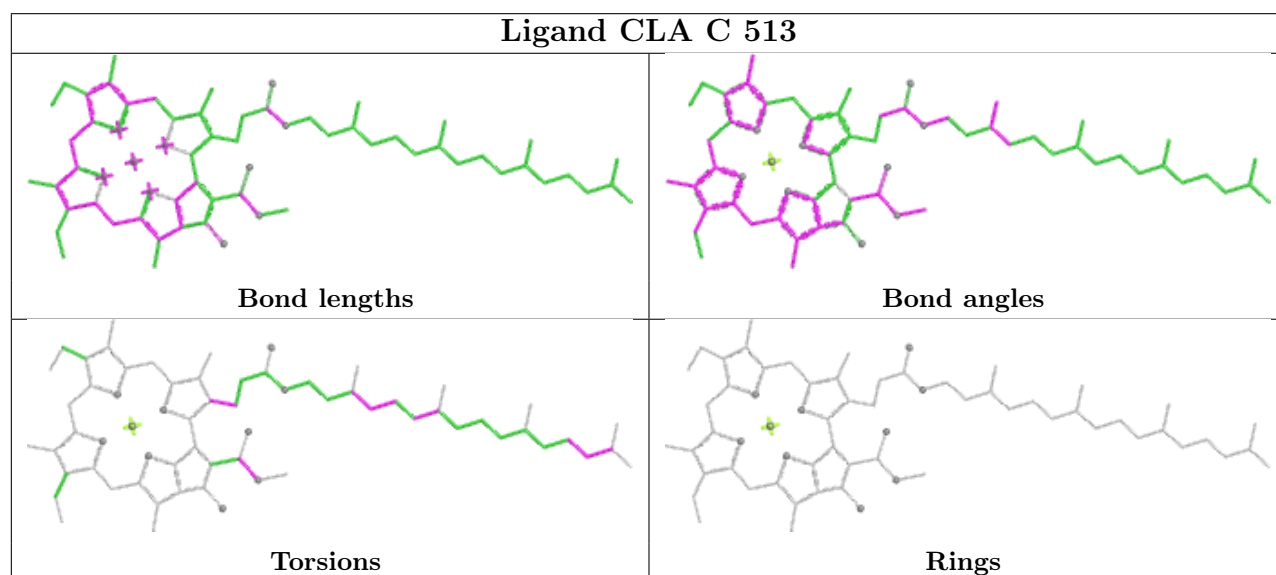
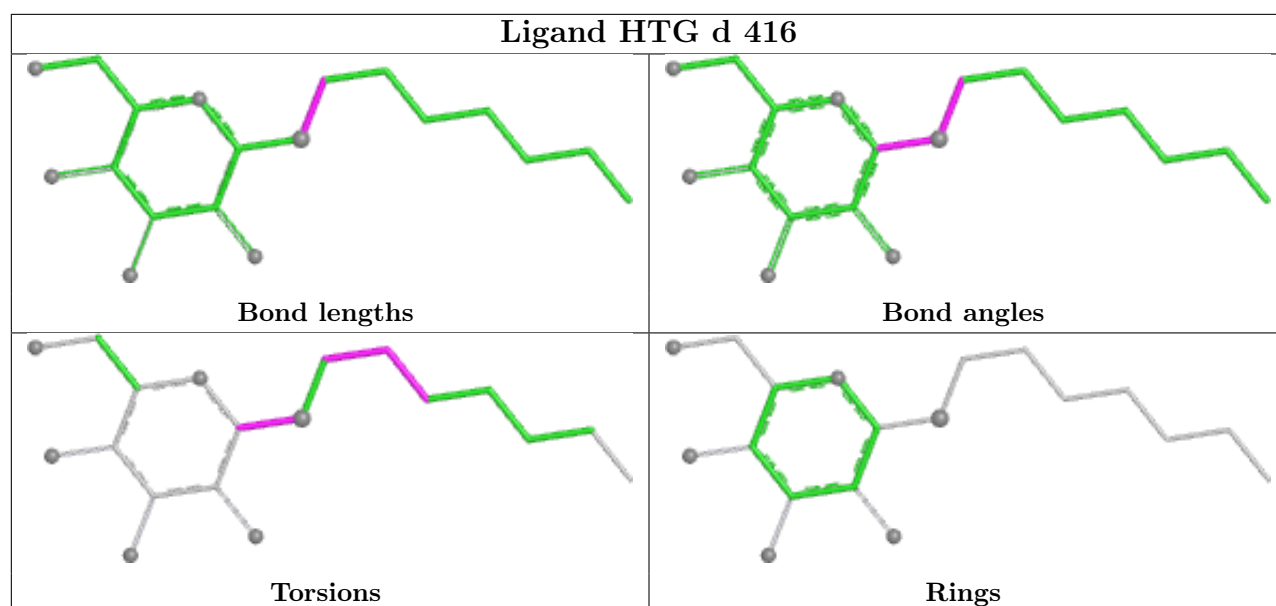
Ligand CLA c 511

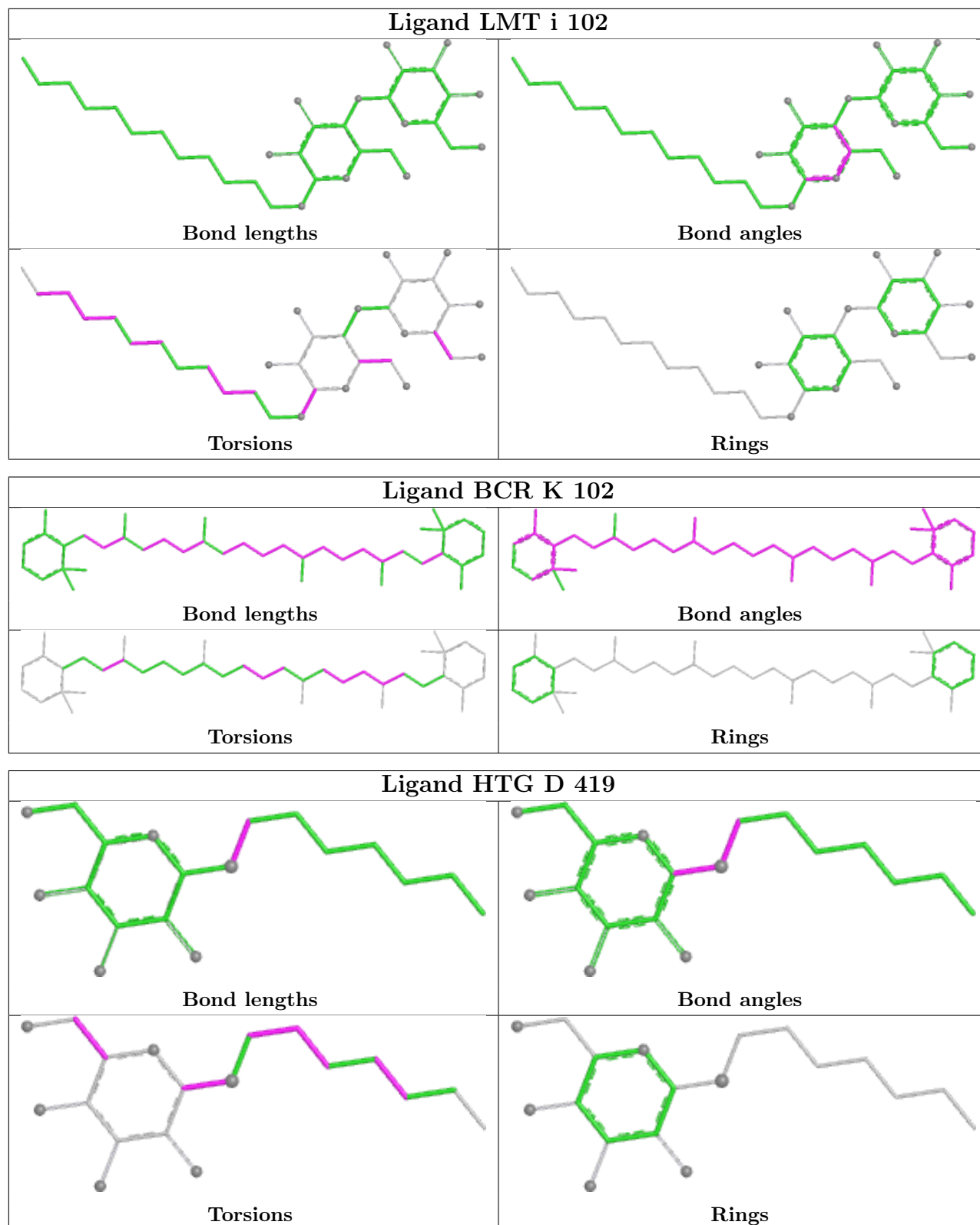


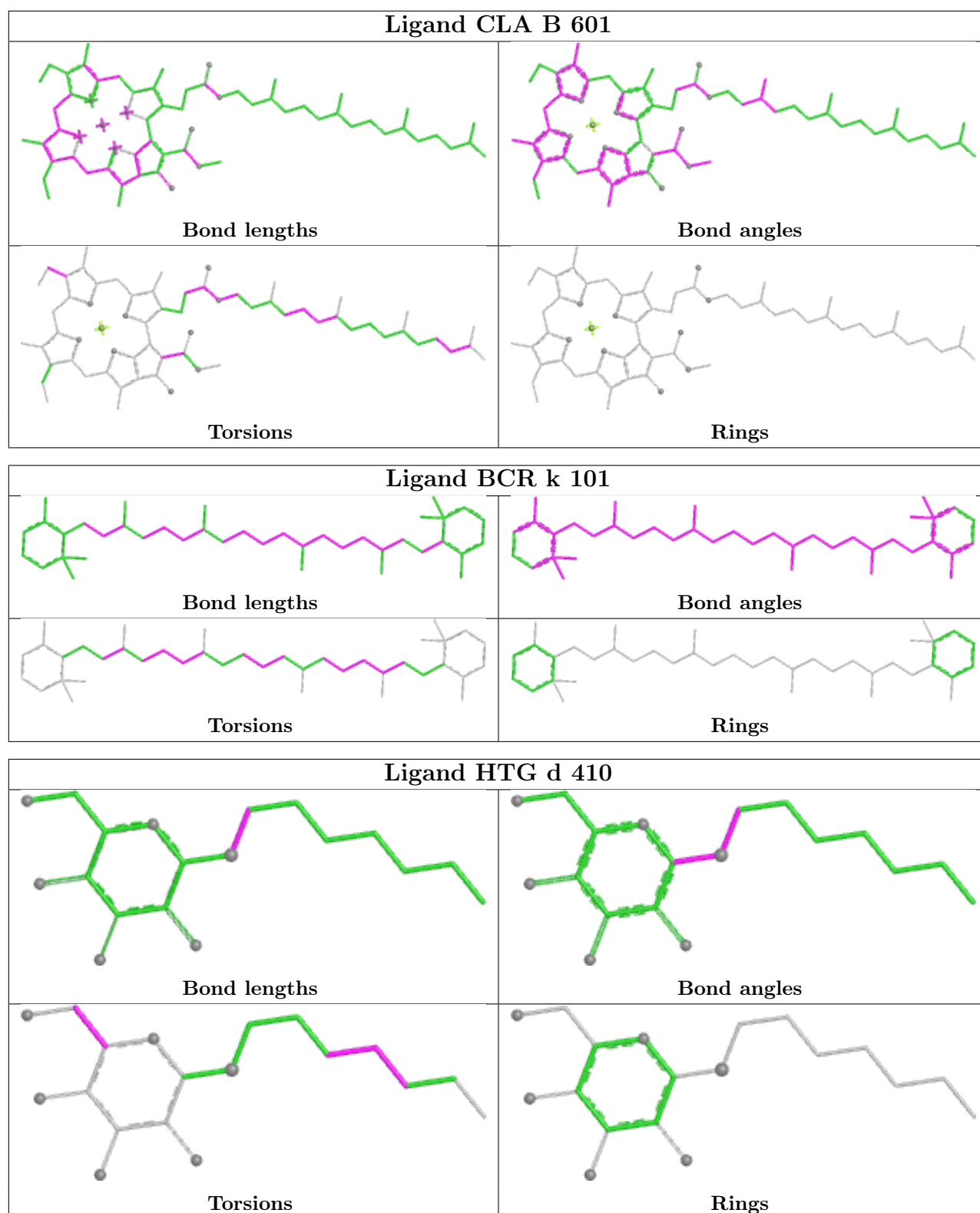


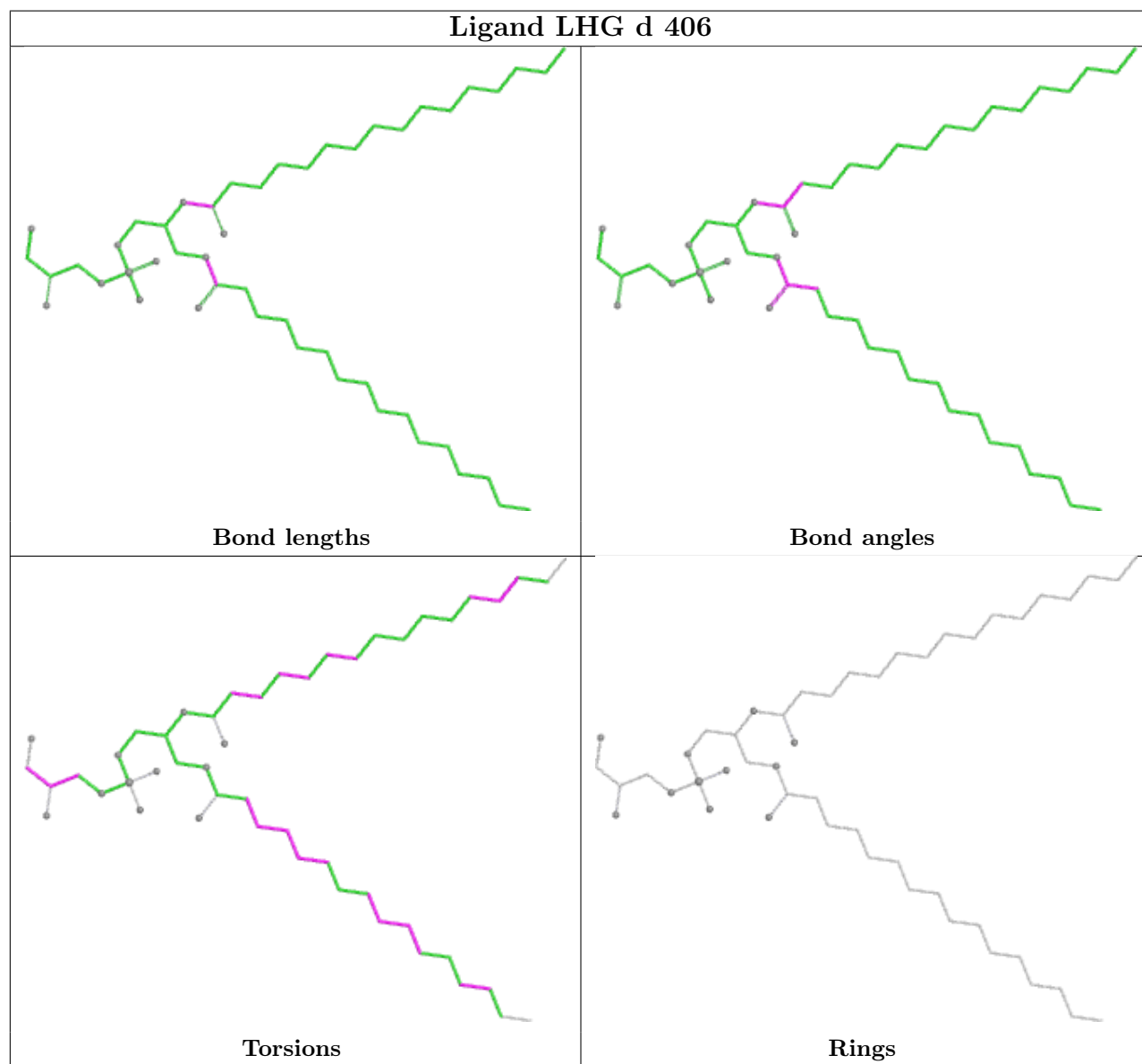
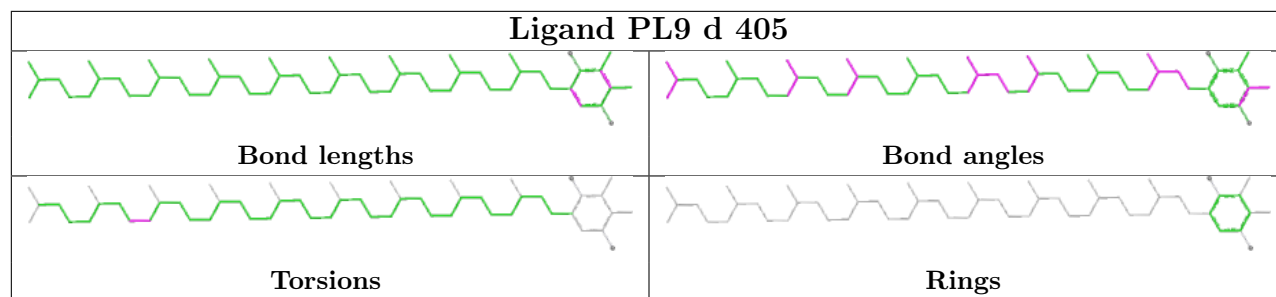




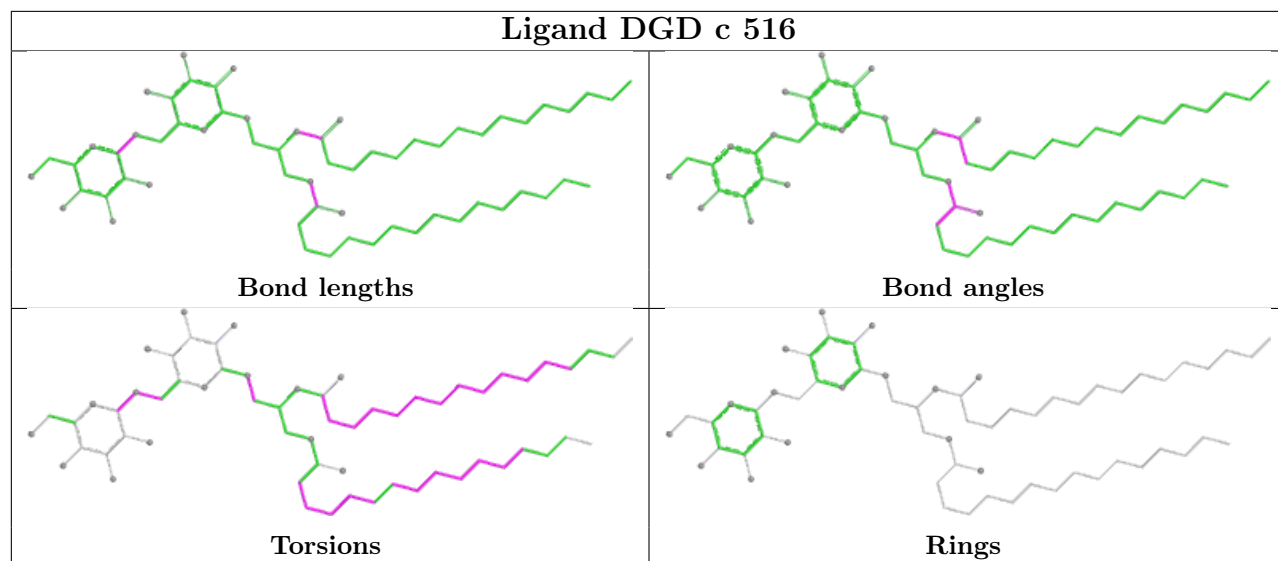




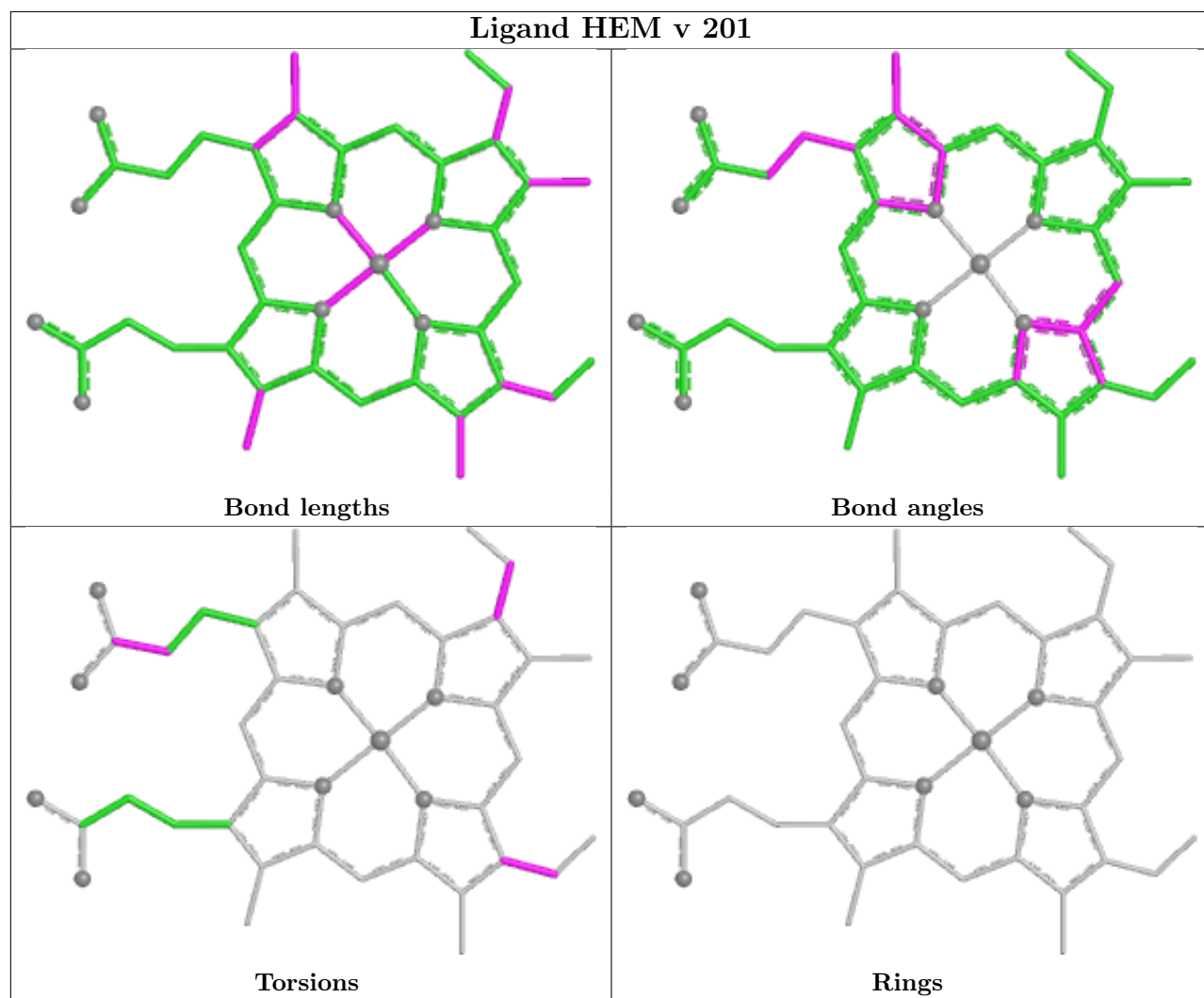


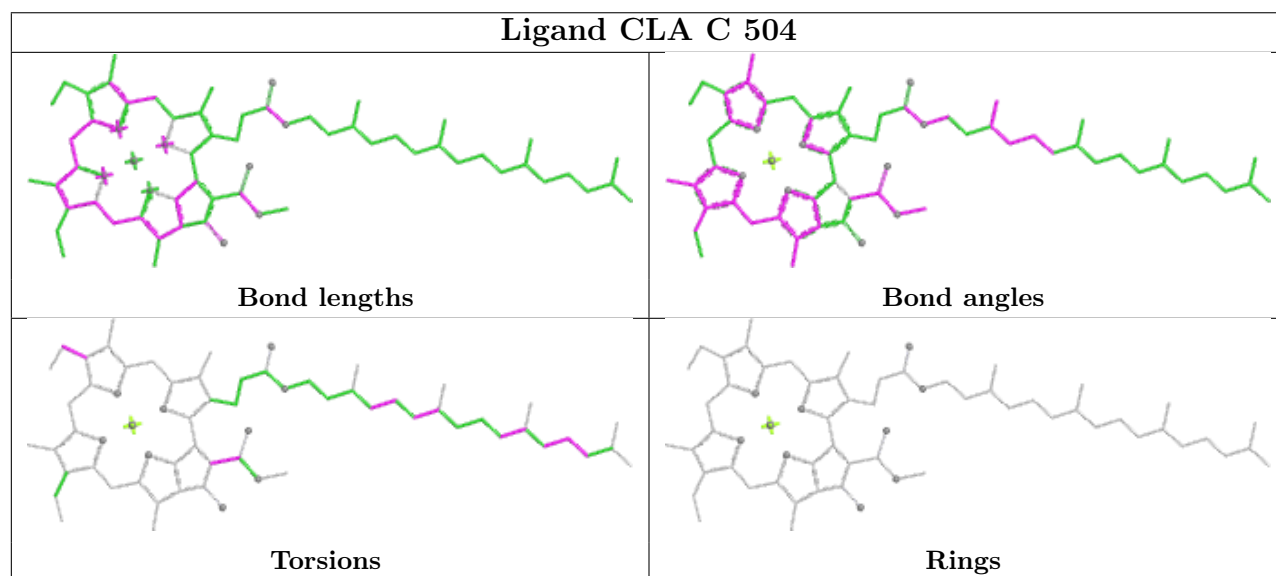
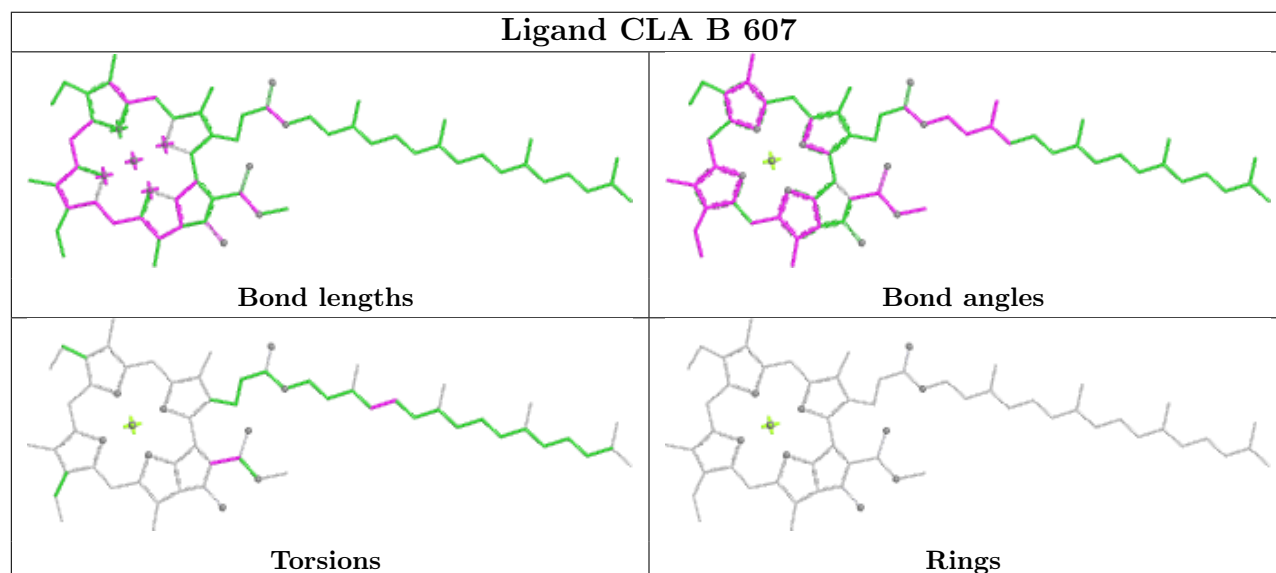
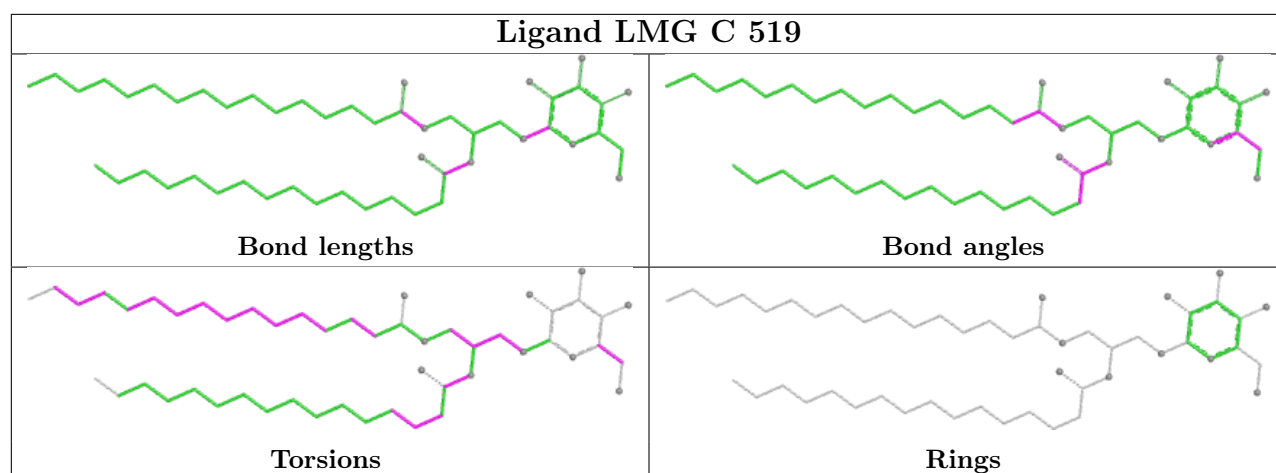


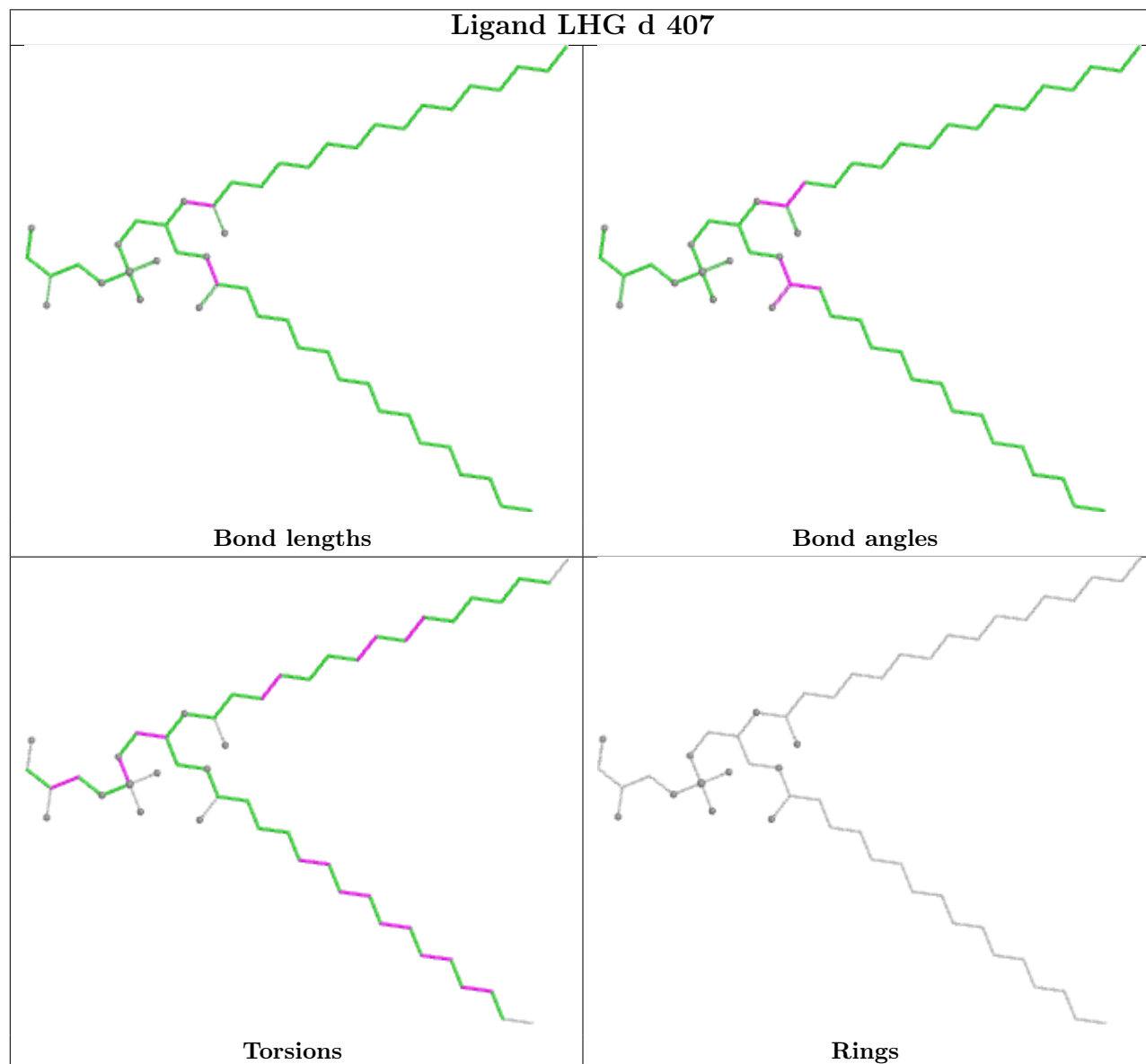
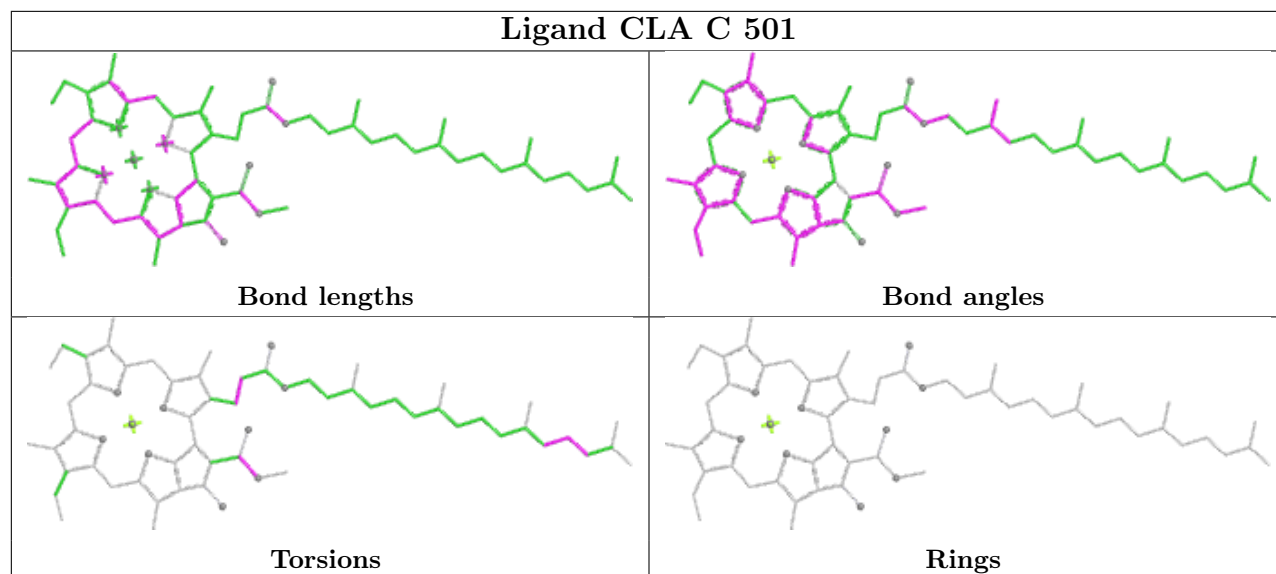
Ligand DGD c 516



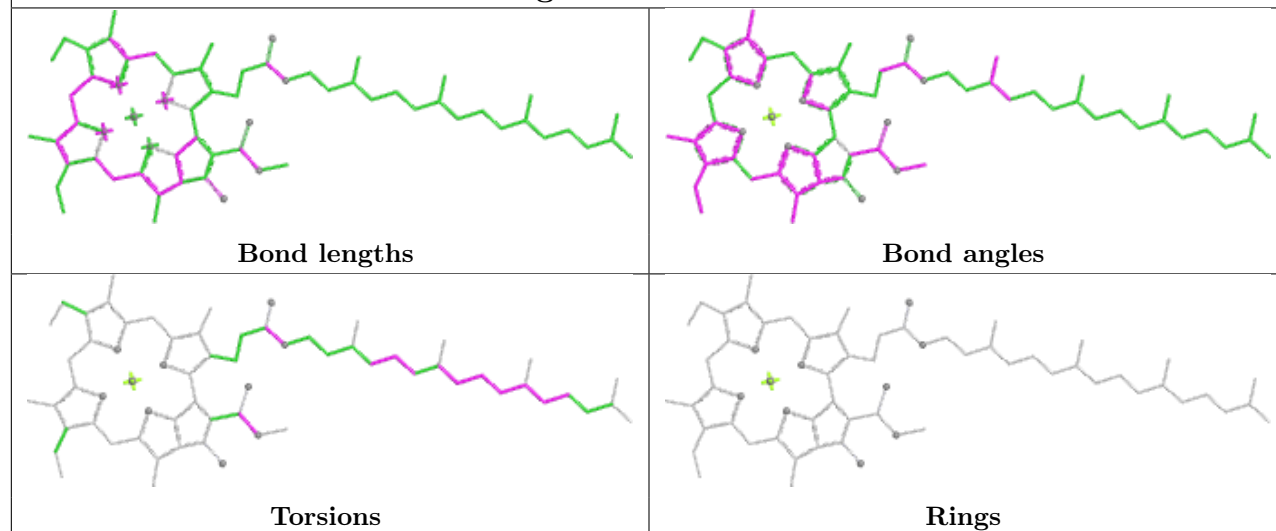
Ligand HEM v 201



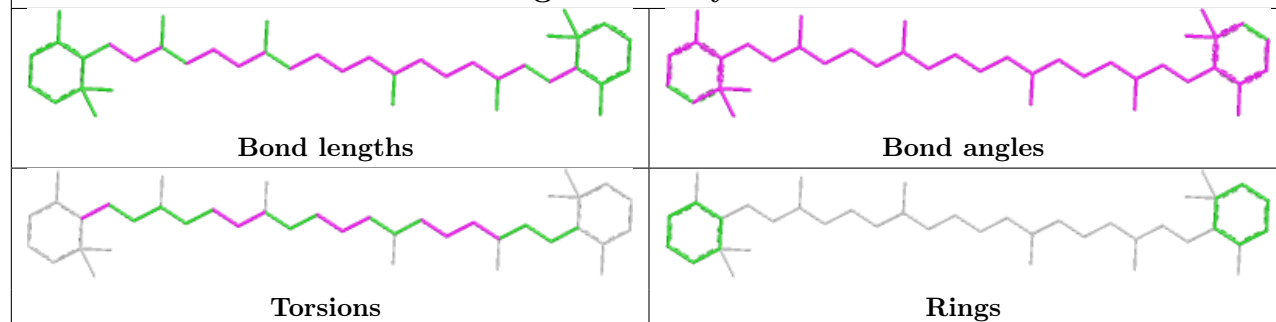




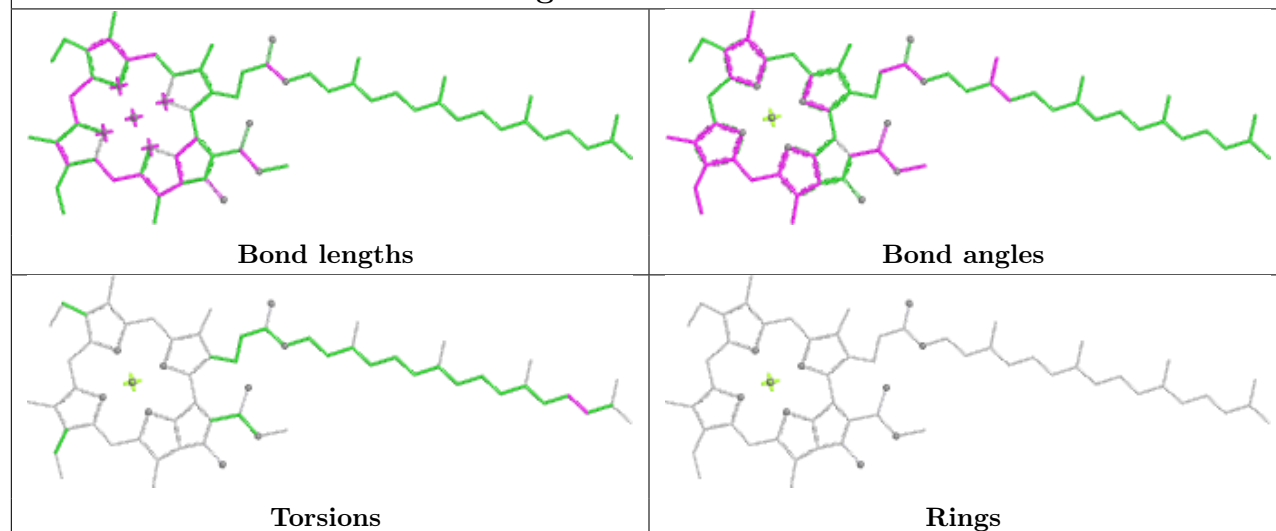
Ligand CLA a 412

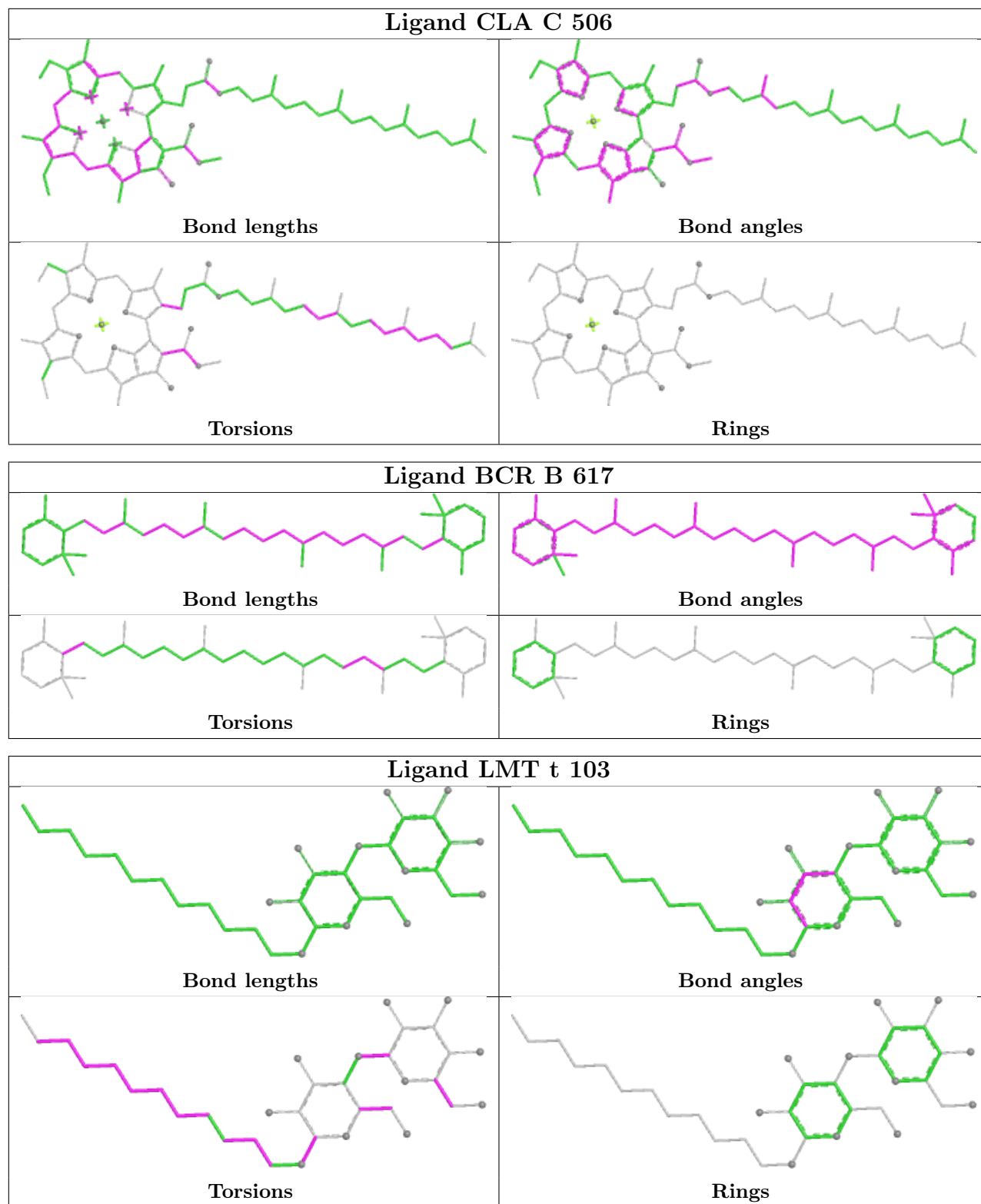


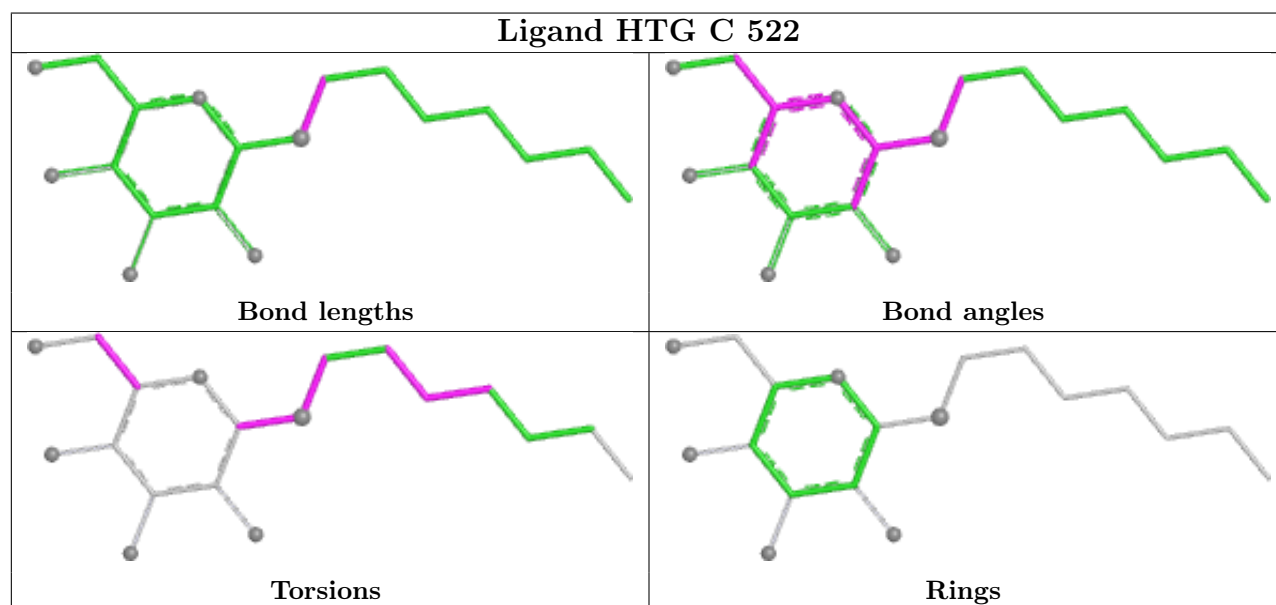
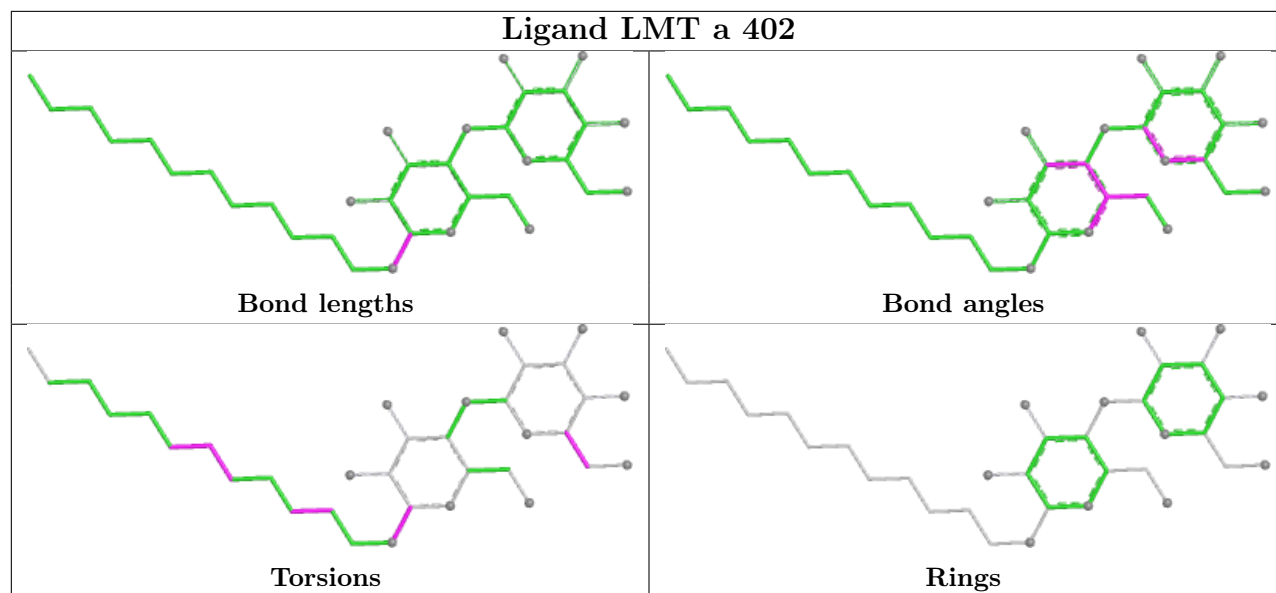
Ligand BCR y 101



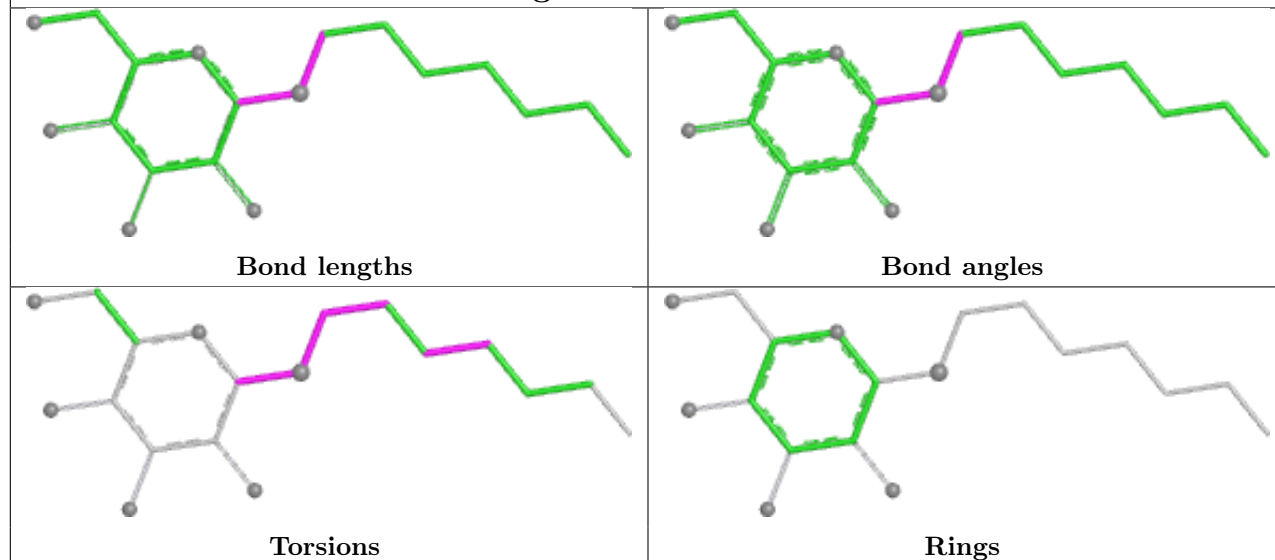
Ligand CLA a 408



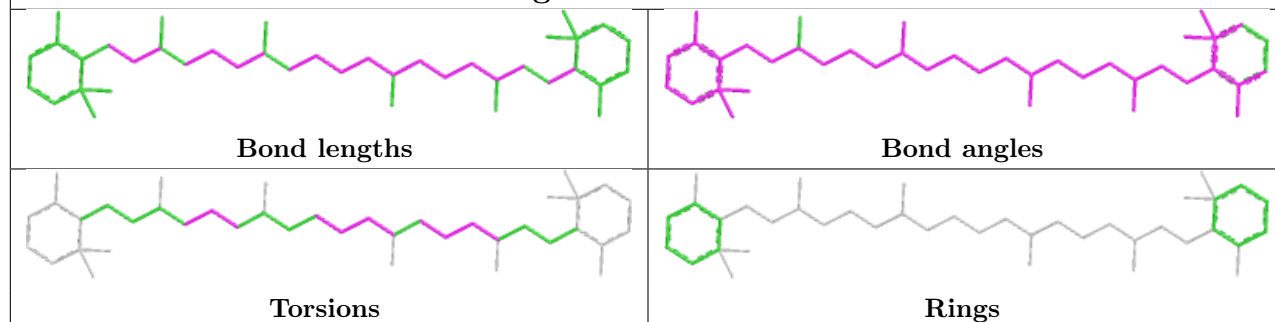




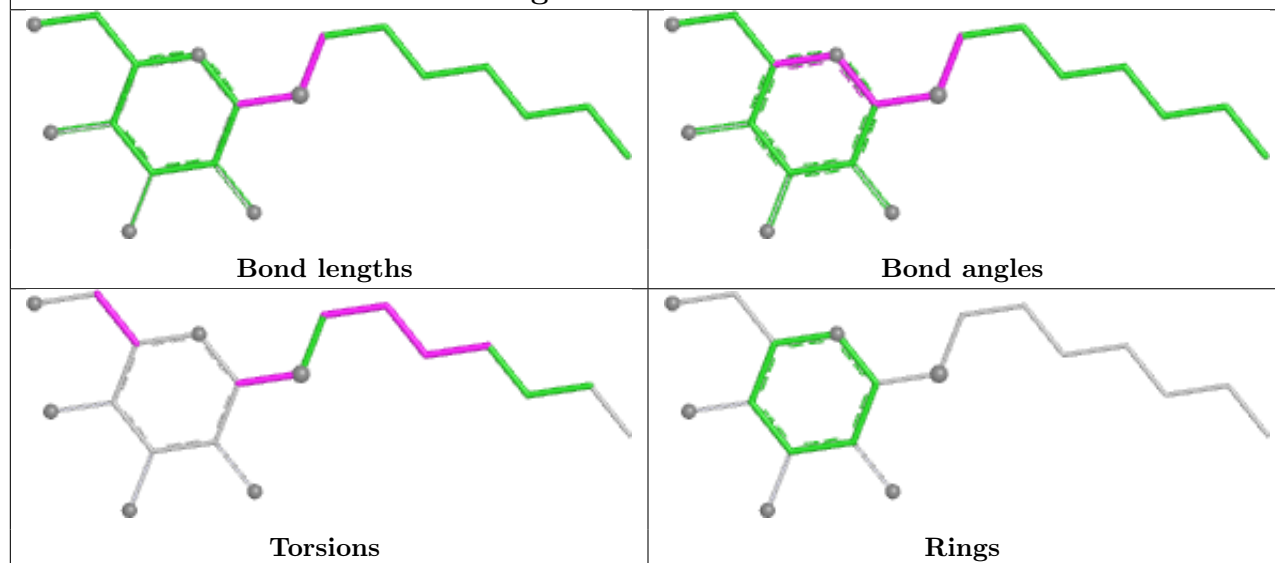
Ligand HTG c 522



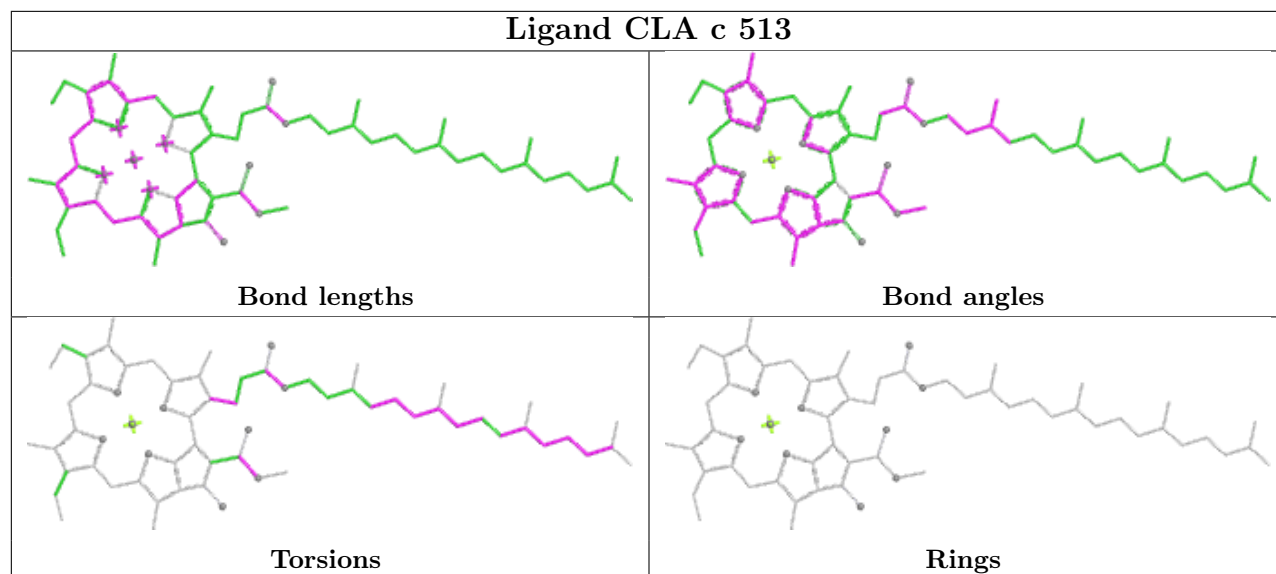
Ligand BCR k 102



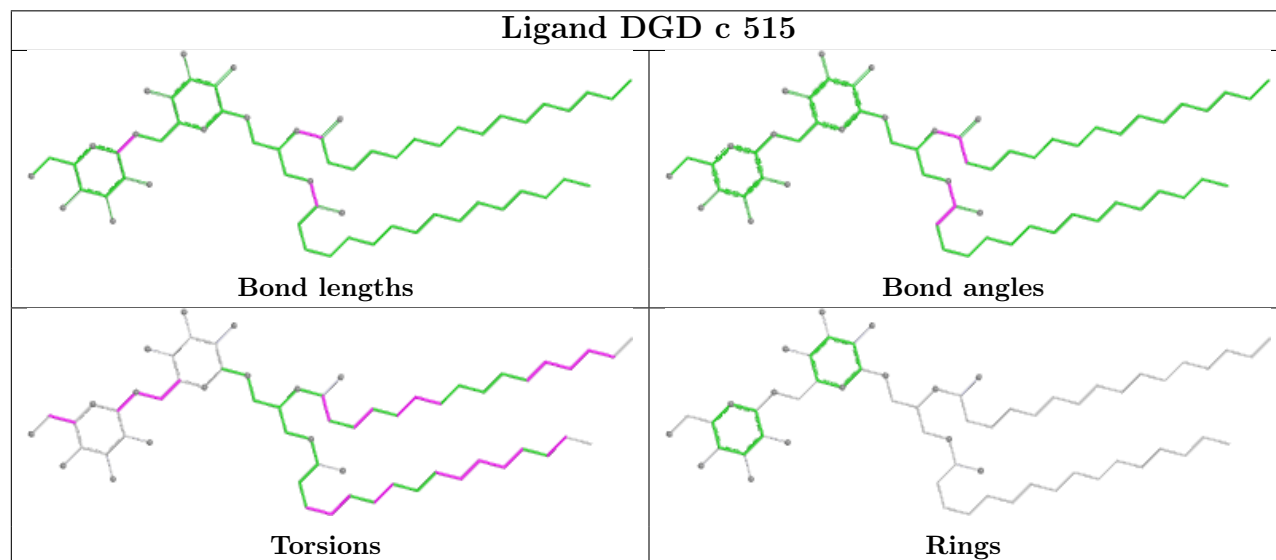
Ligand HTG b 630

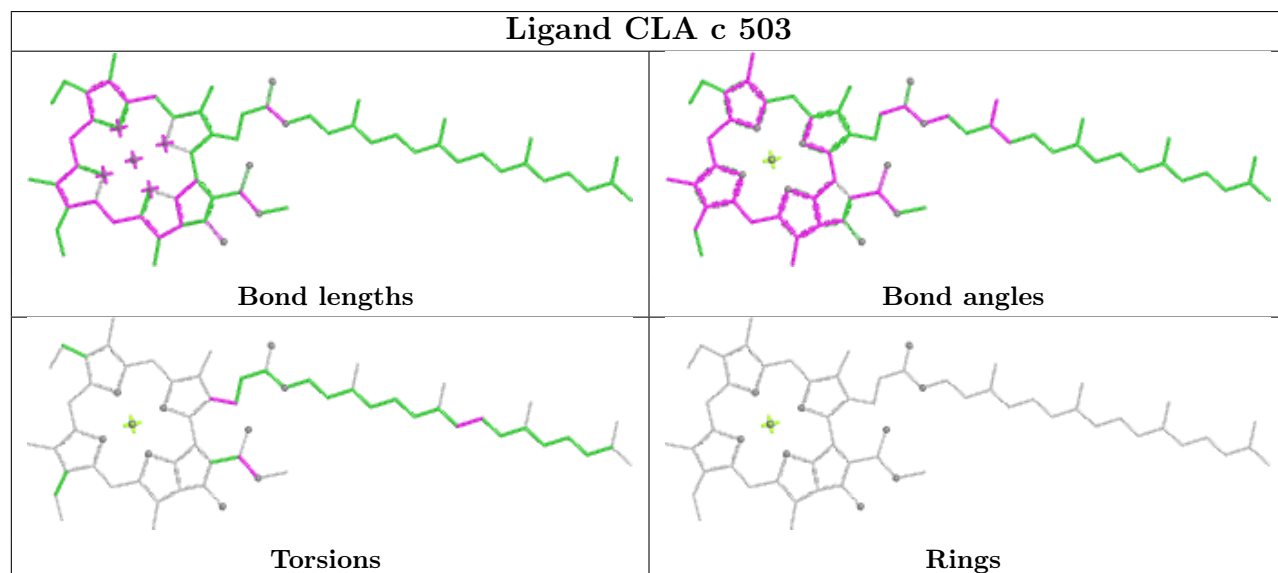
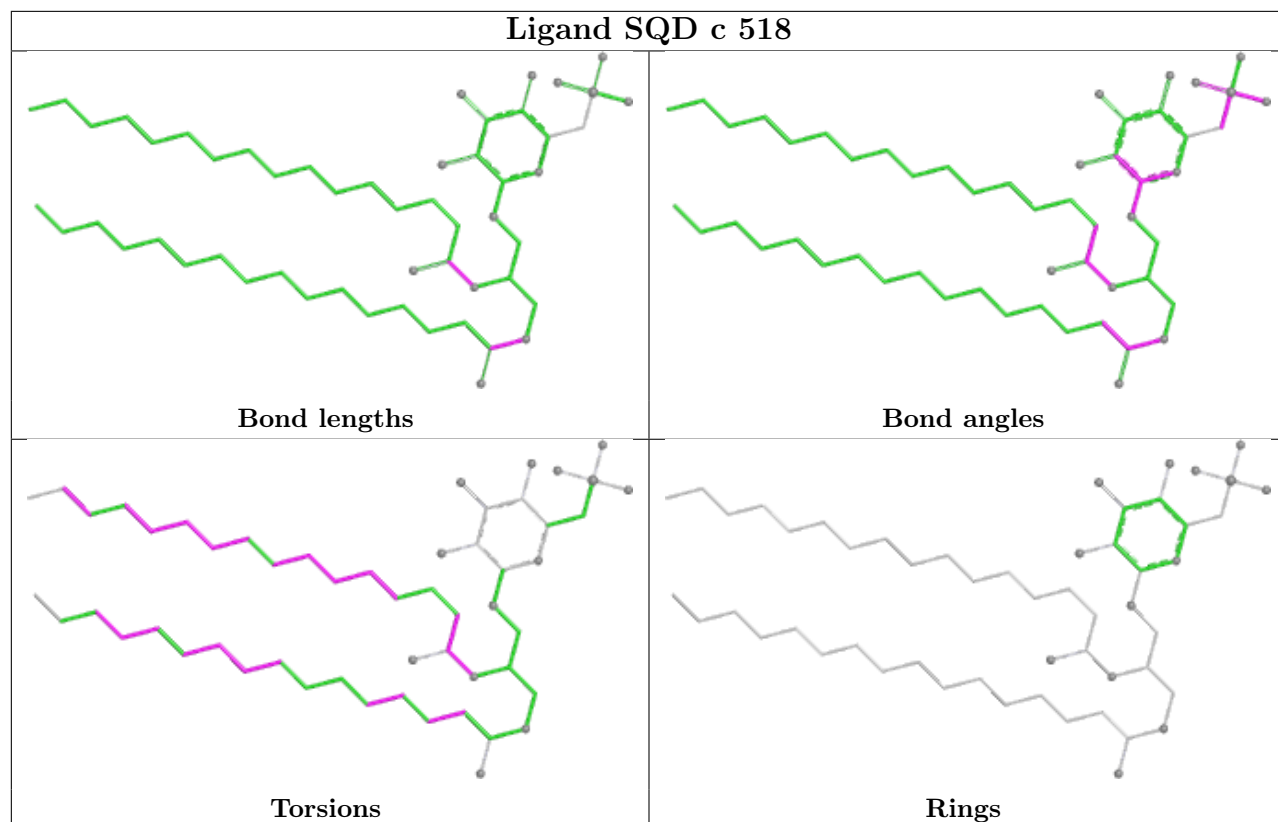


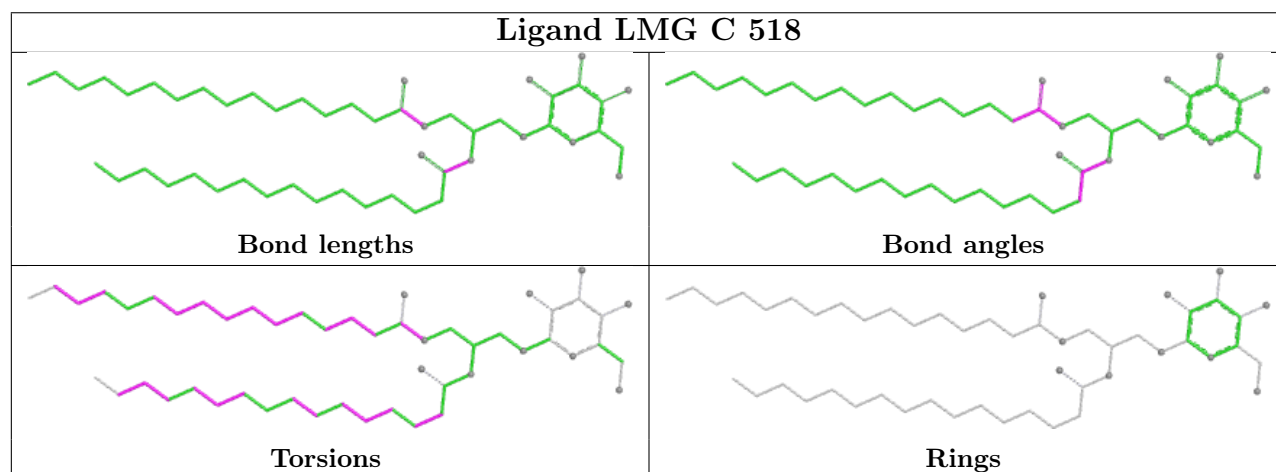
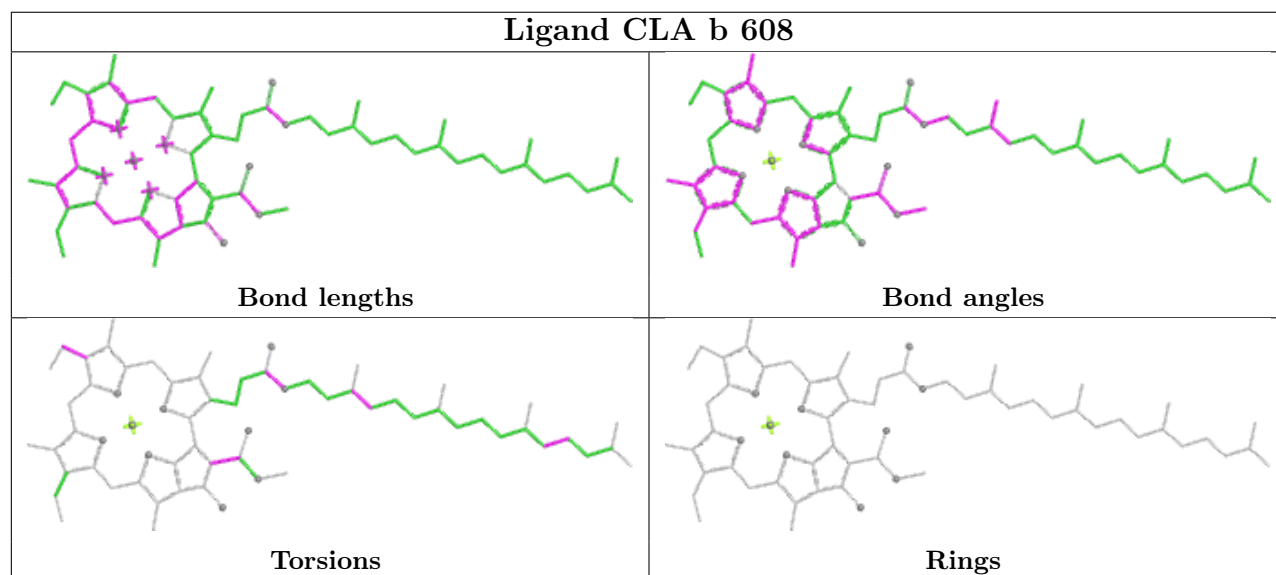
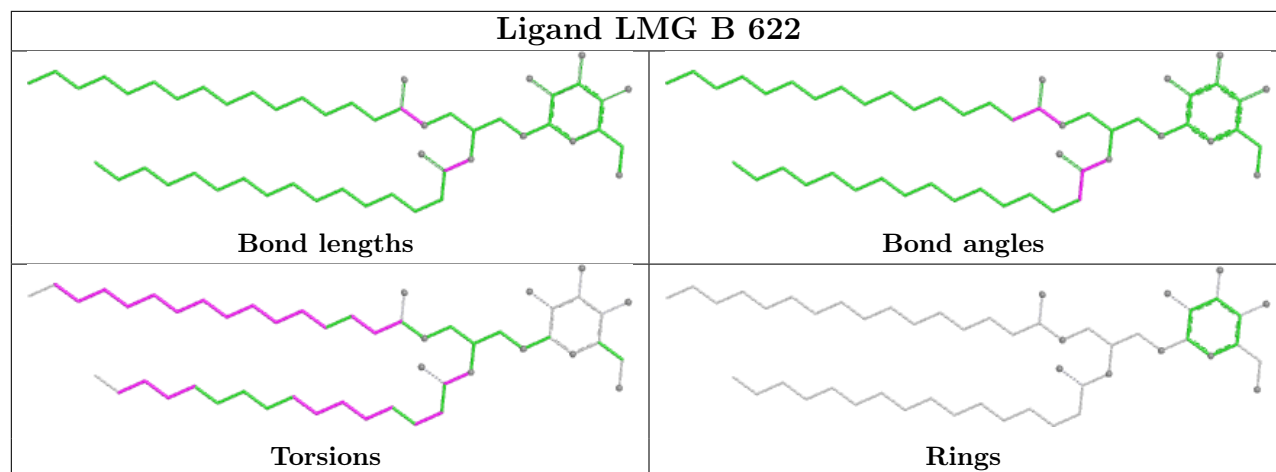
Ligand CLA c 513

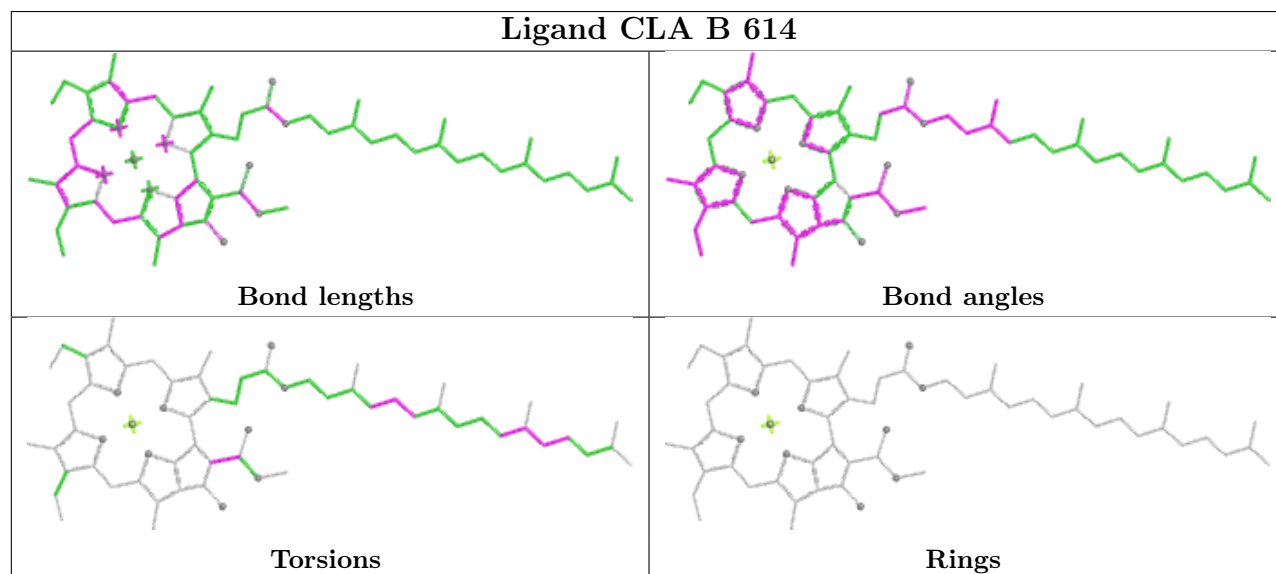
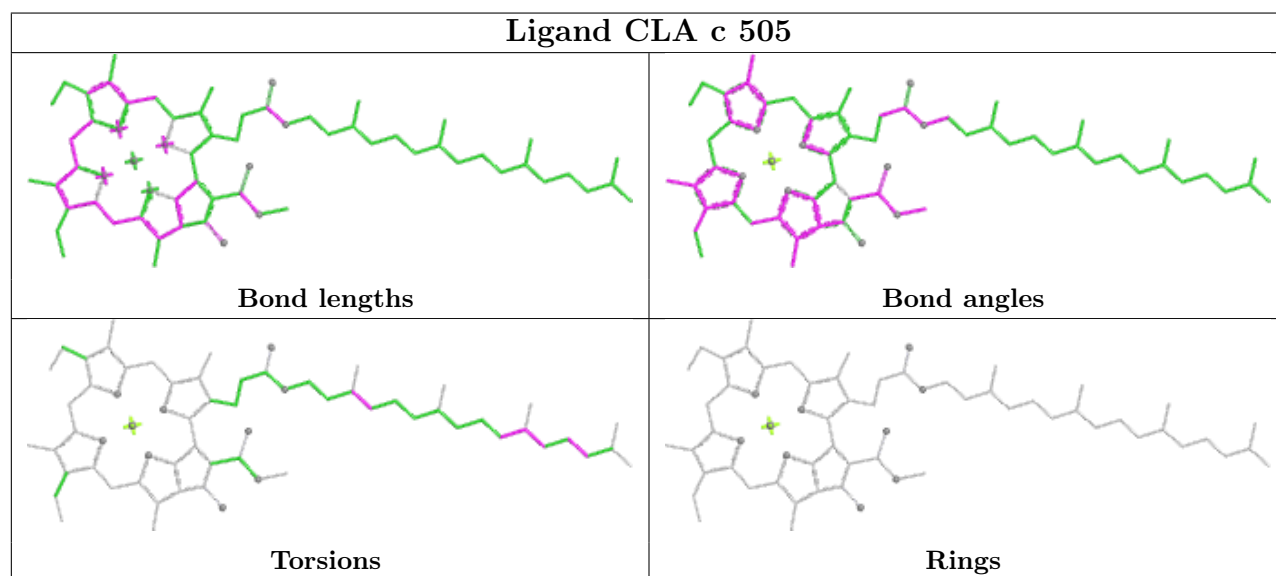
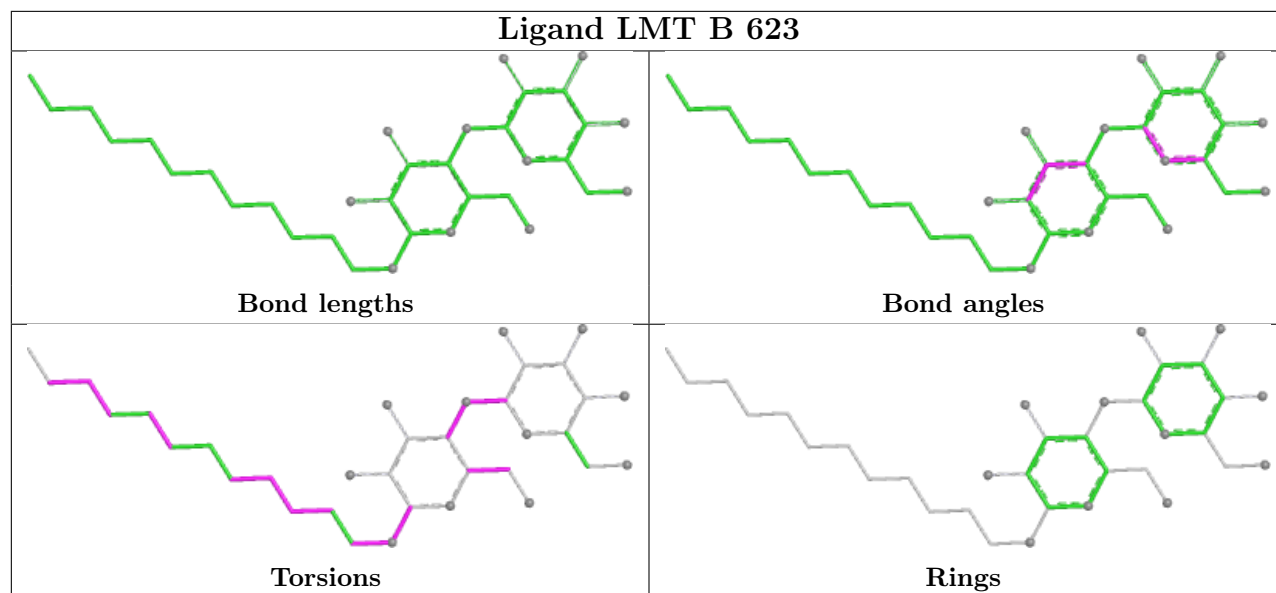


Ligand DGD c 515

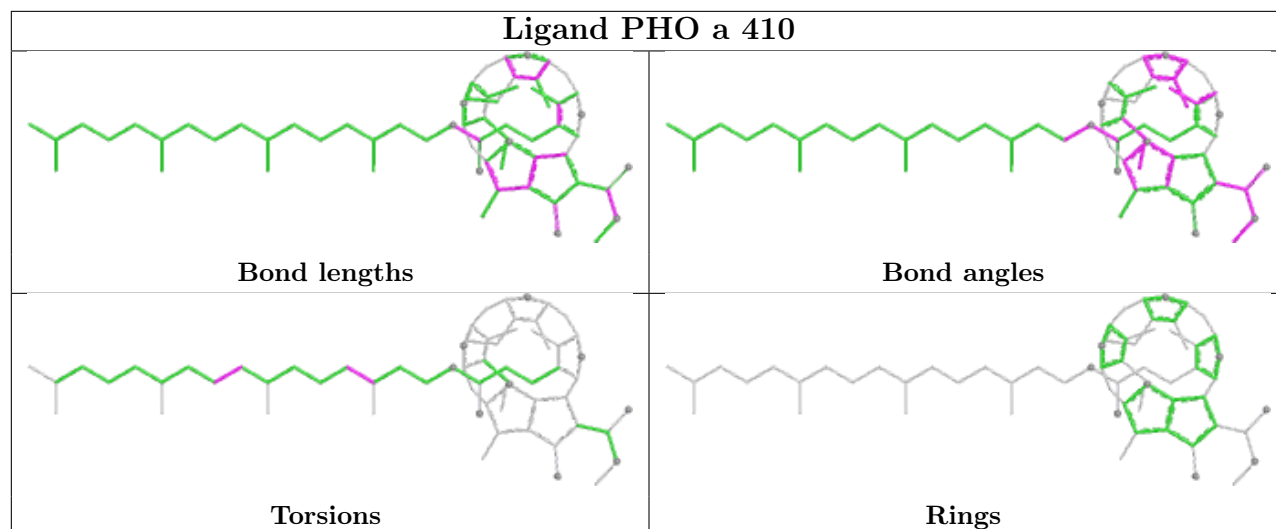




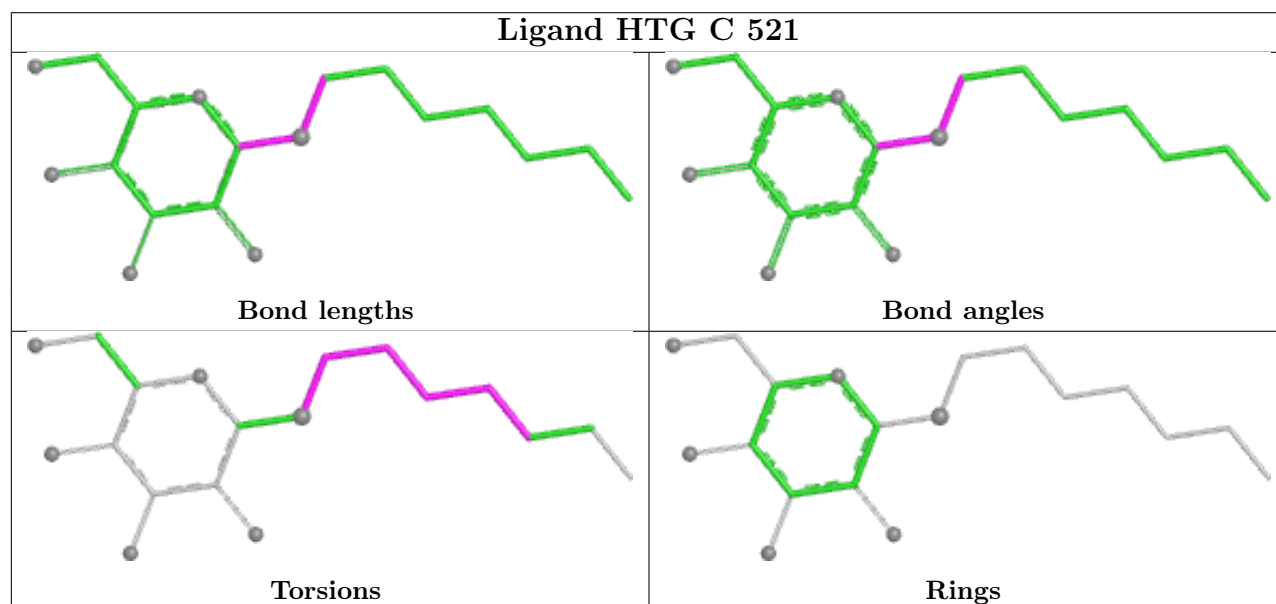




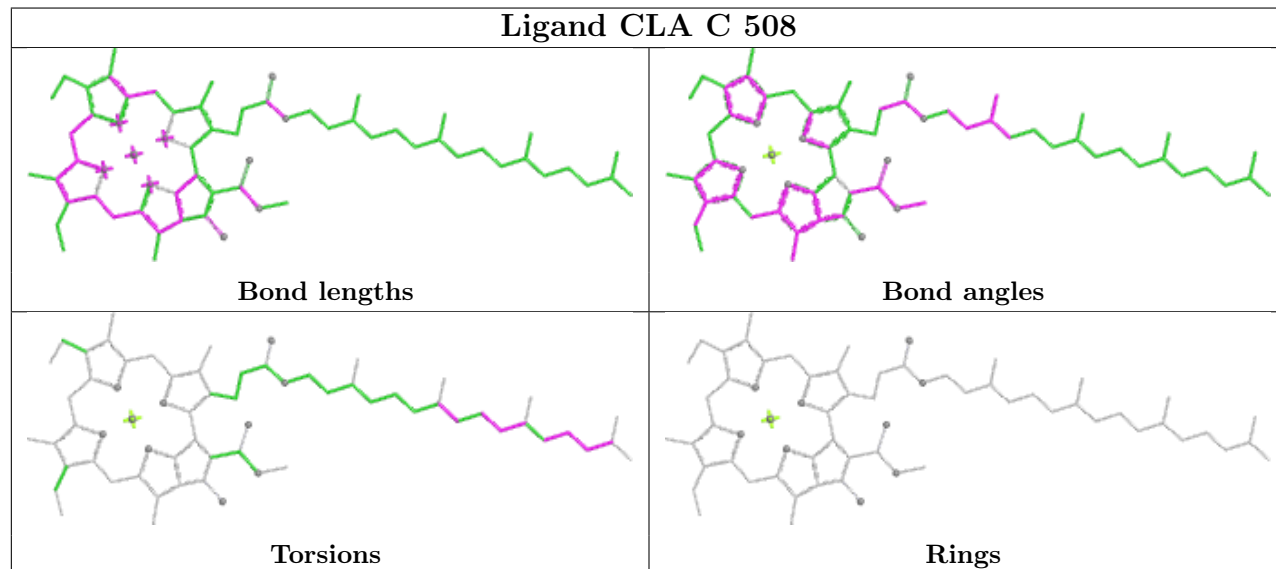
Ligand PHO a 410

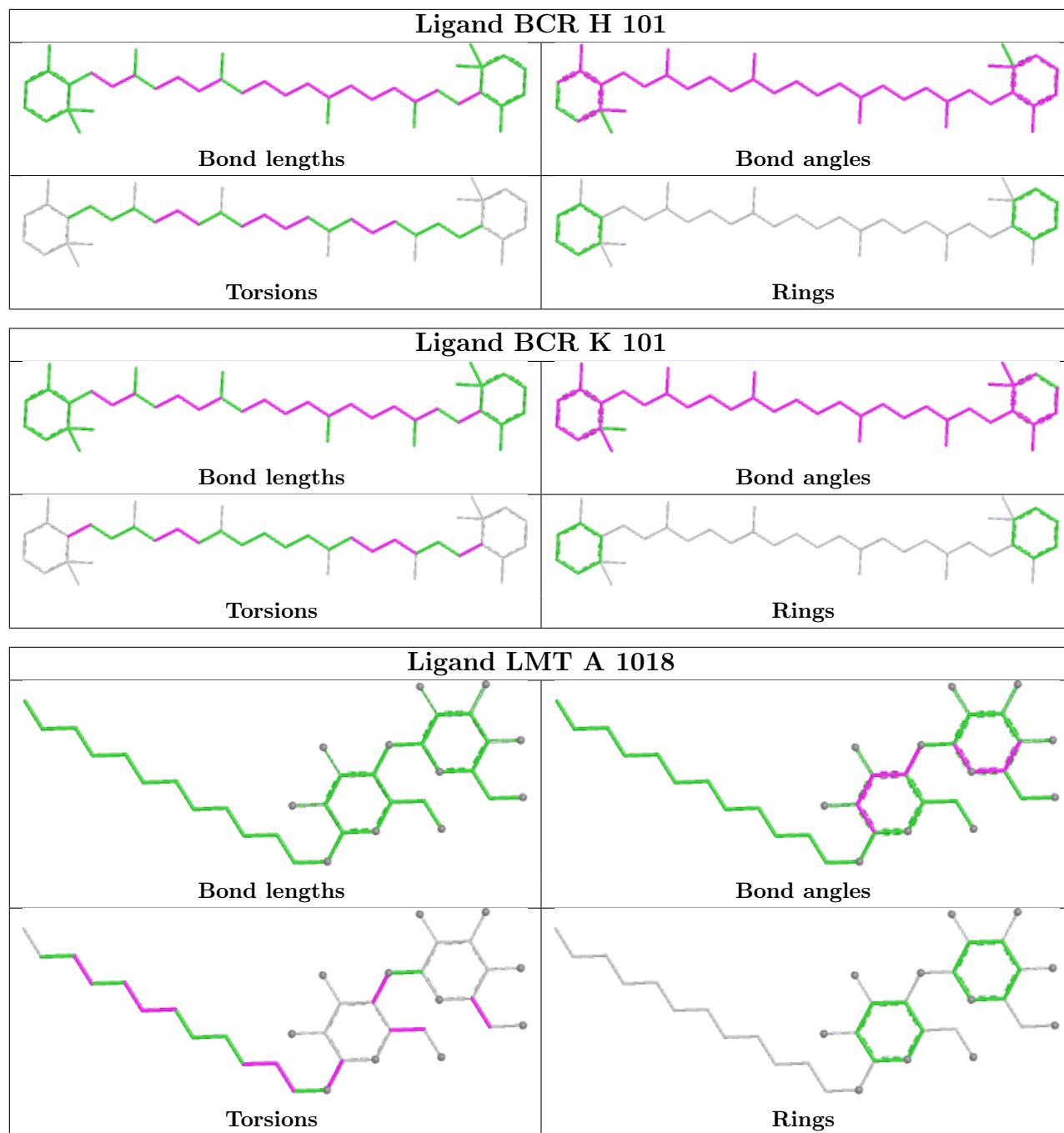


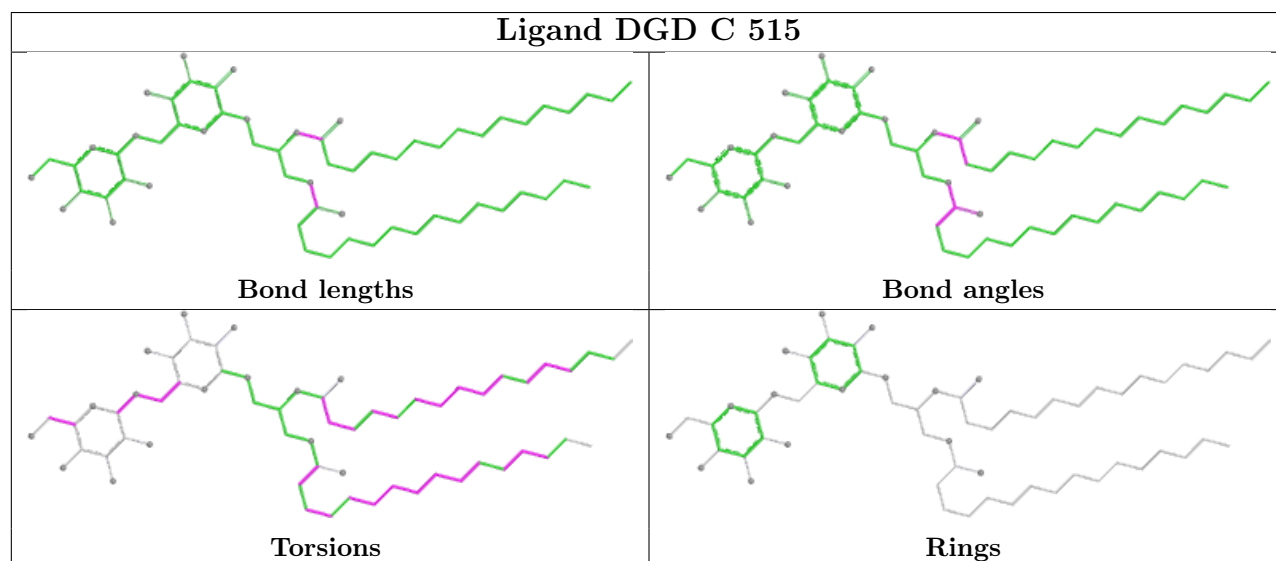
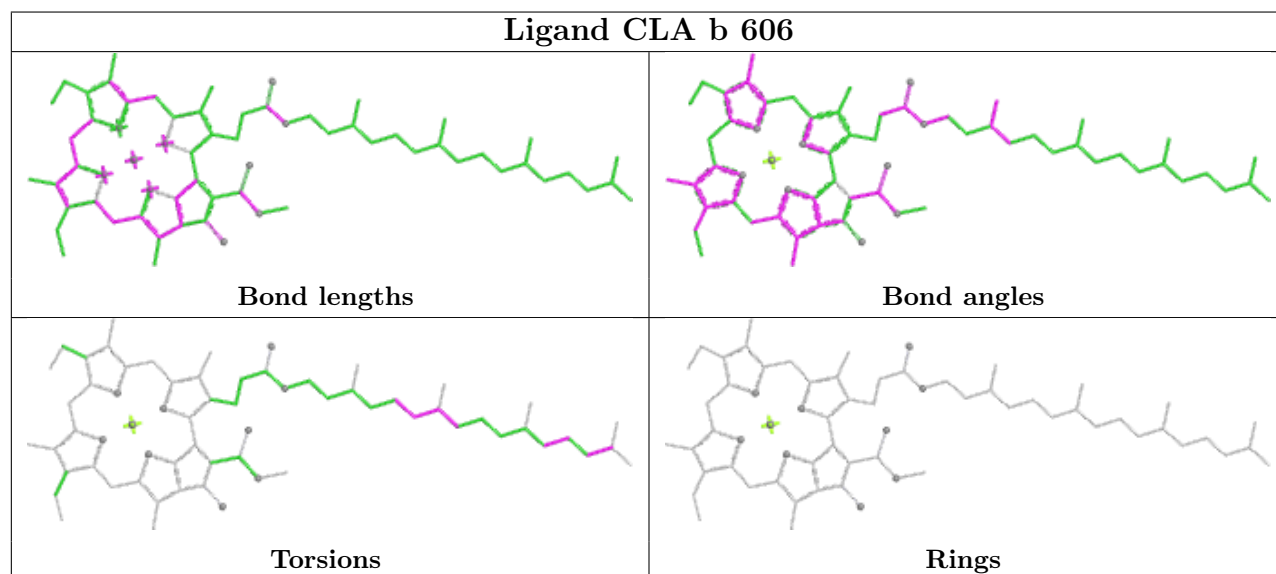
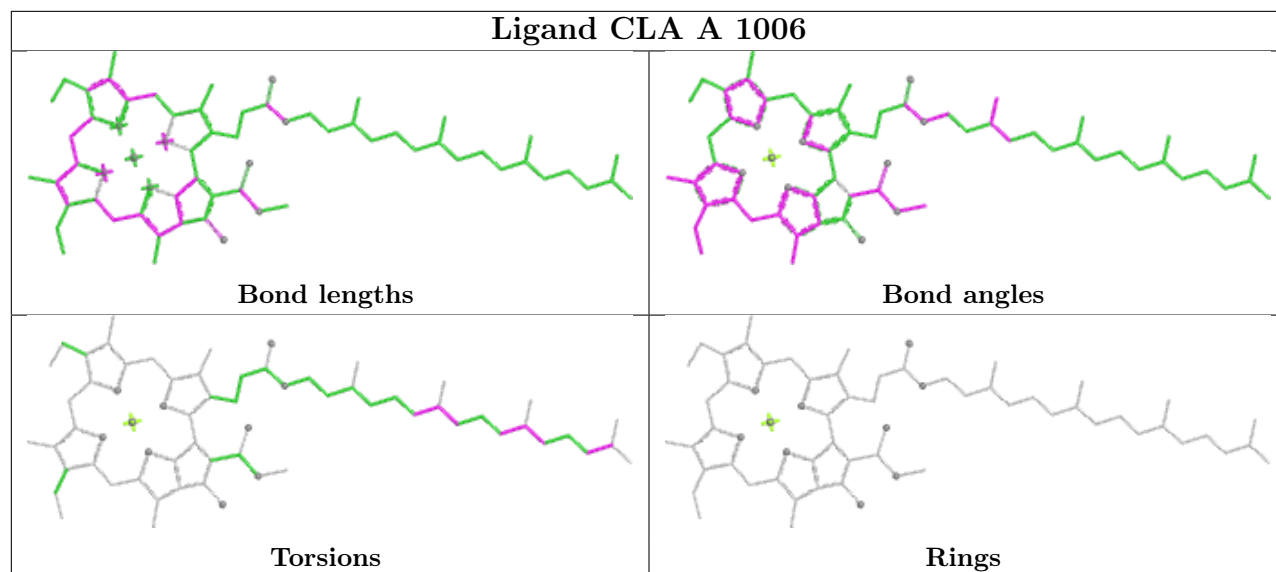
Ligand HTG C 521

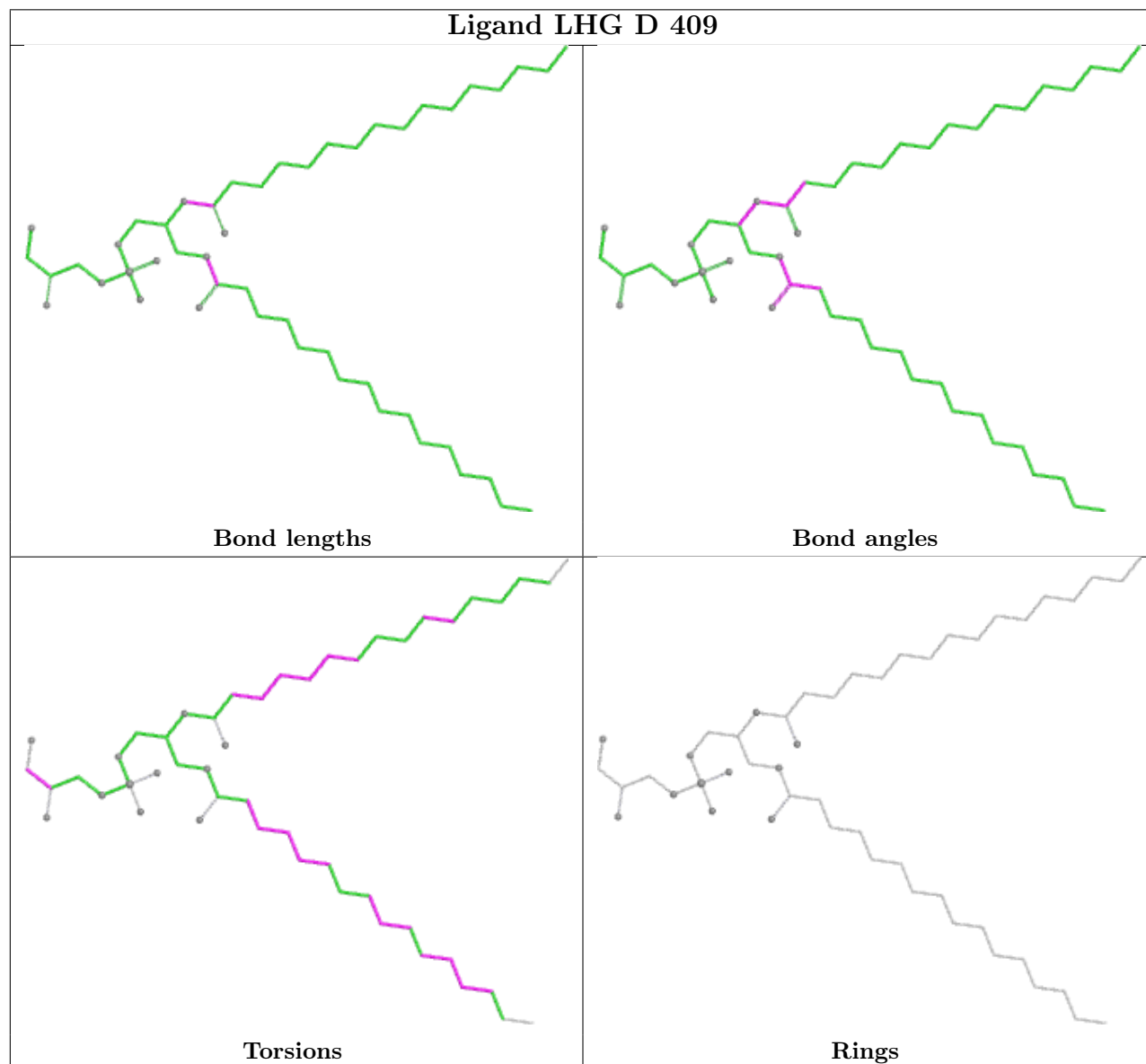
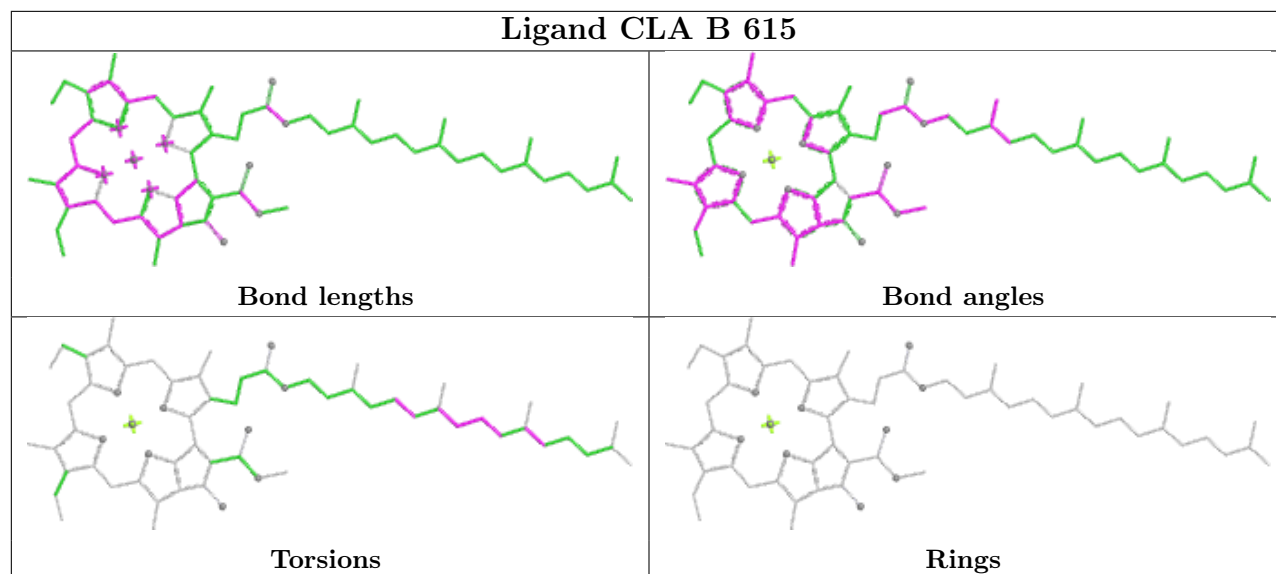


Ligand CLA C 508

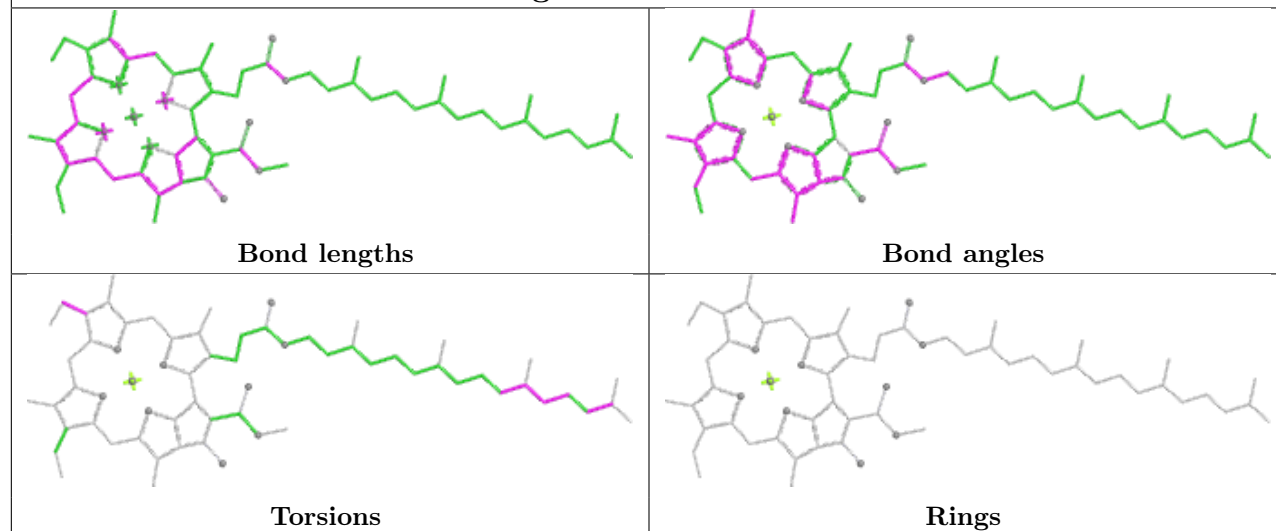




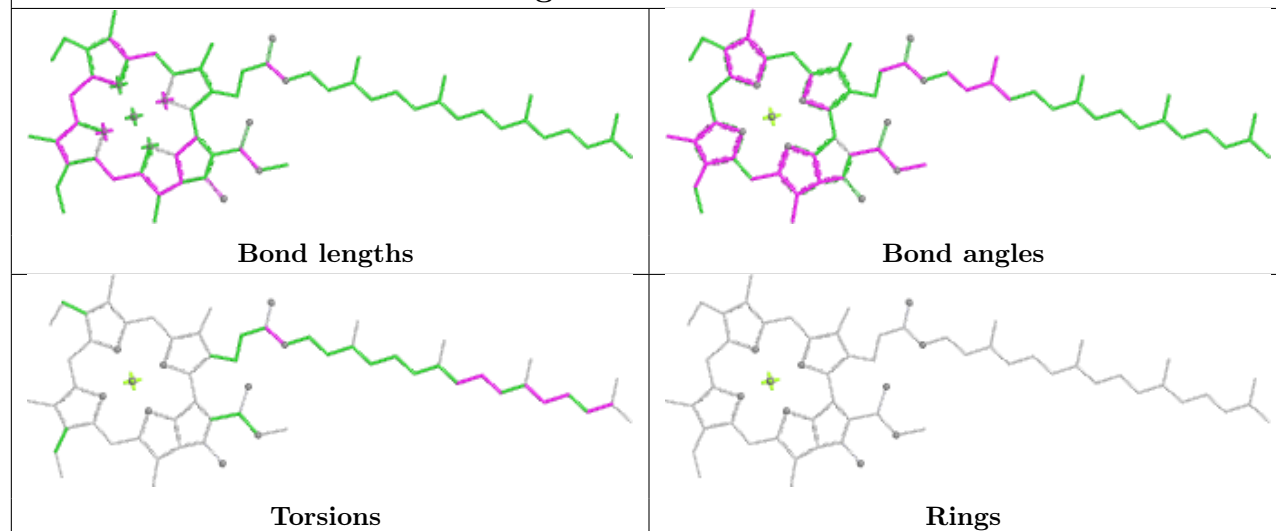




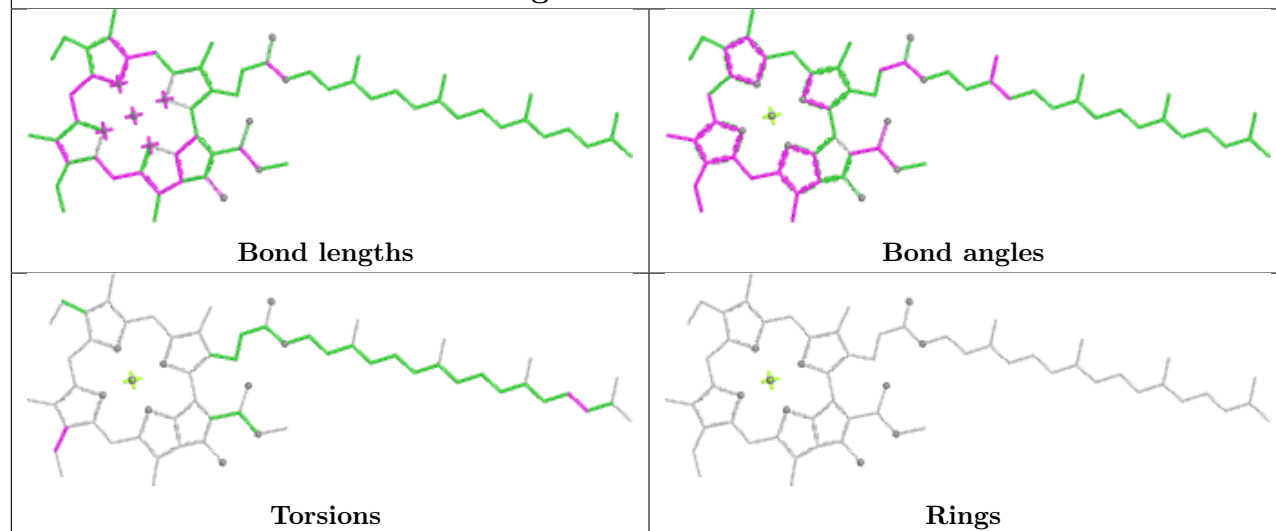
Ligand CLA C 505

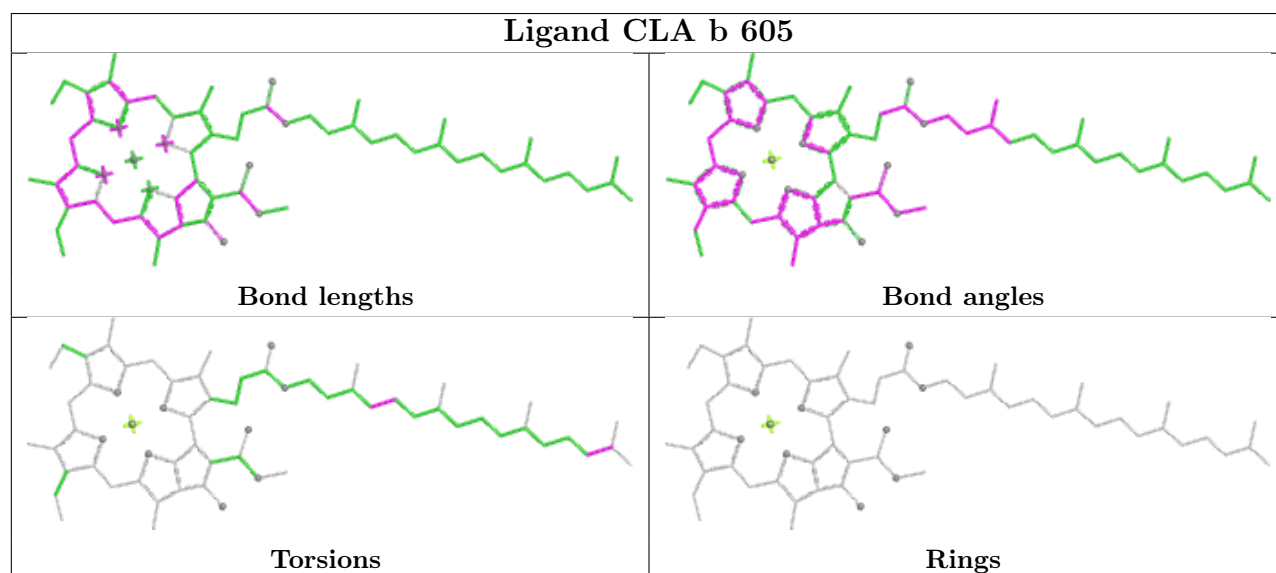
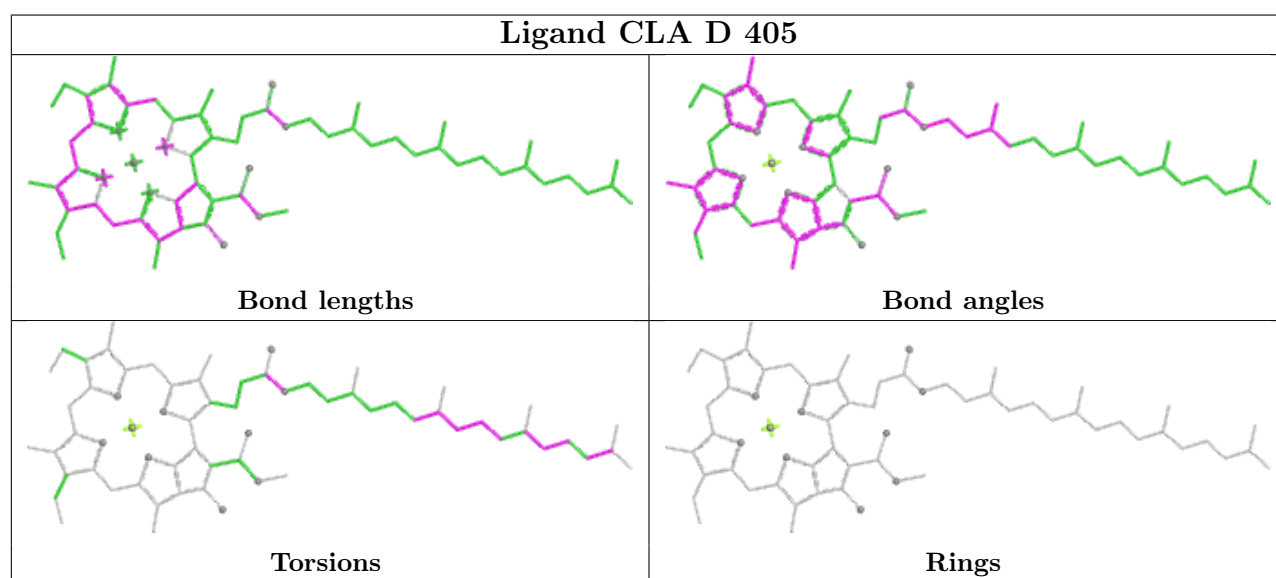
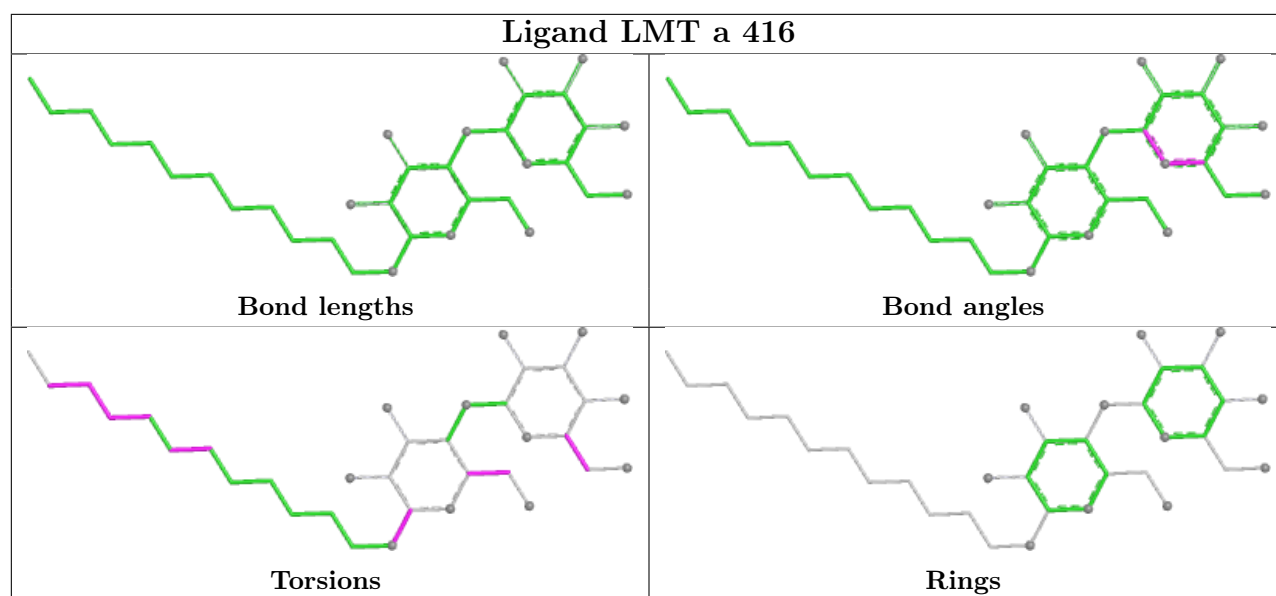


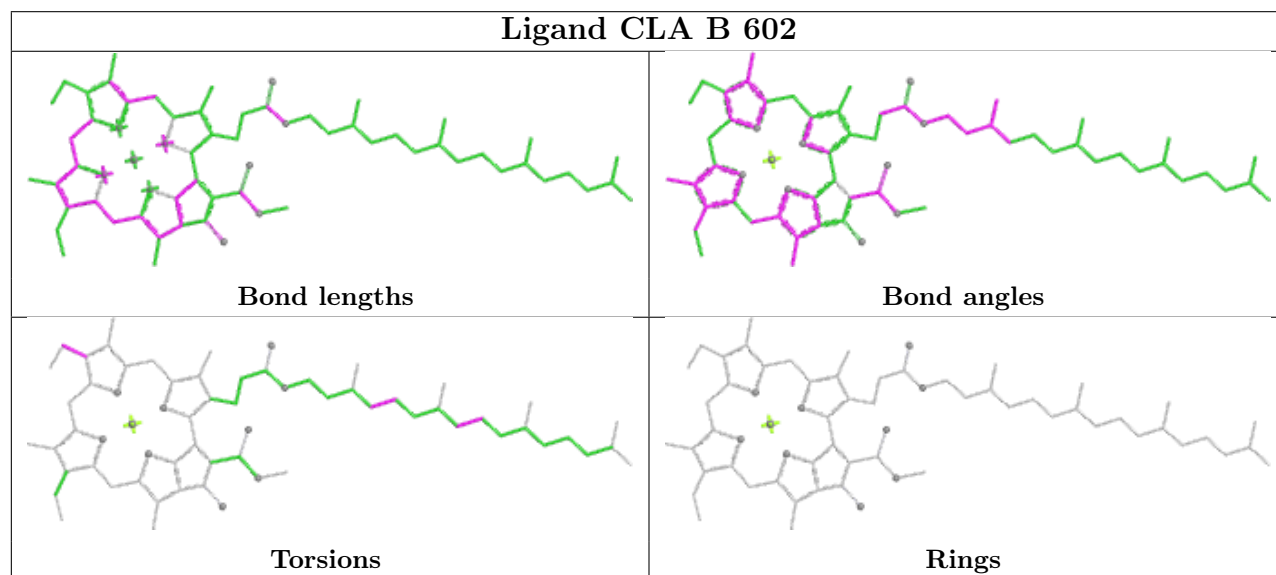
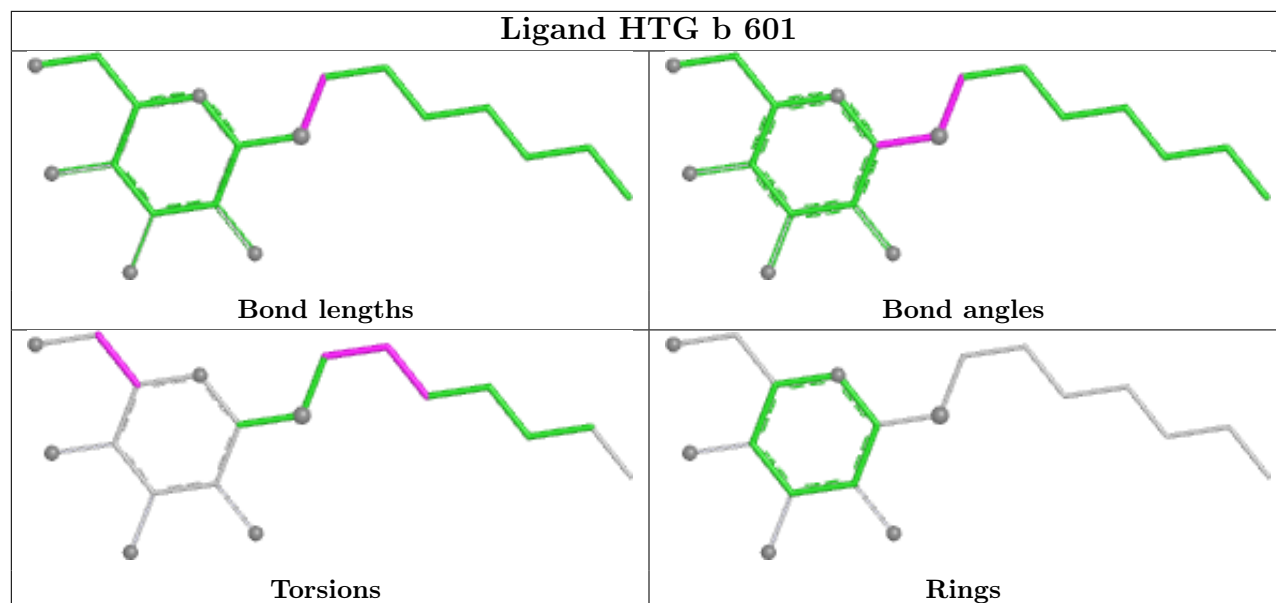
Ligand CLA b 615

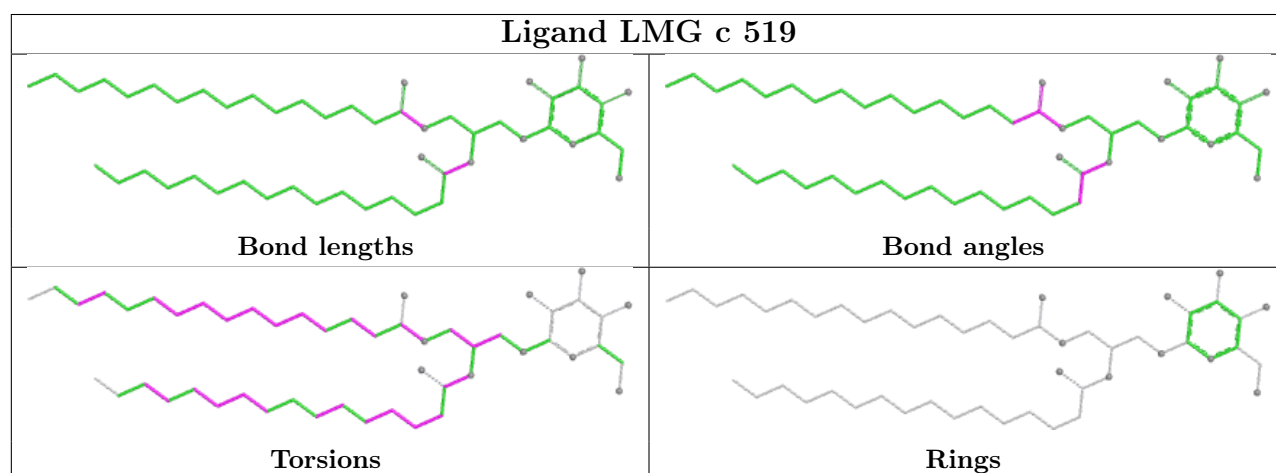
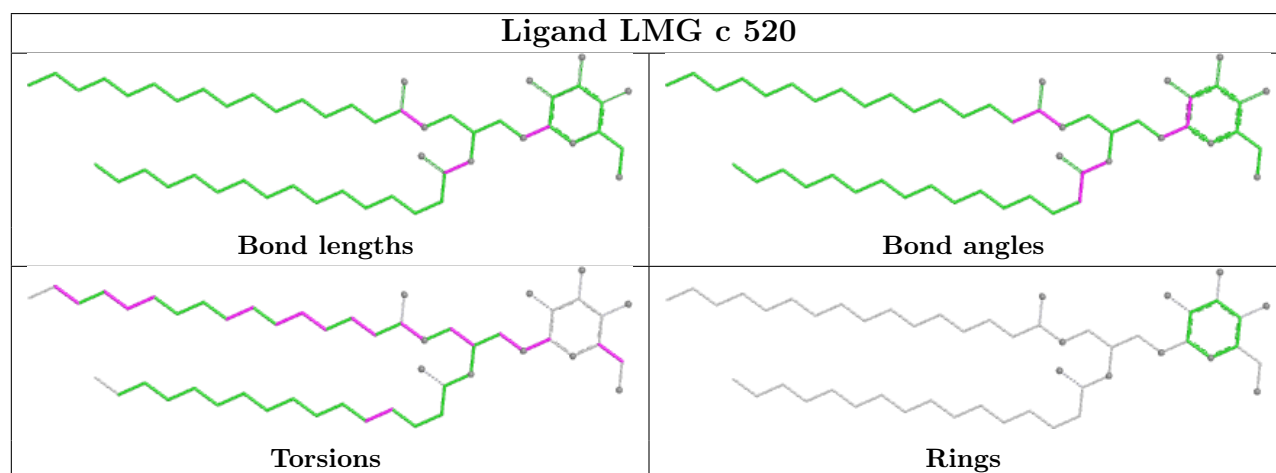
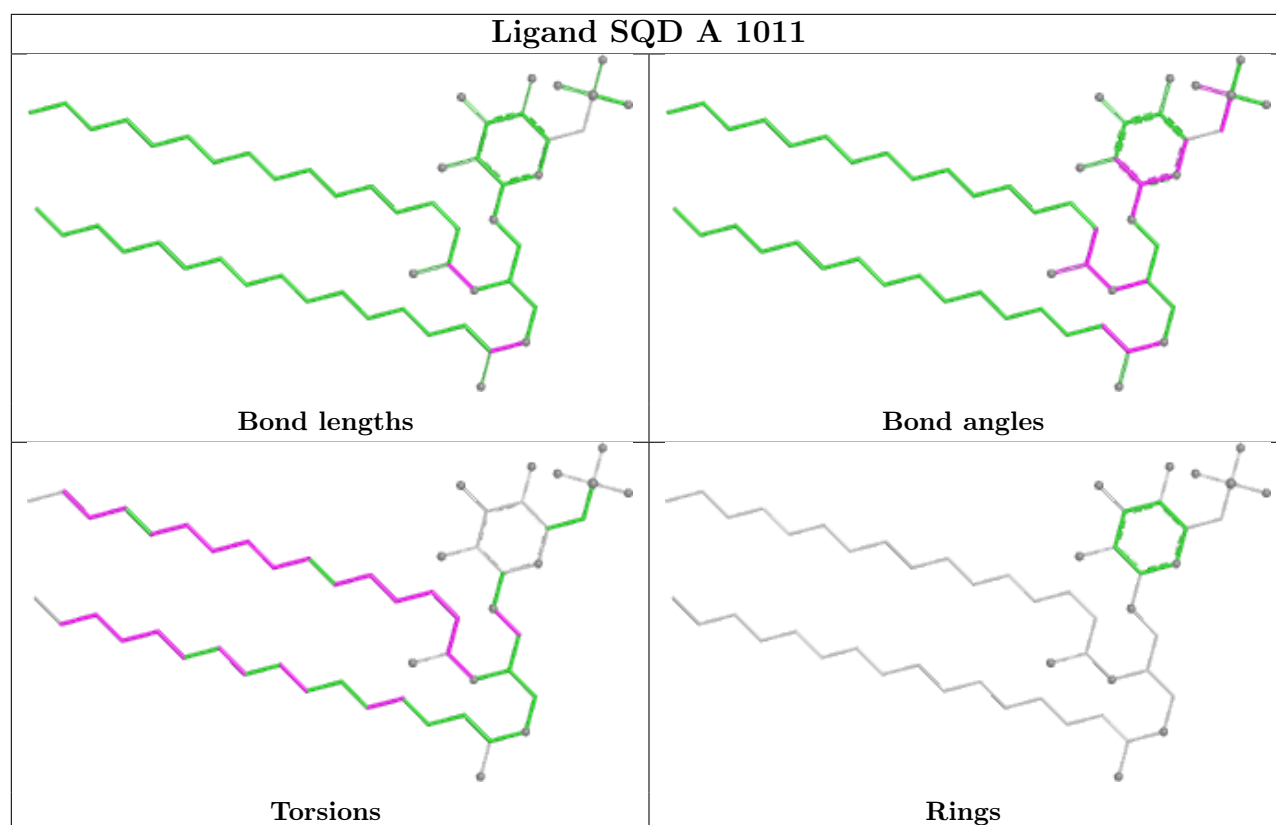


Ligand CLA D 403









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	334/334 (100%)	-0.56	1 (0%) 90 91	16, 25, 41, 64	5 (1%)
1	a	334/334 (100%)	-0.40	2 (0%) 85 87	17, 27, 51, 72	4 (1%)
2	B	505/505 (100%)	-0.41	7 (1%) 73 75	17, 29, 49, 69	10 (1%)
2	b	505/505 (100%)	-0.25	16 (3%) 50 53	17, 31, 59, 88	9 (1%)
3	C	451/451 (100%)	-0.36	4 (0%) 81 83	15, 33, 47, 72	3 (0%)
3	c	450/451 (99%)	-0.11	1 (0%) 91 92	18, 37, 51, 68	2 (0%)
4	D	342/342 (100%)	-0.58	1 (0%) 90 91	18, 26, 39, 88	0
4	d	342/342 (100%)	-0.47	1 (0%) 90 91	21, 29, 46, 80	0
5	E	80/80 (100%)	0.37	6 (7%) 20 21	21, 43, 65, 74	2 (2%)
5	e	78/80 (97%)	0.51	2 (2%) 57 60	35, 47, 68, 75	0
6	F	34/34 (100%)	-0.08	0 100 100	29, 34, 55, 67	0
6	f	32/34 (94%)	0.14	2 (6%) 26 27	33, 40, 69, 78	0
7	H	63/63 (100%)	-0.07	1 (1%) 70 73	21, 36, 45, 54	1 (1%)
7	h	63/63 (100%)	0.12	1 (1%) 70 73	30, 39, 49, 56	0
8	I	35/36 (97%)	0.09	1 (2%) 53 56	32, 37, 71, 87	0
8	i	35/36 (97%)	0.15	2 (5%) 29 31	32, 37, 71, 92	0
9	J	37/37 (100%)	0.16	3 (8%) 18 19	28, 37, 84, 92	0
9	j	37/37 (100%)	0.32	3 (8%) 18 19	33, 44, 68, 75	0
10	K	37/37 (100%)	-0.19	0 100 100	33, 38, 50, 52	0
10	k	37/37 (100%)	0.24	0 100 100	38, 44, 61, 71	0
11	L	37/37 (100%)	-0.43	1 (2%) 56 59	21, 24, 57, 73	0
11	l	37/37 (100%)	-0.43	1 (2%) 56 59	22, 25, 63, 88	0
12	M	33/34 (97%)	-0.40	1 (3%) 52 55	16, 27, 51, 76	1 (3%)
12	m	33/34 (97%)	-0.36	0 100 100	16, 29, 52, 65	1 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.10	9 (3%) 45 47	20, 37, 68, 88	2 (0%)
13	o	243/244 (99%)	0.02	6 (2%) 58 61	24, 38, 68, 78	1 (0%)
14	T	30/31 (96%)	-0.42	1 (3%) 49 51	22, 27, 56, 84	0
14	t	29/31 (93%)	-0.39	1 (3%) 48 50	23, 27, 53, 66	0
15	U	97/97 (100%)	-0.28	0 100 100	24, 31, 48, 66	1 (1%)
15	u	97/97 (100%)	-0.33	0 100 100	24, 32, 42, 71	1 (1%)
16	V	137/137 (100%)	-0.45	0 100 100	21, 30, 43, 62	3 (2%)
16	v	137/137 (100%)	0.02	0 100 100	22, 40, 57, 66	2 (1%)
17	Y	30/30 (100%)	0.29	1 (3%) 49 51	40, 47, 58, 63	0
17	y	30/30 (100%)	0.56	0 100 100	45, 56, 69, 75	0
18	X	40/40 (100%)	0.39	2 (5%) 34 36	33, 40, 65, 80	0
18	x	39/40 (97%)	0.53	3 (7%) 19 21	38, 47, 76, 83	0
19	Z	61/62 (98%)	0.63	6 (9%) 13 13	37, 45, 77, 86	0
19	z	61/62 (98%)	1.15	7 (11%) 9 10	49, 59, 90, 96	0
20	R	34/34 (100%)	2.48	27 (79%) 0 0	71, 86, 100, 101	0
All	All	5280/5296 (99%)	-0.20	120 (2%) 61 64	15, 32, 60, 101	48 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	5.7
7	h	64	ALA	5.2
2	b	486	LEU	4.3
2	b	85	GLY	4.3
20	R	20	VAL	4.2
19	Z	33	TRP	4.1
18	X	41	LEU	4.1
20	R	24	LEU	4.1
5	e	61	ARG	4.0
9	J	5	GLY	4.0
5	e	83	LEU	4.0
20	R	28	VAL	3.9
20	R	35	LEU	3.8
2	b	494	GLY	3.8
20	R	31	VAL	3.6
3	C	23	ALA	3.6
20	R	18	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
13	O	60	ARG	3.3
19	z	61	VAL	3.3
1	a	11	ALA	3.3
5	E	83	LEU	3.3
20	R	23	ILE	3.3
19	z	33	TRP	3.2
13	O	58	ASN	3.2
5	E	4	THR	3.2
7	H	64	ALA	3.2
18	x	2	THR	3.1
2	b	84	THR	3.1
5	E	61	ARG	3.1
20	R	6	LEU	3.1
13	O	35	SER	3.0
9	j	4	GLU	3.0
2	b	491	VAL	3.0
19	z	3	ILE	3.0
2	b	495	PHE	3.0
20	R	7	VAL	2.9
6	f	14	PRO	2.9
20	R	9	LEU	2.9
2	b	86	ILE	2.9
18	X	2	THR	2.9
13	o	58	ASN	2.9
20	R	15	ALA	2.9
20	R	25	PRO	2.8
9	J	4	GLU	2.8
13	O	59	LYS	2.8
2	b	503	THR	2.8
9	J	6	GLY	2.7
20	R	16	ALA	2.7
20	R	10	LEU	2.7
20	R	13	LEU	2.7
3	C	145	SER	2.7
8	I	36	ASP	2.7
3	c	24	THR	2.6
14	T	30	THR	2.6
20	R	34	LEU	2.6
8	i	36	ASP	2.6
2	b	502	VAL	2.6
20	R	5	VAL	2.6
13	O	36	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
20	R	17	GLY	2.6
13	o	246	ALA	2.6
11	l	1	MET	2.5
13	o	35	SER	2.5
2	B	500	GLY	2.5
2	b	505[A]	ARG	2.5
5	E	76	VAL	2.4
19	Z	62	VAL	2.4
2	b	484	PRO	2.4
20	R	27	ALA	2.4
13	o	23	ASP	2.4
14	t	29	ILE	2.4
1	A	11	ALA	2.4
2	b	129	GLY	2.4
20	R	30	GLN	2.4
20	R	12	VAL	2.4
20	R	19	ALA	2.4
6	f	15	ILE	2.4
4	D	12	ARG	2.4
5	E	72	ALA	2.3
9	j	6	GLY	2.3
13	o	60	ARG	2.3
19	z	60	PHE	2.3
19	Z	36	SER	2.3
19	Z	30	PRO	2.3
19	Z	41	PHE	2.3
2	B	86	ILE	2.3
20	R	3	TRP	2.3
2	b	487	SER	2.2
2	b	479	PHE	2.2
19	z	30	PRO	2.2
19	Z	31	GLN	2.2
2	B	495	PHE	2.2
2	b	493	TRP	2.2
5	E	79	PHE	2.2
20	R	14	LEU	2.2
4	d	12	ARG	2.1
13	o	89	SER	2.1
8	i	33	LYS	2.1
2	B	496	TYR	2.1
20	R	26	TYR	2.1
17	Y	19	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
9	j	5	GLY	2.1
11	L	1	MET	2.1
19	z	5	PHE	2.1
18	x	37	VAL	2.1
1	a	251	ALA	2.1
3	C	24	THR	2.1
13	O	28	GLY	2.1
20	R	8	VAL	2.1
13	O	29	ALA	2.1
13	O	246	ALA	2.1
3	C	25	ASN	2.0
13	O	132	ASN	2.0
12	M	33	GLN	2.0
18	x	35	ASP	2.0
2	B	84	THR	2.0
20	R	11	PRO	2.0
2	B	293	ALA	2.0
2	B	484	PRO	2.0
2	b	496	TYR	2.0

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

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
19	FME	Z	1	10/11	0.81	0.16	69,71,74,78	0
19	FME	z	1	10/11	0.81	0.14	87,91,94,95	0
14	FME	t	1	10/11	0.93	0.09	28,30,46,49	0
12	FME	M	1	10/11	0.94	0.08	33,36,43,49	0
14	FME	T	1	10/11	0.95	0.08	27,29,44,46	0
12	FME	m	1	10/11	0.95	0.09	35,38,49,54	0
8	FME	i	1	10/11	0.96	0.07	36,38,40,40	0
8	FME	I	1	10/11	0.97	0.07	34,39,40,40	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	DMS	b	635	4/4	0.59	0.21	66,70,72,74	0
35	HTG	d	416	19/19	0.60	0.17	70,92,94,96	0
32	LMT	a	402	35/35	0.62	0.18	52,65,69,70	0
31	UNL	A	1015	28/-	0.64	0.18	62,73,78,78	0
31	UNL	a	419	30/-	0.64	0.19	62,74,87,89	0
28	SQD	B	620[B]	54/54	0.64	0.18	40,54,66,66	54
28	SQD	B	620[A]	54/54	0.64	0.18	42,56,75,76	54
32	LMT	A	1017	35/35	0.66	0.18	54,72,75,80	0
31	UNL	t	102	16/-	0.66	0.15	68,72,74,74	0
32	LMT	f	103	35/35	0.66	0.17	71,92,104,104	0
31	UNL	y	102	16/-	0.66	0.19	63,65,67,67	0
35	HTG	D	419	19/19	0.67	0.16	59,79,83,84	0
35	HTG	b	630	19/19	0.67	0.20	66,83,88,90	0
34	LHG	e	101	49/49	0.67	0.16	66,97,101,102	0
32	LMT	m	103	35/35	0.68	0.17	55,90,100,101	0
35	HTG	b	602	19/19	0.69	0.16	60,89,94,94	0
33	GOL	d	417	6/6	0.70	0.16	58,61,62,62	0
35	HTG	B	624	19/19	0.70	0.16	58,86,92,92	0
33	GOL	v	204	6/6	0.70	0.15	74,75,76,76	0
32	LMT	A	1018	35/35	0.71	0.16	51,93,113,116	0
32	LMT	C	520	35/35	0.71	0.15	68,75,79,79	0
35	HTG	d	410	19/19	0.71	0.16	74,84,91,91	0
32	LMT	i	102	35/35	0.71	0.16	52,88,111,111	0
31	UNL	K	103	34/-	0.72	0.16	57,76,82,83	0
31	UNL	b	603	16/-	0.72	0.18	64,67,71,71	0
31	UNL	Y	101	16/-	0.72	0.18	66,68,70,70	0
35	HTG	B	629	19/19	0.72	0.14	52,86,90,90	0
35	HTG	D	413	19/19	0.72	0.16	69,80,85,86	0
30	DMS	O	301	4/4	0.73	0.23	72,73,75,76	0
28	SQD	b	623[A]	54/54	0.73	0.17	41,53,70,71	54
33	GOL	b	632	6/6	0.73	0.14	51,56,61,63	0
28	SQD	b	623[B]	54/54	0.73	0.17	49,57,77,80	54
31	UNL	D	414	40/-	0.73	0.16	48,58,72,73	0
35	HTG	c	522	19/19	0.73	0.16	82,85,89,90	0
31	UNL	j	101	16/-	0.73	0.17	58,60,62,63	0
31	UNL	J	102	16/-	0.73	0.16	50,52,58,59	0
31	UNL	d	411	36/-	0.74	0.15	46,56,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LHG	E	101	49/49	0.74	0.15	51,77,83,85	0
32	LMT	M	101	35/35	0.74	0.14	52,85,95,97	0
33	GOL	V	207	6/6	0.74	0.14	60,63,64,64	0
29	LMG	c	521	51/55	0.74	0.17	53,81,93,97	0
31	UNL	b	627	16/-	0.74	0.15	47,48,50,50	0
35	HTG	c	525	19/19	0.75	0.14	76,90,95,96	0
35	HTG	C	522	19/19	0.75	0.16	65,75,80,80	0
29	LMG	Z	101	51/55	0.75	0.17	47,77,104,110	0
33	GOL	D	418	6/6	0.76	0.12	70,72,73,74	0
32	LMT	a	416	35/35	0.76	0.13	73,75,79,79	0
28	SQD	f	102	43/54	0.76	0.17	61,80,89,91	0
32	LMT	b	625	35/35	0.77	0.14	52,82,103,104	0
31	UNL	c	523	32/-	0.77	0.14	63,75,84,87	0
35	HTG	V	202	19/19	0.77	0.16	56,63,77,77	0
29	LMG	c	520	51/55	0.78	0.14	42,74,84,89	0
30	DMS	b	634	4/4	0.78	0.21	61,63,65,68	0
31	UNL	l	101	16/-	0.78	0.16	49,58,68,69	0
32	LMT	t	103	35/35	0.78	0.15	46,75,96,99	0
27	PL9	a	414	55/55	0.78	0.16	53,63,77,78	0
33	GOL	V	204	6/6	0.78	0.15	57,58,59,60	0
29	LMG	C	519	51/55	0.79	0.14	38,74,84,85	0
31	UNL	I	101	13/-	0.79	0.14	54,56,56,57	0
27	PL9	A	1010	55/55	0.79	0.14	43,55,72,72	0
32	LMT	b	631	35/35	0.80	0.15	40,74,94,96	0
35	HTG	C	521	19/19	0.80	0.13	69,71,74,75	0
32	LMT	B	623	35/35	0.80	0.13	48,65,71,72	0
31	UNL	i	101	16/-	0.81	0.15	55,57,62,62	0
30	DMS	V	205	4/4	0.81	0.17	61,62,64,65	0
33	GOL	d	415	6/6	0.81	0.10	63,66,66,67	0
31	UNL	B	625	16/-	0.81	0.13	44,46,52,54	0
30	DMS	a	418	4/4	0.81	0.20	62,63,66,69	0
32	LMT	m	101	35/35	0.82	0.12	38,51,56,57	0
30	DMS	C	525	4/4	0.82	0.19	71,73,73,74	0
30	DMS	B	633	4/4	0.82	0.18	67,69,70,75	0
30	DMS	B	634	4/4	0.82	0.20	54,57,59,59	0
30	DMS	c	528	4/4	0.82	0.24	83,85,86,88	0
31	UNL	B	630	16/-	0.83	0.13	53,56,60,60	0
28	SQD	A	1016	54/54	0.83	0.12	46,60,72,73	0
33	GOL	B	631	6/6	0.84	0.13	56,57,60,62	0
30	DMS	d	413	4/4	0.84	0.17	57,62,62,63	0
29	LMG	A	1012	51/55	0.84	0.12	49,56,67,71	0
30	DMS	C	527	4/4	0.84	0.19	75,75,77,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	GOL	a	420	6/6	0.84	0.12	53,56,57,59	0
31	UNL	X	101	16/-	0.84	0.12	39,43,51,51	0
30	DMS	A	1014	4/4	0.85	0.17	54,54,55,61	0
28	SQD	a	401	54/54	0.85	0.11	42,60,74,76	0
29	LMG	B	622	51/55	0.85	0.11	38,47,58,64	0
32	LMT	M	102	35/35	0.85	0.11	39,58,64,66	0
35	HTG	b	626	19/19	0.85	0.13	43,48,51,51	0
35	HTG	B	628	19/19	0.86	0.13	45,68,72,74	0
31	UNL	L	101	16/-	0.86	0.15	53,56,63,63	0
29	LMG	C	518	51/55	0.86	0.12	36,62,70,70	0
29	LMG	a	415	51/55	0.86	0.10	50,60,70,71	0
31	UNL	d	412	16/-	0.86	0.13	48,53,62,63	0
29	LMG	c	519	51/55	0.86	0.11	45,62,77,80	0
28	SQD	c	518	54/54	0.86	0.13	41,59,74,76	0
35	HTG	o	301	19/19	0.86	0.12	47,49,53,53	0
28	SQD	D	408	43/54	0.87	0.14	41,67,74,76	0
31	UNL	x	101	16/-	0.87	0.11	41,45,59,60	0
30	DMS	b	633	4/4	0.87	0.15	55,55,56,62	0
31	UNL	I	102	13/-	0.87	0.12	55,57,60,60	0
33	GOL	v	203	6/6	0.87	0.11	48,52,53,53	0
30	DMS	O	302	4/4	0.87	0.18	58,59,62,62	0
24	CLA	b	604	65/65	0.87	0.11	40,48,69,70	0
30	DMS	c	527	4/4	0.87	0.15	65,65,66,66	0
33	GOL	A	1019	6/6	0.88	0.14	60,61,62,62	0
26	BCR	d	404	40/40	0.88	0.09	31,36,59,59	0
31	UNL	D	415	16/-	0.88	0.10	39,42,48,49	0
29	LMG	m	102	51/55	0.88	0.10	35,49,57,59	0
33	GOL	V	206	6/6	0.88	0.10	53,56,57,58	0
35	HTG	b	601	19/19	0.89	0.10	44,60,67,67	0
26	BCR	D	406	40/40	0.89	0.10	28,32,50,51	0
30	DMS	C	526	4/4	0.89	0.18	71,71,72,72	0
30	DMS	d	414	4/4	0.89	0.17	58,59,59,60	0
26	BCR	J	101	40/40	0.89	0.08	35,37,41,41	0
30	DMS	D	416	4/4	0.89	0.16	55,55,56,59	0
26	BCR	K	102	40/40	0.89	0.09	39,49,52,52	0
30	DMS	c	526	4/4	0.89	0.18	73,74,74,75	0
24	CLA	c	513	65/65	0.89	0.11	45,54,69,70	0
24	CLA	C	513	65/65	0.90	0.10	41,48,66,68	0
28	SQD	A	1011	54/54	0.90	0.12	43,57,69,69	0
24	CLA	C	506	65/65	0.90	0.09	36,43,73,76	0
26	BCR	h	101	40/40	0.90	0.09	32,39,47,48	0
30	DMS	D	417	4/4	0.90	0.16	57,58,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	k	102	40/40	0.90	0.09	48,54,64,66	0
24	CLA	c	506	65/65	0.90	0.10	38,40,78,81	0
30	DMS	U	201	4/4	0.90	0.14	56,56,58,58	0
29	LMG	D	412	51/55	0.91	0.10	27,38,77,78	0
26	BCR	t	101	40/40	0.91	0.07	26,39,46,47	0
26	BCR	y	101	40/40	0.91	0.08	40,44,46,47	0
24	CLA	B	601	65/65	0.91	0.10	34,42,66,69	0
26	BCR	K	101	40/40	0.91	0.08	32,35,37,38	0
26	BCR	B	618	40/40	0.91	0.07	27,32,41,41	0
29	LMG	d	409	51/55	0.91	0.10	33,42,72,76	0
26	BCR	B	619	40/40	0.91	0.08	31,34,42,43	0
24	CLA	c	512	65/65	0.91	0.10	42,46,65,67	0
26	BCR	k	101	40/40	0.91	0.09	36,45,47,48	0
26	BCR	H	101	40/40	0.91	0.08	27,36,42,42	0
26	BCR	c	514	40/40	0.92	0.08	34,41,43,44	0
24	CLA	c	507	65/65	0.92	0.09	33,34,50,51	0
30	DMS	u	201	4/4	0.92	0.12	56,57,57,59	0
30	DMS	v	202	4/4	0.92	0.14	55,56,58,58	0
26	BCR	T	101	40/40	0.92	0.07	27,37,42,43	0
26	BCR	a	413	40/40	0.92	0.07	24,30,34,34	0
26	BCR	b	622	40/40	0.92	0.08	33,36,40,41	0
34	LHG	d	406	49/49	0.92	0.09	38,41,46,46	0
34	LHG	d	408	49/49	0.92	0.11	32,41,72,74	0
36	DGD	c	516	62/66	0.92	0.09	36,42,75,79	0
36	DGD	h	102	62/66	0.92	0.09	32,38,46,48	0
24	CLA	B	606	65/65	0.93	0.08	27,30,51,53	0
24	CLA	C	512	65/65	0.93	0.08	39,42,71,72	0
30	DMS	B	632	4/4	0.93	0.15	57,58,60,61	0
24	CLA	c	508	65/65	0.93	0.08	32,35,65,72	0
24	CLA	B	616	65/65	0.93	0.10	27,31,79,80	0
30	DMS	C	524	4/4	0.93	0.18	40,41,41,42	0
24	CLA	C	504	65/65	0.93	0.08	27,30,55,57	0
34	LHG	D	409	49/49	0.93	0.09	35,38,43,45	0
34	LHG	D	411	49/49	0.93	0.10	29,38,73,76	0
26	BCR	A	1009	40/40	0.93	0.07	25,29,32,32	0
26	BCR	B	617	40/40	0.93	0.06	28,30,33,33	0
24	CLA	b	612	65/65	0.93	0.08	30,34,37,38	0
24	CLA	b	619	65/65	0.93	0.09	31,35,80,81	0
26	BCR	C	514	40/40	0.93	0.07	31,38,41,41	0
36	DGD	C	515	62/66	0.93	0.08	27,36,63,64	0
36	DGD	H	102	62/66	0.93	0.08	27,34,38,39	0
36	DGD	c	515	62/66	0.93	0.09	28,38,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	501	65/65	0.93	0.08	35,36,43,44	0
24	CLA	c	504	65/65	0.93	0.07	32,35,57,59	0
39	MG	k	103	1/1	0.93	0.06	45,45,45,45	0
24	CLA	C	507	65/65	0.94	0.08	34,37,51,53	0
24	CLA	b	605	65/65	0.94	0.07	29,32,37,37	0
24	CLA	b	609	65/65	0.94	0.07	29,32,65,68	0
24	CLA	C	508	65/65	0.94	0.07	28,31,65,70	0
24	CLA	d	403	65/65	0.94	0.08	31,34,76,77	0
30	DMS	c	529	4/4	0.94	0.17	51,51,53,54	0
25	PHO	a	411	64/64	0.94	0.07	24,30,35,36	0
26	BCR	b	620	40/40	0.94	0.06	28,34,35,35	0
26	BCR	b	621	40/40	0.94	0.06	28,31,41,42	0
24	CLA	C	511	65/65	0.94	0.07	29,35,40,42	0
36	DGD	C	516	62/66	0.94	0.08	28,36,70,72	0
24	CLA	C	505	65/65	0.94	0.07	32,35,44,48	0
24	CLA	c	503	65/65	0.94	0.07	33,39,42,44	0
24	CLA	B	614	65/65	0.94	0.08	24,27,67,68	0
36	DGD	c	517	62/66	0.94	0.08	29,38,64,73	0
24	CLA	c	505	65/65	0.94	0.07	34,36,48,48	0
37	BCT	D	401	4/4	0.94	0.10	37,38,38,41	0
24	CLA	D	405	65/65	0.94	0.08	28,30,70,71	0
24	CLA	c	509	65/65	0.95	0.08	33,35,50,51	0
24	CLA	c	510	65/65	0.95	0.07	33,35,41,43	0
30	DMS	V	203	4/4	0.95	0.11	50,51,51,52	0
24	CLA	c	511	65/65	0.95	0.07	36,39,43,46	0
24	CLA	B	615	65/65	0.95	0.07	27,28,44,46	0
24	CLA	b	608	65/65	0.95	0.07	24,26,35,35	0
24	CLA	A	1008	65/65	0.95	0.08	25,27,79,81	0
25	PHO	D	404	64/64	0.95	0.06	22,25,29,30	0
24	CLA	C	509	65/65	0.95	0.08	28,31,52,53	0
24	CLA	b	613	65/65	0.95	0.07	28,31,38,40	0
24	CLA	b	614	65/65	0.95	0.07	24,26,40,41	0
27	PL9	D	407	55/55	0.95	0.06	21,25,32,33	0
24	CLA	b	615	65/65	0.95	0.07	25,28,32,35	0
27	PL9	d	405	55/55	0.95	0.06	21,27,32,33	0
24	CLA	b	617	65/65	0.95	0.08	24,28,67,68	0
24	CLA	C	510	65/65	0.95	0.06	27,31,38,39	0
24	CLA	C	501	65/65	0.95	0.06	31,35,41,42	0
24	CLA	c	502	65/65	0.95	0.07	28,31,50,51	0
24	CLA	C	503	65/65	0.95	0.06	28,33,36,38	0
24	CLA	B	609	65/65	0.95	0.06	28,31,33,35	0
36	DGD	C	517	62/66	0.95	0.08	24,33,62,69	0

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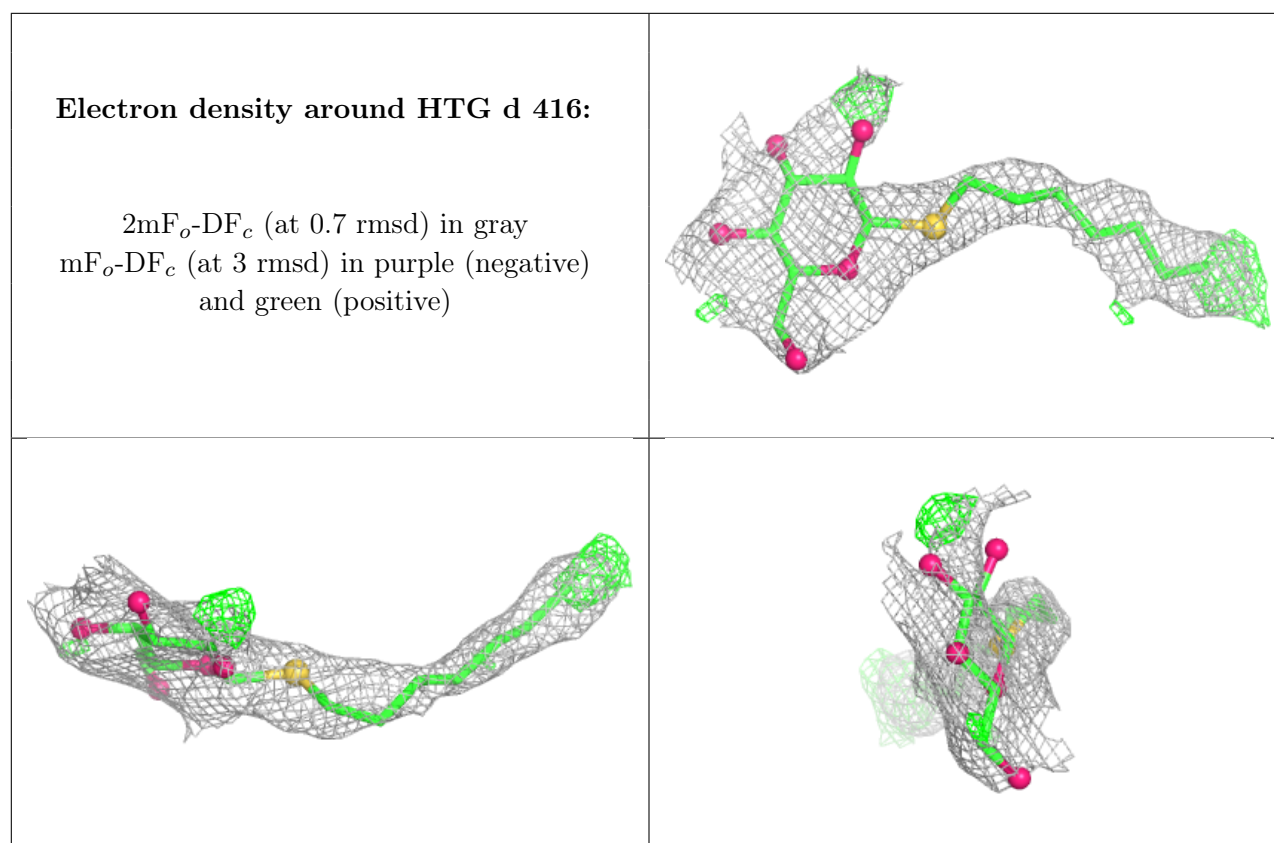
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LHG	D	410	49/49	0.95	0.07	26,30,38,41	0
24	CLA	B	610	65/65	0.95	0.07	24,26,34,36	0
24	CLA	a	409	65/65	0.95	0.08	24,26,85,90	0
34	LHG	b	624	49/49	0.95	0.07	27,32,48,53	0
24	CLA	a	412	65/65	0.95	0.10	26,28,90,92	0
34	LHG	d	407	49/49	0.95	0.07	26,31,40,45	0
24	CLA	B	602	65/65	0.95	0.06	25,27,34,35	0
24	CLA	b	610	65/65	0.96	0.06	23,25,34,35	0
24	CLA	b	611	65/65	0.96	0.06	26,28,38,39	0
24	CLA	B	607	65/65	0.96	0.06	20,22,36,37	0
24	CLA	C	502	65/65	0.96	0.06	26,28,42,44	0
24	CLA	B	608	65/65	0.96	0.06	25,27,31,31	0
25	PHO	A	1007	64/64	0.96	0.05	21,24,26,28	0
24	CLA	D	402	65/65	0.96	0.06	17,20,35,37	0
24	CLA	b	616	65/65	0.96	0.06	25,25,50,52	0
24	CLA	D	403	65/65	0.96	0.05	18,20,29,33	0
34	LHG	B	621	49/49	0.96	0.06	26,32,45,49	0
24	CLA	b	618	65/65	0.96	0.06	30,32,44,46	0
24	CLA	A	1005	65/65	0.96	0.06	17,20,29,33	0
24	CLA	a	407	65/65	0.96	0.06	21,23,30,35	0
30	DMS	b	629	4/4	0.96	0.10	48,49,52,53	0
24	CLA	B	603	65/65	0.96	0.06	25,26,32,34	0
24	CLA	B	611	65/65	0.96	0.06	22,24,36,37	0
24	CLA	B	612	65/65	0.96	0.06	24,26,30,31	0
24	CLA	B	604	65/65	0.96	0.07	22,24,53,55	0
24	CLA	b	606	65/65	0.96	0.06	26,29,35,39	0
30	DMS	B	627	4/4	0.96	0.10	41,41,42,44	0
24	CLA	b	607	65/65	0.96	0.07	24,26,50,51	0
24	CLA	B	605	65/65	0.96	0.06	23,26,31,32	0
37	BCT	d	401	4/4	0.96	0.06	40,40,41,42	0
38	HEM	f	101	43/43	0.96	0.09	42,44,57,63	0
24	CLA	A	1006	65/65	0.96	0.06	22,23,66,69	0
24	CLA	d	402	65/65	0.97	0.06	21,23,39,43	0
30	DMS	b	628	4/4	0.97	0.08	30,31,31,32	0
25	PHO	a	410	64/64	0.97	0.05	22,24,29,31	0
24	CLA	a	408	65/65	0.97	0.05	20,23,31,34	0
24	CLA	B	613	65/65	0.97	0.06	23,25,49,53	0
38	HEM	F	101	43/43	0.97	0.08	39,41,44,46	0
30	DMS	B	626	4/4	0.97	0.07	25,26,26,27	0
38	HEM	v	201	43/43	0.97	0.07	31,32,36,37	0
39	MG	K	104	1/1	0.97	0.03	48,48,48,48	0
39	MG	j	102	1/1	0.97	0.09	37,37,37,37	0

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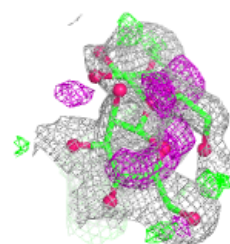
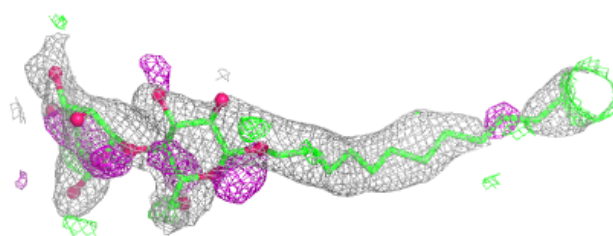
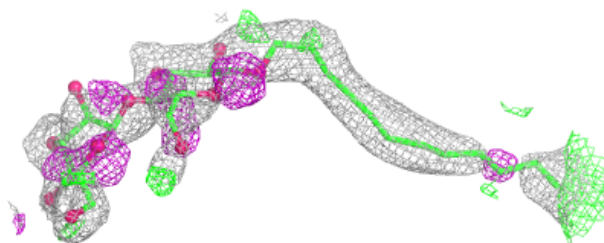
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DMS	c	524	4/4	0.97	0.12	43,43,43,43	0
39	MG	J	103	1/1	0.98	0.03	32,32,32,32	0
38	HEM	V	201	43/43	0.98	0.06	25,26,28,29	0
30	DMS	C	523	4/4	0.98	0.07	36,37,38,38	0
30	DMS	a	417	4/4	0.98	0.07	31,32,33,33	0
21	OER	a	403	10/10	0.99	0.03	27,28,29,31	1
30	DMS	A	1013	4/4	0.99	0.06	29,29,30,31	0
23	CL	a	406	1/1	0.99	0.02	27,27,27,27	0
21	OER	A	1001	10/10	0.99	0.04	24,25,28,28	1
23	CL	a	405	1/1	1.00	0.05	26,26,26,26	0
22	FE2	A	1002	1/1	1.00	0.02	29,29,29,29	0
22	FE2	a	404	1/1	1.00	0.01	29,29,29,29	0
23	CL	A	1003	1/1	1.00	0.05	25,25,25,25	0
23	CL	A	1004	1/1	1.00	0.03	22,22,22,22	0

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

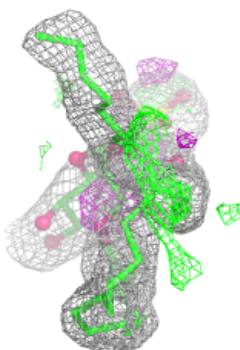
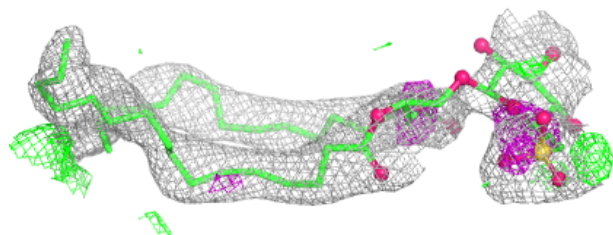
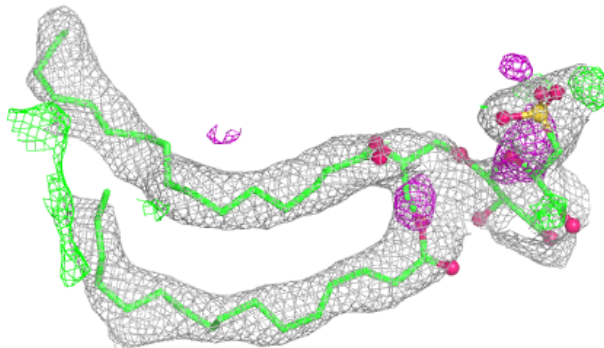


Electron density around LMT a 402:

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

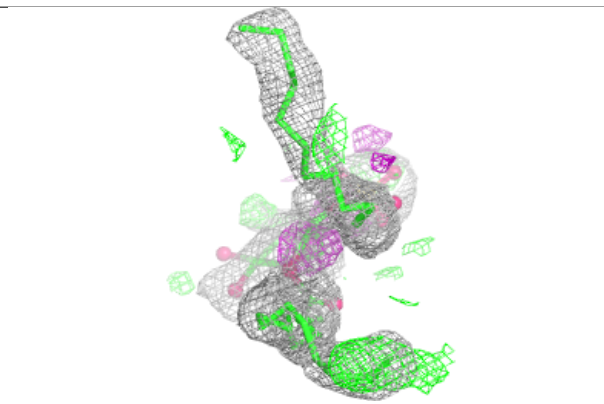
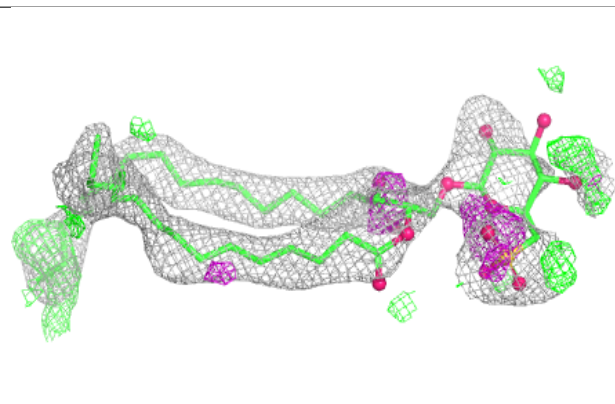
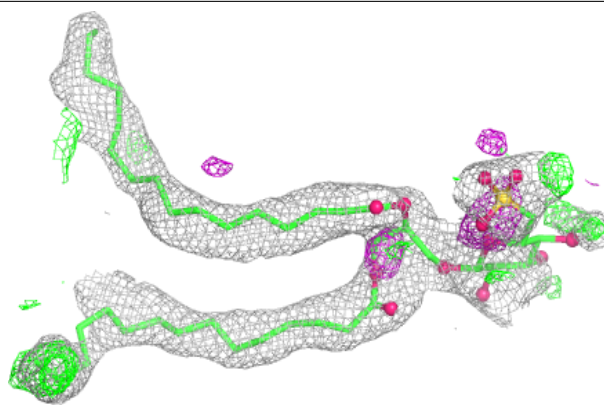
**Electron density around SQD B 620 (B):**

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

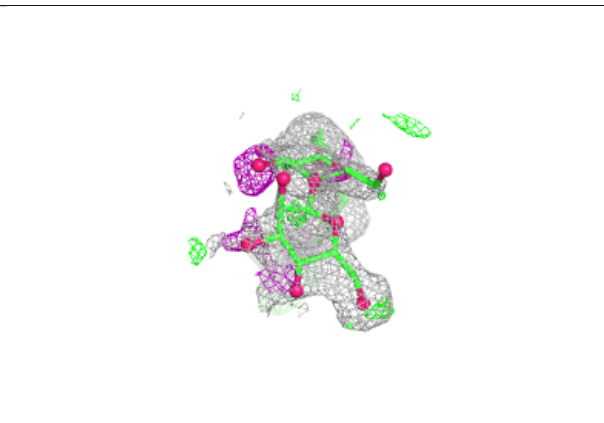
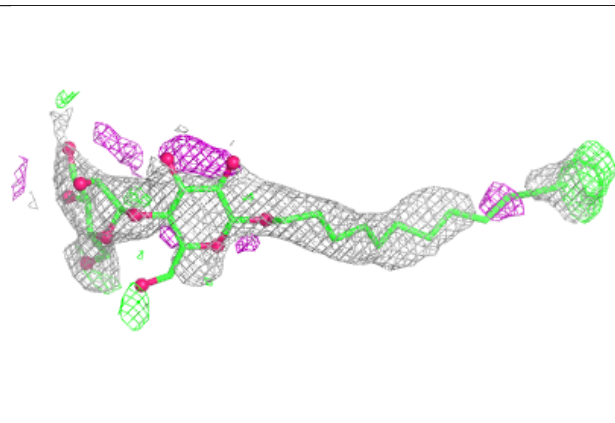
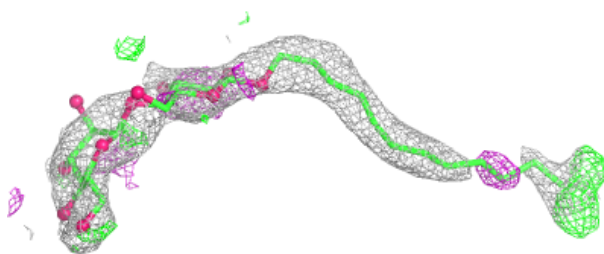


Electron density around SQD B 620 (A):

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

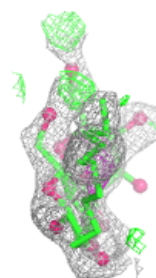
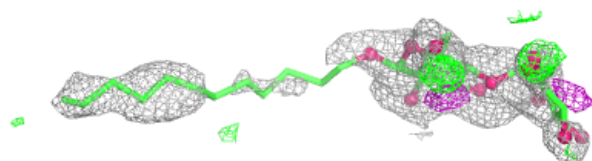
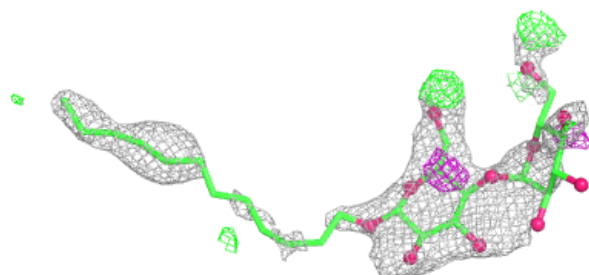
**Electron density around LMT A 1017:**

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

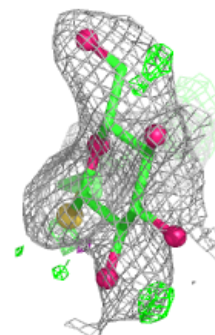
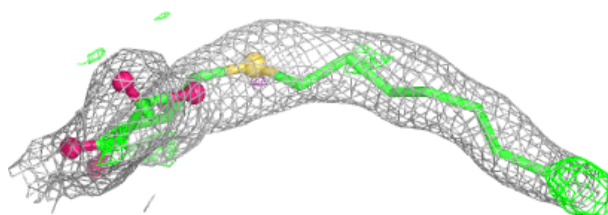


Electron density around LMT f 103:

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

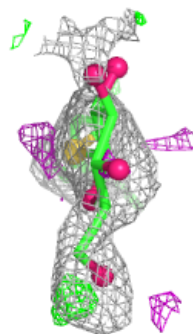
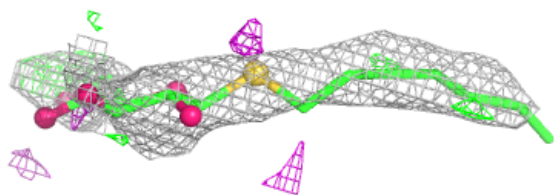
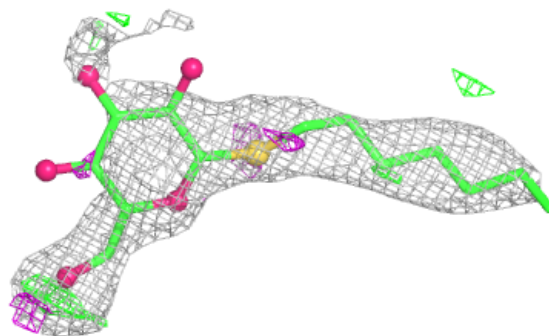
**Electron density around HTG D 419:**

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



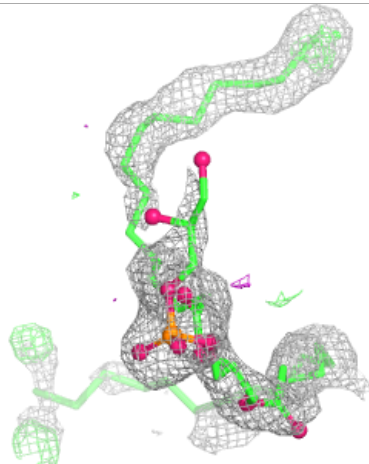
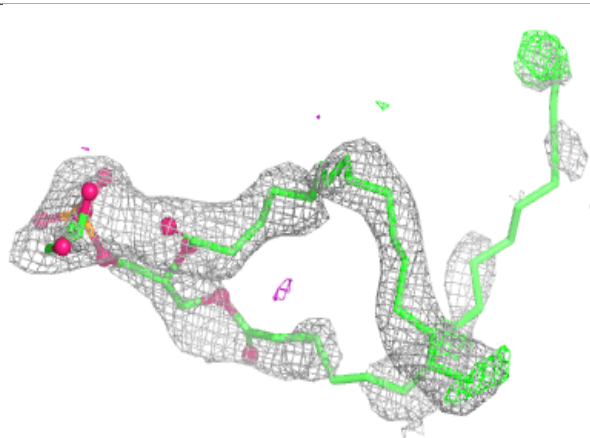
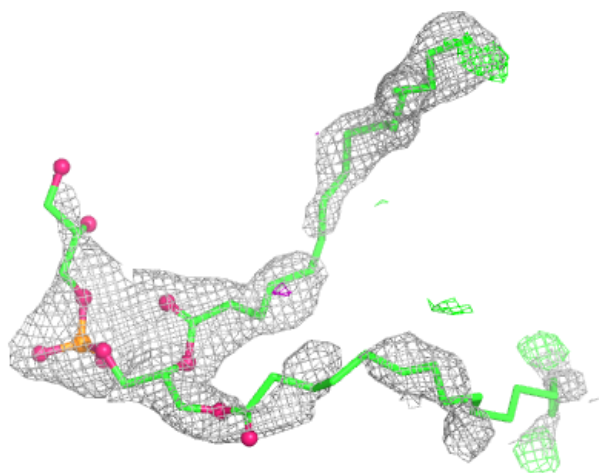
Electron density around HTG b 630:

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



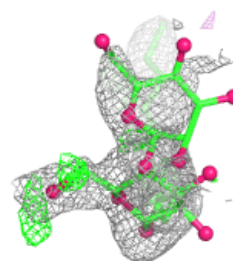
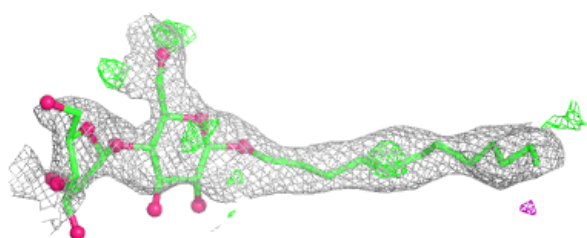
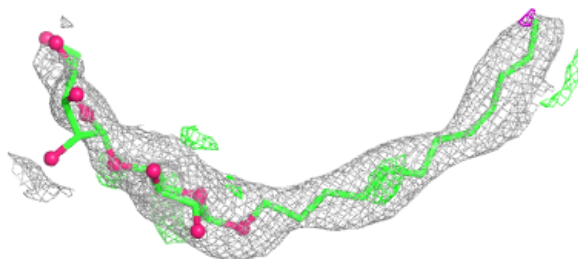
Electron density around LHG e 101:

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

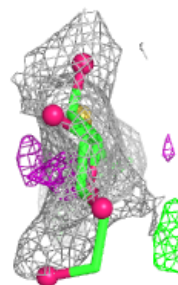
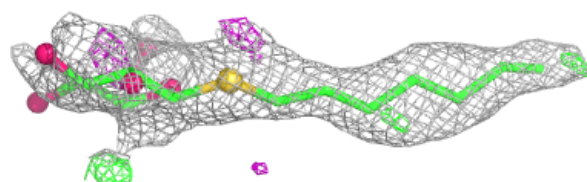
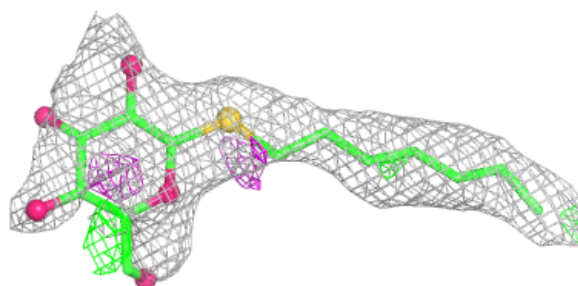


Electron density around LMT m 103:

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

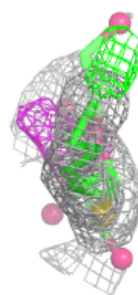
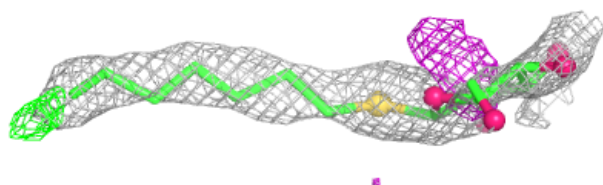
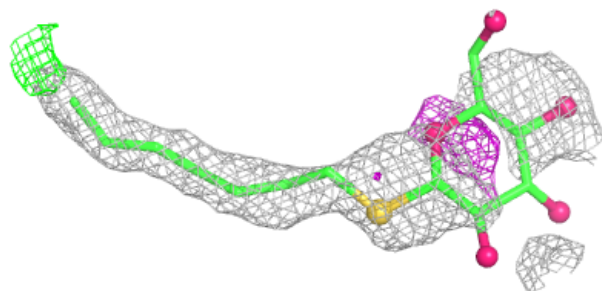
**Electron density around HTG b 602:**

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

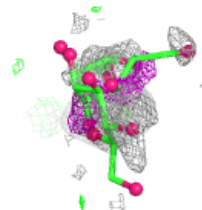
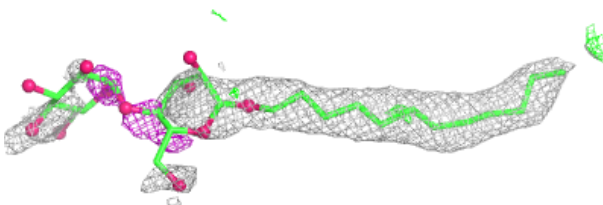
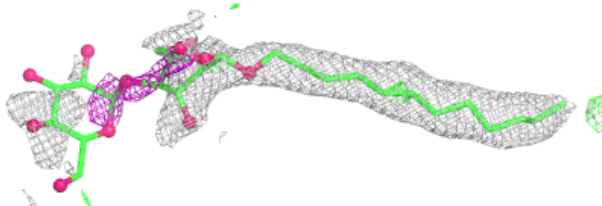


Electron density around HTG B 624:

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

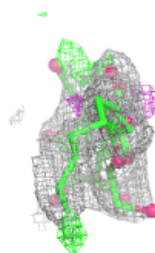
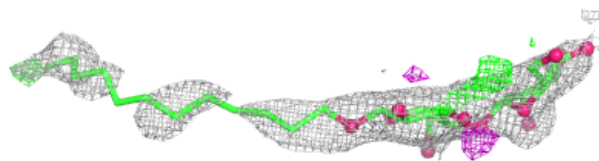
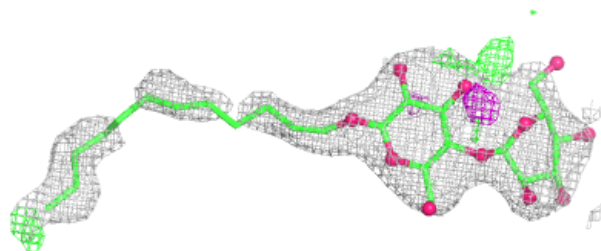
**Electron density around LMT A 1018:**

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

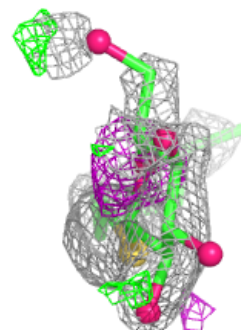
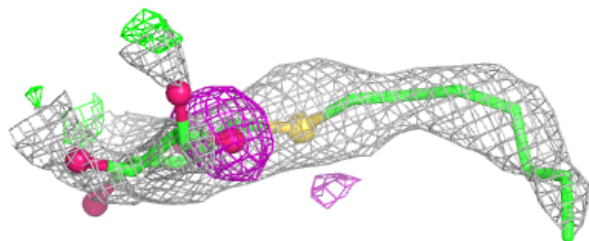
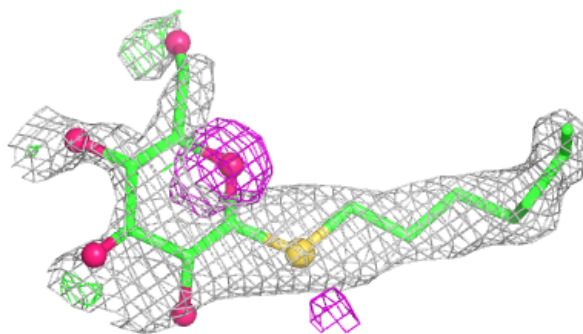


Electron density around LMT C 520:

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

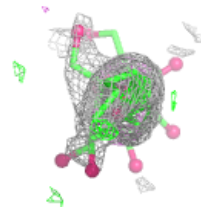
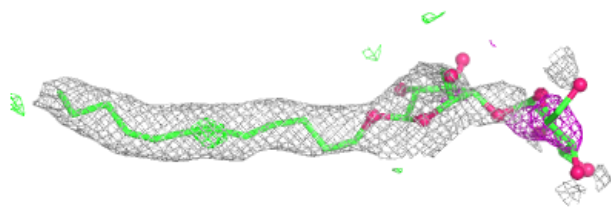
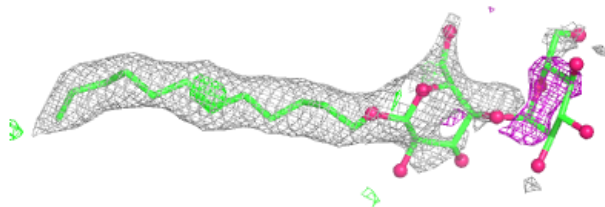
**Electron density around HTG d 410:**

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

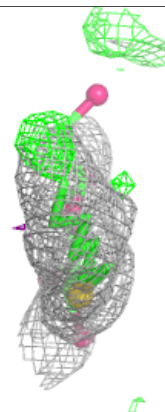
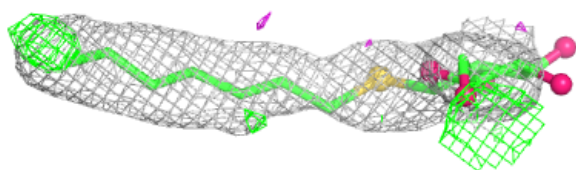
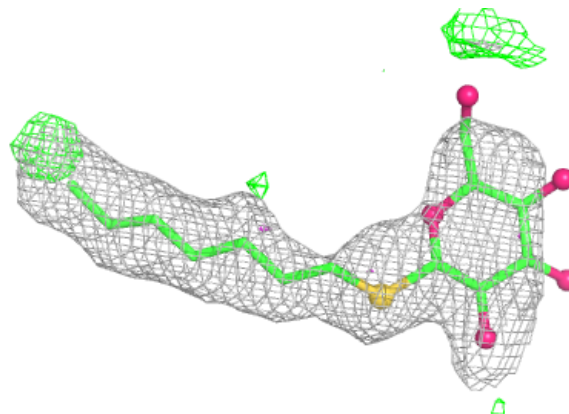


Electron density around LMT i 102:

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

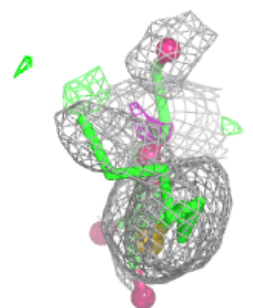
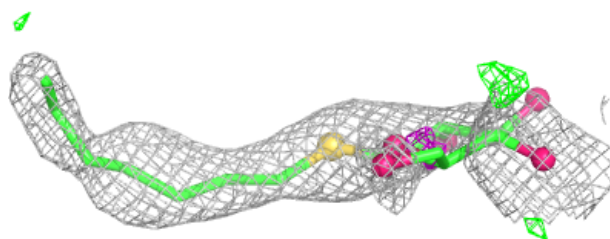
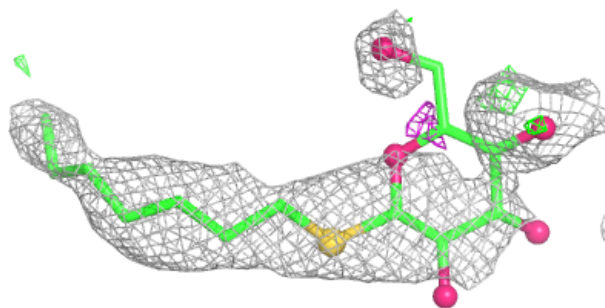
**Electron density around HTG B 629:**

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

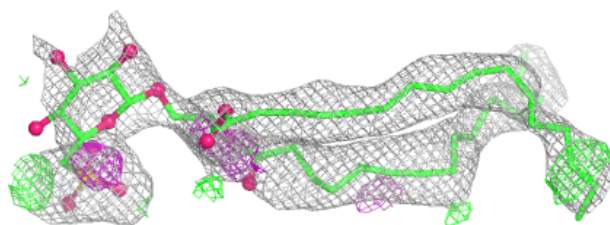
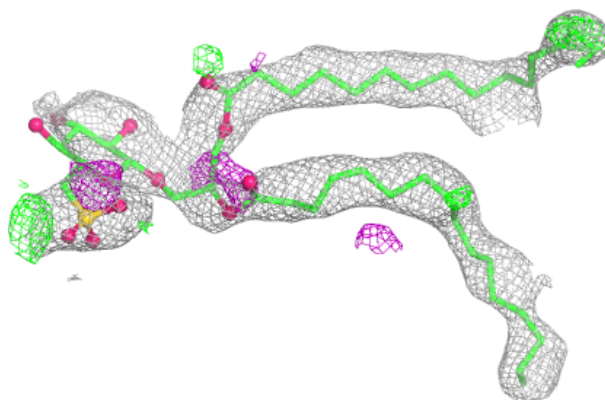


Electron density around HTG D 413:

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

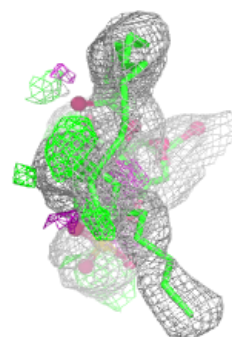
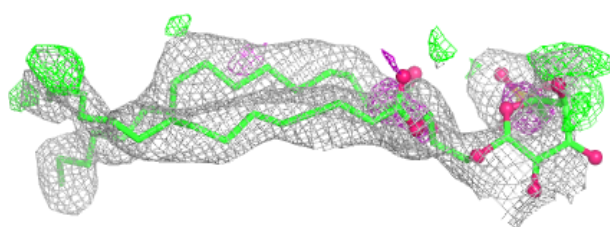
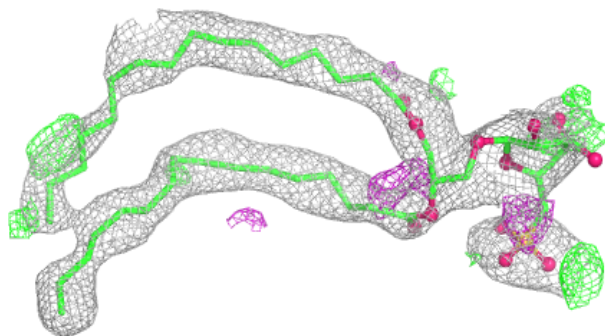
**Electron density around SQD b 623 (A):**

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

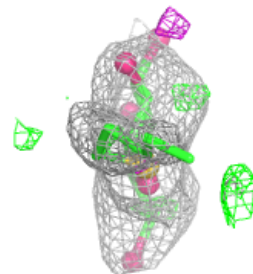
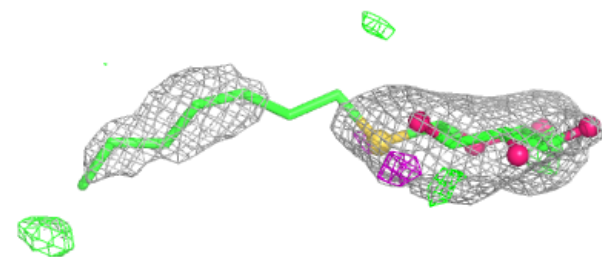
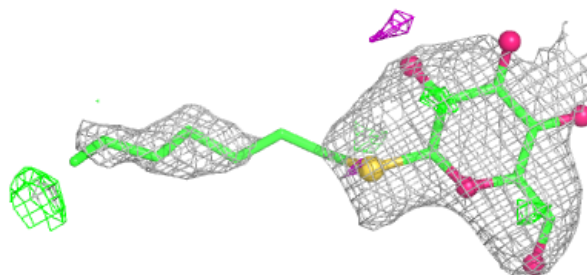


Electron density around SQD b 623 (B):

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

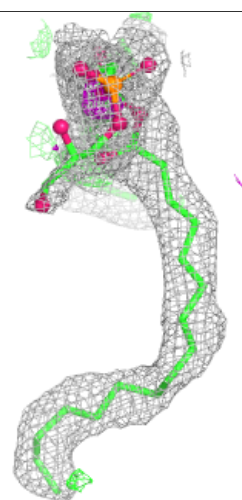
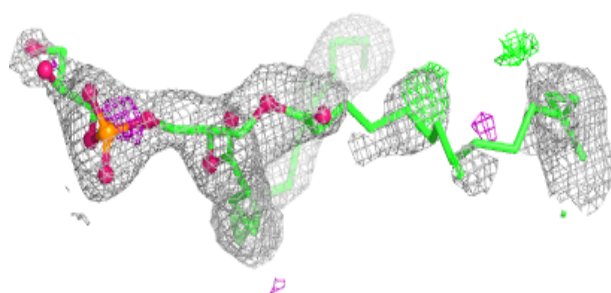
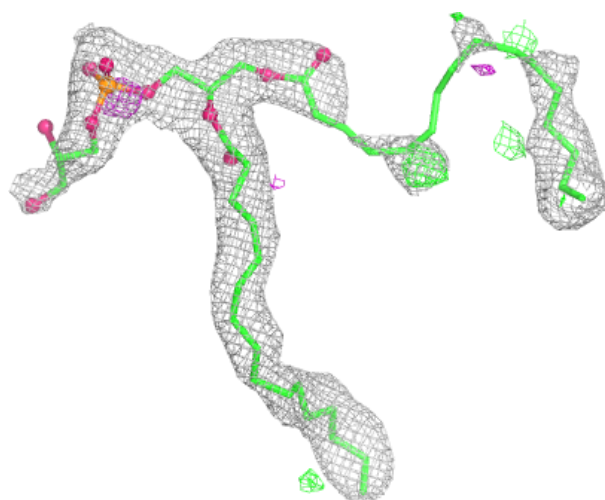
**Electron density around HTG c 522:**

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



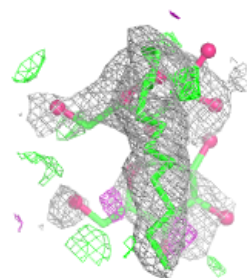
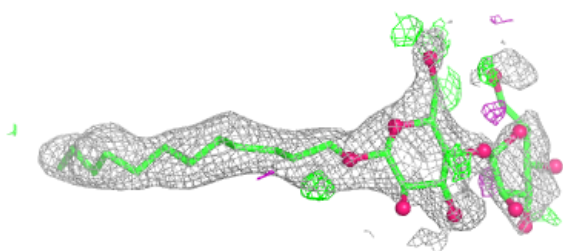
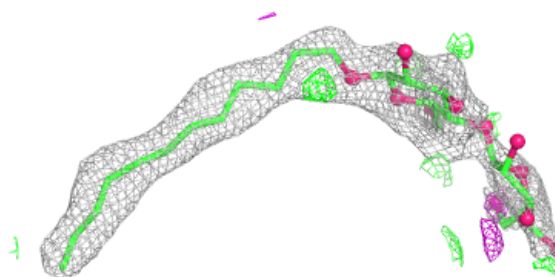
Electron density around LHG E 101:

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

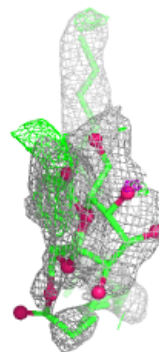
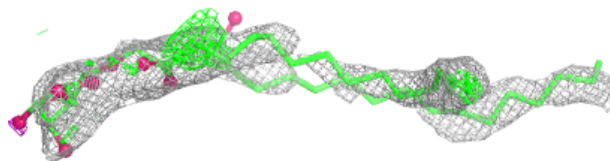
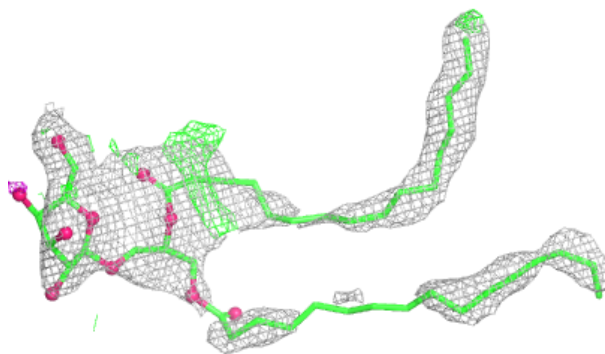


Electron density around LMT M 101:

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

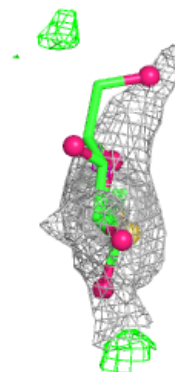
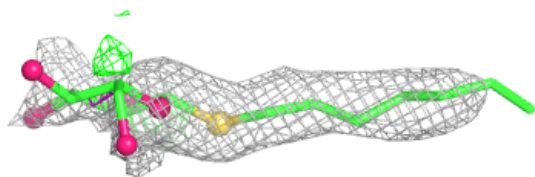
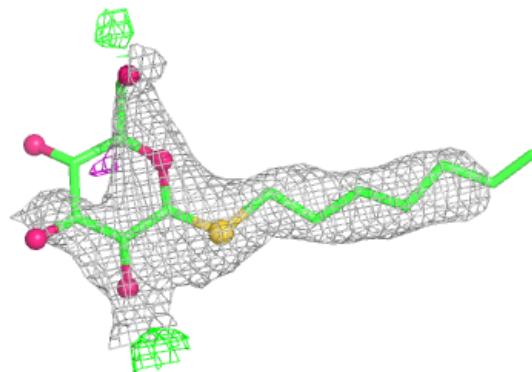
**Electron density around LMG c 521:**

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

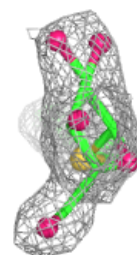
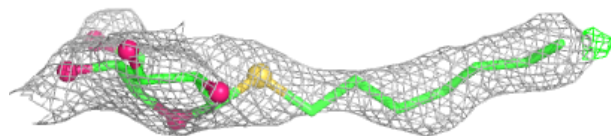
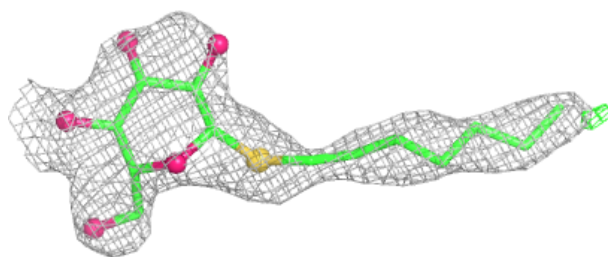


Electron density around HTG c 525:

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

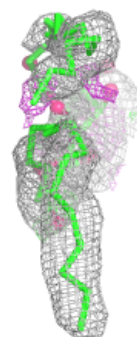
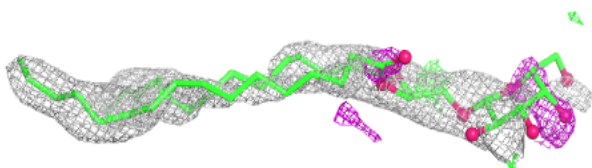
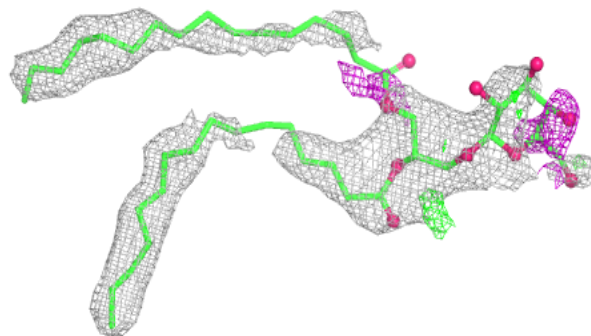
**Electron density around HTG C 522:**

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

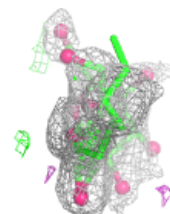
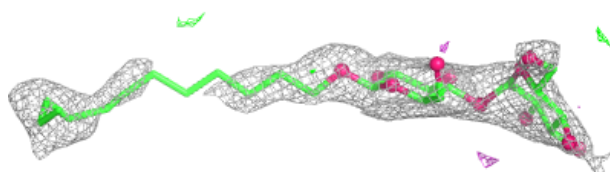
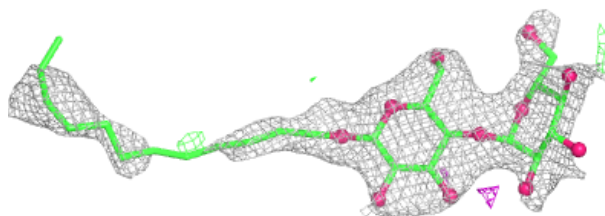


Electron density around LMG Z 101:

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

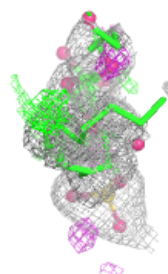
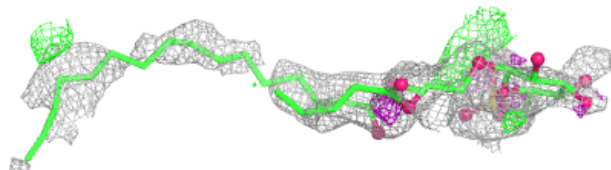
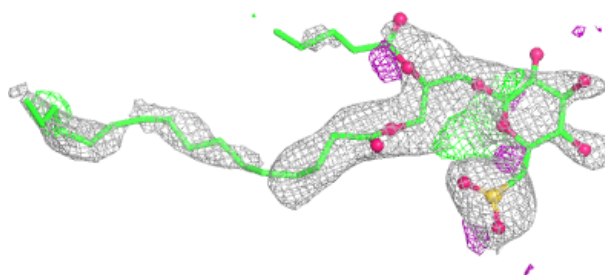
**Electron density around LMT a 416:**

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

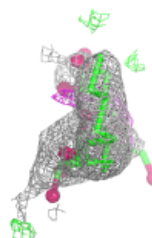
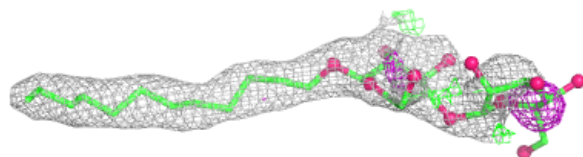
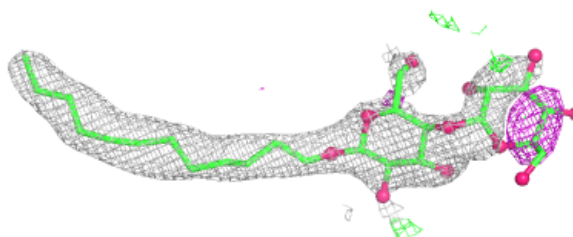


Electron density around SQD f 102:

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

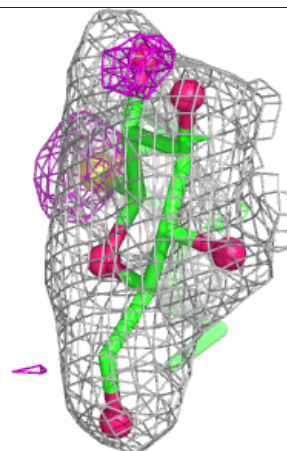
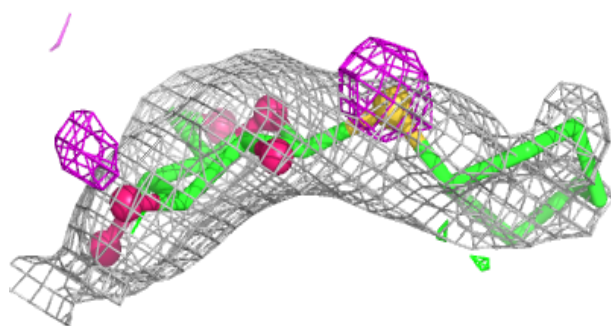
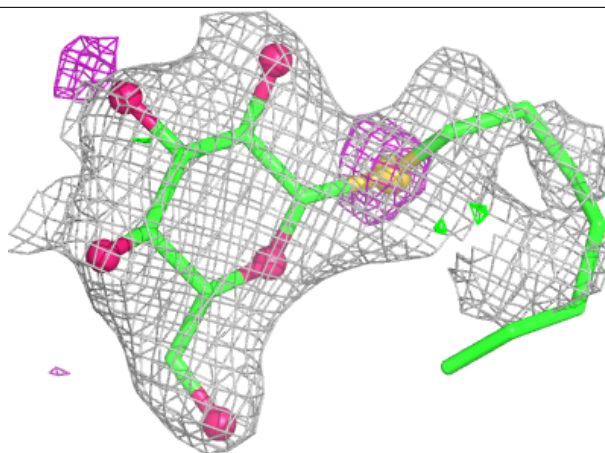
**Electron density around LMT b 625:**

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

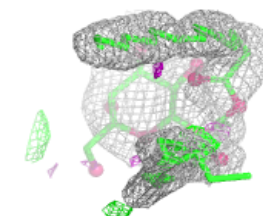
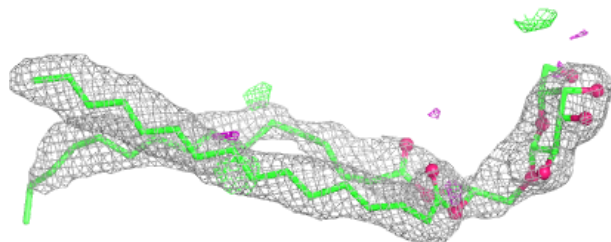
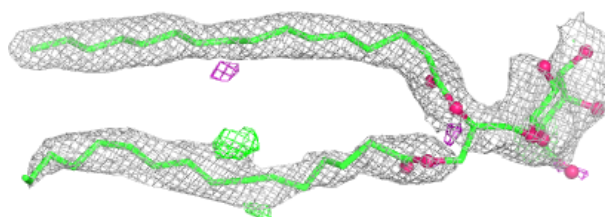


Electron density around HTG V 202:

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

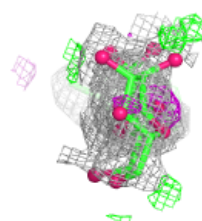
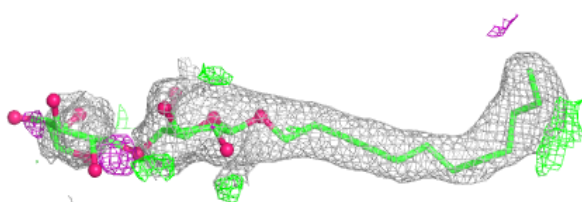
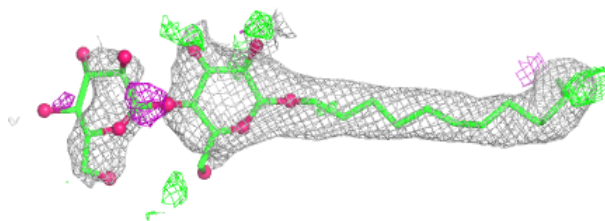
**Electron density around LMG c 520:**

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

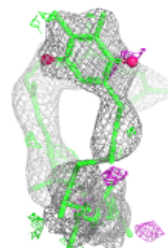
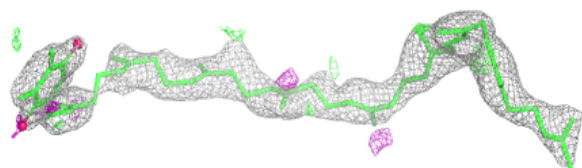
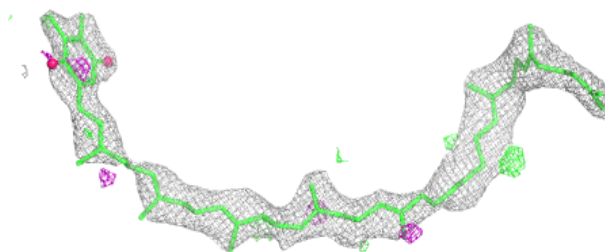


Electron density around LMT t 103:

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

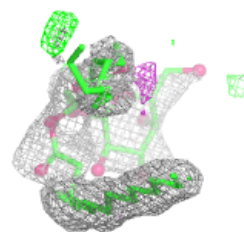
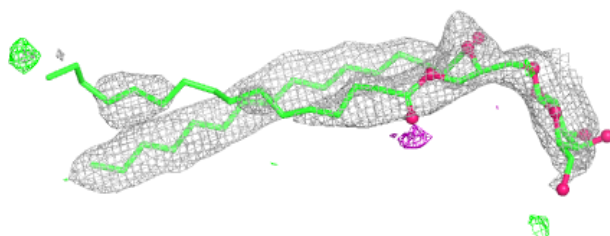
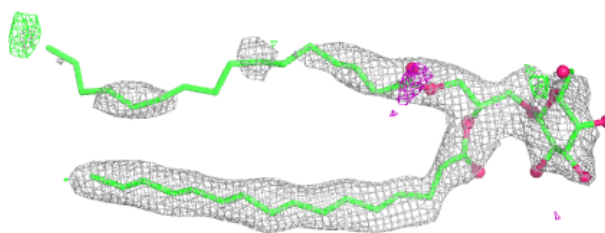
**Electron density around PL9 a 414:**

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

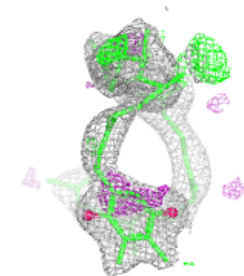
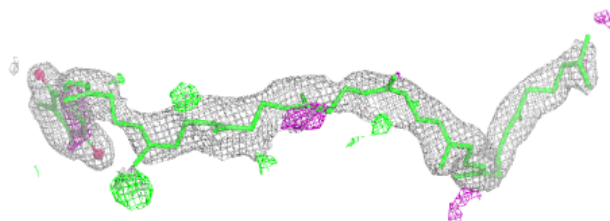
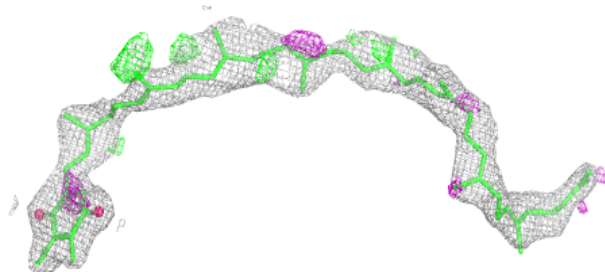


Electron density around LMG C 519:

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

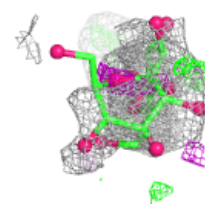
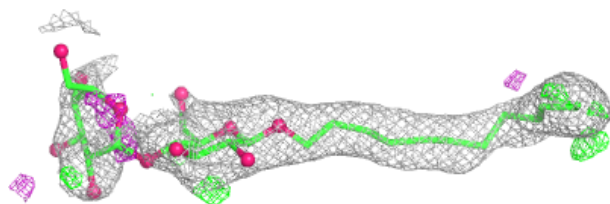
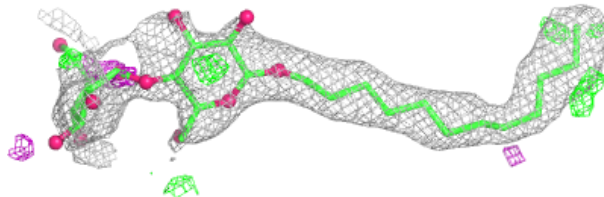
**Electron density around PL9 A 1010:**

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

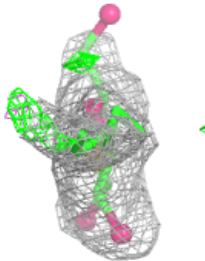
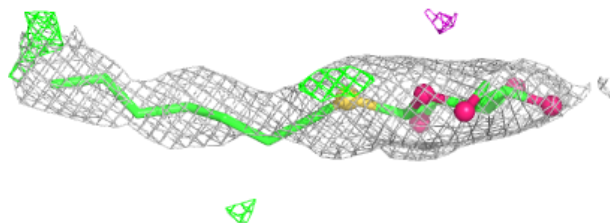
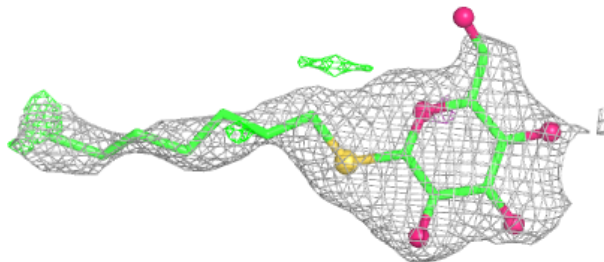


Electron density around LMT b 631:

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

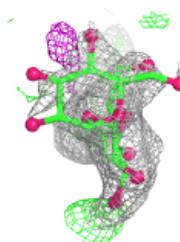
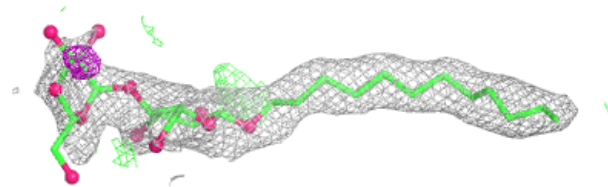
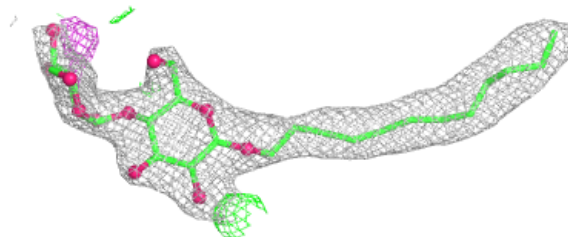
**Electron density around HTG C 521:**

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

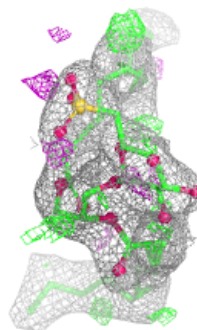
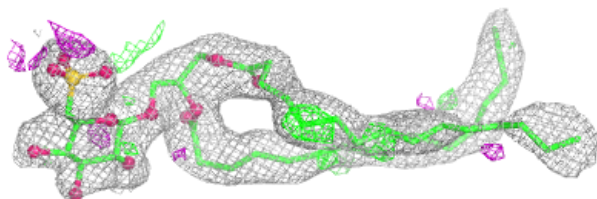
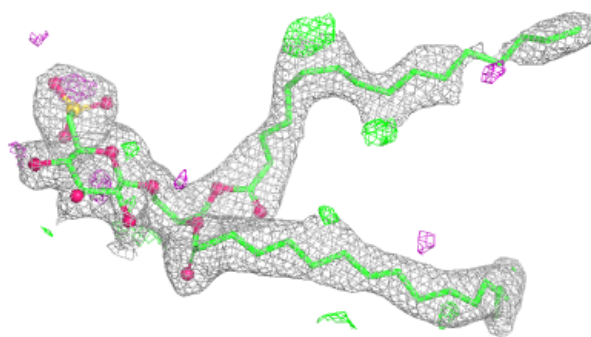


Electron density around LMT B 623:

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

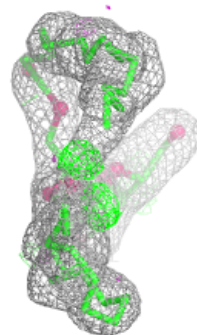
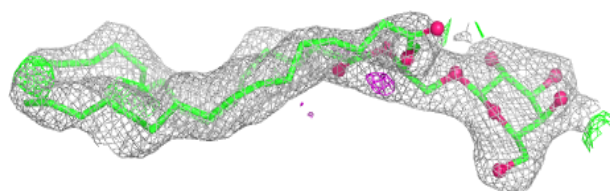
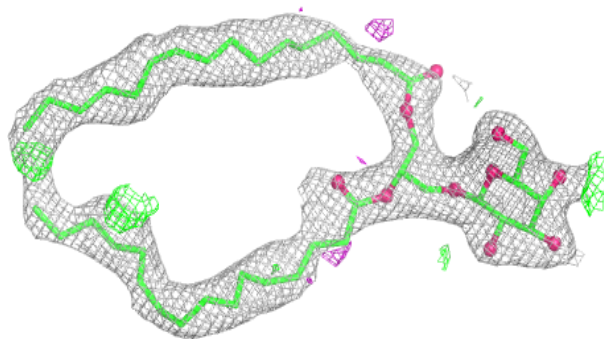
**Electron density around SQD A 1016:**

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

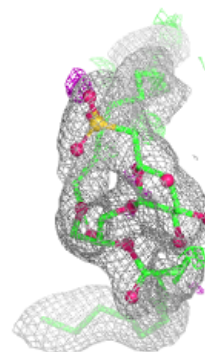
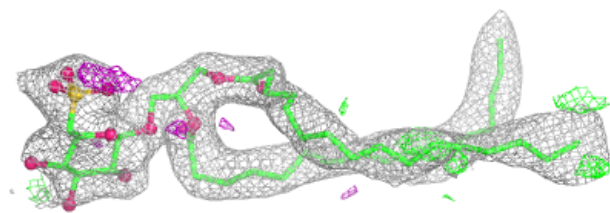
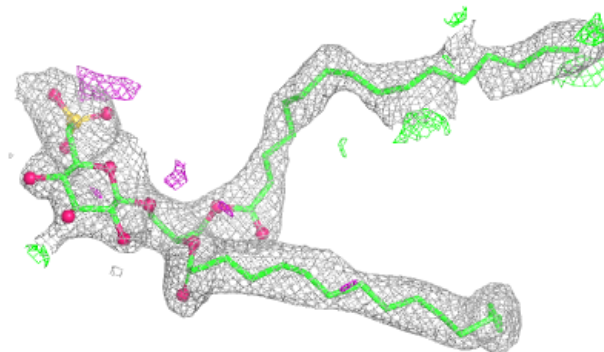


Electron density around LMG A 1012:

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

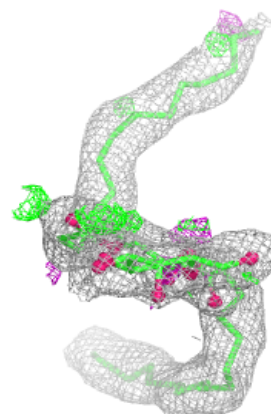
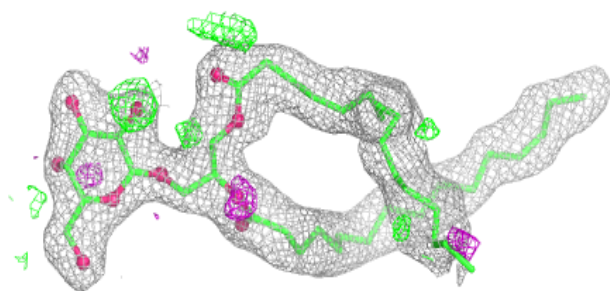
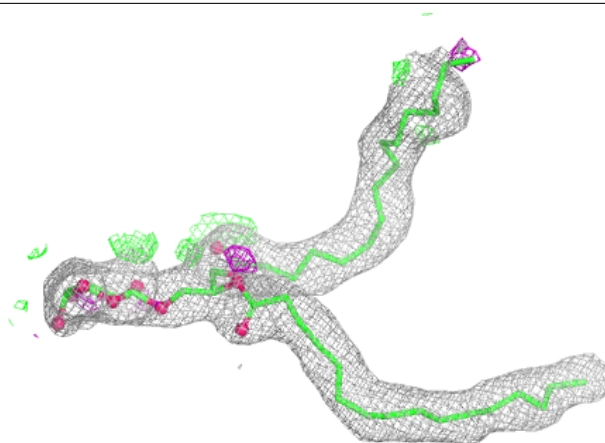
**Electron density around SQD a 401:**

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



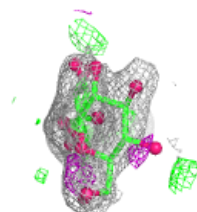
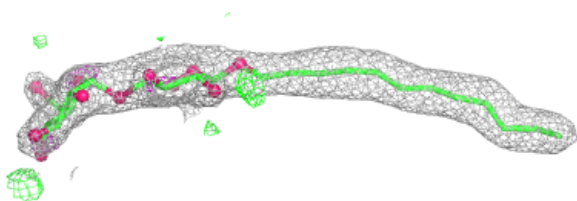
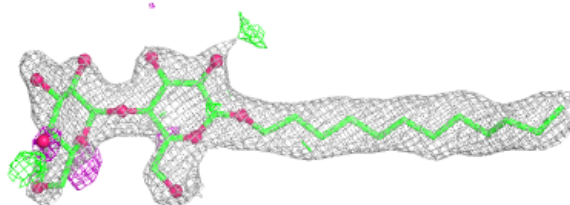
Electron density around LMG B 622:

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

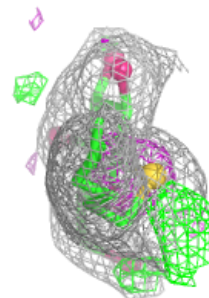
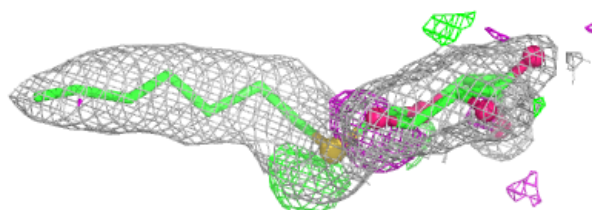
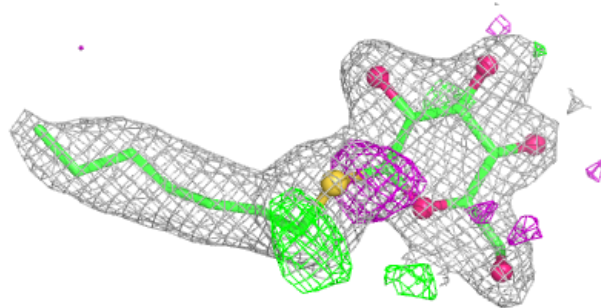


Electron density around LMT M 102:

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

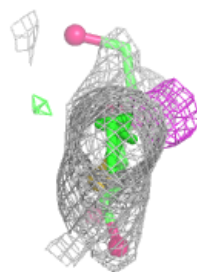
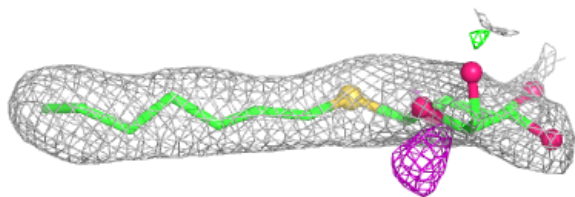
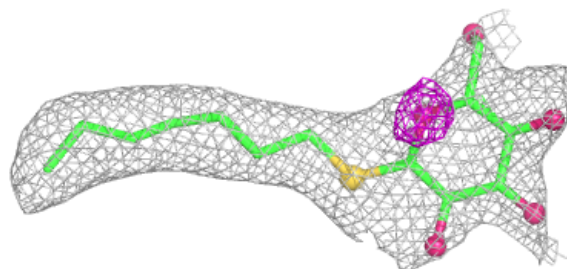
**Electron density around HTG b 626:**

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



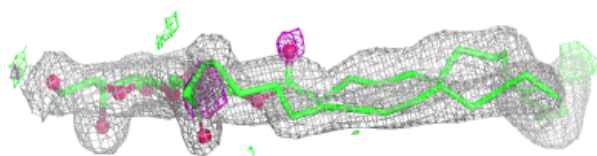
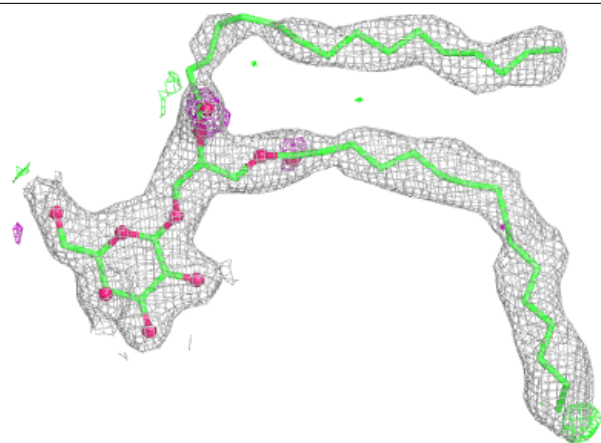
Electron density around HTG B 628:

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

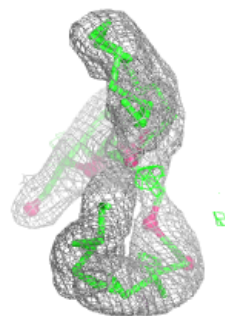
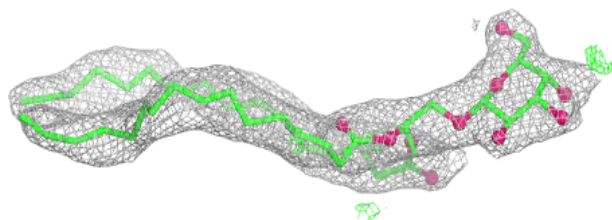
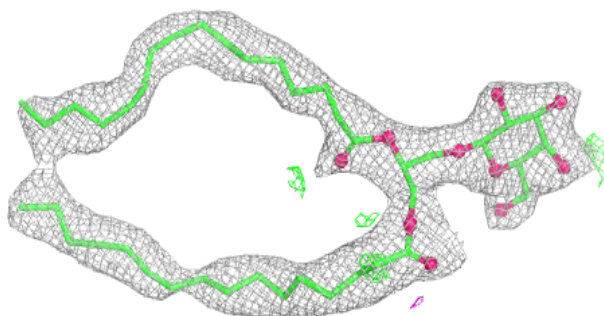


Electron density around LMG C 518:

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

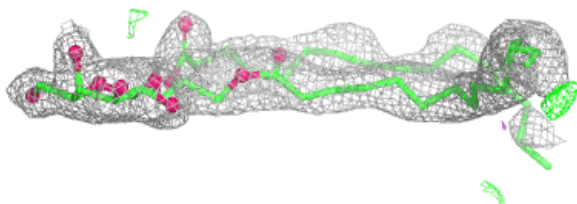
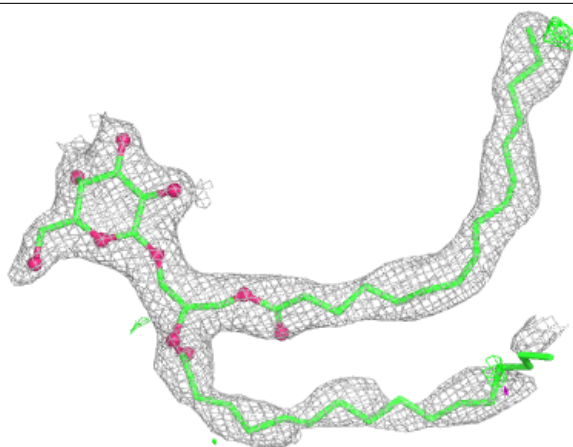
**Electron density around LMG a 415:**

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



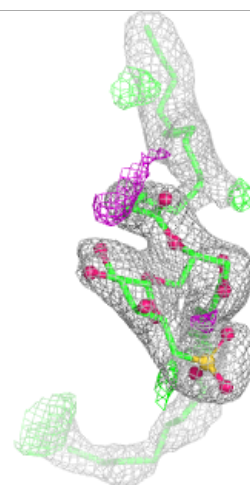
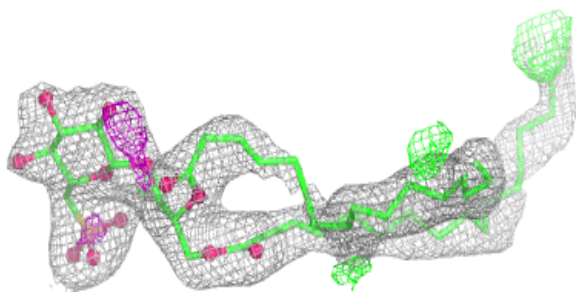
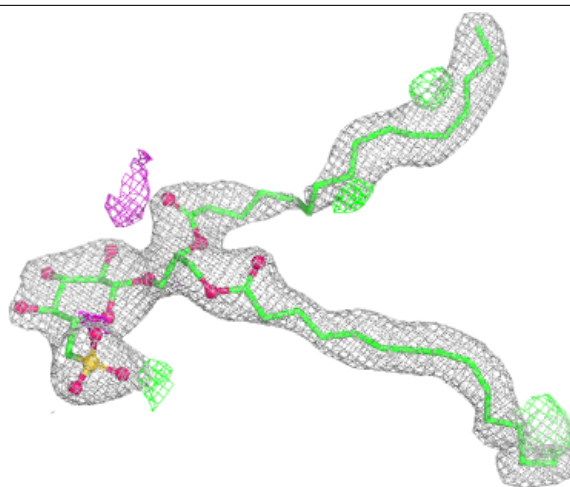
Electron density around LMG c 519:

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



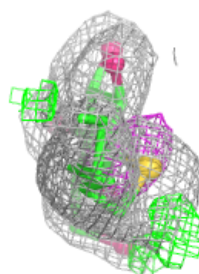
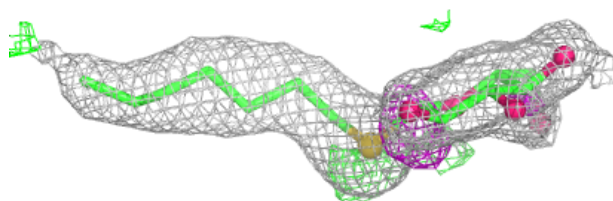
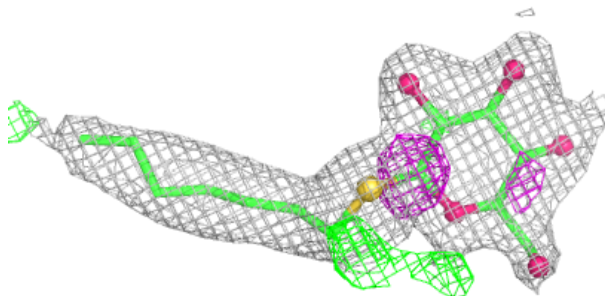
Electron density around SQD c 518:

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

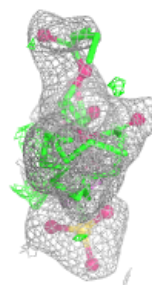
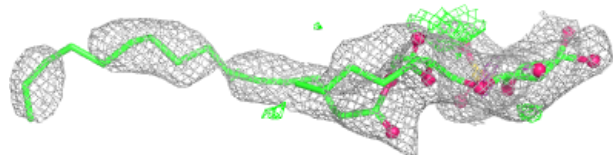
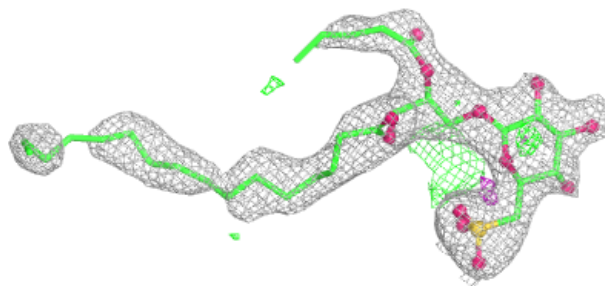


Electron density around HTG o 301:

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

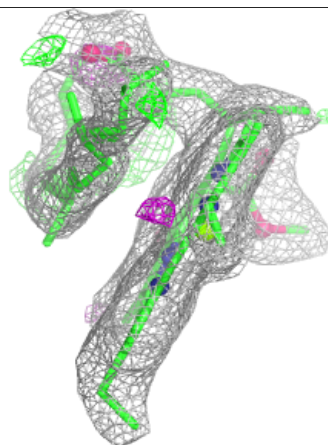
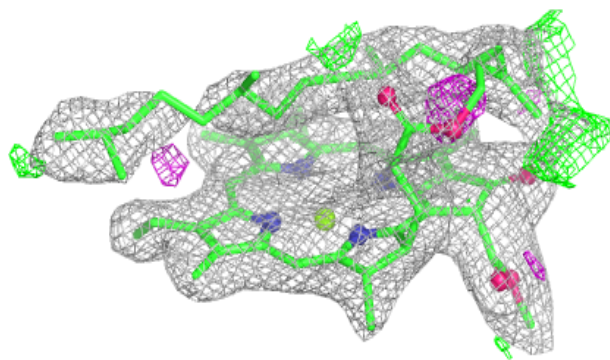
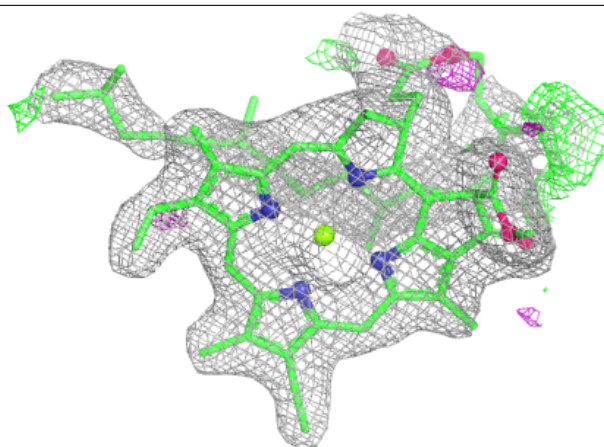
**Electron density around SQD D 408:**

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

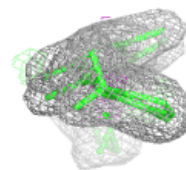
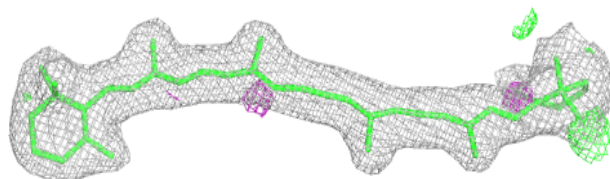
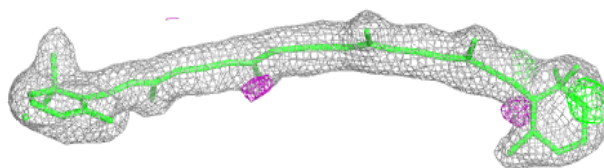


Electron density around CLA b 604:

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

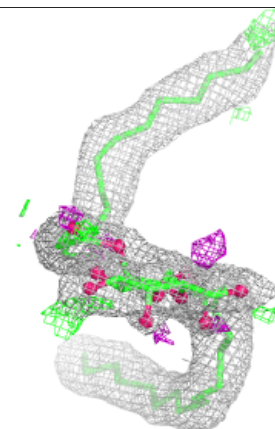
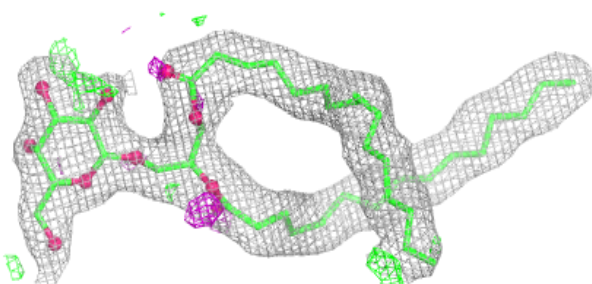
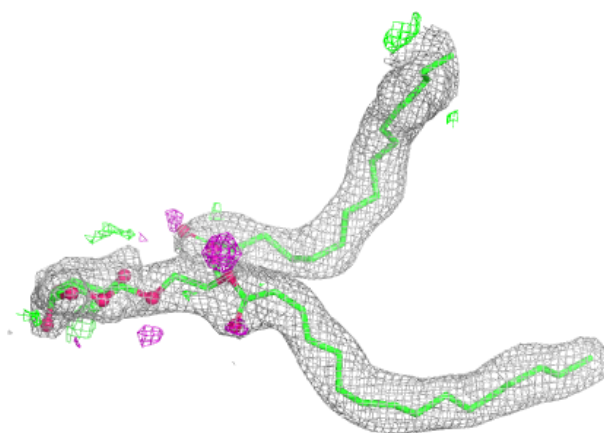
**Electron density around BCR d 404:**

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

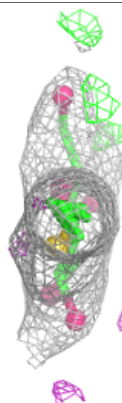
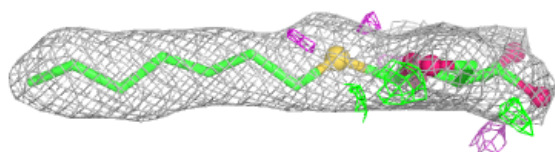
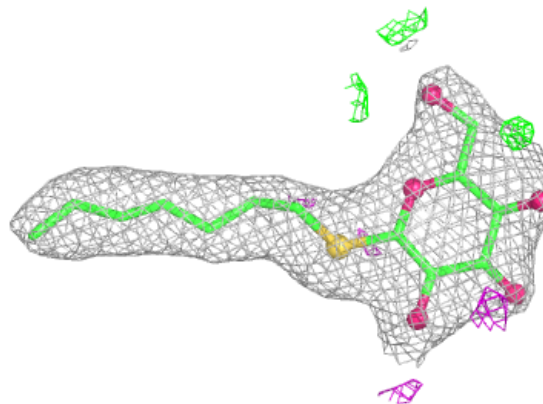


Electron density around LMG m 102:

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

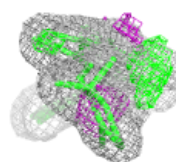
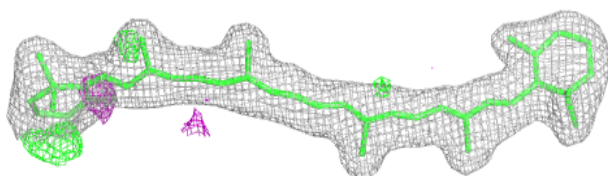
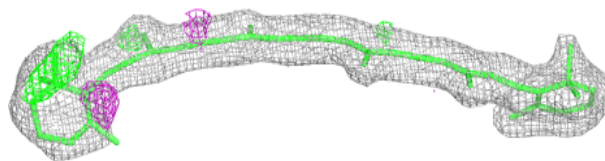
**Electron density around HTG b 601:**

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

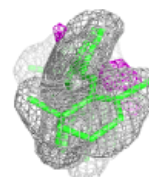
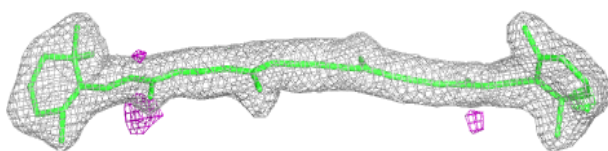
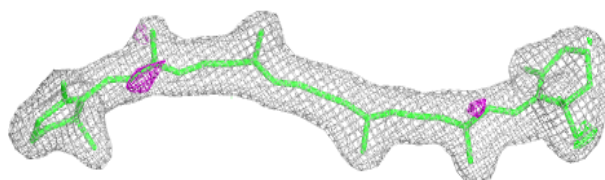


Electron density around BCR D 406:

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

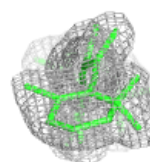
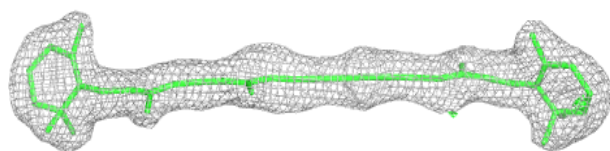
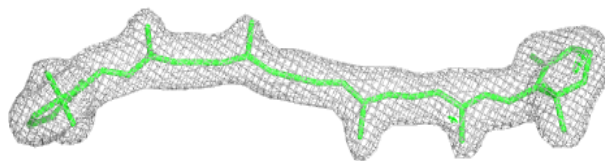
**Electron density around BCR J 101:**

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

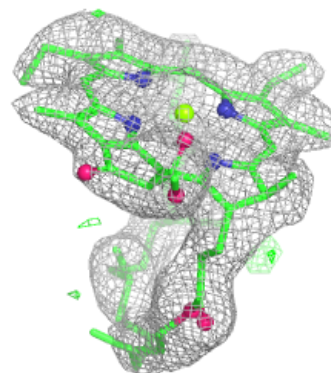
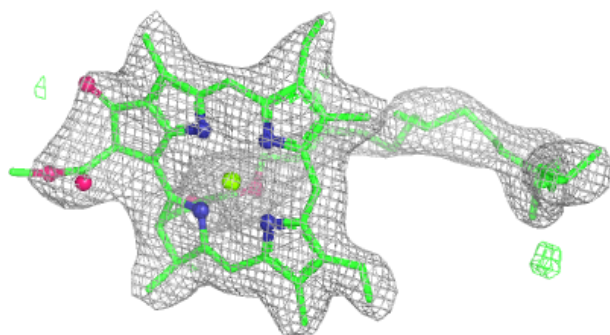
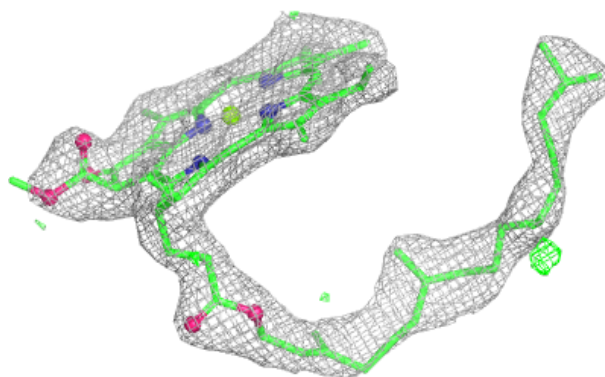


Electron density around BCR K 102:

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

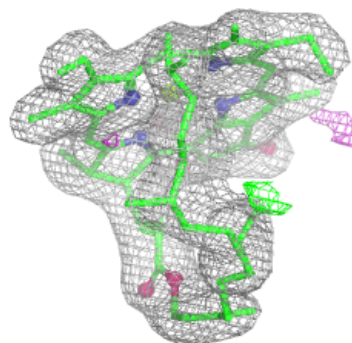
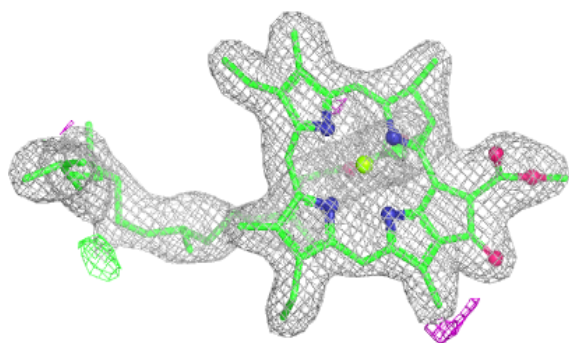
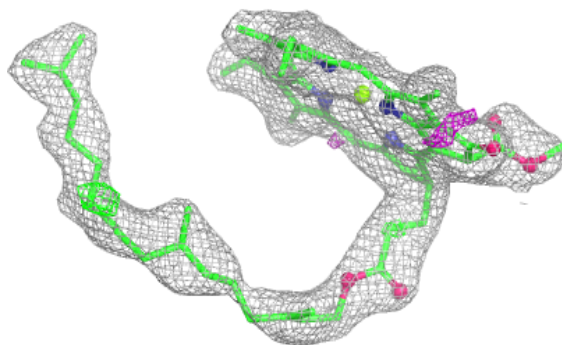
**Electron density around CLA c 513:**

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



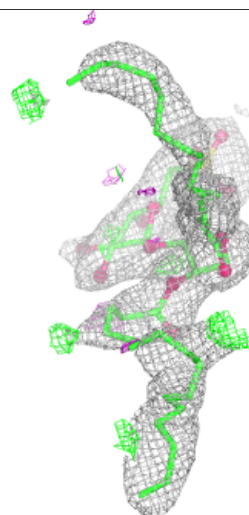
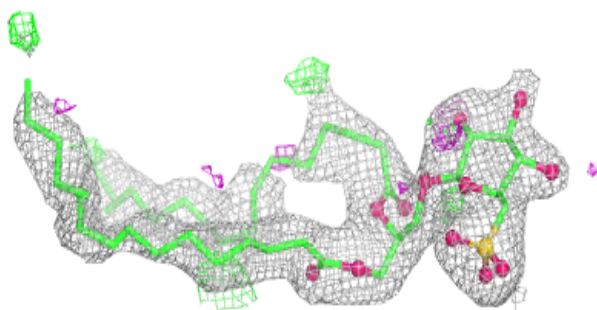
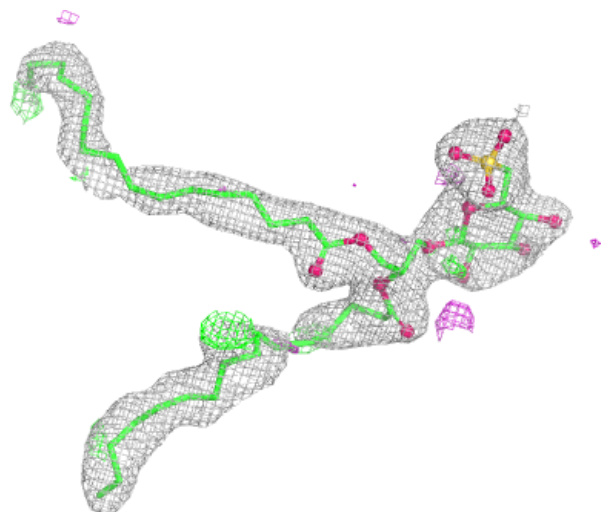
Electron density around CLA C 513:

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



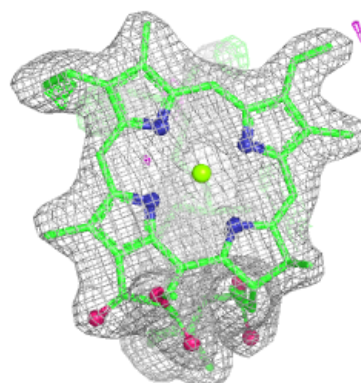
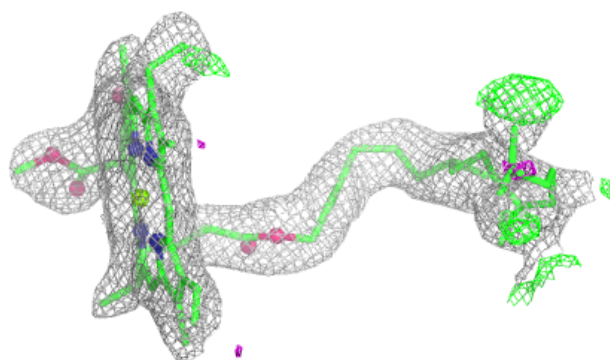
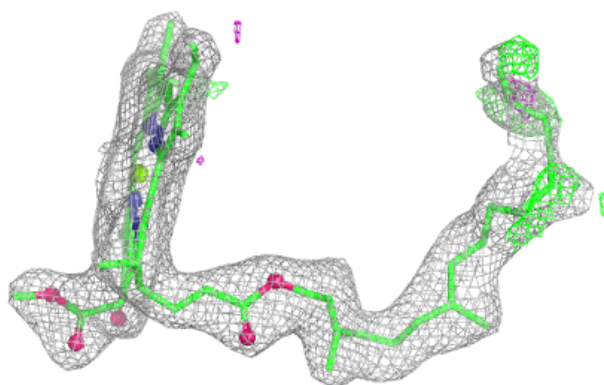
Electron density around SQD A 1011:

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

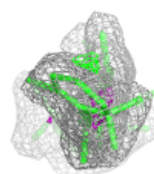
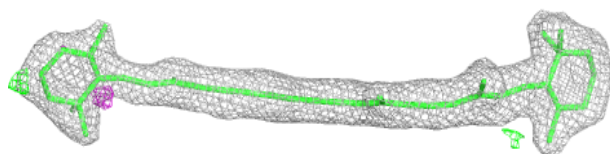


Electron density around CLA C 506:

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

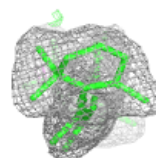
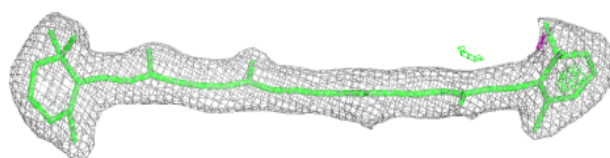
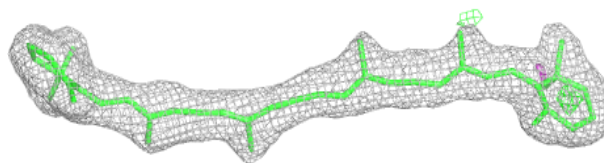
**Electron density around BCR h 101:**

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

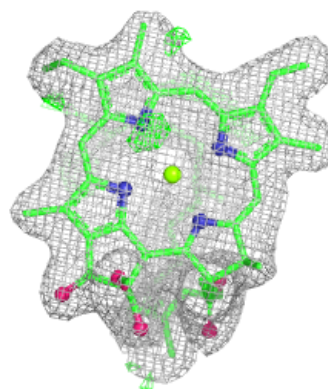
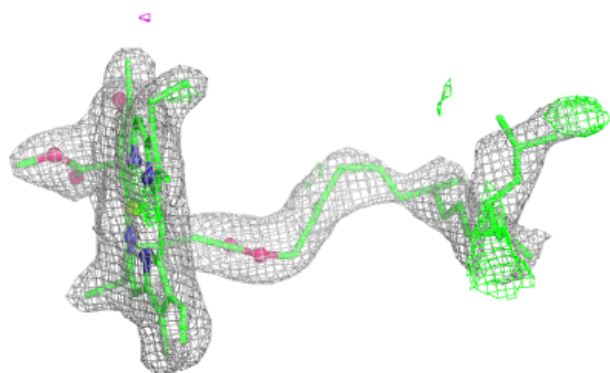
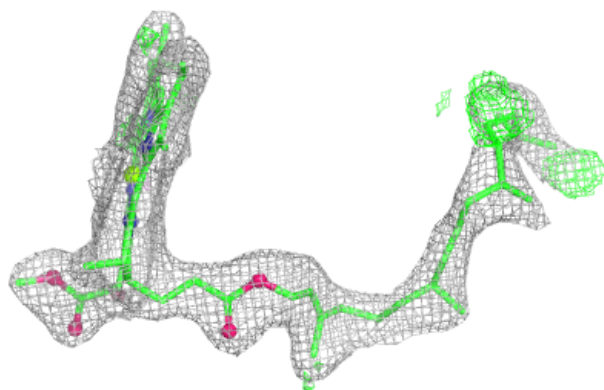


Electron density around BCR k 102:

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

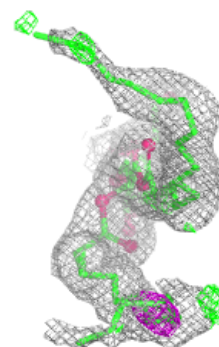
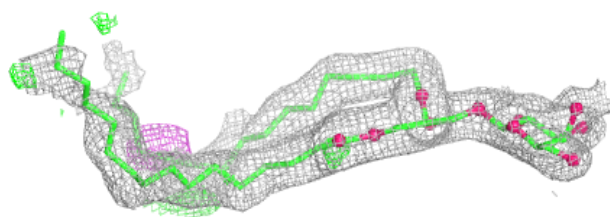
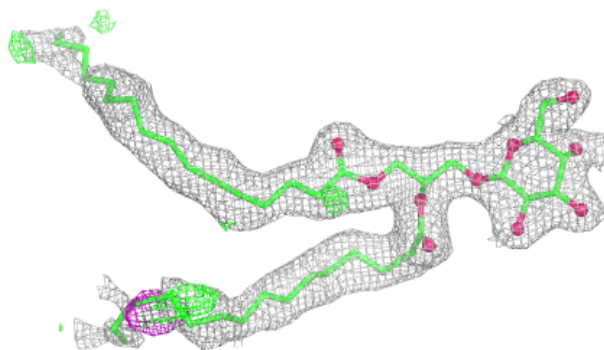
**Electron density around CLA c 506:**

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

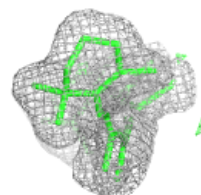
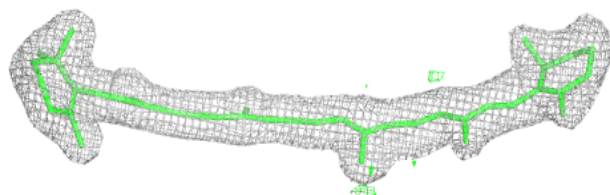
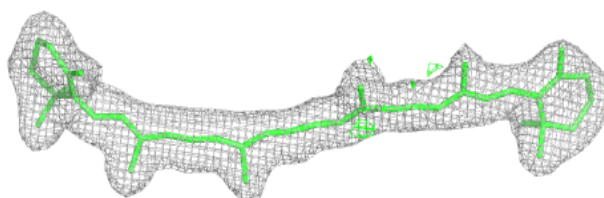


Electron density around LMG D 412:

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

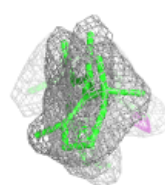
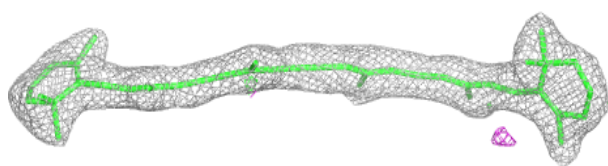
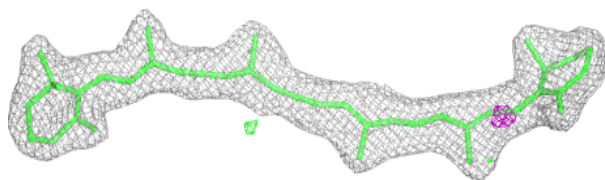
**Electron density around BCR t 101:**

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

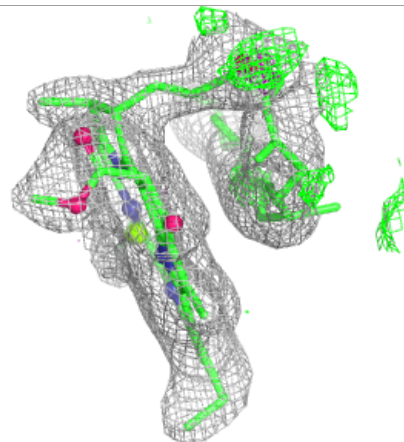
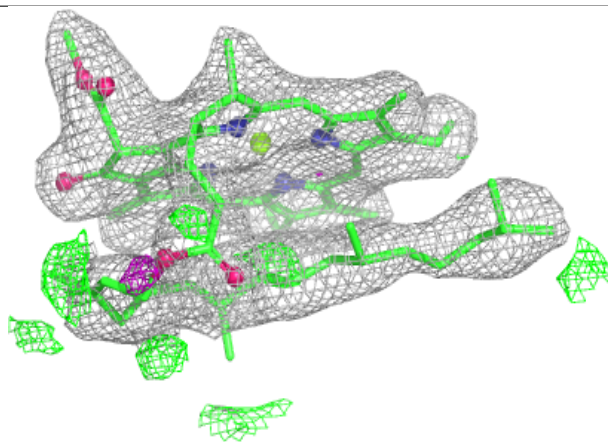
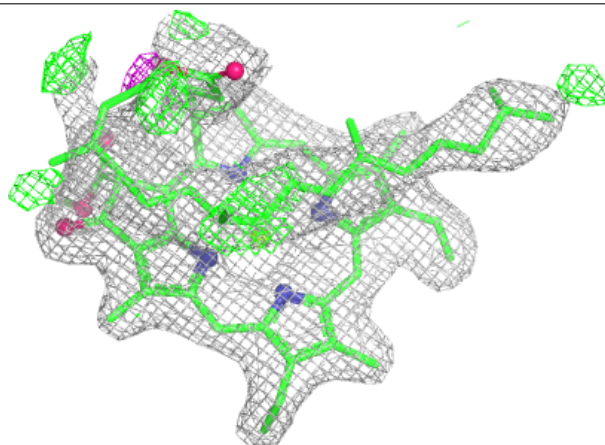


Electron density around BCR y 101:

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

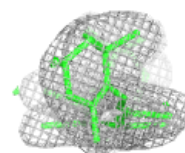
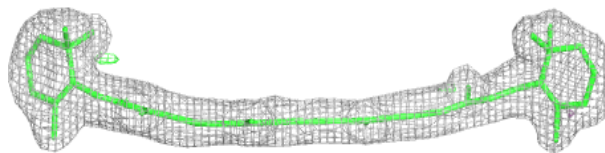
**Electron density around CLA B 601:**

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

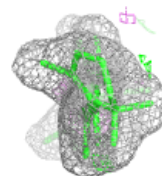
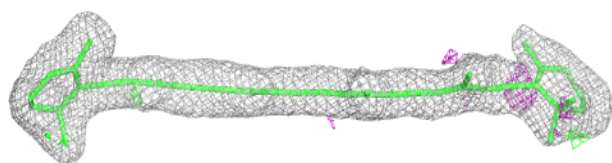
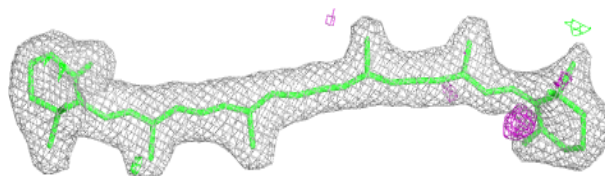


Electron density around BCR K 101:

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

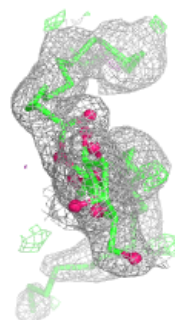
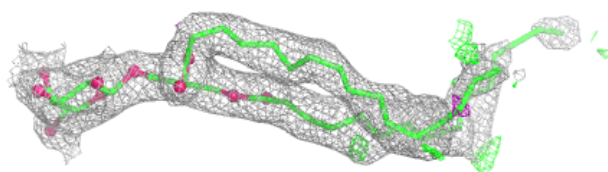
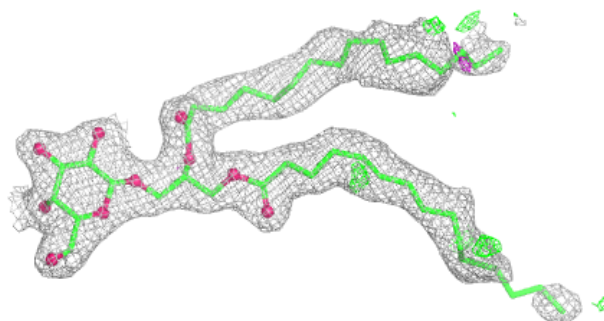
**Electron density around BCR B 618:**

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

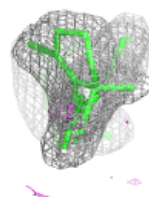
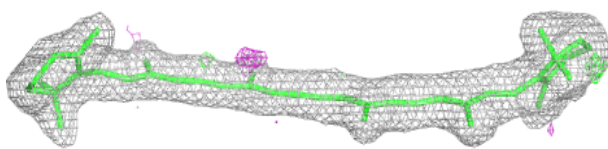
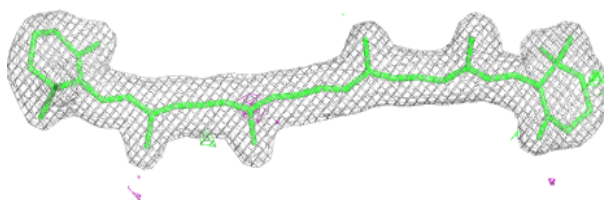


Electron density around LMG d 409:

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

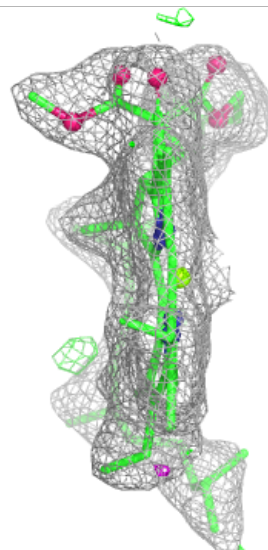
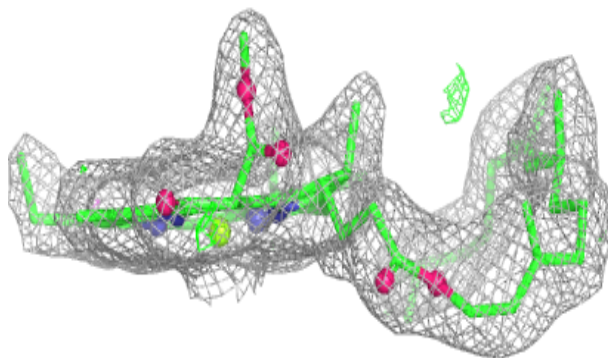
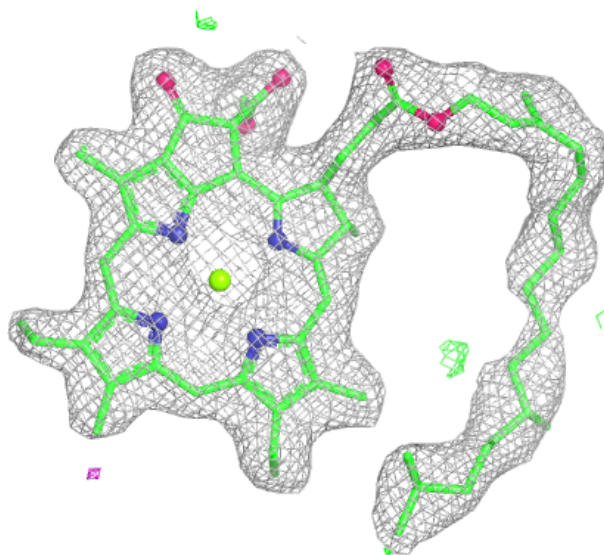
**Electron density around BCR B 619:**

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



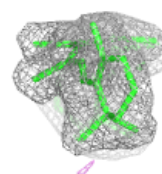
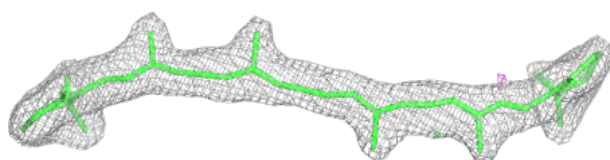
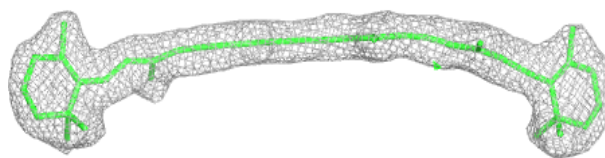
Electron density around CLA c 512:

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

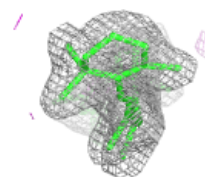
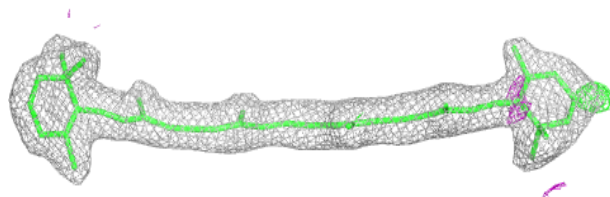
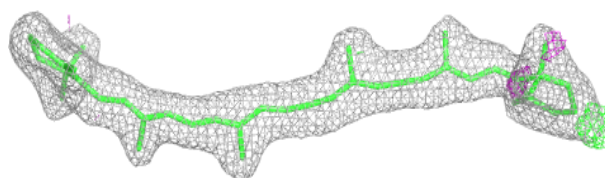


Electron density around BCR k 101:

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

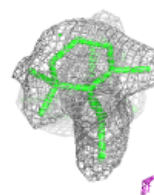
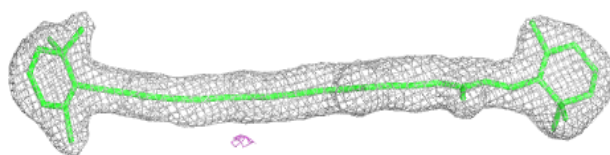
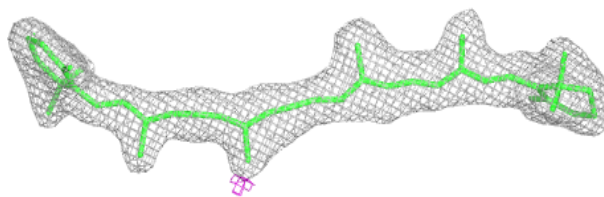
**Electron density around BCR H 101:**

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



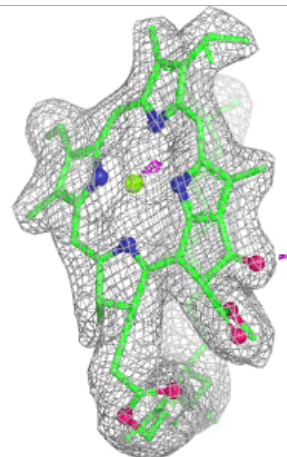
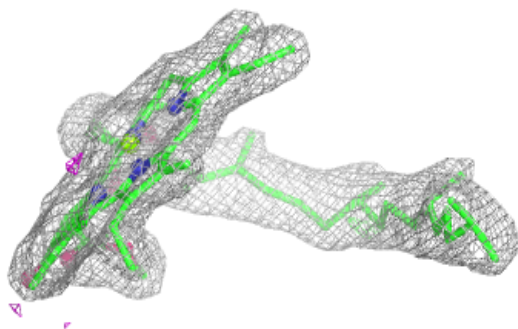
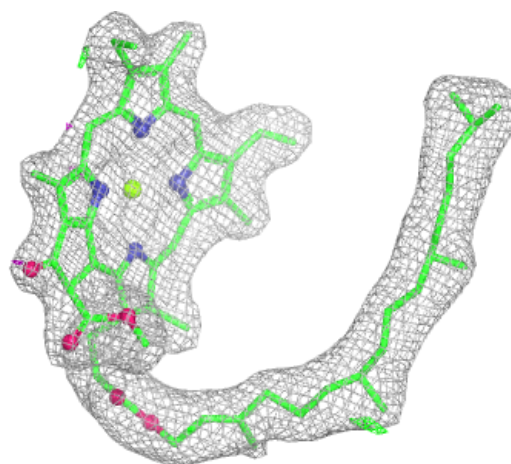
Electron density around BCR c 514:

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



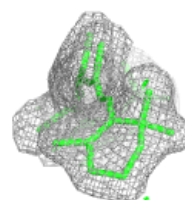
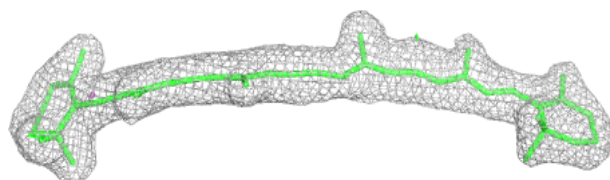
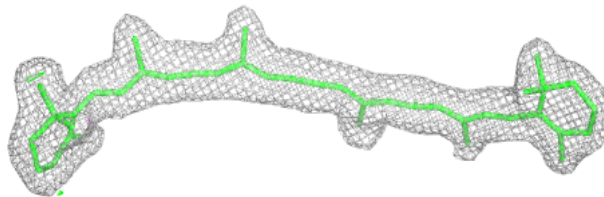
Electron density around CLA c 507:

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

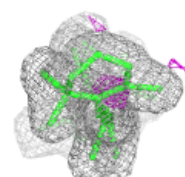
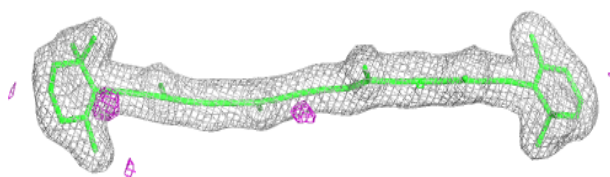
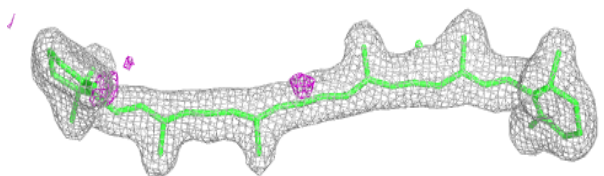


Electron density around BCR T 101:

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

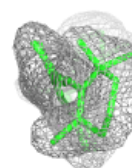
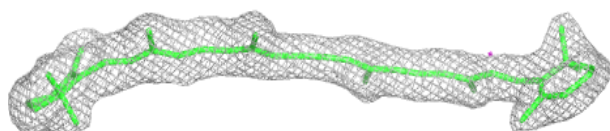
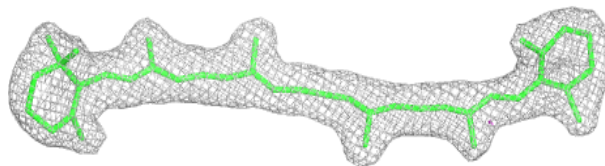
**Electron density around BCR a 413:**

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

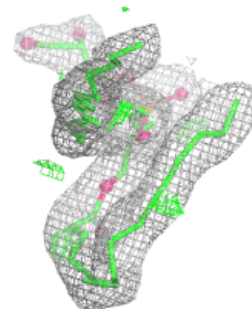
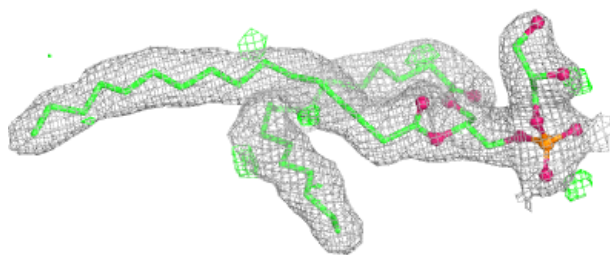
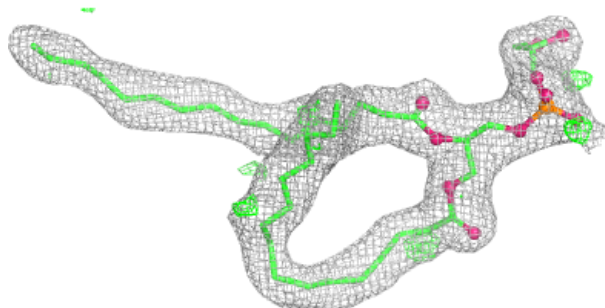


Electron density around BCR b 622:

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

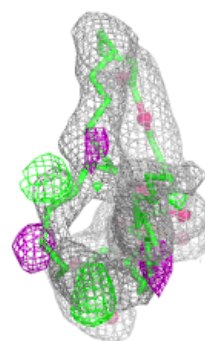
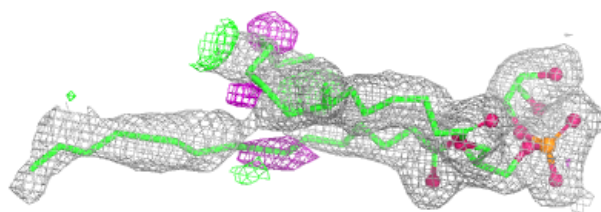
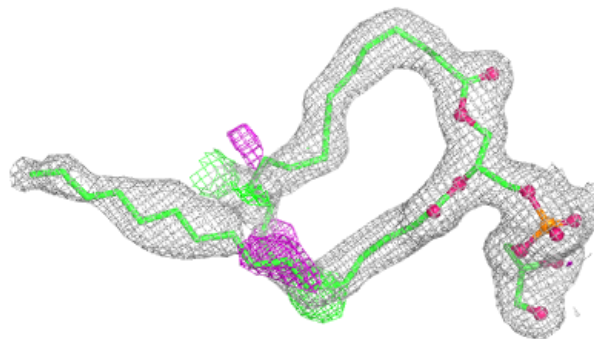
**Electron density around LHG d 406:**

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

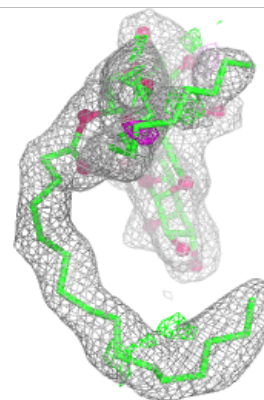
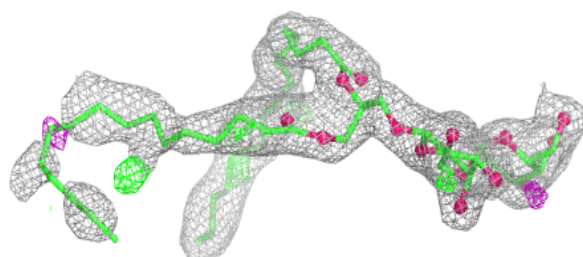
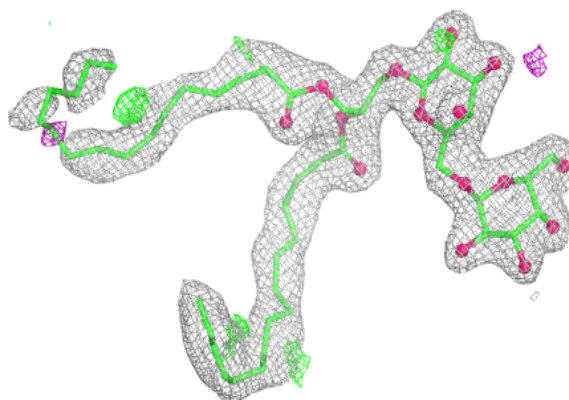


Electron density around LHG d 408:

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

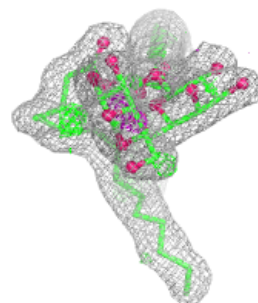
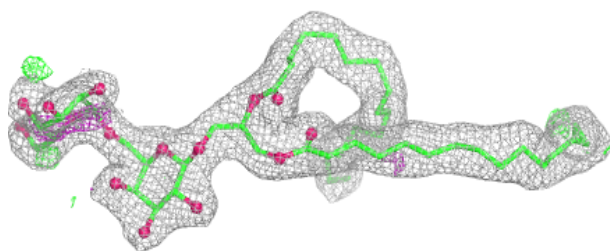
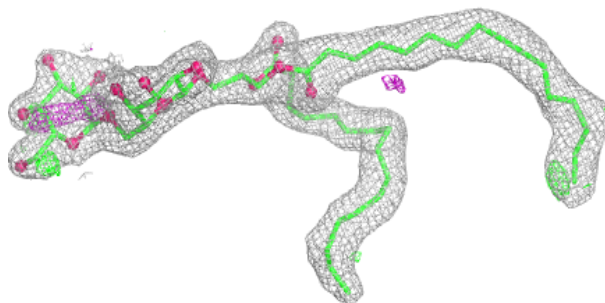
**Electron density around DGD c 516:**

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

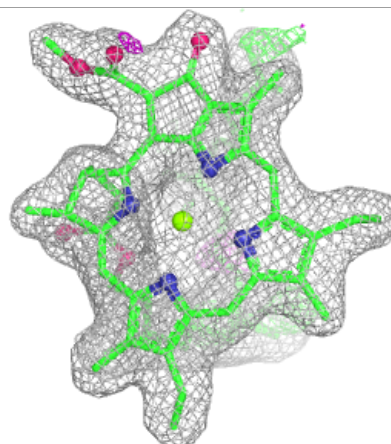
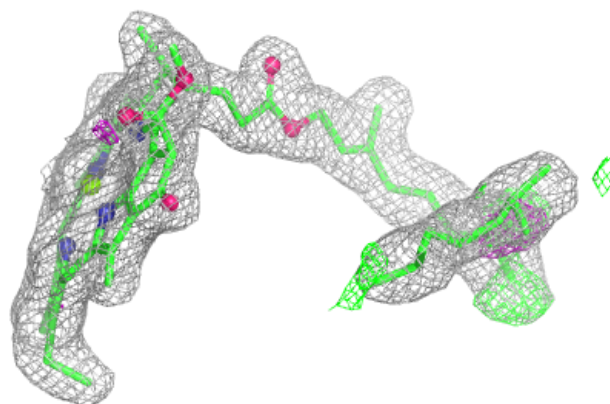
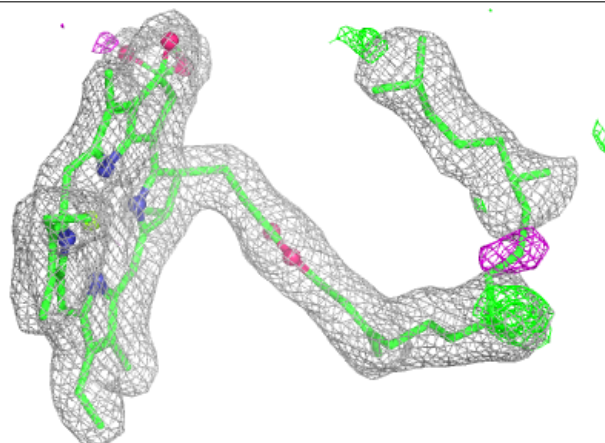


Electron density around DGD h 102:

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

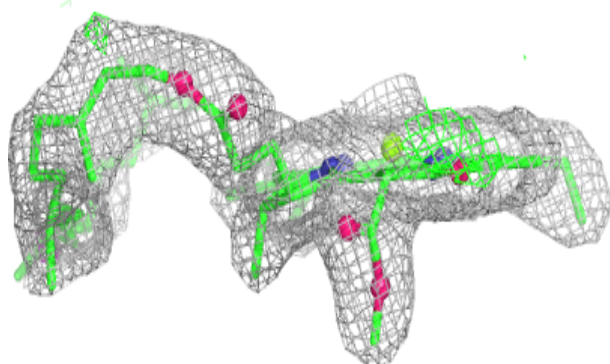
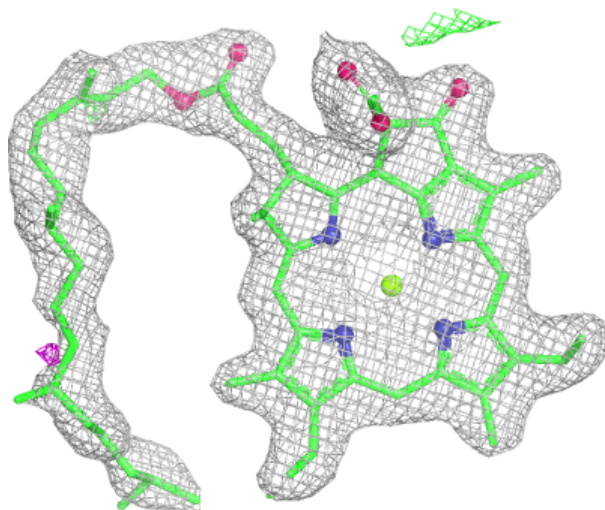
**Electron density around CLA B 606:**

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



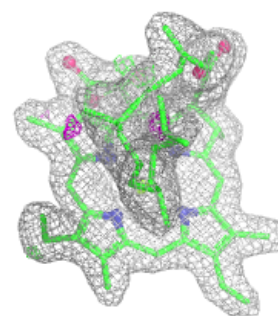
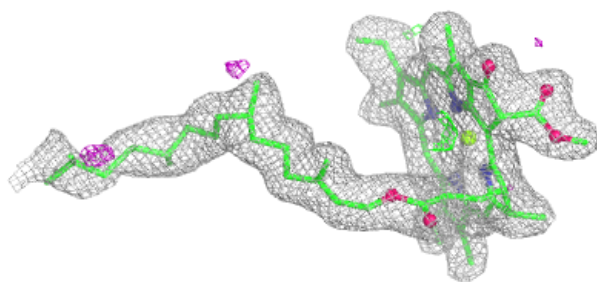
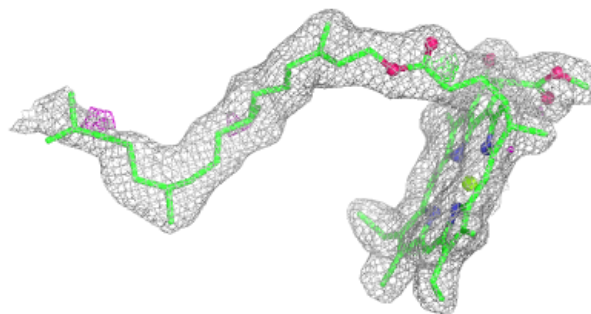
Electron density around CLA C 512:

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



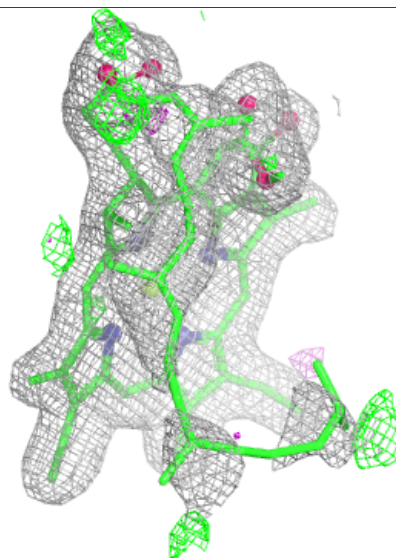
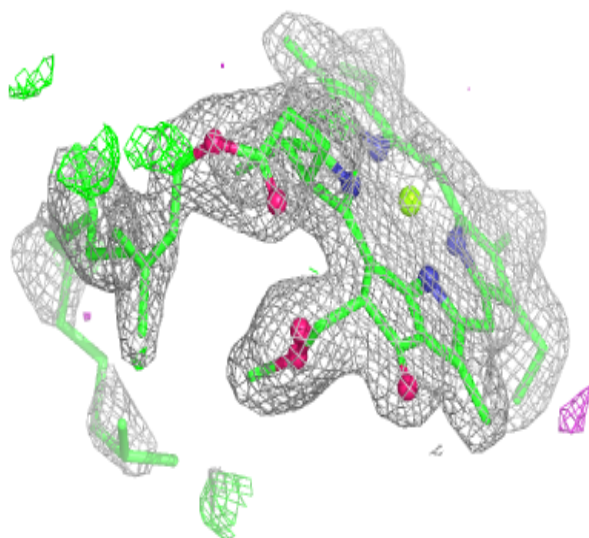
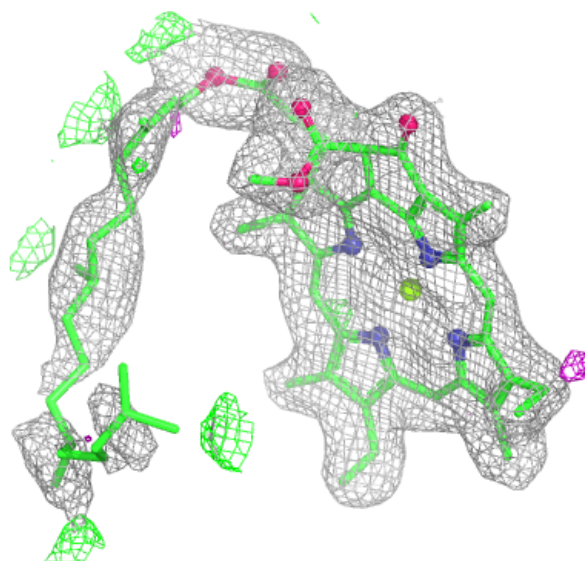
Electron density around CLA c 508:

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



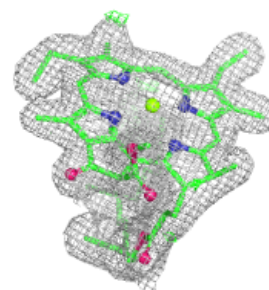
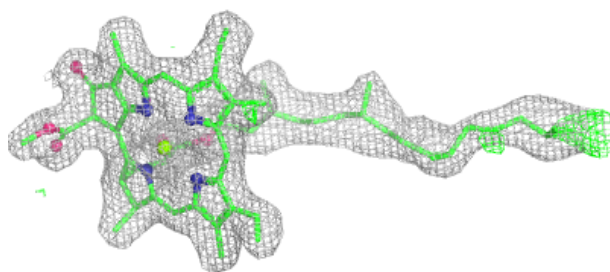
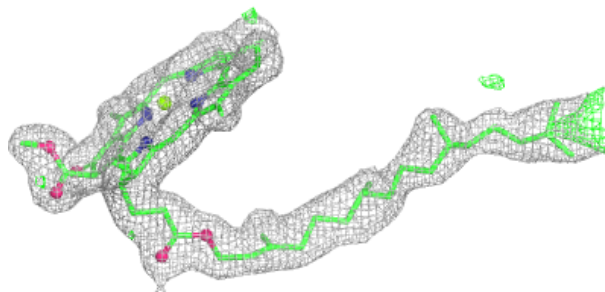
Electron density around CLA B 616:

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

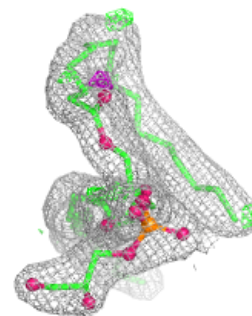
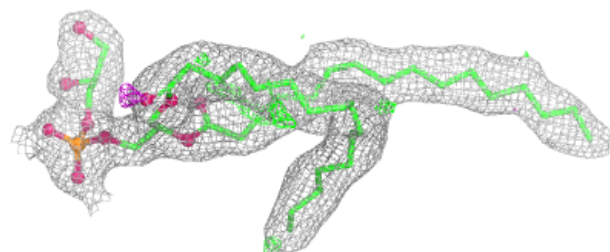
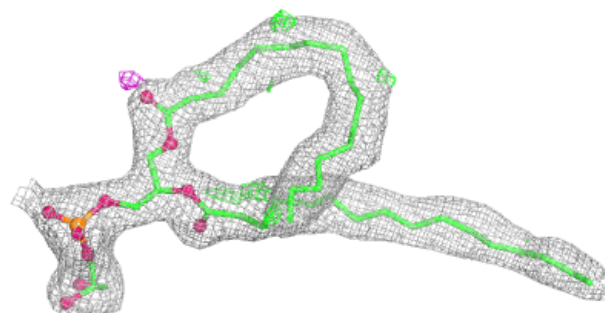


Electron density around CLA C 504:

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

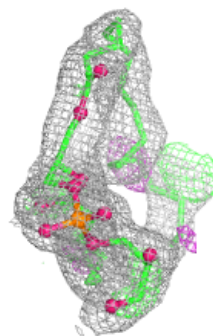
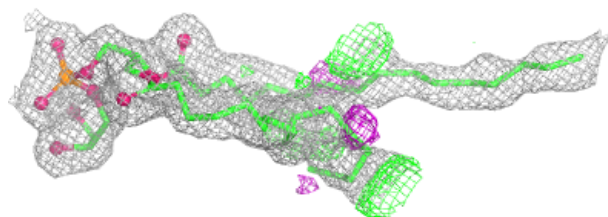
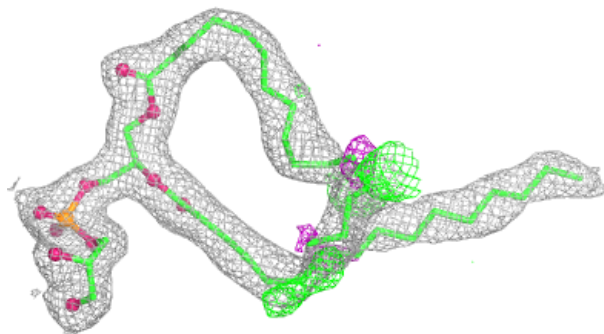
**Electron density around LHG D 409:**

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

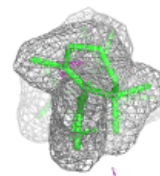
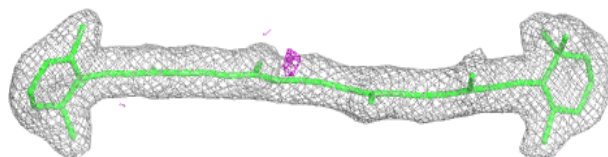
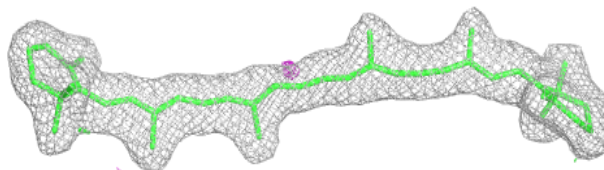


Electron density around LHG D 411:

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

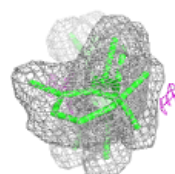
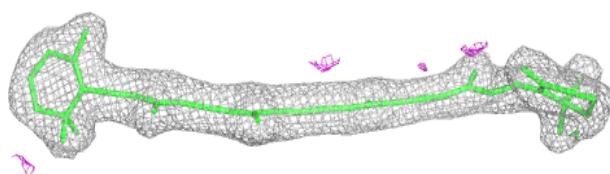
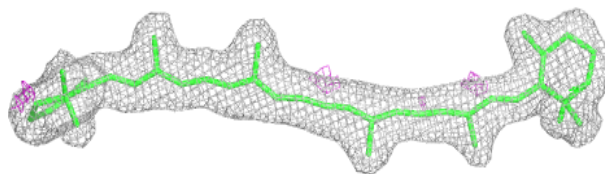
**Electron density around BCR A 1009:**

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

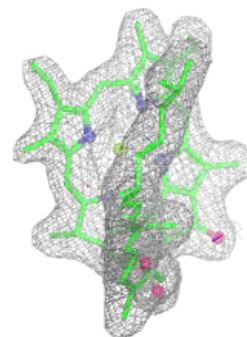
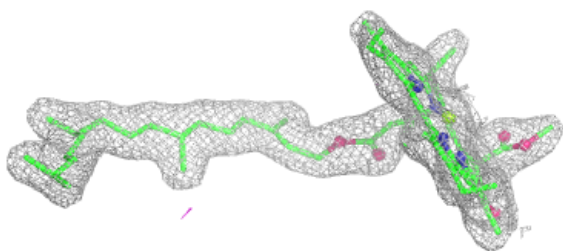
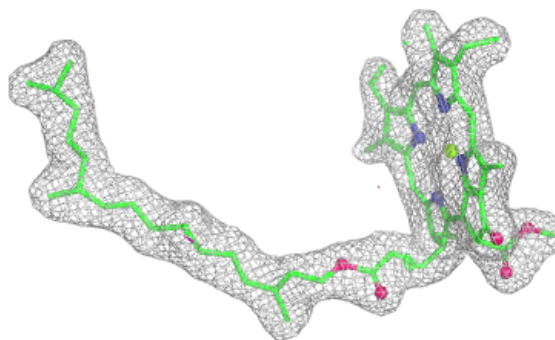


Electron density around BCR B 617:

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

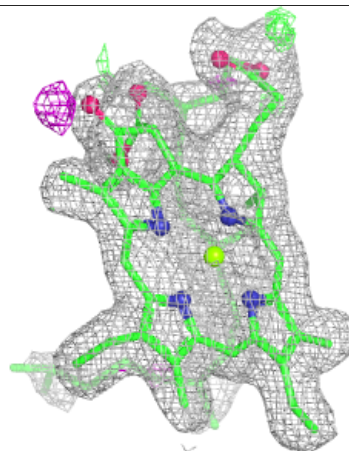
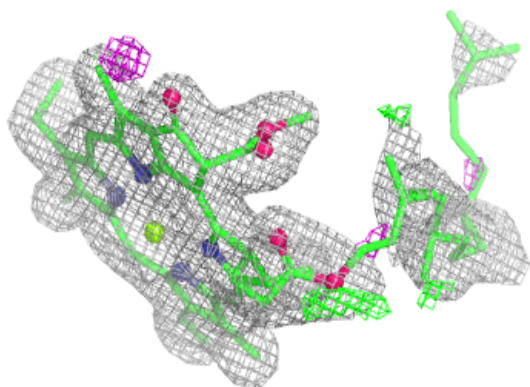
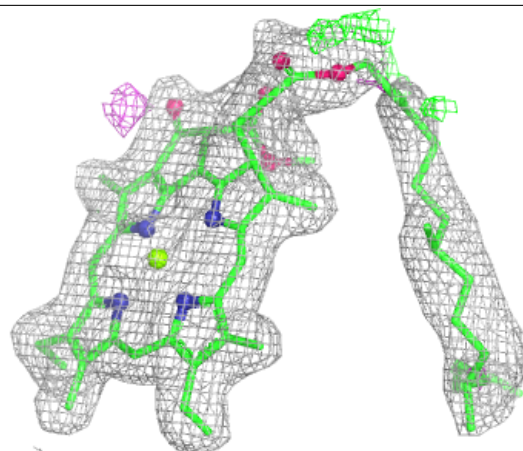
**Electron density around CLA b 612:**

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

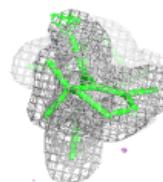
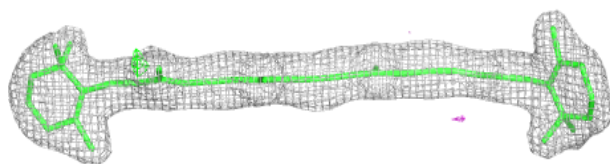
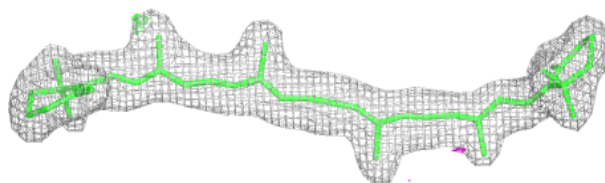


Electron density around CLA b 619:

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

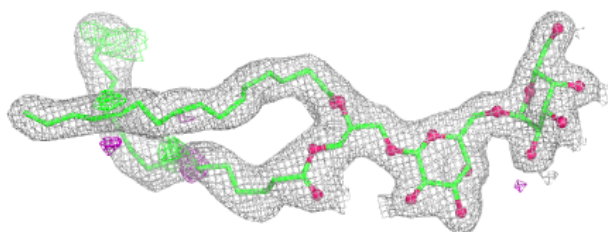
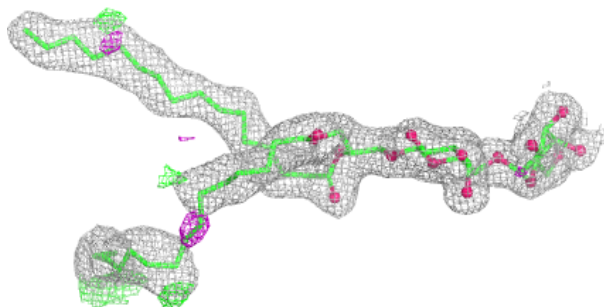
**Electron density around BCR C 514:**

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

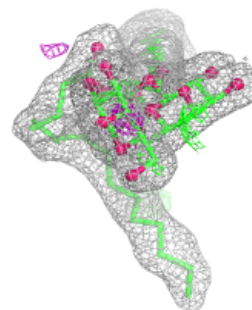
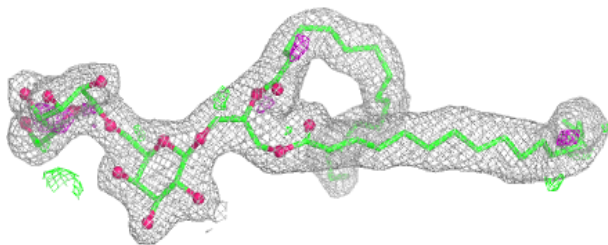
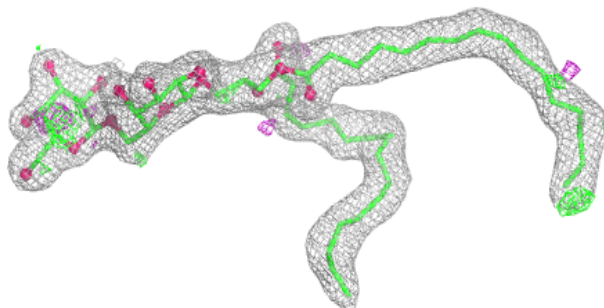


Electron density around DGD C 515:

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

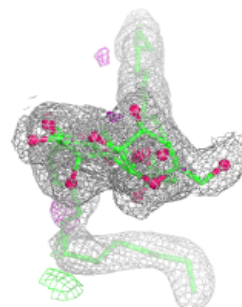
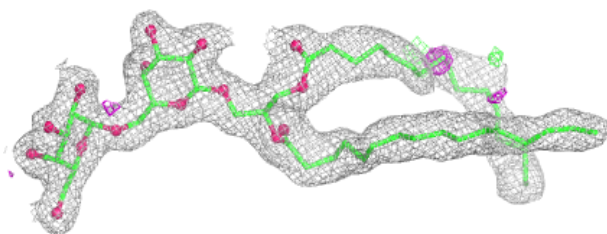
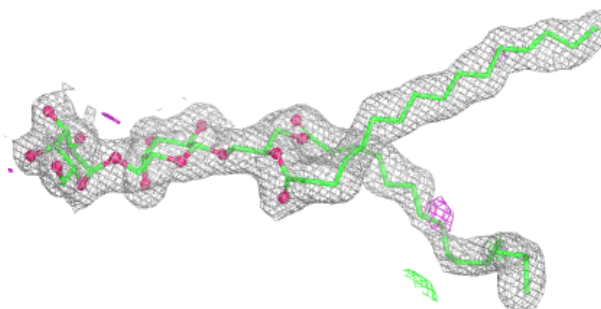
**Electron density around DGD H 102:**

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

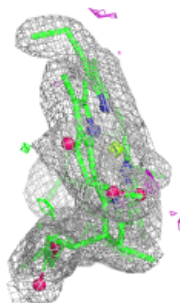
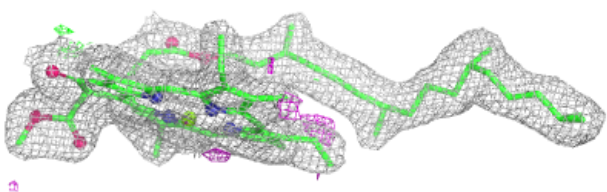
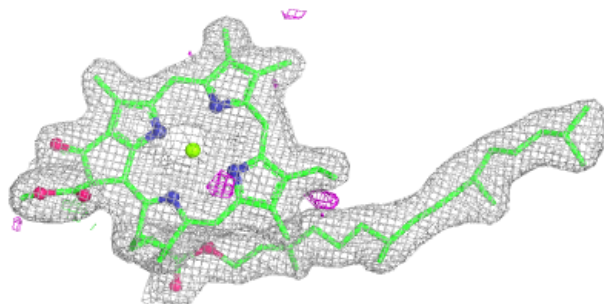


Electron density around DGD c 515:

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

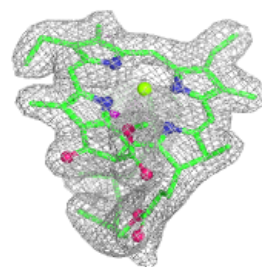
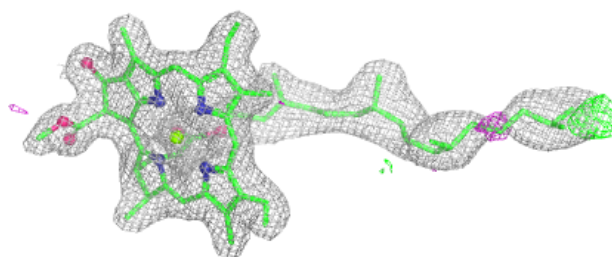
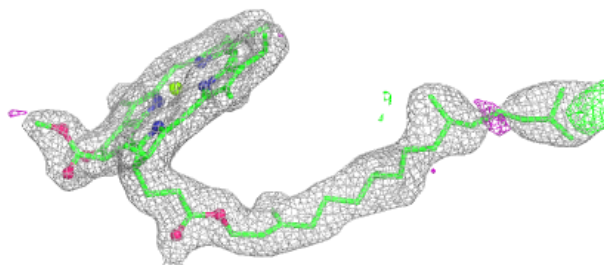
**Electron density around CLA c 501:**

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



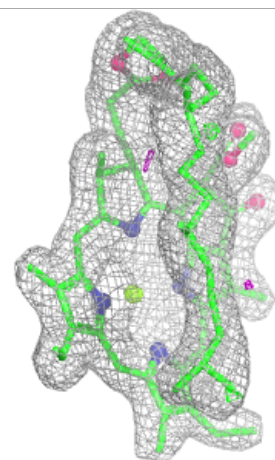
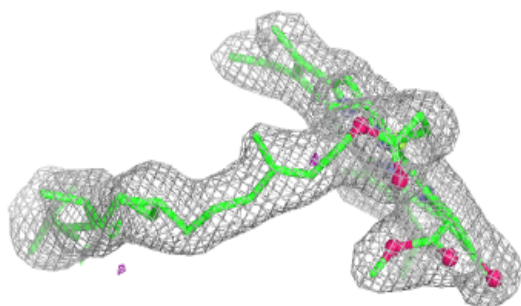
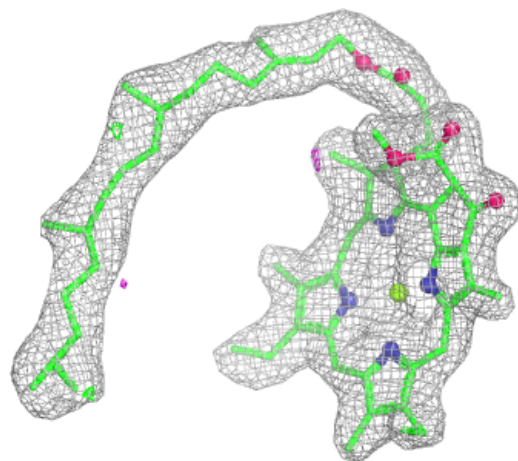
Electron density around CLA c 504:

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



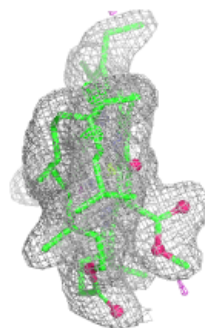
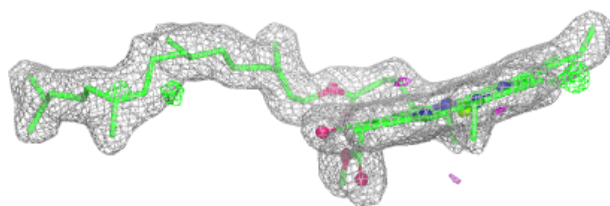
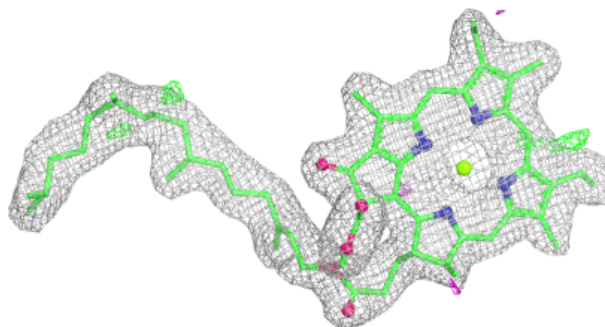
Electron density around CLA C 507:

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

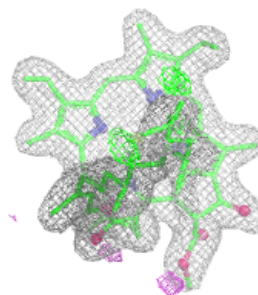
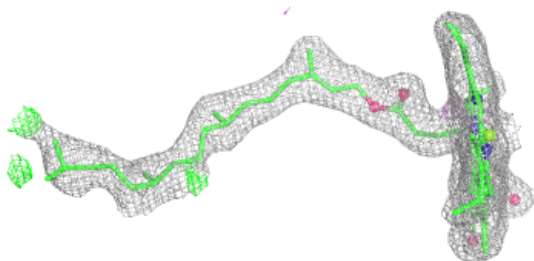
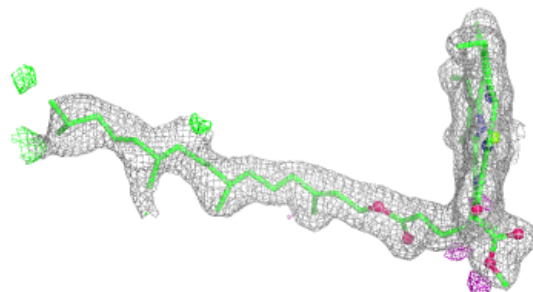


Electron density around CLA b 605:

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

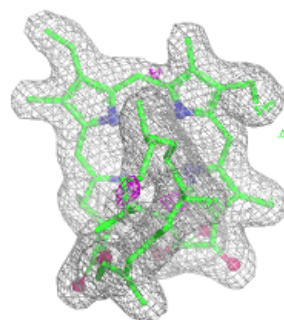
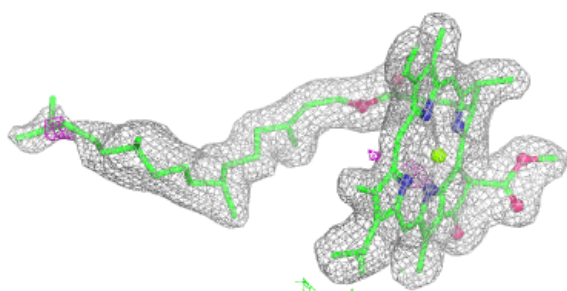
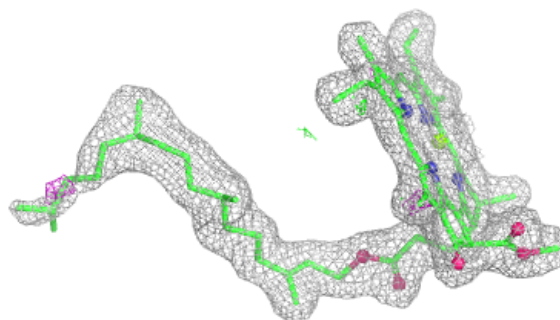
**Electron density around CLA b 609:**

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

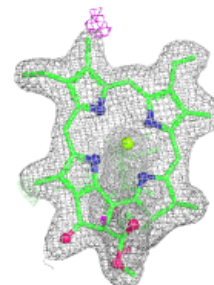
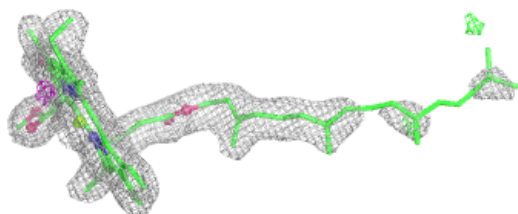
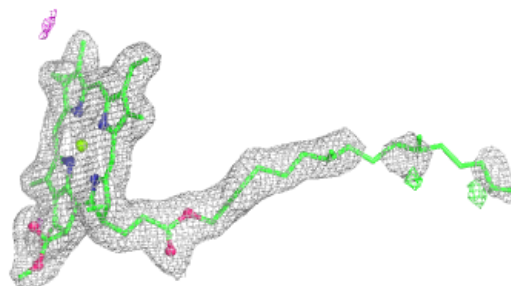


Electron density around CLA C 508:

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

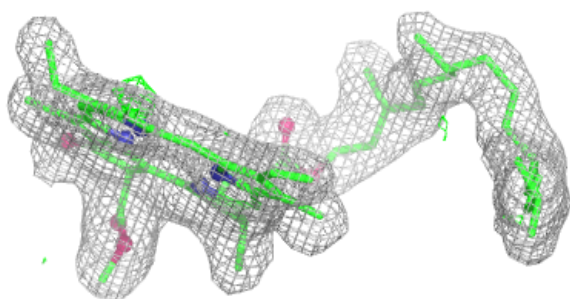
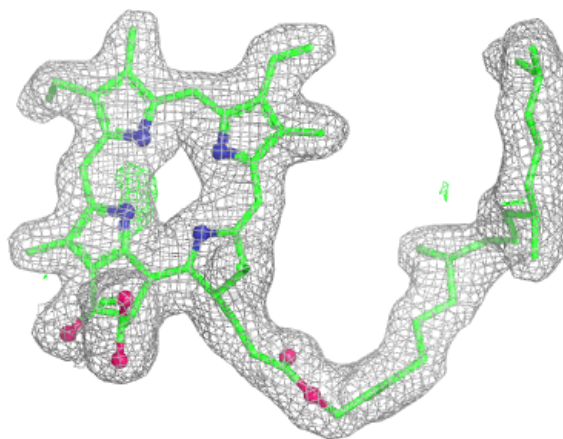
**Electron density around CLA d 403:**

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

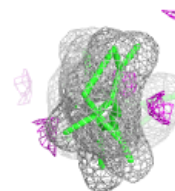
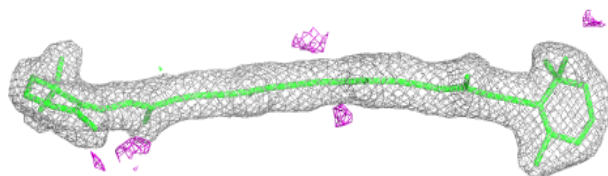
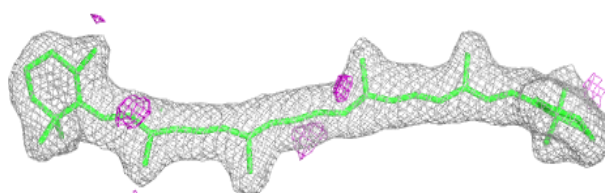


Electron density around PHO a 411:

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

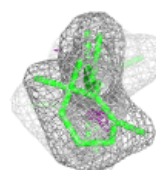
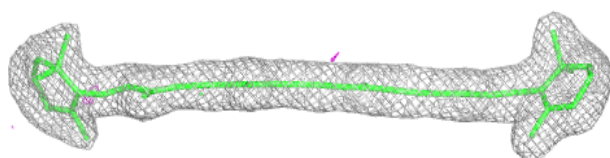
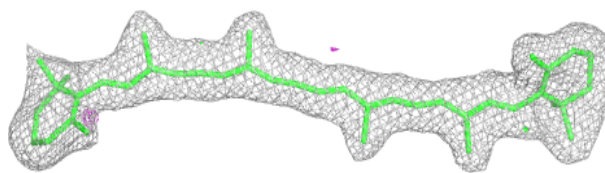
**Electron density around BCR b 620:**

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

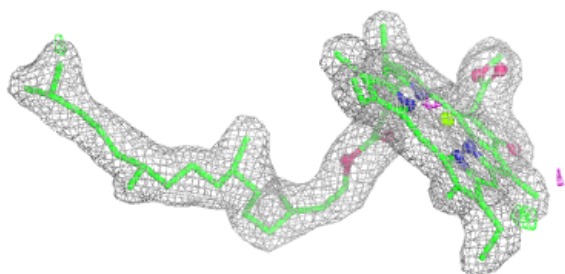
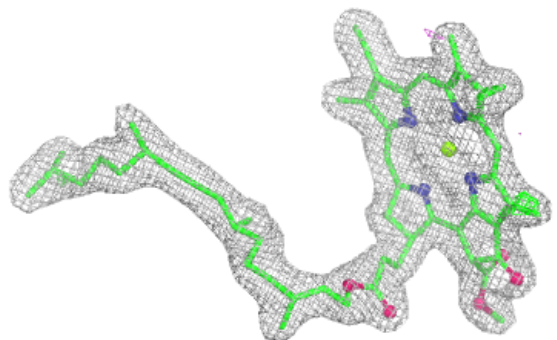


Electron density around BCR b 621:

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

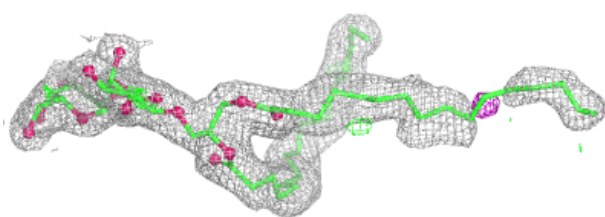
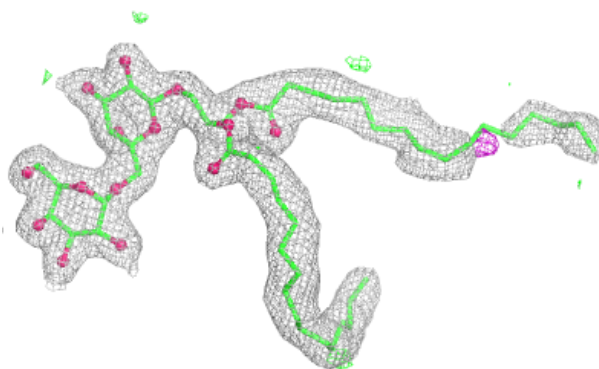
**Electron density around CLA C 511:**

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

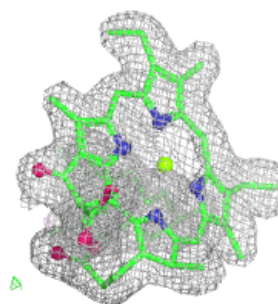
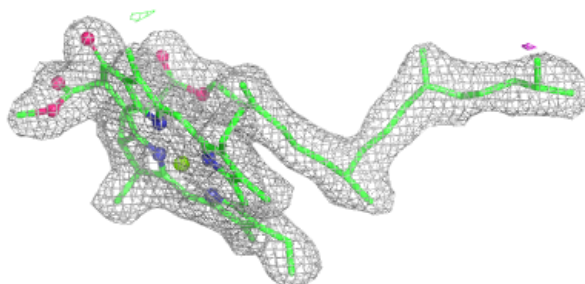
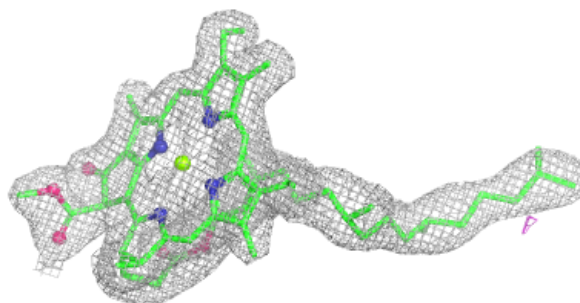


Electron density around DGD C 516:

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

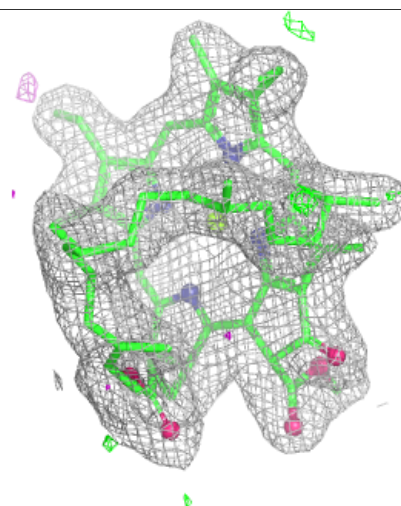
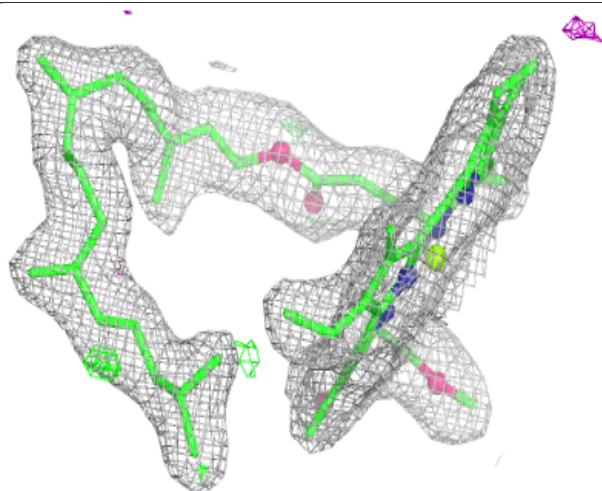
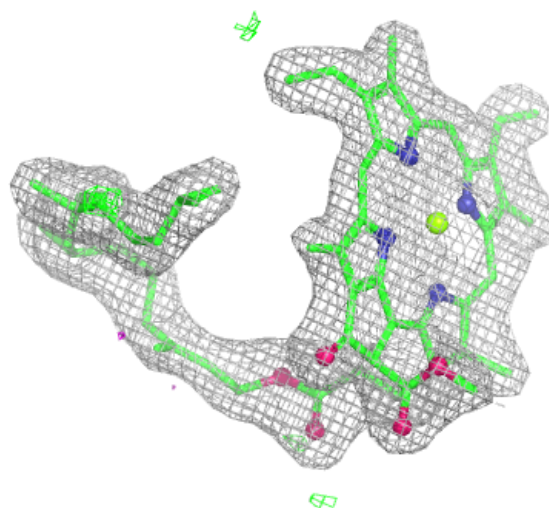
**Electron density around CLA C 505:**

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



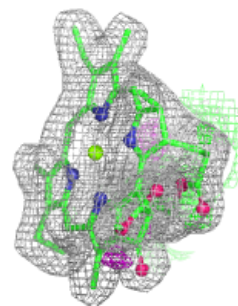
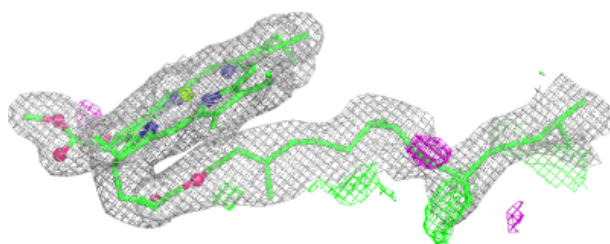
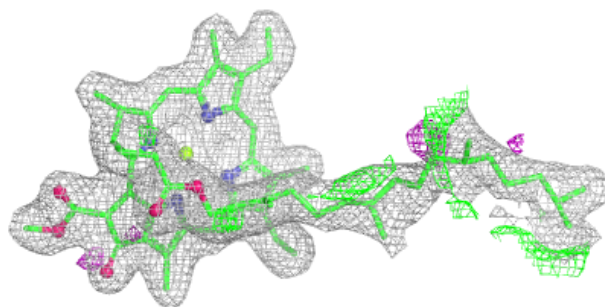
Electron density around CLA c 503:

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

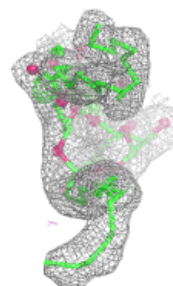
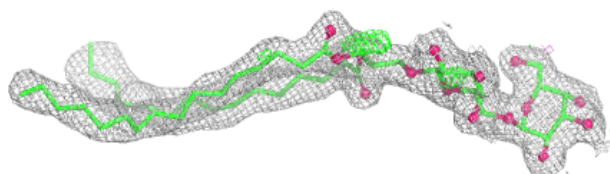
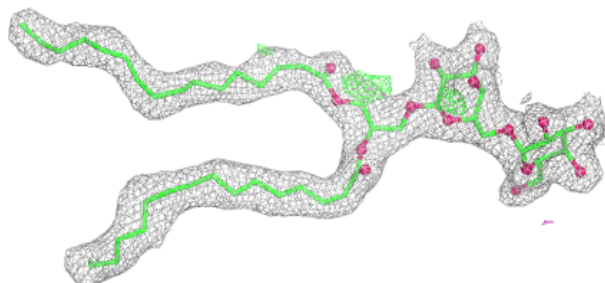


Electron density around CLA B 614:

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

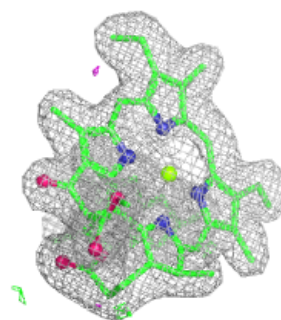
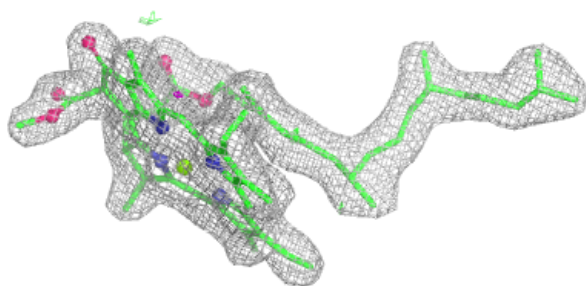
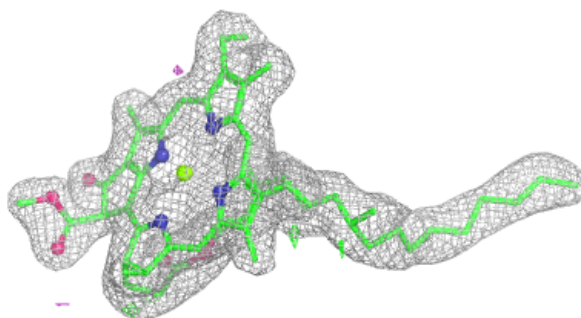
**Electron density around DGD c 517:**

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

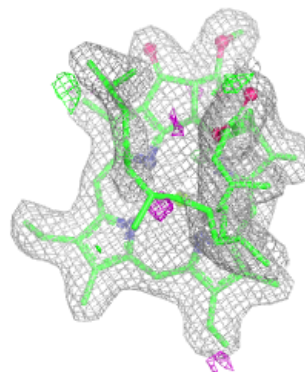
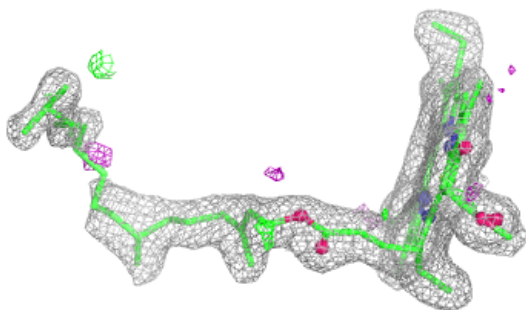
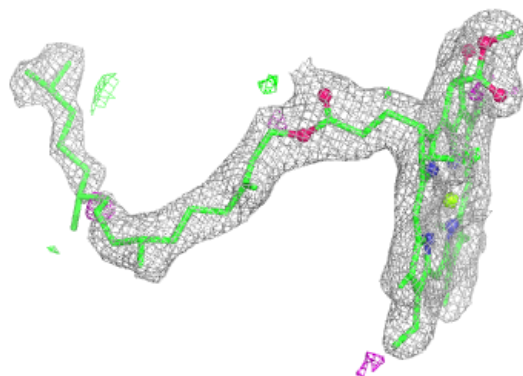


Electron density around CLA c 505:

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

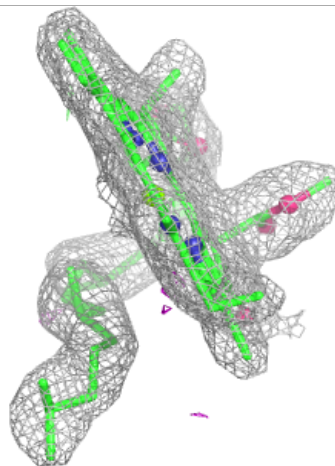
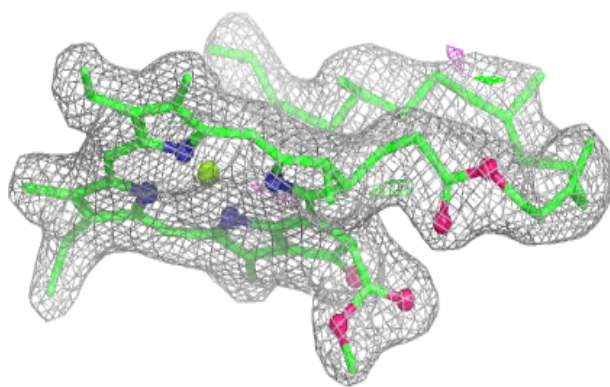
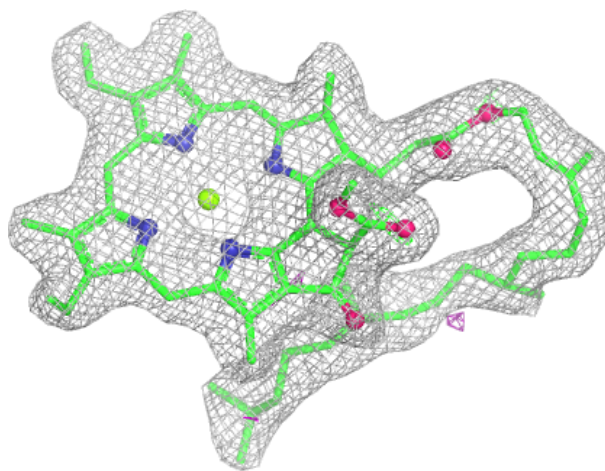
**Electron density around CLA D 405:**

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



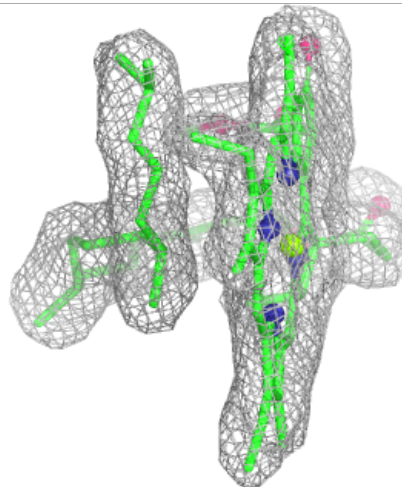
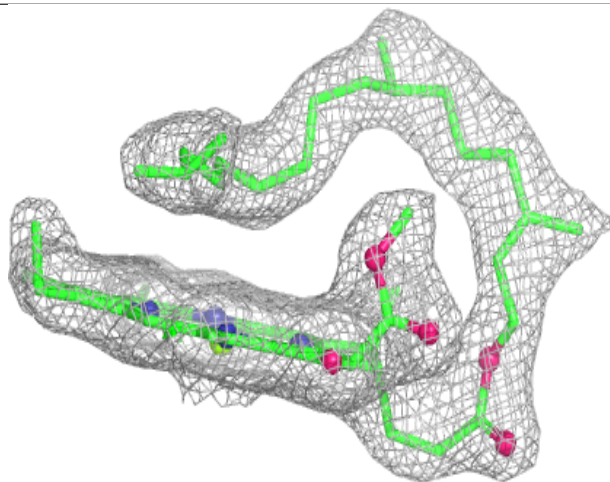
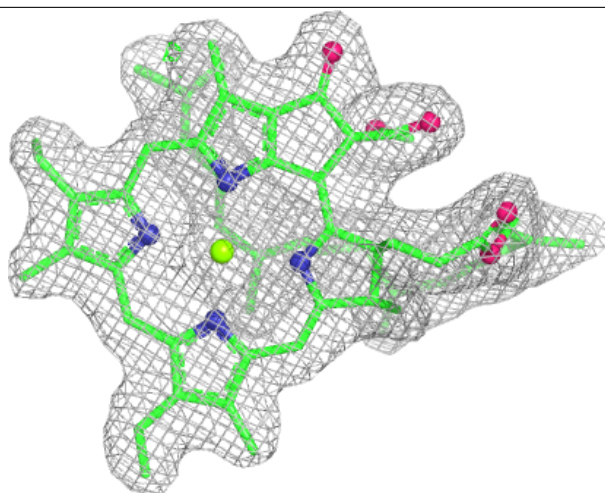
Electron density around CLA c 509:

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



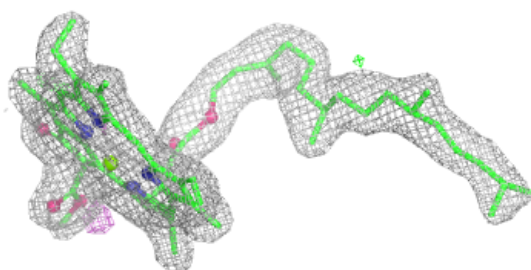
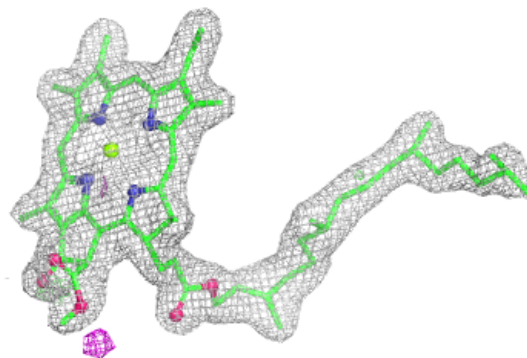
Electron density around CLA c 510:

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



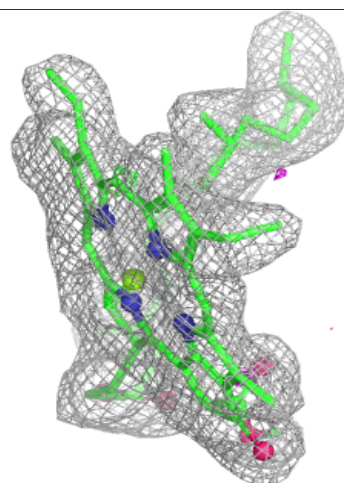
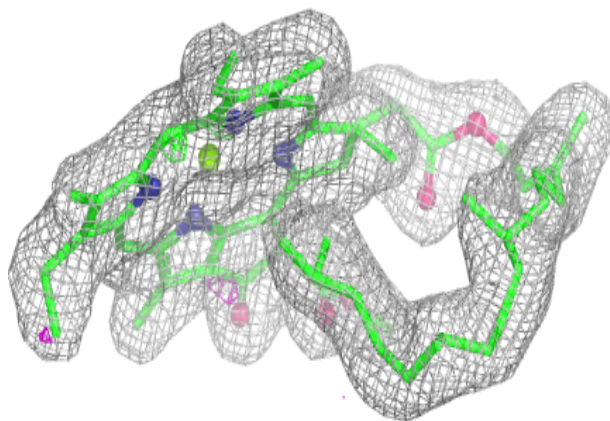
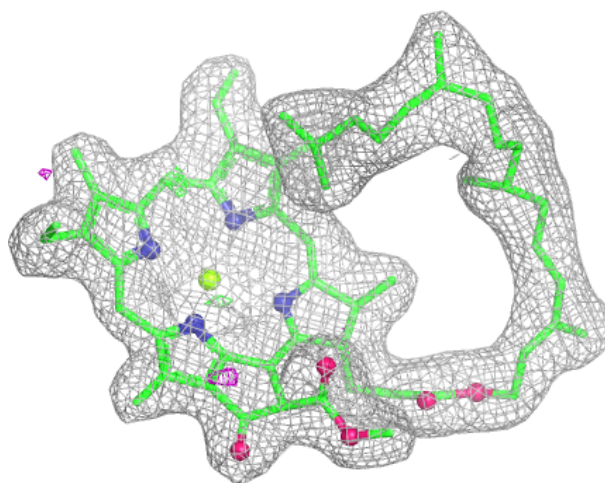
Electron density around CLA c 511:

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



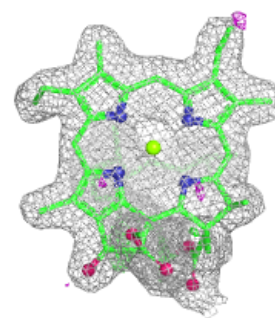
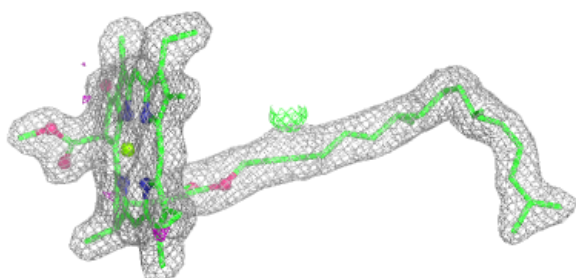
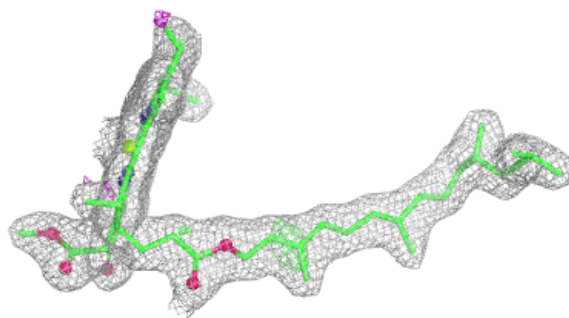
Electron density around CLA B 615:

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

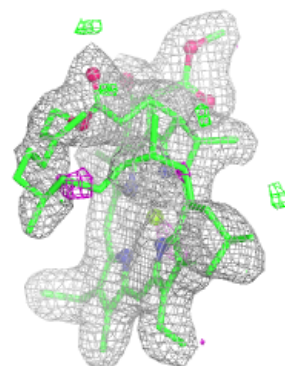
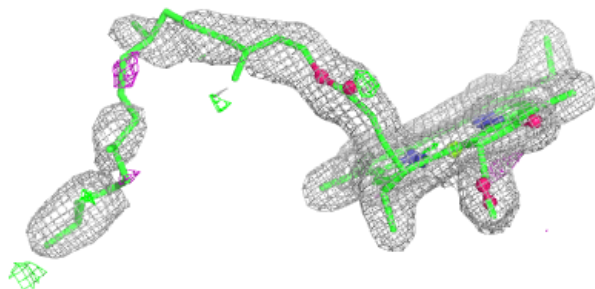
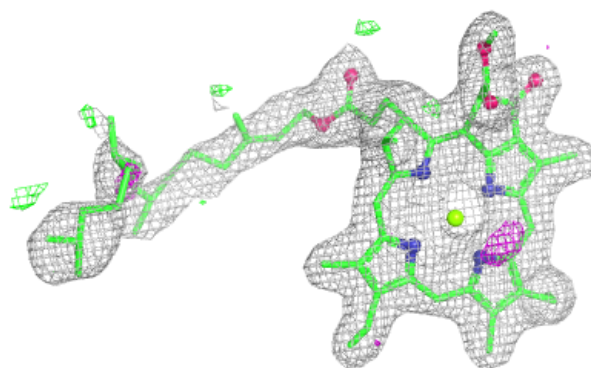


Electron density around CLA b 608:

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

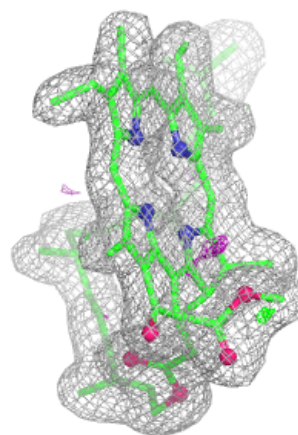
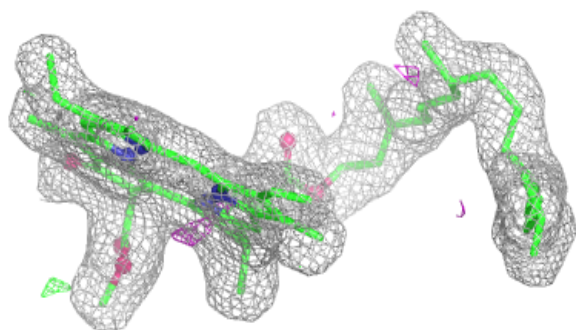
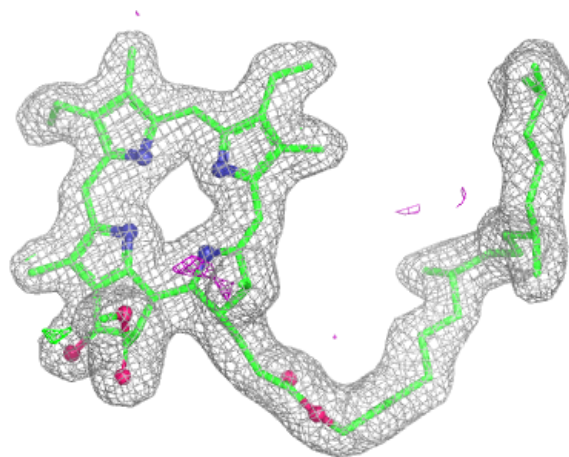
**Electron density around CLA A 1008:**

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



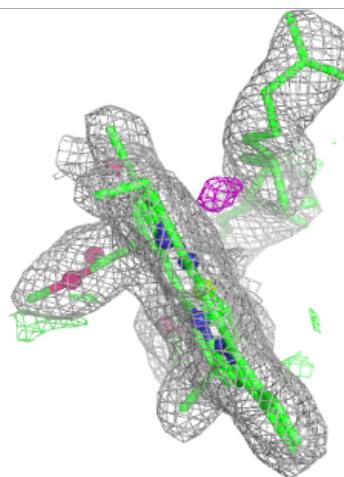
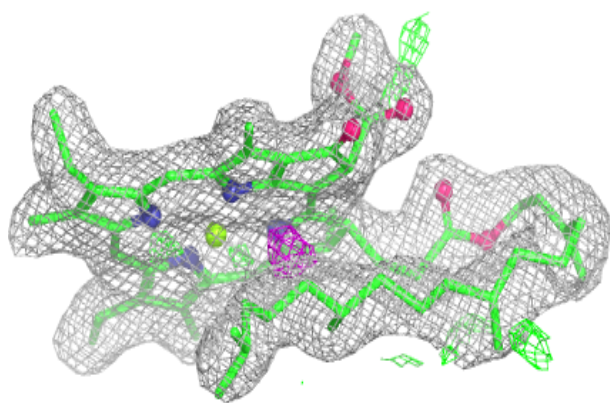
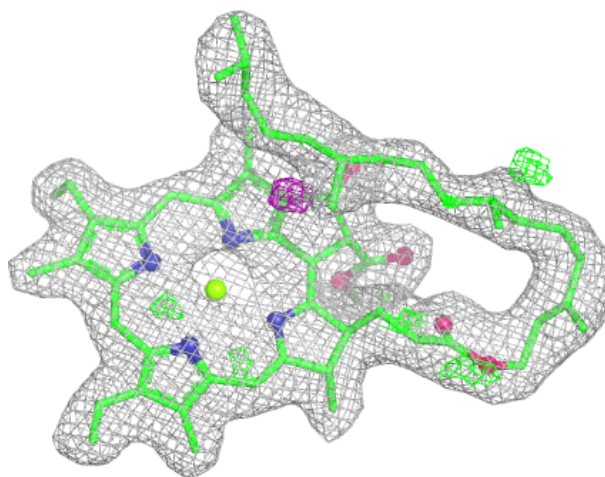
Electron density around PHO D 404:

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



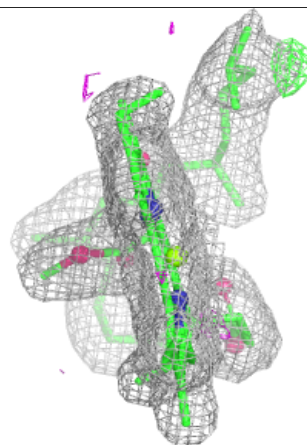
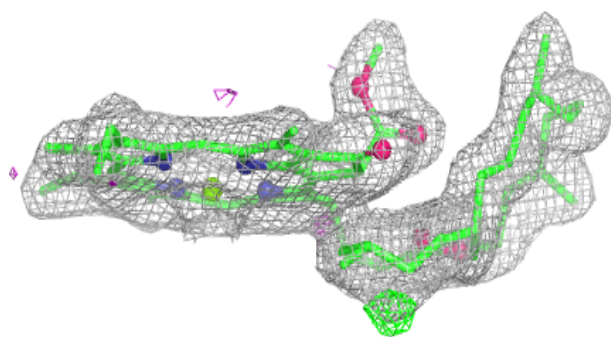
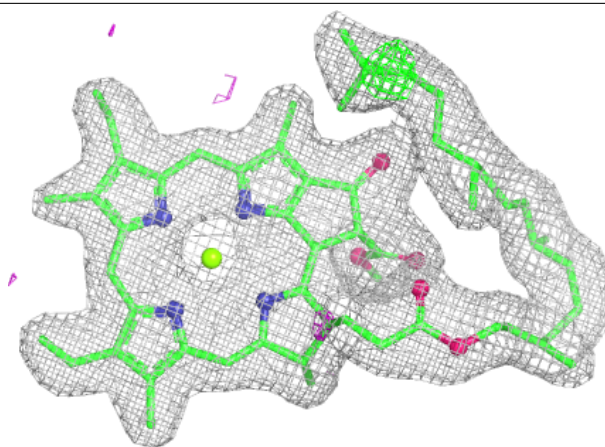
Electron density around CLA C 509:

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



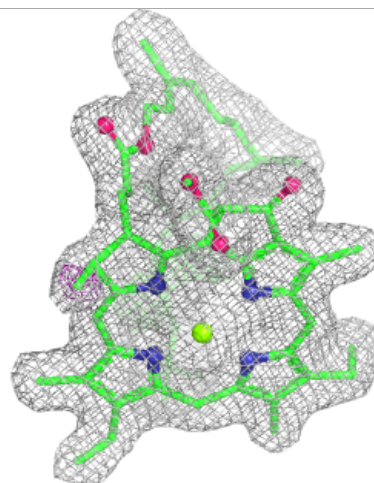
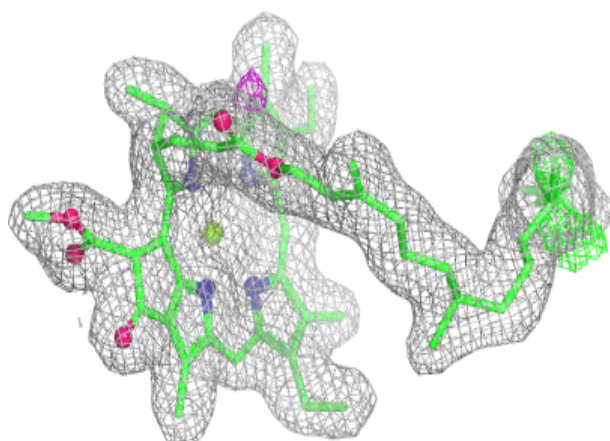
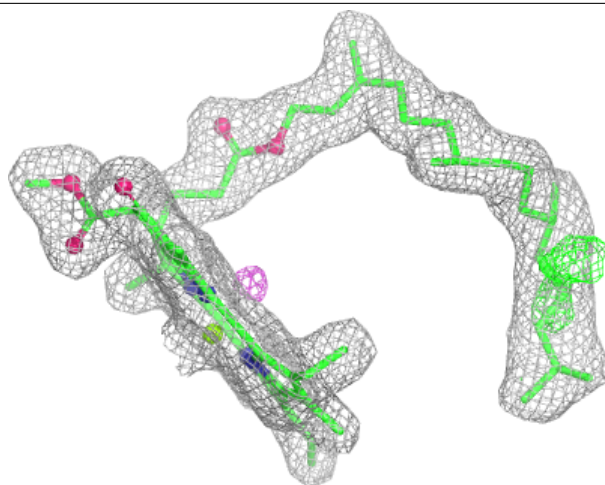
Electron density around CLA b 613:

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



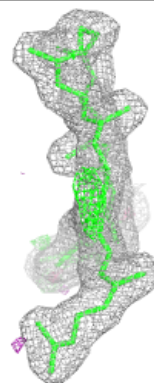
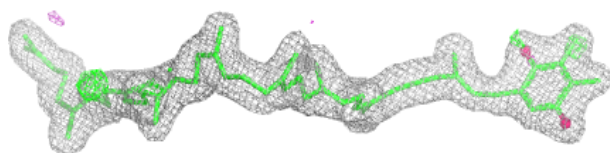
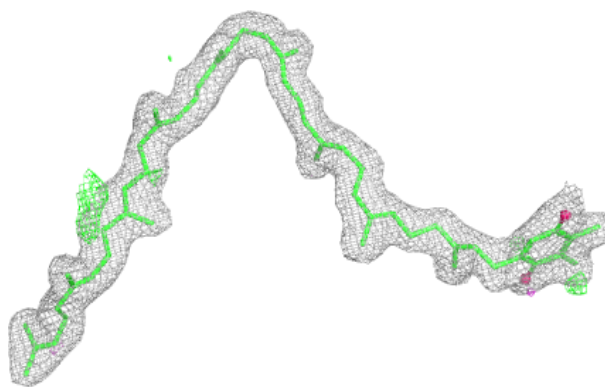
Electron density around CLA b 614:

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

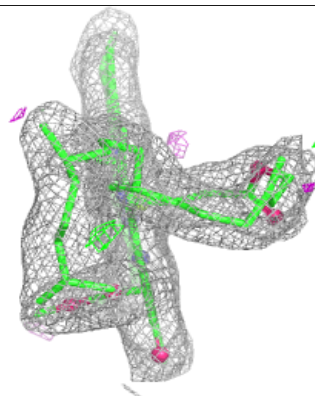
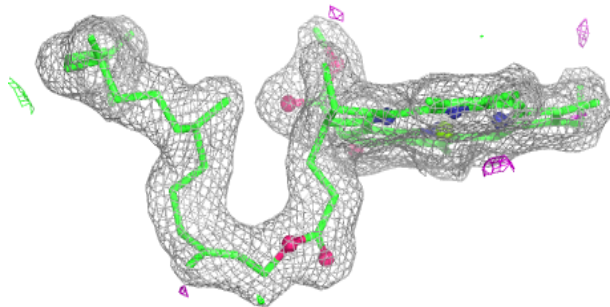
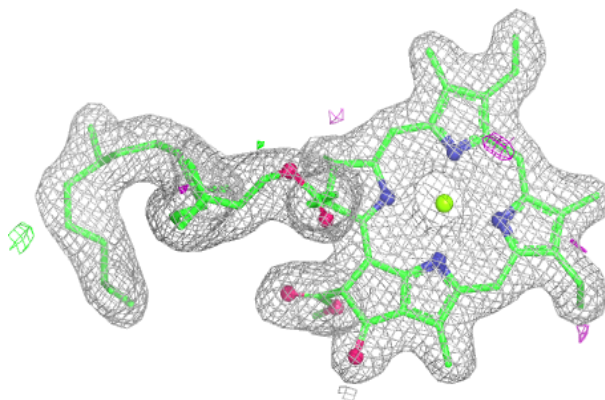


Electron density around PL9 D 407:

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

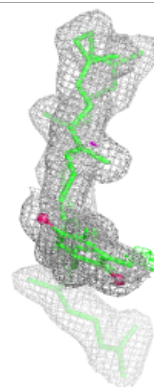
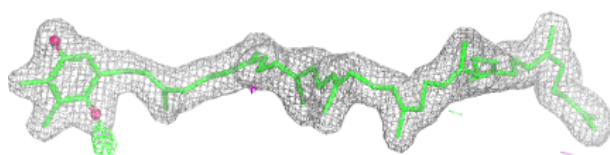
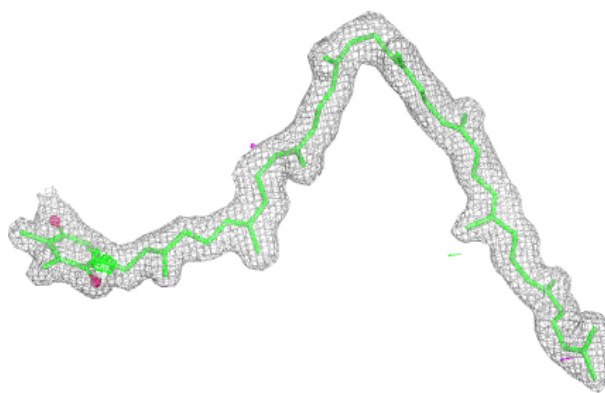
**Electron density around CLA b 615:**

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

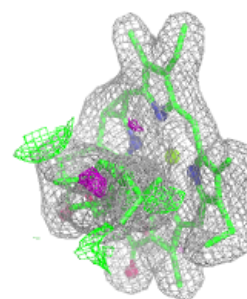
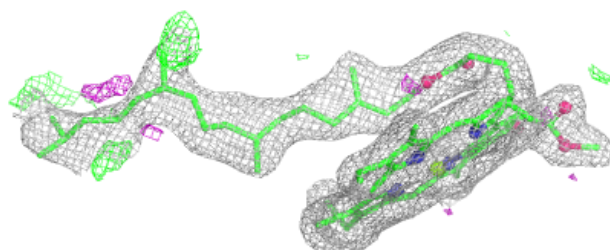
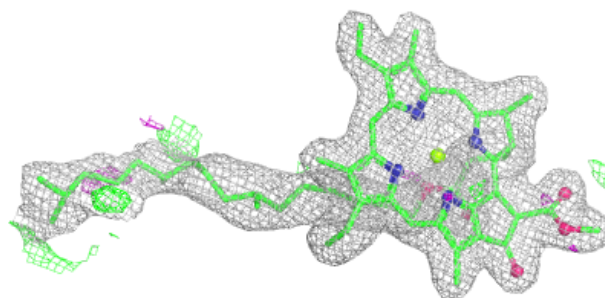


Electron density around PL9 d 405:

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

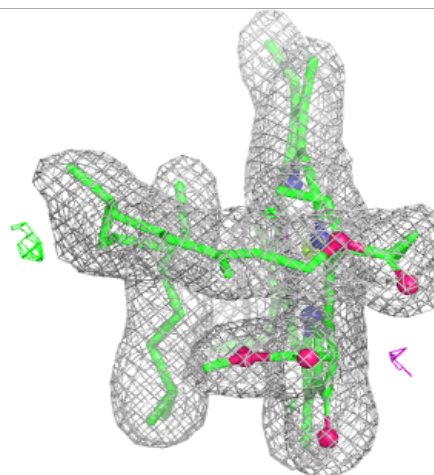
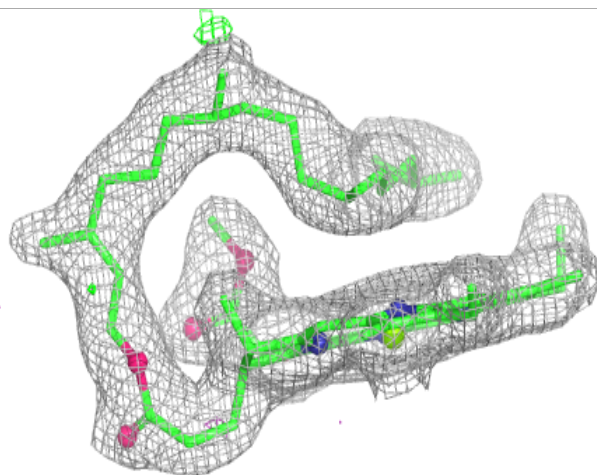
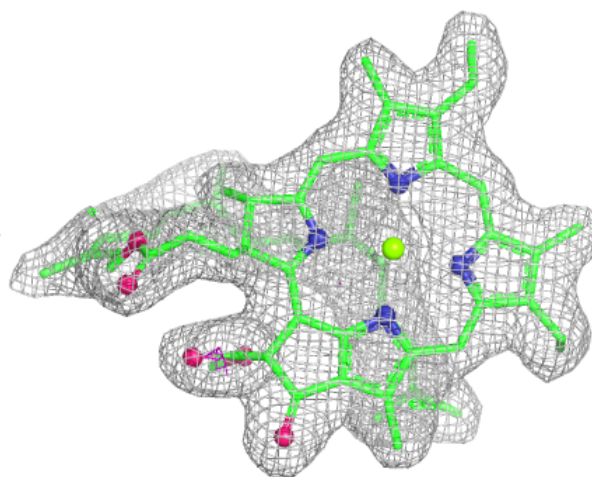
**Electron density around CLA b 617:**

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



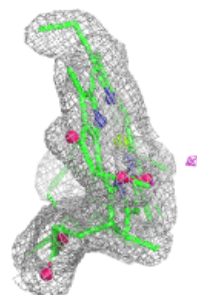
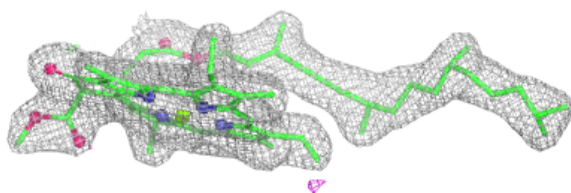
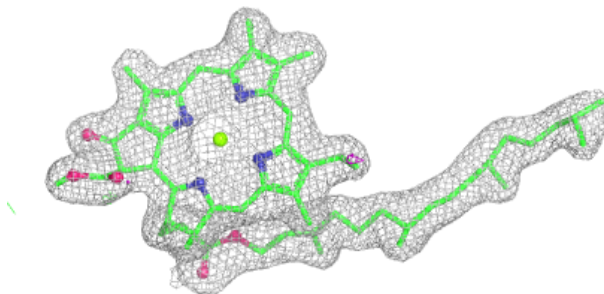
Electron density around CLA C 510:

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

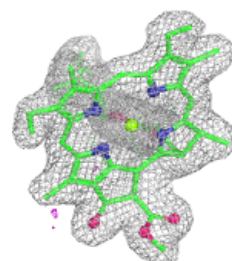
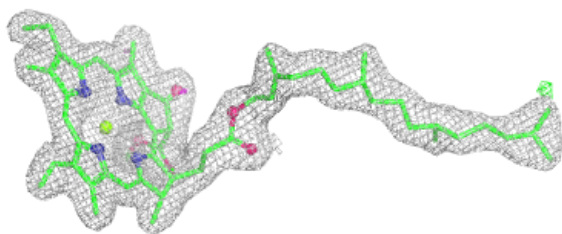
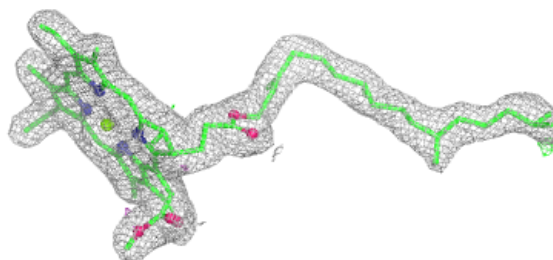


Electron density around CLA C 501:

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

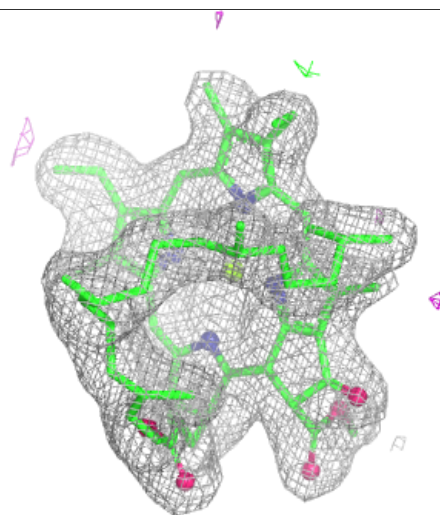
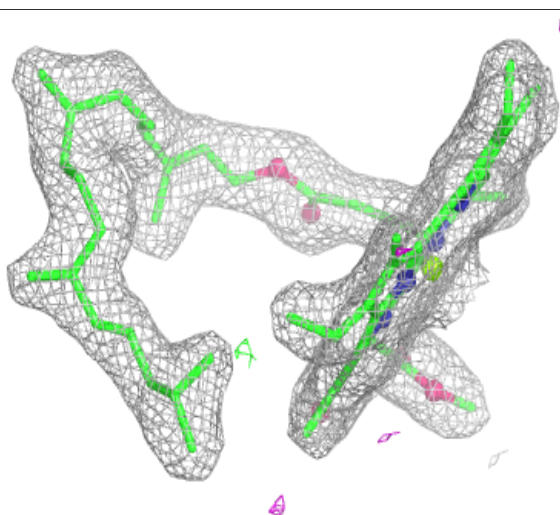
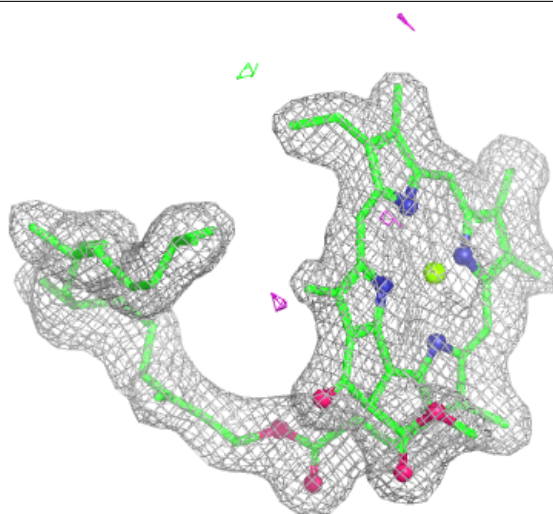
**Electron density around CLA c 502:**

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



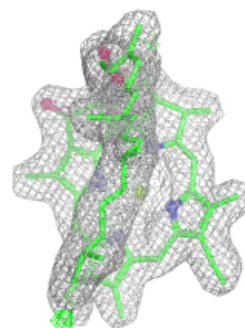
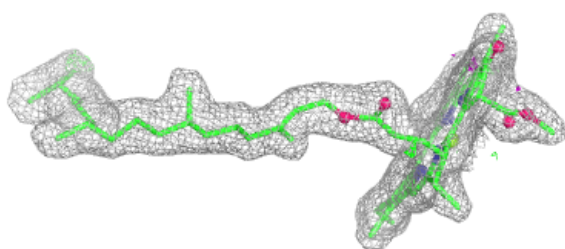
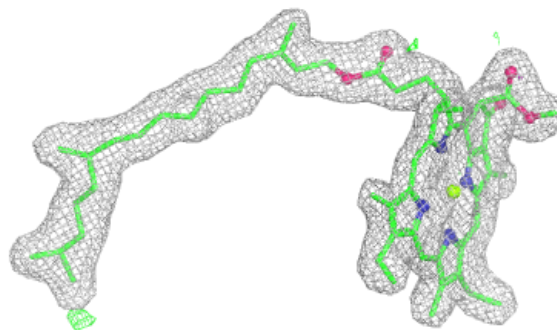
Electron density around CLA C 503:

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

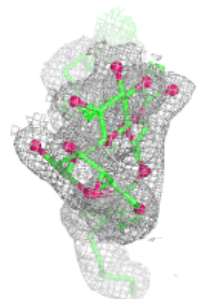
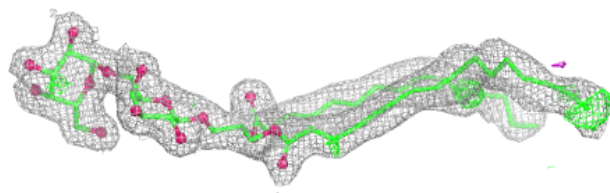
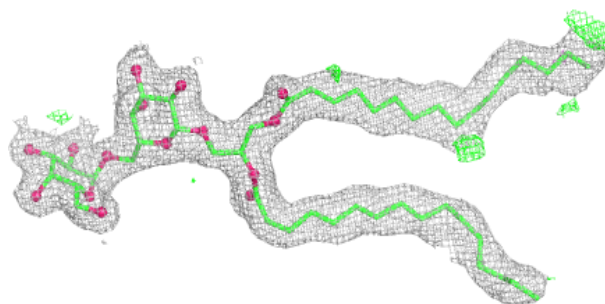


Electron density around CLA B 609:

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

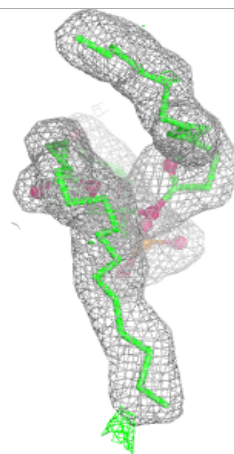
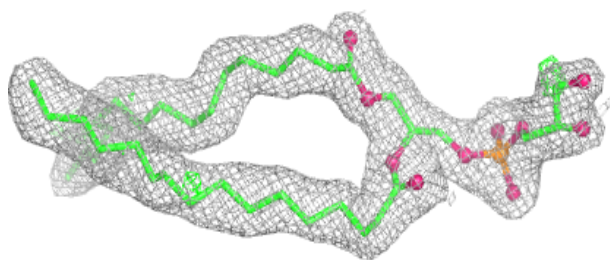
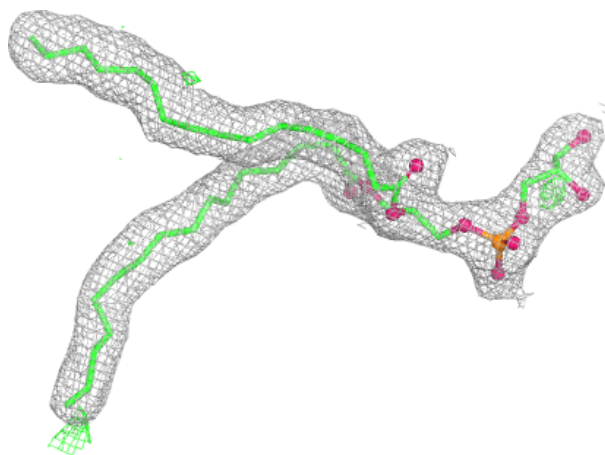
**Electron density around DGD C 517:**

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



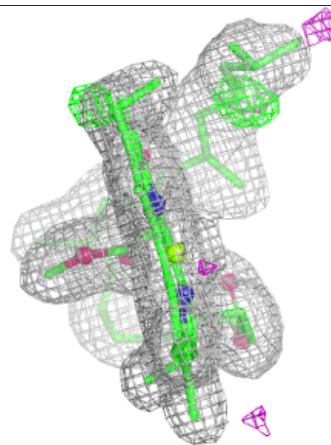
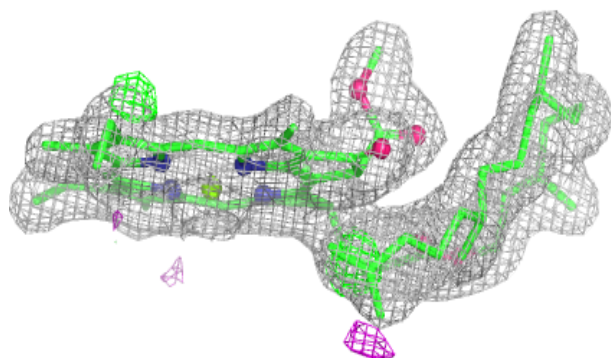
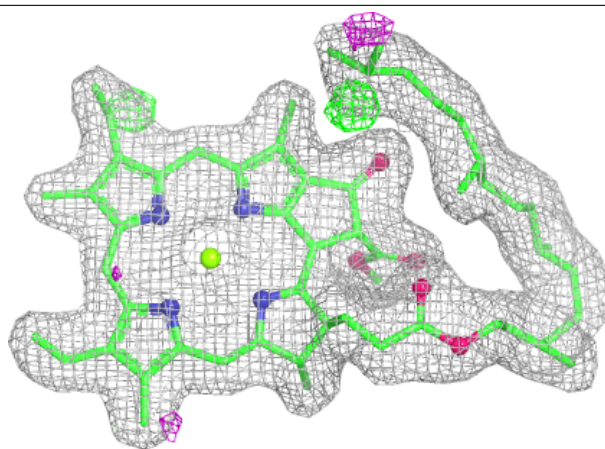
Electron density around LHG D 410:

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



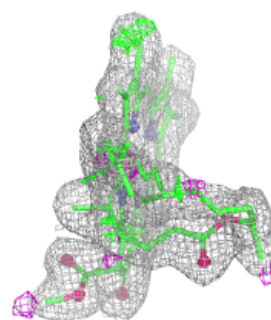
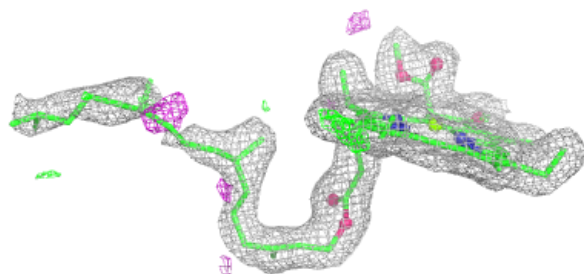
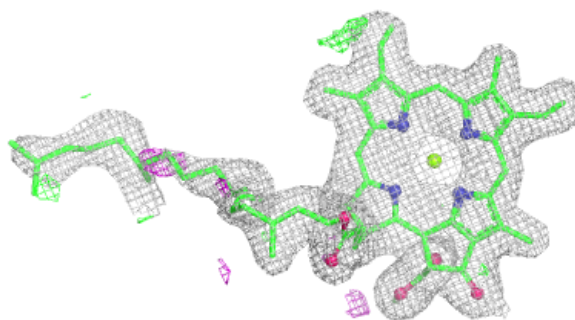
Electron density around CLA B 610:

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



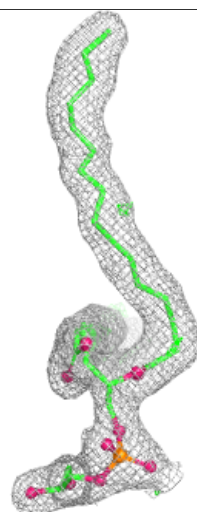
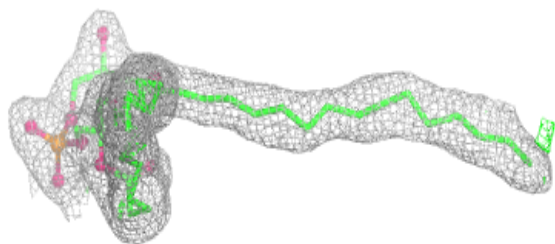
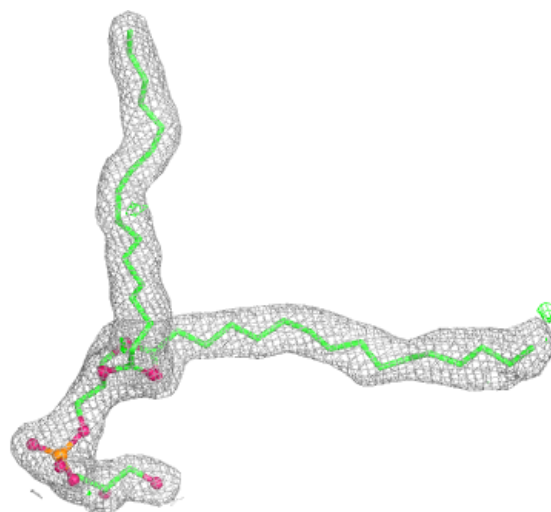
Electron density around CLA a 409:

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



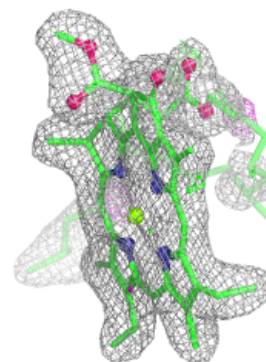
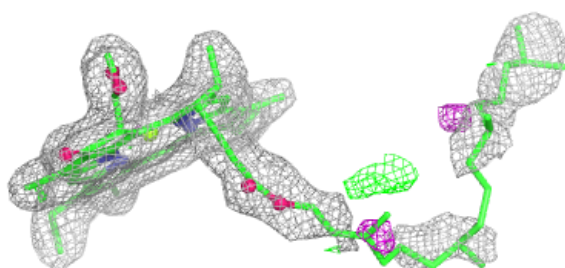
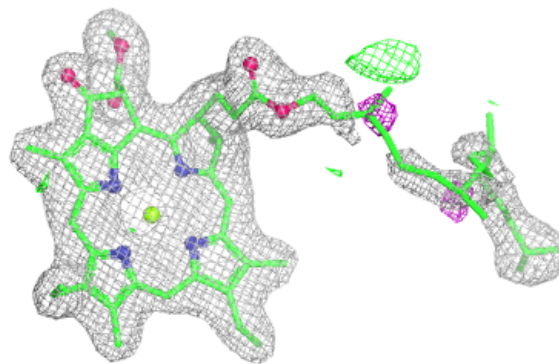
Electron density around LHG b 624:

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

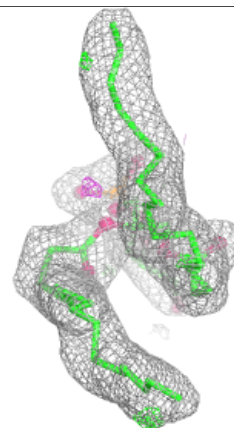
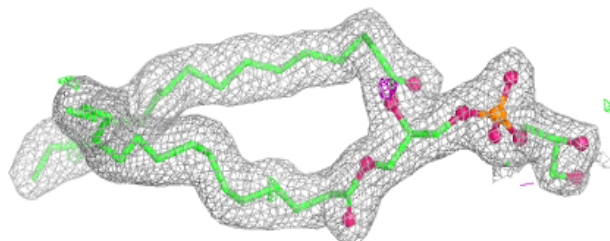
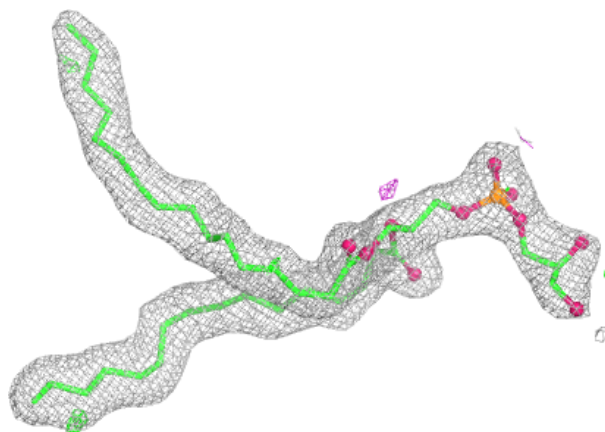


Electron density around CLA a 412:

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

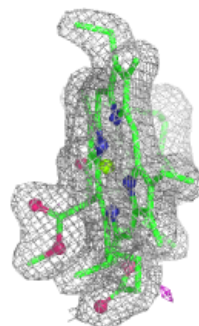
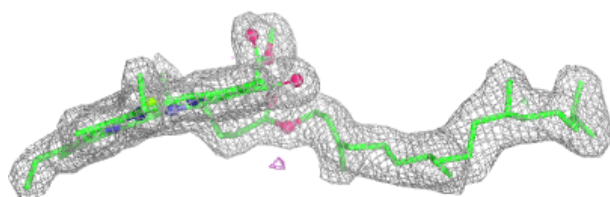
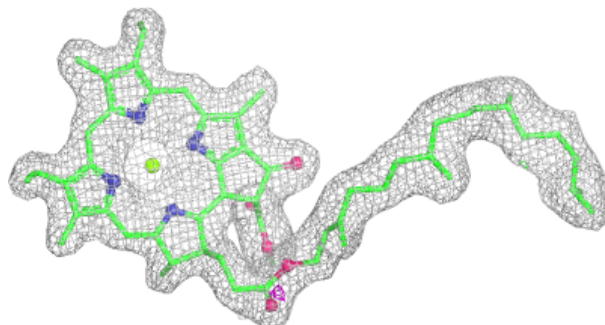
**Electron density around LHG d 407:**

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

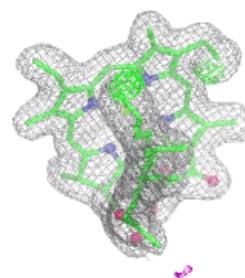
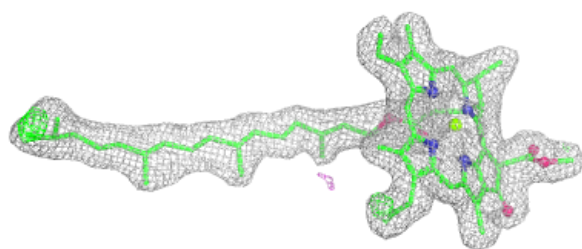
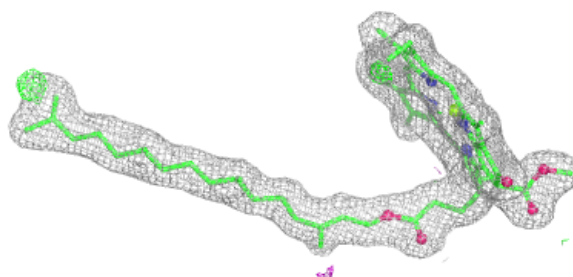


Electron density around CLA B 602:

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

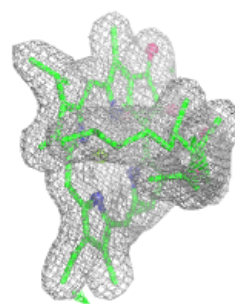
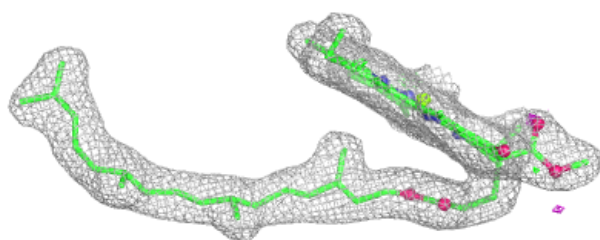
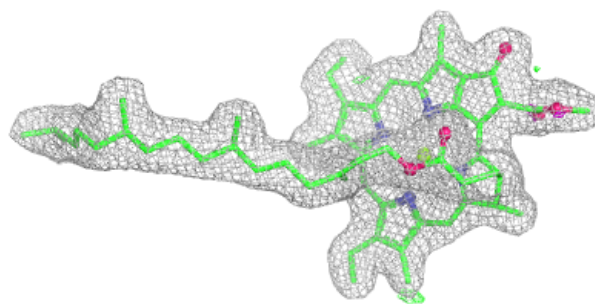
**Electron density around CLA b 610:**

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

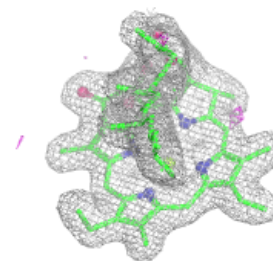
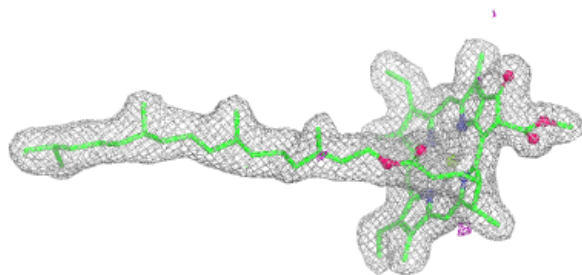
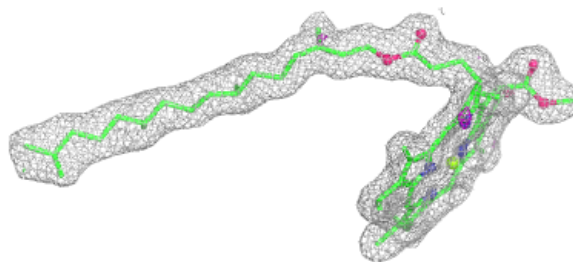


Electron density around CLA b 611:

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

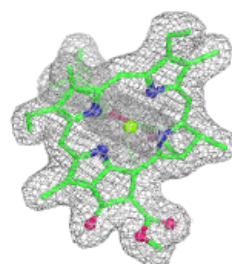
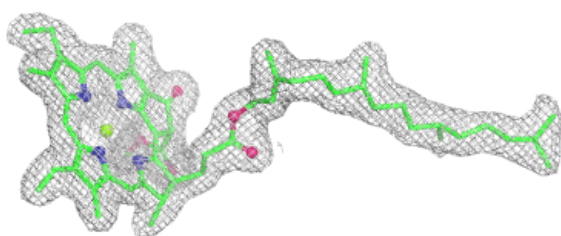
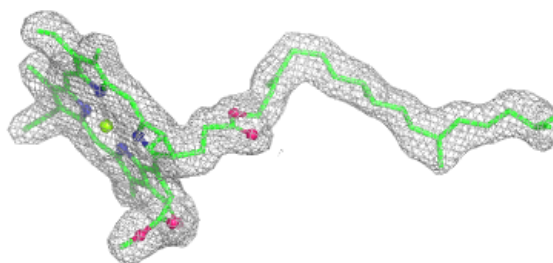
**Electron density around CLA B 607:**

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

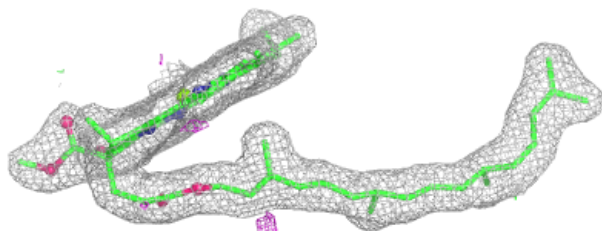
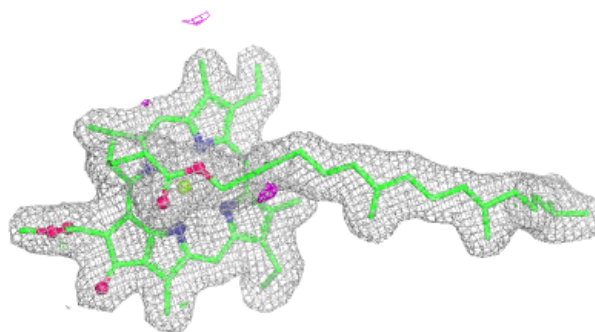


Electron density around CLA C 502:

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

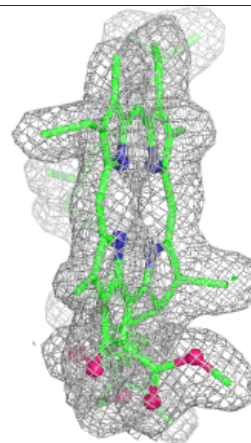
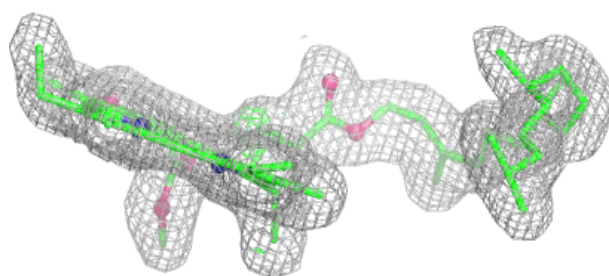
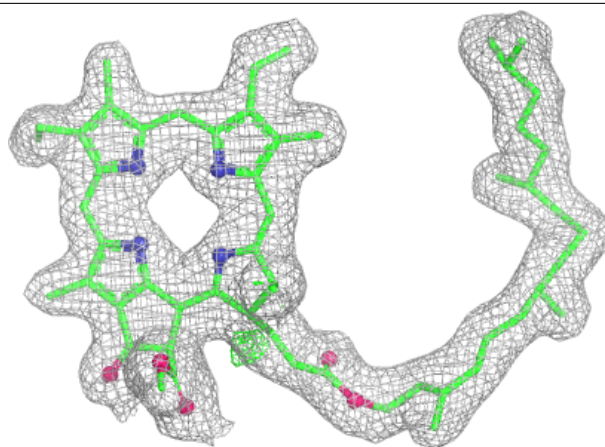
**Electron density around CLA B 608:**

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



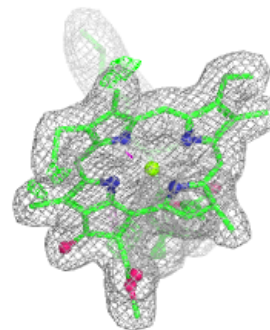
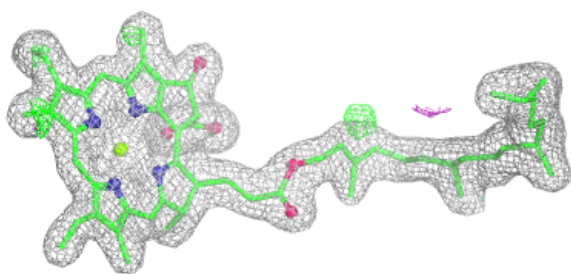
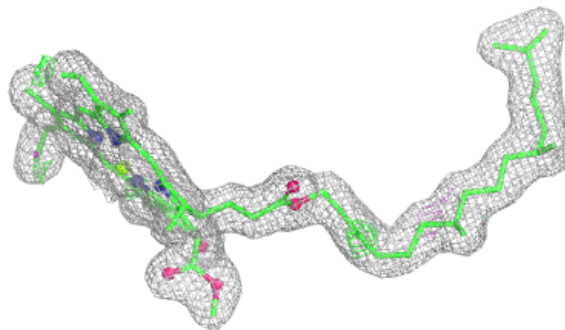
Electron density around PHO A 1007:

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



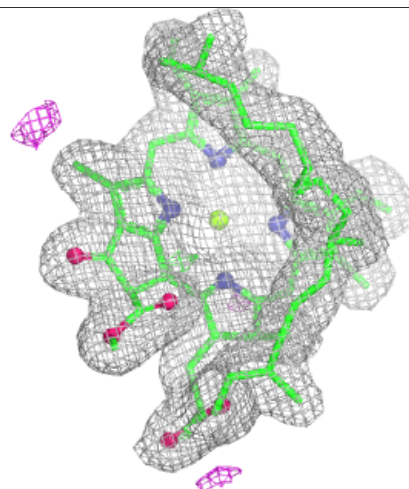
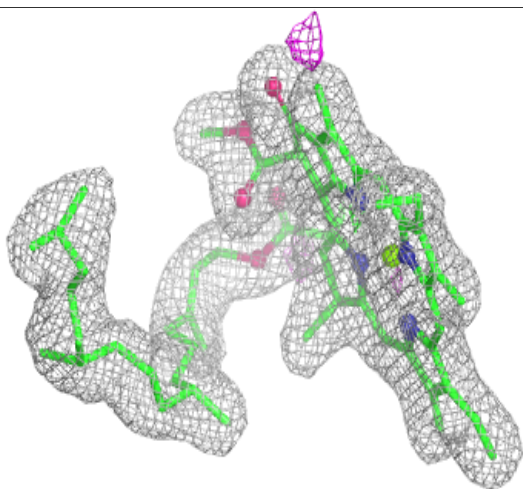
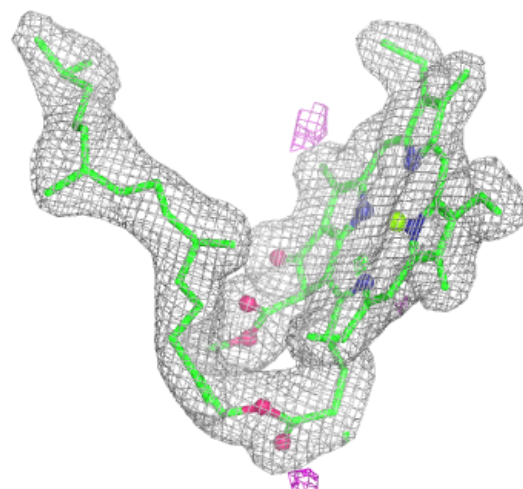
Electron density around CLA D 402:

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



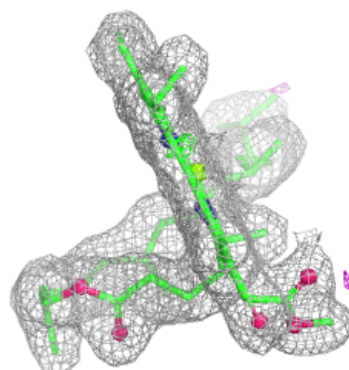
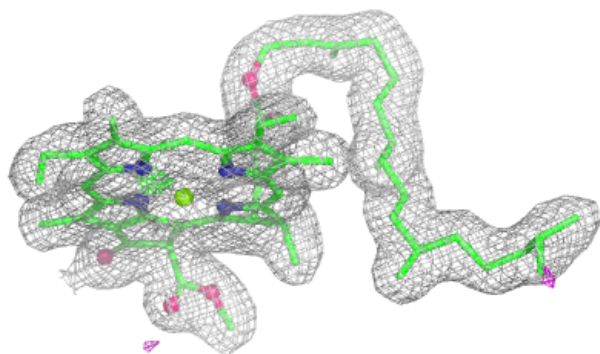
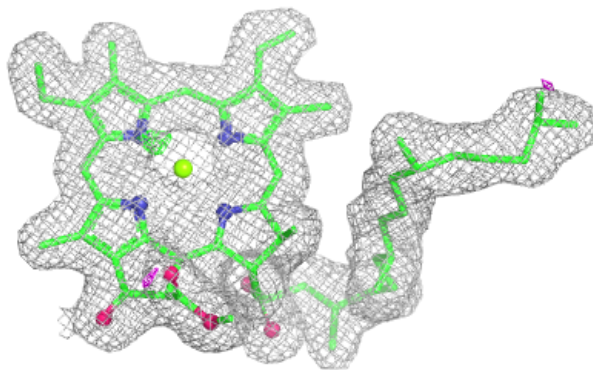
Electron density around CLA b 616:

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



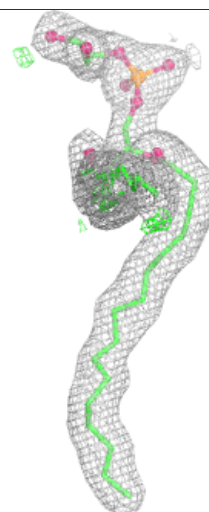
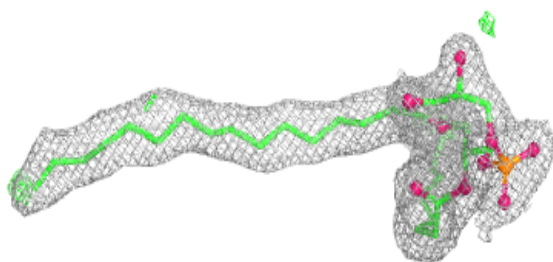
Electron density around CLA D 403:

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



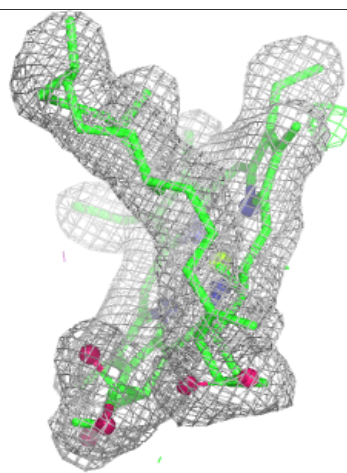
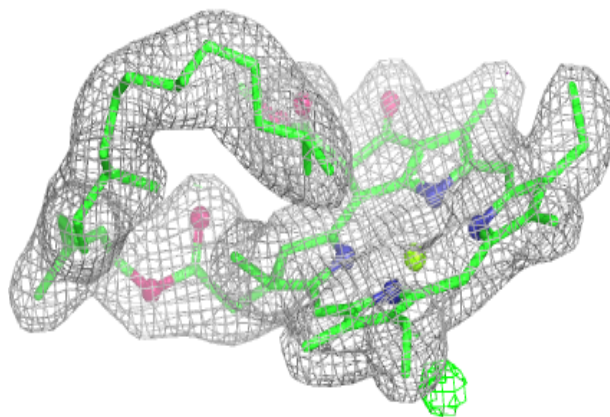
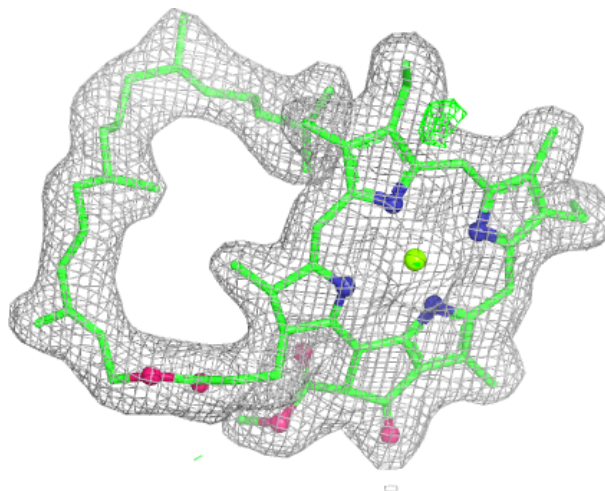
Electron density around LHG B 621:

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



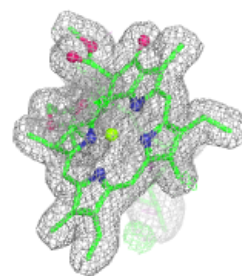
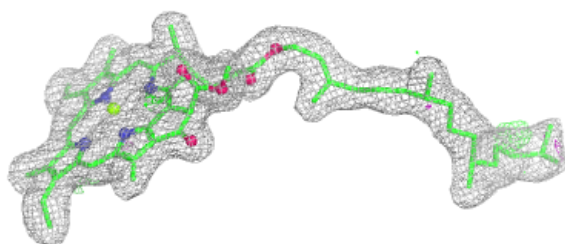
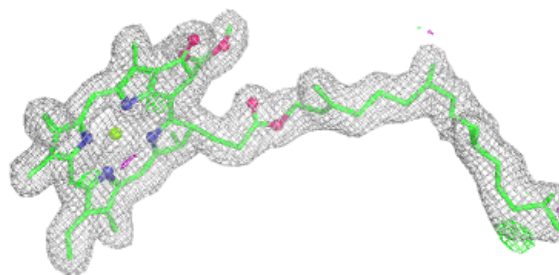
Electron density around CLA b 618:

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

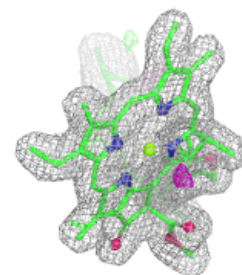
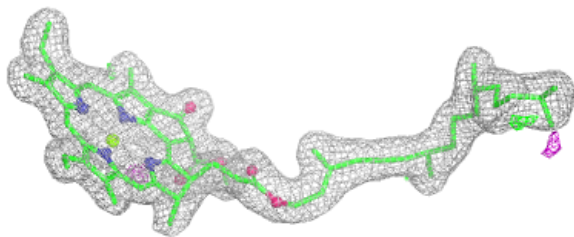
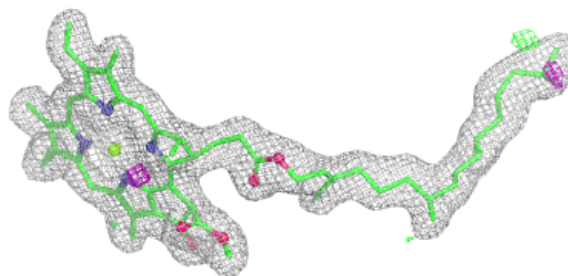


Electron density around CLA A 1005:

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

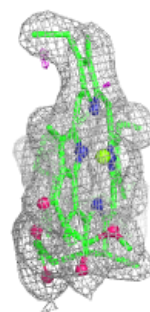
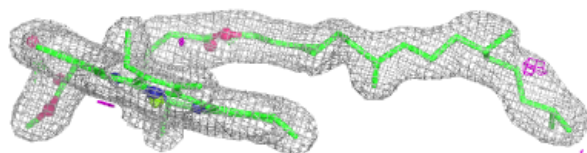
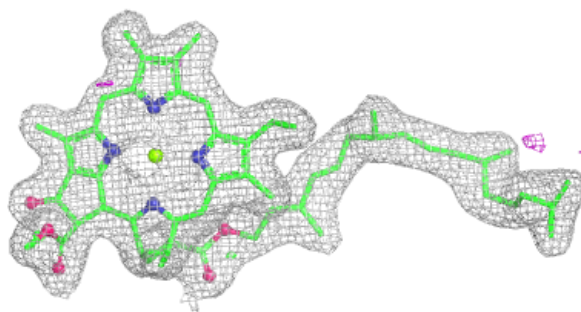
**Electron density around CLA a 407:**

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



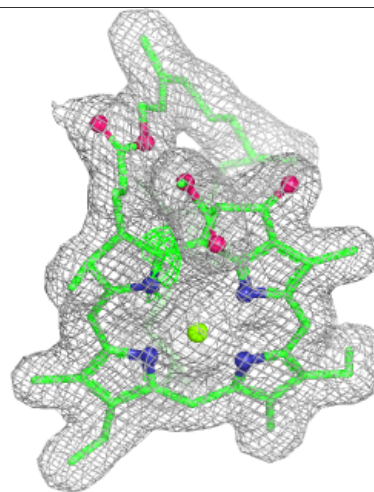
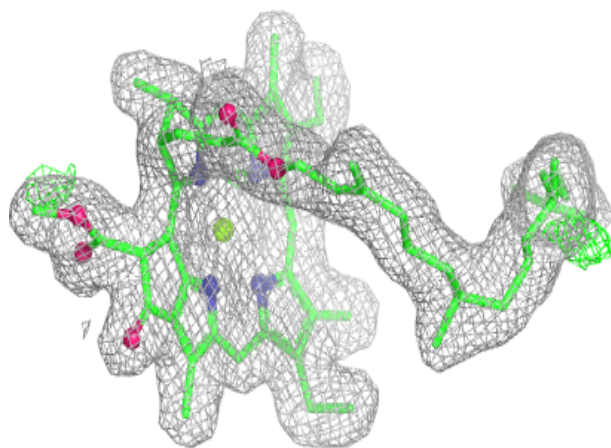
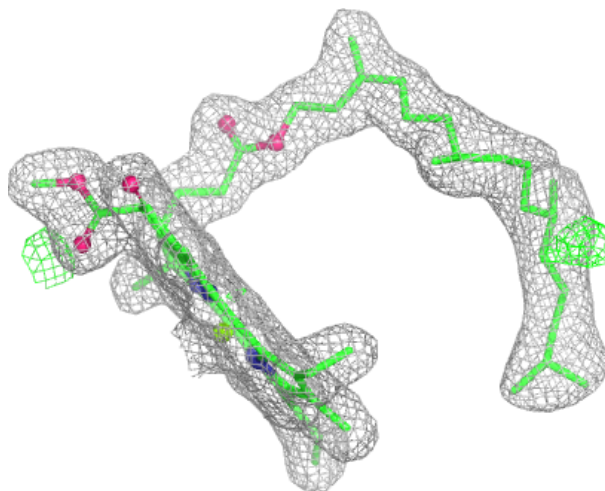
Electron density around CLA B 603:

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



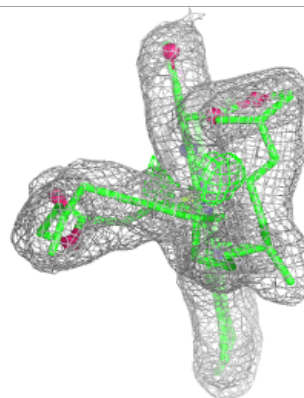
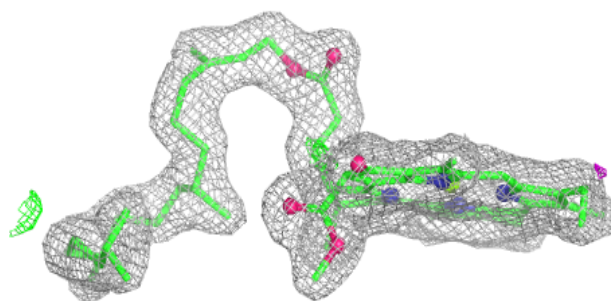
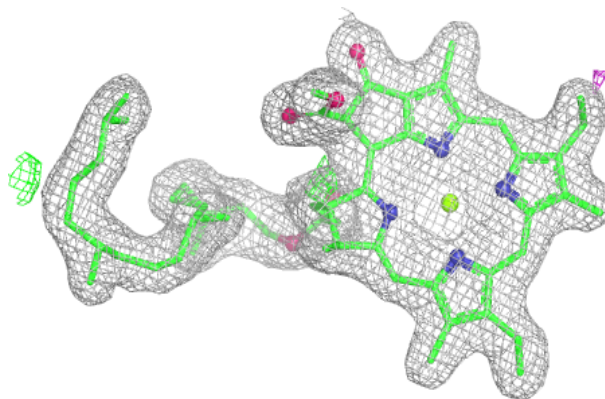
Electron density around CLA B 611:

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

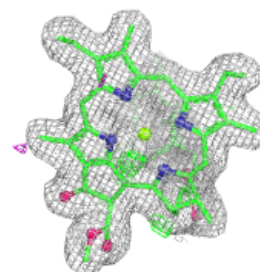
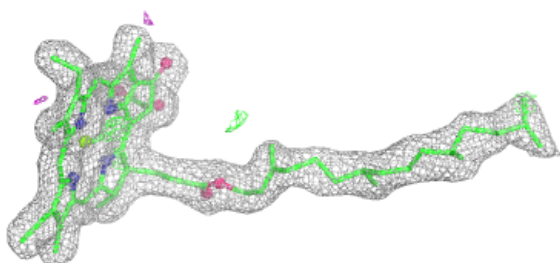
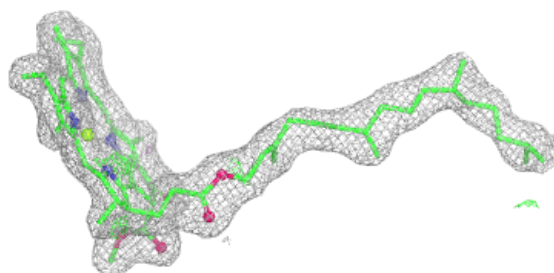


Electron density around CLA B 612:

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

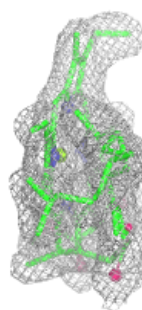
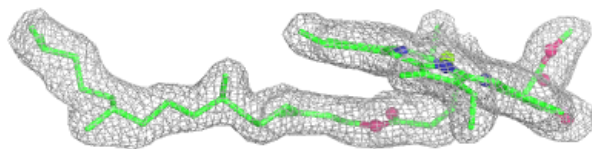
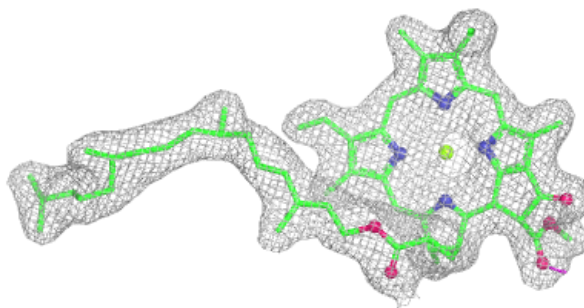
**Electron density around CLA B 604:**

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

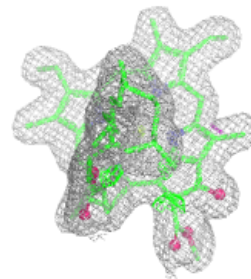
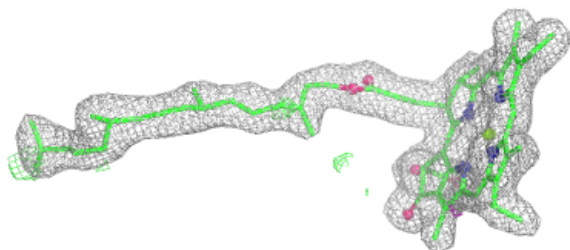
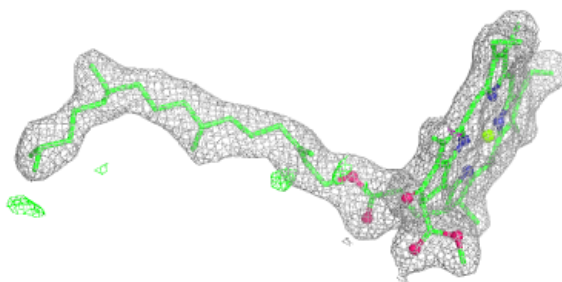


Electron density around CLA b 606:

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

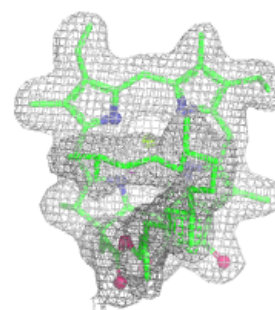
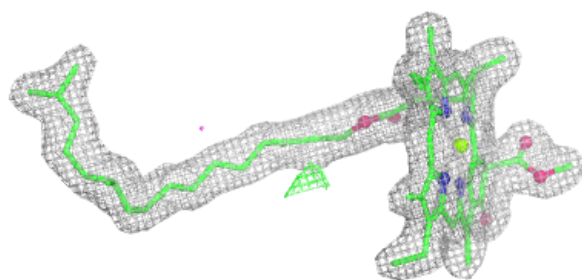
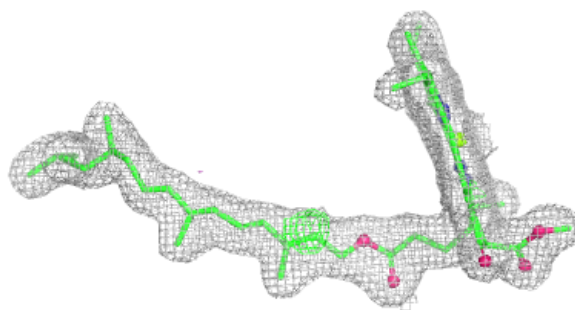
**Electron density around CLA b 607:**

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



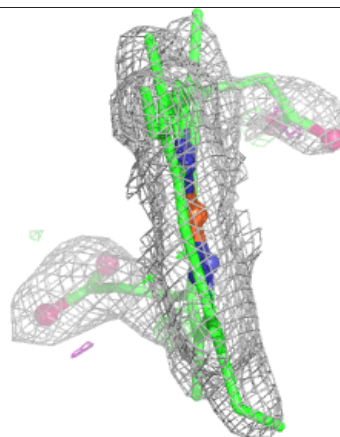
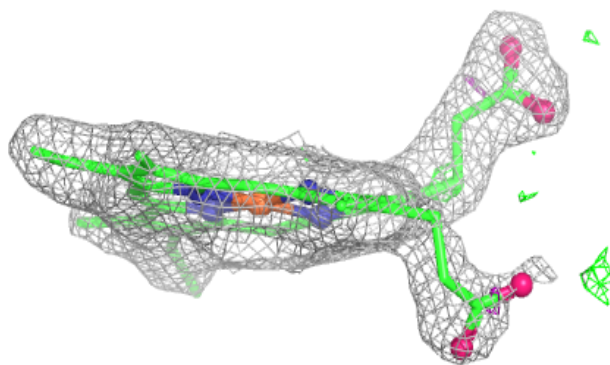
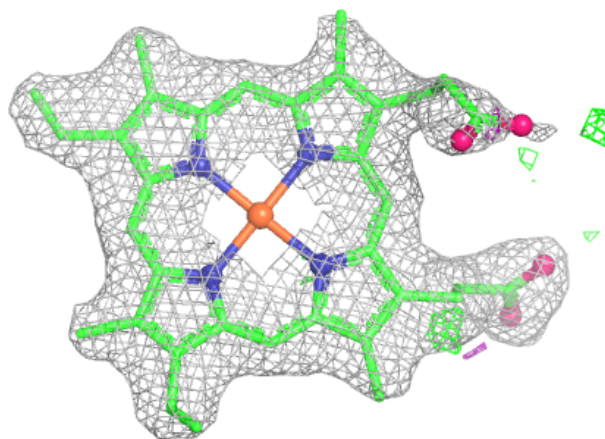
Electron density around CLA B 605:

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



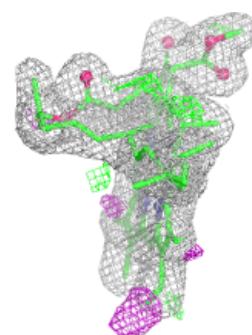
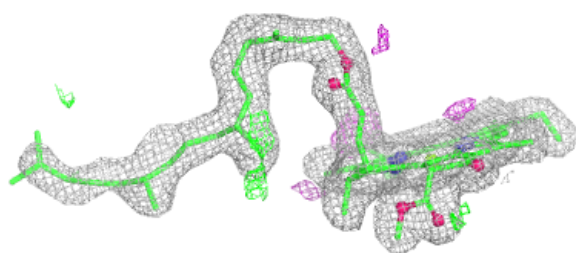
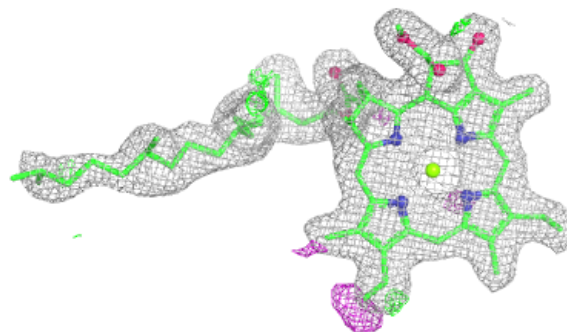
Electron density around HEM f 101:

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

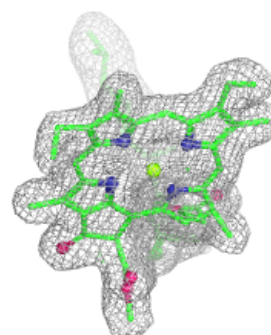
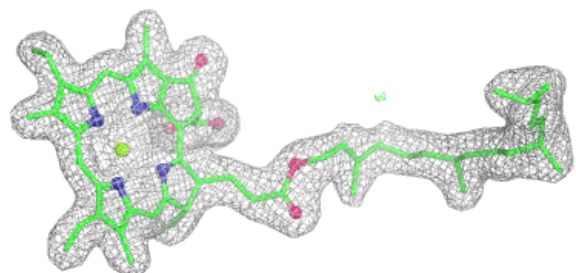
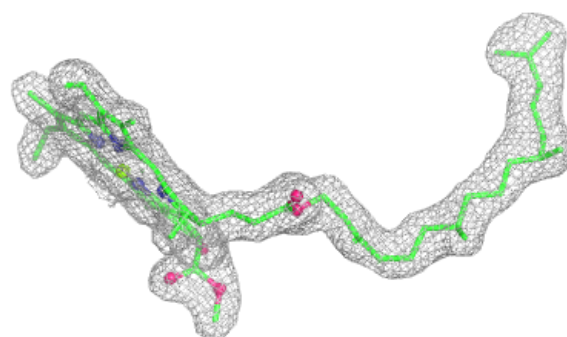


Electron density around CLA A 1006:

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

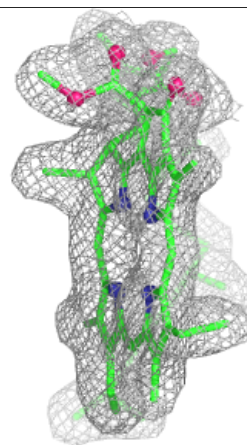
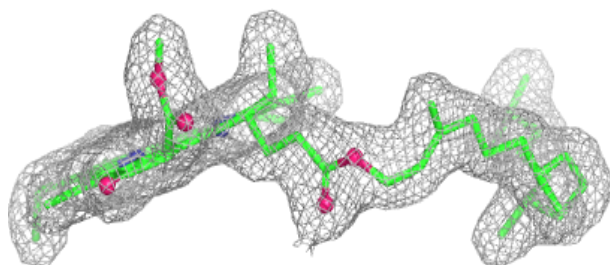
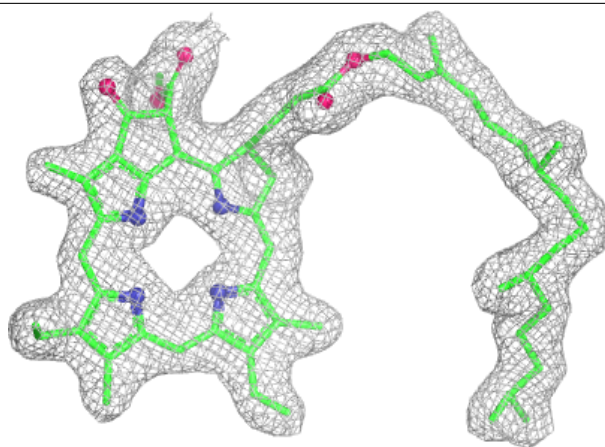
**Electron density around CLA d 402:**

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



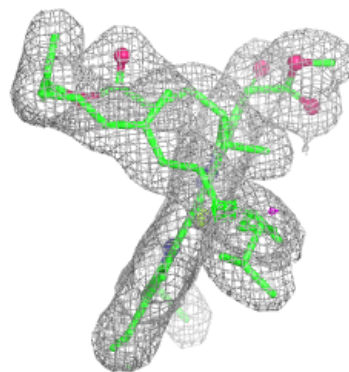
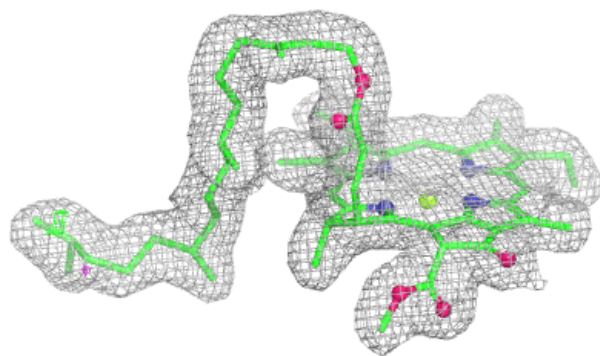
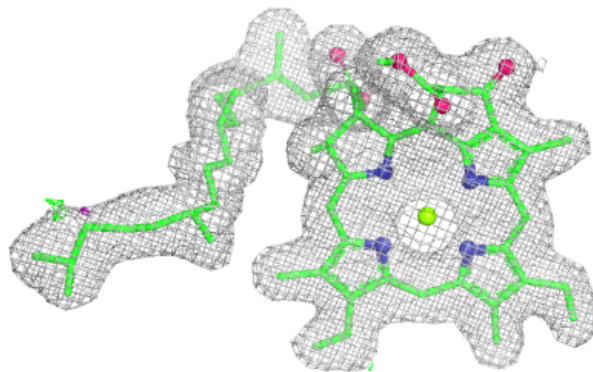
Electron density around PHO a 410:

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



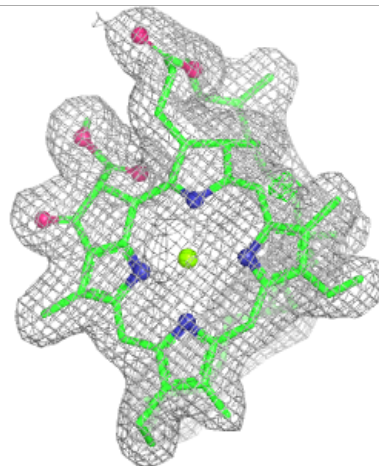
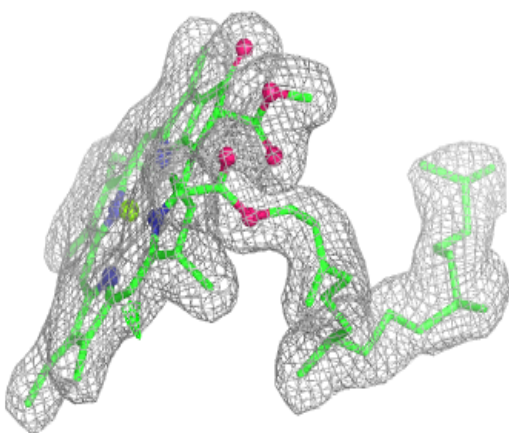
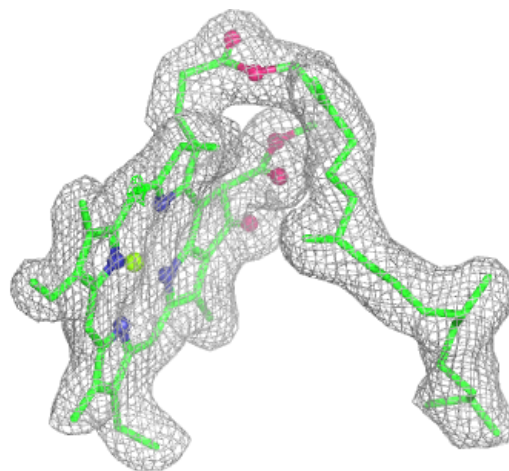
Electron density around CLA a 408:

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



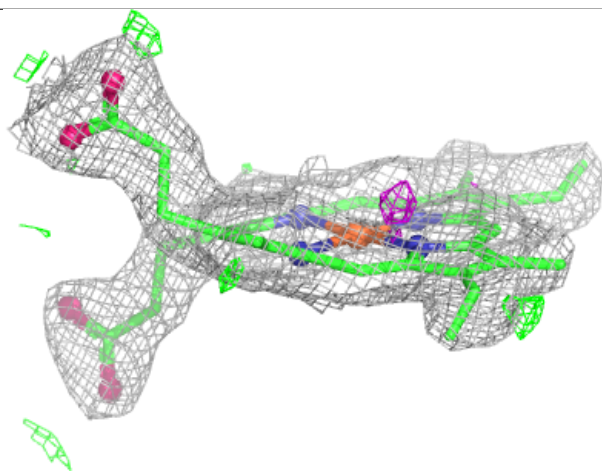
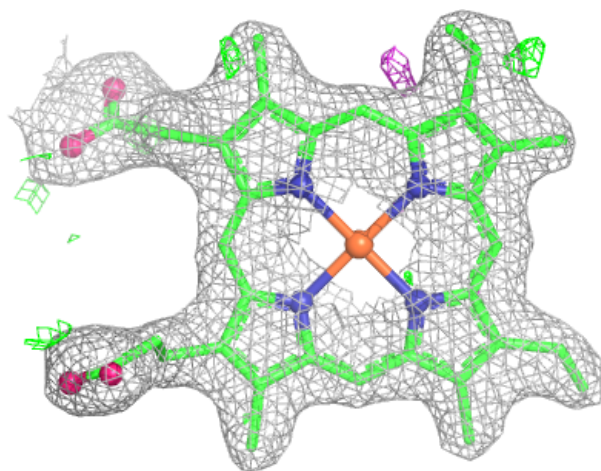
Electron density around CLA B 613:

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



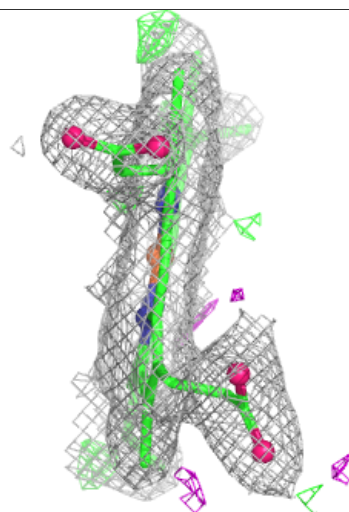
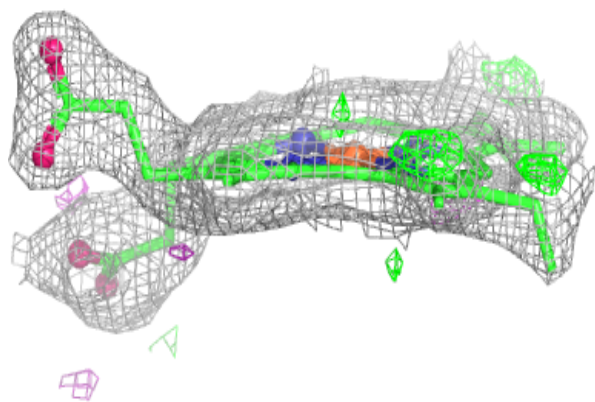
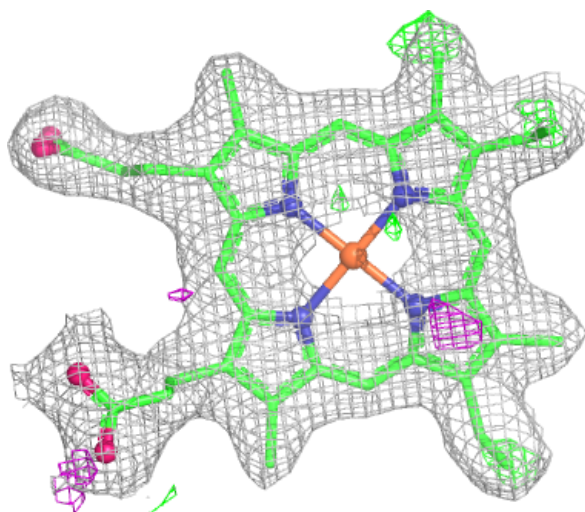
Electron density around HEM F 101:

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



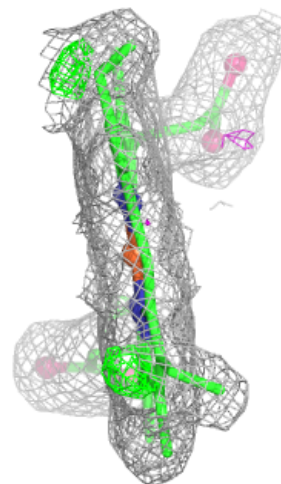
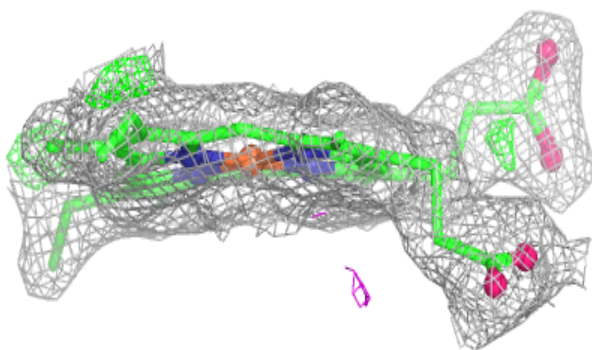
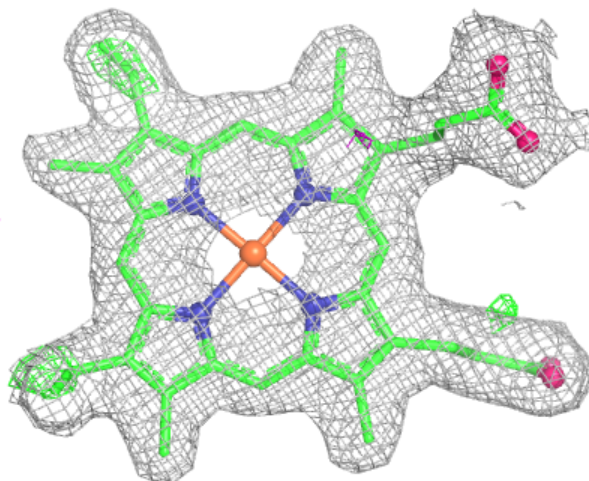
Electron density around HEM v 201:

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



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.